Full wwPDB X-ray Structure Validation Report ⓘ

May 19, 2020 – 08:24 am BST

PDB ID	:	4DV1
Title	:	Crystal structure of the Thermus thermophilus 30S ribosomal subunit with a 16S rRNA mutation, U20G, bound with streptomycin
Authors	:	Demirci, H.; Murphy IV, F.; Murphy, E.; Gregory, S.T.; Dahlberg, A.E.; Jogl, G.
Deposited on	:	2012-02-22
Resolution	:	3.85 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 ⓘ symbol.

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

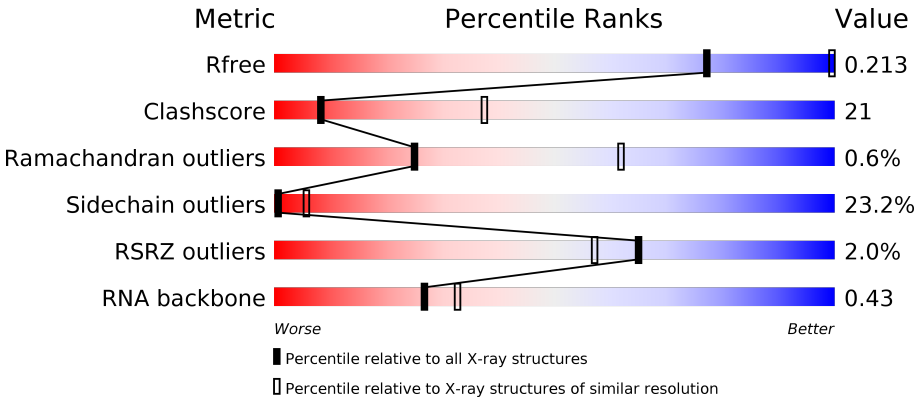
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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	1242 (4.08-3.60)
Clashscore	141614	1004 (4.04-3.64)
Ramachandran outliers	138981	1003 (4.06-3.62)
Sidechain outliers	138945	1266 (4.08-3.60)
RSRZ outliers	127900	1149 (4.08-3.60)
RNA backbone	3102	1038 (4.68-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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% 21% 42% 29% 8%
2	B	256	3% 36% 44% 11% 9%
3	C	239	4% 32% 46% 8% 14%
4	D	209	3% 39% 49% 11%

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Mol	Chain	Length	Quality of chain
5	E	162	42% 39% 11% 7%
6	F	101	37% 53% 10%
7	G	156	4% 44% 44% 10%
8	H	138	46% 41% 13%
9	I	128	% 44% 45% 11%
10	J	105	9% 43% 39% 11% 7%
11	K	129	47% 35% 8% 10%
12	L	135	40% 36% 15% 8%
13	M	126	3% 44% 40% 10% 6%
14	N	61	11% 39% 49% 10%
15	O	89	37% 44% 17%
16	P	88	36% 44% 11% 6%
17	Q	105	35% 44% 14% 6%
18	R	88	% 34% 36% 9% 20%
19	S	93	5% 34% 37% 15% 14%
20	T	106	31% 50% 12% 7%
21	U	27	15% 41% 37% 11% 11%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	PSU	A	1540	-	-	-	X
1	PSU	A	1541	-	-	-	X
23	MG	A	1661	-	-	-	X
23	MG	A	1750	-	-	-	X
23	MG	A	1758	-	-	-	X
23	MG	A	1771	-	-	-	X
23	MG	A	1785	-	-	-	X
23	MG	A	1794	-	-	-	X

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 52297 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	1512	32510	14478	6014	10506	1512	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	G	U	ENGINEERED MUTATION	GB M26923.1
A	1534	C	A	CONFLICT	GB M26923.1
A	1535	A	C	CONFLICT	GB M26923.1

- Molecule 2 is a protein called ribosomal protein S2.

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

- Molecule 3 is a protein called ribosomal protein S3.

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

- Molecule 4 is a protein called ribosomal protein S4.

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

- Molecule 5 is a protein called ribosomal protein S5.

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

- Molecule 6 is a protein called ribosomal protein S6.

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

- Molecule 7 is a protein called ribosomal protein S7.

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

- Molecule 8 is a protein called ribosomal protein S8.

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

- Molecule 9 is a protein called ribosomal protein S9.

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

- Molecule 10 is a protein called ribosomal protein S10.

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

- Molecule 11 is a protein called ribosomal protein S11.

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

- Molecule 12 is a protein called ribosomal protein S12.

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

- Molecule 13 is a protein called ribosomal protein S13.

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

- Molecule 14 is a protein called ribosomal protein S14.

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

- Molecule 15 is a protein called ribosomal protein S15.

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

- Molecule 16 is a protein called ribosomal protein S16.

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

- Molecule 17 is a protein called ribosomal protein S17.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 18 is a protein called ribosomal protein S18.

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

- Molecule 19 is a protein called ribosomal protein S19.

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

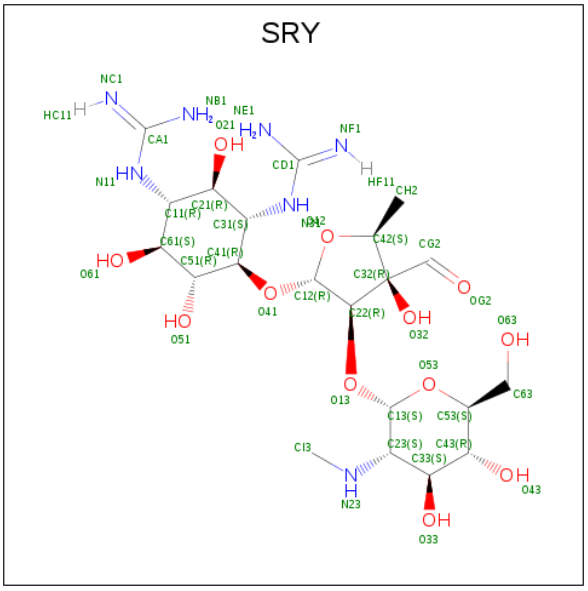
- Molecule 20 is a protein called ribosomal protein S20.

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

- Molecule 21 is a protein called ribosomal protein THX.

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

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



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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	P	1	Total Mg 1 1	0	0
23	J	1	Total Mg 1 1	0	0
23	D	1	Total Mg 1 1	0	0
23	K	1	Total Mg 1 1	0	0
23	E	1	Total Mg 1 1	0	0
23	H	2	Total Mg 2 2	0	0
23	B	1	Total Mg 1 1	0	0
23	I	1	Total Mg 1 1	0	0
23	A	230	Total Mg 230 230	0	0
23	T	2	Total Mg 2 2	0	0
23	N	2	Total Mg 2 2	0	0
23	S	2	Total Mg 2 2	0	0
23	M	2	Total Mg 2 2	0	0

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

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

- Molecule 25 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	396	Total O 396 396	0	0
25	E	6	Total O 6 6	0	0

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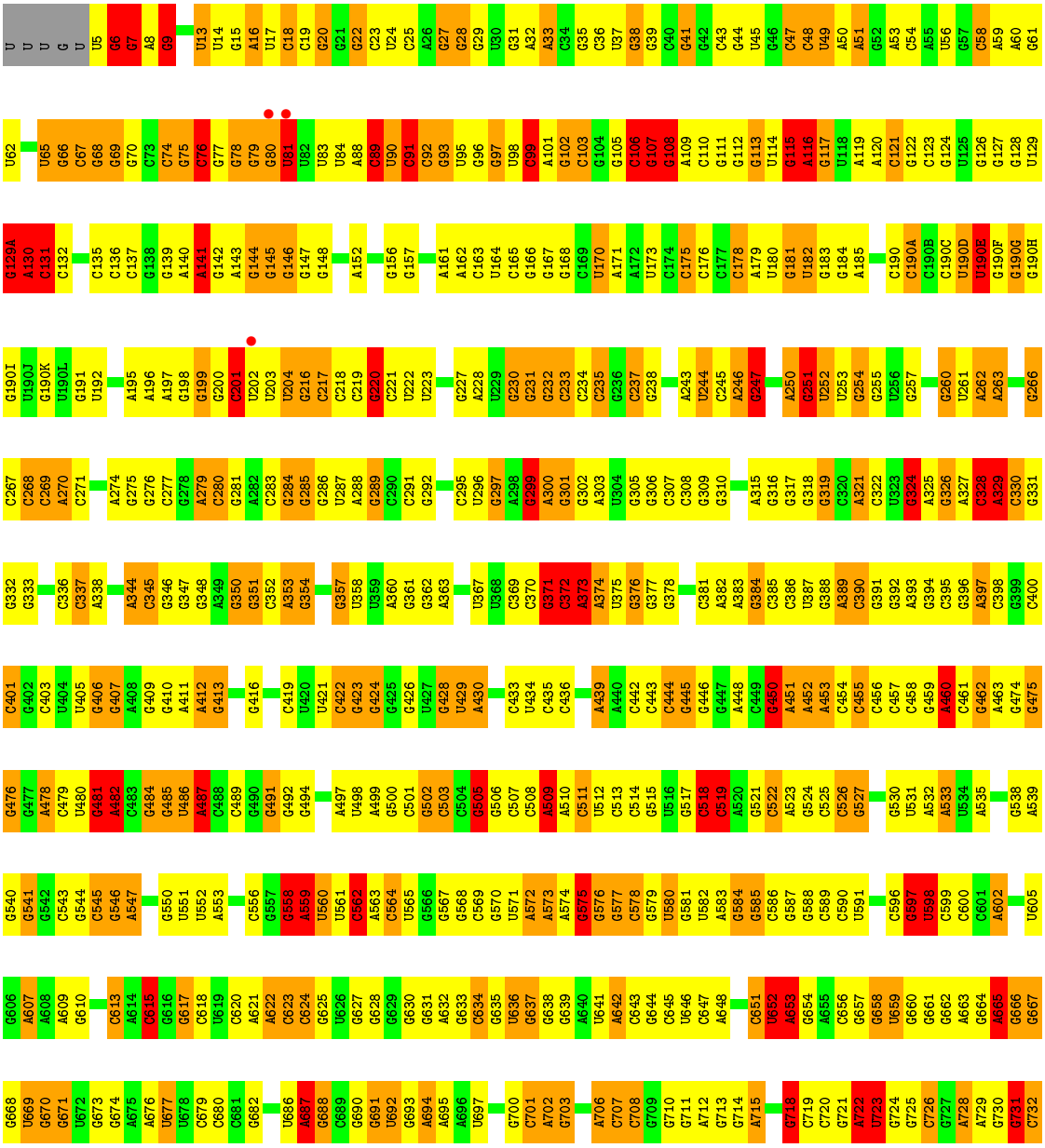
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	G	1	Total O 1 1	0	0
25	J	1	Total O 1 1	0	0
25	N	1	Total O 1 1	0	0
25	Q	1	Total O 1 1	0	0
25	T	3	Total O 3 3	0	0
25	U	1	Total O 1 1	0	0

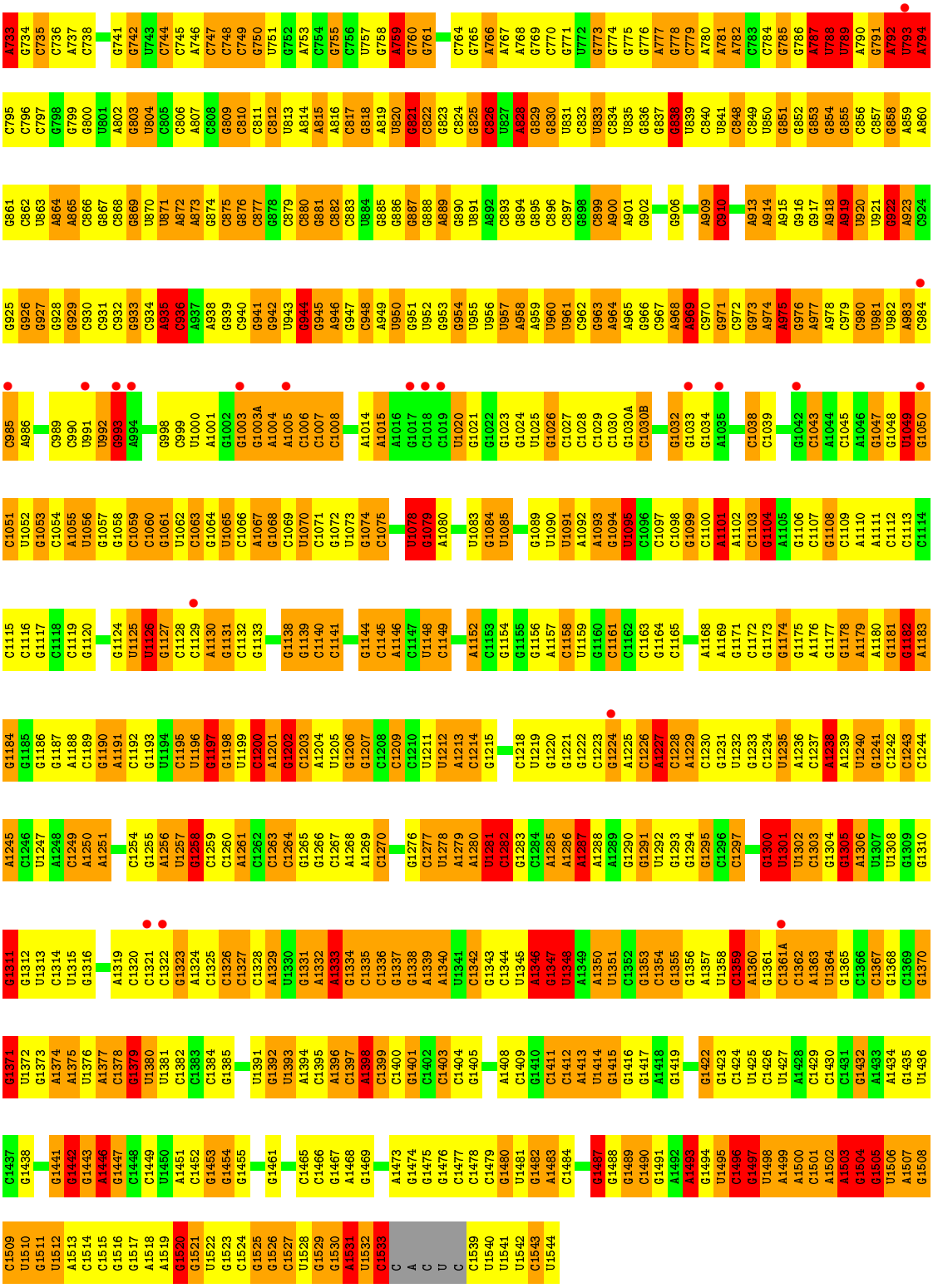
3 Residue-property plots (i)

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

- Molecule 1: 16S rRNA

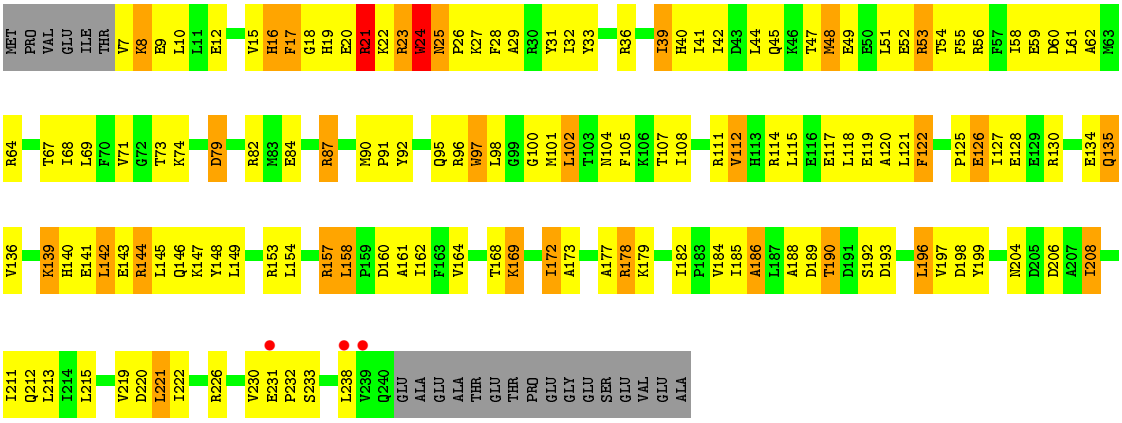
Chain A: 2% 21% 42% 29% 8%





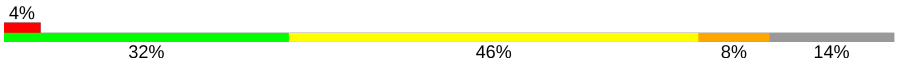
• Molecule 2: ribosomal protein S2

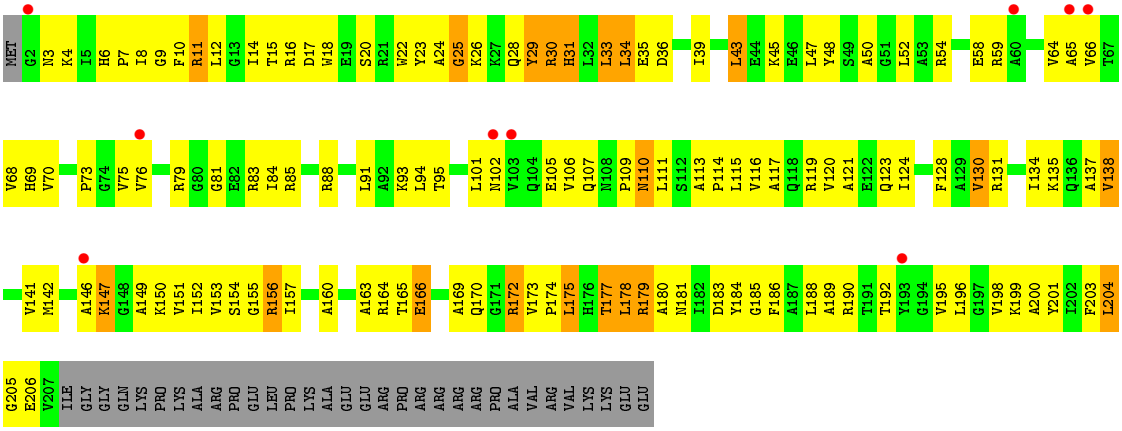
Chain B:



• Molecule 3: ribosomal protein S3

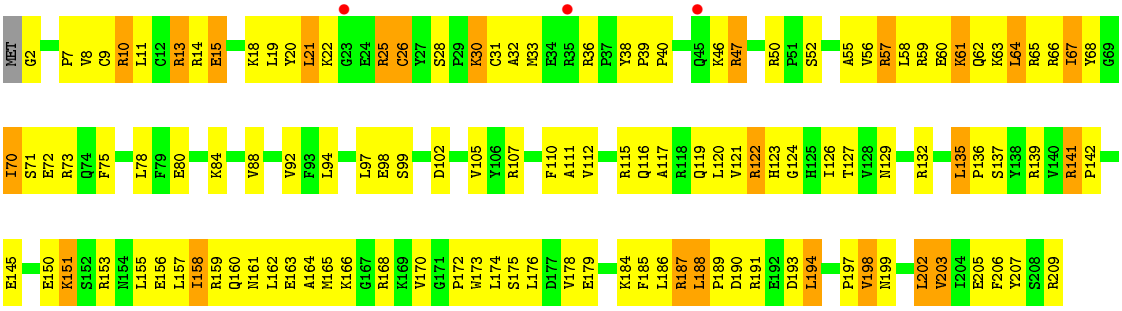
Chain C:





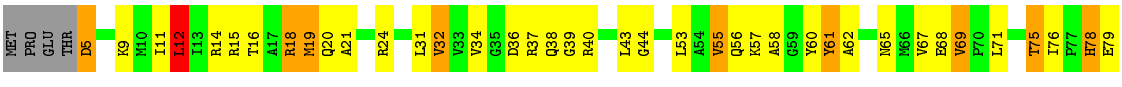
• Molecule 4: ribosomal protein S4

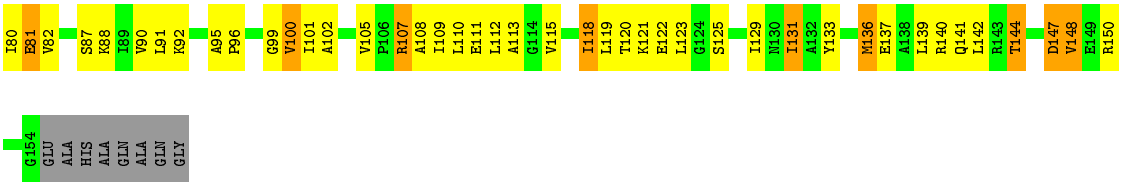
Chain D:



• Molecule 5: ribosomal protein S5

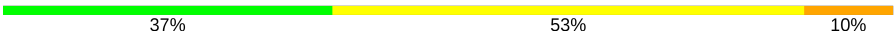
Chain E:

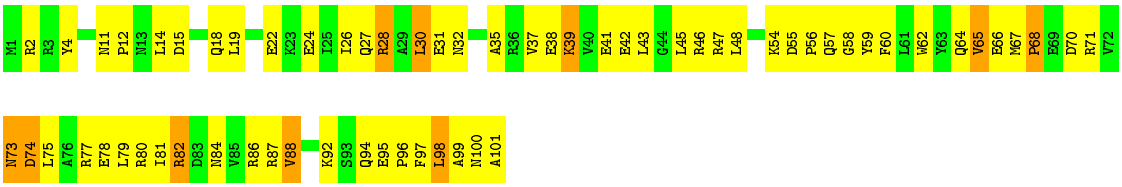




• Molecule 6: ribosomal protein S6

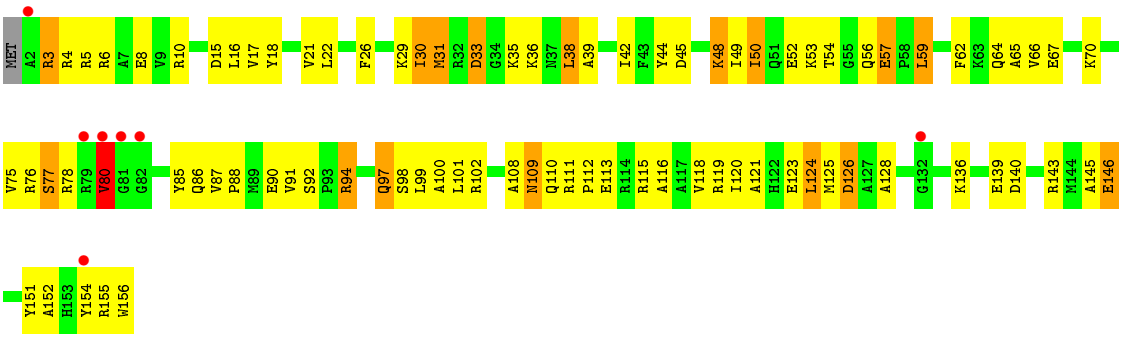
Chain F:





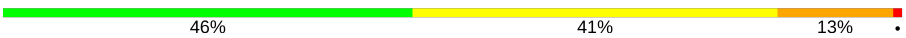
• Molecule 7: ribosomal protein S7

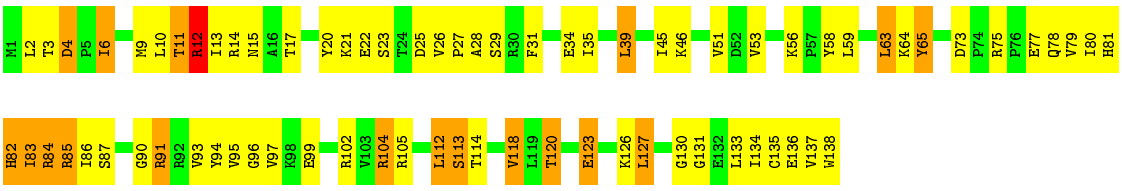
Chain G:



• Molecule 8: ribosomal protein S8

Chain H:

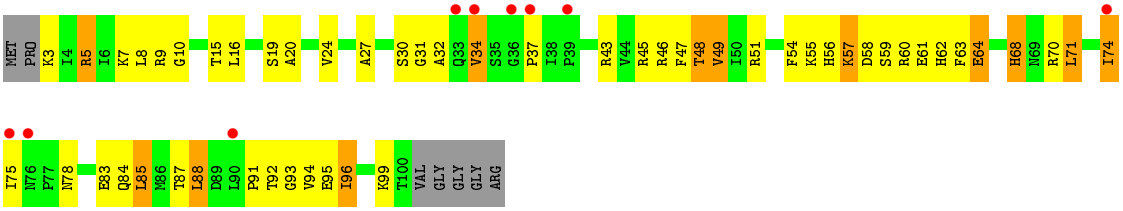




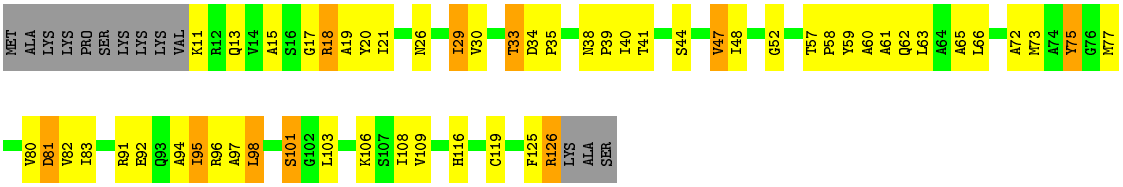
• Molecule 9: ribosomal protein S9

Chain I:

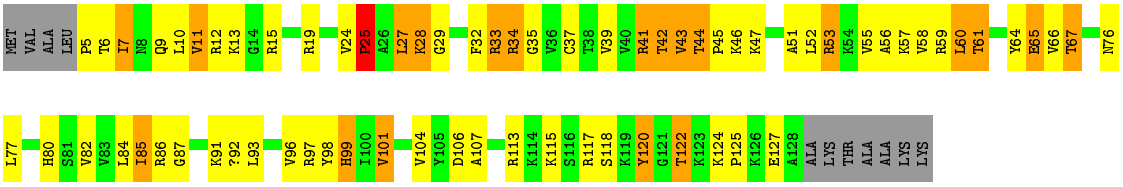
• Molecule 10: ribosomal protein S10



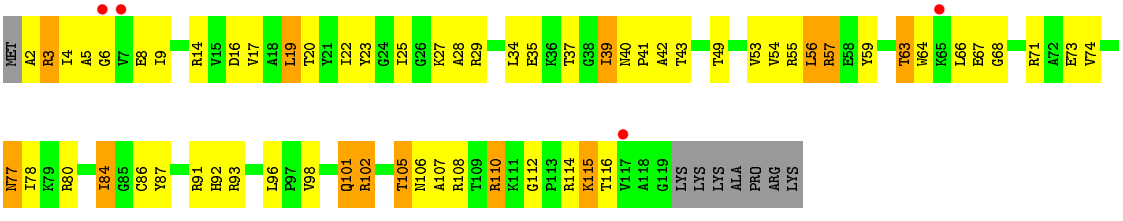
• Molecule 11: ribosomal protein S11



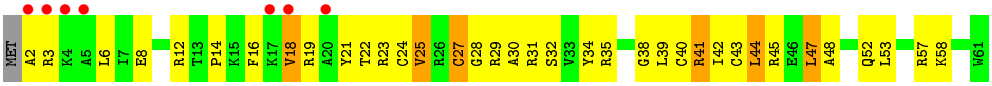
• Molecule 12: ribosomal protein S12



• Molecule 13: ribosomal protein S13

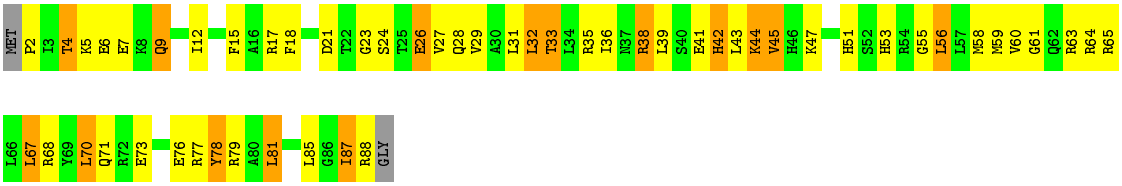


• Molecule 14: ribosomal protein S14



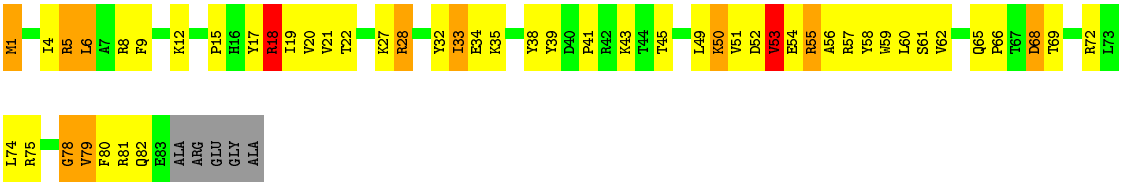
- Molecule 15: ribosomal protein S15

Chain O:



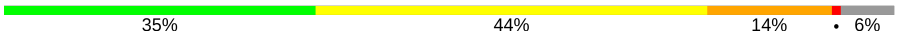
- Molecule 16: ribosomal protein S16

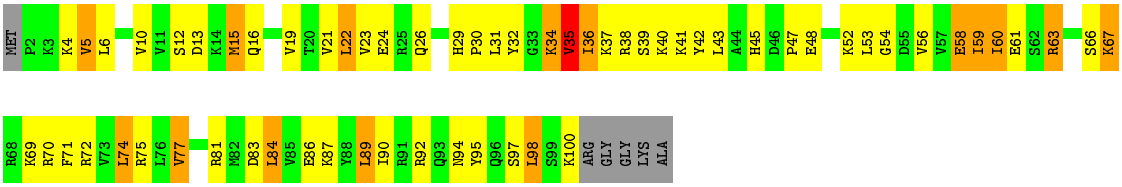
Chain P:



- Molecule 17: ribosomal protein S17

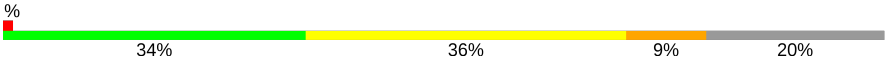
Chain Q:

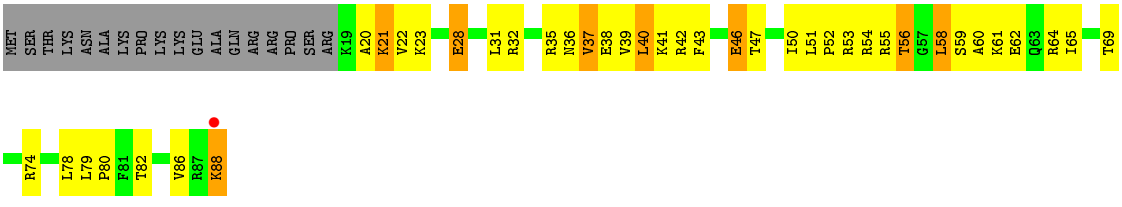




- Molecule 18: ribosomal protein S18

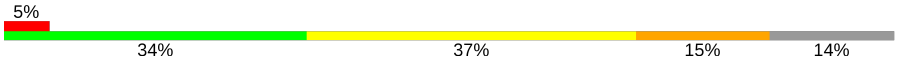
Chain R:

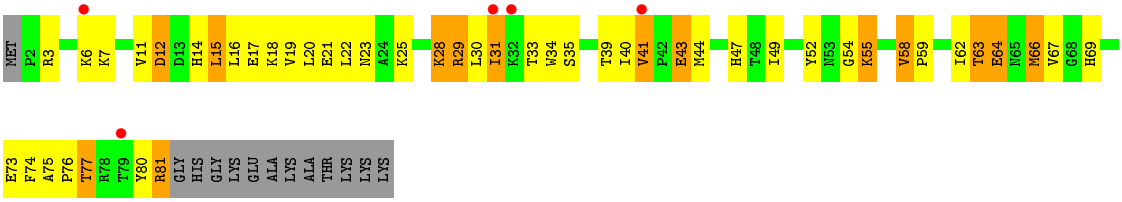




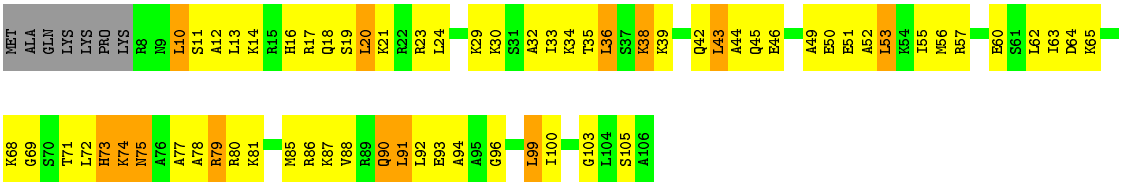
- Molecule 19: ribosomal protein S19

Chain S:

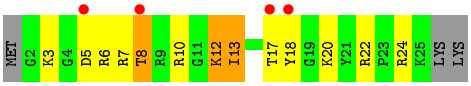




• Molecule 20: ribosomal protein S20



• Molecule 21: ribosomal protein THX



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	403.45Å 403.45Å 173.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.93 – 3.85 34.93 – 3.85	Depositor EDS
% Data completeness (in resolution range)	97.3 (34.93-3.85) 97.1 (34.93-3.85)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.90 (at 3.87Å)	Xtriage
Refinement program	PHENIX dev_978	Depositor
R, R_{free}	0.150 , 0.212 0.151 , 0.213	Depositor DCC
R_{free} test set	6512 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	161.1	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.20 , 133.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	52297	wwPDB-VP
Average B, all atoms (Å^2)	198.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.67% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	1.12	108/36044 (0.3%)	1.81	1604/56250 (2.9%)
2	B	0.63	0/1935	0.79	0/2609
3	C	0.59	0/1636	0.78	1/2205 (0.0%)
4	D	0.69	0/1733	0.89	2/2318 (0.1%)
5	E	0.88	0/1162	1.05	3/1564 (0.2%)
6	F	0.61	0/856	0.79	1/1154 (0.1%)
7	G	0.64	0/1276	0.84	0/1709
8	H	1.01	1/1136 (0.1%)	1.12	2/1527 (0.1%)
9	I	0.61	0/1029	0.82	0/1379
10	J	0.56	0/805	0.80	0/1082
11	K	0.68	0/879	0.89	0/1187
12	L	0.77	0/977	1.01	1/1306 (0.1%)
13	M	0.66	0/947	0.85	0/1270
14	N	0.64	0/501	0.83	0/664
15	O	0.73	0/740	0.91	0/987
16	P	0.77	0/716	1.00	2/963 (0.2%)
17	Q	0.97	0/836	1.14	6/1117 (0.5%)
18	R	0.70	0/579	0.87	1/768 (0.1%)
19	S	0.55	0/661	0.75	0/890
20	T	0.74	0/765	1.00	1/1007 (0.1%)
21	U	0.64	0/212	0.78	0/277
All	All	1.00	109/55425 (0.2%)	1.58	1624/82233 (2.0%)

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
8	H	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
10	J	0	1
12	L	0	1
13	M	0	1
16	P	0	2
20	T	0	1
All	All	0	9

All (109) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1509	C	N3-C4	-10.95	1.26	1.33
1	A	279	A	N9-C4	-10.62	1.31	1.37
1	A	573	A	N7-C5	-8.71	1.34	1.39
1	A	1523	G	N7-C5	-8.10	1.34	1.39
1	A	715	A	N9-C4	-8.01	1.33	1.37
1	A	266	G	N9-C4	-8.00	1.31	1.38
1	A	1513	A	N9-C4	-7.91	1.33	1.37
1	A	279	A	N3-C4	-7.87	1.30	1.34
1	A	1502	A	C5-C6	-7.79	1.34	1.41
1	A	1509	C	N1-C6	-7.73	1.32	1.37
1	A	372	C	C2-O2	7.72	1.31	1.24
1	A	1493	A	N9-C4	7.63	1.42	1.37
1	A	1504	G	N9-C8	-7.34	1.32	1.37
1	A	733	A	N9-C4	-7.22	1.33	1.37
1	A	860	A	N3-C4	-7.14	1.30	1.34
1	A	1521	G	C5-C4	-7.09	1.33	1.38
1	A	715	A	N3-C4	-7.04	1.30	1.34
1	A	569	C	N3-C4	-7.00	1.29	1.33
8	H	135	CYS	CB-SG	-6.93	1.70	1.82
1	A	572	A	N3-C4	-6.81	1.30	1.34
1	A	1523	G	C5-C6	-6.68	1.35	1.42
1	A	372	C	N3-C4	6.46	1.38	1.33
1	A	722	A	N9-C4	-6.44	1.33	1.37
1	A	1501	C	N3-C4	-6.42	1.29	1.33
1	A	1329	A	N7-C5	-6.35	1.35	1.39
1	A	792	A	N9-C4	6.34	1.41	1.37
1	A	1504	G	C6-N1	-6.30	1.35	1.39
1	A	791	G	N9-C4	6.29	1.43	1.38
1	A	1227	A	N9-C4	-6.27	1.34	1.37
1	A	1079	G	N7-C5	-6.27	1.35	1.39
1	A	88	A	N9-C4	6.14	1.41	1.37
1	A	602	A	N9-C4	-6.09	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1377	A	N3-C4	-6.04	1.31	1.34
1	A	1529	G	C6-N1	-6.03	1.35	1.39
1	A	1346	A	C3'-O3'	5.99	1.50	1.42
1	A	828	A	N9-C4	-5.92	1.34	1.37
1	A	1103	C	N3-C4	-5.92	1.29	1.33
1	A	1526	G	N7-C5	-5.89	1.35	1.39
1	A	389	A	N7-C5	-5.87	1.35	1.39
1	A	382	A	N7-C5	-5.86	1.35	1.39
1	A	482	A	N7-C5	-5.85	1.35	1.39
1	A	605	U	N3-C4	-5.82	1.33	1.38
1	A	817	C	N1-C6	-5.81	1.33	1.37
1	A	362	G	N3-C4	-5.79	1.31	1.35
1	A	274	A	N9-C4	-5.78	1.34	1.37
1	A	279	A	N7-C5	-5.76	1.35	1.39
1	A	1504	G	C5-C4	-5.75	1.34	1.38
1	A	1514	C	N3-C4	-5.74	1.29	1.33
1	A	706	A	N3-C4	-5.74	1.31	1.34
1	A	1521	G	N9-C8	-5.72	1.33	1.37
1	A	854	G	C6-N1	-5.71	1.35	1.39
1	A	190(G)	G	N7-C5	-5.69	1.35	1.39
1	A	372	C	C2-N3	5.63	1.40	1.35
1	A	584	G	N7-C5	-5.61	1.35	1.39
1	A	910	C	N3-C4	-5.61	1.30	1.33
1	A	642	A	N7-C5	-5.58	1.35	1.39
1	A	900	A	N7-C5	-5.57	1.35	1.39
1	A	1514	C	N1-C2	-5.57	1.34	1.40
1	A	1510	U	C2-N3	-5.55	1.33	1.37
1	A	291	C	N1-C6	-5.55	1.33	1.37
1	A	1377	A	N9-C4	-5.54	1.34	1.37
1	A	605	U	C2-N3	-5.53	1.33	1.37
1	A	288	A	N9-C4	-5.53	1.34	1.37
1	A	108	G	P-O5'	-5.50	1.54	1.59
1	A	782	A	N7-C5	-5.49	1.35	1.39
1	A	889	A	N9-C4	-5.49	1.34	1.37
1	A	901	A	N9-C4	-5.46	1.34	1.37
1	A	565	U	C2-O2	5.46	1.27	1.22
1	A	1520	G	N3-C4	-5.45	1.31	1.35
1	A	1526	G	C5-C6	-5.43	1.36	1.42
1	A	23	C	N1-C6	-5.43	1.33	1.37
1	A	862	C	C4-C5	-5.42	1.38	1.43
1	A	556	C	N3-C4	-5.42	1.30	1.33
1	A	771	G	N9-C4	-5.42	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	909	A	N7-C5	-5.40	1.36	1.39
1	A	1527	C	C4-C5	-5.39	1.38	1.43
1	A	481	G	N9-C4	5.37	1.42	1.38
1	A	946	A	C6-N1	-5.37	1.31	1.35
1	A	97	G	N9-C4	5.35	1.42	1.38
1	A	1180	A	N9-C4	5.33	1.41	1.37
1	A	329	A	C5-C6	-5.30	1.36	1.41
1	A	791	G	C5-C4	5.30	1.42	1.38
1	A	238	G	C2-N3	-5.29	1.28	1.32
1	A	706	A	N9-C4	-5.24	1.34	1.37
1	A	1329	A	C5-C6	-5.21	1.36	1.41
1	A	1508	G	C6-N1	-5.21	1.35	1.39
1	A	729	A	N9-C4	-5.20	1.34	1.37
1	A	568	G	C6-N1	-5.18	1.35	1.39
1	A	33	A	N3-C4	-5.17	1.31	1.34
1	A	558	G	C5-C6	-5.16	1.37	1.42
1	A	879	C	C4-C5	-5.14	1.38	1.43
1	A	574	A	N3-C4	-5.14	1.31	1.34
1	A	1505	G	N7-C5	-5.14	1.36	1.39
1	A	868	C	N1-C6	-5.13	1.34	1.37
1	A	288	A	C6-N1	-5.12	1.31	1.35
1	A	771	G	N3-C4	-5.10	1.31	1.35
1	A	635	G	C2-N3	-5.09	1.28	1.32
1	A	561	U	N1-C6	-5.08	1.33	1.38
1	A	568	G	N3-C4	-5.07	1.31	1.35
1	A	1396	A	N9-C4	-5.07	1.34	1.37
1	A	917	G	N9-C4	-5.06	1.33	1.38
1	A	574	A	C6-N1	-5.06	1.32	1.35
1	A	1500	A	N3-C4	-5.04	1.31	1.34
1	A	810	C	N1-C6	-5.04	1.34	1.37
1	A	771	G	C5-C6	-5.04	1.37	1.42
1	A	124	G	N3-C4	-5.02	1.31	1.35
1	A	453	A	N9-C4	-5.02	1.34	1.37
1	A	1504	G	N7-C5	-5.01	1.36	1.39
1	A	1401	G	N3-C4	-5.00	1.31	1.35

All (1624) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	573	A	C8-N9-C4	-18.34	98.46	105.80
1	A	1505	G	C8-N9-C4	-15.18	100.33	106.40
1	A	372	C	C6-N1-C2	13.96	125.89	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	279	A	C5-N7-C8	-13.43	97.18	103.90
1	A	481	G	N3-C4-N9	13.26	133.96	126.00
1	A	573	A	N7-C8-N9	13.08	120.34	113.80
1	A	873	A	C8-N9-C4	-12.91	100.64	105.80
1	A	295	C	C6-N1-C2	12.75	125.40	120.30
1	A	1496	C	C6-N1-C2	-12.70	115.22	120.30
1	A	1282	C	C6-N1-C2	-12.62	115.25	120.30
1	A	106	C	C6-N1-C2	-12.58	115.27	120.30
1	A	1370	G	C8-N9-C4	-12.57	101.37	106.40
1	A	1377	A	N1-C6-N6	-12.56	111.06	118.60
1	A	948	C	C6-N1-C2	12.39	125.26	120.30
1	A	310	G	N1-C6-O6	12.37	127.32	119.90
1	A	190(G)	G	N1-C6-O6	12.29	127.27	119.90
1	A	1505	G	N7-C8-N9	12.28	119.24	113.10
1	A	635	G	N1-C6-O6	12.25	127.25	119.90
1	A	326	G	C4-C5-N7	-12.18	105.93	110.80
1	A	279	A	N7-C8-N9	12.15	119.88	113.80
1	A	1181	G	C8-N9-C4	12.02	111.21	106.40
1	A	103	C	C6-N1-C2	-11.98	115.51	120.30
1	A	117	G	C5-C6-N1	-11.89	105.55	111.50
1	A	572	A	N9-C4-C5	11.79	110.52	105.80
1	A	1502	A	C4-C5-N7	11.63	116.52	110.70
1	A	1367	C	C6-N1-C2	-11.52	115.69	120.30
1	A	117	G	N1-C6-O6	11.47	126.78	119.90
1	A	326	G	C5-C6-O6	11.16	135.30	128.60
1	A	190(G)	G	C6-C5-N7	-11.13	123.72	130.40
1	A	331	G	N1-C6-O6	11.11	126.57	119.90
1	A	1370	G	N7-C8-N9	11.10	118.65	113.10
1	A	572	A	N1-C6-N6	-11.01	111.99	118.60
1	A	326	G	N9-C4-C5	10.93	109.77	105.40
1	A	232	G	N9-C4-C5	-10.79	101.08	105.40
1	A	1238	A	N9-C4-C5	10.76	110.11	105.80
1	A	305	G	C8-N9-C4	-10.70	102.12	106.40
1	A	372	C	N1-C2-N3	-10.67	111.73	119.20
1	A	735	C	C6-N1-C2	10.67	124.57	120.30
1	A	928	G	N1-C6-O6	10.62	126.27	119.90
1	A	232	G	C6-C5-N7	-10.51	124.09	130.40
1	A	1403	C	C6-N1-C2	10.48	124.49	120.30
1	A	725	G	C5-C6-O6	-10.44	122.33	128.60
1	A	1238	A	N1-C6-N6	-10.32	112.41	118.60
1	A	232	G	C4-C5-N7	10.30	114.92	110.80
1	A	725	G	C4-C5-N7	10.28	114.91	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1502	A	N1-C6-N6	10.23	124.74	118.60
1	A	1502	A	C5-N7-C8	-10.18	98.81	103.90
1	A	969	A	N1-C6-N6	10.13	124.68	118.60
1	A	565	U	N1-C2-N3	-10.06	108.86	114.90
1	A	815	A	C8-N9-C4	10.05	109.82	105.80
1	A	232	G	N1-C6-O6	10.03	125.92	119.90
1	A	1517	G	C8-N9-C4	-9.98	102.41	106.40
1	A	310	G	C5-C6-O6	-9.87	122.68	128.60
1	A	753	A	C6-N1-C2	-9.86	112.68	118.60
1	A	481	G	C8-N9-C4	9.84	110.34	106.40
1	A	1455	G	N1-C6-O6	9.81	125.78	119.90
1	A	745	C	C6-N1-C2	9.79	124.22	120.30
1	A	238	G	C5-C6-N1	-9.79	106.61	111.50
1	A	299	G	C6-C5-N7	-9.78	124.53	130.40
1	A	1523	G	C8-N9-C4	-9.76	102.50	106.40
1	A	1504	G	N3-C4-C5	-9.74	123.73	128.60
1	A	43	C	C5-C6-N1	-9.73	116.13	121.00
1	A	299	G	N1-C6-O6	9.72	125.73	119.90
1	A	946	A	N1-C6-N6	-9.71	112.77	118.60
1	A	573	A	N9-C4-C5	9.70	109.68	105.80
1	A	238	G	N1-C6-O6	9.65	125.69	119.90
1	A	1329	A	N1-C6-N6	9.65	124.39	118.60
1	A	284	G	N1-C6-O6	9.64	125.69	119.90
1	A	28	G	N1-C6-O6	9.61	125.67	119.90
1	A	715	A	C2-N3-C4	-9.58	105.81	110.60
1	A	1502	A	C6-C5-N7	-9.58	125.59	132.30
1	A	328	C	N3-C2-O2	-9.57	115.20	121.90
1	A	117	G	C8-N9-C1'	-9.57	114.56	127.00
1	A	482	A	N7-C8-N9	9.53	118.56	113.80
1	A	1513	A	C2-N3-C4	-9.52	105.84	110.60
1	A	1249	C	C6-N1-C2	-9.49	116.50	120.30
1	A	190(F)	G	N3-C4-N9	-9.46	120.33	126.00
1	A	830	G	N1-C6-O6	9.45	125.57	119.90
1	A	103	C	N3-C4-C5	-9.41	118.13	121.90
1	A	945	G	C4-C5-C6	-9.37	113.18	118.80
1	A	325	A	N1-C6-N6	-9.37	112.98	118.60
1	A	279	A	C8-N9-C4	-9.35	102.06	105.80
1	A	481	G	N9-C4-C5	-9.34	101.67	105.40
1	A	861	G	C5-C6-N1	9.32	116.16	111.50
1	A	950	U	N3-C4-C5	-9.32	109.01	114.60
1	A	1543	C	N1-C2-O2	9.32	124.49	118.90
17	Q	35	VAL	CB-CA-C	-9.31	93.70	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1339	A	N1-C6-N6	-9.30	113.02	118.60
1	A	1084	G	N3-C4-C5	-9.28	123.96	128.60
1	A	266	G	N3-C4-C5	9.26	133.23	128.60
1	A	1523	G	C5-C6-O6	-9.24	123.06	128.60
1	A	121	C	C6-N1-C2	9.20	123.98	120.30
1	A	944	G	C8-N9-C4	-9.12	102.75	106.40
1	A	1524	C	N3-C4-C5	-9.12	118.25	121.90
1	A	791	G	C8-N9-C4	-9.12	102.75	106.40
1	A	722	A	C2-N3-C4	-9.12	106.04	110.60
1	A	963	G	C8-N9-C4	-9.11	102.76	106.40
1	A	854	G	N1-C2-N3	9.05	129.33	123.90
1	A	88	A	C8-N9-C4	-9.05	102.18	105.80
1	A	117	G	C4-C5-C6	9.05	124.23	118.80
1	A	1347	G	C5-C6-O6	-9.04	123.17	128.60
1	A	635	G	C5-C6-N1	-9.01	107.00	111.50
1	A	790	A	C8-N9-C4	-9.01	102.20	105.80
1	A	283	C	C6-N1-C2	-8.99	116.70	120.30
1	A	1524	C	C6-N1-C2	-8.97	116.71	120.30
1	A	117	G	C6-C5-N7	-8.96	125.02	130.40
1	A	99	C	C6-N1-C2	-8.93	116.73	120.30
1	A	292	G	N1-C6-O6	8.89	125.23	119.90
1	A	305	G	N9-C4-C5	8.87	108.95	105.40
1	A	572	A	C8-N9-C4	-8.87	102.25	105.80
1	A	382	A	C8-N9-C4	-8.86	102.25	105.80
1	A	1079	G	N3-C4-C5	-8.86	124.17	128.60
1	A	326	G	C8-N9-C4	-8.86	102.86	106.40
1	A	16	A	C8-N9-C4	8.83	109.33	105.80
1	A	190(G)	G	C5-C6-N1	-8.81	107.09	111.50
1	A	852	G	C5-C6-N1	-8.79	107.11	111.50
1	A	106	C	N3-C2-O2	-8.78	115.75	121.90
1	A	1237	C	C6-N1-C2	-8.77	116.79	120.30
1	A	289	G	C8-N9-C4	-8.73	102.91	106.40
1	A	1231	G	N1-C6-O6	8.73	125.14	119.90
1	A	137	C	N3-C4-C5	8.69	125.38	121.90
1	A	260	G	C8-N9-C4	-8.68	102.93	106.40
1	A	288	A	C2-N3-C4	-8.67	106.26	110.60
1	A	635	G	N3-C2-N2	-8.65	113.84	119.90
1	A	27	G	N1-C6-O6	8.65	125.09	119.90
1	A	129(A)	G	C4-C5-N7	8.61	114.25	110.80
1	A	852	G	N1-C6-O6	8.61	125.06	119.90
1	A	575	G	C2-N3-C4	-8.60	107.60	111.90
1	A	108	G	N7-C8-N9	8.58	117.39	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	585	G	C8-N9-C4	8.57	109.83	106.40
1	A	946	A	N9-C4-C5	8.56	109.22	105.80
1	A	651	C	C6-N1-C2	8.56	123.72	120.30
1	A	1365	G	C8-N9-C4	-8.55	102.98	106.40
1	A	1526	G	N1-C6-O6	8.55	125.03	119.90
1	A	232	G	C5-C6-O6	-8.53	123.48	128.60
1	A	1403	C	N3-C2-O2	8.53	127.87	121.90
1	A	666	G	C5-C6-N1	-8.50	107.25	111.50
1	A	482	A	N1-C6-N6	8.49	123.69	118.60
1	A	500	G	C8-N9-C4	-8.48	103.01	106.40
1	A	328	C	N1-C2-O2	8.48	123.99	118.90
1	A	481	G	N3-C4-C5	-8.44	124.38	128.60
1	A	730	G	N1-C2-N2	-8.44	108.61	116.20
1	A	600	C	C6-N1-C2	8.44	123.67	120.30
1	A	856	C	N3-C4-C5	-8.41	118.53	121.90
1	A	285	G	N1-C6-O6	8.41	124.94	119.90
1	A	915	A	N1-C6-N6	-8.40	113.56	118.60
1	A	872	A	N1-C6-N6	8.40	123.64	118.60
1	A	569	C	N3-C4-C5	8.38	125.25	121.90
1	A	1332	A	N1-C6-N6	-8.37	113.58	118.60
1	A	326	G	N3-C4-C5	-8.33	124.43	128.60
1	A	131	C	C5-C6-N1	-8.33	116.83	121.00
1	A	1333	A	C8-N9-C4	-8.33	102.47	105.80
1	A	244	U	N1-C2-N3	-8.31	109.91	114.90
1	A	1238	A	C8-N9-C4	-8.30	102.48	105.80
1	A	190(A)	C	C6-N1-C2	-8.29	116.98	120.30
1	A	789	U	C5-C6-N1	8.28	126.84	122.70
1	A	180	U	C2-N1-C1'	8.28	127.64	117.70
1	A	279	A	C6-C5-N7	-8.25	126.53	132.30
1	A	1055	A	N1-C6-N6	-8.23	113.66	118.60
1	A	851	G	C8-N9-C4	-8.21	103.11	106.40
1	A	1354	C	C6-N1-C2	-8.20	117.02	120.30
1	A	1502	A	N9-C4-C5	-8.19	102.52	105.80
1	A	1523	G	N1-C6-O6	8.19	124.81	119.90
1	A	1200	C	C2-N1-C1'	8.19	127.81	118.80
1	A	773	G	C6-C5-N7	-8.18	125.50	130.40
1	A	624	C	C6-N1-C2	8.17	123.57	120.30
1	A	266	G	C2-N3-C4	-8.16	107.82	111.90
1	A	873	A	N9-C4-C5	8.16	109.06	105.80
1	A	482	A	C8-N9-C4	-8.16	102.54	105.80
1	A	1181	G	N7-C8-N9	-8.16	109.02	113.10
1	A	1441	G	C4-C5-N7	-8.13	107.55	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	708	C	C6-N1-C2	8.12	123.55	120.30
1	A	928	G	C6-C5-N7	-8.12	125.53	130.40
1	A	283	C	C2-N1-C1'	8.09	127.70	118.80
1	A	589	C	C5-C6-N1	-8.09	116.96	121.00
1	A	108	G	C8-N9-C4	-8.07	103.17	106.40
1	A	79	G	C8-N9-C4	-8.05	103.18	106.40
1	A	235	C	C6-N1-C2	8.05	123.52	120.30
1	A	700	G	N3-C4-N9	8.04	130.83	126.00
1	A	27	G	C5-C6-O6	-8.03	123.78	128.60
1	A	1529	G	C4-N9-C1'	8.03	136.94	126.50
1	A	331	G	C2-N3-C4	-8.01	107.90	111.90
1	A	1347	G	N9-C4-C5	-8.00	102.20	105.40
1	A	75	G	N3-C4-N9	7.99	130.79	126.00
1	A	1513	A	N1-C2-N3	7.98	133.29	129.30
1	A	950	U	C5-C4-O4	7.98	130.69	125.90
1	A	93	G	C8-N9-C4	7.98	109.59	106.40
1	A	945	G	N1-C2-N3	-7.97	119.12	123.90
1	A	856	C	N1-C2-O2	-7.97	114.12	118.90
1	A	126	G	C8-N9-C4	7.96	109.59	106.40
1	A	372	C	C5-C4-N4	-7.96	114.63	120.20
1	A	292	G	C6-C5-N7	-7.94	125.64	130.40
1	A	931	C	C5-C6-N1	-7.94	117.03	121.00
1	A	279	A	N1-C6-N6	7.93	123.36	118.60
1	A	295	C	N3-C4-C5	7.93	125.07	121.90
1	A	1526	G	C6-C5-N7	-7.93	125.64	130.40
1	A	507	C	C6-N1-C2	-7.89	117.14	120.30
1	A	27	G	C6-C5-N7	-7.89	125.67	130.40
1	A	481	G	C8-N9-C1'	-7.88	116.76	127.00
1	A	1193	G	N1-C6-O6	7.87	124.62	119.90
1	A	1527	C	C5-C4-N4	-7.87	114.69	120.20
1	A	731	G	N1-C6-O6	7.86	124.61	119.90
1	A	251	G	C6-C5-N7	-7.85	125.69	130.40
1	A	795	C	C2-N3-C4	7.84	123.82	119.90
1	A	1530	G	C8-N9-C4	7.84	109.54	106.40
1	A	78	G	N9-C4-C5	-7.84	102.26	105.40
1	A	706	A	C2-N3-C4	-7.84	106.68	110.60
1	A	815	A	N7-C8-N9	-7.84	109.88	113.80
1	A	299	G	C5-C6-O6	-7.81	123.91	128.60
1	A	1329	A	C4-C5-N7	7.81	114.61	110.70
1	A	773	G	C4-C5-N7	7.81	113.92	110.80
1	A	251	G	N1-C6-O6	7.81	124.59	119.90
1	A	1455	G	C6-C5-N7	-7.80	125.72	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	725	G	C5-N7-C8	-7.79	100.40	104.30
1	A	117	G	C4-N9-C1'	7.79	136.63	126.50
1	A	397	A	C8-N9-C4	-7.79	102.69	105.80
1	A	693	G	C4-C5-N7	7.77	113.91	110.80
1	A	854	G	C6-N1-C2	-7.76	120.44	125.10
1	A	1441	G	C5-C6-O6	7.75	133.25	128.60
1	A	936	C	C6-N1-C2	7.75	123.40	120.30
1	A	833	U	N3-C2-O2	-7.74	116.78	122.20
8	H	12	ARG	NE-CZ-NH1	-7.74	116.43	120.30
1	A	234	C	C6-N1-C2	7.74	123.40	120.30
1	A	331	G	C5-C6-N1	-7.74	107.63	111.50
1	A	728	A	C2-N3-C4	-7.73	106.73	110.60
1	A	578	C	C4-C5-C6	7.72	121.26	117.40
1	A	525	C	C6-N1-C2	7.71	123.39	120.30
1	A	18	C	C6-N1-C2	7.71	123.39	120.30
1	A	562	C	N3-C2-O2	-7.71	116.51	121.90
1	A	1187	G	N1-C6-O6	7.70	124.52	119.90
1	A	244	U	C6-N1-C2	7.70	125.62	121.00
1	A	1370	G	C5-N7-C8	-7.70	100.45	104.30
1	A	928	G	C5-C6-O6	-7.69	123.98	128.60
1	A	693	G	C5-C6-O6	-7.68	123.99	128.60
1	A	1523	G	N3-C2-N2	-7.68	114.52	119.90
1	A	811	C	N3-C4-N4	7.67	123.37	118.00
1	A	115	G	C8-N9-C4	7.67	109.47	106.40
1	A	753	A	N1-C2-N3	7.67	133.13	129.30
1	A	201	C	C6-N1-C2	-7.66	117.24	120.30
1	A	605	U	N3-C2-O2	-7.66	116.84	122.20
1	A	15	G	C8-N9-C1'	-7.66	117.05	127.00
1	A	292	G	C5-C6-O6	-7.66	124.01	128.60
1	A	969	A	C2-N3-C4	-7.66	106.77	110.60
1	A	1497	G	C8-N9-C4	-7.65	103.34	106.40
1	A	305	G	N3-C4-N9	-7.65	121.41	126.00
1	A	830	G	C5-C6-N1	-7.65	107.68	111.50
1	A	795	C	N3-C4-C5	-7.64	118.84	121.90
1	A	1531	A	N1-C6-N6	7.64	123.18	118.60
1	A	731	G	C5-C6-O6	-7.63	124.02	128.60
1	A	1209	C	C6-N1-C2	-7.62	117.25	120.30
1	A	735	C	C5-C6-N1	-7.61	117.19	121.00
1	A	190(A)	C	C5-C6-N1	7.61	124.81	121.00
1	A	658	G	C8-N9-C1'	-7.61	117.11	127.00
1	A	1442	G	C4-N9-C1'	7.60	136.38	126.50
1	A	522	C	C5-C6-N1	-7.59	117.20	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1438	G	C5-C6-O6	-7.59	124.05	128.60
1	A	1509	C	C4-C5-C6	7.58	121.19	117.40
1	A	1347	G	C8-N9-C4	7.57	109.43	106.40
1	A	18	C	C5-C6-N1	-7.57	117.22	121.00
1	A	795	C	N3-C4-N4	7.57	123.30	118.00
1	A	1132	C	C6-N1-C2	-7.56	117.28	120.30
1	A	578	C	N3-C4-C5	-7.56	118.88	121.90
1	A	331	G	C6-C5-N7	-7.55	125.87	130.40
1	A	482	A	C6-C5-N7	-7.55	127.02	132.30
1	A	1200	C	N1-C2-O2	7.54	123.42	118.90
1	A	190(F)	G	N3-C4-C5	7.54	132.37	128.60
1	A	253	U	N3-C2-O2	7.53	127.47	122.20
1	A	602	A	C2-N3-C4	-7.53	106.84	110.60
1	A	146	G	N1-C6-O6	7.52	124.41	119.90
1	A	326	G	N1-C6-O6	-7.51	115.39	119.90
1	A	1249	C	C5-C6-N1	7.51	124.75	121.00
1	A	1103	C	C2-N3-C4	-7.50	116.15	119.90
1	A	906	G	N1-C6-O6	7.47	124.38	119.90
1	A	1200	C	C6-N1-C1'	-7.47	111.83	120.80
1	A	279	A	C4-C5-N7	7.46	114.43	110.70
1	A	666	G	N1-C6-O6	7.46	124.38	119.90
1	A	316	G	N3-C4-N9	7.46	130.47	126.00
1	A	1161	C	C6-N1-C2	-7.45	117.32	120.30
1	A	117	G	C2-N3-C4	-7.45	108.17	111.90
1	A	23	C	C5-C6-N1	-7.45	117.27	121.00
1	A	238	G	N3-C2-N2	-7.45	114.68	119.90
1	A	598	U	C5-C6-N1	-7.45	118.97	122.70
1	A	328	C	C2-N1-C1'	7.45	126.99	118.80
1	A	820	U	N1-C2-N3	7.45	119.37	114.90
1	A	28	G	C6-C5-N7	-7.45	125.93	130.40
1	A	890	G	C4-C5-N7	-7.45	107.82	110.80
1	A	1395	C	C6-N1-C2	7.43	123.27	120.30
1	A	1249	C	C2-N1-C1'	7.43	126.97	118.80
1	A	1377	A	N7-C8-N9	-7.43	110.08	113.80
1	A	78	G	C4-C5-N7	7.42	113.77	110.80
1	A	106	C	N1-C2-N3	7.42	124.39	119.20
1	A	1517	G	N7-C8-N9	7.42	116.81	113.10
1	A	1329	A	C5-C6-N6	-7.42	117.77	123.70
1	A	190(G)	G	C4-C5-C6	7.41	123.25	118.80
1	A	875	C	C5-C6-N1	-7.41	117.30	121.00
1	A	482	A	C5-N7-C8	-7.40	100.20	103.90
1	A	950	U	C4-C5-C6	7.40	124.14	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	41	G	C8-N9-C4	-7.40	103.44	106.40
1	A	122	G	N1-C6-O6	7.40	124.34	119.90
1	A	1230	C	C6-N1-C2	-7.40	117.34	120.30
1	A	818	G	N9-C4-C5	7.40	108.36	105.40
1	A	1377	A	C6-C5-N7	7.40	137.48	132.30
1	A	873	A	N7-C8-N9	7.40	117.50	113.80
1	A	283	C	N3-C4-C5	-7.39	118.94	121.90
1	A	944	G	N7-C8-N9	7.38	116.79	113.10
1	A	1158	C	N1-C2-O2	7.38	123.33	118.90
1	A	1074	G	N1-C6-O6	7.38	124.33	119.90
1	A	97	G	C8-N9-C4	-7.37	103.45	106.40
1	A	642	A	C8-N9-C4	-7.36	102.86	105.80
1	A	1443	G	C8-N9-C4	7.36	109.34	106.40
1	A	266	G	C5-N7-C8	-7.36	100.62	104.30
1	A	945	G	C8-N9-C1'	7.36	136.57	127.00
1	A	888	G	C4-C5-C6	7.36	123.22	118.80
1	A	639	G	N1-C2-N3	7.35	128.31	123.90
1	A	669	U	N3-C2-O2	7.35	127.34	122.20
1	A	573	A	C4-C5-C6	7.34	120.67	117.00
1	A	819	A	C8-N9-C4	-7.34	102.86	105.80
1	A	766	A	N1-C6-N6	7.34	123.01	118.60
1	A	804	U	N3-C2-O2	-7.34	117.06	122.20
1	A	642	A	N7-C8-N9	7.33	117.46	113.80
1	A	310	G	C2-N3-C4	-7.33	108.24	111.90
1	A	944	G	N1-C6-O6	-7.32	115.51	119.90
1	A	1442	G	C8-N9-C1'	-7.32	117.49	127.00
1	A	299	G	C4-C5-N7	7.32	113.73	110.80
1	A	1103	C	N3-C4-N4	-7.31	112.88	118.00
1	A	14	U	C6-N1-C2	-7.31	116.61	121.00
1	A	1443	G	N3-C4-C5	7.31	132.26	128.60
1	A	693	G	N9-C4-C5	-7.31	102.48	105.40
1	A	227	G	C4-C5-N7	7.30	113.72	110.80
1	A	1504	G	N1-C6-O6	-7.30	115.52	119.90
1	A	28	G	C4-C5-C6	7.30	123.18	118.80
1	A	296	U	N3-C4-C5	-7.29	110.22	114.60
1	A	1482	G	N3-C4-C5	-7.29	124.95	128.60
1	A	1083	U	N3-C4-C5	-7.29	110.23	114.60
1	A	773	G	N7-C8-N9	7.29	116.74	113.10
1	A	1510	U	N3-C2-O2	-7.29	117.10	122.20
1	A	1501	C	C6-N1-C2	-7.27	117.39	120.30
1	A	730	G	N1-C2-N3	7.26	128.26	123.90
1	A	788	U	C5-C6-N1	7.26	126.33	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	76	C	N3-C4-C5	7.26	124.80	121.90
1	A	1411	C	C6-N1-C2	-7.25	117.40	120.30
1	A	1403	C	N1-C2-N3	-7.25	114.13	119.20
1	A	948	C	N3-C4-C5	7.24	124.80	121.90
1	A	654	G	N3-C4-N9	-7.23	121.66	126.00
1	A	383	A	C8-N9-C4	-7.23	102.91	105.80
1	A	666	G	C2-N3-C4	-7.22	108.29	111.90
1	A	778	G	C5-C6-N1	-7.22	107.89	111.50
1	A	1422	G	N3-C2-N2	-7.22	114.84	119.90
1	A	9	G	C5-C6-O6	-7.22	124.27	128.60
1	A	309	G	N1-C6-O6	7.22	124.23	119.90
1	A	890	G	N9-C4-C5	7.21	108.29	105.40
1	A	1329	A	C6-C5-N7	-7.21	127.25	132.30
1	A	945	G	C6-C5-N7	7.21	134.73	130.40
1	A	232	G	N3-C4-N9	7.21	130.33	126.00
1	A	1526	G	C5-C6-O6	-7.21	124.27	128.60
1	A	310	G	C4-C5-N7	7.20	113.68	110.80
1	A	310	G	N3-C4-C5	7.19	132.20	128.60
1	A	1354	C	N1-C2-O2	7.19	123.22	118.90
1	A	1442	G	N3-C4-C5	-7.19	125.00	128.60
1	A	589	C	C2-N3-C4	-7.19	116.31	119.90
1	A	90	U	C6-N1-C2	-7.18	116.69	121.00
1	A	569	C	C2-N3-C4	-7.18	116.31	119.90
1	A	1483	A	N1-C6-N6	-7.18	114.29	118.60
1	A	1329	A	C5-N7-C8	-7.17	100.31	103.90
1	A	1338	G	N3-C4-C5	-7.17	125.02	128.60
1	A	814	A	C8-N9-C4	7.16	108.66	105.80
1	A	296	U	C4-C5-C6	7.16	123.99	119.70
1	A	873	A	N1-C6-N6	-7.16	114.31	118.60
1	A	800	G	C4-N9-C1'	7.15	135.80	126.50
1	A	1455	G	C2-N3-C4	-7.15	108.33	111.90
1	A	1523	G	C6-C5-N7	-7.14	126.11	130.40
1	A	1377	A	C4-C5-N7	-7.14	107.13	110.70
1	A	1412	C	N3-C2-O2	-7.14	116.90	121.90
1	A	1523	G	N7-C8-N9	7.14	116.67	113.10
1	A	1496	C	N3-C4-C5	-7.13	119.05	121.90
1	A	129(A)	G	C5-N7-C8	-7.13	100.73	104.30
1	A	838	G	C8-N9-C4	7.13	109.25	106.40
1	A	929	G	C2-N3-C4	-7.12	108.34	111.90
1	A	950	U	C6-N1-C2	-7.12	116.73	121.00
1	A	671	G	N1-C6-O6	7.11	124.17	119.90
1	A	1084	G	C8-N9-C4	-7.10	103.56	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1333	A	N9-C4-C5	7.09	108.64	105.80
1	A	564	C	C2-N3-C4	7.09	123.44	119.90
1	A	814	A	N1-C6-N6	7.08	122.85	118.60
1	A	99	C	C5-C6-N1	7.08	124.54	121.00
1	A	1442	G	N3-C4-N9	7.08	130.25	126.00
1	A	266	G	N3-C4-N9	-7.07	121.76	126.00
1	A	1441	G	C5-C6-N1	-7.07	107.97	111.50
1	A	190(E)	U	C5-C6-N1	-7.06	119.17	122.70
1	A	576	G	C4-C5-C6	7.06	123.03	118.80
1	A	336	C	N3-C4-C5	7.06	124.72	121.90
1	A	1504	G	C6-N1-C2	-7.06	120.87	125.10
1	A	400	C	C6-N1-C2	7.04	123.12	120.30
1	A	863	U	N1-C2-N3	7.04	119.12	114.90
1	A	1108	G	N3-C4-C5	-7.02	125.09	128.60
1	A	881	G	C5-C6-O6	-7.02	124.39	128.60
1	A	1103	C	N3-C4-C5	7.02	124.71	121.90
1	A	357	G	N1-C6-O6	7.01	124.11	119.90
1	A	373	A	C5-N7-C8	-7.01	100.39	103.90
1	A	753	A	C4-C5-N7	-7.01	107.20	110.70
1	A	830	G	C4-C5-C6	7.00	123.00	118.80
1	A	899	C	C2-N1-C1'	6.99	126.49	118.80
1	A	589	C	C6-N1-C2	6.99	123.10	120.30
1	A	1049	U	C6-N1-C2	-6.99	116.81	121.00
1	A	723	U	C2-N1-C1'	6.98	126.07	117.70
1	A	56	U	C5-C4-O4	-6.97	121.72	125.90
1	A	729	A	N1-C6-N6	6.97	122.78	118.60
1	A	623	C	C6-N1-C2	6.97	123.09	120.30
1	A	615	C	C5-C6-N1	6.97	124.48	121.00
1	A	15	G	N9-C4-C5	-6.97	102.61	105.40
1	A	773	G	C5-N7-C8	-6.97	100.82	104.30
1	A	1346	A	C5-C6-N1	6.97	121.18	117.70
1	A	607	A	N9-C4-C5	-6.96	103.02	105.80
1	A	283	C	N3-C4-N4	6.96	122.87	118.00
1	A	318	G	N1-C6-O6	6.95	124.07	119.90
20	T	94	ALA	N-CA-C	-6.95	92.24	111.00
16	P	18	ARG	NE-CZ-NH1	-6.95	116.83	120.30
1	A	481	G	C5-C6-O6	-6.94	124.44	128.60
1	A	923	A	C2-N3-C4	-6.94	107.13	110.60
1	A	872	A	N9-C4-C5	-6.94	103.03	105.80
1	A	481	G	N7-C8-N9	-6.93	109.63	113.10
1	A	1165	C	C6-N1-C2	-6.93	117.53	120.30
1	A	190(C)	C	C6-N1-C2	-6.93	117.53	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1347	G	N1-C6-O6	6.93	124.06	119.90
1	A	1258	G	N3-C4-C5	-6.93	125.14	128.60
1	A	1502	A	C2-N3-C4	-6.92	107.14	110.60
1	A	890	G	C5-C6-O6	6.92	132.75	128.60
1	A	667	G	N1-C6-O6	6.92	124.05	119.90
1	A	818	G	C8-N9-C4	-6.91	103.64	106.40
1	A	1438	G	N1-C6-O6	6.91	124.05	119.90
1	A	1350	A	C8-N9-C4	-6.91	103.04	105.80
1	A	819	A	N7-C8-N9	6.90	117.25	113.80
1	A	889	A	C2-N3-C4	-6.90	107.15	110.60
1	A	928	G	C4-C5-N7	6.90	113.56	110.80
1	A	900	A	C2-N3-C4	-6.90	107.15	110.60
1	A	296	U	N1-C2-N3	6.89	119.04	114.90
1	A	253	U	C6-N1-C2	6.88	125.13	121.00
1	A	309	G	C5-C6-O6	-6.88	124.47	128.60
1	A	372	C	C6-N1-C1'	-6.88	112.54	120.80
1	A	950	U	N1-C2-N3	6.88	119.03	114.90
1	A	945	G	C2-N3-C4	6.88	115.34	111.90
1	A	723	U	C5-C6-N1	6.87	126.13	122.70
1	A	860	A	N1-C2-N3	6.87	132.73	129.30
1	A	765	G	C4-C5-N7	6.86	113.55	110.80
1	A	522	C	C2-N1-C1'	-6.85	111.26	118.80
1	A	868	C	N3-C4-C5	6.85	124.64	121.90
1	A	289	G	N7-C8-N9	6.85	116.52	113.10
1	A	1079	G	C4-C5-C6	6.84	122.90	118.80
1	A	450	G	C8-N9-C4	6.83	109.13	106.40
1	A	708	C	N3-C4-C5	6.83	124.63	121.90
1	A	818	G	N3-C4-N9	-6.83	121.90	126.00
1	A	733	A	C2-N3-C4	-6.83	107.19	110.60
1	A	635	G	C2-N3-C4	-6.83	108.49	111.90
1	A	746	A	C8-N9-C4	6.82	108.53	105.80
1	A	852	G	C2-N3-C4	-6.82	108.49	111.90
1	A	1235	U	N1-C2-O2	-6.82	118.03	122.80
1	A	945	G	C5-C6-N1	6.81	114.91	111.50
1	A	771	G	C2-N3-C4	-6.81	108.50	111.90
1	A	93	G	N9-C4-C5	-6.80	102.68	105.40
1	A	773	G	C5-C6-O6	-6.80	124.52	128.60
1	A	1455	G	C4-C5-N7	6.80	113.52	110.80
1	A	53	A	C8-N9-C4	-6.79	103.08	105.80
1	A	718	G	N3-C4-C5	-6.79	125.21	128.60
1	A	1525	G	N9-C4-C5	6.79	108.11	105.40
1	A	950	U	N3-C2-O2	-6.78	117.45	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1392	G	C4-C5-N7	6.78	113.51	110.80
1	A	789	U	C6-N1-C2	-6.78	116.93	121.00
1	A	451	A	C4-C5-C6	-6.78	113.61	117.00
1	A	22	G	C6-C5-N7	-6.77	126.34	130.40
1	A	107	G	N1-C6-O6	6.77	123.96	119.90
1	A	305	G	C8-N9-C1'	6.77	135.80	127.00
1	A	636	U	N3-C4-O4	6.76	124.13	119.40
1	A	577	G	C8-N9-C4	6.75	109.10	106.40
1	A	360	A	C5-N7-C8	-6.74	100.53	103.90
1	A	969	A	C6-C5-N7	-6.74	127.58	132.30
1	A	514	C	C6-N1-C2	-6.74	117.61	120.30
1	A	1345	U	N3-C2-O2	6.74	126.92	122.20
1	A	800	G	C8-N9-C1'	-6.74	118.24	127.00
1	A	851	G	C4-N9-C1'	6.74	135.25	126.50
1	A	1539	C	N3-C4-C5	6.72	124.59	121.90
1	A	963	G	N7-C8-N9	6.72	116.46	113.10
1	A	636	U	N3-C4-C5	-6.72	110.57	114.60
1	A	575	G	C4-C5-N7	6.72	113.49	110.80
1	A	1496	C	C2-N1-C1'	6.72	126.19	118.80
1	A	745	C	N3-C4-C5	6.71	124.58	121.90
1	A	791	G	N3-C4-C5	-6.71	125.24	128.60
1	A	199	G	N1-C6-O6	6.71	123.92	119.90
1	A	401	C	N3-C4-C5	6.71	124.58	121.90
1	A	252	U	C5-C6-N1	-6.71	119.35	122.70
1	A	1116	C	N3-C4-C5	6.71	124.58	121.90
1	A	931	C	C2-N3-C4	-6.70	116.55	119.90
1	A	821	G	C8-N9-C4	6.69	109.08	106.40
1	A	1079	G	C6-C5-N7	-6.69	126.39	130.40
1	A	1079	G	C8-N9-C4	-6.69	103.72	106.40
1	A	1378	C	C6-N1-C2	-6.69	117.62	120.30
1	A	687	A	C8-N9-C4	-6.69	103.13	105.80
1	A	1070	U	N1-C2-N3	6.68	118.91	114.90
1	A	190(F)	G	C4-N9-C1'	-6.68	117.81	126.50
1	A	280	C	C6-N1-C2	6.68	122.97	120.30
1	A	376	G	N7-C8-N9	-6.67	109.76	113.10
1	A	700	G	N3-C2-N2	6.67	124.57	119.90
1	A	1103	C	C5-C6-N1	-6.67	117.67	121.00
1	A	108	G	N1-C6-O6	6.67	123.90	119.90
1	A	1530	G	N3-C4-C5	6.67	131.93	128.60
1	A	1375	A	C5-N7-C8	6.67	107.23	103.90
1	A	129(A)	G	C5-C6-O6	-6.66	124.60	128.60
1	A	29	G	C2-N3-C4	-6.66	108.57	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	59	A	C5-C6-N1	6.66	121.03	117.70
1	A	676	A	C8-N9-C4	6.66	108.46	105.80
1	A	835	U	C5-C4-O4	6.66	129.89	125.90
1	A	530	G	C4-N9-C1'	6.65	135.15	126.50
1	A	1300	G	N1-C6-O6	-6.65	115.91	119.90
1	A	918	A	C6-N1-C2	-6.65	114.61	118.60
1	A	795	C	C5-C6-N1	6.64	124.32	121.00
1	A	43	C	C4-C5-C6	6.64	120.72	117.40
1	A	1531	A	N7-C8-N9	6.64	117.12	113.80
1	A	361	G	C8-N9-C4	6.64	109.06	106.40
1	A	1300	G	C4-C5-N7	-6.64	108.14	110.80
1	A	43	C	C6-N1-C2	6.63	122.95	120.30
1	A	15	G	N1-C6-O6	6.63	123.88	119.90
1	A	326	G	C5-N7-C8	6.63	107.61	104.30
1	A	279	A	C2-N3-C4	-6.62	107.29	110.60
1	A	771	G	N3-C4-C5	6.62	131.91	128.60
1	A	725	G	N1-C6-O6	6.62	123.87	119.90
1	A	373	A	N7-C8-N9	6.62	117.11	113.80
1	A	607	A	C4-C5-N7	6.61	114.00	110.70
1	A	871	U	N1-C2-O2	6.61	127.42	122.80
1	A	176	C	C6-N1-C2	6.59	122.94	120.30
1	A	583	A	N1-C6-N6	6.59	122.56	118.60
1	A	597	G	C6-C5-N7	-6.59	126.44	130.40
1	A	135	C	C5-C6-N1	6.59	124.30	121.00
1	A	316	G	C6-C5-N7	-6.59	126.44	130.40
1	A	577	G	N1-C6-O6	6.59	123.86	119.90
1	A	826	C	C2-N1-C1'	6.59	126.05	118.80
1	A	1487	G	N3-C4-C5	-6.58	125.31	128.60
1	A	108	G	C5-N7-C8	-6.58	101.01	104.30
1	A	572	A	C5-C6-N1	6.57	120.99	117.70
1	A	1332	A	N9-C4-C5	6.57	108.43	105.80
1	A	773	G	N1-C6-O6	6.57	123.84	119.90
1	A	235	C	N3-C4-C5	6.57	124.53	121.90
1	A	287	U	C6-N1-C2	-6.57	117.06	121.00
1	A	299	G	N9-C4-C5	-6.57	102.77	105.40
1	A	1051	C	N3-C4-C5	-6.57	119.27	121.90
1	A	180	U	N3-C4-O4	6.56	123.99	119.40
1	A	1079	G	C4-N9-C1'	6.56	135.03	126.50
1	A	1277	C	C6-N1-C2	-6.56	117.67	120.30
1	A	322	C	C6-N1-C2	6.56	122.92	120.30
1	A	945	G	N1-C6-O6	-6.56	115.96	119.90
1	A	855	G	C5-C6-O6	-6.56	124.66	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1099	G	N1-C6-O6	6.56	123.83	119.90
1	A	1529	G	C8-N9-C1'	-6.56	118.47	127.00
1	A	825	G	C8-N9-C1'	-6.55	118.48	127.00
1	A	1438	G	C4-C5-N7	6.55	113.42	110.80
1	A	1354	C	N3-C2-O2	-6.55	117.32	121.90
1	A	74	C	C2-N1-C1'	6.55	126.00	118.80
1	A	543	C	C6-N1-C2	-6.54	117.68	120.30
1	A	284	G	C5-C6-O6	-6.53	124.68	128.60
1	A	870	U	C5-C6-N1	-6.53	119.43	122.70
1	A	1280	A	N9-C4-C5	6.53	108.41	105.80
1	A	875	C	C6-N1-C2	6.53	122.91	120.30
1	A	373	A	C6-C5-N7	-6.53	127.73	132.30
1	A	245	C	C4-C5-C6	-6.53	114.14	117.40
1	A	372	C	N3-C4-N4	6.52	122.57	118.00
1	A	624	C	N3-C4-C5	6.52	124.51	121.90
1	A	774	G	C6-C5-N7	-6.52	126.49	130.40
1	A	1238	A	C5-C6-N6	6.52	128.91	123.70
1	A	108	G	C4-N9-C1'	6.51	134.97	126.50
1	A	909	A	C8-N9-C4	-6.51	103.19	105.80
1	A	875	C	N3-C4-C5	6.51	124.50	121.90
1	A	1108	G	C4-N9-C1'	6.51	134.97	126.50
1	A	328	C	N3-C4-N4	-6.51	113.45	118.00
1	A	1251	A	C8-N9-C4	-6.50	103.20	105.80
1	A	731	G	C4-C5-N7	6.50	113.40	110.80
1	A	687	A	N3-C4-C5	-6.50	122.25	126.80
1	A	245	C	C5-C6-N1	6.49	124.25	121.00
1	A	1506	U	N1-C2-O2	6.49	127.34	122.80
1	A	285	G	C2-N3-C4	-6.49	108.66	111.90
1	A	1280	A	N1-C6-N6	-6.49	114.71	118.60
1	A	576	G	N1-C2-N3	6.48	127.79	123.90
1	A	1416	G	C4-C5-N7	6.48	113.39	110.80
1	A	54	C	N3-C2-O2	-6.48	117.36	121.90
1	A	873	A	C2-N3-C4	6.47	113.84	110.60
1	A	667	G	C2-N3-C4	-6.47	108.67	111.90
1	A	730	G	N3-C4-C5	-6.47	125.36	128.60
1	A	1504	G	N3-C4-N9	6.47	129.88	126.00
1	A	809	G	N1-C6-O6	6.46	123.78	119.90
1	A	1491	G	C8-N9-C4	-6.46	103.82	106.40
1	A	28	G	C5-C6-N1	-6.46	108.27	111.50
1	A	168	G	C6-C5-N7	-6.46	126.53	130.40
1	A	773	G	C8-N9-C4	-6.45	103.82	106.40
1	A	851	G	N7-C8-N9	6.45	116.33	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1529	G	N3-C4-C5	-6.45	125.37	128.60
1	A	569	C	N1-C2-O2	-6.45	115.03	118.90
1	A	16	A	N7-C8-N9	-6.44	110.58	113.80
1	A	190(F)	G	C8-N9-C1'	6.43	135.36	127.00
1	A	1346	A	P-O3'-C3'	6.43	127.42	119.70
1	A	263	A	C5-C6-N1	6.43	120.92	117.70
1	A	515	G	N1-C6-O6	6.43	123.76	119.90
1	A	227	G	C5-C6-O6	-6.42	124.75	128.60
1	A	975	A	N1-C6-N6	6.42	122.45	118.60
1	A	765	G	C5-N7-C8	-6.42	101.09	104.30
1	A	1187	G	C5-C6-O6	-6.42	124.75	128.60
1	A	253	U	C2-N1-C1'	-6.42	110.00	117.70
1	A	1158	C	C2-N1-C1'	6.42	125.86	118.80
1	A	237	C	C6-N1-C2	-6.42	117.73	120.30
1	A	325	A	N9-C4-C5	6.41	108.36	105.80
1	A	251	G	N3-C4-N9	6.41	129.85	126.00
1	A	1429	C	C6-N1-C2	-6.41	117.74	120.30
1	A	1079	G	N1-C2-N2	-6.40	110.44	116.20
1	A	13	U	N3-C2-O2	-6.40	117.72	122.20
1	A	859	A	N1-C6-N6	6.40	122.44	118.60
1	A	885	G	C6-C5-N7	-6.40	126.56	130.40
1	A	881	G	N1-C6-O6	6.40	123.74	119.90
1	A	1524	C	C2-N1-C1'	6.39	125.83	118.80
1	A	325	A	C5-C6-N6	6.39	128.81	123.70
1	A	1149	C	C6-N1-C2	-6.39	117.74	120.30
1	A	944	G	N3-C4-C5	-6.39	125.41	128.60
1	A	397	A	N7-C8-N9	6.38	116.99	113.80
1	A	503	C	C6-N1-C2	-6.38	117.75	120.30
1	A	948	C	C5-C6-N1	-6.38	117.81	121.00
1	A	238	G	C2-N3-C4	-6.38	108.71	111.90
1	A	814	A	C2-N3-C4	-6.38	107.41	110.60
1	A	1527	C	C6-N1-C2	-6.38	117.75	120.30
1	A	289	G	N1-C2-N3	6.38	127.72	123.90
1	A	1156	G	C8-N9-C4	-6.37	103.85	106.40
1	A	108	G	C6-C5-N7	-6.37	126.58	130.40
1	A	1461	G	C4-C5-N7	6.37	113.35	110.80
1	A	237	C	N3-C2-O2	-6.37	117.44	121.90
1	A	766	A	C8-N9-C4	6.37	108.35	105.80
1	A	875	C	C2-N3-C4	-6.37	116.72	119.90
1	A	735	C	C2-N1-C1'	-6.37	111.80	118.80
1	A	871	U	N1-C2-N3	-6.37	111.08	114.90
1	A	1395	C	C2-N1-C1'	-6.37	111.80	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	825	G	C8-N9-C4	6.36	108.95	106.40
1	A	309	G	C6-C5-N7	-6.36	126.58	130.40
1	A	888	G	C4-N9-C1'	6.36	134.76	126.50
1	A	1517	G	C5-C6-N1	-6.36	108.32	111.50
1	A	297	G	C8-N9-C4	-6.35	103.86	106.40
1	A	753	A	N9-C4-C5	6.35	108.34	105.80
1	A	526	C	N3-C4-C5	6.35	124.44	121.90
1	A	1377	A	N9-C4-C5	6.34	108.34	105.80
1	A	835	U	N1-C2-N3	6.34	118.70	114.90
1	A	852	G	N3-C4-C5	6.34	131.77	128.60
1	A	522	C	N3-C4-N4	-6.34	113.56	118.00
1	A	276	G	C8-N9-C4	6.33	108.93	106.40
1	A	1487	G	C4-N9-C1'	6.33	134.73	126.50
1	A	244	U	N3-C2-O2	6.33	126.63	122.20
1	A	274	A	C8-N9-C4	6.33	108.33	105.80
1	A	308	C	N3-C4-N4	6.33	122.43	118.00
1	A	778	G	C2-N3-C4	-6.32	108.74	111.90
1	A	1344	C	N3-C4-N4	-6.32	113.58	118.00
1	A	131	C	C6-N1-C2	6.32	122.83	120.30
1	A	376	G	C8-N9-C4	6.32	108.93	106.40
1	A	744	C	C6-N1-C2	6.31	122.83	120.30
1	A	190(G)	G	C2-N3-C4	-6.31	108.74	111.90
1	A	79	G	N7-C8-N9	6.31	116.25	113.10
1	A	81	U	C6-N1-C2	-6.31	117.22	121.00
1	A	128	G	N1-C6-O6	6.30	123.68	119.90
1	A	228	A	N1-C6-N6	6.30	122.38	118.60
1	A	730	G	C4-N9-C1'	6.30	134.69	126.50
1	A	880	C	C5-C4-N4	-6.29	115.79	120.20
1	A	916	G	C4-N9-C1'	6.29	134.68	126.50
1	A	652	U	C5-C4-O4	-6.29	122.12	125.90
1	A	260	G	N7-C8-N9	6.29	116.24	113.10
1	A	110	C	N1-C2-O2	6.29	122.67	118.90
1	A	324	G	N3-C4-N9	-6.28	122.23	126.00
1	A	718	G	C4-N9-C1'	6.28	134.67	126.50
1	A	573	A	N3-C4-C5	-6.28	122.40	126.80
1	A	1300	G	C6-C5-N7	6.28	134.17	130.40
1	A	693	G	C6-C5-N7	-6.28	126.63	130.40
1	A	1359	C	C6-N1-C2	-6.27	117.79	120.30
1	A	530	G	C8-N9-C4	-6.27	103.89	106.40
1	A	830	G	C6-C5-N7	-6.27	126.64	130.40
1	A	882	C	C5-C6-N1	-6.27	117.86	121.00
1	A	6	G	C5-C6-N1	-6.27	108.37	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	230	G	N1-C2-N3	6.27	127.66	123.90
1	A	835	U	N3-C2-O2	-6.26	117.81	122.20
1	A	148	G	C8-N9-C4	6.26	108.91	106.40
1	A	117	G	N9-C4-C5	-6.26	102.90	105.40
1	A	295	C	C5-C6-N1	-6.25	117.87	121.00
1	A	730	G	C8-N9-C1'	-6.25	118.87	127.00
1	A	641	U	N3-C2-O2	6.25	126.58	122.20
1	A	1235	U	C6-N1-C2	-6.25	117.25	121.00
1	A	376	G	C5-N7-C8	6.24	107.42	104.30
1	A	1432	G	C5-C6-O6	6.24	132.35	128.60
1	A	91	C	C2-N1-C1'	6.24	125.67	118.80
1	A	122	G	C6-C5-N7	-6.24	126.66	130.40
1	A	1398	A	N1-C2-N3	6.24	132.42	129.30
1	A	945	G	N1-C2-N2	6.24	121.82	116.20
1	A	1043	C	C6-N1-C2	-6.24	117.80	120.30
1	A	220	G	C4-N9-C1'	6.24	134.61	126.50
1	A	1305	G	N1-C6-O6	6.24	123.64	119.90
1	A	888	G	N3-C4-C5	-6.24	125.48	128.60
1	A	828	A	N1-C6-N6	6.23	122.34	118.60
1	A	888	G	C8-N9-C4	-6.23	103.91	106.40
1	A	1332	A	C5-C6-N6	6.23	128.68	123.70
1	A	167	G	N3-C4-C5	-6.23	125.49	128.60
1	A	545	C	N3-C4-C5	-6.23	119.41	121.90
1	A	575	G	N3-C4-C5	6.22	131.71	128.60
1	A	1126	U	C5-C6-N1	6.21	125.81	122.70
1	A	1526	G	C4-C5-N7	6.21	113.29	110.80
1	A	522	C	C6-N1-C2	6.21	122.78	120.30
1	A	577	G	N9-C4-C5	-6.21	102.92	105.40
1	A	199	G	C6-C5-N7	-6.21	126.67	130.40
1	A	1061	G	N1-C6-O6	6.20	123.62	119.90
1	A	41	G	N7-C8-N9	6.20	116.20	113.10
1	A	587	G	C4-C5-N7	-6.20	108.32	110.80
1	A	918	A	C5-C6-N1	6.20	120.80	117.70
1	A	1533	C	C2-N1-C1'	6.20	125.62	118.80
1	A	820	U	N1-C2-O2	-6.20	118.46	122.80
1	A	481	G	C5-N7-C8	6.19	107.40	104.30
1	A	769	G	C8-N9-C4	-6.19	103.92	106.40
1	A	1333	A	C5-C6-N6	6.19	128.65	123.70
1	A	1461	G	N9-C4-C5	-6.19	102.92	105.40
1	A	564	C	N1-C2-N3	-6.19	114.87	119.20
1	A	81	U	C5-C6-N1	6.18	125.79	122.70
1	A	182	U	C5-C6-N1	6.18	125.79	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1281	U	C6-N1-C2	-6.18	117.29	121.00
1	A	585	G	N7-C8-N9	-6.18	110.01	113.10
1	A	1505	G	C5-N7-C8	-6.18	101.21	104.30
1	A	780	A	C6-N1-C2	-6.18	114.89	118.60
1	A	1438	G	C6-C5-N7	-6.18	126.69	130.40
1	A	400	C	N3-C4-C5	6.17	124.37	121.90
1	A	1158	C	N3-C2-O2	-6.17	117.58	121.90
1	A	946	A	C8-N9-C4	-6.17	103.33	105.80
1	A	137	C	C6-N1-C2	6.17	122.77	120.30
1	A	305	G	N3-C2-N2	-6.17	115.58	119.90
1	A	766	A	N9-C4-C5	-6.17	103.33	105.80
1	A	919	A	C2-N3-C4	6.17	113.68	110.60
1	A	97	G	N3-C4-C5	-6.16	125.52	128.60
1	A	570	G	C4-N9-C1'	6.16	134.51	126.50
1	A	1078	U	C5-C6-N1	6.16	125.78	122.70
1	A	693	G	N1-C6-O6	6.16	123.60	119.90
1	A	506	G	N1-C6-O6	-6.16	116.21	119.90
1	A	93	G	N3-C4-N9	6.16	129.69	126.00
1	A	1075	C	C2-N1-C1'	6.16	125.57	118.80
1	A	1100	C	C6-N1-C2	-6.16	117.84	120.30
1	A	119	A	N9-C4-C5	6.15	108.26	105.80
1	A	1332	A	C8-N9-C4	-6.15	103.34	105.80
1	A	333	G	N1-C6-O6	6.15	123.59	119.90
1	A	820	U	C5-C6-N1	-6.15	119.62	122.70
1	A	1282	C	C5-C6-N1	6.15	124.08	121.00
1	A	1505	G	C6-C5-N7	-6.15	126.71	130.40
1	A	247	G	N3-C2-N2	-6.15	115.60	119.90
1	A	1335	C	N3-C2-O2	-6.14	117.60	121.90
1	A	642	A	C5-N7-C8	-6.14	100.83	103.90
1	A	522	C	C5-C4-N4	6.14	124.50	120.20
1	A	1505	G	N9-C4-C5	6.13	107.85	105.40
1	A	1093	A	N1-C6-N6	6.13	122.28	118.60
1	A	562	C	N1-C2-O2	6.13	122.58	118.90
1	A	825	G	N1-C6-O6	6.13	123.58	119.90
1	A	111	G	N3-C4-N9	-6.12	122.33	126.00
1	A	812	C	C5-C4-N4	6.12	124.49	120.20
1	A	180	U	C5-C6-N1	6.12	125.76	122.70
1	A	1354	C	C5-C6-N1	6.12	124.06	121.00
1	A	98	U	C5-C6-N1	6.12	125.76	122.70
1	A	597	G	C4-N9-C1'	6.12	134.45	126.50
1	A	867	G	C2-N3-C4	-6.12	108.84	111.90
1	A	1361(A)	C	C5-C6-N1	6.12	124.06	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	872	A	C2-N3-C4	-6.11	107.54	110.60
1	A	167	G	C8-N9-C4	-6.11	103.95	106.40
1	A	736	C	N3-C4-C5	6.11	124.34	121.90
1	A	901	A	C2-N3-C4	-6.11	107.54	110.60
1	A	654	G	C2-N3-C4	-6.11	108.84	111.90
1	A	896	C	C6-N1-C2	-6.11	117.86	120.30
1	A	711	G	N1-C6-O6	6.11	123.56	119.90
1	A	1467	G	N3-C4-C5	6.11	131.66	128.60
1	A	1347	G	C4-C5-N7	6.10	113.24	110.80
1	A	1476	G	C8-N9-C4	-6.10	103.96	106.40
1	A	1342	C	N3-C4-N4	6.10	122.27	118.00
1	A	570	G	C8-N9-C1'	-6.10	119.07	127.00
1	A	1544	U	N3-C4-O4	6.09	123.67	119.40
1	A	541	G	N1-C6-O6	6.09	123.56	119.90
1	A	303	A	N1-C6-N6	6.09	122.25	118.60
1	A	220	G	C6-C5-N7	-6.09	126.75	130.40
1	A	576	G	C4-N9-C1'	6.09	134.41	126.50
1	A	747	C	C6-N1-C2	6.09	122.73	120.30
1	A	753	A	N3-C4-C5	-6.08	122.54	126.80
1	A	859	A	N7-C8-N9	6.08	116.84	113.80
1	A	659	U	C5-C6-N1	-6.08	119.66	122.70
1	A	651	C	N3-C4-C5	6.08	124.33	121.90
1	A	658	G	N9-C4-C5	-6.08	102.97	105.40
1	A	1415	G	N1-C6-O6	6.08	123.55	119.90
1	A	476	G	C8-N9-C4	-6.07	103.97	106.40
1	A	820	U	C2-N3-C4	-6.07	123.36	127.00
1	A	107	G	C4-C5-N7	6.07	113.23	110.80
1	A	382	A	C6-C5-N7	-6.07	128.05	132.30
1	A	1181	G	C4-N9-C1'	-6.07	118.61	126.50
1	A	1281	U	C5-C6-N1	6.07	125.73	122.70
1	A	79	G	N1-C6-O6	6.07	123.54	119.90
1	A	129(A)	G	N1-C6-O6	6.07	123.54	119.90
1	A	228	A	C2-N3-C4	-6.07	107.57	110.60
1	A	800	G	N1-C2-N3	6.07	127.54	123.90
1	A	283	C	C5-C6-N1	6.07	124.03	121.00
1	A	110	C	N3-C2-O2	-6.06	117.66	121.90
1	A	113	G	C6-C5-N7	-6.06	126.76	130.40
1	A	289	G	C6-C5-N7	-6.06	126.76	130.40
1	A	382	A	N7-C8-N9	6.06	116.83	113.80
1	A	577	G	C4-C5-N7	6.06	113.22	110.80
1	A	773	G	C4-N9-C1'	6.06	134.38	126.50
1	A	190(G)	G	C4-N9-C1'	6.05	134.37	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	53	A	C4-C5-C6	6.05	120.03	117.00
1	A	1379	G	N3-C4-C5	-6.05	125.57	128.60
1	A	1509	C	C5-C6-N1	-6.05	117.97	121.00
1	A	753	A	N1-C6-N6	-6.05	114.97	118.60
1	A	285	G	C6-C5-N7	-6.05	126.77	130.40
1	A	1530	G	N1-C6-O6	6.05	123.53	119.90
1	A	945	G	C4-N9-C1'	-6.04	118.64	126.50
1	A	1374	A	C4-C5-C6	6.04	120.02	117.00
1	A	1377	A	C5-C6-N6	6.04	128.53	123.70
1	A	74	C	C6-N1-C1'	-6.04	113.56	120.80
1	A	928	G	N9-C4-C5	-6.04	102.98	105.40
1	A	899	C	C6-N1-C2	-6.04	117.89	120.30
1	A	916	G	N3-C4-C5	-6.04	125.58	128.60
1	A	926	G	N3-C4-C5	-6.04	125.58	128.60
1	A	726	C	C2-N3-C4	-6.03	116.88	119.90
1	A	654	G	N3-C2-N2	-6.03	115.68	119.90
1	A	558	G	C4-C5-N7	6.03	113.21	110.80
1	A	968	A	N1-C6-N6	6.02	122.21	118.60
1	A	859	A	C5-C6-N6	-6.02	118.88	123.70
1	A	1104	G	N3-C4-N9	6.02	129.61	126.00
1	A	115	G	N7-C8-N9	-6.02	110.09	113.10
1	A	825	G	N9-C4-C5	-6.02	102.99	105.40
1	A	167	G	N1-C6-O6	-6.01	116.29	119.90
1	A	970	C	N1-C2-O2	6.01	122.50	118.90
1	A	597	G	N1-C2-N3	6.00	127.50	123.90
1	A	1056	U	N1-C2-N3	-6.00	111.30	114.90
1	A	9	G	N9-C4-C5	-6.00	103.00	105.40
1	A	450	G	N7-C8-N9	-6.00	110.10	113.10
1	A	658	G	C8-N9-C4	6.00	108.80	106.40
1	A	1523	G	C5-N7-C8	-5.99	101.30	104.30
1	A	777	A	C8-N9-C4	-5.99	103.40	105.80
1	A	731	G	N9-C4-C5	-5.99	103.00	105.40
1	A	969	A	C4-C5-N7	5.99	113.69	110.70
1	A	78	G	C5-C6-O6	-5.99	125.01	128.60
1	A	572	A	C2-N3-C4	5.99	113.59	110.60
1	A	204	U	C2-N1-C1'	5.98	124.88	117.70
1	A	1353	G	C5-C6-N1	5.98	114.49	111.50
1	A	299	G	N3-C4-N9	5.98	129.59	126.00
1	A	1377	A	C6-N1-C2	-5.97	115.02	118.60
1	A	1422	G	C5-C6-N1	-5.97	108.51	111.50
1	A	692	U	N3-C2-O2	-5.97	118.02	122.20
1	A	725	G	C6-C5-N7	-5.97	126.82	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	755	G	C5-C6-N1	5.97	114.49	111.50
1	A	1523	G	C4-C5-N7	5.97	113.19	110.80
1	A	613	C	C6-N1-C2	5.97	122.69	120.30
1	A	1374	A	N1-C2-N3	5.97	132.28	129.30
1	A	1511	G	C4-C5-N7	5.97	113.19	110.80
1	A	521	G	C5-C6-N1	5.96	114.48	111.50
1	A	576	G	N3-C4-C5	-5.96	125.62	128.60
1	A	895	G	C8-N9-C4	-5.96	104.02	106.40
1	A	981	U	N3-C2-O2	5.96	126.37	122.20
1	A	1083	U	C6-N1-C2	-5.95	117.43	121.00
1	A	1237	C	C4-C5-C6	5.95	120.37	117.40
1	A	1446	A	C8-N9-C4	5.94	108.18	105.80
1	A	868	C	C2-N3-C4	-5.94	116.93	119.90
1	A	942	G	N1-C6-O6	5.94	123.47	119.90
1	A	1306	A	C4-C5-C6	5.94	119.97	117.00
1	A	1533	C	C5-C6-N1	5.94	123.97	121.00
1	A	98	U	C6-N1-C2	-5.94	117.44	121.00
1	A	906	G	C6-C5-N7	-5.94	126.84	130.40
1	A	605	U	N1-C2-O2	5.94	126.95	122.80
1	A	1079	G	N3-C4-N9	5.93	129.56	126.00
1	A	751	U	N3-C2-O2	5.93	126.35	122.20
1	A	269	C	C6-N1-C2	-5.92	117.93	120.30
1	A	576	G	C8-N9-C1'	-5.92	119.30	127.00
1	A	1108	G	N3-C4-N9	5.92	129.56	126.00
1	A	1346	A	C6-N1-C2	-5.92	115.05	118.60
1	A	863	U	C4-C5-C6	5.92	123.25	119.70
1	A	1502	A	C5-C6-N6	-5.92	118.97	123.70
1	A	970	C	N3-C2-O2	-5.92	117.76	121.90
1	A	1344	C	C5-C6-N1	-5.92	118.04	121.00
1	A	233	C	N1-C2-O2	5.91	122.45	118.90
1	A	277	C	C6-N1-C2	5.91	122.66	120.30
1	A	1432	G	C5-C6-N1	-5.91	108.55	111.50
1	A	936	C	N1-C2-O2	5.91	122.44	118.90
1	A	372	C	N3-C2-O2	5.91	126.03	121.90
1	A	793	U	C5-C6-N1	5.91	125.65	122.70
1	A	487	A	C8-N9-C4	5.90	108.16	105.80
1	A	23	C	C2-N3-C4	-5.90	116.95	119.90
1	A	670	G	C8-N9-C1'	-5.90	119.33	127.00
1	A	605	U	N3-C4-O4	-5.90	115.27	119.40
1	A	20	G	C2-N3-C4	-5.89	108.95	111.90
1	A	15	G	C4-N9-C1'	5.89	134.16	126.50
1	A	573	A	C6-N1-C2	-5.89	115.07	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1069	C	C6-N1-C2	5.89	122.66	120.30
1	A	1308	U	N3-C2-O2	5.89	126.32	122.20
1	A	1496	C	N3-C2-O2	-5.89	117.78	121.90
1	A	971	G	C4-C5-N7	-5.89	108.44	110.80
1	A	279	A	N1-C2-N3	5.89	132.24	129.30
1	A	697	U	C2-N1-C1'	-5.89	110.64	117.70
1	A	764	C	C6-N1-C2	-5.89	117.94	120.30
1	A	1061	G	C5-C6-N1	-5.89	108.56	111.50
1	A	897	C	N3-C4-N4	5.88	122.12	118.00
1	A	251	G	N9-C4-C5	-5.88	103.05	105.40
1	A	587	G	N1-C6-O6	-5.88	116.37	119.90
1	A	9	G	C8-N9-C1'	-5.88	119.36	127.00
1	A	565	U	C4-C5-C6	-5.88	116.17	119.70
1	A	722	A	C5-N7-C8	-5.88	100.96	103.90
1	A	833	U	N1-C2-O2	5.87	126.91	122.80
1	A	1449	C	C6-N1-C2	5.87	122.65	120.30
1	A	590	C	C6-N1-C2	5.87	122.65	120.30
1	A	779	C	C4-C5-C6	5.87	120.34	117.40
1	A	1467	G	N3-C4-N9	-5.87	122.48	126.00
1	A	454	C	C6-N1-C2	-5.87	117.95	120.30
1	A	116	A	N1-C6-N6	5.87	122.12	118.60
1	A	371	G	C5-C6-N1	5.87	114.43	111.50
1	A	872	A	C6-C5-N7	-5.87	128.19	132.30
1	A	1527	C	C2-N1-C1'	5.87	125.25	118.80
1	A	1441	G	C4-C5-C6	5.86	122.32	118.80
1	A	1195	C	C5-C6-N1	5.86	123.93	121.00
1	A	201	C	C6-N1-C1'	5.86	127.83	120.80
1	A	127	G	N1-C6-O6	5.86	123.42	119.90
1	A	796	C	C6-N1-C2	-5.86	117.96	120.30
17	Q	22	LEU	CA-CB-CG	-5.85	101.84	115.30
1	A	23	C	C4-C5-C6	5.85	120.33	117.40
1	A	530	G	N7-C8-N9	5.85	116.03	113.10
1	A	864	A	N9-C4-C5	5.85	108.14	105.80
1	A	1455	G	C5-C6-N1	-5.85	108.57	111.50
1	A	113	G	N3-C4-N9	5.85	129.51	126.00
1	A	637	G	C8-N9-C1'	-5.85	119.39	127.00
1	A	1093	A	C5-C6-N6	-5.85	119.02	123.70
1	A	1202	G	N1-C6-O6	-5.85	116.39	119.90
1	A	838	G	N7-C8-N9	-5.85	110.18	113.10
1	A	919	A	C8-N9-C4	5.85	108.14	105.80
1	A	1179	A	N1-C6-N6	-5.84	115.09	118.60
1	A	580	U	C4-C5-C6	5.84	123.21	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	521	G	N1-C6-O6	-5.84	116.39	119.90
1	A	654	G	N3-C4-C5	5.84	131.52	128.60
1	A	599	C	N3-C2-O2	5.84	125.99	121.90
1	A	637	G	N3-C4-N9	5.84	129.50	126.00
1	A	766	A	C5-C6-N6	-5.84	119.03	123.70
1	A	220	G	N3-C4-N9	5.84	129.50	126.00
1	A	310	G	C6-C5-N7	-5.83	126.90	130.40
1	A	75	G	N3-C4-C5	-5.83	125.68	128.60
1	A	639	G	N1-C2-N2	-5.83	110.95	116.20
1	A	634	C	N3-C2-O2	-5.83	117.82	121.90
1	A	785	G	N1-C6-O6	5.82	123.39	119.90
1	A	830	G	N3-C2-N2	-5.82	115.82	119.90
1	A	856	C	C4-C5-C6	5.82	120.31	117.40
1	A	1181	G	N3-C4-C5	5.82	131.51	128.60
1	A	636	U	C4-C5-C6	5.82	123.19	119.70
1	A	730	G	C4-C5-C6	5.82	122.29	118.80
17	Q	35	VAL	CG1-CB-CG2	5.82	120.21	110.90
1	A	909	A	C6-N1-C2	-5.81	115.11	118.60
1	A	658	G	C4-N9-C1'	5.80	134.04	126.50
1	A	1416	G	N1-C6-O6	5.80	123.38	119.90
1	A	260	G	N3-C2-N2	-5.80	115.84	119.90
1	A	707	C	C6-N1-C2	5.79	122.62	120.30
1	A	556	C	C5-C6-N1	-5.79	118.11	121.00
1	A	1408	A	N1-C6-N6	5.79	122.07	118.60
1	A	733	A	C8-N9-C4	5.79	108.11	105.80
1	A	305	G	N7-C8-N9	5.79	115.99	113.10
1	A	1063	C	C4-C5-C6	5.79	120.29	117.40
1	A	266	G	C4-C5-N7	5.78	113.11	110.80
1	A	396	G	C6-C5-N7	-5.78	126.93	130.40
1	A	1483	A	N9-C4-C5	5.78	108.11	105.80
1	A	1084	G	N1-C6-O6	-5.77	116.44	119.90
1	A	1107	C	C6-N1-C2	-5.77	117.99	120.30
1	A	119	A	C8-N9-C4	-5.77	103.49	105.80
1	A	794	A	C4-C5-N7	-5.77	107.81	110.70
1	A	1517	G	C4-C5-C6	5.77	122.26	118.80
1	A	719	C	N1-C2-O2	5.77	122.36	118.90
1	A	886	G	C2-N3-C4	-5.77	109.02	111.90
1	A	782	A	C6-N1-C2	-5.77	115.14	118.60
1	A	1503	A	C8-N9-C4	5.77	108.11	105.80
1	A	1446	A	N7-C8-N9	-5.76	110.92	113.80
1	A	331	G	N9-C4-C5	-5.76	103.09	105.40
1	A	1497	G	N7-C8-N9	5.76	115.98	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	575	G	N1-C2-N3	5.76	127.36	123.90
1	A	508	C	N1-C2-O2	5.76	122.36	118.90
1	A	47	C	N3-C2-O2	-5.75	117.87	121.90
1	A	275	G	C8-N9-C4	5.75	108.70	106.40
1	A	1287	A	C8-N9-C4	-5.75	103.50	105.80
1	A	1300	G	C5-C6-O6	5.75	132.05	128.60
1	A	1091	U	N1-C2-O2	5.75	126.83	122.80
1	A	374	A	N1-C6-N6	-5.75	115.15	118.60
1	A	715	A	C5-C6-N1	-5.75	114.83	117.70
1	A	307	C	N1-C2-O2	5.75	122.35	118.90
1	A	637	G	N3-C4-C5	-5.75	125.73	128.60
1	A	509	A	C8-N9-C4	-5.74	103.50	105.80
1	A	1187	G	C4-C5-N7	5.74	113.10	110.80
1	A	220	G	C8-N9-C1'	-5.74	119.54	127.00
1	A	881	G	C6-C5-N7	-5.74	126.96	130.40
1	A	121	C	C5-C6-N1	-5.74	118.13	121.00
1	A	803	G	N1-C2-N2	-5.74	111.04	116.20
1	A	144	G	N1-C6-O6	5.73	123.34	119.90
1	A	1079	G	N1-C2-N3	5.73	127.34	123.90
1	A	103	C	C5-C6-N1	5.73	123.87	121.00
1	A	862	C	C5-C4-N4	-5.73	116.19	120.20
1	A	78	G	C8-N9-C4	5.73	108.69	106.40
1	A	117	G	C8-N9-C4	5.72	108.69	106.40
1	A	578	C	N1-C2-N3	5.72	123.21	119.20
1	A	791	G	N7-C8-N9	5.72	115.96	113.10
1	A	653	A	N1-C6-N6	-5.72	115.17	118.60
1	A	1496	C	C5-C6-N1	5.72	123.86	121.00
1	A	1523	G	N1-C2-N2	5.72	121.34	116.20
1	A	382	A	C4-C5-C6	5.71	119.86	117.00
1	A	308	C	C5-C4-N4	-5.71	116.20	120.20
1	A	15	G	N3-C4-N9	5.71	129.42	126.00
1	A	190(E)	U	C2-N3-C4	-5.71	123.58	127.00
1	A	44	G	C6-C5-N7	-5.70	126.98	130.40
1	A	824	C	N1-C2-O2	-5.70	115.48	118.90
1	A	862	C	C5-C6-N1	5.70	123.85	121.00
1	A	1348	U	C2-N1-C1'	5.70	124.54	117.70
1	A	204	U	C5-C6-N1	5.70	125.55	122.70
1	A	328	C	N3-C4-C5	5.70	124.18	121.90
1	A	190(F)	G	C6-C5-N7	5.69	133.82	130.40
1	A	948	C	C2-N1-C1'	-5.69	112.54	118.80
1	A	657	G	C5-C6-N1	-5.69	108.65	111.50
1	A	1371	G	N3-C4-N9	5.69	129.42	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	742	G	N3-C4-N9	-5.69	122.59	126.00
1	A	519	C	N3-C4-C5	-5.68	119.63	121.90
1	A	6	G	C4-N9-C1'	5.68	133.89	126.50
1	A	1524	C	N3-C4-N4	5.68	121.98	118.00
1	A	397	A	C4-C5-C6	5.68	119.84	117.00
1	A	1337	G	C8-N9-C4	-5.68	104.13	106.40
1	A	27	G	C4-C5-N7	5.68	113.07	110.80
1	A	115	G	P-O3'-C3'	5.68	126.51	119.70
1	A	179	A	N1-C6-N6	5.68	122.01	118.60
1	A	765	G	N1-C6-O6	5.67	123.31	119.90
1	A	1195	C	C6-N1-C2	-5.67	118.03	120.30
1	A	1401	G	C6-C5-N7	-5.67	127.00	130.40
1	A	545	C	C6-N1-C2	-5.67	118.03	120.30
1	A	1238	A	C4-C5-N7	-5.67	107.86	110.70
1	A	1083	U	C4-C5-C6	5.67	123.10	119.70
1	A	1530	G	C4-N9-C1'	-5.67	119.13	126.50
1	A	558	G	C6-C5-N7	-5.67	127.00	130.40
1	A	653	A	N9-C4-C5	5.67	108.07	105.80
1	A	1394	A	N1-C6-N6	-5.67	115.20	118.60
1	A	93	G	N3-C2-N2	5.67	123.87	119.90
1	A	728	A	N1-C2-N3	5.66	132.13	129.30
5	E	12	LEU	CA-CB-CG	5.66	128.31	115.30
6	F	37	VAL	CB-CA-C	-5.66	100.65	111.40
1	A	268	C	N1-C2-O2	5.66	122.29	118.90
1	A	511	C	C5-C6-N1	-5.66	118.17	121.00
1	A	6	G	C6-C5-N7	-5.65	127.01	130.40
1	A	7	G	C6-N1-C2	-5.65	121.71	125.10
1	A	715	A	N1-C2-N3	5.65	132.13	129.30
1	A	9	G	N1-C6-O6	5.65	123.29	119.90
1	A	1264	C	C6-N1-C2	-5.65	118.04	120.30
1	A	29	G	N1-C2-N3	5.65	127.29	123.90
1	A	316	G	C5-C6-O6	-5.65	125.21	128.60
1	A	591	U	C2-N3-C4	-5.65	123.61	127.00
1	A	916	G	C8-N9-C1'	-5.65	119.66	127.00
1	A	577	G	C2-N3-C4	-5.65	109.08	111.90
1	A	122	G	C5-C6-N1	-5.64	108.68	111.50
1	A	1527	C	N3-C4-N4	5.64	121.95	118.00
8	H	4	ASP	CB-CG-OD1	5.64	123.38	118.30
1	A	48	C	C6-N1-C2	5.64	122.56	120.30
1	A	1187	G	C6-C5-N7	-5.64	127.01	130.40
1	A	126	G	N7-C8-N9	-5.64	110.28	113.10
1	A	638	G	C6-C5-N7	-5.64	127.02	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	881	G	C8-N9-C4	5.64	108.66	106.40
1	A	936	C	C5-C6-N1	-5.64	118.18	121.00
1	A	700	G	N9-C4-C5	-5.64	103.14	105.40
1	A	1487	G	C4-C5-C6	5.64	122.18	118.80
1	A	1247	U	C6-N1-C2	-5.64	117.62	121.00
1	A	1353	G	N3-C4-C5	-5.64	125.78	128.60
1	A	1500	A	N1-C6-N6	-5.64	115.22	118.60
1	A	58	C	N3-C4-C5	5.63	124.15	121.90
1	A	190(I)	G	C8-N9-C4	5.63	108.65	106.40
1	A	565	U	C6-N1-C2	5.63	124.38	121.00
1	A	888	G	C4-C5-N7	-5.63	108.55	110.80
1	A	1104	G	C5-C6-O6	-5.63	125.22	128.60
1	A	9	G	N3-C4-N9	5.63	129.38	126.00
1	A	357	G	C8-N9-C4	5.63	108.65	106.40
1	A	790	A	N7-C8-N9	5.63	116.61	113.80
1	A	570	G	N1-C2-N2	-5.63	111.13	116.20
1	A	107	G	C5-C6-O6	-5.63	125.22	128.60
1	A	607	A	N1-C6-N6	5.63	121.98	118.60
1	A	706	A	N1-C2-N3	5.62	132.11	129.30
1	A	572	A	C6-N1-C2	-5.62	115.23	118.60
1	A	931	C	C6-N1-C2	5.62	122.55	120.30
1	A	654	G	N1-C2-N3	5.62	127.27	123.90
1	A	1543	C	N1-C2-N3	-5.62	115.27	119.20
1	A	90	U	C5-C6-N1	5.61	125.51	122.70
1	A	198	G	N1-C6-O6	5.61	123.27	119.90
1	A	1195	C	C2-N1-C1'	5.61	124.97	118.80
1	A	877	C	N1-C2-N3	5.61	123.13	119.20
1	A	106	C	C4-C5-C6	5.60	120.20	117.40
1	A	397	A	N1-C2-N3	5.60	132.10	129.30
1	A	74	C	N1-C2-O2	5.60	122.26	118.90
1	A	1083	U	N3-C4-O4	5.60	123.32	119.40
1	A	852	G	N3-C2-N2	-5.60	115.98	119.90
1	A	88	A	N7-C8-N9	5.60	116.60	113.80
1	A	723	U	N1-C2-O2	5.60	126.72	122.80
1	A	1342	C	C5-C6-N1	5.60	123.80	121.00
1	A	66	G	N1-C6-O6	5.60	123.26	119.90
1	A	66	G	C2-N3-C4	-5.60	109.10	111.90
1	A	310	G	N3-C2-N2	-5.59	115.98	119.90
1	A	190(G)	G	C4-C5-N7	5.59	113.04	110.80
1	A	397	A	C4-N9-C1'	5.59	136.37	126.30
1	A	558	G	N1-C6-O6	5.59	123.25	119.90
1	A	1365	G	N9-C4-C5	5.59	107.64	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1500	A	C6-N1-C2	-5.59	115.25	118.60
1	A	1103	C	N3-C2-O2	-5.59	117.99	121.90
1	A	70	G	N1-C6-O6	5.59	123.25	119.90
1	A	703	G	C4-C5-N7	-5.59	108.56	110.80
1	A	1504	G	N1-C2-N2	-5.58	111.17	116.20
1	A	43	C	C2-N1-C1'	-5.58	112.66	118.80
1	A	297	G	N7-C8-N9	5.58	115.89	113.10
1	A	981	U	C5-C4-O4	-5.58	122.55	125.90
1	A	700	G	N1-C2-N2	-5.58	111.18	116.20
1	A	815	A	N9-C4-C5	-5.58	103.57	105.80
1	A	809	G	C6-C5-N7	-5.58	127.05	130.40
1	A	227	G	N1-C6-O6	5.57	123.24	119.90
1	A	230	G	N1-C2-N2	-5.57	111.18	116.20
1	A	860	A	N9-C4-C5	5.57	108.03	105.80
1	A	1504	G	C4-C5-N7	-5.57	108.57	110.80
1	A	1250	A	N9-C4-C5	5.57	108.03	105.80
1	A	297	G	C6-C5-N7	-5.57	127.06	130.40
1	A	565	U	N3-C4-C5	5.57	117.94	114.60
1	A	658	G	N3-C4-N9	5.57	129.34	126.00
1	A	818	G	N3-C2-N2	-5.57	116.00	119.90
1	A	597	G	N7-C8-N9	5.57	115.88	113.10
1	A	1517	G	C4-N9-C1'	5.57	133.74	126.50
1	A	577	G	C5-C6-O6	-5.56	125.26	128.60
1	A	1237	C	N1-C2-N3	5.56	123.09	119.20
1	A	372	C	N1-C2-O2	5.56	122.24	118.90
1	A	1056	U	N3-C2-O2	5.56	126.09	122.20
1	A	1377	A	C5-N7-C8	5.56	106.68	103.90
1	A	1521	G	C5-C6-N1	5.56	114.28	111.50
1	A	1543	C	C6-N1-C1'	-5.56	114.13	120.80
1	A	632	A	N1-C6-N6	5.55	121.93	118.60
1	A	628	G	N3-C4-C5	-5.55	125.82	128.60
1	A	331	G	C4-C5-C6	5.55	122.13	118.80
1	A	1203	C	C5-C6-N1	5.55	123.78	121.00
1	A	816	A	C2-N3-C4	-5.55	107.83	110.60
1	A	523	A	C2-N3-C4	-5.55	107.83	110.60
1	A	819	A	C4-C5-C6	5.55	119.77	117.00
1	A	292	G	C4-C5-N7	5.54	113.02	110.80
1	A	1345	U	N1-C2-O2	-5.54	118.92	122.80
1	A	923	A	N1-C6-N6	5.54	121.92	118.60
1	A	123	C	N3-C4-C5	-5.54	119.69	121.90
1	A	676	A	N7-C8-N9	-5.54	111.03	113.80
1	A	1231	G	C4-C5-N7	5.54	113.02	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1514	C	C2-N1-C1'	-5.53	112.72	118.80
1	A	43	C	C2-N3-C4	-5.53	117.14	119.90
1	A	171	A	C6-N1-C2	-5.53	115.28	118.60
1	A	1378	C	C5-C6-N1	5.53	123.77	121.00
1	A	885	G	C5-C6-N1	-5.53	108.74	111.50
1	A	894	G	N1-C6-O6	5.53	123.22	119.90
1	A	1338	G	N1-C2-N2	-5.53	111.23	116.20
1	A	13	U	N1-C2-N3	5.52	118.21	114.90
1	A	130	A	C8-N9-C4	5.52	108.01	105.80
1	A	190(G)	G	N7-C8-N9	5.52	115.86	113.10
1	A	790	A	N9-C4-C5	5.52	108.01	105.80
1	A	6	G	N1-C2-N3	5.52	127.21	123.90
1	A	166	G	C8-N9-C4	5.52	108.61	106.40
1	A	337	C	N3-C4-C5	5.52	124.11	121.90
1	A	1441	G	N9-C4-C5	5.52	107.61	105.40
1	A	780	A	N1-C6-N6	-5.52	115.29	118.60
1	A	874	G	C5-C6-O6	-5.52	125.29	128.60
1	A	969	A	C5-N7-C8	-5.52	101.14	103.90
1	A	867	G	N1-C2-N3	5.51	127.21	123.90
1	A	935	A	C5-C6-N1	5.51	120.46	117.70
1	A	505	G	N9-C4-C5	-5.51	103.19	105.40
1	A	407	G	N3-C4-N9	-5.51	122.69	126.00
1	A	785	G	C6-C5-N7	-5.51	127.09	130.40
1	A	1078	U	C6-N1-C2	-5.51	117.69	121.00
1	A	297	G	C4-N9-C1'	5.51	133.66	126.50
1	A	1483	A	C6-N1-C2	-5.51	115.30	118.60
1	A	1487	G	C8-N9-C1'	-5.50	119.84	127.00
1	A	53	A	C6-N1-C2	-5.50	115.30	118.60
1	A	482	A	C5-C6-N6	-5.50	119.30	123.70
1	A	1303	C	C6-N1-C2	5.50	122.50	120.30
1	A	828	A	C2-N3-C4	-5.49	107.85	110.60
1	A	1335	C	C5-C4-N4	5.49	124.04	120.20
1	A	1370	G	C4-C5-N7	5.49	113.00	110.80
1	A	729	A	C5-C6-N6	-5.49	119.31	123.70
1	A	1333	A	N1-C6-N6	-5.49	115.31	118.60
1	A	284	G	C6-C5-N7	-5.49	127.11	130.40
1	A	1189	C	C6-N1-C2	5.49	122.50	120.30
1	A	787	A	C4-C5-C6	5.49	119.74	117.00
1	A	499	A	C8-N9-C4	-5.48	103.61	105.80
1	A	9	G	C6-C5-N7	-5.48	127.11	130.40
1	A	886	G	N1-C2-N3	5.48	127.19	123.90
1	A	946	A	C4-C5-N7	-5.48	107.96	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1392	G	C6-C5-N7	-5.48	127.11	130.40
1	A	589	C	N3-C4-C5	5.48	124.09	121.90
1	A	1230	C	C5-C6-N1	5.48	123.74	121.00
1	A	1454	G	C5-C6-O6	-5.48	125.31	128.60
1	A	303	A	C5-N7-C8	-5.48	101.16	103.90
1	A	825	G	N3-C4-N9	5.48	129.29	126.00
1	A	47	C	C2-N1-C1'	5.47	124.82	118.80
1	A	610	G	C8-N9-C4	-5.47	104.21	106.40
1	A	653	A	C8-N9-C4	-5.47	103.61	105.80
1	A	1067	A	P-O3'-C3'	5.47	126.27	119.70
1	A	1203	C	C6-N1-C2	-5.47	118.11	120.30
1	A	723	U	C6-N1-C2	-5.47	117.72	121.00
1	A	761	G	N1-C2-N2	-5.47	111.28	116.20
1	A	765	G	N3-C4-C5	5.47	131.34	128.60
1	A	58	C	C6-N1-C2	-5.47	118.11	120.30
1	A	289	G	C4-C5-C6	5.47	122.08	118.80
1	A	400	C	C5-C6-N1	-5.47	118.27	121.00
1	A	958	A	N1-C6-N6	-5.47	115.32	118.60
1	A	271	C	C6-N1-C2	-5.46	118.11	120.30
1	A	1531	A	C6-C5-N7	-5.46	128.48	132.30
1	A	309	G	C4-C5-N7	5.46	112.98	110.80
1	A	482	A	C4-C5-N7	5.46	113.43	110.70
1	A	1015	A	N1-C6-N6	-5.46	115.33	118.60
1	A	1502	A	N7-C8-N9	5.46	116.53	113.80
1	A	27	G	C4-N9-C1'	5.46	133.59	126.50
1	A	665	A	C5-C6-N1	5.46	120.43	117.70
1	A	865	A	C8-N9-C4	-5.46	103.62	105.80
1	A	897	C	C5-C4-N4	-5.46	116.38	120.20
1	A	1375	A	N7-C8-N9	-5.46	111.07	113.80
1	A	1331	G	N1-C6-O6	-5.45	116.63	119.90
1	A	732	C	C2-N1-C1'	5.45	124.80	118.80
1	A	1392	G	N9-C4-C5	-5.45	103.22	105.40
1	A	861	G	N1-C6-O6	-5.45	116.63	119.90
1	A	22	G	N1-C6-O6	5.44	123.17	119.90
1	A	585	G	N3-C4-C5	5.44	131.32	128.60
1	A	670	G	N3-C4-N9	5.44	129.26	126.00
1	A	809	G	C5-C6-O6	-5.44	125.33	128.60
1	A	102	G	C8-N9-C4	-5.43	104.23	106.40
1	A	747	C	N3-C4-C5	5.43	124.07	121.90
1	A	1509	C	N3-C2-O2	-5.43	118.10	121.90
1	A	276	G	N1-C6-O6	5.42	123.16	119.90
1	A	80	G	C8-N9-C4	-5.42	104.23	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	251	G	C4-N9-C1'	5.42	133.55	126.50
1	A	823	G	N1-C2-N3	5.42	127.15	123.90
1	A	831	U	C6-N1-C2	-5.42	117.75	121.00
1	A	981	U	N3-C4-O4	5.42	123.19	119.40
5	E	115	VAL	CB-CA-C	-5.42	101.11	111.40
1	A	316	G	N1-C6-O6	5.42	123.15	119.90
1	A	238	G	N3-C4-N9	-5.41	122.75	126.00
1	A	750	G	N1-C6-O6	5.41	123.15	119.90
1	A	568	G	C4-N9-C1'	5.41	133.53	126.50
1	A	797	C	C6-N1-C2	5.41	122.46	120.30
1	A	722	A	N3-C4-C5	5.41	130.58	126.80
1	A	1104	G	N9-C4-C5	-5.41	103.24	105.40
1	A	1231	G	C5-N7-C8	-5.41	101.60	104.30
1	A	1403	C	C2-N3-C4	5.41	122.60	119.90
1	A	139	G	N1-C6-O6	5.40	123.14	119.90
1	A	288	A	C5-C6-N6	5.40	128.02	123.70
1	A	297	G	C4-C5-C6	5.40	122.04	118.80
1	A	502	G	C5-N7-C8	-5.40	101.60	104.30
1	A	199	G	C5-C6-O6	-5.40	125.36	128.60
1	A	1543	C	C2-N1-C1'	5.40	124.74	118.80
1	A	1079	G	C6-N1-C2	-5.39	121.86	125.10
1	A	864	A	N1-C6-N6	-5.39	115.37	118.60
1	A	15	G	C8-N9-C4	5.39	108.56	106.40
1	A	251	G	C8-N9-C1'	-5.39	120.00	127.00
1	A	190(C)	C	N3-C4-C5	-5.38	119.75	121.90
1	A	722	A	C4-C5-N7	5.38	113.39	110.70
1	A	1398	A	N1-C6-N6	-5.38	115.37	118.60
1	A	1514	C	N3-C4-N4	-5.38	114.23	118.00
1	A	671	G	C2-N3-C4	-5.38	109.21	111.90
1	A	7	G	N3-C4-C5	-5.38	125.91	128.60
1	A	331	G	C8-N9-C4	5.38	108.55	106.40
1	A	373	A	N1-C6-N6	5.38	121.83	118.60
1	A	662	G	C5-C6-N1	-5.38	108.81	111.50
1	A	599	C	N1-C2-O2	-5.38	115.67	118.90
1	A	1108	G	C4-C5-C6	5.38	122.03	118.80
4	D	56	VAL	CB-CA-C	-5.38	101.18	111.40
1	A	1504	G	C5-N7-C8	5.37	106.99	104.30
1	A	1524	C	C4-C5-C6	5.37	120.09	117.40
16	P	28	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	A	1224	G	C8-N9-C4	5.37	108.55	106.40
1	A	879	C	C5-C4-N4	-5.37	116.44	120.20
1	A	999	C	C6-N1-C2	-5.37	118.15	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1380	U	C6-N1-C2	-5.37	117.78	121.00
1	A	899	C	C5-C6-N1	5.37	123.68	121.00
1	A	6	G	C2-N3-C4	-5.37	109.22	111.90
1	A	91	C	C6-N1-C1'	-5.36	114.37	120.80
1	A	296	U	N3-C2-O2	-5.36	118.45	122.20
1	A	308	C	C5-C6-N1	5.36	123.68	121.00
1	A	373	A	C8-N9-C4	-5.36	103.66	105.80
1	A	481	G	C2-N3-C4	5.36	114.58	111.90
1	A	451	A	N3-C4-C5	5.36	130.55	126.80
1	A	452	A	N7-C8-N9	-5.36	111.12	113.80
1	A	635	G	C6-C5-N7	-5.36	127.18	130.40
1	A	793	U	C6-N1-C2	-5.36	117.78	121.00
1	A	888	G	C5-C6-N1	-5.36	108.82	111.50
1	A	47	C	C6-N1-C2	-5.36	118.16	120.30
1	A	108	G	C4-C5-N7	5.36	112.94	110.80
1	A	803	G	C5-C6-O6	5.36	131.81	128.60
1	A	666	G	C6-C5-N7	-5.35	127.19	130.40
1	A	190(E)	U	N3-C4-O4	-5.35	115.65	119.40
17	Q	67	LYS	N-CA-C	-5.35	96.55	111.00
1	A	288	A	N3-C4-C5	5.35	130.54	126.80
1	A	1297	C	N3-C4-C5	5.35	124.04	121.90
1	A	1329	A	N7-C8-N9	5.35	116.47	113.80
1	A	730	G	N3-C4-N9	5.34	129.21	126.00
1	A	1508	G	N3-C2-N2	-5.34	116.16	119.90
1	A	882	C	C2-N3-C4	-5.34	117.23	119.90
1	A	1055	A	C4-C5-N7	-5.34	108.03	110.70
1	A	65	U	N3-C4-C5	-5.34	111.40	114.60
1	A	396	G	C4-N9-C1'	5.34	133.44	126.50
1	A	832	C	C2-N3-C4	-5.34	117.23	119.90
1	A	1182	G	N3-C4-N9	5.34	129.20	126.00
1	A	780	A	N9-C4-C5	5.34	107.94	105.80
1	A	171	A	N1-C2-N3	5.33	131.97	129.30
1	A	328	C	C6-N1-C2	-5.33	118.17	120.30
1	A	855	G	C4-C5-N7	5.33	112.93	110.80
1	A	1377	A	C5-C6-N1	5.33	120.37	117.70
1	A	1055	A	C2-N3-C4	5.33	113.27	110.60
1	A	383	A	N7-C8-N9	5.33	116.46	113.80
1	A	190(H)	G	C5-C6-N1	-5.33	108.84	111.50
1	A	733	A	N1-C2-N3	5.33	131.96	129.30
1	A	201	C	N3-C4-C5	-5.32	119.77	121.90
1	A	361	G	N7-C8-N9	-5.32	110.44	113.10
1	A	759	A	C4-C5-C6	5.32	119.66	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1306	A	C5-C6-N1	-5.32	115.04	117.70
1	A	1148	U	C5-C6-N1	5.32	125.36	122.70
1	A	1353	G	C2-N3-C4	5.32	114.56	111.90
1	A	271	C	C5-C6-N1	5.32	123.66	121.00
1	A	378	G	C8-N9-C4	5.32	108.53	106.40
1	A	580	U	C5-C4-O4	5.31	129.09	125.90
1	A	933	G	C6-C5-N7	-5.31	127.22	130.40
1	A	1178	G	N9-C4-C5	5.31	107.52	105.40
1	A	1480	G	C5-C6-O6	5.31	131.78	128.60
1	A	89	C	C5-C6-N1	5.31	123.65	121.00
1	A	324	G	N3-C2-N2	-5.31	116.19	119.90
1	A	882	C	N3-C4-N4	-5.31	114.29	118.00
1	A	119	A	N1-C6-N6	-5.30	115.42	118.60
1	A	667	G	C8-N9-C4	5.30	108.52	106.40
1	A	1334	G	N3-C4-C5	5.30	131.25	128.60
1	A	260	G	N1-C6-O6	5.30	123.08	119.90
1	A	297	G	C5-C6-N1	-5.30	108.85	111.50
1	A	761	G	C6-C5-N7	-5.29	127.22	130.40
1	A	1380	U	N1-C2-N3	5.29	118.08	114.90
1	A	777	A	N7-C8-N9	5.29	116.45	113.80
1	A	851	G	N3-C4-C5	-5.29	125.95	128.60
1	A	811	C	C5-C4-N4	-5.29	116.50	120.20
1	A	79	G	C6-C5-N7	-5.29	127.23	130.40
1	A	573	A	C5-N7-C8	-5.29	101.25	103.90
1	A	700	G	C6-C5-N7	-5.29	127.23	130.40
1	A	1355	G	N1-C6-O6	5.28	123.07	119.90
3	C	25	GLY	N-CA-C	5.28	126.30	113.10
1	A	983	A	C2-N3-C4	5.28	113.24	110.60
1	A	1480	G	N3-C4-C5	-5.28	125.96	128.60
1	A	270	A	C8-N9-C4	-5.28	103.69	105.80
1	A	1509	C	N1-C2-N3	5.28	122.89	119.20
1	A	316	G	N3-C4-C5	-5.28	125.96	128.60
1	A	1333	A	N7-C8-N9	5.27	116.44	113.80
1	A	1416	G	C5-N7-C8	-5.27	101.66	104.30
1	A	360	A	C4-C5-N7	5.27	113.34	110.70
18	R	50	ILE	CB-CA-C	-5.27	101.06	111.60
1	A	946	A	C5-C6-N6	5.27	127.92	123.70
1	A	1504	G	C4-C5-C6	5.27	121.96	118.80
1	A	396	G	N7-C8-N9	5.27	115.73	113.10
1	A	481	G	N3-C2-N2	5.27	123.59	119.90
1	A	577	G	N3-C4-C5	5.27	131.23	128.60
1	A	1517	G	C6-C5-N7	-5.27	127.24	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1126	U	C2-N1-C1'	5.26	124.02	117.70
1	A	180	U	C6-N1-C2	-5.26	117.84	121.00
1	A	559	A	C6-N1-C2	-5.26	115.44	118.60
1	A	181	G	N3-C4-C5	-5.26	125.97	128.60
1	A	1488	G	N9-C4-C5	5.26	107.50	105.40
1	A	97	G	N7-C8-N9	5.26	115.73	113.10
1	A	303	A	C4-C5-N7	5.26	113.33	110.70
1	A	881	G	N9-C4-C5	-5.26	103.30	105.40
1	A	170	U	C2-N1-C1'	-5.25	111.39	117.70
1	A	1229	A	C8-N9-C4	5.25	107.90	105.80
1	A	505	G	C4-C5-N7	5.25	112.90	110.80
1	A	526	C	C2-N3-C4	-5.25	117.27	119.90
1	A	867	G	N1-C6-O6	5.25	123.05	119.90
1	A	105	G	N1-C6-O6	-5.25	116.75	119.90
1	A	926	G	C5-N7-C8	5.25	106.93	104.30
1	A	38	G	C8-N9-C4	5.25	108.50	106.40
1	A	232	G	C8-N9-C1'	-5.25	120.18	127.00
1	A	736	C	N3-C4-N4	-5.24	114.33	118.00
1	A	1107	C	N3-C4-C5	-5.24	119.80	121.90
1	A	1139	G	C8-N9-C4	-5.24	104.30	106.40
1	A	1510	U	C2-N3-C4	-5.24	123.86	127.00
1	A	331	G	C8-N9-C1'	-5.24	120.19	127.00
1	A	362	G	C5-C6-N1	-5.24	108.88	111.50
1	A	1353	G	N1-C6-O6	-5.24	116.76	119.90
1	A	821	G	N7-C8-N9	-5.23	110.48	113.10
1	A	1055	A	C5-N7-C8	5.23	106.52	103.90
1	A	1108	G	C8-N9-C1'	-5.23	120.20	127.00
1	A	1505	G	C4-C5-C6	5.23	121.94	118.80
1	A	826	C	C6-N1-C2	-5.23	118.21	120.30
1	A	518	C	N1-C2-O2	5.22	122.03	118.90
1	A	199	G	C4-C5-N7	5.22	112.89	110.80
1	A	730	G	C5-C6-O6	5.22	131.73	128.60
1	A	288	A	N1-C6-N6	-5.22	115.47	118.60
1	A	935	A	C4-C5-C6	-5.21	114.39	117.00
1	A	872	A	C5-C6-N6	-5.21	119.53	123.70
1	A	1461	G	C5-C6-O6	-5.21	125.47	128.60
1	A	564	C	C6-N1-C1'	-5.21	114.55	120.80
1	A	665	A	C6-N1-C2	-5.21	115.47	118.60
1	A	929	G	C5-C6-N1	-5.21	108.89	111.50
1	A	122	G	C4-C5-N7	5.21	112.88	110.80
1	A	253	U	N1-C2-O2	-5.21	119.15	122.80
1	A	1188	A	C4-C5-C6	5.21	119.61	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	18	C	C4-C5-C6	5.21	120.00	117.40
1	A	103	C	N3-C4-N4	5.21	121.64	118.00
1	A	141	A	C5-N7-C8	-5.21	101.30	103.90
1	A	729	A	C5-N7-C8	-5.21	101.30	103.90
17	Q	98	LEU	CA-CB-CG	5.21	127.28	115.30
1	A	491	G	C8-N9-C1'	-5.21	120.23	127.00
1	A	751	U	C6-N1-C2	5.21	124.12	121.00
1	A	559	A	C5-C6-N1	5.20	120.30	117.70
1	A	1301	U	P-O3'-C3'	5.20	125.94	119.70
1	A	852	G	N3-C4-N9	-5.20	122.88	126.00
1	A	1224	G	N3-C4-C5	5.20	131.20	128.60
1	A	324	G	N1-C2-N2	5.20	120.88	116.20
1	A	887	G	C6-N1-C2	-5.20	121.98	125.10
1	A	1104	G	C4-C5-N7	5.20	112.88	110.80
1	A	1374	A	C5-C6-N1	-5.20	115.10	117.70
1	A	877	C	C5-C6-N1	-5.20	118.40	121.00
1	A	1231	G	C6-C5-N7	-5.19	127.28	130.40
1	A	1533	C	N1-C2-O2	5.19	122.02	118.90
1	A	777	A	C5-N7-C8	-5.19	101.31	103.90
1	A	888	G	N9-C4-C5	5.18	107.47	105.40
1	A	166	G	C5-C6-O6	-5.18	125.49	128.60
1	A	915	A	N9-C4-C5	5.18	107.87	105.80
1	A	508	C	N3-C2-O2	-5.18	118.27	121.90
1	A	881	G	C2-N3-C4	-5.18	109.31	111.90
1	A	1379	G	C2-N3-C4	5.18	114.49	111.90
1	A	190(K)	G	C8-N9-C1'	5.17	133.73	127.00
1	A	1268	A	C2-N3-C4	5.17	113.19	110.60
1	A	691	G	C8-N9-C4	-5.17	104.33	106.40
1	A	1055	A	C5-C6-N1	5.17	120.29	117.70
1	A	1441	G	C8-N9-C4	-5.17	104.33	106.40
1	A	306	G	C8-N9-C4	5.17	108.47	106.40
1	A	444	C	C6-N1-C2	-5.17	118.23	120.30
1	A	970	C	N3-C4-C5	5.17	123.97	121.90
1	A	300	A	C8-N9-C4	-5.17	103.73	105.80
1	A	460	A	C8-N9-C4	-5.16	103.73	105.80
1	A	788	U	N3-C2-O2	5.16	125.81	122.20
1	A	1409	C	C6-N1-C2	-5.16	118.23	120.30
1	A	703	G	C5-C6-O6	5.16	131.70	128.60
1	A	1197	G	N3-C4-N9	5.16	129.10	126.00
1	A	1338	G	N1-C6-O6	-5.16	116.80	119.90
1	A	863	U	C5-C4-O4	5.16	129.00	125.90
1	A	732	C	C6-N1-C1'	-5.16	114.61	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	814	A	N9-C4-C5	-5.16	103.74	105.80
1	A	922	G	C8-N9-C4	-5.16	104.34	106.40
1	A	1454	G	C4-C5-N7	5.16	112.86	110.80
1	A	251	G	C4-C5-N7	5.16	112.86	110.80
1	A	597	G	C4-C5-C6	5.16	121.89	118.80
1	A	867	G	N9-C4-C5	-5.16	103.34	105.40
1	A	318	G	C5-C6-O6	-5.16	125.51	128.60
1	A	700	G	N3-C4-C5	-5.16	126.02	128.60
1	A	822	C	C6-N1-C2	-5.16	118.24	120.30
1	A	1116	C	N1-C2-O2	5.16	121.99	118.90
1	A	1231	G	N7-C8-N9	5.16	115.68	113.10
1	A	565	U	N3-C2-O2	5.15	125.81	122.20
1	A	818	G	C5-C6-N1	-5.15	108.92	111.50
1	A	1231	G	C5-C6-O6	-5.15	125.51	128.60
1	A	804	U	N1-C2-O2	5.15	126.41	122.80
1	A	877	C	C4-C5-C6	5.15	119.97	117.40
1	A	1291	G	C8-N9-C4	-5.15	104.34	106.40
1	A	1311	G	N3-C2-N2	-5.15	116.30	119.90
12	L	85	ILE	CB-CA-C	-5.15	101.31	111.60
1	A	301	G	C8-N9-C4	-5.15	104.34	106.40
17	Q	5	VAL	CB-CA-C	-5.15	101.62	111.40
1	A	156	G	N1-C6-O6	5.14	122.99	119.90
1	A	237	C	N1-C2-N3	5.14	122.80	119.20
1	A	232	G	N3-C2-N2	5.14	123.50	119.90
1	A	869	G	C5-C6-O6	5.14	131.69	128.60
1	A	1099	G	C6-C5-N7	-5.14	127.31	130.40
1	A	1533	C	C6-N1-C1'	-5.14	114.63	120.80
1	A	269	C	N3-C2-O2	-5.14	118.30	121.90
1	A	375	U	C6-N1-C2	-5.14	117.92	121.00
1	A	782	A	N1-C2-N3	5.14	131.87	129.30
1	A	820	U	C4-C5-C6	5.14	122.78	119.70
1	A	1149	C	C5-C6-N1	5.14	123.57	121.00
1	A	1413	A	C6-N1-C2	-5.14	115.52	118.60
1	A	1528	U	C6-N1-C2	5.14	124.08	121.00
1	A	362	G	C5-C6-O6	5.14	131.68	128.60
1	A	769	G	N3-C4-C5	-5.14	126.03	128.60
1	A	511	C	C2-N3-C4	-5.13	117.33	119.90
1	A	596	C	C6-N1-C2	5.13	122.35	120.30
1	A	1461	G	N1-C6-O6	5.13	122.98	119.90
1	A	445	G	N1-C6-O6	5.13	122.98	119.90
1	A	891	U	C6-N1-C2	5.13	124.08	121.00
1	A	462	G	N3-C4-C5	-5.13	126.03	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	558	G	C8-N9-C4	-5.13	104.35	106.40
1	A	993	G	C8-N9-C4	-5.13	104.35	106.40
1	A	1300	G	C5-N7-C8	5.13	106.86	104.30
1	A	1544	U	C5-C4-O4	-5.13	122.82	125.90
1	A	326	G	C4-C5-C6	5.13	121.88	118.80
1	A	668	G	C8-N9-C4	5.13	108.45	106.40
1	A	824	C	C5-C6-N1	-5.13	118.44	121.00
1	A	1531	A	C8-N9-C4	-5.12	103.75	105.80
1	A	51	A	C8-N9-C4	5.12	107.85	105.80
1	A	262	A	N1-C6-N6	-5.12	115.53	118.60
1	A	1331	G	C4-C5-N7	-5.12	108.75	110.80
1	A	1363	A	C8-N9-C4	5.12	107.85	105.80
1	A	665	A	N7-C8-N9	-5.12	111.24	113.80
1	A	668	G	N7-C8-N9	-5.12	110.54	113.10
1	A	780	A	C5-C6-N1	5.12	120.26	117.70
1	A	860	A	C8-N9-C4	-5.12	103.75	105.80
1	A	319	G	C6-C5-N7	-5.12	127.33	130.40
1	A	617	G	C8-N9-C4	5.12	108.45	106.40
1	A	66	G	N3-C2-N2	-5.12	116.32	119.90
1	A	131	C	C4-C5-C6	5.12	119.96	117.40
1	A	587	G	N9-C4-C5	5.12	107.45	105.40
1	A	374	A	C2-N3-C4	5.12	113.16	110.60
1	A	1148	U	N1-C2-O2	5.12	126.38	122.80
1	A	1337	G	N9-C4-C5	5.12	107.45	105.40
1	A	1367	C	C5-C6-N1	5.12	123.56	121.00
1	A	1395	C	C5-C6-N1	-5.12	118.44	121.00
1	A	285	G	C5-C6-N1	-5.11	108.94	111.50
1	A	693	G	N3-C4-N9	5.11	129.07	126.00
1	A	899	C	N3-C4-N4	5.11	121.58	118.00
1	A	1487	G	N3-C4-N9	5.11	129.07	126.00
1	A	482	A	C4-C5-C6	5.11	119.56	117.00
1	A	916	G	N3-C4-N9	5.11	129.06	126.00
1	A	1490	C	C4-C5-C6	-5.11	114.84	117.40
1	A	190(D)	U	C5-C6-N1	-5.11	120.15	122.70
1	A	660	G	C5-C6-O6	-5.11	125.54	128.60
1	A	861	G	C4-C5-C6	-5.11	115.73	118.80
1	A	1543	C	C5-C6-N1	5.11	123.55	121.00
1	A	276	G	C2-N3-C4	-5.10	109.35	111.90
1	A	715	A	N1-C6-N6	5.10	121.66	118.60
1	A	1113	C	C5-C6-N1	5.10	123.55	121.00
1	A	509	A	C3'-C2'-C1'	-5.10	97.42	101.50
1	A	660	G	N1-C6-O6	5.10	122.96	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1181	G	N9-C4-C5	-5.10	103.36	105.40
1	A	317	G	N1-C6-O6	5.10	122.96	119.90
1	A	570	G	N3-C4-N9	5.10	129.06	126.00
1	A	1258	G	N3-C4-N9	5.10	129.06	126.00
1	A	1282	C	N3-C4-C5	-5.10	119.86	121.90
1	A	29	G	C8-N9-C4	5.10	108.44	106.40
1	A	324	G	N1-C6-O6	5.10	122.96	119.90
1	A	7	G	N1-C2-N3	5.10	126.96	123.90
1	A	13	U	C6-N1-C2	-5.10	117.94	121.00
1	A	302	G	C8-N9-C1'	-5.10	120.38	127.00
1	A	1339	A	N9-C4-C5	5.10	107.84	105.80
1	A	1434	A	N1-C6-N6	5.10	121.66	118.60
1	A	546	G	N1-C6-O6	-5.09	116.84	119.90
1	A	141	A	C4-C5-N7	5.09	113.25	110.70
1	A	853	G	C6-C5-N7	-5.09	127.34	130.40
1	A	677	U	N3-C4-C5	-5.09	111.55	114.60
1	A	1203	C	C2-N1-C1'	5.09	124.40	118.80
1	A	416	G	N7-C8-N9	5.08	115.64	113.10
1	A	862	C	C4-C5-C6	-5.08	114.86	117.40
1	A	1333	A	N1-C2-N3	5.08	131.84	129.30
1	A	300	A	C6-N1-C2	-5.08	115.55	118.60
1	A	357	G	C5-C6-N1	-5.08	108.96	111.50
1	A	782	A	C4-C5-C6	5.08	119.54	117.00
1	A	1483	A	C5-C6-N1	5.08	120.24	117.70
1	A	570	G	N1-C2-N3	5.08	126.95	123.90
1	A	708	C	C5-C6-N1	-5.08	118.46	121.00
1	A	899	C	N1-C2-O2	5.08	121.95	118.90
1	A	1305	G	N3-C4-C5	5.08	131.14	128.60
1	A	1308	U	N1-C2-O2	-5.08	119.24	122.80
1	A	227	G	C5-N7-C8	-5.08	101.76	104.30
1	A	1186	G	C5-C6-N1	-5.08	108.96	111.50
1	A	67	C	N3-C4-N4	-5.08	114.45	118.00
1	A	1055	A	N9-C4-C5	5.08	107.83	105.80
1	A	651	C	C5-C6-N1	-5.07	118.46	121.00
1	A	301	G	C4-N9-C1'	5.07	133.09	126.50
1	A	567	G	C4-C5-N7	-5.07	108.77	110.80
1	A	587	G	C5-C6-O6	5.07	131.64	128.60
1	A	788	U	N3-C4-O4	5.07	122.95	119.40
1	A	8	A	N9-C4-C5	5.07	107.83	105.80
1	A	1180	A	C2-N3-C4	5.07	113.13	110.60
1	A	863	U	N1-C2-O2	-5.07	119.25	122.80
1	A	788	U	C2-N3-C4	5.07	130.04	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	812	C	P-O3'-C3'	5.07	125.78	119.70
1	A	1197	G	C4-N9-C1'	5.07	133.09	126.50
1	A	1093	A	C4-C5-N7	5.06	113.23	110.70
1	A	1342	C	C6-N1-C2	-5.06	118.28	120.30
1	A	1430	C	N3-C2-O2	5.06	125.44	121.90
1	A	310	G	N9-C4-C5	-5.06	103.38	105.40
1	A	360	A	C2-N3-C4	-5.06	108.07	110.60
1	A	877	C	C2-N3-C4	-5.06	117.37	119.90
1	A	1191	A	N1-C6-N6	-5.06	115.57	118.60
1	A	324	G	C5-C6-N1	-5.06	108.97	111.50
1	A	794	A	C6-C5-N7	5.06	135.84	132.30
1	A	1359	C	N3-C4-C5	-5.06	119.88	121.90
1	A	116	A	N9-C4-C5	-5.05	103.78	105.80
1	A	660	G	C4-C5-N7	5.05	112.82	110.80
1	A	971	G	N7-C8-N9	-5.05	110.58	113.10
1	A	1338	G	C8-N9-C4	-5.05	104.38	106.40
1	A	799	G	C5-C6-O6	-5.05	125.57	128.60
1	A	858	G	C2-N3-C4	-5.05	109.38	111.90
1	A	326	G	C2-N3-C4	5.04	114.42	111.90
1	A	893	C	N1-C2-N3	-5.04	115.67	119.20
1	A	328	C	C6-N1-C1'	-5.04	114.75	120.80
1	A	1131	G	N3-C4-N9	5.04	129.02	126.00
1	A	120	A	N1-C2-N3	5.04	131.82	129.30
1	A	1116	C	N3-C4-N4	-5.04	114.47	118.00
1	A	1506	U	C2-N1-C1'	5.04	123.75	117.70
1	A	285	G	C4-C5-N7	5.04	112.81	110.80
1	A	764	C	C5-C6-N1	5.04	123.52	121.00
1	A	1347	G	N3-C4-N9	5.04	129.02	126.00
1	A	1100	C	N3-C2-O2	-5.03	118.38	121.90
1	A	923	A	C4-C5-N7	5.03	113.22	110.70
1	A	53	A	N1-C2-N3	5.03	131.81	129.30
1	A	75	G	C8-N9-C1'	-5.03	120.46	127.00
1	A	190(G)	G	C8-N9-C1'	-5.03	120.46	127.00
1	A	615	C	C4-C5-C6	-5.03	114.88	117.40
1	A	1295	G	C8-N9-C4	-5.03	104.39	106.40
1	A	868	C	C5-C4-N4	-5.03	116.68	120.20
1	A	891	U	C5-C6-N1	-5.03	120.19	122.70
1	A	1101	A	N1-C6-N6	5.03	121.62	118.60
1	A	1488	G	C6-N1-C2	-5.03	122.08	125.10
1	A	170	U	N1-C2-O2	-5.03	119.28	122.80
1	A	622	A	C8-N9-C4	5.03	107.81	105.80
1	A	1104	G	C6-C5-N7	-5.02	127.39	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1026	G	C8-N9-C4	5.02	108.41	106.40
1	A	1095	U	C5-C4-O4	-5.02	122.89	125.90
1	A	1412	C	C2-N3-C4	-5.02	117.39	119.90
1	A	288	A	C8-N9-C4	5.02	107.81	105.80
1	A	778	G	N1-C2-N3	5.02	126.91	123.90
1	A	582	U	N3-C2-O2	-5.02	118.69	122.20
1	A	863	U	C6-N1-C1'	5.02	128.23	121.20
1	A	1231	G	C8-N9-C4	-5.02	104.39	106.40
1	A	1543	C	C4-C5-C6	-5.02	114.89	117.40
1	A	232	G	C5-N7-C8	-5.02	101.79	104.30
1	A	325	A	C4-C5-N7	-5.02	108.19	110.70
1	A	687	A	C4-C5-C6	5.02	119.51	117.00
1	A	285	G	N9-C4-C5	-5.02	103.39	105.40
1	A	580	U	C5-C6-N1	-5.02	120.19	122.70
1	A	221	C	N3-C4-C5	5.01	123.91	121.90
1	A	920	U	C5-C4-O4	5.01	128.91	125.90
1	A	1489	G	N1-C2-N3	5.01	126.91	123.90
1	A	1525	G	N3-C2-N2	-5.01	116.39	119.90
1	A	247	G	N1-C6-O6	5.01	122.90	119.90
1	A	1512	U	N1-C2-O2	-5.01	119.30	122.80
1	A	66	G	C6-C5-N7	-5.00	127.40	130.40
1	A	266	G	C5-C6-N1	-5.00	109.00	111.50
1	A	876	G	N1-C2-N3	5.00	126.90	123.90
4	D	30	LYS	N-CA-C	5.00	124.50	111.00
5	E	148	VAL	CB-CA-C	-5.00	101.90	111.40

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	186	ALA	Peptide
2	B	8	LYS	Peptide
8	H	90	GLY	Peptide
10	J	87	THR	Peptide
12	L	25	PRO	Peptide
13	M	105	THR	Peptide
16	P	19	ILE	Peptide
16	P	78	GLY	Peptide
20	T	93	GLU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32510	0	16434	862	0
2	B	1900	0	1951	98	0
3	C	1612	0	1677	122	0
4	D	1703	0	1763	105	0
5	E	1146	0	1207	59	0
6	F	843	0	857	47	0
7	G	1257	0	1296	69	0
8	H	1116	0	1177	60	0
9	I	1010	0	1037	75	0
10	J	792	0	835	49	0
11	K	864	0	881	37	0
12	L	972	0	1058	67	0
13	M	937	0	995	51	0
14	N	492	0	529	49	0
15	O	729	0	768	37	0
16	P	700	0	720	49	0
17	Q	823	0	893	52	0
18	R	574	0	644	41	0
19	S	647	0	673	34	0
20	T	763	0	861	49	0
21	U	208	0	221	15	0
22	A	40	0	37	7	0
23	A	230	0	0	0	0
23	B	1	0	0	0	0
23	D	1	0	0	0	0
23	E	1	0	0	0	0
23	H	2	0	0	0	0
23	I	1	0	0	0	0
23	J	1	0	0	0	0
23	K	1	0	0	0	0
23	M	2	0	0	0	0
23	N	2	0	0	0	0
23	P	1	0	0	0	0
23	S	2	0	0	0	0
23	T	2	0	0	0	0
24	D	1	0	0	0	0
24	N	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	A	396	0	0	4	0
25	E	6	0	0	0	0
25	G	1	0	0	1	0
25	J	1	0	0	0	0
25	N	1	0	0	0	0
25	Q	1	0	0	0	0
25	T	3	0	0	1	0
25	U	1	0	0	0	0
All	All	52297	0	36514	1832	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 21.

All (1832) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1443:G:H5"	1:A:1446:A:H5'	1.37	1.01
1:A:103:C:OP1	20:T:17:ARG:NH1	1.98	0.95
12:L:87:GLY:HA2	12:L:98:TYR:HA	1.50	0.91
1:A:279:A:OP2	17:Q:95:TYR:OH	1.89	0.90
4:D:68:TYR:OH	4:D:98:GLU:OE1	1.91	0.89
1:A:1358:U:H5"	14:N:35:ARG:HG3	1.53	0.89
1:A:1255:G:H2'	1:A:1279:A:H61	1.37	0.88
1:A:1498:UR3:O2'	1:A:1499:A:OP2	1.92	0.88
6:F:100:ASN:HD22	18:R:28:GLU:HG3	1.38	0.87
19:S:33:THR:HG22	19:S:35:SER:H	1.40	0.87
1:A:1316:G:N2	1:A:1319:A:OP2	2.08	0.86
12:L:57:LYS:HD2	12:L:67:THR:HG23	1.57	0.86
7:G:111:ARG:HD3	7:G:112:PRO:HD2	1.58	0.85
1:A:1128:C:OP1	9:I:66:ARG:NH2	2.09	0.85
1:A:235:C:N4	25:A:1969:HOH:O	2.09	0.85
1:A:1412:C:H2'	1:A:1413:A:C8	2.10	0.85
1:A:147:G:H1	1:A:175:C:H42	1.20	0.85
18:R:43:PHE:HD2	18:R:56:THR:HG22	1.42	0.85
6:F:101:ALA:HA	18:R:28:GLU:HB3	1.60	0.84
10:J:31:GLY:HA2	10:J:78:ASN:HB2	1.57	0.84
1:A:419:C:N3	1:A:424:G:N2	2.26	0.84
2:B:17:PHE:HA	2:B:44:LEU:HD11	1.60	0.84
3:C:6:HIS:HD2	3:C:9:GLY:H	1.25	0.83
1:A:1008:C:H42	1:A:1021:G:H22	1.23	0.83
1:A:1125:U:OP2	1:A:1145:C:N4	2.11	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:95:GLU:HG3	6:F:96:PRO:HD2	1.61	0.83
1:A:1376:U:O4	7:G:10:ARG:NH1	2.13	0.82
4:D:64:LEU:HD23	4:D:198:VAL:HG21	1.60	0.82
1:A:998:G:N2	1:A:1043:C:N3	2.28	0.81
8:H:83:ILE:HB	8:H:137:VAL:HG22	1.62	0.81
1:A:1055:A:N6	1:A:1205:U:O2	2.14	0.81
1:A:1124:G:N2	1:A:1126:U:O4	2.13	0.80
1:A:1404:5MC:H1'	1:A:1499:A:C2	2.17	0.80
1:A:113:G:H1'	1:A:354:G:H5'	1.63	0.79
3:C:156:ARG:H	3:C:163:ALA:HA	1.45	0.79
4:D:155:LEU:HB2	4:D:158:ILE:HD11	1.63	0.79
2:B:60:ASP:OD2	2:B:64:ARG:NH2	2.15	0.79
1:A:106:C:H2'	1:A:107:G:H5'	1.65	0.79
10:J:3:LYS:HG2	10:J:75:ILE:HD12	1.65	0.79
7:G:17:VAL:HG12	7:G:18:TYR:HD1	1.48	0.79
2:B:82:ARG:NH1	2:B:92:TYR:OH	2.15	0.79
17:Q:29:HIS:HB2	17:Q:36:ILE:HD13	1.65	0.78
1:A:1007:C:H1'	1:A:1023:G:H1	1.48	0.78
1:A:563:A:N6	25:A:1931:HOH:O	2.13	0.77
5:E:100:VAL:O	5:E:107:ARG:NH2	2.17	0.77
15:O:35:ARG:NH1	15:O:59:MET:SD	2.57	0.77
20:T:44:ALA:HB1	20:T:91:LEU:HB3	1.66	0.77
1:A:936:C:O2	1:A:1382:C:N4	2.16	0.77
1:A:1124:G:N2	1:A:1149:C:N3	2.32	0.77
1:A:613:C:H42	1:A:627:G:H1	1.32	0.76
2:B:157:ARG:HG2	2:B:158:LEU:HD12	1.68	0.76
1:A:1510:U:H2'	1:A:1511:G:C8	2.20	0.76
1:A:584:G:OP2	17:Q:87:LYS:NZ	2.17	0.76
4:D:13:ARG:NH1	4:D:38:TYR:O	2.18	0.76
1:A:1195:C:H3'	1:A:1196:U:H5"	1.67	0.76
3:C:75:VAL:O	3:C:83:ARG:NH1	2.18	0.76
1:A:1426:C:H42	1:A:1474:G:H1	1.32	0.76
1:A:1073:U:OP2	5:E:57:LYS:NZ	2.13	0.76
4:D:190:ASP:H	4:D:193:ASP:HB2	1.51	0.75
1:A:1053:G:H4'	1:A:1054:C:H5'	1.69	0.75
1:A:1266:G:N2	1:A:1269:A:OP2	2.20	0.75
1:A:1130:A:H4'	9:I:20:ARG:HH22	1.52	0.75
6:F:22:GLU:OE2	6:F:82:ARG:NH1	2.19	0.75
1:A:501:C:H2'	1:A:502:G:H8	1.51	0.75
1:A:1255:G:N2	1:A:1259:C:O2	2.18	0.75
1:A:1112:C:O2	3:C:179:ARG:NH1	2.20	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1303:C:H2'	1:A:1304:G:H5'	1.69	0.74
13:M:5:ALA:HB2	13:M:22:ILE:HD13	1.68	0.74
18:R:46:GLU:OE1	18:R:46:GLU:N	2.20	0.74
1:A:1249:C:O2'	9:I:73:GLN:NE2	2.21	0.74
1:A:1255:G:O2'	1:A:1258:G:H1'	1.87	0.74
1:A:409:G:H1	1:A:433:C:H42	1.36	0.74
15:O:6:GLU:OE1	15:O:6:GLU:N	2.17	0.74
21:U:12:LYS:O	21:U:22:ARG:NH1	2.20	0.74
1:A:836:G:OP1	18:R:61:LYS:NZ	2.19	0.73
1:A:1119:C:N3	1:A:1154:G:N2	2.31	0.73
10:J:8:LEU:HB2	10:J:70:ARG:HB2	1.71	0.73
16:P:21:VAL:HG12	16:P:33:ILE:HD12	1.70	0.73
1:A:250:A:H4'	1:A:251:G:O5'	1.88	0.73
1:A:1505:G:H3'	1:A:1505:G:C8	2.24	0.73
12:L:46:LYS:HG2	12:L:47:LYS:H	1.52	0.73
1:A:948:C:H42	1:A:1233:G:H1	1.35	0.73
1:A:953:G:H5'	1:A:965:A:H61	1.54	0.73
4:D:173:TRP:CE2	4:D:189:PRO:HG3	2.24	0.72
3:C:36:ASP:HA	3:C:39:ILE:HD12	1.71	0.72
1:A:1357:A:H2'	1:A:1358:U:C6	2.24	0.72
1:A:1258:G:H1	1:A:1277:C:H42	1.37	0.72
1:A:938:A:H5'	7:G:76:ARG:HH22	1.54	0.72
19:S:11:VAL:HG22	19:S:39:THR:HB	1.72	0.72
21:U:10:ARG:HD3	21:U:13:ILE:HG21	1.70	0.72
9:I:50:LEU:HD11	9:I:81:ILE:HD12	1.71	0.72
1:A:1120:G:N1	1:A:1154:G:N3	2.38	0.72
20:T:12:ALA:HA	25:T:303:HOH:O	1.88	0.72
3:C:25:GLY:H	3:C:28:GLN:HB2	1.53	0.71
19:S:47:HIS:HB2	19:S:49:ILE:HD11	1.72	0.71
1:A:1195:C:H3'	1:A:1196:U:C5'	2.20	0.71
1:A:1328:C:H2'	1:A:1329:A:H8	1.55	0.71
5:E:32:VAL:HG22	5:E:58:ALA:HB1	1.72	0.71
15:O:39:LEU:HD22	15:O:56:LEU:HB2	1.72	0.71
1:A:759:A:H2'	1:A:760:G:H5'	1.71	0.71
7:G:38:LEU:O	7:G:42:ILE:HG13	1.90	0.71
3:C:156:ARG:NH1	3:C:160:ALA:O	2.24	0.71
1:A:106:C:C2'	1:A:107:G:H5'	2.20	0.70
1:A:419:C:H42	1:A:424:G:H1	1.38	0.70
2:B:24:TRP:CZ3	2:B:26:PRO:HA	2.26	0.70
1:A:1240:U:OP2	7:G:116:ALA:N	2.23	0.70
1:A:103:C:P	20:T:17:ARG:HH12	2.14	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1435:G:H2'	1:A:1436:U:C6	2.27	0.70
3:C:6:HIS:CD2	3:C:9:GLY:H	2.08	0.70
1:A:80:G:H1	1:A:89:C:H42	1.40	0.69
2:B:84:GLU:HB3	2:B:219:VAL:HG21	1.75	0.69
12:L:53:ARG:NH1	12:L:92:0TD:OD2	2.25	0.69
1:A:442:C:H42	1:A:492:G:H1	1.41	0.69
1:A:13:U:O2	1:A:914:A:H3'	1.92	0.69
10:J:30:SER:O	10:J:78:ASN:ND2	2.24	0.69
16:P:15:PRO:HG2	16:P:41:PRO:HG3	1.72	0.69
1:A:129(A):G:N3	1:A:190(E):U:H5"	2.07	0.69
1:A:390:C:O3'	16:P:28:ARG:NH2	2.25	0.69
5:E:118:ILE:O	5:E:119:LEU:HD23	1.93	0.69
8:H:120:THR:N	8:H:123:GLU:OE1	2.26	0.69
1:A:517:G:N1	1:A:533:A:OP2	2.24	0.69
1:A:147:G:H1	1:A:175:C:N4	1.91	0.69
2:B:98:LEU:HB2	2:B:101:MET:HG3	1.74	0.68
7:G:16:LEU:HD21	9:I:42:ARG:HG2	1.75	0.68
1:A:1158:C:N3	1:A:1181:G:N2	2.41	0.68
1:A:1103:C:H5'	2:B:98:LEU:HD12	1.76	0.68
14:N:6:LEU:HB3	14:N:23:ARG:NH2	2.09	0.68
9:I:45:ALA:HA	9:I:48:GLU:HB3	1.74	0.68
15:O:12:ILE:HG12	15:O:31:LEU:HD11	1.76	0.68
18:R:32:ARG:HA	18:R:69:THR:HG21	1.76	0.68
8:H:64:LYS:HG3	8:H:79:VAL:HG21	1.74	0.68
15:O:55:GLY:HA2	15:O:58:MET:HE2	1.76	0.68
1:A:1063:C:H2'	1:A:1064:G:C8	2.29	0.68
1:A:978:A:H62	1:A:1360:A:N6	1.92	0.68
1:A:677:U:H3	1:A:713:G:H22	1.39	0.68
4:D:150:GLU:HA	4:D:153:ARG:HE	1.59	0.68
1:A:1412:C:H2'	1:A:1413:A:H8	1.55	0.67
3:C:84:ILE:HG23	3:C:88:ARG:HH21	1.59	0.67
1:A:1048:G:H2'	1:A:1050:G:C8	2.28	0.67
1:A:501:C:H2'	1:A:502:G:C8	2.29	0.67
1:A:615:C:H42	1:A:625:G:H1	1.39	0.67
1:A:1368:G:OP2	9:I:112:LYS:NZ	2.24	0.67
3:C:150:LYS:HE3	3:C:173:VAL:HB	1.76	0.67
3:C:11:ARG:NH1	3:C:177:THR:O	2.20	0.67
4:D:57:ARG:HA	4:D:202:LEU:HD12	1.77	0.67
1:A:1505:G:H8	1:A:1505:G:H3'	1.58	0.67
1:A:789:U:O2'	1:A:791:G:N7	2.27	0.67
4:D:68:TYR:CE2	4:D:97:LEU:HB3	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:U:H4'	20:T:57:ARG:HD2	1.77	0.67
1:A:107:G:C2	1:A:108:G:H1'	2.30	0.67
1:A:501:C:OP1	12:L:117:ARG:NH2	2.28	0.67
1:A:409:G:N2	1:A:433:C:N3	2.36	0.67
1:A:485:G:O2'	1:A:486:U:O5'	2.13	0.67
3:C:142:MET:HA	3:C:146:ALA:HB3	1.77	0.66
1:A:664:G:H22	1:A:741:G:H1	1.43	0.66
3:C:111:LEU:HD13	3:C:204:LEU:HD13	1.78	0.66
12:L:124:LYS:HD2	12:L:125:PRO:HD2	1.76	0.66
1:A:411:A:C5	1:A:413:G:H1'	2.31	0.66
1:A:481:G:HO2'	1:A:482:A:H8	1.41	0.66
3:C:106:VAL:HG12	3:C:109:PRO:HA	1.77	0.66
16:P:53:VAL:O	16:P:56:ALA:N	2.28	0.66
17:Q:87:LYS:HA	17:Q:90:ILE:HD12	1.77	0.66
1:A:1236:A:H4'	1:A:1304:G:H4'	1.77	0.66
22:A:1601:SRY:O61	12:L:46:LYS:HD3	1.95	0.66
9:I:108:VAL:HG12	9:I:109:VAL:H	1.61	0.66
1:A:1245:A:H61	1:A:1292:U:H3	1.43	0.66
1:A:617:G:H1	1:A:623:C:H42	1.44	0.66
14:N:24:CYS:SG	14:N:28:GLY:N	2.68	0.66
1:A:946:A:O2'	1:A:1333:A:N3	2.24	0.66
1:A:968:A:C8	1:A:1062:U:H4'	2.31	0.66
17:Q:34:LYS:HG3	17:Q:35:VAL:N	2.11	0.66
4:D:22:LYS:HB2	4:D:26:CYS:SG	2.36	0.66
13:M:37:THR:O	13:M:55:ARG:NH1	2.27	0.66
5:E:75:THR:OG1	5:E:76:ILE:N	2.29	0.65
3:C:138:VAL:HG13	3:C:151:VAL:HG23	1.77	0.65
11:K:57:THR:HG23	11:K:60:ALA:H	1.62	0.65
13:M:68:GLY:HA2	13:M:71:ARG:HD2	1.76	0.65
1:A:1065:U:H5"	1:A:1190:G:N2	2.12	0.65
1:A:518:C:H5"	1:A:519:C:C6	2.32	0.65
1:A:837:G:H1	1:A:849:C:H42	1.44	0.65
1:A:95:U:H2'	1:A:96:G:H8	1.60	0.65
9:I:26:VAL:HG13	9:I:61:ALA:HB3	1.78	0.65
13:M:14:ARG:HE	13:M:42:ALA:HA	1.61	0.65
17:Q:81:ARG:HB3	17:Q:84:LEU:HD11	1.76	0.65
2:B:185:ILE:HG23	2:B:199:TYR:HB2	1.78	0.65
19:S:22:LEU:HD13	19:S:28:LYS:HD2	1.78	0.65
1:A:1183:A:O2'	1:A:1184:G:OP1	2.14	0.65
4:D:18:LYS:HG2	4:D:33:MET:HG2	1.77	0.65
1:A:527:7MG:H81	1:A:527:7MG:H5"	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:70:LEU:HB3	15:O:78:TYR:HB2	1.79	0.65
1:A:714:G:H2'	1:A:715:A:C8	2.31	0.65
1:A:1290:G:H2'	1:A:1291:G:H8	1.61	0.65
1:A:1008:C:H42	1:A:1021:G:N2	1.94	0.64
1:A:76:C:O2'	1:A:77:G:H5'	1.97	0.64
1:A:547:A:OP2	4:D:2:GLY:N	2.31	0.64
3:C:150:LYS:HG2	3:C:169:ALA:HB2	1.80	0.64
14:N:39:LEU:HD22	14:N:43:CYS:HB3	1.79	0.64
18:R:51:LEU:HD13	18:R:52:PRO:HD2	1.79	0.64
1:A:115:G:O2'	1:A:116:A:OP2	2.12	0.64
1:A:1347:G:N2	1:A:1374:A:OP2	2.19	0.64
3:C:142:MET:HE3	3:C:149:ALA:HB3	1.80	0.64
18:R:59:SER:OG	18:R:60:ALA:N	2.30	0.64
1:A:237:C:OP2	17:Q:40:LYS:NZ	2.16	0.64
3:C:23:TYR:HD2	10:J:95:GLU:HG3	1.63	0.64
12:L:85:ILE:CG2	12:L:98:TYR:HB3	2.28	0.64
15:O:26:GLU:HA	15:O:81:LEU:HD11	1.78	0.64
1:A:539:A:H2'	1:A:540:G:H8	1.62	0.64
1:A:1347:G:H3'	9:I:108:VAL:O	1.97	0.64
1:A:1465:C:H2'	1:A:1466:C:O4'	1.98	0.64
1:A:539:A:H2'	1:A:540:G:C8	2.31	0.64
3:C:130:VAL:O	3:C:134:ILE:HG12	1.98	0.64
5:E:18:ARG:HG2	5:E:19:MET:N	2.12	0.64
6:F:100:ASN:ND2	18:R:28:GLU:HG3	2.12	0.63
1:A:1111:A:N1	3:C:177:THR:OG1	2.32	0.63
1:A:1257:U:H4'	1:A:1258:G:O5'	1.97	0.63
4:D:57:ARG:NH2	5:E:107:ARG:HD3	2.13	0.63
6:F:14:LEU:HD22	6:F:18:GLN:HB3	1.81	0.63
2:B:79:ASP:N	2:B:79:ASP:OD1	2.31	0.63
12:L:27:LEU:C	12:L:29:GLY:H	2.01	0.63
17:Q:40:LYS:HG2	17:Q:42:TYR:CE1	2.33	0.63
9:I:93:ARG:HD2	9:I:97:LYS:NZ	2.14	0.63
20:T:63:ILE:HG21	20:T:81:LYS:HG3	1.80	0.63
1:A:1255:G:H2'	1:A:1279:A:N6	2.12	0.63
8:H:46:LYS:HG3	8:H:64:LYS:HB3	1.81	0.63
18:R:59:SER:N	18:R:62:GLU:OE1	2.32	0.63
1:A:1202:G:O4'	14:N:29:ARG:NH1	2.32	0.62
1:A:1174:G:H2'	1:A:1175:G:H8	1.64	0.62
4:D:191:ARG:HH12	4:D:198:VAL:HG12	1.64	0.62
9:I:53:VAL:HG21	9:I:85:LEU:HD23	1.80	0.62
21:U:10:ARG:HA	21:U:13:ILE:HB	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:47:LEU:HG	3:C:76:VAL:HG11	1.80	0.62
8:H:21:LYS:O	8:H:65:TYR:OH	2.16	0.62
16:P:57:ARG:HH21	16:P:79:VAL:HA	1.63	0.62
20:T:10:LEU:HD13	20:T:12:ALA:H	1.64	0.62
1:A:1242:C:H42	1:A:1295:G:H1	1.46	0.62
1:A:1326:C:OP1	21:U:12:LYS:NZ	2.32	0.62
6:F:14:LEU:HD21	6:F:84:ASN:ND2	2.14	0.62
12:L:117:ARG:HB3	12:L:122:THR:HG23	1.82	0.62
13:M:4:ILE:HG23	13:M:57:ARG:HA	1.81	0.62
15:O:41:GLU:OE2	15:O:44:LYS:NZ	2.33	0.62
1:A:1405:G:H1	1:A:1496:C:H5	1.48	0.62
9:I:10:ARG:HD3	9:I:105:ASP:HB3	1.80	0.62
12:L:84:LEU:HD23	12:L:101:VAL:HG21	1.81	0.62
1:A:973:G:H3'	1:A:974:A:H5"	1.82	0.62
1:A:737:A:O2'	6:F:73:ASN:ND2	2.32	0.62
2:B:24:TRP:HZ3	2:B:29:ALA:HB2	1.64	0.62
12:L:85:ILE:HG21	12:L:98:TYR:HB3	1.80	0.62
1:A:384:G:H2'	1:A:385:C:C6	2.35	0.62
1:A:958:A:O2'	1:A:985:C:O2'	2.17	0.62
6:F:74:ASP:OD1	6:F:74:ASP:N	2.31	0.62
13:M:29:ARG:HD3	13:M:64:TRP:CE2	2.35	0.62
19:S:22:LEU:HD22	19:S:28:LYS:HG3	1.82	0.62
20:T:60:GLU:HG3	20:T:81:LYS:HE3	1.82	0.62
1:A:1028:C:N3	1:A:1034:G:N2	2.47	0.61
1:A:838:G:O6	1:A:848:C:N4	2.33	0.61
18:R:38:GLU:HA	18:R:41:LYS:HE2	1.82	0.61
1:A:731:G:OP1	1:A:766:A:H1'	2.00	0.61
20:T:77:ALA:O	20:T:80:ARG:N	2.34	0.61
1:A:1239:A:H4'	1:A:1240:U:H5"	1.81	0.61
1:A:1300:G:OP2	1:A:1335:C:N4	2.32	0.61
16:P:32:TYR:HE2	16:P:35:LYS:HB2	1.63	0.61
1:A:1030:C:H5	1:A:1030(A):G:C6	2.18	0.61
1:A:1496:C:O2'	1:A:1497:G:O4'	2.17	0.61
5:E:11:ILE:HB	5:E:31:LEU:HB3	1.82	0.61
5:E:147:ASP:O	5:E:150:ARG:HB3	2.01	0.61
1:A:74:C:H42	1:A:96:G:H1	1.48	0.61
20:T:10:LEU:HD22	20:T:11:SER:H	1.66	0.61
1:A:1359:C:O2'	1:A:1361(A):C:N4	2.33	0.61
1:A:1397:C:O2'	1:A:1398:A:OP1	2.19	0.61
7:G:115:ARG:HB2	7:G:118:VAL:HG23	1.81	0.61
1:A:1432:G:O2'	1:A:1468:A:N6	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1504:G:OP1	1:A:1507:A:H4'	2.01	0.61
7:G:48:LYS:HG2	7:G:49:ILE:HD12	1.82	0.61
7:G:78:ARG:HD2	7:G:156:TRP:CE3	2.36	0.61
7:G:88:PRO:HG2	7:G:155:ARG:NH1	2.16	0.61
5:E:65:ASN:ND2	5:E:65:ASN:O	2.34	0.61
6:F:12:PRO:HG3	6:F:57:GLN:HG3	1.83	0.61
1:A:1375:A:H4'	7:G:29:LYS:HE3	1.82	0.61
17:Q:47:PRO:HG2	17:Q:48:GLU:HG2	1.83	0.61
1:A:1243:C:OP2	21:U:10:ARG:NH2	2.32	0.61
16:P:8:ARG:NH1	16:P:15:PRO:HB3	2.16	0.60
1:A:953:G:H2'	1:A:954:G:O4'	2.02	0.60
7:G:30:ILE:HG22	7:G:39:ALA:HB1	1.83	0.60
1:A:935:A:H61	7:G:3:ARG:HG3	1.66	0.60
7:G:70:LYS:HG3	7:G:100:ALA:HB2	1.83	0.60
3:C:26:LYS:HG2	10:J:45:ARG:HH12	1.65	0.60
13:M:16:ASP:OD1	13:M:16:ASP:N	2.26	0.60
1:A:143:A:H2	1:A:220:G:H22	1.47	0.60
3:C:101:LEU:HG	3:C:102:ASN:H	1.66	0.60
6:F:4:TYR:HB2	6:F:65:VAL:HG22	1.82	0.60
14:N:39:LEU:HD13	14:N:43:CYS:HB3	1.82	0.60
1:A:1234:C:H1'	1:A:1364:U:O2	2.01	0.60
4:D:47:ARG:O	4:D:47:ARG:NE	2.33	0.60
10:J:84:GLN:HG3	10:J:85:LEU:HD12	1.83	0.60
1:A:392:G:H2'	1:A:393:A:H8	1.67	0.60
4:D:65:ARG:HB2	4:D:75:PHE:CE1	2.36	0.60
1:A:1346:A:H5"	9:I:120:ARG:HH12	1.66	0.60
9:I:17:VAL:HG21	9:I:80:GLY:HA3	1.83	0.60
1:A:35:G:H2'	1:A:36:C:C6	2.37	0.60
1:A:393:A:OP2	16:P:12:LYS:NZ	2.23	0.60
1:A:1338:G:H2'	1:A:1339:A:C8	2.36	0.60
12:L:6:THR:HG1	12:L:9:GLN:H	1.48	0.60
3:C:150:LYS:HB2	3:C:201:TYR:HB2	1.83	0.60
7:G:108:ALA:HB2	7:G:123:GLU:HG2	1.83	0.60
14:N:8:GLU:O	14:N:12:ARG:N	2.32	0.60
1:A:620:C:H2'	1:A:621:A:O4'	2.02	0.60
1:A:144:G:H1	1:A:178:C:H42	1.49	0.60
2:B:164:VAL:HG23	2:B:186:ALA:HA	1.83	0.60
1:A:102:G:H2'	1:A:103:C:H6	1.65	0.59
1:A:285:G:H2'	1:A:286:G:H8	1.67	0.59
1:A:636:U:H2'	1:A:637:G:C8	2.36	0.59
1:A:826:C:O2	8:H:15:ASN:ND2	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:33:THR:OG1	15:O:63:ARG:NH1	2.31	0.59
1:A:1222:G:OP1	19:S:77:THR:HG21	2.02	0.59
1:A:79:G:C6	1:A:80:G:C6	2.90	0.59
2:B:73:THR:HG23	2:B:95:GLN:O	2.01	0.59
3:C:14:ILE:HD11	14:N:57:ARG:HH22	1.67	0.59
9:I:91:ASP:N	9:I:91:ASP:OD1	2.31	0.59
13:M:101:GLN:OE1	13:M:101:GLN:N	2.34	0.59
14:N:52:GLN:O	14:N:53:LEU:HD23	2.03	0.59
20:T:92:LEU:O	20:T:96:GLY:HA2	2.02	0.59
1:A:571:U:O4	1:A:864:A:N6	2.35	0.59
5:E:144:THR:O	5:E:148:VAL:HG23	2.03	0.59
6:F:35:ALA:HA	6:F:67:MET:HB3	1.83	0.59
15:O:15:PHE:CE2	15:O:85:LEU:HD21	2.38	0.59
1:A:1400:5MC:H3'	1:A:1401:G:H5'	1.85	0.59
1:A:439:A:OP2	1:A:494:G:N1	2.36	0.59
3:C:6:HIS:HD2	3:C:9:GLY:N	1.98	0.59
1:A:1518:MA6:H102	1:A:1519:MA6:H103	1.84	0.59
8:H:73:ASP:OD1	8:H:75:ARG:HB2	2.03	0.59
1:A:913:A:OP2	12:L:91:LYS:NZ	2.36	0.59
1:A:1267:C:N3	1:A:1327:C:O2'	2.36	0.59
1:A:1376:U:H2'	1:A:1377:A:C8	2.38	0.59
1:A:512:U:OP1	4:D:46:LYS:NZ	2.34	0.59
20:T:35:THR:HA	20:T:38:LYS:HE2	1.84	0.59
20:T:50:GLU:HG3	20:T:51:GLU:HG2	1.83	0.59
1:A:1201:A:H4'	1:A:1202:G:O5'	2.03	0.59
1:A:1255:G:C6	1:A:1279:A:N7	2.71	0.59
1:A:578:C:O2'	1:A:728:A:N3	2.35	0.59
1:A:918:A:H2'	1:A:919:A:C8	2.37	0.59
3:C:188:LEU:HD22	3:C:195:VAL:HG22	1.84	0.59
3:C:25:GLY:HA2	3:C:29:TYR:N	2.17	0.59
1:A:1238:A:H5'	1:A:1336:C:H41	1.66	0.58
1:A:109:A:H62	1:A:324:G:H21	1.48	0.58
1:A:394:G:H2'	1:A:395:C:H6	1.68	0.58
3:C:155:GLY:HA2	3:C:164:ARG:O	2.03	0.58
3:C:155:GLY:HA2	3:C:164:ARG:H	1.68	0.58
8:H:123:GLU:HA	8:H:126:LYS:HB3	1.84	0.58
1:A:452:A:O2'	16:P:72:ARG:HD2	2.03	0.58
2:B:162:ILE:O	2:B:185:ILE:HD12	2.03	0.58
20:T:71:THR:O	20:T:72:LEU:HD23	2.03	0.58
3:C:14:ILE:HG22	3:C:15:THR:HG23	1.84	0.58
3:C:6:HIS:CD2	3:C:8:ILE:HB	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:153:VAL:H	3:C:166:GLU:HB3	1.67	0.58
7:G:15:ASP:OD1	7:G:44:TYR:OH	2.21	0.58
12:L:33:ARG:O	12:L:85:ILE:HD12	2.02	0.58
18:R:58:LEU:HD23	18:R:58:LEU:H	1.68	0.58
9:I:19:LEU:HD11	9:I:81:ILE:HA	1.83	0.58
13:M:22:ILE:HD12	13:M:25:ILE:HD12	1.85	0.58
1:A:376:G:O3'	16:P:5:ARG:NH1	2.36	0.58
1:A:200:G:H1	1:A:217:C:H42	1.51	0.58
1:A:407:G:OP1	4:D:115:ARG:NH2	2.31	0.58
1:A:90:U:H2'	1:A:91:C:O4'	2.03	0.58
3:C:123:GLN:O	3:C:128:PHE:HB2	2.03	0.58
13:M:63:THR:HG23	13:M:64:TRP:H	1.68	0.58
16:P:75:ARG:HB2	16:P:80:PHE:HD1	1.69	0.58
20:T:69:GLY:O	20:T:73:HIS:ND1	2.37	0.58
1:A:1255:G:C4	1:A:1279:A:N6	2.71	0.58
1:A:95:U:H2'	1:A:96:G:C8	2.37	0.58
1:A:1007:C:H2'	1:A:1008:C:C5	2.39	0.58
2:B:184:VAL:HG12	2:B:197:VAL:HG13	1.84	0.58
9:I:103:THR:HG22	9:I:104:ARG:O	2.04	0.58
13:M:14:ARG:HB2	13:M:17:VAL:HG23	1.86	0.58
1:A:1360:A:H2	14:N:18:VAL:HB	1.68	0.58
1:A:943:U:C2'	1:A:944:G:H5'	2.34	0.58
14:N:40:CYS:C	14:N:44:LEU:HD22	2.24	0.58
1:A:112:G:O2'	1:A:113:G:H5'	2.04	0.58
1:A:192:U:O4'	20:T:103:GLY:HA2	2.04	0.58
5:E:118:ILE:HG12	5:E:119:LEU:H	1.69	0.58
5:E:105:VAL:HG11	5:E:131:ILE:HG22	1.85	0.58
10:J:57:LYS:NZ	10:J:60:ARG:HH22	2.02	0.58
6:F:80:ARG:HH12	6:F:88:VAL:H	1.51	0.57
1:A:642:A:N3	8:H:113:SER:OG	2.37	0.57
17:Q:24:GLU:HA	17:Q:39:SER:HB3	1.86	0.57
1:A:1030(A):G:H2'	1:A:1030(B):C:H5"	1.86	0.57
1:A:707:C:H2'	1:A:708:C:C6	2.39	0.57
1:A:972:C:OP2	10:J:57:LYS:HE3	2.04	0.57
9:I:15:ALA:HA	9:I:65:VAL:HG12	1.87	0.57
1:A:327:A:O2'	1:A:328:C:O4'	2.22	0.57
3:C:58:GLU:HB3	10:J:92:THR:HG21	1.87	0.57
5:E:102:ALA:HA	5:E:120:THR:HB	1.86	0.57
1:A:1479:C:H2'	1:A:1480:G:H8	1.68	0.57
9:I:16:ARG:HB2	9:I:16:ARG:HH11	1.68	0.57
1:A:1326:C:OP2	21:U:6:ARG:NH2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:836:G:C6	1:A:851:G:C6	2.93	0.57
3:C:180:ALA:HB1	3:C:205:GLY:O	2.05	0.57
6:F:80:ARG:NH1	6:F:88:VAL:H	2.02	0.57
1:A:598:U:H4'	8:H:94:TYR:CD1	2.40	0.57
14:N:24:CYS:SG	14:N:29:ARG:N	2.71	0.57
1:A:1202:G:O2'	14:N:27:CYS:SG	2.62	0.57
1:A:1520:G:H2'	1:A:1521:G:H8	1.68	0.57
1:A:184:G:H2'	1:A:185:A:H8	1.70	0.57
1:A:353:A:H5'	1:A:353:A:H8	1.70	0.57
1:A:451:A:H2	1:A:480:U:C5	2.22	0.57
1:A:452:A:O2'	1:A:453:A:O5'	2.22	0.57
1:A:646:U:H2'	1:A:647:C:C6	2.39	0.57
5:E:99:GLY:O	5:E:101:ILE:HD12	2.03	0.57
9:I:63:ILE:HG21	9:I:77:ILE:HG12	1.86	0.57
16:P:5:ARG:HE	16:P:22:THR:HG21	1.69	0.57
1:A:1379:G:OP2	7:G:6:ARG:NH2	2.38	0.57
2:B:114:ARG:NH1	2:B:117:GLU:OE2	2.33	0.57
17:Q:40:LYS:HE3	17:Q:42:TYR:OH	2.04	0.57
1:A:687:A:H4'	1:A:688:G:O5'	2.04	0.57
1:A:825:G:H1	1:A:875:C:H42	1.52	0.57
3:C:150:LYS:HZ3	3:C:175:LEU:HD11	1.69	0.57
9:I:20:ARG:O	9:I:60:ASP:N	2.38	0.57
1:A:1328:C:H2'	1:A:1329:A:C8	2.37	0.57
1:A:992:U:O2'	1:A:993:G:OP2	2.20	0.57
2:B:19:HIS:CG	2:B:20:GLU:H	2.23	0.57
3:C:10:PHE:CE1	3:C:178:LEU:HD21	2.40	0.57
9:I:93:ARG:HD2	9:I:97:LYS:HZ2	1.68	0.57
16:P:78:GLY:C	16:P:80:PHE:H	2.07	0.57
1:A:1163:C:H2'	1:A:1164:G:C8	2.40	0.57
2:B:118:LEU:HB2	2:B:142:LEU:HD23	1.86	0.57
7:G:26:PHE:HA	7:G:101:LEU:HD23	1.87	0.57
7:G:42:ILE:HG22	7:G:120:ILE:HD12	1.87	0.57
7:G:90:GLU:N	7:G:90:GLU:OE2	2.38	0.57
1:A:1168:A:H2'	1:A:1169:A:C8	2.40	0.56
1:A:129:U:O3'	1:A:129(A):G:H3'	2.04	0.56
3:C:88:ARG:HA	3:C:91:LEU:HB3	1.86	0.56
16:P:4:ILE:HG12	16:P:21:VAL:HG22	1.87	0.56
4:D:60:GLU:HA	4:D:60:GLU:OE1	2.05	0.56
8:H:65:TYR:HA	8:H:79:VAL:HG23	1.87	0.56
1:A:1399:C:O2	1:A:1401:G:C5	2.58	0.56
1:A:914:A:OP1	22:A:1601:SRY:HI33	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:C:OP2	4:D:62:GLN:NE2	2.27	0.56
1:A:975:A:H5'	1:A:975:A:H8	1.70	0.56
1:A:1240:U:OP1	7:G:119:ARG:NH2	2.39	0.56
7:G:50:ILE:O	7:G:54:THR:OG1	2.17	0.56
8:H:2:LEU:HD23	8:H:3:THR:N	2.19	0.56
1:A:1095:U:OP1	1:A:1108:G:N2	2.32	0.56
1:A:411:A:N7	1:A:413:G:H1'	2.20	0.56
4:D:98:GLU:HG2	4:D:189:PRO:HG2	1.87	0.56
9:I:32:ASP:OD2	9:I:33:PHE:N	2.38	0.56
2:B:87:ARG:HH21	2:B:233:SER:HB2	1.68	0.56
10:J:19:SER:HB2	10:J:91:PRO:HG3	1.87	0.56
14:N:39:LEU:HD22	14:N:43:CYS:CB	2.35	0.56
16:P:49:LEU:HD12	16:P:50:LYS:H	1.71	0.56
8:H:91:ARG:NH1	17:Q:32:TYR:O	2.38	0.56
1:A:1281:U:H4'	1:A:1282:C:OP2	2.05	0.56
3:C:35:GLU:O	3:C:39:ILE:HG13	2.06	0.56
5:E:95:ALA:HB1	5:E:96:PRO:HD2	1.87	0.56
9:I:10:ARG:HH21	9:I:11:LYS:HE3	1.71	0.56
1:A:1227:A:O3'	13:M:115:LYS:HG2	2.06	0.56
4:D:61:LYS:HD3	4:D:206:PHE:CE2	2.41	0.56
1:A:1477:C:H2'	1:A:1478:C:H6	1.70	0.56
1:A:613:C:N4	1:A:627:G:H1	2.02	0.56
1:A:83:U:O2'	1:A:84:U:H5'	2.05	0.56
1:A:1198:G:H2'	1:A:1199:U:C6	2.41	0.56
8:H:80:ILE:H	8:H:80:ILE:HD12	1.71	0.56
19:S:64:GLU:O	19:S:67:VAL:HG23	2.06	0.56
1:A:1250:A:H2'	1:A:1251:A:C8	2.41	0.56
1:A:1414:U:H2'	1:A:1415:G:H8	1.70	0.56
1:A:463:A:H2'	1:A:474:G:H8	1.71	0.56
1:A:981:U:H2'	1:A:982:U:C5	2.41	0.56
1:A:1130:A:H4'	9:I:20:ARG:NH2	2.18	0.56
20:T:50:GLU:HA	20:T:100:ILE:HG13	1.88	0.56
20:T:36:LEU:O	20:T:39:LYS:HB3	2.06	0.56
1:A:451:A:N7	1:A:481:G:C2	2.74	0.56
4:D:99:SER:HB2	4:D:139:ARG:HD3	1.87	0.56
12:L:86:ARG:HG3	12:L:86:ARG:HH11	1.71	0.56
1:A:142:G:O2'	1:A:196:A:N1	2.31	0.55
1:A:254:G:OP1	17:Q:67:LYS:O	2.24	0.55
1:A:1103:C:H5'	2:B:98:LEU:CD1	2.36	0.55
1:A:1347:G:O2'	1:A:1348:U:P	2.64	0.55
1:A:651:C:H2'	1:A:652:U:C6	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:C:H2'	1:A:77:G:C8	2.40	0.55
6:F:80:ARG:NH2	6:F:88:VAL:O	2.40	0.55
1:A:562:C:H1'	12:L:15:ARG:HD2	1.88	0.55
1:A:973:G:O3'	14:N:41:ARG:NH2	2.35	0.55
1:A:9:G:OP2	5:E:121:LYS:NZ	2.28	0.55
2:B:178:ARG:HD3	2:B:196:LEU:HD22	1.88	0.55
8:H:63:LEU:H	8:H:63:LEU:HD22	1.71	0.55
8:H:65:TYR:CD1	8:H:65:TYR:N	2.75	0.55
13:M:14:ARG:NE	13:M:42:ALA:HA	2.21	0.55
1:A:235:C:H5'	17:Q:70:ARG:HG2	1.88	0.55
1:A:1020:U:H2'	1:A:1021:G:H8	1.72	0.55
2:B:7:VAL:HG11	2:B:221:LEU:HD23	1.89	0.55
1:A:1071:C:H42	1:A:1104:G:H1	1.53	0.55
1:A:478:A:H2'	1:A:479:C:C6	2.42	0.55
1:A:481:G:O2'	1:A:482:A:H8	1.90	0.55
1:A:1205:U:H5"	3:C:190:ARG:HE	1.71	0.55
4:D:191:ARG:NH1	4:D:198:VAL:HG12	2.21	0.55
6:F:98:LEU:HD22	6:F:101:ALA:HB2	1.88	0.55
3:C:121:ALA:HA	3:C:124:ILE:HD12	1.89	0.55
9:I:86:VAL:HG21	9:I:102:LEU:HD21	1.89	0.55
1:A:974:A:OP2	14:N:41:ARG:NH1	2.40	0.55
1:A:13:U:O4	1:A:20:G:N2	2.34	0.55
1:A:1405:G:N2	1:A:1497:G:C4	2.74	0.55
1:A:1442:G:C2	1:A:1446:A:N7	2.75	0.55
1:A:164:U:H2'	1:A:165:C:C6	2.42	0.55
2:B:53:ARG:HA	2:B:56:ARG:NH1	2.21	0.55
1:A:1279:A:OP2	10:J:9:ARG:NH2	2.40	0.55
12:L:41:ARG:HH12	12:L:43:VAL:HG13	1.72	0.55
1:A:1355:G:H2'	1:A:1356:G:C8	2.41	0.55
1:A:658:G:H2'	1:A:659:U:H6	1.72	0.55
1:A:960:U:H4'	1:A:961:U:C5'	2.37	0.55
6:F:97:PHE:CE2	6:F:99:ALA:HB2	2.42	0.55
8:H:123:GLU:O	8:H:127:LEU:HB2	2.07	0.55
1:A:509:A:H3'	1:A:509:A:C8	2.42	0.55
4:D:55:ALA:O	4:D:59:ARG:HG2	2.06	0.55
1:A:538:G:OP1	12:L:115:LYS:N	2.40	0.55
19:S:21:GLU:O	19:S:25:LYS:HD3	2.06	0.55
5:E:40:ARG:HG2	5:E:68:GLU:HA	1.89	0.55
6:F:4:TYR:CE1	6:F:92:LYS:HG2	2.42	0.55
1:A:1494:G:C2	1:A:1495:U:C5	2.95	0.54
3:C:43:LEU:HD13	3:C:47:LEU:HD13	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:706:A:O2'	11:K:29:ILE:HD11	2.07	0.54
15:O:38:ARG:HB3	15:O:38:ARG:HH11	1.72	0.54
1:A:1007:C:O2'	1:A:1023:G:N2	2.38	0.54
1:A:1068:G:H8	1:A:1068:G:OP2	1.89	0.54
1:A:1419:G:H1	1:A:1481:U:H3	1.55	0.54
1:A:384:G:H2'	1:A:385:C:H6	1.70	0.54
2:B:21:ARG:HA	2:B:39:ILE:HG23	1.89	0.54
3:C:117:ALA:HB2	3:C:200:ALA:HB2	1.89	0.54
3:C:186:PHE:HE1	3:C:199:LYS:HZ2	1.55	0.54
7:G:123:GLU:O	7:G:126:ASP:N	2.39	0.54
8:H:10:LEU:HD22	8:H:83:ILE:HD11	1.89	0.54
11:K:80:VAL:HG21	11:K:103:LEU:HD13	1.89	0.54
17:Q:29:HIS:CE1	17:Q:31:LEU:H	2.24	0.54
1:A:954:G:H21	1:A:1227:A:H62	1.55	0.54
1:A:1376:U:H2'	1:A:1377:A:H8	1.72	0.54
1:A:1413:A:H2	1:A:1487:G:H22	1.53	0.54
1:A:887:G:H1	1:A:910:C:H42	1.55	0.54
2:B:12:GLU:HB2	2:B:213:LEU:HD11	1.89	0.54
4:D:28:SER:O	4:D:30:LYS:N	2.37	0.54
12:L:85:ILE:HG23	12:L:99:HIS:O	2.08	0.54
19:S:18:LYS:O	19:S:22:LEU:HG	2.06	0.54
1:A:451:A:N7	1:A:481:G:N2	2.55	0.54
5:E:109:ILE:HG22	5:E:110:LEU:HD23	1.89	0.54
8:H:4:ASP:OD1	8:H:85:ARG:NH1	2.40	0.54
9:I:19:LEU:HD12	9:I:84:ALA:HB3	1.89	0.54
13:M:86:CYS:SG	13:M:87:TYR:N	2.80	0.54
14:N:23:ARG:NH1	14:N:30:ALA:HB2	2.23	0.54
15:O:61:GLY:O	15:O:65:ARG:HD3	2.06	0.54
17:Q:10:VAL:HG21	17:Q:52:LYS:O	2.08	0.54
20:T:49:ALA:HB3	20:T:99:LEU:HB2	1.90	0.54
2:B:172:ILE:HD12	2:B:173:ALA:H	1.72	0.54
14:N:18:VAL:HG22	14:N:19:ARG:HD2	1.90	0.54
1:A:1004:A:O2'	1:A:1005:A:OP1	2.24	0.54
1:A:1148:U:H2'	1:A:1149:C:O4'	2.07	0.54
1:A:1270:C:HO2'	1:A:1313:U:HO2'	1.43	0.54
1:A:770:C:H42	1:A:809:G:H1	1.55	0.54
1:A:788:U:H5"	1:A:789:U:OP2	2.08	0.54
11:K:66:LEU:HD21	11:K:97:ALA:HB1	1.89	0.54
1:A:474:G:H4'	16:P:81:ARG:HH21	1.72	0.54
1:A:1097:C:H2'	1:A:1098:C:C6	2.42	0.54
1:A:35:G:H2'	1:A:36:C:H6	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:37:ARG:HH22	5:E:111:GLU:HG2	1.73	0.54
9:I:10:ARG:NH1	9:I:105:ASP:OD2	2.40	0.54
11:K:81:ASP:CG	11:K:106:LYS:HB2	2.27	0.54
12:L:87:GLY:H	12:L:99:HIS:H	1.55	0.54
21:U:18:TYR:CG	21:U:24:ARG:HG2	2.43	0.54
1:A:113:G:C1'	1:A:354:G:H5'	2.34	0.54
1:A:130:A:H5'	17:Q:63:ARG:NH2	2.22	0.54
8:H:17:THR:HB	8:H:78:GLN:HE22	1.73	0.54
14:N:39:LEU:HB3	14:N:44:LEU:HD13	1.88	0.54
1:A:1152:A:OP1	10:J:68:HIS:ND1	2.40	0.54
1:A:1301:U:HO2'	1:A:1302:U:C5'	2.21	0.54
1:A:1305:G:N2	1:A:1331:G:H1'	2.23	0.54
22:A:1601:SRY:O21	22:A:1601:SRY:NE1	2.41	0.54
4:D:25:ARG:HA	4:D:28:SER:HB2	1.90	0.54
6:F:11:ASN:HB2	6:F:86:ARG:NE	2.23	0.54
1:A:1049:U:O2'	14:N:3:ARG:NH1	2.41	0.54
1:A:1172:C:H2'	1:A:1173:G:C8	2.43	0.54
1:A:75:G:H2'	1:A:76:C:C6	2.43	0.54
1:A:90:U:C4	1:A:91:C:C4	2.96	0.54
1:A:952:U:H2'	1:A:953:G:H8	1.72	0.54
4:D:8:VAL:O	4:D:11:LEU:N	2.40	0.54
6:F:95:GLU:O	18:R:32:ARG:NH1	2.41	0.54
11:K:40:ILE:HG22	11:K:41:THR:HG23	1.89	0.54
20:T:78:ALA:HA	20:T:81:LYS:HD3	1.90	0.54
1:A:792:A:N6	1:A:794:A:C2	2.76	0.53
13:M:39:ILE:HD12	13:M:40:ASN:H	1.74	0.53
17:Q:56:VAL:O	17:Q:77:VAL:HG23	2.08	0.53
1:A:1056:U:O2'	1:A:1057:G:H5'	2.08	0.53
1:A:1290:G:H2'	1:A:1291:G:C8	2.41	0.53
1:A:369:C:H42	1:A:392:G:H1	1.55	0.53
1:A:757:U:H2'	1:A:758:G:O4'	2.06	0.53
2:B:97:TRP:HZ2	2:B:102:LEU:HD13	1.72	0.53
4:D:187:ARG:NH1	4:D:188:LEU:HD23	2.24	0.53
4:D:63:LYS:O	4:D:67:ILE:HG13	2.08	0.53
10:J:16:LEU:HD21	10:J:94:VAL:HA	1.90	0.53
1:A:1006:C:H2'	1:A:1007:C:C6	2.43	0.53
2:B:16:HIS:CD2	2:B:204:ASN:H	2.27	0.53
15:O:21:ASP:OD1	15:O:24:SER:OG	2.20	0.53
19:S:69:HIS:HB3	19:S:73:GLU:CD	2.28	0.53
1:A:1329:A:P	13:M:28:ALA:HB3	2.49	0.53
3:C:188:LEU:HD23	3:C:196:LEU:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:9:PHE:CE2	16:P:18:ARG:HD2	2.43	0.53
17:Q:81:ARG:NH2	17:Q:83:ASP:OD2	2.41	0.53
1:A:1258:G:H1	1:A:1277:C:N4	2.03	0.53
1:A:1531:A:O5'	1:A:1531:A:H8	1.91	0.53
1:A:372:C:H1'	1:A:373:A:OP2	2.09	0.53
1:A:914:A:P	22:A:1601:SRY:HI33	2.49	0.53
1:A:1104:G:O5'	2:B:111:ARG:HD2	2.08	0.53
4:D:10:ARG:HA	4:D:13:ARG:HG2	1.89	0.53
1:A:1163:C:H2'	1:A:1164:G:H8	1.74	0.53
1:A:17:U:H2'	1:A:18:C:C6	2.43	0.53
1:A:200:G:H2'	1:A:201:C:O2	2.07	0.53
7:G:139:GLU:O	7:G:143:ARG:HB3	2.09	0.53
8:H:87:SER:HA	8:H:93:VAL:HG23	1.90	0.53
1:A:505:G:H1	1:A:526:C:H42	1.57	0.53
1:A:965:A:C2	1:A:969:A:C2	2.97	0.53
7:G:5:ARG:NH2	25:G:201:HOH:O	2.37	0.53
8:H:85:ARG:NE	8:H:87:SER:O	2.42	0.53
1:A:1061:G:H1'	10:J:56:HIS:CE1	2.44	0.53
13:M:96:LEU:O	13:M:110:ARG:NH1	2.41	0.53
15:O:2:PRO:O	15:O:38:ARG:NH2	2.41	0.53
1:A:1145:C:H1'	1:A:1146:A:N7	2.24	0.53
1:A:451:A:N6	1:A:481:G:C4	2.77	0.53
4:D:162:LEU:HA	4:D:165:MET:HB2	1.90	0.53
1:A:775:G:C2'	1:A:776:G:H5'	2.39	0.53
3:C:180:ALA:CB	3:C:203:PHE:HE1	2.22	0.53
3:C:81:GLY:O	3:C:84:ILE:HG22	2.08	0.53
4:D:190:ASP:OD1	4:D:191:ARG:N	2.42	0.53
5:E:122:GLU:O	5:E:123:LEU:HD23	2.09	0.53
8:H:9:MET:O	8:H:13:ILE:HD12	2.09	0.53
1:A:392:G:H2'	1:A:393:A:C8	2.44	0.53
3:C:66:VAL:HG12	3:C:68:VAL:HG23	1.91	0.53
6:F:67:MET:HB2	6:F:68:PRO:HD2	1.90	0.53
7:G:140:ASP:HA	7:G:143:ARG:HD2	1.89	0.53
15:O:18:PHE:CZ	15:O:21:ASP:HB2	2.44	0.53
16:P:68:ASP:OD1	16:P:68:ASP:N	2.42	0.53
18:R:46:GLU:CD	18:R:46:GLU:H	2.10	0.53
1:A:1014:A:H2'	1:A:1015:A:O4'	2.08	0.52
1:A:1204:A:C5	1:A:1205:U:C5	2.97	0.52
1:A:1278:U:H4'	1:A:1279:A:N3	2.24	0.52
1:A:1392:G:N2	1:A:1502:A:H8	2.07	0.52
1:A:1493:A:H2'	1:A:1494:G:H8	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:42:GLU:OE1	6:F:59:TYR:OH	2.15	0.52
12:L:6:THR:OG1	12:L:9:GLN:N	2.37	0.52
14:N:40:CYS:O	14:N:44:LEU:N	2.30	0.52
16:P:9:PHE:HE2	16:P:18:ARG:HD2	1.74	0.52
1:A:1064:G:N2	1:A:1191:A:OP2	2.36	0.52
1:A:1354:C:H2'	1:A:1355:G:H8	1.74	0.52
1:A:1392:G:H21	1:A:1502:A:H8	1.57	0.52
1:A:463:A:OP1	16:P:75:ARG:NH1	2.37	0.52
1:A:760:G:H2'	1:A:761:G:O4'	2.08	0.52
1:A:1057:G:H5"	3:C:154:SER:HB2	1.92	0.52
13:M:59:TYR:O	13:M:63:THR:HG22	2.09	0.52
1:A:1218:C:H2'	1:A:1219:U:C6	2.45	0.52
1:A:1355:G:H2'	1:A:1356:G:H8	1.73	0.52
1:A:403:C:O2'	4:D:122:ARG:NH1	2.43	0.52
13:M:22:ILE:HG22	13:M:23:TYR:N	2.25	0.52
14:N:2:ALA:HB2	14:N:28:GLY:HA3	1.91	0.52
1:A:1525:G:H2'	1:A:1526:G:H8	1.74	0.52
1:A:89:C:H2'	1:A:90:U:C6	2.44	0.52
3:C:11:ARG:NH1	3:C:178:LEU:HA	2.24	0.52
4:D:119:GLN:HG3	4:D:123:HIS:CD2	2.44	0.52
7:G:80:VAL:HG11	7:G:154:TYR:HE2	1.75	0.52
8:H:114:THR:HG22	8:H:131:GLY:HA3	1.92	0.52
8:H:6:ILE:HB	8:H:85:ARG:NH1	2.24	0.52
4:D:10:ARG:O	4:D:13:ARG:HG2	2.08	0.52
10:J:8:LEU:HD21	10:J:96:ILE:HG23	1.90	0.52
13:M:2:ALA:O	13:M:4:ILE:HD12	2.10	0.52
14:N:24:CYS:O	14:N:28:GLY:HA2	2.10	0.52
22:A:1601:SRY:O21	22:A:1601:SRY:NB1	2.42	0.52
1:A:75:G:C6	1:A:96:G:N1	2.77	0.52
1:A:767:A:H2'	1:A:768:A:O4'	2.09	0.52
2:B:136:VAL:O	2:B:140:HIS:ND1	2.41	0.52
4:D:13:ARG:NH2	4:D:40:PRO:HA	2.25	0.52
6:F:41:GLU:O	6:F:62:TRP:HB3	2.09	0.52
6:F:2:ARG:O	6:F:66:GLU:HA	2.09	0.52
6:F:70:ASP:OD1	6:F:71:ARG:HG2	2.09	0.52
13:M:74:VAL:O	13:M:78:ILE:HG13	2.10	0.52
1:A:1101:A:H4'	1:A:1102:A:O5'	2.10	0.52
1:A:130:A:H5'	17:Q:63:ARG:CZ	2.40	0.52
1:A:372:C:H4'	1:A:373:A:O5'	2.10	0.52
1:A:371:G:O2'	1:A:372:C:H5'	2.10	0.52
1:A:37:U:H2'	1:A:38:G:O4'	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:975:A:H4'	1:A:976:G:O5'	2.09	0.52
8:H:82:HIS:CE1	8:H:138:TRP:NE1	2.77	0.52
8:H:86:ILE:HG21	8:H:133:LEU:HD13	1.91	0.52
9:I:48:GLU:N	9:I:49:PRO:HD2	2.25	0.52
1:A:463:A:H1'	16:P:82:GLN:HG3	1.92	0.52
5:E:20:GLN:CD	5:E:21:ALA:H	2.13	0.52
1:A:1256:A:H4'	1:A:1257:U:O5'	2.10	0.52
1:A:1328:C:OP2	21:U:7:ARG:NH1	2.43	0.52
1:A:609:A:N6	25:A:2089:HOH:O	2.42	0.52
1:A:644:G:C5	1:A:645:C:C5	2.98	0.52
2:B:168:THR:HG22	2:B:169:LYS:HD2	1.92	0.52
5:E:69:VAL:HG21	5:E:113:ALA:HB1	1.92	0.52
12:L:86:ARG:HG3	12:L:86:ARG:NH1	2.23	0.52
17:Q:58:GLU:HB3	17:Q:74:LEU:HB3	1.92	0.52
1:A:411:A:H62	1:A:413:G:N2	2.08	0.52
1:A:721:G:C6	1:A:733:A:C2	2.98	0.52
8:H:12:ARG:NH1	8:H:27:PRO:HD3	2.24	0.52
8:H:82:HIS:CE1	8:H:138:TRP:CD1	2.98	0.52
3:C:23:TYR:CD2	10:J:95:GLU:HG3	2.44	0.52
1:A:1197:G:H5"	1:A:1198:G:OP2	2.11	0.51
1:A:1404:5MC:H1'	1:A:1499:A:H2	1.73	0.51
1:A:269:C:H2'	1:A:270:A:C8	2.45	0.51
2:B:27:LYS:HD3	2:B:193:ASP:OD1	2.10	0.51
2:B:59:GLU:HB2	2:B:221:LEU:HD11	1.92	0.51
3:C:36:ASP:O	3:C:39:ILE:HB	2.11	0.51
4:D:163:GLU:HG3	4:D:166:LYS:HE2	1.91	0.51
9:I:50:LEU:O	9:I:53:VAL:HG12	2.10	0.51
1:A:1052:U:C2	1:A:1200:C:N4	2.78	0.51
1:A:422:C:H4'	1:A:423:G:O5'	2.10	0.51
25:A:2110:HOH:O	2:B:96:ARG:HG2	2.11	0.51
11:K:72:ALA:HA	11:K:75:TYR:HB2	1.91	0.51
1:A:750:G:N3	15:O:23:GLY:HA3	2.25	0.51
1:A:757:U:H5"	1:A:822:C:O2	2.10	0.51
1:A:974:A:H8	1:A:974:A:OP1	1.94	0.51
2:B:55:PHE:HA	2:B:58:ILE:HD12	1.91	0.51
5:E:5:ASP:OD1	5:E:5:ASP:N	2.43	0.51
14:N:47:LEU:O	14:N:53:LEU:HG	2.11	0.51
1:A:1357:A:H2'	1:A:1358:U:H6	1.71	0.51
1:A:633:G:H2'	1:A:634:C:C6	2.46	0.51
2:B:68:ILE:H	2:B:90:MET:HG2	1.74	0.51
3:C:26:LYS:HG2	10:J:45:ARG:NH1	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:72:ALA:HB1	11:K:77:MET:HG3	1.93	0.51
17:Q:66:SER:H	17:Q:69:LYS:HB2	1.74	0.51
8:H:82:HIS:CE1	8:H:138:TRP:HE1	2.28	0.51
1:A:1030:C:N3	1:A:1032:G:N1	2.58	0.51
1:A:1172:C:H2'	1:A:1173:G:H8	1.76	0.51
1:A:230:G:H2'	1:A:231:G:O4'	2.11	0.51
3:C:120:VAL:HG12	3:C:124:ILE:HD11	1.92	0.51
7:G:145:ALA:O	7:G:146:GLU:HG2	2.10	0.51
10:J:91:PRO:HB2	10:J:94:VAL:HG13	1.91	0.51
1:A:658:G:H1	1:A:747:C:H42	1.59	0.51
3:C:16:ARG:HG3	3:C:17:ASP:H	1.76	0.51
8:H:27:PRO:HA	8:H:58:TYR:CD2	2.45	0.51
1:A:1029:C:N3	1:A:1033:G:N2	2.58	0.51
1:A:1095:U:H5"	1:A:1109:C:O2	2.11	0.51
1:A:279:A:OP1	1:A:280:C:O2'	2.17	0.51
1:A:710:G:H5"	6:F:54:LYS:HE3	1.91	0.51
4:D:31:CYS:C	4:D:33:MET:H	2.13	0.51
5:E:39:GLY:O	5:E:69:VAL:HG23	2.11	0.51
12:L:6:THR:HG23	12:L:9:GLN:OE1	2.10	0.51
15:O:56:LEU:O	15:O:60:VAL:HG23	2.10	0.51
1:A:1094:G:O2'	1:A:1108:G:N2	2.44	0.51
1:A:575:G:OP1	1:A:575:G:H4'	2.11	0.51
2:B:18:GLY:HA2	2:B:42:ILE:HG12	1.93	0.51
4:D:111:ALA:HA	4:D:161:ASN:ND2	2.25	0.51
8:H:20:TYR:CE2	8:H:75:ARG:HD2	2.45	0.51
20:T:43:LEU:HD12	20:T:52:ALA:HA	1.93	0.51
1:A:1302:U:O4	13:M:14:ARG:NH1	2.44	0.51
1:A:1505:G:C3'	1:A:1505:G:C8	2.91	0.51
1:A:552:U:H2'	1:A:553:A:C8	2.46	0.51
2:B:161:ALA:HB1	2:B:185:ILE:HD11	1.92	0.51
1:A:1368:G:OP1	9:I:111:ARG:NH1	2.44	0.51
9:I:118:LYS:O	9:I:120:ARG:N	2.43	0.51
11:K:95:ILE:HA	11:K:98:LEU:CD1	2.41	0.51
12:L:87:GLY:HA2	12:L:98:TYR:CA	2.32	0.51
1:A:1003:G:H2'	1:A:1003(A):G:C8	2.46	0.50
1:A:1120:G:H22	1:A:1154:G:H1'	1.75	0.50
1:A:789:U:H2'	1:A:791:G:OP2	2.11	0.50
1:A:984:C:N3	1:A:1221:G:N2	2.54	0.50
2:B:49:GLU:O	2:B:52:GLU:HB3	2.11	0.50
3:C:116:VAL:O	3:C:120:VAL:HG23	2.11	0.50
7:G:77:SER:HA	7:G:86:GLN:HA	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:53:VAL:O	16:P:55:ARG:N	2.44	0.50
17:Q:4:LYS:HG3	17:Q:5:VAL:N	2.24	0.50
1:A:1074:G:C6	1:A:1075:C:C4	2.99	0.50
1:A:738:C:OP1	6:F:92:LYS:HD3	2.11	0.50
3:C:121:ALA:HB1	3:C:189:ALA:HB2	1.91	0.50
3:C:30:ARG:HG2	3:C:31:HIS:H	1.76	0.50
8:H:104:ARG:CZ	8:H:138:TRP:CZ2	2.95	0.50
9:I:53:VAL:HG22	9:I:92:TYR:CZ	2.46	0.50
15:O:39:LEU:CD2	15:O:56:LEU:HB2	2.41	0.50
17:Q:13:ASP:O	17:Q:15:MET:N	2.44	0.50
1:A:299:G:H2'	1:A:300:A:C8	2.47	0.50
1:A:93:G:C2	1:A:95:U:C2	2.99	0.50
10:J:37:PRO:HA	10:J:71:LEU:H	1.75	0.50
1:A:502:G:C2	1:A:503:C:C2	2.99	0.50
1:A:803:G:C6	1:A:804:U:C4	2.99	0.50
1:A:882:C:O2'	1:A:883:C:H5'	2.11	0.50
5:E:44:GLY:HA3	5:E:62:ALA:HB2	1.93	0.50
7:G:62:PHE:O	7:G:66:VAL:HG23	2.11	0.50
8:H:25:ASP:OD1	8:H:25:ASP:N	2.44	0.50
20:T:29:LYS:O	20:T:32:ALA:HB3	2.11	0.50
1:A:1112:C:H1'	3:C:179:ARG:HH12	1.76	0.50
1:A:962:C:H1'	1:A:1201:A:N1	2.26	0.50
1:A:1411:C:H42	1:A:1489:G:H1	1.60	0.50
1:A:247:G:OP2	17:Q:100:LYS:HD3	2.11	0.50
1:A:909:A:H2'	1:A:910:C:O4'	2.11	0.50
3:C:142:MET:CE	3:C:170:GLN:HB2	2.42	0.50
4:D:7:PRO:HB2	4:D:10:ARG:HG2	1.92	0.50
8:H:84:ARG:HD2	8:H:85:ARG:O	2.12	0.50
9:I:61:ALA:HB1	9:I:63:ILE:HG12	1.94	0.50
1:A:1279:A:OP1	10:J:7:LYS:NZ	2.45	0.50
12:L:117:ARG:NH2	12:L:124:LYS:HD3	2.27	0.50
19:S:34:TRP:HA	19:S:52:TYR:HB3	1.92	0.50
1:A:1211:U:O2'	1:A:1212:U:OP2	2.26	0.50
1:A:435:C:H2'	1:A:436:C:H6	1.77	0.50
4:D:173:TRP:NE1	4:D:189:PRO:HG3	2.25	0.50
5:E:81:GLU:OE2	5:E:81:GLU:N	2.38	0.50
7:G:57:GLU:OE1	7:G:59:LEU:HB3	2.11	0.50
16:P:53:VAL:O	16:P:54:GLU:C	2.50	0.50
16:P:74:LEU:HD22	16:P:79:VAL:HG21	1.94	0.50
18:R:58:LEU:N	18:R:58:LEU:HD23	2.26	0.50
1:A:1078:U:H5"	1:A:1079:G:OP2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1526:G:O2'	1:A:1527:C:H5'	2.12	0.50
1:A:299:G:C6	1:A:300:A:C6	2.99	0.50
1:A:741:G:H2'	1:A:742:G:O4'	2.12	0.50
6:F:97:PHE:HE2	6:F:99:ALA:HB2	1.76	0.50
1:A:932:C:H5'	7:G:4:ARG:HG2	1.94	0.50
11:K:92:GLU:HG3	11:K:96:ARG:NH1	2.26	0.50
1:A:559:A:O2'	1:A:560:U:OP2	2.24	0.50
4:D:170:VAL:HG11	4:D:175:SER:HA	1.92	0.50
1:A:1229:A:OP1	13:M:116:THR:OG1	2.26	0.50
1:A:232:G:H2'	1:A:233:C:H6	1.77	0.50
1:A:90:U:O4	1:A:91:C:N4	2.45	0.50
15:O:33:THR:HG21	15:O:85:LEU:HD13	1.94	0.50
1:A:450:G:OP1	16:P:43:LYS:NZ	2.45	0.50
17:Q:58:GLU:O	17:Q:59:ILE:HD13	2.12	0.50
20:T:35:THR:HA	20:T:38:LYS:NZ	2.27	0.50
20:T:50:GLU:HG3	20:T:51:GLU:H	1.77	0.50
1:A:1483:A:H2'	1:A:1484:C:O4'	2.12	0.49
1:A:945:G:N1	1:A:1337:G:C2	2.80	0.49
4:D:155:LEU:HB2	4:D:158:ILE:CD1	2.37	0.49
7:G:65:ALA:HB2	7:G:128:ALA:HB2	1.94	0.49
11:K:30:VAL:HG21	11:K:65:ALA:HA	1.94	0.49
12:L:77:LEU:HD21	12:L:107:ALA:HB2	1.92	0.49
1:A:1310:G:OP1	13:M:77:ASN:ND2	2.44	0.49
14:N:39:LEU:HD13	14:N:43:CYS:C	2.33	0.49
15:O:6:GLU:HA	15:O:9:GLN:HB2	1.94	0.49
1:A:1119:C:H42	1:A:1154:G:H1	1.60	0.49
1:A:948:C:N4	1:A:1233:G:H1	2.07	0.49
1:A:1301:U:HO2'	1:A:1302:U:P	2.34	0.49
1:A:337:C:H2'	1:A:338:A:C8	2.46	0.49
1:A:394:G:H2'	1:A:395:C:C6	2.47	0.49
1:A:429:U:H1'	1:A:430:A:H5"	1.95	0.49
1:A:954:G:C5	1:A:955:U:C4	3.00	0.49
7:G:115:ARG:HD2	7:G:118:VAL:HG21	1.94	0.49
8:H:4:ASP:OD2	8:H:85:ARG:NH1	2.45	0.49
12:L:19:ARG:HD2	12:L:19:ARG:H	1.77	0.49
17:Q:22:LEU:HD12	17:Q:23:VAL:H	1.77	0.49
1:A:1285:A:H4'	1:A:1286:A:O5'	2.12	0.49
1:A:942:G:H21	9:I:124:GLN:HE22	1.59	0.49
1:A:1174:G:H2'	1:A:1175:G:C8	2.45	0.49
1:A:1258:G:OP2	1:A:1258:G:H8	1.96	0.49
1:A:922:G:C6	1:A:923:A:C6	3.01	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:945:G:C6	1:A:1337:G:C2	3.00	0.49
1:A:954:G:N2	1:A:1227:A:H62	2.11	0.49
2:B:177:ALA:HB1	2:B:182:ILE:HB	1.94	0.49
5:E:43:LEU:HD22	5:E:136:MET:HG2	1.93	0.49
10:J:71:LEU:HD22	10:J:71:LEU:N	2.26	0.49
12:L:59:ARG:NH1	12:L:65:GLU:HB3	2.27	0.49
1:A:1220:G:H2'	1:A:1221:G:O4'	2.13	0.49
1:A:49:U:H5"	1:A:49:U:H6	1.76	0.49
1:A:533:A:O2'	1:A:535:A:OP2	2.28	0.49
1:A:983:A:OP1	14:N:3:ARG:NH2	2.44	0.49
3:C:25:GLY:N	3:C:28:GLN:HB2	2.26	0.49
4:D:63:LYS:NZ	4:D:197:PRO:O	2.40	0.49
5:E:43:LEU:HD11	5:E:133:TYR:HD2	1.77	0.49
11:K:17:GLY:HA2	11:K:35:PRO:HG3	1.95	0.49
1:A:232:G:H1'	1:A:262:A:N1	2.28	0.49
1:A:748:C:H4'	1:A:749:C:O5'	2.12	0.49
3:C:50:ALA:HB2	3:C:75:VAL:HB	1.95	0.49
6:F:62:TRP:CH2	6:F:64:GLN:HB2	2.46	0.49
1:A:967:5MC:H4'	9:I:128:ARG:NE	2.26	0.49
19:S:80:TYR:CG	19:S:81:ARG:N	2.81	0.49
1:A:1326:C:H5"	21:U:18:TYR:O	2.12	0.49
1:A:1403:C:H2'	1:A:1404:5MC:C6	2.48	0.49
1:A:443:C:H2'	1:A:444:C:H6	1.78	0.49
1:A:942:G:C2	1:A:943:U:C2	3.00	0.49
1:A:737:A:H1'	6:F:73:ASN:HD21	1.78	0.49
7:G:87:VAL:HG13	7:G:151:TYR:HB3	1.93	0.49
4:D:57:ARG:NH2	4:D:205:GLU:OE2	2.46	0.49
6:F:60:PHE:CZ	18:R:78:LEU:HD21	2.48	0.49
11:K:62:GLN:O	11:K:66:LEU:HG	2.13	0.49
13:M:84:ILE:HG13	13:M:86:CYS:H	1.78	0.49
20:T:75:ASN:OD1	20:T:75:ASN:N	2.46	0.49
1:A:344:A:H4'	1:A:345:C:OP2	2.13	0.49
2:B:143:GLU:O	2:B:147:LYS:HG3	2.12	0.49
2:B:184:VAL:O	2:B:198:ASP:HB2	2.12	0.49
12:L:27:LEU:C	12:L:29:GLY:N	2.66	0.49
15:O:76:GLU:N	15:O:79:ARG:HH21	2.10	0.49
16:P:57:ARG:HH21	16:P:79:VAL:CA	2.24	0.49
19:S:63:THR:HG22	19:S:64:GLU:H	1.77	0.49
1:A:1206:G:H2'	1:A:1207:2MG:C8	2.48	0.49
1:A:691:G:H2'	1:A:692:U:H6	1.77	0.49
7:G:88:PRO:HG2	7:G:155:ARG:HH12	1.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:881:G:OP2	12:L:12:ARG:NH2	2.46	0.49
15:O:36:ILE:HG13	15:O:59:MET:HE3	1.94	0.49
18:R:61:LYS:O	18:R:65:ILE:HG13	2.13	0.49
1:A:485:G:O2'	1:A:486:U:P	2.71	0.48
1:A:67:C:H2'	1:A:68:G:C8	2.48	0.48
3:C:6:HIS:NE2	3:C:8:ILE:HB	2.28	0.48
9:I:8:GLY:HA2	9:I:79:LEU:HD12	1.94	0.48
1:A:1190:G:OP1	3:C:4:LYS:HA	2.13	0.48
1:A:161:A:N1	1:A:347:G:O2'	2.42	0.48
1:A:27:G:H2'	1:A:28:G:O4'	2.14	0.48
4:D:141:ARG:HG2	4:D:142:PRO:HD2	1.95	0.48
13:M:5:ALA:CB	13:M:22:ILE:HD13	2.40	0.48
1:A:1203:C:OP1	14:N:2:ALA:N	2.46	0.48
16:P:6:LEU:HD12	16:P:6:LEU:HA	1.60	0.48
3:C:137:ALA:O	3:C:141:VAL:HG23	2.12	0.48
3:C:10:PHE:CD1	3:C:178:LEU:HD21	2.48	0.48
5:E:142:LEU:HA	5:E:142:LEU:HD23	1.60	0.48
5:E:82:VAL:O	5:E:88:LYS:HA	2.14	0.48
8:H:34:GLU:HB3	8:H:118:VAL:HG21	1.94	0.48
10:J:34:VAL:HG22	10:J:74:ILE:HG23	1.95	0.48
18:R:39:VAL:HG13	18:R:40:LEU:HD23	1.96	0.48
1:A:217:C:H2'	1:A:218:C:H6	1.77	0.48
1:A:455:C:H2'	1:A:456:C:H6	1.78	0.48
1:A:828:A:OP1	1:A:828:A:H4'	2.14	0.48
4:D:8:VAL:HG11	4:D:21:LEU:HB2	1.93	0.48
12:L:58:VAL:O	12:L:65:GLU:HA	2.13	0.48
1:A:452:A:O2'	1:A:453:A:O4'	2.29	0.48
1:A:484:G:H5'	1:A:486:U:H1'	1.95	0.48
1:A:517:G:H5'	1:A:519:C:C2	2.49	0.48
3:C:147:LYS:HB3	3:C:203:PHE:CE2	2.48	0.48
12:L:56:ALA:O	12:L:58:VAL:HG23	2.12	0.48
20:T:35:THR:HA	20:T:38:LYS:CE	2.43	0.48
1:A:1426:C:H2'	1:A:1427:U:H6	1.78	0.48
1:A:502:G:P	12:L:118:SER:HG	2.36	0.48
1:A:76:C:H2'	1:A:77:G:H8	1.77	0.48
1:A:781:A:C4	1:A:802:A:C2	3.02	0.48
1:A:191:G:H1'	20:T:105:SER:HA	1.94	0.48
20:T:51:GLU:O	20:T:55:ILE:HG12	2.13	0.48
1:A:1520:G:O2'	1:A:1521:G:H5'	2.14	0.48
1:A:695:A:C2	1:A:787:A:H1'	2.49	0.48
1:A:865:A:H8	1:A:865:A:O5'	1.97	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:12:LEU:HD22	3:C:18:TRP:CD1	2.48	0.48
4:D:156:GLU:HG3	4:D:160:GLN:HE22	1.78	0.48
4:D:9:CYS:SG	4:D:31:CYS:O	2.72	0.48
9:I:50:LEU:HD23	9:I:85:LEU:HD21	1.95	0.48
13:M:108:ARG:HD3	13:M:114:ARG:NH2	2.29	0.48
1:A:1020:U:C2	1:A:1021:G:C8	3.02	0.48
1:A:1126:U:H3	1:A:1149:C:H1'	1.79	0.48
1:A:1363:A:H4'	1:A:1364:U:H5"	1.93	0.48
1:A:1373:G:H5"	7:G:36:LYS:HD3	1.95	0.48
1:A:1508:G:C5	1:A:1509:C:C5	3.01	0.48
1:A:35:G:C6	1:A:36:C:N4	2.81	0.48
12:L:84:LEU:O	12:L:101:VAL:HG23	2.14	0.48
16:P:51:VAL:HG12	16:P:53:VAL:N	2.29	0.48
1:A:721:G:H4'	1:A:722:A:O4'	2.13	0.48
1:A:79:G:N1	1:A:80:G:C6	2.82	0.48
1:A:956:U:H4'	19:S:80:TYR:HE1	1.79	0.48
2:B:47:THR:HG22	2:B:51:LEU:HD12	1.96	0.48
6:F:28:ARG:O	6:F:32:ASN:HB2	2.13	0.48
10:J:5:ARG:HG3	10:J:5:ARG:H	1.44	0.48
15:O:26:GLU:OE2	15:O:77:ARG:HD2	2.13	0.48
16:P:58:TYR:CD1	16:P:58:TYR:C	2.85	0.48
16:P:8:ARG:CZ	16:P:15:PRO:HB3	2.44	0.48
18:R:43:PHE:CD2	18:R:56:THR:HG22	2.33	0.48
1:A:113:G:H2'	1:A:114:U:C6	2.49	0.48
1:A:1130:A:N6	1:A:1144:G:H21	2.12	0.48
1:A:949:A:C2	1:A:1233:G:N3	2.82	0.48
1:A:1240:U:H5	7:G:109:ASN:HD21	1.59	0.48
1:A:1254:C:H2'	1:A:1255:G:C8	2.49	0.48
1:A:1242:C:N4	1:A:1295:G:H1	2.09	0.48
1:A:411:A:N6	1:A:413:G:N3	2.61	0.48
1:A:785:G:C2	1:A:786:G:C8	3.02	0.48
1:A:946:A:H2'	1:A:947:G:C8	2.49	0.48
2:B:84:GLU:O	2:B:87:ARG:HB2	2.14	0.48
7:G:66:VAL:HG12	7:G:70:LYS:HZ3	1.78	0.48
9:I:104:ARG:HD2	9:I:105:ASP:H	1.79	0.48
14:N:39:LEU:CD2	14:N:43:CYS:HB3	2.44	0.48
1:A:1510:U:H2'	1:A:1511:G:H8	1.75	0.47
1:A:478:A:H2'	1:A:479:C:H6	1.79	0.47
1:A:837:G:H1	1:A:849:C:N4	2.11	0.47
7:G:31:MET:HB2	7:G:35:LYS:O	2.14	0.47
10:J:46:ARG:HD2	10:J:64:GLU:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1191:A:H2'	1:A:1192:C:C6	2.49	0.47
1:A:376:G:H2'	1:A:377:G:H8	1.79	0.47
1:A:505:G:C6	1:A:535:A:C2	3.01	0.47
1:A:679:C:H2'	1:A:680:C:C6	2.48	0.47
1:A:975:A:O2'	14:N:32:SER:HB2	2.15	0.47
2:B:95:GLN:HG3	2:B:148:TYR:HA	1.95	0.47
7:G:17:VAL:HG12	7:G:18:TYR:CD1	2.39	0.47
1:A:933:G:OP2	7:G:3:ARG:HB3	2.15	0.47
17:Q:38:ARG:HA	17:Q:38:ARG:HD3	1.55	0.47
1:A:1452:C:H4'	1:A:1453:G:O5'	2.14	0.47
1:A:558:G:H5"	1:A:559:A:H3'	1.95	0.47
1:A:663:A:H2'	1:A:664:G:O4'	2.14	0.47
1:A:691:G:H2'	1:A:692:U:C6	2.49	0.47
1:A:90:U:C4	1:A:91:C:N4	2.83	0.47
1:A:943:U:H2'	1:A:944:G:H5'	1.96	0.47
1:A:976:G:OP2	1:A:1358:U:H1'	2.14	0.47
2:B:36:ARG:CG	2:B:41:ILE:HD11	2.45	0.47
1:A:1191:A:H5"	3:C:4:LYS:NZ	2.29	0.47
4:D:8:VAL:O	4:D:10:ARG:N	2.47	0.47
11:K:39:PRO:O	11:K:40:ILE:HD13	2.14	0.47
15:O:70:LEU:HD22	15:O:70:LEU:HA	1.38	0.47
1:A:968:A:OP1	1:A:968:A:H8	1.98	0.47
16:P:43:LYS:HB2	16:P:43:LYS:HE2	1.72	0.47
1:A:1004:A:O2'	1:A:1005:A:P	2.71	0.47
1:A:1120:G:C2	1:A:1154:G:N3	2.82	0.47
1:A:956:U:H2'	1:A:957:U:O4'	2.15	0.47
2:B:96:ARG:HH12	2:B:172:ILE:HD11	1.80	0.47
3:C:84:ILE:HG23	3:C:88:ARG:NH2	2.28	0.47
6:F:48:LEU:HG	6:F:57:GLN:HA	1.96	0.47
9:I:114:TYR:H	9:I:114:TYR:HD2	1.60	0.47
9:I:6:GLY:HA3	9:I:83:ARG:HB3	1.97	0.47
19:S:11:VAL:HG13	19:S:39:THR:O	2.15	0.47
1:A:1263:C:H2'	1:A:1264:C:O4'	2.14	0.47
1:A:1301:U:O2'	1:A:1302:U:O5'	2.30	0.47
1:A:1442:G:C6	1:A:1446:A:N6	2.78	0.47
1:A:1493:A:H2'	1:A:1494:G:C8	2.49	0.47
1:A:979:C:H42	14:N:18:VAL:HG23	1.78	0.47
2:B:71:VAL:HB	2:B:164:VAL:HG12	1.96	0.47
3:C:110:ASN:OD1	3:C:110:ASN:N	2.47	0.47
3:C:22:TRP:CD1	3:C:59:ARG:HG2	2.50	0.47
9:I:79:LEU:HD13	9:I:83:ARG:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:29:VAL:O	15:O:33:THR:HB	2.14	0.47
20:T:87:LYS:HD3	20:T:90:GLN:HE21	1.79	0.47
1:A:1392:G:C2'	1:A:1393:U:H5'	2.45	0.47
1:A:484:G:O2'	1:A:485:G:OP2	2.22	0.47
2:B:112:VAL:HG23	2:B:149:LEU:HD13	1.96	0.47
2:B:17:PHE:HD1	2:B:18:GLY:N	2.13	0.47
3:C:130:VAL:HG11	3:C:157:ILE:HG23	1.97	0.47
7:G:75:VAL:HG22	7:G:88:PRO:HA	1.96	0.47
14:N:41:ARG:HG3	14:N:42:ILE:N	2.30	0.47
16:P:78:GLY:C	16:P:80:PHE:N	2.66	0.47
1:A:1007:C:O2	1:A:1023:G:N1	2.48	0.47
1:A:1500:A:OP2	1:A:1505:G:OP1	2.33	0.47
1:A:877:C:O2	8:H:3:THR:HG21	2.15	0.47
1:A:75:G:C6	1:A:96:G:C6	3.02	0.47
2:B:122:PHE:CZ	2:B:139:LYS:HE2	2.50	0.47
1:A:653:A:O4'	8:H:56:LYS:HE2	2.14	0.47
13:M:108:ARG:NH2	13:M:112:GLY:O	2.48	0.47
19:S:41:VAL:HG23	19:S:44:MET:HG3	1.96	0.47
1:A:60:A:H4'	1:A:61:G:O5'	2.15	0.47
1:A:837:G:C2	1:A:850:U:O2	2.68	0.47
1:A:853:G:C2	1:A:854:G:C8	3.03	0.47
1:A:952:U:H2'	1:A:953:G:C8	2.49	0.47
2:B:196:LEU:HD23	2:B:196:LEU:HA	1.66	0.47
3:C:190:ARG:HG3	3:C:195:VAL:HB	1.96	0.47
4:D:102:ASP:HB3	4:D:136:PRO:HB3	1.96	0.47
8:H:96:GLY:HA2	8:H:130:GLY:HA3	1.96	0.47
10:J:51:ARG:HG3	10:J:59:SER:HB2	1.97	0.47
10:J:61:GLU:OE1	14:N:45:ARG:NH1	2.47	0.47
19:S:34:TRP:HD1	19:S:52:TYR:CG	2.32	0.47
1:A:1339:A:H5"	1:A:1340:A:OP2	2.14	0.47
1:A:260:G:C4	1:A:261:U:C5	3.03	0.47
1:A:344:A:H5'	1:A:345:C:C5	2.50	0.47
1:A:219:C:O2'	1:A:381:C:H5'	2.15	0.47
1:A:690:G:C6	1:A:691:G:C6	3.03	0.47
7:G:57:GLU:HG3	7:G:57:GLU:H	1.48	0.47
9:I:75:ASP:O	9:I:78:LYS:HB3	2.15	0.47
11:K:65:ALA:HB1	11:K:98:LEU:HB3	1.97	0.47
13:M:105:THR:O	13:M:107:ALA:N	2.48	0.47
18:R:55:ARG:HB3	18:R:55:ARG:CZ	2.45	0.47
1:A:1070:U:O2	1:A:1106:G:C2	2.69	0.47
1:A:1499:A:H1'	1:A:1520:G:OP1	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:694:A:N1	1:A:787:A:O2'	2.46	0.47
1:A:792:A:O2'	1:A:793:U:OP2	2.23	0.47
1:A:986:A:H1'	19:S:54:GLY:O	2.15	0.47
3:C:36:ASP:HA	3:C:39:ILE:CD1	2.43	0.47
6:F:38:GLU:HB2	6:F:64:GLN:O	2.15	0.47
14:N:23:ARG:HH12	14:N:30:ALA:HB2	1.80	0.47
16:P:60:LEU:HD23	16:P:60:LEU:HA	1.73	0.47
17:Q:61:GLU:HA	17:Q:71:PHE:CE1	2.50	0.47
21:U:12:LYS:HB3	21:U:22:ARG:HD2	1.97	0.47
1:A:1145:C:H1'	1:A:1146:A:C8	2.49	0.46
1:A:1303:C:H2'	1:A:1304:G:C5'	2.42	0.46
1:A:1347:G:O2'	1:A:1348:U:O5'	2.33	0.46
1:A:1373:G:H5"	7:G:36:LYS:HB2	1.97	0.46
1:A:315:A:O2'	1:A:330:C:O2'	2.26	0.46
2:B:119:GLU:HG3	2:B:142:LEU:HD11	1.97	0.46
2:B:7:VAL:HG21	2:B:221:LEU:HD23	1.97	0.46
4:D:124:GLY:O	4:D:132:ARG:HG3	2.16	0.46
8:H:31:PHE:O	8:H:35:ILE:HG12	2.15	0.46
11:K:47:VAL:HG12	11:K:48:ILE:N	2.30	0.46
1:A:131:C:H2'	1:A:132:C:C6	2.50	0.46
1:A:1399:C:C2	1:A:1401:G:C4	3.04	0.46
1:A:457:C:H2'	1:A:458:C:C6	2.50	0.46
1:A:544:G:C5	1:A:545:C:C5	3.02	0.46
1:A:953:G:C5'	1:A:965:A:H61	2.23	0.46
3:C:172:ARG:NH1	3:C:172:ARG:HB2	2.29	0.46
4:D:187:ARG:CZ	4:D:188:LEU:HB2	2.45	0.46
4:D:61:LYS:HE2	4:D:72:GLU:OE1	2.15	0.46
9:I:111:ARG:HH11	9:I:113:LYS:HA	1.80	0.46
1:A:1232:U:H5"	9:I:124:GLN:O	2.15	0.46
12:L:11:VAL:HG22	17:Q:29:HIS:CD2	2.51	0.46
1:A:1325:C:H4'	21:U:17:THR:HG21	1.97	0.46
1:A:102:G:H2'	1:A:103:C:C6	2.49	0.46
1:A:1003:G:N2	1:A:1039:C:N3	2.62	0.46
1:A:1261:A:H1'	1:A:1283:G:H5"	1.96	0.46
2:B:115:LEU:HD23	2:B:153:ARG:NE	2.30	0.46
2:B:82:ARG:HB2	2:B:82:ARG:NH1	2.30	0.46
6:F:12:PRO:HD3	6:F:58:GLY:HA2	1.97	0.46
13:M:17:VAL:O	13:M:20:THR:HB	2.14	0.46
15:O:17:ARG:HB2	15:O:18:PHE:CD2	2.51	0.46
17:Q:10:VAL:HG23	17:Q:54:GLY:H	1.79	0.46
1:A:707:C:H4'	11:K:20:TYR:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:113:ALA:HA	3:C:116:VAL:HG23	1.96	0.46
17:Q:40:LYS:HE3	17:Q:42:TYR:CZ	2.50	0.46
19:S:29:ARG:H	19:S:29:ARG:HD2	1.80	0.46
1:A:1030:C:N4	1:A:1032:G:O6	2.47	0.46
1:A:1065:U:C5	1:A:1190:G:H1'	2.50	0.46
1:A:268:C:H2'	1:A:269:C:H6	1.80	0.46
3:C:147:LYS:HZ3	3:C:203:PHE:HE2	1.63	0.46
7:G:16:LEU:HD11	9:I:45:ALA:HB2	1.97	0.46
12:L:60:LEU:HD13	12:L:60:LEU:HA	1.60	0.46
18:R:53:ARG:NH1	18:R:58:LEU:O	2.49	0.46
19:S:15:LEU:O	19:S:19:VAL:HG12	2.16	0.46
1:A:1003:G:H22	1:A:1039:C:H42	1.64	0.46
1:A:1124:G:H5"	1:A:1125:U:OP1	2.15	0.46
1:A:406:G:H21	4:D:119:GLN:HE22	1.63	0.46
1:A:666:G:H5'	1:A:726:C:H1'	1.96	0.46
2:B:24:TRP:CE3	2:B:26:PRO:HA	2.51	0.46
7:G:50:ILE:HD11	7:G:125:MET:HB2	1.97	0.46
8:H:77:GLU:HG2	8:H:78:GLN:N	2.30	0.46
16:P:17:TYR:HD1	16:P:39:TYR:HD2	1.63	0.46
1:A:184:G:H2'	1:A:185:A:C8	2.48	0.46
1:A:792:A:N6	1:A:794:A:N1	2.63	0.46
1:A:986:A:O2'	19:S:52:TYR:OH	2.26	0.46
4:D:15:GLU:CD	4:D:59:ARG:HH21	2.18	0.46
4:D:64:LEU:HD22	4:D:67:ILE:HD12	1.98	0.46
1:A:935:A:N6	7:G:3:ARG:HG3	2.29	0.46
1:A:691:G:H3'	11:K:26:ASN:HD21	1.79	0.46
12:L:25:PRO:C	12:L:27:LEU:N	2.64	0.46
1:A:452:A:HO2'	1:A:453:A:C4'	2.29	0.46
1:A:694:A:C2	1:A:695:A:H1'	2.50	0.46
1:A:792:A:C6	1:A:794:A:C2	3.04	0.46
1:A:781:A:C5	1:A:802:A:C2	3.04	0.46
1:A:881:G:OP1	12:L:13:LYS:NZ	2.48	0.46
3:C:105:GLU:O	3:C:107:GLN:NE2	2.49	0.46
9:I:19:LEU:HD11	9:I:81:ILE:HD13	1.98	0.46
12:L:25:PRO:HB3	12:L:27:LEU:HD12	1.98	0.46
1:A:269:C:H2'	1:A:270:A:H8	1.80	0.46
1:A:370:C:N3	1:A:392:G:C2	2.84	0.46
1:A:788:U:H3'	1:A:789:U:O4'	2.16	0.46
2:B:125:PRO:HG2	2:B:126:GLU:OE1	2.16	0.46
3:C:142:MET:HE1	3:C:170:GLN:HB2	1.98	0.46
3:C:70:VAL:O	3:C:106:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:107:ARG:NH1	4:D:194:LEU:HD11	2.31	0.46
4:D:30:LYS:O	4:D:32:ALA:N	2.48	0.46
5:E:110:LEU:HD12	5:E:118:ILE:HG21	1.98	0.46
12:L:44:THR:HA	12:L:45:PRO:HD3	1.54	0.46
12:L:82:VAL:O	12:L:106:ASP:HB2	2.16	0.46
1:A:1323:G:H2'	1:A:1324:A:C8	2.51	0.46
1:A:1542:U:H2'	1:A:1543:C:C6	2.51	0.46
1:A:268:C:H2'	1:A:269:C:C6	2.51	0.46
1:A:701:C:O2'	1:A:702:A:OP2	2.24	0.46
1:A:738:C:P	6:F:92:LYS:HD3	2.56	0.46
1:A:78:G:N1	1:A:92:C:C4	2.84	0.46
1:A:923:A:O4'	1:A:1398:A:C2	2.68	0.46
1:A:940:C:H2'	1:A:941:G:O4'	2.16	0.46
10:J:27:ALA:O	10:J:31:GLY:N	2.44	0.46
11:K:94:ALA:O	11:K:98:LEU:HD12	2.16	0.46
13:M:91:ARG:HB3	13:M:98:VAL:HG22	1.97	0.46
18:R:54:ARG:HB2	18:R:54:ARG:HE	1.58	0.46
1:A:1060:C:C2	1:A:1198:G:C2	3.04	0.45
1:A:350:G:O2'	1:A:351:G:H5'	2.16	0.45
1:A:389:A:C6	1:A:390:C:H1'	2.51	0.45
1:A:459:G:H1'	1:A:463:A:H61	1.81	0.45
1:A:479:C:H2'	1:A:480:U:O4'	2.16	0.45
1:A:806:C:H2'	1:A:807:A:H8	1.81	0.45
1:A:942:G:N2	1:A:943:U:C2	2.83	0.45
2:B:97:TRP:CZ2	2:B:102:LEU:HD13	2.51	0.45
2:B:44:LEU:O	2:B:47:THR:HB	2.16	0.45
2:B:52:GLU:HG2	2:B:56:ARG:HH22	1.81	0.45
7:G:17:VAL:HG11	7:G:44:TYR:CE2	2.51	0.45
9:I:8:GLY:H	9:I:83:ARG:NH1	2.14	0.45
10:J:57:LYS:HG3	10:J:58:ASP:OD2	2.15	0.45
1:A:345:C:OP2	1:A:345:C:H6	1.98	0.45
1:A:485:G:HO2'	1:A:486:U:P	2.39	0.45
1:A:945:G:N1	1:A:1337:G:N2	2.63	0.45
4:D:94:LEU:O	4:D:97:LEU:HB2	2.17	0.45
10:J:8:LEU:HA	10:J:95:GLU:O	2.16	0.45
1:A:1360:A:C2	14:N:18:VAL:HB	2.49	0.45
15:O:85:LEU:HD23	15:O:85:LEU:N	2.31	0.45
1:A:1267:C:O2'	21:U:20:LYS:HG3	2.16	0.45
1:A:1482:G:HO2'	1:A:1483:A:H8	1.62	0.45
1:A:152:A:N6	1:A:170:U:C2	2.85	0.45
1:A:337:C:H2'	1:A:338:A:H8	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:A:HO2'	1:A:453:A:C5'	2.30	0.45
1:A:833:U:H2'	1:A:834:C:C6	2.50	0.45
4:D:112:VAL:HG23	4:D:116:GLN:OE1	2.16	0.45
4:D:194:LEU:HD13	4:D:194:LEU:HA	1.63	0.45
6:F:26:ILE:O	6:F:30:LEU:HD12	2.16	0.45
1:A:983:A:P	14:N:3:ARG:HH22	2.39	0.45
17:Q:74:LEU:HD22	17:Q:74:LEU:HA	1.66	0.45
1:A:1014:A:N6	1:A:1015:A:N1	2.64	0.45
1:A:1048:G:H2'	1:A:1050:G:H8	1.81	0.45
1:A:1053:G:OP1	1:A:1054:C:H5"	2.16	0.45
1:A:1094:G:OP2	1:A:1095:U:H5	2.00	0.45
1:A:459:G:H1'	1:A:463:A:N6	2.32	0.45
1:A:550:G:C5	1:A:551:U:C5	3.04	0.45
1:A:671:G:H1	1:A:735:C:H42	1.63	0.45
2:B:74:LYS:NZ	2:B:206:ASP:OD1	2.35	0.45
5:E:123:LEU:HA	5:E:123:LEU:HD23	1.55	0.45
5:E:55:VAL:HG12	5:E:56:GLN:N	2.32	0.45
1:A:825:G:H21	8:H:11:THR:HG21	1.80	0.45
9:I:32:ASP:HB3	9:I:35:GLU:OE1	2.16	0.45
10:J:20:ALA:O	10:J:24:VAL:HG12	2.16	0.45
14:N:3:ARG:HE	14:N:6:LEU:HD23	1.82	0.45
1:A:977:A:H8	1:A:1223:C:N3	2.14	0.45
1:A:951:G:OP2	13:M:102:ARG:NH2	2.47	0.45
1:A:75:G:O6	1:A:96:G:C6	2.70	0.45
3:C:150:LYS:NZ	3:C:175:LEU:HD11	2.30	0.45
4:D:102:ASP:HA	4:D:121:VAL:HG21	1.99	0.45
4:D:13:ARG:HB2	4:D:38:TYR:O	2.16	0.45
7:G:5:ARG:HB3	7:G:6:ARG:H	1.62	0.45
8:H:4:ASP:CG	8:H:85:ARG:HH11	2.20	0.45
9:I:118:LYS:C	9:I:120:ARG:H	2.19	0.45
18:R:56:THR:HB	18:R:58:LEU:CD2	2.46	0.45
1:A:1422:G:C2	1:A:1423:G:C8	3.05	0.45
1:A:718:G:O6	18:R:74:ARG:NH1	2.48	0.45
1:A:723:U:O2	1:A:723:U:H2'	2.16	0.45
1:A:89:C:H2'	1:A:90:U:O4'	2.16	0.45
1:A:77:G:C6	1:A:93:G:N1	2.85	0.45
2:B:231:GLU:HB3	2:B:232:PRO:HD2	1.99	0.45
3:C:175:LEU:HD22	3:C:201:TYR:CD2	2.52	0.45
1:A:880:C:OP2	12:L:6:THR:HG21	2.17	0.45
17:Q:59:ILE:HG23	17:Q:71:PHE:HB3	1.98	0.45
20:T:16:HIS:CE1	20:T:20:LEU:HD11	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:45:GLN:N	20:T:45:GLN:OE1	2.49	0.45
1:A:1058:G:H2'	1:A:1059:C:C6	2.51	0.45
1:A:1089:G:C6	1:A:1090:U:C4	3.05	0.45
1:A:1202:G:H2'	1:A:1203:C:O4'	2.16	0.45
1:A:1351:U:H4'	7:G:33:ASP:OD2	2.17	0.45
1:A:435:C:H2'	1:A:436:C:C6	2.51	0.45
1:A:661:G:H1	1:A:744:C:H42	1.63	0.45
1:A:975:A:H5'	1:A:975:A:C8	2.49	0.45
3:C:30:ARG:H	3:C:30:ARG:HD3	1.80	0.45
3:C:85:ARG:HH11	3:C:88:ARG:HH12	1.63	0.45
5:E:36:ASP:C	5:E:38:GLN:H	2.19	0.45
5:E:92:LYS:O	5:E:118:ILE:HG12	2.17	0.45
9:I:86:VAL:HG23	9:I:96:LEU:HD22	1.98	0.45
12:L:42:THR:HA	12:L:53:ARG:O	2.16	0.45
13:M:23:TYR:HB3	13:M:67:GLU:HA	1.98	0.45
14:N:16:PHE:HD1	14:N:19:ARG:NE	2.15	0.45
1:A:977:A:H8	1:A:1223:C:C4	2.34	0.45
1:A:1267:C:O2	21:U:20:LYS:HD2	2.16	0.45
1:A:1511:G:H2'	1:A:1512:U:O4'	2.15	0.45
1:A:457:C:H2'	1:A:458:C:H6	1.82	0.45
1:A:79:G:C2	1:A:80:G:C4	3.05	0.45
4:D:173:TRP:CE2	4:D:174:LEU:HD11	2.51	0.45
5:E:11:ILE:HB	5:E:31:LEU:CB	2.46	0.45
9:I:20:ARG:HB2	9:I:60:ASP:HB3	1.99	0.45
12:L:92:0TD:N	12:L:92:0TD:OD1	2.49	0.45
18:R:56:THR:HB	18:R:58:LEU:HD21	1.99	0.45
1:A:1338:G:C6	1:A:1339:A:C6	3.05	0.45
1:A:489:C:OP1	4:D:132:ARG:NH2	2.49	0.45
1:A:6:G:O2'	1:A:7:G:H5'	2.17	0.45
1:A:922:G:C2	1:A:1396:A:C6	3.05	0.45
1:A:946:A:N1	1:A:1236:A:C2	2.85	0.45
3:C:175:LEU:HG	3:C:175:LEU:H	1.46	0.45
1:A:620:C:N1	4:D:135:LEU:HD13	2.31	0.45
4:D:20:TYR:HA	4:D:26:CYS:SG	2.57	0.45
8:H:112:LEU:HD12	8:H:112:LEU:H	1.82	0.45
8:H:6:ILE:HG13	8:H:31:PHE:HE2	1.81	0.45
8:H:20:TYR:HA	8:H:65:TYR:CE2	2.52	0.45
11:K:44:SER:H	11:K:47:VAL:HB	1.81	0.45
13:M:102:ARG:HG3	13:M:102:ARG:O	2.17	0.45
13:M:105:THR:OG1	13:M:106:ASN:HB2	2.16	0.45
13:M:27:LYS:HA	13:M:27:LYS:HD2	1.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:34:LEU:HD13	13:M:41:PRO:HA	1.99	0.45
14:N:41:ARG:HG3	14:N:42:ILE:H	1.82	0.45
1:A:974:A:P	14:N:41:ARG:HH22	2.39	0.45
16:P:39:TYR:HE2	16:P:41:PRO:HB3	1.82	0.45
18:R:22:VAL:HG23	18:R:56:THR:HA	1.99	0.45
18:R:60:ALA:O	18:R:64:ARG:HG3	2.17	0.45
1:A:1202:G:C4	14:N:42:ILE:HD12	2.52	0.45
1:A:456:C:C2	1:A:457:C:C5	3.04	0.45
1:A:92:C:H2'	1:A:93:G:H8	1.81	0.45
4:D:159:ARG:O	4:D:163:GLU:HB2	2.17	0.45
4:D:31:CYS:SG	4:D:31:CYS:O	2.75	0.45
1:A:1080:A:H5"	5:E:16:THR:OG1	2.17	0.45
18:R:43:PHE:O	18:R:51:LEU:HD23	2.16	0.45
19:S:15:LEU:HD12	19:S:16:LEU:N	2.32	0.45
20:T:30:LYS:O	20:T:33:ILE:HB	2.17	0.45
1:A:1342:C:H2'	1:A:1343:G:C8	2.51	0.44
6:F:27:GLN:O	6:F:31:GLU:HG3	2.17	0.44
7:G:121:ALA:O	7:G:124:LEU:HD12	2.16	0.44
9:I:6:GLY:CA	9:I:83:ARG:HB3	2.46	0.44
11:K:125:PHE:C	11:K:126:ARG:HG3	2.37	0.44
1:A:1265:G:C6	1:A:1266:G:C6	3.05	0.44
1:A:1329:A:OP1	13:M:28:ALA:HB3	2.17	0.44
1:A:450:G:N7	1:A:481:G:O6	2.50	0.44
1:A:517:G:H5'	1:A:519:C:O2	2.16	0.44
3:C:150:LYS:HG2	3:C:169:ALA:CB	2.46	0.44
14:N:39:LEU:CD1	14:N:43:CYS:HB3	2.47	0.44
17:Q:43:LEU:HD23	17:Q:43:LEU:HA	1.69	0.44
18:R:52:PRO:O	18:R:56:THR:OG1	2.29	0.44
20:T:51:GLU:HG2	20:T:51:GLU:H	1.56	0.44
1:A:1196:U:H3'	1:A:1196:U:OP1	2.18	0.44
1:A:328:C:O2	1:A:328:C:H2'	2.17	0.44
1:A:370:C:H2'	1:A:371:G:O4'	2.17	0.44
1:A:451:A:H2	1:A:480:U:C4	2.35	0.44
1:A:575:G:HO2'	1:A:821:G:H5'	1.82	0.44
1:A:401:C:H1'	1:A:622:A:H1'	1.99	0.44
1:A:712:A:H2'	1:A:713:G:O4'	2.18	0.44
1:A:665:A:H2'	1:A:732:C:O2	2.17	0.44
1:A:92:C:O2'	1:A:93:G:H5'	2.17	0.44
3:C:181:ASN:O	3:C:181:ASN:ND2	2.50	0.44
1:A:546:G:OP1	4:D:73:ARG:HG2	2.16	0.44
5:E:65:ASN:OD1	5:E:140:ARG:NH2	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:73:ASN:HD22	6:F:73:ASN:N	2.14	0.44
7:G:88:PRO:HG2	7:G:155:ARG:CZ	2.47	0.44
12:L:120:TYR:CD2	12:L:120:TYR:N	2.85	0.44
15:O:29:VAL:HG11	15:O:67:LEU:HD21	1.98	0.44
1:A:1423:G:N2	1:A:1477:C:O2	2.40	0.44
1:A:1532:U:H2'	1:A:1533:C:H3'	2.00	0.44
1:A:279:A:H8	1:A:279:A:H5'	1.82	0.44
1:A:411:A:H62	1:A:413:G:H21	1.65	0.44
10:J:57:LYS:HE2	10:J:57:LYS:HB2	1.86	0.44
12:L:24:VAL:HG13	12:L:98:TYR:HE2	1.81	0.44
13:M:3:ARG:HA	13:M:8:GLU:O	2.17	0.44
1:A:1391:U:H2'	1:A:1392:G:C8	2.53	0.44
1:A:1400:5MC:H3'	1:A:1401:G:C5'	2.46	0.44
1:A:429:U:H4'	1:A:430:A:O5'	2.17	0.44
1:A:602:A:C2	1:A:637:G:C2	3.06	0.44
1:A:658:G:H2'	1:A:659:U:C6	2.52	0.44
1:A:803:G:O5'	1:A:803:G:H8	1.99	0.44
1:A:829:G:O2'	1:A:830:G:H5'	2.18	0.44
2:B:100:GLY:O	2:B:104:ASN:N	2.49	0.44
2:B:114:ARG:NE	2:B:141:GLU:OE2	2.46	0.44
2:B:139:LYS:HZ2	2:B:143:GLU:HG3	1.82	0.44
2:B:36:ARG:HG3	2:B:41:ILE:HD11	1.99	0.44
8:H:28:ALA:HB2	8:H:59:LEU:HG	1.99	0.44
9:I:5:TYR:CE2	9:I:18:PHE:HE2	2.35	0.44
12:L:28:LYS:HG3	12:L:33:ARG:NH1	2.32	0.44
12:L:34:ARG:HG3	12:L:34:ARG:O	2.18	0.44
12:L:24:VAL:HG13	12:L:98:TYR:CE2	2.53	0.44
1:A:263:A:OP2	20:T:79:ARG:NH1	2.48	0.44
1:A:1235:U:O3'	21:U:3:LYS:HB2	2.18	0.44
1:A:1342:C:H2'	1:A:1343:G:H8	1.82	0.44
1:A:1540:PSU:HN1	1:A:1541:PSU:HN1	1.64	0.44
1:A:222:U:H2'	1:A:223:U:C6	2.53	0.44
1:A:642:A:C5	1:A:643:C:C5	3.05	0.44
2:B:54:THR:OG1	2:B:199:TYR:HB3	2.17	0.44
6:F:4:TYR:HE1	6:F:92:LYS:HG2	1.79	0.44
12:L:5:PRO:HG2	12:L:10:LEU:HD11	1.99	0.44
17:Q:95:TYR:O	17:Q:97:SER:N	2.50	0.44
1:A:956:U:HO2'	19:S:80:TYR:HD1	1.63	0.44
1:A:538:G:OP2	12:L:115:LYS:HB2	2.17	0.44
1:A:695:A:OP2	11:K:52:GLY:HA3	2.18	0.44
2:B:31:TYR:CD2	2:B:31:TYR:N	2.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:48:MET:HA	2:B:51:LEU:HB2	1.99	0.44
1:A:410:G:OP2	4:D:25:ARG:HG3	2.17	0.44
7:G:50:ILE:HD13	7:G:50:ILE:HA	1.61	0.44
8:H:134:ILE:HA	8:H:134:ILE:HD13	1.70	0.44
1:A:1004:A:HO2'	1:A:1005:A:P	2.41	0.44
1:A:1424:C:H2'	1:A:1425:U:H6	1.83	0.44
1:A:815:A:N6	1:A:1509:C:H1'	2.33	0.44
1:A:69:G:H1	1:A:99:C:H42	1.66	0.44
1:A:838:G:C2	1:A:849:C:C2	3.05	0.44
2:B:87:ARG:HB3	2:B:87:ARG:HH11	1.82	0.44
15:O:42:HIS:CD2	15:O:43:LEU:HD23	2.53	0.44
17:Q:29:HIS:HA	17:Q:30:PRO:HD3	1.57	0.44
17:Q:58:GLU:HB3	17:Q:74:LEU:CB	2.47	0.44
17:Q:83:ASP:N	17:Q:83:ASP:OD1	2.50	0.44
1:A:1014:A:H4'	19:S:14:HIS:CD2	2.53	0.44
19:S:18:LYS:HD2	19:S:31:ILE:HD11	2.00	0.44
20:T:53:LEU:HD22	20:T:56:MET:HE2	2.00	0.44
1:A:1072:G:C6	1:A:1073:U:C4	3.06	0.44
1:A:1494:G:C2	1:A:1495:U:C4	3.05	0.44
1:A:1496:C:O2'	1:A:1497:G:O5'	2.35	0.44
1:A:61:G:H2'	1:A:62:U:O4'	2.18	0.44
2:B:15:VAL:HG11	2:B:213:LEU:HD12	2.00	0.44
3:C:11:ARG:HD3	3:C:181:ASN:HA	1.99	0.44
3:C:7:PRO:HG2	3:C:184:TYR:CD1	2.53	0.44
4:D:105:VAL:HG13	4:D:110:PHE:HB2	1.99	0.44
4:D:70:ILE:HD13	4:D:70:ILE:HA	1.63	0.44
4:D:98:GLU:OE2	4:D:107:ARG:NE	2.50	0.44
6:F:78:GLU:O	6:F:81:ILE:HG22	2.18	0.44
11:K:73:MET:HG3	11:K:103:LEU:HD21	1.98	0.44
1:A:1228:C:O3'	13:M:116:THR:HG23	2.18	0.44
13:M:19:LEU:HD11	13:M:56:LEU:CD1	2.48	0.44
15:O:17:ARG:HD3	15:O:26:GLU:OE2	2.18	0.44
17:Q:22:LEU:HD12	17:Q:22:LEU:HA	1.52	0.44
1:A:1244:C:H42	1:A:1293:G:H1	1.64	0.43
1:A:1426:C:H2'	1:A:1427:U:C6	2.52	0.43
1:A:16:A:O2'	1:A:17:U:H5'	2.18	0.43
1:A:434:U:H2'	1:A:435:C:C6	2.53	0.43
1:A:667:G:H4'	15:O:51:HIS:ND1	2.32	0.43
1:A:673:G:H2'	1:A:674:G:C8	2.53	0.43
1:A:838:G:N2	1:A:849:C:C2	2.86	0.43
2:B:62:ALA:HB1	2:B:222:ILE:HG23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:22:TRP:CH2	3:C:33:LEU:HD21	2.53	0.43
5:E:110:LEU:HD23	5:E:110:LEU:N	2.33	0.43
6:F:11:ASN:HA	6:F:12:PRO:HD2	1.73	0.43
8:H:35:ILE:HG12	8:H:35:ILE:H	1.61	0.43
10:J:5:ARG:HD3	10:J:99:LYS:HB3	1.98	0.43
12:L:113:ARG:HH12	12:L:115:LYS:HB3	1.83	0.43
12:L:51:ALA:O	12:L:52:LEU:HD23	2.18	0.43
19:S:43:GLU:OE1	19:S:43:GLU:N	2.49	0.43
20:T:65:LYS:O	20:T:68:LYS:HB3	2.18	0.43
1:A:1293:G:H2'	1:A:1294:G:O4'	2.18	0.43
1:A:77:G:C6	1:A:93:G:C6	3.06	0.43
3:C:173:VAL:HG12	3:C:175:LEU:HD23	2.00	0.43
4:D:57:ARG:HG3	4:D:202:LEU:CD1	2.48	0.43
8:H:12:ARG:HH11	8:H:26:VAL:HA	1.82	0.43
11:K:38:ASN:HA	11:K:39:PRO:HD3	1.66	0.43
12:L:53:ARG:HG2	12:L:93:LEU:HD11	2.00	0.43
1:A:1133:G:N2	1:A:1141:C:N3	2.63	0.43
1:A:146:G:C2	1:A:147:G:C4	3.06	0.43
1:A:1498:UR3:H6	1:A:1498:UR3:O5'	2.18	0.43
1:A:448:A:P	1:A:485:G:H22	2.40	0.43
1:A:679:C:H2'	1:A:680:C:H6	1.83	0.43
3:C:114:PRO:N	3:C:185:GLY:HA3	2.33	0.43
5:E:90:VAL:O	5:E:91:LEU:HD23	2.19	0.43
1:A:1178:G:P	9:I:97:LYS:HZ3	2.41	0.43
1:A:109:A:H2'	1:A:326:G:N2	2.33	0.43
1:A:357:G:C2	1:A:358:U:C5	3.07	0.43
1:A:445:G:H2'	1:A:446:G:H8	1.83	0.43
1:A:83:U:C2'	1:A:84:U:H5'	2.48	0.43
1:A:959:A:O2'	1:A:984:C:O2'	2.34	0.43
3:C:73:PRO:HG3	3:C:105:GLU:OE1	2.19	0.43
5:E:90:VAL:C	5:E:91:LEU:HD23	2.39	0.43
7:G:124:LEU:HG	7:G:124:LEU:H	1.44	0.43
15:O:85:LEU:HB2	15:O:87:ILE:HD12	2.01	0.43
17:Q:63:ARG:HH11	17:Q:63:ARG:CB	2.32	0.43
21:U:5:ASP:O	21:U:8:THR:OG1	2.35	0.43
1:A:1084:G:O2'	1:A:1085:U:OP1	2.34	0.43
1:A:1226:C:H4'	1:A:1227:A:OP1	2.18	0.43
1:A:1474:G:H2'	1:A:1475:G:C8	2.54	0.43
1:A:321:A:N6	1:A:329:A:OP2	2.49	0.43
1:A:90:U:C4	1:A:91:C:C5	3.06	0.43
1:A:946:A:C6	1:A:1236:A:C2	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:964:A:O2'	10:J:55:LYS:NZ	2.22	0.43
4:D:25:ARG:HA	4:D:28:SER:H	1.83	0.43
4:D:30:LYS:C	4:D:32:ALA:H	2.20	0.43
7:G:17:VAL:HG21	7:G:44:TYR:CZ	2.53	0.43
8:H:53:VAL:HB	8:H:58:TYR:CD1	2.54	0.43
9:I:48:GLU:HA	9:I:51:ARG:HD2	2.00	0.43
9:I:17:VAL:HG22	9:I:63:ILE:HD12	2.00	0.43
13:M:16:ASP:HB3	13:M:34:LEU:HD12	1.99	0.43
1:A:1054:C:OP1	1:A:1197:G:OP1	2.37	0.43
1:A:1301:U:O2'	1:A:1302:U:P	2.77	0.43
1:A:279:A:C8	1:A:279:A:H5'	2.53	0.43
1:A:410:G:N1	1:A:429:U:O2	2.51	0.43
1:A:920:U:H2'	1:A:921:U:C6	2.54	0.43
2:B:54:THR:O	2:B:58:ILE:HG13	2.19	0.43
4:D:119:GLN:HG3	4:D:123:HIS:NE2	2.33	0.43
8:H:17:THR:HG22	8:H:63:LEU:HG	2.01	0.43
1:A:1117:G:H5"	9:I:104:ARG:NH2	2.33	0.43
12:L:59:ARG:HH11	12:L:59:ARG:HA	1.84	0.43
15:O:4:THR:O	15:O:7:GLU:HB2	2.19	0.43
17:Q:6:LEU:O	17:Q:58:GLU:HG3	2.17	0.43
20:T:50:GLU:H	20:T:50:GLU:HG2	1.34	0.43
20:T:33:ILE:HG12	20:T:62:LEU:CD2	2.48	0.43
1:A:1008:C:N4	1:A:1021:G:H22	2.04	0.43
1:A:1347:G:H2'	1:A:1373:G:C6	2.53	0.43
1:A:1521:G:H2'	1:A:1522:U:C6	2.54	0.43
1:A:190:C:O2'	1:A:190(A):C:H5'	2.18	0.43
1:A:284:G:H2'	1:A:285:G:C8	2.53	0.43
1:A:391:G:C6	1:A:392:G:C5	3.07	0.43
2:B:188:ALA:HB1	2:B:192:SER:OG	2.18	0.43
4:D:126:ILE:O	4:D:132:ARG:HA	2.18	0.43
4:D:88:VAL:O	4:D:92:VAL:HG23	2.17	0.43
10:J:8:LEU:CD2	10:J:96:ILE:HG23	2.49	0.43
12:L:35:GLY:HA3	12:L:60:LEU:HD13	2.00	0.43
17:Q:40:LYS:HG3	17:Q:41:LYS:N	2.33	0.43
18:R:37:VAL:HG13	18:R:41:LYS:HD3	2.00	0.43
18:R:88:LYS:NZ	18:R:88:LYS:HB3	2.33	0.43
19:S:58:VAL:HA	19:S:59:PRO:HD3	1.66	0.43
1:A:1094:G:O2'	1:A:1095:U:OP1	2.37	0.43
1:A:1112:C:H1'	3:C:179:ARG:NH1	2.33	0.43
22:A:1601:SRY:C22	22:A:1601:SRY:HI32	2.49	0.43
4:D:190:ASP:HB3	4:D:193:ASP:OD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:100:ASN:HB2	18:R:23:LYS:HD2	1.99	0.43
9:I:89:ASN:HB3	9:I:92:TYR:HB2	2.01	0.43
10:J:88:LEU:HD23	10:J:88:LEU:HA	1.85	0.43
13:M:92:HIS:CD2	13:M:98:VAL:HG21	2.53	0.43
1:A:1326:C:H2'	1:A:1327:C:C6	2.53	0.43
1:A:927:G:O2'	1:A:1503:A:N7	2.46	0.43
1:A:854:G:H3'	1:A:871:U:O4	2.18	0.43
2:B:226:ARG:HB2	2:B:226:ARG:HE	1.64	0.43
4:D:187:ARG:NH2	4:D:188:LEU:O	2.51	0.43
5:E:43:LEU:HD11	5:E:133:TYR:CD2	2.53	0.43
17:Q:89:LEU:HD23	17:Q:89:LEU:HA	1.77	0.43
19:S:75:ALA:HA	19:S:76:PRO:HD2	1.82	0.43
1:A:1157:A:H4'	1:A:1158:C:O4'	2.18	0.43
1:A:1384:C:H2'	1:A:1385:G:C8	2.54	0.43
1:A:585:G:C6	1:A:586:C:C4	3.06	0.43
1:A:1206:G:H4'	3:C:192:THR:O	2.19	0.43
4:D:11:LEU:HD13	4:D:66:ARG:CD	2.49	0.43
9:I:104:ARG:HD2	9:I:105:ASP:N	2.34	0.43
9:I:36:TYR:CD2	9:I:37:PHE:CE2	3.07	0.43
11:K:101:SER:HG	11:K:103:LEU:H	1.65	0.43
11:K:58:PRO:O	11:K:61:ALA:HB3	2.19	0.43
12:L:98:TYR:CD1	12:L:98:TYR:N	2.87	0.43
1:A:1303:C:C2'	1:A:1304:G:H5'	2.44	0.42
1:A:1502:A:H2	1:A:1505:G:H1	1.66	0.42
1:A:24:U:H2'	1:A:25:C:C6	2.54	0.42
1:A:386:C:C2'	1:A:387:U:H5'	2.49	0.42
1:A:474:G:C2	1:A:475:G:N7	2.87	0.42
1:A:77:G:N1	1:A:93:G:C6	2.87	0.42
1:A:865:A:C6	1:A:866:C:C4	3.07	0.42
11:K:33:THR:HB	11:K:39:PRO:HA	2.01	0.42
12:L:115:LYS:HD2	12:L:115:LYS:HA	1.87	0.42
14:N:44:LEU:O	14:N:48:ALA:HB2	2.19	0.42
16:P:41:PRO:O	16:P:43:LYS:HD3	2.19	0.42
1:A:1060:C:N3	1:A:1198:G:C6	2.87	0.42
1:A:113:G:H2'	1:A:114:U:H6	1.84	0.42
1:A:448:A:C4	1:A:487:A:C2	3.07	0.42
1:A:981:U:H2'	1:A:982:U:C6	2.54	0.42
3:C:113:ALA:N	3:C:114:PRO:HD2	2.33	0.42
4:D:18:LYS:HB3	4:D:20:TYR:HE2	1.84	0.42
5:E:100:VAL:HG12	5:E:118:ILE:HG22	2.01	0.42
15:O:15:PHE:HE2	15:O:85:LEU:HD21	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:G:H1'	17:Q:16:GLN:OE1	2.19	0.42
1:A:1092:A:H1'	1:A:1183:A:N6	2.34	0.42
1:A:1376:U:C2	1:A:1377:A:N7	2.87	0.42
1:A:1518:MA6:H102	1:A:1519:MA6:C6	2.49	0.42
1:A:825:G:H1	1:A:875:C:N4	2.16	0.42
1:A:833:U:H2'	1:A:834:C:H6	1.84	0.42
2:B:91:PRO:HA	2:B:154:LEU:HD12	2.01	0.42
5:E:139:LEU:HA	5:E:139:LEU:HD23	1.59	0.42
7:G:136:LYS:HE2	7:G:136:LYS:HB2	1.76	0.42
7:G:152:ALA:HA	7:G:155:ARG:CZ	2.49	0.42
5:E:78:HIS:ND1	8:H:104:ARG:HG3	2.33	0.42
10:J:15:THR:HG21	10:J:93:GLY:HA3	2.00	0.42
16:P:4:ILE:HA	16:P:20:VAL:O	2.19	0.42
20:T:18:GLN:O	20:T:21:LYS:HB2	2.18	0.42
1:A:1201:A:H1'	1:A:1202:G:OP2	2.20	0.42
1:A:1213:A:N6	1:A:1215:G:N3	2.67	0.42
1:A:1479:C:H2'	1:A:1480:G:C8	2.52	0.42
1:A:200:G:N2	1:A:218:C:C2	2.87	0.42
1:A:279:A:H5"	1:A:281:G:O4'	2.18	0.42
1:A:162:A:H1'	1:A:348:G:O2'	2.19	0.42
1:A:945:G:O6	1:A:1236:A:N1	2.52	0.42
2:B:115:LEU:HD11	2:B:146:GLN:HG3	2.02	0.42
2:B:25:ASN:C	2:B:25:ASN:HD22	2.22	0.42
3:C:106:VAL:CG1	3:C:109:PRO:HA	2.45	0.42
3:C:94:LEU:HD13	3:C:94:LEU:HA	1.73	0.42
5:E:11:ILE:HG22	5:E:12:LEU:N	2.33	0.42
5:E:31:LEU:HA	5:E:31:LEU:HD23	1.54	0.42
8:H:39:LEU:HA	8:H:39:LEU:HD13	1.72	0.42
11:K:34:ASP:HA	11:K:35:PRO:HD3	1.81	0.42
13:M:6:GLY:O	13:M:67:GLU:HG2	2.19	0.42
13:M:23:TYR:CZ	13:M:71:ARG:HG2	2.55	0.42
1:A:1241:G:H2'	1:A:1242:C:H6	1.84	0.42
1:A:1249:C:H2'	1:A:1250:A:H5'	2.01	0.42
1:A:1361(A):C:O2'	1:A:1362:C:H6	2.01	0.42
1:A:216:G:H2'	1:A:217:C:C6	2.54	0.42
1:A:217:C:H2'	1:A:218:C:C6	2.54	0.42
1:A:647:C:H2'	1:A:648:A:C8	2.55	0.42
2:B:108:ILE:HD13	2:B:108:ILE:HA	1.83	0.42
2:B:28:PHE:HD2	2:B:32:ILE:HD11	1.84	0.42
3:C:135:LYS:HB3	3:C:135:LYS:HE2	1.84	0.42
4:D:57:ARG:NH1	4:D:202:LEU:HD11	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:76:ILE:HD12	5:E:76:ILE:N	2.34	0.42
9:I:15:ALA:CB	9:I:65:VAL:HG12	2.48	0.42
10:J:37:PRO:HB2	10:J:70:ARG:HB3	2.02	0.42
17:Q:29:HIS:C	17:Q:29:HIS:ND1	2.73	0.42
18:R:53:ARG:NH1	18:R:59:SER:HA	2.34	0.42
19:S:39:THR:HG22	19:S:40:ILE:O	2.18	0.42
20:T:53:LEU:HA	20:T:53:LEU:HD22	1.79	0.42
20:T:88:VAL:O	20:T:92:LEU:HD23	2.20	0.42
1:A:1328:C:C2	1:A:1329:A:C8	3.08	0.42
1:A:219:C:C4	1:A:220:G:C8	3.07	0.42
1:A:460:A:C6	1:A:462:G:C5	3.08	0.42
2:B:157:ARG:HG2	2:B:158:LEU:N	2.34	0.42
4:D:156:GLU:O	4:D:160:GLN:NE2	2.53	0.42
4:D:172:PRO:HD2	4:D:173:TRP:CZ3	2.55	0.42
1:A:7:G:O6	5:E:92:LYS:HE3	2.19	0.42
7:G:10:ARG:HB2	7:G:10:ARG:NH1	2.34	0.42
11:K:48:ILE:HD13	11:K:63:LEU:HB3	2.02	0.42
11:K:19:ALA:HB2	11:K:80:VAL:CG1	2.50	0.42
14:N:12:ARG:HD2	14:N:14:PRO:HG3	2.02	0.42
15:O:28:GLN:O	15:O:32:LEU:HB2	2.19	0.42
16:P:38:TYR:O	16:P:49:LEU:HD12	2.20	0.42
19:S:30:LEU:HB3	19:S:31:ILE:H	1.67	0.42
1:A:132:C:O3'	20:T:74:LYS:NZ	2.43	0.42
1:A:809:G:C6	1:A:810:C:C5	3.08	0.42
3:C:175:LEU:HD22	3:C:201:TYR:CE2	2.54	0.42
6:F:79:LEU:HD23	6:F:79:LEU:HA	1.80	0.42
8:H:95:VAL:HB	8:H:99:GLU:HB2	2.01	0.42
9:I:79:LEU:O	9:I:83:ARG:HB2	2.20	0.42
9:I:50:LEU:HD21	9:I:85:LEU:HD11	2.02	0.42
11:K:18:ARG:HB2	11:K:33:THR:HG23	2.01	0.42
10:J:49:VAL:CG1	14:N:41:ARG:HB2	2.50	0.42
16:P:65:GLN:HA	16:P:66:PRO:HD2	1.84	0.42
20:T:33:ILE:HG12	20:T:62:LEU:HD23	2.01	0.42
1:A:1276:G:H2'	1:A:1277:C:C6	2.55	0.42
1:A:33:A:N3	12:L:32:PHE:HE2	2.17	0.42
3:C:17:ASP:O	3:C:54:ARG:NH2	2.53	0.42
11:K:21:ILE:HD12	11:K:95:ILE:HG12	2.02	0.42
13:M:92:HIS:NE2	13:M:98:VAL:HG21	2.35	0.42
17:Q:24:GLU:HG2	17:Q:39:SER:HB3	2.02	0.42
1:A:1138:G:O2'	1:A:1140:C:H5'	2.20	0.42
1:A:232:G:H2'	1:A:233:C:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:G:C4	1:A:36:C:C5	3.07	0.42
1:A:707:C:O3'	11:K:20:TYR:HE2	2.03	0.42
3:C:134:ILE:N	3:C:134:ILE:HD13	2.34	0.42
3:C:155:GLY:HA3	3:C:163:ALA:HB1	2.02	0.42
13:M:40:ASN:ND2	13:M:43:THR:HG23	2.35	0.42
16:P:53:VAL:HG23	16:P:54:GLU:H	1.84	0.42
1:A:522:C:H5"	12:L:120:TYR:OH	2.19	0.42
1:A:538:G:P	12:L:115:LYS:HB2	2.60	0.42
1:A:980:C:C5	1:A:981:U:C4	3.08	0.42
3:C:180:ALA:HB1	3:C:203:PHE:HE1	1.85	0.42
6:F:55:ASP:HA	6:F:56:PRO:HD3	1.83	0.42
1:A:1321:C:H5'	13:M:87:TYR:CE2	2.54	0.42
18:R:32:ARG:HA	18:R:69:THR:CG2	2.46	0.42
19:S:12:ASP:H	19:S:15:LEU:HD11	1.84	0.42
1:A:1474:G:H2'	1:A:1475:G:H8	1.85	0.41
22:A:1601:SRY:H22	22:A:1601:SRY:HI32	2.02	0.41
1:A:460:A:OP1	1:A:460:A:H8	2.03	0.41
1:A:663:A:H5"	18:R:61:LYS:HE3	2.01	0.41
4:D:11:LEU:HD13	4:D:66:ARG:HD3	2.02	0.41
14:N:41:ARG:HA	14:N:44:LEU:HB2	2.02	0.41
16:P:39:TYR:CZ	16:P:41:PRO:HA	2.55	0.41
1:A:1198:G:H2'	1:A:1199:U:C5	2.56	0.41
1:A:1347:G:H2'	1:A:1373:G:O6	2.20	0.41
1:A:491:G:C4	1:A:492:G:C8	3.07	0.41
1:A:778:G:C5	1:A:779:C:C5	3.08	0.41
1:A:78:G:C5	1:A:79:G:N7	2.88	0.41
1:A:960:U:H4'	1:A:961:U:O5'	2.21	0.41
1:A:9:G:OP1	5:E:122:GLU:HG3	2.19	0.41
2:B:23:ARG:O	2:B:24:TRP:CD1	2.74	0.41
3:C:150:LYS:HG3	3:C:173:VAL:HG21	2.01	0.41
4:D:206:PHE:CE2	4:D:207:TYR:CE2	3.08	0.41
9:I:96:LEU:HA	9:I:99:LEU:HD12	2.01	0.41
16:P:50:LYS:HE2	16:P:50:LYS:HB2	1.81	0.41
16:P:51:VAL:HG12	16:P:52:ASP:C	2.40	0.41
17:Q:26:GLN:HG2	17:Q:37:LYS:HB2	2.01	0.41
18:R:20:ALA:HA	18:R:21:LYS:NZ	2.35	0.41
20:T:10:LEU:HD22	20:T:11:SER:N	2.32	0.41
1:A:1060:C:H4'	10:J:51:ARG:HB3	2.01	0.41
1:A:1061:G:C6	1:A:1197:G:C6	3.08	0.41
1:A:1354:C:H2'	1:A:1355:G:C8	2.54	0.41
1:A:1497:G:H2'	1:A:1498:UR3:H5'	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:172:ILE:H	2:B:172:ILE:HG13	1.46	0.41
4:D:117:ALA:O	4:D:121:VAL:HG23	2.21	0.41
4:D:199:ASN:ND2	4:D:202:LEU:HD23	2.36	0.41
4:D:205:GLU:CD	5:E:100:VAL:HG23	2.40	0.41
5:E:18:ARG:HE	5:E:18:ARG:HB3	1.45	0.41
3:C:26:LYS:HG2	10:J:45:ARG:HH22	1.85	0.41
1:A:881:G:P	12:L:12:ARG:HH22	2.43	0.41
12:L:37:CYS:SG	12:L:56:ALA:HB1	2.61	0.41
15:O:38:ARG:O	15:O:41:GLU:HB3	2.20	0.41
1:A:1098:C:H2'	1:A:1099:G:O4'	2.21	0.41
1:A:1277:C:H1'	1:A:1282:C:H1'	2.02	0.41
1:A:1350:A:OP2	9:I:118:LYS:HD3	2.19	0.41
1:A:1516:G:N2	1:A:1519:MA6:OP2	2.47	0.41
1:A:412:A:O2'	1:A:413:G:O4'	2.37	0.41
1:A:929:G:H2'	1:A:930:C:O4'	2.20	0.41
1:A:986:A:C6	1:A:1220:G:C6	3.09	0.41
2:B:135:GLN:HB2	2:B:135:GLN:HE21	1.55	0.41
2:B:189:ASP:OD1	2:B:189:ASP:N	2.53	0.41
2:B:22:LYS:HB2	2:B:22:LYS:HE2	1.90	0.41
2:B:40:HIS:HD1	2:B:190:THR:HG21	1.85	0.41
3:C:116:VAL:O	3:C:119:ARG:HB3	2.20	0.41
4:D:157:LEU:HA	4:D:157:LEU:HD23	1.81	0.41
5:E:71:LEU:HD11	5:E:113:ALA:O	2.20	0.41
5:E:75:THR:C	5:E:76:ILE:HD12	2.41	0.41
1:A:1092:A:H5"	7:G:4:ARG:CZ	2.50	0.41
1:A:1346:A:C5'	9:I:120:ARG:HH12	2.30	0.41
19:S:66:MET:H	19:S:66:MET:HG2	1.63	0.41
1:A:101:A:C2	1:A:102:G:C8	3.09	0.41
1:A:1133:G:N2	1:A:1141:C:C2	2.84	0.41
1:A:1306:A:C6	1:A:1332:A:C8	3.07	0.41
1:A:682:G:N2	1:A:708:C:O2	2.51	0.41
1:A:837:G:N2	1:A:850:U:C2	2.89	0.41
1:A:89:C:N3	1:A:90:U:C4	2.89	0.41
2:B:105:PHE:HA	2:B:105:PHE:HD1	1.71	0.41
2:B:73:THR:HG22	2:B:73:THR:O	2.21	0.41
5:E:11:ILE:HD12	5:E:11:ILE:HG23	1.67	0.41
7:G:30:ILE:HD13	7:G:30:ILE:HA	1.74	0.41
7:G:94:ARG:HA	7:G:97:GLN:HB2	2.02	0.41
10:J:48:THR:HB	10:J:62:HIS:CD2	2.55	0.41
11:K:15:ALA:HA	11:K:77:MET:HA	2.02	0.41
16:P:32:TYR:CD1	16:P:32:TYR:N	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:73:HIS:HB3	20:T:74:LYS:H	1.56	0.41
1:A:1277:C:O2'	1:A:1279:A:H1'	2.20	0.41
1:A:1314:C:H2'	1:A:1315:U:C6	2.56	0.41
1:A:1367:C:H5'	10:J:60:ARG:NH1	2.36	0.41
1:A:1372:U:H2'	1:A:1373:G:H5'	2.02	0.41
1:A:146:G:N2	1:A:147:G:C4	2.88	0.41
1:A:284:G:H2'	1:A:285:G:H8	1.84	0.41
1:A:544:G:C6	1:A:545:C:C4	3.08	0.41
2:B:220:ASP:HA	2:B:230:VAL:HG21	2.02	0.41
3:C:59:ARG:O	10:J:92:THR:HG23	2.21	0.41
4:D:174:LEU:HA	4:D:184:LYS:O	2.20	0.41
4:D:58:LEU:HD22	4:D:58:LEU:HA	1.74	0.41
9:I:49:PRO:O	9:I:53:VAL:HB	2.21	0.41
10:J:10:GLY:HA3	10:J:16:LEU:HD11	2.02	0.41
10:J:32:ALA:O	10:J:34:VAL:HG23	2.20	0.41
18:R:36:ASN:OD1	18:R:39:VAL:HG12	2.21	0.41
18:R:37:VAL:O	18:R:40:LEU:N	2.54	0.41
1:A:1061:G:H5"	1:A:1062:U:OP2	2.21	0.41
1:A:1109:C:H2'	1:A:1110:A:O4'	2.21	0.41
1:A:1254:C:H2'	1:A:1255:G:H8	1.86	0.41
1:A:1360:A:H8	1:A:1361:G:O4'	2.04	0.41
1:A:1473:A:H2'	1:A:1474:G:O4'	2.21	0.41
1:A:389:A:C5	1:A:390:C:H1'	2.56	0.41
1:A:79:G:H2'	1:A:80:G:C8	2.55	0.41
1:A:969:A:H5'	1:A:969:A:H8	1.85	0.41
1:A:986:A:H4'	19:S:55:LYS:NZ	2.36	0.41
2:B:208:ILE:HG12	2:B:211:ILE:HD11	2.03	0.41
3:C:24:ALA:HB1	3:C:28:GLN:HB2	2.03	0.41
4:D:64:LEU:HD22	4:D:64:LEU:HA	1.83	0.41
5:E:9:LYS:NZ	5:E:108:ALA:HA	2.36	0.41
7:G:140:ASP:HA	7:G:143:ARG:CD	2.50	0.41
9:I:111:ARG:NH1	9:I:113:LYS:HA	2.36	0.41
9:I:89:ASN:O	9:I:92:TYR:HB2	2.21	0.41
11:K:92:GLU:HG3	11:K:96:ARG:HH11	1.85	0.41
16:P:58:TYR:CD1	16:P:59:TRP:N	2.88	0.41
20:T:53:LEU:HA	20:T:56:MET:HE2	2.03	0.41
1:A:1004:A:H1'	1:A:1038:C:H42	1.84	0.41
1:A:1056:U:H5'	3:C:163:ALA:HB2	2.02	0.41
1:A:144:G:H2'	1:A:145:G:O4'	2.21	0.41
1:A:426:G:OP1	4:D:38:TYR:OH	2.28	0.41
1:A:413:G:H2'	1:A:428:G:N2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:U:H3'	1:A:81:U:C6	2.55	0.41
3:C:174:PRO:HB2	3:C:177:THR:HG22	2.03	0.41
3:C:195:VAL:O	3:C:196:LEU:HD23	2.21	0.41
4:D:151:LYS:H	4:D:151:LYS:HD2	1.84	0.41
8:H:82:HIS:ND1	8:H:138:TRP:NE1	2.69	0.41
11:K:20:TYR:CD1	11:K:83:ILE:HB	2.55	0.41
13:M:108:ARG:HD3	13:M:114:ARG:HH21	1.85	0.41
16:P:78:GLY:HA2	16:P:80:PHE:H	1.86	0.41
1:A:998:G:H1	1:A:1043:C:H42	1.69	0.41
1:A:1091:U:O2	1:A:1093:A:H8	2.03	0.41
1:A:1196:U:OP1	1:A:1197:G:H5'	2.20	0.41
1:A:1393:U:HO2'	1:A:1501:C:HO2'	1.69	0.41
1:A:1417:G:O5'	1:A:1417:G:H8	2.04	0.41
1:A:1507:A:H2'	1:A:1508:G:O4'	2.21	0.41
1:A:35:G:C4	1:A:550:G:N2	2.88	0.41
1:A:363:A:OP2	12:L:61:THR:HG21	2.21	0.41
1:A:963:G:N2	1:A:973:G:C5	2.89	0.41
2:B:25:ASN:HD21	2:B:27:LYS:HG3	1.86	0.41
3:C:151:VAL:HG12	3:C:152:ILE:N	2.35	0.41
3:C:43:LEU:HD13	3:C:47:LEU:CD1	2.51	0.41
8:H:95:VAL:O	8:H:131:GLY:N	2.43	0.41
9:I:49:PRO:HD3	9:I:101:PHE:CE2	2.56	0.41
1:A:974:A:P	14:N:41:ARG:HH12	2.44	0.41
16:P:1:MET:HE3	16:P:1:MET:HB3	1.91	0.41
1:A:1060:C:H2'	1:A:1061:G:H8	1.86	0.41
1:A:1287:A:H2'	1:A:1288:A:C8	2.56	0.41
1:A:1356:G:H2'	1:A:1357:A:C8	2.56	0.41
1:A:1351:U:H3	1:A:1371:G:H1	1.67	0.41
1:A:140:A:H2'	1:A:141:A:O4'	2.21	0.41
1:A:363:A:OP2	12:L:34:ARG:HG2	2.20	0.41
1:A:371:G:C2'	1:A:372:C:H5'	2.51	0.41
1:A:669:U:H2'	1:A:670:G:H8	1.86	0.41
1:A:922:G:H5"	1:A:922:G:H8	1.86	0.41
2:B:130:ARG:HD2	2:B:134:GLU:OE2	2.21	0.41
2:B:215:LEU:HD23	2:B:215:LEU:HA	1.73	0.41
4:D:72:GLU:O	4:D:72:GLU:HG3	2.21	0.41
1:A:1075:C:H5"	2:B:179:LYS:NZ	2.36	0.41
1:A:1347:G:N2	1:A:1373:G:H2'	2.36	0.41
1:A:1399:C:H4'	1:A:1400:5MC:H5"	2.02	0.41
1:A:297:G:N2	1:A:300:A:OP2	2.53	0.41
1:A:114:U:H1'	1:A:353:A:H1'	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:G:H21	4:D:119:GLN:NE2	2.18	0.41
1:A:837:G:N2	1:A:850:U:O2	2.54	0.41
1:A:830:G:N2	1:A:857:C:C2	2.89	0.41
1:A:946:A:H2'	1:A:947:G:H8	1.85	0.41
1:A:954:G:C6	1:A:955:U:C4	3.09	0.41
5:E:131:ILE:HD13	5:E:131:ILE:HA	1.55	0.41
1:A:939:G:H5"	7:G:102:ARG:NH1	2.36	0.41
8:H:83:ILE:HG21	8:H:83:ILE:HD13	1.74	0.41
12:L:7:ILE:HD13	12:L:7:ILE:HA	1.40	0.41
14:N:25:VAL:HG12	14:N:38:GLY:O	2.21	0.41
15:O:43:LEU:HD11	15:O:53:HIS:HA	2.02	0.41
16:P:34:GLU:OE2	16:P:55:ARG:HD2	2.21	0.41
17:Q:31:LEU:HA	17:Q:31:LEU:HD12	1.75	0.41
17:Q:4:LYS:O	17:Q:60:ILE:HD13	2.22	0.41
20:T:14:LYS:HA	20:T:17:ARG:NH2	2.36	0.41
20:T:20:LEU:O	20:T:23:ARG:HB3	2.20	0.41
1:A:1425:U:H2'	1:A:1426:C:C6	2.56	0.40
1:A:597:G:C4	1:A:644:G:C2	3.09	0.40
1:A:925:G:C2	1:A:927:G:C8	3.09	0.40
3:C:22:TRP:HH2	3:C:33:LEU:HD21	1.84	0.40
3:C:52:LEU:O	3:C:115:LEU:HD21	2.21	0.40
6:F:4:TYR:CD1	6:F:92:LYS:HA	2.56	0.40
7:G:64:GLN:HA	7:G:67:GLU:HB3	2.03	0.40
10:J:49:VAL:HG23	14:N:34:TYR:OH	2.21	0.40
10:J:7:LYS:HD3	10:J:9:ARG:HE	1.86	0.40
1:A:720:C:H5"	18:R:52:PRO:HA	2.03	0.40
18:R:79:LEU:CD2	18:R:80:PRO:HD2	2.51	0.40
1:A:1090:U:O2'	1:A:1091:U:H5'	2.20	0.40
1:A:1214:C:H3'	1:A:1215:G:H8	1.86	0.40
1:A:1447:G:N3	1:A:1447:G:H2'	2.36	0.40
1:A:246:A:O3'	1:A:247:G:H4'	2.21	0.40
1:A:285:G:C4	1:A:286:G:C8	3.09	0.40
1:A:373:A:H1'	1:A:481:G:H1'	2.02	0.40
1:A:775:G:H2'	1:A:776:G:H5'	2.03	0.40
2:B:144:ARG:HG3	2:B:145:LEU:N	2.36	0.40
4:D:111:ALA:HA	4:D:161:ASN:HD22	1.85	0.40
7:G:70:LYS:NZ	7:G:97:GLN:HA	2.36	0.40
9:I:15:ALA:CA	9:I:65:VAL:HG12	2.51	0.40
11:K:82:VAL:HB	11:K:108:ILE:CD1	2.51	0.40
1:A:1000:U:H2'	1:A:1001:A:C8	2.56	0.40
1:A:1125:U:P	1:A:1145:C:H41	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1053:G:O2'	1:A:1199:U:H5	2.04	0.40
1:A:820:U:H4'	1:A:821:G:OP2	2.20	0.40
1:A:899:C:H2'	1:A:900:A:O4'	2.20	0.40
1:A:919:A:O5'	1:A:919:A:H8	2.04	0.40
2:B:117:GLU:O	2:B:120:ALA:HB3	2.21	0.40
3:C:20:SER:HB3	3:C:22:TRP:NE1	2.37	0.40
4:D:164:ALA:O	4:D:168:ARG:HD2	2.21	0.40
6:F:39:LYS:HB2	6:F:39:LYS:NZ	2.37	0.40
8:H:39:LEU:HB3	8:H:45:ILE:HG12	2.04	0.40
13:M:40:ASN:HB3	13:M:43:THR:HG23	2.03	0.40
20:T:36:LEU:HA	20:T:36:LEU:HD23	1.68	0.40
1:A:1005:A:N6	1:A:1024:G:O2'	2.55	0.40
1:A:1181:G:C4	1:A:1182:G:N1	2.90	0.40
1:A:1311:G:N2	1:A:1327:C:C2	2.89	0.40
1:A:1311:G:N3	1:A:1311:G:H2'	2.36	0.40
1:A:1519:MA6:H8	1:A:1519:MA6:O5'	2.20	0.40
1:A:474:G:N2	1:A:475:G:C5	2.90	0.40
1:A:580:U:H2'	1:A:581:G:O4'	2.21	0.40
1:A:633:G:H2'	1:A:634:C:H6	1.86	0.40
1:A:778:G:C6	1:A:779:C:C4	3.10	0.40
1:A:79:G:C2	1:A:80:G:C5	3.10	0.40
3:C:34:LEU:HG	14:N:25:VAL:HG11	2.03	0.40
3:C:58:GLU:H	3:C:65:ALA:HB3	1.86	0.40
5:E:61:TYR:HD2	5:E:61:TYR:HA	1.77	0.40
7:G:21:VAL:HG22	7:G:21:VAL:H	1.57	0.40
7:G:75:VAL:HG13	7:G:87:VAL:C	2.41	0.40
9:I:104:ARG:NH1	9:I:105:ASP:O	2.54	0.40
10:J:16:LEU:HB3	10:J:70:ARG:HE	1.85	0.40
13:M:34:LEU:HD23	13:M:34:LEU:HA	1.58	0.40
17:Q:6:LEU:HD13	17:Q:23:VAL:HG11	2.02	0.40
17:Q:29:HIS:CE1	17:Q:32:TYR:H	2.40	0.40
1:A:1047:G:C2'	1:A:1048:G:H5'	2.51	0.40
1:A:1126:U:H2'	1:A:1127:G:H5'	2.03	0.40
1:A:1179:A:OP2	9:I:93:ARG:NH1	2.54	0.40
1:A:1290:G:O2'	1:A:1291:G:H5'	2.21	0.40
1:A:136:C:H1'	16:P:1:MET:HG3	2.03	0.40
1:A:1478:C:O2	1:A:1478:C:H2'	2.22	0.40
1:A:260:G:C6	1:A:261:U:C4	3.10	0.40
1:A:75:G:O2'	1:A:76:C:H5'	2.21	0.40
1:A:945:G:H2'	1:A:945:G:N3	2.36	0.40
3:C:93:LYS:O	3:C:94:LEU:HD13	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:203:VAL:O	4:D:206:PHE:HB3	2.21	0.40
18:R:62:GLU:O	18:R:65:ILE:N	2.55	0.40
19:S:74:PHE:N	19:S:74:PHE:CD1	2.90	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%)	200 (86%)	30 (13%)	2 (1%)	17 53
3	C	204/239 (85%)	179 (88%)	25 (12%)	0	100 100
4	D	206/209 (99%)	186 (90%)	20 (10%)	0	100 100
5	E	148/162 (91%)	136 (92%)	11 (7%)	1 (1%)	22 59
6	F	99/101 (98%)	90 (91%)	8 (8%)	1 (1%)	15 51
7	G	153/156 (98%)	136 (89%)	16 (10%)	1 (1%)	22 59
8	H	136/138 (99%)	129 (95%)	7 (5%)	0	100 100
9	I	125/128 (98%)	114 (91%)	10 (8%)	1 (1%)	19 56
10	J	96/105 (91%)	82 (85%)	13 (14%)	1 (1%)	15 51
11	K	114/129 (88%)	103 (90%)	11 (10%)	0	100 100
12	L	121/135 (90%)	107 (88%)	12 (10%)	2 (2%)	9 42
13	M	116/126 (92%)	103 (89%)	12 (10%)	1 (1%)	17 53
14	N	58/61 (95%)	49 (84%)	9 (16%)	0	100 100
15	O	85/89 (96%)	80 (94%)	4 (5%)	1 (1%)	13 48
16	P	81/88 (92%)	75 (93%)	5 (6%)	1 (1%)	13 48
17	Q	97/105 (92%)	89 (92%)	8 (8%)	0	100 100
18	R	68/88 (77%)	59 (87%)	9 (13%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
19	S	78/93 (84%)	67 (86%)	10 (13%)	1 (1%)	12 46
20	T	97/106 (92%)	85 (88%)	11 (11%)	1 (1%)	15 51
21	U	22/27 (82%)	20 (91%)	2 (9%)	0	100 100
All	All	2336/2541 (92%)	2089 (89%)	233 (10%)	14 (1%)	25 62

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	S	31	ILE
12	L	28	LYS
2	B	21	ARG
2	B	24	TRP
9	I	119	ALA
20	T	99	LEU
5	E	129	ILE
16	P	53	VAL
7	G	80	VAL
6	F	68	PRO
10	J	34	VAL
13	M	84	ILE
12	L	25	PRO
15	O	45	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	202/220 (92%)	158 (78%)	44 (22%)	1 7
3	C	160/188 (85%)	129 (81%)	31 (19%)	1 9
4	D	180/181 (99%)	136 (76%)	44 (24%)	0 5
5	E	115/123 (94%)	83 (72%)	32 (28%)	0 3
6	F	90/90 (100%)	70 (78%)	20 (22%)	1 7
7	G	126/127 (99%)	96 (76%)	30 (24%)	0 5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	H	119/119 (100%)	91 (76%)	28 (24%)	1 5
9	I	98/99 (99%)	76 (78%)	22 (22%)	1 6
10	J	87/92 (95%)	71 (82%)	16 (18%)	1 11
11	K	88/99 (89%)	71 (81%)	17 (19%)	1 10
12	L	103/110 (94%)	75 (73%)	28 (27%)	0 3
13	M	94/101 (93%)	74 (79%)	20 (21%)	1 7
14	N	49/50 (98%)	39 (80%)	10 (20%)	1 8
15	O	79/80 (99%)	56 (71%)	23 (29%)	0 2
16	P	72/74 (97%)	57 (79%)	15 (21%)	1 8
17	Q	94/97 (97%)	71 (76%)	23 (24%)	0 5
18	R	61/77 (79%)	47 (77%)	14 (23%)	1 6
19	S	71/80 (89%)	51 (72%)	20 (28%)	0 2
20	T	76/82 (93%)	55 (72%)	21 (28%)	0 3
21	U	19/22 (86%)	16 (84%)	3 (16%)	2 16
All	All	1983/2111 (94%)	1522 (77%)	461 (23%)	1 6

All (461) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	8	LYS
2	B	9	GLU
2	B	10	LEU
2	B	16	HIS
2	B	17	PHE
2	B	21	ARG
2	B	23	ARG
2	B	24	TRP
2	B	25	ASN
2	B	33	TYR
2	B	39	ILE
2	B	45	GLN
2	B	48	MET
2	B	53	ARG
2	B	61	LEU
2	B	67	THR
2	B	69	LEU
2	B	79	ASP

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Mol	Chain	Res	Type
2	B	87	ARG
2	B	97	TRP
2	B	102	LEU
2	B	107	THR
2	B	112	VAL
2	B	121	LEU
2	B	122	PHE
2	B	126	GLU
2	B	127	ILE
2	B	128	GLU
2	B	135	GLN
2	B	139	LYS
2	B	142	LEU
2	B	144	ARG
2	B	157	ARG
2	B	158	LEU
2	B	160	ASP
2	B	169	LYS
2	B	172	ILE
2	B	178	ARG
2	B	190	THR
2	B	196	LEU
2	B	208	ILE
2	B	212	GLN
2	B	221	LEU
2	B	238	LEU
3	C	3	ASN
3	C	11	ARG
3	C	29	TYR
3	C	30	ARG
3	C	31	HIS
3	C	33	LEU
3	C	34	LEU
3	C	43	LEU
3	C	45	LYS
3	C	48	TYR
3	C	64	VAL
3	C	69	HIS
3	C	79	ARG
3	C	95	THR
3	C	110	ASN
3	C	130	VAL

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Mol	Chain	Res	Type
3	C	131	ARG
3	C	138	VAL
3	C	147	LYS
3	C	156	ARG
3	C	165	THR
3	C	166	GLU
3	C	172	ARG
3	C	175	LEU
3	C	177	THR
3	C	178	LEU
3	C	179	ARG
3	C	183	ASP
3	C	198	VAL
3	C	204	LEU
3	C	206	GLU
4	D	10	ARG
4	D	13	ARG
4	D	14	ARG
4	D	15	GLU
4	D	19	LEU
4	D	21	LEU
4	D	25	ARG
4	D	26	CYS
4	D	36	ARG
4	D	39	PRO
4	D	47	ARG
4	D	50	ARG
4	D	52	SER
4	D	57	ARG
4	D	61	LYS
4	D	64	LEU
4	D	67	ILE
4	D	70	ILE
4	D	71	SER
4	D	78	LEU
4	D	80	GLU
4	D	84	LYS
4	D	120	LEU
4	D	122	ARG
4	D	127	THR
4	D	129	ASN
4	D	135	LEU

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Mol	Chain	Res	Type
4	D	137	SER
4	D	141	ARG
4	D	145	GLU
4	D	151	LYS
4	D	158	ILE
4	D	176	LEU
4	D	178	VAL
4	D	179	GLU
4	D	185	PHE
4	D	186	LEU
4	D	187	ARG
4	D	188	LEU
4	D	194	LEU
4	D	198	VAL
4	D	202	LEU
4	D	203	VAL
4	D	209	ARG
5	E	5	ASP
5	E	12	LEU
5	E	14	ARG
5	E	15	ARG
5	E	18	ARG
5	E	19	MET
5	E	24	ARG
5	E	32	VAL
5	E	34	VAL
5	E	53	LEU
5	E	55	VAL
5	E	60	TYR
5	E	61	TYR
5	E	67	VAL
5	E	69	VAL
5	E	75	THR
5	E	78	HIS
5	E	79	GLU
5	E	80	ILE
5	E	81	GLU
5	E	87	SER
5	E	100	VAL
5	E	107	ARG
5	E	112	LEU
5	E	118	ILE

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Mol	Chain	Res	Type
5	E	125	SER
5	E	131	ILE
5	E	136	MET
5	E	137	GLU
5	E	141	GLN
5	E	144	THR
5	E	147	ASP
6	F	15	ASP
6	F	19	LEU
6	F	24	GLU
6	F	28	ARG
6	F	30	LEU
6	F	39	LYS
6	F	43	LEU
6	F	45	LEU
6	F	46	ARG
6	F	47	ARG
6	F	65	VAL
6	F	73	ASN
6	F	74	ASP
6	F	75	LEU
6	F	77	ARG
6	F	82	ARG
6	F	87	ARG
6	F	88	VAL
6	F	94	GLN
6	F	98	LEU
7	G	3	ARG
7	G	8	GLU
7	G	22	LEU
7	G	30	ILE
7	G	31	MET
7	G	33	ASP
7	G	38	LEU
7	G	45	ASP
7	G	48	LYS
7	G	50	ILE
7	G	52	GLU
7	G	53	LYS
7	G	56	GLN
7	G	57	GLU
7	G	59	LEU

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Mol	Chain	Res	Type
7	G	77	SER
7	G	80	VAL
7	G	85	TYR
7	G	91	VAL
7	G	92	SER
7	G	94	ARG
7	G	97	GLN
7	G	98	SER
7	G	99	LEU
7	G	109	ASN
7	G	110	GLN
7	G	113	GLU
7	G	124	LEU
7	G	126	ASP
7	G	146	GLU
8	H	6	ILE
8	H	11	THR
8	H	12	ARG
8	H	14	ARG
8	H	22	GLU
8	H	23	SER
8	H	29	SER
8	H	39	LEU
8	H	51	VAL
8	H	63	LEU
8	H	65	TYR
8	H	81	HIS
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	105	ARG
8	H	112	LEU
8	H	113	SER
8	H	118	VAL
8	H	120	THR
8	H	123	GLU
8	H	127	LEU

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Mol	Chain	Res	Type
8	H	136	GLU
9	I	3	GLN
9	I	14	VAL
9	I	16	ARG
9	I	29	ASN
9	I	35	GLU
9	I	38	GLN
9	I	48	GLU
9	I	53	VAL
9	I	58	HIS
9	I	70	LYS
9	I	79	LEU
9	I	83	ARG
9	I	87	GLN
9	I	91	ASP
9	I	92	TYR
9	I	104	ARG
9	I	109	VAL
9	I	111	ARG
9	I	113	LYS
9	I	114	TYR
9	I	118	LYS
9	I	121	ARG
10	J	5	ARG
10	J	43	ARG
10	J	47	PHE
10	J	48	THR
10	J	49	VAL
10	J	54	PHE
10	J	57	LYS
10	J	63	PHE
10	J	64	GLU
10	J	68	HIS
10	J	71	LEU
10	J	74	ILE
10	J	83	GLU
10	J	85	LEU
10	J	88	LEU
10	J	96	ILE
11	K	11	LYS
11	K	13	GLN
11	K	18	ARG

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Mol	Chain	Res	Type
11	K	29	ILE
11	K	33	THR
11	K	47	VAL
11	K	59	TYR
11	K	75	TYR
11	K	81	ASP
11	K	91	ARG
11	K	95	ILE
11	K	98	LEU
11	K	101	SER
11	K	109	VAL
11	K	116	HIS
11	K	119	CYS
11	K	126	ARG
12	L	7	ILE
12	L	11	VAL
12	L	27	LEU
12	L	33	ARG
12	L	34	ARG
12	L	39	VAL
12	L	41	ARG
12	L	42	THR
12	L	43	VAL
12	L	44	THR
12	L	53	ARG
12	L	55	VAL
12	L	60	LEU
12	L	61	THR
12	L	64	TYR
12	L	65	GLU
12	L	66	VAL
12	L	67	THR
12	L	76	ASN
12	L	80	HIS
12	L	96	VAL
12	L	97	ARG
12	L	99	HIS
12	L	101	VAL
12	L	104	VAL
12	L	120	TYR
12	L	122	THR
12	L	127	GLU

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Mol	Chain	Res	Type
13	M	3	ARG
13	M	9	ILE
13	M	19	LEU
13	M	35	GLU
13	M	39	ILE
13	M	49	THR
13	M	53	VAL
13	M	54	VAL
13	M	56	LEU
13	M	57	ARG
13	M	63	THR
13	M	66	LEU
13	M	73	GLU
13	M	77	ASN
13	M	80	ARG
13	M	93	ARG
13	M	101	GLN
13	M	102	ARG
13	M	110	ARG
13	M	115	LYS
14	N	18	VAL
14	N	21	TYR
14	N	22	THR
14	N	25	VAL
14	N	27	CYS
14	N	31	ARG
14	N	41	ARG
14	N	44	LEU
14	N	47	LEU
14	N	58	LYS
15	O	4	THR
15	O	5	LYS
15	O	9	GLN
15	O	26	GLU
15	O	27	VAL
15	O	32	LEU
15	O	33	THR
15	O	38	ARG
15	O	42	HIS
15	O	44	LYS
15	O	45	VAL
15	O	47	LYS

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Mol	Chain	Res	Type
15	O	56	LEU
15	O	64	ARG
15	O	67	LEU
15	O	68	ARG
15	O	70	LEU
15	O	71	GLN
15	O	73	GLU
15	O	78	TYR
15	O	81	LEU
15	O	87	ILE
15	O	88	ARG
16	P	1	MET
16	P	5	ARG
16	P	6	LEU
16	P	18	ARG
16	P	27	LYS
16	P	33	ILE
16	P	45	THR
16	P	50	LYS
16	P	53	VAL
16	P	55	ARG
16	P	61	SER
16	P	62	VAL
16	P	68	ASP
16	P	69	THR
16	P	79	VAL
17	Q	12	SER
17	Q	15	MET
17	Q	19	VAL
17	Q	21	VAL
17	Q	34	LYS
17	Q	35	VAL
17	Q	36	ILE
17	Q	45	HIS
17	Q	53	LEU
17	Q	58	GLU
17	Q	59	ILE
17	Q	60	ILE
17	Q	63	ARG
17	Q	72	ARG
17	Q	74	LEU
17	Q	75	ARG

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Mol	Chain	Res	Type
17	Q	77	VAL
17	Q	84	LEU
17	Q	86	GLU
17	Q	89	LEU
17	Q	92	ARG
17	Q	94	ASN
17	Q	98	LEU
18	R	21	LYS
18	R	28	GLU
18	R	31	LEU
18	R	35	ARG
18	R	37	VAL
18	R	40	LEU
18	R	42	ARG
18	R	46	GLU
18	R	47	THR
18	R	56	THR
18	R	58	LEU
18	R	82	THR
18	R	86	VAL
18	R	88	LYS
19	S	3	ARG
19	S	6	LYS
19	S	7	LYS
19	S	12	ASP
19	S	15	LEU
19	S	17	GLU
19	S	20	LEU
19	S	23	ASN
19	S	28	LYS
19	S	29	ARG
19	S	41	VAL
19	S	43	GLU
19	S	55	LYS
19	S	58	VAL
19	S	62	ILE
19	S	63	THR
19	S	64	GLU
19	S	66	MET
19	S	77	THR
19	S	81	ARG
20	T	10	LEU

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Mol	Chain	Res	Type
20	T	13	LEU
20	T	19	SER
20	T	20	LEU
20	T	24	LEU
20	T	34	LYS
20	T	36	LEU
20	T	38	LYS
20	T	42	GLN
20	T	43	LEU
20	T	46	GLU
20	T	53	LEU
20	T	64	ASP
20	T	73	HIS
20	T	74	LYS
20	T	75	ASN
20	T	79	ARG
20	T	85	MET
20	T	86	ARG
20	T	90	GLN
20	T	91	LEU
21	U	8	THR
21	U	12	LYS
21	U	13	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	25	ASN
3	C	6	HIS
4	D	119	GLN
6	F	73	ASN
6	F	100	ASN
7	G	110	GLN
9	I	73	GLN
15	O	46	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1508/1522 (99%)	390 (25%)	45 (2%)

All (390) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	7	G
1	A	9	G
1	A	19	C
1	A	22	G
1	A	31	G
1	A	32	A
1	A	39	G
1	A	41	G
1	A	45	U
1	A	47	C
1	A	48	C
1	A	49	U
1	A	50	A
1	A	51	A
1	A	58	C
1	A	66	G
1	A	68	G
1	A	69	G
1	A	76	C
1	A	81	U
1	A	89	C
1	A	91	C
1	A	92	C
1	A	97	G
1	A	99	C
1	A	106	C
1	A	107	G
1	A	108	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	141	A
1	A	145	G
1	A	157	G
1	A	163	C
1	A	175	C
1	A	178	C
1	A	182	U

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Mol	Chain	Res	Type
1	A	183	G
1	A	190(D)	U
1	A	190(E)	U
1	A	190(G)	G
1	A	195	A
1	A	197	A
1	A	199	G
1	A	201	C
1	A	202	U
1	A	203	U
1	A	204	U
1	A	216	G
1	A	217	C
1	A	220	G
1	A	231	G
1	A	243	A
1	A	244	U
1	A	246	A
1	A	247	G
1	A	251	G
1	A	252	U
1	A	254	G
1	A	257	G
1	A	266	G
1	A	267	C
1	A	289	G
1	A	299	G
1	A	301	G
1	A	319	G
1	A	321	A
1	A	324	G
1	A	328	C
1	A	329	A
1	A	330	C
1	A	332	G
1	A	344	A
1	A	345	C
1	A	346	G
1	A	350	G
1	A	351	G
1	A	352	C
1	A	353	A

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Mol	Chain	Res	Type
1	A	354	G
1	A	367	U
1	A	371	G
1	A	372	C
1	A	373	A
1	A	374	A
1	A	384	G
1	A	388	G
1	A	390	C
1	A	397	A
1	A	398	C
1	A	405	U
1	A	406	G
1	A	412	A
1	A	413	G
1	A	421	U
1	A	422	C
1	A	423	G
1	A	424	G
1	A	429	U
1	A	430	A
1	A	439	A
1	A	450	G
1	A	455	C
1	A	460	A
1	A	461	C
1	A	475	G
1	A	476	G
1	A	478	A
1	A	481	G
1	A	482	A
1	A	485	G
1	A	486	U
1	A	487	A
1	A	497	A
1	A	498	U
1	A	505	G
1	A	509	A
1	A	510	A
1	A	511	C
1	A	513	C
1	A	518	C

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Mol	Chain	Res	Type
1	A	519	C
1	A	524	G
1	A	527	7MG
1	A	531	U
1	A	532	A
1	A	533	A
1	A	541	G
1	A	547	A
1	A	558	G
1	A	559	A
1	A	560	U
1	A	562	C
1	A	564	C
1	A	572	A
1	A	573	A
1	A	575	G
1	A	576	G
1	A	577	G
1	A	579	G
1	A	588	G
1	A	597	G
1	A	598	U
1	A	607	A
1	A	615	C
1	A	618	C
1	A	624	C
1	A	630	G
1	A	631	G
1	A	652	U
1	A	653	A
1	A	656	C
1	A	665	A
1	A	686	U
1	A	687	A
1	A	688	G
1	A	694	A
1	A	701	C
1	A	702	A
1	A	703	G
1	A	718	G
1	A	722	A
1	A	723	U

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Mol	Chain	Res	Type
1	A	724	G
1	A	731	G
1	A	733	A
1	A	734	G
1	A	749	C
1	A	755	G
1	A	759	A
1	A	760	G
1	A	773	G
1	A	777	A
1	A	781	A
1	A	782	A
1	A	784	C
1	A	787	A
1	A	788	U
1	A	789	U
1	A	792	A
1	A	793	U
1	A	794	A
1	A	813	U
1	A	817	C
1	A	818	G
1	A	821	G
1	A	826	C
1	A	828	A
1	A	829	G
1	A	838	G
1	A	839	U
1	A	840	C
1	A	841	U
1	A	848	C
1	A	855	G
1	A	858	G
1	A	869	G
1	A	872	A
1	A	873	A
1	A	876	G
1	A	889	A
1	A	902	G
1	A	910	C
1	A	914	A
1	A	919	A

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Mol	Chain	Res	Type
1	A	922	G
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	936	C
1	A	941	G
1	A	944	G
1	A	950	U
1	A	954	G
1	A	957	U
1	A	960	U
1	A	961	U
1	A	964	A
1	A	966	M2G
1	A	969	A
1	A	971	G
1	A	973	G
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	980	C
1	A	985	C
1	A	989	C
1	A	990	C
1	A	991	U
1	A	992	U
1	A	993	G
1	A	1003	G
1	A	1003(A)	G
1	A	1005	A
1	A	1006	C
1	A	1007	C
1	A	1008	C
1	A	1020	U
1	A	1025	U
1	A	1026	G
1	A	1027	C
1	A	1030(B)	C
1	A	1032	G
1	A	1038	C

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Mol	Chain	Res	Type
1	A	1045	C
1	A	1047	G
1	A	1050	G
1	A	1051	C
1	A	1053	G
1	A	1059	C
1	A	1060	C
1	A	1065	U
1	A	1066	C
1	A	1068	G
1	A	1078	U
1	A	1079	G
1	A	1085	U
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1104	G
1	A	1115	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	1138	G
1	A	1139	G
1	A	1140	C
1	A	1141	C
1	A	1144	G
1	A	1145	C
1	A	1146	A
1	A	1152	A
1	A	1159	U
1	A	1161	C
1	A	1171	G
1	A	1174	G
1	A	1176	A
1	A	1177	G
1	A	1183	A
1	A	1184	G
1	A	1190	G
1	A	1196	U

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Mol	Chain	Res	Type
1	A	1197	G
1	A	1198	G
1	A	1200	C
1	A	1201	A
1	A	1202	G
1	A	1206	G
1	A	1207	2MG
1	A	1209	C
1	A	1212	U
1	A	1213	A
1	A	1214	C
1	A	1224	G
1	A	1225	A
1	A	1226	C
1	A	1227	A
1	A	1228	C
1	A	1238	A
1	A	1240	U
1	A	1241	G
1	A	1243	C
1	A	1245	A
1	A	1257	U
1	A	1258	G
1	A	1260	C
1	A	1261	A
1	A	1263	C
1	A	1270	C
1	A	1278	U
1	A	1279	A
1	A	1280	A
1	A	1281	U
1	A	1282	C
1	A	1286	A
1	A	1287	A
1	A	1297	C
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1305	G
1	A	1311	G
1	A	1312	G
1	A	1320	C

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Mol	Chain	Res	Type
1	A	1322	C
1	A	1323	G
1	A	1326	C
1	A	1327	C
1	A	1334	G
1	A	1336	C
1	A	1340	A
1	A	1346	A
1	A	1347	G
1	A	1348	U
1	A	1351	U
1	A	1353	G
1	A	1359	C
1	A	1360	A
1	A	1362	C
1	A	1364	U
1	A	1370	G
1	A	1371	G
1	A	1378	C
1	A	1379	G
1	A	1381	U
1	A	1393	U
1	A	1397	C
1	A	1398	A
1	A	1399	C
1	A	1414	U
1	A	1441	G
1	A	1442	G
1	A	1446	A
1	A	1447	G
1	A	1451	A
1	A	1453	G
1	A	1454	G
1	A	1469	G
1	A	1487	G
1	A	1490	C
1	A	1493	A
1	A	1495	U
1	A	1496	C
1	A	1497	G
1	A	1498	UR3
1	A	1499	A

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Mol	Chain	Res	Type
1	A	1503	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1507	A
1	A	1515	C
1	A	1520	G
1	A	1529	G
1	A	1530	G
1	A	1531	A
1	A	1532	U
1	A	1533	C

All (45) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U
1	A	65	U
1	A	115	G
1	A	129(A)	G
1	A	173	U
1	A	181	G
1	A	243	A
1	A	250	A
1	A	251	G
1	A	328	C
1	A	372	C
1	A	428	G
1	A	429	U
1	A	484	G
1	A	485	G
1	A	509	A
1	A	518	C
1	A	559	A
1	A	597	G
1	A	687	A
1	A	701	C
1	A	748	C
1	A	812	C
1	A	913	A
1	A	960	U
1	A	975	A

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Mol	Chain	Res	Type
1	A	992	U
1	A	1004	A
1	A	1049	U
1	A	1065	U
1	A	1067	A
1	A	1139	G
1	A	1145	C
1	A	1182	G
1	A	1183	A
1	A	1201	A
1	A	1256	A
1	A	1257	U
1	A	1285	A
1	A	1301	U
1	A	1333	A
1	A	1346	A
1	A	1347	G
1	A	1380	U
1	A	1505	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	M2G	A	966	1	20,27,28	1.75	4 (20%)	22,40,43	2.17	4 (18%)
1	5MC	A	1400	1	15,22,23	1.02	1 (6%)	19,32,35	1.15	2 (10%)
1	MA6	A	1519	1	19,26,27	2.00	5 (26%)	18,38,41	0.80	0
1	5MC	A	1407	1	15,22,23	1.69	3 (20%)	19,32,35	0.88	1 (5%)
1	2MG	A	1207	1	19,26,27	2.41	4 (21%)	21,38,41	2.07	3 (14%)
1	PSU	A	516	1	17,21,22	1.35	2 (11%)	20,30,33	3.86	6 (30%)
1	PSU	A	1540	1	17,21,22	1.14	1 (5%)	20,30,33	3.53	7 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	UR3	A	1498	1	14,22,23	1.16	1 (7%)	15,32,35	1.13	1 (6%)
1	4OC	A	1402	1	16,23,24	1.19	2 (12%)	17,32,35	0.78	0
1	7MG	A	527	1	22,26,27	1.91	6 (27%)	28,39,42	1.69	4 (14%)
1	PSU	A	1541	1	17,21,22	1.03	1 (5%)	20,30,33	3.22	5 (25%)
1	5MC	A	967	1	15,22,23	1.00	1 (6%)	19,32,35	1.08	1 (5%)
12	0TD	L	92	12	4,9,10	1.10	0	3,11,13	3.74	2 (66%)
1	MA6	A	1518	1	19,26,27	1.63	3 (15%)	18,38,41	1.46	2 (11%)
1	5MC	A	1404	1	15,22,23	1.29	2 (13%)	19,32,35	1.21	2 (10%)

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	M2G	A	966	1	-	4/7/29/30	0/3/3/3
1	5MC	A	1400	1	-	2/5/25/26	0/2/2/2
1	MA6	A	1519	1	-	5/7/29/30	0/3/3/3
1	5MC	A	1407	1	-	0/5/25/26	0/2/2/2
1	2MG	A	1207	1	-	2/5/27/28	0/3/3/3
1	PSU	A	516	1	-	0/7/25/26	0/2/2/2
1	PSU	A	1540	1	-	3/7/25/26	0/2/2/2
1	UR3	A	1498	1	-	3/5/25/26	0/2/2/2
1	4OC	A	1402	1	-	5/9/29/30	0/2/2/2
1	7MG	A	527	1	-	2/7/37/38	0/3/3/3
1	PSU	A	1541	1	-	1/7/25/26	0/2/2/2
1	5MC	A	967	1	-	1/5/25/26	0/2/2/2
12	0TD	L	92	12	-	2/3/12/14	-
1	MA6	A	1518	1	-	5/7/29/30	0/3/3/3
1	5MC	A	1404	1	-	0/5/25/26	0/2/2/2

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1207	2MG	C2-N2	7.34	1.40	1.34
1	A	1207	2MG	C6-N1	6.10	1.43	1.33
1	A	1407	5MC	C5-C4	5.20	1.49	1.41
1	A	1519	MA6	C6-N1	5.18	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	966	M2G	C6-N1	4.50	1.40	1.33
1	A	527	7MG	C8-N9	-4.37	1.35	1.45
1	A	527	7MG	C4-N3	4.26	1.39	1.34
1	A	1519	MA6	C2-N1	4.18	1.41	1.33
1	A	516	PSU	C4-N3	4.08	1.40	1.33
1	A	1518	MA6	C4-N3	3.95	1.41	1.35
1	A	966	M2G	C4-N3	3.84	1.41	1.35
1	A	1540	PSU	C4-N3	3.71	1.39	1.33
1	A	1518	MA6	C9-N6	3.60	1.54	1.45
1	A	1404	5MC	C5-C4	3.58	1.46	1.41
1	A	1541	PSU	C4-N3	3.56	1.39	1.33
1	A	1518	MA6	C6-N1	3.43	1.38	1.33
1	A	966	M2G	C2-N2	3.08	1.39	1.34
1	A	527	7MG	C2-N2	3.07	1.40	1.33
1	A	1498	UR3	C4-N3	-3.06	1.33	1.38
1	A	1402	4OC	C2-N3	2.96	1.44	1.38
1	A	1519	MA6	C5-C4	2.94	1.48	1.40
1	A	1207	2MG	C4-N3	2.90	1.40	1.35
1	A	527	7MG	CM7-N7	-2.83	1.41	1.46
1	A	1519	MA6	C9-N6	2.64	1.51	1.45
1	A	966	M2G	O6-C6	-2.45	1.18	1.24
1	A	967	5MC	C4-N4	2.44	1.40	1.34
1	A	1519	MA6	C4-N3	2.43	1.39	1.35
1	A	527	7MG	C2-N1	-2.41	1.31	1.35
1	A	516	PSU	O4'-C1'	-2.41	1.41	1.44
1	A	1407	5MC	C2-N3	2.38	1.42	1.38
1	A	1207	2MG	C2-N1	2.31	1.41	1.34
1	A	527	7MG	O6-C6	-2.23	1.18	1.24
1	A	1404	5MC	C6-C5	-2.21	1.34	1.40
1	A	1407	5MC	C4-N4	2.15	1.39	1.34
1	A	1402	4OC	CM4-N4	2.10	1.48	1.45
1	A	1400	5MC	C5-C4	2.03	1.44	1.41

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	516	PSU	N1-C2-N3	-13.59	117.63	128.43
1	A	1540	PSU	N1-C2-N3	-11.62	119.20	128.43
1	A	1541	PSU	N1-C2-N3	-10.00	120.48	128.43
1	A	516	PSU	C4-N3-C2	7.79	121.72	115.14
1	A	1207	2MG	C5-C6-N1	-7.52	113.14	123.43
1	A	1540	PSU	C4-N3-C2	7.11	121.14	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1541	PSU	C4-N3-C2	7.02	121.07	115.14
1	A	966	M2G	C5-C6-N1	-6.74	114.22	123.43
1	A	966	M2G	C6-N1-C2	5.79	123.08	116.18
1	A	1541	PSU	C5-C4-N3	-5.71	118.00	125.36
1	A	527	7MG	N3-C4-N9	5.42	133.87	126.91
12	L	92	0TD	CSB-SB-CB	-5.26	91.51	101.85
1	A	1518	MA6	C1'-N9-C4	-4.96	117.92	126.64
1	A	516	PSU	C5-C4-N3	-4.67	119.34	125.36
1	A	527	7MG	N7-C8-N9	4.26	109.47	103.38
1	A	1540	PSU	C5-C4-N3	-4.20	119.95	125.36
1	A	527	7MG	C5-C4-N3	-4.18	119.67	126.49
1	A	1207	2MG	C6-N1-C2	4.02	122.39	115.18
1	A	516	PSU	C6-N1-C2	3.59	121.29	115.36
1	A	1540	PSU	C5-C1'-C2'	-3.58	108.92	115.32
1	A	1404	5MC	N4-C4-N3	-3.48	112.12	117.03
1	A	1540	PSU	O4'-C1'-C5	3.47	115.31	109.93
12	L	92	0TD	CB-CA-N	-3.45	101.75	109.10
1	A	967	5MC	C2-N3-C4	2.87	119.48	116.02
1	A	1540	PSU	C6-N1-C2	2.80	119.99	115.36
1	A	1207	2MG	C4-C5-N7	2.79	112.31	109.40
1	A	966	M2G	N3-C2-N2	2.70	119.92	117.18
1	A	1400	5MC	C2-N3-C4	2.69	119.26	116.02
1	A	516	PSU	C5-C6-N1	-2.65	121.18	124.44
1	A	1541	PSU	C4-C5-C1'	2.62	126.07	121.12
1	A	1498	UR3	C3'-C2'-C1'	2.57	104.85	100.98
1	A	1518	MA6	N1-C6-N6	-2.54	114.38	117.06
1	A	1541	PSU	C6-N1-C2	2.45	119.39	115.36
1	A	1540	PSU	O4'-C1'-C2'	2.33	108.43	104.66
1	A	966	M2G	C4-C5-N7	2.31	111.80	109.40
1	A	516	PSU	O4'-C1'-C2'	2.24	108.28	104.66
1	A	1404	5MC	C5-C4-N3	2.20	124.73	121.26
1	A	1407	5MC	N4-C4-N3	-2.19	113.94	117.03
1	A	1400	5MC	CM5-C5-C6	2.12	123.16	118.68
1	A	527	7MG	C2-N3-C4	2.04	119.52	113.89

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1519	MA6	C5-C6-N6-C9
1	A	1519	MA6	N1-C6-N6-C9
1	A	1207	2MG	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	A	1207	2MG	C3'-C4'-C5'-O5'
1	A	1540	PSU	O4'-C1'-C5-C6
1	A	1498	UR3	O4'-C1'-N1-C6
1	A	1402	4OC	O4'-C4'-C5'-O5'
1	A	1402	4OC	C3'-C4'-C5'-O5'
1	A	1402	4OC	O4'-C1'-N1-C6
1	A	1402	4OC	N3-C4-N4-CM4
1	A	1402	4OC	C5-C4-N4-CM4
1	A	1541	PSU	C2'-C1'-C5-C6
1	A	967	5MC	C2'-C1'-N1-C6
1	A	1518	MA6	C5-C6-N6-C9
1	A	1518	MA6	O4'-C4'-C5'-O5'
1	A	1400	5MC	O4'-C4'-C5'-O5'
1	A	1400	5MC	C3'-C4'-C5'-O5'
1	A	1518	MA6	C3'-C4'-C5'-O5'
1	A	1498	UR3	C3'-C4'-C5'-O5'
1	A	1518	MA6	N1-C6-N6-C9
1	A	1519	MA6	O4'-C4'-C5'-O5'
1	A	1498	UR3	O4'-C4'-C5'-O5'
1	A	1519	MA6	C5-C6-N6-C10
1	A	966	M2G	N3-C2-N2-CM2
1	A	1519	MA6	C3'-C4'-C5'-O5'
1	A	966	M2G	N3-C2-N2-CM1
1	A	966	M2G	N1-C2-N2-CM2
1	A	527	7MG	C3'-C4'-C5'-O5'
1	A	966	M2G	N1-C2-N2-CM1
1	A	1540	PSU	C2'-C1'-C5-C6
1	A	1518	MA6	C5-C6-N6-C10
1	A	527	7MG	O4'-C4'-C5'-O5'
1	A	1540	PSU	O4'-C1'-C5-C4
12	L	92	0TD	CA-CB-SB-CSB
12	L	92	0TD	CG-CB-SB-CSB

There are no ring outliers.

11 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1400	5MC	3	0
1	A	1519	MA6	4	0
1	A	1207	2MG	1	0
1	A	1540	PSU	1	0
1	A	1498	UR3	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	527	7MG	1	0
1	A	1541	PSU	1	0
1	A	967	5MC	1	0
12	L	92	0TD	2	0
1	A	1518	MA6	2	0
1	A	1404	5MC	3	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 250 ligands modelled in this entry, 249 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	SRY	A	1601	-	40,42,42	2.37	13 (32%)	49,63,63	2.27	13 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	SRY	A	1601	-	-	5/20/87/87	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	1601	SRY	CD1-N31	9.33	1.49	1.33
22	A	1601	SRY	CA1-N11	5.93	1.43	1.33
22	A	1601	SRY	O53-C53	-3.40	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	1601	SRY	C11-N11	-3.34	1.40	1.45
22	A	1601	SRY	C23-N23	-2.85	1.42	1.47
22	A	1601	SRY	C21-C11	-2.84	1.47	1.53
22	A	1601	SRY	CA1-NB1	2.65	1.45	1.34
22	A	1601	SRY	CD1-NE1	2.40	1.44	1.34
22	A	1601	SRY	O51-C51	-2.37	1.37	1.43
22	A	1601	SRY	C32-CG2	-2.35	1.48	1.52
22	A	1601	SRY	O43-C43	-2.23	1.37	1.43
22	A	1601	SRY	C21-C31	-2.22	1.48	1.53
22	A	1601	SRY	O32-C32	-2.17	1.40	1.44

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	1601	SRY	C12-O42-C42	-5.92	99.07	108.38
22	A	1601	SRY	C13-O13-C22	-5.92	105.98	116.25
22	A	1601	SRY	C61-C11-N11	-5.88	99.52	110.62
22	A	1601	SRY	O41-C12-O42	-4.32	106.75	111.43
22	A	1601	SRY	C43-C33-C23	-4.14	104.28	110.34
22	A	1601	SRY	CI3-N23-C23	-4.10	108.41	114.38
22	A	1601	SRY	O13-C13-C23	3.60	114.44	108.24
22	A	1601	SRY	C12-O41-C41	-3.04	110.45	117.96
22	A	1601	SRY	C21-C31-N31	2.99	116.27	110.62
22	A	1601	SRY	O13-C13-O53	-2.14	104.69	110.67
22	A	1601	SRY	O32-C32-C22	2.04	116.35	111.62
22	A	1601	SRY	C61-C51-C41	2.01	114.27	109.68
22	A	1601	SRY	OG2-CG2-C32	-2.01	119.64	124.27

There are no chirality outliers.

All (5) torsion outliers are listed below:

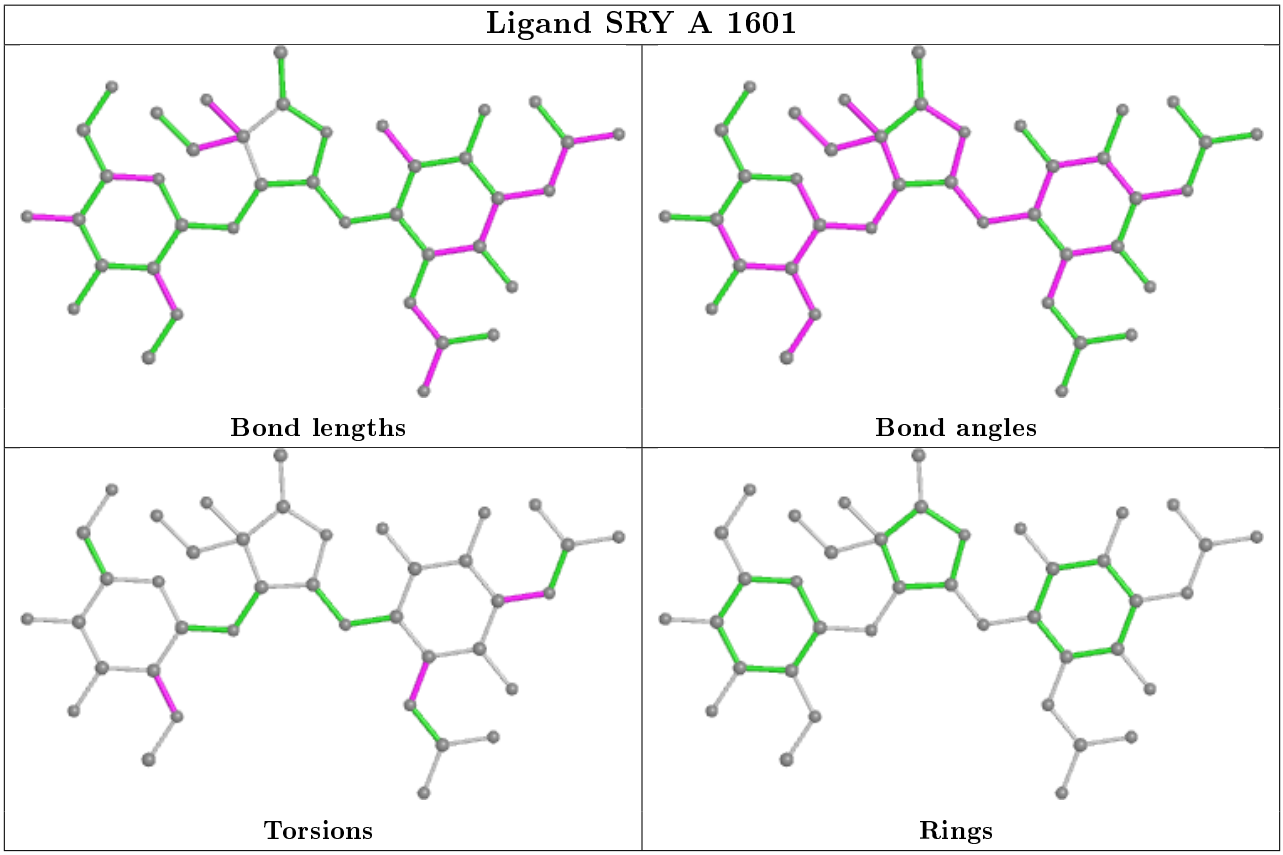
Mol	Chain	Res	Type	Atoms
22	A	1601	SRY	C13-C23-N23-CI3
22	A	1601	SRY	C41-C31-N31-CD1
22	A	1601	SRY	C21-C31-N31-CD1
22	A	1601	SRY	C21-C11-N11-CA1
22	A	1601	SRY	C61-C11-N11-CA1

There are no ring outliers.

1 monomer is involved in 7 short contacts:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1498/1522 (98%)	-0.37	23 (1%) 73 66	106, 179, 327, 407	0
2	B	234/256 (91%)	-0.58	3 (1%) 77 70	145, 211, 332, 358	0
3	C	206/239 (86%)	-0.31	9 (4%) 34 29	181, 265, 316, 365	0
4	D	208/209 (99%)	-0.43	3 (1%) 75 67	124, 193, 249, 283	0
5	E	150/162 (92%)	-0.67	0 100 100	104, 150, 199, 232	0
6	F	101/101 (100%)	-0.71	0 100 100	155, 212, 246, 277	0
7	G	155/156 (99%)	-0.42	7 (4%) 33 28	172, 228, 288, 335	0
8	H	138/138 (100%)	-0.77	0 100 100	94, 135, 187, 218	0
9	I	127/128 (99%)	-0.37	1 (0%) 86 80	201, 250, 303, 322	0
10	J	98/105 (93%)	0.04	9 (9%) 9 7	220, 277, 355, 391	0
11	K	116/129 (89%)	-0.70	0 100 100	130, 171, 224, 258	0
12	L	123/135 (91%)	-0.54	0 100 100	107, 175, 218, 248	0
13	M	118/126 (93%)	-0.47	4 (3%) 45 37	162, 214, 254, 309	0
14	N	60/61 (98%)	0.14	7 (11%) 4 4	187, 249, 314, 329	0
15	O	87/89 (97%)	-0.54	0 100 100	113, 171, 213, 232	0
16	P	83/88 (94%)	-0.58	0 100 100	130, 180, 220, 274	0
17	Q	99/105 (94%)	-0.65	0 100 100	116, 150, 201, 232	0
18	R	70/88 (79%)	-0.63	1 (1%) 75 67	116, 183, 245, 259	0
19	S	80/93 (86%)	0.11	5 (6%) 20 15	234, 284, 341, 352	0
20	T	99/106 (93%)	-0.69	0 100 100	124, 172, 240, 267	0
21	U	24/27 (88%)	0.57	4 (16%) 1 2	198, 248, 286, 302	0
All	All	3874/4063 (95%)	-0.43	76 (1%) 65 57	94, 194, 306, 407	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	G	81	GLY	5.3
19	S	79	THR	5.2
1	A	1018	C	5.1
4	D	35	ARG	4.8
10	J	34	VAL	4.4
3	C	65	ALA	4.2
1	A	1019	C	4.2
3	C	193	TYR	4.1
1	A	1042	G	4.1
10	J	39	PRO	3.8
21	U	8	THR	3.8
1	A	1129	C	3.7
14	N	17	LYS	3.7
10	J	37	PRO	3.7
1	A	81	U	3.7
10	J	33	GLN	3.6
3	C	66	VAL	3.6
1	A	993	G	3.5
14	N	5	ALA	3.4
3	C	102	ASN	3.4
1	A	202	U	3.2
1	A	1224	G	3.2
1	A	1005	A	3.2
1	A	984	C	3.1
3	C	60	ALA	3.1
3	C	103	VAL	3.0
1	A	1017	G	3.0
10	J	90	LEU	2.9
7	G	2	ALA	2.9
1	A	1322	C	2.8
18	R	88	LYS	2.8
21	U	5	ASP	2.7
7	G	132	GLY	2.7
19	S	31	ILE	2.7
19	S	6	LYS	2.7
10	J	75	ILE	2.6
7	G	82	GLY	2.6
1	A	793	U	2.6
14	N	18	VAL	2.6
2	B	239	VAL	2.6
1	A	1033	G	2.5
3	C	76	VAL	2.5
21	U	17	THR	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	238	LEU	2.5
1	A	1361(A)	C	2.5
14	N	2	ALA	2.5
10	J	74	ILE	2.4
2	B	231	GLU	2.4
10	J	76	ASN	2.4
14	N	20	ALA	2.4
19	S	41	VAL	2.3
1	A	991	U	2.3
3	C	2	GLY	2.3
13	M	7	VAL	2.3
7	G	154	TYR	2.3
13	M	65	LYS	2.2
1	A	1321	C	2.2
1	A	994	A	2.2
14	N	3	ARG	2.2
21	U	18	TYR	2.2
3	C	146	ALA	2.2
4	D	45	GLN	2.2
7	G	79	ARG	2.2
19	S	32	LYS	2.2
1	A	1035	A	2.1
4	D	23	GLY	2.1
1	A	985	C	2.1
13	M	117	VAL	2.1
1	A	1003	G	2.1
9	I	110	GLU	2.1
1	A	80	G	2.1
1	A	1050	G	2.1
13	M	6	GLY	2.0
7	G	80	VAL	2.0
14	N	4	LYS	2.0
10	J	36	GLY	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	PSU	A	1540	20/21	0.78	0.63	235,263,334,335	0
1	PSU	A	1541	20/21	0.79	0.41	297,305,321,325	0
1	PSU	A	516	20/21	0.92	0.16	163,188,214,220	0
1	2MG	A	1207	24/25	0.93	0.33	231,289,310,316	0
1	5MC	A	1400	21/22	0.94	0.23	142,169,178,182	0
1	MA6	A	1519	24/25	0.94	0.20	144,181,202,206	0
1	UR3	A	1498	21/22	0.95	0.20	160,183,204,223	0
1	M2G	A	966	25/26	0.95	0.17	177,182,207,211	0
1	5MC	A	967	21/22	0.95	0.14	182,192,200,205	0
1	4OC	A	1402	22/23	0.96	0.19	150,156,180,192	0
12	0TD	L	92	10/11	0.96	0.28	121,166,173,350	0
1	7MG	A	527	24/25	0.97	0.15	125,146,165,180	0
1	5MC	A	1407	21/22	0.97	0.15	171,191,202,207	0
1	MA6	A	1518	24/25	0.97	0.12	151,187,221,227	0
1	5MC	A	1404	21/22	0.97	0.13	166,182,196,204	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
23	MG	P	101	1/1	0.30	0.34	122,122,122,122	0
23	MG	A	1758	1/1	0.60	0.75	128,128,128,128	0
23	MG	A	1757	1/1	0.64	0.30	143,143,143,143	0
23	MG	S	102	1/1	0.67	0.16	156,156,156,156	0
23	MG	A	1681	1/1	0.67	0.11	243,243,243,243	0
23	MG	A	1785	1/1	0.69	1.14	142,142,142,142	0
23	MG	A	1784	1/1	0.70	0.40	145,145,145,145	0
23	MG	A	1771	1/1	0.70	0.70	138,138,138,138	0
23	MG	A	1672	1/1	0.72	0.26	102,102,102,102	0
23	MG	A	1730	1/1	0.74	0.39	134,134,134,134	0
23	MG	A	1794	1/1	0.75	0.71	206,206,206,206	0
23	MG	A	1773	1/1	0.76	0.12	162,162,162,162	0
23	MG	A	1667	1/1	0.76	0.39	143,143,143,143	0
23	MG	A	1661	1/1	0.76	0.58	124,124,124,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	MG	A	1782	1/1	0.77	0.28	131,131,131,131	0
23	MG	A	1738	1/1	0.78	0.24	123,123,123,123	0
23	MG	A	1750	1/1	0.78	0.50	125,125,125,125	0
23	MG	A	1659	1/1	0.78	0.38	142,142,142,142	0
23	MG	A	1707	1/1	0.79	0.28	120,120,120,120	0
23	MG	A	1714	1/1	0.80	0.21	143,143,143,143	0
23	MG	A	1712	1/1	0.80	0.30	138,138,138,138	0
23	MG	A	1727	1/1	0.81	0.17	138,138,138,138	0
23	MG	A	1825	1/1	0.82	0.15	377,377,377,377	0
23	MG	N	103	1/1	0.82	0.28	156,156,156,156	0
23	MG	A	1723	1/1	0.82	0.33	109,109,109,109	0
23	MG	A	1760	1/1	0.83	0.24	130,130,130,130	0
23	MG	A	1620	1/1	0.83	0.82	197,197,197,197	0
23	MG	A	1827	1/1	0.84	0.29	391,391,391,391	0
23	MG	A	1739	1/1	0.85	0.19	162,162,162,162	0
23	MG	A	1668	1/1	0.86	0.94	173,173,173,173	0
23	MG	A	1776	1/1	0.86	0.21	111,111,111,111	0
23	MG	A	1817	1/1	0.86	0.11	197,197,197,197	0
23	MG	A	1787	1/1	0.87	0.32	102,102,102,102	0
23	MG	A	1783	1/1	0.87	0.79	133,133,133,133	0
23	MG	A	1828	1/1	0.87	0.19	356,356,356,356	0
23	MG	A	1673	1/1	0.87	0.17	118,118,118,118	0
23	MG	A	1736	1/1	0.87	0.28	125,125,125,125	0
23	MG	A	1779	1/1	0.87	0.22	146,146,146,146	0
23	MG	A	1819	1/1	0.88	0.15	483,483,483,483	0
23	MG	A	1701	1/1	0.88	0.29	129,129,129,129	0
23	MG	A	1699	1/1	0.88	0.15	135,135,135,135	0
23	MG	A	1737	1/1	0.88	0.37	140,140,140,140	0
23	MG	A	1774	1/1	0.88	0.50	128,128,128,128	0
23	MG	A	1718	1/1	0.88	0.37	144,144,144,144	0
23	MG	A	1607	1/1	0.88	0.10	161,161,161,161	0
23	MG	A	1703	1/1	0.88	0.46	180,180,180,180	0
23	MG	A	1731	1/1	0.89	0.29	148,148,148,148	0
23	MG	A	1778	1/1	0.89	0.11	156,156,156,156	0
23	MG	A	1777	1/1	0.89	0.16	107,107,107,107	0
23	MG	N	102	1/1	0.89	0.18	214,214,214,214	0
23	MG	A	1759	1/1	0.89	0.41	161,161,161,161	0
23	MG	A	1655	1/1	0.89	0.31	181,181,181,181	0
23	MG	A	1664	1/1	0.89	0.44	226,226,226,226	0
23	MG	A	1675	1/1	0.89	0.35	121,121,121,121	0
23	MG	A	1694	1/1	0.89	0.74	180,180,180,180	0
23	MG	A	1683	1/1	0.89	0.11	422,422,422,422	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	MG	A	1775	1/1	0.90	0.70	123,123,123,123	0
23	MG	A	1710	1/1	0.90	0.11	161,161,161,161	0
23	MG	A	1688	1/1	0.90	0.21	301,301,301,301	0
23	MG	A	1651	1/1	0.90	0.44	140,140,140,140	0
23	MG	A	1765	1/1	0.90	0.14	372,372,372,372	0
23	MG	A	1697	1/1	0.90	0.38	135,135,135,135	0
23	MG	A	1786	1/1	0.91	0.15	145,145,145,145	0
23	MG	A	1793	1/1	0.91	0.19	302,302,302,302	0
23	MG	A	1728	1/1	0.91	0.16	150,150,150,150	0
23	MG	A	1735	1/1	0.91	0.23	155,155,155,155	0
23	MG	A	1772	1/1	0.91	0.18	121,121,121,121	0
23	MG	A	1645	1/1	0.91	0.12	146,146,146,146	0
23	MG	A	1816	1/1	0.91	0.08	262,262,262,262	0
23	MG	A	1639	1/1	0.91	0.24	126,126,126,126	0
23	MG	A	1626	1/1	0.91	0.34	118,118,118,118	0
23	MG	A	1715	1/1	0.92	0.35	151,151,151,151	0
23	MG	A	1751	1/1	0.92	0.33	133,133,133,133	0
23	MG	A	1734	1/1	0.92	0.33	163,163,163,163	0
23	MG	A	1692	1/1	0.92	0.70	142,142,142,142	0
23	MG	A	1621	1/1	0.92	0.20	166,166,166,166	0
23	MG	A	1637	1/1	0.92	0.19	143,143,143,143	0
23	MG	A	1658	1/1	0.92	0.41	146,146,146,146	0
23	MG	A	1653	1/1	0.92	0.53	185,185,185,185	0
23	MG	A	1831	1/1	0.92	0.24	484,484,484,484	0
23	MG	A	1744	1/1	0.92	0.25	176,176,176,176	0
23	MG	A	1813	1/1	0.92	0.22	146,146,146,146	0
23	MG	A	1815	1/1	0.93	0.22	190,190,190,190	0
23	MG	A	1647	1/1	0.93	0.19	180,180,180,180	0
23	MG	A	1829	1/1	0.93	0.09	323,323,323,323	0
23	MG	A	1650	1/1	0.93	0.22	155,155,155,155	0
23	MG	A	1685	1/1	0.93	0.09	263,263,263,263	0
23	MG	A	1696	1/1	0.93	0.23	245,245,245,245	0
23	MG	I	201	1/1	0.93	0.29	204,204,204,204	0
23	MG	A	1720	1/1	0.93	0.23	139,139,139,139	0
23	MG	A	1749	1/1	0.93	0.65	126,126,126,126	0
23	MG	K	201	1/1	0.93	0.08	181,181,181,181	0
23	MG	A	1640	1/1	0.93	0.36	129,129,129,129	0
23	MG	A	1768	1/1	0.94	0.04	550,550,550,550	0
23	MG	A	1745	1/1	0.94	0.28	235,235,235,235	0
23	MG	E	201	1/1	0.94	0.09	435,435,435,435	0
23	MG	A	1822	1/1	0.94	0.15	374,374,374,374	0
23	MG	A	1676	1/1	0.94	0.32	133,133,133,133	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	MG	A	1796	1/1	0.94	0.33	372,372,372,372	0
23	MG	A	1781	1/1	0.94	0.34	145,145,145,145	0
23	MG	A	1788	1/1	0.94	0.17	156,156,156,156	0
23	MG	A	1702	1/1	0.94	0.09	126,126,126,126	0
23	MG	B	301	1/1	0.94	0.44	181,181,181,181	0
23	MG	A	1635	1/1	0.95	0.35	214,214,214,214	0
23	MG	A	1762	1/1	0.95	0.30	109,109,109,109	0
23	MG	A	1755	1/1	0.95	0.21	190,190,190,190	0
23	MG	A	1704	1/1	0.95	0.29	118,118,118,118	0
23	MG	A	1767	1/1	0.95	0.28	327,327,327,327	0
23	MG	A	1665	1/1	0.95	0.04	247,247,247,247	0
22	SRY	A	1601	40/40	0.95	0.20	123,154,201,206	0
23	MG	A	1656	1/1	0.95	0.34	173,173,173,173	0
23	MG	A	1604	1/1	0.95	0.17	133,133,133,133	0
23	MG	A	1713	1/1	0.95	0.22	133,133,133,133	0
23	MG	A	1622	1/1	0.95	0.68	138,138,138,138	0
23	MG	A	1693	1/1	0.95	0.17	179,179,179,179	0
23	MG	A	1618	1/1	0.95	0.22	152,152,152,152	0
23	MG	A	1820	1/1	0.95	0.11	265,265,265,265	0
23	MG	A	1802	1/1	0.95	0.20	457,457,457,457	0
23	MG	A	1705	1/1	0.95	0.27	153,153,153,153	0
23	MG	A	1741	1/1	0.95	0.17	145,145,145,145	0
23	MG	A	1789	1/1	0.95	0.16	152,152,152,152	0
23	MG	A	1663	1/1	0.95	0.38	138,138,138,138	0
23	MG	S	101	1/1	0.95	0.32	138,138,138,138	0
23	MG	A	1695	1/1	0.95	0.12	245,245,245,245	0
23	MG	A	1660	1/1	0.95	0.07	194,194,194,194	0
23	MG	A	1641	1/1	0.95	0.10	134,134,134,134	0
23	MG	A	1810	1/1	0.96	0.14	117,117,117,117	0
23	MG	A	1804	1/1	0.96	0.30	420,420,420,420	0
23	MG	A	1689	1/1	0.96	0.57	151,151,151,151	0
23	MG	A	1716	1/1	0.96	0.30	121,121,121,121	0
23	MG	M	201	1/1	0.96	0.41	163,163,163,163	0
23	MG	A	1708	1/1	0.96	0.19	119,119,119,119	0
23	MG	A	1800	1/1	0.96	0.23	400,400,400,400	0
23	MG	A	1809	1/1	0.96	0.23	281,281,281,281	0
23	MG	A	1742	1/1	0.96	0.11	134,134,134,134	0
23	MG	A	1670	1/1	0.96	0.36	173,173,173,173	0
23	MG	A	1766	1/1	0.96	0.19	220,220,220,220	0
23	MG	A	1654	1/1	0.96	0.18	201,201,201,201	0
23	MG	A	1722	1/1	0.96	0.20	116,116,116,116	0
23	MG	A	1615	1/1	0.96	0.34	129,129,129,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	MG	A	1652	1/1	0.96	0.32	141,141,141,141	0
23	MG	A	1748	1/1	0.96	0.20	204,204,204,204	0
23	MG	A	1769	1/1	0.96	0.25	209,209,209,209	0
23	MG	J	201	1/1	0.97	0.21	138,138,138,138	0
23	MG	A	1686	1/1	0.97	0.14	150,150,150,150	0
23	MG	A	1808	1/1	0.97	0.20	444,444,444,444	0
23	MG	A	1679	1/1	0.97	0.46	133,133,133,133	0
23	MG	H	202	1/1	0.97	0.16	137,137,137,137	0
23	MG	A	1790	1/1	0.97	0.23	148,148,148,148	0
23	MG	A	1721	1/1	0.97	0.23	135,135,135,135	0
23	MG	A	1623	1/1	0.97	0.14	170,170,170,170	0
23	MG	A	1807	1/1	0.97	0.39	427,427,427,427	0
23	MG	A	1780	1/1	0.97	0.11	111,111,111,111	0
23	MG	A	1603	1/1	0.97	0.12	128,128,128,128	0
23	MG	A	1617	1/1	0.97	0.21	129,129,129,129	0
23	MG	A	1632	1/1	0.97	0.16	91,91,91,91	0
23	MG	A	1624	1/1	0.97	0.28	210,210,210,210	0
23	MG	A	1798	1/1	0.97	0.39	454,454,454,454	0
23	MG	A	1814	1/1	0.97	0.08	128,128,128,128	0
23	MG	A	1706	1/1	0.97	0.26	163,163,163,163	0
23	MG	A	1791	1/1	0.97	0.11	144,144,144,144	0
23	MG	A	1611	1/1	0.97	0.04	223,223,223,223	0
23	MG	A	1657	1/1	0.97	0.14	177,177,177,177	0
23	MG	A	1756	1/1	0.97	0.29	213,213,213,213	0
23	MG	A	1616	1/1	0.97	0.13	107,107,107,107	0
23	MG	A	1614	1/1	0.97	0.15	94,94,94,94	0
23	MG	A	1746	1/1	0.97	0.12	282,282,282,282	0
23	MG	A	1634	1/1	0.97	0.09	112,112,112,112	0
23	MG	A	1631	1/1	0.97	0.19	127,127,127,127	0
23	MG	A	1732	1/1	0.97	0.16	131,131,131,131	0
23	MG	H	201	1/1	0.97	0.41	131,131,131,131	0
23	MG	A	1764	1/1	0.97	0.15	308,308,308,308	0
23	MG	A	1625	1/1	0.97	0.20	134,134,134,134	0
23	MG	A	1763	1/1	0.97	0.08	181,181,181,181	0
23	MG	A	1743	1/1	0.97	0.29	183,183,183,183	0
23	MG	A	1629	1/1	0.97	0.11	125,125,125,125	0
23	MG	A	1608	1/1	0.97	0.19	118,118,118,118	0
23	MG	A	1826	1/1	0.97	0.28	458,458,458,458	0
23	MG	A	1799	1/1	0.97	0.25	242,242,242,242	0
23	MG	M	202	1/1	0.97	0.67	148,148,148,148	0
23	MG	A	1648	1/1	0.98	0.24	230,230,230,230	0
23	MG	A	1811	1/1	0.98	0.34	346,346,346,346	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	MG	A	1666	1/1	0.98	0.15	187,187,187,187	0
23	MG	T	201	1/1	0.98	0.18	142,142,142,142	0
23	MG	A	1724	1/1	0.98	0.09	176,176,176,176	0
23	MG	A	1671	1/1	0.98	0.12	208,208,208,208	0
23	MG	A	1691	1/1	0.98	0.14	187,187,187,187	0
23	MG	A	1797	1/1	0.98	0.14	429,429,429,429	0
23	MG	A	1709	1/1	0.98	0.10	141,141,141,141	0
23	MG	A	1638	1/1	0.98	0.27	170,170,170,170	0
23	MG	A	1818	1/1	0.98	0.55	483,483,483,483	0
23	MG	D	302	1/1	0.98	0.16	186,186,186,186	0
23	MG	A	1830	1/1	0.98	0.16	494,494,494,494	0
23	MG	A	1717	1/1	0.98	0.17	110,110,110,110	0
23	MG	A	1680	1/1	0.98	0.41	306,306,306,306	0
23	MG	A	1803	1/1	0.98	0.18	342,342,342,342	0
23	MG	A	1662	1/1	0.98	0.12	162,162,162,162	0
23	MG	A	1602	1/1	0.98	0.28	180,180,180,180	0
23	MG	A	1795	1/1	0.98	0.10	457,457,457,457	0
23	MG	A	1753	1/1	0.98	0.06	118,118,118,118	0
23	MG	A	1606	1/1	0.98	0.24	126,126,126,126	0
23	MG	A	1684	1/1	0.98	0.09	124,124,124,124	0
23	MG	A	1687	1/1	0.98	0.17	96,96,96,96	0
23	MG	A	1610	1/1	0.98	0.12	193,193,193,193	0
23	MG	A	1646	1/1	0.98	0.06	131,131,131,131	0
23	MG	A	1711	1/1	0.98	0.31	187,187,187,187	0
23	MG	A	1754	1/1	0.98	0.26	177,177,177,177	0
23	MG	A	1609	1/1	0.98	0.19	155,155,155,155	0
23	MG	A	1801	1/1	0.98	0.11	423,423,423,423	0
23	MG	A	1733	1/1	0.98	0.05	126,126,126,126	0
23	MG	A	1649	1/1	0.98	0.10	192,192,192,192	0
23	MG	A	1752	1/1	0.98	0.21	147,147,147,147	0
23	MG	A	1740	1/1	0.98	0.22	123,123,123,123	0
23	MG	A	1805	1/1	0.98	0.10	426,426,426,426	0
23	MG	A	1729	1/1	0.98	0.40	123,123,123,123	0
23	MG	A	1698	1/1	0.98	0.19	131,131,131,131	0
23	MG	T	202	1/1	0.98	0.24	450,450,450,450	0
23	MG	A	1627	1/1	0.98	0.12	160,160,160,160	0
23	MG	A	1700	1/1	0.98	0.13	134,134,134,134	0
23	MG	A	1612	1/1	0.99	0.07	123,123,123,123	0
23	MG	A	1677	1/1	0.99	0.18	191,191,191,191	0
24	ZN	N	101	1/1	0.99	0.19	336,336,336,336	0
23	MG	A	1682	1/1	0.99	0.12	365,365,365,365	0
23	MG	A	1619	1/1	0.99	0.35	253,253,253,253	0

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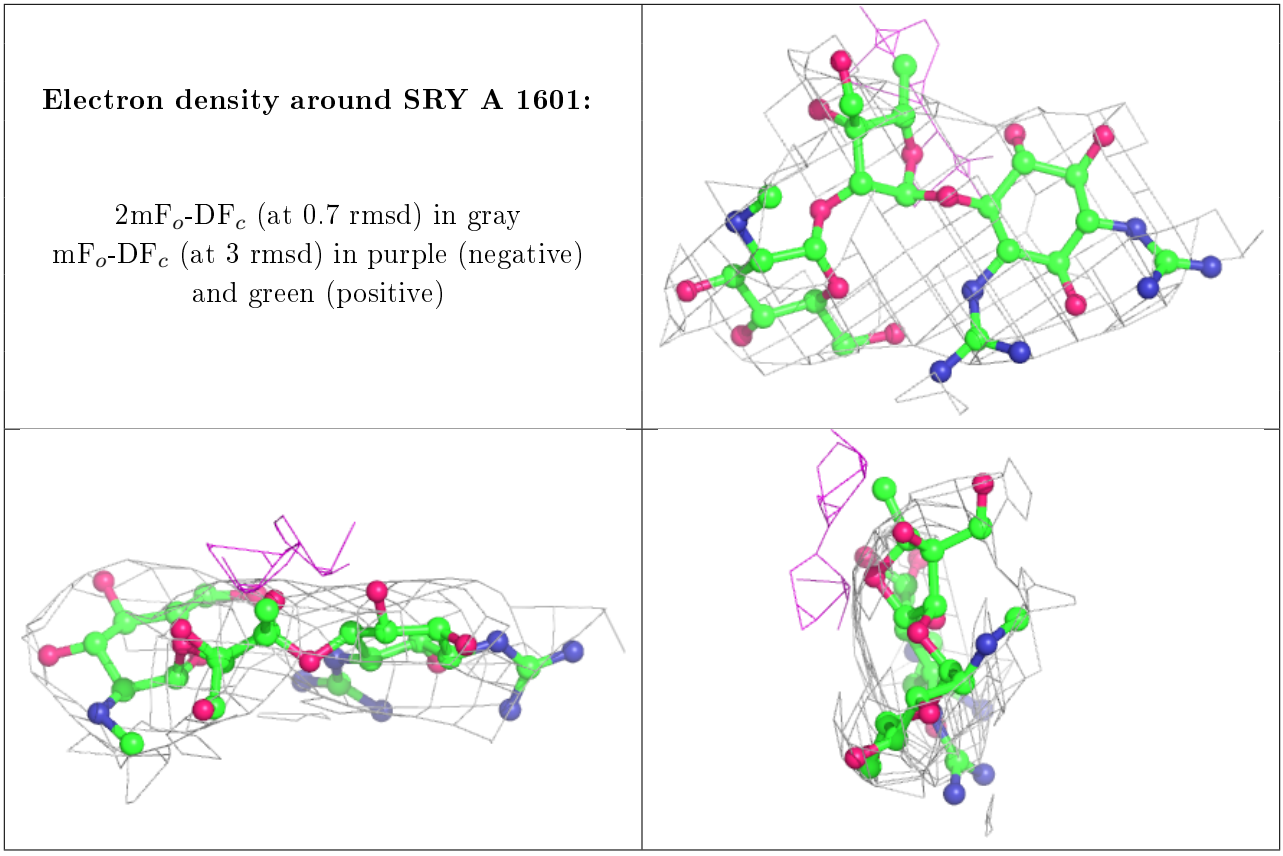
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	MG	A	1747	1/1	0.99	0.18	296,296,296,296	0
23	MG	A	1690	1/1	0.99	0.20	216,216,216,216	0
23	MG	A	1761	1/1	0.99	0.13	158,158,158,158	0
23	MG	A	1636	1/1	0.99	0.70	186,186,186,186	0
23	MG	A	1726	1/1	0.99	0.18	130,130,130,130	0
23	MG	A	1806	1/1	0.99	0.16	392,392,392,392	0
23	MG	A	1792	1/1	0.99	0.20	127,127,127,127	0
23	MG	A	1643	1/1	0.99	0.30	135,135,135,135	0
23	MG	A	1613	1/1	0.99	0.20	126,126,126,126	0
23	MG	A	1644	1/1	0.99	0.16	175,175,175,175	0
23	MG	A	1824	1/1	0.99	0.18	366,366,366,366	0
23	MG	A	1628	1/1	0.99	0.45	191,191,191,191	0
23	MG	A	1821	1/1	0.99	0.18	236,236,236,236	0
24	ZN	D	301	1/1	0.99	0.32	159,159,159,159	0
23	MG	A	1633	1/1	0.99	0.43	125,125,125,125	0
23	MG	A	1725	1/1	0.99	0.14	153,153,153,153	0
23	MG	A	1674	1/1	0.99	0.16	112,112,112,112	0
23	MG	A	1719	1/1	0.99	0.17	105,105,105,105	0
23	MG	A	1630	1/1	0.99	0.13	92,92,92,92	0
23	MG	A	1605	1/1	0.99	0.08	148,148,148,148	0
23	MG	A	1642	1/1	0.99	0.17	107,107,107,107	0
23	MG	A	1812	1/1	0.99	0.08	226,226,226,226	0
23	MG	A	1678	1/1	0.99	0.10	136,136,136,136	0
23	MG	A	1669	1/1	0.99	0.29	138,138,138,138	0
23	MG	A	1770	1/1	0.99	0.26	141,141,141,141	0
23	MG	A	1823	1/1	1.00	0.14	194,194,194,194	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around SRY A 1601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.