Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:59 PM GMT

PDB ID	:	4DR1
Title	:	Crystal structure of the apo 30S ribosomal subunit from Thermus thermophilus (HB8)
Authors	:	Demirci, H.; Murphy IV, F.; Murphy, E.; Gregory, S.T.; Dahlberg, A.E.; Jogl, G.
Deposited on	:	2012-02-16
Resolution	:	3.60 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

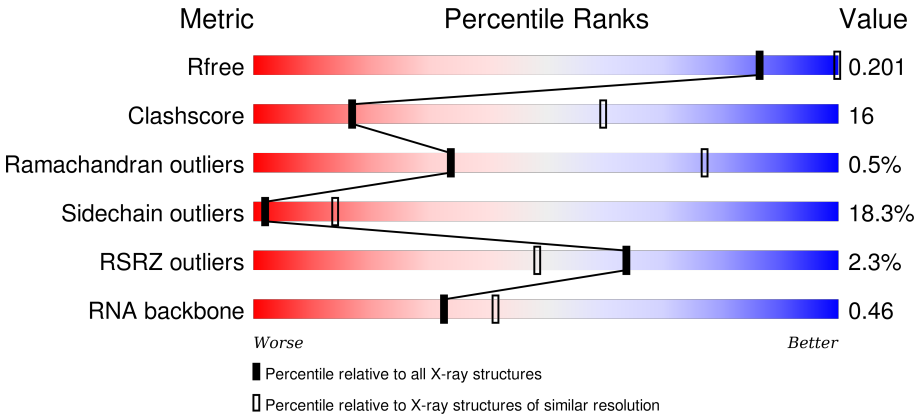
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance

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

The reported resolution of this entry is 3.60 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}	91344	1408 (3.80-3.40)
Clashscore	102246	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)
RSRZ outliers	91569	1003 (3.78-3.42)
RNA backbone	2183	1058 (4.40-2.80)

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. 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% 27% 43% 23% 6%
2	B	256	48% 33% 10% 9%
3	C	239	6% 43% 34% 8% 14%
4	D	209	% 54% 35% 11%

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Mol	Chain	Length	Quality of chain
5	E	162	49% 35% 7% 7%
6	F	101	60% 32% 8%
7	G	156	5% 57% 37% 6%
8	H	138	50% 42% 8%
9	I	128	3% 45% 43% 11%
10	J	105	13% 50% 35% 9% 7%
11	K	129	52% 31% 7% 10%
12	L	135	42% 41% 9% 8%
13	M	126	3% 35% 48% 10% 6%
14	N	61	7% 34% 56% 8%
15	O	89	% 46% 40% 10%
16	P	88	45% 43% 6% 6%
17	Q	105	42% 43% 9% 6%
18	R	88	% 43% 32% 5% 20%
19	S	93	4% 49% 31% 5% 14%
20	T	106	% 46% 39% 8% 7%
21	U	27	22% 48% 33% 7% 11%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	MG	A	1636	-	-	-	X
22	MG	A	1643	-	-	-	X
22	MG	A	1649	-	-	-	X
22	MG	A	1653	-	-	-	X
22	MG	A	1679	-	-	-	X
22	MG	A	1719	-	-	-	X
22	MG	A	1734	-	-	-	X
22	MG	A	1735	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	MG	A	1746	-	-	-	X
22	MG	A	1748	-	-	-	X
22	MG	A	1751	-	-	-	X
22	MG	A	1767	-	-	-	X
22	MG	A	1770	-	-	-	X
22	MG	A	1773	-	-	-	X
22	MG	A	1797	-	-	-	X
22	MG	A	1807	-	-	-	X
22	MG	A	1810	-	-	-	X
22	MG	A	1820	-	-	-	X
22	MG	A	1822	-	-	-	X
22	MG	A	1826	-	-	-	X
22	MG	A	1836	-	-	-	X
22	MG	B	301	-	-	-	X
22	MG	B	302	-	-	-	X
22	MG	C	302	-	-	-	X
22	MG	D	302	-	-	-	X

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 52227 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	1512	32644	14540	6039	10547	1518	0	6	0

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a protein called 30S 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 30S 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 30S 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 30S ribosomal protein S5.

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

- Molecule 6 is a protein called 30S 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 30S 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 30S 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 30S 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 30S 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 30S 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 30S 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 30S 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 30S 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 30S 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 30S 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 30S 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 30S 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 30S ribosomal protein S19.

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

- Molecule 20 is a protein called 30S ribosomal protein S20.

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

- Molecule 21 is a protein called 30S ribosomal protein THX.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	P	2	Total 2	Mg 2	0	0
22	Q	1	Total 1	Mg 1	0	0
22	D	4	Total 4	Mg 4	0	0
22	E	1	Total 1	Mg 1	0	0
22	B	2	Total 2	Mg 2	0	0
22	C	3	Total 3	Mg 3	0	0
22	A	239	Total 239	Mg 239	0	0
22	L	1	Total 1	Mg 1	0	0
22	F	1	Total 1	Mg 1	0	0

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

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

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

- Molecule 24 is water.

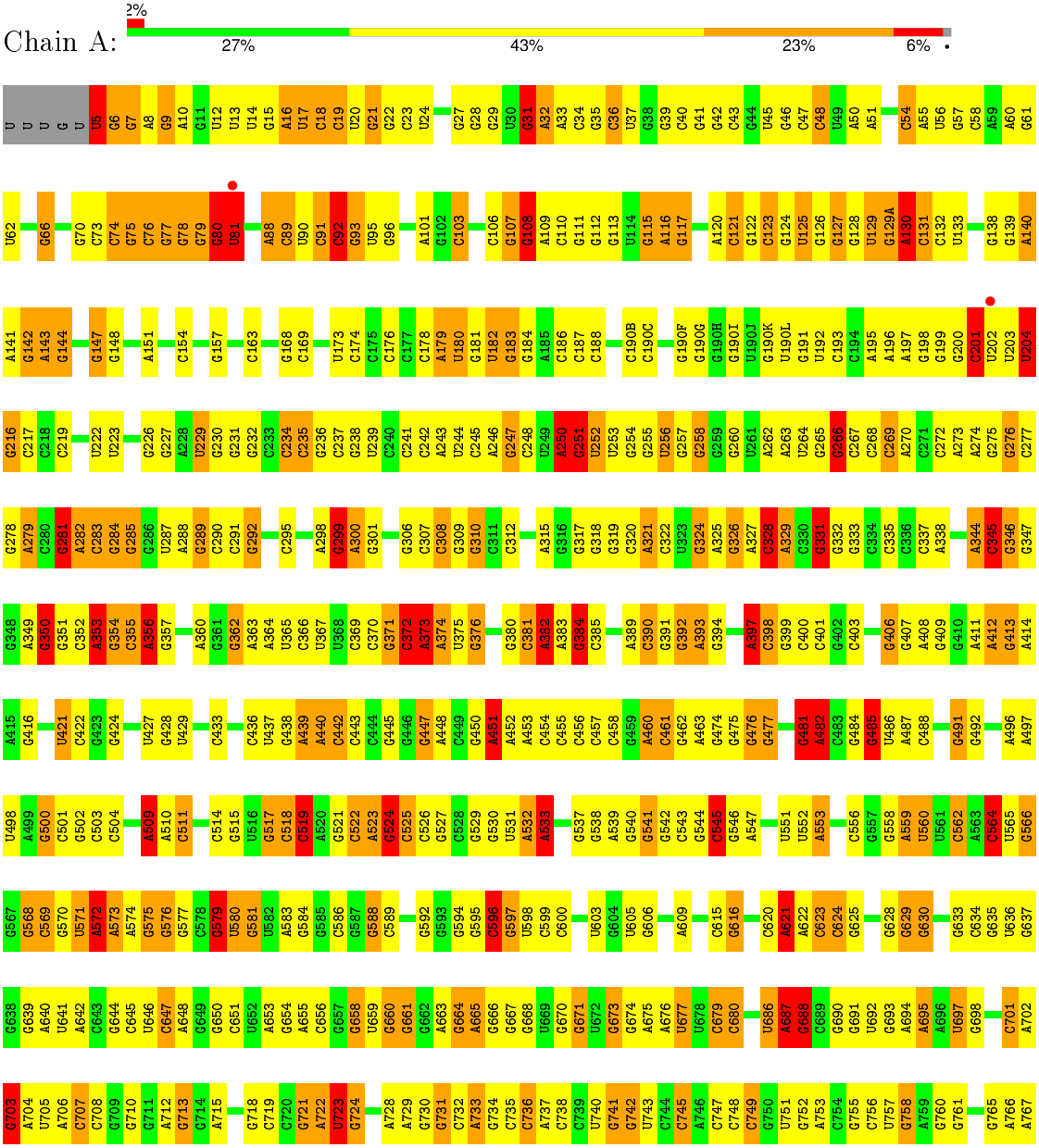
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	232	Total O 232 232	0	0
24	E	3	Total O 3 3	0	0
24	L	1	Total O 1 1	0	0
24	Q	1	Total O 1 1	0	0
24	T	2	Total O 2 2	0	0

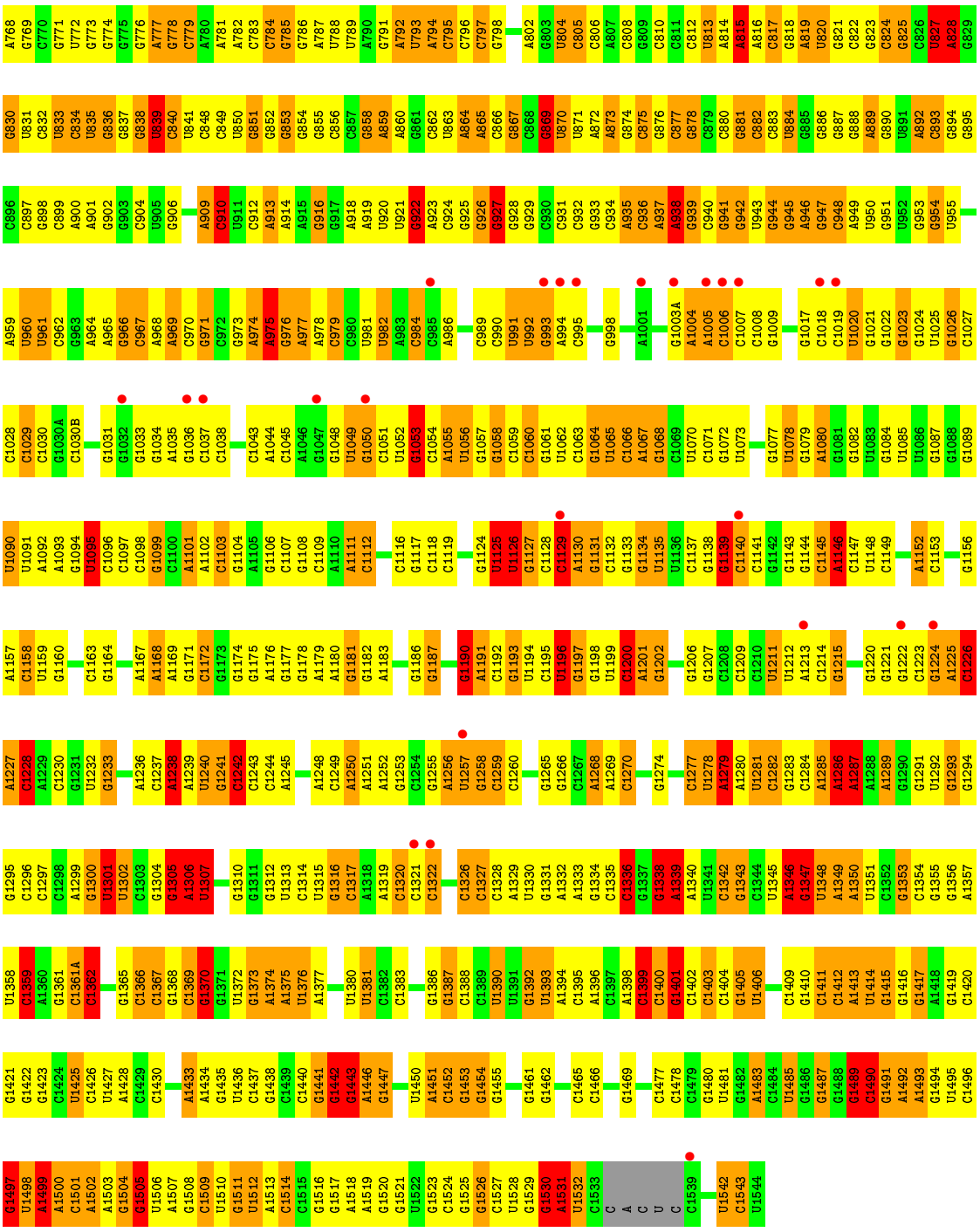
3 Residue-property plots (i)

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

- Molecule 1: 16S rRNA

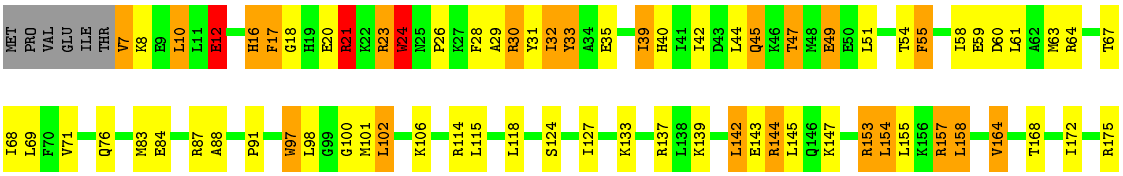
Chain A:





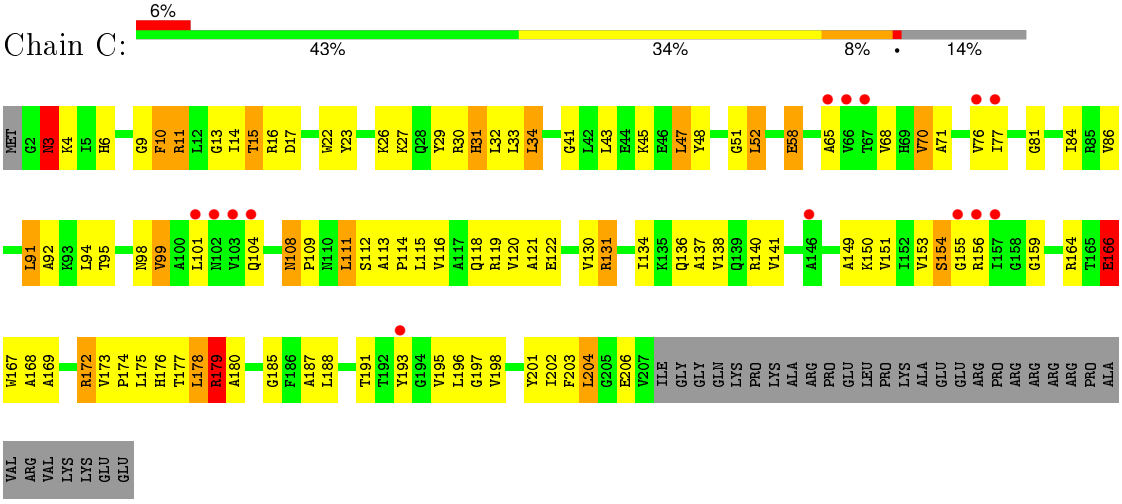
• Molecule 2: 30S ribosomal protein S2

Chain B:



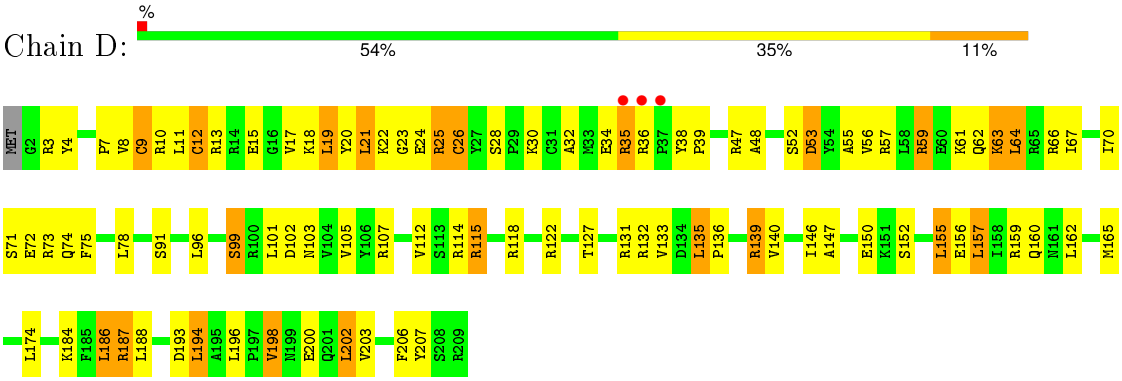
• Molecule 3: 30S ribosomal protein S3

Chain C:



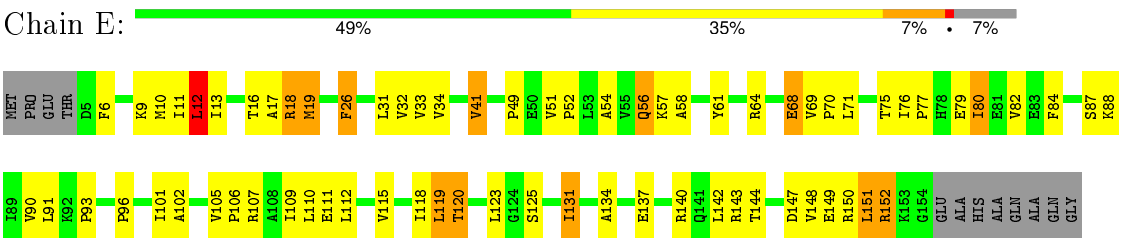
• Molecule 4: 30S ribosomal protein S4

Chain D:



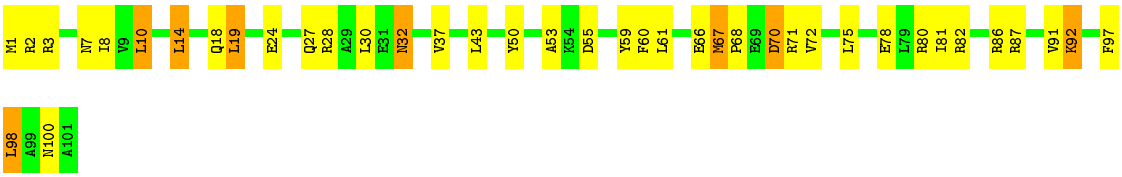
• Molecule 5: 30S ribosomal protein S5

Chain E:



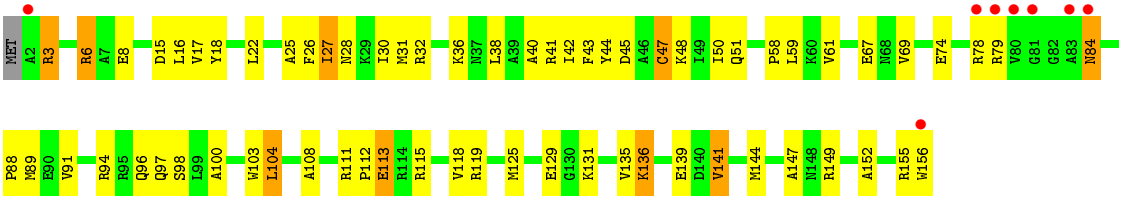
• Molecule 6: 30S ribosomal protein S6

Chain F:



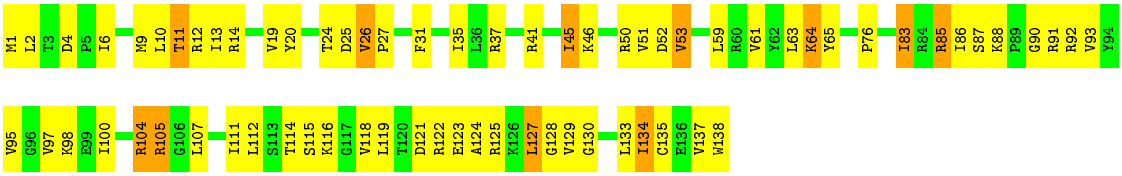
• Molecule 7: 30S ribosomal protein S7

Chain G:



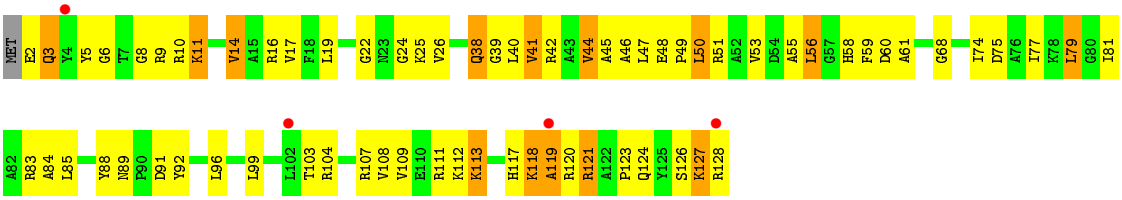
• Molecule 8: 30S ribosomal protein S8

Chain H:



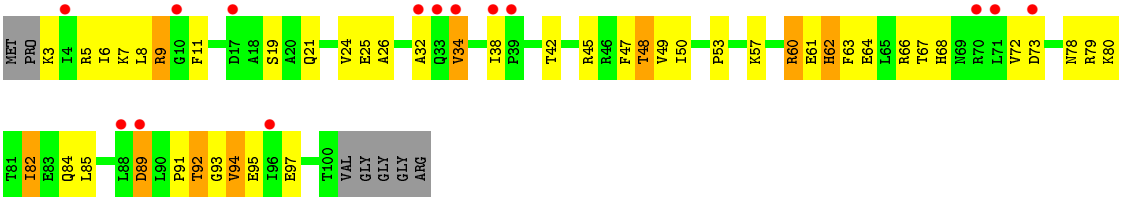
• Molecule 9: 30S ribosomal protein S9

Chain I:



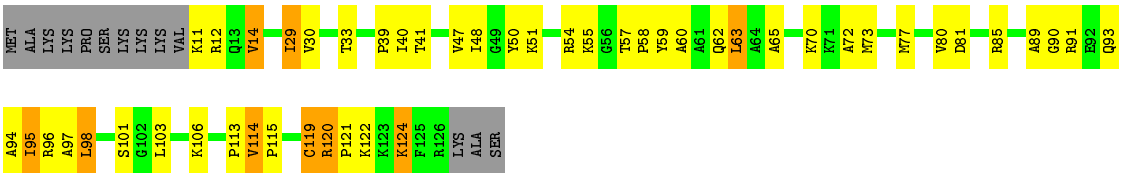
• Molecule 10: 30S ribosomal protein S10

Chain J:



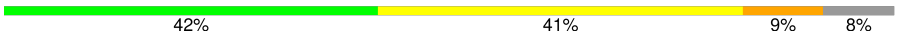
• Molecule 11: 30S ribosomal protein S11

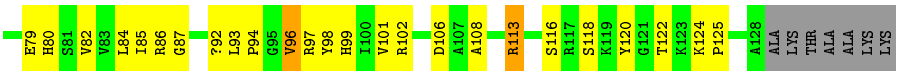
Chain K:



• Molecule 12: 30S ribosomal protein S12

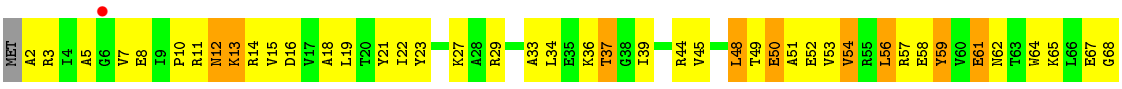
Chain L:





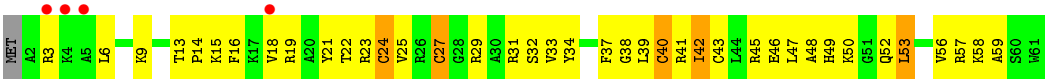
• Molecule 13: 30S ribosomal protein S13

Chain M:



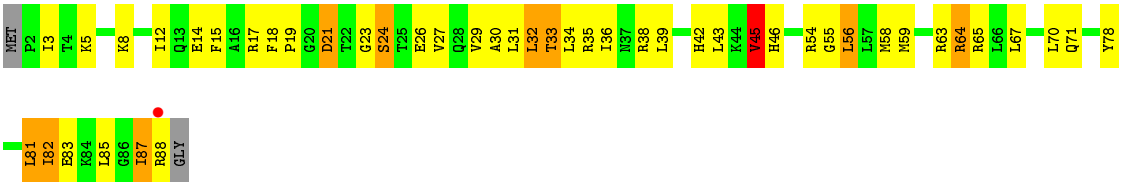
• Molecule 14: 30S ribosomal protein S14

Chain N:



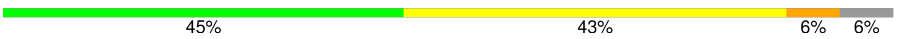
• Molecule 15: 30S ribosomal protein S15

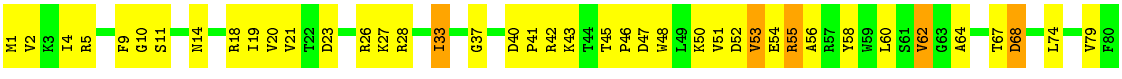
Chain O:



• Molecule 16: 30S ribosomal protein S16

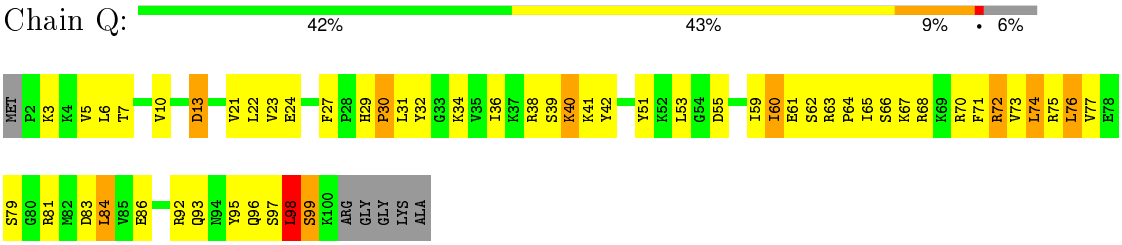
Chain P:





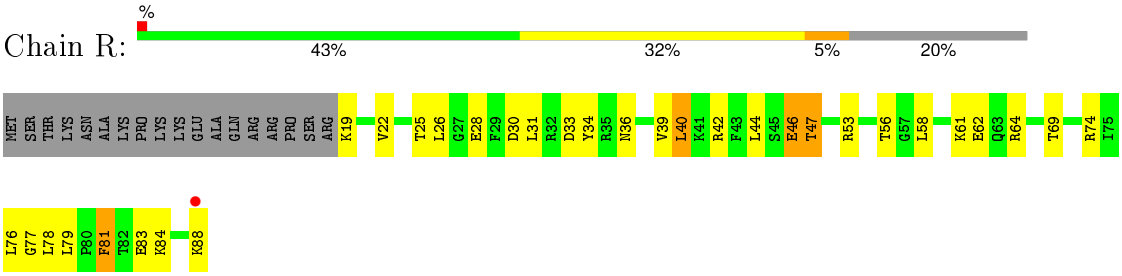
• Molecule 17: 30S ribosomal protein S17

Chain Q:



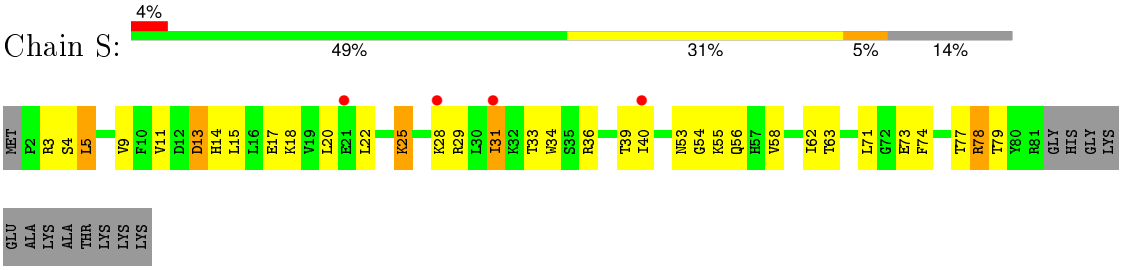
• Molecule 18: 30S ribosomal protein S18

Chain R:



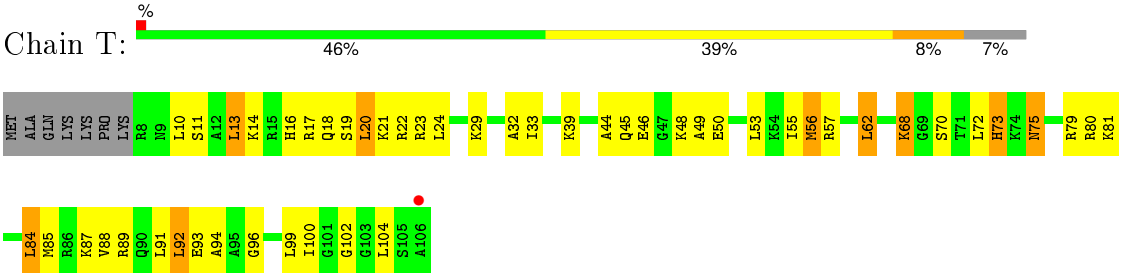
• Molecule 19: 30S ribosomal protein S19

Chain S:



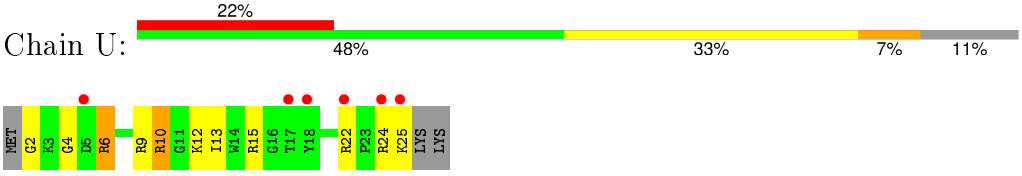
• Molecule 20: 30S ribosomal protein S20

Chain T:



• Molecule 21: 30S ribosomal protein THX

Chain U:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	403.04Å 403.04Å 174.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.64 – 3.60 34.64 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.2 (34.64-3.60) 99.0 (34.64-3.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.81 (at 3.56Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_978)	Depositor
R, R_{free}	0.157 , 0.207 0.158 , 0.201	Depositor DCC
R_{free} test set	8156 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	138.5	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 139.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 163418 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	52227	wwPDB-VP
Average B, all atoms (Å^2)	167.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.87% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, MA6, 0TD, MG, 2MG, 5MC, UR3, 4OC, M2G, 7MG, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	1.11	101/36139 (0.3%)	1.77	1380/56396 (2.4%)
2	B	0.72	1/1935 (0.1%)	0.89	0/2609
3	C	0.55	1/1636 (0.1%)	0.80	4/2205 (0.2%)
4	D	0.68	1/1733 (0.1%)	0.86	2/2318 (0.1%)
5	E	0.93	0/1162	1.07	3/1564 (0.2%)
6	F	0.59	0/856	0.81	1/1154 (0.1%)
7	G	0.60	0/1276	0.76	0/1709
8	H	0.99	1/1136 (0.1%)	1.07	0/1527
9	I	0.60	0/1029	0.80	0/1379
10	J	0.59	0/805	0.81	0/1082
11	K	0.70	0/879	0.90	0/1187
12	L	0.77	0/977	1.00	0/1306
13	M	0.60	0/947	0.81	0/1270
14	N	0.56	0/501	0.84	0/664
15	O	0.76	0/740	0.96	2/987 (0.2%)
16	P	0.76	0/716	0.96	1/963 (0.1%)
17	Q	0.91	0/836	1.16	3/1117 (0.3%)
18	R	0.77	2/579 (0.3%)	0.91	0/768
19	S	0.49	0/661	0.76	0/890
20	T	0.67	0/765	0.95	1/1007 (0.1%)
21	U	0.56	0/212	0.81	0/277
All	All	0.99	107/55520 (0.2%)	1.55	1397/82379 (1.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	2
8	H	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
17	Q	0	1
20	T	0	2
All	All	0	7

All (107) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	279	A	N9-C4	-13.91	1.29	1.37
1	A	817	C	N1-C6	-9.69	1.31	1.37
1	A	279	A	N3-C4	-9.58	1.29	1.34
1	A	1509	C	N1-C6	-9.55	1.31	1.37
1	A	822	C	N1-C6	-8.43	1.32	1.37
1	A	1508	G	N7-C5	-8.42	1.34	1.39
1	A	852	G	C6-O6	8.29	1.31	1.24
4	D	12	CYS	CB-SG	8.16	1.96	1.82
1	A	107	G	C5-C6	-8.01	1.34	1.42
1	A	130	A	N9-C4	-7.98	1.33	1.37
1	A	80	G	N9-C4	7.40	1.43	1.38
1	A	569	C	N3-C4	-7.36	1.28	1.33
1	A	482	A	N7-C5	-7.33	1.34	1.39
1	A	860	A	N3-C4	-7.29	1.30	1.34
1	A	1502	A	N9-C4	-7.29	1.33	1.37
1	A	1079	G	N7-C5	-7.16	1.34	1.39
1	A	1377	A	N9-C4	-7.15	1.33	1.37
1	A	573	A	N7-C5	-7.07	1.35	1.39
1	A	279	A	N7-C5	-7.01	1.35	1.39
1	A	589	C	N1-C6	-6.93	1.32	1.37
1	A	573	A	N9-C4	6.92	1.42	1.37
1	A	858	G	C5-C6	-6.88	1.35	1.42
1	A	564	C	N1-C6	-6.81	1.33	1.37
1	A	858	G	N1-C2	6.80	1.43	1.37
1	A	858	G	N7-C5	-6.79	1.35	1.39
1	A	882	C	N1-C6	-6.79	1.33	1.37
8	H	135	CYS	CB-SG	-6.76	1.70	1.82
1	A	828	A	N9-C4	-6.70	1.33	1.37
1	A	715	A	N9-C4	-6.69	1.33	1.37
1	A	1500	A	C6-N1	-6.68	1.30	1.35
1	A	1508	G	N9-C8	-6.68	1.33	1.37
1	A	574	A	C5-C4	-6.66	1.34	1.38
1	A	266	G	N7-C5	-6.62	1.35	1.39
1	A	569	C	N1-C6	-6.54	1.33	1.37
1	A	288	A	N9-C4	-6.49	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	572	A	C6-N1	-6.44	1.31	1.35
1	A	1502	A	C5-C6	-6.34	1.35	1.41
1	A	654	G	N9-C4	-6.34	1.32	1.38
1	A	574	A	C6-N1	-6.25	1.31	1.35
1	A	1501	C	N1-C6	-6.25	1.33	1.37
1	A	568	G	C6-N1	-6.21	1.35	1.39
1	A	1401	G	N3-C4	-6.20	1.31	1.35
1	A	595	G	N9-C8	-6.19	1.33	1.37
1	A	279	A	C5-C6	-6.14	1.35	1.41
1	A	1501	C	N3-C4	-6.14	1.29	1.33
1	A	1248	A	N9-C4	6.12	1.41	1.37
1	A	1377	A	N3-C4	-6.09	1.31	1.34
1	A	817	C	N3-C4	-6.09	1.29	1.33
1	A	918	A	N7-C5	-6.08	1.35	1.39
1	A	835	U	C4-O4	6.03	1.28	1.23
1	A	889	A	N3-C4	-6.02	1.31	1.34
1	A	16	A	C6-N1	-5.93	1.31	1.35
1	A	125	U	C2-N3	-5.91	1.33	1.37
1	A	1394	A	N9-C4	-5.89	1.34	1.37
1	A	79	G	N9-C4	5.88	1.42	1.38
1	A	1401	G	C5-C4	-5.82	1.34	1.38
1	A	107	G	N7-C5	-5.81	1.35	1.39
1	A	586	C	N1-C6	-5.76	1.33	1.37
1	A	1346	A	C3'-O3'	5.75	1.50	1.42
1	A	596	C	N1-C6	-5.72	1.33	1.37
1	A	1502	A	N7-C5	-5.71	1.35	1.39
1	A	16	A	N3-C4	-5.67	1.31	1.34
1	A	753	A	N3-C4	-5.65	1.31	1.34
1	A	655	A	C6-N6	-5.64	1.29	1.33
1	A	920	U	C4-O4	5.61	1.28	1.23
2	B	12	GLU	CG-CD	5.57	1.60	1.51
1	A	882	C	N3-C4	-5.56	1.30	1.33
1	A	1146	A	N9-C4	-5.50	1.34	1.37
1	A	1500	A	N3-C4	-5.50	1.31	1.34
1	A	1301	U	C3'-O3'	5.48	1.49	1.42
1	A	108	G	N9-C8	5.46	1.41	1.37
1	A	151	A	N9-C4	-5.45	1.34	1.37
1	A	266	G	N9-C4	-5.45	1.33	1.38
1	A	1502	A	N3-C4	-5.43	1.31	1.34
1	A	130	A	N3-C4	-5.42	1.31	1.34
1	A	1514	C	N1-C6	-5.40	1.33	1.37
1	A	635	G	N3-C4	-5.39	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	266	G	C5-C6	-5.37	1.36	1.42
1	A	566	G	N7-C5	-5.34	1.36	1.39
1	A	364	A	N7-C5	-5.33	1.36	1.39
1	A	23	C	N1-C6	-5.31	1.33	1.37
1	A	1306	A	N7-C5	-5.30	1.36	1.39
1	A	1377	A	C6-N1	-5.26	1.31	1.35
3	C	3	ASN	CB-CG	5.25	1.63	1.51
1	A	834	C	N1-C6	-5.24	1.34	1.37
18	R	46	GLU	CG-CD	5.23	1.59	1.51
1	A	856	C	N1-C6	-5.23	1.34	1.37
1	A	363	A	N9-C4	-5.22	1.34	1.37
1	A	281	G	C3'-O3'	5.19	1.49	1.42
1	A	553	A	N9-C4	-5.17	1.34	1.37
1	A	722	A	C5-C6	-5.14	1.36	1.41
1	A	1500	A	C5-C4	-5.14	1.35	1.38
1	A	824	C	N1-C6	-5.13	1.34	1.37
1	A	729	A	N7-C5	-5.12	1.36	1.39
1	A	117	G	C5-C6	-5.12	1.37	1.42
1	A	1370	G	N9-C4	5.11	1.42	1.38
1	A	572	A	C6-N6	-5.09	1.29	1.33
1	A	888	G	C2-N3	-5.09	1.28	1.32
1	A	574	A	N3-C4	-5.09	1.31	1.34
1	A	797	C	N1-C6	-5.08	1.34	1.37
18	R	46	GLU	CB-CG	5.07	1.61	1.52
1	A	1300	G	C3'-O3'	5.06	1.49	1.42
1	A	1509	C	N3-C4	-5.03	1.30	1.33
1	A	852	G	C5-C4	5.03	1.41	1.38
1	A	393	A	N9-C4	-5.02	1.34	1.37
1	A	665	A	N9-C4	-5.02	1.34	1.37
1	A	860	A	N9-C4	-5.01	1.34	1.37

All (1397) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	117	G	N1-C6-O6	21.97	133.08	119.90
1	A	858	G	N1-C6-O6	19.43	131.56	119.90
1	A	117	G	C6-C5-N7	-18.81	119.11	130.40
1	A	279	A	C5-N7-C8	-17.11	95.35	103.90
1	A	579	G	N1-C6-O6	15.79	129.37	119.90
1	A	852	G	C5-C6-N1	-15.70	103.65	111.50
1	A	858	G	C5-C6-O6	-15.38	119.37	128.60
1	A	266	G	C6-C5-N7	-14.92	121.45	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	279	A	C2-N3-C4	-14.56	103.32	110.60
1	A	266	G	C5-N7-C8	-14.52	97.04	104.30
1	A	266	G	C4-C5-N7	14.31	116.53	110.80
1	A	107	G	C4-C5-N7	13.90	116.36	110.80
1	A	279	A	N7-C8-N9	13.86	120.73	113.80
1	A	232	G	N1-C6-O6	13.85	128.21	119.90
1	A	117	G	C2-N3-C4	-13.17	105.32	111.90
1	A	1200	C	C2-N1-C1'	13.16	133.28	118.80
1	A	948	C	C6-N1-C2	13.07	125.53	120.30
1	A	279	A	N1-C6-N6	13.01	126.40	118.60
1	A	117	G	C5-C6-N1	-12.91	105.04	111.50
1	A	266	G	N1-C6-O6	12.62	127.47	119.90
1	A	1181	G	C8-N9-C4	12.56	111.42	106.40
1	A	1502	A	C5-N7-C8	-12.55	97.62	103.90
1	A	266	G	N7-C8-N9	12.52	119.36	113.10
1	A	117	G	N9-C4-C5	-12.37	100.45	105.40
1	A	572	A	N1-C6-N6	-12.36	111.18	118.60
1	A	232	G	N9-C4-C5	-12.22	100.51	105.40
1	A	481	G	N3-C4-N9	12.10	133.26	126.00
1	A	573	A	C8-N9-C4	-12.06	100.97	105.80
1	A	599	C	C6-N1-C2	12.02	125.11	120.30
1	A	277	C	C6-N1-C2	11.80	125.02	120.30
1	A	858	G	C4-C5-N7	11.62	115.45	110.80
1	A	858	G	C6-C5-N7	-11.60	123.44	130.40
1	A	858	G	C5-N7-C8	-11.56	98.52	104.30
1	A	279	A	C5-C6-N1	-11.47	111.97	117.70
1	A	238	G	C5-C6-N1	-11.46	105.77	111.50
1	A	1531	A	N1-C6-N6	11.46	125.47	118.60
1	A	722	A	C2-N3-C4	-11.42	104.89	110.60
1	A	117	G	C4-C5-N7	11.40	115.36	110.80
1	A	80	G	N3-C4-C5	-11.37	122.91	128.60
1	A	858	G	N7-C8-N9	11.36	118.78	113.10
1	A	1080	A	N1-C6-N6	-11.33	111.80	118.60
1	A	1200	C	N1-C2-O2	11.25	125.65	118.90
1	A	117	G	C5-C6-O6	-11.22	121.87	128.60
1	A	80	G	C8-N9-C4	-11.22	101.91	106.40
1	A	331	G	N1-C6-O6	11.20	126.62	119.90
1	A	117	G	C4-C5-C6	11.20	125.52	118.80
1	A	279	A	C6-C5-N7	-11.06	124.56	132.30
1	A	1370	G	C8-N9-C4	-11.04	101.99	106.40
1	A	1505	G	C8-N9-C4	-11.03	101.99	106.40
1	A	107	G	C5-C6-O6	-10.95	122.03	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	289	G	N1-C6-O6	10.85	126.41	119.90
1	A	1502	A	C4-C5-N7	10.69	116.04	110.70
1	A	107	G	N1-C6-O6	10.67	126.30	119.90
1	A	107	G	C6-C5-N7	-10.67	124.00	130.40
1	A	1369	C	C6-N1-C2	-10.66	116.04	120.30
1	A	881	G	N1-C6-O6	10.64	126.28	119.90
1	A	852	G	C2-N3-C4	-10.57	106.61	111.90
1	A	858	G	C2-N3-C4	-10.36	106.72	111.90
1	A	279	A	C8-N9-C4	-10.22	101.71	105.80
1	A	79	G	C2-N3-C4	10.17	116.98	111.90
1	A	366	C	N1-C2-O2	10.16	125.00	118.90
1	A	1200	C	C6-N1-C1'	-10.16	108.61	120.80
1	A	579	G	C6-C5-N7	-10.15	124.31	130.40
1	A	774	G	N1-C6-O6	10.12	125.97	119.90
1	A	635	G	N1-C6-O6	10.06	125.93	119.90
1	A	873	A	C8-N9-C4	-10.04	101.79	105.80
1	A	635	G	C5-C6-N1	-10.01	106.49	111.50
1	A	858	G	N3-C2-N2	-9.90	112.97	119.90
1	A	624	C	C6-N1-C2	9.89	124.26	120.30
1	A	964	A	C8-N9-C4	-9.88	101.85	105.80
1	A	572	A	N9-C4-C5	9.86	109.74	105.80
1	A	279	A	C4-C5-N7	9.81	115.61	110.70
1	A	851	G	C6-C5-N7	-9.75	124.55	130.40
1	A	190(G)	G	N1-C6-O6	9.70	125.72	119.90
1	A	117	G	C8-N9-C1'	-9.67	114.43	127.00
1	A	774	G	C4-C5-N7	9.65	114.66	110.80
1	A	232	G	C6-C5-N7	-9.62	124.63	130.40
1	A	851	G	C4-N9-C1'	9.62	139.01	126.50
1	A	15	G	N1-C6-O6	9.62	125.67	119.90
1	A	266	G	C5-C6-O6	-9.59	122.85	128.60
1	A	1502	A	N7-C8-N9	9.56	118.58	113.80
1	A	859	A	N1-C2-N3	9.52	134.06	129.30
1	A	1490	C	C5-C6-N1	9.46	125.73	121.00
1	A	773	G	C5-C6-O6	-9.45	122.93	128.60
1	A	856	C	N3-C4-C5	-9.40	118.14	121.90
1	A	281	G	N1-C6-O6	9.39	125.54	119.90
1	A	1490	C	C4-C5-C6	-9.37	112.71	117.40
1	A	730	G	C4-C5-N7	-9.33	107.07	110.80
1	A	481	G	C8-N9-C4	9.33	110.13	106.40
1	A	295	C	C6-N1-C2	9.32	124.03	120.30
1	A	945	G	C5-C6-O6	-9.31	123.01	128.60
1	A	573	A	N9-C4-C5	9.30	109.52	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	946	A	C6-N1-C2	-9.30	113.02	118.60
1	A	568	G	N1-C6-O6	-9.29	114.33	119.90
1	A	1347	G	C8-N9-C4	9.28	110.11	106.40
1	A	283	C	C6-N1-C2	-9.28	116.59	120.30
1	A	573	A	C4-C5-C6	9.28	121.64	117.00
1	A	825	G	C8-N9-C4	9.27	110.11	106.40
1	A	858	G	C8-N9-C4	-9.24	102.70	106.40
1	A	107	G	N9-C4-C5	-9.23	101.71	105.40
1	A	753	A	N1-C2-N3	9.22	133.91	129.30
1	A	1502	A	C6-C5-N7	-9.21	125.85	132.30
1	A	481	G	N9-C4-C5	-9.20	101.72	105.40
1	A	945	G	C4-C5-N7	9.16	114.46	110.80
1	A	1200	C	C5-C6-N1	9.16	125.58	121.00
1	A	20	U	C5-C6-N1	-9.15	118.12	122.70
1	A	481	G	C5-C6-O6	-9.14	123.11	128.60
1	A	1377	A	N1-C6-N6	-9.13	113.12	118.60
1	A	232	G	C4-C5-N7	9.11	114.44	110.80
1	A	1502	A	N1-C6-N6	9.11	124.06	118.60
1	A	29	G	C2-N3-C4	-9.10	107.35	111.90
1	A	76	C	N1-C2-O2	-9.04	113.47	118.90
1	A	122	G	N1-C6-O6	9.04	125.33	119.90
1	A	1370	G	N7-C8-N9	9.04	117.62	113.10
1	A	660	G	N1-C6-O6	9.03	125.32	119.90
1	A	283	C	C5-C6-N1	9.03	125.51	121.00
17	Q	98	LEU	CA-CB-CG	9.03	136.06	115.30
1	A	579	G	C5-C6-N1	-9.00	107.00	111.50
1	A	654	G	C2-N3-C4	-8.98	107.41	111.90
1	A	292	G	N1-C6-O6	8.97	125.28	119.90
1	A	789	U	N3-C4-C5	-8.96	109.22	114.60
1	A	936	C	C6-N1-C2	8.95	123.88	120.30
1	A	247	G	N1-C6-O6	8.94	125.26	119.90
1	A	328	C	N1-C2-O2	8.92	124.25	118.90
1	A	91	C	C6-N1-C2	8.91	123.86	120.30
1	A	1412	C	C6-N1-C2	-8.90	116.74	120.30
1	A	815	A	N7-C8-N9	-8.89	109.35	113.80
1	A	328	C	N3-C4-N4	-8.86	111.80	118.00
1	A	789	U	N1-C2-N3	8.85	120.21	114.90
1	A	836	G	N1-C6-O6	8.84	125.20	119.90
1	A	774	G	C5-C6-O6	-8.82	123.31	128.60
1	A	835	U	C4-C5-C6	8.80	124.98	119.70
1	A	1339	A	N1-C6-N6	-8.78	113.33	118.60
1	A	372	C	C6-N1-C2	8.77	123.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	922	G	N1-C6-O6	8.74	125.15	119.90
1	A	1181	G	N7-C8-N9	-8.72	108.74	113.10
1	A	825	G	C5-C6-O6	-8.71	123.37	128.60
1	A	309	G	C5-C6-O6	-8.70	123.38	128.60
1	A	482	A	N1-C6-N6	8.69	123.81	118.60
1	A	117	G	C4-N9-C1'	8.62	137.71	126.50
1	A	773	G	N1-C6-O6	8.58	125.05	119.90
1	A	256	U	C5-C4-O4	-8.56	120.76	125.90
1	A	815	A	C8-N9-C4	8.52	109.21	105.80
1	A	454	C	N1-C2-O2	8.52	124.01	118.90
1	A	509	A	C8-N9-C4	-8.52	102.39	105.80
1	A	1531	A	N7-C8-N9	8.51	118.05	113.80
1	A	482	A	N7-C8-N9	8.50	118.05	113.80
1	A	89	C	C6-N1-C2	-8.49	116.91	120.30
1	A	862	C	C5-C4-N4	-8.47	114.27	120.20
1	A	281	G	C8-N9-C1'	-8.45	116.01	127.00
1	A	79	G	N3-C4-C5	-8.45	124.38	128.60
1	A	1327	C	C5-C6-N1	-8.45	116.78	121.00
1	A	856	C	N1-C2-O2	-8.44	113.84	118.90
1	A	600	C	C5-C6-N1	-8.41	116.79	121.00
1	A	310	G	C5-C6-O6	-8.39	123.56	128.60
1	A	888	G	C5-C6-N1	-8.39	107.30	111.50
1	A	1317	C	C6-N1-C2	8.39	123.66	120.30
1	A	592	G	C5-C6-N1	-8.37	107.32	111.50
1	A	777	A	C8-N9-C4	-8.37	102.45	105.80
1	A	805	C	N3-C4-C5	8.36	125.24	121.90
1	A	284	G	N1-C6-O6	8.35	124.91	119.90
1	A	922	G	C4-N9-C1'	8.34	137.34	126.50
1	A	931	C	C5-C6-N1	-8.32	116.84	121.00
1	A	1327	C	C6-N1-C2	8.32	123.63	120.30
1	A	579	G	C5-C6-O6	-8.30	123.62	128.60
1	A	1350	A	C8-N9-C4	-8.29	102.48	105.80
1	A	144	G	N1-C6-O6	8.27	124.86	119.90
1	A	28	G	N1-C6-O6	8.24	124.84	119.90
1	A	143	A	C5-C6-N1	-8.23	113.58	117.70
1	A	922	G	C6-C5-N7	-8.20	125.48	130.40
1	A	920	U	C5-C4-O4	8.19	130.81	125.90
1	A	1531	A	C6-C5-N7	-8.18	126.57	132.30
1	A	835	U	C5-C4-O4	8.16	130.80	125.90
1	A	881	G	C8-N9-C4	8.16	109.67	106.40
1	A	851	G	C8-N9-C1'	-8.16	116.39	127.00
1	A	92	C	N1-C2-O2	8.15	123.79	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	628	G	N3-C4-C5	-8.14	124.53	128.60
1	A	529	G	N1-C6-O6	8.14	124.78	119.90
1	A	595	G	C5-N7-C8	8.13	108.36	104.30
1	A	830	G	C5-C6-N1	-8.12	107.44	111.50
1	A	774	G	C6-C5-N7	-8.12	125.53	130.40
1	A	703	G	C5-C6-O6	8.12	133.47	128.60
1	A	331	G	C6-C5-N7	-8.11	125.53	130.40
1	A	317	G	N1-C6-O6	8.08	124.75	119.90
1	A	277	C	C5-C6-N1	-8.08	116.96	121.00
1	A	328	C	N3-C4-C5	8.06	125.12	121.90
1	A	789	U	C5-C4-O4	8.06	130.74	125.90
1	A	833	U	C5-C4-O4	8.05	130.73	125.90
1	A	851	G	N1-C6-O6	8.03	124.72	119.90
1	A	128	G	N1-C6-O6	8.03	124.72	119.90
1	A	562	C	N1-C2-O2	8.01	123.71	118.90
1	A	1532	U	C4-C5-C6	-7.98	114.91	119.70
1	A	919	A	C8-N9-C4	7.97	108.99	105.80
1	A	651	C	N3-C2-O2	7.96	127.47	121.90
1	A	29	G	N1-C2-N3	7.95	128.67	123.90
1	A	735	C	C6-N1-C2	7.95	123.48	120.30
1	A	931	C	C2-N3-C4	-7.95	115.93	119.90
1	A	852	G	N1-C6-O6	7.93	124.66	119.90
4	D	12	CYS	CA-CB-SG	7.93	128.28	114.00
1	A	125	U	C5-C6-N1	-7.91	118.75	122.70
1	A	789	U	C6-N1-C2	-7.91	116.26	121.00
1	A	281	G	N9-C4-C5	-7.90	102.24	105.40
1	A	637	G	C8-N9-C4	7.90	109.56	106.40
1	A	285	G	N1-C2-N3	7.89	128.63	123.90
1	A	569	C	C5-C6-N1	-7.89	117.06	121.00
1	A	944	G	C8-N9-C4	-7.89	103.24	106.40
1	A	835	U	N3-C4-C5	-7.89	109.87	114.60
1	A	288	A	C8-N9-C4	7.87	108.95	105.80
1	A	935	A	N1-C6-N6	-7.87	113.88	118.60
1	A	1528	U	C5-C6-N1	-7.87	118.77	122.70
1	A	722	A	N1-C6-N6	7.86	123.32	118.60
1	A	1403	C	C2-N1-C1'	7.85	127.43	118.80
1	A	945	G	C5-N7-C8	-7.84	100.38	104.30
1	A	805	C	C6-N1-C2	7.81	123.42	120.30
1	A	285	G	C2-N3-C4	-7.80	108.00	111.90
1	A	736	C	N3-C2-O2	-7.80	116.44	121.90
1	A	922	G	C4-C5-C6	7.80	123.48	118.80
1	A	817	C	C5-C6-N1	-7.79	117.10	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	482	A	C6-C5-N7	-7.78	126.85	132.30
1	A	154	C	C5-C4-N4	-7.78	114.75	120.20
1	A	389	A	C4-C5-N7	-7.78	106.81	110.70
1	A	389	A	N1-C6-N6	-7.78	113.93	118.60
1	A	635	G	C2-N3-C4	-7.78	108.01	111.90
1	A	1306	A	N7-C8-N9	7.78	117.69	113.80
1	A	572	A	C5-C6-N1	7.77	121.58	117.70
1	A	176	C	C6-N1-C2	7.75	123.40	120.30
1	A	129	U	N3-C4-C5	-7.73	109.96	114.60
1	A	266	G	C8-N9-C4	-7.70	103.32	106.40
1	A	21	G	C5-C6-N1	-7.70	107.65	111.50
1	A	922	G	C5-C6-N1	-7.69	107.66	111.50
1	A	851	G	C4-C5-C6	7.68	123.41	118.80
1	A	647	C	C6-N1-C2	7.67	123.37	120.30
1	A	1511	G	N1-C6-O6	-7.67	115.30	119.90
1	A	817	C	C6-N1-C2	7.66	123.36	120.30
1	A	232	G	C5-C6-O6	-7.65	124.01	128.60
1	A	108	G	C8-N9-C4	-7.63	103.35	106.40
1	A	862	C	N3-C4-C5	7.63	124.95	121.90
1	A	730	G	N9-C4-C5	7.62	108.45	105.40
1	A	1528	U	C6-N1-C2	7.62	125.57	121.00
1	A	901	A	C2-N3-C4	-7.59	106.80	110.60
1	A	971	G	C8-N9-C4	7.59	109.44	106.40
1	A	753	A	N1-C6-N6	-7.58	114.05	118.60
1	A	970	C	N1-C2-O2	7.56	123.44	118.90
1	A	232	G	C6-N1-C2	7.56	129.64	125.10
1	A	89	C	C5-C6-N1	7.56	124.78	121.00
1	A	1530	G	N3-C4-C5	7.54	132.37	128.60
1	A	1080	A	N9-C4-C5	7.53	108.81	105.80
1	A	279	A	N3-C4-C5	7.53	132.07	126.80
1	A	573	A	N3-C4-C5	-7.53	121.53	126.80
1	A	328	C	N3-C2-O2	-7.53	116.63	121.90
1	A	389	A	C5-C6-N6	7.52	129.72	123.70
1	A	1490	C	N3-C4-C5	7.52	124.91	121.90
1	A	568	G	C5-C6-O6	7.50	133.10	128.60
1	A	858	G	N3-C4-C5	7.50	132.35	128.60
1	A	584	G	C5-C6-O6	-7.48	124.11	128.60
1	A	403	C	C4-C5-C6	7.48	121.14	117.40
1	A	279	A	N3-C4-N9	-7.47	121.42	127.40
1	A	1158	C	C6-N1-C2	-7.47	117.31	120.30
1	A	922	G	C8-N9-C1'	-7.47	117.29	127.00
1	A	318	G	N3-C2-N2	-7.46	114.67	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1350	A	N7-C8-N9	7.46	117.53	113.80
1	A	232	G	C5-C6-N1	-7.46	107.77	111.50
17	Q	84	LEU	CA-CB-CG	-7.46	98.15	115.30
1	A	1372	U	C5-C6-N1	7.46	126.43	122.70
1	A	108	G	N7-C8-N9	7.45	116.83	113.10
1	A	445	G	N1-C6-O6	7.45	124.37	119.90
1	A	108	G	C5-N7-C8	-7.45	100.58	104.30
1	A	870	U	N1-C2-N3	-7.44	110.44	114.90
1	A	1377	A	C5-C6-N6	7.43	129.65	123.70
1	A	382	A	C8-N9-C4	-7.43	102.83	105.80
1	A	9	G	N1-C6-O6	7.43	124.36	119.90
1	A	916	G	C6-N1-C2	-7.42	120.65	125.10
1	A	19	C	N3-C4-C5	7.42	124.87	121.90
1	A	241	C	C5-C6-N1	-7.42	117.29	121.00
1	A	1238	A	C8-N9-C4	-7.42	102.83	105.80
1	A	1377	A	C2-N3-C4	-7.41	106.89	110.60
1	A	78	G	N1-C6-O6	7.40	124.34	119.90
1	A	642	A	C6-N1-C2	-7.40	114.16	118.60
1	A	1338	G	N1-C6-O6	-7.39	115.47	119.90
1	A	122	G	C5-C6-N1	-7.38	107.81	111.50
1	A	886	G	N1-C6-O6	7.38	124.33	119.90
1	A	667	G	N1-C6-O6	7.37	124.32	119.90
1	A	481	G	N7-C8-N9	-7.37	109.42	113.10
1	A	1411	C	C6-N1-C2	-7.37	117.35	120.30
1	A	580	U	N3-C4-C5	-7.36	110.19	114.60
1	A	16	A	N7-C8-N9	-7.36	110.12	113.80
1	A	530	G	C4-N9-C1'	7.35	136.06	126.50
1	A	128	G	C5-C6-O6	-7.35	124.19	128.60
1	A	299	G	N1-C6-O6	7.34	124.31	119.90
1	A	389	A	N9-C4-C5	7.33	108.73	105.80
1	A	576	G	N3-C4-C5	-7.33	124.93	128.60
1	A	16	A	C8-N9-C4	7.33	108.73	105.80
1	A	481	G	C2-N3-C4	7.33	115.56	111.90
1	A	1505	G	N9-C4-C5	7.33	108.33	105.40
1	A	460	A	C8-N9-C4	-7.33	102.87	105.80
1	A	789	U	C4-C5-C6	7.32	124.09	119.70
1	A	266	G	C4-N9-C1'	7.32	136.01	126.50
1	A	447	G	C5-C6-O6	7.31	132.98	128.60
1	A	1532	U	N3-C2-O2	7.30	127.31	122.20
1	A	1502	A	C2-N3-C4	-7.30	106.95	110.60
1	A	589	C	C5-C6-N1	-7.30	117.35	121.00
1	A	753	A	N9-C4-C5	7.29	108.72	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1365	G	C8-N9-C4	-7.29	103.48	106.40
1	A	676	A	C8-N9-C4	7.29	108.72	105.80
1	A	640	A	C6-N1-C2	-7.29	114.23	118.60
1	A	18	C	C6-N1-C2	7.29	123.22	120.30
1	A	730	G	N1-C6-O6	-7.29	115.53	119.90
1	A	753	A	C6-N1-C2	-7.28	114.23	118.60
1	A	769	G	C8-N9-C4	7.28	109.31	106.40
1	A	32	A	N1-C2-N3	7.28	132.94	129.30
1	A	127	G	N1-C6-O6	7.28	124.27	119.90
1	A	281	G	C6-C5-N7	-7.28	126.03	130.40
1	A	579	G	C2-N3-C4	-7.28	108.26	111.90
1	A	979	C	C6-N1-C2	-7.27	117.39	120.30
1	A	1287	A	C5-C6-N6	7.27	129.52	123.70
1	A	1377	A	N1-C2-N3	7.25	132.93	129.30
1	A	252	U	C5-C6-N1	-7.25	119.08	122.70
1	A	482	A	C4-C5-C6	7.25	120.62	117.00
1	A	76	C	C6-N1-C1'	7.25	129.50	120.80
1	A	1361(A)	C	C5-C6-N1	7.25	124.62	121.00
1	A	525	C	C6-N1-C2	7.25	123.20	120.30
1	A	308	C	N1-C2-O2	7.24	123.24	118.90
1	A	1350	A	C5-N7-C8	-7.23	100.28	103.90
1	A	76	C	C2-N1-C1'	-7.21	110.87	118.80
1	A	238	G	C2-N3-C4	-7.21	108.30	111.90
1	A	730	G	N1-C2-N3	7.21	128.22	123.90
1	A	723	U	C5-C6-N1	7.20	126.30	122.70
1	A	1478	C	C6-N1-C2	-7.19	117.42	120.30
1	A	777	A	N7-C8-N9	7.19	117.40	113.80
1	A	529	G	C5-C6-N1	-7.19	107.91	111.50
1	A	1531	A	C5-N7-C8	-7.17	100.31	103.90
1	A	481	G	N3-C4-C5	-7.16	125.02	128.60
1	A	552	U	N1-C2-N3	7.13	119.18	114.90
1	A	676	A	N7-C8-N9	-7.12	110.24	113.80
1	A	1347	G	N9-C4-C5	-7.12	102.55	105.40
1	A	1531	A	C4-C5-N7	7.12	114.26	110.70
1	A	190(G)	G	C6-C5-N7	-7.10	126.14	130.40
1	A	74	C	C6-N1-C2	-7.09	117.46	120.30
1	A	875	C	C2-N3-C4	-7.09	116.35	119.90
1	A	724	G	C5-C6-O6	-7.09	124.35	128.60
1	A	1461	G	C8-N9-C4	7.09	109.23	106.40
1	A	238	G	N1-C6-O6	7.09	124.15	119.90
1	A	487	A	C8-N9-C4	7.08	108.63	105.80
1	A	331	G	C5-C6-N1	-7.08	107.96	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1287	A	N1-C6-N6	-7.07	114.36	118.60
1	A	110	C	C6-N1-C2	7.07	123.13	120.30
1	A	239	U	N3-C4-C5	-7.07	110.36	114.60
5	E	41	VAL	CB-CA-C	-7.05	98.01	111.40
1	A	1295	G	C8-N9-C4	-7.03	103.59	106.40
1	A	852	G	C6-N1-C2	7.03	129.32	125.10
1	A	1080	A	C4-C5-N7	-7.03	107.19	110.70
1	A	820	U	N1-C2-O2	-7.02	117.88	122.80
1	A	875	C	N3-C4-C5	7.02	124.71	121.90
1	A	703	G	C4-C5-N7	-7.01	107.99	110.80
1	A	870	U	N1-C2-O2	7.01	127.71	122.80
1	A	569	C	C6-N1-C2	7.00	123.10	120.30
1	A	660	G	C5-C6-N1	-7.00	108.00	111.50
1	A	1505	G	N7-C8-N9	7.00	116.60	113.10
1	A	773	G	C4-C5-N7	7.00	113.60	110.80
1	A	318	G	N1-C6-O6	6.99	124.10	119.90
1	A	107	G	C5-N7-C8	-6.98	100.81	104.30
1	A	1390	U	N3-C4-C5	-6.98	110.41	114.60
1	A	1108	G	C8-N9-C4	-6.98	103.61	106.40
1	A	201	C	C6-N1-C2	-6.97	117.51	120.30
1	A	946	A	C5-C6-N1	6.96	121.18	117.70
1	A	912	C	N3-C4-N4	6.96	122.87	118.00
1	A	281	G	C5-C6-O6	-6.96	124.42	128.60
1	A	723	U	C2-N1-C1'	6.96	126.05	117.70
1	A	250	A	N1-C6-N6	6.96	122.77	118.60
1	A	558	G	N1-C6-O6	6.96	124.07	119.90
1	A	1403	C	C6-N1-C1'	-6.96	112.45	120.80
1	A	289	G	C5-C6-O6	-6.95	124.43	128.60
1	A	835	U	N3-C2-O2	-6.95	117.33	122.20
1	A	288	A	N3-C4-C5	6.95	131.66	126.80
1	A	723	U	N1-C2-O2	6.95	127.66	122.80
1	A	357	G	N1-C6-O6	6.94	124.06	119.90
1	A	596	C	C6-N1-C2	6.94	123.07	120.30
1	A	615	C	C6-N1-C2	-6.93	117.53	120.30
1	A	306	G	N3-C2-N2	-6.93	115.05	119.90
1	A	80	G	C4-N9-C1'	6.92	135.50	126.50
1	A	595	G	N3-C4-C5	-6.92	125.14	128.60
1	A	7	G	C4-C5-N7	-6.92	108.03	110.80
1	A	488	C	N3-C4-C5	6.91	124.67	121.90
1	A	29	G	C5-C6-N1	-6.91	108.05	111.50
1	A	722	A	C5-C6-N1	-6.91	114.25	117.70
1	A	481	G	C8-N9-C1'	-6.90	118.03	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	291	C	N3-C4-C5	6.89	124.66	121.90
1	A	482	A	C8-N9-C4	-6.89	103.04	105.80
1	A	326	G	C4-C5-N7	-6.87	108.05	110.80
1	A	281	G	C4-N9-C1'	6.86	135.41	126.50
1	A	558	G	C6-C5-N7	-6.86	126.29	130.40
1	A	570	G	C4-N9-C1'	6.85	135.40	126.50
1	A	373	A	N1-C2-N3	6.84	132.72	129.30
1	A	693	G	N1-C6-O6	6.84	124.00	119.90
1	A	400	C	N3-C4-N4	-6.83	113.22	118.00
1	A	1338	G	C5-C6-O6	6.83	132.70	128.60
1	A	774	G	C5-N7-C8	-6.83	100.89	104.30
1	A	1452	C	N1-C2-O2	6.82	122.99	118.90
1	A	599	C	N3-C2-O2	6.82	126.67	121.90
1	A	813	U	C5-C4-O4	-6.82	121.81	125.90
1	A	724	G	C4-C5-N7	6.82	113.53	110.80
1	A	147	G	N1-C6-O6	6.81	123.99	119.90
1	A	485	G	C4-C5-N7	-6.80	108.08	110.80
1	A	875	C	C5-C6-N1	-6.80	117.60	121.00
3	C	32	LEU	CA-CB-CG	6.80	130.93	115.30
1	A	873	A	C2-N3-C4	6.79	114.00	110.60
5	E	119	LEU	CA-CB-CG	-6.78	99.70	115.30
1	A	569	C	N3-C4-N4	-6.78	113.26	118.00
1	A	852	G	N3-C4-C5	6.78	131.99	128.60
1	A	783	C	N3-C4-C5	6.78	124.61	121.90
1	A	595	G	C4-C5-C6	6.77	122.86	118.80
1	A	126	G	C8-N9-C4	6.76	109.11	106.40
1	A	854	G	C6-C5-N7	-6.75	126.35	130.40
1	A	32	A	C4-C5-C6	6.75	120.38	117.00
1	A	389	A	N1-C2-N3	6.75	132.68	129.30
1	A	292	G	C6-C5-N7	-6.75	126.35	130.40
1	A	1441	G	C5-C6-N1	-6.74	108.13	111.50
1	A	1395	C	C6-N1-C2	6.74	123.00	120.30
1	A	242	C	C5-C6-N1	-6.74	117.63	121.00
1	A	573	A	C4-C5-N7	-6.73	107.33	110.70
1	A	881	G	C5-C6-O6	-6.72	124.57	128.60
1	A	1242	C	N3-C4-N4	-6.72	113.29	118.00
1	A	628	G	N3-C4-N9	6.72	130.03	126.00
1	A	779	C	N1-C2-O2	-6.71	114.87	118.90
1	A	769	G	N1-C6-O6	6.71	123.93	119.90
1	A	235	C	C6-N1-C2	6.71	122.98	120.30
1	A	715	A	C2-N3-C4	-6.70	107.25	110.60
1	A	1490	C	C5-C4-N4	-6.70	115.51	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	553	A	C8-N9-C4	6.70	108.48	105.80
1	A	881	G	C2-N3-C4	-6.70	108.55	111.90
1	A	1405	G	C8-N9-C4	6.70	109.08	106.40
1	A	648	A	C8-N9-C4	6.69	108.48	105.80
1	A	910	C	C6-N1-C2	6.69	122.97	120.30
1	A	1346	A	C5-C6-N1	6.69	121.04	117.70
1	A	756	C	C6-N1-C2	6.68	122.97	120.30
1	A	1413	A	N7-C8-N9	6.68	117.14	113.80
1	A	1508	G	N7-C8-N9	6.68	116.44	113.10
1	A	865	A	C6-N1-C2	-6.68	114.59	118.60
1	A	854	G	N1-C2-N3	6.67	127.90	123.90
1	A	964	A	N9-C4-C5	6.67	108.47	105.80
1	A	595	G	C4-C5-N7	-6.66	108.14	110.80
1	A	23	C	C5-C6-N1	-6.66	117.67	121.00
1	A	874	G	N1-C6-O6	6.65	123.89	119.90
1	A	835	U	N1-C2-N3	6.65	118.89	114.90
1	A	791	G	C4-C5-C6	6.65	122.79	118.80
1	A	644	G	C4-C5-N7	6.64	113.46	110.80
1	A	1543	C	N1-C2-O2	6.64	122.89	118.90
1	A	1347	G	N3-C4-N9	6.64	129.99	126.00
1	A	599	C	N3-C4-C5	6.64	124.56	121.90
1	A	730	G	C5-C6-O6	6.63	132.58	128.60
1	A	92	C	N3-C2-O2	-6.63	117.26	121.90
1	A	1299	A	C8-N9-C4	-6.63	103.15	105.80
1	A	788	U	N3-C4-O4	6.62	124.03	119.40
1	A	941	G	N1-C6-O6	6.61	123.86	119.90
1	A	856	C	C4-C5-C6	6.61	120.70	117.40
1	A	288	A	C2-N3-C4	-6.60	107.30	110.60
1	A	184	G	N1-C6-O6	6.59	123.85	119.90
1	A	1305	G	C4-C5-N7	-6.58	108.17	110.80
1	A	723	U	C6-N1-C2	-6.57	117.06	121.00
1	A	1080	A	C5-C6-N6	6.57	128.96	123.70
1	A	1346	A	P-O3'-C3'	6.57	127.59	119.70
1	A	117	G	N1-C2-N3	6.57	127.84	123.90
1	A	773	G	N9-C4-C5	-6.57	102.77	105.40
1	A	285	G	N1-C6-O6	6.57	123.84	119.90
1	A	1335	C	N1-C2-O2	6.57	122.84	118.90
1	A	1064	G	C2-N3-C4	-6.56	108.62	111.90
1	A	586	C	C6-N1-C2	6.56	122.92	120.30
1	A	574	A	N7-C8-N9	-6.56	110.52	113.80
1	A	40	C	C6-N1-C2	6.56	122.92	120.30
1	A	836	G	C8-N9-C4	6.55	109.02	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	865	A	C5-C6-N1	6.55	120.98	117.70
5	E	12	LEU	CA-CB-CG	6.55	130.37	115.30
1	A	825	G	N1-C6-O6	6.55	123.83	119.90
1	A	589	C	C2-N3-C4	-6.55	116.63	119.90
1	A	238	G	N3-C2-N2	-6.54	115.32	119.90
1	A	769	G	C5-C6-O6	-6.54	124.68	128.60
1	A	595	G	C8-N9-C1'	-6.53	118.51	127.00
1	A	830	G	C4-C5-N7	-6.53	108.19	110.80
1	A	1339	A	C2-N3-C4	6.53	113.87	110.60
1	A	147	G	C5-C6-N1	-6.53	108.23	111.50
6	F	98	LEU	CA-CB-CG	-6.53	100.28	115.30
1	A	814	A	C8-N9-C4	6.52	108.41	105.80
1	A	1228	C	N1-C2-O2	6.52	122.81	118.90
1	A	873	A	N7-C8-N9	6.51	117.06	113.80
1	A	1289	A	C8-N9-C4	-6.51	103.19	105.80
1	A	884	U	C5-C6-N1	-6.51	119.44	122.70
1	A	637	G	C8-N9-C1'	-6.51	118.54	127.00
1	A	734	G	N1-C6-O6	6.50	123.80	119.90
1	A	890	G	C4-C5-N7	-6.50	108.20	110.80
1	A	268	C	N3-C4-C5	-6.49	119.31	121.90
1	A	1305	G	N9-C4-C5	6.49	108.00	105.40
1	A	366	C	N3-C2-O2	-6.48	117.36	121.90
1	A	773	G	C6-C5-N7	-6.48	126.51	130.40
1	A	10	A	C2-N3-C4	-6.48	107.36	110.60
1	A	28	G	C5-C6-O6	-6.48	124.71	128.60
1	A	241	C	N1-C2-O2	-6.48	115.01	118.90
1	A	552	U	C2-N3-C4	-6.48	123.11	127.00
1	A	75	G	C8-N9-C4	6.47	108.99	106.40
1	A	1462	G	N1-C6-O6	6.47	123.78	119.90
1	A	269	C	N3-C2-O2	-6.46	117.38	121.90
1	A	1095	U	C6-N1-C2	6.46	124.87	121.00
1	A	836	G	C5-C6-N1	-6.46	108.27	111.50
1	A	574	A	C8-N9-C4	6.45	108.38	105.80
1	A	138	G	N7-C8-N9	-6.45	109.88	113.10
1	A	873	A	C5-C6-N1	6.45	120.92	117.70
1	A	839	U	N1-C2-O2	6.45	127.31	122.80
1	A	81	U	C6-N1-C2	-6.44	117.13	121.00
1	A	1526	G	N1-C6-O6	6.44	123.76	119.90
1	A	1317	C	N1-C2-O2	6.44	122.76	118.90
1	A	1190	G	P-O3'-C3'	6.43	127.42	119.70
1	A	123	C	N3-C4-C5	-6.43	119.33	121.90
1	A	295	C	C5-C6-N1	-6.43	117.78	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	948	C	C2-N1-C1'	-6.43	111.72	118.80
1	A	723	U	N3-C2-O2	-6.43	117.70	122.20
1	A	1497	G	C8-N9-C4	-6.42	103.83	106.40
1	A	877	C	N1-C2-O2	-6.41	115.05	118.90
1	A	58	C	C6-N1-C2	-6.41	117.73	120.30
1	A	713	G	C8-N9-C4	-6.41	103.84	106.40
1	A	734	G	C5-C6-O6	-6.40	124.76	128.60
1	A	32	A	C6-N1-C2	-6.40	114.76	118.60
1	A	269	C	C4-C5-C6	6.40	120.60	117.40
1	A	730	G	C6-N1-C2	-6.40	121.26	125.10
1	A	331	G	C4-C5-C6	6.39	122.64	118.80
1	A	850	U	C5-C4-O4	6.39	129.74	125.90
1	A	1107	C	C6-N1-C2	-6.39	117.74	120.30
1	A	1153	C	C6-N1-C2	6.39	122.86	120.30
1	A	654	G	N3-C4-C5	6.39	131.79	128.60
1	A	579	G	C4-C5-N7	6.39	113.35	110.80
1	A	154	C	N3-C4-C5	6.38	124.45	121.90
1	A	936	C	C5-C6-N1	-6.38	117.81	121.00
1	A	333	G	N1-C6-O6	6.38	123.73	119.90
1	A	867	G	N1-C6-O6	6.38	123.73	119.90
1	A	722	A	C6-C5-N7	-6.38	127.84	132.30
1	A	450	G	C4-C5-N7	-6.37	108.25	110.80
1	A	882	C	N1-C2-N3	6.37	123.66	119.20
1	A	541	G	N1-C6-O6	6.37	123.72	119.90
1	A	13	U	N3-C4-O4	6.36	123.85	119.40
1	A	138	G	C8-N9-C4	6.36	108.94	106.40
1	A	606	G	C4-C5-N7	-6.36	108.26	110.80
1	A	1413	A	C8-N9-C4	-6.36	103.26	105.80
1	A	767	A	C5-C6-N1	6.35	120.88	117.70
1	A	1361(A)	C	N1-C2-O2	6.35	122.71	118.90
1	A	922	G	N1-C2-N3	6.34	127.71	123.90
1	A	232	G	N3-C4-N9	6.34	129.80	126.00
1	A	600	C	C2-N3-C4	-6.34	116.73	119.90
1	A	1347	G	N7-C8-N9	-6.33	109.93	113.10
1	A	640	A	N1-C2-N3	6.33	132.47	129.30
1	A	1478	C	C5-C6-N1	6.33	124.17	121.00
1	A	447	G	C4-C5-N7	-6.33	108.27	110.80
1	A	1338	G	N1-C2-N3	6.33	127.70	123.90
1	A	403	C	C5-C6-N1	-6.32	117.84	121.00
1	A	913	A	N1-C6-N6	-6.32	114.81	118.60
1	A	1274	G	C8-N9-C4	-6.32	103.87	106.40
1	A	606	G	C5-C6-N1	-6.31	108.34	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1531	A	C5-C6-N1	-6.31	114.54	117.70
1	A	27	G	C5-C6-O6	-6.31	124.82	128.60
1	A	80	G	N3-C4-N9	6.31	129.78	126.00
1	A	660	G	C2-N3-C4	-6.30	108.75	111.90
1	A	400	C	N3-C4-C5	6.30	124.42	121.90
1	A	306	G	C8-N9-C4	6.29	108.92	106.40
1	A	481	G	C5-N7-C8	6.29	107.45	104.30
1	A	54	C	N3-C2-O2	-6.29	117.50	121.90
1	A	565	U	N3-C2-O2	6.29	126.60	122.20
1	A	450	G	C8-N9-C4	6.28	108.91	106.40
1	A	823	G	N1-C2-N3	6.28	127.67	123.90
1	A	400	C	C5-C6-N1	-6.28	117.86	121.00
1	A	1332	A	N1-C6-N6	-6.28	114.83	118.60
1	A	242	C	C6-N1-C2	6.28	122.81	120.30
1	A	712	A	C2-N3-C4	-6.27	107.46	110.60
1	A	331	G	N9-C4-C5	-6.26	102.89	105.40
1	A	1487	G	N1-C6-O6	-6.26	116.14	119.90
1	A	18	C	C5-C6-N1	-6.26	117.87	121.00
1	A	289	G	C6-C5-N7	-6.26	126.64	130.40
1	A	859	A	C6-N1-C2	-6.26	114.84	118.60
1	A	1392	G	C6-C5-N7	-6.26	126.64	130.40
1	A	1447	G	C4-C5-N7	6.26	113.30	110.80
1	A	117	G	C5-N7-C8	-6.25	101.17	104.30
1	A	331	G	C8-N9-C1'	-6.25	118.87	127.00
1	A	1181	G	N9-C4-C5	-6.25	102.90	105.40
1	A	526	C	C6-N1-C2	6.25	122.80	120.30
1	A	306	G	N1-C6-O6	6.25	123.65	119.90
1	A	276	G	C8-N9-C4	6.25	108.90	106.40
1	A	301	G	C8-N9-C4	-6.24	103.90	106.40
1	A	581	G	N3-C4-N9	-6.24	122.25	126.00
1	A	1082	G	N1-C6-O6	6.24	123.64	119.90
1	A	1375	A	N1-C6-N6	-6.24	114.86	118.60
1	A	815	A	C5-N7-C8	6.24	107.02	103.90
1	A	7	G	N9-C4-C5	6.23	107.89	105.40
1	A	190(C)	C	C6-N1-C2	-6.23	117.81	120.30
1	A	945	G	C5-C6-N1	6.23	114.61	111.50
1	A	1377	A	N9-C4-C5	6.23	108.29	105.80
1	A	795	C	C6-N1-C2	6.22	122.79	120.30
1	A	287	U	N3-C4-C5	-6.22	110.87	114.60
1	A	1524	C	C6-N1-C2	-6.22	117.81	120.30
1	A	80	G	N7-C8-N9	6.22	116.21	113.10
1	A	522	C	C6-N1-C2	6.22	122.79	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	92	C	C2-N1-C1'	6.21	125.64	118.80
1	A	817	C	C6-N1-C1'	-6.21	113.35	120.80
1	A	946	A	N1-C2-N3	6.21	132.40	129.30
1	A	851	G	N3-C4-N9	6.21	129.72	126.00
1	A	34	C	N3-C2-O2	6.20	126.24	121.90
1	A	964	A	N7-C8-N9	6.20	116.90	113.80
1	A	147	G	C2-N3-C4	-6.20	108.80	111.90
1	A	190(G)	G	C5-C6-N1	-6.19	108.40	111.50
1	A	1238	A	N9-C4-C5	6.19	108.28	105.80
1	A	1490	C	N1-C2-O2	6.19	122.61	118.90
1	A	860	A	N1-C2-N3	6.19	132.40	129.30
1	A	1377	A	N3-C4-N9	-6.18	122.45	127.40
1	A	1433	A	N1-C6-N6	-6.18	114.89	118.60
1	A	36	C	C6-N1-C2	-6.18	117.83	120.30
1	A	971	G	N1-C6-O6	6.18	123.61	119.90
1	A	1413	A	C5-N7-C8	-6.18	100.81	103.90
1	A	307	C	C5-C6-N1	6.18	124.09	121.00
1	A	1126	U	C5-C6-N1	6.18	125.79	122.70
1	A	9	G	C5-C6-O6	-6.17	124.90	128.60
1	A	238	G	C4-C5-C6	6.17	122.50	118.80
1	A	721	G	C4-N9-C1'	6.17	134.53	126.50
1	A	32	A	C6-C5-N7	-6.17	127.98	132.30
1	A	250	A	C2-N3-C4	-6.17	107.51	110.60
1	A	912	C	C5-C4-N4	-6.17	115.88	120.20
1	A	876	G	C5-C6-O6	-6.17	124.90	128.60
1	A	328	C	C4-C5-C6	-6.16	114.32	117.40
1	A	623	C	N3-C4-C5	6.16	124.36	121.90
1	A	1230	C	C5-C6-N1	6.16	124.08	121.00
1	A	796	C	C5-C6-N1	-6.16	117.92	121.00
1	A	565	U	C5-C4-O4	-6.15	122.21	125.90
1	A	595	G	N3-C4-N9	6.15	129.69	126.00
1	A	24	U	C6-N1-C2	6.15	124.69	121.00
1	A	1079	G	C8-N9-C4	-6.15	103.94	106.40
1	A	948	C	N3-C4-C5	6.15	124.36	121.90
1	A	710	G	N1-C6-O6	6.14	123.59	119.90
1	A	1058	G	C5-C6-O6	6.14	132.28	128.60
1	A	252	U	N1-C2-N3	6.13	118.58	114.90
1	A	942	G	C6-C5-N7	-6.13	126.72	130.40
1	A	247	G	N3-C4-C5	6.13	131.66	128.60
1	A	252	U	C4-C5-C6	6.13	123.38	119.70
1	A	232	G	C8-N9-C4	6.12	108.85	106.40
1	A	621	A	C5-N7-C8	-6.12	100.84	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	869	G	N3-C4-C5	6.12	131.66	128.60
1	A	1386	G	N7-C8-N9	-6.12	110.04	113.10
1	A	1240	U	C5-C4-O4	6.11	129.57	125.90
1	A	1200	C	N3-C2-O2	-6.11	117.63	121.90
1	A	661	G	C5-C6-N1	-6.10	108.45	111.50
1	A	694	A	N1-C6-N6	6.10	122.26	118.60
1	A	227	G	N1-C6-O6	6.10	123.56	119.90
1	A	722	A	N1-C2-N3	6.10	132.35	129.30
1	A	128	G	C6-C5-N7	-6.10	126.74	130.40
1	A	523	A	C2-N3-C4	-6.10	107.55	110.60
1	A	1512	U	N3-C4-C5	-6.09	110.94	114.60
1	A	687	A	P-O3'-C3'	6.09	127.01	119.70
1	A	928	G	N1-C6-O6	6.09	123.55	119.90
1	A	1530	G	C8-N9-C4	6.09	108.83	106.40
1	A	289	G	N3-C2-N2	-6.08	115.64	119.90
1	A	190(I)	G	C8-N9-C4	6.08	108.83	106.40
1	A	126	G	C5-C6-N1	-6.08	108.46	111.50
1	A	309	G	C4-C5-N7	6.08	113.23	110.80
1	A	1107	C	N3-C4-C5	-6.08	119.47	121.90
1	A	130	A	C2-N3-C4	-6.07	107.56	110.60
1	A	816	A	C2-N3-C4	-6.07	107.56	110.60
1	A	1307	U	N3-C2-O2	-6.07	117.95	122.20
1	A	1442	G	N3-C4-N9	6.07	129.64	126.00
1	A	281	G	P-O3'-C3'	6.07	126.98	119.70
1	A	456	C	N1-C2-O2	6.07	122.54	118.90
1	A	558	G	C5-C6-O6	-6.07	124.96	128.60
1	A	660	G	C6-C5-N7	-6.07	126.76	130.40
1	A	128	G	C4-C5-N7	6.06	113.23	110.80
1	A	1508	G	C8-N9-C4	-6.06	103.97	106.40
1	A	168	G	C6-C5-N7	-6.06	126.76	130.40
1	A	1299	A	N7-C8-N9	6.06	116.83	113.80
1	A	79	G	C8-N9-C4	-6.06	103.98	106.40
1	A	661	G	C8-N9-C4	-6.06	103.98	106.40
1	A	715	A	C8-N9-C4	6.06	108.22	105.80
1	A	250	A	C5-C6-N1	-6.05	114.67	117.70
1	A	265	G	C2-N3-C4	-6.05	108.87	111.90
1	A	854	G	C4-C5-C6	6.05	122.43	118.80
1	A	901	A	C5-C6-N6	6.05	128.54	123.70
1	A	1490	C	C2-N1-C1'	6.05	125.46	118.80
1	A	353	A	N1-C6-N6	-6.05	114.97	118.60
1	A	190(B)	C	C5-C6-N1	6.04	124.02	121.00
1	A	1376	U	C5-C6-N1	-6.04	119.68	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	828	A	N1-C6-N6	6.04	122.22	118.60
1	A	1099	G	N1-C6-O6	6.04	123.52	119.90
1	A	656	C	N3-C4-C5	6.04	124.31	121.90
1	A	817	C	C4-C5-C6	6.04	120.42	117.40
1	A	1346	A	C6-N1-C2	-6.03	114.98	118.60
1	A	944	G	C5-C6-O6	6.03	132.22	128.60
1	A	392	G	C6-C5-N7	-6.02	126.79	130.40
1	A	1336	C	N1-C2-O2	6.02	122.51	118.90
1	A	179	A	N1-C6-N6	6.02	122.21	118.60
1	A	232	G	C8-N9-C1'	-6.02	119.18	127.00
1	A	1327	C	C2-N1-C1'	-6.02	112.18	118.80
1	A	1353	G	C5-C6-N1	6.02	114.51	111.50
1	A	1178	G	N9-C4-C5	6.01	107.80	105.40
1	A	795	C	N3-C2-O2	6.01	126.11	121.90
1	A	888	G	N3-C2-N2	-6.00	115.70	119.90
1	A	1301	U	P-O3'-C3'	6.00	126.91	119.70
1	A	529	G	C4-C5-C6	6.00	122.40	118.80
1	A	786	G	N1-C6-O6	6.00	123.50	119.90
1	A	1421	G	C8-N9-C4	-6.00	104.00	106.40
1	A	132	C	C4-C5-C6	5.99	120.40	117.40
1	A	375	U	N1-C2-N3	5.99	118.50	114.90
3	C	47	LEU	CA-CB-CG	5.99	129.08	115.30
1	A	20	U	C4-C5-C6	5.99	123.29	119.70
1	A	91	C	N3-C2-O2	5.99	126.09	121.90
1	A	117	G	N3-C4-N9	5.99	129.59	126.00
1	A	43	C	C6-N1-C2	5.99	122.69	120.30
1	A	157	G	C5-C6-N1	-5.98	108.51	111.50
1	A	241	C	C2-N3-C4	-5.98	116.91	119.90
1	A	661	G	N1-C6-O6	5.98	123.49	119.90
1	A	932	C	N3-C2-O2	-5.98	117.71	121.90
1	A	851	G	N7-C8-N9	5.98	116.09	113.10
1	A	1367	C	C6-N1-C2	-5.98	117.91	120.30
1	A	108	G	N3-C4-N9	-5.98	122.42	126.00
1	A	810	C	N3-C4-N4	5.98	122.18	118.00
1	A	854	G	C2-N3-C4	-5.98	108.91	111.90
1	A	292	G	C5-C6-O6	-5.97	125.02	128.60
1	A	680	C	C6-N1-C2	5.97	122.69	120.30
1	A	833	U	N3-C4-C5	-5.97	111.02	114.60
1	A	698	G	N3-C4-C5	-5.97	125.62	128.60
20	T	94	ALA	N-CA-C	-5.97	94.89	111.00
1	A	698	G	C4-N9-C1'	5.96	134.25	126.50
1	A	326	G	C5-C6-O6	5.96	132.18	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1376	U	C5-C4-O4	5.96	129.48	125.90
1	A	360	A	C5-N7-C8	-5.95	100.92	103.90
1	A	595	G	C4-N9-C1'	5.95	134.24	126.50
1	A	1416	G	C8-N9-C4	-5.95	104.02	106.40
1	A	722	A	N9-C4-C5	-5.95	103.42	105.80
1	A	62	U	N3-C4-C5	-5.95	111.03	114.60
1	A	1296	C	N3-C4-C5	-5.95	119.52	121.90
1	A	1374	A	N1-C2-N3	5.95	132.27	129.30
1	A	637	G	N9-C4-C5	-5.94	103.02	105.40
1	A	190(C)	C	N3-C4-C5	-5.94	119.52	121.90
1	A	654	G	C5-N7-C8	-5.94	101.33	104.30
1	A	893	C	C6-N1-C2	-5.94	117.92	120.30
1	A	80	G	C4-C5-C6	5.94	122.36	118.80
1	A	325	A	N9-C4-C5	5.93	108.17	105.80
1	A	559	A	C6-N1-C2	-5.93	115.04	118.60
1	A	863	U	C5-C4-O4	5.93	129.46	125.90
1	A	29	G	N1-C6-O6	5.93	123.46	119.90
1	A	509	A	N7-C8-N9	5.93	116.77	113.80
1	A	882	C	C4-C5-C6	5.93	120.37	117.40
1	A	774	G	N9-C4-C5	-5.93	103.03	105.40
1	A	1293	G	C8-N9-C4	-5.92	104.03	106.40
1	A	938	A	N1-C6-N6	-5.92	115.05	118.60
1	A	1353	G	N1-C6-O6	-5.92	116.35	119.90
1	A	605	U	N3-C4-C5	-5.92	111.05	114.60
1	A	658	G	C8-N9-C1'	-5.92	119.31	127.00
1	A	642	A	C5-C6-N1	5.91	120.66	117.70
1	A	644	G	C5-C6-O6	-5.91	125.05	128.60
1	A	802	A	C5-C6-N6	-5.91	118.97	123.70
1	A	345	C	C6-N1-C2	-5.91	117.94	120.30
1	A	17	U	C4-C5-C6	5.91	123.24	119.70
1	A	575	G	C6-N1-C2	-5.91	121.56	125.10
1	A	703	G	N9-C4-C5	5.91	107.76	105.40
1	A	66	G	N3-C2-N2	-5.90	115.77	119.90
1	A	924	C	N3-C2-O2	5.90	126.03	121.90
1	A	138	G	C5-N7-C8	5.90	107.25	104.30
1	A	306	G	C5-C6-N1	-5.89	108.55	111.50
1	A	570	G	N3-C4-C5	-5.89	125.65	128.60
1	A	579	G	C4-C5-C6	5.89	122.34	118.80
1	A	616	G	C5-C6-N1	-5.89	108.55	111.50
1	A	916	G	C5-C6-O6	-5.89	125.06	128.60
1	A	942	G	C4-N9-C1'	5.89	134.16	126.50
1	A	16	A	C2-N3-C4	-5.89	107.66	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	878	G	C5-C6-O6	-5.88	125.07	128.60
1	A	693	G	C6-C5-N7	-5.88	126.87	130.40
1	A	650	G	C8-N9-C4	5.88	108.75	106.40
1	A	897	C	N3-C2-O2	-5.88	117.79	121.90
1	A	1523	G	N3-C2-N2	-5.88	115.79	119.90
1	A	519	C	C6-N1-C2	5.88	122.65	120.30
3	C	101	LEU	CA-CB-CG	5.87	128.81	115.30
1	A	317	G	C6-C5-N7	-5.87	126.88	130.40
1	A	636	U	C4-C5-C6	5.87	123.22	119.70
1	A	677	U	C5-C6-N1	-5.87	119.77	122.70
1	A	1196	U	N3-C2-O2	-5.87	118.09	122.20
1	A	648	A	N7-C8-N9	-5.87	110.87	113.80
1	A	1376	U	N3-C2-O2	-5.86	118.10	122.20
1	A	603	U	C4-C5-C6	5.86	123.22	119.70
1	A	5	U	N1-C2-O2	5.86	126.90	122.80
1	A	1268	A	N9-C4-C5	5.86	108.14	105.80
1	A	867	G	C6-C5-N7	-5.86	126.89	130.40
1	A	771	G	C5-C6-O6	-5.86	125.09	128.60
1	A	1386	G	C8-N9-C4	5.85	108.74	106.40
1	A	439	A	C8-N9-C4	-5.85	103.46	105.80
1	A	877	C	N1-C2-N3	5.85	123.30	119.20
1	A	904	C	N3-C4-C5	5.85	124.24	121.90
1	A	70	G	N1-C6-O6	5.84	123.41	119.90
1	A	281	G	C4-C5-N7	5.84	113.14	110.80
1	A	285	G	C5-C6-N1	-5.84	108.58	111.50
1	A	283	C	C2-N1-C1'	5.84	125.22	118.80
1	A	1129	C	C6-N1-C2	-5.84	117.97	120.30
1	A	941	G	C2-N3-C4	-5.83	108.99	111.90
1	A	1532	U	C5-C6-N1	5.82	125.61	122.70
1	A	450	G	C5-N7-C8	5.82	107.21	104.30
1	A	1087	G	N1-C6-O6	5.82	123.39	119.90
1	A	15	G	C5-C6-N1	-5.82	108.59	111.50
1	A	279	A	N1-C2-N3	5.82	132.21	129.30
1	A	277	C	C2-N1-C1'	-5.81	112.40	118.80
1	A	107	G	N1-C2-N3	-5.81	120.41	123.90
1	A	1087	G	N3-C4-C5	5.81	131.51	128.60
1	A	1178	G	C8-N9-C4	-5.81	104.08	106.40
1	A	575	G	N1-C2-N3	5.80	127.38	123.90
1	A	1200	C	C6-N1-C2	-5.79	117.98	120.30
1	A	482	A	C5-N7-C8	-5.79	101.00	103.90
1	A	584	G	N1-C6-O6	5.79	123.37	119.90
1	A	530	G	C8-N9-C1'	-5.78	119.48	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	572	A	C6-N1-C2	-5.78	115.13	118.60
1	A	745	C	N3-C4-C5	5.78	124.21	121.90
1	A	1108	G	N3-C4-C5	-5.78	125.71	128.60
1	A	1240	U	C4-C5-C6	5.78	123.17	119.70
1	A	318	G	C5-C6-N1	-5.77	108.61	111.50
1	A	241	C	C4-C5-C6	5.77	120.28	117.40
1	A	1499	A	N7-C8-N9	-5.76	110.92	113.80
1	A	1524	C	N3-C4-C5	-5.76	119.60	121.90
1	A	573	A	C2-N3-C4	5.76	113.48	110.60
1	A	1414	U	N3-C2-O2	-5.76	118.17	122.20
1	A	380	G	C4-C5-N7	-5.76	108.50	110.80
1	A	599	C	N1-C2-N3	-5.76	115.17	119.20
1	A	1268	A	C8-N9-C4	-5.76	103.50	105.80
1	A	729	A	N1-C6-N6	5.75	122.05	118.60
1	A	603	U	N3-C4-C5	-5.75	111.15	114.60
1	A	1425	U	C5-C4-O4	5.75	129.35	125.90
1	A	1447	G	C5-N7-C8	-5.75	101.43	104.30
1	A	248	C	C4-C5-C6	5.75	120.27	117.40
1	A	1499	A	C8-N9-C4	5.75	108.10	105.80
1	A	450	G	N7-C8-N9	-5.74	110.23	113.10
1	A	1511	G	C5-C6-O6	5.74	132.05	128.60
1	A	804	U	N3-C2-O2	-5.74	118.18	122.20
1	A	445	G	C6-C5-N7	-5.74	126.96	130.40
1	A	877	C	C2-N3-C4	-5.74	117.03	119.90
1	A	524	G	C4-N9-C1'	5.73	133.95	126.50
1	A	600	C	C4-C5-C6	5.73	120.27	117.40
1	A	1343	G	N3-C2-N2	-5.73	115.89	119.90
1	A	840	C	N1-C2-O2	5.73	122.34	118.90
1	A	895	G	C4-C5-N7	5.73	113.09	110.80
1	A	306	G	N3-C4-C5	5.73	131.46	128.60
1	A	230	G	N1-C2-N3	5.72	127.33	123.90
1	A	460	A	N3-C4-C5	-5.72	122.79	126.80
1	A	1131	G	N1-C6-O6	5.72	123.33	119.90
1	A	1390	U	C4-C5-C6	5.72	123.14	119.70
1	A	34	C	C2-N1-C1'	-5.72	112.51	118.80
1	A	942	G	N1-C6-O6	5.72	123.33	119.90
1	A	825	G	N9-C4-C5	-5.72	103.11	105.40
1	A	283	C	C2-N3-C4	5.71	122.76	119.90
1	A	666	G	C5-C6-N1	-5.71	108.64	111.50
1	A	19	C	C2-N3-C4	-5.71	117.05	119.90
1	A	947	G	C8-N9-C4	5.71	108.68	106.40
1	A	1287	A	C4-C5-N7	-5.71	107.85	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	948	C	C5-C6-N1	-5.70	118.15	121.00
1	A	260	G	C6-C5-N7	-5.70	126.98	130.40
1	A	1277	C	C6-N1-C2	-5.70	118.02	120.30
1	A	758	G	C5-C6-O6	-5.70	125.18	128.60
1	A	854	G	C4-N9-C1'	5.69	133.90	126.50
1	A	798	G	N1-C2-N3	5.69	127.31	123.90
1	A	830	G	C4-C5-C6	5.69	122.21	118.80
1	A	854	G	C8-N9-C1'	-5.69	119.61	127.00
1	A	1370	G	N3-C4-C5	-5.69	125.76	128.60
1	A	586	C	C5-C6-N1	-5.68	118.16	121.00
1	A	111	G	N3-C4-N9	-5.68	122.59	126.00
1	A	325	A	N1-C6-N6	-5.68	115.19	118.60
1	A	1305	G	C8-N9-C4	-5.68	104.13	106.40
1	A	190(F)	G	N3-C4-C5	5.68	131.44	128.60
1	A	279	A	C4-C5-C6	5.68	119.84	117.00
1	A	1193	G	N1-C6-O6	5.68	123.31	119.90
1	A	1542	U	C6-N1-C2	5.68	124.41	121.00
1	A	129	U	C2-N3-C4	5.67	130.41	127.00
1	A	75	G	N7-C8-N9	-5.67	110.26	113.10
1	A	765	G	N1-C6-O6	5.67	123.30	119.90
1	A	881	G	N3-C2-N2	-5.67	115.93	119.90
1	A	851	G	N3-C4-C5	-5.67	125.76	128.60
1	A	767	A	C6-N1-C2	-5.67	115.20	118.60
1	A	970	C	N3-C2-O2	-5.67	117.93	121.90
1	A	673	G	N1-C6-O6	5.67	123.30	119.90
1	A	1058	G	C4-C5-N7	-5.67	108.53	110.80
1	A	1200	C	C5-C4-N4	-5.66	116.24	120.20
1	A	777	A	C5-N7-C8	-5.66	101.07	103.90
1	A	5	U	P-O3'-C3'	5.65	126.48	119.70
1	A	898	G	C8-N9-C4	5.65	108.66	106.40
1	A	916	G	N1-C2-N3	5.65	127.29	123.90
1	A	533	A	C8-N9-C4	-5.65	103.54	105.80
1	A	78	G	C6-N1-C2	5.65	128.49	125.10
1	A	661	G	N7-C8-N9	5.64	115.92	113.10
1	A	892	A	N1-C2-N3	5.64	132.12	129.30
1	A	1233	G	C2-N3-C4	-5.64	109.08	111.90
1	A	1483	A	C8-N9-C4	5.64	108.06	105.80
1	A	283	C	N3-C4-C5	-5.64	119.64	121.90
1	A	300	A	C8-N9-C4	-5.64	103.54	105.80
1	A	860	A	C8-N9-C4	-5.64	103.55	105.80
1	A	929	G	C2-N3-C4	-5.64	109.08	111.90
1	A	749	C	C5-C6-N1	5.64	123.82	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	92	C	C6-N1-C1'	-5.63	114.04	120.80
1	A	355	C	C6-N1-C2	-5.63	118.05	120.30
1	A	133	U	N3-C2-O2	-5.63	118.26	122.20
1	A	234	C	C5-C4-N4	-5.63	116.26	120.20
1	A	412	A	C8-N9-C4	5.63	108.05	105.80
1	A	1268	A	C6-N1-C2	-5.63	115.22	118.60
1	A	107	G	N3-C4-N9	5.62	129.37	126.00
1	A	667	G	C5-C6-O6	-5.62	125.23	128.60
1	A	881	G	N9-C4-C5	-5.62	103.15	105.40
1	A	1306	A	C8-N9-C4	-5.62	103.55	105.80
1	A	1334	G	C8-N9-C4	5.62	108.65	106.40
1	A	867	G	C4-C5-N7	5.62	113.05	110.80
1	A	1405	G	N3-C4-C5	5.62	131.41	128.60
1	A	75	G	C4-N9-C1'	-5.62	119.20	126.50
1	A	752	G	C5-C6-N1	-5.62	108.69	111.50
1	A	250	A	N9-C4-C5	-5.61	103.55	105.80
1	A	564	C	N1-C2-O2	5.61	122.27	118.90
1	A	816	A	N1-C2-N3	5.61	132.10	129.30
1	A	599	C	C5-C4-N4	-5.61	116.28	120.20
1	A	588	G	C2-N3-C4	-5.61	109.10	111.90
1	A	256	U	N1-C2-N3	-5.60	111.54	114.90
1	A	878	G	N1-C6-O6	5.60	123.26	119.90
1	A	628	G	C4-N9-C1'	5.60	133.78	126.50
1	A	724	G	N9-C4-C5	-5.60	103.16	105.40
1	A	1193	G	C5-C6-N1	-5.60	108.70	111.50
1	A	77	G	N9-C4-C5	-5.60	103.16	105.40
1	A	1067	A	C2-N3-C4	5.60	113.40	110.60
1	A	1523	G	N9-C4-C5	5.60	107.64	105.40
1	A	1060	C	C2-N1-C1'	5.59	124.95	118.80
1	A	655	A	C8-N9-C4	5.59	108.03	105.80
1	A	1242	C	C5-C4-N4	5.59	124.11	120.20
1	A	36	C	N3-C4-C5	-5.58	119.67	121.90
1	A	309	G	N1-C6-O6	5.58	123.25	119.90
1	A	1131	G	N7-C8-N9	5.58	115.89	113.10
1	A	1469	G	N7-C8-N9	5.58	115.89	113.10
1	A	1103	C	C5-C6-N1	-5.58	118.21	121.00
1	A	1502	A	C8-N9-C4	-5.58	103.57	105.80
1	A	982	U	C6-N1-C2	-5.58	117.65	121.00
1	A	1233	G	N9-C4-C5	-5.58	103.17	105.40
1	A	1084	G	N3-C4-C5	-5.58	125.81	128.60
1	A	855	G	N1-C6-O6	-5.57	116.56	119.90
1	A	858	G	N1-C2-N2	5.57	121.22	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	853	G	C6-C5-N7	-5.57	127.06	130.40
1	A	1112	C	C5-C6-N1	-5.57	118.21	121.00
1	A	630	G	C5-C6-N1	-5.57	108.72	111.50
1	A	1366	C	C6-N1-C2	-5.57	118.07	120.30
1	A	73	C	C6-N1-C2	-5.57	118.07	120.30
1	A	476	G	N1-C6-O6	5.57	123.24	119.90
1	A	909	A	C6-N1-C2	-5.57	115.26	118.60
1	A	1172	C	C2-N1-C1'	-5.56	112.69	118.80
1	A	12	U	N3-C4-O4	5.55	123.29	119.40
1	A	703	G	C8-N9-C4	-5.55	104.18	106.40
1	A	1233	G	C4-C5-N7	5.55	113.02	110.80
1	A	1532	U	N3-C4-C5	5.55	117.93	114.60
1	A	199	G	C2-N3-C4	-5.55	109.13	111.90
1	A	73	C	N1-C2-O2	-5.54	115.57	118.90
1	A	788	U	N3-C4-C5	-5.54	111.27	114.60
1	A	862	C	C6-N1-C2	5.54	122.52	120.30
1	A	140	A	C8-N9-C4	-5.54	103.58	105.80
1	A	438	G	C5-C6-O6	5.54	131.92	128.60
1	A	1442	G	C4-N9-C1'	5.54	133.70	126.50
1	A	819	A	C5-C6-N1	-5.54	114.93	117.70
1	A	75	G	N3-C4-C5	5.53	131.37	128.60
1	A	641	U	C2-N1-C1'	5.53	124.34	117.70
1	A	804	U	N1-C2-N3	5.53	118.22	114.90
1	A	183	G	C6-C5-N7	-5.52	127.08	130.40
1	A	204	U	C2-N1-C1'	5.52	124.33	117.70
1	A	688	G	N1-C6-O6	5.52	123.21	119.90
1	A	229	U	N3-C4-C5	-5.52	111.29	114.60
1	A	247	G	C5-C6-O6	-5.52	125.29	128.60
1	A	931	C	C4-C5-C6	5.52	120.16	117.40
1	A	366	C	C2-N1-C1'	5.52	124.87	118.80
1	A	1370	G	C4-N9-C1'	5.52	133.67	126.50
1	A	637	G	N3-C4-N9	5.51	129.31	126.00
1	A	1497	G	N3-C4-C5	-5.51	125.84	128.60
1	A	580	U	C4-C5-C6	5.51	123.01	119.70
1	A	9	G	C6-C5-N7	-5.50	127.10	130.40
1	A	1078	U	C6-N1-C2	-5.50	117.70	121.00
1	A	120	A	N1-C2-N3	5.50	132.05	129.30
1	A	1060	C	N1-C2-O2	5.50	122.20	118.90
1	A	1107	C	C5-C6-N1	5.50	123.75	121.00
1	A	1386	G	N3-C2-N2	-5.49	116.06	119.90
1	A	1373	G	N3-C4-N9	5.49	129.29	126.00
1	A	201	C	C2-N1-C1'	5.49	124.84	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	433	C	C6-N1-C2	-5.49	118.11	120.30
1	A	636	U	N3-C4-O4	5.49	123.24	119.40
1	A	530	G	C8-N9-C4	-5.49	104.21	106.40
1	A	1372	U	C6-N1-C2	-5.49	117.71	121.00
1	A	300	A	N9-C4-C5	5.48	107.99	105.80
1	A	823	G	C2-N3-C4	-5.48	109.16	111.90
1	A	481	G	N1-C6-O6	5.48	123.19	119.90
1	A	1335	C	N3-C2-O2	-5.48	118.06	121.90
1	A	1349	A	N1-C6-N6	-5.48	115.31	118.60
1	A	406	G	N1-C6-O6	5.48	123.19	119.90
1	A	971	G	C5-C6-N1	-5.48	108.76	111.50
1	A	392	G	C4-C5-C6	5.47	122.08	118.80
1	A	573	A	C5-N7-C8	5.47	106.64	103.90
1	A	625	G	N3-C4-C5	-5.47	125.86	128.60
1	A	365	U	C2-N1-C1'	5.47	124.27	117.70
1	A	835	U	C5-C6-N1	-5.47	119.96	122.70
1	A	485	G	C5-N7-C8	5.47	107.03	104.30
1	A	931	C	N1-C2-N3	5.47	123.03	119.20
1	A	664	G	C5-C6-O6	5.47	131.88	128.60
1	A	1395	C	N1-C2-O2	-5.47	115.62	118.90
1	A	1447	G	N1-C6-O6	5.46	123.18	119.90
1	A	779	C	C4-C5-C6	5.46	120.13	117.40
1	A	7	G	C2-N3-C4	5.45	114.63	111.90
1	A	918	A	C6-N1-C2	-5.45	115.33	118.60
1	A	588	G	C5-C6-N1	-5.45	108.77	111.50
1	A	864	A	C5-C6-N1	-5.45	114.97	117.70
1	A	530	G	N7-C8-N9	5.45	115.83	113.10
1	A	1452	C	N1-C2-N3	-5.45	115.39	119.20
1	A	256	U	N3-C4-O4	5.45	123.21	119.40
1	A	1328	C	N3-C4-C5	5.45	124.08	121.90
1	A	609	A	N1-C6-N6	5.44	121.87	118.60
1	A	1053	G	C8-N9-C4	5.44	108.58	106.40
1	A	301	G	N7-C8-N9	5.44	115.82	113.10
1	A	583	A	C5-C6-N6	-5.44	119.35	123.70
1	A	913	A	N9-C4-C5	5.43	107.97	105.80
1	A	860	A	C6-N1-C2	-5.43	115.34	118.60
1	A	1340	A	C2-N3-C4	-5.43	107.89	110.60
1	A	440	A	C8-N9-C4	-5.43	103.63	105.80
1	A	621	A	N7-C8-N9	5.43	116.51	113.80
1	A	944	G	N9-C4-C5	5.43	107.57	105.40
1	A	1530	G	C4-N9-C1'	-5.43	119.44	126.50
1	A	768	A	N1-C2-N3	5.42	132.01	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1361(A)	C	C5-C4-N4	-5.42	116.40	120.20
1	A	397	A	C6-N1-C2	-5.42	115.35	118.60
1	A	573	A	C5-C6-N6	5.42	128.04	123.70
1	A	890	G	C5-C6-N1	-5.42	108.79	111.50
1	A	1107	C	C2-N3-C4	5.42	122.61	119.90
1	A	204	U	C5-C6-N1	5.42	125.41	122.70
1	A	718	G	N1-C6-O6	5.42	123.15	119.90
1	A	169	C	N3-C4-C5	-5.41	119.73	121.90
1	A	190(G)	G	C2-N3-C4	-5.41	109.19	111.90
1	A	1442	G	C8-N9-C1'	-5.41	119.97	127.00
1	A	1469	G	C5-N7-C8	-5.41	101.59	104.30
1	A	269	C	C5-C6-N1	-5.41	118.30	121.00
1	A	310	G	N1-C6-O6	5.41	123.14	119.90
1	A	898	G	N7-C8-N9	-5.41	110.40	113.10
1	A	629	G	N3-C4-C5	-5.40	125.90	128.60
1	A	808	C	N3-C4-C5	5.40	124.06	121.90
1	A	124	G	N1-C6-O6	-5.40	116.66	119.90
1	A	247	G	C2-N3-C4	-5.40	109.20	111.90
1	A	881	G	N7-C8-N9	-5.40	110.40	113.10
1	A	142	G	N3-C4-C5	-5.40	125.90	128.60
1	A	1299	A	C4-N9-C1'	5.40	136.01	126.30
1	A	830	G	N9-C4-C5	5.39	107.56	105.40
1	A	892	A	C2-N3-C4	-5.39	107.90	110.60
1	A	78	G	C5-C6-N1	-5.39	108.81	111.50
1	A	1158	C	N3-C4-C5	-5.38	119.75	121.90
1	A	89	C	C2-N1-C1'	5.38	124.72	118.80
1	A	266	G	C4-C5-C6	5.38	122.03	118.80
1	A	266	G	C2-N3-C4	-5.38	109.21	111.90
1	A	852	G	N3-C4-N9	-5.38	122.78	126.00
1	A	1226	C	N1-C2-O2	5.38	122.12	118.90
1	A	853	G	C4-C5-C6	5.38	122.03	118.80
1	A	945	G	N7-C8-N9	5.38	115.79	113.10
1	A	14	U	N3-C4-O4	5.37	123.16	119.40
1	A	900	A	N1-C2-N3	5.37	131.99	129.30
1	A	1268	A	N1-C2-N3	5.37	131.99	129.30
1	A	285	G	N3-C2-N2	-5.37	116.14	119.90
1	A	1135	U	C2-N1-C1'	5.37	124.14	117.70
1	A	1336	C	C2-N1-C1'	5.37	124.70	118.80
1	A	1383	C	C6-N1-C2	-5.36	118.16	120.30
1	A	728	A	C5-C6-N6	-5.36	119.41	123.70
1	A	581	G	N3-C4-C5	5.36	131.28	128.60
1	A	556	C	N3-C4-C5	5.36	124.04	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1347	G	C5-C6-O6	-5.36	125.39	128.60
1	A	281	G	N3-C4-N9	5.36	129.21	126.00
1	A	18	C	C2-N3-C4	-5.36	117.22	119.90
1	A	326	G	N1-C6-O6	-5.36	116.69	119.90
1	A	882	C	C6-N1-C2	-5.36	118.16	120.30
1	A	55	A	C6-N1-C2	-5.35	115.39	118.60
1	A	721	G	C8-N9-C1'	-5.35	120.04	127.00
1	A	123	C	C6-N1-C2	-5.35	118.16	120.30
1	A	168	G	C4-N9-C1'	5.35	133.45	126.50
1	A	839	U	C2-N1-C1'	5.35	124.12	117.70
1	A	944	G	N1-C6-O6	-5.35	116.69	119.90
1	A	376	G	C5-N7-C8	5.35	106.97	104.30
1	A	1064	G	N1-C2-N3	5.35	127.11	123.90
1	A	664	G	C4-C5-N7	-5.34	108.66	110.80
1	A	552	U	C5-C6-N1	-5.34	120.03	122.70
1	A	1134	G	C8-N9-C4	-5.34	104.26	106.40
1	A	416	G	C6-C5-N7	-5.34	127.20	130.40
1	A	509	A	N3-C4-C5	-5.34	123.06	126.80
1	A	570	G	C8-N9-C4	-5.33	104.27	106.40
1	A	32	A	N3-C4-N9	5.33	131.67	127.40
1	A	588	G	N1-C2-N3	5.33	127.10	123.90
1	A	1306	A	C5-C6-N1	-5.33	115.03	117.70
1	A	1455	G	N1-C6-O6	5.33	123.10	119.90
15	O	23	GLY	N-CA-C	5.33	126.44	113.10
1	A	1078	U	C5-C6-N1	5.33	125.36	122.70
1	A	1392	G	C4-N9-C1'	5.33	133.43	126.50
1	A	623	C	C6-N1-C2	5.32	122.43	120.30
1	A	779	C	N1-C2-N3	5.32	122.93	119.20
1	A	871	U	N1-C2-N3	-5.32	111.71	114.90
1	A	375	U	C6-N1-C2	-5.32	117.81	121.00
1	A	1259	C	N1-C2-O2	5.32	122.09	118.90
1	A	1306	A	C5-N7-C8	-5.32	101.24	103.90
1	A	509	A	C6-N1-C2	-5.32	115.41	118.60
1	A	107	G	N3-C2-N2	5.32	123.62	119.90
1	A	331	G	C5-C6-O6	-5.32	125.41	128.60
1	A	703	G	N3-C4-C5	-5.32	125.94	128.60
1	A	982	U	N3-C2-O2	-5.32	118.48	122.20
1	A	697	U	N3-C4-O4	-5.32	115.68	119.40
1	A	893	C	N1-C2-O2	5.32	122.09	118.90
1	A	969	A	N1-C6-N6	5.32	121.79	118.60
1	A	1531	A	C8-N9-C4	-5.31	103.67	105.80
1	A	9	G	N9-C4-C5	-5.31	103.28	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	251	G	N7-C8-N9	5.31	115.76	113.10
1	A	901	A	N1-C2-N3	5.31	131.96	129.30
1	A	1399	C	N1-C2-O2	-5.31	115.71	118.90
1	A	878	G	C4-C5-N7	5.31	112.92	110.80
1	A	747	C	C2-N3-C4	-5.31	117.25	119.90
1	A	487	A	N7-C8-N9	-5.30	111.15	113.80
1	A	855	G	N7-C8-N9	-5.30	110.45	113.10
1	A	491	G	N1-C6-O6	5.30	123.08	119.90
1	A	742	G	C8-N9-C4	-5.30	104.28	106.40
1	A	894	G	C4-C5-N7	5.30	112.92	110.80
1	A	733	A	N1-C2-N3	5.30	131.95	129.30
1	A	636	U	N3-C4-C5	-5.30	111.42	114.60
1	A	1282	C	C6-N1-C2	-5.30	118.18	120.30
1	A	1452	C	C6-N1-C1'	-5.29	114.45	120.80
1	A	238	G	N1-C2-N3	5.29	127.08	123.90
1	A	871	U	N1-C2-O2	5.29	126.50	122.80
3	C	179	ARG	N-CA-C	-5.29	96.72	111.00
1	A	545	C	C6-N1-C2	-5.29	118.19	120.30
1	A	1293	G	C5-C6-N1	-5.29	108.86	111.50
1	A	1279	A	C4-C5-C6	5.29	119.64	117.00
1	A	335	C	N1-C2-O2	-5.28	115.73	118.90
1	A	753	A	C4-C5-N7	-5.28	108.06	110.70
1	A	776	G	N3-C4-C5	5.28	131.24	128.60
1	A	350	G	C5-N7-C8	-5.28	101.66	104.30
1	A	447	G	N1-C6-O6	-5.28	116.73	119.90
1	A	1305	G	C5-C6-N1	-5.28	108.86	111.50
1	A	1525	G	N1-C2-N3	5.28	127.07	123.90
1	A	688	G	C6-C5-N7	-5.28	127.23	130.40
1	A	307	C	N3-C4-N4	5.28	121.69	118.00
1	A	570	G	C8-N9-C1'	-5.28	120.14	127.00
1	A	975	A	C6-N1-C2	5.28	121.77	118.60
1	A	628	G	C4-C5-C6	5.27	121.97	118.80
1	A	705	U	N1-C2-N3	5.27	118.06	114.90
1	A	1417	G	N9-C4-C5	5.27	107.51	105.40
1	A	1125	U	C5-C4-O4	-5.27	122.74	125.90
1	A	894	G	C6-C5-N7	-5.27	127.24	130.40
1	A	1249	C	C6-N1-C2	-5.27	118.19	120.30
1	A	1532	U	N1-C2-N3	-5.27	111.74	114.90
1	A	32	A	N1-C6-N6	5.27	121.76	118.60
17	Q	99	SER	N-CA-C	5.27	125.22	111.00
1	A	899	C	C2-N1-C1'	5.26	124.59	118.80
1	A	825	G	N7-C8-N9	-5.26	110.47	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1333	A	C4-C5-C6	5.26	119.63	117.00
1	A	511	C	C5-C6-N1	-5.26	118.37	121.00
1	A	1531	A	N9-C4-C5	-5.25	103.70	105.80
1	A	667	G	C6-C5-N7	-5.25	127.25	130.40
1	A	1350	A	C4-C5-N7	5.25	113.33	110.70
1	A	1417	G	C8-N9-C4	-5.25	104.30	106.40
1	A	772	U	C5-C6-N1	-5.25	120.08	122.70
1	A	260	G	N1-C6-O6	5.25	123.05	119.90
1	A	1248	A	C2-N3-C4	5.25	113.22	110.60
1	A	247	G	C4-C5-N7	5.24	112.90	110.80
1	A	277	C	N3-C4-C5	5.24	124.00	121.90
1	A	324	G	N1-C6-O6	5.24	123.05	119.90
1	A	686	U	N3-C2-O2	-5.24	118.53	122.20
1	A	788	U	C2-N1-C1'	5.24	123.99	117.70
1	A	679	C	C6-N1-C2	5.24	122.40	120.30
1	A	860	A	N7-C8-N9	5.24	116.42	113.80
1	A	126	G	N9-C4-C5	-5.24	103.30	105.40
1	A	288	A	N3-C4-N9	-5.24	123.21	127.40
1	A	876	G	C8-N9-C4	5.24	108.50	106.40
1	A	575	G	C5-C6-O6	-5.23	125.46	128.60
1	A	1187	G	C8-N9-C4	-5.23	104.31	106.40
1	A	736	C	C2-N3-C4	-5.23	117.28	119.90
1	A	810	C	C5-C4-N4	-5.23	116.54	120.20
1	A	728	A	C5-N7-C8	-5.23	101.28	103.90
1	A	787	A	C5-N7-C8	-5.23	101.28	103.90
1	A	460	A	C2-N3-C4	5.22	113.21	110.60
1	A	251	G	C6-C5-N7	-5.22	127.27	130.40
1	A	290	C	C5-C4-N4	-5.22	116.54	120.20
1	A	778	G	N1-C2-N3	5.22	127.03	123.90
1	A	1362	C	C6-N1-C2	-5.22	118.21	120.30
1	A	878	G	C5-N7-C8	-5.22	101.69	104.30
1	A	1377	A	C4-C5-N7	-5.22	108.09	110.70
1	A	1508	G	C6-C5-N7	-5.22	127.27	130.40
1	A	248	C	N1-C2-O2	-5.21	115.77	118.90
1	A	635	G	N3-C2-N2	-5.21	116.25	119.90
1	A	169	C	C6-N1-C2	-5.21	118.22	120.30
1	A	860	A	C4-C5-C6	5.21	119.61	117.00
1	A	360	A	C2-N3-C4	-5.21	108.00	110.60
1	A	710	G	C5-C6-O6	-5.21	125.47	128.60
1	A	712	A	N1-C2-N3	5.21	131.91	129.30
1	A	1441	G	C5-C6-O6	5.21	131.73	128.60
1	A	1353	G	C8-N9-C4	-5.21	104.32	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	728	A	N1-C6-N6	5.21	121.72	118.60
1	A	1056	U	N3-C2-O2	5.21	125.84	122.20
1	A	686	U	N1-C2-N3	5.21	118.02	114.90
1	A	1125	U	N1-C2-N3	-5.21	111.78	114.90
1	A	864	A	C5-C6-N6	5.20	127.86	123.70
1	A	1394	A	C4-C5-N7	5.20	113.30	110.70
1	A	476	G	N9-C4-C5	-5.20	103.32	105.40
1	A	1052	U	C6-N1-C2	-5.20	117.88	121.00
1	A	408	A	C8-N9-C4	-5.20	103.72	105.80
1	A	640	A	C8-N9-C4	-5.20	103.72	105.80
1	A	384	G	N3-C4-N9	5.20	129.12	126.00
1	A	1215	G	C4-N9-C1'	5.20	133.25	126.50
1	A	1383	C	N3-C4-C5	-5.20	119.82	121.90
1	A	833	U	C4-C5-C6	5.19	122.81	119.70
1	A	1029	C	C6-N1-C2	-5.19	118.22	120.30
1	A	1387	G	N1-C2-N3	5.19	127.02	123.90
1	A	17	U	C5-C6-N1	-5.19	120.10	122.70
1	A	921	U	N3-C4-C5	-5.19	111.49	114.60
1	A	1300	G	P-O3'-C3'	5.19	125.92	119.70
1	A	229	U	N1-C2-N3	5.18	118.01	114.90
1	A	184	G	C5-C6-O6	-5.18	125.49	128.60
1	A	1156	G	C8-N9-C4	-5.18	104.33	106.40
4	D	198	VAL	CB-CA-C	-5.18	101.56	111.40
1	A	129	U	C5-C4-O4	5.18	129.01	125.90
1	A	144	G	N3-C4-C5	5.18	131.19	128.60
1	A	820	U	N1-C2-N3	5.18	118.01	114.90
1	A	19	C	C5-C4-N4	-5.17	116.58	120.20
1	A	93	G	C4-C5-N7	5.17	112.87	110.80
1	A	199	G	N1-C6-O6	5.17	123.00	119.90
1	A	876	G	C4-C5-N7	5.17	112.87	110.80
1	A	1051	C	C6-N1-C2	-5.17	118.23	120.30
1	A	808	C	C6-N1-C2	5.17	122.37	120.30
1	A	31	G	N9-C4-C5	-5.17	103.33	105.40
1	A	79	G	C4-C5-N7	-5.17	108.73	110.80
1	A	139	G	N1-C6-O6	5.17	123.00	119.90
1	A	670	G	N1-C6-O6	5.17	123.00	119.90
1	A	942	G	C8-N9-C1'	-5.17	120.29	127.00
1	A	1090	U	N3-C4-C5	-5.17	111.50	114.60
1	A	932	C	C2-N1-C1'	5.16	124.48	118.80
1	A	827	U	N1-C2-N3	5.16	118.00	114.90
1	A	1359	C	C6-N1-C2	-5.16	118.24	120.30
1	A	1239	A	C2-N3-C4	-5.16	108.02	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	193	C	C5-C6-N1	-5.16	118.42	121.00
1	A	363	A	C2-N3-C4	-5.16	108.02	110.60
1	A	874	G	C5-C6-O6	-5.16	125.51	128.60
1	A	852	G	C5-C6-O6	5.15	131.69	128.60
1	A	1390	U	C6-N1-C2	-5.15	117.91	121.00
1	A	32	A	C4-N9-C1'	5.15	135.57	126.30
1	A	579	G	C5-N7-C8	-5.15	101.72	104.30
1	A	1200	C	N3-C4-N4	5.15	121.61	118.00
1	A	1386	G	C4-C5-N7	-5.15	108.74	110.80
1	A	654	G	N1-C2-N3	5.15	126.99	123.90
1	A	1139	G	N9-C4-C5	5.15	107.46	105.40
1	A	309	G	N9-C4-C5	-5.15	103.34	105.40
1	A	1289	A	C2-N3-C4	5.15	113.17	110.60
1	A	1403	C	N3-C4-N4	5.15	121.60	118.00
1	A	1469	G	C4-C5-N7	5.15	112.86	110.80
1	A	264	U	N1-C2-N3	5.15	117.99	114.90
1	A	948	C	N3-C2-O2	5.15	125.50	121.90
1	A	315	A	N1-C2-N3	5.14	131.87	129.30
1	A	656	C	C2-N3-C4	-5.14	117.33	119.90
1	A	927	G	C5-C6-N1	-5.14	108.93	111.50
1	A	1084	G	C4-C5-N7	-5.14	108.74	110.80
1	A	372	C	C6-N1-C1'	-5.14	114.63	120.80
1	A	840	C	C2-N1-C1'	5.14	124.45	118.80
1	A	916	G	N3-C4-N9	5.14	129.08	126.00
1	A	365	U	C6-N1-C1'	-5.14	114.01	121.20
1	A	851	G	C8-N9-C4	-5.14	104.35	106.40
1	A	1370	G	C5-N7-C8	-5.14	101.73	104.30
1	A	697	U	C5-C4-O4	5.13	128.98	125.90
1	A	1353	G	N3-C4-C5	-5.13	126.03	128.60
1	A	245	C	N3-C4-C5	5.13	123.95	121.90
1	A	1373	G	N3-C4-C5	-5.13	126.03	128.60
1	A	932	C	C6-N1-C2	-5.13	118.25	120.30
1	A	747	C	C5-C6-N1	-5.13	118.44	121.00
1	A	912	C	N1-C2-O2	-5.13	115.82	118.90
1	A	872	A	C6-C5-N7	-5.13	128.71	132.30
1	A	906	G	N1-C6-O6	5.13	122.97	119.90
1	A	1139	G	C4-C5-N7	-5.13	108.75	110.80
1	A	686	U	C4-C5-C6	5.12	122.78	119.70
1	A	859	A	C8-N9-C4	-5.12	103.75	105.80
1	A	877	C	C4-C5-C6	5.12	119.96	117.40
1	A	881	G	C6-C5-N7	-5.12	127.33	130.40
1	A	121	C	C6-N1-C2	5.12	122.35	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	73	C	C5-C6-N1	5.12	123.56	121.00
1	A	814	A	N7-C8-N9	-5.12	111.24	113.80
1	A	110	C	N3-C2-O2	5.12	125.48	121.90
1	A	1491	G	N1-C6-O6	-5.12	116.83	119.90
1	A	126	G	C2-N3-C4	-5.12	109.34	111.90
1	A	1333	A	N1-C2-N3	5.12	131.86	129.30
1	A	127	G	C5-C6-O6	-5.12	125.53	128.60
1	A	948	C	N1-C2-N3	-5.12	115.62	119.20
1	A	1505	G	P-O3'-C3'	5.12	125.84	119.70
1	A	625	G	C5-C6-O6	-5.11	125.53	128.60
1	A	707	C	N3-C2-O2	5.11	125.48	121.90
1	A	791	G	C6-C5-N7	-5.11	127.33	130.40
1	A	635	G	N3-C4-C5	5.11	131.16	128.60
1	A	275	G	N1-C6-O6	5.11	122.97	119.90
1	A	666	G	N1-C6-O6	5.11	122.97	119.90
1	A	728	A	C4-C5-N7	5.11	113.25	110.70
1	A	1443	G	N3-C4-C5	5.11	131.15	128.60
1	A	1286	A	C8-N9-C4	-5.10	103.76	105.80
1	A	761	G	C2-N3-C4	-5.10	109.35	111.90
1	A	875	C	C6-N1-C2	5.10	122.34	120.30
1	A	74	C	C5-C6-N1	5.10	123.55	121.00
1	A	886	G	C5-C6-O6	-5.10	125.54	128.60
1	A	635	G	C6-C5-N7	-5.10	127.34	130.40
1	A	660	G	N9-C4-C5	-5.10	103.36	105.40
1	A	1477	C	C6-N1-C2	-5.10	118.26	120.30
1	A	230	G	N1-C2-N2	-5.09	111.61	116.20
1	A	1332	A	C5-C6-N6	5.09	127.78	123.70
1	A	103	C	C6-N1-C2	-5.09	118.26	120.30
1	A	784	C	N1-C2-N3	5.09	122.76	119.20
1	A	1190	G	C5-C6-N1	-5.09	108.95	111.50
1	A	143	A	N1-C6-N6	5.09	121.65	118.60
1	A	642	A	C8-N9-C4	-5.09	103.76	105.80
1	A	1287	A	N9-C4-C5	5.09	107.84	105.80
1	A	1383	C	N3-C4-N4	5.09	121.56	118.00
16	P	60	LEU	CA-CB-CG	-5.09	103.60	115.30
1	A	942	G	C5-C6-N1	-5.09	108.96	111.50
1	A	362	G	C5-C6-N1	-5.09	108.96	111.50
1	A	920	U	N3-C4-C5	-5.09	111.55	114.60
1	A	1339	A	N9-C4-C5	5.09	107.83	105.80
1	A	1342	C	N1-C2-O2	-5.09	115.85	118.90
1	A	229	U	C6-N1-C2	-5.08	117.95	121.00
1	A	1327	C	N3-C4-C5	5.08	123.93	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	23	C	C4-C5-C6	5.08	119.94	117.40
1	A	703	G	C4-C5-C6	5.08	121.85	118.80
1	A	719	C	C5-C6-N1	-5.08	118.46	121.00
1	A	840	C	C6-N1-C2	-5.08	118.27	120.30
1	A	1543	C	N1-C2-N3	-5.08	115.64	119.20
1	A	132	C	N1-C2-N3	5.08	122.75	119.20
1	A	529	G	C6-C5-N7	-5.08	127.35	130.40
1	A	668	G	C8-N9-C4	5.08	108.43	106.40
1	A	29	G	C4-C5-C6	5.08	121.85	118.80
1	A	32	A	C5-C6-N6	-5.08	119.64	123.70
1	A	916	G	C5-C6-N1	5.08	114.04	111.50
1	A	1295	G	N3-C4-N9	-5.08	122.95	126.00
1	A	292	G	C8-N9-C1'	-5.07	120.41	127.00
1	A	671	G	N1-C6-O6	5.07	122.94	119.90
1	A	477	G	N1-C6-O6	5.07	122.94	119.90
1	A	703	G	C5-N7-C8	5.07	106.83	104.30
1	A	906	G	C6-C5-N7	-5.07	127.36	130.40
1	A	745	C	C6-N1-C2	5.07	122.33	120.30
1	A	327	A	C5-C6-N1	5.07	120.23	117.70
1	A	935	A	C6-C5-N7	5.07	135.85	132.30
1	A	1403	C	C5-C4-N4	-5.07	116.65	120.20
1	A	522	C	C5-C6-N1	-5.07	118.47	121.00
1	A	856	C	N1-C2-N3	5.07	122.75	119.20
1	A	1412	C	C2-N1-C1'	5.07	124.37	118.80
1	A	356	A	N1-C6-N6	-5.06	115.57	118.60
1	A	1369	C	C5-C6-N1	5.06	123.53	121.00
1	A	201	C	N3-C2-O2	-5.06	118.36	121.90
1	A	589	C	C6-N1-C2	5.05	122.32	120.30
1	A	78	G	N3-C4-C5	5.05	131.13	128.60
1	A	869	G	C5-C6-N1	-5.05	108.97	111.50
1	A	500	G	N1-C6-O6	5.05	122.93	119.90
1	A	605	U	C4-C5-C6	5.05	122.73	119.70
1	A	707	C	N1-C2-O2	-5.05	115.87	118.90
1	A	894	G	C2-N3-C4	-5.05	109.38	111.90
1	A	1388	C	C6-N1-C2	5.05	122.32	120.30
15	O	24	SER	CB-CA-C	-5.05	100.50	110.10
1	A	768	A	C6-N1-C2	-5.05	115.57	118.60
1	A	1167	A	C8-N9-C4	-5.05	103.78	105.80
1	A	201	C	N1-C2-O2	5.05	121.93	118.90
1	A	353	A	N9-C4-C5	5.05	107.82	105.80
1	A	523	A	C8-N9-C4	5.05	107.82	105.80
1	A	381	C	N3-C4-C5	5.04	123.92	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	232	G	N1-C2-N3	-5.04	120.88	123.90
1	A	651	C	N1-C2-O2	-5.04	115.88	118.90
1	A	832	C	C5-C4-N4	-5.04	116.67	120.20
1	A	919	A	N7-C8-N9	-5.04	111.28	113.80
1	A	17	U	N3-C4-O4	5.04	122.93	119.40
1	A	920	U	C6-N1-C1'	5.04	128.26	121.20
1	A	333	G	C5-C6-N1	-5.04	108.98	111.50
1	A	366	C	C6-N1-C1'	-5.04	114.75	120.80
1	A	521	G	N1-C6-O6	-5.04	116.88	119.90
1	A	88	A	C2-N3-C4	5.04	113.12	110.60
1	A	639	G	N1-C2-N3	5.04	126.92	123.90
1	A	1059	C	C6-N1-C2	5.04	122.31	120.30
1	A	122	G	C6-C5-N7	-5.04	127.38	130.40
1	A	174	C	C5-C4-N4	-5.04	116.67	120.20
1	A	922	G	N3-C4-C5	-5.04	126.08	128.60
1	A	1338	G	N1-C2-N2	-5.03	111.67	116.20
1	A	1452	C	C2-N3-C4	5.03	122.42	119.90
1	A	1489	G	N1-C6-O6	-5.03	116.88	119.90
1	A	28	G	C6-C5-N7	-5.03	127.38	130.40
1	A	559	A	N3-C4-C5	-5.03	123.28	126.80
1	A	299	G	C6-C5-N7	-5.03	127.38	130.40
1	A	667	G	C8-N9-C1'	-5.03	120.47	127.00
1	A	1215	G	C8-N9-C4	-5.03	104.39	106.40
1	A	123	C	C4-C5-C6	5.03	119.91	117.40
1	A	1080	A	C6-C5-N7	5.03	135.82	132.30
1	A	1405	G	N7-C8-N9	-5.03	110.59	113.10
1	A	236	G	N3-C2-N2	5.02	123.42	119.90
1	A	237	C	N3-C4-C5	5.02	123.91	121.90
1	A	715	A	N3-C4-C5	5.02	130.32	126.80
1	A	1366	C	C5-C6-N1	5.02	123.51	121.00
1	A	1336	C	N3-C2-O2	-5.02	118.39	121.90
1	A	1412	C	N3-C2-O2	-5.02	118.39	121.90
1	A	300	A	N1-C2-N3	5.02	131.81	129.30
1	A	806	C	N3-C4-C5	5.02	123.91	121.90
1	A	791	G	C8-N9-C4	-5.02	104.39	106.40
1	A	1393	U	C5-C4-O4	-5.02	122.89	125.90
1	A	1462	G	C5-C6-O6	-5.02	125.59	128.60
1	A	234	C	N3-C4-C5	5.01	123.91	121.90
1	A	20	U	C2-N3-C4	-5.01	123.99	127.00
1	A	1441	G	N9-C4-C5	5.01	107.41	105.40
1	A	1524	C	C4-C5-C6	5.01	119.90	117.40
1	A	451	A	C4-C5-C6	-5.01	114.50	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	236	G	N1-C6-O6	-5.00	116.90	119.90
1	A	566	G	C8-N9-C4	-5.00	104.40	106.40
1	A	852	G	C4-C5-C6	5.00	121.80	118.80

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	166	GLU	Peptide
3	C	179	ARG	Peptide
8	H	27	PRO	Peptide
8	H	90	GLY	Peptide
17	Q	13	ASP	Peptide
20	T	11	SER	Peptide
20	T	93	GLU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32644	0	16505	666	0
2	B	1900	0	1951	78	0
3	C	1612	0	1677	80	0
4	D	1703	0	1763	72	0
5	E	1146	0	1207	47	0
6	F	843	0	857	27	0
7	G	1257	0	1296	51	0
8	H	1116	0	1177	54	0
9	I	1010	0	1037	75	0
10	J	792	0	835	44	0
11	K	864	0	881	37	0
12	L	972	0	1058	59	0
13	M	937	0	995	50	0
14	N	492	0	529	35	0
15	O	729	0	768	38	0
16	P	700	0	720	25	0
17	Q	823	0	893	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	R	574	0	644	27	0
19	S	647	0	673	24	0
20	T	763	0	861	33	0
21	U	208	0	221	14	0
22	A	239	0	0	0	0
22	B	2	0	0	0	0
22	C	3	0	0	0	0
22	D	4	0	0	0	0
22	E	1	0	0	0	0
22	F	1	0	0	0	0
22	L	1	0	0	0	0
22	P	2	0	0	0	0
22	Q	1	0	0	0	0
23	D	1	0	0	0	0
23	N	1	0	0	0	0
24	A	232	0	0	12	0
24	E	3	0	0	0	0
24	L	1	0	0	0	0
24	Q	1	0	0	0	0
24	T	2	0	0	0	0
All	All	52227	0	36548	1427	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 16.

All (1427) 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:1195:C:H3'	1:A:1196:U:H5"	1.46	0.95
20:T:100:ILE:HG22	20:T:102:GLY:H	1.32	0.90
12:L:41:ARG:HH21	12:L:43:VAL:HG13	1.36	0.90
1:A:103:C:OP1	20:T:17:ARG:NH1	2.03	0.90
1:A:279:A:OP2	17:Q:95:TYR:OH	1.90	0.88
3:C:137:ALA:HA	3:C:140:ARG:HD2	1.55	0.87
1:A:1060:C:OP1	14:N:45:ARG:NH2	2.07	0.87
2:B:114:ARG:HH11	2:B:118:LEU:HD21	1.41	0.85
1:A:992:U:H3	1:A:1044:A:H62	1.25	0.85
1:A:664:G:H22	1:A:741:G:H1	1.23	0.84
12:L:27:LEU:O	12:L:29:GLY:N	2.10	0.83
1:A:144:G:H1	1:A:178:C:H42	1.25	0.83
8:H:83:ILE:HG12	8:H:137:VAL:HG22	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:G:HO2'	1:A:482:A:H8	1.27	0.82
1:A:1417:G:O2'	1:A:1483:A:N6	2.13	0.82
17:Q:81:ARG:HE	17:Q:84:LEU:HD12	1.45	0.81
1:A:1497:G:H2'	1:A:1498:UR3:H5'	1.61	0.81
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.64	0.80
3:C:6:HIS:HD2	3:C:9:GLY:H	1.27	0.80
8:H:4:ASP:OD2	8:H:85:ARG:NH1	2.15	0.79
1:A:1347:G:H1'	1:A:1348:U:H5	1.48	0.79
1:A:1368:G:H5"	9:I:112:LYS:HB3	1.64	0.79
17:Q:66:SER:O	17:Q:70:ARG:NH1	2.16	0.79
9:I:25:LYS:NZ	9:I:60:ASP:OD2	2.15	0.78
1:A:1316:G:N2	1:A:1319:A:OP2	2.16	0.78
1:A:1406:U:O2'	1:A:1517[B]:G:N2	2.16	0.78
10:J:47:PHE:HB3	14:N:34:TYR:HE2	1.49	0.77
1:A:1111:A:H61	3:C:177:THR:HB	1.49	0.77
5:E:11:ILE:HB	5:E:31:LEU:HB3	1.65	0.77
1:A:1356:G:H2'	1:A:1357:A:C8	2.20	0.77
15:O:33:THR:OG1	15:O:63:ARG:NH1	2.18	0.77
1:A:1240:U:OP1	7:G:119:ARG:NH2	2.17	0.77
3:C:156:ARG:NH1	3:C:193:TYR:O	2.17	0.77
4:D:11:LEU:HD13	4:D:66:ARG:HD2	1.67	0.76
20:T:56:MET:HG3	20:T:88:VAL:HG21	1.66	0.76
6:F:70:ASP:N	6:F:70:ASP:OD1	2.15	0.76
1:A:1126:U:O4	1:A:1127:G:N2	2.19	0.75
1:A:1125:U:OP2	1:A:1145:C:N4	2.19	0.75
12:L:25:PRO:C	12:L:27:LEU:H	1.88	0.75
10:J:49:VAL:HG13	14:N:41:ARG:HB2	1.69	0.75
6:F:97:PHE:HE1	18:R:61:LYS:HE2	1.51	0.75
1:A:869:G:N7	24:A:2109:HOH:O	2.19	0.75
10:J:50:ILE:HA	10:J:60:ARG:HB3	1.68	0.75
1:A:1195:C:H3'	1:A:1196:U:C5'	2.16	0.74
1:A:1504:G:OP1	1:A:1507:A:H4'	1.87	0.74
12:L:24:VAL:HG13	12:L:98:TYR:HE2	1.51	0.74
15:O:17:ARG:HH11	15:O:17:ARG:HG3	1.52	0.74
6:F:10:LEU:HD12	6:F:59:TYR:HB3	1.69	0.74
1:A:979:C:O2	1:A:1317:C:N4	2.19	0.74
12:L:27:LEU:HB3	12:L:28:LYS:HG2	1.69	0.74
1:A:1145:C:O2'	1:A:1146:A:O5'	2.06	0.74
3:C:150:LYS:HB3	3:C:201:TYR:HB2	1.68	0.74
3:C:180:ALA:HB1	3:C:203:PHE:HE1	1.51	0.74
3:C:13:GLY:HA3	14:N:57:ARG:HH21	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:64:GLU:OE2	10:J:66:ARG:NH2	2.20	0.73
17:Q:29:HIS:CG	17:Q:30:PRO:HD2	2.24	0.73
1:A:269:C:H2'	1:A:270:A:C8	2.24	0.73
10:J:82:ILE:HA	10:J:85:LEU:HB2	1.68	0.72
2:B:55:PHE:HD2	2:B:58:ILE:HD12	1.54	0.72
1:A:1147:C:H4'	9:I:5:TYR:HE1	1.54	0.72
17:Q:62:SER:OG	17:Q:72:ARG:HG3	1.89	0.72
1:A:1152:A:OP1	10:J:68:HIS:ND1	2.22	0.72
9:I:126:SER:OG	9:I:127:LYS:N	2.21	0.72
3:C:112:SER:HB3	3:C:115:LEU:HD12	1.71	0.72
1:A:1125:U:H3	10:J:5:ARG:HH21	1.37	0.72
4:D:61:LYS:NZ	4:D:62:GLN:OE1	2.18	0.72
15:O:56:LEU:HA	15:O:59:MET:HE2	1.71	0.72
2:B:91:PRO:HG2	2:B:155:LEU:HD23	1.73	0.71
1:A:951:G:OP2	13:M:102:ARG:NH2	2.23	0.71
20:T:50:GLU:HA	20:T:100:ILE:HG13	1.72	0.71
7:G:17:VAL:HG12	7:G:18:TYR:HD1	1.55	0.71
1:A:975:A:H5'	1:A:975:A:H8	1.55	0.71
10:J:61:GLU:OE1	14:N:45:ARG:NH1	2.24	0.71
1:A:1256:A:O2'	1:A:1257:U:OP2	2.08	0.71
1:A:1049:U:O2'	14:N:3:ARG:NH1	2.24	0.71
3:C:52:LEU:HD12	3:C:68:VAL:HG13	1.72	0.71
1:A:250:A:H4'	1:A:251:G:O5'	1.91	0.71
1:A:95:U:H2'	1:A:96:G:H8	1.55	0.70
1:A:1510:U:H2'	1:A:1511:G:C8	2.26	0.70
3:C:179:ARG:HD3	3:C:206:GLU:HG3	1.73	0.70
9:I:50:LEU:HD11	9:I:81:ILE:HD13	1.72	0.70
1:A:1435:G:H2'	1:A:1436:U:C6	2.26	0.70
1:A:1257:U:O2'	1:A:1258:G:OP2	2.08	0.70
9:I:46:ALA:HB2	9:I:74:ILE:HG23	1.73	0.70
18:R:46:GLU:CD	18:R:46:GLU:H	1.95	0.69
4:D:22:LYS:HB2	4:D:26:CYS:SG	2.31	0.69
10:J:21:GLN:NE2	10:J:25:GLU:OE2	2.25	0.69
5:E:144:THR:O	5:E:148:VAL:HG23	1.91	0.69
12:L:53:ARG:NH1	12:L:92:0TD:OD2	2.24	0.69
3:C:150:LYS:HG3	3:C:169:ALA:HB2	1.73	0.69
3:C:26:LYS:O	3:C:30:ARG:NH1	2.25	0.69
1:A:452:A:O2'	1:A:453:A:O4'	2.08	0.69
1:A:1222:G:OP2	1:A:1322:C:N4	2.26	0.69
7:G:16:LEU:HD12	9:I:44:VAL:HG12	1.74	0.69
1:A:1497:G:C2'	1:A:1498:UR3:H5'	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:G:OP1	4:D:10:ARG:NH2	2.26	0.68
16:P:68:ASP:OD1	16:P:68:ASP:N	2.26	0.68
13:M:16:ASP:OD1	13:M:16:ASP:N	2.26	0.68
1:A:1414:U:H2'	1:A:1415:G:C8	2.28	0.68
3:C:131:ARG:HA	3:C:134:ILE:HD12	1.76	0.68
16:P:9:PHE:HD1	16:P:18:ARG:HG3	1.59	0.68
1:A:1349:A:P	9:I:118:LYS:HZ1	2.17	0.67
1:A:1305:G:N2	1:A:1331:G:H1'	2.09	0.67
13:M:11:ARG:HG3	13:M:12:ASN:HB2	1.75	0.67
8:H:10:LEU:HD22	8:H:83:ILE:HD13	1.77	0.67
1:A:1399:C:H4'	1:A:1400:5MC:H5"	1.76	0.67
1:A:1443:G:H5"	1:A:1446:A:H5'	1.76	0.67
1:A:263:A:OP2	20:T:79:ARG:NH1	2.27	0.67
9:I:55:ALA:HB1	9:I:59:PHE:HB2	1.76	0.67
15:O:12:ILE:HG12	15:O:31:LEU:HD11	1.76	0.67
3:C:23:TYR:OH	10:J:9:ARG:NH1	2.26	0.67
1:A:1255:G:C6	1:A:1279:A:N7	2.63	0.67
6:F:14:LEU:HD13	6:F:18:GLN:HB3	1.77	0.67
1:A:1338:G:H2'	1:A:1339:A:C8	2.30	0.67
1:A:113:G:H1'	1:A:354:G:H5'	1.78	0.66
1:A:1498:UR3:O4'	1:A:1519[A]:MA6:H2	1.96	0.66
1:A:103:C:P	20:T:17:ARG:HH12	2.18	0.66
1:A:1190:G:OP1	3:C:4:LYS:HA	1.95	0.66
1:A:1144:G:N2	1:A:1145:C:O2	2.28	0.66
15:O:55:GLY:HA2	15:O:58:MET:HE2	1.78	0.66
1:A:1128:C:O2'	1:A:1130:A:N7	2.28	0.66
10:J:61:GLU:OE2	14:N:58:LYS:NZ	2.28	0.66
8:H:20:TYR:CE1	8:H:76:PRO:HD2	2.31	0.66
1:A:1148:U:H2'	1:A:1149:C:O4'	1.96	0.66
1:A:966:M2G:HM22	1:A:967:5MC:C2	2.30	0.66
1:A:281:G:O2'	1:A:282:A:OP2	2.07	0.66
1:A:269:C:H2'	1:A:270:A:H8	1.61	0.65
20:T:100:ILE:HG22	20:T:102:GLY:N	2.09	0.65
1:A:77:G:H2'	1:A:78:G:C8	2.30	0.65
1:A:560:U:H5'	1:A:566:G:N2	2.12	0.65
15:O:33:THR:HG21	15:O:85:LEU:HD13	1.77	0.65
1:A:1222:G:OP1	19:S:77:THR:HG21	1.95	0.65
1:A:443:C:H42	1:A:491:G:H1	1.45	0.65
5:E:80:ILE:HG22	8:H:104:ARG:HH21	1.60	0.65
1:A:407:G:OP1	4:D:115:ARG:NH1	2.29	0.65
17:Q:95:TYR:HA	17:Q:98:LEU:HD11	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1255:G:O2'	1:A:1258:G:H1'	1.97	0.65
11:K:40:ILE:HG22	11:K:41:THR:HG23	1.79	0.65
20:T:39:LYS:HG2	20:T:55:ILE:HD13	1.77	0.65
21:U:6:ARG:HD2	21:U:15:ARG:NH2	2.11	0.65
14:N:18:VAL:HG23	14:N:19:ARG:HG3	1.79	0.65
1:A:858:G:N7	24:A:2109:HOH:O	2.29	0.64
1:A:1049:U:H4'	1:A:1050:G:O5'	1.97	0.64
1:A:76:C:H2'	1:A:77:G:H8	1.61	0.64
3:C:41:GLY:O	3:C:45:LYS:HG2	1.97	0.64
2:B:21:ARG:HA	2:B:39:ILE:HA	1.80	0.64
8:H:85:ARG:NE	8:H:87:SER:O	2.31	0.64
3:C:108:ASN:HB3	3:C:111:LEU:HB2	1.80	0.64
1:A:89:C:H2'	1:A:90:U:H6	1.62	0.64
1:A:427:U:OP1	4:D:13:ARG:NH2	2.31	0.64
1:A:517:G:N1	1:A:533:A:OP2	2.29	0.64
1:A:1387:G:O2'	24:A:2061:HOH:O	2.14	0.64
13:M:15:VAL:HG21	13:M:48:LEU:HD21	1.80	0.63
7:G:40:ALA:HB3	9:I:41:VAL:HG21	1.80	0.63
8:H:104:ARG:HG2	8:H:104:ARG:HH11	1.62	0.63
11:K:57:THR:HG23	11:K:60:ALA:H	1.62	0.63
1:A:328:C:O2	1:A:328:C:H2'	1.96	0.63
1:A:707:C:H2'	1:A:708:C:C6	2.32	0.63
7:G:84:ASN:OD1	7:G:84:ASN:N	2.30	0.63
11:K:29:ILE:HG12	11:K:30:VAL:N	2.13	0.63
16:P:21:VAL:HG12	16:P:33:ILE:HD12	1.81	0.63
20:T:46:GLU:OE1	20:T:48:LYS:NZ	2.32	0.63
1:A:686:U:HO2'	1:A:687:A:H8	1.45	0.63
10:J:50:ILE:H	10:J:50:ILE:HD12	1.62	0.63
1:A:553:A:O2'	12:L:29:GLY:O	2.16	0.63
3:C:154:SER:OG	3:C:155:GLY:N	2.29	0.63
12:L:27:LEU:C	12:L:29:GLY:H	1.95	0.62
1:A:1128:C:H5'	9:I:16:ARG:HH12	1.63	0.62
11:K:48:ILE:HD12	11:K:63:LEU:HB2	1.81	0.62
1:A:864:A:H2'	1:A:865:A:C8	2.35	0.62
13:M:117:VAL:HG12	13:M:118:ALA:H	1.64	0.62
7:G:91:VAL:HG11	7:G:96:GLN:HG3	1.81	0.62
1:A:310:G:OP2	16:P:27:LYS:NZ	2.25	0.62
15:O:45:VAL:HB	15:O:46:HIS:ND1	2.13	0.62
1:A:1143:G:H2'	1:A:1144:G:C8	2.35	0.62
1:A:1064:G:N2	1:A:1190:G:O2'	2.33	0.62
1:A:537:G:OP1	12:L:113:ARG:NH2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:137:ALA:O	3:C:141:VAL:HG23	1.99	0.62
4:D:64:LEU:HD23	4:D:198:VAL:HG21	1.81	0.62
3:C:33:LEU:HD21	14:N:53:LEU:HD22	1.82	0.62
1:A:77:G:C6	1:A:93:G:N1	2.68	0.62
1:A:1148:U:H1'	9:I:16:ARG:HH21	1.64	0.62
1:A:1373:G:H5"	7:G:36:LYS:HE3	1.82	0.62
12:L:5:PRO:HG2	12:L:15:ARG:NH2	2.14	0.62
2:B:240:GLN:OE1	2:B:240:GLN:N	2.31	0.62
1:A:1164:G:H1	1:A:1172:C:H42	1.47	0.62
4:D:23:GLY:HA3	4:D:112:VAL:HG12	1.81	0.62
1:A:967:5MC:O2'	9:I:128:ARG:NH1	2.33	0.61
1:A:1090:U:H2'	1:A:1091:U:H6	1.65	0.61
1:A:501:C:H2'	1:A:502:G:C8	2.35	0.61
1:A:673:G:H2'	1:A:674:G:C8	2.34	0.61
4:D:107:ARG:HH12	4:D:114:ARG:HH21	1.47	0.61
1:A:1349:A:OP1	9:I:118:LYS:NZ	2.32	0.61
1:A:707:C:H2'	1:A:708:C:H6	1.65	0.61
19:S:11:VAL:HG22	19:S:39:THR:HB	1.82	0.61
1:A:1513:A:H2'	1:A:1514:C:C6	2.36	0.61
9:I:24:GLY:HA3	9:I:56:LEU:HD23	1.83	0.61
16:P:74:LEU:O	16:P:79:VAL:HG23	2.01	0.61
5:E:88:LYS:HB3	5:E:123:LEU:HB2	1.82	0.61
1:A:1499:A:H1'	1:A:1520[A]:G:H5'	1.81	0.61
15:O:87:ILE:HG22	15:O:88:ARG:H	1.64	0.61
1:A:1224:G:N2	1:A:1362:C:O2	2.33	0.61
1:A:1143:G:H2'	1:A:1144:G:H8	1.64	0.61
14:N:39:LEU:HD22	14:N:43:CYS:HB3	1.81	0.61
1:A:827:U:H5"	1:A:828:A:OP2	2.00	0.61
1:A:1291:G:H2'	1:A:1292:U:C6	2.35	0.61
12:L:25:PRO:HB2	12:L:64:TYR:HE2	1.66	0.61
1:A:858:G:O6	24:A:2107:HOH:O	2.16	0.61
17:Q:74:LEU:HD23	17:Q:75:ARG:HG2	1.83	0.61
1:A:1101:A:H4'	1:A:1102:A:O5'	1.99	0.61
1:A:1368:G:OP2	9:I:112:LYS:HD3	2.01	0.61
1:A:130:A:H5'	17:Q:63:ARG:HE	1.66	0.61
2:B:223:ILE:HD13	2:B:230:VAL:HG21	1.82	0.61
1:A:1020:U:H2'	1:A:1021:G:H8	1.66	0.61
1:A:1314:C:H2'	1:A:1315:U:C6	2.35	0.60
1:A:1305:G:OP1	21:U:2:GLY:N	2.34	0.60
3:C:22:TRP:HA	10:J:93:GLY:HA2	1.83	0.60
4:D:78:LEU:HD21	4:D:96:LEU:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1006:C:H42	1:A:1022:G:H22	1.47	0.60
1:A:581:G:N7	24:A:1973:HOH:O	2.31	0.60
4:D:187:ARG:NH2	4:D:188:LEU:HB2	2.17	0.60
9:I:26:VAL:HG13	9:I:61:ALA:HB3	1.83	0.60
16:P:43:LYS:HG2	16:P:48:TRP:CD2	2.36	0.60
1:A:76:C:H42	1:A:95:U:H3	1.49	0.60
16:P:4:ILE:HG12	16:P:21:VAL:HG22	1.82	0.60
5:E:33:VAL:HG11	5:E:109:ILE:HA	1.82	0.60
9:I:45:ALA:HA	9:I:48:GLU:HB2	1.82	0.60
1:A:1347:G:H3'	9:I:108:VAL:O	2.02	0.60
7:G:17:VAL:HG12	7:G:18:TYR:CD1	2.34	0.60
2:B:16:HIS:CD2	2:B:204:ASN:H	2.19	0.60
1:A:992:U:H3	1:A:1044:A:N6	1.97	0.60
15:O:29:VAL:HG11	15:O:67:LEU:HD21	1.83	0.60
1:A:89:C:H2'	1:A:90:U:O4'	2.00	0.60
7:G:38:LEU:O	7:G:42:ILE:HG13	2.02	0.60
1:A:1392:G:H21	1:A:1502:A:H8	1.47	0.60
1:A:1349:A:C2	1:A:1374:A:C4	2.90	0.60
11:K:62:GLN:HG3	11:K:97:ALA:HB2	1.83	0.60
8:H:116:LYS:NZ	8:H:127:LEU:HD12	2.17	0.60
13:M:96:LEU:O	13:M:110:ARG:NH1	2.35	0.60
20:T:81:LYS:O	20:T:85:MET:HG3	2.01	0.60
2:B:63:MET:HB3	2:B:225:ALA:HB1	1.83	0.60
3:C:31:HIS:HA	3:C:34:LEU:HB2	1.84	0.60
1:A:204:U:H4'	1:A:216:G:OP1	2.02	0.59
6:F:55:ASP:HB3	6:F:86:ARG:HH12	1.66	0.59
1:A:89:C:H2'	1:A:90:U:C6	2.38	0.59
20:T:33:ILE:HD13	20:T:62:LEU:HB3	1.84	0.59
5:E:32:VAL:HB	5:E:58:ALA:HB1	1.83	0.59
1:A:1366:C:H2'	1:A:1367:C:H6	1.67	0.59
1:A:757:U:H2'	1:A:758:G:O4'	2.01	0.59
1:A:973:G:H3'	1:A:974:A:H5"	1.84	0.59
8:H:41:ARG:NH1	8:H:123:GLU:OE2	2.35	0.59
14:N:6:LEU:HB3	14:N:23:ARG:NH2	2.17	0.59
6:F:78:GLU:HA	6:F:81:ILE:HD12	1.83	0.59
1:A:235:C:N4	24:A:1988:HOH:O	2.36	0.59
1:A:1443:G:C5'	1:A:1446:A:H5'	2.33	0.59
20:T:92:LEU:O	20:T:96:GLY:HA2	2.03	0.59
1:A:345:C:OP2	1:A:345:C:H6	1.85	0.59
1:A:1301:U:O2'	1:A:1302:U:O5'	2.20	0.59
10:J:79:ARG:NH1	10:J:79:ARG:HA	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:7:VAL:HG11	2:B:221:LEU:HD23	1.83	0.59
11:K:94:ALA:O	11:K:98:LEU:HB2	2.03	0.59
5:E:77:PRO:HD2	5:E:142:LEU:HD13	1.85	0.59
1:A:390:C:O3'	16:P:28:ARG:NH2	2.36	0.59
1:A:1009:G:H1	1:A:1020:U:H3	1.51	0.58
1:A:737:A:H2'	1:A:738:C:C6	2.37	0.58
19:S:5:LEU:HB2	19:S:9:VAL:HG22	1.84	0.58
1:A:35:G:O2'	12:L:118:SER:O	2.21	0.58
18:R:22:VAL:HG23	18:R:56:THR:HA	1.84	0.58
1:A:1313:U:O4	19:S:4:SER:OG	2.12	0.58
1:A:5:U:H4'	1:A:6:G:O5'	2.02	0.58
12:L:28:LYS:C	12:L:30:ALA:H	2.04	0.58
3:C:134:ILE:HG23	3:C:151:VAL:HB	1.85	0.58
2:B:91:PRO:HG2	2:B:155:LEU:CD2	2.33	0.58
1:A:1048:G:H1	1:A:1209:C:H42	1.50	0.58
1:A:1409:C:H2'	1:A:1410:G:C8	2.37	0.58
14:N:27:CYS:HB2	14:N:43:CYS:SG	2.33	0.58
1:A:216:G:H2'	1:A:217:C:C6	2.37	0.58
18:R:47:THR:HA	18:R:83:GLU:HB2	1.85	0.58
1:A:1126:U:O2'	1:A:1127:G:OP1	2.19	0.58
1:A:344:A:H5'	1:A:345:C:C5	2.38	0.58
2:B:97:TRP:HZ2	2:B:102:LEU:HD22	1.69	0.58
17:Q:24:GLU:HG2	17:Q:39:SER:HB3	1.86	0.58
8:H:25:ASP:OD1	8:H:25:ASP:N	2.36	0.58
1:A:1225:A:N3	1:A:1225:A:H2'	2.19	0.58
1:A:1347:G:O2'	1:A:1348:U:P	2.62	0.58
12:L:87:GLY:HA2	12:L:98:TYR:HA	1.85	0.58
3:C:179:ARG:HG3	3:C:179:ARG:HH11	1.68	0.58
4:D:107:ARG:HH21	4:D:194:LEU:HD12	1.67	0.58
9:I:8:GLY:HA3	9:I:79:LEU:HB3	1.84	0.58
15:O:39:LEU:HD13	15:O:56:LEU:HB2	1.86	0.58
4:D:187:ARG:CZ	4:D:188:LEU:HB2	2.34	0.58
11:K:80:VAL:HG21	11:K:103:LEU:HD13	1.86	0.58
16:P:19:ILE:HD12	16:P:37:GLY:HA3	1.86	0.58
1:A:836:G:C6	1:A:851:G:C6	2.92	0.58
4:D:15:GLU:O	4:D:17:VAL:HG23	2.04	0.58
1:A:1347:G:O6	9:I:10:ARG:NH2	2.29	0.58
9:I:19:LEU:HD23	9:I:61:ALA:HB2	1.84	0.58
3:C:155:GLY:HA2	3:C:164:ARG:H	1.69	0.58
1:A:324:G:OP1	20:T:22:ARG:NH1	2.37	0.58
9:I:117:HIS:NE2	9:I:123:PRO:HB3	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:C:H2'	1:A:458:C:H6	1.68	0.58
1:A:858:G:O6	1:A:869:G:C8	2.57	0.58
3:C:138:VAL:HG13	3:C:149:ALA:HB3	1.85	0.58
1:A:372:C:H4'	1:A:373:A:O5'	2.03	0.58
1:A:90:U:O2'	1:A:91:C:H5'	2.04	0.57
15:O:21:ASP:OD1	15:O:24:SER:OG	2.22	0.57
1:A:967:5MC:H4'	9:I:128:ARG:HG3	1.85	0.57
1:A:1243:C:H42	1:A:1294:G:H1	1.52	0.57
1:A:937:A:N6	1:A:1345:U:O4	2.37	0.57
9:I:10:ARG:HG2	9:I:75:ASP:HB2	1.85	0.57
1:A:580:U:H2'	1:A:581:G:O4'	2.05	0.57
1:A:1106:G:H5"	3:C:172:ARG:HB3	1.85	0.57
1:A:91:C:HO2'	1:A:92:C:H6	1.52	0.57
1:A:442:C:H42	1:A:492:G:H1	1.52	0.57
1:A:299:G:H2'	1:A:300:A:C8	2.40	0.57
16:P:2:VAL:O	16:P:64:ALA:HA	2.04	0.57
8:H:31:PHE:O	8:H:35:ILE:HG12	2.04	0.57
1:A:579:G:H4'	15:O:54:ARG:HH21	1.69	0.57
12:L:25:PRO:C	12:L:27:LEU:N	2.56	0.57
1:A:235:C:H5'	17:Q:70:ARG:HG2	1.87	0.57
2:B:88:ALA:HB2	2:B:219:VAL:HG13	1.87	0.57
1:A:1118:C:H5'	9:I:104:ARG:HG3	1.87	0.57
1:A:633:G:H2'	1:A:634:C:C6	2.40	0.57
20:T:49:ALA:HB3	20:T:99:LEU:HD12	1.87	0.57
20:T:75:ASN:OD1	20:T:75:ASN:N	2.36	0.57
1:A:298:A:N6	24:A:2058:HOH:O	2.08	0.57
9:I:117:HIS:HB2	9:I:121:ARG:HG2	1.86	0.57
17:Q:63:ARG:HG2	17:Q:64:PRO:HD2	1.87	0.57
14:N:24:CYS:HA	14:N:38:GLY:O	2.05	0.57
1:A:129:U:O3'	1:A:129(A):G:H3'	2.05	0.57
1:A:384:G:H2'	1:A:385:C:C6	2.40	0.57
1:A:509:A:H3'	1:A:509:A:C8	2.39	0.57
1:A:1511:G:H2'	1:A:1512:U:O4'	2.05	0.57
11:K:65:ALA:HB1	11:K:98:LEU:HD23	1.87	0.57
1:A:1139:G:H4'	1:A:1140:C:C5'	2.35	0.57
12:L:124:LYS:HD2	12:L:125:PRO:HD2	1.87	0.57
1:A:975:A:H5'	1:A:975:A:C8	2.38	0.56
3:C:153:VAL:HG12	3:C:196:LEU:HD22	1.87	0.56
1:A:1139:G:H4'	1:A:1140:C:O5'	2.05	0.56
1:A:569:C:H42	1:A:881:G:H1	1.53	0.56
3:C:14:ILE:HG22	3:C:15:THR:HG23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1129:C:H4'	1:A:1130:A:OP2	2.05	0.56
1:A:1225:A:H5'	1:A:1226:C:OP2	2.05	0.56
4:D:55:ALA:O	4:D:59:ARG:HG2	2.06	0.56
9:I:38:GLN:OE1	9:I:39:GLY:N	2.37	0.56
10:J:50:ILE:HG13	10:J:60:ARG:HD3	1.86	0.56
2:B:55:PHE:CD2	2:B:58:ILE:HD12	2.38	0.56
1:A:1112:C:H1'	3:C:179:ARG:NH2	2.20	0.56
19:S:53:ASN:ND2	19:S:56:GLN:HB2	2.20	0.56
12:L:102:ARG:NH2	12:L:108:ALA:O	2.24	0.56
3:C:180:ALA:CB	3:C:203:PHE:HE1	2.18	0.56
1:A:758:G:C8	24:A:1974:HOH:O	2.59	0.56
6:F:100:ASN:O	18:R:28:GLU:HG3	2.06	0.56
3:C:43:LEU:HA	3:C:47:LEU:HD13	1.87	0.56
5:E:93:PRO:HD2	8:H:105:ARG:HH21	1.69	0.56
3:C:29:TYR:HE1	10:J:11:PHE:HE1	1.54	0.56
12:L:25:PRO:HA	12:L:27:LEU:H	1.71	0.56
12:L:24:VAL:HG13	12:L:98:TYR:CE2	2.36	0.56
1:A:532:A:H2'	1:A:533:A:H5"	1.87	0.56
1:A:792:A:H4'	1:A:793:U:O5'	2.06	0.56
1:A:1437:C:H2'	1:A:1438:G:H8	1.71	0.56
1:A:481:G:O2'	1:A:482:A:H8	1.86	0.56
13:M:99:ARG:HB2	13:M:101:GLN:NE2	2.21	0.56
1:A:451:A:N6	1:A:481:G:C4	2.73	0.56
5:E:17:ALA:HB2	5:E:26:PHE:HD2	1.71	0.56
1:A:254:G:OP1	17:Q:67:LYS:O	2.23	0.56
1:A:45:U:H2'	1:A:46:G:C8	2.41	0.56
4:D:162:LEU:HA	4:D:165:MET:HB2	1.88	0.56
10:J:63:PHE:HB3	14:N:57:ARG:O	2.05	0.56
12:L:113:ARG:NH1	12:L:116:SER:H	2.03	0.56
2:B:47:THR:OG1	2:B:202:PRO:O	2.23	0.56
7:G:115:ARG:HB2	7:G:118:VAL:HG23	1.88	0.56
1:A:1516[B]:G:N2	1:A:1519[B]:MA6:OP2	2.34	0.55
1:A:1393:U:HO2'	1:A:1501:C:HO2'	1.50	0.55
1:A:411:A:N7	1:A:413:G:N3	2.55	0.55
5:E:101:ILE:O	5:E:120:THR:HB	2.06	0.55
2:B:28:PHE:HD2	2:B:32:ILE:HD11	1.71	0.55
13:M:90:LEU:HD23	13:M:93:ARG:HD2	1.88	0.55
3:C:58:GLU:HB3	10:J:92:THR:HG21	1.88	0.55
8:H:87:SER:HA	8:H:93:VAL:HG13	1.87	0.55
1:A:1392:G:N2	1:A:1502:A:H8	2.04	0.55
10:J:48:THR:HA	10:J:62:HIS:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:9:ARG:HE	21:U:22:ARG:HG3	1.70	0.55
6:F:97:PHE:CE1	18:R:61:LYS:HE2	2.39	0.55
1:A:869:G:H5"	1:A:870:U:OP1	2.06	0.55
8:H:104:ARG:HG3	8:H:138:TRP:CD2	2.41	0.55
1:A:500:G:C6	1:A:546:G:C2	2.95	0.55
17:Q:60:ILE:HD13	17:Q:61:GLU:N	2.22	0.55
1:A:1347:G:O2'	1:A:1348:U:OP2	2.25	0.55
1:A:544:G:OP1	4:D:62:GLN:NE2	2.37	0.55
7:G:18:TYR:HE2	7:G:59:LEU:HA	1.72	0.55
4:D:9:CYS:O	4:D:12:CYS:HB2	2.06	0.55
1:A:1509:C:H42	1:A:1526:G:H1	1.53	0.55
9:I:112:LYS:HA	9:I:119:ALA:HB2	1.89	0.55
3:C:150:LYS:HB2	3:C:173:VAL:HG21	1.88	0.55
9:I:50:LEU:HB3	9:I:55:ALA:HB3	1.89	0.55
1:A:1128:C:H5'	9:I:16:ARG:NH1	2.21	0.55
1:A:1006:C:H2'	1:A:1007:C:H6	1.71	0.55
1:A:1028:C:H42	1:A:1033:G:H1	1.55	0.55
1:A:401:C:O2'	1:A:621:A:N3	2.31	0.55
7:G:111:ARG:HG2	7:G:112:PRO:HD2	1.87	0.55
20:T:68:LYS:HE3	20:T:68:LYS:HA	1.88	0.55
17:Q:29:HIS:CD2	17:Q:30:PRO:HD2	2.42	0.55
1:A:1256:A:H4'	1:A:1257:U:O5'	2.05	0.55
1:A:1130:A:O2'	9:I:3:GLN:NE2	2.24	0.55
1:A:353:A:H5'	1:A:353:A:H8	1.72	0.55
3:C:172:ARG:NH2	3:C:174:PRO:HG3	2.21	0.55
9:I:48:GLU:N	9:I:49:PRO:HD2	2.22	0.55
8:H:121:ASP:OD2	8:H:122:ARG:N	2.38	0.55
14:N:50:LYS:HG2	14:N:52:GLN:HE21	1.72	0.55
1:A:948:C:OP2	13:M:108:ARG:HB2	2.07	0.55
1:A:1403:C:H1'	1:A:1500:A:N1	2.22	0.55
13:M:62:ASN:N	13:M:62:ASN:OD1	2.39	0.55
10:J:79:ARG:NH1	10:J:82:ILE:HB	2.21	0.55
3:C:154:SER:HB3	3:C:197:GLY:H	1.72	0.55
20:T:45:GLN:HA	20:T:91:LEU:HD12	1.87	0.55
10:J:6:ILE:HD13	10:J:72:VAL:HB	1.88	0.55
8:H:118:VAL:C	8:H:119:LEU:HD23	2.27	0.55
1:A:1531:A:O5'	1:A:1531:A:H8	1.90	0.55
4:D:35:ARG:O	4:D:36:ARG:HG3	2.07	0.54
12:L:5:PRO:HG2	12:L:15:ARG:HH22	1.71	0.54
4:D:174:LEU:O	4:D:186:LEU:HD11	2.07	0.54
15:O:30:ALA:HA	15:O:85:LEU:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:16:HIS:NE2	20:T:20:LEU:HD21	2.22	0.54
1:A:1286:A:H2'	1:A:1287:A:H4'	1.88	0.54
18:R:74:ARG:HB3	18:R:81:PHE:CE1	2.42	0.54
1:A:451:A:OP1	1:A:451:A:H8	1.90	0.54
1:A:707:C:OP1	11:K:85:ARG:NH1	2.41	0.54
1:A:706:A:O2'	11:K:29:ILE:HD11	2.07	0.54
1:A:974:A:OP2	14:N:29:ARG:NH2	2.40	0.54
3:C:58:GLU:H	3:C:65:ALA:HB3	1.73	0.54
1:A:243:A:C2	1:A:246:A:C8	2.96	0.54
13:M:86:CYS:SG	13:M:87:TYR:N	2.81	0.54
1:A:1193:G:H2'	1:A:1194:U:H6	1.73	0.54
1:A:1417:G:HO2'	1:A:1483:A:N6	2.05	0.54
1:A:1048:G:H5"	14:N:3:ARG:HD2	1.89	0.54
15:O:18:PHE:HD1	15:O:19:PRO:O	1.91	0.54
1:A:581:G:C8	24:A:1973:HOH:O	2.60	0.54
12:L:93:LEU:HD12	12:L:96:VAL:HG21	1.88	0.54
1:A:1359:C:H1'	1:A:1361(A):C:H41	1.72	0.54
4:D:18:LYS:HE2	4:D:20:TYR:HE2	1.72	0.54
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.42	0.54
1:A:594:G:H1	1:A:645:C:H42	1.56	0.54
3:C:112:SER:O	3:C:116:VAL:HG23	2.08	0.54
1:A:1065:U:H5"	1:A:1190:G:N2	2.23	0.54
1:A:998:G:N2	1:A:1043:C:O2	2.41	0.54
3:C:91:LEU:HD21	3:C:99:VAL:HG22	1.89	0.54
5:E:71:LEU:HD21	5:E:115:VAL:HG22	1.90	0.54
8:H:2:LEU:C	8:H:2:LEU:HD23	2.28	0.54
1:A:1191:A:H2'	1:A:1192:C:C6	2.42	0.54
1:A:1008:C:H42	1:A:1021:G:H1	1.55	0.54
13:M:5:ALA:HB3	13:M:8:GLU:HG3	1.90	0.54
5:E:84:PHE:HB2	5:E:134:ALA:HB2	1.90	0.54
7:G:69:VAL:HG21	7:G:104:LEU:HD21	1.90	0.54
16:P:52:ASP:OD2	16:P:55:ARG:HB2	2.08	0.54
1:A:103:C:OP2	20:T:14:LYS:HD2	2.08	0.53
3:C:6:HIS:CD2	3:C:9:GLY:H	2.16	0.53
1:A:130:A:C8	17:Q:63:ARG:HG3	2.43	0.53
1:A:500:G:C5	1:A:546:G:N2	2.77	0.53
1:A:1281:U:H5'	1:A:1282:C:H5	1.72	0.53
1:A:1198:G:H2'	1:A:1199:U:C6	2.43	0.53
1:A:77:G:C4	1:A:93:G:N2	2.77	0.53
1:A:353:A:H5'	1:A:353:A:C8	2.43	0.53
1:A:1304:G:OP2	24:A:2087:HOH:O	2.19	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:26:PHE:O	7:G:30:ILE:HG13	2.08	0.53
1:A:946:A:H2'	1:A:947:G:C8	2.43	0.53
1:A:279:A:H8	1:A:279:A:H5'	1.73	0.53
2:B:158:LEU:H	2:B:158:LEU:HD12	1.73	0.53
8:H:9:MET:HG3	8:H:26:VAL:HG21	1.89	0.53
13:M:13:LYS:O	13:M:45:VAL:HG23	2.07	0.53
18:R:53:ARG:NH1	18:R:58:LEU:O	2.38	0.53
1:A:660:G:H1	1:A:745:C:H42	1.56	0.53
1:A:1343:G:H1'	9:I:121:ARG:NH1	2.23	0.53
1:A:192:U:H5'	20:T:102:GLY:O	2.09	0.53
1:A:1145:C:HO2'	1:A:1146:A:P	2.30	0.53
1:A:1139:G:H4'	1:A:1140:C:H5'	1.91	0.53
1:A:596:C:C2'	1:A:597:G:H5'	2.38	0.53
9:I:22:GLY:HA3	9:I:60:ASP:HB2	1.90	0.53
1:A:503:C:H2'	1:A:504:C:C6	2.44	0.53
17:Q:31:LEU:HD23	17:Q:32:TYR:CE2	2.44	0.53
15:O:78:TYR:CZ	15:O:82:ILE:HD12	2.44	0.53
6:F:8:ILE:HB	6:F:61:LEU:HB2	1.90	0.53
12:L:69:TYR:HE2	12:L:71:PRO:HA	1.73	0.53
1:A:1305:G:O2'	1:A:1306:A:H8	1.91	0.53
4:D:36:ARG:HG2	4:D:38:TYR:CZ	2.44	0.53
1:A:141:A:H1'	1:A:182:U:O2	2.09	0.53
9:I:88:TYR:HD2	9:I:89:ASN:HB2	1.74	0.53
1:A:1004:A:H5"	1:A:1025:U:C4	2.44	0.53
1:A:1116:C:O2'	9:I:108:VAL:HG21	2.09	0.52
19:S:77:THR:HG22	19:S:78:ARG:HD2	1.91	0.52
15:O:24:SER:HB2	15:O:27:VAL:HG23	1.91	0.52
1:A:1499:A:H1'	1:A:1520[A]:G:OP1	2.09	0.52
1:A:1442:G:C2	1:A:1446:A:N7	2.77	0.52
1:A:383:A:C6	1:A:384:G:H1'	2.44	0.52
1:A:76:C:H2'	1:A:77:G:C8	2.43	0.52
4:D:127:THR:HB	4:D:147:ALA:HB3	1.91	0.52
3:C:11:ARG:HA	3:C:178:LEU:HD11	1.90	0.52
1:A:95:U:H2'	1:A:96:G:C8	2.41	0.52
1:A:866:C:H2'	1:A:867:G:O4'	2.08	0.52
12:L:82:VAL:HG13	12:L:106:ASP:OD1	2.09	0.52
13:M:2:ALA:O	13:M:10:PRO:HD2	2.10	0.52
1:A:80:G:H2'	1:A:81:U:H5'	1.91	0.52
4:D:72:GLU:OE1	4:D:207:TYR:OH	2.27	0.52
11:K:70:LYS:HA	11:K:73:MET:HG2	1.92	0.52
12:L:35:GLY:HA3	12:L:60:LEU:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:116:VAL:HG21	3:C:202:ILE:HD11	1.92	0.52
11:K:48:ILE:CD1	11:K:63:LEU:HB2	2.39	0.52
15:O:26:GLU:HA	15:O:81:LEU:HD11	1.92	0.52
1:A:943:U:H1'	9:I:124:GLN:HE22	1.74	0.52
1:A:968:A:C8	1:A:1062:U:H4'	2.44	0.52
13:M:54:VAL:HG22	13:M:58:GLU:OE1	2.10	0.52
4:D:146:ILE:HD12	4:D:146:ILE:N	2.24	0.52
1:A:1061:G:H1	1:A:1195:C:H42	1.58	0.52
1:A:1349:A:OP1	9:I:120:ARG:HB2	2.09	0.52
3:C:174:PRO:HB2	3:C:177:THR:CG2	2.40	0.52
9:I:19:LEU:HD22	9:I:59:PHE:HD2	1.75	0.52
4:D:36:ARG:HG2	4:D:38:TYR:OH	2.09	0.52
2:B:200:ILE:HG12	2:B:202:PRO:HD3	1.92	0.52
4:D:3:ARG:HH22	4:D:74:GLN:NE2	2.07	0.52
13:M:57:ARG:O	13:M:61:GLU:HB2	2.10	0.52
14:N:50:LYS:HB3	14:N:52:GLN:HG3	1.92	0.52
1:A:1403:C:H1'	1:A:1500:A:C2	2.45	0.52
1:A:1250:A:C6	1:A:1251:A:C6	2.97	0.52
1:A:1073:U:OP2	5:E:57:LYS:NZ	2.35	0.52
11:K:72:ALA:HB1	11:K:77:MET:HG3	1.92	0.52
14:N:48:ALA:HB1	14:N:56:VAL:HG11	1.92	0.52
1:A:501:C:H2'	1:A:502:G:H8	1.74	0.52
13:M:3:ARG:HA	13:M:8:GLU:O	2.10	0.52
1:A:943:U:H2'	1:A:944:G:H5'	1.92	0.52
17:Q:93:GLN:HG2	17:Q:96:GLN:HE21	1.75	0.52
1:A:960:U:H4'	1:A:961:U:C5'	2.40	0.52
4:D:152:SER:O	4:D:155:LEU:HB2	2.09	0.51
8:H:114:THR:HG21	8:H:129:VAL:HG23	1.91	0.51
18:R:58:LEU:HD22	18:R:62:GLU:HB3	1.92	0.51
1:A:677:U:H3	1:A:713:G:H22	1.58	0.51
1:A:143:A:O3'	1:A:144:G:H8	1.93	0.51
11:K:14:VAL:HG11	11:K:40:ILE:HD11	1.90	0.51
14:N:29:ARG:HB3	14:N:33:VAL:HG22	1.91	0.51
5:E:142:LEU:O	5:E:143:ARG:HD3	2.10	0.51
1:A:1117:G:H5"	9:I:104:ARG:NH2	2.25	0.51
1:A:838:G:H2'	1:A:839:U:H5"	1.91	0.51
1:A:1201:A:H4'	1:A:1202:G:O5'	2.10	0.51
1:A:1055:A:N7	1:A:1200:C:N4	2.54	0.51
10:J:32:ALA:O	10:J:34:VAL:HG23	2.09	0.51
1:A:1518[B]:MA6:H102	1:A:1519[B]:MA6:H103	1.91	0.51
1:A:1374:A:C4	1:A:1375:A:C8	2.99	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:79:ARG:HA	10:J:79:ARG:CZ	2.40	0.51
1:A:476:G:H2'	1:A:477:G:C8	2.45	0.51
1:A:695:A:H61	1:A:797:C:H1'	1.75	0.51
1:A:1376:U:OP1	7:G:98:SER:OG	2.16	0.51
1:A:1068:G:H8	1:A:1068:G:OP2	1.92	0.51
7:G:108:ALA:O	7:G:119:ARG:HB3	2.10	0.51
1:A:721:G:OP2	18:R:53:ARG:HG3	2.11	0.51
1:A:1004:A:H5"	1:A:1025:U:C5	2.46	0.51
6:F:91:VAL:HG12	6:F:92:LYS:O	2.11	0.51
1:A:1327:C:OP2	21:U:12:LYS:NZ	2.42	0.51
1:A:540:G:H2'	1:A:541:G:C8	2.45	0.51
1:A:1026:G:O6	1:A:1035:A:N6	2.36	0.51
12:L:87:GLY:H	12:L:99:HIS:H	1.59	0.51
4:D:78:LEU:HD21	4:D:96:LEU:CB	2.40	0.51
1:A:1006:C:H2'	1:A:1007:C:C6	2.46	0.51
1:A:1003(A):G:C5	1:A:1004:A:H1'	2.45	0.51
4:D:102:ASP:OD1	4:D:103:ASN:N	2.44	0.51
7:G:78:ARG:HG3	7:G:156:TRP:CE3	2.45	0.51
15:O:29:VAL:O	15:O:33:THR:HB	2.10	0.51
3:C:51:GLY:O	3:C:71:ALA:N	2.26	0.51
2:B:23:ARG:O	2:B:24:TRP:HD1	1.94	0.51
15:O:14:GLU:HG3	15:O:15:PHE:CD1	2.45	0.51
17:Q:65:ILE:N	17:Q:65:ILE:HD12	2.26	0.51
1:A:278:G:C6	17:Q:95:TYR:HD2	2.28	0.51
3:C:130:VAL:HG22	3:C:134:ILE:HD11	1.93	0.51
1:A:503:C:H2'	1:A:504:C:H6	1.76	0.51
1:A:337:C:H2'	1:A:338:A:C8	2.45	0.51
4:D:101:LEU:O	4:D:105:VAL:HG23	2.11	0.51
10:J:89:ASP:HB2	10:J:91:PRO:HD2	1.92	0.51
10:J:19:SER:HB2	10:J:91:PRO:HG3	1.93	0.51
1:A:1008:C:N4	1:A:1021:G:H1	2.09	0.51
1:A:216:G:H2'	1:A:217:C:H6	1.75	0.51
1:A:1175:G:H2'	1:A:1176:A:C8	2.45	0.51
17:Q:63:ARG:HG2	17:Q:64:PRO:CD	2.40	0.51
11:K:47:VAL:HG12	11:K:48:ILE:HG23	1.92	0.51
4:D:107:ARG:HH12	4:D:114:ARG:NH2	2.08	0.51
1:A:976:G:OP1	14:N:32:SER:HB2	2.10	0.51
20:T:23:ARG:HG2	20:T:24:LEU:HD12	1.93	0.51
1:A:1359:C:O2'	1:A:1361:G:N7	2.43	0.51
20:T:89:ARG:NH2	20:T:104:LEU:HB3	2.26	0.51
1:A:1034:G:H2'	1:A:1035:A:H8	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:104:ARG:HG2	8:H:104:ARG:NH1	2.26	0.51
4:D:107:ARG:NH1	4:D:114:ARG:HH21	2.08	0.51
18:R:28:GLU:N	18:R:28:GLU:OE1	2.44	0.51
2:B:213:LEU:HD23	2:B:214:ILE:HD13	1.92	0.51
3:C:114:PRO:O	3:C:118:GLN:HG3	2.11	0.51
1:A:1518[B]:MA6:H93	1:A:1519[B]:MA6:N1	2.26	0.50
9:I:112:LYS:HE2	9:I:113:LYS:O	2.11	0.50
1:A:1305:G:O2'	1:A:1306:A:P	2.69	0.50
16:P:53:VAL:O	16:P:56:ALA:N	2.44	0.50
1:A:1369:C:H2'	1:A:1370:G:C8	2.46	0.50
1:A:106:C:C2'	1:A:107:G:H5'	2.41	0.50
8:H:114:THR:HG22	8:H:130:GLY:O	2.10	0.50
1:A:633:G:H2'	1:A:634:C:H6	1.76	0.50
1:A:943:U:C2'	1:A:944:G:H5'	2.42	0.50
1:A:514:C:H2'	1:A:515:G:C8	2.46	0.50
1:A:1133:G:H1	1:A:1141:C:H42	1.59	0.50
1:A:92:C:O2'	1:A:93:G:H5'	2.12	0.50
11:K:50:TYR:CE2	11:K:54:ARG:HD2	2.46	0.50
1:A:858:G:O2'	1:A:859:A:H5'	2.11	0.50
1:A:1305:G:H22	1:A:1331:G:H1'	1.76	0.50
1:A:491:G:C2	1:A:492:G:C8	2.99	0.50
18:R:74:ARG:HD3	18:R:81:PHE:HA	1.92	0.50
1:A:691:G:H2'	1:A:692:U:C6	2.46	0.50
1:A:41:G:H2'	1:A:42:G:C8	2.46	0.50
1:A:1530:G:OP1	1:A:1530:G:H4'	2.11	0.50
12:L:42:THR:HG22	12:L:52:LEU:HB3	1.93	0.50
10:J:79:ARG:HH12	10:J:82:ILE:HB	1.76	0.50
17:Q:40:LYS:HE2	17:Q:42:TYR:CZ	2.47	0.50
5:E:118:ILE:HG12	5:E:119:LEU:N	2.26	0.50
1:A:1131:G:H2'	1:A:1132:C:C6	2.47	0.50
1:A:457:C:H2'	1:A:458:C:C6	2.46	0.50
2:B:84:GLU:HB3	2:B:219:VAL:HG21	1.93	0.50
3:C:70:VAL:HG21	3:C:76:VAL:HG21	1.93	0.50
4:D:19:LEU:HB3	4:D:67:ILE:HG12	1.94	0.50
1:A:981:U:H5'	14:N:21:TYR:CZ	2.47	0.50
1:A:374:A:H2'	1:A:374:A:N3	2.26	0.50
13:M:48:LEU:HB3	13:M:53:VAL:HG23	1.94	0.50
3:C:114:PRO:HA	3:C:185:GLY:HA3	1.94	0.50
1:A:1260:C:O5'	1:A:1284:C:H4'	2.12	0.50
7:G:47:CYS:HA	7:G:50:ILE:HG22	1.94	0.50
12:L:7:ILE:O	12:L:10:LEU:N	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1406:U:H4'	1:A:1518[B]:MA6:H1'	1.94	0.50
1:A:1399:C:O2	1:A:1401:G:C5	2.65	0.50
1:A:1221:G:OP1	19:S:36:ARG:HD3	2.11	0.50
1:A:819:A:H4'	1:A:820:U:OP2	2.11	0.50
1:A:1409:C:H2'	1:A:1410:G:H8	1.77	0.49
1:A:421:U:H5'	1:A:422:C:H5	1.77	0.49
2:B:153:ARG:HB3	2:B:154:LEU:HD23	1.94	0.49
1:A:56:U:H2'	1:A:57:G:H8	1.76	0.49
1:A:661:G:H8	1:A:661:G:H5"	1.77	0.49
1:A:1305:G:O2'	1:A:1306:A:O5'	2.30	0.49
2:B:188:ALA:O	2:B:202:PRO:HA	2.12	0.49
1:A:321:A:H2'	1:A:322:C:H6	1.77	0.49
7:G:22:LEU:HD13	7:G:97:GLN:NE2	2.27	0.49
5:E:76:ILE:HG23	5:E:142:LEU:CD1	2.41	0.49
1:A:736:C:H2'	1:A:737:A:C8	2.47	0.49
1:A:514:C:H2'	1:A:515:G:H8	1.76	0.49
1:A:17:U:H2'	1:A:18:C:C6	2.48	0.49
15:O:34:LEU:HD23	15:O:34:LEU:C	2.32	0.49
1:A:92:C:O2	1:A:93:G:C8	2.65	0.49
12:L:113:ARG:HH11	12:L:116:SER:H	1.60	0.49
1:A:1366:C:H2'	1:A:1367:C:C6	2.45	0.49
4:D:21:LEU:HD11	4:D:67:ILE:HA	1.95	0.49
4:D:25:ARG:O	4:D:25:ARG:HG2	2.11	0.49
1:A:701:C:H5"	1:A:703:G:H5'	1.94	0.49
18:R:25:THR:HG22	18:R:42:ARG:HH22	1.77	0.49
3:C:202:ILE:HG22	3:C:204:LEU:HD23	1.95	0.49
1:A:77:G:H2'	1:A:78:G:H8	1.77	0.49
1:A:966:M2G:C5	1:A:967:5MC:HM52	2.48	0.49
2:B:16:HIS:NE2	2:B:204:ASN:N	2.60	0.49
1:A:371:G:O2'	1:A:372:C:H5'	2.11	0.49
5:E:82:VAL:HG12	5:E:134:ALA:HB1	1.94	0.49
1:A:1077:G:N2	1:A:1080:A:OP2	2.43	0.49
1:A:742:G:H2'	1:A:743:U:O4'	2.12	0.49
12:L:84:LEU:HD23	12:L:101:VAL:HG21	1.93	0.49
1:A:266:G:H5"	1:A:266:G:H8	1.77	0.49
1:A:858:G:O6	1:A:869:G:N7	2.45	0.49
3:C:130:VAL:HG21	3:C:153:VAL:HG21	1.94	0.49
3:C:77:ILE:HD13	3:C:84:ILE:HD12	1.94	0.49
12:L:27:LEU:HD23	12:L:28:LYS:HE2	1.95	0.49
3:C:167:TRP:HE3	3:C:168:ALA:H	1.58	0.49
1:A:688:G:O2'	1:A:704:A:N1	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:692:U:OP1	11:K:124:LYS:HE3	2.12	0.49
1:A:78:G:N2	1:A:79:G:H1'	2.28	0.49
1:A:1305:G:O2'	1:A:1306:A:C8	2.65	0.49
9:I:48:GLU:OE1	9:I:51:ARG:NH1	2.45	0.49
7:G:78:ARG:HG3	7:G:156:TRP:HE3	1.78	0.49
1:A:349:A:H2'	1:A:350:G:H5"	1.95	0.49
1:A:1168:A:H2'	1:A:1169:A:C8	2.47	0.49
1:A:731:G:O2'	1:A:732:C:H5'	2.12	0.49
1:A:1465:C:H2'	1:A:1466:C:O4'	2.13	0.49
15:O:18:PHE:CZ	15:O:21:ASP:HB2	2.47	0.49
1:A:463:A:H2'	1:A:474:G:O4'	2.12	0.49
1:A:815:A:N3	1:A:1527:C:O2'	2.34	0.49
2:B:157:ARG:HG2	2:B:158:LEU:N	2.28	0.49
18:R:39:VAL:HG13	18:R:40:LEU:HD23	1.95	0.49
1:A:1480:G:C6	1:A:1481:U:C4	3.00	0.49
1:A:571:U:H5"	1:A:572:A:OP2	2.13	0.49
4:D:157:LEU:O	4:D:160:GLN:HB2	2.12	0.49
1:A:758:G:N7	24:A:1974:HOH:O	2.33	0.49
5:E:69:VAL:HG12	5:E:71:LEU:HG	1.94	0.49
1:A:1201:A:H4'	1:A:1202:G:C5'	2.42	0.49
2:B:17:PHE:HD1	2:B:18:GLY:N	2.11	0.49
1:A:887:G:H1	1:A:910:C:H42	1.61	0.49
1:A:723:U:O2	1:A:723:U:H2'	2.13	0.49
1:A:279:A:C8	1:A:279:A:H5'	2.48	0.48
1:A:1516[A]:G:N1	1:A:1519[A]:MA6:OP2	2.46	0.48
1:A:1346:A:O2'	1:A:1347:G:OP2	2.24	0.48
15:O:55:GLY:O	15:O:59:MET:HG3	2.13	0.48
1:A:77:G:N2	1:A:78:G:C4	2.81	0.48
1:A:79:G:C2	1:A:80:G:N7	2.81	0.48
10:J:42:THR:HG23	10:J:67:THR:O	2.13	0.48
1:A:686:U:O2'	1:A:687:A:H8	1.94	0.48
14:N:37:PHE:C	14:N:39:LEU:H	2.15	0.48
6:F:53:ALA:HB3	6:F:86:ARG:CZ	2.43	0.48
1:A:986:A:H1'	19:S:55:LYS:HA	1.95	0.48
1:A:1269:A:N1	1:A:1312:G:O2'	2.41	0.48
19:S:18:LYS:HD3	19:S:31:ILE:HD11	1.94	0.48
1:A:646:U:H2'	1:A:647:C:C6	2.48	0.48
1:A:60:A:P	1:A:331:G:H22	2.36	0.48
1:A:1111:A:N6	3:C:177:THR:HB	2.24	0.48
1:A:1191:A:H2'	1:A:1192:C:H6	1.76	0.48
1:A:1158:C:N3	1:A:1181:G:N2	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:G:N3	1:A:66:G:H2'	2.28	0.48
15:O:17:ARG:HG3	15:O:17:ARG:NH1	2.23	0.48
9:I:19:LEU:HD22	9:I:59:PHE:CD2	2.48	0.48
1:A:500:G:H2'	1:A:501:C:C6	2.48	0.48
1:A:737:A:H2'	1:A:738:C:H6	1.77	0.48
8:H:100:ILE:HG23	8:H:112:LEU:HD11	1.95	0.48
16:P:10:GLY:HA3	16:P:14:ASN:O	2.12	0.48
1:A:1520[A]:G:H2'	1:A:1521:G:H8	1.78	0.48
1:A:77:G:O2'	1:A:78:G:H5'	2.13	0.48
3:C:27:LYS:HA	3:C:30:ARG:HH12	1.78	0.48
1:A:828:A:H4'	1:A:828:A:OP1	2.14	0.48
9:I:8:GLY:HA2	9:I:79:LEU:HD13	1.95	0.48
1:A:937:A:H5"	1:A:938:A:OP2	2.13	0.48
1:A:7:G:H5'	1:A:298:A:H5'	1.95	0.48
3:C:29:TYR:HE1	10:J:11:PHE:CE1	2.31	0.48
7:G:26:PHE:CE2	7:G:30:ILE:HD11	2.49	0.48
1:A:1425:U:H2'	1:A:1426:C:H6	1.77	0.48
1:A:1425:U:H2'	1:A:1426:C:C6	2.48	0.48
1:A:130:A:H5'	17:Q:63:ARG:NE	2.29	0.48
7:G:91:VAL:CG1	7:G:96:GLN:HG3	2.43	0.48
15:O:87:ILE:HG22	15:O:88:ARG:N	2.28	0.48
1:A:1526:G:H2'	1:A:1527:C:H6	1.79	0.48
3:C:121:ALA:HB2	3:C:187:ALA:HB1	1.95	0.48
1:A:933:G:O6	7:G:3:ARG:NH2	2.46	0.48
1:A:219:C:O2'	1:A:381:C:H5'	2.13	0.48
1:A:381:C:H2'	1:A:382:A:O4'	2.14	0.48
12:L:25:PRO:CA	12:L:27:LEU:H	2.26	0.48
9:I:111:ARG:O	9:I:113:LYS:HD2	2.13	0.48
1:A:320:C:O2'	1:A:1435:G:H1'	2.14	0.48
15:O:64:ARG:HG3	15:O:88:ARG:NH1	2.29	0.48
4:D:57:ARG:HG3	4:D:202:LEU:HD13	1.96	0.48
1:A:142:G:N3	1:A:196:A:H2	2.12	0.48
6:F:80:ARG:HH11	6:F:80:ARG:HG2	1.78	0.48
1:A:1326:C:OP2	21:U:6:ARG:NH2	2.47	0.48
1:A:253:U:H2'	1:A:254:G:H8	1.79	0.48
3:C:91:LEU:HD23	3:C:92:ALA:N	2.29	0.48
17:Q:59:ILE:HG23	17:Q:71:PHE:HB3	1.96	0.48
1:A:551:U:O2'	12:L:86:ARG:HD2	2.14	0.48
19:S:25:LYS:HD2	19:S:25:LYS:N	2.28	0.48
2:B:59:GLU:HB2	2:B:221:LEU:HD11	1.96	0.48
4:D:18:LYS:HE2	4:D:20:TYR:CE2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:C:OP2	12:L:69:TYR:OH	2.28	0.48
1:A:960:U:H1'	1:A:1223:C:H5'	1.96	0.48
1:A:362:G:OP1	12:L:61:THR:HG22	2.14	0.48
1:A:448:A:P	1:A:485:G:H22	2.37	0.48
1:A:1493:A:H2'	1:A:1494:G:H8	1.79	0.48
2:B:217:ARG:HD3	2:B:217:ARG:HA	1.58	0.48
1:A:1057:G:C4	1:A:1058:G:C8	3.02	0.48
21:U:6:ARG:NH1	21:U:15:ARG:HH12	2.11	0.48
1:A:1053:G:HO2'	1:A:1199:U:H5	1.60	0.48
1:A:41:G:H2'	1:A:42:G:H8	1.79	0.48
1:A:321:A:H2'	1:A:322:C:C6	2.48	0.48
5:E:137:GLU:HG2	5:E:140:ARG:HH11	1.79	0.48
2:B:115:LEU:HD13	2:B:145:LEU:HB3	1.95	0.48
9:I:126:SER:HB2	9:I:127:LYS:HD2	1.96	0.48
1:A:1063:C:OP2	1:A:1064:G:O2'	2.30	0.48
7:G:144:MET:O	7:G:147:ALA:HB3	2.12	0.48
5:E:18:ARG:HG2	5:E:19:MET:N	2.25	0.48
12:L:28:LYS:HG3	12:L:33:ARG:CZ	2.44	0.47
1:A:1498:UR3:O2'	1:A:1499:A:OP2	2.21	0.47
3:C:15:THR:HG21	3:C:179:ARG:O	2.14	0.47
1:A:1305:G:H3'	21:U:4:GLY:O	2.14	0.47
1:A:18:C:H2'	1:A:19:C:O4'	2.14	0.47
13:M:33:ALA:O	13:M:37:THR:OG1	2.16	0.47
1:A:664:G:OP1	18:R:64:ARG:HD2	2.14	0.47
1:A:1126:U:H6	1:A:1126:U:O5'	1.97	0.47
1:A:75:G:C2	1:A:96:G:C2	3.01	0.47
1:A:79:G:H5'	1:A:80:G:OP2	2.13	0.47
1:A:835:U:H3	1:A:851:G:H1	1.62	0.47
1:A:346:G:H2'	1:A:347:G:O4'	2.14	0.47
1:A:1097:C:H2'	1:A:1098:C:C6	2.49	0.47
1:A:1098:C:H2'	1:A:1099:G:O4'	2.14	0.47
1:A:1258:G:H2'	1:A:1259:C:C6	2.49	0.47
18:R:76:LEU:HD23	18:R:76:LEU:HA	1.56	0.47
2:B:71:VAL:HB	2:B:164:VAL:HG12	1.97	0.47
1:A:1498:UR3:C4'	1:A:1519[A]:MA6:H2	2.43	0.47
1:A:1354:C:H2'	1:A:1355:G:H8	1.80	0.47
4:D:187:ARG:HD2	4:D:187:ARG:HA	1.43	0.47
1:A:476:G:H2'	1:A:477:G:H8	1.78	0.47
1:A:337:C:H2'	1:A:338:A:H8	1.78	0.47
16:P:58:TYR:CE1	16:P:62:VAL:HG21	2.48	0.47
12:L:46:LYS:NZ	12:L:47:LYS:HE2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:G:H2'	1:A:22:G:C8	2.49	0.47
1:A:675:A:O2'	11:K:114:VAL:O	2.31	0.47
1:A:1451:A:H5"	1:A:1452:C:H5	1.79	0.47
14:N:40:CYS:H	14:N:43:CYS:HB2	1.78	0.47
18:R:39:VAL:CG1	18:R:40:LEU:HD23	2.44	0.47
1:A:1211:U:H1'	1:A:1213:A:N3	2.30	0.47
12:L:85:ILE:HG23	12:L:98:TYR:HB3	1.95	0.47
1:A:78:G:N1	1:A:92:C:N4	2.62	0.47
2:B:223:ILE:HG13	2:B:223:ILE:H	1.59	0.47
2:B:98:LEU:HB2	2:B:101:MET:CG	2.45	0.47
1:A:1118:C:H1'	1:A:1179:A:C4	2.49	0.47
13:M:19:LEU:O	13:M:22:ILE:HG13	2.14	0.47
3:C:11:ARG:HB3	3:C:16:ARG:HB2	1.95	0.47
1:A:833:U:H2'	1:A:834:C:C6	2.49	0.47
1:A:1126:U:HO2'	1:A:1127:G:P	2.37	0.47
9:I:5:TYR:CD2	9:I:6:GLY:N	2.82	0.47
1:A:1093:A:N3	1:A:1109:C:O2'	2.44	0.47
1:A:1250:A:H4'	9:I:68:GLY:N	2.30	0.47
11:K:93:GLN:HA	11:K:96:ARG:HG3	1.96	0.47
20:T:10:LEU:O	20:T:13:LEU:HD12	2.14	0.47
1:A:255:G:C2	1:A:272:C:C2	3.03	0.47
5:E:87:SER:HB3	5:E:131:ILE:HD13	1.96	0.47
1:A:1516[A]:G:H2'	1:A:1518[A]:MA6:OP2	2.15	0.47
11:K:114:VAL:HG23	11:K:115:PRO:HD2	1.97	0.47
13:M:36:LYS:HB2	13:M:59:TYR:CE2	2.50	0.47
1:A:778:G:H2'	1:A:779:C:O4'	2.13	0.47
8:H:86:ILE:HG21	8:H:133:LEU:HD22	1.96	0.47
1:A:1435:G:H2'	1:A:1436:U:H6	1.79	0.47
11:K:70:LYS:NZ	11:K:70:LYS:HB3	2.30	0.47
15:O:14:GLU:HG3	15:O:15:PHE:CE1	2.50	0.47
4:D:184:LYS:HE3	4:D:184:LYS:HB2	1.74	0.47
17:Q:22:LEU:HA	17:Q:22:LEU:HD12	1.58	0.47
17:Q:83:ASP:N	17:Q:83:ASP:OD1	2.46	0.47
1:A:1405:G:O2'	1:A:1518[A]:MA6:O2'	2.28	0.47
1:A:1313:U:H5	19:S:4:SER:HB2	1.79	0.47
2:B:218:ALA:O	2:B:222:ILE:HG13	2.14	0.47
2:B:219:VAL:HA	2:B:222:ILE:HD12	1.97	0.47
2:B:215:LEU:HD23	2:B:215:LEU:HA	1.72	0.47
10:J:64:GLU:HG2	14:N:59:ALA:HA	1.96	0.46
1:A:542:G:H2'	1:A:543:C:H6	1.80	0.46
15:O:12:ILE:HG23	15:O:27:VAL:HG11	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:60:ALA:HA	11:K:63:LEU:HD12	1.97	0.46
1:A:502:G:H2'	1:A:503:C:O4'	2.15	0.46
1:A:1402:4OC:O2	1:A:1500:A:N1	2.48	0.46
7:G:69:VAL:HG12	7:G:100:ALA:HA	1.97	0.46
2:B:24:TRP:HZ3	2:B:29:ALA:HB2	1.80	0.46
1:A:186:C:H2'	1:A:187:C:C6	2.49	0.46
4:D:132:ARG:HG3	4:D:133:VAL:N	2.29	0.46
1:A:925:G:C2	1:A:927:G:C8	3.03	0.46
17:Q:97:SER:O	17:Q:98:LEU:HD12	2.14	0.46
12:L:28:LYS:C	12:L:30:ALA:N	2.69	0.46
15:O:42:HIS:CD2	15:O:43:LEU:HD23	2.50	0.46
1:A:1063:C:H2'	1:A:1064:G:C8	2.49	0.46
18:R:40:LEU:HB3	18:R:79:LEU:HD11	1.97	0.46
6:F:2:ARG:O	6:F:66:GLU:HA	2.15	0.46
7:G:41:ARG:HH11	7:G:41:ARG:HB3	1.80	0.46
17:Q:27:PHE:CE1	17:Q:36:ILE:HD11	2.50	0.46
1:A:451:A:OP1	1:A:451:A:C8	2.67	0.46
7:G:16:LEU:HD21	9:I:42:ARG:HG2	1.97	0.46
1:A:1070:U:H2'	1:A:1071:C:H6	1.80	0.46
13:M:97:PRO:HB2	13:M:101:GLN:OE1	2.15	0.46
2:B:30:ARG:HD2	2:B:31:TYR:CZ	2.49	0.46
20:T:84:LEU:HD23	20:T:84:LEU:HA	1.78	0.46
1:A:78:G:H1	1:A:92:C:N4	2.14	0.46
4:D:64:LEU:HD12	4:D:75:PHE:CZ	2.50	0.46
2:B:98:LEU:O	2:B:101:MET:HG3	2.16	0.46
1:A:299:G:C6	1:A:300:A:C6	3.03	0.46
19:S:28:LYS:HG2	19:S:29:ARG:H	1.81	0.46
4:D:70:ILE:HG22	4:D:71:SER:O	2.16	0.46
1:A:283:C:C2	1:A:284:G:C8	3.02	0.46
11:K:58:PRO:HD3	11:K:89:ALA:HB1	1.96	0.46
13:M:88:ARG:NH1	19:S:3:ARG:HH21	2.14	0.46
3:C:174:PRO:HB2	3:C:177:THR:HG22	1.96	0.46
4:D:61:LYS:HZ2	4:D:62:GLN:N	2.13	0.46
7:G:51:GLN:HB2	7:G:58:PRO:HD3	1.97	0.46
9:I:2:GLU:HG3	9:I:3:GLN:N	2.31	0.46
21:U:6:ARG:CZ	21:U:15:ARG:HH12	2.29	0.46
1:A:532:A:O2'	1:A:533:A:OP1	2.20	0.46
1:A:1242:C:OP1	21:U:10:ARG:NH1	2.45	0.46
4:D:4:TYR:OH	4:D:7:PRO:O	2.24	0.46
5:E:51:VAL:HB	5:E:52:PRO:HD3	1.97	0.46
1:A:131:C:O2	1:A:262:A:H2	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:GLU:HG2	2:B:40:HIS:HD2	1.79	0.46
8:H:111:ILE:HG22	8:H:134:ILE:HD12	1.96	0.46
1:A:1005:A:H1'	1:A:1026:G:H22	1.81	0.46
10:J:57:LYS:O	10:J:60:ARG:NH1	2.48	0.46
2:B:51:LEU:O	2:B:55:PHE:HB2	2.15	0.46
9:I:88:TYR:CD2	9:I:89:ASN:HB2	2.49	0.46
1:A:1305:G:C8	1:A:1305:G:OP2	2.68	0.46
1:A:1063:C:C6	1:A:1064:G:C8	3.04	0.46
1:A:687:A:H4'	1:A:688:G:O5'	2.16	0.46
4:D:70:ILE:HG22	4:D:71:SER:N	2.30	0.46
1:A:1037:C:H2'	1:A:1038:C:C6	2.51	0.46
1:A:397:A:H5'	1:A:398:C:OP1	2.15	0.46
1:A:1499:A:C1'	1:A:1520[A]:G:H5'	2.46	0.46
5:E:12:LEU:HD13	5:E:31:LEU:HB2	1.96	0.46
1:A:1443:G:H5"	1:A:1446:A:OP1	2.16	0.46
9:I:39:GLY:O	9:I:40:LEU:HD23	2.16	0.46
3:C:71:ALA:HB1	3:C:109:PRO:HG3	1.97	0.46
1:A:1186:G:H2'	1:A:1187:G:O4'	2.15	0.46
1:A:824:C:H2'	1:A:825:G:C8	2.50	0.46
1:A:1035:A:H2'	1:A:1036:G:C8	2.50	0.46
1:A:1257:U:H4'	1:A:1258:G:O5'	2.15	0.46
13:M:48:LEU:HD12	13:M:53:VAL:HG23	1.98	0.46
1:A:1301:U:HO2'	1:A:1302:U:P	2.38	0.46
6:F:28:ARG:O	6:F:32:ASN:HB2	2.16	0.46
12:L:58:VAL:HG12	12:L:59:ARG:O	2.15	0.46
7:G:18:TYR:OH	7:G:58:PRO:HG2	2.16	0.46
14:N:24:CYS:HB2	14:N:39:LEU:C	2.36	0.46
2:B:223:ILE:O	2:B:227:GLY:N	2.48	0.46
10:J:48:THR:OG1	10:J:62:HIS:CD2	2.69	0.46
1:A:949:A:C2	1:A:1233:G:N3	2.84	0.46
1:A:222:U:H2'	1:A:223:U:C6	2.50	0.46
12:L:27:LEU:HG	12:L:28:LYS:H	1.81	0.46
1:A:1504:G:H4'	1:A:1505:G:H5'	1.98	0.46
1:A:75:G:N1	1:A:96:G:C6	2.83	0.46
2:B:84:GLU:OE1	2:B:216:SER:HA	2.16	0.46
21:U:13:ILE:HG22	21:U:22:ARG:CZ	2.46	0.46
14:N:46:GLU:O	14:N:49:HIS:HB2	2.15	0.46
1:A:1197:G:H5"	24:A:2066:HOH:O	2.16	0.45
19:S:39:THR:HG22	19:S:40:ILE:O	2.16	0.45
5:E:17:ALA:CB	5:E:26:PHE:HD2	2.29	0.45
1:A:880:C:OP1	12:L:8:ASN:ND2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:922:G:C2	1:A:1396:A:C6	3.04	0.45
1:A:200:G:H2'	1:A:201:C:C6	2.50	0.45
1:A:679:C:H2'	1:A:680:C:C6	2.51	0.45
8:H:86:ILE:HG22	8:H:87:SER:N	2.31	0.45
1:A:1330:U:H2'	1:A:1331:G:H5'	1.99	0.45
1:A:1065:U:H4'	1:A:1066:C:O5'	2.16	0.45
1:A:436:C:H5'	4:D:156:GLU:OE1	2.16	0.45
3:C:81:GLY:O	3:C:84:ILE:HG22	2.17	0.45
13:M:39:ILE:HG23	13:M:52:GLU:OE2	2.15	0.45
1:A:1228:C:O3'	13:M:116:THR:HG23	2.16	0.45
1:A:1196:U:OP1	1:A:1197:G:H5'	2.17	0.45
1:A:1355:G:H2'	1:A:1356:G:C8	2.51	0.45
3:C:112:SER:O	3:C:115:LEU:HB2	2.15	0.45
1:A:1485:U:H2'	1:A:1485:U:O2	2.16	0.45
11:K:85:ARG:HD3	11:K:113:PRO:HD3	1.98	0.45
14:N:32:SER:O	14:N:40:CYS:HB2	2.16	0.45
8:H:105:ARG:HA	8:H:105:ARG:HD3	1.77	0.45
7:G:22:LEU:O	7:G:25:ALA:HB3	2.16	0.45
2:B:133:LYS:O	2:B:137:ARG:HG3	2.16	0.45
1:A:892:A:H2'	1:A:893:C:C6	2.51	0.45
5:E:105:VAL:HB	5:E:106:PRO:HD3	1.99	0.45
19:S:74:PHE:N	19:S:74:PHE:CD1	2.84	0.45
1:A:455:C:H6	1:A:455:C:O5'	1.99	0.45
1:A:35:G:H2'	1:A:36:C:C6	2.51	0.45
1:A:959:A:H3'	1:A:960:U:H5"	1.98	0.45
13:M:88:ARG:HG3	13:M:98:VAL:HG13	1.97	0.45
17:Q:5:VAL:O	17:Q:6:LEU:HD23	2.15	0.45
8:H:46:LYS:HG3	8:H:64:LYS:HB3	1.98	0.45
2:B:20:GLU:HB2	2:B:190:THR:HB	1.98	0.45
1:A:544:G:C6	1:A:545:C:C4	3.05	0.45
12:L:48:PRO:HG2	12:L:92:0TD:H3	1.98	0.45
1:A:1057:G:H4'	3:C:154:SER:HG	1.81	0.45
15:O:45:VAL:HG12	15:O:46:HIS:H	1.80	0.45
10:J:24:VAL:HG13	10:J:34:VAL:HG11	1.98	0.45
7:G:94:ARG:O	7:G:97:GLN:HB3	2.16	0.45
1:A:731:G:OP1	1:A:766:A:H1'	2.17	0.45
1:A:109:A:H2'	1:A:326:G:N2	2.31	0.45
6:F:67:MET:HE1	6:F:71:ARG:HB2	1.98	0.45
15:O:29:VAL:HG13	15:O:63:ARG:HG3	1.99	0.45
1:A:79:G:C5	1:A:91:C:N3	2.84	0.45
1:A:1306:A:C2	1:A:1307:U:H1'	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:53:VAL:O	16:P:55:ARG:N	2.49	0.45
1:A:1412:C:H2'	1:A:1413:A:C8	2.52	0.45
13:M:50:GLU:HG3	13:M:51:ALA:N	2.32	0.45
20:T:70:SER:HA	20:T:73:HIS:CD2	2.51	0.45
13:M:27:LYS:HA	13:M:27:LYS:HD2	1.53	0.45
10:J:50:ILE:CD1	10:J:50:ILE:H	2.28	0.45
3:C:116:VAL:O	3:C:120:VAL:HG23	2.16	0.45
1:A:328:C:O2'	1:A:329:A:OP2	2.27	0.45
5:E:93:PRO:HD2	8:H:105:ARG:NH2	2.31	0.45
1:A:1509:C:N4	1:A:1526:G:H1	2.15	0.45
1:A:909:A:H2'	1:A:910:C:O4'	2.17	0.45
12:L:46:LYS:HD2	12:L:94:PRO:CG	2.47	0.45
10:J:7:LYS:HB3	10:J:97:GLU:HB2	1.99	0.45
16:P:4:ILE:HG21	16:P:74:LEU:HD11	1.98	0.45
8:H:1:MET:HG2	8:H:2:LEU:N	2.32	0.45
12:L:60:LEU:HA	12:L:60:LEU:HD13	1.68	0.45
1:A:1381:U:N1	7:G:156:TRP:HH2	2.15	0.45
17:Q:21:VAL:O	17:Q:41:LYS:HA	2.16	0.45
7:G:135:VAL:HG12	7:G:139:GLU:OE2	2.17	0.45
2:B:114:ARG:HD2	2:B:118:LEU:HG	1.99	0.45
4:D:203:VAL:O	4:D:206:PHE:HB3	2.17	0.45
9:I:17:VAL:HG11	9:I:81:ILE:HA	1.99	0.45
6:F:86:ARG:O	6:F:87:ARG:HG2	2.16	0.45
18:R:58:LEU:HA	18:R:58:LEU:HD23	1.60	0.45
1:A:140:A:H2'	1:A:141:A:O4'	2.17	0.45
1:A:273:A:N6	1:A:274:A:C6	2.85	0.45
7:G:44:TYR:O	7:G:48:LYS:HG3	2.17	0.45
20:T:56:MET:HG2	20:T:84:LEU:HD13	1.99	0.45
1:A:1190:G:O3'	3:C:3:ASN:HB2	2.17	0.45
4:D:155:LEU:HD23	4:D:156:GLU:H	1.82	0.45
20:T:92:LEU:HA	20:T:92:LEU:HD22	1.60	0.45
3:C:10:PHE:CE2	3:C:178:LEU:HB2	2.51	0.45
1:A:475:G:C4	1:A:476:G:C8	3.05	0.44
19:S:18:LYS:O	19:S:22:LEU:HG	2.16	0.44
17:Q:10:VAL:HG23	17:Q:55:ASP:O	2.17	0.44
7:G:27:ILE:HD11	7:G:43:PHE:HB3	1.98	0.44
1:A:1305:G:H5"	21:U:4:GLY:HA3	1.99	0.44
1:A:112:G:O2'	1:A:113:G:H5'	2.18	0.44
5:E:76:ILE:HG23	5:E:142:LEU:HD11	1.99	0.44
1:A:253:U:H2'	1:A:254:G:C8	2.53	0.44
7:G:113:GLU:HG2	7:G:113:GLU:H	1.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:40:LYS:HG2	17:Q:42:TYR:CE1	2.52	0.44
2:B:10:LEU:C	2:B:12:GLU:H	2.20	0.44
11:K:119:CYS:O	11:K:121:PRO:HD3	2.18	0.44
6:F:98:LEU:HA	6:F:98:LEU:HD23	1.68	0.44
2:B:51:LEU:HG	2:B:201:ILE:HG23	1.99	0.44
1:A:1278:U:H5'	1:A:1279:A:O4'	2.16	0.44
1:A:976:G:C8	1:A:1358:U:O2	2.70	0.44
2:B:100:GLY:N	2:B:176:GLU:OE2	2.39	0.44
1:A:1241:G:H2'	1:A:1242:C:H6	1.82	0.44
3:C:187:ALA:HB3	3:C:198:VAL:HB	1.99	0.44
3:C:172:ARG:CZ	3:C:172:ARG:HB2	2.47	0.44
1:A:130:A:H1'	1:A:263:A:O2'	2.18	0.44
1:A:106:C:O2'	1:A:107:G:H5'	2.18	0.44
1:A:1211:U:H1'	1:A:1213:A:C2	2.52	0.44
1:A:376:G:OP2	16:P:67:THR:HG21	2.17	0.44
1:A:518:C:H4'	1:A:519:C:O5'	2.16	0.44
1:A:629:G:H2'	1:A:630:G:O4'	2.18	0.44
7:G:74:GLU:O	7:G:88:PRO:HA	2.16	0.44
5:E:110:LEU:HA	5:E:110:LEU:HD23	1.59	0.44
1:A:858:G:C6	1:A:869:G:C8	3.05	0.44
8:H:116:LYS:HZ2	8:H:127:LEU:HD12	1.80	0.44
2:B:97:TRP:CZ2	2:B:101:MET:HB2	2.52	0.44
1:A:955:U:H1'	1:A:1227:A:H61	1.83	0.44
2:B:87:ARG:HH21	2:B:219:VAL:HB	1.82	0.44
2:B:24:TRP:CZ3	2:B:26:PRO:HA	2.51	0.44
1:A:877:C:O2'	1:A:878:G:H5'	2.17	0.44
4:D:61:LYS:HD3	4:D:206:PHE:CE2	2.53	0.44
3:C:167:TRP:HE3	3:C:168:ALA:N	2.16	0.44
1:A:1191:A:C4	1:A:1192:C:C5	3.06	0.44
1:A:1157:A:H4'	1:A:1158:C:O5'	2.17	0.44
17:Q:31:LEU:HA	17:Q:31:LEU:HD12	1.83	0.44
7:G:47:CYS:O	7:G:50:ILE:HG22	2.18	0.44
13:M:88:ARG:HH11	19:S:3:ARG:HH21	1.66	0.44
1:A:824:C:H2'	1:A:825:G:H8	1.83	0.44
17:Q:76:LEU:HD11	17:Q:79:SER:HB2	1.98	0.44
11:K:91:ARG:HH12	18:R:88:LYS:NZ	2.15	0.44
1:A:1505:G:H3'	1:A:1505:G:C8	2.52	0.44
1:A:407:G:N2	1:A:436:C:C2	2.85	0.44
1:A:1250:A:O2'	9:I:68:GLY:HA2	2.18	0.44
1:A:540:G:H2'	1:A:541:G:H8	1.80	0.44
1:A:447:G:H2'	1:A:485:G:N2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1244:C:H42	1:A:1293:G:H1	1.66	0.44
12:L:27:LEU:C	12:L:29:GLY:N	2.61	0.44
4:D:8:VAL:O	4:D:11:LEU:N	2.37	0.44
1:A:92:C:H2'	1:A:93:G:C8	2.53	0.44
4:D:187:ARG:HH22	4:D:188:LEU:HD12	1.82	0.44
1:A:1241:G:H2'	1:A:1242:C:C6	2.53	0.44
8:H:119:LEU:HD12	8:H:124:ALA:HA	1.99	0.44
20:T:20:LEU:O	20:T:23:ARG:HB3	2.18	0.44
1:A:1450:U:O2'	1:A:1451:A:H8	2.01	0.44
1:A:1237:C:N4	1:A:1336:C:O2	2.51	0.44
2:B:139:LYS:NZ	2:B:143:GLU:HG3	2.33	0.44
4:D:99:SER:HB3	4:D:139:ARG:HG3	1.99	0.44
1:A:393:A:C2	1:A:394:G:C8	3.06	0.44
1:A:234:C:H2'	1:A:235:C:C6	2.53	0.44
8:H:20:TYR:HA	8:H:65:TYR:CZ	2.52	0.44
1:A:560:U:H5'	1:A:566:G:C2	2.52	0.44
1:A:440:A:H5'	1:A:442:C:OP2	2.18	0.44
1:A:243:A:H4'	1:A:244:U:H5"	2.00	0.44
12:L:82:VAL:O	12:L:106:ASP:HB2	2.18	0.44
15:O:81:LEU:HA	15:O:81:LEU:HD23	1.79	0.44
1:A:959:A:O2'	1:A:984:C:O2'	2.34	0.44
1:A:820:U:H4'	1:A:821:G:OP2	2.18	0.44
19:S:73:GLU:HB2	19:S:74:PHE:CE1	2.53	0.44
13:M:107:ALA:HB3	13:M:111:LYS:HE3	2.00	0.44
12:L:41:ARG:HG2	12:L:42:THR:N	2.33	0.43
3:C:134:ILE:HG21	3:C:167:TRP:O	2.18	0.43
1:A:1285:A:H4'	1:A:1286:A:O5'	2.18	0.43
4:D:24:GLU:HG2	4:D:25:ARG:H	1.83	0.43
4:D:47:ARG:HG2	4:D:48:ALA:N	2.33	0.43
1:A:229:U:O2'	16:P:23:ASP:HB2	2.18	0.43
17:Q:81:ARG:HE	17:Q:84:LEU:CD1	2.24	0.43
9:I:10:ARG:O	9:I:11:LYS:C	2.57	0.43
1:A:88:A:H2'	1:A:89:C:O4'	2.18	0.43
9:I:79:LEU:HA	9:I:79:LEU:HD23	1.88	0.43
13:M:8:GLU:HG3	13:M:22:ILE:HG23	1.99	0.43
1:A:945:G:O6	1:A:1236:A:N1	2.50	0.43
1:A:1265:G:C6	1:A:1266:G:C6	3.06	0.43
6:F:7:ASN:HD21	18:R:34:TYR:HE1	1.66	0.43
20:T:29:LYS:O	20:T:32:ALA:HB3	2.17	0.43
15:O:85:LEU:HD23	15:O:85:LEU:HA	1.65	0.43
2:B:187:LEU:HD22	2:B:187:LEU:HA	1.73	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:A:O2'	1:A:453:A:O5'	2.35	0.43
13:M:12:ASN:N	13:M:45:VAL:HB	2.33	0.43
6:F:14:LEU:HB2	6:F:19:LEU:HD12	2.00	0.43
8:H:104:ARG:HG3	8:H:138:TRP:CE3	2.53	0.43
1:A:1071:C:O2'	1:A:1072:G:H5'	2.17	0.43
12:L:124:LYS:HA	12:L:125:PRO:HD3	1.84	0.43
1:A:376:G:H5"	16:P:5:ARG:HD2	1.99	0.43
2:B:144:ARG:O	2:B:147:LYS:HB3	2.18	0.43
12:L:6:THR:H	12:L:9:GLN:HB2	1.82	0.43
2:B:185:ILE:HA	2:B:199:TYR:O	2.19	0.43
7:G:129:GLU:OE1	7:G:131:LYS:HE2	2.18	0.43
2:B:114:ARG:NH1	2:B:118:LEU:HD21	2.21	0.43
1:A:1497:G:O2'	1:A:1518[A]:MA6:H92	2.18	0.43
10:J:53:PRO:HA	14:N:41:ARG:NH2	2.34	0.43
1:A:79:G:C4	1:A:91:C:O2	2.71	0.43
1:A:93:G:O2'	1:A:95:U:H5'	2.17	0.43
4:D:35:ARG:N	4:D:35:ARG:HD2	2.33	0.43
1:A:1226:C:H2'	13:M:103:THR:OG1	2.19	0.43
8:H:124:ALA:O	8:H:128:GLY:N	2.49	0.43
1:A:539:A:H2'	1:A:540:G:C8	2.54	0.43
1:A:1493:A:H2'	1:A:1494:G:C8	2.54	0.43
8:H:50:ARG:HA	8:H:59:LEU:HD23	2.00	0.43
1:A:1029:C:H2'	1:A:1030:C:H6	1.83	0.43
8:H:13:ILE:HG21	8:H:13:ILE:HD13	1.72	0.43
1:A:1119:C:OP1	9:I:9:ARG:NH2	2.51	0.43
3:C:159:GLY:HA2	3:C:193:TYR:CG	2.54	0.43
1:A:1148:U:O2'	9:I:14:VAL:HG21	2.19	0.43
4:D:38:TYR:HB2	4:D:39:PRO:HD2	2.00	0.43
11:K:59:TYR:CE1	11:K:63:LEU:HD21	2.54	0.43
1:A:981:U:H5'	14:N:21:TYR:CE1	2.54	0.43
13:M:36:LYS:HB2	13:M:59:TYR:HE2	1.83	0.43
1:A:115:G:O2'	1:A:116:A:OP2	2.24	0.43
2:B:233:SER:HA	2:B:234:PRO:HD3	1.91	0.43
12:L:31:PRO:HB2	12:L:32:PHE:CD2	2.54	0.43
1:A:1018:C:H2'	1:A:1019:C:O4'	2.18	0.43
11:K:95:ILE:H	11:K:95:ILE:HG13	1.51	0.43
12:L:120:TYR:CD2	12:L:120:TYR:N	2.86	0.43
1:A:1355:G:H2'	1:A:1356:G:H8	1.83	0.43
1:A:1145:C:HO2'	1:A:1146:A:C5'	2.28	0.43
1:A:858:G:C6	1:A:869:G:N7	2.87	0.43
3:C:27:LYS:O	3:C:30:ARG:NH2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1329:A:H2'	1:A:1330:U:O4'	2.18	0.43
1:A:1091:U:O2	1:A:1093:A:C8	2.71	0.43
5:E:76:ILE:H	5:E:76:ILE:HG13	1.38	0.43
1:A:60:A:H4'	1:A:61:G:O5'	2.18	0.43
1:A:524:G:H2'	1:A:525:C:C6	2.53	0.43
1:A:355:C:C4	1:A:356:A:N7	2.86	0.43
13:M:78:ILE:O	13:M:81:LEU:HD12	2.18	0.43
2:B:60:ASP:CG	2:B:64:ARG:HH12	2.16	0.43
17:Q:38:ARG:HA	17:Q:38:ARG:HD3	1.57	0.43
7:G:6:ARG:O	7:G:6:ARG:HG3	2.17	0.43
4:D:15:GLU:HB3	4:D:63:LYS:HD3	2.00	0.43
1:A:1437:C:H2'	1:A:1438:G:C8	2.53	0.43
7:G:88:PRO:O	7:G:89:MET:HB3	2.19	0.43
1:A:953:G:H2'	1:A:954:G:O4'	2.19	0.43
5:E:56:GLN:NE2	5:E:56:GLN:HA	2.34	0.43
11:K:106:LYS:HD2	11:K:106:LYS:HA	1.85	0.43
2:B:191:ASP:N	2:B:191:ASP:OD1	2.50	0.43
2:B:54:THR:O	2:B:58:ILE:HG13	2.19	0.43
3:C:23:TYR:HE1	10:J:67:THR:HG23	1.83	0.43
1:A:344:A:H5'	1:A:345:C:H5	1.81	0.43
8:H:45:ILE:HD12	8:H:61:VAL:HG13	2.01	0.43
2:B:142:LEU:HD23	2:B:142:LEU:HA	1.83	0.43
17:Q:29:HIS:ND1	17:Q:30:PRO:HD2	2.33	0.43
1:A:1255:G:N2	1:A:1283:G:H1'	2.34	0.43
1:A:1007:C:O2	1:A:1023:G:N1	2.51	0.43
9:I:8:GLY:CA	9:I:79:LEU:HB3	2.49	0.43
1:A:509:A:C3'	1:A:509:A:C8	3.02	0.43
1:A:986:A:H1'	19:S:54:GLY:O	2.18	0.43
1:A:991:U:O2	1:A:993:G:H8	2.02	0.43
13:M:23:TYR:HB2	13:M:67:GLU:OE2	2.18	0.43
18:R:26:LEU:HA	18:R:26:LEU:HD12	1.62	0.43
4:D:53:ASP:OD1	4:D:53:ASP:N	2.51	0.43
18:R:31:LEU:HD23	18:R:31:LEU:HA	1.63	0.43
2:B:76:GLN:HG3	2:B:206:ASP:CG	2.39	0.43
2:B:187:LEU:HD22	2:B:201:ILE:O	2.19	0.43
9:I:19:LEU:HD12	9:I:84:ALA:HB3	2.01	0.43
8:H:104:ARG:CZ	8:H:138:TRP:CZ2	3.02	0.43
1:A:436:C:H2'	1:A:437:U:H6	1.83	0.43
1:A:1089:G:C6	1:A:1090:U:C4	3.07	0.43
14:N:37:PHE:C	14:N:39:LEU:N	2.72	0.43
1:A:620:C:H2'	1:A:621:A:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:70:ILE:HA	12:L:71:PRO:HD3	1.70	0.43
8:H:134:ILE:H	8:H:134:ILE:HG13	1.61	0.43
7:G:15:ASP:OD1	7:G:44:TYR:OH	2.37	0.43
2:B:83:MET:SD	2:B:234:PRO:HB2	2.59	0.43
4:D:52:SER:O	4:D:56:VAL:HG23	2.19	0.43
14:N:14:PRO:O	14:N:15:LYS:HB3	2.18	0.43
1:A:990:C:H5'	1:A:1017:G:O2'	2.19	0.43
2:B:55:PHE:HD2	2:B:55:PHE:HA	1.66	0.42
1:A:1063:C:H2'	1:A:1064:G:H8	1.83	0.42
4:D:23:GLY:CA	4:D:112:VAL:HG12	2.47	0.42
21:U:10:ARG:O	21:U:13:ILE:HG12	2.19	0.42
1:A:1251:A:H2'	1:A:1252:A:C8	2.54	0.42
1:A:1238:A:OP1	1:A:1336:C:N4	2.52	0.42
1:A:451:A:N7	1:A:481:G:C2	2.86	0.42
16:P:18:ARG:O	16:P:20:VAL:HG23	2.19	0.42
21:U:6:ARG:HD2	21:U:15:ARG:HH22	1.83	0.42
1:A:474:G:N1	1:A:475:G:C5	2.87	0.42
5:E:69:VAL:HA	5:E:70:PRO:HD3	1.76	0.42
1:A:1202:G:C4	14:N:42:ILE:HD12	2.54	0.42
1:A:56:U:H2'	1:A:57:G:C8	2.53	0.42
7:G:152:ALA:O	7:G:155:ARG:HG2	2.20	0.42
13:M:68:GLY:HA2	13:M:71:ARG:HD2	2.01	0.42
1:A:481:G:O2'	1:A:482:A:C8	2.65	0.42
1:A:1350:A:OP2	9:I:118:LYS:HE3	2.19	0.42
9:I:113:LYS:H	9:I:119:ALA:HA	1.84	0.42
1:A:79:G:C4	1:A:91:C:C2	3.07	0.42
9:I:89:ASN:HB3	9:I:92:TYR:CD1	2.54	0.42
1:A:1190:G:O2'	1:A:1191:A:OP2	2.37	0.42
14:N:24:CYS:HB3	14:N:40:CYS:HB3	1.99	0.42
13:M:8:GLU:CD	13:M:22:ILE:HA	2.40	0.42
1:A:1491:G:N2	1:A:1492:A:H62	2.16	0.42
12:L:47:LYS:H	12:L:47:LYS:HG3	1.51	0.42
5:E:51:VAL:O	5:E:54:ALA:HB3	2.19	0.42
8:H:11:THR:O	8:H:12:ARG:C	2.58	0.42
19:S:17:GLU:HA	19:S:20:LEU:HG	2.00	0.42
8:H:53:VAL:HG12	8:H:53:VAL:O	2.19	0.42
5:E:31:LEU:HA	5:E:31:LEU:HD23	1.54	0.42
1:A:79:G:H2'	1:A:79:G:N3	2.34	0.42
20:T:44:ALA:HB1	20:T:92:LEU:HD23	2.02	0.42
1:A:1526:G:C4	1:A:1527:C:C5	3.08	0.42
20:T:87:LYS:O	20:T:91:LEU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:5:VAL:C	17:Q:6:LEU:HD23	2.39	0.42
1:A:190(K):G:H2'	1:A:190(L):U:C6	2.55	0.42
1:A:197:A:H1'	1:A:198:G:O4'	2.20	0.42
13:M:65:LYS:H	13:M:65:LYS:HG2	1.36	0.42
12:L:41:ARG:HE	12:L:43:VAL:HG22	1.84	0.42
1:A:1321:C:C5	1:A:1322:C:C2	3.08	0.42
1:A:443:C:N4	1:A:491:G:H1	2.13	0.42
1:A:1232:U:H5"	9:I:124:GLN:O	2.19	0.42
6:F:67:MET:HB2	6:F:68:PRO:HD2	2.02	0.42
1:A:1427:U:H2'	1:A:1428:A:C8	2.54	0.42
1:A:1440:C:H2'	1:A:1441:G:O4'	2.19	0.42
7:G:28:ASN:O	7:G:31:MET:HB3	2.19	0.42
1:A:784:C:H2'	1:A:785:G:O4'	2.19	0.42
8:H:10:LEU:HA	8:H:10:LEU:HD23	1.70	0.42
8:H:127:LEU:HA	8:H:127:LEU:HD13	1.73	0.42
1:A:391:G:C6	1:A:392:G:C5	3.07	0.42
3:C:113:ALA:N	3:C:114:PRO:HD2	2.34	0.42
1:A:284:G:H2'	1:A:285:G:C8	2.54	0.42
13:M:77:ASN:O	13:M:80:ARG:HB3	2.19	0.42
11:K:120:ARG:HG2	11:K:120:ARG:HH11	1.85	0.42
16:P:43:LYS:HG2	16:P:48:TRP:CG	2.55	0.42
8:H:100:ILE:HD12	8:H:125:ARG:HG3	2.01	0.42
7:G:104:LEU:HD22	7:G:104:LEU:HA	1.81	0.42
10:J:19:SER:CB	10:J:91:PRO:HG3	2.50	0.42
2:B:18:GLY:HA3	2:B:42:ILE:H	1.85	0.42
18:R:33:ASP:OD2	18:R:36:ASN:N	2.52	0.42
2:B:184:VAL:HG12	2:B:197:VAL:HG13	2.01	0.42
5:E:151:LEU:HD23	5:E:151:LEU:HA	1.65	0.42
1:A:77:G:C2	1:A:78:G:C4	3.08	0.42
1:A:1095:U:H2'	1:A:1096:C:C6	2.54	0.42
1:A:36:C:C4	1:A:37:U:C5	3.08	0.42
1:A:690:G:H2'	1:A:691:G:O4'	2.19	0.42
1:A:16:A:HO2'	1:A:1080:A:HO2'	1.65	0.42
13:M:34:LEU:HD13	13:M:39:ILE:HB	2.02	0.42
13:M:49:THR:HB	13:M:52:GLU:H	1.85	0.42
1:A:31:G:N2	1:A:48:C:OP1	2.45	0.42
2:B:45:GLN:O	2:B:49:GLU:HG3	2.20	0.42
4:D:30:LYS:O	4:D:32:ALA:N	2.53	0.42
2:B:33:TYR:C	2:B:33:TYR:CD2	2.93	0.42
1:A:1220:G:H5'	19:S:34:TRP:O	2.20	0.42
1:A:1255:G:C6	1:A:1283:G:C2	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:G:N1	1:A:80:G:N7	2.68	0.42
1:A:1329:A:C5'	13:M:29:ARG:HD2	2.49	0.42
10:J:48:THR:OG1	10:J:62:HIS:HB3	2.20	0.42
12:L:67:THR:O	12:L:96:VAL:HG12	2.20	0.42
1:A:540:G:C4	1:A:541:G:C8	3.08	0.42
4:D:28:SER:O	4:D:30:LYS:N	2.51	0.42
5:E:102:ALA:HB3	5:E:107:ARG:HB2	2.02	0.42
1:A:940:C:H2'	1:A:941:G:O4'	2.20	0.42
1:A:1368:G:H5'	9:I:112:LYS:O	2.19	0.42
1:A:923:A:O2'	1:A:1399:C:OP2	2.25	0.42
1:A:1148:U:H4'	9:I:14:VAL:HG11	2.02	0.42
1:A:1103:C:H2'	1:A:1104:G:O4'	2.20	0.42
1:A:461:C:H4'	1:A:462:G:OP2	2.20	0.42
15:O:34:LEU:HD23	15:O:35:ARG:N	2.35	0.42
16:P:50:LYS:HG2	16:P:51:VAL:H	1.85	0.42
1:A:1433:A:N6	1:A:1434:A:C6	2.88	0.42
1:A:1453:G:H2'	1:A:1454:G:O4'	2.20	0.42
7:G:103:TRP:CZ2	7:G:141:VAL:HG21	2.54	0.42
13:M:21:TYR:N	13:M:21:TYR:CD2	2.87	0.42
5:E:11:ILE:HG22	5:E:12:LEU:N	2.34	0.41
1:A:502:G:P	12:L:118:SER:HG	2.43	0.41
11:K:98:LEU:HA	11:K:98:LEU:HD22	1.68	0.41
1:A:938:A:C6	1:A:939:G:C5	3.08	0.41
5:E:119:LEU:HD23	5:E:119:LEU:HA	1.50	0.41
1:A:794:A:N6	1:A:795:C:N4	2.68	0.41
1:A:830:G:C6	1:A:831:U:C4	3.08	0.41
5:E:10:MET:SD	5:E:13:ILE:HG23	2.60	0.41
8:H:107:LEU:N	8:H:107:LEU:HD23	2.35	0.41
7:G:136:LYS:HB3	7:G:136:LYS:NZ	2.35	0.41
5:E:112:LEU:HA	5:E:112:LEU:HD23	1.51	0.41
1:A:191:G:O2'	20:T:102:GLY:O	2.17	0.41
9:I:118:LYS:HZ2	9:I:118:LYS:HG3	1.57	0.41
5:E:148:VAL:O	5:E:152:ARG:HG3	2.20	0.41
1:A:1342:C:H2'	1:A:1343:G:C8	2.55	0.41
7:G:22:LEU:HD12	7:G:22:LEU:HA	1.74	0.41
4:D:24:GLU:O	4:D:25:ARG:HB3	2.20	0.41
8:H:59:LEU:HA	8:H:59:LEU:HD23	1.81	0.41
1:A:173:U:H6	1:A:198:G:HO2'	1.67	0.41
11:K:33:THR:HB	11:K:39:PRO:HA	2.02	0.41
1:A:804:U:H5"	1:A:805:C:OP2	2.20	0.41
17:Q:51:TYR:CE1	17:Q:73:VAL:HB	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:38:ARG:HD3	15:O:38:ARG:HA	1.62	0.41
1:A:79:G:N2	1:A:80:G:C8	2.88	0.41
9:I:46:ALA:HB1	9:I:77:ILE:HG21	2.02	0.41
3:C:164:ARG:NH1	3:C:166:GLU:OE1	2.51	0.41
7:G:40:ALA:CB	9:I:41:VAL:HG21	2.48	0.41
17:Q:3:LYS:HD3	17:Q:61:GLU:O	2.19	0.41
2:B:71:VAL:O	2:B:164:VAL:HA	2.19	0.41
3:C:119:ARG:O	3:C:122:GLU:HB2	2.20	0.41
1:A:1419:G:H2'	1:A:1420:C:C6	2.55	0.41
20:T:18:GLN:O	20:T:21:LYS:HB2	2.20	0.41
1:A:1543:C:H6	1:A:1543:C:O5'	2.03	0.41
8:H:4:ASP:CG	8:H:85:ARG:NH1	2.72	0.41
15:O:32:LEU:HD12	15:O:63:ARG:HB2	2.01	0.41
3:C:153:VAL:HG12	3:C:154:SER:H	1.84	0.41
11:K:47:VAL:HG12	11:K:48:ILE:N	2.34	0.41
2:B:16:HIS:CE1	2:B:210:SER:HB2	2.56	0.41
1:A:1180:A:OP1	9:I:103:THR:OG1	2.33	0.41
8:H:121:ASP:HB2	8:H:125:ARG:NH2	2.35	0.41
1:A:107:G:C2	1:A:108:G:H1'	2.56	0.41
1:A:266:G:C8	1:A:266:G:H5"	2.56	0.41
11:K:51:LYS:O	11:K:55:LYS:HE2	2.20	0.41
1:A:1270:C:OP2	21:U:24:ARG:NH2	2.53	0.41
13:M:56:LEU:HD23	13:M:56:LEU:HA	1.62	0.41
13:M:12:ASN:H	13:M:45:VAL:HB	1.85	0.41
1:A:966:M2G:HM22	1:A:967:5MC:O2	2.20	0.41
6:F:67:MET:HE3	6:F:67:MET:HB2	1.91	0.41
1:A:123:C:OP1	1:A:312:C:H5'	2.21	0.41
10:J:26:ALA:HB1	10:J:84:GLN:HB3	2.03	0.41
16:P:40:ASP:HA	16:P:41:PRO:HD3	1.82	0.41
9:I:53:VAL:HB	9:I:92:TYR:CZ	2.56	0.41
4:D:194:LEU:HB3	4:D:196:LEU:HG	2.02	0.41
1:A:881:G:OP2	12:L:12:ARG:NH2	2.53	0.41
10:J:6:ILE:HG22	10:J:8:LEU:HD21	2.03	0.41
1:A:369:C:O2'	1:A:370:C:H5'	2.21	0.41
1:A:1053:G:O2'	1:A:1199:U:H5	2.04	0.41
13:M:71:ARG:HG2	13:M:71:ARG:NH1	2.36	0.41
1:A:622:A:C8	1:A:623:C:C6	3.08	0.41
19:S:13:ASP:N	19:S:13:ASP:OD2	2.51	0.41
1:A:1354:C:H2'	1:A:1355:G:C8	2.54	0.41
1:A:1152:A:OP1	10:J:68:HIS:CE1	2.74	0.41
1:A:1415:G:H1	1:A:1485:U:H3	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:115:ARG:HB2	7:G:118:VAL:CG2	2.50	0.41
1:A:1201:A:H4'	1:A:1202:G:H5"	2.03	0.41
10:J:91:PRO:HB2	10:J:94:VAL:HB	2.03	0.41
1:A:661:G:H5"	1:A:661:G:C8	2.55	0.41
1:A:1213:A:N6	1:A:1215:G:N3	2.69	0.41
1:A:927:G:H1	1:A:1390:U:H3	1.67	0.41
6:F:1:MET:HB3	6:F:66:GLU:HG2	2.02	0.41
6:F:67:MET:SD	6:F:72:VAL:HG23	2.61	0.41
5:E:10:MET:O	5:E:10:MET:HE3	2.20	0.41
1:A:883:C:C2	1:A:884:U:C5	3.09	0.41
1:A:1422:G:C2	1:A:1423:G:N7	2.88	0.41
5:E:9:LYS:NZ	5:E:111:GLU:OE1	2.53	0.41
1:A:1027:C:N4	1:A:1034:G:H1	2.19	0.41
1:A:95:U:O2'	1:A:96:G:H5'	2.21	0.41
1:A:125:U:O3'	1:A:633:G:N2	2.54	0.41
1:A:257:G:C6	1:A:258:G:N7	2.89	0.41
1:A:179:A:H2'	1:A:180:U:C6	2.55	0.41
18:R:19:LYS:HE3	18:R:19:LYS:HB2	1.76	0.41
5:E:68:GLU:HG3	5:E:68:GLU:O	2.21	0.41
15:O:32:LEU:HD22	15:O:32:LEU:HA	1.72	0.41
1:A:1026:G:N7	1:A:1027:C:C4	2.89	0.41
10:J:50:ILE:CA	10:J:60:ARG:HB3	2.45	0.41
9:I:50:LEU:HA	9:I:53:VAL:HG22	2.03	0.41
14:N:16:PHE:HB2	14:N:19:ARG:HD2	2.03	0.41
1:A:427:U:OP2	4:D:36:ARG:NH2	2.54	0.41
9:I:8:GLY:HA2	9:I:79:LEU:CD1	2.51	0.41
1:A:620:C:N1	4:D:135:LEU:HD13	2.35	0.41
7:G:111:ARG:NH1	7:G:113:GLU:OE2	2.54	0.41
1:A:1402:4OC:H2'	1:A:1403:C:H6	1.84	0.41
13:M:84:ILE:HG13	13:M:86:CYS:H	1.86	0.41
1:A:659:U:H2'	1:A:660:G:C8	2.56	0.41
1:A:564:C:C5	17:Q:31:LEU:HD21	2.56	0.41
11:K:90:GLY:HA2	11:K:93:GLN:HB2	2.01	0.41
6:F:27:GLN:HA	6:F:30:LEU:HD12	2.03	0.41
17:Q:7:THR:O	17:Q:23:VAL:HG13	2.20	0.41
1:A:292:G:H1	1:A:308:C:H42	1.69	0.41
1:A:1495:U:H2'	1:A:1496:C:C6	2.56	0.41
1:A:1401:G:O6	1:A:1504:G:N2	2.54	0.41
12:L:85:ILE:CG2	12:L:98:TYR:HB3	2.50	0.41
17:Q:63:ARG:HA	17:Q:64:PRO:HD3	1.85	0.41
4:D:155:LEU:HD23	4:D:156:GLU:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1320:C:N4	19:S:36:ARG:HG3	2.36	0.41
4:D:135:LEU:HA	4:D:136:PRO:HD3	1.92	0.41
1:A:1003(A):G:H2'	1:A:1004:A:H4'	2.03	0.41
1:A:147:G:N2	1:A:148:G:C4	2.89	0.41
1:A:276:G:O3'	17:Q:68:ARG:NH1	2.51	0.41
2:B:68:ILE:HG21	2:B:68:ILE:HD13	1.74	0.41
5:E:61:TYR:HA	5:E:61:TYR:HD1	1.72	0.41
2:B:187:LEU:HD12	2:B:205:ASP:HA	2.03	0.40
9:I:53:VAL:HG21	9:I:85:LEU:HD21	2.03	0.40
1:A:1163:C:N3	1:A:1174:G:C2	2.89	0.40
1:A:1134:G:H1	1:A:1140:C:H42	1.67	0.40
8:H:100:ILE:HG13	8:H:100:ILE:H	1.68	0.40
8:H:100:ILE:CG2	8:H:112:LEU:HD11	2.51	0.40
2:B:158:LEU:H	2:B:158:LEU:CD1	2.32	0.40
1:A:398:C:O2'	1:A:399:G:H5'	2.21	0.40
1:A:794:A:C6	1:A:795:C:C4	3.09	0.40
1:A:256:U:H2'	1:A:257:G:C8	2.57	0.40
1:A:977:A:H2'	1:A:978:A:H5"	2.04	0.40
1:A:926:G:N2	1:A:1542:U:OP1	2.44	0.40
2:B:182:ILE:HA	2:B:183:PRO:HD3	1.86	0.40
5:E:90:VAL:O	5:E:91:LEU:HD23	2.21	0.40
1:A:1532:U:O5'	1:A:1532:U:H6	2.04	0.40
1:A:875:C:O2'	8:H:14:ARG:NH1	2.54	0.40
3:C:136:GLN:O	3:C:140:ARG:HG3	2.21	0.40
15:O:39:LEU:HD23	15:O:43:LEU:HG	2.03	0.40
1:A:1277:C:O2'	1:A:1279:A:H1'	2.21	0.40
1:A:1163:C:H2'	1:A:1164:G:O4'	2.22	0.40
2:B:97:TRP:HZ3	2:B:176:GLU:OE2	2.04	0.40
1:A:1221:G:H4'	19:S:53:ASN:O	2.21	0.40
2:B:23:ARG:O	2:B:24:TRP:CD1	2.73	0.40
11:K:50:TYR:CD2	11:K:54:ARG:HD2	2.57	0.40
6:F:68:PRO:HG2	6:F:71:ARG:HG3	2.03	0.40
2:B:231:GLU:HB3	2:B:232:PRO:HD2	2.02	0.40
1:A:523:A:H8	1:A:523:A:O5'	2.04	0.40
16:P:45:THR:HB	16:P:46:PRO:HD2	2.04	0.40
1:A:127:G:N2	1:A:234:C:O2	2.52	0.40
1:A:979:C:OP1	1:A:1222:G:O6	2.40	0.40
15:O:36:ILE:HD13	15:O:59:MET:HE3	2.03	0.40
1:A:1056:U:H2'	1:A:1057:G:H8	1.87	0.40
1:A:1338:G:C6	1:A:1339:A:C6	3.10	0.40
1:A:344:A:H4'	1:A:345:C:OP2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:881:G:H2'	1:A:882:C:O4'	2.21	0.40
10:J:89:ASP:CB	10:J:91:PRO:HD2	2.52	0.40
2:B:33:TYR:HD2	2:B:33:TYR:O	2.03	0.40
1:A:1489:G:H2'	1:A:1490:C:C6	2.56	0.40
1:A:397:A:N3	1:A:397:A:H3'	2.35	0.40
1:A:825:G:H21	8:H:11:THR:HG21	1.86	0.40
6:F:60:PHE:CZ	18:R:78:LEU:HD21	2.56	0.40
11:K:11:LYS:HE2	11:K:11:LYS:HB3	1.87	0.40
4:D:200:GLU:CD	4:D:200:GLU:H	2.24	0.40
1:A:663:A:H2'	1:A:664:G:O4'	2.22	0.40
1:A:1404:5MC:H1'	1:A:1499:A:C2	2.57	0.40
1:A:1255:G:H22	1:A:1283:G:H1'	1.87	0.40
1:A:74:C:C4	1:A:75:G:N7	2.90	0.40
5:E:80:ILE:CG2	8:H:104:ARG:HH21	2.32	0.40
1:A:35:G:C6	1:A:36:C:N4	2.89	0.40
4:D:114:ARG:HG3	4:D:114:ARG:HH11	1.86	0.40
8:H:116:LYS:HD2	8:H:129:VAL:HG11	2.03	0.40
1:A:1179:A:H2'	1:A:1180:A:O4'	2.20	0.40
1:A:376:G:P	16:P:67:THR:HG21	2.61	0.40
5:E:102:ALA:O	5:E:107:ARG:NH1	2.54	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%)	208 (90%)	22 (10%)	2 (1%)	21 67
3	C	204/239 (85%)	180 (88%)	23 (11%)	1 (0%)	34 77
4	D	206/209 (99%)	196 (95%)	10 (5%)	0	100 100
5	E	148/162 (91%)	140 (95%)	8 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
7	G	153/156 (98%)	136 (89%)	17 (11%)	0	100	100
8	H	136/138 (99%)	132 (97%)	4 (3%)	0	100	100
9	I	125/128 (98%)	114 (91%)	10 (8%)	1 (1%)	24	69
10	J	96/105 (91%)	79 (82%)	16 (17%)	1 (1%)	19	66
11	K	114/129 (88%)	100 (88%)	14 (12%)	0	100	100
12	L	121/135 (90%)	109 (90%)	10 (8%)	2 (2%)	11	55
13	M	116/126 (92%)	103 (89%)	12 (10%)	1 (1%)	21	67
14	N	58/61 (95%)	51 (88%)	7 (12%)	0	100	100
15	O	85/89 (96%)	77 (91%)	7 (8%)	1 (1%)	16	62
16	P	81/88 (92%)	77 (95%)	4 (5%)	0	100	100
17	Q	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
18	R	68/88 (77%)	63 (93%)	5 (7%)	0	100	100
19	S	78/93 (84%)	72 (92%)	5 (6%)	1 (1%)	15	60
20	T	97/106 (92%)	85 (88%)	11 (11%)	1 (1%)	19	66
21	U	22/27 (82%)	21 (96%)	1 (4%)	0	100	100
All	All	2336/2541 (92%)	2128 (91%)	197 (8%)	11 (0%)	34	77

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	21	ARG
19	S	31	ILE
12	L	28	LYS
2	B	24	TRP
20	T	73	HIS
9	I	119	ALA
12	L	51	ALA
3	C	86	VAL
10	J	34	VAL
13	M	7	VAL
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%)	160 (79%)	42 (21%)	1 10
3	C	160/188 (85%)	130 (81%)	30 (19%)	2 13
4	D	180/181 (99%)	150 (83%)	30 (17%)	3 19
5	E	115/123 (94%)	91 (79%)	24 (21%)	1 10
6	F	90/90 (100%)	77 (86%)	13 (14%)	4 26
7	G	126/127 (99%)	109 (86%)	17 (14%)	5 29
8	H	119/119 (100%)	94 (79%)	25 (21%)	1 10
9	I	98/99 (99%)	77 (79%)	21 (21%)	1 9
10	J	87/92 (95%)	72 (83%)	15 (17%)	2 17
11	K	88/99 (89%)	75 (85%)	13 (15%)	4 25
12	L	103/110 (94%)	82 (80%)	21 (20%)	1 11
13	M	94/101 (93%)	72 (77%)	22 (23%)	1 7
14	N	49/50 (98%)	38 (78%)	11 (22%)	1 8
15	O	79/80 (99%)	63 (80%)	16 (20%)	1 11
16	P	72/74 (97%)	59 (82%)	13 (18%)	2 15
17	Q	94/97 (97%)	80 (85%)	14 (15%)	4 25
18	R	61/77 (79%)	54 (88%)	7 (12%)	7 36
19	S	71/80 (89%)	59 (83%)	12 (17%)	2 18
20	T	76/82 (93%)	63 (83%)	13 (17%)	2 18
21	U	19/22 (86%)	16 (84%)	3 (16%)	3 22
All	All	1983/2111 (94%)	1621 (82%)	362 (18%)	2 14

All (362) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	7	VAL
2	B	8	LYS
2	B	10	LEU

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Mol	Chain	Res	Type
2	B	12	GLU
2	B	16	HIS
2	B	17	PHE
2	B	21	ARG
2	B	23	ARG
2	B	24	TRP
2	B	30	ARG
2	B	32	ILE
2	B	33	TYR
2	B	39	ILE
2	B	44	LEU
2	B	45	GLN
2	B	47	THR
2	B	49	GLU
2	B	55	PHE
2	B	61	LEU
2	B	67	THR
2	B	69	LEU
2	B	97	TRP
2	B	102	LEU
2	B	106	LYS
2	B	124	SER
2	B	127	ILE
2	B	142	LEU
2	B	144	ARG
2	B	153	ARG
2	B	154	LEU
2	B	157	ARG
2	B	158	LEU
2	B	164	VAL
2	B	168	THR
2	B	172	ILE
2	B	175	ARG
2	B	178	ARG
2	B	200	ILE
2	B	217	ARG
2	B	223	ILE
2	B	235	SER
2	B	239	VAL
3	C	3	ASN
3	C	10	PHE
3	C	11	ARG

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Mol	Chain	Res	Type
3	C	15	THR
3	C	17	ASP
3	C	31	HIS
3	C	34	LEU
3	C	48	TYR
3	C	52	LEU
3	C	58	GLU
3	C	70	VAL
3	C	91	LEU
3	C	94	LEU
3	C	95	THR
3	C	98	ASN
3	C	99	VAL
3	C	104	GLN
3	C	108	ASN
3	C	111	LEU
3	C	131	ARG
3	C	154	SER
3	C	166	GLU
3	C	172	ARG
3	C	175	LEU
3	C	176	HIS
3	C	178	LEU
3	C	188	LEU
3	C	191	THR
3	C	195	VAL
3	C	204	LEU
4	D	9	CYS
4	D	19	LEU
4	D	21	LEU
4	D	25	ARG
4	D	26	CYS
4	D	34	GLU
4	D	35	ARG
4	D	53	ASP
4	D	59	ARG
4	D	63	LYS
4	D	64	LEU
4	D	73	ARG
4	D	91	SER
4	D	99	SER
4	D	115	ARG

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Mol	Chain	Res	Type
4	D	118	ARG
4	D	122	ARG
4	D	131	ARG
4	D	135	LEU
4	D	139	ARG
4	D	140	VAL
4	D	150	GLU
4	D	155	LEU
4	D	157	LEU
4	D	159	ARG
4	D	186	LEU
4	D	187	ARG
4	D	193	ASP
4	D	194	LEU
4	D	202	LEU
5	E	6	PHE
5	E	12	LEU
5	E	16	THR
5	E	18	ARG
5	E	19	MET
5	E	26	PHE
5	E	34	VAL
5	E	41	VAL
5	E	49	PRO
5	E	56	GLN
5	E	64	ARG
5	E	68	GLU
5	E	75	THR
5	E	79	GLU
5	E	80	ILE
5	E	96	PRO
5	E	120	THR
5	E	125	SER
5	E	131	ILE
5	E	147	ASP
5	E	149	GLU
5	E	150	ARG
5	E	151	LEU
5	E	152	ARG
6	F	3	ARG
6	F	10	LEU
6	F	14	LEU

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Mol	Chain	Res	Type
6	F	19	LEU
6	F	24	GLU
6	F	32	ASN
6	F	37	VAL
6	F	43	LEU
6	F	67	MET
6	F	70	ASP
6	F	75	LEU
6	F	82	ARG
6	F	92	LYS
7	G	3	ARG
7	G	6	ARG
7	G	8	GLU
7	G	27	ILE
7	G	32	ARG
7	G	45	ASP
7	G	47	CYS
7	G	61	VAL
7	G	67	GLU
7	G	79	ARG
7	G	84	ASN
7	G	104	LEU
7	G	113	GLU
7	G	125	MET
7	G	136	LYS
7	G	141	VAL
7	G	149	ARG
8	H	6	ILE
8	H	11	THR
8	H	19	VAL
8	H	24	THR
8	H	26	VAL
8	H	37	ARG
8	H	45	ILE
8	H	51	VAL
8	H	52	ASP
8	H	53	VAL
8	H	63	LEU
8	H	64	LYS
8	H	83	ILE
8	H	85	ARG
8	H	88	LYS

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Mol	Chain	Res	Type
8	H	91	ARG
8	H	92	ARG
8	H	95	VAL
8	H	97	VAL
8	H	98	LYS
8	H	104	ARG
8	H	105	ARG
8	H	115	SER
8	H	127	LEU
8	H	134	ILE
9	I	3	GLN
9	I	11	LYS
9	I	14	VAL
9	I	38	GLN
9	I	41	VAL
9	I	44	VAL
9	I	47	LEU
9	I	50	LEU
9	I	56	LEU
9	I	58	HIS
9	I	79	LEU
9	I	83	ARG
9	I	91	ASP
9	I	96	LEU
9	I	99	LEU
9	I	107	ARG
9	I	109	VAL
9	I	113	LYS
9	I	118	LYS
9	I	121	ARG
9	I	127	LYS
10	J	3	LYS
10	J	9	ARG
10	J	38	ILE
10	J	45	ARG
10	J	48	THR
10	J	60	ARG
10	J	62	HIS
10	J	73	ASP
10	J	78	ASN
10	J	80	LYS
10	J	82	ILE

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Mol	Chain	Res	Type
10	J	89	ASP
10	J	92	THR
10	J	94	VAL
10	J	95	GLU
11	K	12	ARG
11	K	14	VAL
11	K	29	ILE
11	K	63	LEU
11	K	81	ASP
11	K	95	ILE
11	K	98	LEU
11	K	101	SER
11	K	114	VAL
11	K	119	CYS
11	K	120	ARG
11	K	122	LYS
11	K	124	LYS
12	L	7	ILE
12	L	16	GLU
12	L	18	VAL
12	L	20	LYS
12	L	33	ARG
12	L	34	ARG
12	L	36	VAL
12	L	41	ARG
12	L	42	THR
12	L	43	VAL
12	L	47	LYS
12	L	55	VAL
12	L	59	ARG
12	L	61	THR
12	L	67	THR
12	L	79	GLU
12	L	80	HIS
12	L	96	VAL
12	L	97	ARG
12	L	113	ARG
12	L	122	THR
13	M	12	ASN
13	M	13	LYS
13	M	14	ARG
13	M	37	THR

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Mol	Chain	Res	Type
13	M	44	ARG
13	M	48	LEU
13	M	50	GLU
13	M	54	VAL
13	M	56	LEU
13	M	59	TYR
13	M	61	GLU
13	M	64	TRP
13	M	70	LEU
13	M	73	GLU
13	M	81	LEU
13	M	103	THR
13	M	105	THR
13	M	108	ARG
13	M	109	THR
13	M	110	ARG
13	M	113	PRO
13	M	114	ARG
14	N	9	LYS
14	N	13	THR
14	N	22	THR
14	N	24	CYS
14	N	25	VAL
14	N	27	CYS
14	N	31	ARG
14	N	40	CYS
14	N	42	ILE
14	N	47	LEU
14	N	53	LEU
15	O	3	ILE
15	O	5	LYS
15	O	8	LYS
15	O	21	ASP
15	O	32	LEU
15	O	33	THR
15	O	45	VAL
15	O	56	LEU
15	O	64	ARG
15	O	65	ARG
15	O	70	LEU
15	O	71	GLN
15	O	81	LEU

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Mol	Chain	Res	Type
15	O	82	ILE
15	O	83	GLU
15	O	87	ILE
16	P	1	MET
16	P	11	SER
16	P	26	ARG
16	P	33	ILE
16	P	42	ARG
16	P	47	ASP
16	P	53	VAL
16	P	54	GLU
16	P	55	ARG
16	P	62	VAL
16	P	68	ASP
16	P	81	ARG
16	P	82	GLN
17	Q	13	ASP
17	Q	30	PRO
17	Q	34	LYS
17	Q	40	LYS
17	Q	53	LEU
17	Q	60	ILE
17	Q	72	ARG
17	Q	74	LEU
17	Q	76	LEU
17	Q	77	VAL
17	Q	86	GLU
17	Q	92	ARG
17	Q	98	LEU
17	Q	99	SER
18	R	30	ASP
18	R	40	LEU
18	R	44	LEU
18	R	47	THR
18	R	69	THR
18	R	81	PHE
18	R	84	LYS
19	S	5	LEU
19	S	13	ASP
19	S	14	HIS
19	S	15	LEU
19	S	25	LYS

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Mol	Chain	Res	Type
19	S	33	THR
19	S	58	VAL
19	S	62	ILE
19	S	63	THR
19	S	71	LEU
19	S	78	ARG
19	S	79	THR
20	T	13	LEU
20	T	19	SER
20	T	20	LEU
20	T	53	LEU
20	T	56	MET
20	T	57	ARG
20	T	62	LEU
20	T	68	LYS
20	T	72	LEU
20	T	75	ASN
20	T	80	ARG
20	T	84	LEU
20	T	92	LEU
21	U	6	ARG
21	U	10	ARG
21	U	25	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	40	HIS
2	B	204	ASN
3	C	6	HIS
4	D	42	GLN
5	E	72	GLN
6	F	13	ASN
9	I	3	GLN
9	I	73	GLN
9	I	124	GLN
10	J	62	HIS
14	N	52	GLN
17	Q	96	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1504/1522 (98%)	339 (22%)	51 (3%)

All (339) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	8	A
1	A	9	G
1	A	31	G
1	A	32	A
1	A	33	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	50	A
1	A	51	A
1	A	54	C
1	A	80	G
1	A	81	U
1	A	92	C
1	A	101	A
1	A	108	G
1	A	115	G
1	A	116	A
1	A	117	G
1	A	121	C
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	163	C
1	A	180	U
1	A	181	G
1	A	182	U
1	A	183	G
1	A	188	C
1	A	195	A
1	A	201	C
1	A	202	U
1	A	203	U
1	A	204	U
1	A	216	G
1	A	226	G
1	A	231	G

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Mol	Chain	Res	Type
1	A	247	G
1	A	250	A
1	A	251	G
1	A	252	U
1	A	258	G
1	A	266	G
1	A	267	C
1	A	281	G
1	A	282	A
1	A	289	G
1	A	299	G
1	A	319	G
1	A	321	A
1	A	328	C
1	A	329	A
1	A	331	G
1	A	332	G
1	A	344	A
1	A	345	C
1	A	346	G
1	A	350	G
1	A	351	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	356	A
1	A	367	U
1	A	371	G
1	A	372	C
1	A	373	A
1	A	374	A
1	A	382	A
1	A	384	G
1	A	390	C
1	A	397	A
1	A	398	C
1	A	406	G
1	A	409	G
1	A	412	A
1	A	413	G
1	A	414	A
1	A	421	U

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Mol	Chain	Res	Type
1	A	424	G
1	A	429	U
1	A	439	A
1	A	442	C
1	A	451	A
1	A	460	A
1	A	461	C
1	A	481	G
1	A	482	A
1	A	485	G
1	A	486	U
1	A	496	A
1	A	497	A
1	A	498	U
1	A	509	A
1	A	510	A
1	A	511	C
1	A	517	G
1	A	518	C
1	A	519	C
1	A	524	G
1	A	527	7MG
1	A	531	U
1	A	532	A
1	A	533	A
1	A	538	G
1	A	545	C
1	A	547	A
1	A	559	A
1	A	560	U
1	A	562	C
1	A	564	C
1	A	568	G
1	A	571	U
1	A	572	A
1	A	573	A
1	A	576	G
1	A	577	G
1	A	579	G
1	A	588	G
1	A	596	C
1	A	597	G

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Mol	Chain	Res	Type
1	A	598	U
1	A	616	G
1	A	621	A
1	A	624	C
1	A	653	A
1	A	658	G
1	A	665	A
1	A	671	G
1	A	687	A
1	A	688	G
1	A	695	A
1	A	697	U
1	A	701	C
1	A	702	A
1	A	703	G
1	A	722	A
1	A	723	U
1	A	724	G
1	A	731	G
1	A	733	A
1	A	740	U
1	A	741	G
1	A	749	C
1	A	751	U
1	A	755	G
1	A	760	G
1	A	777	A
1	A	781	A
1	A	782	A
1	A	785	G
1	A	792	A
1	A	793	U
1	A	794	A
1	A	812	C
1	A	813	U
1	A	815	A
1	A	817	C
1	A	818	G
1	A	827	U
1	A	828	A
1	A	837	G
1	A	838	G

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Mol	Chain	Res	Type
1	A	839	U
1	A	840	C
1	A	841	U
1	A	848	C
1	A	849	C
1	A	853	G
1	A	869	G
1	A	873	A
1	A	889	A
1	A	902	G
1	A	910	C
1	A	914	A
1	A	916	G
1	A	922	G
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	936	C
1	A	937	A
1	A	938	A
1	A	939	G
1	A	942	G
1	A	950	U
1	A	954	G
1	A	961	U
1	A	962	C
1	A	966	M2G
1	A	967	5MC
1	A	969	A
1	A	971	G
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	982	U
1	A	984	C
1	A	989	C
1	A	991	U
1	A	992	U
1	A	993	G
1	A	994	A

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Mol	Chain	Res	Type
1	A	995	C
1	A	1004	A
1	A	1005	A
1	A	1006	C
1	A	1020	U
1	A	1023	G
1	A	1024	G
1	A	1026	G
1	A	1030(B)	C
1	A	1031	G
1	A	1045	C
1	A	1050	G
1	A	1053	G
1	A	1054	C
1	A	1055	A
1	A	1065	U
1	A	1066	C
1	A	1068	G
1	A	1078	U
1	A	1085	U
1	A	1092	A
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1111	A
1	A	1124	G
1	A	1125	U
1	A	1126	U
1	A	1127	G
1	A	1129	C
1	A	1130	A
1	A	1135	U
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1140	C
1	A	1146	A
1	A	1152	A
1	A	1159	U
1	A	1160	G
1	A	1168	A
1	A	1171	G

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Mol	Chain	Res	Type
1	A	1177	G
1	A	1183	A
1	A	1191	A
1	A	1196	U
1	A	1197	G
1	A	1200	C
1	A	1201	A
1	A	1202	G
1	A	1206	G
1	A	1207	2MG
1	A	1211	U
1	A	1212	U
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	1241	G
1	A	1242	C
1	A	1245	A
1	A	1250	A
1	A	1253	G
1	A	1256	A
1	A	1257	U
1	A	1258	G
1	A	1268	A
1	A	1270	C
1	A	1278	U
1	A	1279	A
1	A	1280	A
1	A	1281	U
1	A	1286	A
1	A	1287	A
1	A	1289	A
1	A	1297	C
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1305	G
1	A	1306	A

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Mol	Chain	Res	Type
1	A	1307	U
1	A	1310	G
1	A	1316	G
1	A	1320	C
1	A	1322	C
1	A	1326	C
1	A	1336	C
1	A	1338	G
1	A	1339	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	1362	C
1	A	1370	G
1	A	1381	U
1	A	1398	A
1	A	1399	C
1	A	1400	5MC
1	A	1401	G
1	A	1406	U
1	A	1411	C
1	A	1415	G
1	A	1430	C
1	A	1442	G
1	A	1443	G
1	A	1446	A
1	A	1447	G
1	A	1451	A
1	A	1453	G
1	A	1454	G
1	A	1485	U
1	A	1487	G
1	A	1489	G
1	A	1490	C
1	A	1492	A
1	A	1493	A
1	A	1497	G
1	A	1498	UR3
1	A	1499	A

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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	1529	G
1	A	1530	G
1	A	1531	A

All (51) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U
1	A	92	C
1	A	115	G
1	A	129(A)	G
1	A	181	G
1	A	204	U
1	A	250	A
1	A	251	G
1	A	281	G
1	A	328	C
1	A	350	G
1	A	353	A
1	A	372	C
1	A	428	G
1	A	484	G
1	A	485	G
1	A	496	A
1	A	509	A
1	A	518	C
1	A	532	A
1	A	559	A
1	A	575	G
1	A	687	A
1	A	701	C
1	A	748	C
1	A	792	A
1	A	812	C
1	A	913	A
1	A	960	U
1	A	965	A
1	A	992	U

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Mol	Chain	Res	Type
1	A	1049	U
1	A	1065	U
1	A	1067	A
1	A	1126	U
1	A	1129	C
1	A	1139	G
1	A	1145	C
1	A	1182	G
1	A	1190	G
1	A	1201	A
1	A	1256	A
1	A	1257	U
1	A	1285	A
1	A	1300	G
1	A	1301	U
1	A	1305	G
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)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	2MG	A	1207	1	17,26,27	2.44	4 (23%)	21,38,41	2.11	3 (14%)
1	5MC	A	1400	1	13,22,23	1.24	2 (15%)	15,32,35	1.08	1 (6%)
1	4OC	A	1402	1	13,23,24	1.08	2 (15%)	18,32,35	1.00	1 (5%)
1	5MC	A	1404	1	13,22,23	1.48	2 (15%)	15,32,35	1.20	2 (13%)
1	5MC	A	1407	1	13,22,23	1.63	2 (15%)	15,32,35	1.08	1 (6%)
1	UR3	A	1498	1	12,22,23	1.52	2 (16%)	16,32,35	1.49	2 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	MA6	A	1518[A]	1	16,26,27	0.96	1 (6%)	18,38,41	1.24	2 (11%)
1	MA6	A	1518[B]	1	16,26,27	1.20	1 (6%)	18,38,41	1.29	3 (16%)
1	MA6	A	1519[A]	1	16,26,27	0.96	1 (6%)	18,38,41	1.35	3 (16%)
1	MA6	A	1519[B]	1	16,26,27	1.48	4 (25%)	18,38,41	1.14	2 (11%)
1	PSU	A	1540	1	13,21,22	1.05	1 (7%)	18,30,33	4.17	6 (33%)
1	PSU	A	1541	1	13,21,22	1.16	1 (7%)	18,30,33	4.03	5 (27%)
1	PSU	A	516	1,22	13,21,22	0.91	1 (7%)	18,30,33	3.79	5 (27%)
1	7MG	A	527	1,22	19,26,27	2.53	6 (31%)	24,39,42	1.72	6 (25%)
1	M2G	A	966	1	17,27,28	1.37	3 (17%)	22,40,43	1.96	1 (4%)
1	5MC	A	967	1	13,22,23	1.13	1 (7%)	15,32,35	0.99	2 (13%)
12	0TD	L	92	12	4,9,10	1.01	0	4,11,13	3.49	3 (75%)

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

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

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	7MG	C8-N9	-6.30	1.36	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1498	UR3	C6-N1	-3.82	1.30	1.35
1	A	527	7MG	CM7-N7	-3.01	1.40	1.46
1	A	527	7MG	O6-C6	-2.92	1.17	1.24
1	A	1498	UR3	C4-N3	-2.37	1.34	1.38
1	A	1407	5MC	C6-C5	-2.26	1.34	1.40
1	A	1402	4OC	C4-N3	-2.15	1.30	1.34
1	A	527	7MG	C8-N7	-2.06	1.34	1.43
1	A	1518[A]	MA6	C2-N1	2.01	1.37	1.33
1	A	1400	5MC	CM5-C5	2.07	1.55	1.51
1	A	1404	5MC	C6-N1	2.08	1.38	1.35
1	A	966	M2G	C4-N3	2.12	1.39	1.35
1	A	966	M2G	C2-N2	2.12	1.38	1.34
1	A	1402	4OC	C5-C4	2.17	1.44	1.39
1	A	1207	2MG	C2-N1	2.19	1.42	1.34
1	A	1519[A]	MA6	C2-N1	2.32	1.38	1.33
1	A	967	5MC	C6-N1	2.42	1.38	1.35
1	A	1519[B]	MA6	C2-N1	2.53	1.38	1.33
1	A	1518[B]	MA6	C6-N1	2.56	1.37	1.34
1	A	1519[B]	MA6	C2-N3	2.59	1.36	1.32
1	A	1519[B]	MA6	C4-N3	2.65	1.39	1.35
1	A	516	PSU	C4-N3	2.66	1.38	1.33
1	A	1519[B]	MA6	C6-N1	2.70	1.37	1.34
1	A	1400	5MC	C6-N1	3.08	1.39	1.35
1	A	1541	PSU	C4-N3	3.22	1.39	1.33
1	A	1540	PSU	C4-N3	3.31	1.39	1.33
1	A	966	M2G	C6-N1	4.11	1.40	1.33
1	A	1207	2MG	C4-N3	4.17	1.42	1.35
1	A	1404	5MC	C5-C4	4.57	1.48	1.41
1	A	1407	5MC	C5-C4	4.62	1.48	1.41
1	A	527	7MG	C2-N2	4.65	1.43	1.34
1	A	527	7MG	C4-N3	5.19	1.41	1.34
1	A	1207	2MG	C2-N2	5.41	1.40	1.34
1	A	1207	2MG	C6-N1	6.57	1.45	1.33

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1540	PSU	N1-C2-N3	-14.96	118.79	128.33
1	A	1541	PSU	N1-C2-N3	-14.72	118.94	128.33
1	A	516	PSU	N1-C2-N3	-13.66	119.62	128.33
1	A	966	M2G	C5-C6-N1	-7.98	112.67	123.59
1	A	1207	2MG	C5-C6-N1	-7.43	113.44	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	L	92	0TD	CSB-SB-CB	-5.62	90.94	101.54
1	A	527	7MG	C5-C4-N3	-5.58	121.38	126.82
1	A	1402	4OC	CM4-N4-C4	-3.57	119.89	122.98
1	A	1404	5MC	N4-C4-N3	-3.42	111.99	116.95
1	A	1540	PSU	C5-C1'-C2'	-3.31	109.65	115.52
12	L	92	0TD	CB-CA-N	-3.22	102.69	109.66
1	A	1407	5MC	N4-C4-N3	-3.10	112.45	116.95
1	A	527	7MG	C4-N9-C1'	-2.79	119.98	126.70
1	A	1518[B]	MA6	N1-C6-N6	-2.69	114.12	117.05
1	A	967	5MC	N4-C4-N3	-2.34	113.55	116.95
1	A	1540	PSU	C5-C6-N1	-2.29	121.16	124.39
12	L	92	0TD	O-C-CA	-2.29	119.39	125.44
1	A	1498	UR3	C5-C4-N3	-2.26	112.68	117.45
1	A	1518[A]	MA6	C1'-N9-C4	-2.25	123.55	126.94
1	A	1519[A]	MA6	C2'-C1'-N9	-2.13	111.03	114.29
1	A	516	PSU	C5-C6-N1	-2.11	121.41	124.39
1	A	527	7MG	N1-C2-N3	-2.02	122.23	125.53
1	A	1404	5MC	C5-C4-N3	2.01	124.63	121.27
1	A	1519[B]	MA6	N3-C2-N1	2.08	130.49	128.89
1	A	967	5MC	CM5-C5-C6	2.09	122.83	118.62
1	A	527	7MG	C6-N1-C2	2.17	118.95	115.94
1	A	527	7MG	N2-C2-N1	2.19	120.83	117.20
1	A	1518[B]	MA6	C2-N1-C6	2.37	116.48	111.43
1	A	1519[B]	MA6	C2-N1-C6	2.42	116.58	111.43
1	A	1540	PSU	O4'-C1'-C2'	2.44	107.21	104.73
1	A	1207	2MG	C4-C5-N7	2.44	111.72	109.48
1	A	1519[A]	MA6	C2-N1-C6	2.44	116.63	111.43
1	A	1518[B]	MA6	N3-C2-N1	2.53	130.83	128.89
1	A	1541	PSU	C5-C1'-C2'	2.63	120.18	115.52
1	A	1541	PSU	O4'-C1'-C2'	2.66	107.44	104.73
1	A	527	7MG	N3-C4-N9	2.86	131.05	126.75
1	A	1400	5MC	CM5-C5-C6	2.98	124.62	118.62
1	A	516	PSU	C6-N1-C2	3.07	120.41	115.47
1	A	1498	UR3	C6-C5-C4	3.24	123.34	117.28
1	A	1518[A]	MA6	C2-N1-C6	3.33	118.53	111.43
1	A	1541	PSU	C6-N1-C2	3.40	120.93	115.47
1	A	516	PSU	O4'-C1'-C2'	3.41	108.20	104.73
1	A	1540	PSU	C6-N1-C2	3.49	121.07	115.47
1	A	1519[A]	MA6	N3-C2-N1	3.72	131.75	128.89
1	A	1207	2MG	C6-N1-C2	4.73	122.19	115.31
1	A	1541	PSU	C4-N3-C2	6.25	120.64	115.25
1	A	516	PSU	C4-N3-C2	6.28	120.68	115.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1540	PSU	C4-N3-C2	6.85	121.17	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1400	5MC	1	0
1	A	1402	4OC	2	0
1	A	1404	5MC	1	0
1	A	1498	UR3	5	0
1	A	1518[A]	MA6	3	0
1	A	1518[B]	MA6	3	0
1	A	1519[A]	MA6	3	0
1	A	1519[B]	MA6	3	0
1	A	966	M2G	3	0
1	A	967	5MC	5	0
12	L	92	0TD	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 256 ligands modelled in this entry, 256 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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%)	-0.29	27 (1%) 71 58	85, 149, 294, 392	0
2	B	234/256 (91%)	-0.54	0 100 100	107, 163, 248, 282	0
3	C	206/239 (86%)	0.04	14 (6%) 20 13	167, 228, 284, 310	0
4	D	208/209 (99%)	-0.38	3 (1%) 78 65	105, 155, 204, 238	0
5	E	150/162 (92%)	-0.57	0 100 100	80, 121, 160, 178	0
6	F	101/101 (100%)	-0.63	0 100 100	122, 176, 205, 223	0
7	G	155/156 (99%)	-0.27	8 (5%) 31 22	135, 193, 257, 275	0
8	H	138/138 (100%)	-0.66	0 100 100	74, 109, 147, 192	0
9	I	127/128 (99%)	-0.16	4 (3%) 52 38	151, 217, 251, 272	0
10	J	98/105 (93%)	0.47	14 (14%) 4 3	190, 234, 309, 344	0
11	K	116/129 (89%)	-0.50	0 100 100	118, 148, 198, 218	0
12	L	123/135 (91%)	-0.45	0 100 100	86, 150, 190, 221	0
13	M	118/126 (93%)	-0.22	4 (3%) 49 35	138, 184, 221, 319	0
14	N	60/61 (98%)	0.15	4 (6%) 21 13	167, 208, 268, 285	0
15	O	87/89 (97%)	-0.46	1 (1%) 82 70	93, 134, 179, 189	0
16	P	83/88 (94%)	-0.51	0 100 100	102, 145, 176, 226	0
17	Q	99/105 (94%)	-0.55	0 100 100	95, 123, 167, 189	0
18	R	70/88 (79%)	-0.53	1 (1%) 78 65	110, 146, 206, 216	0
19	S	80/93 (86%)	0.27	4 (5%) 32 22	198, 244, 285, 305	0
20	T	99/106 (93%)	-0.59	1 (1%) 84 73	113, 150, 202, 238	0
21	U	24/27 (88%)	1.23	6 (25%) 1 1	167, 192, 215, 235	0
All	All	3874/4063 (95%)	-0.31	91 (2%) 64 48	74, 160, 266, 392	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	993	G	7.7
1	A	1018	C	5.9
14	N	4	LYS	5.1
1	A	1129	C	5.0
1	A	994	A	4.8
7	G	2	ALA	4.8
1	A	1019	C	4.5
21	U	18	TYR	4.3
10	J	39	PRO	4.3
3	C	157	ILE	4.2
10	J	34	VAL	4.0
3	C	66	VAL	3.9
13	M	117	VAL	3.8
3	C	193	TYR	3.7
10	J	33	GLN	3.7
21	U	17	THR	3.7
1	A	1006	C	3.5
1	A	1050	G	3.5
1	A	202	U	3.5
21	U	24	ARG	3.5
1	A	1005	A	3.4
7	G	80	VAL	3.4
1	A	1001	A	3.4
3	C	102	ASN	3.4
7	G	81	GLY	3.4
14	N	3	ARG	3.3
13	M	118	ALA	3.3
3	C	156	ARG	3.2
14	N	5	ALA	3.2
3	C	103	VAL	3.2
4	D	35	ARG	3.2
4	D	37	PRO	3.0
1	A	1140	C	3.0
3	C	65	ALA	2.9
10	J	71	LEU	2.9
1	A	1257	U	2.9
3	C	77	ILE	2.9
20	T	106	ALA	2.8
3	C	104	GLN	2.8
1	A	985	C	2.8
4	D	36	ARG	2.7
3	C	155	GLY	2.6
1	A	1037	C	2.6

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Mol	Chain	Res	Type	RSRZ
3	C	76	VAL	2.6
9	I	4	TYR	2.6
10	J	89	ASP	2.6
1	A	81	U	2.6
1	A	1007	C	2.6
21	U	5	ASP	2.6
10	J	17	ASP	2.5
1	A	995	C	2.4
1	A	1036	G	2.4
1	A	1322	C	2.4
3	C	67	THR	2.4
19	S	40	ILE	2.4
1	A	1003(A)	G	2.4
1	A	1032	G	2.3
10	J	4	ILE	2.3
1	A	1321	C	2.3
19	S	21	GLU	2.3
3	C	101	LEU	2.3
1	A	1213	A	2.3
21	U	25	LYS	2.3
10	J	73	ASP	2.3
1	A	1047	G	2.3
13	M	6	GLY	2.3
21	U	22	ARG	2.3
7	G	156	TRP	2.2
10	J	32	ALA	2.2
3	C	146	ALA	2.2
7	G	83	ALA	2.2
19	S	31	ILE	2.2
10	J	38	ILE	2.2
19	S	28	LYS	2.2
1	A	1539	C	2.2
7	G	79	ARG	2.2
10	J	10	GLY	2.2
7	G	78	ARG	2.1
9	I	128	ARG	2.1
10	J	96	ILE	2.1
9	I	102	LEU	2.1
18	R	88	LYS	2.1
10	J	88	LEU	2.1
1	A	1224	G	2.1
9	I	119	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
14	N	18	VAL	2.1
7	G	84	ASN	2.0
13	M	119	GLY	2.0
10	J	70	ARG	2.0
15	O	88	ARG	2.0
1	A	1222	G	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{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	LLDF	B-factors(Å^2)	Q<0.9
1	MA6	A	1518[A]	24/25	0.96	0.23	-	115,120,128,130	24
12	0TD	L	92	10/11	0.97	0.42	-	150,171,185,382	0
1	5MC	A	1407	21/22	0.95	0.21	-	134,175,190,192	0
1	2MG	A	1207	24/25	0.90	0.15	-	207,227,293,300	0
1	5MC	A	1400	21/22	0.96	0.19	-	114,137,145,148	0
1	MA6	A	1519[A]	24/25	0.96	0.29	-	109,121,132,133	24
1	M2G	A	966	25/26	0.96	0.16	-	153,180,185,193	0
1	5MC	A	1404	21/22	0.94	0.18	-	118,133,162,167	0
1	PSU	A	516	20/21	0.90	0.14	-	138,167,192,192	0
1	5MC	A	967	21/22	0.95	0.13	-	152,157,177,181	0
1	PSU	A	1541	20/21	0.84	0.36	-	211,234,251,253	0
1	UR3	A	1498	21/22	0.95	0.25	-	118,145,161,171	0
1	7MG	A	527	24/25	0.94	0.15	-	128,140,159,170	0
1	PSU	A	1540	20/21	0.79	0.58	-	239,244,264,268	0
1	MA6	A	1518[B]	24/25	0.96	0.23	-	116,127,138,148	24
1	MA6	A	1519[B]	24/25	0.96	0.29	-	107,127,131,133	24
1	4OC	A	1402	22/23	0.96	0.20	-	122,134,156,160	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{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	LLDF	B-factors(Å^2)	Q<0.9
22	MG	A	1810	1/1	0.93	0.63	19.03	150,150,150,150	0
22	MG	D	302	1/1	0.92	0.53	10.88	109,109,109,109	0
22	MG	A	1649	1/1	0.99	0.47	10.37	165,165,165,165	0
22	MG	B	301	1/1	0.97	0.57	10.23	120,120,120,120	0
22	MG	C	302	1/1	0.95	0.57	8.77	172,172,172,172	0
22	MG	A	1734	1/1	0.94	0.26	7.04	101,101,101,101	0
22	MG	A	1748	1/1	0.94	0.30	5.94	116,116,116,116	0
22	MG	A	1836	1/1	0.97	0.33	5.74	109,109,109,109	0
22	MG	A	1826	1/1	0.98	0.42	5.26	104,104,104,104	0
22	MG	A	1797	1/1	0.95	0.46	5.10	163,163,163,163	0
22	MG	A	1746	1/1	0.94	0.37	4.72	91,91,91,91	0
22	MG	A	1653	1/1	0.94	0.23	4.68	114,114,114,114	0
22	MG	A	1636	1/1	0.96	0.23	4.64	203,203,203,203	0
22	MG	A	1767	1/1	0.92	0.39	4.55	104,104,104,104	0
22	MG	A	1735	1/1	0.87	0.29	3.79	112,112,112,112	0
22	MG	A	1770	1/1	0.92	0.24	3.79	100,100,100,100	0
22	MG	A	1679	1/1	0.98	0.38	3.29	138,138,138,138	0
22	MG	A	1820	1/1	0.90	0.28	3.26	148,148,148,148	0
22	MG	A	1643	1/1	0.94	0.29	3.26	111,111,111,111	0
22	MG	A	1773	1/1	0.86	0.56	3.06	128,128,128,128	0
22	MG	B	302	1/1	0.83	0.33	3.03	185,185,185,185	0
22	MG	A	1751	1/1	0.98	0.25	2.63	125,125,125,125	0
22	MG	A	1719	1/1	0.88	0.20	2.63	267,267,267,267	0
22	MG	A	1807	1/1	0.89	0.23	2.49	106,106,106,106	0
22	MG	A	1814	1/1	0.98	0.23	1.98	250,250,250,250	0
22	MG	A	1607	1/1	0.98	0.26	1.58	107,107,107,107	0
22	MG	A	1611	1/1	0.99	0.23	1.25	90,90,90,90	0
22	MG	L	201	1/1	0.80	0.37	1.24	140,140,140,140	0
22	MG	D	303	1/1	0.94	0.23	1.11	122,122,122,122	0
22	MG	A	1663	1/1	0.93	0.18	1.11	102,102,102,102	0
23	ZN	N	101	1/1	0.91	0.19	0.82	319,319,319,319	0
22	MG	A	1727	1/1	0.97	0.15	0.77	118,118,118,118	0
22	MG	A	1699	1/1	0.98	0.21	0.72	113,113,113,113	0
22	MG	A	1622	1/1	0.93	0.22	0.70	146,146,146,146	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
23	ZN	D	301	1/1	0.99	0.34	0.50	130,130,130,130	0
22	MG	A	1822	1/1	0.76	0.47	0.49	136,136,136,136	0
22	MG	A	1712	1/1	0.97	0.18	0.47	182,182,182,182	0
22	MG	A	1617	1/1	0.95	0.24	0.38	84,84,84,84	0
22	MG	A	1774	1/1	0.95	0.14	0.33	167,167,167,167	0
22	MG	A	1763	1/1	0.97	0.13	0.28	90,90,90,90	0
22	MG	A	1811	1/1	0.97	0.15	0.14	165,165,165,165	0
22	MG	A	1623	1/1	0.99	0.17	0.09	91,91,91,91	0
22	MG	A	1631	1/1	0.97	0.16	-0.11	123,123,123,123	0
22	MG	A	1658	1/1	0.92	0.18	-0.28	92,92,92,92	0
22	MG	A	1724	1/1	0.94	0.14	-0.42	132,132,132,132	0
22	MG	A	1759	1/1	0.97	0.20	-0.43	132,132,132,132	0
22	MG	A	1823	1/1	0.91	0.24	-0.76	123,123,123,123	0
22	MG	C	301	1/1	0.82	0.14	-0.78	139,139,139,139	0
22	MG	A	1796	1/1	0.98	0.10	-0.79	98,98,98,98	0
22	MG	A	1809	1/1	0.98	0.11	-0.80	133,133,133,133	0
22	MG	A	1705	1/1	0.96	0.14	-1.02	157,157,157,157	0
22	MG	A	1697	1/1	0.98	0.11	-1.13	183,183,183,183	0
22	MG	A	1616	1/1	0.97	0.15	-1.14	92,92,92,92	0
22	MG	A	1837	1/1	1.00	0.06	-1.17	156,156,156,156	0
22	MG	C	303	1/1	0.98	0.11	-1.26	175,175,175,175	0
22	MG	A	1641	1/1	0.98	0.14	-1.40	80,80,80,80	0
22	MG	A	1672	1/1	0.92	0.10	-1.62	164,164,164,164	0
22	MG	A	1711	1/1	0.98	0.11	-1.62	101,101,101,101	0
22	MG	A	1633	1/1	0.97	0.12	-1.71	112,112,112,112	0
22	MG	A	1723	1/1	0.89	0.12	-1.80	114,114,114,114	0
22	MG	A	1665	1/1	0.99	0.12	-2.13	127,127,127,127	0
22	MG	A	1813	1/1	0.97	0.12	-2.65	264,264,264,264	0
22	MG	A	1715	1/1	0.98	0.10	-3.79	114,114,114,114	0
22	MG	A	1646	1/1	0.98	0.06	-6.74	84,84,84,84	0
22	MG	A	1804	1/1	0.89	0.50	-	121,121,121,121	0
22	MG	A	1731	1/1	0.89	0.12	-	140,140,140,140	0
22	MG	A	1733	1/1	0.85	0.10	-	261,261,261,261	0
22	MG	A	1620	1/1	0.99	0.21	-	101,101,101,101	0
22	MG	A	1718	1/1	0.98	0.23	-	301,301,301,301	0
22	MG	A	1771	1/1	0.79	0.31	-	105,105,105,105	0
22	MG	A	1638	1/1	1.00	0.30	-	76,76,76,76	0
22	MG	A	1831	1/1	0.80	0.16	-	121,121,121,121	0
22	MG	A	1668	1/1	0.98	0.08	-	129,129,129,129	0
22	MG	A	1830	1/1	0.89	0.24	-	114,114,114,114	0
22	MG	A	1756	1/1	0.75	0.23	-	122,122,122,122	0
22	MG	A	1669	1/1	0.85	0.27	-	136,136,136,136	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
22	MG	A	1614	1/1	0.95	0.15	-	160,160,160,160	0
22	MG	A	1717	1/1	0.96	0.17	-	131,131,131,131	0
22	MG	A	1608	1/1	0.94	0.11	-	146,146,146,146	0
22	MG	A	1613	1/1	0.97	0.07	-	153,153,153,153	0
22	MG	A	1683	1/1	0.98	0.26	-	186,186,186,186	0
22	MG	A	1772	1/1	0.68	0.94	-	108,108,108,108	0
22	MG	A	1760	1/1	0.96	0.31	-	143,143,143,143	0
22	MG	A	1619	1/1	0.87	0.28	-	121,121,121,121	0
22	MG	A	1698	1/1	0.83	0.27	-	99,99,99,99	0
22	MG	A	1793	1/1	0.64	0.21	-	176,176,176,176	0
22	MG	A	1709	1/1	0.72	0.34	-	132,132,132,132	0
22	MG	A	1621	1/1	0.98	0.46	-	143,143,143,143	0
22	MG	A	1740	1/1	0.93	0.52	-	86,86,86,86	0
22	MG	A	1721	1/1	0.66	0.29	-	154,154,154,154	0
22	MG	A	1757	1/1	0.90	0.50	-	102,102,102,102	0
22	MG	A	1635	1/1	0.98	0.52	-	221,221,221,221	0
22	MG	A	1808	1/1	0.95	0.07	-	141,141,141,141	0
22	MG	A	1673	1/1	1.00	0.07	-	141,141,141,141	0
22	MG	A	1787	1/1	0.72	0.49	-	126,126,126,126	0
22	MG	A	1775	1/1	0.90	0.59	-	132,132,132,132	0
22	MG	A	1685	1/1	0.80	0.24	-	111,111,111,111	0
22	MG	A	1681	1/1	0.74	0.25	-	121,121,121,121	0
22	MG	A	1781	1/1	0.54	0.24	-	123,123,123,123	0
22	MG	A	1824	1/1	0.76	0.43	-	127,127,127,127	0
22	MG	A	1776	1/1	0.75	0.47	-	98,98,98,98	0
22	MG	A	1601	1/1	0.91	0.32	-	132,132,132,132	0
22	MG	A	1647	1/1	0.95	0.23	-	132,132,132,132	0
22	MG	A	1755	1/1	0.97	0.36	-	139,139,139,139	0
22	MG	A	1692	1/1	0.88	0.11	-	131,131,131,131	0
22	MG	A	1602	1/1	0.98	0.50	-	152,152,152,152	0
22	MG	A	1671	1/1	0.98	0.15	-	119,119,119,119	0
22	MG	A	1786	1/1	0.93	0.15	-	174,174,174,174	0
22	MG	A	1839	1/1	0.91	0.18	-	138,138,138,138	0
22	MG	A	1682	1/1	0.95	0.25	-	156,156,156,156	0
22	MG	A	1716	1/1	0.83	1.05	-	211,211,211,211	0
22	MG	A	1750	1/1	0.83	0.38	-	149,149,149,149	0
22	MG	A	1604	1/1	0.99	0.22	-	137,137,137,137	0
22	MG	A	1729	1/1	0.97	0.13	-	112,112,112,112	0
22	MG	A	1707	1/1	0.94	0.22	-	143,143,143,143	0
22	MG	A	1639	1/1	0.85	0.28	-	105,105,105,105	0
22	MG	A	1829	1/1	0.90	0.65	-	97,97,97,97	0
22	MG	A	1798	1/1	0.92	0.34	-	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
22	MG	A	1741	1/1	0.91	0.51	-	127,127,127,127	0
22	MG	A	1684	1/1	0.93	0.18	-	145,145,145,145	0
22	MG	P	102	1/1	0.51	0.22	-	119,119,119,119	0
22	MG	A	1801	1/1	0.63	0.68	-	142,142,142,142	0
22	MG	A	1696	1/1	0.96	0.40	-	174,174,174,174	0
22	MG	A	1816	1/1	0.82	0.38	-	149,149,149,149	0
22	MG	A	1753	1/1	0.87	0.18	-	138,138,138,138	0
22	MG	A	1659	1/1	0.96	0.17	-	112,112,112,112	0
22	MG	A	1689	1/1	0.94	0.17	-	270,270,270,270	0
22	MG	A	1651	1/1	0.95	0.20	-	132,132,132,132	0
22	MG	A	1782	1/1	0.80	0.53	-	148,148,148,148	0
22	MG	A	1743	1/1	0.93	0.38	-	104,104,104,104	0
22	MG	A	1834	1/1	0.71	0.18	-	146,146,146,146	0
22	MG	A	1664	1/1	0.85	0.29	-	115,115,115,115	0
22	MG	A	1799	1/1	0.88	0.29	-	157,157,157,157	0
22	MG	A	1785	1/1	0.72	0.82	-	82,82,82,82	0
22	MG	A	1722	1/1	0.96	0.12	-	88,88,88,88	0
22	MG	A	1703	1/1	0.88	0.60	-	120,120,120,120	0
22	MG	A	1606	1/1	0.99	0.11	-	101,101,101,101	0
22	MG	A	1732	1/1	0.90	0.69	-	138,138,138,138	0
22	MG	E	201	1/1	0.90	0.09	-	146,146,146,146	0
22	MG	A	1662	1/1	0.79	0.27	-	151,151,151,151	0
22	MG	A	1805	1/1	0.95	0.55	-	138,138,138,138	0
22	MG	A	1675	1/1	0.84	0.12	-	143,143,143,143	0
22	MG	A	1738	1/1	0.80	0.50	-	122,122,122,122	0
22	MG	A	1838	1/1	0.62	0.89	-	144,144,144,144	0
22	MG	A	1634	1/1	0.72	0.92	-	124,124,124,124	0
22	MG	A	1701	1/1	0.98	0.23	-	134,134,134,134	0
22	MG	A	1788	1/1	0.92	0.31	-	115,115,115,115	0
22	MG	A	1778	1/1	0.89	0.38	-	136,136,136,136	0
22	MG	A	1714	1/1	0.99	0.32	-	146,146,146,146	0
22	MG	A	1821	1/1	0.89	0.18	-	144,144,144,144	0
22	MG	F	201	1/1	0.96	0.29	-	134,134,134,134	0
22	MG	A	1817	1/1	0.76	0.42	-	127,127,127,127	0
22	MG	D	304	1/1	0.85	0.13	-	112,112,112,112	0
22	MG	Q	201	1/1	0.94	0.18	-	116,116,116,116	0
22	MG	A	1769	1/1	0.88	0.60	-	145,145,145,145	0
22	MG	A	1766	1/1	0.99	0.18	-	134,134,134,134	0
22	MG	A	1720	1/1	0.85	0.37	-	150,150,150,150	0
22	MG	A	1674	1/1	0.88	0.43	-	155,155,155,155	0
22	MG	A	1628	1/1	0.93	0.34	-	89,89,89,89	0
22	MG	A	1655	1/1	0.98	0.22	-	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
22	MG	A	1752	1/1	0.98	0.12	-	122,122,122,122	0
22	MG	A	1789	1/1	0.92	0.63	-	134,134,134,134	0
22	MG	A	1666	1/1	0.91	0.21	-	120,120,120,120	0
22	MG	A	1754	1/1	0.47	0.59	-	130,130,130,130	0
22	MG	A	1713	1/1	0.98	0.17	-	122,122,122,122	0
22	MG	A	1818	1/1	0.66	0.94	-	129,129,129,129	0
22	MG	A	1791	1/1	0.89	0.32	-	147,147,147,147	0
22	MG	A	1730	1/1	0.84	0.24	-	124,124,124,124	0
22	MG	A	1710	1/1	0.96	0.32	-	208,208,208,208	0
22	MG	A	1708	1/1	0.96	0.09	-	152,152,152,152	0
22	MG	A	1676	1/1	0.95	0.19	-	153,153,153,153	0
22	MG	A	1736	1/1	0.73	0.40	-	121,121,121,121	0
22	MG	A	1678	1/1	0.92	0.12	-	98,98,98,98	0
22	MG	A	1827	1/1	0.98	0.23	-	140,140,140,140	0
22	MG	A	1704	1/1	0.91	0.05	-	178,178,178,178	0
22	MG	A	1657	1/1	0.99	0.17	-	170,170,170,170	0
22	MG	A	1745	1/1	0.45	0.45	-	132,132,132,132	0
22	MG	A	1629	1/1	0.80	0.13	-	208,208,208,208	0
22	MG	A	1627	1/1	0.95	0.68	-	98,98,98,98	0
22	MG	A	1758	1/1	0.47	0.75	-	139,139,139,139	0
22	MG	A	1686	1/1	0.96	0.23	-	112,112,112,112	0
22	MG	A	1690	1/1	0.88	0.34	-	179,179,179,179	0
22	MG	A	1642	1/1	0.98	0.17	-	119,119,119,119	0
22	MG	A	1694	1/1	0.99	0.11	-	133,133,133,133	0
22	MG	A	1742	1/1	0.85	0.38	-	108,108,108,108	0
22	MG	A	1780	1/1	0.97	0.26	-	136,136,136,136	0
22	MG	A	1794	1/1	0.70	0.97	-	150,150,150,150	0
22	MG	A	1706	1/1	0.79	0.44	-	148,148,148,148	0
22	MG	A	1783	1/1	0.89	0.25	-	142,142,142,142	0
22	MG	A	1777	1/1	0.96	0.39	-	94,94,94,94	0
22	MG	A	1670	1/1	0.93	0.45	-	108,108,108,108	0
22	MG	A	1737	1/1	0.91	0.17	-	145,145,145,145	0
22	MG	A	1819	1/1	0.88	0.30	-	132,132,132,132	0
22	MG	A	1667	1/1	0.70	0.24	-	102,102,102,102	0
22	MG	A	1640	1/1	0.97	0.32	-	202,202,202,202	0
22	MG	A	1765	1/1	0.77	0.49	-	113,113,113,113	0
22	MG	A	1728	1/1	0.95	0.26	-	150,150,150,150	0
22	MG	A	1609	1/1	0.98	0.29	-	106,106,106,106	0
22	MG	A	1612	1/1	0.96	0.11	-	194,194,194,194	0
22	MG	A	1800	1/1	0.95	0.20	-	126,126,126,126	0
22	MG	A	1784	1/1	0.90	0.99	-	149,149,149,149	0
22	MG	A	1661	1/1	0.99	0.23	-	154,154,154,154	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
22	MG	A	1739	1/1	0.89	0.57	-	116,116,116,116	0
22	MG	A	1680	1/1	0.97	0.09	-	275,275,275,275	0
22	MG	A	1615	1/1	0.97	0.06	-	123,123,123,123	0
22	MG	A	1749	1/1	0.99	0.10	-	111,111,111,111	0
22	MG	A	1806	1/1	0.57	0.34	-	157,157,157,157	0
22	MG	A	1825	1/1	0.49	0.23	-	132,132,132,132	0
22	MG	A	1762	1/1	0.94	0.17	-	118,118,118,118	0
22	MG	A	1625	1/1	0.93	0.53	-	61,61,61,61	0
22	MG	A	1644	1/1	0.97	0.21	-	105,105,105,105	0
22	MG	A	1687	1/1	0.88	1.23	-	130,130,130,130	0
22	MG	A	1637	1/1	1.00	0.14	-	85,85,85,85	0
22	MG	A	1654	1/1	0.95	0.05	-	126,126,126,126	0
22	MG	A	1693	1/1	0.94	0.71	-	176,176,176,176	0
22	MG	A	1618	1/1	0.97	0.42	-	123,123,123,123	0
22	MG	A	1790	1/1	0.94	0.16	-	130,130,130,130	0
22	MG	A	1702	1/1	0.98	0.12	-	143,143,143,143	0
22	MG	A	1632	1/1	0.86	0.30	-	113,113,113,113	0
22	MG	D	305	1/1	0.67	0.85	-	123,123,123,123	0
22	MG	A	1652	1/1	0.98	0.12	-	93,93,93,93	0
22	MG	A	1792	1/1	0.98	0.07	-	127,127,127,127	0
22	MG	A	1835	1/1	0.88	0.26	-	149,149,149,149	0
22	MG	A	1828	1/1	0.55	1.29	-	154,154,154,154	0
22	MG	A	1677	1/1	0.87	0.19	-	130,130,130,130	0
22	MG	A	1630	1/1	0.93	0.26	-	123,123,123,123	0
22	MG	A	1605	1/1	0.95	1.01	-	109,109,109,109	0
22	MG	A	1744	1/1	0.94	0.70	-	133,133,133,133	0
22	MG	A	1726	1/1	0.98	0.26	-	341,341,341,341	0
22	MG	A	1650	1/1	0.92	0.22	-	121,121,121,121	0
22	MG	A	1802	1/1	0.89	0.21	-	122,122,122,122	0
22	MG	A	1761	1/1	0.93	0.54	-	129,129,129,129	0
22	MG	A	1725	1/1	0.90	0.44	-	115,115,115,115	0
22	MG	A	1832	1/1	0.76	0.17	-	118,118,118,118	0
22	MG	A	1691	1/1	0.81	0.23	-	128,128,128,128	0
22	MG	A	1688	1/1	0.99	0.10	-	169,169,169,169	0
22	MG	A	1603	1/1	0.93	0.23	-	121,121,121,121	0
22	MG	A	1803	1/1	0.95	0.13	-	160,160,160,160	0
22	MG	A	1645	1/1	0.96	0.50	-	90,90,90,90	0
22	MG	A	1648	1/1	0.95	0.50	-	226,226,226,226	0
22	MG	A	1624	1/1	0.84	0.43	-	124,124,124,124	0
22	MG	A	1764	1/1	0.72	0.29	-	126,126,126,126	0
22	MG	A	1833	1/1	0.70	0.09	-	112,112,112,112	0
22	MG	A	1795	1/1	0.97	0.54	-	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
22	MG	A	1815	1/1	0.99	0.08	-	202,202,202,202	0
22	MG	A	1656	1/1	0.98	0.23	-	124,124,124,124	0
22	MG	A	1768	1/1	0.97	0.31	-	92,92,92,92	0
22	MG	A	1610	1/1	0.91	0.23	-	111,111,111,111	0
22	MG	A	1695	1/1	0.99	0.19	-	167,167,167,167	0
22	MG	A	1626	1/1	0.93	0.22	-	172,172,172,172	0
22	MG	A	1660	1/1	0.99	0.10	-	122,122,122,122	0
22	MG	A	1812	1/1	0.95	0.11	-	228,228,228,228	0
22	MG	A	1747	1/1	0.98	0.21	-	138,138,138,138	0
22	MG	A	1700	1/1	0.92	0.21	-	129,129,129,129	0
22	MG	P	101	1/1	0.93	0.35	-	86,86,86,86	0
22	MG	A	1779	1/1	0.93	0.24	-	115,115,115,115	0

6.5 Other polymers (i)

There are no such residues in this entry.