Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:59 PM GMT

PDB ID	:	4DUZ
Title	:	Crystal structure of the Thermus thermophilus 30S ribosomal subunit with a 16S rRNA mutation, U13C, bound with streptomycin
Authors	:	Demirci, H.; Murphy IV, F.; Murphy, E.; Gregory, S.T.; Dahlberg, A.E.; Jogl, G.
Deposited on	:	2012-02-22
Resolution	:	3.65 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:

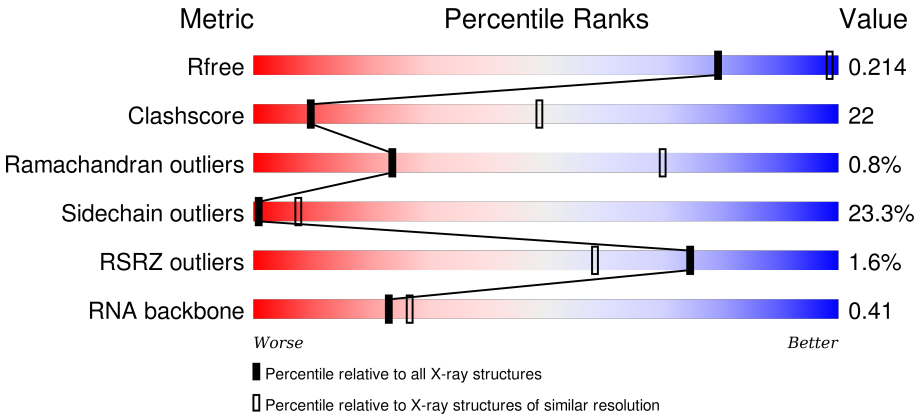
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.65 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	1010 (3.82-3.50)
Clashscore	102246	1125 (3.82-3.50)
Ramachandran outliers	100387	1079 (3.82-3.50)
Sidechain outliers	100360	1078 (3.82-3.50)
RSRZ outliers	91569	1017 (3.82-3.50)
RNA backbone	2183	1066 (4.52-2.80)

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	% 15% 41% 32% 11% •
2	B	256	33% 48% 9% • 9%
3	C	239	5% 31% 44% 11% 14%
4	D	209	% 49% 38% 11% •

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Mol	Chain	Length	Quality of chain
5	E	162	40% 43% 9% 7%
6	F	101	45% 48% 8%
7	G	156	2% 50% 42% 6%
8	H	138	32% 49% 18%
9	I	128	2% 43% 48% 8%
10	J	105	7% 28% 50% 16% 7%
11	K	129	39% 39% 12% 10%
12	L	135	42% 31% 18% 8%
13	M	126	2% 40% 44% 10% 6%
14	N	61	3% 41% 44% 13%
15	O	89	35% 47% 16%
16	P	88	42% 38% 13% 6%
17	Q	105	38% 37% 17% 6%
18	R	88	27% 41% 10% 20%
19	S	93	4% 41% 32% 12% 14%
20	T	106	% 45% 33% 15% 7%
21	U	27	19% 33% 44% 11% 11%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	MG	A	1613	-	-	-	X
23	MG	A	1641	-	-	-	X
23	MG	A	1666	-	-	-	X
23	MG	A	1690	-	-	-	X
23	MG	A	1691	-	-	-	X
23	MG	A	1699	-	-	-	X
23	MG	A	1708	-	-	-	X
23	MG	A	1724	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	MG	A	1726	-	-	-	X
23	MG	A	1728	-	-	-	X
23	MG	A	1731	-	-	-	X
23	MG	A	1732	-	-	-	X
23	MG	A	1747	-	-	-	X
23	MG	A	1761	-	-	-	X
23	MG	A	1768	-	-	-	X
23	MG	A	1779	-	-	-	X
23	MG	A	1788	-	-	-	X
23	MG	A	1828	-	-	-	X
23	MG	A	1843	-	-	-	X
23	MG	A	1846	-	-	-	X
23	MG	A	1848	-	-	-	X
23	MG	B	301	-	-	-	X
23	MG	H	203	-	-	-	X
23	MG	M	202	-	-	-	X
23	MG	T	1202	-	-	-	X

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 52289 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	32507	14477	6012	10506	1512	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	C	U	ENGINEERED MUTATION	GB M26923.1
A	1534	C	A	CONFLICT	GB M26923.1
A	1535	A	C	CONFLICT	GB M26923.1

- Molecule 2 is a protein called ribosomal protein S2.

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

- Molecule 3 is a protein called ribosomal protein S3.

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

- Molecule 4 is a protein called ribosomal protein S4.

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

- Molecule 5 is a protein called ribosomal protein S5.

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

- Molecule 6 is a protein called ribosomal protein S6.

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

- Molecule 7 is a protein called ribosomal protein S7.

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

- Molecule 8 is a protein called ribosomal protein S8.

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

- Molecule 9 is a protein called ribosomal protein S9.

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

- Molecule 10 is a protein called ribosomal protein S10.

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

- Molecule 11 is a protein called ribosomal protein S11.

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

- Molecule 12 is a protein called ribosomal protein S12.

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

- Molecule 13 is a protein called ribosomal protein S13.

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

- Molecule 14 is a protein called ribosomal protein S14.

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

- Molecule 15 is a protein called ribosomal protein S15.

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

- Molecule 16 is a protein called ribosomal protein S16.

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

- Molecule 17 is a protein called ribosomal protein S17.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 18 is a protein called ribosomal protein S18.

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

- Molecule 19 is a protein called ribosomal protein S19.

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

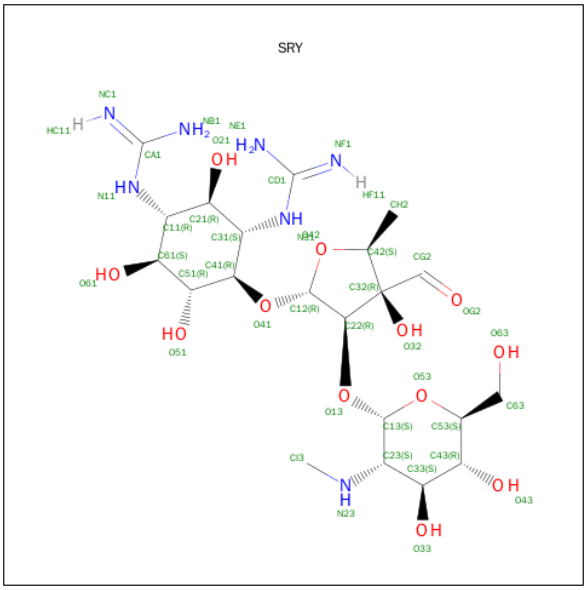
- Molecule 20 is a protein called ribosomal protein S20.

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

- Molecule 21 is a protein called ribosomal protein THX.

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

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



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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	P	2	Total Mg 2 2	0	0
23	J	1	Total Mg 1 1	0	0
23	Q	2	Total Mg 2 2	0	0
23	D	1	Total Mg 1 1	0	0
23	E	1	Total Mg 1 1	0	0
23	H	4	Total Mg 4 4	0	0
23	B	2	Total Mg 2 2	0	0
23	A	249	Total Mg 249 249	0	0
23	T	2	Total Mg 2 2	0	0
23	S	1	Total Mg 1 1	0	0
23	M	2	Total Mg 2 2	0	0

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

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

- Molecule 25 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	369	Total O 369 369	0	0
25	D	1	Total O 1 1	0	0
25	E	6	Total O 6 6	0	0
25	G	1	Total O 1 1	0	0

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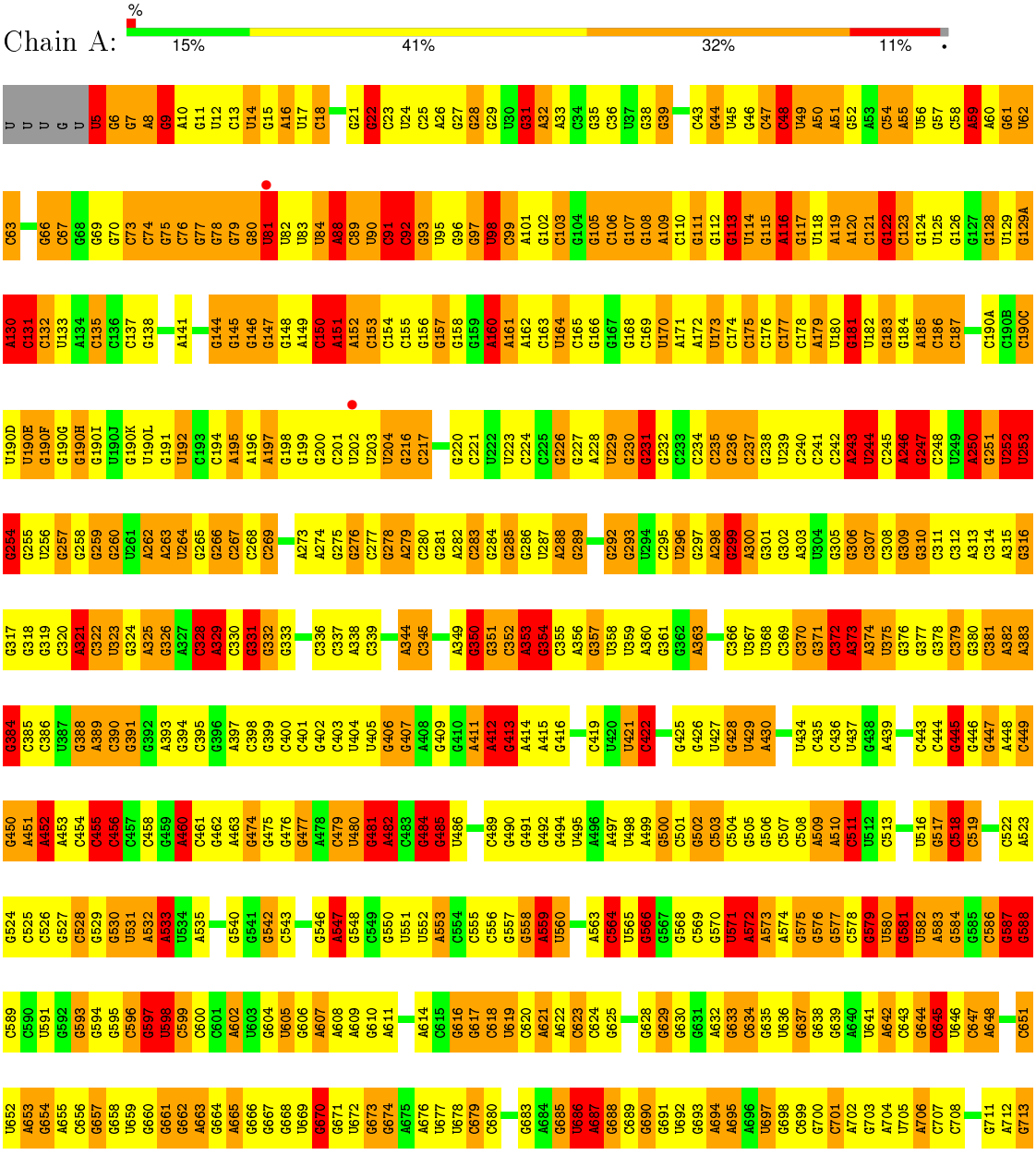
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	L	1	Total O 1 1	0	0
25	P	1	Total O 1 1	0	0
25	Q	4	Total O 4 4	0	0
25	T	2	Total O 2 2	0	0

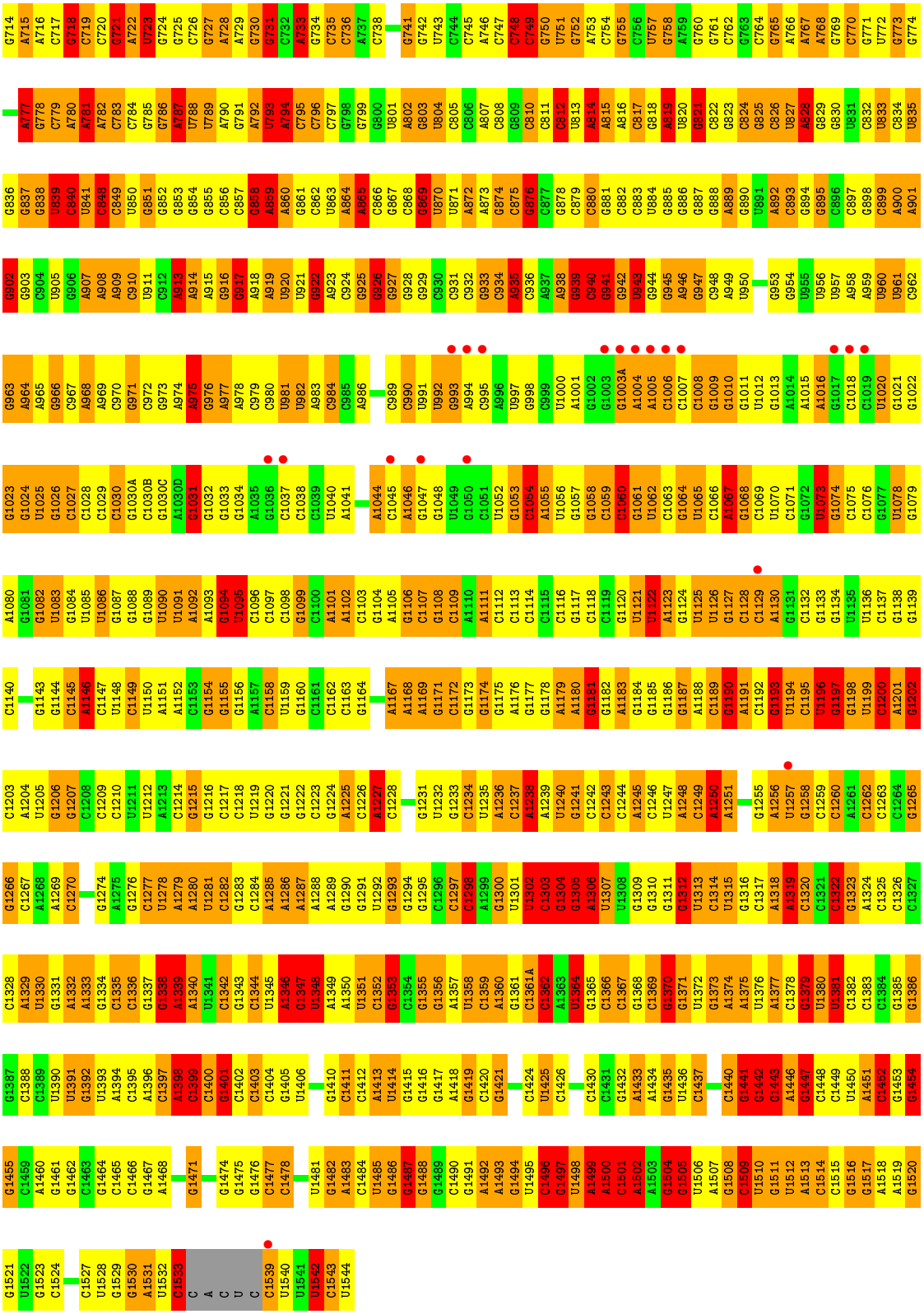
3 Residue-property plots (i)

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

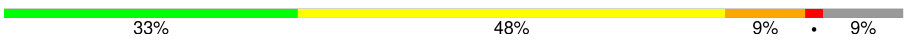
Chain A:

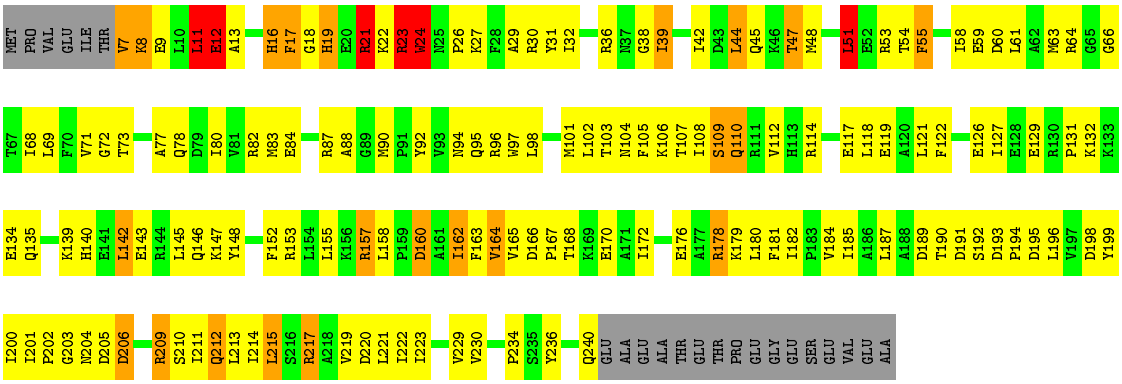




• Molecule 2: ribosomal protein S2

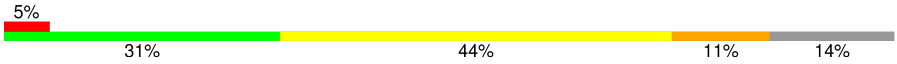
Chain B:

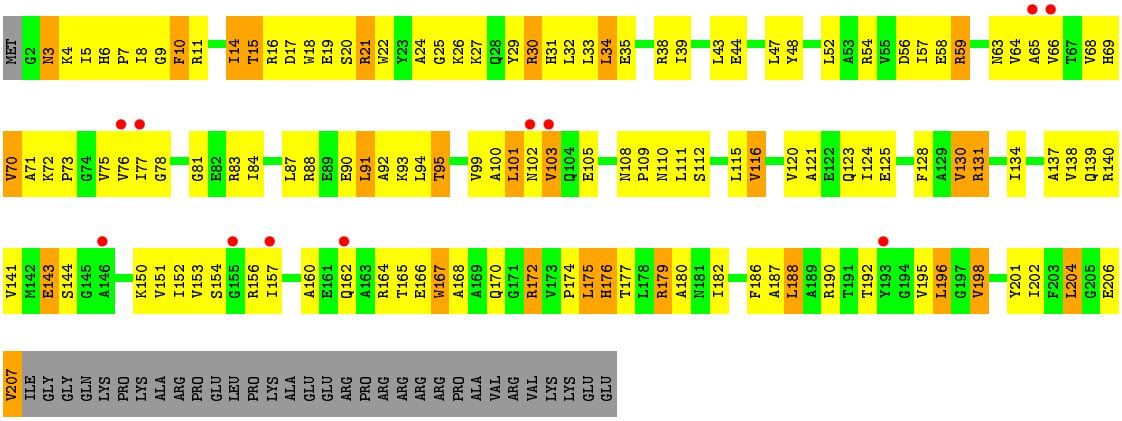




• Molecule 3: ribosomal protein S3

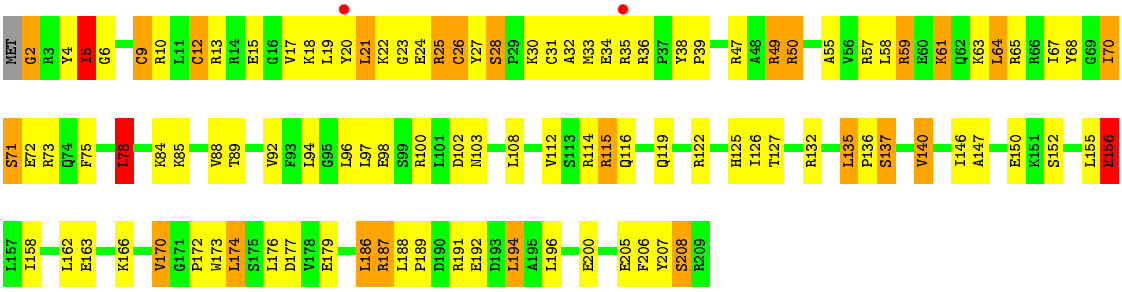
Chain C:





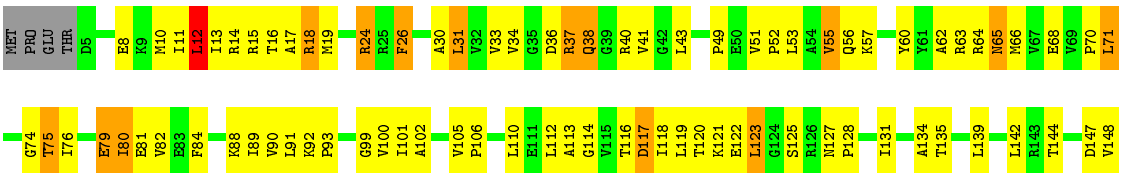
• Molecule 4: ribosomal protein S4

Chain D:



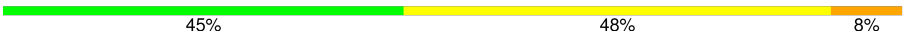
• Molecule 5: ribosomal protein S5

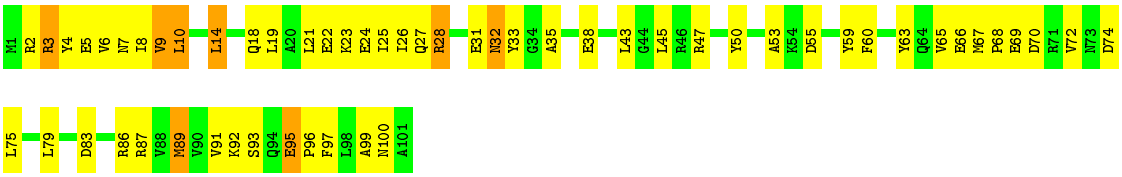
Chain E:



- Molecule 6: ribosomal protein S6

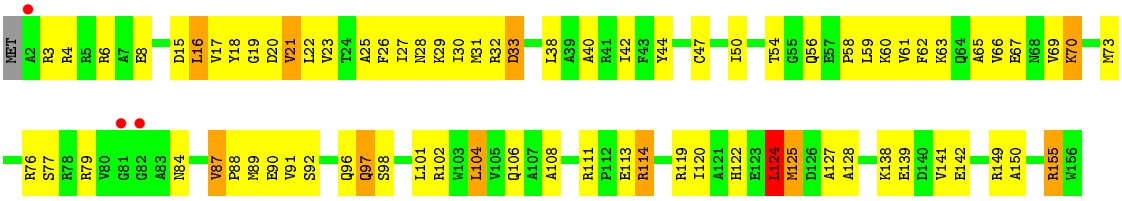
Chain F:





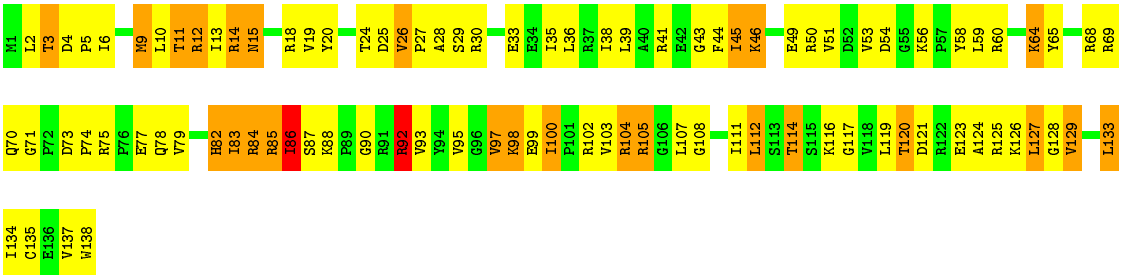
- Molecule 7: ribosomal protein S7

Chain G:



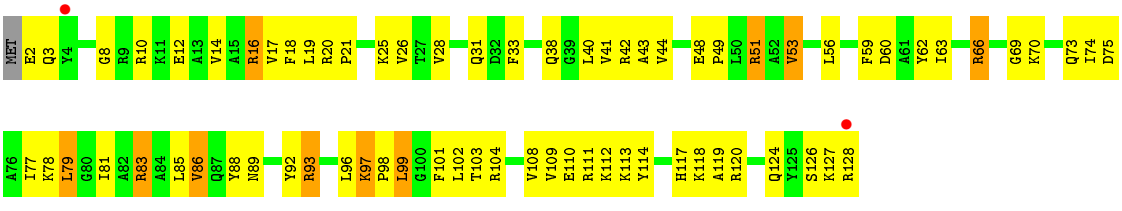
- Molecule 8: ribosomal protein S8

Chain H:



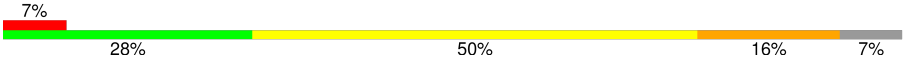
- Molecule 9: ribosomal protein S9

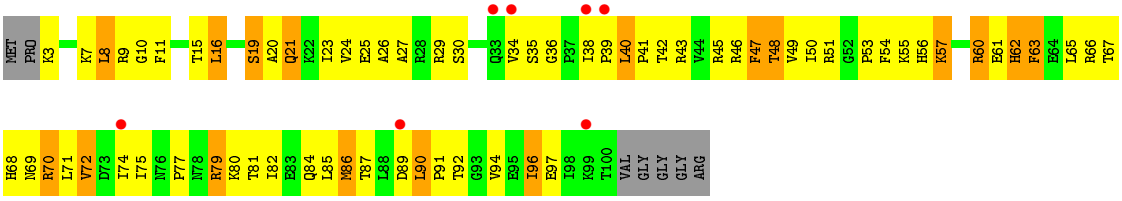
Chain I:



- Molecule 10: ribosomal protein S10

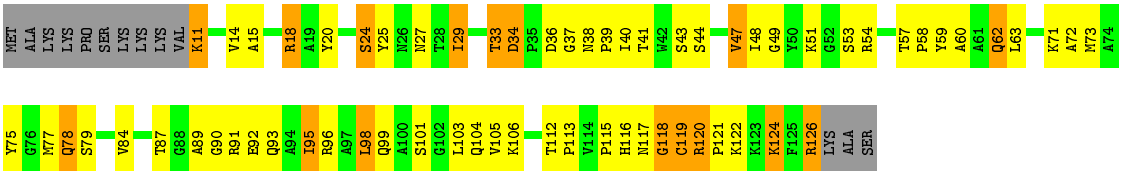
Chain J:





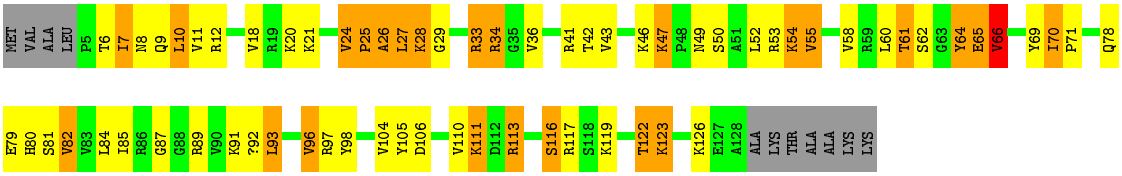
• Molecule 11: ribosomal protein S11

Chain K:



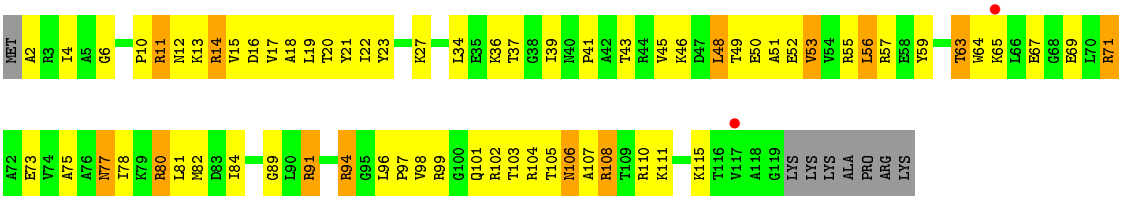
• Molecule 12: ribosomal protein S12

Chain L:



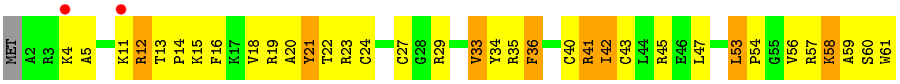
• Molecule 13: ribosomal protein S13

Chain M:



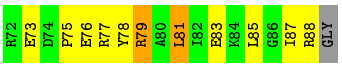
• Molecule 14: ribosomal protein S14

Chain N:



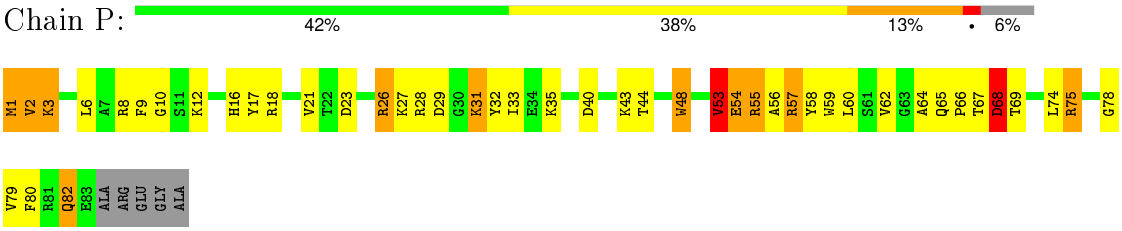
• Molecule 15: ribosomal protein S15

Chain O:



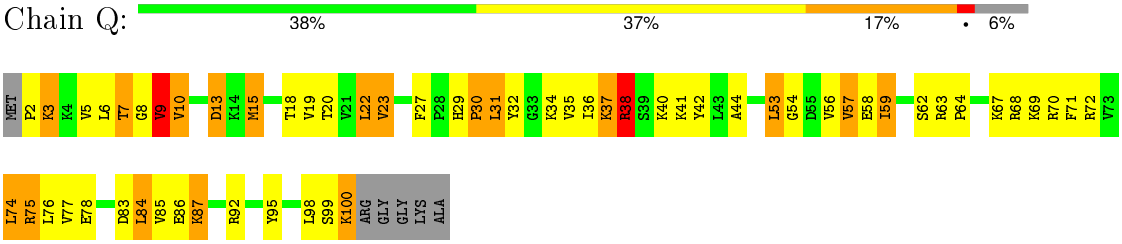
• Molecule 16: ribosomal protein S16

Chain P:



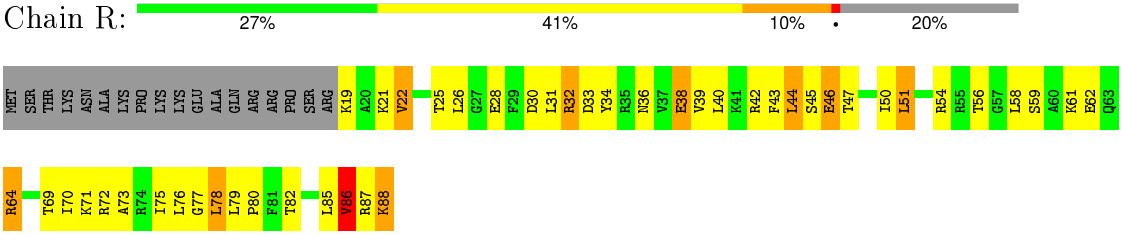
• Molecule 17: ribosomal protein S17

Chain Q:



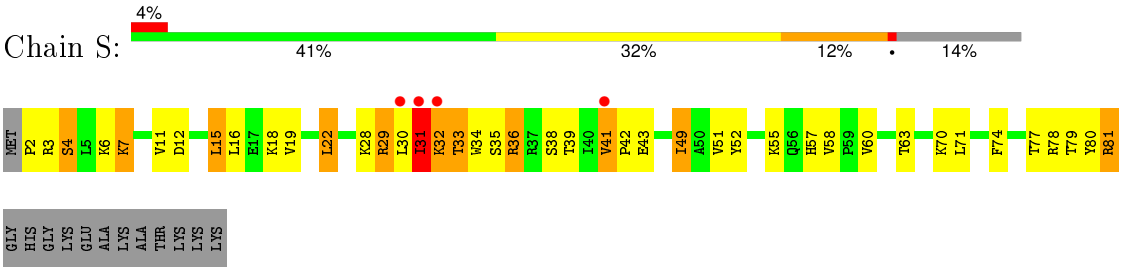
• Molecule 18: ribosomal protein S18

Chain R:



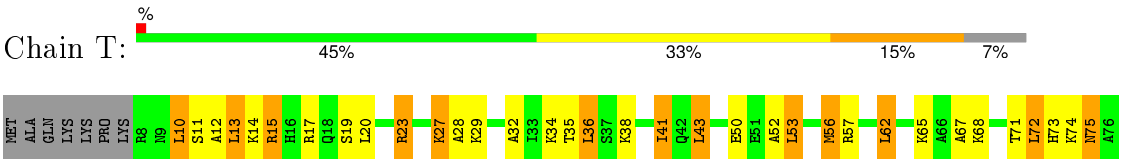
• Molecule 19: ribosomal protein S19

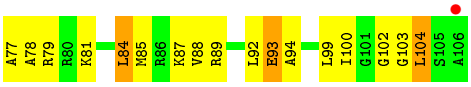
Chain S:



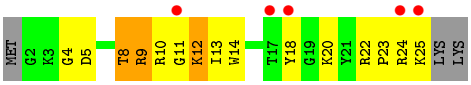
• Molecule 20: ribosomal protein S20

Chain T:





• Molecule 21: ribosomal protein THX



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	402.52Å 402.52Å 173.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.56 – 3.65 34.56 – 3.65	Depositor EDS
% Data completeness (in resolution range)	95.6 (34.56-3.65) 95.4 (34.56-3.65)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.27 (at 3.66Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_978)	Depositor
R, R_{free}	0.156 , 0.216 0.158 , 0.214	Depositor DCC
R_{free} test set	7502 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	141.1	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 133.4	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 150416 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	52289	wwPDB-VP
Average B, all atoms (Å^2)	172.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.07% 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, M2G, MA6, 0TD, MG, 2MG, 5MC, UR3, 4OC, SRY, 7MG, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	1.30	226/36040 (0.6%)	2.04	2283/56243 (4.1%)
2	B	0.77	0/1935	0.97	6/2609 (0.2%)
3	C	0.62	0/1636	0.84	1/2205 (0.0%)
4	D	0.77	1/1733 (0.1%)	0.97	4/2318 (0.2%)
5	E	1.01	1/1162 (0.1%)	1.13	1/1564 (0.1%)
6	F	0.73	0/856	0.88	0/1154
7	G	0.74	0/1276	0.89	1/1709 (0.1%)
8	H	1.12	0/1136	1.23	4/1527 (0.3%)
9	I	0.63	0/1029	0.86	1/1379 (0.1%)
10	J	0.58	0/805	0.85	1/1082 (0.1%)
11	K	0.76	1/879 (0.1%)	1.01	3/1187 (0.3%)
12	L	0.91	0/977	1.13	3/1306 (0.2%)
13	M	0.70	0/947	0.93	0/1270
14	N	0.67	1/501 (0.2%)	0.86	0/664
15	O	0.84	0/740	1.03	3/987 (0.3%)
16	P	0.92	1/716 (0.1%)	1.10	1/963 (0.1%)
17	Q	1.09	1/836 (0.1%)	1.23	5/1117 (0.4%)
18	R	0.81	0/579	0.99	1/768 (0.1%)
19	S	0.64	0/661	0.88	0/890
20	T	0.79	0/765	1.05	3/1007 (0.3%)
21	U	0.57	0/212	0.92	0/277
All	All	1.15	232/55421 (0.4%)	1.77	2321/82226 (2.8%)

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

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

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Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	2
8	H	0	2
10	J	0	2
12	L	0	3
15	O	0	1
17	Q	0	1
18	R	0	1
20	T	0	1
All	All	0	19

All (232) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	279	A	N9-C4	-12.51	1.30	1.37
1	A	130	A	N3-C4	-10.46	1.28	1.34
1	A	828	A	N9-C4	-9.94	1.31	1.37
1	A	946	A	N3-C4	-9.94	1.28	1.34
1	A	819	A	N3-C4	-9.27	1.29	1.34
1	A	298	A	N3-C4	-8.91	1.29	1.34
1	A	279	A	N7-C5	-8.63	1.34	1.39
1	A	1377	A	N9-C4	-8.55	1.32	1.37
1	A	130	A	N9-C4	-8.48	1.32	1.37
1	A	563	A	N3-C4	-8.15	1.29	1.34
1	A	868	C	N1-C6	-8.11	1.32	1.37
1	A	860	A	N9-C4	-8.10	1.32	1.37
1	A	329	A	N9-C4	-7.97	1.33	1.37
1	A	1500	A	C6-N1	-7.64	1.30	1.35
1	A	833	U	C4-O4	7.61	1.29	1.23
1	A	915	A	N9-C4	-7.49	1.33	1.37
1	A	320	C	N1-C6	-7.29	1.32	1.37
1	A	779	C	N1-C6	-7.29	1.32	1.37
1	A	1520	G	N9-C4	-7.29	1.32	1.38
1	A	1243	C	N1-C6	-7.21	1.32	1.37
1	A	788	U	C2-N3	7.20	1.42	1.37
1	A	722	A	N9-C4	-7.19	1.33	1.37
1	A	931	C	N3-C4	-7.18	1.28	1.33
1	A	564	C	N1-C6	-7.15	1.32	1.37
1	A	946	A	C6-N1	-7.12	1.30	1.35
1	A	583	A	N9-C4	-7.08	1.33	1.37
1	A	279	A	C5-C6	-7.05	1.34	1.41
1	A	874	G	N9-C8	-6.97	1.32	1.37
1	A	589	C	N1-C6	-6.97	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	12	CYS	CB-SG	6.97	1.94	1.82
1	A	817	C	N1-C6	-6.94	1.32	1.37
1	A	1502	A	C5-C6	-6.92	1.34	1.41
1	A	602	A	N9-C4	-6.92	1.33	1.37
1	A	880	C	N3-C4	-6.84	1.29	1.33
1	A	108	G	N9-C8	6.82	1.42	1.37
1	A	566	G	N7-C5	-6.82	1.35	1.39
1	A	872	A	N7-C5	-6.80	1.35	1.39
1	A	576	G	N3-C4	-6.79	1.30	1.35
1	A	266	G	N9-C4	-6.75	1.32	1.38
1	A	706	A	N9-C4	-6.75	1.33	1.37
1	A	897	C	N3-C4	-6.73	1.29	1.33
1	A	533	A	N9-C4	6.72	1.41	1.37
1	A	117	G	C5-C4	6.72	1.43	1.38
1	A	131	C	N3-C4	-6.71	1.29	1.33
1	A	581	G	N7-C5	-6.67	1.35	1.39
1	A	16	A	N9-C4	-6.67	1.33	1.37
1	A	586	C	N1-C6	-6.65	1.33	1.37
1	A	729	A	N9-C4	-6.65	1.33	1.37
1	A	1078	U	C4-O4	-6.65	1.18	1.23
1	A	715	A	N9-C4	-6.65	1.33	1.37
1	A	856	C	N1-C6	-6.63	1.33	1.37
1	A	566	G	N3-C4	-6.61	1.30	1.35
1	A	569	C	N3-C4	-6.60	1.29	1.33
1	A	654	G	N9-C4	-6.56	1.32	1.38
1	A	152	A	N9-C4	-6.53	1.33	1.37
1	A	1346	A	C3'-O3'	6.53	1.51	1.42
1	A	1499	A	N7-C5	-6.47	1.35	1.39
1	A	1497	G	N7-C5	-6.46	1.35	1.39
1	A	124	G	N3-C4	-6.44	1.30	1.35
1	A	1509	C	N3-C4	-6.38	1.29	1.33
1	A	451	A	N9-C4	-6.37	1.34	1.37
1	A	1502	A	N3-C4	-6.28	1.31	1.34
1	A	109	A	N9-C4	-6.28	1.34	1.37
1	A	570	G	C5-C4	-6.27	1.33	1.38
1	A	869	G	C8-N7	-6.26	1.27	1.30
1	A	1338	G	C6-N1	-6.24	1.35	1.39
1	A	944	G	C6-N1	-6.22	1.35	1.39
1	A	600	C	N1-C6	-6.21	1.33	1.37
1	A	563	A	N9-C4	-6.18	1.34	1.37
1	A	1504	G	N7-C5	-6.16	1.35	1.39
1	A	730	G	N9-C8	-6.15	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	897	C	N1-C6	-6.14	1.33	1.37
1	A	1513	A	N3-C4	-6.14	1.31	1.34
1	A	1523	G	C5-C4	-6.11	1.34	1.38
1	A	676	A	N9-C4	-6.09	1.34	1.37
1	A	572	A	C6-N1	-6.07	1.31	1.35
17	Q	23	VAL	CB-CG1	-6.05	1.40	1.52
1	A	1329	A	N7-C5	-6.02	1.35	1.39
1	A	1501	C	N3-C4	-6.02	1.29	1.33
1	A	654	G	N3-C4	-6.01	1.31	1.35
1	A	357	G	N9-C8	-6.00	1.33	1.37
1	A	144	G	N1-C2	5.98	1.42	1.37
1	A	1442	G	N9-C4	5.95	1.42	1.38
1	A	572	A	C5-C4	-5.95	1.34	1.38
1	A	822	C	N1-C6	-5.95	1.33	1.37
1	A	124	G	C6-N1	-5.93	1.35	1.39
1	A	1499	A	C5-C6	-5.92	1.35	1.41
1	A	812	C	N1-C6	-5.91	1.33	1.37
1	A	730	G	C6-N1	-5.89	1.35	1.39
1	A	1243	C	N3-C4	-5.89	1.29	1.33
1	A	574	A	N9-C4	-5.89	1.34	1.37
1	A	822	C	C4-C5	-5.87	1.38	1.43
14	N	27	CYS	CB-SG	-5.86	1.72	1.81
1	A	570	G	N1-C2	-5.86	1.33	1.37
1	A	1079	G	N7-C5	-5.86	1.35	1.39
1	A	1524	C	N1-C6	-5.86	1.33	1.37
1	A	61	G	N3-C4	-5.84	1.31	1.35
1	A	1394	A	N9-C4	-5.84	1.34	1.37
1	A	722	A	C5-C6	-5.83	1.35	1.41
1	A	874	G	C5-C4	-5.83	1.34	1.38
1	A	633	G	C5-C4	-5.81	1.34	1.38
1	A	574	A	N3-C4	-5.80	1.31	1.34
1	A	1513	A	N9-C4	-5.80	1.34	1.37
1	A	357	G	N3-C4	-5.78	1.31	1.35
1	A	300	A	N3-C4	-5.78	1.31	1.34
1	A	190(G)	G	N7-C5	-5.78	1.35	1.39
1	A	1079	G	C6-N1	-5.77	1.35	1.39
1	A	1520	G	N7-C5	-5.77	1.35	1.39
1	A	1076	C	N3-C4	-5.76	1.29	1.33
1	A	1064	G	N9-C4	-5.76	1.33	1.38
1	A	746	A	N3-C4	-5.75	1.31	1.34
1	A	329	A	C5-C6	-5.70	1.35	1.41
1	A	1523	G	C5-C6	-5.69	1.36	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	802	A	N9-C4	-5.68	1.34	1.37
1	A	625	G	C6-N1	-5.67	1.35	1.39
1	A	1146	A	N9-C4	-5.66	1.34	1.37
1	A	605	U	C4-O4	5.64	1.28	1.23
1	A	559	A	N3-C4	-5.62	1.31	1.34
1	A	1500	A	N3-C4	-5.62	1.31	1.34
1	A	826	C	N1-C6	-5.60	1.33	1.37
1	A	460	A	N9-C4	5.60	1.41	1.37
1	A	11	G	C6-N1	-5.59	1.35	1.39
1	A	328	C	N3-C4	-5.59	1.30	1.33
1	A	909	A	N9-C4	-5.59	1.34	1.37
1	A	1524	C	C4'-C3'	-5.59	1.47	1.52
1	A	780	A	N3-C4	-5.59	1.31	1.34
1	A	885	G	C2-N3	-5.59	1.28	1.32
1	A	922	G	C6-N1	-5.59	1.35	1.39
1	A	901	A	N9-C4	-5.59	1.34	1.37
1	A	151	A	N9-C4	-5.58	1.34	1.37
1	A	803	G	N1-C2	-5.58	1.33	1.37
1	A	117	G	C6-O6	5.57	1.29	1.24
1	A	1329	A	C5-C6	-5.56	1.36	1.41
1	A	1520	G	C5-C6	-5.56	1.36	1.42
1	A	733	A	N9-C4	-5.55	1.34	1.37
1	A	765	G	N9-C4	-5.55	1.33	1.38
1	A	1078	U	C4-C5	-5.54	1.38	1.43
1	A	144	G	C6-N1	5.54	1.43	1.39
1	A	571	U	N1-C2	-5.54	1.33	1.38
1	A	926	G	N9-C4	5.54	1.42	1.38
1	A	1080	A	C6-N1	-5.52	1.31	1.35
1	A	807	A	N3-C4	-5.51	1.31	1.34
1	A	1520	G	C5-C4	-5.51	1.34	1.38
1	A	577	G	N9-C4	-5.50	1.33	1.38
1	A	1377	A	N3-C4	-5.50	1.31	1.34
1	A	905	U	N1-C2	-5.49	1.33	1.38
1	A	703	G	C6-O6	5.49	1.29	1.24
1	A	828	A	N3-C4	-5.47	1.31	1.34
1	A	1520	G	N3-C4	-5.47	1.31	1.35
1	A	240	C	N1-C6	-5.46	1.33	1.37
1	A	742	G	C5-C4	-5.45	1.34	1.38
1	A	1248	A	N9-C4	5.43	1.41	1.37
1	A	727	G	C6-N1	-5.42	1.35	1.39
1	A	880	C	N1-C6	-5.42	1.33	1.37
1	A	372	C	N3-C4	5.41	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	243	A	N7-C5	-5.41	1.36	1.39
1	A	1332	A	N9-C4	5.40	1.41	1.37
1	A	1515	C	C4-C5	-5.39	1.38	1.43
1	A	97	G	N9-C4	5.38	1.42	1.38
1	A	794	A	C5-C6	5.38	1.45	1.41
1	A	1306	A	N9-C8	-5.38	1.33	1.37
1	A	88	A	N9-C4	5.37	1.41	1.37
11	K	119	CYS	CB-SG	-5.37	1.73	1.81
1	A	819	A	C6-N1	-5.37	1.31	1.35
1	A	1370	G	N9-C4	5.35	1.42	1.38
5	E	33	VAL	CA-CB	-5.35	1.43	1.54
1	A	730	G	N3-C4	-5.35	1.31	1.35
1	A	303	A	N9-C4	-5.34	1.34	1.37
1	A	873	A	N9-C4	5.34	1.41	1.37
16	P	48	TRP	CB-CG	-5.34	1.40	1.50
1	A	129(A)	G	C2-N3	5.33	1.37	1.32
1	A	1377	A	C6-N1	-5.33	1.31	1.35
1	A	1502	A	N9-C4	-5.32	1.34	1.37
1	A	1401	G	N7-C5	-5.32	1.36	1.39
1	A	701	C	C3'-O3'	5.31	1.49	1.42
1	A	116	A	N9-C4	-5.30	1.34	1.37
1	A	287	U	C2-O2	-5.30	1.17	1.22
1	A	1338	G	N1-C2	-5.30	1.33	1.37
1	A	109	A	N3-C4	-5.29	1.31	1.34
1	A	90	U	C2-N3	5.28	1.41	1.37
1	A	819	A	N9-C4	-5.28	1.34	1.37
1	A	1504	G	C5-C4	-5.28	1.34	1.38
1	A	1502	A	N7-C5	-5.27	1.36	1.39
1	A	575	G	C6-N1	-5.27	1.35	1.39
1	A	1064	G	N3-C4	-5.26	1.31	1.35
1	A	944	G	N1-C2	-5.26	1.33	1.37
1	A	863	U	N1-C2	-5.26	1.33	1.38
1	A	913	A	C3'-O3'	5.25	1.49	1.42
1	A	812	C	C3'-O3'	5.25	1.49	1.42
1	A	525	C	N1-C6	-5.25	1.34	1.37
1	A	54	C	N3-C4	-5.24	1.30	1.33
1	A	728	A	C6-N6	-5.24	1.29	1.33
1	A	583	A	N3-C4	-5.22	1.31	1.34
1	A	828	A	N7-C5	-5.22	1.36	1.39
1	A	586	C	N3-C4	-5.21	1.30	1.33
1	A	1501	C	C2-N3	-5.20	1.31	1.35
1	A	279	A	N3-C4	-5.18	1.31	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	715	A	N3-C4	-5.18	1.31	1.34
1	A	889	A	N7-C5	-5.17	1.36	1.39
1	A	703	G	N3-C4	-5.17	1.31	1.35
1	A	611	A	N9-C4	-5.17	1.34	1.37
1	A	807	A	N9-C4	-5.17	1.34	1.37
1	A	606	G	N9-C4	5.16	1.42	1.38
1	A	802	A	C5-C4	-5.16	1.35	1.38
1	A	1442	G	N3-C4	5.16	1.39	1.35
1	A	922	G	N1-C2	-5.14	1.33	1.37
1	A	621	A	N7-C5	-5.14	1.36	1.39
1	A	746	A	N9-C4	-5.13	1.34	1.37
1	A	742	G	N3-C4	-5.12	1.31	1.35
1	A	109	A	N7-C5	-5.12	1.36	1.39
1	A	117	G	N1-C2	5.09	1.41	1.37
1	A	285	G	C6-O6	5.09	1.28	1.24
1	A	300	A	N9-C4	-5.09	1.34	1.37
1	A	931	C	C2-N3	-5.09	1.31	1.35
1	A	1516	G	N9-C4	5.08	1.42	1.38
1	A	230	G	C6-O6	5.08	1.28	1.24
1	A	1307	U	N1-C2	5.07	1.43	1.38
1	A	635	G	N3-C4	-5.06	1.31	1.35
1	A	1403	C	C1'-N1	-5.06	1.39	1.46
1	A	587	G	N1-C2	-5.06	1.33	1.37
1	A	674	G	N9-C4	-5.05	1.33	1.38
1	A	322	C	N1-C6	-5.05	1.34	1.37
1	A	945	G	N9-C8	5.05	1.41	1.37
1	A	374	A	N7-C5	5.04	1.42	1.39
1	A	742	G	N1-C2	-5.03	1.33	1.37
1	A	814	A	N9-C4	-5.03	1.34	1.37
1	A	120	A	C6-N1	-5.02	1.32	1.35
1	A	243	A	C3'-O3'	5.02	1.49	1.42
1	A	130	A	C6-N1	-5.01	1.32	1.35
1	A	474	G	N9-C4	-5.00	1.33	1.38
1	A	575	G	C6-O6	-5.00	1.19	1.24
1	A	120	A	N9-C8	-5.00	1.33	1.37

All (2321) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	279	A	C5-N7-C8	-16.40	95.70	103.90
1	A	873	A	C8-N9-C4	-15.88	99.45	105.80
1	A	279	A	N1-C6-N6	15.42	127.85	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1505	G	C8-N9-C4	-14.85	100.46	106.40
1	A	329	A	C2-N3-C4	-14.28	103.46	110.60
1	A	1403	C	C6-N1-C2	14.19	125.98	120.30
1	A	824	C	C6-N1-C2	13.94	125.88	120.30
1	A	599	C	C6-N1-C2	13.56	125.72	120.30
1	A	703	G	C4-C5-N7	-13.28	105.49	110.80
1	A	122	G	N1-C6-O6	13.12	127.78	119.90
1	A	285	G	N1-C6-O6	13.11	127.77	119.90
1	A	279	A	N7-C8-N9	12.79	120.20	113.80
1	A	117	G	C5-C6-N1	-12.77	105.11	111.50
1	A	28	G	N1-C6-O6	12.76	127.55	119.90
1	A	572	A	N1-C6-N6	-12.68	110.99	118.60
1	A	867	G	N1-C6-O6	12.63	127.48	119.90
1	A	266	G	N3-C4-C5	12.62	134.91	128.60
1	A	281	G	N1-C6-O6	12.62	127.47	119.90
1	A	676	A	C8-N9-C4	12.56	110.83	105.80
1	A	117	G	C6-C5-N7	-12.39	122.97	130.40
1	A	1403	C	N3-C2-O2	12.38	130.56	121.90
1	A	279	A	C6-C5-N7	-12.26	123.72	132.30
1	A	130	A	N1-C2-N3	12.17	135.39	129.30
1	A	572	A	N9-C4-C5	12.17	110.67	105.80
1	A	117	G	N1-C6-O6	12.09	127.16	119.90
1	A	945	G	C5-C6-N1	12.06	117.53	111.50
1	A	266	G	N3-C4-N9	-12.01	118.79	126.00
1	A	92	C	C4-C5-C6	11.97	123.39	117.40
1	A	279	A	C4-C5-N7	11.97	116.68	110.70
1	A	824	C	C5-C6-N1	-11.96	115.02	121.00
1	A	232	G	N1-C6-O6	11.93	127.06	119.90
1	A	931	C	C5-C6-N1	-11.89	115.05	121.00
1	A	794	A	C2-N3-C4	11.87	116.53	110.60
1	A	117	G	C4-C5-C6	11.82	125.89	118.80
1	A	579	G	N1-C6-O6	11.80	126.98	119.90
1	A	1329	A	N1-C6-N6	11.78	125.67	118.60
1	A	285	G	C5-C6-N1	-11.76	105.62	111.50
1	A	1080	A	N1-C6-N6	-11.72	111.56	118.60
1	A	945	G	C5-C6-O6	-11.72	121.57	128.60
1	A	1108	G	C8-N9-C4	-11.71	101.72	106.40
1	A	718	G	C8-N9-C4	-11.70	101.72	106.40
1	A	525	C	C6-N1-C2	11.67	124.97	120.30
1	A	117	G	C8-N9-C1'	-11.67	111.83	127.00
1	A	481	G	N3-C4-N9	11.62	132.97	126.00
1	A	285	G	C2-N3-C4	-11.56	106.12	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	852	G	C5-C6-N1	-11.55	105.72	111.50
1	A	731	G	N1-C6-O6	11.50	126.80	119.90
1	A	722	A	C2-N3-C4	-11.48	104.86	110.60
1	A	1200	C	C2-N1-C1'	11.47	131.42	118.80
1	A	819	A	C8-N9-C4	-11.27	101.29	105.80
1	A	1455	G	N1-C6-O6	11.27	126.66	119.90
1	A	814	A	C2-N3-C4	-11.18	105.01	110.60
1	A	1442	G	N3-C4-N9	11.15	132.69	126.00
1	A	635	G	C2-N3-C4	-11.13	106.33	111.90
1	A	933	G	N1-C6-O6	11.10	126.56	119.90
1	A	635	G	C5-C6-N1	-11.07	105.97	111.50
1	A	703	G	N9-C4-C5	11.04	109.82	105.40
1	A	295	C	C6-N1-C2	10.99	124.70	120.30
1	A	117	G	C4-N9-C1'	10.95	140.74	126.50
1	A	144	G	N1-C6-O6	10.95	126.47	119.90
1	A	1499	A	N1-C6-N6	10.89	125.14	118.60
1	A	259	G	C2-N3-C4	-10.87	106.47	111.90
1	A	933	G	C6-C5-N7	-10.79	123.92	130.40
1	A	801	U	C5-C6-N1	-10.78	117.31	122.70
1	A	833	U	N3-C4-C5	-10.73	108.16	114.60
1	A	255	G	N1-C6-O6	10.72	126.33	119.90
1	A	757	U	N3-C4-C5	-10.71	108.17	114.60
1	A	299	G	N1-C6-O6	10.69	126.32	119.90
1	A	107	G	C4-C5-N7	10.69	115.08	110.80
1	A	257	G	N3-C4-N9	10.68	132.41	126.00
1	A	596	C	C6-N1-C2	10.68	124.57	120.30
1	A	1460	A	N1-C6-N6	10.67	125.00	118.60
1	A	1496	C	C5-C6-N1	10.66	126.33	121.00
1	A	122	G	C5-C6-N1	-10.65	106.17	111.50
1	A	79	G	C8-N9-C4	-10.63	102.15	106.40
1	A	572	A	C8-N9-C4	-10.61	101.56	105.80
1	A	868	C	C4-C5-C6	10.61	122.70	117.40
1	A	329	A	C8-N9-C4	10.58	110.03	105.80
1	A	718	G	N7-C8-N9	10.58	118.39	113.10
1	A	266	G	C2-N3-C4	-10.58	106.61	111.90
1	A	605	U	N3-C4-C5	-10.55	108.27	114.60
1	A	1502	A	C5-N7-C8	-10.53	98.63	103.90
1	A	606	G	C8-N9-C4	-10.53	102.19	106.40
1	A	185	A	C8-N9-C4	10.53	110.01	105.80
1	A	599	C	N3-C4-C5	10.52	126.11	121.90
1	A	819	A	N9-C4-C5	10.52	110.01	105.80
1	A	928	G	N1-C6-O6	10.51	126.21	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	569	C	C5-C6-N1	-10.43	115.79	121.00
1	A	1200	C	C6-N1-C2	-10.40	116.14	120.30
1	A	703	G	C5-C6-O6	10.38	134.83	128.60
1	A	1080	A	C5-C6-N6	10.37	132.00	123.70
1	A	616	G	C5-C6-N1	-10.35	106.32	111.50
1	A	1082	G	C8-N9-C4	10.32	110.53	106.40
1	A	577	G	C8-N9-C4	10.31	110.53	106.40
1	A	745	C	N3-C4-C5	10.31	126.03	121.90
1	A	778	G	N1-C6-O6	10.30	126.08	119.90
1	A	730	G	C4-C5-N7	-10.27	106.69	110.80
1	A	797	C	C6-N1-C2	10.27	124.41	120.30
1	A	232	G	C6-C5-N7	-10.26	124.24	130.40
1	A	132	C	C2-N3-C4	-10.24	114.78	119.90
1	A	107	G	C6-C5-N7	-10.23	124.26	130.40
1	A	825	G	N1-C6-O6	10.22	126.03	119.90
1	A	1080	A	N9-C4-C5	10.18	109.87	105.80
1	A	1197	G	N9-C4-C5	-10.17	101.33	105.40
1	A	451	A	C8-N9-C4	10.16	109.87	105.80
1	A	828	A	C2-N3-C4	-10.14	105.53	110.60
1	A	130	A	C2-N3-C4	-10.12	105.54	110.60
1	A	1442	G	N3-C4-C5	-10.11	123.55	128.60
1	A	1362	C	C6-N1-C2	-10.10	116.26	120.30
1	A	922	G	N3-C4-C5	-10.08	123.56	128.60
1	A	1515	C	C6-N1-C2	-10.03	116.29	120.30
1	A	232	G	C2-N3-C4	-9.97	106.92	111.90
1	A	1500	A	C8-N9-C4	-9.97	101.81	105.80
1	A	546	G	N3-C4-N9	9.96	131.98	126.00
1	A	1505	G	N7-C8-N9	9.95	118.07	113.10
1	A	719	C	N1-C2-O2	9.95	124.87	118.90
1	A	703	G	N3-C4-C5	-9.94	123.63	128.60
1	A	875	C	C6-N1-C2	9.93	124.27	120.30
1	A	190(G)	G	C6-C5-N7	-9.92	124.45	130.40
1	A	577	G	C5-C6-O6	-9.88	122.67	128.60
1	A	455	C	N1-C2-O2	9.87	124.82	118.90
1	A	558	G	N1-C6-O6	9.82	125.79	119.90
1	A	1342	C	N3-C2-O2	9.81	128.77	121.90
1	A	132	C	C5-C6-N1	-9.80	116.10	121.00
1	A	628	G	N3-C4-C5	-9.79	123.71	128.60
1	A	944	G	N3-C4-C5	-9.78	123.71	128.60
1	A	303	A	C2-N3-C4	-9.78	105.71	110.60
1	A	600	C	C6-N1-C2	9.77	124.21	120.30
1	A	703	G	C8-N9-C4	-9.76	102.50	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	945	G	C2-N3-C4	9.76	116.78	111.90
1	A	941	G	N1-C6-O6	9.74	125.75	119.90
1	A	91	C	N1-C2-O2	-9.74	113.06	118.90
1	A	944	G	N1-C6-O6	-9.71	114.08	119.90
1	A	298	A	C6-N1-C2	-9.70	112.78	118.60
1	A	597	G	N1-C2-N2	-9.67	107.49	116.20
1	A	1502	A	C6-C5-N7	-9.66	125.53	132.30
1	A	1238	A	N9-C4-C5	9.65	109.66	105.80
1	A	175	C	C6-N1-C2	9.65	124.16	120.30
1	A	933	G	C5-C6-O6	-9.65	122.81	128.60
1	A	481	G	C8-N9-C4	9.63	110.25	106.40
1	A	898	G	C5-C6-O6	9.62	134.37	128.60
1	A	1059	C	C6-N1-C2	9.61	124.14	120.30
1	A	938	A	N1-C6-N6	-9.58	112.85	118.60
1	A	1377	A	C2-N3-C4	-9.58	105.81	110.60
1	A	292	G	N1-C6-O6	9.57	125.64	119.90
1	A	764	C	N3-C4-C5	9.55	125.72	121.90
1	A	27	G	C5-C6-O6	-9.54	122.88	128.60
1	A	706	A	C2-N3-C4	-9.53	105.84	110.60
1	A	281	G	C5-C6-O6	-9.52	122.89	128.60
1	A	190(G)	G	N1-C6-O6	9.52	125.61	119.90
1	A	245	C	C5-C4-N4	-9.51	113.55	120.20
1	A	876	G	C2-N3-C4	-9.50	107.15	111.90
1	A	735	C	C6-N1-C2	9.48	124.09	120.30
1	A	767	A	N1-C6-N6	-9.48	112.91	118.60
1	A	825	G	C8-N9-C4	9.48	110.19	106.40
1	A	931	C	C2-N3-C4	-9.47	115.16	119.90
1	A	602	A	C8-N9-C4	9.46	109.58	105.80
1	A	1497	G	C6-C5-N7	-9.46	124.73	130.40
1	A	108	G	N3-C4-C5	9.44	133.32	128.60
1	A	31	G	C4-C5-N7	-9.41	107.03	110.80
1	A	823	G	C2-N3-C4	-9.39	107.20	111.90
1	A	1342	C	N1-C2-O2	-9.39	113.27	118.90
1	A	805	C	N3-C4-C5	9.38	125.65	121.90
1	A	901	A	C2-N3-C4	-9.38	105.91	110.60
1	A	676	A	N7-C8-N9	-9.36	109.12	113.80
1	A	852	G	C2-N3-C4	-9.34	107.23	111.90
1	A	232	G	N9-C4-C5	-9.33	101.67	105.40
1	A	795	C	N3-C4-C5	-9.32	118.17	121.90
1	A	778	G	C2-N3-C4	-9.31	107.25	111.90
1	A	1523	G	C8-N9-C4	-9.31	102.68	106.40
1	A	482	A	N1-C6-N6	9.30	124.18	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	460	A	C8-N9-C4	-9.30	102.08	105.80
1	A	27	G	N1-C6-O6	9.29	125.48	119.90
1	A	577	G	N9-C4-C5	-9.29	101.68	105.40
1	A	1346	A	N1-C6-N6	-9.29	113.03	118.60
1	A	1087	G	N1-C6-O6	9.28	125.47	119.90
1	A	858	G	C4-C5-N7	9.27	114.51	110.80
1	A	605	U	C4-C5-C6	9.25	125.25	119.70
1	A	822	C	N3-C4-N4	9.24	124.47	118.00
1	A	1370	G	C8-N9-C4	-9.23	102.71	106.40
1	A	230	G	N1-C6-O6	9.21	125.43	119.90
1	A	130	A	C4-C5-C6	9.21	121.60	117.00
1	A	1348	U	C2-N1-C1'	9.21	128.75	117.70
1	A	614	A	C8-N9-C4	-9.20	102.12	105.80
1	A	605	U	N1-C2-N3	9.18	120.41	114.90
1	A	255	G	C6-C5-N7	-9.18	124.89	130.40
1	A	824	C	C2-N3-C4	-9.18	115.31	119.90
1	A	779	C	C5-C6-N1	-9.17	116.41	121.00
1	A	230	G	C8-N9-C4	9.14	110.06	106.40
1	A	943	U	N3-C2-O2	-9.14	115.80	122.20
1	A	915	A	C2-N3-C4	-9.13	106.04	110.60
1	A	32	A	N1-C2-N3	9.12	133.86	129.30
1	A	625	G	N3-C4-C5	-9.12	124.04	128.60
1	A	874	G	C5-C6-O6	-9.10	123.14	128.60
1	A	1434	A	N1-C6-N6	9.09	124.05	118.60
1	A	1502	A	C2-N3-C4	-9.08	106.06	110.60
1	A	474	G	N1-C6-O6	9.04	125.32	119.90
1	A	873	A	N9-C4-C5	9.03	109.41	105.80
1	A	546	G	N3-C4-C5	-9.03	124.08	128.60
1	A	876	G	C4-C5-N7	9.02	114.41	110.80
1	A	132	C	C4-C5-C6	9.01	121.91	117.40
1	A	944	G	C5-C6-O6	8.99	134.00	128.60
1	A	1236	A	N1-C2-N3	-8.99	124.81	129.30
1	A	820	U	N1-C2-O2	-8.98	116.51	122.80
1	A	606	G	N3-C4-C5	-8.98	124.11	128.60
1	A	481	G	N9-C4-C5	-8.97	101.81	105.40
1	A	1502	A	N7-C8-N9	8.97	118.28	113.80
1	A	129(A)	G	N9-C4-C5	-8.94	101.83	105.40
1	A	856	C	C4-C5-C6	8.93	121.87	117.40
1	A	565	U	C5-C4-O4	-8.93	120.54	125.90
1	A	635	G	N1-C2-N3	8.92	129.25	123.90
1	A	589	C	C5-C6-N1	-8.92	116.54	121.00
1	A	190(C)	C	C6-N1-C2	-8.91	116.73	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	328	C	N1-C2-O2	8.90	124.24	118.90
1	A	1462	G	N1-C6-O6	8.90	125.24	119.90
1	A	873	A	N1-C6-N6	-8.89	113.26	118.60
1	A	52	G	C6-C5-N7	-8.89	125.06	130.40
1	A	232	G	C5-C6-N1	-8.89	107.05	111.50
1	A	703	G	C5-N7-C8	8.89	108.75	104.30
1	A	1329	A	C6-C5-N7	-8.87	126.09	132.30
1	A	278	G	C4-C5-N7	-8.84	107.26	110.80
1	A	867	G	C6-C5-N7	-8.84	125.09	130.40
1	A	310	G	C5-C6-O6	-8.84	123.30	128.60
1	A	731	G	C5-C6-O6	-8.84	123.30	128.60
1	A	948	C	N3-C4-C5	8.84	125.43	121.90
1	A	78	G	C4-C5-N7	8.83	114.33	110.80
1	A	1249	C	C6-N1-C2	-8.83	116.77	120.30
1	A	298	A	N1-C2-N3	8.83	133.71	129.30
1	A	873	A	N7-C8-N9	8.82	118.21	113.80
1	A	260	G	C8-N9-C4	-8.82	102.87	106.40
1	A	820	U	N1-C2-N3	8.82	120.19	114.90
1	A	575	G	C6-N1-C2	-8.81	119.81	125.10
1	A	576	G	N3-C4-C5	-8.80	124.20	128.60
1	A	876	G	N1-C2-N3	8.81	129.18	123.90
1	A	316	G	C6-C5-N7	-8.80	125.12	130.40
1	A	525	C	C5-C4-N4	-8.77	114.06	120.20
1	A	329	A	N3-C4-C5	8.77	132.94	126.80
1	A	1516	G	N3-C4-C5	-8.77	124.22	128.60
1	A	228	A	C8-N9-C4	-8.75	102.30	105.80
1	A	753	A	C6-N1-C2	-8.74	113.36	118.60
1	A	577	G	C4-C5-N7	8.73	114.29	110.80
1	A	926	G	N3-C4-C5	-8.72	124.24	128.60
1	A	238	G	C5-C6-N1	-8.72	107.14	111.50
1	A	804	U	N3-C4-C5	-8.72	109.37	114.60
1	A	770	C	C5-C6-N1	-8.72	116.64	121.00
1	A	1108	G	N3-C4-C5	-8.71	124.24	128.60
1	A	230	G	N9-C4-C5	-8.71	101.92	105.40
1	A	824	C	N3-C4-C5	8.69	125.38	121.90
1	A	328	C	N3-C4-N4	-8.68	111.93	118.00
1	A	569	C	C4-C5-C6	8.67	121.74	117.40
1	A	730	G	C5-C6-O6	8.67	133.80	128.60
1	A	814	A	C8-N9-C4	8.67	109.27	105.80
1	A	277	C	C6-N1-C2	8.66	123.77	120.30
1	A	851	G	C4-N9-C1'	8.66	137.76	126.50
1	A	745	C	C6-N1-C2	8.65	123.76	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	856	C	N3-C4-C5	-8.65	118.44	121.90
1	A	860	A	C2-N3-C4	-8.65	106.28	110.60
1	A	43	C	C6-N1-C2	8.64	123.76	120.30
1	A	529	G	N1-C6-O6	8.64	125.08	119.90
1	A	720	C	N1-C2-O2	8.63	124.08	118.90
1	A	599	C	N3-C2-O2	8.62	127.94	121.90
1	A	255	G	N9-C4-C5	-8.62	101.95	105.40
1	A	577	G	N1-C6-O6	8.62	125.07	119.90
1	A	1371	G	C8-N9-C4	-8.62	102.95	106.40
1	A	59	A	C5-C6-N1	8.61	122.00	117.70
1	A	15	G	C8-N9-C4	8.60	109.84	106.40
1	A	854	G	N1-C2-N2	-8.60	108.46	116.20
1	A	690	G	C5-C6-O6	8.58	133.75	128.60
1	A	1502	A	C4-C5-N7	8.58	114.99	110.70
1	A	874	G	N1-C6-O6	8.56	125.04	119.90
1	A	577	G	N3-C4-C5	8.56	132.88	128.60
1	A	1390	U	N3-C4-C5	-8.56	109.47	114.60
1	A	137	C	N3-C4-C5	8.55	125.32	121.90
1	A	16	A	C2-N3-C4	-8.54	106.33	110.60
1	A	872	A	N1-C6-N6	8.54	123.72	118.60
1	A	729	A	C2-N3-C4	-8.53	106.33	110.60
1	A	1107	C	C6-N1-C2	-8.52	116.89	120.30
1	A	1102	A	C8-N9-C4	8.52	109.21	105.80
1	A	46	G	C5-C6-N1	-8.52	107.24	111.50
1	A	523	A	C8-N9-C4	8.51	109.21	105.80
1	A	771	G	C4-C5-N7	8.51	114.20	110.80
1	A	111	G	N1-C2-N2	8.50	123.85	116.20
1	A	128	G	N1-C6-O6	8.50	125.00	119.90
8	H	12	ARG	NE-CZ-NH1	-8.50	116.05	120.30
1	A	1149	C	C6-N1-C2	-8.48	116.91	120.30
1	A	54	C	C6-N1-C2	-8.47	116.91	120.30
1	A	1302	U	C5-C6-N1	-8.47	118.46	122.70
1	A	235	C	C6-N1-C2	8.47	123.69	120.30
1	A	1486	G	N1-C6-O6	8.46	124.98	119.90
1	A	14	U	N1-C2-N3	8.46	119.97	114.90
1	A	1452	C	C6-N1-C2	8.46	123.68	120.30
1	A	1380	U	N3-C2-O2	-8.45	116.29	122.20
1	A	259	G	C5-C6-N1	-8.44	107.28	111.50
1	A	1333	A	N1-C2-N3	8.42	133.51	129.30
1	A	787	A	N1-C6-N6	8.41	123.65	118.60
1	A	1530	G	N1-C6-O6	8.40	124.94	119.90
1	A	169	C	N3-C4-C5	-8.40	118.54	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	580	U	N3-C4-C5	-8.40	109.56	114.60
1	A	833	U	C5-C4-O4	8.40	130.94	125.90
1	A	939	G	C4-C5-N7	-8.40	107.44	110.80
1	A	1403	C	N1-C2-N3	-8.40	113.32	119.20
1	A	600	C	C5-C6-N1	-8.39	116.80	121.00
1	A	621	A	C8-N9-C4	-8.39	102.44	105.80
1	A	794	A	C5-N7-C8	8.39	108.09	103.90
1	A	23	C	N3-C4-C5	-8.39	118.55	121.90
1	A	788	U	N3-C4-O4	8.38	125.27	119.40
1	A	970	C	N1-C2-O2	8.38	123.93	118.90
1	A	547	A	C5-C6-N6	-8.38	117.00	123.70
1	A	27	G	C4-C5-N7	8.37	114.15	110.80
1	A	795	C	C2-N3-C4	8.37	124.09	119.90
1	A	117	G	C2-N3-C4	-8.37	107.72	111.90
1	A	1516	G	C8-N9-C4	-8.37	103.05	106.40
1	A	1369	C	C6-N1-C2	-8.36	116.95	120.30
1	A	1355	G	N3-C4-C5	-8.35	124.42	128.60
1	A	1442	G	C2-N3-C4	8.34	116.07	111.90
1	A	786	G	N1-C6-O6	8.34	124.91	119.90
1	A	1105	A	C8-N9-C4	-8.34	102.46	105.80
1	A	108	G	N3-C4-N9	-8.33	121.00	126.00
1	A	1240	U	C5-C4-O4	8.33	130.90	125.90
4	D	78	LEU	CA-CB-CG	-8.33	96.14	115.30
1	A	23	C	C6-N1-C2	-8.33	116.97	120.30
1	A	901	A	N1-C2-N3	8.32	133.46	129.30
1	A	1348	U	N3-C4-O4	8.32	125.23	119.40
1	A	279	A	C5-C6-N6	-8.32	117.04	123.70
1	A	98	U	C5-C6-N1	8.32	126.86	122.70
1	A	1197	G	C5-C6-O6	-8.32	123.61	128.60
1	A	372	C	C6-N1-C2	8.31	123.62	120.30
1	A	558	G	C5-C6-O6	-8.31	123.61	128.60
1	A	1388	C	N1-C2-O2	-8.30	113.92	118.90
1	A	259	G	N3-C4-C5	8.29	132.75	128.60
1	A	170	U	N1-C2-O2	-8.29	117.00	122.80
1	A	1516	G	N3-C4-N9	8.29	130.97	126.00
1	A	924	C	C6-N1-C2	-8.29	116.99	120.30
1	A	175	C	N3-C4-C5	8.28	125.21	121.90
1	A	812	C	C4-C5-C6	8.28	121.54	117.40
1	A	255	G	C5-C6-O6	-8.28	123.63	128.60
17	Q	31	LEU	CA-CB-CG	-8.28	96.26	115.30
1	A	78	G	C5-C6-N1	8.26	115.63	111.50
1	A	1064	G	C2-N3-C4	-8.23	107.78	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	484	G	C4-C5-N7	-8.23	107.51	110.80
1	A	144	G	N3-C4-C5	8.22	132.71	128.60
1	A	278	G	N1-C6-O6	-8.22	114.97	119.90
1	A	919	A	C8-N9-C4	8.22	109.09	105.80
1	A	1307	U	N1-C2-O2	8.21	128.55	122.80
1	A	762	C	C5-C4-N4	-8.21	114.45	120.20
1	A	871	U	N1-C2-O2	8.21	128.54	122.80
1	A	1377	A	N1-C6-N6	-8.20	113.68	118.60
1	A	1531	A	N7-C8-N9	8.21	117.90	113.80
1	A	628	G	N3-C4-N9	8.20	130.92	126.00
1	A	1079	G	C5-C6-O6	8.19	133.52	128.60
1	A	1108	G	N7-C8-N9	8.19	117.19	113.10
1	A	546	G	C4-N9-C1'	8.17	137.13	126.50
1	A	569	C	C2-N3-C4	-8.17	115.81	119.90
1	A	283	C	N3-C4-C5	-8.16	118.64	121.90
1	A	825	G	N3-C2-N2	-8.16	114.19	119.90
1	A	307	C	C5-C6-N1	8.16	125.08	121.00
1	A	909	A	C5-C6-N6	-8.16	117.18	123.70
1	A	1262	C	C6-N1-C2	-8.15	117.04	120.30
1	A	572	A	C5-C6-N1	8.15	121.77	117.70
1	A	1435	G	N1-C6-O6	8.15	124.79	119.90
1	A	129(A)	G	C8-N9-C1'	-8.13	116.43	127.00
1	A	851	G	C6-C5-N7	-8.13	125.52	130.40
1	A	658	G	N1-C2-N3	8.13	128.78	123.90
1	A	890	G	N1-C6-O6	-8.13	115.02	119.90
1	A	230	G	C5-C6-N1	-8.12	107.44	111.50
1	A	1385	G	N1-C6-O6	-8.12	115.03	119.90
1	A	79	G	N7-C8-N9	8.11	117.16	113.10
1	A	1030	C	C6-N1-C2	-8.11	117.06	120.30
1	A	1377	A	N1-C2-N3	8.10	133.35	129.30
1	A	583	A	C8-N9-C4	8.09	109.04	105.80
1	A	1339	A	N1-C6-N6	-8.09	113.75	118.60
1	A	939	G	N3-C4-C5	-8.09	124.56	128.60
1	A	1447	G	C4-C5-N7	8.08	114.03	110.80
1	A	579	G	C2-N3-C4	-8.08	107.86	111.90
1	A	729	A	C5-N7-C8	-8.07	99.86	103.90
1	A	75	G	C4-N9-C1'	8.07	136.99	126.50
1	A	931	C	N3-C4-N4	-8.07	112.35	118.00
1	A	1471	G	C8-N9-C4	8.07	109.63	106.40
1	A	621	A	N7-C8-N9	8.07	117.83	113.80
1	A	247	G	N1-C6-O6	8.06	124.74	119.90
1	A	671	G	C5-C6-N1	-8.06	107.47	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	98	U	C6-N1-C2	-8.04	116.17	121.00
1	A	1523	G	C5-C6-O6	-8.04	123.78	128.60
1	A	1200	C	N1-C2-O2	8.03	123.72	118.90
1	A	1307	U	N3-C2-O2	-8.03	116.58	122.20
1	A	111	G	N3-C4-N9	-8.03	121.19	126.00
1	A	1442	G	C4-N9-C1'	8.02	136.93	126.50
1	A	944	G	C8-N9-C4	-8.02	103.19	106.40
1	A	92	C	C5-C6-N1	-8.01	117.00	121.00
1	A	1236	A	C6-N1-C2	8.01	123.41	118.60
1	A	400	C	N3-C4-N4	-8.00	112.40	118.00
1	A	525	C	N3-C2-O2	8.00	127.50	121.90
1	A	667	G	N1-C6-O6	8.00	124.70	119.90
1	A	826	C	C6-N1-C2	7.99	123.50	120.30
1	A	830	G	C5-C6-N1	-7.98	107.51	111.50
1	A	1464	G	N1-C6-O6	7.98	124.69	119.90
1	A	778	G	C5-C6-N1	-7.98	107.51	111.50
1	A	1441	G	C4-C5-N7	-7.97	107.61	110.80
1	A	880	C	C5-C6-N1	-7.97	117.02	121.00
1	A	1499	A	C5-C6-N6	-7.96	117.33	123.70
1	A	690	G	N1-C6-O6	-7.96	115.12	119.90
1	A	674	G	C2-N3-C4	-7.96	107.92	111.90
1	A	771	G	N9-C4-C5	-7.96	102.22	105.40
1	A	597	G	N1-C2-N3	7.94	128.66	123.90
1	A	1421	G	C8-N9-C4	-7.94	103.22	106.40
1	A	123	C	C6-N1-C2	-7.93	117.13	120.30
1	A	1531	A	C8-N9-C4	-7.93	102.63	105.80
1	A	1502	A	N1-C6-N6	7.93	123.36	118.60
1	A	46	G	N3-C2-N2	-7.93	114.35	119.90
1	A	90	U	C6-N1-C2	-7.93	116.24	121.00
1	A	654	G	N3-C4-N9	-7.91	121.25	126.00
1	A	881	G	C6-C5-N7	-7.91	125.65	130.40
1	A	1383	C	N3-C4-N4	7.91	123.54	118.00
1	A	257	G	C6-C5-N7	-7.91	125.65	130.40
1	A	75	G	N3-C4-C5	-7.90	124.65	128.60
1	A	559	A	C4-C5-C6	7.90	120.95	117.00
1	A	90	U	C5-C6-N1	7.89	126.65	122.70
1	A	941	G	C5-C6-O6	-7.89	123.87	128.60
1	A	1496	C	C6-N1-C2	-7.88	117.15	120.30
1	A	881	G	N1-C6-O6	7.88	124.63	119.90
1	A	593	G	C2-N3-C4	-7.88	107.96	111.90
1	A	5	U	C2-N1-C1'	7.87	127.15	117.70
1	A	38	G	N3-C4-C5	7.87	132.54	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1079	G	N1-C6-O6	-7.87	115.18	119.90
1	A	556	C	C6-N1-C2	7.86	123.44	120.30
1	A	29	G	C2-N3-C4	-7.85	107.97	111.90
1	A	1370	G	N3-C4-C5	-7.84	124.68	128.60
1	A	1054	C	C5-C6-N1	7.84	124.92	121.00
1	A	317	G	C4-C5-N7	7.84	113.93	110.80
1	A	454	C	N1-C2-O2	7.83	123.60	118.90
1	A	111	G	N1-C6-O6	7.83	124.60	119.90
1	A	157	G	C5-C6-N1	-7.83	107.58	111.50
1	A	120	A	C2-N3-C4	-7.82	106.69	110.60
1	A	451	A	N9-C4-C5	-7.82	102.67	105.80
1	A	746	A	N1-C2-N3	7.82	133.21	129.30
1	A	814	A	N1-C6-N6	7.82	123.29	118.60
1	A	575	G	C5-C6-O6	-7.81	123.91	128.60
1	A	661	G	N1-C6-O6	7.81	124.58	119.90
1	A	819	A	N1-C2-N3	7.81	133.20	129.30
1	A	130	A	C6-C5-N7	-7.80	126.84	132.30
1	A	939	G	C6-N1-C2	-7.80	120.42	125.10
1	A	1064	G	N1-C2-N3	7.80	128.58	123.90
1	A	259	G	N3-C4-N9	-7.80	121.32	126.00
1	A	373	A	C8-N9-C4	-7.79	102.69	105.80
1	A	14	U	C6-N1-C2	-7.78	116.33	121.00
1	A	138	G	C8-N9-C4	7.78	109.51	106.40
1	A	52	G	C4-C5-N7	7.77	113.91	110.80
1	A	131	C	N3-C2-O2	-7.77	116.46	121.90
1	A	1527	C	N3-C4-C5	7.77	125.01	121.90
1	A	864	A	C5-C6-N1	-7.77	113.82	117.70
1	A	185	A	N7-C8-N9	-7.76	109.92	113.80
1	A	1362	C	C5-C6-N1	7.76	124.88	121.00
1	A	1231	G	C5-C6-N1	-7.75	107.62	111.50
1	A	1516	G	C6-C5-N7	-7.75	125.75	130.40
1	A	1197	G	N3-C4-N9	7.75	130.65	126.00
1	A	939	G	N1-C6-O6	-7.74	115.25	119.90
1	A	724	G	N9-C4-C5	-7.74	102.30	105.40
1	A	1197	G	C8-N9-C4	7.74	109.50	106.40
1	A	593	G	C5-C6-N1	-7.74	107.63	111.50
1	A	900	A	N1-C2-N3	7.73	133.17	129.30
1	A	852	G	N1-C6-O6	7.73	124.54	119.90
1	A	872	A	C6-C5-N7	-7.73	126.89	132.30
1	A	27	G	C5-N7-C8	-7.73	100.44	104.30
1	A	1086	U	C6-N1-C2	7.72	125.64	121.00
1	A	236	G	N1-C6-O6	-7.72	115.27	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	228	A	N9-C4-C5	7.71	108.89	105.80
4	D	174	LEU	CB-CG-CD2	-7.71	97.89	111.00
1	A	943	U	N1-C2-O2	7.71	128.20	122.80
1	A	1200	C	N3-C2-O2	-7.70	116.51	121.90
1	A	310	G	C8-N9-C4	7.70	109.48	106.40
1	A	794	A	C4-C5-N7	-7.70	106.85	110.70
1	A	898	G	C4-C5-N7	-7.69	107.72	110.80
1	A	934	C	C6-N1-C2	7.69	123.38	120.30
1	A	78	G	N9-C4-C5	-7.68	102.33	105.40
1	A	1348	U	C5-C6-N1	7.67	126.54	122.70
1	A	1244	C	C6-N1-C2	-7.67	117.23	120.30
1	A	111	G	N3-C2-N2	-7.67	114.53	119.90
1	A	940	C	N3-C4-C5	7.67	124.97	121.90
1	A	1062	U	C5-C4-O4	7.67	130.50	125.90
1	A	559	A	C8-N9-C4	-7.67	102.73	105.80
1	A	862	C	N3-C4-C5	7.66	124.96	121.90
1	A	589	C	C2-N3-C4	-7.66	116.07	119.90
1	A	880	C	C2-N3-C4	-7.65	116.08	119.90
1	A	546	G	C8-N9-C1'	-7.65	117.06	127.00
1	A	814	A	N1-C2-N3	7.65	133.12	129.30
1	A	703	G	C4-C5-C6	7.64	123.39	118.80
1	A	693	G	N9-C4-C5	-7.64	102.34	105.40
1	A	1234	C	C6-N1-C2	7.64	123.36	120.30
1	A	257	G	C5-C6-O6	-7.64	124.02	128.60
1	A	801	U	C6-N1-C2	7.63	125.58	121.00
1	A	1102	A	N7-C8-N9	-7.63	109.99	113.80
1	A	862	C	C5-C4-N4	-7.62	114.86	120.20
1	A	1304	G	N1-C6-O6	-7.62	115.33	119.90
1	A	278	G	C5-C6-O6	7.62	133.17	128.60
1	A	372	C	C6-N1-C1'	-7.61	111.67	120.80
1	A	602	A	C2-N3-C4	-7.61	106.80	110.60
1	A	817	C	C5-C4-N4	-7.61	114.87	120.20
1	A	629	G	N3-C4-C5	-7.61	124.80	128.60
1	A	788	U	N3-C2-O2	7.61	127.52	122.20
1	A	575	G	C5-C6-N1	7.60	115.30	111.50
1	A	308	C	C5-C4-N4	-7.60	114.88	120.20
1	A	651	C	C5-C6-N1	-7.59	117.20	121.00
1	A	947	G	C2-N3-C4	-7.59	108.11	111.90
1	A	1181	G	C8-N9-C4	7.59	109.44	106.40
1	A	730	G	N1-C6-O6	-7.58	115.35	119.90
1	A	660	G	N9-C4-C5	-7.58	102.37	105.40
1	A	1447	G	C5-N7-C8	-7.57	100.51	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	767	A	N9-C4-C5	7.57	108.83	105.80
1	A	941	G	C6-C5-N7	-7.57	125.86	130.40
1	A	1334	G	C8-N9-C4	7.57	109.43	106.40
1	A	257	G	C4-N9-C1'	7.57	136.34	126.50
1	A	287	U	N1-C2-N3	7.57	119.44	114.90
1	A	881	G	C5-C6-O6	-7.56	124.06	128.60
1	A	255	G	N3-C4-N9	7.56	130.53	126.00
1	A	1088	G	N1-C6-O6	7.56	124.43	119.90
1	A	945	G	N1-C2-N2	7.56	123.00	116.20
1	A	754	C	C6-N1-C2	-7.54	117.28	120.30
1	A	909	A	N1-C6-N6	7.54	123.13	118.60
1	A	260	G	N7-C8-N9	7.54	116.87	113.10
1	A	654	G	N3-C4-C5	7.54	132.37	128.60
1	A	1187	G	C8-N9-C4	-7.54	103.39	106.40
1	A	839	U	N1-C2-O2	7.53	128.07	122.80
1	A	1187	G	C4-N9-C1'	7.53	136.29	126.50
1	A	576	G	C4-C5-C6	7.53	123.32	118.80
1	A	255	G	C8-N9-C1'	-7.53	117.22	127.00
1	A	306	G	N3-C2-N2	-7.53	114.63	119.90
1	A	456	C	N3-C4-C5	7.53	124.91	121.90
1	A	975	A	N1-C6-N6	7.53	123.12	118.60
1	A	1312	G	C4-C5-N7	7.52	113.81	110.80
1	A	583	A	N7-C8-N9	-7.52	110.04	113.80
1	A	24	U	C5-C4-O4	-7.52	121.39	125.90
1	A	474	G	C4-C5-N7	7.52	113.81	110.80
1	A	606	G	C4-C5-N7	-7.51	107.80	110.80
1	A	804	U	C6-N1-C2	-7.51	116.50	121.00
1	A	727	G	C4-C5-N7	-7.51	107.80	110.80
1	A	372	C	C5-C4-N4	-7.50	114.95	120.20
1	A	721	G	C4-N9-C1'	7.50	136.25	126.50
1	A	1530	G	N3-C4-C5	7.50	132.35	128.60
1	A	1197	G	N1-C6-O6	7.50	124.40	119.90
1	A	108	G	C5-N7-C8	-7.49	100.55	104.30
1	A	257	G	N9-C4-C5	-7.49	102.40	105.40
1	A	1238	A	C5-C6-N6	7.49	129.69	123.70
1	A	46	G	N1-C6-O6	7.49	124.39	119.90
1	A	774	G	C6-C5-N7	-7.49	125.91	130.40
1	A	674	G	C8-N9-C4	7.48	109.39	106.40
1	A	243	A	P-O3'-C3'	7.47	128.67	119.70
1	A	712	A	C2-N3-C4	-7.47	106.86	110.60
1	A	117	G	N1-C2-N3	7.47	128.38	123.90
1	A	577	G	C2-N3-C4	-7.46	108.17	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1306	A	N1-C6-N6	7.46	123.08	118.60
1	A	107	G	C5-N7-C8	-7.46	100.57	104.30
1	A	1235	U	C5-C4-O4	-7.45	121.43	125.90
1	A	858	G	N3-C2-N2	7.45	125.11	119.90
1	A	833	U	C4-C5-C6	7.44	124.17	119.70
1	A	131	C	C2-N3-C4	-7.42	116.19	119.90
1	A	310	G	N1-C6-O6	7.42	124.35	119.90
1	A	597	G	C4-N9-C1'	7.42	136.14	126.50
1	A	575	G	N1-C2-N3	7.41	128.34	123.90
1	A	1347	G	C8-N9-C4	7.41	109.36	106.40
1	A	606	G	N9-C4-C5	7.40	108.36	105.40
1	A	777	A	C8-N9-C4	-7.39	102.84	105.80
1	A	253	U	N1-C2-O2	-7.39	117.63	122.80
1	A	1361(A)	C	N1-C2-O2	7.39	123.33	118.90
1	A	867	G	C5-C6-O6	-7.39	124.17	128.60
1	A	622	A	C8-N9-C4	7.38	108.75	105.80
1	A	1512	U	N1-C2-O2	-7.38	117.63	122.80
1	A	625	G	C8-N9-C4	-7.38	103.45	106.40
1	A	941	G	C4-C5-N7	7.38	113.75	110.80
1	A	1332	A	N1-C6-N6	-7.38	114.17	118.60
1	A	589	C	C4-C5-C6	7.38	121.09	117.40
1	A	1452	C	N1-C2-N3	-7.38	114.04	119.20
1	A	285	G	C6-C5-N7	-7.37	125.98	130.40
1	A	257	G	C8-N9-C1'	-7.37	117.42	127.00
1	A	389	A	C8-N9-C4	-7.37	102.85	105.80
1	A	825	G	C2-N3-C4	-7.37	108.21	111.90
1	A	576	G	C4-N9-C1'	7.37	136.08	126.50
1	A	1338	G	N1-C6-O6	-7.37	115.48	119.90
1	A	451	A	N3-C4-C5	7.37	131.96	126.80
1	A	1346	A	P-O3'-C3'	7.36	128.54	119.70
1	A	770	C	N3-C4-N4	-7.36	112.85	118.00
1	A	1414	U	N3-C4-C5	-7.36	110.18	114.60
1	A	1455	G	C5-C6-N1	-7.36	107.82	111.50
1	A	230	G	C2-N3-C4	-7.36	108.22	111.90
1	A	391	G	C8-N9-C4	7.36	109.34	106.40
1	A	174	C	N3-C4-C5	7.35	124.84	121.90
1	A	724	G	C4-C5-N7	7.35	113.74	110.80
1	A	1505	G	N9-C4-C5	7.35	108.34	105.40
1	A	581	G	C2-N3-C4	-7.34	108.23	111.90
1	A	89	C	C5-C6-N1	7.34	124.67	121.00
1	A	722	A	N3-C4-C5	7.34	131.94	126.80
1	A	1179	A	C8-N9-C4	-7.34	102.86	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	451	A	C4-C5-C6	-7.33	113.33	117.00
1	A	1209	C	C6-N1-C2	-7.33	117.37	120.30
1	A	727	G	C5-C6-O6	7.33	133.00	128.60
1	A	66	G	C8-N9-C4	-7.33	103.47	106.40
1	A	283	C	C6-N1-C2	-7.33	117.37	120.30
1	A	308	C	N1-C2-O2	7.32	123.29	118.90
1	A	357	G	C8-N9-C4	7.32	109.33	106.40
1	A	316	G	N3-C4-C5	-7.32	124.94	128.60
1	A	741	G	C6-C5-N7	7.32	134.79	130.40
1	A	237	C	N3-C4-C5	-7.32	118.97	121.90
1	A	228	A	N3-C4-N9	-7.31	121.55	127.40
1	A	928	G	C5-C6-O6	-7.31	124.21	128.60
1	A	916	G	C8-N9-C4	-7.31	103.48	106.40
1	A	8	A	C8-N9-C4	-7.30	102.88	105.80
1	A	108	G	N3-C2-N2	-7.30	114.79	119.90
1	A	257	G	C4-C5-N7	7.30	113.72	110.80
1	A	120	A	C5-C6-N6	7.29	129.53	123.70
1	A	783	C	C6-N1-C2	7.29	123.22	120.30
1	A	869	G	N1-C6-O6	7.29	124.27	119.90
1	A	122	G	C6-C5-N7	-7.29	126.03	130.40
1	A	128	G	C5-C6-O6	-7.29	124.23	128.60
1	A	751	U	C6-N1-C2	7.29	125.37	121.00
1	A	822	C	C5-C4-N4	-7.29	115.10	120.20
1	A	1416	G	N1-C6-O6	7.29	124.27	119.90
1	A	599	C	C5-C4-N4	-7.28	115.10	120.20
1	A	43	C	C5-C6-N1	-7.28	117.36	121.00
1	A	944	G	N9-C4-C5	7.27	108.31	105.40
1	A	703	G	C5-C6-N1	-7.27	107.87	111.50
1	A	838	G	C8-N9-C4	7.26	109.31	106.40
1	A	945	G	C4-C5-N7	7.26	113.70	110.80
1	A	1200	C	C5-C6-N1	7.26	124.63	121.00
1	A	635	G	C4-C5-C6	7.26	123.16	118.80
1	A	788	U	C5-C6-N1	7.26	126.33	122.70
1	A	329	A	N9-C4-C5	-7.26	102.90	105.80
1	A	480	U	N3-C4-C5	-7.26	110.25	114.60
1	A	1364	U	N3-C2-O2	-7.25	117.13	122.20
1	A	1516	G	N7-C8-N9	7.25	116.72	113.10
1	A	81	U	C5-C6-N1	7.25	126.32	122.70
1	A	584	G	C5-C6-O6	-7.24	124.26	128.60
1	A	1442	G	C8-N9-C1'	-7.24	117.59	127.00
1	A	22	G	C6-C5-N7	-7.23	126.06	130.40
1	A	563	A	C8-N9-C4	-7.23	102.91	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	899	C	N1-C2-O2	-7.22	114.56	118.90
1	A	1338	G	N1-C2-N2	-7.22	109.70	116.20
1	A	259	G	N1-C6-O6	7.21	124.23	119.90
1	A	103	C	N3-C4-C5	-7.21	119.02	121.90
1	A	779	C	C4-C5-C6	7.20	121.00	117.40
1	A	553	A	C5-C6-N1	7.20	121.30	117.70
1	A	1265	G	C8-N9-C4	-7.20	103.52	106.40
1	A	754	C	C2-N1-C1'	7.20	126.72	118.80
1	A	1455	G	C6-C5-N7	-7.20	126.08	130.40
1	A	757	U	C4-C5-C6	7.19	124.02	119.70
1	A	945	G	C4-C5-C6	-7.19	114.49	118.80
1	A	266	G	C5-N7-C8	-7.19	100.71	104.30
1	A	1373	G	N3-C4-N9	7.19	130.31	126.00
1	A	238	G	C6-C5-N7	-7.18	126.09	130.40
1	A	1195	C	C6-N1-C2	7.18	123.17	120.30
1	A	642	A	C6-N1-C2	-7.18	114.29	118.60
1	A	28	G	C5-C6-N1	-7.17	107.91	111.50
1	A	820	U	C4-C5-C6	7.17	124.00	119.70
1	A	946	A	C6-N1-C2	-7.17	114.30	118.60
1	A	132	C	N1-C2-N3	7.17	124.22	119.20
1	A	99	C	C6-N1-C2	-7.17	117.43	120.30
1	A	898	G	N1-C6-O6	-7.17	115.60	119.90
1	A	868	C	N3-C4-C5	-7.16	119.03	121.90
1	A	97	G	C8-N9-C4	-7.16	103.54	106.40
1	A	228	A	C5-C6-N6	7.16	129.43	123.70
1	A	122	G	C2-N3-C4	-7.16	108.32	111.90
1	A	482	A	N7-C8-N9	7.16	117.38	113.80
1	A	117	G	N3-C4-N9	7.15	130.29	126.00
1	A	1249	C	C5-C6-N1	7.15	124.58	121.00
1	A	28	G	N3-C2-N2	-7.15	114.90	119.90
1	A	1329	A	C4-C5-N7	7.15	114.27	110.70
1	A	278	G	C6-C5-N7	7.14	134.68	130.40
1	A	860	A	C5-N7-C8	-7.14	100.33	103.90
1	A	47	C	N3-C2-O2	-7.13	116.91	121.90
1	A	1084	G	N3-C4-N9	7.13	130.28	126.00
1	A	1083	U	C5-C4-O4	-7.13	121.62	125.90
1	A	1187	G	C6-C5-N7	-7.12	126.13	130.40
1	A	686	U	C5-C6-N1	-7.12	119.14	122.70
1	A	722	A	N1-C6-N6	7.12	122.87	118.60
1	A	736	C	N3-C2-O2	-7.12	116.92	121.90
1	A	851	G	C8-N9-C1'	-7.11	117.75	127.00
1	A	660	G	C8-N9-C4	7.11	109.25	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1084	G	N3-C4-C5	-7.11	125.05	128.60
1	A	1158	C	C6-N1-C2	-7.11	117.46	120.30
1	A	1197	G	C8-N9-C1'	-7.11	117.76	127.00
1	A	238	G	N1-C6-O6	7.11	124.16	119.90
1	A	263	A	C2-N3-C4	7.10	114.15	110.60
1	A	721	G	C8-N9-C1'	-7.10	117.77	127.00
1	A	938	A	C5-C6-N6	7.10	129.38	123.70
1	A	876	G	N1-C2-N2	-7.10	109.81	116.20
1	A	1200	C	C6-N1-C1'	-7.10	112.28	120.80
1	A	1196	U	N1-C2-O2	7.10	127.77	122.80
1	A	559	A	N1-C2-N3	7.09	132.85	129.30
1	A	1317	C	C6-N1-C2	7.08	123.13	120.30
1	A	129(A)	G	C6-C5-N7	-7.08	126.15	130.40
1	A	1323	G	C8-N9-C4	7.08	109.23	106.40
1	A	741	G	N1-C6-O6	-7.08	115.65	119.90
1	A	555	C	C2-N3-C4	-7.08	116.36	119.90
1	A	1478	C	C6-N1-C2	-7.07	117.47	120.30
1	A	624	C	C6-N1-C2	7.07	123.13	120.30
1	A	285	G	N1-C2-N3	7.07	128.14	123.90
1	A	283	C	C5-C6-N1	7.07	124.53	121.00
1	A	1235	U	N1-C2-O2	-7.06	117.86	122.80
1	A	801	U	C2-N1-C1'	-7.06	109.22	117.70
1	A	810	C	C5-C4-N4	-7.06	115.26	120.20
1	A	1380	U	C5-C4-O4	7.06	130.14	125.90
1	A	579	G	C6-C5-N7	-7.06	126.17	130.40
1	A	108	G	N1-C2-N2	7.06	122.55	116.20
1	A	876	G	C6-C5-N7	-7.06	126.17	130.40
1	A	686	U	C4-C5-C6	7.05	123.93	119.70
1	A	111	G	N3-C4-C5	7.05	132.12	128.60
1	A	474	G	C2-N3-C4	-7.05	108.37	111.90
1	A	281	G	C4-C5-N7	7.04	113.62	110.80
1	A	898	G	N3-C4-N9	-7.04	121.77	126.00
1	A	648	A	N1-C2-N3	7.04	132.82	129.30
1	A	481	G	N7-C8-N9	-7.04	109.58	113.10
1	A	801	U	C2-N3-C4	-7.04	122.78	127.00
1	A	38	G	C4-N9-C1'	-7.02	117.37	126.50
1	A	474	G	N9-C4-C5	-7.01	102.59	105.40
1	A	1497	G	N1-C6-O6	7.01	124.11	119.90
1	A	1500	A	N1-C6-N6	-7.01	114.39	118.60
1	A	558	G	C6-C5-N7	-7.01	126.19	130.40
1	A	876	G	N9-C4-C5	-7.01	102.60	105.40
1	A	646	U	N3-C2-O2	-7.01	117.30	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	16	A	N3-C4-C5	7.00	131.70	126.80
1	A	482	A	C6-C5-N7	-7.00	127.40	132.30
1	A	1238	A	C4-C5-N7	-7.00	107.20	110.70
1	A	693	G	C8-N9-C4	7.00	109.20	106.40
1	A	867	G	N9-C4-C5	-7.00	102.60	105.40
1	A	1397	C	C2-N3-C4	7.00	123.40	119.90
1	A	573	A	C8-N9-C4	-7.00	103.00	105.80
1	A	721	G	N3-C4-N9	6.99	130.20	126.00
1	A	660	G	C2-N3-C4	-6.99	108.41	111.90
1	A	400	C	N3-C4-C5	6.99	124.69	121.90
1	A	303	A	N1-C2-N3	6.98	132.79	129.30
1	A	929	G	C2-N3-C4	-6.98	108.41	111.90
1	A	137	C	C6-N1-C2	6.97	123.09	120.30
1	A	635	G	N1-C6-O6	6.97	124.08	119.90
1	A	780	A	C6-N1-C2	-6.96	114.42	118.60
1	A	660	G	C4-C5-N7	6.96	113.58	110.80
1	A	558	G	C4-C5-N7	6.95	113.58	110.80
1	A	117	G	N9-C4-C5	-6.95	102.62	105.40
1	A	460	A	C2-N3-C4	6.95	114.08	110.60
1	A	614	A	N7-C8-N9	6.95	117.28	113.80
1	A	671	G	C8-N9-C4	6.94	109.18	106.40
1	A	898	G	N9-C4-C5	6.94	108.18	105.40
1	A	559	A	N7-C8-N9	6.94	117.27	113.80
1	A	317	G	N1-C6-O6	6.93	124.06	119.90
1	A	1087	G	N9-C4-C5	-6.93	102.63	105.40
1	A	905	U	N3-C2-O2	6.93	127.05	122.20
1	A	602	A	N7-C8-N9	-6.93	110.33	113.80
1	A	719	C	N3-C2-O2	-6.93	117.05	121.90
1	A	1452	C	C6-N1-C1'	-6.93	112.49	120.80
1	A	823	G	N1-C2-N2	-6.92	109.97	116.20
1	A	823	G	N1-C2-N3	6.92	128.05	123.90
1	A	279	A	C8-N9-C4	-6.92	103.03	105.80
1	A	663	A	N7-C8-N9	-6.92	110.34	113.80
1	A	875	C	C5-C6-N1	-6.92	117.54	121.00
1	A	186	C	N3-C4-C5	6.92	124.67	121.90
1	A	238	G	C2-N3-C4	-6.92	108.44	111.90
1	A	75	G	C8-N9-C1'	-6.91	118.02	127.00
1	A	812	C	N3-C4-C5	-6.91	119.14	121.90
1	A	372	C	N3-C4-N4	6.91	122.83	118.00
1	A	670	G	C4-N9-C1'	6.90	135.47	126.50
1	A	1106	G	C4-C5-N7	6.90	113.56	110.80
1	A	235	C	N3-C4-C5	6.90	124.66	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	757	U	N3-C4-O4	6.90	124.23	119.40
1	A	1098	C	C6-N1-C2	6.89	123.06	120.30
1	A	886	G	N3-C2-N2	-6.89	115.08	119.90
1	A	190(G)	G	C4-N9-C1'	6.89	135.46	126.50
1	A	412	A	C8-N9-C4	6.88	108.55	105.80
1	A	1031	G	C8-N9-C4	-6.88	103.65	106.40
1	A	1187	G	N7-C8-N9	6.88	116.54	113.10
1	A	1193	G	N1-C6-O6	6.88	124.03	119.90
1	A	13	C	N1-C2-O2	6.88	123.03	118.90
1	A	583	A	N1-C2-N3	6.88	132.74	129.30
1	A	858	G	N9-C4-C5	-6.87	102.65	105.40
1	A	326	G	C4-C5-N7	-6.86	108.06	110.80
1	A	1385	G	C4-C5-N7	-6.86	108.06	110.80
1	A	257	G	N3-C4-C5	-6.86	125.17	128.60
1	A	25	C	N3-C4-C5	6.86	124.64	121.90
1	A	295	C	C5-C6-N1	-6.86	117.57	121.00
1	A	24	U	N1-C2-O2	-6.86	118.00	122.80
1	A	449	C	C6-N1-C2	-6.86	117.56	120.30
1	A	874	G	N3-C4-C5	-6.86	125.17	128.60
1	A	963	G	C5-C6-N1	-6.86	108.07	111.50
1	A	22	G	N7-C8-N9	6.85	116.53	113.10
1	A	874	G	N3-C4-N9	6.85	130.11	126.00
1	A	1108	G	C4-C5-C6	6.85	122.91	118.80
1	A	373	A	N9-C4-C5	6.84	108.54	105.80
1	A	1370	G	C4-N9-C1'	6.84	135.39	126.50
1	A	236	G	N3-C2-N2	6.83	124.68	119.90
1	A	456	C	N1-C2-O2	6.83	123.00	118.90
1	A	460	A	N7-C8-N9	6.83	117.22	113.80
1	A	107	G	N1-C6-O6	6.83	124.00	119.90
1	A	1339	A	C5-C6-N1	6.83	121.11	117.70
1	A	1237	C	C4-C5-C6	6.83	120.81	117.40
1	A	93	G	N1-C6-O6	-6.82	115.81	119.90
1	A	1122	U	C5-C6-N1	6.82	126.11	122.70
1	A	1281	U	C6-N1-C2	-6.82	116.91	121.00
1	A	1318	A	C8-N9-C4	6.82	108.53	105.80
1	A	774	G	N1-C6-O6	6.82	123.99	119.90
1	A	819	A	N7-C8-N9	6.82	117.21	113.80
1	A	642	A	N1-C2-N3	6.81	132.71	129.30
1	A	1080	A	C8-N9-C4	-6.81	103.08	105.80
1	A	155	C	N3-C4-C5	-6.81	119.18	121.90
1	A	879	C	C6-N1-C2	6.81	123.02	120.30
1	A	382	A	C8-N9-C4	-6.80	103.08	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	77	G	N1-C6-O6	6.80	123.98	119.90
1	A	724	G	C5-C6-O6	-6.80	124.52	128.60
1	A	1375	A	C8-N9-C4	6.80	108.52	105.80
1	A	229	U	N1-C2-N3	6.80	118.98	114.90
1	A	274	A	N7-C8-N9	-6.79	110.40	113.80
1	A	1274	G	C8-N9-C4	-6.79	103.68	106.40
1	A	770	C	C6-N1-C2	6.79	123.02	120.30
1	A	1377	A	N3-C4-N9	-6.79	121.97	127.40
1	A	1425	U	C5-C4-O4	6.79	129.97	125.90
1	A	5	U	N3-C4-O4	6.79	124.15	119.40
1	A	793	U	N1-C2-O2	6.79	127.55	122.80
1	A	1374	A	C5-C6-N1	-6.79	114.31	117.70
1	A	481	G	N3-C4-C5	-6.79	125.21	128.60
1	A	277	C	C5-C6-N1	-6.79	117.61	121.00
1	A	357	G	C8-N9-C1'	-6.79	118.18	127.00
1	A	563	A	C5-N7-C8	-6.78	100.51	103.90
1	A	911	U	C5-C6-N1	-6.78	119.31	122.70
1	A	1108	G	C4-N9-C1'	6.78	135.31	126.50
1	A	28	G	C5-C6-O6	-6.78	124.53	128.60
1	A	651	C	C6-N1-C2	6.78	123.01	120.30
1	A	765	G	N3-C4-C5	6.78	131.99	128.60
1	A	727	G	C5-N7-C8	6.78	107.69	104.30
1	A	1414	U	C4-C5-C6	6.78	123.77	119.70
1	A	540	G	N1-C6-O6	6.77	123.96	119.90
1	A	32	A	C6-N1-C2	-6.77	114.54	118.60
1	A	970	C	N3-C2-O2	-6.77	117.16	121.90
1	A	547	A	N1-C6-N6	6.77	122.66	118.60
1	A	1355	G	N3-C4-N9	6.76	130.06	126.00
1	A	384	G	N3-C4-C5	-6.76	125.22	128.60
1	A	771	G	C8-N9-C4	6.76	109.10	106.40
1	A	131	C	N1-C2-N3	6.76	123.93	119.20
1	A	711	G	C5-C6-N1	6.76	114.88	111.50
1	A	780	A	N1-C2-N3	6.76	132.68	129.30
1	A	901	A	C5-C6-N6	6.76	129.11	123.70
1	A	1435	G	C2-N3-C4	-6.76	108.52	111.90
1	A	565	U	N3-C4-O4	6.75	124.13	119.40
1	A	851	G	N3-C4-N9	6.75	130.05	126.00
1	A	1340	A	N1-C2-N3	6.75	132.67	129.30
1	A	316	G	C4-C5-C6	6.75	122.85	118.80
1	A	879	C	N3-C4-C5	6.74	124.60	121.90
1	A	235	C	N3-C4-N4	-6.74	113.28	118.00
1	A	190(G)	G	N7-C8-N9	6.73	116.47	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	298	A	N9-C4-C5	6.73	108.49	105.80
1	A	15	G	N9-C4-C5	-6.73	102.71	105.40
1	A	305	G	C8-N9-C4	-6.73	103.71	106.40
1	A	5	U	C6-N1-C1'	-6.72	111.79	121.20
1	A	18	C	N1-C2-O2	6.72	122.93	118.90
1	A	752	G	N3-C4-C5	6.72	131.96	128.60
1	A	674	G	N3-C4-C5	6.71	131.96	128.60
1	A	297	G	N1-C6-O6	6.71	123.93	119.90
1	A	12	U	C5-C6-N1	-6.71	119.35	122.70
1	A	971	G	C5-C6-N1	-6.71	108.14	111.50
1	A	621	A	C6-C5-N7	-6.71	127.61	132.30
1	A	623	C	C6-N1-C2	6.71	122.98	120.30
1	A	718	G	C4-N9-C1'	6.71	135.22	126.50
1	A	556	C	N3-C4-C5	6.71	124.58	121.90
1	A	890	G	C5-C6-O6	6.71	132.62	128.60
1	A	794	A	N7-C8-N9	-6.70	110.45	113.80
1	A	922	G	C8-N9-C4	-6.70	103.72	106.40
1	A	1318	A	C4-C5-C6	-6.70	113.65	117.00
1	A	666	G	N1-C6-O6	6.70	123.92	119.90
1	A	260	G	N3-C4-N9	-6.70	121.98	126.00
1	A	525	C	N3-C4-N4	6.70	122.69	118.00
1	A	579	G	C5-C6-N1	-6.70	108.15	111.50
1	A	1375	A	N7-C8-N9	-6.70	110.45	113.80
1	A	52	G	N1-C6-O6	6.69	123.91	119.90
1	A	559	A	C6-C5-N7	-6.69	127.62	132.30
1	A	113	G	C4-C5-N7	6.69	113.48	110.80
1	A	316	G	N3-C4-N9	6.69	130.01	126.00
1	A	814	A	N9-C4-C5	-6.69	103.12	105.80
1	A	812	C	N1-C2-N3	6.68	123.88	119.20
1	A	720	C	N3-C2-O2	-6.68	117.22	121.90
1	A	1329	A	C5-C6-N6	-6.67	118.36	123.70
1	A	90	U	N3-C4-O4	6.67	124.07	119.40
1	A	328	C	N3-C2-O2	-6.67	117.23	121.90
1	A	1167	A	C8-N9-C4	-6.67	103.13	105.80
1	A	706	A	N3-C4-C5	6.67	131.47	126.80
1	A	933	G	C4-C5-C6	6.66	122.80	118.80
1	A	305	G	C6-C5-N7	-6.66	126.40	130.40
1	A	658	G	N1-C2-N2	-6.66	110.21	116.20
1	A	455	C	N3-C2-O2	-6.66	117.24	121.90
1	A	881	G	N1-C2-N3	6.66	127.89	123.90
1	A	1383	C	C6-N1-C2	-6.66	117.64	120.30
1	A	54	C	N3-C2-O2	-6.65	117.24	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	950	U	C5-C4-O4	6.65	129.89	125.90
1	A	890	G	C4-C5-N7	-6.65	108.14	110.80
1	A	1462	G	C5-C6-O6	-6.65	124.61	128.60
1	A	49	U	N3-C2-O2	6.65	126.85	122.20
1	A	616	G	N1-C6-O6	6.65	123.89	119.90
1	A	484	G	C5-N7-C8	6.64	107.62	104.30
1	A	10	A	N1-C2-N3	6.64	132.62	129.30
1	A	743	U	N3-C4-C5	-6.64	110.62	114.60
1	A	621	A	C5-N7-C8	-6.64	100.58	103.90
1	A	1370	G	N7-C8-N9	6.64	116.42	113.10
1	A	16	A	C5-C6-N1	-6.64	114.38	117.70
1	A	730	G	C5-N7-C8	6.63	107.62	104.30
1	A	570	G	N3-C4-C5	-6.63	125.28	128.60
1	A	661	G	N3-C2-N2	-6.63	115.26	119.90
1	A	839	U	C2-N1-C1'	6.63	125.66	117.70
1	A	1146	A	C8-N9-C4	6.62	108.45	105.80
1	A	919	A	C4-C5-C6	-6.62	113.69	117.00
1	A	88	A	C8-N9-C4	-6.62	103.15	105.80
1	A	1477	C	C6-N1-C2	-6.62	117.65	120.30
1	A	948	C	C6-N1-C2	6.61	122.94	120.30
1	A	540	G	C5-C6-O6	-6.60	124.64	128.60
1	A	389	A	N9-C4-C5	6.60	108.44	105.80
1	A	928	G	C4-C5-N7	6.60	113.44	110.80
1	A	892	A	C2-N3-C4	-6.59	107.30	110.60
1	A	1231	G	N1-C6-O6	6.59	123.86	119.90
1	A	524	G	N1-C6-O6	6.59	123.85	119.90
1	A	697	U	N3-C4-O4	-6.59	114.79	119.40
1	A	852	G	N3-C4-C5	6.59	131.89	128.60
1	A	1082	G	N7-C8-N9	-6.58	109.81	113.10
1	A	778	G	C8-N9-C4	6.58	109.03	106.40
1	A	190(G)	G	C4-C5-C6	6.58	122.75	118.80
1	A	824	C	C2-N1-C1'	-6.58	111.56	118.80
20	T	94	ALA	N-CA-C	-6.58	93.24	111.00
1	A	252	U	C5-C6-N1	-6.57	119.41	122.70
1	A	400	C	N1-C2-O2	6.57	122.84	118.90
1	A	331	G	C6-C5-N7	-6.56	126.46	130.40
1	A	1332	A	C5-C6-N6	6.56	128.95	123.70
1	A	851	G	N1-C6-O6	6.56	123.84	119.90
1	A	596	C	N1-C2-N3	-6.56	114.61	119.20
1	A	168	G	C4-N9-C1'	6.55	135.02	126.50
1	A	869	G	N9-C4-C5	-6.55	102.78	105.40
1	A	1317	C	N1-C2-O2	6.55	122.83	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	864	A	C5-C6-N6	6.55	128.94	123.70
1	A	1496	C	C2-N3-C4	6.55	123.18	119.90
1	A	1266	G	N3-C4-C5	6.55	131.88	128.60
1	A	597	G	C8-N9-C1'	-6.55	118.49	127.00
1	A	317	G	C2-N3-C4	-6.54	108.63	111.90
1	A	583	A	C2-N3-C4	-6.54	107.33	110.60
1	A	297	G	C6-C5-N7	-6.54	126.48	130.40
1	A	113	G	C5-N7-C8	-6.53	101.03	104.30
1	A	975	A	C5-N7-C8	-6.53	100.64	103.90
1	A	45	U	C5-C6-N1	-6.53	119.44	122.70
1	A	45	U	C4-C5-C6	6.53	123.62	119.70
1	A	316	G	C8-N9-C4	-6.53	103.79	106.40
1	A	361	G	N1-C6-O6	-6.53	115.98	119.90
1	A	922	G	C4-N9-C1'	6.53	134.99	126.50
1	A	144	G	C5-C6-O6	-6.53	124.69	128.60
1	A	481	G	C8-N9-C1'	-6.53	118.52	127.00
1	A	597	G	N3-C4-C5	-6.53	125.34	128.60
1	A	389	A	C4-C5-N7	-6.52	107.44	110.70
1	A	530	G	C4-N9-C1'	6.52	134.98	126.50
1	A	357	G	N1-C6-O6	6.52	123.81	119.90
1	A	523	A	C2-N3-C4	-6.51	107.34	110.60
1	A	606	G	C5-C6-O6	6.51	132.51	128.60
1	A	897	C	N3-C2-O2	-6.51	117.34	121.90
1	A	829	G	C8-N9-C4	6.51	109.00	106.40
1	A	1087	G	C2-N3-C4	-6.51	108.64	111.90
1	A	296	U	N1-C2-N3	6.51	118.81	114.90
1	A	867	G	C2-N3-C4	-6.51	108.64	111.90
1	A	285	G	C4-C5-C6	6.51	122.70	118.80
1	A	303	A	N1-C6-N6	6.51	122.50	118.60
1	A	786	G	C5-C6-O6	-6.50	124.70	128.60
1	A	882	C	C4-C5-C6	6.50	120.65	117.40
1	A	928	G	N9-C4-C5	-6.50	102.80	105.40
1	A	1520	G	N3-C4-C5	6.50	131.85	128.60
1	A	1340	A	C2-N3-C4	-6.50	107.35	110.60
1	A	146	G	N3-C2-N2	-6.50	115.35	119.90
1	A	721	G	C6-C5-N7	-6.50	126.50	130.40
1	A	1078	U	C5-C6-N1	6.50	125.95	122.70
1	A	1447	G	N7-C8-N9	6.50	116.35	113.10
1	A	378	G	C8-N9-C4	6.49	109.00	106.40
1	A	926	G	N3-C4-N9	6.49	129.89	126.00
1	A	946	A	N1-C2-N3	6.49	132.54	129.30
1	A	1086	U	N1-C2-N3	-6.49	111.01	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	129(A)	G	C4-N9-C1'	6.48	134.93	126.50
1	A	1394	A	N1-C6-N6	-6.48	114.71	118.60
1	A	78	G	N3-C2-N2	6.48	124.43	119.90
1	A	103	C	C6-N1-C2	-6.48	117.71	120.30
1	A	107	G	N7-C8-N9	6.48	116.34	113.10
1	A	1514	C	C6-N1-C2	-6.48	117.71	120.30
1	A	524	G	C5-C6-O6	-6.48	124.72	128.60
1	A	621	A	N1-C6-N6	6.47	122.48	118.60
1	A	812	C	P-O3'-C3'	6.47	127.47	119.70
1	A	129(A)	G	N3-C4-N9	6.47	129.88	126.00
1	A	273	A	C5-C6-N1	6.47	120.94	117.70
1	A	663	A	C8-N9-C4	6.47	108.39	105.80
1	A	22	G	C4-N9-C1'	6.47	134.91	126.50
1	A	1468	A	C6-N1-C2	-6.47	114.72	118.60
1	A	260	G	C5-N7-C8	-6.47	101.07	104.30
1	A	935	A	N1-C6-N6	-6.47	114.72	118.60
1	A	858	G	C5-N7-C8	-6.46	101.07	104.30
1	A	697	U	C2-N1-C1'	-6.46	109.95	117.70
1	A	854	G	N1-C2-N3	6.45	127.77	123.90
1	A	1073	U	N3-C4-O4	6.45	123.92	119.40
1	A	693	G	N3-C4-N9	6.45	129.87	126.00
1	A	1070	U	N3-C2-O2	-6.45	117.69	122.20
1	A	899	C	N3-C2-O2	6.44	126.41	121.90
1	A	413	G	C2-N3-C4	6.44	115.12	111.90
1	A	1156	G	C8-N9-C4	-6.44	103.83	106.40
1	A	1460	A	C6-C5-N7	-6.44	127.79	132.30
1	A	1475	G	C5-C6-N1	-6.44	108.28	111.50
7	G	124	LEU	CA-CB-CG	-6.44	100.50	115.30
1	A	1497	G	C4-C5-C6	6.44	122.66	118.80
1	A	48	C	C6-N1-C2	6.43	122.87	120.30
1	A	771	G	C5-C6-O6	-6.43	124.74	128.60
1	A	1385	G	C5-C6-O6	6.43	132.46	128.60
1	A	774	G	C4-C5-N7	6.43	113.37	110.80
1	A	74	C	C2-N1-C1'	6.43	125.87	118.80
1	A	52	G	C5-N7-C8	-6.43	101.09	104.30
1	A	24	U	N3-C2-O2	6.42	126.70	122.20
1	A	77	G	C6-C5-N7	-6.42	126.55	130.40
1	A	945	G	C5-N7-C8	-6.42	101.09	104.30
1	A	531	U	N3-C2-O2	-6.42	117.71	122.20
1	A	753	A	C5-C6-N1	6.42	120.91	117.70
1	A	796	C	C5-C6-N1	-6.42	117.79	121.00
1	A	671	G	C2-N3-C4	-6.41	108.69	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1497	G	C5-C6-N1	-6.41	108.29	111.50
1	A	888	G	N3-C2-N2	-6.41	115.41	119.90
1	A	1203	C	C5-C6-N1	6.41	124.21	121.00
1	A	1203	C	C6-N1-C2	-6.41	117.74	120.30
8	H	86	ILE	CG1-CB-CG2	-6.41	97.30	111.40
1	A	255	G	C4-N9-C1'	6.41	134.83	126.50
1	A	325	A	N1-C6-N6	-6.40	114.76	118.60
1	A	723	U	C6-N1-C2	-6.40	117.16	121.00
1	A	917	G	N1-C6-O6	6.40	123.74	119.90
1	A	880	C	C4-C5-C6	6.40	120.60	117.40
1	A	28	G	C6-C5-N7	-6.39	126.56	130.40
1	A	827	U	C2-N1-C1'	6.39	125.37	117.70
1	A	939	G	C5-N7-C8	6.39	107.50	104.30
1	A	320	C	N1-C2-N3	6.39	123.67	119.20
1	A	445	G	C8-N9-C4	-6.39	103.84	106.40
1	A	1499	A	C6-C5-N7	-6.39	127.83	132.30
1	A	810	C	N3-C2-O2	6.38	126.37	121.90
20	T	43	LEU	CA-CB-CG	-6.38	100.62	115.30
1	A	299	G	C5-C6-O6	-6.38	124.77	128.60
1	A	474	G	N3-C4-C5	6.38	131.79	128.60
1	A	635	G	C6-C5-N7	-6.38	126.57	130.40
1	A	639	G	N1-C2-N3	6.38	127.73	123.90
1	A	531	U	C5-C4-O4	6.38	129.72	125.90
1	A	801	U	N3-C4-O4	-6.38	114.94	119.40
1	A	31	G	C5-C6-O6	6.37	132.42	128.60
1	A	1500	A	N9-C4-C5	6.37	108.35	105.80
1	A	107	G	C5-C6-O6	-6.37	124.78	128.60
1	A	452	A	C8-N9-C4	6.37	108.35	105.80
1	A	690	G	C4-C5-N7	-6.37	108.25	110.80
1	A	854	G	C6-N1-C2	-6.37	121.28	125.10
1	A	8	A	N9-C4-C5	6.37	108.35	105.80
1	A	656	C	C2-N3-C4	-6.37	116.72	119.90
1	A	1374	A	C4-C5-C6	6.37	120.18	117.00
1	A	690	G	N9-C4-C5	6.36	107.95	105.40
1	A	1483	A	N1-C6-N6	-6.36	114.78	118.60
1	A	722	A	C5-C6-N1	-6.36	114.52	117.70
1	A	871	U	N3-C2-O2	-6.36	117.75	122.20
1	A	1303	C	N1-C2-O2	6.36	122.71	118.90
1	A	825	G	N7-C8-N9	-6.35	109.92	113.10
1	A	939	G	C5-C6-N1	6.35	114.68	111.50
1	A	28	G	C4-C5-C6	6.35	122.61	118.80
1	A	157	G	N1-C6-O6	6.35	123.71	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1306	A	C5-C6-N1	-6.35	114.52	117.70
1	A	153	C	N3-C4-C5	-6.35	119.36	121.90
1	A	293	G	C5-C6-N1	-6.35	108.33	111.50
1	A	897	C	C2-N3-C4	-6.35	116.72	119.90
1	A	607	A	C2-N3-C4	-6.35	107.43	110.60
1	A	130	A	C5-N7-C8	-6.34	100.73	103.90
1	A	292	G	C8-N9-C4	6.34	108.94	106.40
1	A	559	A	C4-N9-C1'	6.34	137.71	126.30
1	A	278	G	C5-N7-C8	6.33	107.47	104.30
1	A	752	G	C5-C6-N1	-6.33	108.33	111.50
1	A	1238	A	N1-C6-N6	-6.33	114.80	118.60
1	A	1475	G	N1-C6-O6	6.33	123.70	119.90
1	A	277	C	C2-N1-C1'	-6.33	111.84	118.80
1	A	862	C	N1-C2-N3	-6.33	114.77	119.20
1	A	855	G	C2-N3-C4	-6.33	108.74	111.90
1	A	454	C	C5-C6-N1	6.32	124.16	121.00
1	A	1294	G	C8-N9-C4	-6.32	103.87	106.40
1	A	247	G	C5-C6-O6	-6.32	124.81	128.60
1	A	274	A	C8-N9-C4	6.32	108.33	105.80
1	A	380	G	C5-C6-N1	-6.32	108.34	111.50
1	A	604	G	C4-C5-N7	-6.32	108.27	110.80
1	A	747	C	N3-C4-C5	6.32	124.43	121.90
1	A	1434	A	N9-C4-C5	-6.32	103.27	105.80
1	A	131	C	C5-C6-N1	-6.31	117.84	121.00
1	A	596	C	N1-C2-O2	6.31	122.69	118.90
1	A	10	A	C2-N3-C4	-6.31	107.44	110.60
1	A	288	A	C8-N9-C4	6.31	108.32	105.80
1	A	1391	U	N1-C2-O2	6.31	127.22	122.80
1	A	588	G	C8-N9-C4	6.31	108.92	106.40
1	A	752	G	C2-N3-C4	-6.31	108.75	111.90
1	A	1499	A	N9-C4-C5	-6.31	103.28	105.80
1	A	1502	A	C8-N9-C4	-6.31	103.28	105.80
1	A	1155	G	C8-N9-C4	-6.31	103.88	106.40
1	A	1082	G	N9-C4-C5	-6.30	102.88	105.40
1	A	867	G	C5-C6-N1	-6.30	108.35	111.50
1	A	310	G	N9-C4-C5	-6.30	102.88	105.40
1	A	546	G	C6-C5-N7	-6.29	126.62	130.40
1	A	881	G	C2-N3-C4	-6.29	108.75	111.90
1	A	929	G	N1-C2-N3	6.29	127.67	123.90
1	A	1375	A	N1-C6-N6	-6.29	114.83	118.60
1	A	245	C	N3-C4-N4	6.29	122.40	118.00
1	A	1181	G	N7-C8-N9	-6.29	109.96	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	237	C	C4-C5-C6	6.29	120.54	117.40
1	A	511	C	N3-C4-C5	6.29	124.41	121.90
1	A	878	G	C4-C5-N7	6.29	113.31	110.80
1	A	703	G	C4-N9-C1'	6.28	134.67	126.50
1	A	130	A	N1-C6-N6	6.28	122.37	118.60
1	A	963	G	C8-N9-C4	-6.28	103.89	106.40
1	A	1262	C	N3-C4-C5	-6.28	119.39	121.90
1	A	841	U	C5-C6-N1	6.28	125.84	122.70
1	A	147	G	N1-C6-O6	6.28	123.67	119.90
1	A	687	A	P-O3'-C3'	6.28	127.23	119.70
1	A	893	C	N1-C2-O2	6.28	122.67	118.90
1	A	860	A	N1-C2-N3	6.27	132.43	129.30
1	A	1106	G	C5-N7-C8	-6.26	101.17	104.30
1	A	599	C	N1-C2-O2	-6.26	115.14	118.90
1	A	778	G	N9-C4-C5	-6.26	102.89	105.40
1	A	221	C	N3-C4-C5	6.26	124.40	121.90
12	L	26	ALA	N-CA-C	-6.26	94.10	111.00
1	A	661	G	C5-C6-N1	-6.26	108.37	111.50
1	A	723	U	C5-C6-N1	6.26	125.83	122.70
1	A	91	C	C2-N1-C1'	-6.26	111.92	118.80
1	A	851	G	N3-C4-C5	-6.26	125.47	128.60
1	A	975	A	C5-C6-N1	-6.26	114.57	117.70
1	A	179	A	C6-N1-C2	-6.25	114.85	118.60
1	A	671	G	N1-C6-O6	6.25	123.65	119.90
1	A	263	A	N1-C6-N6	-6.25	114.85	118.60
1	A	574	A	N3-C4-N9	-6.25	122.40	127.40
1	A	741	G	C5-C6-N1	6.25	114.62	111.50
1	A	884	U	C5-C6-N1	-6.25	119.58	122.70
1	A	232	G	C8-N9-C4	6.25	108.90	106.40
1	A	1455	G	C4-C5-N7	6.24	113.30	110.80
1	A	1441	G	C5-C6-O6	6.24	132.34	128.60
17	Q	9	VAL	CB-CA-C	-6.24	99.54	111.40
1	A	279	A	C2-N3-C4	-6.24	107.48	110.60
1	A	262	A	N1-C6-N6	-6.24	114.86	118.60
1	A	474	G	C6-C5-N7	-6.24	126.66	130.40
1	A	1305	G	N1-C6-O6	6.23	123.64	119.90
1	A	93	G	C5-C6-N1	6.23	114.62	111.50
2	B	51	LEU	CA-CB-CG	-6.23	100.97	115.30
1	A	1158	C	N3-C4-C5	-6.23	119.41	121.90
1	A	1542	U	C2-N1-C1'	-6.23	110.23	117.70
1	A	799	G	C4-C5-N7	6.23	113.29	110.80
1	A	1366	C	C5-C6-N1	6.23	124.11	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	579	G	C5-C6-O6	-6.22	124.87	128.60
1	A	1443	G	C8-N9-C4	6.22	108.89	106.40
1	A	481	G	N3-C2-N2	6.21	124.25	119.90
1	A	584	G	C5-C6-N1	6.21	114.61	111.50
1	A	563	A	N7-C8-N9	6.21	116.91	113.80
1	A	1515	C	C5-C6-N1	6.21	124.11	121.00
1	A	416	G	N1-C6-O6	6.21	123.62	119.90
1	A	75	G	N3-C4-N9	6.21	129.72	126.00
1	A	224	C	C5-C6-N1	-6.20	117.90	121.00
1	A	731	G	C4-C5-N7	6.20	113.28	110.80
1	A	933	G	C4-C5-N7	6.20	113.28	110.80
1	A	70	G	N1-C6-O6	6.20	123.62	119.90
1	A	192	U	C6-N1-C2	6.20	124.72	121.00
1	A	833	U	N1-C2-N3	6.19	118.62	114.90
1	A	1434	A	C5-C6-N6	-6.19	118.75	123.70
12	L	66	VAL	CB-CA-C	-6.19	99.63	111.40
1	A	1197	G	C4-C5-N7	6.19	113.28	110.80
1	A	718	G	C6-C5-N7	-6.19	126.69	130.40
1	A	98	U	N3-C4-C5	-6.19	110.89	114.60
1	A	1383	C	N3-C4-C5	-6.19	119.42	121.90
1	A	1231	G	C2-N3-C4	-6.19	108.81	111.90
1	A	144	G	N3-C2-N2	-6.18	115.57	119.90
1	A	481	G	C5-C6-O6	-6.18	124.89	128.60
1	A	581	G	N3-C4-N9	-6.18	122.29	126.00
1	A	787	A	C5-C6-N6	-6.18	118.75	123.70
1	A	614	A	N1-C2-N3	6.18	132.39	129.30
1	A	28	G	C2-N3-C4	-6.18	108.81	111.90
1	A	1348	U	C6-N1-C1'	-6.18	112.55	121.20
1	A	628	G	N3-C2-N2	6.17	124.22	119.90
1	A	47	C	C4-C5-C6	6.17	120.49	117.40
1	A	604	G	N7-C8-N9	-6.17	110.02	113.10
1	A	1346	A	C6-C5-N7	6.17	136.62	132.30
1	A	46	G	C4-C5-C6	6.17	122.50	118.80
1	A	146	G	N1-C6-O6	6.17	123.60	119.90
1	A	232	G	C4-C5-C6	6.17	122.50	118.80
1	A	1488	G	C8-N9-C4	6.17	108.87	106.40
1	A	1380	U	N1-C2-N3	6.16	118.60	114.90
1	A	827	U	N3-C2-O2	-6.16	117.89	122.20
1	A	316	G	C4-N9-C1'	6.16	134.50	126.50
1	A	570	G	C2-N3-C4	6.15	114.98	111.90
1	A	144	G	C2-N3-C4	-6.15	108.82	111.90
1	A	850	U	C5-C4-O4	6.15	129.59	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	975	A	C2-N3-C4	-6.15	107.52	110.60
1	A	1513	A	N9-C4-C5	6.15	108.26	105.80
5	E	12	LEU	CA-CB-CG	6.15	129.45	115.30
1	A	1370	G	N1-C6-O6	6.15	123.59	119.90
1	A	285	G	C8-N9-C4	6.15	108.86	106.40
1	A	525	C	N1-C2-N3	-6.15	114.89	119.20
1	A	833	U	C6-N1-C2	-6.15	117.31	121.00
1	A	1401	G	C8-N9-C4	-6.14	103.94	106.40
1	A	238	G	N7-C8-N9	6.14	116.17	113.10
1	A	932	C	N3-C2-O2	-6.14	117.60	121.90
1	A	1352	C	C6-N1-C2	-6.14	117.84	120.30
1	A	1455	G	C5-N7-C8	-6.14	101.23	104.30
1	A	747	C	C2-N3-C4	-6.14	116.83	119.90
1	A	876	G	C5-N7-C8	-6.14	101.23	104.30
1	A	524	G	C6-C5-N7	-6.14	126.72	130.40
1	A	1234	C	C5-C4-N4	-6.14	115.91	120.20
1	A	670	G	N1-C6-O6	6.13	123.58	119.90
1	A	731	G	C6-C5-N7	-6.13	126.72	130.40
1	A	854	G	N3-C4-C5	-6.13	125.53	128.60
1	A	599	C	C2-N3-C4	-6.13	116.83	119.90
1	A	232	G	C4-C5-N7	6.13	113.25	110.80
1	A	237	C	N3-C2-O2	-6.13	117.61	121.90
1	A	263	A	N1-C2-N3	-6.13	126.23	129.30
1	A	445	G	C5-C6-N1	-6.13	108.43	111.50
1	A	1079	G	C8-N9-C4	-6.13	103.95	106.40
1	A	661	G	C2-N3-C4	-6.13	108.84	111.90
1	A	610	G	C4-N9-C1'	6.13	134.47	126.50
1	A	221	C	N3-C4-N4	-6.12	113.71	118.00
1	A	1533	C	C6-N1-C2	-6.12	117.85	120.30
1	A	301	G	N1-C2-N3	6.12	127.57	123.90
1	A	160	A	C8-N9-C4	-6.12	103.35	105.80
1	A	599	C	C5-C6-N1	-6.12	117.94	121.00
1	A	331	G	C8-N9-C1'	-6.12	119.05	127.00
1	A	566	G	C5-C6-N1	-6.12	108.44	111.50
1	A	1373	G	N3-C4-C5	-6.12	125.54	128.60
1	A	722	A	C4-C5-N7	6.11	113.75	110.70
1	A	350	G	C2-N3-C4	-6.11	108.85	111.90
1	A	489	C	N3-C2-O2	6.10	126.17	121.90
1	A	1329	A	C5-N7-C8	-6.10	100.85	103.90
1	A	865	A	C5-C6-N1	6.10	120.75	117.70
1	A	357	G	C4-C5-C6	6.10	122.46	118.80
1	A	1249	C	C2-N1-C1'	6.10	125.51	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	66	G	N3-C2-N2	-6.09	115.63	119.90
1	A	38	G	N3-C4-N9	-6.09	122.35	126.00
1	A	1379	G	N3-C4-C5	-6.09	125.56	128.60
1	A	1399	C	N1-C2-N3	6.09	123.46	119.20
1	A	654	G	C2-N3-C4	-6.09	108.86	111.90
1	A	941	G	C5-N7-C8	-6.08	101.26	104.30
1	A	46	G	C4-C5-N7	-6.08	108.37	110.80
1	A	277	C	N3-C4-N4	-6.08	113.74	118.00
1	A	316	G	N1-C6-O6	6.08	123.55	119.90
1	A	730	G	N1-C2-N3	6.08	127.55	123.90
1	A	107	G	N9-C4-C5	-6.08	102.97	105.40
1	A	232	G	C8-N9-C1'	-6.08	119.09	127.00
1	A	108	G	C4-C5-N7	6.08	113.23	110.80
1	A	1332	A	C8-N9-C4	-6.08	103.37	105.80
1	A	625	G	C4-N9-C1'	6.07	134.40	126.50
1	A	1531	A	C5-N7-C8	-6.07	100.86	103.90
1	A	855	G	C5-C6-N1	-6.07	108.46	111.50
1	A	1333	A	C4-C5-C6	6.07	120.03	117.00
1	A	153	C	C6-N1-C2	-6.07	117.87	120.30
1	A	366	C	N3-C2-O2	-6.07	117.65	121.90
1	A	917	G	C6-C5-N7	-6.07	126.76	130.40
1	A	284	G	C5-C6-O6	-6.06	124.96	128.60
1	A	452	A	C2-N3-C4	-6.06	107.57	110.60
1	A	816	A	C2-N3-C4	-6.06	107.57	110.60
1	A	867	G	C4-C5-N7	6.06	113.22	110.80
1	A	523	A	N7-C8-N9	-6.06	110.77	113.80
1	A	854	G	N3-C4-N9	6.06	129.63	126.00
1	A	617	G	N3-C4-N9	6.06	129.63	126.00
1	A	832	C	N1-C2-O2	-6.06	115.27	118.90
1	A	893	C	N3-C2-O2	-6.06	117.66	121.90
1	A	895	G	N1-C2-N3	6.06	127.53	123.90
1	A	75	G	C4-C5-C6	6.06	122.43	118.80
1	A	580	U	C6-N1-C2	-6.06	117.37	121.00
1	A	884	U	C6-N1-C2	6.06	124.63	121.00
1	A	1347	G	N7-C8-N9	-6.05	110.07	113.10
1	A	264	U	N1-C2-O2	-6.05	118.56	122.80
1	A	892	A	C8-N9-C4	6.05	108.22	105.80
1	A	944	G	N1-C2-N2	-6.05	110.76	116.20
1	A	730	G	N9-C4-C5	6.05	107.82	105.40
1	A	1391	U	N1-C2-N3	-6.04	111.27	114.90
1	A	1235	U	N3-C4-O4	6.04	123.63	119.40
1	A	1390	U	C5-C4-O4	6.04	129.53	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	502	G	N1-C6-O6	6.04	123.52	119.90
1	A	1080	A	N3-C4-N9	-6.04	122.57	127.40
1	A	628	G	N1-C2-N2	-6.04	110.77	116.20
17	Q	84	LEU	CA-CB-CG	-6.04	101.41	115.30
1	A	175	C	C5-C6-N1	-6.04	117.98	121.00
1	A	9	G	N1-C6-O6	6.03	123.52	119.90
1	A	764	C	C5-C4-N4	-6.03	115.98	120.20
1	A	1460	A	C5-C6-N6	-6.03	118.88	123.70
1	A	1533	C	C2-N1-C1'	6.03	125.43	118.80
1	A	29	G	N1-C2-N3	6.03	127.52	123.90
1	A	788	U	C2-N3-C4	6.03	130.62	127.00
1	A	316	G	N7-C8-N9	6.02	116.11	113.10
1	A	98	U	C2-N3-C4	6.02	130.61	127.00
1	A	723	U	C2-N1-C1'	6.02	124.93	117.70
1	A	1482	G	C4-N9-C1'	6.02	134.33	126.50
1	A	124	G	C8-N9-C4	-6.02	103.99	106.40
1	A	755	G	N3-C4-C5	-6.02	125.59	128.60
1	A	854	G	N1-C6-O6	-6.02	116.29	119.90
1	A	1236	A	N1-C6-N6	6.01	122.21	118.60
1	A	860	A	N1-C6-N6	6.01	122.21	118.60
1	A	634	C	C6-N1-C2	-6.01	117.90	120.30
1	A	835	U	N3-C2-O2	-6.01	117.99	122.20
1	A	629	G	N3-C4-N9	6.00	129.60	126.00
1	A	683	G	C4-C5-N7	-6.00	108.40	110.80
1	A	275	G	C8-N9-C4	6.00	108.80	106.40
1	A	280	C	N3-C4-N4	-6.00	113.80	118.00
1	A	309	G	N3-C4-N9	6.00	129.60	126.00
1	A	817	C	N3-C4-N4	6.00	122.20	118.00
2	B	23	ARG	N-CA-C	-6.00	94.79	111.00
1	A	255	G	C4-C5-N7	6.00	113.20	110.80
1	A	482	A	C4-C5-C6	6.00	120.00	117.00
1	A	664	G	C5-C6-O6	6.00	132.20	128.60
1	A	1239	A	C8-N9-C4	6.00	108.20	105.80
1	A	712	A	N1-C2-N3	5.99	132.29	129.30
1	A	698	G	C4-N9-C1'	5.99	134.28	126.50
1	A	282	A	N1-C6-N6	-5.98	115.01	118.60
1	A	1102	A	C5-N7-C8	5.98	106.89	103.90
1	A	25	C	C5-C4-N4	-5.98	116.01	120.20
1	A	799	G	C5-C6-O6	-5.98	125.01	128.60
1	A	183	G	C6-C5-N7	-5.98	126.81	130.40
1	A	1078	U	N3-C2-O2	-5.98	118.02	122.20
1	A	755	G	C4-N9-C1'	5.97	134.27	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1078	U	C6-N1-C2	-5.97	117.42	121.00
1	A	281	G	C6-C5-N7	-5.97	126.82	130.40
1	A	1307	U	C2-N1-C1'	5.97	124.86	117.70
1	A	936	C	C5-C6-N1	-5.97	118.02	121.00
1	A	372	C	N1-C2-N3	-5.96	115.03	119.20
1	A	1380	U	N3-C4-O4	-5.96	115.22	119.40
1	A	746	A	C2-N3-C4	-5.96	107.62	110.60
1	A	765	G	C2-N3-C4	-5.96	108.92	111.90
1	A	1471	G	C2-N3-C4	-5.96	108.92	111.90
1	A	784	C	N1-C2-O2	-5.96	115.33	118.90
1	A	819	A	N1-C6-N6	-5.96	115.03	118.60
1	A	1293	G	C8-N9-C4	-5.96	104.02	106.40
1	A	1509	C	C6-N1-C2	-5.96	117.92	120.30
1	A	266	G	C5-C6-O6	5.96	132.17	128.60
1	A	480	U	C4-C5-C6	5.96	123.27	119.70
1	A	851	G	N7-C8-N9	5.96	116.08	113.10
1	A	862	C	N3-C2-O2	5.96	126.07	121.90
1	A	74	C	C6-N1-C1'	-5.95	113.66	120.80
1	A	303	A	C5-C6-N1	-5.95	114.73	117.70
1	A	786	G	C4-C5-N7	5.95	113.18	110.80
1	A	666	G	C5-C6-N1	-5.95	108.53	111.50
1	A	825	G	C5-C6-O6	-5.94	125.03	128.60
1	A	1344	C	N3-C4-C5	5.94	124.28	121.90
1	A	1371	G	N7-C8-N9	5.94	116.07	113.10
1	A	1520	G	C5-C6-O6	-5.94	125.04	128.60
1	A	388	G	C8-N9-C4	5.94	108.78	106.40
1	A	317	G	C6-C5-N7	-5.94	126.84	130.40
1	A	788	U	N3-C4-C5	-5.94	111.04	114.60
1	A	229	U	C4-C5-C6	5.94	123.26	119.70
1	A	818	G	N3-C4-N9	-5.94	122.44	126.00
1	A	670	G	C8-N9-C1'	-5.93	119.28	127.00
1	A	931	C	N3-C4-C5	5.93	124.27	121.90
1	A	90	U	N3-C4-C5	-5.93	111.04	114.60
1	A	922	G	N3-C4-N9	5.93	129.56	126.00
1	A	422	C	N1-C2-O2	5.93	122.46	118.90
1	A	559	A	N3-C4-C5	-5.93	122.65	126.80
1	A	228	A	N7-C8-N9	5.93	116.76	113.80
1	A	868	C	C5-C6-N1	-5.93	118.04	121.00
1	A	1388	C	N3-C2-O2	5.93	126.05	121.90
1	A	484	G	N1-C6-O6	-5.92	116.35	119.90
1	A	80	G	C8-N9-C4	-5.92	104.03	106.40
1	A	864	A	C6-N1-C2	5.92	122.15	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	762	C	C4-C5-C6	-5.92	114.44	117.40
1	A	230	G	C8-N9-C1'	-5.92	119.31	127.00
1	A	1520	G	C5-N7-C8	-5.92	101.34	104.30
1	A	1149	C	C2-N1-C1'	5.92	125.31	118.80
1	A	761	G	C2-N3-C4	-5.91	108.94	111.90
1	A	147	G	C8-N9-C4	5.91	108.76	106.40
1	A	1381	U	N1-C2-N3	-5.90	111.36	114.90
1	A	228	A	C2-N3-C4	-5.90	107.65	110.60
1	A	556	C	C5-C6-N1	-5.90	118.05	121.00
1	A	43	C	N3-C4-C5	5.90	124.26	121.90
1	A	296	U	C5-C6-N1	-5.90	119.75	122.70
1	A	1248	A	C2-N3-C4	5.90	113.55	110.60
1	A	1187	G	N1-C6-O6	5.90	123.44	119.90
1	A	283	C	C2-N3-C4	5.89	122.85	119.90
1	A	839	U	C6-N1-C1'	-5.89	112.95	121.20
1	A	936	C	C4-C5-C6	5.89	120.35	117.40
1	A	1302	U	C2-N3-C4	-5.89	123.47	127.00
1	A	894	G	C2-N3-C4	-5.89	108.95	111.90
1	A	169	C	C4-C5-C6	5.89	120.34	117.40
1	A	773	G	N1-C2-N3	5.89	127.43	123.90
1	A	292	G	N9-C4-C5	-5.89	103.05	105.40
1	A	1322	C	C2-N1-C1'	5.89	125.28	118.80
1	A	1520	G	N3-C4-N9	-5.89	122.47	126.00
1	A	551	U	C5-C6-N1	-5.88	119.76	122.70
1	A	1203	C	N3-C4-C5	-5.88	119.55	121.90
1	A	1375	A	C5-N7-C8	5.88	106.84	103.90
1	A	570	G	C4-N9-C1'	5.88	134.15	126.50
1	A	141	A	N1-C6-N6	5.88	122.13	118.60
1	A	657	G	N1-C6-O6	5.88	123.43	119.90
1	A	774	G	C5-C6-O6	-5.88	125.07	128.60
1	A	361	G	C5-C6-N1	5.88	114.44	111.50
1	A	887	G	N1-C2-N2	-5.88	110.91	116.20
1	A	147	G	C5-C6-O6	-5.87	125.08	128.60
1	A	893	C	C2-N1-C1'	5.87	125.26	118.80
1	A	777	A	N1-C6-N6	-5.87	115.08	118.60
1	A	318	G	N1-C2-N3	5.86	127.42	123.90
1	A	810	C	N3-C4-N4	5.86	122.11	118.00
1	A	882	C	C5-C6-N1	-5.86	118.07	121.00
1	A	1367	C	C6-N1-C2	-5.86	117.95	120.30
1	A	236	G	C5-C6-O6	5.86	132.12	128.60
1	A	326	G	N3-C4-C5	-5.86	125.67	128.60
1	A	808	C	C6-N1-C2	5.86	122.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1306	A	C8-N9-C1'	-5.86	117.16	127.70
1	A	1441	G	N9-C4-C5	5.85	107.74	105.40
1	A	190(I)	G	C8-N9-C4	5.85	108.74	106.40
1	A	701	C	P-O3'-C3'	5.85	126.72	119.70
2	B	16	HIS	N-CA-C	5.85	126.80	111.00
1	A	241	C	C4-C5-C6	5.85	120.33	117.40
1	A	245	C	C6-N1-C2	5.85	122.64	120.30
11	K	118	GLY	N-CA-C	5.85	127.71	113.10
1	A	307	C	N3-C4-N4	5.84	122.09	118.00
1	A	671	G	N3-C4-C5	5.84	131.52	128.60
1	A	848	C	N3-C4-C5	5.84	124.24	121.90
1	A	1496	C	C2-N1-C1'	5.84	125.23	118.80
1	A	51	A	C5-N7-C8	-5.84	100.98	103.90
1	A	1300	G	C8-N9-C4	5.84	108.74	106.40
1	A	328	C	N3-C4-C5	5.84	124.23	121.90
1	A	745	C	C2-N3-C4	-5.84	116.98	119.90
1	A	938	A	N9-C4-C5	5.84	108.13	105.80
1	A	760	G	C2-N3-C4	-5.83	108.98	111.90
1	A	168	G	N3-C4-N9	5.83	129.50	126.00
1	A	916	G	N7-C8-N9	5.83	116.02	113.10
1	A	995	C	N1-C2-O2	5.83	122.40	118.90
1	A	373	A	C6-N1-C2	-5.83	115.10	118.60
1	A	388	G	N3-C4-N9	5.83	129.50	126.00
1	A	1132	C	C6-N1-C2	-5.83	117.97	120.30
1	A	581	G	N3-C4-C5	5.82	131.51	128.60
1	A	719	C	C6-N1-C1'	-5.82	113.81	120.80
1	A	129	U	N3-C4-C5	-5.82	111.11	114.60
1	A	283	C	N1-C2-O2	5.82	122.39	118.90
1	A	199	G	N3-C2-N2	-5.81	115.83	119.90
1	A	975	A	C4-C5-N7	5.81	113.61	110.70
1	A	1311	G	N3-C2-N2	-5.81	115.83	119.90
1	A	229	U	N3-C4-C5	-5.81	111.11	114.60
1	A	754	C	N3-C2-O2	-5.81	117.83	121.90
1	A	1499	A	C4-C5-N7	5.81	113.61	110.70
1	A	542	G	C8-N9-C4	-5.81	104.08	106.40
1	A	1087	G	C8-N9-C4	5.81	108.72	106.40
1	A	253	U	N3-C2-O2	5.80	126.26	122.20
1	A	777	A	N9-C4-C5	5.80	108.12	105.80
1	A	1238	A	N1-C2-N3	5.80	132.20	129.30
1	A	287	U	C6-N1-C2	-5.80	117.52	121.00
1	A	1462	G	C2-N3-C4	-5.80	109.00	111.90
1	A	591	U	C5-C6-N1	-5.80	119.80	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	661	G	N7-C8-N9	5.80	116.00	113.10
1	A	506	G	C2-N3-C4	-5.80	109.00	111.90
1	A	852	G	C8-N9-C4	5.80	108.72	106.40
1	A	400	C	C6-N1-C2	5.80	122.62	120.30
1	A	607	A	C5-N7-C8	-5.80	101.00	103.90
1	A	887	G	N1-C2-N3	5.79	127.38	123.90
1	A	33	A	C8-N9-C4	5.79	108.12	105.80
1	A	242	C	C6-N1-C2	5.79	122.62	120.30
1	A	1121	U	N3-C4-O4	5.79	123.45	119.40
1	A	1122	U	C6-N1-C2	-5.79	117.53	121.00
1	A	246	A	C8-N9-C4	-5.79	103.49	105.80
1	A	670	G	C6-C5-N7	-5.79	126.93	130.40
1	A	694	A	C5-C6-N1	-5.79	114.81	117.70
1	A	765	G	N1-C6-O6	5.79	123.37	119.90
1	A	1390	U	C4-C5-C6	5.79	123.17	119.70
1	A	1543	C	N1-C2-N3	-5.79	115.15	119.20
1	A	670	G	N3-C4-C5	-5.78	125.71	128.60
1	A	389	A	N3-C4-C5	-5.78	122.75	126.80
1	A	460	A	N3-C4-C5	-5.78	122.75	126.80
1	A	557	G	C5-C6-N1	-5.78	108.61	111.50
1	A	876	G	N1-C6-O6	5.78	123.37	119.90
10	J	40	LEU	CA-CB-CG	5.78	128.58	115.30
1	A	76	C	C5-C6-N1	-5.77	118.11	121.00
1	A	129(A)	G	N1-C6-O6	5.77	123.36	119.90
1	A	781	A	C5-N7-C8	-5.77	101.01	103.90
1	A	5	U	P-O3'-C3'	5.77	126.63	119.70
1	A	1414	U	C5-C4-O4	5.77	129.36	125.90
1	A	547	A	C4-C5-N7	5.77	113.59	110.70
1	A	77	G	C5-C6-O6	-5.77	125.14	128.60
1	A	542	G	N3-C4-C5	-5.77	125.72	128.60
1	A	1087	G	N3-C4-C5	5.77	131.48	128.60
1	A	1108	G	N9-C4-C5	5.76	107.71	105.40
1	A	789	U	C6-N1-C2	-5.76	117.54	121.00
1	A	1054	C	C4-C5-C6	-5.76	114.52	117.40
1	A	576	G	C8-N9-C4	-5.76	104.10	106.40
1	A	605	U	C6-N1-C2	-5.76	117.54	121.00
1	A	1332	A	C4-C5-N7	-5.76	107.82	110.70
1	A	1508	G	C8-N9-C4	-5.76	104.10	106.40
1	A	91	C	C6-N1-C1'	5.75	127.70	120.80
1	A	1080	A	C4-C5-N7	-5.75	107.82	110.70
1	A	1539	C	C6-N1-C2	5.75	122.60	120.30
1	A	779	C	N1-C2-O2	-5.75	115.45	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1202	G	N3-C4-C5	-5.75	125.72	128.60
1	A	336	C	N3-C4-N4	5.75	122.02	118.00
1	A	1195	C	N3-C2-O2	5.75	125.92	121.90
1	A	1377	A	C5-C6-N6	5.75	128.30	123.70
1	A	1528	U	C6-N1-C2	5.75	124.45	121.00
1	A	99	C	C2-N1-C1'	5.75	125.12	118.80
1	A	113	G	C6-C5-N7	-5.75	126.95	130.40
1	A	317	G	N9-C4-C5	-5.75	103.10	105.40
8	H	92	ARG	CG-CD-NE	5.75	123.87	111.80
1	A	108	G	N7-C8-N9	5.75	115.97	113.10
1	A	31	G	C5-N7-C8	5.74	107.17	104.30
1	A	276	G	C8-N9-C4	5.74	108.70	106.40
1	A	703	G	C2-N3-C4	5.74	114.77	111.90
1	A	474	G	C5-C6-O6	-5.74	125.16	128.60
1	A	604	G	C5-N7-C8	5.74	107.17	104.30
1	A	656	C	C5-C6-N1	-5.74	118.13	121.00
1	A	890	G	C6-C5-N7	5.74	133.84	130.40
15	O	36	ILE	CB-CA-C	-5.74	100.13	111.60
15	O	56	LEU	CA-CB-CG	-5.74	102.10	115.30
1	A	480	U	C5-C4-O4	5.74	129.34	125.90
1	A	93	G	N3-C2-N2	5.73	123.91	119.90
1	A	931	C	C4-C5-C6	5.73	120.27	117.40
1	A	597	G	C6-N1-C2	-5.72	121.67	125.10
1	A	1311	G	C5-C6-N1	-5.72	108.64	111.50
1	A	157	G	N3-C2-N2	-5.72	115.89	119.90
1	A	27	G	C6-C5-N7	-5.72	126.97	130.40
1	A	751	U	N1-C2-N3	-5.72	111.47	114.90
1	A	245	C	N3-C2-O2	5.72	125.90	121.90
1	A	862	C	C6-N1-C2	5.72	122.59	120.30
1	A	925	G	N3-C2-N2	5.72	123.90	119.90
1	A	723	U	N1-C2-O2	5.72	126.80	122.80
1	A	119	A	N9-C4-C5	5.72	108.09	105.80
1	A	1390	U	N1-C2-O2	-5.72	118.80	122.80
1	A	11	G	N1-C2-N3	5.71	127.33	123.90
1	A	116	A	C5-C6-N1	-5.71	114.84	117.70
1	A	660	G	N1-C6-O6	5.71	123.33	119.90
1	A	1067	A	P-O3'-C3'	5.71	126.56	119.70
1	A	107	G	N3-C2-N2	5.71	123.90	119.90
1	A	905	U	C2-N1-C1'	-5.71	110.84	117.70
1	A	569	C	N3-C4-N4	-5.71	114.00	118.00
1	A	22	G	C8-N9-C4	-5.71	104.12	106.40
1	A	157	G	N3-C4-N9	-5.71	122.58	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	240	C	C5-C4-N4	-5.71	116.21	120.20
1	A	1087	G	C4-C5-N7	5.71	113.08	110.80
1	A	1149	C	C5-C6-N1	5.71	123.85	121.00
1	A	217	C	C5-C6-N1	5.70	123.85	121.00
1	A	616	G	C2-N3-C4	-5.70	109.05	111.90
1	A	658	G	C8-N9-C4	5.70	108.68	106.40
1	A	137	C	N3-C4-N4	-5.70	114.01	118.00
1	A	579	G	N1-C2-N3	5.70	127.32	123.90
1	A	1353	G	C5-C6-N1	5.70	114.35	111.50
1	A	945	G	C8-N9-C4	-5.70	104.12	106.40
1	A	309	G	C6-C5-N7	-5.70	126.98	130.40
1	A	943	U	C2-N1-C1'	5.70	124.53	117.70
1	A	1298	C	N1-C2-O2	5.70	122.32	118.90
1	A	481	G	C5-N7-C8	5.69	107.15	104.30
1	A	130	A	N7-C8-N9	5.69	116.65	113.80
1	A	595	G	N1-C6-O6	-5.69	116.48	119.90
1	A	946	A	N1-C6-N6	-5.69	115.18	118.60
1	A	1095	U	C6-N1-C2	5.69	124.42	121.00
1	A	1197	G	C6-C5-N7	-5.69	126.98	130.40
1	A	1523	G	N3-C2-N2	-5.69	115.92	119.90
1	A	697	U	C5-C6-N1	-5.69	119.86	122.70
1	A	1381	U	C6-N1-C2	5.69	124.42	121.00
1	A	1524	C	N3-C4-C5	-5.69	119.62	121.90
1	A	122	G	N3-C4-C5	5.69	131.44	128.60
1	A	778	G	N3-C4-C5	5.69	131.44	128.60
1	A	1352	C	C5-C6-N1	5.69	123.84	121.00
1	A	1388	C	C2-N1-C1'	-5.69	112.55	118.80
1	A	15	G	N1-C6-O6	5.68	123.31	119.90
1	A	168	G	C8-N9-C1'	-5.68	119.61	127.00
1	A	244	U	C5-C6-N1	-5.68	119.86	122.70
1	A	307	C	C5-C4-N4	-5.68	116.22	120.20
1	A	168	G	N3-C4-C5	-5.68	125.76	128.60
1	A	1338	G	C5-C6-O6	5.68	132.01	128.60
1	A	250	A	C2-N3-C4	-5.68	107.76	110.60
1	A	586	C	C5-C6-N1	-5.68	118.16	121.00
1	A	659	U	C5-C6-N1	-5.68	119.86	122.70
1	A	922	G	N1-C6-O6	-5.68	116.49	119.90
4	D	94	LEU	CA-CB-CG	-5.68	102.25	115.30
1	A	273	A	N1-C6-N6	-5.67	115.19	118.60
1	A	1392	G	C8-N9-C1'	-5.67	119.62	127.00
1	A	416	G	C5-C6-O6	-5.67	125.20	128.60
1	A	502	G	C5-C6-O6	-5.67	125.20	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	119	A	C6-N1-C2	-5.67	115.20	118.60
1	A	769	G	C5-C6-O6	-5.67	125.20	128.60
1	A	1447	G	C8-N9-C4	-5.67	104.13	106.40
1	A	598	U	C6-N1-C2	5.67	124.40	121.00
1	A	373	A	N7-C8-N9	5.67	116.63	113.80
1	A	1087	G	C6-C5-N7	-5.67	127.00	130.40
1	A	1193	G	C5-C6-N1	-5.67	108.67	111.50
1	A	721	G	C4-C5-C6	5.67	122.20	118.80
1	A	931	C	N1-C2-N3	5.67	123.17	119.20
1	A	944	G	C4-C5-N7	-5.67	108.53	110.80
1	A	1084	G	C5-C6-O6	-5.67	125.20	128.60
1	A	1488	G	N7-C8-N9	-5.67	110.27	113.10
1	A	1516	G	C4-N9-C1'	5.67	133.86	126.50
1	A	662	G	C8-N9-C4	5.66	108.67	106.40
1	A	660	G	N1-C2-N2	-5.66	111.11	116.20
1	A	285	G	N3-C4-C5	5.66	131.43	128.60
1	A	888	G	C4-C5-N7	-5.66	108.54	110.80
1	A	885	G	C5-C6-N1	-5.66	108.67	111.50
1	A	1334	G	N7-C8-N9	-5.66	110.27	113.10
1	A	741	G	C4-N9-C1'	-5.65	119.15	126.50
1	A	888	G	C5-C6-N1	-5.65	108.67	111.50
1	A	661	G	C8-N9-C4	-5.65	104.14	106.40
1	A	1312	G	C5-N7-C8	-5.65	101.47	104.30
1	A	1360	A	C8-N9-C4	-5.65	103.54	105.80
1	A	452	A	N3-C4-C5	5.64	130.75	126.80
1	A	805	C	N1-C2-O2	5.64	122.29	118.90
1	A	768	A	C6-N1-C2	-5.64	115.21	118.60
1	A	770	C	C2-N3-C4	-5.64	117.08	119.90
1	A	779	C	C2-N3-C4	-5.64	117.08	119.90
1	A	874	G	C8-N9-C1'	-5.64	119.67	127.00
1	A	635	G	C8-N9-C1'	-5.64	119.67	127.00
1	A	862	C	C4-C5-C6	-5.64	114.58	117.40
1	A	888	G	N9-C4-C5	5.64	107.66	105.40
1	A	111	G	C5-C6-O6	-5.64	125.22	128.60
1	A	580	U	N3-C4-O4	5.64	123.35	119.40
1	A	373	A	N1-C2-N3	5.63	132.12	129.30
1	A	575	G	C4-C5-N7	5.63	113.05	110.80
1	A	597	G	N3-C2-N2	5.63	123.84	119.90
1	A	577	G	C4-N9-C1'	-5.63	119.18	126.50
1	A	1031	G	N7-C8-N9	5.63	115.92	113.10
1	A	474	G	C8-N9-C4	5.63	108.65	106.40
1	A	751	U	N3-C2-O2	5.63	126.14	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	872	A	C5-C6-N6	-5.63	119.20	123.70
1	A	1312	G	C5-C6-O6	-5.63	125.22	128.60
1	A	223	U	N1-C2-O2	-5.63	118.86	122.80
1	A	801	U	N3-C4-C5	5.63	117.98	114.60
1	A	885	G	N3-C4-C5	5.63	131.41	128.60
1	A	1330	U	N1-C2-O2	5.63	126.74	122.80
1	A	1361(A)	C	C5-C4-N4	-5.63	116.26	120.20
1	A	26	A	N1-C2-N3	5.62	132.11	129.30
1	A	79	G	N1-C6-O6	5.62	123.27	119.90
1	A	106	C	C6-N1-C2	-5.62	118.05	120.30
1	A	856	C	N1-C2-O2	-5.62	115.53	118.90
1	A	80	G	N1-C6-O6	5.62	123.27	119.90
1	A	120	A	C4-C5-N7	-5.62	107.89	110.70
4	D	12	CYS	CA-CB-SG	5.62	124.11	114.00
1	A	1392	G	C4-N9-C1'	5.62	133.80	126.50
1	A	723	U	N3-C2-O2	-5.61	118.27	122.20
1	A	1468	A	N1-C6-N6	-5.61	115.23	118.60
1	A	580	U	N1-C2-N3	5.61	118.27	114.90
1	A	934	C	C5-C6-N1	-5.61	118.19	121.00
1	A	1542	U	C5-C4-O4	5.61	129.26	125.90
1	A	326	G	C5-N7-C8	5.60	107.10	104.30
1	A	485	G	C4-N9-C1'	-5.60	119.22	126.50
1	A	670	G	N3-C4-N9	5.60	129.36	126.00
1	A	1078	U	C2-N1-C1'	5.60	124.42	117.70
1	A	565	U	N1-C2-N3	-5.59	111.54	114.90
1	A	644	G	N1-C6-O6	5.59	123.26	119.90
1	A	1447	G	C5-C6-N1	5.59	114.30	111.50
1	A	93	G	N3-C4-C5	-5.59	125.80	128.60
1	A	597	G	N3-C4-N9	5.59	129.35	126.00
1	A	1516	G	C4-C5-C6	5.59	122.15	118.80
1	A	1240	U	N3-C4-O4	-5.59	115.49	119.40
1	A	781	A	C2-N3-C4	-5.59	107.81	110.60
1	A	1073	U	N3-C4-C5	-5.59	111.25	114.60
1	A	920	U	N3-C4-C5	-5.58	111.25	114.60
1	A	685	G	C2-N3-C4	-5.58	109.11	111.90
1	A	73	C	C5-C6-N1	5.58	123.79	121.00
1	A	308	C	N1-C2-N3	-5.58	115.29	119.20
1	A	651	C	C4-C5-C6	5.58	120.19	117.40
1	A	853	G	C6-C5-N7	-5.58	127.05	130.40
1	A	25	C	C6-N1-C2	5.58	122.53	120.30
1	A	482	A	C5-N7-C8	-5.58	101.11	103.90
1	A	1238	A	C8-N9-C4	-5.57	103.57	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	120	A	N1-C6-N6	-5.57	115.26	118.60
1	A	750	G	C6-N1-C2	-5.57	121.76	125.10
1	A	878	G	C5-C6-O6	-5.57	125.26	128.60
1	A	1462	G	C8-N9-C4	5.57	108.63	106.40
1	A	254	G	C8-N9-C4	5.56	108.62	106.40
1	A	518	C	N1-C2-O2	5.56	122.24	118.90
1	A	779	C	C6-N1-C2	5.56	122.53	120.30
1	A	1313	U	N3-C4-O4	5.56	123.29	119.40
1	A	1370	G	C5-C6-O6	-5.56	125.26	128.60
1	A	931	C	N3-C2-O2	-5.56	118.01	121.90
1	A	1335	C	N3-C4-C5	5.56	124.12	121.90
1	A	1517	G	N3-C4-C5	5.56	131.38	128.60
1	A	52	G	N3-C4-N9	5.56	129.33	126.00
1	A	458	C	N1-C2-O2	-5.55	115.57	118.90
1	A	647	C	C6-N1-C2	5.55	122.52	120.30
1	A	867	G	C8-N9-C1'	-5.55	119.78	127.00
1	A	121	C	C6-N1-C2	-5.55	118.08	120.30
1	A	637	G	N3-C4-N9	5.55	129.33	126.00
1	A	909	A	C4-C5-N7	5.55	113.48	110.70
1	A	485	G	N1-C6-O6	5.55	123.23	119.90
1	A	885	G	N1-C6-O6	5.55	123.23	119.90
1	A	1528	U	N3-C4-C5	5.55	117.93	114.60
1	A	58	C	C6-N1-C2	-5.54	118.08	120.30
1	A	129(A)	G	C4-C5-N7	5.54	113.02	110.80
1	A	353	A	N1-C6-N6	-5.54	115.27	118.60
1	A	1302	U	N1-C2-N3	5.54	118.23	114.90
1	A	1107	C	C5-C6-N1	5.54	123.77	121.00
1	A	1325	C	C5-C4-N4	-5.54	116.32	120.20
1	A	1370	G	N3-C4-N9	5.54	129.32	126.00
1	A	190(G)	G	C5-C6-N1	-5.54	108.73	111.50
1	A	1231	G	C6-C5-N7	-5.54	127.08	130.40
1	A	485	G	C5-C6-N1	-5.54	108.73	111.50
1	A	14	U	N3-C2-O2	-5.53	118.33	122.20
1	A	50	A	C8-N9-C4	5.53	108.01	105.80
1	A	559	A	C6-N1-C2	-5.53	115.28	118.60
1	A	605	U	N3-C4-O4	5.53	123.27	119.40
1	A	1442	G	C5-C6-O6	-5.53	125.28	128.60
1	A	576	G	C8-N9-C1'	-5.53	119.81	127.00
1	A	604	G	C8-N9-C4	5.53	108.61	106.40
1	A	963	G	N1-C6-O6	5.53	123.22	119.90
1	A	131	C	N3-C4-N4	-5.53	114.13	118.00
1	A	407	G	N3-C4-C5	5.53	131.36	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	854	G	N3-C2-N2	5.52	123.77	119.90
1	A	863	U	C2-N1-C1'	-5.52	111.07	117.70
1	A	1442	G	C5-C6-N1	5.52	114.26	111.50
1	A	571	U	N1-C2-O2	-5.52	118.94	122.80
1	A	760	G	N7-C8-N9	-5.52	110.34	113.10
1	A	1276	G	N1-C6-O6	5.52	123.21	119.90
1	A	489	C	C6-N1-C2	5.52	122.51	120.30
1	A	597	G	N1-C6-O6	-5.51	116.59	119.90
1	A	629	G	C4-N9-C1'	5.51	133.67	126.50
1	A	717	C	N3-C2-O2	5.51	125.76	121.90
1	A	1082	G	C5-C6-O6	-5.51	125.29	128.60
1	A	828	A	N1-C2-N3	5.51	132.06	129.30
1	A	1435	G	N3-C4-C5	5.51	131.35	128.60
1	A	1053	G	C5-N7-C8	5.50	107.05	104.30
1	A	1306	A	N9-C4-C5	-5.50	103.60	105.80
1	A	1329	A	C2-N3-C4	-5.50	107.85	110.60
1	A	238	G	C5-N7-C8	-5.50	101.55	104.30
1	A	619	U	N1-C2-N3	5.50	118.20	114.90
1	A	697	U	C5-C4-O4	5.50	129.20	125.90
1	A	1270	C	C6-N1-C2	5.50	122.50	120.30
1	A	237	C	C6-N1-C2	-5.50	118.10	120.30
1	A	1262	C	C5-C6-N1	5.50	123.75	121.00
1	A	266	G	C5-C6-N1	-5.49	108.75	111.50
1	A	27	G	N7-C8-N9	5.49	115.85	113.10
1	A	354	G	C8-N9-C4	-5.49	104.20	106.40
1	A	1196	U	N3-C2-O2	-5.49	118.36	122.20
1	A	925	G	N3-C4-N9	5.49	129.29	126.00
1	A	93	G	N3-C4-N9	5.49	129.29	126.00
1	A	190(D)	U	C5-C6-N1	-5.49	119.96	122.70
1	A	917	G	C4-C5-C6	5.49	122.09	118.80
1	A	1009	G	C8-N9-C4	-5.49	104.20	106.40
1	A	123	C	C5-C6-N1	5.49	123.74	121.00
1	A	107	G	N3-C4-N9	5.49	129.29	126.00
1	A	119	A	C5-C6-N1	5.49	120.44	117.70
1	A	1487	G	C8-N9-C4	-5.49	104.21	106.40
1	A	840	C	C2-N1-C1'	5.48	124.83	118.80
1	A	350	G	N3-C4-N9	-5.48	122.71	126.00
1	A	1088	G	N3-C4-N9	-5.48	122.71	126.00
1	A	293	G	N1-C6-O6	5.48	123.19	119.90
1	A	546	G	N1-C2-N2	-5.48	111.27	116.20
1	A	247	G	C6-C5-N7	-5.48	127.11	130.40
1	A	1520	G	C4-C5-N7	5.48	112.99	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	879	C	C2-N1-C1'	-5.48	112.78	118.80
1	A	273	A	C6-N1-C2	-5.47	115.31	118.60
1	A	929	G	N1-C6-O6	5.47	123.19	119.90
1	A	1452	C	N1-C2-O2	5.47	122.18	118.90
1	A	23	C	C4-C5-C6	5.47	120.14	117.40
1	A	228	A	N1-C6-N6	-5.47	115.32	118.60
1	A	789	U	C5-C6-N1	5.47	125.43	122.70
1	A	901	A	C5-C6-N1	-5.47	114.97	117.70
1	A	1353	G	N3-C4-C5	-5.47	125.87	128.60
1	A	282	A	C2-N3-C4	5.46	113.33	110.60
1	A	317	G	C5-C6-O6	-5.46	125.32	128.60
1	A	389	A	C4-C5-C6	5.46	119.73	117.00
1	A	550	G	N1-C2-N3	5.46	127.18	123.90
1	A	571	U	N3-C2-O2	5.46	126.03	122.20
1	A	31	G	N9-C4-C5	5.46	107.58	105.40
1	A	721	G	N3-C4-C5	-5.46	125.87	128.60
1	A	55	A	C6-N1-C2	-5.46	115.32	118.60
1	A	925	G	N1-C2-N2	-5.46	111.28	116.20
1	A	1189	C	C6-N1-C2	5.46	122.48	120.30
1	A	120	A	N1-C2-N3	5.46	132.03	129.30
1	A	329	A	N1-C6-N6	5.46	121.88	118.60
1	A	484	G	C2-N3-C4	5.46	114.63	111.90
1	A	910	C	C2-N3-C4	-5.46	117.17	119.90
1	A	289	G	N1-C2-N3	5.46	127.17	123.90
1	A	299	G	C6-C5-N7	-5.46	127.13	130.40
1	A	59	A	C5-C6-N6	-5.45	119.34	123.70
1	A	793	U	N1-C2-N3	-5.45	111.63	114.90
1	A	1240	U	N1-C2-N3	5.45	118.17	114.90
1	A	5	U	C5-C4-O4	-5.45	122.63	125.90
1	A	99	C	N3-C2-O2	-5.45	118.08	121.90
1	A	606	G	C2-N3-C4	5.45	114.62	111.90
1	A	606	G	N1-C6-O6	-5.45	116.63	119.90
1	A	778	G	C6-C5-N7	-5.45	127.13	130.40
1	A	804	U	C5-C4-O4	5.45	129.17	125.90
1	A	818	G	N3-C4-C5	5.45	131.32	128.60
1	A	661	G	C5-N7-C8	-5.45	101.58	104.30
1	A	771	G	C2-N3-C4	-5.45	109.18	111.90
1	A	1361(A)	C	N3-C4-C5	5.45	124.08	121.90
1	A	1361(A)	C	C4-C5-C6	-5.45	114.68	117.40
1	A	447	G	C8-N9-C1'	-5.44	119.93	127.00
1	A	878	G	C6-C5-N7	-5.44	127.14	130.40
1	A	1079	G	N3-C2-N2	5.44	123.71	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1455	G	N7-C8-N9	5.44	115.82	113.10
1	A	1306	A	C4-C5-C6	5.44	119.72	117.00
1	A	1421	G	N7-C8-N9	5.44	115.82	113.10
1	A	452	A	C5-C6-N1	-5.44	114.98	117.70
1	A	38	G	C8-N9-C1'	5.43	134.07	127.00
1	A	314	C	C6-N1-C2	5.43	122.47	120.30
1	A	872	A	C4-C5-N7	5.43	113.42	110.70
1	A	1104	G	N9-C4-C5	5.43	107.57	105.40
1	A	84	U	N3-C4-O4	5.43	123.20	119.40
1	A	794	A	C6-C5-N7	5.43	136.10	132.30
1	A	638	G	N1-C6-O6	5.43	123.16	119.90
1	A	1374	A	N1-C2-N3	5.43	132.01	129.30
1	A	1105	A	N7-C8-N9	5.43	116.51	113.80
1	A	45	U	C5-C4-O4	5.43	129.16	125.90
1	A	229	U	C6-N1-C2	-5.43	117.74	121.00
1	A	366	C	C2-N1-C1'	5.43	124.77	118.80
1	A	391	G	N7-C8-N9	-5.43	110.39	113.10
1	A	654	G	C4-N9-C1'	-5.43	119.45	126.50
1	A	919	A	N9-C4-C5	-5.43	103.63	105.80
2	B	12	GLU	N-CA-C	5.43	125.65	111.00
1	A	476	G	N9-C4-C5	-5.42	103.23	105.40
1	A	1413	A	C5-N7-C8	-5.42	101.19	103.90
1	A	1461	G	C8-N9-C4	5.42	108.57	106.40
1	A	1074	G	C5-C6-O6	5.42	131.85	128.60
1	A	44	G	N9-C4-C5	-5.42	103.23	105.40
1	A	477	G	N1-C6-O6	5.42	123.15	119.90
1	A	1087	G	C5-C6-N1	-5.42	108.79	111.50
1	A	1403	C	C2-N3-C4	5.42	122.61	119.90
1	A	855	G	N3-C4-C5	5.42	131.31	128.60
12	L	85	ILE	CB-CA-C	-5.42	100.76	111.60
1	A	553	A	N1-C6-N6	-5.42	115.35	118.60
1	A	830	G	C2-N3-C4	-5.42	109.19	111.90
1	A	1373	G	N3-C2-N2	5.42	123.69	119.90
1	A	1344	C	C2-N3-C4	-5.42	117.19	119.90
1	A	303	A	C8-N9-C4	5.41	107.97	105.80
1	A	504	C	C6-N1-C2	-5.41	118.13	120.30
1	A	600	C	C4-C5-C6	5.41	120.11	117.40
1	A	733	A	C2-N3-C4	-5.41	107.89	110.60
1	A	797	C	N3-C4-C5	5.41	124.06	121.90
1	A	320	C	C4-C5-C6	5.41	120.10	117.40
1	A	133	U	N3-C2-O2	-5.41	118.42	122.20
1	A	328	C	C2-N1-C1'	5.41	124.75	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	419	C	C6-N1-C2	5.41	122.46	120.30
1	A	576	G	N9-C4-C5	5.41	107.56	105.40
1	A	1432	G	N1-C6-O6	-5.40	116.66	119.90
20	T	62	LEU	CB-CG-CD2	-5.40	101.82	111.00
1	A	76	C	C2-N3-C4	-5.40	117.20	119.90
1	A	895	G	N1-C2-N2	-5.40	111.34	116.20
1	A	1406	U	N3-C4-O4	5.40	123.18	119.40
1	A	154	C	N3-C4-N4	5.40	121.78	118.00
1	A	190(F)	G	C4-N9-C1'	-5.40	119.48	126.50
1	A	947	G	N9-C4-C5	-5.40	103.24	105.40
1	A	1266	G	C4-N9-C1'	-5.40	119.48	126.50
1	A	1088	G	N3-C4-C5	5.40	131.30	128.60
1	A	175	C	C2-N3-C4	-5.39	117.20	119.90
1	A	787	A	N9-C4-C5	-5.39	103.64	105.80
1	A	76	C	N3-C4-N4	-5.39	114.23	118.00
1	A	1543	C	N1-C2-O2	5.39	122.13	118.90
1	A	296	U	C4-C5-C6	5.39	122.93	119.70
1	A	889	A	C8-N9-C4	-5.39	103.64	105.80
1	A	947	G	C6-C5-N7	-5.39	127.17	130.40
1	A	1295	G	C8-N9-C4	-5.39	104.25	106.40
1	A	129(A)	G	C8-N9-C4	5.38	108.55	106.40
1	A	663	A	N1-C6-N6	-5.38	115.37	118.60
1	A	78	G	C4-C5-C6	-5.38	115.57	118.80
1	A	718	G	C5-N7-C8	-5.38	101.61	104.30
1	A	774	G	N7-C8-N9	5.38	115.79	113.10
1	A	302	G	C8-N9-C4	5.38	108.55	106.40
1	A	47	C	N1-C2-O2	5.38	122.13	118.90
1	A	292	G	C5-C6-O6	-5.38	125.37	128.60
1	A	872	A	C4-C5-C6	5.38	119.69	117.00
1	A	963	G	N7-C8-N9	5.38	115.79	113.10
1	A	117	G	N1-C2-N2	-5.38	111.36	116.20
1	A	555	C	N3-C4-C5	5.38	124.05	121.90
1	A	245	C	N3-C4-C5	5.37	124.05	121.90
1	A	363	A	N1-C6-N6	-5.37	115.38	118.60
1	A	460	A	C4-N9-C1'	5.37	135.97	126.30
1	A	829	G	N3-C4-N9	5.37	129.22	126.00
1	A	944	G	C4-N9-C1'	5.37	133.49	126.50
1	A	38	G	C8-N9-C4	5.37	108.55	106.40
1	A	451	A	C4-C5-N7	5.37	113.39	110.70
1	A	480	U	C6-N1-C2	-5.37	117.78	121.00
1	A	664	G	N1-C6-O6	-5.37	116.68	119.90
1	A	1088	G	N3-C2-N2	-5.37	116.14	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	44	LEU	CA-CB-CG	-5.37	102.95	115.30
1	A	308	C	C6-N1-C1'	-5.37	114.36	120.80
1	A	576	G	N1-C2-N3	5.37	127.12	123.90
1	A	1179	A	N9-C4-C5	5.37	107.95	105.80
1	A	31	G	N7-C8-N9	-5.37	110.42	113.10
1	A	413	G	C5-C6-O6	-5.37	125.38	128.60
1	A	571	U	C5-C4-O4	-5.37	122.68	125.90
1	A	324	G	C5-C6-N1	-5.36	108.82	111.50
1	A	535	A	C4-C5-C6	5.36	119.68	117.00
1	A	642	A	C8-N9-C4	-5.36	103.66	105.80
1	A	645	C	C5-C6-N1	5.36	123.68	121.00
1	A	79	G	C5-C6-N1	-5.36	108.82	111.50
1	A	762	C	N3-C4-C5	5.36	124.05	121.90
1	A	363	A	N3-C4-N9	-5.36	123.11	127.40
1	A	787	A	C8-N9-C4	5.36	107.94	105.80
1	A	105	G	N1-C2-N3	5.36	127.11	123.90
1	A	451	A	C2-N3-C4	-5.36	107.92	110.60
1	A	866	C	C5-C6-N1	-5.36	118.32	121.00
1	A	74	C	N3-C4-N4	5.36	121.75	118.00
1	A	983	A	C2-N3-C4	5.36	113.28	110.60
1	A	1190	G	P-O3'-C3'	5.36	126.13	119.70
1	A	1513	A	C8-N9-C4	-5.36	103.66	105.80
1	A	329	A	N7-C8-N9	-5.35	111.12	113.80
1	A	131	C	C4-C5-C6	5.35	120.08	117.40
1	A	1116	C	N3-C4-C5	5.35	124.04	121.90
1	A	617	G	C8-N9-C1'	-5.35	120.05	127.00
1	A	913	A	C8-N9-C4	-5.35	103.66	105.80
1	A	1234	C	N1-C2-N3	-5.35	115.45	119.20
1	A	1397	C	N1-C2-N3	-5.35	115.45	119.20
1	A	1530	G	C8-N9-C4	5.35	108.54	106.40
1	A	183	G	N7-C8-N9	5.35	115.77	113.10
1	A	679	C	N3-C4-C5	5.35	124.04	121.90
1	A	760	G	C5-C6-N1	-5.35	108.83	111.50
1	A	1330	U	C2-N1-C1'	5.35	124.11	117.70
1	A	16	A	C6-N1-C2	5.34	121.81	118.60
1	A	565	U	C6-N1-C2	5.34	124.21	121.00
1	A	1486	G	N3-C4-C5	5.34	131.27	128.60
1	A	326	G	C2-N3-C4	5.34	114.57	111.90
1	A	28	G	N1-C2-N3	5.34	127.11	123.90
1	A	376	G	C4-C5-N7	-5.34	108.66	110.80
1	A	377	G	C6-C5-N7	-5.34	127.20	130.40
1	A	741	G	N7-C8-N9	-5.34	110.43	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1199	U	C6-N1-C2	-5.34	117.80	121.00
1	A	610	G	C8-N9-C1'	-5.34	120.06	127.00
1	A	1209	C	N3-C4-C5	-5.34	119.77	121.90
1	A	147	G	N9-C4-C5	-5.33	103.27	105.40
1	A	52	G	N7-C8-N9	5.33	115.77	113.10
1	A	765	G	C5-C6-N1	-5.33	108.83	111.50
1	A	1109	C	N1-C2-O2	5.33	122.10	118.90
1	A	1305	G	P-O3'-C3'	5.33	126.10	119.70
1	A	454	C	C2-N1-C1'	5.33	124.66	118.80
1	A	865	A	N1-C6-N6	-5.33	115.40	118.60
1	A	922	G	C6-N1-C2	-5.33	121.90	125.10
1	A	641	U	N1-C2-N3	5.33	118.10	114.90
1	A	866	C	C2-N3-C4	-5.33	117.24	119.90
1	A	264	U	C2-N1-C1'	-5.33	111.31	117.70
1	A	285	G	N9-C4-C5	-5.33	103.27	105.40
1	A	381	C	N1-C2-O2	5.33	122.10	118.90
1	A	727	G	N1-C6-O6	-5.33	116.70	119.90
1	A	753	A	N1-C2-N3	5.33	131.96	129.30
1	A	305	G	C4-C5-C6	5.32	121.99	118.80
1	A	826	C	C5-C6-N1	-5.32	118.34	121.00
1	A	887	G	C2-N3-C4	-5.32	109.24	111.90
1	A	600	C	C2-N3-C4	-5.32	117.24	119.90
1	A	686	U	N1-C2-N3	5.32	118.09	114.90
1	A	551	U	C6-N1-C2	5.32	124.19	121.00
1	A	1158	C	C5-C4-N4	5.32	123.92	120.20
1	A	144	G	C5-C6-N1	-5.31	108.84	111.50
1	A	186	C	N3-C2-O2	-5.31	118.18	121.90
1	A	266	G	C8-N9-C1'	5.31	133.91	127.00
1	A	794	A	N3-C4-C5	-5.31	123.08	126.80
1	A	1528	U	N1-C2-O2	5.31	126.52	122.80
1	A	1542	U	C5-C6-N1	-5.31	120.04	122.70
1	A	928	G	C6-C5-N7	-5.31	127.21	130.40
1	A	181	G	C6-C5-N7	-5.31	127.22	130.40
1	A	616	G	C4-C5-C6	5.31	121.99	118.80
1	A	812	C	C6-N1-C2	-5.31	118.18	120.30
1	A	43	C	C2-N3-C4	-5.31	117.25	119.90
1	A	1060	C	C2-N3-C4	-5.31	117.25	119.90
1	A	1390	U	C6-N1-C1'	5.31	128.63	121.20
1	A	284	G	N1-C6-O6	5.30	123.08	119.90
1	A	767	A	C6-N1-C2	-5.30	115.42	118.60
1	A	240	C	N3-C4-N4	5.30	121.71	118.00
1	A	641	U	N3-C2-O2	-5.30	118.49	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1203	C	C2-N1-C1'	5.30	124.63	118.80
1	A	186	C	N1-C2-O2	5.30	122.08	118.90
1	A	975	A	C6-N1-C2	5.30	121.78	118.60
1	A	900	A	C2-N3-C4	-5.29	107.95	110.60
1	A	183	G	C8-N9-C4	-5.29	104.28	106.40
1	A	598	U	C2-N1-C1'	-5.29	111.35	117.70
1	A	853	G	N1-C6-O6	5.29	123.08	119.90
1	A	382	A	C5-N7-C8	-5.29	101.25	103.90
1	A	851	G	C4-C5-C6	5.29	121.97	118.80
1	A	352	C	N3-C2-O2	-5.29	118.20	121.90
1	A	1069	C	N1-C2-O2	5.29	122.07	118.90
1	A	311	C	C6-N1-C2	-5.29	118.19	120.30
1	A	617	G	N1-C6-O6	5.29	123.07	119.90
1	A	62	U	C5-C6-N1	-5.29	120.06	122.70
1	A	302	G	N7-C8-N9	-5.29	110.46	113.10
1	A	353	A	C5-C6-N6	5.29	127.93	123.70
1	A	1330	U	N3-C2-O2	-5.29	118.50	122.20
1	A	1385	G	N9-C4-C5	5.29	107.52	105.40
3	C	175	LEU	CA-CB-CG	5.29	127.46	115.30
1	A	253	U	C5-C4-O4	-5.29	122.73	125.90
1	A	508	C	N3-C4-C5	5.28	124.01	121.90
1	A	1521	G	C5-C6-N1	5.28	114.14	111.50
1	A	372	C	C2-N1-C1'	5.28	124.61	118.80
1	A	547	A	C5-C6-N1	5.28	120.34	117.70
1	A	190(G)	G	C8-N9-C4	-5.28	104.29	106.40
1	A	572	A	C2-N3-C4	5.28	113.24	110.60
1	A	721	G	N1-C6-O6	5.28	123.07	119.90
1	A	130	A	C5-C6-N1	-5.28	115.06	117.70
1	A	301	G	N7-C8-N9	5.28	115.74	113.10
1	A	823	G	C8-N9-C4	5.28	108.51	106.40
1	A	1468	A	N7-C8-N9	-5.28	111.16	113.80
1	A	301	G	C8-N9-C4	-5.27	104.29	106.40
1	A	672	U	C2-N1-C1'	-5.27	111.37	117.70
1	A	718	G	N3-C4-C5	-5.27	125.96	128.60
1	A	859	A	C8-N9-C4	-5.27	103.69	105.80
1	A	1485	U	N3-C2-O2	5.27	125.89	122.20
1	A	299	G	C5-C6-N1	-5.27	108.86	111.50
1	A	329	A	N1-C2-N3	5.27	131.94	129.30
1	A	572	A	C6-N1-C2	-5.27	115.44	118.60
1	A	1329	A	C4-C5-C6	5.27	119.64	117.00
1	A	1433	A	C6-N1-C2	-5.27	115.44	118.60
17	Q	38	ARG	NE-CZ-NH2	-5.27	117.66	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	576	G	C4-C5-N7	-5.27	108.69	110.80
1	A	1266	G	N3-C4-N9	-5.27	122.84	126.00
1	A	306	G	N1-C2-N2	5.27	120.94	116.20
1	A	547	A	N9-C4-C5	-5.27	103.69	105.80
1	A	1289	A	N1-C6-N6	-5.27	115.44	118.60
1	A	281	G	N3-C2-N2	-5.27	116.21	119.90
1	A	484	G	C6-C5-N7	5.26	133.56	130.40
1	A	667	G	C6-C5-N7	-5.26	127.24	130.40
1	A	1490	C	C6-N1-C2	-5.26	118.20	120.30
1	A	1496	C	C4-C5-C6	-5.26	114.77	117.40
1	A	242	C	C5-C4-N4	-5.26	116.52	120.20
1	A	416	G	C6-C5-N7	-5.26	127.25	130.40
1	A	762	C	C5-C6-N1	5.26	123.63	121.00
1	A	1441	G	C5-C6-N1	-5.26	108.87	111.50
1	A	1454	G	C8-N9-C4	-5.26	104.30	106.40
1	A	31	G	N3-C4-N9	-5.26	122.84	126.00
1	A	262	A	C5-C6-N6	5.26	127.91	123.70
1	A	1462	G	N9-C4-C5	-5.26	103.30	105.40
1	A	177	C	N1-C2-O2	5.26	122.05	118.90
1	A	1356	G	N1-C6-O6	-5.26	116.75	119.90
1	A	1486	G	C5-C6-N1	-5.26	108.87	111.50
1	A	388	G	C8-N9-C1'	-5.25	120.17	127.00
1	A	1099	G	N3-C4-N9	-5.25	122.85	126.00
1	A	241	C	N1-C2-O2	-5.25	115.75	118.90
1	A	695	A	N1-C2-N3	5.25	131.93	129.30
1	A	1091	U	C2-N1-C1'	5.25	124.00	117.70
1	A	531	U	N1-C2-N3	5.25	118.05	114.90
1	A	913	A	P-O3'-C3'	5.25	126.00	119.70
1	A	31	G	C6-C5-N7	5.25	133.55	130.40
1	A	331	G	N1-C6-O6	5.25	123.05	119.90
1	A	500	G	N3-C4-C5	5.25	131.22	128.60
1	A	528	C	C6-N1-C2	-5.25	118.20	120.30
1	A	774	G	C5-N7-C8	-5.25	101.68	104.30
1	A	1500	A	C6-N1-C2	-5.25	115.45	118.60
1	A	642	A	N9-C4-C5	5.24	107.90	105.80
1	A	729	A	N1-C2-N3	5.24	131.92	129.30
1	A	749	C	C5-C6-N1	5.24	123.62	121.00
1	A	876	G	C5-C6-O6	-5.24	125.45	128.60
1	A	931	C	C2-N1-C1'	-5.24	113.03	118.80
11	K	98	LEU	CA-CB-CG	-5.24	103.24	115.30
1	A	945	G	N1-C2-N3	-5.24	120.75	123.90
1	A	97	G	N7-C8-N9	5.24	115.72	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	162	A	C8-N9-C4	-5.24	103.70	105.80
1	A	382	A	N7-C8-N9	5.24	116.42	113.80
1	A	755	G	C8-N9-C1'	-5.24	120.19	127.00
1	A	628	G	C2-N3-C4	5.24	114.52	111.90
1	A	858	G	N1-C2-N2	-5.24	111.49	116.20
1	A	1210	C	C5-C6-N1	5.24	123.62	121.00
1	A	908	A	C8-N9-C4	-5.24	103.71	105.80
1	A	945	G	N3-C2-N2	-5.24	116.23	119.90
1	A	1180	A	C2-N3-C4	5.24	113.22	110.60
1	A	1462	G	N3-C4-C5	5.24	131.22	128.60
1	A	924	C	C5-C6-N1	5.23	123.62	121.00
1	A	16	A	N3-C4-N9	-5.23	123.22	127.40
1	A	1416	G	C4-C5-N7	5.23	112.89	110.80
1	A	1482	G	C8-N9-C1'	-5.23	120.20	127.00
1	A	1513	A	C6-N1-C2	-5.23	115.46	118.60
1	A	254	G	N1-C2-N2	-5.23	111.49	116.20
1	A	1078	U	N1-C2-O2	5.23	126.46	122.80
1	A	713	G	N3-C4-C5	-5.23	125.99	128.60
1	A	331	G	N9-C4-C5	-5.23	103.31	105.40
1	A	1492	A	C8-N9-C4	5.23	107.89	105.80
1	A	190(H)	G	C5-C6-N1	-5.22	108.89	111.50
1	A	523	A	C5-C6-N1	-5.22	115.09	117.70
1	A	745	C	C5-C4-N4	-5.22	116.54	120.20
1	A	760	G	C8-N9-C4	5.22	108.49	106.40
1	A	870	U	C6-N1-C2	5.22	124.13	121.00
1	A	350	G	N3-C4-C5	5.22	131.21	128.60
1	A	863	U	C6-N1-C1'	5.22	128.51	121.20
1	A	629	G	N1-C2-N2	-5.22	111.50	116.20
1	A	374	A	C8-N9-C4	5.22	107.89	105.80
1	A	658	G	C8-N9-C1'	-5.22	120.22	127.00
1	A	829	G	N9-C4-C5	-5.22	103.31	105.40
1	A	971	G	N1-C6-O6	5.22	123.03	119.90
1	A	450	G	C4-C5-N7	-5.21	108.71	110.80
1	A	506	G	C4-C5-N7	5.21	112.89	110.80
1	A	821	G	C5-C6-O6	-5.21	125.47	128.60
1	A	1521	G	N3-C4-C5	-5.21	125.99	128.60
1	A	190(G)	G	C8-N9-C1'	-5.21	120.23	127.00
1	A	1475	G	N3-C2-N2	-5.21	116.25	119.90
1	A	292	G	C8-N9-C1'	-5.21	120.23	127.00
1	A	190(F)	G	N3-C4-N9	-5.21	122.88	126.00
1	A	722	A	C5-N7-C8	-5.21	101.30	103.90
1	A	1187	G	C4-C5-C6	5.21	121.92	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1312	G	N7-C8-N9	5.21	115.70	113.10
1	A	758	G	C2-N3-C4	-5.20	109.30	111.90
1	A	824	C	N1-C2-O2	-5.20	115.78	118.90
2	B	21	ARG	N-CA-C	5.20	125.05	111.00
15	O	63	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	A	321	A	N1-C6-N6	5.20	121.72	118.60
1	A	559	A	N1-C6-N6	5.20	121.72	118.60
1	A	1202	G	N3-C4-N9	5.20	129.12	126.00
1	A	1332	A	N9-C4-C5	5.20	107.88	105.80
1	A	153	C	N3-C4-N4	5.20	121.64	118.00
1	A	328	C	C5-C4-N4	5.20	123.84	120.20
1	A	1451	A	C8-N9-C4	5.20	107.88	105.80
1	A	625	G	N3-C4-N9	5.20	129.12	126.00
1	A	919	A	N1-C2-N3	-5.20	126.70	129.30
1	A	240	C	N3-C2-O2	5.20	125.54	121.90
1	A	279	A	C5-C6-N1	-5.20	115.10	117.70
1	A	574	A	C5-C6-N6	5.20	127.86	123.70
1	A	1053	G	C4-C5-N7	-5.20	108.72	110.80
1	A	84	U	C2-N1-C1'	5.19	123.93	117.70
1	A	157	G	N3-C4-C5	5.19	131.20	128.60
1	A	279	A	C4-C5-C6	5.19	119.60	117.00
1	A	281	G	N3-C4-C5	5.19	131.20	128.60
1	A	146	G	C5-C6-N1	-5.19	108.91	111.50
1	A	580	U	N1-C2-O2	-5.19	119.17	122.80
1	A	895	G	C6-C5-N7	-5.19	127.29	130.40
1	A	617	G	C6-C5-N7	-5.19	127.29	130.40
1	A	1360	A	N9-C4-C5	5.19	107.88	105.80
1	A	59	A	C6-N1-C2	-5.19	115.49	118.60
1	A	617	G	N9-C4-C5	-5.18	103.33	105.40
1	A	947	G	C8-N9-C4	5.18	108.47	106.40
1	A	138	G	N7-C8-N9	-5.18	110.51	113.10
1	A	377	G	C4-N9-C1'	5.18	133.24	126.50
1	A	888	G	N1-C2-N3	5.18	127.01	123.90
1	A	129	U	C4-C5-C6	5.18	122.81	119.70
1	A	1290	G	N1-C6-O6	5.18	123.01	119.90
1	A	47	C	N3-C4-C5	-5.18	119.83	121.90
1	A	915	A	N3-C4-C5	5.18	130.42	126.80
1	A	255	G	C4-C5-C6	5.17	121.91	118.80
1	A	812	C	N3-C2-O2	-5.17	118.28	121.90
1	A	828	A	N3-C4-C5	5.17	130.42	126.80
1	A	1234	C	N3-C4-N4	5.17	121.62	118.00
1	A	239	U	C4-C5-C6	5.17	122.80	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1059	C	C5-C6-N1	-5.17	118.41	121.00
1	A	947	G	N1-C6-O6	5.17	123.00	119.90
1	A	1338	G	N3-C2-N2	5.17	123.52	119.90
1	A	1403	C	N3-C4-N4	5.17	121.62	118.00
1	A	170	U	N3-C2-O2	5.17	125.82	122.20
1	A	1370	G	C6-C5-N7	-5.17	127.30	130.40
1	A	376	G	N9-C4-C5	5.17	107.47	105.40
1	A	909	A	C6-N1-C2	-5.17	115.50	118.60
17	Q	99	SER	N-CA-C	5.17	124.95	111.00
1	A	1084	G	C4-N9-C1'	5.17	133.22	126.50
1	A	1416	G	C6-C5-N7	-5.17	127.30	130.40
1	A	564	C	N3-C4-N4	5.16	121.61	118.00
1	A	764	C	C4-C5-C6	-5.16	114.82	117.40
1	A	869	G	C4-C5-N7	5.16	112.87	110.80
1	A	44	G	C8-N9-C1'	-5.16	120.29	127.00
1	A	869	G	C5-C6-O6	-5.16	125.50	128.60
1	A	1510	U	C6-N1-C1'	-5.16	113.97	121.20
1	A	1511	G	N1-C6-O6	-5.16	116.80	119.90
1	A	584	G	C2-N3-C4	5.16	114.48	111.90
1	A	784	C	N1-C2-N3	5.16	122.81	119.20
1	A	1196	U	C2-N1-C1'	5.16	123.89	117.70
1	A	1319	A	C5-C6-N1	-5.16	115.12	117.70
1	A	67	C	C6-N1-C2	-5.16	118.24	120.30
1	A	187	C	N3-C4-C5	-5.16	119.84	121.90
1	A	383	A	C5-C6-N6	-5.16	119.58	123.70
1	A	818	G	N3-C2-N2	-5.16	116.29	119.90
1	A	1523	G	N1-C6-O6	5.16	122.99	119.90
11	K	87	THR	CB-CA-C	-5.16	97.68	111.60
1	A	518	C	N3-C2-O2	-5.15	118.29	121.90
1	A	818	G	N1-C6-O6	5.15	122.99	119.90
1	A	1084	G	C6-N1-C2	-5.15	122.01	125.10
1	A	533	A	C8-N9-C4	-5.15	103.74	105.80
1	A	1338	G	N3-C4-C5	-5.15	126.02	128.60
1	A	309	G	C5-C6-O6	-5.15	125.51	128.60
1	A	586	C	C2-N3-C4	-5.15	117.32	119.90
1	A	1314	C	N3-C4-N4	5.15	121.61	118.00
16	P	68	ASP	CB-CG-OD1	-5.15	113.67	118.30
1	A	633	G	N3-C2-N2	5.15	123.50	119.90
1	A	795	C	N3-C4-N4	5.15	121.60	118.00
1	A	1236	A	N9-C4-C5	-5.15	103.74	105.80
1	A	1265	G	N7-C8-N9	5.15	115.67	113.10
1	A	372	C	N1-C2-O2	5.14	121.99	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	799	G	C6-C5-N7	-5.14	127.31	130.40
1	A	859	A	N7-C8-N9	5.14	116.37	113.80
1	A	1194	U	C6-N1-C2	-5.14	117.91	121.00
1	A	59	A	C5-N7-C8	-5.14	101.33	103.90
1	A	59	A	C4-C5-N7	5.14	113.27	110.70
1	A	148	G	C5-C6-N1	5.14	114.07	111.50
1	A	1111	A	N1-C6-N6	-5.14	115.52	118.60
1	A	1468	A	C4-C5-N7	-5.14	108.13	110.70
1	A	70	G	C5-C6-O6	-5.14	125.52	128.60
1	A	154	C	C5-C4-N4	-5.14	116.60	120.20
1	A	1187	G	C8-N9-C1'	-5.14	120.32	127.00
8	H	13	ILE	CG1-CB-CG2	-5.14	100.09	111.40
1	A	1455	G	C5-C6-O6	-5.14	125.52	128.60
1	A	1520	G	N3-C2-N2	-5.14	116.30	119.90
1	A	63	C	N3-C2-O2	5.14	125.50	121.90
1	A	239	U	N3-C4-C5	-5.14	111.52	114.60
1	A	256	U	C5-C4-O4	-5.14	122.82	125.90
1	A	637	G	C8-N9-C4	5.14	108.45	106.40
1	A	819	A	C5-C6-N6	5.14	127.81	123.70
1	A	1129	C	N3-C2-O2	-5.14	118.30	121.90
1	A	297	G	C2-N3-C4	-5.13	109.33	111.90
1	A	1377	A	N3-C4-C5	5.13	130.40	126.80
1	A	132	C	N3-C2-O2	-5.13	118.31	121.90
1	A	318	G	C4-C5-C6	5.13	121.88	118.80
1	A	492	G	C5-C6-N1	-5.13	108.93	111.50
1	A	577	G	C5-N7-C8	-5.13	101.73	104.30
1	A	825	G	C5-C6-N1	-5.13	108.94	111.50
1	A	1455	G	C2-N3-C4	-5.13	109.33	111.90
1	A	357	G	N7-C8-N9	-5.13	110.53	113.10
1	A	874	G	N3-C2-N2	-5.13	116.31	119.90
1	A	122	G	C6-N1-C2	5.13	128.18	125.10
1	A	1447	G	C4-C5-C6	-5.13	115.72	118.80
1	A	237	C	N1-C2-N3	5.13	122.79	119.20
1	A	1227	A	C8-N9-C4	-5.13	103.75	105.80
1	A	1348	U	N3-C4-C5	-5.13	111.52	114.60
1	A	1398	A	N1-C2-N3	5.13	131.86	129.30
1	A	894	G	C4-C5-N7	5.12	112.85	110.80
1	A	231	G	N3-C4-C5	-5.12	126.04	128.60
1	A	305	G	N7-C8-N9	5.12	115.66	113.10
1	A	523	A	N3-C4-C5	5.12	130.38	126.80
1	A	587	G	C8-N9-C4	-5.12	104.35	106.40
1	A	818	G	N1-C2-N2	5.12	120.81	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	574	A	N1-C6-N6	-5.12	115.53	118.60
1	A	781	A	C4-C5-N7	5.12	113.26	110.70
1	A	288	A	C2-N3-C4	-5.12	108.04	110.60
1	A	305	G	C5-C6-N1	-5.12	108.94	111.50
1	A	602	A	N3-C4-C5	5.12	130.38	126.80
1	A	665	A	N1-C6-N6	-5.12	115.53	118.60
1	A	9	G	C6-C5-N7	-5.11	127.33	130.40
1	A	157	G	C2-N3-C4	-5.11	109.34	111.90
1	A	670	G	C4-C5-C6	5.11	121.87	118.80
1	A	760	G	N3-C4-C5	5.11	131.16	128.60
1	A	1460	A	C4-C5-N7	5.11	113.26	110.70
1	A	1521	G	C6-N1-C2	-5.11	122.03	125.10
1	A	375	U	N1-C2-N3	5.11	117.96	114.90
1	A	416	G	C4-C5-N7	5.11	112.84	110.80
1	A	572	A	C8-N9-C1'	5.11	136.89	127.70
1	A	794	A	N1-C6-N6	-5.11	115.54	118.60
1	A	1312	G	C6-C5-N7	-5.11	127.34	130.40
1	A	586	C	C4-C5-C6	5.11	119.95	117.40
1	A	1306	A	C6-C5-N7	-5.11	128.73	132.30
1	A	902	G	C8-N9-C4	5.10	108.44	106.40
1	A	79	G	N3-C2-N2	-5.10	116.33	119.90
1	A	975	A	N3-C4-C5	5.10	130.37	126.80
1	A	995	C	C2-N1-C1'	5.10	124.41	118.80
1	A	1505	G	N3-C4-C5	-5.10	126.05	128.60
1	A	1364	U	N1-C2-O2	5.10	126.37	122.80
1	A	1371	G	N3-C4-C5	-5.10	126.05	128.60
1	A	1452	C	C5-C4-N4	-5.10	116.63	120.20
1	A	646	U	C4-C5-C6	5.10	122.76	119.70
1	A	907	A	N1-C2-N3	5.10	131.85	129.30
1	A	185	A	N9-C4-C5	-5.10	103.76	105.80
1	A	52	G	C5-C6-O6	-5.09	125.54	128.60
1	A	325	A	C6-N1-C2	-5.09	115.54	118.60
1	A	1437	C	C2-N3-C4	5.09	122.45	119.90
1	A	883	C	C6-N1-C2	-5.09	118.26	120.30
1	A	1083	U	N3-C4-O4	5.09	122.96	119.40
1	A	1468	A	C5-N7-C8	5.09	106.44	103.90
1	A	257	G	N1-C6-O6	5.08	122.95	119.90
1	A	729	A	C4-C5-N7	5.08	113.24	110.70
1	A	190(F)	G	C8-N9-C1'	5.08	133.61	127.00
1	A	1435	G	C5-C6-N1	-5.08	108.96	111.50
1	A	111	G	C8-N9-C1'	5.08	133.60	127.00
1	A	660	G	C5-C6-O6	-5.08	125.55	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	666	G	C8-N9-C1'	-5.08	120.39	127.00
1	A	1434	A	C6-C5-N7	-5.08	128.75	132.30
1	A	9	G	C5-C6-O6	-5.08	125.55	128.60
1	A	331	G	C4-N9-C1'	5.08	133.10	126.50
1	A	724	G	C8-N9-C4	5.08	108.43	106.40
1	A	119	A	C8-N9-C4	-5.07	103.77	105.80
1	A	624	C	C5-C4-N4	-5.07	116.65	120.20
1	A	946	A	N9-C4-C5	5.07	107.83	105.80
1	A	1250	A	C4-C5-C6	5.07	119.54	117.00
1	A	1502	A	N1-C2-N3	5.07	131.84	129.30
1	A	145	G	N1-C6-O6	5.07	122.94	119.90
1	A	389	A	N1-C6-N6	-5.07	115.56	118.60
1	A	833	U	C6-N1-C1'	5.07	128.30	121.20
1	A	874	G	C4-C5-C6	5.07	121.84	118.80
1	A	901	A	N3-C4-N9	-5.07	123.35	127.40
1	A	557	G	N1-C2-N3	5.06	126.94	123.90
9	I	56	LEU	CA-CB-CG	5.06	126.95	115.30
1	A	573	A	N7-C8-N9	5.06	116.33	113.80
1	A	257	G	N3-C2-N2	5.06	123.44	119.90
1	A	1079	G	N3-C4-C5	-5.06	126.07	128.60
18	R	44	LEU	CB-CG-CD2	-5.06	102.40	111.00
1	A	760	G	N3-C4-N9	-5.06	122.97	126.00
1	A	292	G	C6-C5-N7	-5.06	127.37	130.40
1	A	635	G	C8-N9-C4	5.06	108.42	106.40
1	A	1195	C	C5-C4-N4	-5.06	116.66	120.20
1	A	1399	C	C2-N3-C4	-5.05	117.37	119.90
1	A	1515	C	C5-C4-N4	-5.05	116.66	120.20
1	A	1094	G	C4-C5-N7	5.05	112.82	110.80
1	A	1414	U	N1-C2-N3	5.05	117.93	114.90
1	A	123	C	C2-N3-C4	5.05	122.43	119.90
1	A	916	G	C5-N7-C8	-5.05	101.77	104.30
1	A	648	A	C6-N1-C2	-5.05	115.57	118.60
1	A	866	C	N3-C4-C5	5.05	123.92	121.90
1	A	902	G	C5-C6-N1	5.05	114.02	111.50
1	A	522	C	C2-N1-C1'	-5.05	113.25	118.80
1	A	881	G	C4-C5-C6	5.05	121.83	118.80
1	A	1416	G	C5-C6-O6	-5.05	125.57	128.60
1	A	1455	G	C8-N9-C4	-5.05	104.38	106.40
1	A	890	G	N7-C8-N9	-5.04	110.58	113.10
1	A	1386	G	N7-C8-N9	-5.04	110.58	113.10
1	A	752	G	N3-C4-N9	-5.04	122.97	126.00
1	A	1325	C	N3-C4-N4	5.04	121.53	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1370	G	C2-N3-C4	5.04	114.42	111.90
1	A	743	U	C4-C5-C6	5.04	122.72	119.70
1	A	14	U	C5-C4-O4	5.04	128.92	125.90
1	A	1373	G	C8-N9-C1'	-5.04	120.45	127.00
1	A	893	C	C6-N1-C2	-5.04	118.28	120.30
1	A	895	G	C4-N9-C1'	5.04	133.05	126.50
1	A	1339	A	C6-C5-N7	5.04	135.82	132.30
1	A	363	A	N9-C4-C5	5.03	107.81	105.80
1	A	5	U	C5-C6-N1	5.03	125.22	122.70
1	A	62	U	C4-C5-C6	5.03	122.72	119.70
1	A	1502	A	C4-N9-C1'	5.03	135.35	126.30
1	A	1543	C	C5-C6-N1	5.03	123.51	121.00
1	A	292	G	C5-C6-N1	-5.03	108.99	111.50
1	A	481	G	C2-N3-C4	5.03	114.41	111.90
1	A	52	G	N1-C2-N2	-5.03	111.68	116.20
1	A	530	G	C8-N9-C1'	-5.02	120.47	127.00
1	A	665	A	C6-N1-C2	-5.02	115.59	118.60
1	A	695	A	C5-N7-C8	-5.02	101.39	103.90
1	A	748	C	C6-N1-C2	-5.02	118.29	120.30
1	A	376	G	N3-C2-N2	-5.02	116.39	119.90
1	A	761	G	N9-C4-C5	-5.02	103.39	105.40
1	A	309	G	C6-N1-C2	-5.02	122.09	125.10
1	A	24	U	C2-N3-C4	-5.02	123.99	127.00
1	A	1172	C	C6-N1-C2	5.02	122.31	120.30
1	A	622	A	N7-C8-N9	-5.02	111.29	113.80
1	A	477	G	C5-C6-N1	-5.01	108.99	111.50
1	A	915	A	C8-N9-C4	5.01	107.81	105.80
1	A	235	C	C5-C6-N1	-5.01	118.49	121.00
1	A	608	A	N9-C4-C5	5.01	107.81	105.80
1	A	80	G	N7-C8-N9	5.01	115.61	113.10
1	A	130	A	C6-N1-C2	-5.01	115.59	118.60
1	A	1058	G	C4-C5-N7	-5.01	108.80	110.80
1	A	1062	U	N3-C4-O4	-5.01	115.89	119.40
1	A	306	G	N1-C6-O6	5.01	122.91	119.90
1	A	280	C	C5-C4-N4	5.01	123.71	120.20
1	A	507	C	N3-C4-C5	5.01	123.90	121.90
1	A	656	C	N3-C4-C5	5.01	123.90	121.90
1	A	679	C	N1-C2-O2	5.01	121.91	118.90
1	A	852	G	N1-C2-N3	5.01	126.91	123.90
1	A	400	C	C5-C6-N1	-5.01	118.50	121.00
1	A	125	U	C5-C6-N1	-5.00	120.20	122.70
1	A	125	U	N1-C2-N3	5.00	117.90	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	190(G)	G	C4-C5-N7	5.00	112.80	110.80
1	A	553	A	N7-C8-N9	-5.00	111.30	113.80
1	A	628	G	C4-N9-C1'	5.00	133.00	126.50
1	A	762	C	N3-C4-N4	5.00	121.50	118.00
1	A	1365	G	N3-C2-N2	-5.00	116.40	119.90
1	A	150	C	C5-C4-N4	-5.00	116.70	120.20
1	A	322	C	N3-C4-C5	-5.00	119.90	121.90
1	A	829	G	C8-N9-C1'	-5.00	120.50	127.00

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	11	LEU	Peptide
2	B	77	ALA	Peptide
2	B	8	LYS	Peptide
3	C	166	GLU	Peptide
3	C	179	ARG	Peptide
3	C	24	ALA	Peptide
4	D	2	GLY	Peptide
4	D	28	SER	Peptide
8	H	27	PRO	Peptide
8	H	90	GLY	Peptide
10	J	86	MET	Peptide
10	J	90	LEU	Peptide
12	L	24	VAL	Peptide
12	L	27	LEU	Peptide
12	L	91	LYS	Peptide
15	O	2	PRO	Peptide
17	Q	13	ASP	Peptide
18	R	86	VAL	Peptide
20	T	93	GLU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32507	0	16434	989	0
2	B	1900	0	1951	109	0
3	C	1612	0	1677	103	0
4	D	1703	0	1763	90	0
5	E	1146	0	1207	63	0
6	F	843	0	857	50	0
7	G	1257	0	1296	63	0
8	H	1116	0	1177	83	0
9	I	1010	0	1037	69	0
10	J	792	0	835	54	0
11	K	864	0	881	48	0
12	L	972	0	1058	49	0
13	M	937	0	995	50	0
14	N	492	0	529	45	0
15	O	729	0	768	48	0
16	P	700	0	720	39	0
17	Q	823	0	893	59	0
18	R	574	0	644	38	0
19	S	647	0	673	33	0
20	T	763	0	861	41	0
21	U	208	0	221	18	0
22	A	40	0	37	5	0
23	A	249	0	0	0	0
23	B	2	0	0	0	0
23	D	1	0	0	0	0
23	E	1	0	0	0	0
23	H	4	0	0	0	0
23	J	1	0	0	0	0
23	M	2	0	0	0	0
23	P	2	0	0	0	0
23	Q	2	0	0	0	0
23	S	1	0	0	0	0
23	T	2	0	0	0	0
24	D	1	0	0	0	0
24	N	1	0	0	0	0
25	A	369	0	0	20	0
25	D	1	0	0	0	0
25	E	6	0	0	0	0
25	G	1	0	0	0	0
25	L	1	0	0	0	0
25	P	1	0	0	0	0
25	Q	4	0	0	0	0
25	T	2	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	52289	0	36514	1932	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

All (1932) 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:1433:A:N7	1:A:1467:G:N2	2.15	0.95
12:L:24:VAL:HG12	12:L:26:ALA:H	1.33	0.93
17:Q:29:HIS:CD2	17:Q:32:TYR:H	1.88	0.92
1:A:1240:U:OP1	7:G:119:ARG:NH2	2.02	0.92
19:S:11:VAL:HG22	19:S:39:THR:HB	1.49	0.92
10:J:15:THR:HG22	10:J:94:VAL:HG13	1.54	0.90
1:A:1249:C:O2'	9:I:73:GLN:NE2	2.05	0.90
1:A:427:U:OP1	4:D:13:ARG:NH2	2.05	0.89
10:J:38:ILE:HD11	10:J:71:LEU:HB2	1.54	0.89
1:A:279:A:OP2	17:Q:95:TYR:OH	1.90	0.89
9:I:126:SER:OG	9:I:127:LYS:N	2.06	0.88
1:A:1061:G:H1	1:A:1195:C:H42	1.20	0.88
1:A:1316:G:N2	1:A:1319:A:OP2	2.07	0.87
3:C:150:LYS:HB3	3:C:201:TYR:HB2	1.57	0.85
1:A:1195:C:H3'	1:A:1196:U:H5"	1.55	0.85
1:A:310:G:OP2	16:P:27:LYS:NZ	2.09	0.85
7:G:155:ARG:HA	7:G:155:ARG:HH11	1.42	0.84
8:H:82:HIS:HE1	8:H:84:ARG:HB2	1.42	0.84
1:A:1055:A:O2'	3:C:156:ARG:NH1	2.10	0.84
1:A:384:G:H2'	1:A:385:C:C6	2.13	0.83
1:A:1338:G:H2'	1:A:1339:A:C8	2.14	0.83
8:H:69:ARG:NH2	8:H:75:ARG:O	2.12	0.82
2:B:109:SER:HA	2:B:112:VAL:HG23	1.61	0.82
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.60	0.82
17:Q:29:HIS:HD2	17:Q:32:TYR:H	1.26	0.82
1:A:986:A:O2'	19:S:52:TYR:OH	1.98	0.82
11:K:57:THR:HG23	11:K:60:ALA:H	1.44	0.81
8:H:9:MET:HG3	8:H:26:VAL:HG21	1.60	0.81
1:A:1112:C:H1'	3:C:179:ARG:HH22	1.45	0.81
1:A:869:G:N7	25:A:2219:HOH:O	2.12	0.81
1:A:1055:A:N7	1:A:1200:C:N4	2.29	0.81
3:C:153:VAL:HG12	3:C:154:SER:H	1.46	0.80
12:L:25:PRO:HB3	12:L:27:LEU:HD22	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1047:G:H5"	14:N:4:LYS:HD3	1.63	0.80
1:A:407:G:OP1	4:D:115:ARG:NH1	2.15	0.80
1:A:517:G:N1	1:A:533:A:OP2	2.13	0.80
13:M:91:ARG:HB3	13:M:98:VAL:HG22	1.63	0.80
1:A:1257:U:H4'	1:A:1258:G:O5'	1.78	0.79
1:A:1009:G:H1	1:A:1020:U:H3	1.28	0.79
4:D:13:ARG:HD2	4:D:38:TYR:O	1.82	0.79
3:C:14:ILE:HB	3:C:15:THR:HG23	1.64	0.79
1:A:1101:A:H4'	1:A:1102:A:O5'	1.82	0.79
1:A:1125:U:OP2	1:A:1145:C:N4	2.16	0.79
1:A:1347:G:H3'	9:I:108:VAL:O	1.82	0.78
1:A:1130:A:H4'	9:I:20:ARG:HH22	1.48	0.78
11:K:40:ILE:HG22	11:K:41:THR:HG23	1.65	0.78
15:O:25:THR:HG21	15:O:70:LEU:HD23	1.65	0.78
1:A:190(A):C:H42	1:A:190(H):G:H1	1.32	0.77
1:A:1309:G:OP2	13:M:99:ARG:NH2	2.17	0.77
5:E:11:ILE:HB	5:E:31:LEU:HB3	1.67	0.77
1:A:1412:C:H2'	1:A:1413:A:C8	2.19	0.77
1:A:91:C:C5	1:A:92:C:H5	2.03	0.77
1:A:337:C:H2'	1:A:338:A:H8	1.49	0.77
1:A:967:5MC:H4'	9:I:128:ARG:HG3	1.66	0.76
1:A:1368:G:H5"	9:I:112:LYS:HB3	1.68	0.76
15:O:33:THR:HG23	15:O:63:ARG:NH1	2.00	0.76
6:F:33:TYR:CD1	6:F:75:LEU:HA	2.20	0.76
3:C:92:ALA:HB2	3:C:99:VAL:HG12	1.67	0.76
12:L:27:LEU:C	12:L:29:GLY:H	1.87	0.75
7:G:18:TYR:HD2	7:G:59:LEU:HD13	1.50	0.75
3:C:27:LYS:O	3:C:30:ARG:NH2	2.19	0.75
1:A:92:C:O2'	1:A:93:G:H5'	1.85	0.75
8:H:2:LEU:HD23	8:H:3:THR:N	2.02	0.75
3:C:17:ASP:O	3:C:54:ARG:NH2	2.19	0.75
4:D:64:LEU:HA	4:D:67:ILE:HD12	1.68	0.75
1:A:1435:G:H2'	1:A:1436:U:C6	2.22	0.75
1:A:1369:C:H2'	1:A:1370:G:C8	2.22	0.74
1:A:1128:C:O2'	1:A:1130:A:OP2	2.04	0.74
1:A:1113:C:H42	1:A:1187:G:H1	1.34	0.74
8:H:114:THR:HB	8:H:116:LYS:H	1.50	0.74
1:A:1073:U:OP2	5:E:57:LYS:NZ	2.15	0.74
10:J:47:PHE:HB3	14:N:34:TYR:HE2	1.52	0.74
9:I:108:VAL:HG12	9:I:109:VAL:H	1.52	0.73
1:A:1368:G:O2'	10:J:46:ARG:NH2	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:15:GLU:OE2	4:D:59:ARG:NH2	2.20	0.73
1:A:474:G:H2'	1:A:475:G:H8	1.52	0.73
1:A:1285:A:H4'	1:A:1286:A:O5'	1.88	0.73
7:G:27:ILE:HD12	7:G:40:ALA:HA	1.71	0.73
1:A:1504:G:OP1	1:A:1507:A:H4'	1.88	0.73
15:O:6:GLU:HA	15:O:9:GLN:HB2	1.69	0.73
7:G:15:ASP:HB3	7:G:19:GLY:H	1.54	0.73
1:A:793:U:O2'	1:A:794:A:O5'	2.07	0.73
2:B:158:LEU:H	2:B:158:LEU:HD12	1.54	0.73
10:J:9:ARG:HH21	10:J:97:GLU:HG3	1.53	0.72
3:C:58:GLU:H	3:C:65:ALA:HB3	1.54	0.72
13:M:22:ILE:HG22	13:M:23:TYR:H	1.53	0.72
13:M:75:ALA:HA	13:M:78:ILE:HD12	1.71	0.72
1:A:1342:C:H2'	1:A:1343:G:H8	1.54	0.72
11:K:121:PRO:HG2	11:K:126:ARG:HG2	1.72	0.72
3:C:88:ARG:HA	3:C:91:LEU:HD23	1.71	0.72
12:L:87:GLY:HA2	12:L:98:TYR:HA	1.71	0.72
3:C:188:LEU:HD21	3:C:195:VAL:HG13	1.71	0.72
3:C:48:TYR:HA	3:C:52:LEU:HD23	1.70	0.72
1:A:1086:U:H3	1:A:1099:G:H22	1.35	0.72
6:F:33:TYR:HD1	6:F:75:LEU:HA	1.52	0.72
2:B:213:LEU:HD23	2:B:214:ILE:HD13	1.72	0.71
16:P:57:ARG:HG3	16:P:79:VAL:HG12	1.72	0.71
11:K:43:SER:HB2	11:K:47:VAL:HG11	1.71	0.71
1:A:926:G:N2	1:A:1542:U:OP1	2.23	0.71
2:B:205:ASP:OD1	2:B:206:ASP:N	2.24	0.71
1:A:1059:C:N4	1:A:1198:G:O6	2.14	0.71
1:A:91:C:C6	1:A:92:C:H5	2.08	0.71
1:A:1347:G:O2'	1:A:1348:U:O5'	2.08	0.71
1:A:547:A:OP2	4:D:2:GLY:N	2.24	0.71
10:J:63:PHE:HB3	14:N:57:ARG:O	1.91	0.71
1:A:827:U:H5'	1:A:828:A:OP2	1.92	0.70
18:R:73:ALA:HB3	18:R:79:LEU:HD12	1.73	0.70
1:A:750:G:H1'	15:O:23:GLY:H	1.56	0.70
1:A:1057:G:H5"	3:C:154:SER:HB2	1.73	0.70
8:H:26:VAL:HG13	8:H:59:LEU:HB2	1.73	0.70
14:N:18:VAL:HG22	14:N:19:ARG:HD2	1.74	0.70
1:A:1234:C:H1'	1:A:1364:U:O2	1.91	0.70
20:T:56:MET:HE2	20:T:85:MET:HA	1.73	0.70
4:D:22:LYS:HB2	4:D:26:CYS:SG	2.31	0.70
8:H:4:ASP:OD2	8:H:85:ARG:NH1	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:26:GLU:HG3	15:O:81:LEU:HG	1.74	0.70
1:A:1175:G:H2'	1:A:1176:A:C8	2.26	0.70
1:A:1200:C:O2	1:A:1205:U:N3	2.25	0.69
1:A:992:U:O2'	1:A:993:G:OP2	2.10	0.69
1:A:716:A:H1'	11:K:118:GLY:HA2	1.73	0.69
15:O:70:LEU:HB3	15:O:78:TYR:HB2	1.74	0.69
1:A:337:C:H2'	1:A:338:A:C8	2.28	0.69
1:A:1111:A:H61	3:C:177:THR:HG22	1.57	0.69
6:F:69:GLU:N	6:F:69:GLU:OE1	2.24	0.69
1:A:964:A:O2'	10:J:55:LYS:NZ	2.16	0.69
3:C:5:ILE:HD11	3:C:10:PHE:HD2	1.55	0.69
1:A:1347:G:H1'	1:A:1348:U:H5	1.57	0.69
21:U:5:ASP:HB3	21:U:8:THR:OG1	1.92	0.69
1:A:1158:C:N3	1:A:1181:G:N2	2.41	0.69
15:O:12:ILE:HG12	15:O:31:LEU:HD11	1.75	0.69
3:C:156:ARG:HB3	3:C:196:LEU:HD22	1.73	0.69
1:A:93:G:C2	1:A:95:U:C2	2.81	0.69
1:A:1400:5MC:H3'	1:A:1401:G:H5'	1.75	0.69
8:H:38:ILE:HD13	8:H:41:ARG:NH2	2.08	0.69
1:A:1090:U:H2'	1:A:1091:U:H6	1.57	0.69
1:A:718:G:C8	1:A:718:G:H5"	2.28	0.69
1:A:1397:C:O2'	1:A:1398:A:OP1	2.07	0.69
1:A:80:G:H22	1:A:89:C:H42	1.40	0.69
1:A:485:G:O2'	1:A:486:U:OP2	2.10	0.69
9:I:48:GLU:OE1	9:I:51:ARG:NH1	2.23	0.69
1:A:93:G:H2'	1:A:95:U:C6	2.28	0.69
9:I:21:PRO:HA	9:I:59:PHE:HA	1.75	0.69
7:G:22:LEU:HD23	7:G:62:PHE:HE2	1.58	0.68
17:Q:29:HIS:HD2	17:Q:32:TYR:N	1.91	0.68
14:N:16:PHE:HB2	14:N:19:ARG:HD3	1.75	0.68
11:K:101:SER:OG	11:K:103:LEU:N	2.26	0.68
18:R:59:SER:H	18:R:62:GLU:HB2	1.58	0.68
13:M:59:TYR:O	13:M:63:THR:OG1	2.10	0.68
11:K:90:GLY:HA2	11:K:93:GLN:HB2	1.76	0.68
12:L:53:ARG:NH1	12:L:92:0TD:OD2	2.27	0.68
1:A:112:G:C2'	1:A:113:G:H5'	2.24	0.68
1:A:1130:A:H4'	9:I:20:ARG:NH2	2.09	0.68
1:A:250:A:H4'	1:A:251:G:O5'	1.94	0.68
17:Q:31:LEU:HD23	17:Q:32:TYR:CE2	2.29	0.68
1:A:9:G:OP1	5:E:122:GLU:HG3	1.94	0.68
1:A:28:G:O2'	1:A:296:U:OP1	2.10	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:838:G:H2'	1:A:839:U:H5"	1.74	0.68
1:A:1349:A:OP2	9:I:118:LYS:HD3	1.94	0.68
1:A:1278:U:H4'	1:A:1279:A:N3	2.10	0.67
2:B:132:LYS:NZ	2:B:135:GLN:OE1	2.20	0.67
1:A:1510:U:H2'	1:A:1511:G:C8	2.30	0.67
22:A:1601:SRY:H12	22:A:1601:SRY:O63	1.95	0.67
17:Q:62:SER:OG	17:Q:72:ARG:HG2	1.94	0.67
1:A:345:C:H6	1:A:345:C:OP2	1.77	0.67
1:A:21:G:H2'	1:A:22:G:C8	2.29	0.67
1:A:90:U:C4	1:A:91:C:N4	2.62	0.67
1:A:90:U:O4	1:A:91:C:N4	2.27	0.67
7:G:16:LEU:HD23	9:I:42:ARG:HG2	1.75	0.67
5:E:110:LEU:HD13	5:E:118:ILE:HD13	1.77	0.67
1:A:679:C:H2'	1:A:680:C:H6	1.60	0.67
17:Q:38:ARG:HD2	17:Q:38:ARG:N	2.09	0.67
1:A:1356:G:H2'	1:A:1357:A:C8	2.30	0.67
11:K:93:GLN:HA	11:K:96:ARG:HD3	1.76	0.67
14:N:24:CYS:HB3	14:N:33:VAL:HG12	1.75	0.67
3:C:39:ILE:HD12	3:C:57:ILE:HD13	1.77	0.67
2:B:101:MET:HA	2:B:108:ILE:HG13	1.77	0.66
1:A:1442:G:N2	1:A:1447:G:N7	2.37	0.66
1:A:1492:A:H2'	1:A:1493:A:H4'	1.77	0.66
1:A:819:A:H8	1:A:819:A:H5'	1.60	0.66
1:A:992:U:H3	1:A:1044:A:H62	1.44	0.66
15:O:12:ILE:HD11	15:O:31:LEU:HD21	1.78	0.66
9:I:8:GLY:HA2	9:I:79:LEU:HD12	1.77	0.66
1:A:1305:G:H5"	21:U:4:GLY:HA3	1.77	0.66
13:M:19:LEU:HD21	13:M:56:LEU:HD11	1.78	0.66
1:A:914:A:OP1	22:A:1601:SRY:HI33	1.94	0.66
14:N:40:CYS:HB3	14:N:43:CYS:SG	2.35	0.66
1:A:484:G:O2'	1:A:485:G:OP2	2.11	0.66
1:A:1147:C:O2	9:I:16:ARG:NH2	2.26	0.66
1:A:1367:C:H5'	10:J:60:ARG:NH2	2.11	0.66
6:F:67:MET:HB2	6:F:68:PRO:HD2	1.77	0.66
7:G:70:LYS:HG2	7:G:96:GLN:HB3	1.78	0.66
13:M:19:LEU:O	13:M:22:ILE:HG13	1.94	0.66
1:A:1191:A:OP1	3:C:3:ASN:ND2	2.29	0.66
1:A:902:G:H2'	1:A:903:G:H8	1.59	0.66
10:J:49:VAL:HG13	14:N:41:ARG:HB2	1.76	0.66
1:A:1181:G:O2'	1:A:1182:G:O4'	2.12	0.66
3:C:110:ASN:HD22	3:C:140:ARG:HB3	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:67:THR:HG22	16:P:69:THR:H	1.60	0.66
1:A:1376:U:OP1	7:G:98:SER:OG	2.08	0.66
1:A:78:G:N1	1:A:92:C:C4	2.64	0.66
1:A:1118:C:H1'	1:A:1179:A:C4	2.30	0.66
13:M:11:ARG:HA	13:M:45:VAL:HG11	1.77	0.66
10:J:8:LEU:HD13	10:J:20:ALA:HB2	1.76	0.65
7:G:18:TYR:CD2	7:G:59:LEU:HD13	2.30	0.65
1:A:1243:C:OP2	21:U:10:ARG:NH2	2.29	0.65
3:C:131:ARG:HA	3:C:134:ILE:HD12	1.78	0.65
3:C:93:LYS:HG2	3:C:94:LEU:HD22	1.77	0.65
1:A:916:G:H2'	1:A:917:G:H8	1.62	0.65
1:A:946:A:H2'	1:A:947:G:C8	2.30	0.65
1:A:1201:A:H4'	1:A:1202:G:H5'	1.78	0.65
1:A:1323:G:OP2	19:S:3:ARG:NH1	2.29	0.65
19:S:16:LEU:HA	19:S:19:VAL:HG12	1.77	0.65
21:U:9:ARG:HH22	21:U:23:PRO:HD2	1.61	0.65
3:C:83:ARG:O	3:C:87:LEU:HB2	1.97	0.65
7:G:26:PHE:HD1	7:G:101:LEU:HD22	1.61	0.65
14:N:21:TYR:HB2	14:N:23:ARG:HG2	1.79	0.65
16:P:75:ARG:HB2	16:P:80:PHE:CD1	2.30	0.65
2:B:132:LYS:HA	2:B:135:GLN:HB3	1.77	0.65
1:A:617:G:H1	1:A:623:C:H42	1.44	0.65
6:F:32:ASN:ND2	6:F:32:ASN:O	2.27	0.65
8:H:82:HIS:CE1	8:H:84:ARG:HB2	2.27	0.65
1:A:1343:G:H2'	1:A:1344:C:C6	2.32	0.65
1:A:144:G:H1	1:A:178:C:H42	1.43	0.65
1:A:1513:A:N6	25:A:2057:HOH:O	2.30	0.65
1:A:1255:G:O2'	1:A:1258:G:N3	2.30	0.65
16:P:75:ARG:HB2	16:P:80:PHE:HD1	1.62	0.65
1:A:263:A:OP2	20:T:79:ARG:NH1	2.29	0.65
2:B:97:TRP:HZ2	2:B:102:LEU:HD13	1.62	0.64
19:S:18:LYS:O	19:S:22:LEU:HB2	1.97	0.64
6:F:2:ARG:O	6:F:66:GLU:HA	1.98	0.64
1:A:1143:G:H2'	1:A:1144:G:H8	1.61	0.64
17:Q:75:ARG:HB2	17:Q:75:ARG:HH11	1.63	0.64
12:L:113:ARG:HH22	12:L:116:SER:H	1.45	0.64
2:B:209:ARG:HH11	2:B:209:ARG:HG3	1.63	0.64
1:A:93:G:N2	1:A:95:U:H1'	2.12	0.64
1:A:414:A:OP2	1:A:428:G:N2	2.20	0.64
1:A:1496:C:O2'	1:A:1497:G:H5"	1.98	0.64
1:A:1391:U:H2'	1:A:1392:G:C8	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:131:PRO:HG2	2:B:134:GLU:HG3	1.80	0.64
9:I:97:LYS:HB2	9:I:102:LEU:HD12	1.80	0.64
3:C:167:TRP:HE3	3:C:168:ALA:N	1.95	0.64
1:A:243:A:H4'	1:A:244:U:O5'	1.98	0.64
1:A:679:C:H2'	1:A:680:C:C6	2.33	0.63
7:G:90:GLU:HG2	7:G:91:VAL:H	1.63	0.63
17:Q:29:HIS:CG	17:Q:30:PRO:HD2	2.33	0.63
1:A:1342:C:H2'	1:A:1343:G:C8	2.34	0.63
1:A:839:U:H5'	1:A:840:C:H5	1.64	0.63
17:Q:18:THR:HG23	17:Q:69:LYS:HE3	1.79	0.63
1:A:184:G:H2'	1:A:185:A:H8	1.63	0.63
3:C:58:GLU:HB3	10:J:92:THR:HG21	1.81	0.63
1:A:718:G:H8	1:A:718:G:H5"	1.63	0.63
1:A:945:G:O6	1:A:1236:A:N1	2.31	0.63
8:H:103:VAL:HG12	8:H:108:GLY:HA3	1.79	0.63
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.34	0.63
9:I:25:LYS:HG3	9:I:60:ASP:OD1	1.98	0.63
1:A:1442:G:N7	1:A:1446:A:N6	2.47	0.63
1:A:434:U:H2'	1:A:435:C:C6	2.34	0.63
1:A:1128:C:OP1	9:I:66:ARG:NH1	2.30	0.63
1:A:837:G:H1	1:A:849:C:H42	1.47	0.63
1:A:1417:G:O2'	1:A:1483:A:N6	2.31	0.63
1:A:1359:C:OP2	14:N:35:ARG:NH1	2.31	0.63
18:R:30:ASP:HB3	18:R:33:ASP:HB2	1.80	0.63
2:B:142:LEU:HD13	2:B:146:GLN:HE22	1.63	0.63
4:D:68:TYR:OH	4:D:98:GLU:OE1	2.11	0.63
10:J:36:GLY:HA2	10:J:72:VAL:HG13	1.79	0.63
1:A:802:A:H2'	1:A:803:G:O4'	1.99	0.62
5:E:60:TYR:CE1	5:E:64:ARG:HD2	2.34	0.62
1:A:633:G:H2'	1:A:634:C:C6	2.34	0.62
5:E:65:ASN:ND2	5:E:65:ASN:O	2.32	0.62
1:A:795:C:H5"	1:A:796:C:OP2	1.99	0.62
1:A:1358:U:O2'	1:A:1359:C:OP1	2.17	0.62
1:A:481:G:HO2'	1:A:482:A:H8	1.43	0.62
2:B:21:ARG:HA	2:B:39:ILE:HA	1.82	0.62
1:A:1251:A:H4'	9:I:12:GLU:OE2	1.99	0.62
1:A:1286:A:H2'	1:A:1287:A:H4'	1.79	0.62
1:A:1255:G:O2'	1:A:1258:G:H1'	1.99	0.62
1:A:474:G:H2'	1:A:475:G:C8	2.35	0.62
4:D:31:CYS:C	4:D:33:MET:H	2.03	0.62
1:A:501:C:H2'	1:A:502:G:C8	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:G:H2'	1:A:300:A:C8	2.35	0.62
12:L:27:LEU:C	12:L:29:GLY:N	2.53	0.62
1:A:1255:G:H2'	1:A:1279:A:H61	1.64	0.62
15:O:33:THR:HA	15:O:63:ARG:HH11	1.64	0.62
2:B:12:GLU:HG2	2:B:213:LEU:HD22	1.80	0.62
1:A:1004:A:H5'	1:A:1025:U:H3	1.65	0.62
1:A:190(E):U:O2'	17:Q:63:ARG:NH2	2.32	0.62
1:A:235:C:H5'	17:Q:70:ARG:HG2	1.80	0.62
19:S:80:TYR:CE1	19:S:81:ARG:HB3	2.34	0.62
1:A:1420:C:H2'	1:A:1421:G:H8	1.65	0.62
1:A:1068:G:H8	1:A:1068:G:OP2	1.82	0.62
1:A:393:A:OP2	16:P:12:LYS:NZ	2.29	0.62
1:A:825:G:H21	8:H:11:THR:HG21	1.65	0.62
3:C:75:VAL:O	3:C:83:ARG:HD3	2.00	0.62
1:A:184:G:H2'	1:A:185:A:C8	2.35	0.62
9:I:26:VAL:HB	9:I:33:PHE:HB2	1.82	0.62
15:O:33:THR:HA	15:O:63:ARG:NH1	2.15	0.61
2:B:73:THR:HG21	2:B:96:ARG:HD2	1.81	0.61
1:A:738:C:OP1	6:F:92:LYS:HD3	1.99	0.61
14:N:16:PHE:HD1	14:N:19:ARG:HH11	1.48	0.61
1:A:14:U:O2	1:A:16:A:C8	2.53	0.61
1:A:1143:G:H2'	1:A:1144:G:C8	2.35	0.61
4:D:64:LEU:HD22	4:D:64:LEU:O	2.00	0.61
2:B:16:HIS:HB3	2:B:210:SER:HB2	1.83	0.61
2:B:30:ARG:HG3	2:B:31:TYR:CD2	2.35	0.61
1:A:1400:5MC:H3'	1:A:1401:G:C5'	2.31	0.61
1:A:1179:A:H2'	1:A:1180:A:O4'	2.01	0.61
1:A:633:G:H2'	1:A:634:C:H6	1.65	0.61
13:M:34:LEU:HD13	13:M:41:PRO:HA	1.82	0.61
1:A:815:A:N6	1:A:1509:C:H1'	2.15	0.61
16:P:6:LEU:HD23	16:P:17:TYR:CD2	2.35	0.61
6:F:70:ASP:N	6:F:70:ASP:OD1	2.33	0.61
1:A:93:G:H2'	1:A:95:U:H6	1.62	0.61
8:H:119:LEU:HD12	8:H:124:ALA:HB2	1.83	0.61
6:F:10:LEU:HD12	6:F:59:TYR:HB3	1.81	0.61
7:G:27:ILE:HA	7:G:30:ILE:HD12	1.80	0.61
1:A:1241:G:H2'	1:A:1242:C:H6	1.65	0.61
1:A:79:G:C6	1:A:80:G:C6	2.88	0.61
5:E:17:ALA:HA	5:E:26:PHE:HB3	1.80	0.61
19:S:36:ARG:HB3	19:S:51:VAL:HG11	1.83	0.61
16:P:68:ASP:OD1	16:P:68:ASP:N	2.28	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:33:THR:HG23	15:O:63:ARG:HH12	1.64	0.61
2:B:96:ARG:HE	2:B:97:TRP:H	1.49	0.61
1:A:685:G:O2'	1:A:686:U:H5"	2.01	0.61
3:C:14:ILE:O	3:C:16:ARG:N	2.27	0.61
1:A:1063:C:H2'	1:A:1064:G:C8	2.36	0.61
1:A:1190:G:O3'	3:C:3:ASN:HB2	2.01	0.60
3:C:134:ILE:O	3:C:138:VAL:HG23	2.01	0.60
1:A:518:C:H2'	1:A:530:G:C8	2.35	0.60
1:A:1182:G:H4'	1:A:1183:A:H5'	1.83	0.60
1:A:902:G:H2'	1:A:903:G:C8	2.35	0.60
7:G:65:ALA:HB1	7:G:127:ALA:HB3	1.83	0.60
1:A:527:7MG:H81	1:A:527:7MG:H5"	1.81	0.60
4:D:15:GLU:HG2	4:D:63:LYS:HG3	1.82	0.60
4:D:26:CYS:HA	4:D:31:CYS:HB2	1.82	0.60
11:K:58:PRO:HD3	11:K:89:ALA:HB1	1.83	0.60
10:J:16:LEU:HD13	10:J:68:HIS:HB2	1.83	0.60
10:J:27:ALA:HA	10:J:81:THR:HG23	1.83	0.60
12:L:10:LEU:HD12	17:Q:32:TYR:CZ	2.37	0.60
2:B:82:ARG:HG2	2:B:92:TYR:CE1	2.36	0.60
20:T:65:LYS:O	20:T:68:LYS:HB2	2.02	0.60
7:G:108:ALA:O	7:G:119:ARG:HB3	2.01	0.60
5:E:90:VAL:O	5:E:91:LEU:HD23	2.01	0.60
8:H:46:LYS:HG3	8:H:64:LYS:HB2	1.84	0.60
5:E:74:GLY:HA3	5:E:116:THR:HG22	1.82	0.60
1:A:429:U:OP1	4:D:36:ARG:NH1	2.32	0.60
1:A:1059:C:N3	1:A:1198:G:N1	2.32	0.60
21:U:8:THR:HG22	21:U:9:ARG:H	1.67	0.60
1:A:1236:A:H4'	1:A:1304:G:H4'	1.84	0.60
1:A:355:C:H5'	1:A:389:A:OP2	2.00	0.60
4:D:125:HIS:HD1	4:D:152:SER:HG	1.50	0.60
18:R:46:GLU:OE2	18:R:86:VAL:HG23	2.02	0.60
1:A:135:C:O2	16:P:1:MET:HB2	2.01	0.59
1:A:864:A:H2'	1:A:865:A:C8	2.37	0.59
1:A:1005:A:N6	1:A:1024:G:O2'	2.35	0.59
1:A:112:G:H2'	1:A:113:G:H5'	1.83	0.59
5:E:81:GLU:HG3	5:E:90:VAL:HG22	1.84	0.59
1:A:1441:G:H4'	1:A:1442:G:C5	2.37	0.59
1:A:706:A:O2'	11:K:29:ILE:HD11	2.02	0.59
1:A:1126:U:N3	1:A:1149:C:H1'	2.17	0.59
1:A:757:U:H2'	1:A:758:G:O4'	2.02	0.59
1:A:1145:C:HO2'	1:A:1146:A:P	2.25	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:G:H2'	1:A:80:G:C8	2.37	0.59
12:L:66:VAL:HG11	12:L:98:TYR:CE1	2.38	0.59
3:C:6:HIS:HD2	3:C:9:GLY:H	1.49	0.59
12:L:110:VAL:HA	12:L:111:LYS:HE3	1.83	0.59
13:M:22:ILE:HG22	13:M:23:TYR:N	2.17	0.59
5:E:121:LYS:HG2	5:E:123:LEU:CD2	2.32	0.59
1:A:673:G:H5'	6:F:87:ARG:HD2	1.83	0.59
13:M:96:LEU:HB3	13:M:97:PRO:HD2	1.84	0.59
5:E:37:ARG:HB3	5:E:37:ARG:HH11	1.66	0.59
1:A:76:C:H2'	1:A:77:G:C8	2.37	0.59
2:B:142:LEU:HD13	2:B:146:GLN:NE2	2.18	0.59
20:T:12:ALA:HA	25:T:1302:HOH:O	2.02	0.59
1:A:1410:G:H2'	1:A:1411:C:H6	1.67	0.59
1:A:1391:U:H2'	1:A:1392:G:H8	1.66	0.59
3:C:180:ALA:HB1	3:C:182:ILE:HG13	1.83	0.59
1:A:113:G:H1'	1:A:354:G:H5'	1.85	0.59
12:L:28:LYS:HE3	12:L:33:ARG:HH12	1.67	0.59
1:A:835:U:OP1	18:R:64:ARG:NH2	2.34	0.59
20:T:50:GLU:HA	20:T:100:ILE:HG13	1.85	0.59
1:A:1145:C:O2'	1:A:1146:A:O5'	2.18	0.59
9:I:43:ALA:HA	9:I:74:ILE:HD13	1.83	0.59
1:A:819:A:H5'	1:A:819:A:C8	2.37	0.59
8:H:95:VAL:HB	8:H:99:GLU:HB2	1.85	0.59
1:A:160:A:O2'	1:A:161:A:OP1	2.21	0.59
5:E:71:LEU:HD21	5:E:113:ALA:O	2.03	0.59
1:A:92:C:O2	1:A:93:G:C8	2.56	0.58
11:K:78:GLN:HA	11:K:103:LEU:HD22	1.84	0.58
1:A:758:G:C8	25:A:2216:HOH:O	2.52	0.58
3:C:202:ILE:HG22	3:C:204:LEU:HD23	1.85	0.58
13:M:48:LEU:HD12	13:M:53:VAL:HG23	1.85	0.58
1:A:1241:G:H2'	1:A:1242:C:C6	2.38	0.58
10:J:48:THR:HA	10:J:62:HIS:HB3	1.85	0.58
11:K:73:MET:HG2	11:K:103:LEU:HD21	1.85	0.58
1:A:62:U:H2'	1:A:63:C:C6	2.39	0.58
1:A:1009:G:N2	1:A:1010:G:H1'	2.18	0.58
14:N:16:PHE:HD1	14:N:19:ARG:NH1	2.01	0.58
6:F:53:ALA:HB3	6:F:86:ARG:NE	2.19	0.58
1:A:966:M2G:HM22	1:A:967:5MC:C2	2.39	0.58
1:A:839:U:H5'	1:A:840:C:C5	2.38	0.58
1:A:108:G:C6	20:T:15:ARG:HG2	2.38	0.58
1:A:1028:C:H2'	1:A:1029:C:H6	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:20:TYR:HA	8:H:65:TYR:CZ	2.38	0.58
1:A:692:U:OP1	11:K:124:LYS:NZ	2.32	0.58
1:A:1516:G:H1'	1:A:1519:MA6:H101	1.86	0.58
1:A:620:C:N1	4:D:135:LEU:HD13	2.19	0.58
1:A:80:G:N2	1:A:89:C:H42	2.01	0.58
1:A:90:U:N3	1:A:91:C:N3	2.52	0.58
1:A:1114:C:O2	14:N:60:SER:OG	2.21	0.58
3:C:64:VAL:HG11	3:C:99:VAL:HG23	1.85	0.58
1:A:1399:C:H4'	1:A:1400:5MC:H5"	1.85	0.58
1:A:1266:G:N2	1:A:1269:A:OP2	2.35	0.58
1:A:653:A:O4'	8:H:56:LYS:HE2	2.04	0.58
1:A:938:A:H5'	7:G:76:ARG:HH22	1.69	0.58
18:R:38:GLU:OE1	18:R:38:GLU:HA	2.03	0.58
1:A:1402:4OC:HM22	1:A:1403:C:H5'	1.85	0.58
1:A:1498:UR3:O2'	1:A:1499:A:OP2	2.14	0.58
4:D:127:THR:HB	4:D:147:ALA:HB3	1.86	0.58
1:A:95:U:H2'	1:A:96:G:H8	1.68	0.58
1:A:975:A:H4'	1:A:976:G:O5'	2.02	0.58
8:H:51:VAL:HG11	8:H:60:ARG:HG2	1.84	0.58
12:L:6:THR:OG1	12:L:9:GLN:HG3	2.04	0.58
1:A:1123:A:H2	10:J:39:PRO:HG3	1.68	0.58
7:G:27:ILE:CD1	7:G:40:ALA:HA	2.34	0.57
1:A:677:U:H3	1:A:713:G:H22	1.52	0.57
1:A:279:A:H8	1:A:279:A:H5'	1.68	0.57
10:J:77:PRO:HB2	10:J:82:ILE:HD11	1.84	0.57
1:A:1476:G:H2'	1:A:1477:C:C6	2.39	0.57
1:A:411:A:N7	1:A:413:G:N3	2.52	0.57
1:A:780:A:O2'	1:A:781:A:H5"	2.05	0.57
1:A:707:C:H2'	1:A:708:C:C6	2.39	0.57
16:P:53:VAL:O	16:P:56:ALA:N	2.37	0.57
1:A:1163:C:H2'	1:A:1164:G:O4'	2.04	0.57
1:A:827:U:H3'	1:A:870:U:O4	2.05	0.57
1:A:1497:G:H2'	1:A:1498:UR3:H5'	1.85	0.57
10:J:11:PHE:CE2	10:J:65:LEU:HD21	2.39	0.57
11:K:54:ARG:O	11:K:57:THR:HG22	2.04	0.57
1:A:909:A:H2'	1:A:910:C:O4'	2.03	0.57
1:A:966:M2G:HM22	1:A:967:5MC:H1'	1.87	0.57
8:H:114:THR:HB	8:H:116:LYS:N	2.19	0.57
1:A:451:A:N6	1:A:481:G:C4	2.72	0.57
1:A:714:G:H2'	1:A:715:A:C8	2.39	0.57
16:P:10:GLY:HA3	16:P:16:HIS:H	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1206:G:H2'	1:A:1207:2MG:C8	2.40	0.57
1:A:88:A:H2'	1:A:89:C:C6	2.40	0.57
10:J:62:HIS:O	14:N:59:ALA:HB3	2.04	0.57
1:A:750:G:O2'	15:O:21:ASP:OD2	2.23	0.57
5:E:80:ILE:HG12	5:E:81:GLU:N	2.16	0.57
1:A:243:A:C2	1:A:246:A:C8	2.92	0.57
1:A:80:G:H22	1:A:89:C:N4	2.02	0.57
1:A:552:U:H2'	1:A:553:A:C8	2.40	0.57
1:A:571:U:H5"	1:A:572:A:OP2	2.05	0.57
1:A:1372:U:H2'	1:A:1373:G:O4'	2.05	0.57
1:A:93:G:H21	1:A:95:U:H1'	1.68	0.57
1:A:481:G:O2'	1:A:482:A:H8	1.88	0.57
1:A:384:G:H2'	1:A:385:C:H6	1.64	0.57
11:K:47:VAL:HG12	11:K:48:ILE:HG13	1.87	0.57
9:I:79:LEU:O	9:I:83:ARG:HG2	2.05	0.57
4:D:187:ARG:NE	4:D:188:LEU:H	2.02	0.57
3:C:112:SER:O	3:C:115:LEU:HB2	2.04	0.57
13:M:49:THR:HG22	13:M:51:ALA:H	1.70	0.57
15:O:4:THR:HG23	15:O:7:GLU:HB2	1.86	0.57
1:A:858:G:O6	1:A:869:G:C8	2.58	0.56
8:H:6:ILE:HB	8:H:85:ARG:NH1	2.20	0.56
1:A:1403:C:O2'	1:A:1404:5MC:H5'	2.05	0.56
1:A:1238:A:H5'	1:A:1336:C:H41	1.70	0.56
1:A:321:A:H2'	1:A:322:C:H6	1.70	0.56
5:E:76:ILE:O	5:E:93:PRO:HB3	2.04	0.56
12:L:93:LEU:O	12:L:96:VAL:HG23	2.05	0.56
4:D:98:GLU:HG2	4:D:189:PRO:HG3	1.87	0.56
12:L:69:TYR:HE2	12:L:71:PRO:HA	1.68	0.56
21:U:9:ARG:HH22	21:U:23:PRO:CD	2.17	0.56
1:A:9:G:OP2	5:E:121:LYS:NZ	2.31	0.56
1:A:838:G:H1	1:A:848:C:H42	1.53	0.56
1:A:390:C:O3'	16:P:28:ARG:NH2	2.38	0.56
6:F:4:TYR:CE1	6:F:92:LYS:HG2	2.40	0.56
1:A:687:A:C2	1:A:704:A:C5	2.93	0.56
11:K:104:GLN:HG2	11:K:106:LYS:NZ	2.20	0.56
1:A:1267:C:O2'	21:U:20:LYS:HG3	2.06	0.56
13:M:12:ASN:H	13:M:45:VAL:HB	1.69	0.56
4:D:191:ARG:O	4:D:194:LEU:HD12	2.05	0.56
3:C:123:GLN:HE21	3:C:128:PHE:HD2	1.53	0.56
1:A:31:G:O2'	1:A:48:C:N4	2.38	0.56
2:B:68:ILE:O	2:B:90:MET:HB3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:95:TYR:HA	17:Q:98:LEU:CD1	2.36	0.56
1:A:1195:C:H3'	1:A:1196:U:C5'	2.32	0.56
1:A:1204:A:H2'	1:A:1205:U:H5'	1.87	0.56
1:A:1323:G:H2'	1:A:1324:A:C8	2.40	0.56
1:A:694:A:N1	1:A:787:A:O2'	2.39	0.56
1:A:60:A:P	1:A:331:G:H22	2.29	0.56
12:L:7:ILE:O	12:L:11:VAL:HG23	2.06	0.56
15:O:32:LEU:HD12	15:O:63:ARG:HB2	1.88	0.56
9:I:17:VAL:HG22	9:I:63:ILE:HD12	1.88	0.56
5:E:152:ARG:NE	8:H:44:PHE:HE1	2.04	0.56
15:O:16:ALA:HB1	15:O:21:ASP:HB3	1.87	0.56
1:A:1089:G:C6	1:A:1090:U:N3	2.74	0.56
19:S:31:ILE:HG22	19:S:49:ILE:HG12	1.88	0.56
5:E:116:THR:HG23	5:E:117:ASP:OD2	2.06	0.56
1:A:412:A:H1'	4:D:35:ARG:HH21	1.70	0.56
20:T:81:LYS:O	20:T:85:MET:HG3	2.06	0.56
13:M:49:THR:HB	13:M:52:GLU:H	1.70	0.56
1:A:126:G:OP1	1:A:605:U:O2'	2.21	0.56
1:A:56:U:H2'	1:A:57:G:H8	1.71	0.56
13:M:14:ARG:HH11	13:M:14:ARG:HG2	1.70	0.56
14:N:24:CYS:H	14:N:33:VAL:HG11	1.71	0.56
4:D:57:ARG:HB3	4:D:206:PHE:HB2	1.88	0.56
9:I:89:ASN:O	9:I:92:TYR:HB2	2.05	0.56
1:A:200:G:H1	1:A:217:C:H42	1.54	0.56
1:A:397:A:O2'	1:A:399:G:OP2	2.20	0.56
2:B:36:ARG:O	2:B:39:ILE:HG12	2.06	0.55
1:A:758:G:N7	25:A:2216:HOH:O	2.37	0.55
2:B:178:ARG:NH1	8:H:71:GLY:O	2.39	0.55
1:A:1280:A:N7	10:J:40:LEU:HD22	2.21	0.55
5:E:15:ARG:HG3	5:E:15:ARG:HH11	1.72	0.55
4:D:15:GLU:O	4:D:17:VAL:N	2.39	0.55
3:C:167:TRP:HE3	3:C:168:ALA:H	1.51	0.55
1:A:501:C:H2'	1:A:502:G:H8	1.69	0.55
1:A:1188:A:O3'	14:N:58:LYS:NZ	2.38	0.55
1:A:1352:C:H2'	1:A:1353:G:C8	2.41	0.55
1:A:463:A:H2'	1:A:474:G:O4'	2.05	0.55
1:A:1004:A:H5'	1:A:1025:U:N3	2.21	0.55
3:C:77:ILE:HG22	3:C:81:GLY:HA2	1.88	0.55
7:G:38:LEU:O	7:G:42:ILE:HG13	2.07	0.55
1:A:1113:C:N4	1:A:1187:G:H1	2.02	0.55
8:H:86:ILE:HG21	8:H:133:LEU:HD13	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1361(A):C:C2'	1:A:1362:C:H5"	2.36	0.55
17:Q:15:MET:HB3	17:Q:18:THR:HB	1.88	0.55
1:A:629:G:H2'	1:A:630:G:O4'	2.07	0.55
1:A:1496:C:O2'	1:A:1497:G:O4'	2.24	0.55
17:Q:5:VAL:C	17:Q:6:LEU:HD23	2.27	0.55
1:A:858:G:N7	25:A:2220:HOH:O	2.33	0.55
4:D:18:LYS:HB3	4:D:20:TYR:HE2	1.72	0.55
13:M:12:ASN:N	13:M:45:VAL:HB	2.22	0.55
2:B:180:LEU:HB2	2:B:182:ILE:CD1	2.37	0.55
1:A:1395:C:C2'	1:A:1396:A:H5'	2.37	0.55
1:A:1228:C:OP1	13:M:108:ARG:NH2	2.39	0.55
9:I:48:GLU:N	9:I:49:PRO:HD2	2.22	0.55
2:B:24:TRP:CZ3	2:B:26:PRO:HA	2.42	0.55
16:P:53:VAL:O	16:P:55:ARG:N	2.39	0.55
2:B:72:GLY:HA3	2:B:165:VAL:HG22	1.87	0.55
16:P:2:VAL:O	16:P:64:ALA:HA	2.07	0.55
1:A:1054:C:H3'	1:A:1054:C:H6	1.71	0.55
1:A:89:C:H2'	1:A:90:U:O4'	2.07	0.55
1:A:1284:C:OP2	1:A:1285:A:O2'	2.22	0.55
1:A:1191:A:H2'	1:A:1192:C:H6	1.72	0.55
1:A:1117:G:H5"	9:I:104:ARG:NH2	2.22	0.55
1:A:322:C:C2'	1:A:323:U:H5'	2.37	0.55
5:E:79:GLU:HB3	5:E:92:LYS:HA	1.88	0.55
1:A:933:G:OP2	7:G:3:ARG:HB2	2.06	0.55
2:B:45:GLN:O	2:B:48:MET:HB2	2.06	0.55
13:M:11:ARG:HG3	13:M:12:ASN:N	2.22	0.55
2:B:71:VAL:O	2:B:164:VAL:HA	2.07	0.55
16:P:9:PHE:HD2	16:P:18:ARG:HG3	1.72	0.55
2:B:119:GLU:OE1	2:B:153:ARG:NH2	2.40	0.55
4:D:9:CYS:O	4:D:12:CYS:HB2	2.07	0.55
1:A:838:G:C2'	1:A:839:U:H5"	2.37	0.55
17:Q:7:THR:HA	17:Q:57:VAL:O	2.07	0.55
18:R:44:LEU:HD21	18:R:70:ILE:HD13	1.89	0.55
20:T:11:SER:HA	20:T:13:LEU:HD11	1.89	0.55
1:A:1282:C:H2'	1:A:1283:G:O4'	2.06	0.54
1:A:1217:C:OP1	14:N:5:ALA:HB1	2.06	0.54
1:A:350:G:H5"	1:A:350:G:H8	1.72	0.54
10:J:25:GLU:HB3	10:J:29:ARG:HH21	1.72	0.54
11:K:62:GLN:HG3	11:K:63:LEU:N	2.21	0.54
1:A:1430:C:C2	1:A:1471:G:N2	2.76	0.54
17:Q:8:GLY:O	17:Q:56:VAL:HA	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:39:LEU:HB3	15:O:56:LEU:HD13	1.88	0.54
1:A:580:U:H2'	1:A:581:G:O4'	2.07	0.54
1:A:1305:G:N2	1:A:1331:G:H1'	2.22	0.54
1:A:1414:U:H2'	1:A:1415:G:H8	1.73	0.54
4:D:102:ASP:OD1	4:D:103:ASN:N	2.37	0.54
1:A:1095:U:OP1	1:A:1108:G:N2	2.33	0.54
3:C:156:ARG:NH1	3:C:160:ALA:O	2.41	0.54
1:A:1443:G:H5'	1:A:1446:A:H5'	1.88	0.54
10:J:53:PRO:HA	14:N:41:ARG:HH22	1.72	0.54
5:E:75:THR:HB	5:E:117:ASP:O	2.08	0.54
1:A:620:C:H2'	1:A:621:A:O4'	2.07	0.54
1:A:1403:C:C5	1:A:1404:5MC:HM52	2.43	0.54
1:A:1171:G:H2'	1:A:1172:C:H6	1.73	0.54
11:K:92:GLU:O	11:K:95:ILE:HG13	2.08	0.54
1:A:781:A:C5	1:A:802:A:C2	2.96	0.54
17:Q:9:VAL:HG12	17:Q:54:GLY:HA2	1.89	0.54
12:L:54:LYS:HB3	12:L:70:ILE:HD12	1.90	0.54
1:A:1298:C:O2'	7:G:114:ARG:NH1	2.41	0.54
2:B:17:PHE:HD1	2:B:18:GLY:N	2.04	0.54
4:D:35:ARG:O	4:D:36:ARG:HG3	2.07	0.54
4:D:15:GLU:C	4:D:17:VAL:H	2.09	0.54
3:C:6:HIS:CD2	3:C:9:GLY:H	2.25	0.54
3:C:120:VAL:O	3:C:124:ILE:HG12	2.07	0.54
5:E:34:VAL:HG12	5:E:62:ALA:HB1	1.89	0.54
1:A:35:G:H2'	1:A:36:C:H6	1.72	0.54
15:O:22:THR:O	15:O:27:VAL:HG11	2.07	0.54
1:A:984:C:H42	1:A:1221:G:H1	1.55	0.54
9:I:89:ASN:O	9:I:92:TYR:N	2.37	0.54
1:A:1302:U:H5"	25:A:2227:HOH:O	2.07	0.54
1:A:735:C:H1'	18:R:75:ILE:HD12	1.90	0.54
1:A:858:G:N7	25:A:2218:HOH:O	2.40	0.54
1:A:1347:G:H1'	1:A:1348:U:C5	2.41	0.54
1:A:447:G:N1	1:A:485:G:O2'	2.40	0.54
1:A:526:C:O3'	22:A:1601:SRY:HI31	2.07	0.54
1:A:1361(A):C:O2'	1:A:1362:C:H6	1.91	0.54
13:M:16:ASP:N	13:M:16:ASP:OD1	2.40	0.54
1:A:815:A:H62	1:A:1509:C:H1'	1.72	0.54
1:A:1518:MA6:H102	1:A:1519:MA6:H103	1.90	0.54
1:A:173:U:H6	1:A:198:G:HO2'	1.56	0.54
1:A:1061:G:H1	1:A:1195:C:N4	1.98	0.54
1:A:1065:U:H5	1:A:1190:G:C4	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:C:OP2	12:L:116:SER:HB3	2.07	0.54
1:A:369:C:OP2	1:A:388:G:N2	2.39	0.54
2:B:184:VAL:HG23	2:B:198:ASP:H	1.73	0.54
1:A:1367:C:OP2	9:I:112:LYS:NZ	2.41	0.54
4:D:9:CYS:SG	4:D:31:CYS:O	2.65	0.54
2:B:21:ARG:HG2	2:B:23:ARG:HH11	1.73	0.54
2:B:105:PHE:HE2	2:B:157:ARG:HA	1.73	0.53
3:C:110:ASN:ND2	3:C:140:ARG:HB3	2.22	0.53
16:P:75:ARG:HH11	16:P:75:ARG:HG3	1.72	0.53
13:M:14:ARG:HG2	13:M:14:ARG:NH1	2.23	0.53
1:A:1424:C:H2'	1:A:1425:U:H6	1.73	0.53
1:A:532:A:O2'	1:A:533:A:OP1	2.22	0.53
7:G:26:PHE:CD1	7:G:101:LEU:HD22	2.43	0.53
10:J:82:ILE:HA	10:J:85:LEU:HD12	1.90	0.53
2:B:88:ALA:HB2	2:B:219:VAL:HG13	1.90	0.53
18:R:36:ASN:O	18:R:40:LEU:HG	2.08	0.53
1:A:558:G:H5"	1:A:559:A:H3'	1.89	0.53
1:A:90:U:C4	1:A:91:C:C4	2.96	0.53
21:U:13:ILE:HA	21:U:22:ARG:NH1	2.23	0.53
1:A:1511:G:H2'	1:A:1512:U:O4'	2.09	0.53
1:A:1518:MA6:H2'	1:A:1519:MA6:C8	2.38	0.53
1:A:620:C:C2	4:D:135:LEU:HD13	2.43	0.53
1:A:973:G:O2'	14:N:29:ARG:NH2	2.40	0.53
1:A:564:C:C5	17:Q:31:LEU:HD21	2.43	0.53
1:A:1504:G:C3'	1:A:1505:G:H5'	2.37	0.53
9:I:103:THR:HG22	9:I:104:ARG:O	2.08	0.53
1:A:394:G:H2'	1:A:395:C:C6	2.44	0.53
1:A:321:A:C2	1:A:333:G:C2	2.96	0.53
17:Q:40:LYS:HD3	17:Q:42:TYR:CZ	2.43	0.53
1:A:254:G:OP1	17:Q:67:LYS:O	2.25	0.53
1:A:381:C:H2'	1:A:382:A:O4'	2.08	0.53
1:A:1502:A:H2'	1:A:1504:G:C8	2.42	0.53
15:O:22:THR:OG1	15:O:23:GLY:N	2.40	0.53
10:J:8:LEU:HD23	10:J:96:ILE:HG23	1.88	0.53
3:C:87:LEU:HD22	3:C:101:LEU:HD11	1.89	0.53
1:A:1008:C:H42	1:A:1021:G:H1	1.56	0.53
4:D:174:LEU:C	4:D:186:LEU:HD21	2.29	0.53
1:A:462:G:H21	16:P:82:GLN:HE21	1.57	0.53
1:A:954:G:H21	1:A:1227:A:H62	1.55	0.53
1:A:1392:G:H2'	1:A:1393:U:H6	1.74	0.53
1:A:1404:5MC:H2'	1:A:1405:G:O4'	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1539:C:H2'	1:A:1540:PSU:H6	1.73	0.53
1:A:49:U:O2'	1:A:50:A:H2'	2.08	0.53
11:K:41:THR:HG21	11:K:71:LYS:HB3	1.90	0.53
4:D:31:CYS:SG	4:D:31:CYS:O	2.66	0.53
2:B:23:ARG:O	2:B:24:TRP:HD1	1.91	0.53
18:R:39:VAL:HG13	18:R:40:LEU:HD23	1.91	0.53
6:F:95:GLU:HG3	6:F:96:PRO:HD2	1.90	0.53
7:G:54:THR:HG22	7:G:56:GLN:H	1.74	0.53
13:M:107:ALA:HB3	13:M:111:LYS:HE3	1.89	0.53
8:H:53:VAL:HB	8:H:58:TYR:CD1	2.44	0.53
17:Q:27:PHE:CZ	17:Q:36:ILE:HD11	2.43	0.53
1:A:405:U:O4	4:D:2:GLY:HA3	2.08	0.53
1:A:1007:C:H2'	1:A:1008:C:C5	2.43	0.53
1:A:1403:C:H2'	1:A:1404:5MC:C6	2.44	0.53
2:B:223:ILE:HG21	2:B:230:VAL:HB	1.90	0.53
1:A:1532:U:H2'	1:A:1533:C:H3'	1.91	0.53
8:H:15:ASN:N	8:H:15:ASN:OD1	2.41	0.53
1:A:117:G:O5'	1:A:117:G:H8	1.92	0.53
10:J:7:LYS:HA	10:J:71:LEU:HD13	1.91	0.53
1:A:976:G:OP2	1:A:1358:U:H1'	2.08	0.53
2:B:82:ARG:HG2	2:B:92:TYR:HE1	1.73	0.53
4:D:173:TRP:HB2	4:D:187:ARG:O	2.09	0.53
1:A:1448:C:H2'	1:A:1449:C:H6	1.74	0.53
1:A:596:C:C2'	1:A:597:G:H5'	2.38	0.53
1:A:383:A:C6	1:A:384:G:H1'	2.44	0.53
1:A:1198:G:H2'	1:A:1199:U:C6	2.43	0.52
9:I:118:LYS:O	9:I:120:ARG:N	2.39	0.52
7:G:73:MET:SD	7:G:90:GLU:HA	2.49	0.52
1:A:685:G:C2'	1:A:686:U:H5"	2.38	0.52
2:B:180:LEU:HB2	2:B:182:ILE:HD12	1.90	0.52
13:M:99:ARG:HB2	13:M:101:GLN:HE22	1.73	0.52
10:J:51:ARG:CZ	10:J:61:GLU:HB2	2.38	0.52
1:A:673:G:H2'	1:A:674:G:C8	2.44	0.52
1:A:560:U:H5'	1:A:566:G:N2	2.24	0.52
15:O:87:ILE:HG22	15:O:88:ARG:N	2.23	0.52
2:B:21:ARG:HG3	2:B:22:LYS:H	1.73	0.52
5:E:84:PHE:HB2	5:E:134:ALA:HB2	1.91	0.52
20:T:71:THR:O	20:T:72:LEU:HD23	2.09	0.52
1:A:921:U:O2'	5:E:19:MET:O	2.17	0.52
13:M:23:TYR:CZ	13:M:71:ARG:HD3	2.44	0.52
14:N:21:TYR:CD1	14:N:21:TYR:N	2.77	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:838:G:N2	1:A:849:C:C2	2.77	0.52
1:A:1305:G:H3'	21:U:4:GLY:O	2.10	0.52
16:P:6:LEU:HD23	16:P:17:TYR:CG	2.45	0.52
6:F:53:ALA:HB3	6:F:86:ARG:HE	1.73	0.52
8:H:97:VAL:HG12	8:H:98:LYS:HD3	1.92	0.52
2:B:19:HIS:CE1	2:B:204:ASN:ND2	2.77	0.52
17:Q:6:LEU:O	17:Q:58:GLU:HA	2.09	0.52
1:A:1517:G:H5"	25:A:2084:HOH:O	2.08	0.52
7:G:62:PHE:CE2	7:G:66:VAL:HG21	2.44	0.52
1:A:1006:C:H41	1:A:1024:G:H21	1.56	0.52
1:A:1121:U:H2'	1:A:1122:U:C6	2.45	0.52
1:A:1144:G:N2	1:A:1146:A:H62	2.07	0.52
1:A:1177:G:N2	1:A:1181:G:O6	2.43	0.52
1:A:1359:C:H1'	1:A:1361(A):C:H41	1.74	0.52
1:A:1305:G:OP2	1:A:1305:G:C8	2.63	0.52
16:P:75:ARG:O	16:P:75:ARG:HG2	2.09	0.52
13:M:52:GLU:HG2	13:M:55:ARG:HH21	1.75	0.52
1:A:170:U:O2'	1:A:171:A:H5'	2.08	0.52
9:I:2:GLU:HG3	9:I:3:GLN:OE1	2.09	0.52
10:J:91:PRO:O	10:J:94:VAL:HG22	2.10	0.52
12:L:66:VAL:HG11	12:L:98:TYR:HE1	1.75	0.52
2:B:189:ASP:HB3	2:B:203:GLY:O	2.10	0.52
5:E:24:ARG:HB2	5:E:26:PHE:HE2	1.75	0.52
1:A:1403:C:C6	1:A:1404:5MC:HM52	2.45	0.52
1:A:1171:G:H2'	1:A:1172:C:C6	2.45	0.52
1:A:191:G:N2	20:T:103:GLY:O	2.42	0.52
1:A:1347:G:O2'	1:A:1348:U:P	2.68	0.52
1:A:79:G:C2	1:A:80:G:C4	2.98	0.52
1:A:1505:G:H3'	1:A:1505:G:C8	2.44	0.52
2:B:12:GLU:HA	2:B:12:GLU:OE1	2.09	0.52
8:H:11:THR:OG1	8:H:14:ARG:NH1	2.32	0.52
8:H:64:LYS:HG2	8:H:79:VAL:HG21	1.91	0.52
4:D:25:ARG:C	4:D:27:TYR:H	2.09	0.52
1:A:248:C:O2'	1:A:283:C:H4'	2.09	0.52
7:G:60:LYS:HD2	7:G:63:LYS:HE2	1.90	0.52
16:P:21:VAL:HG21	16:P:59:TRP:CD1	2.44	0.52
3:C:30:ARG:HD3	3:C:30:ARG:H	1.75	0.52
1:A:1012:U:H2'	1:A:1013:G:C8	2.45	0.52
1:A:385:C:H2'	1:A:386:C:C6	2.44	0.51
1:A:581:G:O3'	15:O:64:ARG:NH2	2.43	0.51
1:A:436:C:H2'	1:A:437:U:H6	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:62:SER:OG	12:L:64:TYR:HB2	2.09	0.51
1:A:83:U:C2'	1:A:84:U:H5'	2.40	0.51
1:A:1248:A:N3	9:I:70:LYS:HE3	2.25	0.51
1:A:316:G:H1	1:A:337:C:H42	1.59	0.51
11:K:58:PRO:HA	11:K:90:GLY:HA3	1.91	0.51
6:F:97:PHE:H	18:R:32:ARG:HH12	1.59	0.51
1:A:8:A:N7	4:D:208:SER:OG	2.44	0.51
1:A:445:G:O5'	1:A:445:G:H8	1.91	0.51
1:A:833:U:H2'	1:A:834:C:C6	2.45	0.51
16:P:26:ARG:HD2	16:P:31:LYS:O	2.10	0.51
1:A:1347:G:N2	1:A:1373:G:H2'	2.25	0.51
15:O:26:GLU:OE1	15:O:77:ARG:HD2	2.10	0.51
1:A:251:G:H4'	1:A:252:U:OP1	2.07	0.51
17:Q:74:LEU:HD22	17:Q:75:ARG:HG2	1.91	0.51
8:H:100:ILE:HG23	8:H:112:LEU:HD21	1.93	0.51
6:F:7:ASN:HB2	6:F:89:MET:O	2.09	0.51
19:S:12:ASP:CG	19:S:38:SER:HB3	2.30	0.51
13:M:2:ALA:O	13:M:10:PRO:HD2	2.10	0.51
1:A:1222:G:OP1	19:S:77:THR:HG21	2.11	0.51
8:H:86:ILE:HG21	8:H:133:LEU:HB3	1.92	0.51
1:A:1395:C:O2'	1:A:1396:A:H5'	2.10	0.51
20:T:10:LEU:HD13	20:T:11:SER:N	2.24	0.51
2:B:139:LYS:O	2:B:143:GLU:HG3	2.09	0.51
19:S:4:SER:O	19:S:6:LYS:NZ	2.44	0.51
8:H:9:MET:CG	8:H:26:VAL:HG21	2.37	0.51
1:A:704:A:C2	1:A:705:U:H1'	2.45	0.51
1:A:690:G:H2'	1:A:691:G:O4'	2.09	0.51
1:A:425:G:H2'	1:A:426:G:H5'	1.92	0.51
20:T:17:ARG:O	20:T:20:LEU:HB2	2.10	0.51
1:A:278:G:C6	17:Q:95:TYR:HD2	2.27	0.51
9:I:42:ARG:NH2	9:I:75:ASP:OD1	2.43	0.51
1:A:838:G:H1	1:A:848:C:N4	2.08	0.51
2:B:157:ARG:H	2:B:157:ARG:HD2	1.75	0.51
1:A:118:U:H3'	1:A:288:A:H61	1.76	0.51
12:L:126:LYS:HD2	12:L:126:LYS:N	2.26	0.51
1:A:428:G:H4'	1:A:429:U:O5'	2.11	0.51
1:A:938:A:H5'	7:G:76:ARG:HH12	1.75	0.51
1:A:1424:C:H2'	1:A:1425:U:C6	2.45	0.51
1:A:510:A:H5"	1:A:511:C:P	2.51	0.51
10:J:42:THR:HG23	10:J:67:THR:O	2.10	0.51
18:R:76:LEU:HB3	18:R:78:LEU:HD21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:100:ASN:ND2	6:F:100:ASN:O	2.43	0.51
8:H:84:ARG:O	8:H:135:CYS:HB2	2.11	0.51
2:B:189:ASP:O	2:B:192:SER:OG	2.29	0.51
1:A:1329:A:H2'	1:A:1330:U:H6	1.76	0.51
18:R:46:GLU:OE2	18:R:85:LEU:HD12	2.10	0.51
1:A:106:C:O2	1:A:379:C:H4'	2.11	0.51
11:K:104:GLN:HB3	11:K:106:LYS:HE2	1.92	0.51
1:A:935:A:N6	7:G:3:ARG:HG3	2.25	0.51
2:B:217:ARG:O	2:B:220:ASP:HB2	2.10	0.51
1:A:647:C:H2'	1:A:648:A:H8	1.76	0.51
1:A:857:C:H3'	25:A:2218:HOH:O	2.09	0.51
3:C:91:LEU:HG	3:C:99:VAL:HG11	1.92	0.51
1:A:344:A:H5'	1:A:345:C:C5	2.45	0.51
3:C:172:ARG:NH2	3:C:174:PRO:HG3	2.26	0.51
1:A:836:G:OP1	18:R:61:LYS:NZ	2.37	0.51
1:A:1186:G:H2'	1:A:1187:G:O4'	2.10	0.51
1:A:1243:C:H5"	21:U:8:THR:CG2	2.41	0.51
1:A:976:G:H4'	1:A:977:A:OP1	2.11	0.51
1:A:1360:A:OP2	14:N:35:ARG:NH2	2.44	0.51
1:A:216:G:C2	1:A:217:C:C4	2.99	0.51
1:A:1095:U:P	1:A:1108:G:H22	2.34	0.51
1:A:60:A:H4'	1:A:61:G:O5'	2.10	0.50
15:O:15:PHE:CD2	15:O:30:ALA:HB2	2.46	0.50
1:A:731:G:OP1	1:A:766:A:H1'	2.11	0.50
1:A:1366:C:H2'	1:A:1367:C:H6	1.76	0.50
7:G:91:VAL:HG12	7:G:92:SER:N	2.27	0.50
1:A:235:C:N4	25:A:1970:HOH:O	2.44	0.50
1:A:60:A:O5'	1:A:331:G:N2	2.44	0.50
1:A:1450:U:H2'	1:A:1452:C:N4	2.26	0.50
1:A:1255:G:H2'	1:A:1279:A:N6	2.24	0.50
1:A:1447:G:N3	1:A:1447:G:H2'	2.25	0.50
1:A:321:A:H2'	1:A:322:C:C6	2.46	0.50
3:C:66:VAL:HG12	3:C:68:VAL:HG23	1.93	0.50
18:R:22:VAL:HG23	18:R:56:THR:HA	1.92	0.50
7:G:69:VAL:HG21	7:G:104:LEU:HD21	1.92	0.50
2:B:240:GLN:OE1	2:B:240:GLN:N	2.45	0.50
1:A:92:C:H2'	1:A:93:G:H8	1.76	0.50
4:D:21:LEU:HD21	4:D:67:ILE:O	2.11	0.50
1:A:826:C:H2'	1:A:827:U:H6	1.76	0.50
1:A:957:U:O2'	1:A:959:A:N7	2.38	0.50
1:A:390:C:H2'	1:A:391:G:C8	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:70:VAL:HG13	3:C:72:LYS:H	1.76	0.50
1:A:91:C:C6	1:A:92:C:C5	2.96	0.50
1:A:1303:C:H2'	1:A:1304:G:H5'	1.93	0.50
1:A:782:A:H2'	1:A:783:C:O4'	2.12	0.50
1:A:481:G:O2'	1:A:482:A:C8	2.58	0.50
6:F:4:TYR:HB2	6:F:65:VAL:CG2	2.41	0.50
6:F:91:VAL:HG12	6:F:92:LYS:O	2.12	0.50
10:J:29:ARG:NH1	10:J:84:GLN:OE1	2.35	0.50
2:B:122:PHE:CE2	2:B:139:LYS:HD3	2.46	0.50
1:A:1332:A:H2'	1:A:1333:A:C8	2.47	0.50
1:A:157:G:H2'	1:A:158:G:H8	1.75	0.50
1:A:1543:C:H6	1:A:1543:C:O5'	1.95	0.50
8:H:50:ARG:HA	8:H:59:LEU:HD23	1.92	0.50
19:S:22:LEU:HD21	19:S:28:LYS:HB2	1.92	0.50
12:L:111:LYS:H	12:L:111:LYS:HE3	1.75	0.50
10:J:65:LEU:HD23	10:J:66:ARG:N	2.27	0.50
20:T:29:LYS:O	20:T:32:ALA:HB3	2.12	0.50
1:A:1500:A:H5"	1:A:1501:C:OP2	2.12	0.50
5:E:51:VAL:N	5:E:52:PRO:HD2	2.27	0.50
1:A:778:G:H2'	1:A:779:C:O4'	2.11	0.50
1:A:781:A:C4	1:A:802:A:C2	3.00	0.50
1:A:455:C:C2'	1:A:456:C:H5'	2.42	0.50
1:A:721:G:C6	1:A:733:A:C2	3.00	0.50
7:G:79:ARG:HB2	7:G:84:ASN:CG	2.32	0.50
12:L:82:VAL:O	12:L:106:ASP:HB2	2.11	0.50
1:A:1494:G:C2	1:A:1495:U:C4	3.00	0.50
8:H:2:LEU:HD23	8:H:3:THR:H	1.75	0.50
8:H:124:ALA:O	8:H:128:GLY:N	2.45	0.50
2:B:97:TRP:HH2	2:B:176:GLU:CD	2.14	0.50
4:D:152:SER:O	4:D:155:LEU:HB2	2.12	0.50
1:A:1016:A:O2'	1:A:1217:C:O2	2.29	0.50
1:A:5:U:H4'	1:A:6:G:O5'	2.11	0.50
1:A:1486:G:H2'	1:A:1487:G:O4'	2.12	0.49
1:A:1040:U:H2'	1:A:1041:A:H8	1.76	0.49
1:A:77:G:N1	1:A:93:G:C5	2.80	0.49
15:O:2:PRO:O	15:O:3:ILE:HG13	2.11	0.49
1:A:353:A:H8	1:A:353:A:H5'	1.77	0.49
1:A:1046:A:H3'	1:A:1047:G:H8	1.78	0.49
1:A:78:G:C6	1:A:92:C:N4	2.80	0.49
1:A:95:U:O2'	1:A:96:G:H5'	2.12	0.49
1:A:1370:G:C2	1:A:1371:G:N7	2.80	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:120:THR:HG23	8:H:123:GLU:OE1	2.12	0.49
1:A:1442:G:C5	1:A:1446:A:N6	2.80	0.49
1:A:677:U:H2'	1:A:678:U:H6	1.76	0.49
6:F:23:LYS:O	6:F:27:GLN:HG2	2.12	0.49
1:A:583:A:H2'	1:A:584:G:O4'	2.12	0.49
1:A:1392:G:H21	1:A:1502:A:H8	1.59	0.49
1:A:978:A:O2'	1:A:1322:C:N3	2.44	0.49
4:D:102:ASP:HB3	4:D:136:PRO:HB3	1.94	0.49
1:A:149:A:H2'	1:A:150:C:C6	2.47	0.49
1:A:156:G:H1	1:A:165:C:H42	1.59	0.49
5:E:149:GLU:O	5:E:153:LYS:HB2	2.12	0.49
1:A:75:G:N1	1:A:96:G:C6	2.80	0.49
1:A:865:A:O5'	1:A:865:A:H8	1.96	0.49
1:A:1126:U:H3	1:A:1149:C:H1'	1.77	0.49
1:A:908:A:C2	1:A:909:A:C4	3.00	0.49
2:B:18:GLY:HA3	2:B:42:ILE:H	1.76	0.49
1:A:98:U:H2'	1:A:99:C:C6	2.48	0.49
3:C:18:TRP:CD1	14:N:54:PRO:HA	2.47	0.49
1:A:705:U:H5"	1:A:706:A:OP2	2.13	0.49
1:A:35:G:H2'	1:A:36:C:C6	2.48	0.49
1:A:409:G:OP1	4:D:24:GLU:O	2.31	0.49
1:A:790:A:H3'	1:A:791:G:C8	2.48	0.49
3:C:43:LEU:HD23	3:C:47:LEU:HD13	1.94	0.49
9:I:18:PHE:CD1	9:I:62:TYR:HD2	2.31	0.49
8:H:20:TYR:HA	8:H:65:TYR:CE2	2.48	0.49
16:P:10:GLY:CA	16:P:16:HIS:H	2.26	0.49
8:H:121:ASP:HB2	8:H:125:ARG:NH2	2.28	0.49
1:A:325:A:H2'	1:A:326:G:O4'	2.13	0.49
1:A:997:U:H2'	1:A:998:G:O4'	2.13	0.49
5:E:99:GLY:O	5:E:101:ILE:HG12	2.12	0.49
21:U:18:TYR:CD2	21:U:24:ARG:HA	2.48	0.49
12:L:78:GLN:HG2	12:L:81:SER:HB3	1.95	0.49
3:C:152:ILE:HG22	3:C:153:VAL:O	2.13	0.49
8:H:28:ALA:CB	8:H:59:LEU:HG	2.43	0.49
9:I:108:VAL:HG12	9:I:109:VAL:N	2.23	0.49
1:A:1513:A:H2'	1:A:1514:C:C6	2.47	0.49
1:A:1347:G:O6	9:I:10:ARG:NH2	2.37	0.49
1:A:825:G:H2'	1:A:826:C:O4'	2.13	0.49
14:N:12:ARG:HG2	14:N:14:PRO:HD3	1.94	0.49
10:J:24:VAL:HG22	10:J:72:VAL:HG11	1.95	0.49
11:K:27:ASN:ND2	11:K:29:ILE:HG22	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1030:C:H2'	1:A:1030(A):G:C8	2.48	0.49
1:A:688:G:H1	1:A:699:C:H42	1.60	0.49
9:I:99:LEU:HB3	9:I:101:PHE:CD1	2.47	0.49
1:A:186:C:H2'	1:A:187:C:C6	2.47	0.49
1:A:7:G:H5'	1:A:298:A:H5'	1.94	0.49
8:H:45:ILE:O	8:H:45:ILE:HG12	2.08	0.49
8:H:41:ARG:NH1	8:H:123:GLU:OE2	2.42	0.49
3:C:35:GLU:O	3:C:39:ILE:HG13	2.13	0.49
1:A:673:G:H5'	6:F:87:ARG:CD	2.42	0.49
7:G:65:ALA:HB2	7:G:128:ALA:HB2	1.95	0.49
1:A:1005:A:H8	1:A:1006:C:C6	2.31	0.49
2:B:59:GLU:HB2	2:B:221:LEU:HD21	1.94	0.49
3:C:164:ARG:HG2	3:C:165:THR:N	2.27	0.49
11:K:84:VAL:HG11	11:K:91:ARG:HD3	1.95	0.49
1:A:1250:A:H2	1:A:1353:G:H21	1.61	0.48
8:H:11:THR:O	8:H:12:ARG:C	2.50	0.48
18:R:73:ALA:CB	18:R:79:LEU:HD12	2.42	0.48
7:G:91:VAL:HG11	7:G:96:GLN:HG3	1.95	0.48
10:J:82:ILE:HD12	10:J:82:ILE:H	1.77	0.48
15:O:5:LYS:O	15:O:8:LYS:N	2.44	0.48
1:A:149:A:H2'	1:A:150:C:H6	1.78	0.48
1:A:1351:U:H4'	7:G:33:ASP:OD2	2.13	0.48
1:A:1173:G:C6	1:A:1174:G:C5	3.01	0.48
12:L:34:ARG:HB2	12:L:105:TYR:CE1	2.47	0.48
6:F:9:VAL:HG13	6:F:60:PHE:CD2	2.48	0.48
1:A:411:A:H62	1:A:413:G:N2	2.11	0.48
1:A:1412:C:H2'	1:A:1413:A:H8	1.75	0.48
1:A:338:A:C2	1:A:339:C:C2	3.01	0.48
1:A:1399:C:C6	1:A:1502:A:N6	2.81	0.48
1:A:1074:G:O4'	2:B:104:ASN:HB2	2.12	0.48
1:A:654:G:H2'	1:A:655:A:C8	2.48	0.48
9:I:111:ARG:HH22	10:J:62:HIS:HE1	1.60	0.48
1:A:122:G:C2	1:A:123:C:C2	3.01	0.48
12:L:113:ARG:HH12	12:L:116:SER:N	2.12	0.48
1:A:1023:G:H3'	1:A:1024:G:C5'	2.43	0.48
3:C:20:SER:O	14:N:54:PRO:HB3	2.14	0.48
1:A:1291:G:H2'	1:A:1292:U:C6	2.48	0.48
1:A:1054:C:OP1	1:A:1197:G:OP1	2.31	0.48
3:C:153:VAL:HG12	3:C:154:SER:N	2.23	0.48
12:L:27:LEU:CA	12:L:29:GLY:H	2.27	0.48
1:A:91:C:C5	1:A:92:C:C5	2.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:67:GLU:OE1	13:M:71:ARG:NH2	2.47	0.48
8:H:86:ILE:HG22	8:H:87:SER:N	2.28	0.48
2:B:17:PHE:CD1	2:B:18:GLY:N	2.81	0.48
1:A:954:G:N2	1:A:1227:A:H62	2.11	0.48
1:A:1502:A:H2'	1:A:1504:G:N7	2.28	0.48
1:A:688:G:H2'	1:A:689:C:H6	1.78	0.48
1:A:765:G:C6	1:A:812:C:C2	3.01	0.48
20:T:67:ALA:HB2	20:T:77:ALA:HB2	1.95	0.48
2:B:160:ASP:N	2:B:160:ASP:OD2	2.46	0.48
17:Q:29:HIS:CD2	17:Q:31:LEU:H	2.31	0.48
8:H:104:ARG:HG2	8:H:104:ARG:HH11	1.78	0.48
1:A:1413:A:C2	1:A:1488:G:C2	3.01	0.48
3:C:44:GLU:HG3	3:C:52:LEU:HD22	1.96	0.48
14:N:15:LYS:HE2	14:N:16:PHE:CZ	2.49	0.48
1:A:344:A:H5'	1:A:345:C:H5	1.78	0.48
6:F:35:ALA:HA	6:F:67:MET:HB3	1.95	0.48
17:Q:63:ARG:HG2	17:Q:64:PRO:N	2.29	0.48
1:A:373:A:H1'	1:A:481:G:N3	2.27	0.48
13:M:34:LEU:CD1	13:M:41:PRO:HA	2.42	0.48
1:A:1265:G:C6	1:A:1266:G:C6	3.01	0.48
4:D:170:VAL:HG13	4:D:174:LEU:HB2	1.95	0.48
1:A:953:G:H2'	1:A:954:G:O4'	2.12	0.48
3:C:73:PRO:HG3	3:C:105:GLU:CD	2.33	0.48
1:A:259:G:H2'	1:A:260:G:O4'	2.13	0.48
5:E:11:ILE:HG22	5:E:12:LEU:HD13	1.95	0.48
1:A:78:G:C2	1:A:92:C:C2	3.02	0.48
18:R:45:SER:HB3	18:R:47:THR:O	2.14	0.48
3:C:71:ALA:HB1	3:C:109:PRO:HB3	1.96	0.48
18:R:25:THR:OG1	18:R:25:THR:O	2.14	0.48
1:A:1426:C:H42	1:A:1474:G:H1	1.61	0.48
2:B:172:ILE:H	2:B:172:ILE:HD12	1.78	0.48
1:A:1255:G:C8	1:A:1279:A:N6	2.78	0.48
20:T:84:LEU:O	20:T:88:VAL:HG23	2.14	0.48
2:B:38:GLY:O	2:B:39:ILE:HD13	2.14	0.48
13:M:16:ASP:HB3	13:M:34:LEU:HD12	1.95	0.48
1:A:1265:G:H2'	1:A:1266:G:O4'	2.14	0.48
2:B:47:THR:OG1	2:B:202:PRO:O	2.32	0.48
13:M:37:THR:HB	13:M:39:ILE:HG13	1.95	0.48
6:F:6:VAL:HB	6:F:63:TYR:HB2	1.96	0.48
1:A:429:U:H1'	1:A:430:A:H5"	1.96	0.48
14:N:16:PHE:CD1	14:N:19:ARG:NH1	2.82	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:22:LEU:O	7:G:25:ALA:HB3	2.14	0.48
13:M:52:GLU:HG2	13:M:55:ARG:NH2	2.29	0.48
4:D:61:LYS:HE2	4:D:72:GLU:OE2	2.13	0.48
2:B:44:LEU:HD23	2:B:44:LEU:HA	1.67	0.48
1:A:880:C:OP1	12:L:12:ARG:NH1	2.46	0.48
10:J:69:ASN:C	10:J:70:ARG:HG2	2.34	0.48
13:M:17:VAL:O	13:M:20:THR:HB	2.13	0.48
1:A:267:C:H2'	1:A:268:C:C6	2.49	0.48
4:D:88:VAL:O	4:D:92:VAL:HG23	2.13	0.48
1:A:1346:A:O2'	1:A:1347:G:OP2	2.26	0.48
1:A:919:A:O2'	1:A:920:U:H5'	2.14	0.48
5:E:36:ASP:C	5:E:38:GLN:H	2.18	0.48
1:A:1082:G:O2'	1:A:1083:U:H5'	2.14	0.48
1:A:1201:A:H4'	1:A:1202:G:C5'	2.44	0.47
1:A:93:G:C2	1:A:95:U:N1	2.82	0.47
1:A:1368:G:OP2	9:I:112:LYS:HD3	2.14	0.47
4:D:15:GLU:O	4:D:17:VAL:HG13	2.14	0.47
21:U:5:ASP:O	21:U:11:GLY:HA3	2.14	0.47
17:Q:44:ALA:HB1	17:Q:72:ARG:HA	1.95	0.47
1:A:299:G:C6	1:A:300:A:C6	3.02	0.47
4:D:187:ARG:HD2	4:D:187:ARG:HA	1.65	0.47
1:A:267:C:H2'	1:A:268:C:H6	1.79	0.47
1:A:402:G:C6	1:A:403:C:C4	3.02	0.47
21:U:10:ARG:HA	21:U:13:ILE:HB	1.96	0.47
1:A:1314:C:H41	19:S:6:LYS:NZ	2.11	0.47
1:A:766:A:C8	1:A:814:A:N6	2.82	0.47
1:A:357:G:H1'	1:A:368:U:O2	2.14	0.47
5:E:127:ASN:HA	5:E:128:PRO:HD3	1.75	0.47
15:O:18:PHE:HD1	15:O:19:PRO:O	1.97	0.47
1:A:594:G:H1	1:A:645:C:H42	1.62	0.47
3:C:139:GLN:O	3:C:143:GLU:HB2	2.14	0.47
1:A:858:G:C8	25:A:2218:HOH:O	2.56	0.47
10:J:50:ILE:HG22	10:J:60:ARG:HD3	1.96	0.47
1:A:939:G:H5"	7:G:102:ARG:NH1	2.30	0.47
1:A:581:G:C8	25:A:2214:HOH:O	2.66	0.47
1:A:236:G:H2'	1:A:237:C:O4'	2.13	0.47
12:L:47:LYS:HE2	12:L:47:LYS:HB2	1.56	0.47
1:A:767:A:H2'	1:A:768:A:O4'	2.14	0.47
1:A:1009:G:N2	1:A:1020:U:O2	2.48	0.47
1:A:96:G:H2'	1:A:97:G:C8	2.49	0.47
9:I:112:LYS:HG2	9:I:113:LYS:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:13:ILE:HG22	21:U:14:TRP:N	2.29	0.47
1:A:976:G:N7	1:A:1358:U:N3	2.61	0.47
3:C:94:LEU:HA	3:C:94:LEU:HD13	1.67	0.47
1:A:632:A:H2'	1:A:633:G:H5'	1.96	0.47
1:A:1007:C:H2'	1:A:1008:C:H5	1.77	0.47
1:A:1028:C:N4	1:A:1034:G:H21	2.13	0.47
1:A:103:C:O2'	1:A:172:A:N1	2.31	0.47
18:R:43:PHE:O	18:R:51:LEU:HB2	2.15	0.47
5:E:40:ARG:HB3	5:E:66:MET:HE2	1.96	0.47
1:A:925:G:C2	1:A:927:G:C8	3.02	0.47
1:A:407:G:O2'	4:D:116:GLN:HG3	2.13	0.47
5:E:31:LEU:HA	5:E:31:LEU:HD23	1.55	0.47
1:A:88:A:H2'	1:A:89:C:H6	1.78	0.47
1:A:1368:G:C5'	9:I:112:LYS:HB3	2.42	0.47
1:A:1361(A):C:HO2'	1:A:1362:C:H5"	1.79	0.47
1:A:1361(A):C:O2'	1:A:1362:C:O4'	2.32	0.47
1:A:781:A:H2'	1:A:782:A:H5'	1.96	0.47
12:L:55:VAL:HG12	12:L:69:TYR:HA	1.95	0.47
5:E:152:ARG:CZ	8:H:44:PHE:HE1	2.28	0.47
1:A:103:C:OP1	20:T:17:ARG:NH1	2.47	0.47
5:E:52:PRO:O	5:E:55:VAL:HG12	2.14	0.47
1:A:788:U:H2'	1:A:789:U:O4'	2.14	0.47
2:B:126:GLU:HA	2:B:129:GLU:HG3	1.96	0.47
1:A:1144:G:H22	1:A:1146:A:H62	1.62	0.47
1:A:941:G:C6	1:A:942:G:C8	3.03	0.47
1:A:959:A:HO2'	1:A:984:C:HO2'	1.58	0.47
21:U:12:LYS:HB3	21:U:22:ARG:HD2	1.96	0.47
1:A:123:C:OP1	1:A:312:C:H5'	2.14	0.47
1:A:130:A:H1'	1:A:263:A:O2'	2.15	0.47
1:A:106:C:C2'	1:A:107:G:H5'	2.45	0.47
4:D:174:LEU:O	4:D:186:LEU:HD11	2.14	0.47
1:A:778:G:H8	1:A:778:G:O5'	1.96	0.47
4:D:23:GLY:HA3	4:D:112:VAL:HG12	1.96	0.47
4:D:140:VAL:HG11	4:D:146:ILE:HD11	1.96	0.47
17:Q:87:LYS:HE3	17:Q:87:LYS:HA	1.97	0.47
20:T:36:LEU:HA	20:T:36:LEU:HD23	1.49	0.47
4:D:32:ALA:O	4:D:36:ARG:N	2.48	0.47
15:O:33:THR:O	15:O:36:ILE:HB	2.15	0.47
10:J:47:PHE:HB3	14:N:34:TYR:CE2	2.42	0.47
18:R:79:LEU:HD23	18:R:80:PRO:HD2	1.96	0.47
1:A:1003(A):G:H3'	1:A:1004:A:H5"	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:81:GLU:CD	5:E:88:LYS:HE3	2.35	0.47
3:C:59:ARG:HE	3:C:59:ARG:HB2	1.60	0.47
2:B:98:LEU:HB2	2:B:101:MET:HG3	1.96	0.47
1:A:1117:G:N2	1:A:1180:A:O2'	2.47	0.47
3:C:167:TRP:CE3	3:C:168:ALA:N	2.75	0.47
1:A:1022:G:H2'	1:A:1023:G:H5"	1.97	0.47
1:A:62:U:H2'	1:A:63:C:H6	1.78	0.47
5:E:84:PHE:CB	5:E:134:ALA:HB2	2.45	0.47
1:A:1106:G:H5"	3:C:172:ARG:HB3	1.96	0.47
1:A:766:A:OP2	25:A:2188:HOH:O	2.21	0.47
1:A:1074:G:C6	1:A:1075:C:C4	3.02	0.47
4:D:100:ARG:NH1	4:D:137:SER:HA	2.30	0.47
11:K:98:LEU:HA	11:K:98:LEU:HD12	1.54	0.47
8:H:36:LEU:HA	8:H:36:LEU:HD23	1.72	0.47
1:A:1240:U:C2	7:G:32:ARG:HD2	2.50	0.47
3:C:54:ARG:H	3:C:69:HIS:HB2	1.79	0.47
20:T:52:ALA:O	20:T:56:MET:HB2	2.15	0.47
20:T:56:MET:HG3	20:T:88:VAL:HG21	1.97	0.47
1:A:1357:A:H5"	1:A:1358:U:OP2	2.15	0.47
16:P:67:THR:HG22	16:P:69:THR:N	2.27	0.47
18:R:46:GLU:OE2	18:R:86:VAL:N	2.30	0.47
1:A:707:C:H5"	11:K:20:TYR:CD2	2.50	0.47
1:A:953:G:C5'	1:A:965:A:H61	2.27	0.47
1:A:309:G:O2'	1:A:607:A:N1	2.48	0.47
1:A:824:C:H42	1:A:876:G:H1	1.63	0.47
1:A:723:U:O2	1:A:723:U:H2'	2.14	0.47
5:E:139:LEU:HA	5:E:139:LEU:HD23	1.61	0.47
1:A:941:G:C2	1:A:1343:G:C2	3.03	0.47
9:I:96:LEU:HB3	9:I:102:LEU:HG	1.97	0.47
4:D:61:LYS:HD3	4:D:206:PHE:CE2	2.49	0.47
1:A:1262:C:H2'	1:A:1263:C:C6	2.50	0.47
13:M:4:ILE:HG23	13:M:57:ARG:HA	1.97	0.47
2:B:55:PHE:HA	2:B:58:ILE:HG12	1.95	0.47
12:L:93:LEU:HD12	12:L:96:VAL:HG21	1.95	0.47
1:A:1358:U:H5"	14:N:35:ARG:HG3	1.96	0.47
1:A:1361:G:O5'	1:A:1361:G:H8	1.98	0.47
7:G:26:PHE:HA	7:G:101:LEU:HD13	1.96	0.47
1:A:160:A:HO2'	1:A:161:A:P	2.37	0.47
9:I:63:ILE:HG21	9:I:77:ILE:HG12	1.96	0.47
1:A:1314:C:H2'	1:A:1315:U:C6	2.50	0.47
1:A:699:C:C2'	1:A:700:G:H5'	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:34:ASP:O	11:K:37:GLY:N	2.31	0.47
6:F:24:GLU:HG3	6:F:28:ARG:HD2	1.97	0.47
1:A:328:C:O2	1:A:328:C:H2'	2.15	0.47
17:Q:84:LEU:HD23	17:Q:84:LEU:HA	1.49	0.47
1:A:1053:G:HO2'	1:A:1199:U:H5	1.62	0.46
8:H:73:ASP:HA	8:H:74:PRO:HD2	1.68	0.46
8:H:28:ALA:HB2	8:H:59:LEU:HG	1.98	0.46
1:A:1109:C:OP2	3:C:176:HIS:ND1	2.47	0.46
1:A:1361(A):C:H2'	1:A:1362:C:H5"	1.97	0.46
2:B:103:THR:N	2:B:176:GLU:OE1	2.47	0.46
5:E:117:ASP:OD2	5:E:117:ASP:N	2.48	0.46
1:A:44:G:N2	1:A:399:G:C4	2.83	0.46
1:A:1450:U:H2'	1:A:1452:C:H41	1.78	0.46
19:S:12:ASP:OD2	19:S:35:SER:OG	2.32	0.46
1:A:942:G:N3	1:A:943:U:C6	2.83	0.46
1:A:839:U:C5'	1:A:840:C:H5	2.28	0.46
17:Q:75:ARG:HB2	17:Q:75:ARG:NH1	2.30	0.46
2:B:30:ARG:HG3	2:B:31:TYR:CE2	2.49	0.46
1:A:204:U:H4'	1:A:216:G:OP1	2.14	0.46
1:A:509:A:H5"	4:D:55:ALA:HB2	1.97	0.46
12:L:117:ARG:HB3	12:L:122:THR:O	2.15	0.46
1:A:1381:U:C5	1:A:1382:C:C5	3.03	0.46
1:A:192:U:H4'	20:T:57:ARG:HD2	1.97	0.46
6:F:33:TYR:CD1	6:F:75:LEU:HD23	2.50	0.46
3:C:91:LEU:O	3:C:95:THR:HG23	2.16	0.46
14:N:21:TYR:HD1	14:N:21:TYR:N	2.12	0.46
11:K:18:ARG:HB3	11:K:33:THR:HG23	1.96	0.46
4:D:61:LYS:HD2	4:D:207:TYR:OH	2.16	0.46
1:A:150:C:H2'	1:A:151:A:O5'	2.16	0.46
9:I:99:LEU:HD13	9:I:101:PHE:HE1	1.80	0.46
5:E:8:GLU:OE1	5:E:63:ARG:NH2	2.49	0.46
1:A:657:G:H4'	15:O:28:GLN:HG3	1.96	0.46
1:A:411:A:C5	1:A:413:G:N3	2.84	0.46
8:H:69:ARG:N	8:H:74:PRO:O	2.46	0.46
9:I:20:ARG:O	9:I:60:ASP:N	2.49	0.46
11:K:101:SER:HG	11:K:103:LEU:H	1.59	0.46
1:A:130:A:C8	17:Q:63:ARG:HG3	2.50	0.46
19:S:31:ILE:HA	19:S:31:ILE:HD13	1.78	0.46
1:A:369:C:C2'	1:A:370:C:H5'	2.45	0.46
1:A:1126:U:H2'	1:A:1127:G:H5'	1.97	0.46
4:D:173:TRP:O	4:D:186:LEU:HG	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:39:LEU:HD13	15:O:56:LEU:HB2	1.97	0.46
1:A:436:C:C2	1:A:437:U:C5	3.04	0.46
1:A:353:A:H5'	1:A:353:A:C8	2.50	0.46
1:A:374:A:H2'	1:A:375:U:C6	2.51	0.46
1:A:101:A:H2'	1:A:102:G:H8	1.81	0.46
3:C:34:LEU:HD22	3:C:38:ARG:HE	1.80	0.46
1:A:1347:G:H22	1:A:1374:A:P	2.39	0.46
1:A:1374:A:C4	1:A:1375:A:C8	3.03	0.46
1:A:1064:G:N2	1:A:1190:G:H2'	2.31	0.46
1:A:837:G:H1	1:A:849:C:N4	2.13	0.46
17:Q:74:LEU:HB3	17:Q:75:ARG:HG2	1.97	0.46
1:A:695:A:C2	1:A:787:A:H1'	2.51	0.46
8:H:97:VAL:O	8:H:100:ILE:HG13	2.16	0.46
13:M:77:ASN:O	13:M:80:ARG:HB3	2.16	0.46
1:A:1305:G:O2'	1:A:1306:A:P	2.73	0.46
1:A:1237:C:N4	1:A:1336:C:O2	2.48	0.46
4:D:100:ARG:HH12	4:D:137:SER:HB3	1.81	0.46
1:A:748:C:H4'	1:A:749:C:O5'	2.16	0.46
1:A:547:A:H4'	1:A:548:G:O5'	2.15	0.46
20:T:84:LEU:HD22	20:T:88:VAL:CG2	2.46	0.46
8:H:38:ILE:HD13	8:H:41:ARG:HH21	1.78	0.46
12:L:92:0TD:N	12:L:92:0TD:OD1	2.44	0.46
1:A:235:C:C5'	17:Q:70:ARG:HG2	2.45	0.46
2:B:87:ARG:HH21	2:B:219:VAL:HG12	1.79	0.46
1:A:131:C:O2	1:A:262:A:H2	1.97	0.46
1:A:195:A:H5'	1:A:196:A:OP2	2.15	0.46
16:P:60:LEU:HD23	16:P:60:LEU:HA	1.56	0.46
1:A:1249:C:HO2'	9:I:73:GLN:NE2	2.10	0.46
15:O:32:LEU:HD22	15:O:32:LEU:HA	1.76	0.46
15:O:36:ILE:HG12	15:O:59:MET:HG2	1.98	0.46
1:A:1287:A:H2	1:A:1353:G:N3	2.13	0.46
8:H:86:ILE:HD12	8:H:86:ILE:HG23	1.66	0.46
1:A:1191:A:C4	1:A:1192:C:C5	3.04	0.46
1:A:1117:G:H4'	9:I:104:ARG:NH1	2.30	0.46
1:A:1410:G:C4	1:A:1411:C:C5	3.04	0.46
1:A:620:C:H2'	1:A:621:A:C8	2.51	0.46
1:A:460:A:C6	1:A:462:G:C6	3.04	0.46
4:D:205:GLU:O	4:D:208:SER:HB3	2.16	0.46
1:A:413:G:H3'	1:A:413:G:C8	2.51	0.46
10:J:38:ILE:HD11	10:J:71:LEU:N	2.30	0.46
1:A:1337:G:H5"	1:A:1338:G:OP1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:15:GLU:CD	4:D:59:ARG:HH21	2.18	0.46
1:A:1175:G:H2'	1:A:1176:A:H8	1.78	0.46
1:A:1064:G:OP1	1:A:1386:G:H4'	2.16	0.46
1:A:1189:C:H4'	3:C:10:PHE:CE2	2.50	0.46
5:E:118:ILE:O	5:E:119:LEU:HD23	2.15	0.46
1:A:977:A:O2'	1:A:978:A:H5"	2.16	0.46
1:A:394:G:H2'	1:A:395:C:H6	1.79	0.46
4:D:155:LEU:HD23	4:D:156:GLU:N	2.30	0.46
16:P:8:ARG:HG2	16:P:10:GLY:H	1.80	0.46
1:A:509:A:O2'	1:A:510:A:OP1	2.21	0.46
6:F:8:ILE:HD13	6:F:26:ILE:HD13	1.96	0.46
1:A:179:A:H2'	1:A:180:U:H6	1.81	0.46
3:C:25:GLY:HA2	3:C:29:TYR:HB2	1.97	0.46
1:A:316:G:OP2	1:A:351:G:O2'	2.34	0.46
2:B:201:ILE:HG21	2:B:214:ILE:HG21	1.98	0.46
16:P:74:LEU:HD22	16:P:79:VAL:HG21	1.98	0.46
1:A:1090:U:H2'	1:A:1091:U:C6	2.45	0.46
9:I:49:PRO:O	9:I:53:VAL:HB	2.16	0.46
1:A:181:G:C6	1:A:194:C:N3	2.84	0.46
1:A:106:C:H2'	1:A:107:G:O4'	2.15	0.46
9:I:17:VAL:HG11	9:I:81:ILE:HA	1.98	0.46
1:A:197:A:N3	1:A:198:G:H1'	2.30	0.46
20:T:20:LEU:O	20:T:23:ARG:HB3	2.16	0.46
1:A:668:G:H1'	15:O:46:HIS:HD2	1.81	0.46
7:G:138:LYS:HE2	7:G:139:GLU:HG3	1.98	0.46
17:Q:31:LEU:HA	17:Q:31:LEU:HD12	1.55	0.45
1:A:1338:G:C6	1:A:1339:A:C6	3.04	0.45
9:I:66:ARG:HB2	9:I:66:ARG:HE	1.43	0.45
1:A:750:G:N3	15:O:23:GLY:HA3	2.30	0.45
19:S:28:LYS:HD3	19:S:31:ILE:HG12	1.98	0.45
1:A:699:C:H2'	1:A:700:G:H5'	1.97	0.45
1:A:972:C:H4'	10:J:57:LYS:CD	2.46	0.45
1:A:1151:A:H5"	10:J:41:PRO:HA	1.98	0.45
2:B:155:LEU:HA	2:B:155:LEU:HD23	1.74	0.45
4:D:78:LEU:HD21	4:D:96:LEU:HB3	1.98	0.45
1:A:1193:G:H2'	1:A:1194:U:H6	1.81	0.45
1:A:190(K):G:H2'	1:A:190(L):U:C6	2.52	0.45
20:T:43:LEU:HG	20:T:43:LEU:H	1.40	0.45
1:A:411:A:N6	1:A:413:G:C2	2.84	0.45
4:D:30:LYS:O	4:D:32:ALA:N	2.49	0.45
1:A:1279:A:OP2	10:J:9:ARG:NH1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:17:ASP:OD1	3:C:21:ARG:NH1	2.49	0.45
1:A:1392:G:O2'	1:A:1393:U:H5'	2.17	0.45
14:N:14:PRO:O	14:N:15:LYS:HB3	2.16	0.45
8:H:87:SER:HA	8:H:93:VAL:HG23	1.98	0.45
19:S:49:ILE:O	19:S:60:VAL:HG12	2.16	0.45
1:A:372:C:H4'	1:A:373:A:O5'	2.16	0.45
1:A:738:C:P	6:F:92:LYS:HD3	2.56	0.45
1:A:518:C:H1'	12:L:50:SER:HB3	1.98	0.45
8:H:25:ASP:OD1	8:H:60:ARG:HD3	2.15	0.45
1:A:331:G:H5'	25:A:1996:HOH:O	2.16	0.45
1:A:200:G:H2'	1:A:201:C:O4'	2.17	0.45
1:A:1107:C:C4	1:A:1108:G:C8	3.04	0.45
1:A:735:C:H5'	18:R:71:LYS:HD3	1.98	0.45
8:H:97:VAL:HG23	8:H:129:VAL:O	2.16	0.45
12:L:58:VAL:O	12:L:65:GLU:HA	2.16	0.45
19:S:74:PHE:N	19:S:74:PHE:CD1	2.85	0.45
1:A:1053:G:O2'	1:A:1199:U:H5	1.99	0.45
1:A:1046:A:H5'	1:A:1047:G:OP2	2.17	0.45
1:A:1435:G:O5'	1:A:1435:G:H8	2.00	0.45
1:A:1221:G:C4	1:A:1222:G:C8	3.04	0.45
1:A:980:C:H3'	1:A:981:U:H6	1.81	0.45
1:A:1359:C:P	14:N:35:ARG:HH11	2.40	0.45
1:A:234:C:H2'	1:A:235:C:C6	2.52	0.45
1:A:1216:G:H5"	14:N:5:ALA:HB2	1.98	0.45
1:A:597:G:H2'	1:A:598:U:H5'	1.99	0.45
1:A:647:C:H2'	1:A:648:A:C8	2.52	0.45
1:A:98:U:H2'	1:A:99:C:H6	1.80	0.45
4:D:177:ASP:OD2	4:D:179:GLU:HB2	2.16	0.45
5:E:89:ILE:HG21	5:E:135:THR:HA	1.99	0.45
7:G:87:VAL:HA	7:G:88:PRO:HD3	1.71	0.45
1:A:1124:G:H5'	10:J:35:SER:O	2.17	0.45
9:I:93:ARG:HB3	9:I:93:ARG:HH11	1.81	0.45
1:A:958:A:C5	19:S:55:LYS:HB2	2.50	0.45
1:A:986:A:H4'	19:S:55:LYS:NZ	2.32	0.45
12:L:25:PRO:HB3	12:L:27:LEU:CD2	2.42	0.45
1:A:1348:U:O2'	9:I:120:ARG:HD2	2.16	0.45
7:G:17:VAL:HG12	7:G:18:TYR:HD1	1.82	0.45
7:G:40:ALA:CB	9:I:41:VAL:HG21	2.47	0.45
1:A:1064:G:H1'	1:A:1190:G:H21	1.81	0.45
1:A:978:A:OP1	1:A:1361:G:N2	2.46	0.45
1:A:1417:G:N2	1:A:1484:C:C4	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:U:O2'	1:A:84:U:H5'	2.16	0.45
20:T:20:LEU:HD13	20:T:20:LEU:HA	1.66	0.45
6:F:5:GLU:OE1	18:R:34:TYR:OH	2.24	0.45
1:A:1465:C:H2'	1:A:1466:C:O4'	2.16	0.45
1:A:1092:A:H5'	7:G:4:ARG:NH1	2.31	0.45
2:B:194:PRO:HA	2:B:200:ILE:HD11	1.98	0.45
3:C:179:ARG:HD2	3:C:206:GLU:HG3	1.98	0.45
1:A:1102:A:H2'	1:A:1103:C:H6	1.82	0.45
17:Q:37:LYS:C	17:Q:38:ARG:HD2	2.36	0.45
3:C:101:LEU:HD23	3:C:102:ASN:H	1.82	0.45
2:B:24:TRP:HA	2:B:191:ASP:HA	1.99	0.45
3:C:116:VAL:HG21	3:C:202:ILE:HD11	1.97	0.45
1:A:509:A:OP2	25:A:2198:HOH:O	2.21	0.45
1:A:654:G:H2'	1:A:655:A:H8	1.81	0.45
1:A:1292:U:H2'	1:A:1293:G:H8	1.81	0.45
7:G:138:LYS:HG2	7:G:139:GLU:N	2.31	0.45
11:K:11:LYS:NZ	11:K:11:LYS:HB2	2.31	0.45
20:T:75:ASN:O	20:T:78:ALA:N	2.49	0.45
6:F:33:TYR:HD1	6:F:75:LEU:HD23	1.81	0.45
1:A:1504:G:H4'	1:A:1505:G:H5'	1.97	0.45
1:A:1507:A:C2	1:A:1508:G:C4	3.05	0.45
1:A:1094:G:OP2	1:A:1095:U:C5	2.69	0.45
1:A:1226:C:H4'	1:A:1227:A:OP1	2.16	0.45
1:A:425:G:C2'	1:A:426:G:H5'	2.47	0.45
17:Q:77:VAL:HG12	17:Q:78:GLU:N	2.30	0.45
1:A:922:G:C6	1:A:923:A:C6	3.05	0.45
13:M:106:ASN:N	13:M:106:ASN:OD1	2.49	0.45
8:H:104:ARG:HG3	8:H:138:TRP:CD2	2.51	0.45
13:M:94:ARG:HB3	13:M:96:LEU:CD1	2.46	0.45
1:A:105:G:H2'	1:A:106:C:C6	2.51	0.45
1:A:62:U:O2'	1:A:379:C:O2	2.29	0.45
1:A:578:C:H2'	1:A:579:G:O4'	2.16	0.45
1:A:734:G:H21	18:R:75:ILE:HD13	1.82	0.45
7:G:120:ILE:O	7:G:124:LEU:HB2	2.17	0.45
15:O:79:ARG:O	15:O:83:GLU:HG2	2.17	0.45
1:A:128:G:O3'	17:Q:3:LYS:NZ	2.49	0.45
1:A:1320:C:OP1	19:S:70:LYS:HE2	2.17	0.45
5:E:82:VAL:HG12	5:E:82:VAL:O	2.15	0.45
12:L:123:LYS:HG2	12:L:123:LYS:H	1.45	0.45
12:L:11:VAL:H	12:L:11:VAL:HG23	1.40	0.45
7:G:15:ASP:OD2	7:G:16:LEU:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1189:C:P	10:J:51:ARG:HH22	2.40	0.45
19:S:28:LYS:HG2	19:S:29:ARG:H	1.82	0.45
1:A:1410:G:C4	1:A:1491:G:N2	2.85	0.45
2:B:215:LEU:HD23	2:B:215:LEU:HA	1.58	0.45
1:A:110:C:H2'	1:A:111:G:O4'	2.16	0.45
1:A:586:C:OP1	17:Q:34:LYS:NZ	2.50	0.45
4:D:126:ILE:HD13	4:D:126:ILE:HA	1.70	0.45
1:A:1054:C:H3'	1:A:1054:C:C6	2.52	0.45
1:A:1060:C:OP1	14:N:45:ARG:NH2	2.50	0.45
1:A:1047:G:H2'	1:A:1048:G:H5'	1.99	0.45
1:A:78:G:H5'	1:A:79:G:OP2	2.16	0.45
1:A:90:U:C4	1:A:91:C:N3	2.85	0.45
1:A:1400:5MC:H4'	1:A:1544:U:C5	2.52	0.45
13:M:78:ILE:HA	13:M:81:LEU:HD23	1.97	0.45
2:B:189:ASP:OD1	2:B:205:ASP:HB3	2.16	0.45
1:A:113:G:H2'	1:A:114:U:C6	2.52	0.45
1:A:113:G:C2	1:A:315:A:N1	2.85	0.45
1:A:1361(A):C:HO2'	1:A:1362:C:H6	1.64	0.45
7:G:70:LYS:NZ	7:G:97:GLN:HA	2.32	0.45
1:A:946:A:H2'	1:A:947:G:H8	1.79	0.45
1:A:1008:C:O4'	1:A:1023:G:N2	2.50	0.45
1:A:1476:G:H2'	1:A:1477:C:H6	1.81	0.45
2:B:47:THR:O	2:B:51:LEU:HB2	2.17	0.45
5:E:13:ILE:HG22	5:E:30:ALA:HA	1.99	0.45
6:F:99:ALA:HB2	18:R:31:LEU:HG	1.99	0.45
3:C:7:PRO:HB3	3:C:11:ARG:HH21	1.81	0.45
3:C:26:LYS:HD3	3:C:26:LYS:HA	1.81	0.45
1:A:942:G:C2	1:A:943:U:C6	3.05	0.45
16:P:57:ARG:HG3	16:P:79:VAL:CG1	2.45	0.45
14:N:12:ARG:HB3	14:N:13:THR:H	1.50	0.45
15:O:81:LEU:HA	15:O:81:LEU:HD23	1.78	0.45
9:I:2:GLU:OE2	9:I:3:GLN:NE2	2.50	0.45
16:P:21:VAL:HG21	16:P:59:TRP:CG	2.52	0.45
1:A:1133:G:C2	1:A:1134:G:C8	3.05	0.45
1:A:1494:G:H2'	1:A:1495:U:H6	1.81	0.45
1:A:247:G:OP2	17:Q:100:LYS:HD2	2.16	0.45
1:A:452:A:C2	1:A:453:A:C4	3.05	0.45
1:A:1418:A:H61	1:A:1482:G:H1'	1.81	0.45
1:A:81:U:H3'	1:A:81:U:H6	1.82	0.45
1:A:428:G:C5	1:A:430:A:C6	3.05	0.44
1:A:1349:A:H2'	1:A:1350:A:O4'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:C:N3	1:A:90:U:N3	2.65	0.44
3:C:10:PHE:C	3:C:10:PHE:CD1	2.91	0.44
1:A:559:A:H4'	1:A:560:U:O5'	2.17	0.44
1:A:1031:G:C8	1:A:1032:G:N7	2.85	0.44
3:C:130:VAL:HG11	3:C:157:ILE:HG23	1.99	0.44
1:A:725:G:O2'	1:A:726:C:H5'	2.17	0.44
7:G:58:PRO:O	7:G:61:VAL:HB	2.17	0.44
4:D:163:GLU:HG3	4:D:166:LYS:HE3	1.99	0.44
1:A:960:U:H1'	1:A:1223:C:H5'	1.99	0.44
1:A:429:U:H4'	1:A:430:A:O5'	2.17	0.44
1:A:674:G:H5'	6:F:50:TYR:CE2	2.52	0.44
20:T:13:LEU:HG	20:T:13:LEU:H	1.51	0.44
1:A:1232:U:H5"	9:I:124:GLN:O	2.17	0.44
7:G:20:ASP:OD1	7:G:21:VAL:N	2.50	0.44
11:K:15:ALA:HA	11:K:77:MET:HA	1.97	0.44
12:L:84:LEU:HB3	12:L:104:VAL:HG11	1.99	0.44
1:A:96:G:H2'	1:A:97:G:H8	1.82	0.44
14:N:19:ARG:H	14:N:19:ARG:HG2	1.46	0.44
3:C:90:GLU:OE1	3:C:93:LYS:HD2	2.18	0.44
1:A:371:G:O2'	1:A:372:C:H5'	2.17	0.44
1:A:918:A:H2'	1:A:919:A:C8	2.53	0.44
1:A:108:G:O6	20:T:15:ARG:HG2	2.17	0.44
2:B:184:VAL:HG22	2:B:198:ASP:OD2	2.17	0.44
4:D:65:ARG:HG3	4:D:70:ILE:HG22	1.99	0.44
1:A:1454:G:H2'	1:A:1455:G:H8	1.82	0.44
8:H:111:ILE:HG22	8:H:134:ILE:HB	1.99	0.44
19:S:11:VAL:HA	19:S:38:SER:HB2	2.00	0.44
12:L:25:PRO:C	12:L:27:LEU:HB2	2.37	0.44
1:A:80:G:N2	1:A:90:U:H3	2.16	0.44
1:A:1250:A:O2'	1:A:1370:G:O2'	2.29	0.44
5:E:90:VAL:O	5:E:120:THR:HA	2.17	0.44
1:A:1355:G:H2'	1:A:1356:G:H8	1.83	0.44
1:A:1497:G:C2'	1:A:1498:UR3:H5'	2.47	0.44
1:A:1067:A:H4'	1:A:1068:G:O5'	2.17	0.44
1:A:1008:C:N4	1:A:1021:G:H1	2.14	0.44
1:A:98:U:C2	1:A:99:C:C5	3.05	0.44
1:A:961:U:H2'	1:A:962:C:O4'	2.18	0.44
6:F:14:LEU:HD13	6:F:18:GLN:HB3	1.99	0.44
3:C:32:LEU:HG	3:C:59:ARG:NH1	2.33	0.44
8:H:100:ILE:CG2	8:H:112:LEU:HD21	2.48	0.44
1:A:1494:G:C2	1:A:1495:U:C5	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:22:LEU:HD22	17:Q:41:LYS:HG3	1.99	0.44
17:Q:10:VAL:HG22	17:Q:10:VAL:O	2.17	0.44
1:A:1060:C:O2	10:J:56:HIS:NE2	2.51	0.44
1:A:532:A:H2'	1:A:533:A:C5'	2.47	0.44
1:A:80:G:H1	1:A:89:C:H42	1.65	0.44
1:A:914:A:P	22:A:1601:SRY:HI33	2.57	0.44
2:B:96:ARG:NE	2:B:97:TRP:H	2.13	0.44
1:A:434:U:C4	1:A:435:C:N4	2.85	0.44
1:A:1477:C:H2'	1:A:1478:C:H6	1.82	0.44
10:J:10:GLY:O	10:J:67:THR:HA	2.17	0.44
15:O:14:GLU:HG2	15:O:15:PHE:CE1	2.53	0.44
2:B:107:THR:HG23	2:B:110:GLN:OE1	2.17	0.44
1:A:413:G:H3'	1:A:413:G:H8	1.82	0.44
12:L:25:PRO:CA	12:L:27:LEU:HB2	2.48	0.44
13:M:67:GLU:O	13:M:71:ARG:HG2	2.17	0.44
14:N:20:ALA:C	14:N:21:TYR:HD1	2.21	0.44
4:D:22:LYS:HG3	4:D:26:CYS:SG	2.57	0.44
1:A:1064:G:H21	1:A:1190:G:H2'	1.82	0.44
1:A:250:A:O4'	1:A:252:U:C6	2.71	0.44
1:A:1329:A:H2'	1:A:1330:U:O4'	2.18	0.44
6:F:4:TYR:CZ	6:F:72:VAL:HG21	2.52	0.44
6:F:22:GLU:O	6:F:26:ILE:HG13	2.17	0.44
1:A:972:C:H4'	10:J:57:LYS:HG2	2.00	0.44
1:A:874:G:C2'	1:A:875:C:H5'	2.48	0.44
1:A:230:G:H2'	1:A:231:G:O4'	2.18	0.44
2:B:162:ILE:O	2:B:185:ILE:HD12	2.18	0.44
1:A:869:G:C5	25:A:2219:HOH:O	2.67	0.44
5:E:11:ILE:HA	5:E:11:ILE:HD13	1.74	0.44
1:A:89:C:N3	1:A:90:U:C2	2.86	0.44
1:A:1392:G:H2'	1:A:1393:U:C6	2.53	0.44
1:A:1189:C:H4'	3:C:10:PHE:HE2	1.83	0.44
5:E:90:VAL:C	5:E:91:LEU:HD23	2.38	0.44
1:A:1358:U:H3'	1:A:1359:C:C5	2.53	0.44
1:A:978:A:C6	1:A:1318:A:C6	3.06	0.44
1:A:1420:C:H2'	1:A:1421:G:C8	2.47	0.44
16:P:1:MET:O	16:P:3:LYS:HG2	2.17	0.44
1:A:1154:G:C6	1:A:1155:G:C5	3.06	0.44
1:A:59:A:H3'	1:A:331:G:N2	2.33	0.44
5:E:152:ARG:HB3	8:H:43:GLY:HA3	1.99	0.44
6:F:95:GLU:O	18:R:32:ARG:NH1	2.51	0.44
1:A:103:C:OP2	20:T:14:LYS:HD2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1245:A:H5"	1:A:1246:C:OP2	2.18	0.44
18:R:25:THR:OG1	18:R:42:ARG:NH1	2.50	0.44
1:A:956:U:C2	1:A:1225:A:C2	3.06	0.44
1:A:1032:G:O5'	1:A:1032:G:H8	2.00	0.44
11:K:24:SER:OG	11:K:25:TYR:N	2.49	0.44
4:D:4:TYR:C	4:D:5:ILE:HG13	2.38	0.44
1:A:257:G:H1	1:A:269:C:H42	1.66	0.44
19:S:41:VAL:HB	19:S:42:PRO:HD2	1.99	0.44
1:A:772:U:H2'	1:A:773:G:O4'	2.18	0.44
2:B:61:LEU:HG	2:B:66:GLY:HA3	1.99	0.44
8:H:82:HIS:CD2	8:H:138:TRP:NE1	2.86	0.44
1:A:858:G:O6	25:A:2220:HOH:O	2.21	0.44
1:A:78:G:C6	1:A:92:C:C4	3.06	0.44
1:A:93:G:N2	1:A:95:U:C2	2.86	0.44
1:A:979:C:C5	1:A:980:C:C4	3.06	0.44
1:A:1093:A:N3	1:A:1109:C:O2'	2.43	0.44
1:A:312:C:H2'	1:A:313:A:O4'	2.18	0.44
2:B:97:TRP:CH2	2:B:176:GLU:CD	2.90	0.44
6:F:32:ASN:HD22	6:F:32:ASN:C	2.17	0.44
1:A:619:U:C4	4:D:135:LEU:HD21	2.53	0.44
4:D:207:TYR:HD2	4:D:207:TYR:HA	1.64	0.44
2:B:217:ARG:HD3	2:B:217:ARG:HA	1.76	0.44
15:O:75:PRO:O	15:O:79:ARG:HD3	2.18	0.44
12:L:8:ASN:OD1	17:Q:34:LYS:HE2	2.17	0.44
11:K:38:ASN:HA	11:K:39:PRO:HD3	1.58	0.44
1:A:643:C:C2'	1:A:644:G:H5'	2.47	0.44
17:Q:53:LEU:HA	17:Q:53:LEU:HD13	1.56	0.44
10:J:38:ILE:HD11	10:J:71:LEU:H	1.83	0.43
1:A:1492:A:C2'	1:A:1493:A:H4'	2.45	0.43
1:A:192:U:H5'	20:T:102:GLY:O	2.18	0.43
2:B:212:GLN:C	2:B:212:GLN:HE21	2.21	0.43
4:D:84:LYS:HE2	4:D:84:LYS:HB3	1.88	0.43
1:A:1255:G:N2	1:A:1259:C:O2	2.46	0.43
1:A:1250:A:C6	1:A:1251:A:C6	3.07	0.43
8:H:119:LEU:HD12	8:H:124:ALA:CB	2.47	0.43
1:A:113:G:H2'	1:A:114:U:H6	1.82	0.43
4:D:135:LEU:H	4:D:135:LEU:HG	1.64	0.43
11:K:18:ARG:HB3	11:K:20:TYR:HE1	1.83	0.43
1:A:128:G:OP1	17:Q:2:PRO:HD2	2.18	0.43
1:A:145:G:H1	1:A:177:C:H42	1.65	0.43
2:B:147:LYS:HZ2	2:B:148:TYR:HE2	1.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:G:H21	4:D:119:GLN:HE22	1.64	0.43
8:H:107:LEU:HD23	8:H:107:LEU:N	2.34	0.43
1:A:966:M2G:HM22	1:A:967:5MC:O2	2.18	0.43
6:F:33:TYR:HD1	6:F:75:LEU:CA	2.28	0.43
6:F:33:TYR:CE1	6:F:75:LEU:HA	2.52	0.43
1:A:1500:A:OP2	1:A:1505:G:OP1	2.36	0.43
1:A:939:G:H2'	1:A:940:C:C6	2.53	0.43
8:H:86:ILE:CG2	8:H:133:LEU:HB3	2.47	0.43
7:G:22:LEU:HA	7:G:22:LEU:HD12	1.69	0.43
1:A:114:U:O2'	1:A:115:G:H5'	2.18	0.43
9:I:86:VAL:HG23	9:I:96:LEU:HD22	2.00	0.43
1:A:16:A:C2	1:A:920:U:C2	3.07	0.43
1:A:253:U:H2'	1:A:254:G:H8	1.82	0.43
3:C:43:LEU:O	3:C:47:LEU:HB2	2.18	0.43
1:A:109:A:C6	1:A:326:G:C6	3.06	0.43
1:A:892:A:C2	1:A:907:A:C4	3.07	0.43
7:G:28:ASN:HA	7:G:31:MET:HE2	2.00	0.43
1:A:359:U:H2'	1:A:360:A:C8	2.54	0.43
13:M:65:LYS:HE3	13:M:69:GLU:HG2	2.00	0.43
15:O:40:SER:O	15:O:44:LYS:HG2	2.18	0.43
1:A:1026:G:C8	1:A:1027:C:C5	3.07	0.43
1:A:1199:U:H4'	10:J:54:PHE:CD1	2.53	0.43
3:C:153:VAL:HA	3:C:198:VAL:HG12	1.99	0.43
8:H:85:ARG:NE	8:H:87:SER:O	2.51	0.43
1:A:1089:G:C2	1:A:1097:C:C2	3.06	0.43
11:K:18:ARG:CB	11:K:33:THR:HG23	2.49	0.43
2:B:87:ARG:O	2:B:223:ILE:HD11	2.18	0.43
17:Q:23:VAL:HG21	17:Q:42:TYR:CD1	2.53	0.43
1:A:599:C:O2'	8:H:129:VAL:HG12	2.17	0.43
1:A:157:G:H2'	1:A:158:G:C8	2.54	0.43
17:Q:22:LEU:HA	17:Q:22:LEU:HD22	1.69	0.43
1:A:728:A:C8	15:O:54:ARG:NH1	2.86	0.43
2:B:166:ASP:OD1	2:B:167:PRO:HD2	2.18	0.43
7:G:47:CYS:O	7:G:50:ILE:HB	2.19	0.43
1:A:1277:C:O2'	1:A:1279:A:H1'	2.18	0.43
1:A:1255:G:H22	1:A:1283:G:H1'	1.83	0.43
1:A:518:C:H4'	1:A:519:C:O5'	2.18	0.43
18:R:46:GLU:HG3	18:R:47:THR:N	2.31	0.43
1:A:445:G:H2'	1:A:446:G:C8	2.53	0.43
20:T:29:LYS:HB2	20:T:29:LYS:HE2	1.58	0.43
1:A:455:C:H2'	1:A:456:C:H5'	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:29:HIS:ND1	17:Q:30:PRO:HD2	2.33	0.43
1:A:1060:C:C2'	1:A:1061:G:H5'	2.49	0.43
1:A:115:G:O2'	1:A:116:A:OP2	2.22	0.43
2:B:101:MET:O	2:B:105:PHE:HA	2.17	0.43
1:A:1330:U:H2'	1:A:1331:G:H5'	2.00	0.43
19:S:22:LEU:HD11	19:S:31:ILE:HG13	2.01	0.43
19:S:31:ILE:HG23	19:S:32:LYS:N	2.33	0.43
1:A:500:G:C6	1:A:501:C:N4	2.87	0.43
6:F:91:VAL:HG13	18:R:72:ARG:NH2	2.34	0.43
1:A:1516:G:O5'	1:A:1516:G:H8	2.02	0.43
12:L:69:TYR:CE2	12:L:71:PRO:HA	2.51	0.43
15:O:87:ILE:HG22	15:O:88:ARG:HB2	2.01	0.43
6:F:27:GLN:O	6:F:31:GLU:HG3	2.19	0.43
1:A:257:G:H2'	1:A:258:G:O4'	2.19	0.43
4:D:13:ARG:NH2	4:D:36:ARG:HH22	2.17	0.43
7:G:155:ARG:HA	7:G:155:ARG:NH1	2.22	0.43
1:A:1181:G:C5	1:A:1182:G:C6	3.07	0.43
19:S:33:THR:O	19:S:51:VAL:HA	2.18	0.43
11:K:27:ASN:HD22	11:K:29:ILE:HG22	1.83	0.43
1:A:1148:U:H2'	1:A:1149:C:H6	1.84	0.43
5:E:37:ARG:O	5:E:114:GLY:HA3	2.19	0.43
1:A:509:A:H3'	1:A:509:A:C8	2.53	0.43
1:A:1150:U:O4	1:A:1151:A:N6	2.50	0.43
5:E:11:ILE:HG22	5:E:12:LEU:N	2.33	0.43
4:D:17:VAL:HG21	4:D:63:LYS:HD3	2.01	0.43
1:A:1028:C:O2'	1:A:1029:C:H5'	2.18	0.43
3:C:76:VAL:HG11	3:C:103:VAL:HG11	2.00	0.43
3:C:76:VAL:HG12	3:C:77:ILE:HD13	2.01	0.43
1:A:836:G:C6	1:A:851:G:C6	3.06	0.43
1:A:593:G:H2'	1:A:594:G:O4'	2.19	0.43
1:A:587:G:O2'	1:A:588:G:OP2	2.32	0.43
4:D:4:TYR:HE2	4:D:6:GLY:C	2.22	0.43
14:N:53:LEU:HD12	14:N:56:VAL:HG21	2.01	0.43
1:A:949:A:C2	1:A:1233:G:N3	2.87	0.43
1:A:428:G:H1'	1:A:429:U:OP2	2.19	0.43
1:A:1060:C:C2	1:A:1198:G:C2	3.07	0.43
1:A:1255:G:N1	1:A:1283:G:C2	2.87	0.43
1:A:1287:A:H2'	1:A:1288:A:C8	2.53	0.43
1:A:940:C:H5"	1:A:941:G:OP2	2.19	0.43
11:K:48:ILE:HG22	11:K:49:GLY:H	1.83	0.43
8:H:6:ILE:O	8:H:10:LEU:HG	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:8:THR:HG22	21:U:9:ARG:N	2.33	0.43
1:A:1328:C:C2'	1:A:1329:A:H5'	2.49	0.43
1:A:500:G:C6	1:A:501:C:C4	3.07	0.43
2:B:17:PHE:HA	2:B:44:LEU:HD11	2.00	0.43
2:B:44:LEU:HA	2:B:47:THR:HB	2.01	0.43
1:A:253:U:H2'	1:A:254:G:C8	2.54	0.43
20:T:53:LEU:HA	20:T:53:LEU:HD22	1.81	0.43
1:A:528:C:H41	12:L:49:ASN:CG	2.21	0.43
1:A:860:A:H2'	1:A:861:G:O4'	2.19	0.43
16:P:32:TYR:CE2	16:P:35:LYS:HB2	2.54	0.43
6:F:79:LEU:HD23	6:F:79:LEU:HA	1.66	0.43
1:A:413:G:O6	4:D:36:ARG:NE	2.52	0.43
4:D:38:TYR:HB2	4:D:39:PRO:HD2	2.01	0.43
1:A:1200:C:OP1	1:A:1201:A:H2'	2.19	0.43
1:A:92:C:C2	1:A:93:G:C8	3.06	0.43
8:H:10:LEU:HD22	8:H:83:ILE:HD12	1.99	0.43
4:D:68:TYR:CD2	4:D:97:LEU:HD22	2.54	0.43
1:A:299:G:O5'	1:A:299:G:H8	2.02	0.43
17:Q:6:LEU:HD23	17:Q:6:LEU:N	2.34	0.43
1:A:1015:A:H2'	1:A:1016:A:O4'	2.19	0.43
10:J:26:ALA:HA	10:J:29:ARG:CZ	2.49	0.43
19:S:6:LYS:HB3	19:S:7:LYS:H	1.31	0.43
3:C:18:TRP:NE1	14:N:54:PRO:HA	2.34	0.43
1:A:1225:A:N3	1:A:1225:A:H2'	2.33	0.43
1:A:968:A:C8	1:A:1062:U:H4'	2.53	0.43
1:A:662:G:H2'	1:A:663:A:C8	2.54	0.43
13:M:13:LYS:HB2	13:M:18:ALA:HB2	2.01	0.42
9:I:118:LYS:C	9:I:120:ARG:H	2.21	0.42
1:A:1368:G:OP1	9:I:111:ARG:NH2	2.47	0.42
11:K:44:SER:H	11:K:47:VAL:HB	1.83	0.42
1:A:39:G:O6	1:A:547:A:H2'	2.18	0.42
9:I:97:LYS:N	9:I:98:PRO:HD2	2.34	0.42
8:H:65:TYR:HA	8:H:79:VAL:HG23	1.99	0.42
1:A:1033:G:H2'	1:A:1034:G:O4'	2.19	0.42
4:D:173:TRP:C	4:D:186:LEU:HG	2.39	0.42
1:A:197:A:H1'	1:A:198:G:O4'	2.19	0.42
5:E:51:VAL:HG12	5:E:52:PRO:HD3	2.01	0.42
1:A:265:G:H2'	1:A:267:C:C5	2.54	0.42
17:Q:20:THR:HG22	17:Q:41:LYS:HG2	2.01	0.42
6:F:3:ARG:NE	6:F:38:GLU:OE2	2.51	0.42
11:K:115:PRO:C	11:K:117:ASN:H	2.21	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:A:H2'	25:A:2149:HOH:O	2.17	0.42
16:P:43:LYS:HE2	16:P:43:LYS:HB2	1.90	0.42
14:N:36:PHE:CD1	14:N:36:PHE:C	2.92	0.42
2:B:114:ARG:HH21	2:B:118:LEU:HD21	1.84	0.42
1:A:1057:G:C4	1:A:1058:G:C8	3.07	0.42
3:C:8:ILE:HG23	3:C:16:ARG:HG2	2.02	0.42
1:A:74:C:H2'	1:A:75:G:C8	2.54	0.42
1:A:1260:C:O5'	1:A:1284:C:H4'	2.20	0.42
1:A:793:U:HO2'	1:A:794:A:C5'	2.26	0.42
13:M:36:LYS:HD2	13:M:59:TYR:OH	2.18	0.42
1:A:1357:A:H2'	1:A:1358:U:C6	2.54	0.42
2:B:98:LEU:HB2	2:B:101:MET:CG	2.50	0.42
1:A:503:C:O5'	1:A:503:C:H6	2.03	0.42
13:M:15:VAL:HG12	13:M:34:LEU:HD11	2.00	0.42
1:A:935:A:H61	7:G:3:ARG:HG3	1.83	0.42
11:K:95:ILE:O	11:K:99:GLN:HG3	2.19	0.42
15:O:85:LEU:HD23	15:O:85:LEU:HA	1.54	0.42
3:C:73:PRO:HG3	3:C:105:GLU:OE1	2.19	0.42
3:C:34:LEU:HD13	3:C:38:ARG:HE	1.84	0.42
1:A:146:G:N2	1:A:147:G:C4	2.87	0.42
11:K:112:THR:HA	11:K:113:PRO:HD2	1.91	0.42
1:A:575:G:O2'	1:A:821:G:H5'	2.19	0.42
6:F:45:LEU:HD23	6:F:45:LEU:HA	1.87	0.42
8:H:104:ARG:HG2	8:H:104:ARG:NH1	2.35	0.42
1:A:1200:C:O2	1:A:1200:C:H2'	2.20	0.42
12:L:98:TYR:CD1	12:L:98:TYR:N	2.87	0.42
11:K:48:ILE:HG13	11:K:48:ILE:H	1.42	0.42
1:A:993:G:N3	1:A:993:G:H2'	2.35	0.42
13:M:94:ARG:HB3	13:M:96:LEU:HD12	2.00	0.42
1:A:107:G:N2	1:A:108:G:H1'	2.35	0.42
1:A:197:A:H4'	1:A:198:G:O5'	2.20	0.42
10:J:19:SER:O	10:J:23:ILE:HG12	2.19	0.42
3:C:137:ALA:O	3:C:141:VAL:HG23	2.19	0.42
2:B:54:THR:OG1	2:B:199:TYR:HB3	2.20	0.42
8:H:105:ARG:HD3	8:H:105:ARG:HA	1.79	0.42
20:T:41:ILE:HA	20:T:41:ILE:HD12	1.67	0.42
12:L:7:ILE:O	12:L:10:LEU:N	2.52	0.42
4:D:30:LYS:C	4:D:32:ALA:H	2.21	0.42
1:A:96:G:C2	1:A:97:G:C4	3.08	0.42
8:H:83:ILE:HG22	8:H:83:ILE:O	2.18	0.42
1:A:975:A:H5'	1:A:975:A:H8	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:678:U:H1'	1:A:777:A:O3'	2.20	0.42
2:B:7:VAL:HG11	2:B:221:LEU:HB2	2.01	0.42
2:B:193:ASP:HA	2:B:194:PRO:HD2	1.72	0.42
1:A:586:C:C2'	1:A:587:G:H5'	2.49	0.42
1:A:81:U:H5'	1:A:82:U:OP1	2.20	0.42
1:A:643:C:H2'	1:A:644:G:H5'	2.01	0.42
1:A:229:U:H4'	16:P:33:ILE:HD13	2.00	0.42
2:B:78:GLN:HB2	2:B:94:ASN:OD1	2.19	0.42
1:A:1168:A:H2'	1:A:1169:A:C8	2.54	0.42
1:A:811:C:H4'	1:A:900:A:N6	2.34	0.42
1:A:285:G:O2'	1:A:286:G:H5'	2.20	0.42
5:E:112:LEU:HA	5:E:112:LEU:HD23	1.87	0.42
1:A:1057:G:C5	1:A:1058:G:N7	2.88	0.42
1:A:981:U:H5"	1:A:982:U:O5'	2.19	0.42
14:N:18:VAL:O	14:N:20:ALA:N	2.53	0.42
3:C:10:PHE:C	3:C:10:PHE:HD1	2.23	0.42
5:E:88:LYS:HB3	5:E:123:LEU:HB2	2.02	0.42
1:A:1510:U:H2'	1:A:1511:G:H8	1.81	0.42
1:A:1095:U:H2'	1:A:1096:C:O4'	2.19	0.42
1:A:558:G:C5'	1:A:559:A:H3'	2.48	0.42
11:K:72:ALA:HB1	11:K:77:MET:CG	2.50	0.42
1:A:152:A:OP2	1:A:153:C:N4	2.43	0.42
1:A:602:A:C2	1:A:637:G:C2	3.08	0.42
20:T:27:LYS:HG3	20:T:28:ALA:N	2.33	0.42
5:E:147:ASP:O	5:E:150:ARG:HB3	2.19	0.42
1:A:1144:G:C2	1:A:1145:C:O2	2.72	0.42
9:I:12:GLU:O	9:I:12:GLU:HG2	2.19	0.42
13:M:6:GLY:O	13:M:67:GLU:HG2	2.20	0.42
1:A:826:C:H2'	1:A:827:U:C6	2.54	0.42
1:A:1089:G:C6	1:A:1090:U:C4	3.08	0.42
1:A:687:A:C2	1:A:704:A:C6	3.08	0.42
15:O:4:THR:OG1	15:O:5:LYS:N	2.52	0.42
1:A:1226:C:N4	13:M:104:ARG:HG3	2.35	0.42
1:A:1540:PSU:O4	1:A:1540:PSU:H2'	2.19	0.42
1:A:1030(A):G:N3	1:A:1030(C):G:OP2	2.53	0.42
1:A:402:G:C6	1:A:403:C:C5	3.08	0.42
1:A:960:U:H4'	1:A:961:U:C5'	2.50	0.42
1:A:229:U:O2'	16:P:23:ASP:HB2	2.19	0.42
1:A:175:C:H2'	1:A:176:C:H6	1.85	0.42
2:B:11:LEU:O	2:B:13:ALA:N	2.51	0.42
1:A:276:G:O3'	17:Q:68:ARG:NH1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1215:G:H2'	1:A:1215:G:N3	2.34	0.42
6:F:43:LEU:HA	6:F:43:LEU:HD13	1.83	0.42
1:A:279:A:C8	1:A:279:A:H5'	2.53	0.42
13:M:18:ALA:O	13:M:21:TYR:HB2	2.20	0.42
15:O:70:LEU:HD22	15:O:70:LEU:HA	1.46	0.42
1:A:1089:G:C6	1:A:1090:U:C2	3.08	0.42
18:R:59:SER:N	18:R:62:GLU:OE1	2.53	0.42
2:B:73:THR:HG23	2:B:95:GLN:O	2.20	0.42
16:P:75:ARG:C	16:P:78:GLY:H	2.23	0.42
1:A:371:G:C2'	1:A:372:C:H5'	2.49	0.42
12:L:28:LYS:HD2	12:L:33:ARG:NH2	2.35	0.42
1:A:579:G:H2'	1:A:580:U:C6	2.54	0.42
18:R:51:LEU:HB3	18:R:56:THR:HG23	2.01	0.42
6:F:9:VAL:HG13	6:F:60:PHE:CE2	2.54	0.42
1:A:81:U:H3'	1:A:81:U:C6	2.55	0.42
17:Q:20:THR:CG2	17:Q:41:LYS:HG2	2.49	0.42
16:P:40:ASP:HB3	16:P:48:TRP:HB2	2.01	0.42
15:O:61:GLY:O	15:O:65:ARG:HD2	2.19	0.42
7:G:122:HIS:O	7:G:125:MET:HG3	2.19	0.42
18:R:87:ARG:HB3	18:R:88:LYS:H	1.67	0.42
11:K:120:ARG:HD3	11:K:120:ARG:HH11	1.65	0.42
1:A:226:G:N2	25:A:2108:HOH:O	2.13	0.42
1:A:1056:U:H2'	1:A:1057:G:H8	1.84	0.42
1:A:1058:G:C6	1:A:1059:C:C4	3.07	0.42
1:A:89:C:C2	1:A:90:U:C2	3.07	0.42
3:C:99:VAL:HG22	3:C:100:ALA:O	2.19	0.42
14:N:40:CYS:HB3	14:N:43:CYS:H	1.83	0.42
3:C:78:GLY:HA3	3:C:83:ARG:HB2	2.01	0.42
17:Q:15:MET:CB	17:Q:18:THR:HB	2.50	0.42
1:A:785:G:H2'	1:A:786:G:H5'	2.02	0.42
2:B:126:GLU:HG2	2:B:129:GLU:HB2	2.00	0.42
1:A:922:G:N1	1:A:923:A:C2	2.88	0.42
20:T:34:LYS:O	20:T:38:LYS:HE3	2.19	0.42
13:M:99:ARG:NH1	19:S:2:PRO:HD3	2.35	0.42
8:H:114:THR:OG1	8:H:117:GLY:O	2.24	0.42
4:D:18:LYS:HG3	4:D:33:MET:HE2	2.01	0.42
1:A:1303:C:C2'	1:A:1304:G:H5'	2.50	0.42
13:M:107:ALA:CB	13:M:111:LYS:HE3	2.49	0.42
8:H:97:VAL:HG23	8:H:129:VAL:C	2.40	0.42
1:A:510:A:P	25:A:2199:HOH:O	2.77	0.42
15:O:14:GLU:HG2	15:O:15:PHE:HE1	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:C:H2'	1:A:444:C:H6	1.85	0.42
1:A:479:C:H2'	1:A:480:U:O4'	2.20	0.42
2:B:145:LEU:HA	2:B:145:LEU:HD23	1.66	0.42
17:Q:29:HIS:CD2	17:Q:32:TYR:N	2.67	0.42
1:A:404:U:H2'	1:A:405:U:H6	1.85	0.42
3:C:32:LEU:O	3:C:35:GLU:HB3	2.20	0.42
2:B:176:GLU:O	2:B:179:LYS:N	2.52	0.42
1:A:1329:A:H2'	1:A:1330:U:C6	2.55	0.42
1:A:1008:C:O5'	1:A:1008:C:H6	2.03	0.42
1:A:597:G:H2'	1:A:598:U:C5'	2.49	0.42
15:O:87:ILE:CG2	15:O:88:ARG:N	2.83	0.42
17:Q:59:ILE:CG2	17:Q:71:PHE:HD1	2.33	0.42
5:E:102:ALA:HB1	5:E:106:PRO:HB2	2.02	0.42
1:A:651:C:O2'	1:A:652:U:H5'	2.20	0.42
1:A:494:G:HO2'	1:A:495:U:H6	1.63	0.42
1:A:1371:G:H4'	9:I:69:GLY:HA3	2.01	0.41
1:A:1190:G:OP1	3:C:4:LYS:HA	2.19	0.41
1:A:1089:G:O6	1:A:1090:U:N3	2.52	0.41
6:F:50:TYR:HE1	18:R:77:GLY:HA2	1.82	0.41
1:A:1419:G:C6	1:A:1420:C:C4	3.08	0.41
1:A:791:G:N2	1:A:792:A:H62	2.18	0.41
3:C:139:GLN:HG2	3:C:170:GLN:OE1	2.20	0.41
1:A:1150:U:H4'	10:J:41:PRO:HG3	2.01	0.41
16:P:58:TYR:CD1	16:P:58:TYR:C	2.93	0.41
18:R:54:ARG:HE	18:R:54:ARG:HB2	1.48	0.41
10:J:48:THR:OG1	10:J:62:HIS:CD2	2.73	0.41
7:G:15:ASP:OD1	7:G:18:TYR:HB2	2.20	0.41
4:D:21:LEU:HA	4:D:21:LEU:HD22	1.93	0.41
1:A:393:A:C2	1:A:394:G:C8	3.07	0.41
1:A:194:C:O3'	20:T:68:LYS:HE2	2.20	0.41
1:A:164:U:H2'	1:A:165:C:C6	2.55	0.41
1:A:642:A:C5	1:A:643:C:C4	3.09	0.41
2:B:83:MET:SD	2:B:234:PRO:HB2	2.61	0.41
1:A:1378:C:H2'	1:A:1379:G:O4'	2.20	0.41
10:J:38:ILE:HD12	10:J:38:ILE:O	2.20	0.41
1:A:958:A:H1'	19:S:55:LYS:HD3	2.01	0.41
3:C:179:ARG:HD2	3:C:207:VAL:HA	2.01	0.41
1:A:76:C:H2'	1:A:77:G:H8	1.82	0.41
1:A:982:U:O2	1:A:1222:G:N2	2.53	0.41
1:A:1063:C:H2'	1:A:1064:G:H8	1.82	0.41
1:A:113:G:C2	1:A:315:A:C2	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:838:G:C3'	1:A:839:U:H5"	2.51	0.41
1:A:1442:G:C6	1:A:1446:A:N7	2.88	0.41
9:I:8:GLY:N	9:I:83:ARG:HD2	2.35	0.41
1:A:901:A:N7	1:A:902:G:H1'	2.34	0.41
1:A:921:U:O2'	5:E:18:ARG:HG3	2.20	0.41
7:G:88:PRO:O	7:G:89:MET:HB3	2.21	0.41
1:A:892:A:C5	1:A:893:C:C4	3.07	0.41
1:A:859:A:H2'	1:A:860:A:O4'	2.19	0.41
4:D:49:ARG:HG3	4:D:50:ARG:N	2.36	0.41
1:A:1218:C:H2'	1:A:1219:U:C6	2.55	0.41
8:H:9:MET:HE3	8:H:9:MET:HB3	2.00	0.41
1:A:75:G:C6	1:A:96:G:C6	3.09	0.41
9:I:111:ARG:HD2	14:N:61:TRP:OXT	2.20	0.41
7:G:18:TYR:HD1	7:G:18:TYR:N	2.18	0.41
7:G:16:LEU:HD11	9:I:44:VAL:HB	2.02	0.41
4:D:68:TYR:CE2	4:D:97:LEU:HB3	2.54	0.41
2:B:84:GLU:HB3	2:B:219:VAL:HG21	2.01	0.41
1:A:1031:G:H8	1:A:1031:G:H3'	1.85	0.41
6:F:14:LEU:HD22	6:F:18:GLN:OE1	2.20	0.41
1:A:329:A:C5	1:A:332:G:C6	3.09	0.41
2:B:29:ALA:HA	2:B:32:ILE:HG13	2.01	0.41
8:H:92:ARG:HH11	8:H:92:ARG:CG	2.33	0.41
4:D:158:ILE:HD13	4:D:158:ILE:HA	1.69	0.41
19:S:11:VAL:HG12	19:S:15:LEU:HD11	2.02	0.41
16:P:74:LEU:O	16:P:79:VAL:HG23	2.20	0.41
8:H:119:LEU:HB3	8:H:123:GLU:HB3	2.02	0.41
5:E:80:ILE:O	5:E:80:ILE:HG23	2.21	0.41
22:A:1601:SRY:C22	22:A:1601:SRY:HI32	2.50	0.41
3:C:172:ARG:HH22	3:C:174:PRO:HG3	1.85	0.41
3:C:29:TYR:CE2	3:C:33:LEU:HD11	2.56	0.41
10:J:43:ARG:HD3	10:J:45:ARG:NH2	2.36	0.41
1:A:1312:G:N2	1:A:1313:U:H1'	2.36	0.41
14:N:4:LYS:HE2	14:N:4:LYS:HB3	1.89	0.41
7:G:18:TYR:N	7:G:18:TYR:CD1	2.89	0.41
1:A:941:G:C6	1:A:942:G:N7	2.89	0.41
1:A:1397:C:HO2'	1:A:1398:A:P	2.37	0.41
1:A:526:C:OP1	1:A:913:A:H3'	2.21	0.41
2:B:97:TRP:CZ2	2:B:101:MET:HB2	2.55	0.41
1:A:451:A:OP1	1:A:451:A:H8	2.04	0.41
1:A:1267:C:O2	21:U:20:LYS:HD2	2.20	0.41
1:A:1040:U:O4	1:A:1041:A:N6	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:U:C2'	1:A:265:G:H5'	2.49	0.41
2:B:163:PHE:HA	2:B:185:ILE:O	2.20	0.41
1:A:642:A:C6	1:A:643:C:C4	3.08	0.41
1:A:1345:U:C2	1:A:1377:A:C2	3.09	0.41
8:H:30:ARG:O	8:H:33:GLU:N	2.54	0.41
2:B:181:PHE:CD2	8:H:70:GLN:HB3	2.56	0.41
1:A:132:C:H4'	20:T:74:LYS:HD2	2.03	0.41
1:A:427:U:OP2	4:D:36:ARG:NH2	2.53	0.41
1:A:1091:U:O2	1:A:1093:A:C8	2.74	0.41
18:R:58:LEU:HB3	18:R:62:GLU:HB3	2.03	0.41
1:A:977:A:C2'	1:A:978:A:H5"	2.50	0.41
3:C:138:VAL:HG22	3:C:151:VAL:HG23	2.02	0.41
17:Q:18:THR:HG22	17:Q:19:VAL:N	2.35	0.41
1:A:730:G:C5	1:A:731:G:H1'	2.56	0.41
1:A:1494:G:H2'	1:A:1495:U:C6	2.56	0.41
1:A:1481:U:O2'	1:A:1482:G:H5'	2.21	0.41
1:A:1071:C:H5"	5:E:49:PRO:HG2	2.02	0.41
8:H:77:GLU:HG2	8:H:78:GLN:H	1.84	0.41
1:A:421:U:H5'	1:A:422:C:H5	1.86	0.41
20:T:89:ARG:NH2	20:T:104:LEU:HB3	2.36	0.41
1:A:490:G:C6	1:A:491:G:N7	2.88	0.41
1:A:1256:A:H4'	1:A:1257:U:O5'	2.19	0.41
1:A:77:G:N1	1:A:93:G:C6	2.89	0.41
1:A:78:G:O6	1:A:92:C:N4	2.54	0.41
7:G:15:ASP:OD2	7:G:44:TYR:OH	2.39	0.41
4:D:64:LEU:CD1	4:D:75:PHE:HZ	2.34	0.41
8:H:120:THR:HG23	8:H:123:GLU:CD	2.41	0.41
5:E:118:ILE:HG12	5:E:119:LEU:N	2.35	0.41
8:H:65:TYR:CD1	8:H:65:TYR:N	2.88	0.41
5:E:52:PRO:HG2	5:E:53:LEU:H	1.86	0.41
3:C:108:ASN:N	3:C:109:PRO:HD3	2.35	0.41
1:A:403:C:OP1	4:D:137:SER:OG	2.29	0.41
1:A:727:G:H4'	1:A:741:G:H22	1.86	0.41
2:B:211:ILE:O	2:B:215:LEU:HB2	2.20	0.41
14:N:42:ILE:HG13	14:N:42:ILE:H	1.64	0.41
1:A:982:U:O2	1:A:1222:G:N1	2.54	0.41
21:U:13:ILE:HA	21:U:22:ARG:HH12	1.86	0.41
1:A:1181:G:HO2'	1:A:1182:G:C1'	2.32	0.41
8:H:124:ALA:HA	8:H:127:LEU:HB2	2.03	0.41
1:A:116:A:O5'	1:A:116:A:H8	2.04	0.41
1:A:1442:G:C5	1:A:1446:A:C6	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:617:G:N2	1:A:618:C:N3	2.69	0.41
16:P:53:VAL:O	16:P:54:GLU:C	2.59	0.41
20:T:10:LEU:HD22	20:T:10:LEU:HA	1.57	0.41
11:K:99:GLN:OE1	11:K:105:VAL:HG21	2.21	0.41
15:O:15:PHE:CZ	15:O:85:LEU:HD21	2.56	0.41
1:A:1001:A:H61	1:A:1041:A:N6	2.19	0.41
1:A:791:G:H2'	1:A:792:A:C8	2.56	0.41
9:I:99:LEU:HB3	9:I:101:PHE:CE1	2.55	0.41
1:A:1247:U:O2	1:A:1291:G:N1	2.54	0.41
2:B:152:PHE:CE1	2:B:155:LEU:HD12	2.55	0.41
2:B:80:ILE:HD12	2:B:212:GLN:HG3	2.02	0.41
20:T:74:LYS:HA	20:T:74:LYS:HD3	1.71	0.41
1:A:306:G:H2'	1:A:307:C:H6	1.85	0.41
16:P:65:GLN:HA	16:P:66:PRO:HD2	1.97	0.41
13:M:82:MET:HA	13:M:89:GLY:HA3	2.03	0.41
3:C:186:PHE:CD2	3:C:187:ALA:N	2.88	0.41
5:E:131:ILE:HD13	5:E:131:ILE:HA	1.95	0.41
4:D:28:SER:O	4:D:30:LYS:N	2.46	0.41
1:A:1111:A:N6	3:C:177:THR:HG22	2.31	0.41
1:A:1064:G:H1'	1:A:1190:G:N2	2.37	0.41
1:A:1189:C:H5"	1:A:1190:G:OP2	2.21	0.41
1:A:990:C:C4	1:A:1216:G:N2	2.89	0.41
17:Q:59:ILE:CG2	17:Q:71:PHE:CD1	3.04	0.41
1:A:652:U:O4	1:A:752:G:O2'	2.28	0.41
1:A:448:A:C2	1:A:449:C:C4	3.09	0.41
5:E:142:LEU:HD23	5:E:142:LEU:HA	1.81	0.41
1:A:1205:U:H2'	1:A:1206:G:C8	2.56	0.40
1:A:966:M2G:N3	1:A:966:M2G:H2'	2.36	0.40
1:A:1368:G:OP2	9:I:114:TYR:N	2.54	0.40
1:A:1037:C:H2'	1:A:1038:C:C5	2.57	0.40
1:A:370:C:C2'	1:A:371:G:H5'	2.50	0.40
1:A:234:C:H2'	1:A:235:C:H6	1.87	0.40
1:A:16:A:C2	1:A:920:U:O2	2.74	0.40
1:A:707:C:H5"	11:K:20:TYR:HD2	1.84	0.40
11:K:59:TYR:O	11:K:62:GLN:N	2.51	0.40
1:A:1245:A:N1	1:A:1293:G:C2	2.89	0.40
1:A:401:C:H2'	1:A:402:G:C8	2.57	0.40
1:A:374:A:C6	1:A:375:U:C4	3.09	0.40
15:O:45:VAL:HG12	15:O:46:HIS:H	1.87	0.40
7:G:47:CYS:HA	7:G:50:ILE:HG12	2.03	0.40
3:C:121:ALA:O	3:C:125:GLU:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:222:ILE:HG21	2:B:222:ILE:HD13	1.85	0.40
3:C:179:ARG:HD3	3:C:179:ARG:HA	1.84	0.40
1:A:1250:A:H2	1:A:1353:G:N2	2.19	0.40
11:K:47:VAL:HG12	11:K:48:ILE:N	2.36	0.40
17:Q:72:ARG:HH11	17:Q:72:ARG:HD2	1.70	0.40
1:A:976:G:C8	1:A:1358:U:C2	3.09	0.40
1:A:1440:C:C2'	1:A:1441:G:H5'	2.51	0.40
1:A:1516:G:H1'	1:A:1519:MA6:C10	2.51	0.40
1:A:582:U:OP1	15:O:64:ARG:NH2	2.53	0.40
6:F:97:PHE:H	18:R:32:ARG:NH1	2.17	0.40
12:L:46:LYS:CG	12:L:47:LYS:H	2.35	0.40
2:B:114:ARG:O	2:B:117:GLU:HG2	2.21	0.40
1:A:636:U:H2'	1:A:637:G:C8	2.56	0.40
5:E:105:VAL:HB	5:E:106:PRO:HD3	2.04	0.40
1:A:17:U:H2'	1:A:18:C:C6	2.56	0.40
1:A:363:A:OP1	12:L:61:THR:OG1	2.30	0.40
1:A:1248:A:C6	1:A:1249:C:N4	2.90	0.40
1:A:389:A:H2'	1:A:390:C:H5'	2.03	0.40
1:A:734:G:H21	18:R:75:ILE:CD1	2.35	0.40
1:A:735:C:O2'	1:A:736:C:H5'	2.21	0.40
1:A:7:G:H5'	1:A:298:A:O4'	2.22	0.40
2:B:69:LEU:HB3	2:B:162:ILE:HD12	2.03	0.40
20:T:73:HIS:HB3	20:T:74:LYS:H	1.48	0.40
1:A:448:A:C2	1:A:449:C:C5	3.10	0.40
1:A:810:C:O2	1:A:899:C:N4	2.54	0.40
2:B:60:ASP:O	2:B:64:ARG:HG3	2.21	0.40
9:I:28:VAL:O	9:I:31:GLN:N	2.54	0.40
1:A:1375:A:H4'	7:G:29:LYS:NZ	2.36	0.40
9:I:112:LYS:HG3	9:I:117:HIS:O	2.22	0.40
3:C:59:ARG:HG3	3:C:63:ASN:O	2.21	0.40
19:S:28:LYS:CD	19:S:31:ILE:HG12	2.51	0.40
1:A:803:G:H2'	1:A:804:U:O4'	2.22	0.40
1:A:451:A:OP1	1:A:451:A:C8	2.75	0.40
7:G:150:ALA:HA	11:K:59:TYR:CD2	2.56	0.40
1:A:669:U:H2'	1:A:670:G:C8	2.56	0.40
1:A:1314:C:H41	19:S:6:LYS:HZ2	1.69	0.40
1:A:357:G:C2	1:A:358:U:C5	3.09	0.40
20:T:53:LEU:HD12	20:T:102:GLY:H	1.86	0.40
1:A:1219:U:C4	1:A:1220:G:N7	2.89	0.40
8:H:137:VAL:HG12	8:H:138:TRP:N	2.36	0.40
9:I:75:ASP:OD2	9:I:78:LYS:HE3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1504:G:C4'	1:A:1505:G:H5'	2.51	0.40
1:A:981:U:H4'	14:N:21:TYR:CE2	2.56	0.40
1:A:1162:C:C2	1:A:1175:G:C2	3.09	0.40
12:L:53:ARG:HD3	12:L:93:LEU:CD2	2.52	0.40
1:A:1148:U:H4'	9:I:14:VAL:HG11	2.04	0.40
4:D:172:PRO:HD2	4:D:173:TRP:CE3	2.56	0.40
10:J:21:GLN:O	10:J:25:GLU:HG3	2.22	0.40
1:A:179:A:H2'	1:A:180:U:C6	2.56	0.40
4:D:70:ILE:HG23	4:D:71:SER:N	2.36	0.40
8:H:92:ARG:HH11	8:H:92:ARG:HG3	1.86	0.40
1:A:542:G:O2'	1:A:543:C:H5'	2.21	0.40
2:B:27:LYS:HB3	2:B:27:LYS:HE2	1.78	0.40
1:A:1297:C:H6	1:A:1297:C:OP2	2.05	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%)	203 (88%)	25 (11%)	4 (2%)	11 57
3	C	204/239 (85%)	175 (86%)	28 (14%)	1 (0%)	34 77
4	D	206/209 (99%)	190 (92%)	14 (7%)	2 (1%)	19 66
5	E	148/162 (91%)	138 (93%)	9 (6%)	1 (1%)	26 72
6	F	99/101 (98%)	90 (91%)	9 (9%)	0	100 100
7	G	153/156 (98%)	133 (87%)	20 (13%)	0	100 100
8	H	136/138 (99%)	127 (93%)	9 (7%)	0	100 100
9	I	125/128 (98%)	113 (90%)	11 (9%)	1 (1%)	24 70
10	J	96/105 (91%)	73 (76%)	19 (20%)	4 (4%)	3 36
11	K	114/129 (88%)	104 (91%)	10 (9%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
12	L	121/135 (90%)	109 (90%)	10 (8%)	2 (2%)	11 57
13	M	116/126 (92%)	105 (90%)	10 (9%)	1 (1%)	21 68
14	N	58/61 (95%)	53 (91%)	5 (9%)	0	100 100
15	O	85/89 (96%)	75 (88%)	10 (12%)	0	100 100
16	P	81/88 (92%)	75 (93%)	5 (6%)	1 (1%)	16 63
17	Q	97/105 (92%)	88 (91%)	9 (9%)	0	100 100
18	R	68/88 (77%)	62 (91%)	6 (9%)	0	100 100
19	S	78/93 (84%)	70 (90%)	7 (9%)	1 (1%)	15 61
20	T	97/106 (92%)	79 (81%)	17 (18%)	1 (1%)	19 66
21	U	22/27 (82%)	19 (86%)	3 (14%)	0	100 100
All	All	2336/2541 (92%)	2081 (89%)	236 (10%)	19 (1%)	24 70

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	21	ARG
2	B	24	TRP
3	C	15	THR
12	L	28	LYS
19	S	31	ILE
10	J	79	ARG
10	J	86	MET
4	D	156	GLU
20	T	99	LEU
2	B	12	GLU
9	I	119	ALA
4	D	5	ILE
12	L	25	PRO
10	J	34	VAL
5	E	70	PRO
2	B	229	VAL
13	M	84	ILE
16	P	53	VAL
10	J	72	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%)	163 (81%)	39 (19%)	2 13
3	C	160/188 (85%)	125 (78%)	35 (22%)	1 9
4	D	180/181 (99%)	139 (77%)	41 (23%)	1 8
5	E	115/123 (94%)	88 (76%)	27 (24%)	1 7
6	F	90/90 (100%)	74 (82%)	16 (18%)	2 16
7	G	126/127 (99%)	104 (82%)	22 (18%)	2 17
8	H	119/119 (100%)	80 (67%)	39 (33%)	0 2
9	I	98/99 (99%)	82 (84%)	16 (16%)	3 20
10	J	87/92 (95%)	66 (76%)	21 (24%)	1 7
11	K	88/99 (89%)	66 (75%)	22 (25%)	1 6
12	L	103/110 (94%)	69 (67%)	34 (33%)	0 2
13	M	94/101 (93%)	70 (74%)	24 (26%)	1 6
14	N	49/50 (98%)	38 (78%)	11 (22%)	1 8
15	O	79/80 (99%)	61 (77%)	18 (23%)	1 8
16	P	72/74 (97%)	57 (79%)	15 (21%)	1 10
17	Q	94/97 (97%)	71 (76%)	23 (24%)	1 7
18	R	61/77 (79%)	45 (74%)	16 (26%)	0 5
19	S	71/80 (89%)	50 (70%)	21 (30%)	0 4
20	T	76/82 (93%)	57 (75%)	19 (25%)	1 6
21	U	19/22 (86%)	15 (79%)	4 (21%)	1 10
All	All	1983/2111 (94%)	1520 (77%)	463 (23%)	1 8

All (463) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	7	VAL
2	B	8	LYS
2	B	9	GLU

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Mol	Chain	Res	Type
2	B	11	LEU
2	B	12	GLU
2	B	17	PHE
2	B	19	HIS
2	B	23	ARG
2	B	24	TRP
2	B	39	ILE
2	B	47	THR
2	B	51	LEU
2	B	53	ARG
2	B	55	PHE
2	B	63	MET
2	B	106	LYS
2	B	109	SER
2	B	110	GLN
2	B	121	LEU
2	B	127	ILE
2	B	140	HIS
2	B	142	LEU
2	B	157	ARG
2	B	160	ASP
2	B	162	ILE
2	B	164	VAL
2	B	168	THR
2	B	170	GLU
2	B	178	ARG
2	B	187	LEU
2	B	190	THR
2	B	195	ASP
2	B	196	LEU
2	B	206	ASP
2	B	209	ARG
2	B	212	GLN
2	B	215	LEU
2	B	217	ARG
2	B	236	TYR
3	C	3	ASN
3	C	10	PHE
3	C	14	ILE
3	C	19	GLU
3	C	21	ARG
3	C	22	TRP

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Mol	Chain	Res	Type
3	C	30	ARG
3	C	31	HIS
3	C	34	LEU
3	C	56	ASP
3	C	59	ARG
3	C	70	VAL
3	C	84	ILE
3	C	91	LEU
3	C	95	THR
3	C	101	LEU
3	C	103	VAL
3	C	111	LEU
3	C	116	VAL
3	C	130	VAL
3	C	131	ARG
3	C	143	GLU
3	C	144	SER
3	C	162	GLN
3	C	167	TRP
3	C	172	ARG
3	C	175	LEU
3	C	176	HIS
3	C	188	LEU
3	C	190	ARG
3	C	192	THR
3	C	196	LEU
3	C	198	VAL
3	C	204	LEU
3	C	207	VAL
4	D	5	ILE
4	D	9	CYS
4	D	10	ARG
4	D	19	LEU
4	D	21	LEU
4	D	25	ARG
4	D	26	CYS
4	D	34	GLU
4	D	47	ARG
4	D	49	ARG
4	D	50	ARG
4	D	58	LEU
4	D	59	ARG

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Mol	Chain	Res	Type
4	D	61	LYS
4	D	64	LEU
4	D	70	ILE
4	D	71	SER
4	D	73	ARG
4	D	78	LEU
4	D	85	LYS
4	D	89	THR
4	D	108	LEU
4	D	114	ARG
4	D	115	ARG
4	D	122	ARG
4	D	132	ARG
4	D	135	LEU
4	D	137	SER
4	D	140	VAL
4	D	150	GLU
4	D	156	GLU
4	D	162	LEU
4	D	170	VAL
4	D	176	LEU
4	D	186	LEU
4	D	187	ARG
4	D	192	GLU
4	D	194	LEU
4	D	196	LEU
4	D	200	GLU
4	D	208	SER
5	E	10	MET
5	E	12	LEU
5	E	14	ARG
5	E	16	THR
5	E	18	ARG
5	E	24	ARG
5	E	26	PHE
5	E	31	LEU
5	E	37	ARG
5	E	38	GLN
5	E	41	VAL
5	E	43	LEU
5	E	55	VAL
5	E	56	GLN

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Mol	Chain	Res	Type
5	E	65	ASN
5	E	68	GLU
5	E	71	LEU
5	E	75	THR
5	E	79	GLU
5	E	80	ILE
5	E	100	VAL
5	E	117	ASP
5	E	123	LEU
5	E	125	SER
5	E	144	THR
5	E	148	VAL
5	E	149	GLU
6	F	3	ARG
6	F	9	VAL
6	F	10	LEU
6	F	14	LEU
6	F	19	LEU
6	F	21	LEU
6	F	25	ILE
6	F	28	ARG
6	F	32	ASN
6	F	47	ARG
6	F	55	ASP
6	F	74	ASP
6	F	83	ASP
6	F	89	MET
6	F	93	SER
6	F	95	GLU
7	G	6	ARG
7	G	8	GLU
7	G	16	LEU
7	G	21	VAL
7	G	23	VAL
7	G	33	ASP
7	G	67	GLU
7	G	70	LYS
7	G	77	SER
7	G	87	VAL
7	G	97	GLN
7	G	104	LEU
7	G	106	GLN

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Mol	Chain	Res	Type
7	G	111	ARG
7	G	113	GLU
7	G	114	ARG
7	G	124	LEU
7	G	125	MET
7	G	141	VAL
7	G	142	GLU
7	G	149	ARG
7	G	155	ARG
8	H	3	THR
8	H	5	PRO
8	H	9	MET
8	H	11	THR
8	H	14	ARG
8	H	15	ASN
8	H	18	ARG
8	H	19	VAL
8	H	24	THR
8	H	26	VAL
8	H	29	SER
8	H	35	ILE
8	H	39	LEU
8	H	45	ILE
8	H	46	LYS
8	H	49	GLU
8	H	54	ASP
8	H	64	LYS
8	H	68	ARG
8	H	82	HIS
8	H	83	ILE
8	H	84	ARG
8	H	85	ARG
8	H	86	ILE
8	H	88	LYS
8	H	92	ARG
8	H	97	VAL
8	H	98	LYS
8	H	100	ILE
8	H	102	ARG
8	H	104	ARG
8	H	105	ARG
8	H	112	LEU

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Mol	Chain	Res	Type
8	H	114	THR
8	H	120	THR
8	H	126	LYS
8	H	127	LEU
8	H	129	VAL
8	H	133	LEU
9	I	16	ARG
9	I	19	LEU
9	I	38	GLN
9	I	40	LEU
9	I	51	ARG
9	I	53	VAL
9	I	66	ARG
9	I	79	LEU
9	I	83	ARG
9	I	85	LEU
9	I	86	VAL
9	I	88	TYR
9	I	93	ARG
9	I	97	LYS
9	I	99	LEU
9	I	110	GLU
10	J	3	LYS
10	J	8	LEU
10	J	16	LEU
10	J	19	SER
10	J	21	GLN
10	J	30	SER
10	J	47	PHE
10	J	48	THR
10	J	57	LYS
10	J	60	ARG
10	J	62	HIS
10	J	63	PHE
10	J	70	ARG
10	J	74	ILE
10	J	75	ILE
10	J	79	ARG
10	J	80	LYS
10	J	87	THR
10	J	89	ASP
10	J	90	LEU

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Mol	Chain	Res	Type
10	J	96	ILE
11	K	11	LYS
11	K	14	VAL
11	K	18	ARG
11	K	24	SER
11	K	29	ILE
11	K	33	THR
11	K	34	ASP
11	K	36	ASP
11	K	47	VAL
11	K	51	LYS
11	K	53	SER
11	K	62	GLN
11	K	75	TYR
11	K	78	GLN
11	K	79	SER
11	K	95	ILE
11	K	116	HIS
11	K	119	CYS
11	K	120	ARG
11	K	122	LYS
11	K	124	LYS
11	K	126	ARG
12	L	7	ILE
12	L	10	LEU
12	L	18	VAL
12	L	20	LYS
12	L	21	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	52	LEU
12	L	54	LYS
12	L	55	VAL
12	L	60	LEU
12	L	61	THR
12	L	64	TYR
12	L	65	GLU

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Mol	Chain	Res	Type
12	L	66	VAL
12	L	70	ILE
12	L	79	GLU
12	L	80	HIS
12	L	82	VAL
12	L	89	ARG
12	L	93	LEU
12	L	96	VAL
12	L	97	ARG
12	L	111	LYS
12	L	113	ARG
12	L	116	SER
12	L	119	LYS
12	L	122	THR
12	L	123	LYS
13	M	11	ARG
13	M	14	ARG
13	M	27	LYS
13	M	43	THR
13	M	46	LYS
13	M	48	LEU
13	M	50	GLU
13	M	53	VAL
13	M	56	LEU
13	M	63	THR
13	M	64	TRP
13	M	71	ARG
13	M	73	GLU
13	M	77	ASN
13	M	80	ARG
13	M	91	ARG
13	M	94	ARG
13	M	102	ARG
13	M	103	THR
13	M	105	THR
13	M	106	ASN
13	M	108	ARG
13	M	110	ARG
13	M	115	LYS
14	N	11	LYS
14	N	12	ARG
14	N	21	TYR

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Mol	Chain	Res	Type
14	N	22	THR
14	N	33	VAL
14	N	36	PHE
14	N	41	ARG
14	N	42	ILE
14	N	47	LEU
14	N	53	LEU
14	N	58	LYS
15	O	4	THR
15	O	9	GLN
15	O	13	GLN
15	O	22	THR
15	O	28	GLN
15	O	32	LEU
15	O	34	LEU
15	O	39	LEU
15	O	47	LYS
15	O	65	ARG
15	O	66	LEU
15	O	67	LEU
15	O	70	LEU
15	O	71	GLN
15	O	73	GLU
15	O	76	GLU
15	O	79	ARG
15	O	81	LEU
16	P	1	MET
16	P	2	VAL
16	P	3	LYS
16	P	26	ARG
16	P	29	ASP
16	P	31	LYS
16	P	44	THR
16	P	53	VAL
16	P	54	GLU
16	P	55	ARG
16	P	57	ARG
16	P	62	VAL
16	P	68	ASP
16	P	75	ARG
16	P	82	GLN
17	Q	3	LYS

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Mol	Chain	Res	Type
17	Q	7	THR
17	Q	9	VAL
17	Q	10	VAL
17	Q	13	ASP
17	Q	15	MET
17	Q	22	LEU
17	Q	30	PRO
17	Q	35	VAL
17	Q	37	LYS
17	Q	38	ARG
17	Q	53	LEU
17	Q	57	VAL
17	Q	59	ILE
17	Q	74	LEU
17	Q	75	ARG
17	Q	76	LEU
17	Q	83	ASP
17	Q	85	VAL
17	Q	86	GLU
17	Q	87	LYS
17	Q	92	ARG
17	Q	100	LYS
18	R	19	LYS
18	R	21	LYS
18	R	22	VAL
18	R	26	LEU
18	R	28	GLU
18	R	32	ARG
18	R	38	GLU
18	R	46	GLU
18	R	50	ILE
18	R	51	LEU
18	R	64	ARG
18	R	69	THR
18	R	78	LEU
18	R	82	THR
18	R	86	VAL
18	R	88	LYS
19	S	4	SER
19	S	7	LYS
19	S	15	LEU
19	S	22	LEU

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Mol	Chain	Res	Type
19	S	29	ARG
19	S	30	LEU
19	S	31	ILE
19	S	32	LYS
19	S	33	THR
19	S	34	TRP
19	S	36	ARG
19	S	41	VAL
19	S	43	GLU
19	S	49	ILE
19	S	57	HIS
19	S	58	VAL
19	S	63	THR
19	S	71	LEU
19	S	78	ARG
19	S	79	THR
19	S	81	ARG
20	T	10	LEU
20	T	13	LEU
20	T	15	ARG
20	T	19	SER
20	T	23	ARG
20	T	27	LYS
20	T	35	THR
20	T	36	LEU
20	T	41	ILE
20	T	53	LEU
20	T	56	MET
20	T	62	LEU
20	T	72	LEU
20	T	75	ASN
20	T	84	LEU
20	T	87	LYS
20	T	92	LEU
20	T	93	GLU
20	T	104	LEU
21	U	8	THR
21	U	9	ARG
21	U	12	LYS
21	U	25	LYS

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

Mol	Chain	Res	Type
2	B	19	HIS
3	C	6	HIS
3	C	110	ASN
4	D	119	GLN
5	E	20	GLN
7	G	28	ASN
8	H	82	HIS
9	I	73	GLN
9	I	117	HIS
16	P	82	GLN
17	Q	29	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1508/1522 (99%)	409 (27%)	57 (3%)

All (409) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	7	G
1	A	9	G
1	A	22	G
1	A	31	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	51	A
1	A	54	C
1	A	55	A
1	A	59	A
1	A	66	G
1	A	67	C
1	A	69	G
1	A	73	C
1	A	81	U
1	A	88	A
1	A	91	C
1	A	92	C
1	A	98	U

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Mol	Chain	Res	Type
1	A	113	G
1	A	114	U
1	A	115	G
1	A	116	A
1	A	120	A
1	A	121	C
1	A	122	G
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	135	C
1	A	151	A
1	A	160	A
1	A	161	A
1	A	163	C
1	A	164	U
1	A	166	G
1	A	173	U
1	A	181	G
1	A	182	U
1	A	183	G
1	A	190(C)	C
1	A	190(E)	U
1	A	190(F)	G
1	A	195	A
1	A	197	A
1	A	202	U
1	A	203	U
1	A	204	U
1	A	216	G
1	A	220	G
1	A	226	G
1	A	227	G
1	A	231	G
1	A	244	U
1	A	247	G
1	A	251	G
1	A	252	U
1	A	253	U
1	A	254	G
1	A	266	G
1	A	267	C

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Mol	Chain	Res	Type
1	A	269	C
1	A	289	G
1	A	292	G
1	A	293	G
1	A	299	G
1	A	319	G
1	A	321	A
1	A	323	U
1	A	328	C
1	A	329	A
1	A	330	C
1	A	331	G
1	A	332	G
1	A	344	A
1	A	345	C
1	A	349	A
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	370	C
1	A	371	G
1	A	373	A
1	A	379	C
1	A	384	G
1	A	390	C
1	A	398	C
1	A	406	G
1	A	411	A
1	A	412	A
1	A	413	G
1	A	415	A
1	A	421	U
1	A	422	C
1	A	428	G
1	A	429	U
1	A	430	A
1	A	439	A
1	A	445	G

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Mol	Chain	Res	Type
1	A	450	G
1	A	452	A
1	A	455	C
1	A	456	C
1	A	460	A
1	A	461	C
1	A	477	G
1	A	479	C
1	A	481	G
1	A	482	A
1	A	485	G
1	A	497	A
1	A	498	U
1	A	499	A
1	A	503	C
1	A	505	G
1	A	509	A
1	A	510	A
1	A	511	C
1	A	513	C
1	A	516	PSU
1	A	517	G
1	A	518	C
1	A	519	C
1	A	531	U
1	A	532	A
1	A	533	A
1	A	547	A
1	A	559	A
1	A	560	U
1	A	564	C
1	A	566	G
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	581	G
1	A	582	U
1	A	587	G

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Mol	Chain	Res	Type
1	A	588	G
1	A	597	G
1	A	598	U
1	A	609	A
1	A	616	G
1	A	618	C
1	A	645	C
1	A	653	A
1	A	661	G
1	A	665	A
1	A	670	G
1	A	673	G
1	A	686	U
1	A	687	A
1	A	688	G
1	A	697	U
1	A	701	C
1	A	702	A
1	A	718	G
1	A	719	C
1	A	721	G
1	A	722	A
1	A	723	U
1	A	731	G
1	A	749	C
1	A	751	U
1	A	755	G
1	A	770	C
1	A	777	A
1	A	781	A
1	A	782	A
1	A	787	A
1	A	792	A
1	A	793	U
1	A	794	A
1	A	813	U
1	A	814	A
1	A	815	A
1	A	817	C
1	A	819	A
1	A	821	G
1	A	828	A

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Mol	Chain	Res	Type
1	A	837	G
1	A	839	U
1	A	840	C
1	A	841	U
1	A	848	C
1	A	849	C
1	A	858	G
1	A	859	A
1	A	865	A
1	A	869	G
1	A	872	A
1	A	876	G
1	A	889	A
1	A	895	G
1	A	902	G
1	A	914	A
1	A	917	G
1	A	922	G
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	939	G
1	A	940	C
1	A	941	G
1	A	942	G
1	A	943	U
1	A	960	U
1	A	961	U
1	A	963	G
1	A	964	A
1	A	966	M2G
1	A	968	A
1	A	969	A
1	A	971	G
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	981	U
1	A	982	U
1	A	984	C

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Mol	Chain	Res	Type
1	A	989	C
1	A	990	C
1	A	991	U
1	A	992	U
1	A	993	G
1	A	994	A
1	A	1000	U
1	A	1003(A)	G
1	A	1004	A
1	A	1005	A
1	A	1006	C
1	A	1008	C
1	A	1010	G
1	A	1011	G
1	A	1016	A
1	A	1018	C
1	A	1020	U
1	A	1023	G
1	A	1024	G
1	A	1025	U
1	A	1026	G
1	A	1027	C
1	A	1030(B)	C
1	A	1031	G
1	A	1044	A
1	A	1045	C
1	A	1046	A
1	A	1052	U
1	A	1054	C
1	A	1055	A
1	A	1060	C
1	A	1061	G
1	A	1065	U
1	A	1066	C
1	A	1068	G
1	A	1073	U
1	A	1078	U
1	A	1085	U
1	A	1090	U
1	A	1092	A
1	A	1094	G
1	A	1095	U

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Mol	Chain	Res	Type
1	A	1101	A
1	A	1120	G
1	A	1122	U
1	A	1123	A
1	A	1125	U
1	A	1126	U
1	A	1127	G
1	A	1128	C
1	A	1129	C
1	A	1130	A
1	A	1136	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	1154	G
1	A	1159	U
1	A	1160	G
1	A	1167	A
1	A	1168	A
1	A	1169	A
1	A	1171	G
1	A	1174	G
1	A	1178	G
1	A	1181	G
1	A	1183	A
1	A	1184	G
1	A	1185	G
1	A	1190	G
1	A	1191	A
1	A	1193	G
1	A	1196	U
1	A	1197	G
1	A	1198	G
1	A	1200	C
1	A	1201	A
1	A	1202	G
1	A	1206	G
1	A	1207	2MG
1	A	1212	U

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Mol	Chain	Res	Type
1	A	1214	C
1	A	1215	G
1	A	1224	G
1	A	1225	A
1	A	1227	A
1	A	1238	A
1	A	1241	G
1	A	1245	A
1	A	1250	A
1	A	1251	A
1	A	1256	A
1	A	1257	U
1	A	1258	G
1	A	1260	C
1	A	1270	C
1	A	1277	C
1	A	1278	U
1	A	1279	A
1	A	1280	A
1	A	1281	U
1	A	1282	C
1	A	1286	A
1	A	1287	A
1	A	1297	C
1	A	1298	C
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1303	C
1	A	1304	G
1	A	1305	G
1	A	1306	A
1	A	1307	U
1	A	1310	G
1	A	1312	G
1	A	1315	U
1	A	1319	A
1	A	1320	C
1	A	1322	C
1	A	1326	C
1	A	1335	C
1	A	1336	C

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Mol	Chain	Res	Type
1	A	1338	G
1	A	1339	A
1	A	1340	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	1364	U
1	A	1370	G
1	A	1379	G
1	A	1381	U
1	A	1398	A
1	A	1399	C
1	A	1400	5MC
1	A	1401	G
1	A	1411	C
1	A	1419	G
1	A	1437	C
1	A	1440	C
1	A	1441	G
1	A	1442	G
1	A	1443	G
1	A	1446	A
1	A	1447	G
1	A	1451	A
1	A	1452	C
1	A	1453	G
1	A	1454	G
1	A	1485	U
1	A	1487	G
1	A	1493	A
1	A	1494	G
1	A	1496	C
1	A	1497	G
1	A	1498	UR3
1	A	1499	A
1	A	1500	A
1	A	1501	C
1	A	1502	A
1	A	1504	G

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Mol	Chain	Res	Type
1	A	1505	G
1	A	1506	U
1	A	1509	C
1	A	1520	G
1	A	1529	G
1	A	1530	G
1	A	1531	A
1	A	1533	C
1	A	1542	U

All (57) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U
1	A	91	C
1	A	115	G
1	A	129(A)	G
1	A	150	C
1	A	160	A
1	A	181	G
1	A	202	U
1	A	203	U
1	A	204	U
1	A	243	A
1	A	246	A
1	A	250	A
1	A	251	G
1	A	329	A
1	A	350	G
1	A	372	C
1	A	428	G
1	A	429	U
1	A	484	G
1	A	509	A
1	A	518	C
1	A	532	A
1	A	559	A
1	A	686	U
1	A	687	A
1	A	701	C
1	A	718	G
1	A	733	A

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Mol	Chain	Res	Type
1	A	748	C
1	A	777	A
1	A	792	A
1	A	812	C
1	A	819	A
1	A	913	A
1	A	960	U
1	A	975	A
1	A	992	U
1	A	1004	A
1	A	1065	U
1	A	1067	A
1	A	1139	G
1	A	1145	C
1	A	1190	G
1	A	1196	U
1	A	1201	A
1	A	1256	A
1	A	1257	U
1	A	1279	A
1	A	1285	A
1	A	1300	G
1	A	1305	G
1	A	1346	A
1	A	1347	G
1	A	1358	U
1	A	1380	U
1	A	1505	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	2MG	A	1207	1	17,26,27	2.00	3 (17%)	21,38,41	2.16	4 (19%)
1	5MC	A	1400	1	13,22,23	1.00	1 (7%)	15,32,35	1.17	3 (20%)
1	4OC	A	1402	1	13,23,24	1.12	1 (7%)	18,32,35	0.73	0
1	5MC	A	1404	1	13,22,23	0.98	1 (7%)	15,32,35	0.76	0
1	5MC	A	1407	1	13,22,23	1.67	3 (23%)	15,32,35	1.14	2 (13%)
1	UR3	A	1498	1	12,22,23	2.64	4 (33%)	16,32,35	1.58	2 (12%)
1	MA6	A	1518	1	16,26,27	1.94	5 (31%)	18,38,41	2.32	4 (22%)
1	MA6	A	1519	1	16,26,27	3.46	7 (43%)	18,38,41	1.25	2 (11%)
1	PSU	A	1540	1	13,21,22	1.32	2 (15%)	18,30,33	4.57	5 (27%)
1	PSU	A	1541	1	13,21,22	1.19	1 (7%)	18,30,33	3.91	6 (33%)
1	PSU	A	516	1,23	13,21,22	1.28	2 (15%)	18,30,33	4.09	5 (27%)
1	7MG	A	527	1	19,26,27	2.63	6 (31%)	24,39,42	1.83	6 (25%)
1	M2G	A	966	1	17,27,28	1.78	3 (17%)	22,40,43	2.23	5 (22%)
1	5MC	A	967	1	13,22,23	1.00	0	15,32,35	0.98	1 (6%)
12	0TD	L	92	12	4,9,10	1.21	0	4,11,13	4.22	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	1	-	0/7/29/30	0/3/3/3
1	MA6	A	1519	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	1,23	-	0/7/25/26	0/2/2/2
1	7MG	A	527	1	-	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 (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1498	UR3	C6-N1	-6.98	1.26	1.35
1	A	527	7MG	C8-N9	-6.70	1.35	1.45
1	A	1498	UR3	C4-N3	-4.31	1.31	1.38
1	A	527	7MG	CM7-N7	-3.06	1.40	1.46
1	A	527	7MG	O6-C6	-2.97	1.17	1.24
1	A	1407	5MC	C6-C5	-2.63	1.33	1.40
1	A	1540	PSU	C5-C1'	-2.63	1.49	1.52
1	A	1498	UR3	C6-C5	-2.47	1.32	1.38
1	A	516	PSU	O4'-C1'	-2.27	1.40	1.44
1	A	527	7MG	C8-N7	-2.17	1.33	1.43
1	A	1404	5MC	C6-C5	-2.01	1.34	1.40
1	A	1518	MA6	C5-N7	2.01	1.46	1.39
1	A	1407	5MC	O4'-C1'	2.04	1.43	1.41
1	A	1400	5MC	C6-N1	2.06	1.38	1.35
1	A	1498	UR3	O3'-C3'	2.15	1.48	1.43
1	A	1207	2MG	C2-N1	2.27	1.42	1.34
1	A	966	M2G	C2-N2	2.51	1.39	1.34
1	A	1519	MA6	C9-N6	2.64	1.52	1.45
1	A	1518	MA6	C9-N6	2.77	1.52	1.45
1	A	1519	MA6	C2-N3	2.89	1.37	1.32
1	A	1402	4OC	CM4-N4	2.92	1.50	1.45
1	A	1519	MA6	C2-N1	2.92	1.39	1.33
1	A	1519	MA6	C5-C4	2.93	1.47	1.40
1	A	1518	MA6	C6-N1	3.11	1.38	1.34
1	A	516	PSU	C4-N3	3.14	1.38	1.33
1	A	1518	MA6	C5-C4	3.16	1.47	1.40
1	A	1519	MA6	C5-N7	3.22	1.50	1.39
1	A	1540	PSU	C4-N3	3.33	1.39	1.33
1	A	1541	PSU	C4-N3	3.54	1.39	1.33
1	A	966	M2G	C4-N3	4.21	1.42	1.35
1	A	1207	2MG	C2-N2	4.27	1.39	1.34
1	A	1518	MA6	C2-N1	4.38	1.42	1.33
1	A	966	M2G	C6-N1	4.53	1.41	1.33
1	A	1407	5MC	C5-C4	4.62	1.48	1.41
1	A	527	7MG	C4-N3	4.71	1.40	1.34
1	A	527	7MG	C2-N2	5.58	1.45	1.34
1	A	1207	2MG	C6-N1	6.04	1.44	1.33
1	A	1519	MA6	C4-N3	8.28	1.47	1.35
1	A	1519	MA6	C6-N1	8.72	1.45	1.34

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	-15.15	118.67	128.33
1	A	516	PSU	N1-C2-N3	-14.59	119.03	128.33
1	A	1541	PSU	N1-C2-N3	-13.89	119.47	128.33
1	A	966	M2G	C5-C6-N1	-7.85	112.86	123.59
1	A	1207	2MG	C5-C6-N1	-7.74	113.01	123.59
1	A	1540	PSU	C5-C1'-C2'	-7.56	102.09	115.52
1	A	1518	MA6	C1'-N9-C4	-6.87	116.57	126.94
1	A	527	7MG	C5-C4-N3	-6.28	120.70	126.82
12	L	92	0TD	CSB-SB-CB	-5.79	90.61	101.54
12	L	92	0TD	CB-CA-N	-5.09	98.64	109.66
1	A	1518	MA6	N1-C6-N6	-4.25	112.42	117.05
1	A	1519	MA6	C1'-N9-C4	-3.52	121.63	126.94
1	A	966	M2G	N1-C2-N2	-3.31	113.43	117.16
12	L	92	0TD	C-CA-N	-3.03	103.51	109.83
1	A	1407	5MC	N4-C4-N3	-2.59	113.20	116.95
1	A	527	7MG	C4-N9-C1'	-2.57	120.51	126.70
1	A	1400	5MC	N4-C4-N3	-2.47	113.37	116.95
1	A	1207	2MG	CM2-N2-C2	-2.44	120.31	123.07
1	A	1498	UR3	C5-C4-N3	-2.40	112.38	117.45
1	A	527	7MG	N1-C2-N3	-2.34	121.70	125.53
1	A	516	PSU	C5-C6-N1	-2.29	121.16	124.39
1	A	966	M2G	C2-N3-C4	-2.03	112.64	115.09
1	A	1540	PSU	O4'-C1'-C2'	2.02	106.78	104.73
1	A	1541	PSU	C5-C1'-C2'	2.07	119.19	115.52
1	A	1407	5MC	C5-C4-N3	2.11	124.80	121.27
1	A	527	7MG	N2-C2-N1	2.14	120.74	117.20
1	A	1541	PSU	C4-C5-C1'	2.23	125.30	121.23
1	A	527	7MG	C2-N3-C4	2.27	121.16	114.53
1	A	1400	5MC	CM5-C5-C6	2.29	123.23	118.62
1	A	966	M2G	C4-C5-N7	2.34	111.63	109.48
1	A	1400	5MC	C5-C4-N3	2.41	125.30	121.27
1	A	1207	2MG	C4-C5-N7	2.67	111.93	109.48
1	A	1541	PSU	C6-N1-C2	2.73	119.86	115.47
1	A	516	PSU	C6-N1-C2	2.79	119.95	115.47
1	A	967	5MC	CM5-C5-C6	2.95	124.55	118.62
1	A	1518	MA6	C2-N1-C6	3.06	117.94	111.43
1	A	527	7MG	N3-C4-N9	3.07	131.37	126.75
1	A	1519	MA6	C2-N1-C6	3.09	118.01	111.43
1	A	516	PSU	O4'-C1'-C2'	3.09	107.88	104.73
1	A	1541	PSU	O4'-C1'-C2'	3.28	108.07	104.73
1	A	1540	PSU	C6-N1-C2	3.29	120.76	115.47
1	A	966	M2G	N3-C2-N2	3.44	121.06	117.16
1	A	1518	MA6	N3-C2-N1	3.69	131.72	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1498	UR3	C6-C5-C4	3.96	124.69	117.28
1	A	1207	2MG	C6-N1-C2	4.11	121.29	115.31
1	A	1541	PSU	C4-N3-C2	6.88	121.19	115.25
1	A	1540	PSU	C4-N3-C2	7.58	121.80	115.25
1	A	516	PSU	C4-N3-C2	7.85	122.03	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1207	2MG	1	0
1	A	1400	5MC	4	0
1	A	1402	4OC	1	0
1	A	1404	5MC	5	0
1	A	1498	UR3	3	0
1	A	1518	MA6	2	0
1	A	1519	MA6	4	0
1	A	1540	PSU	2	0
1	A	527	7MG	1	0
1	A	966	M2G	4	0
1	A	967	5MC	4	0
12	L	92	0TD	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 270 ligands modelled in this entry, 269 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	SRY	A	1601	-	33,42,42	1.47	6 (18%)	36,63,63	1.95	12 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	SRY	A	1601	-	-	0/16/87/87	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	1601	SRY	O53-C53	-3.23	1.36	1.44
22	A	1601	SRY	C23-N23	-3.05	1.42	1.47
22	A	1601	SRY	C11-N11	-2.71	1.42	1.47
22	A	1601	SRY	O51-C51	-2.48	1.37	1.43
22	A	1601	SRY	O32-C32	-2.40	1.40	1.44
22	A	1601	SRY	C21-C11	-2.14	1.48	1.53

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	1601	SRY	C13-O53-C53	-4.37	105.25	113.75
22	A	1601	SRY	O42-C12-C22	-3.57	103.92	107.42
22	A	1601	SRY	C13-O13-C22	-3.50	110.01	116.30
22	A	1601	SRY	C33-C43-C53	-3.46	104.16	110.20
22	A	1601	SRY	C61-C11-N11	-2.70	103.40	111.38
22	A	1601	SRY	C43-C33-C23	-2.68	106.72	110.43
22	A	1601	SRY	O13-C13-O53	-2.49	104.37	110.68
22	A	1601	SRY	O43-C43-C53	2.08	114.75	109.24
22	A	1601	SRY	O13-C22-C32	2.20	116.81	111.52
22	A	1601	SRY	O33-C33-C23	2.41	114.58	109.66
22	A	1601	SRY	C63-C53-C43	2.54	119.28	113.02
22	A	1601	SRY	O41-C41-C51	2.98	114.85	107.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	1601	SRY	5	0

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%)	-0.38	22 (1%) 76 61	91, 154, 301, 391	0
2	B	234/256 (91%)	-0.58	0 100 100	125, 174, 266, 283	0
3	C	206/239 (86%)	-0.09	11 (5%) 30 18	181, 240, 279, 300	0
4	D	208/209 (99%)	-0.50	2 (0%) 84 71	112, 159, 214, 231	0
5	E	150/162 (92%)	-0.61	0 100 100	80, 126, 173, 210	0
6	F	101/101 (100%)	-0.69	0 100 100	123, 174, 206, 235	0
7	G	155/156 (99%)	-0.42	3 (1%) 70 53	151, 198, 247, 296	0
8	H	138/138 (100%)	-0.72	0 100 100	81, 110, 145, 193	0
9	I	127/128 (99%)	-0.27	2 (1%) 74 58	154, 229, 263, 300	0
10	J	98/105 (93%)	0.25	7 (7%) 19 10	217, 246, 300, 348	0
11	K	116/129 (89%)	-0.64	0 100 100	117, 150, 194, 234	0
12	L	123/135 (91%)	-0.47	0 100 100	87, 145, 186, 245	0
13	M	118/126 (93%)	-0.30	2 (1%) 73 56	136, 183, 220, 242	0
14	N	60/61 (98%)	0.11	2 (3%) 50 33	184, 226, 269, 294	0
15	O	87/89 (97%)	-0.56	0 100 100	87, 137, 178, 199	0
16	P	83/88 (94%)	-0.57	0 100 100	117, 152, 181, 207	0
17	Q	99/105 (94%)	-0.66	0 100 100	89, 128, 163, 183	0
18	R	70/88 (79%)	-0.70	0 100 100	113, 150, 199, 218	0
19	S	80/93 (86%)	0.17	4 (5%) 32 20	180, 242, 278, 303	0
20	T	99/106 (93%)	-0.64	1 (1%) 84 71	117, 155, 206, 236	0
21	U	24/27 (88%)	1.01	5 (20%) 1 1	154, 205, 230, 236	0
All	All	3874/4063 (95%)	-0.40	61 (1%) 74 58	80, 165, 269, 391	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
21	U	17	THR	4.8
1	A	994	A	4.5
3	C	193	TYR	4.5
1	A	1037	C	4.3
1	A	1019	C	4.3
1	A	1129	C	4.3
1	A	1539	C	4.2
1	A	1018	C	4.1
10	J	39	PRO	4.1
10	J	33	GLN	3.8
3	C	103	VAL	3.8
3	C	65	ALA	3.7
3	C	102	ASN	3.6
1	A	993	G	3.5
21	U	25	LYS	3.5
21	U	18	TYR	3.4
1	A	1017	G	3.3
3	C	155	GLY	3.2
1	A	1005	A	3.2
7	G	81	GLY	3.2
14	N	11	LYS	3.0
7	G	2	ALA	3.0
13	M	117	VAL	2.9
1	A	1006	C	2.9
14	N	4	LYS	2.8
19	S	30	LEU	2.8
1	A	1045	C	2.8
19	S	31	ILE	2.8
1	A	1007	C	2.8
3	C	66	VAL	2.8
1	A	1050	G	2.7
1	A	202	U	2.7
19	S	32	LYS	2.7
1	A	1004	A	2.7
1	A	995	C	2.6
10	J	34	VAL	2.5
10	J	99	LYS	2.5
1	A	1036	G	2.4
10	J	74	ILE	2.4
13	M	65	LYS	2.3
3	C	157	ILE	2.3
1	A	1257	U	2.3
21	U	24	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1047	G	2.3
1	A	1003(A)	G	2.3
3	C	162	GLN	2.2
7	G	82	GLY	2.2
3	C	76	VAL	2.2
20	T	106	ALA	2.2
4	D	20	TYR	2.2
1	A	81	U	2.2
1	A	1003	G	2.2
10	J	38	ILE	2.1
19	S	41	VAL	2.1
9	I	128	ARG	2.1
3	C	146	ALA	2.1
3	C	77	ILE	2.1
9	I	4	TYR	2.1
21	U	11	GLY	2.0
4	D	35	ARG	2.0
10	J	89	ASP	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	2MG	A	1207	24/25	0.90	0.27	-	233,253,259,266	0
1	5MC	A	1404	21/22	0.95	0.17	-	140,150,159,171	0
1	5MC	A	967	21/22	0.96	0.14	-	145,164,179,184	0
1	5MC	A	1400	21/22	0.94	0.18	-	123,161,167,168	0
1	7MG	A	527	24/25	0.97	0.14	-	118,132,143,146	0
1	MA6	A	1519	24/25	0.97	0.14	-	126,149,157,161	0
1	M2G	A	966	25/26	0.94	0.19	-	141,169,180,185	0
1	UR3	A	1498	21/22	0.92	0.25	-	130,151,177,185	0
1	PSU	A	516	20/21	0.94	0.10	-	126,162,186,188	0
1	PSU	A	1540	20/21	0.79	0.68	-	251,258,331,332	0
1	MA6	A	1518	24/25	0.95	0.13	-	138,166,194,200	0
1	4OC	A	1402	22/23	0.95	0.19	-	130,148,159,165	0
12	0TD	L	92	10/11	0.96	0.31	-	111,148,156,269	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	PSU	A	1541	20/21	0.76	0.46	-	257,268,323,323	0
1	5MC	A	1407	21/22	0.96	0.12	-	163,173,184,184	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
23	MG	A	1779	1/1	0.87	0.80	89.76	119,119,119,119	0
23	MG	A	1726	1/1	0.96	0.37	21.98	121,121,121,121	0
23	MG	H	203	1/1	0.96	0.89	17.31	111,111,111,111	0
23	MG	A	1728	1/1	0.94	0.39	15.09	156,156,156,156	0
23	MG	B	301	1/1	0.92	0.57	11.87	159,159,159,159	0
23	MG	T	1202	1/1	0.93	0.37	9.51	330,330,330,330	0
23	MG	A	1761	1/1	0.87	0.36	8.25	163,163,163,163	0
23	MG	A	1690	1/1	0.92	0.30	8.12	138,138,138,138	0
23	MG	A	1691	1/1	0.87	0.41	7.93	331,331,331,331	0
23	MG	A	1848	1/1	0.98	0.28	7.23	278,278,278,278	0
23	MG	A	1768	1/1	0.97	0.26	7.16	118,118,118,118	0
23	MG	A	1846	1/1	0.92	0.33	7.08	228,228,228,228	0
23	MG	A	1732	1/1	0.87	0.28	6.25	101,101,101,101	0
23	MG	A	1613	1/1	0.97	0.28	5.44	177,177,177,177	0
23	MG	A	1666	1/1	0.94	0.30	5.34	168,168,168,168	0
23	MG	A	1641	1/1	0.88	0.29	5.26	149,149,149,149	0
23	MG	A	1788	1/1	0.93	0.22	4.98	112,112,112,112	0
23	MG	A	1731	1/1	0.91	0.44	4.48	118,118,118,118	0
23	MG	M	202	1/1	0.98	0.45	4.45	137,137,137,137	0
23	MG	A	1708	1/1	0.82	0.28	4.23	115,115,115,115	0
23	MG	A	1699	1/1	0.94	0.28	3.98	130,130,130,130	0
23	MG	A	1843	1/1	0.98	0.18	3.92	380,380,380,380	0
23	MG	A	1828	1/1	0.96	0.29	3.85	409,409,409,409	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
23	MG	A	1747	1/1	0.82	0.15	3.37	104,104,104,104	0
23	MG	A	1724	1/1	0.94	0.34	2.87	128,128,128,128	0
23	MG	A	1715	1/1	0.99	0.18	1.59	134,134,134,134	0
23	MG	A	1656	1/1	0.94	0.17	1.39	143,143,143,143	0
23	MG	A	1706	1/1	0.94	0.19	1.32	167,167,167,167	0
23	MG	A	1737	1/1	0.68	0.39	1.27	158,158,158,158	0
23	MG	A	1781	1/1	0.92	0.18	1.23	101,101,101,101	0
23	MG	A	1663	1/1	0.96	0.23	1.08	141,141,141,141	0
23	MG	A	1609	1/1	0.99	0.19	0.65	126,126,126,126	0
23	MG	D	302	1/1	0.96	0.17	0.52	124,124,124,124	0
23	MG	A	1683	1/1	0.81	0.24	0.36	272,272,272,272	0
23	MG	A	1739	1/1	0.93	0.24	0.33	117,117,117,117	0
22	SRY	A	1601	40/40	0.96	0.19	0.27	103,141,162,165	0
23	MG	A	1786	1/1	0.94	0.26	0.21	155,155,155,155	0
23	MG	A	1765	1/1	0.91	0.28	0.08	139,139,139,139	0
23	MG	A	1754	1/1	0.99	0.15	0.07	122,122,122,122	0
23	MG	A	1614	1/1	0.96	0.20	-0.02	94,94,94,94	0
23	MG	A	1687	1/1	0.97	0.18	-0.09	114,114,114,114	0
23	MG	A	1682	1/1	0.92	0.24	-0.10	185,185,185,185	0
23	MG	A	1709	1/1	0.97	0.17	-0.16	102,102,102,102	0
24	ZN	D	301	1/1	1.00	0.31	-0.35	125,125,125,125	0
23	MG	A	1773	1/1	0.97	0.17	-0.37	334,334,334,334	0
23	MG	A	1827	1/1	0.99	0.17	-0.37	134,134,134,134	0
23	MG	A	1646	1/1	0.90	0.11	-0.41	148,148,148,148	0
23	MG	T	1201	1/1	0.98	0.18	-0.44	81,81,81,81	0
23	MG	A	1736	1/1	0.98	0.11	-0.48	109,109,109,109	0
23	MG	A	1808	1/1	0.97	0.14	-0.61	139,139,139,139	0
23	MG	A	1702	1/1	0.94	0.20	-0.68	116,116,116,116	0
23	MG	A	1630	1/1	0.95	0.11	-0.86	116,116,116,116	0
24	ZN	N	101	1/1	0.95	0.14	-0.91	395,395,395,395	0
23	MG	A	1685	1/1	0.91	0.13	-0.95	127,127,127,127	0
23	MG	A	1672	1/1	0.99	0.12	-1.01	167,167,167,167	0
23	MG	A	1825	1/1	0.98	0.13	-1.17	314,314,314,314	0
23	MG	A	1751	1/1	0.98	0.07	-1.26	257,257,257,257	0
23	MG	A	1842	1/1	0.98	0.17	-1.28	159,159,159,159	0
23	MG	A	1749	1/1	0.94	0.07	-1.34	142,142,142,142	0
23	MG	A	1633	1/1	0.99	0.13	-1.39	91,91,91,91	0
23	MG	A	1649	1/1	0.99	0.12	-1.42	206,206,206,206	0
23	MG	A	1807	1/1	0.98	0.14	-1.43	99,99,99,99	0
23	MG	A	1628	1/1	0.98	0.12	-1.72	131,131,131,131	0
23	MG	A	1674	1/1	0.99	0.11	-2.06	113,113,113,113	0
23	MG	A	1721	1/1	0.91	0.10	-2.50	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
23	MG	A	1688	1/1	0.98	0.11	-2.78	116,116,116,116	0
23	MG	A	1841	1/1	0.98	0.11	-3.01	274,274,274,274	0
23	MG	A	1635	1/1	0.98	0.07	-3.51	89,89,89,89	0
23	MG	A	1650	1/1	0.98	0.10	-3.73	138,138,138,138	0
23	MG	A	1753	1/1	0.98	0.11	-4.06	265,265,265,265	0
23	MG	A	1804	1/1	0.94	0.21	-	146,146,146,146	0
23	MG	A	1822	1/1	0.98	0.19	-	265,265,265,265	0
23	MG	A	1790	1/1	0.88	0.34	-	133,133,133,133	0
23	MG	A	1681	1/1	0.97	0.06	-	226,226,226,226	0
23	MG	A	1729	1/1	0.95	0.30	-	162,162,162,162	0
23	MG	P	102	1/1	0.65	0.47	-	115,115,115,115	0
23	MG	A	1686	1/1	0.98	0.15	-	184,184,184,184	0
23	MG	A	1616	1/1	0.92	0.24	-	95,95,95,95	0
23	MG	A	1662	1/1	0.96	0.11	-	148,148,148,148	0
23	MG	A	1610	1/1	0.92	0.34	-	106,106,106,106	0
23	MG	A	1659	1/1	0.96	0.15	-	154,154,154,154	0
23	MG	A	1803	1/1	0.68	0.22	-	103,103,103,103	0
23	MG	A	1844	1/1	0.97	0.14	-	199,199,199,199	0
23	MG	A	1839	1/1	0.99	0.21	-	116,116,116,116	0
23	MG	A	1833	1/1	0.80	0.12	-	189,189,189,189	0
23	MG	A	1809	1/1	0.96	0.21	-	118,118,118,118	0
23	MG	A	1824	1/1	0.94	0.22	-	485,485,485,485	0
23	MG	A	1796	1/1	0.92	0.14	-	137,137,137,137	0
23	MG	A	1636	1/1	0.99	0.42	-	167,167,167,167	0
23	MG	A	1678	1/1	0.98	0.11	-	146,146,146,146	0
23	MG	A	1805	1/1	0.99	0.15	-	105,105,105,105	0
23	MG	A	1743	1/1	0.95	1.00	-	129,129,129,129	0
23	MG	A	1767	1/1	0.98	0.24	-	132,132,132,132	0
23	MG	A	1705	1/1	0.96	0.25	-	127,127,127,127	0
23	MG	M	201	1/1	0.86	0.46	-	139,139,139,139	0
23	MG	A	1750	1/1	0.90	0.12	-	158,158,158,158	0
23	MG	A	1622	1/1	0.99	0.16	-	156,156,156,156	0
23	MG	A	1665	1/1	0.93	0.09	-	247,247,247,247	0
23	MG	A	1652	1/1	0.94	0.60	-	126,126,126,126	0
23	MG	Q	202	1/1	0.79	0.36	-	89,89,89,89	0
23	MG	H	204	1/1	0.67	1.00	-	125,125,125,125	0
23	MG	A	1637	1/1	0.96	0.65	-	177,177,177,177	0
23	MG	A	1694	1/1	0.91	0.27	-	141,141,141,141	0
23	MG	A	1838	1/1	0.79	0.38	-	427,427,427,427	0
23	MG	A	1607	1/1	0.93	0.07	-	183,183,183,183	0
23	MG	A	1692	1/1	0.91	0.23	-	117,117,117,117	0
23	MG	A	1617	1/1	0.96	0.14	-	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
23	MG	A	1697	1/1	0.91	0.18	-	260,260,260,260	0
23	MG	A	1791	1/1	0.49	0.45	-	138,138,138,138	0
23	MG	A	1707	1/1	0.57	0.33	-	117,117,117,117	0
23	MG	A	1648	1/1	0.88	0.33	-	144,144,144,144	0
23	MG	A	1710	1/1	0.78	0.68	-	98,98,98,98	0
23	MG	A	1723	1/1	0.95	0.17	-	102,102,102,102	0
23	MG	A	1654	1/1	0.90	0.12	-	176,176,176,176	0
23	MG	A	1621	1/1	0.94	0.16	-	109,109,109,109	0
23	MG	A	1821	1/1	0.96	0.21	-	315,315,315,315	0
23	MG	A	1802	1/1	0.94	0.11	-	139,139,139,139	0
23	MG	A	1797	1/1	0.79	0.85	-	140,140,140,140	0
23	MG	A	1671	1/1	0.88	0.50	-	135,135,135,135	0
23	MG	A	1818	1/1	0.91	0.19	-	423,423,423,423	0
23	MG	A	1717	1/1	0.98	0.14	-	107,107,107,107	0
23	MG	A	1611	1/1	0.98	0.12	-	174,174,174,174	0
23	MG	A	1644	1/1	0.98	0.30	-	127,127,127,127	0
23	MG	A	1603	1/1	0.93	0.25	-	135,135,135,135	0
23	MG	A	1689	1/1	0.95	0.26	-	336,336,336,336	0
23	MG	A	1785	1/1	0.92	0.09	-	137,137,137,137	0
23	MG	A	1801	1/1	0.88	0.25	-	105,105,105,105	0
23	MG	A	1798	1/1	0.79	0.26	-	131,131,131,131	0
23	MG	A	1727	1/1	0.74	0.49	-	116,116,116,116	0
23	MG	A	1816	1/1	0.99	0.08	-	179,179,179,179	0
23	MG	A	1673	1/1	0.71	0.39	-	99,99,99,99	0
23	MG	Q	201	1/1	0.91	0.32	-	118,118,118,118	0
23	MG	A	1760	1/1	0.96	0.17	-	139,139,139,139	0
23	MG	A	1774	1/1	0.97	0.10	-	496,496,496,496	0
23	MG	A	1675	1/1	0.96	0.15	-	113,113,113,113	0
23	MG	A	1713	1/1	0.89	0.28	-	110,110,110,110	0
23	MG	A	1693	1/1	0.99	0.08	-	134,134,134,134	0
23	MG	A	1769	1/1	0.90	1.33	-	157,157,157,157	0
23	MG	A	1620	1/1	0.95	0.59	-	166,166,166,166	0
23	MG	A	1772	1/1	0.99	0.30	-	243,243,243,243	0
23	MG	A	1703	1/1	0.91	0.26	-	121,121,121,121	0
23	MG	A	1782	1/1	0.69	0.43	-	123,123,123,123	0
23	MG	A	1742	1/1	0.75	0.49	-	151,151,151,151	0
23	MG	A	1677	1/1	0.98	0.21	-	149,149,149,149	0
23	MG	A	1735	1/1	0.93	0.12	-	112,112,112,112	0
23	MG	A	1812	1/1	0.98	0.19	-	202,202,202,202	0
23	MG	A	1668	1/1	0.76	0.44	-	191,191,191,191	0
23	MG	A	1787	1/1	0.84	0.28	-	145,145,145,145	0
23	MG	A	1704	1/1	0.90	0.29	-	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
23	MG	A	1623	1/1	0.96	0.15	-	100,100,100,100	0
23	MG	A	1795	1/1	0.97	0.34	-	127,127,127,127	0
23	MG	A	1740	1/1	0.92	0.15	-	112,112,112,112	0
23	MG	A	1719	1/1	0.86	0.26	-	143,143,143,143	0
23	MG	A	1757	1/1	0.92	0.26	-	122,122,122,122	0
23	MG	A	1618	1/1	0.99	0.14	-	139,139,139,139	0
23	MG	A	1836	1/1	0.99	0.07	-	201,201,201,201	0
23	MG	A	1725	1/1	0.98	0.30	-	89,89,89,89	0
23	MG	A	1759	1/1	0.93	0.25	-	161,161,161,161	0
23	MG	A	1640	1/1	0.80	0.39	-	107,107,107,107	0
23	MG	A	1608	1/1	0.97	0.33	-	112,112,112,112	0
23	MG	A	1793	1/1	0.87	0.51	-	139,139,139,139	0
23	MG	A	1847	1/1	0.68	0.43	-	418,418,418,418	0
23	MG	A	1835	1/1	0.93	0.15	-	166,166,166,166	0
23	MG	A	1700	1/1	0.96	0.10	-	144,144,144,144	0
23	MG	A	1800	1/1	0.78	0.57	-	105,105,105,105	0
23	MG	A	1823	1/1	0.98	0.19	-	307,307,307,307	0
23	MG	A	1602	1/1	0.77	0.33	-	198,198,198,198	0
23	MG	A	1813	1/1	0.95	0.27	-	371,371,371,371	0
23	MG	B	302	1/1	0.70	0.11	-	112,112,112,112	0
23	MG	A	1642	1/1	0.97	0.19	-	249,249,249,249	0
23	MG	A	1820	1/1	0.98	0.08	-	176,176,176,176	0
23	MG	A	1792	1/1	0.78	0.48	-	136,136,136,136	0
23	MG	H	202	1/1	0.94	0.31	-	83,83,83,83	0
23	MG	A	1776	1/1	0.92	0.14	-	135,135,135,135	0
23	MG	A	1758	1/1	0.80	0.34	-	106,106,106,106	0
23	MG	A	1789	1/1	0.91	0.39	-	137,137,137,137	0
23	MG	A	1819	1/1	0.93	0.18	-	309,309,309,309	0
23	MG	A	1657	1/1	0.96	0.09	-	177,177,177,177	0
23	MG	A	1799	1/1	0.93	0.40	-	117,117,117,117	0
23	MG	A	1634	1/1	0.94	0.31	-	101,101,101,101	0
23	MG	A	1605	1/1	0.99	0.08	-	107,107,107,107	0
23	MG	A	1849	1/1	0.97	0.29	-	399,399,399,399	0
23	MG	A	1670	1/1	0.97	0.54	-	130,130,130,130	0
23	MG	A	1806	1/1	0.89	0.30	-	128,128,128,128	0
23	MG	A	1667	1/1	0.87	0.29	-	114,114,114,114	0
23	MG	A	1752	1/1	0.96	0.13	-	148,148,148,148	0
23	MG	A	1730	1/1	0.96	0.15	-	144,144,144,144	0
23	MG	A	1748	1/1	0.88	0.23	-	144,144,144,144	0
23	MG	A	1777	1/1	0.58	0.29	-	132,132,132,132	0
23	MG	A	1655	1/1	0.98	0.14	-	161,161,161,161	0
23	MG	A	1811	1/1	0.96	0.24	-	226,226,226,226	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
23	MG	A	1712	1/1	0.98	0.12	-	128,128,128,128	0
23	MG	A	1755	1/1	0.84	0.38	-	122,122,122,122	0
23	MG	A	1780	1/1	0.98	0.24	-	105,105,105,105	0
23	MG	J	201	1/1	0.92	0.41	-	128,128,128,128	0
23	MG	A	1771	1/1	0.90	0.22	-	348,348,348,348	0
23	MG	A	1653	1/1	0.97	0.11	-	124,124,124,124	0
23	MG	A	1661	1/1	0.51	0.91	-	118,118,118,118	0
23	MG	A	1794	1/1	0.61	0.51	-	117,117,117,117	0
23	MG	A	1679	1/1	0.93	0.59	-	125,125,125,125	0
23	MG	A	1783	1/1	0.73	0.39	-	91,91,91,91	0
23	MG	A	1615	1/1	0.92	0.43	-	121,121,121,121	0
23	MG	A	1837	1/1	0.96	0.36	-	350,350,350,350	0
23	MG	A	1680	1/1	0.90	0.28	-	190,190,190,190	0
23	MG	A	1714	1/1	0.92	0.10	-	112,112,112,112	0
23	MG	A	1763	1/1	0.87	0.47	-	290,290,290,290	0
23	MG	A	1734	1/1	0.95	0.12	-	145,145,145,145	0
23	MG	A	1762	1/1	0.96	0.55	-	172,172,172,172	0
23	MG	A	1629	1/1	0.96	0.55	-	97,97,97,97	0
23	MG	A	1744	1/1	0.85	0.42	-	115,115,115,115	0
23	MG	P	101	1/1	0.74	0.39	-	93,93,93,93	0
23	MG	A	1764	1/1	0.31	0.47	-	122,122,122,122	0
23	MG	A	1651	1/1	0.81	0.32	-	144,144,144,144	0
23	MG	A	1612	1/1	0.97	0.42	-	128,128,128,128	0
23	MG	A	1625	1/1	0.96	0.14	-	206,206,206,206	0
23	MG	A	1829	1/1	0.99	0.09	-	180,180,180,180	0
23	MG	A	1830	1/1	0.78	0.37	-	114,114,114,114	0
23	MG	A	1741	1/1	0.67	0.56	-	105,105,105,105	0
23	MG	A	1695	1/1	0.97	0.07	-	146,146,146,146	0
23	MG	A	1834	1/1	0.90	0.06	-	204,204,204,204	0
23	MG	S	101	1/1	0.77	0.20	-	130,130,130,130	0
23	MG	A	1606	1/1	0.98	0.16	-	117,117,117,117	0
23	MG	A	1766	1/1	0.79	0.36	-	114,114,114,114	0
23	MG	A	1733	1/1	0.74	0.57	-	124,124,124,124	0
23	MG	A	1632	1/1	0.90	0.24	-	103,103,103,103	0
23	MG	A	1638	1/1	0.91	0.27	-	136,136,136,136	0
23	MG	A	1716	1/1	0.80	0.49	-	111,111,111,111	0
23	MG	A	1832	1/1	0.97	0.20	-	148,148,148,148	0
23	MG	A	1840	1/1	0.99	0.17	-	100,100,100,100	0
23	MG	A	1639	1/1	0.99	0.32	-	139,139,139,139	0
23	MG	A	1647	1/1	0.96	0.20	-	146,146,146,146	0
23	MG	A	1660	1/1	0.94	0.21	-	211,211,211,211	0
23	MG	A	1626	1/1	0.98	0.18	-	162,162,162,162	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
23	MG	A	1831	1/1	0.95	0.23	-	114,114,114,114	0
23	MG	A	1701	1/1	0.83	0.30	-	133,133,133,133	0
23	MG	A	1746	1/1	0.81	0.19	-	145,145,145,145	0
23	MG	H	201	1/1	0.86	0.39	-	85,85,85,85	0
23	MG	E	201	1/1	0.98	0.07	-	167,167,167,167	0
23	MG	A	1784	1/1	0.97	1.02	-	125,125,125,125	0
23	MG	A	1815	1/1	0.90	0.39	-	406,406,406,406	0
23	MG	A	1745	1/1	0.94	0.60	-	179,179,179,179	0
23	MG	A	1658	1/1	0.92	0.24	-	148,148,148,148	0
23	MG	A	1645	1/1	0.99	0.12	-	144,144,144,144	0
23	MG	A	1684	1/1	0.98	0.38	-	242,242,242,242	0
23	MG	A	1720	1/1	0.94	0.19	-	115,115,115,115	0
23	MG	A	1826	1/1	0.96	0.29	-	366,366,366,366	0
23	MG	A	1722	1/1	0.95	0.18	-	117,117,117,117	0
23	MG	A	1627	1/1	0.94	0.20	-	130,130,130,130	0
23	MG	A	1624	1/1	0.90	0.35	-	214,214,214,214	0
23	MG	A	1756	1/1	0.92	0.30	-	120,120,120,120	0
23	MG	A	1604	1/1	0.92	0.27	-	103,103,103,103	0
23	MG	A	1817	1/1	0.93	0.18	-	354,354,354,354	0
23	MG	A	1696	1/1	0.76	0.85	-	138,138,138,138	0
23	MG	A	1698	1/1	0.73	0.36	-	115,115,115,115	0
23	MG	A	1664	1/1	0.88	0.29	-	180,180,180,180	0
23	MG	A	1814	1/1	0.98	0.15	-	254,254,254,254	0
23	MG	A	1738	1/1	0.90	0.20	-	112,112,112,112	0
23	MG	A	1850	1/1	0.89	0.23	-	314,314,314,314	0
23	MG	A	1810	1/1	0.98	0.15	-	190,190,190,190	0
23	MG	A	1845	1/1	0.97	0.15	-	341,341,341,341	0
23	MG	A	1775	1/1	0.97	0.25	-	135,135,135,135	0
23	MG	A	1718	1/1	0.86	0.14	-	145,145,145,145	0
23	MG	A	1643	1/1	0.98	0.14	-	85,85,85,85	0
23	MG	A	1619	1/1	0.98	0.14	-	150,150,150,150	0
23	MG	A	1711	1/1	0.84	0.34	-	121,121,121,121	0
23	MG	A	1770	1/1	0.99	0.10	-	215,215,215,215	0
23	MG	A	1778	1/1	0.89	0.16	-	180,180,180,180	0
23	MG	A	1631	1/1	1.00	0.11	-	102,102,102,102	0
23	MG	A	1676	1/1	0.99	0.19	-	109,109,109,109	0
23	MG	A	1669	1/1	0.99	0.45	-	131,131,131,131	0

6.5 Other polymers (i)

There are no such residues in this entry.