Full wwPDB X-ray Structure Validation Report ⓘ

Feb 10, 2025 – 02:12 PM EST

PDB ID	:	4DV3
Title	:	Crystal structure of the Thermus thermophilus 30S ribosomal subunit with a 16S rRNA mutation, C912A, 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	:	3.55 Å(reported)

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

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

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

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

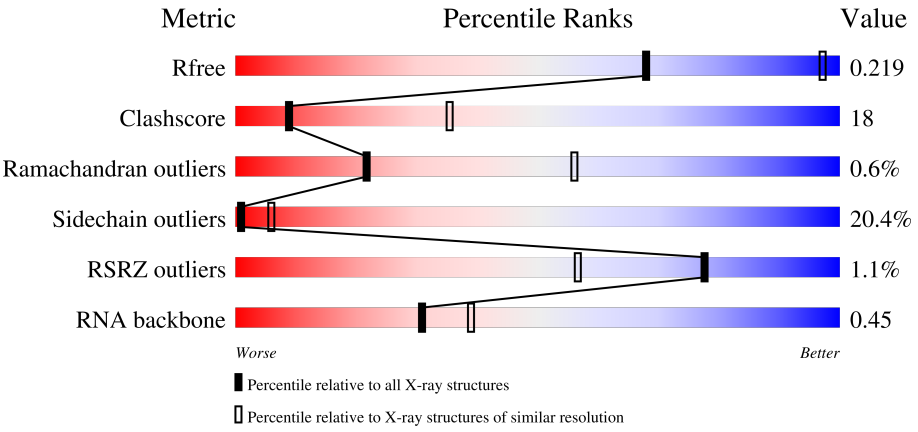
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 3.55 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}	164625	1272 (3.60-3.48)
Clashscore	180529	1360 (3.60-3.48)
Ramachandran outliers	177936	1347 (3.60-3.48)
Sidechain outliers	177891	1348 (3.60-3.48)
RSRZ outliers	164620	1271 (3.60-3.48)
RNA backbone	3690	1090 (4.02-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1522	% 23% 41% 28% 8%
2	B	256	41% 38% 11% 9%
3	C	239	% 38% 38% 10% 14%

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Mol	Chain	Length	Quality of chain
4	D	209	4% 55% 35% 9%
5	E	162	41% 40% 10% 7%
6	F	101	46% 46% 9%
7	G	156	% 49% 41% 9%
8	H	138	45% 40% 14%
9	I	128	2% 38% 53% 8%
10	J	105	3% 36% 49% 9% 7%
11	K	129	% 46% 38% 6% 10%
12	L	135	% 44% 36% 11% 8%
13	M	126	2% 43% 36% 15% 6%
14	N	61	2% 43% 46% 10%
15	O	89	51% 42% 6%
16	P	88	38% 45% 11% 6%
17	Q	105	30% 52% 11% 6%
18	R	88	41% 31% 8% 20%
19	S	93	4% 45% 31% 10% 14%
20	T	106	% 40% 43% 10% 7%
21	U	27	4% 41% 33% 15% 11%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	MG	A	1670	-	-	-	X
23	MG	A	1742	-	-	-	X
23	MG	A	1750	-	-	-	X
23	MG	M	203	-	-	-	X

2 Entry composition (i)

There are 25 unique types of molecules in this entry. The entry contains 52302 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
1	A	1512	Total	C	N	O	P	0	0	0
			32509	14478	6013	10506	1512			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	912	A	C	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
2	B	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			

- Molecule 3 is a protein called ribosomal protein S3.

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

- Molecule 4 is a protein called ribosomal protein S4.

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

- 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			

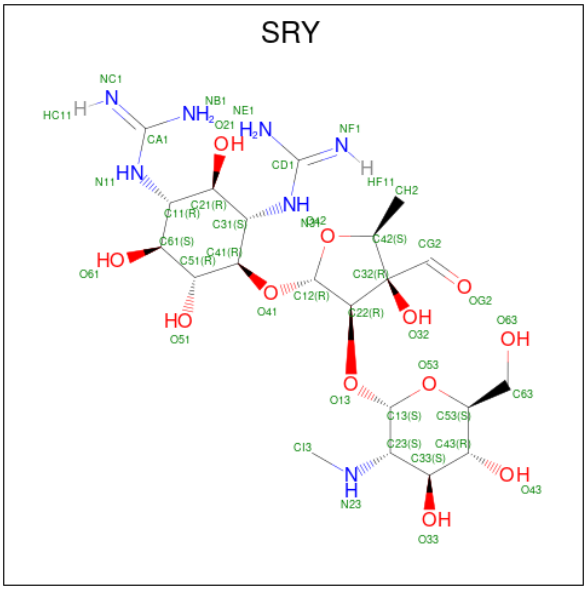
- Molecule 20 is a protein called ribosomal protein S20.

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	A	259	Total Mg 259 259	0	0
23	B	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	J	2	Total Mg 2 2	0	0
23	K	1	Total Mg 1 1	0	0
23	M	3	Total Mg 3 3	0	0
23	N	1	Total Mg 1 1	0	0
23	P	3	Total Mg 3 3	0	0
23	Q	2	Total Mg 2 2	0	0
23	S	1	Total Mg 1 1	0	0
23	T	1	Total Mg 1 1	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

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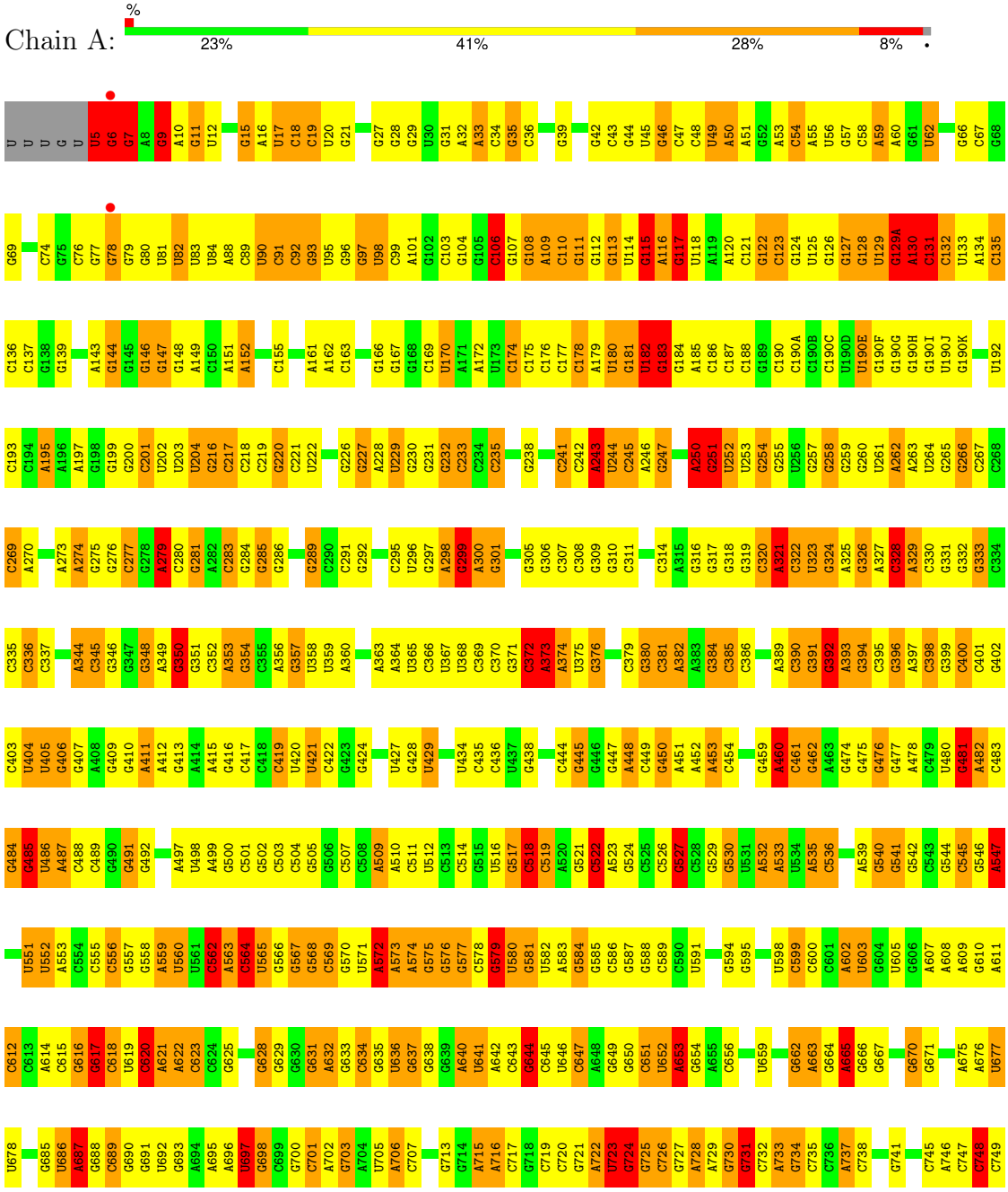
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	E	6	Total O 6 6	0	0
25	J	1	Total O 1 1	0	0
25	L	1	Total O 1 1	0	0
25	Q	1	Total O 1 1	0	0
25	T	2	Total O 2 2	0	0
25	U	1	Total O 1 1	0	0

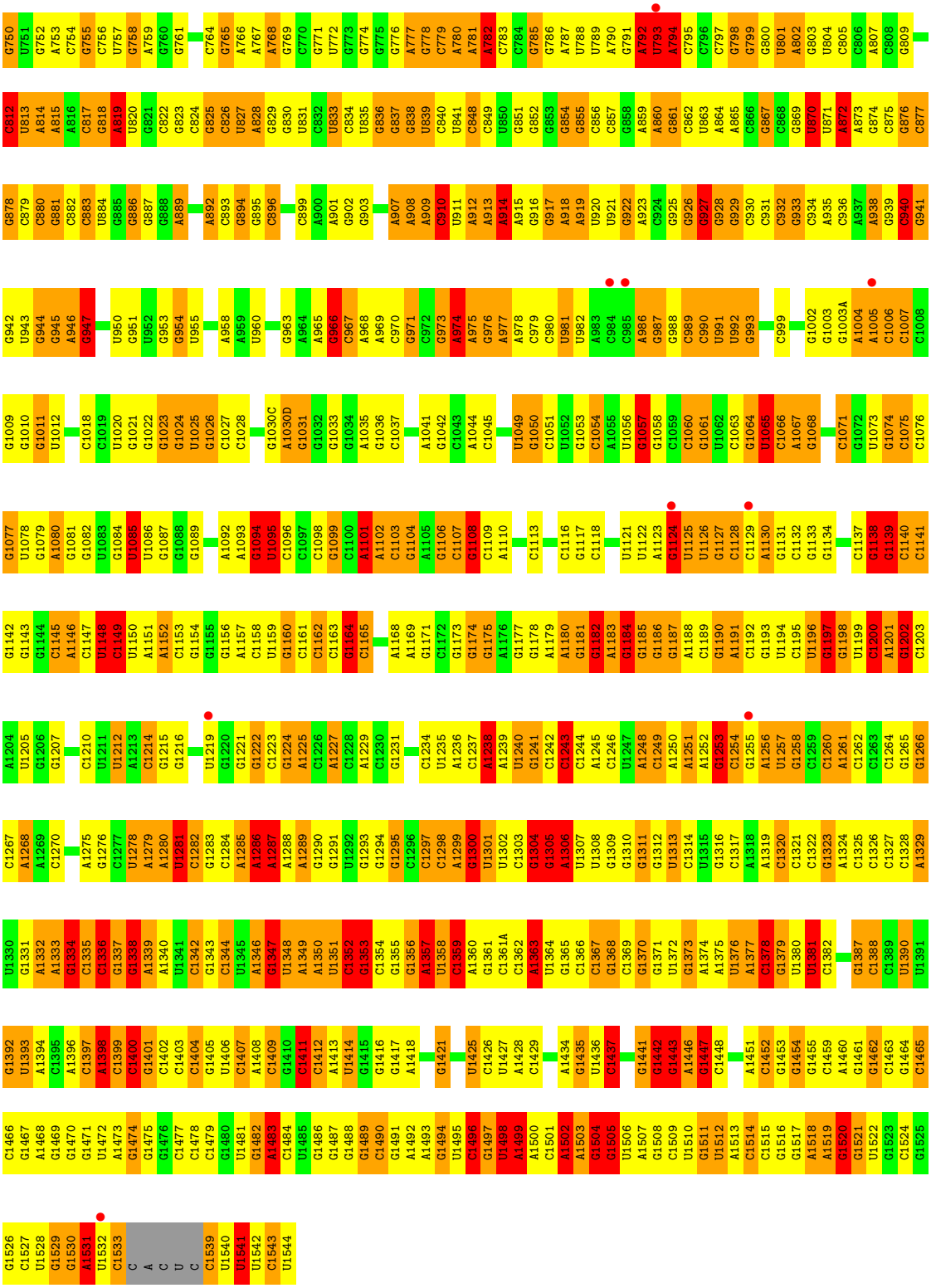
3 Residue-property plots (i)

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

- Molecule 1: 16S rRNA

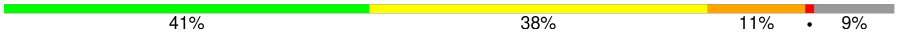
Chain A:

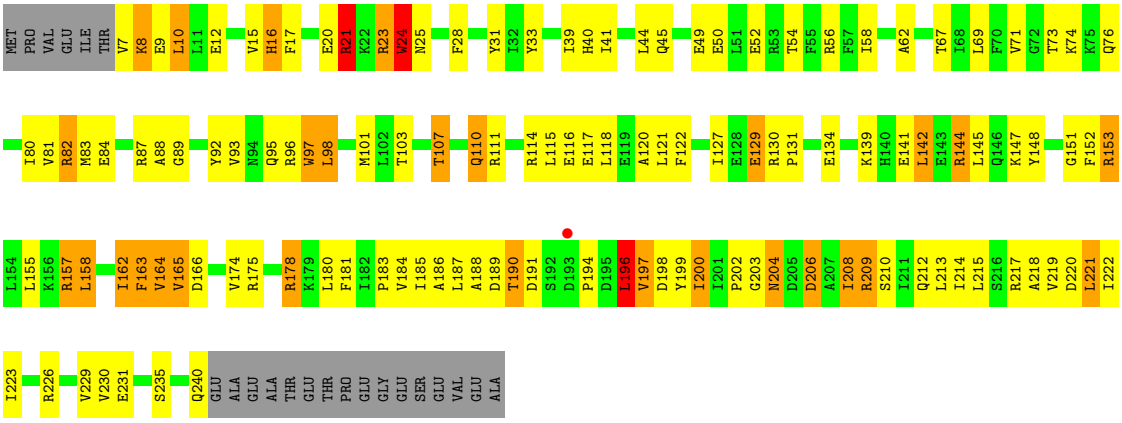




• Molecule 2: ribosomal protein S2

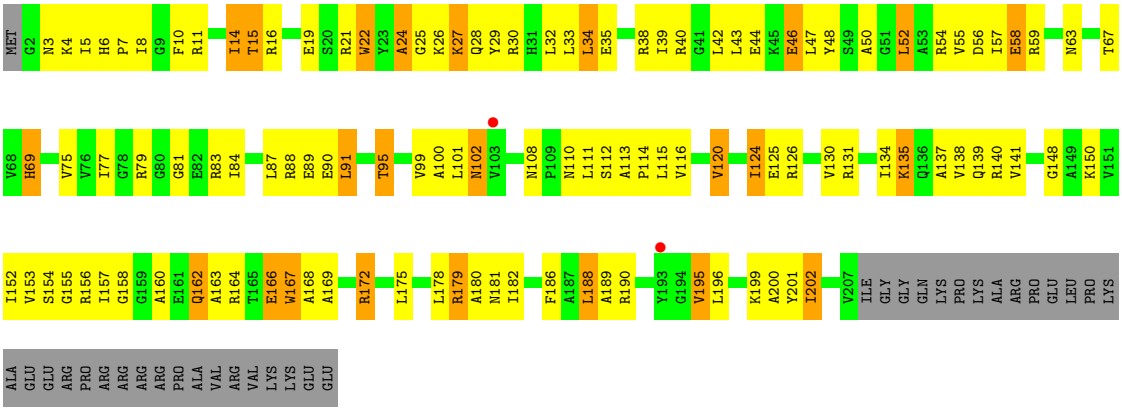
Chain B:





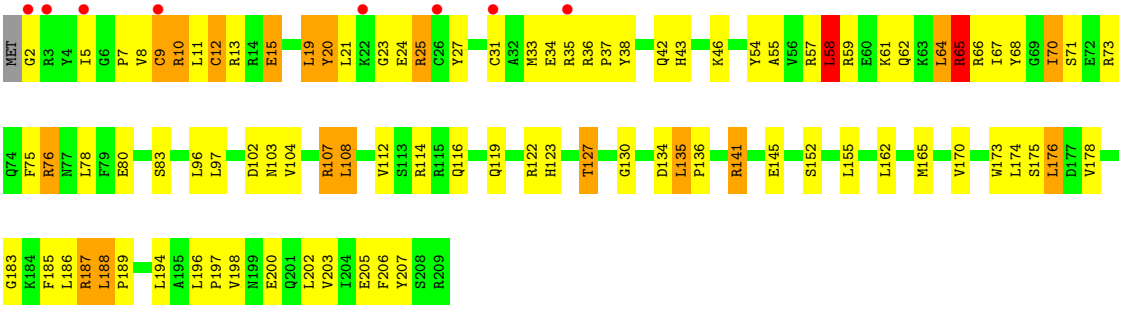
• Molecule 3: ribosomal protein S3

Chain C:



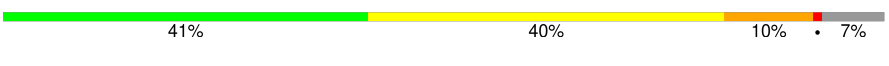
• Molecule 4: ribosomal protein S4

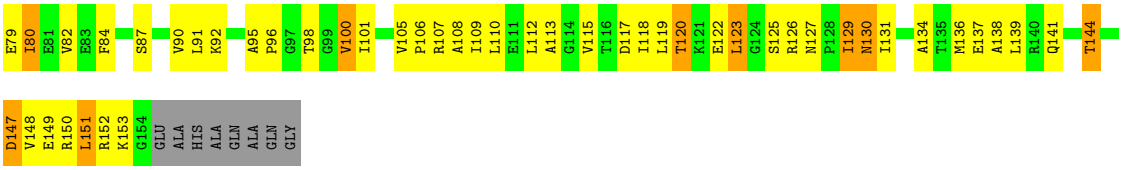
Chain D:



• Molecule 5: ribosomal protein S5

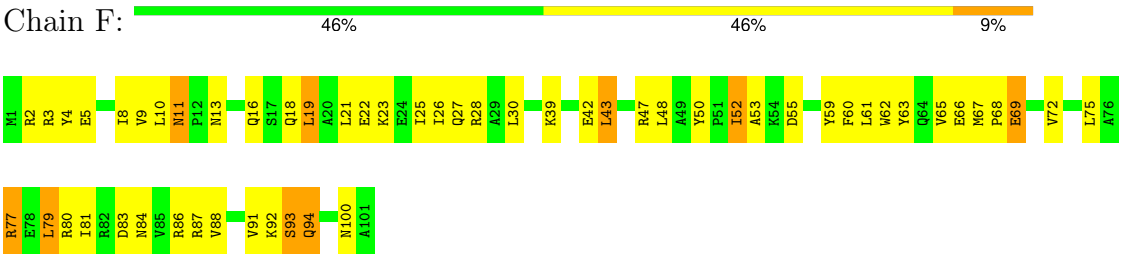
Chain E:





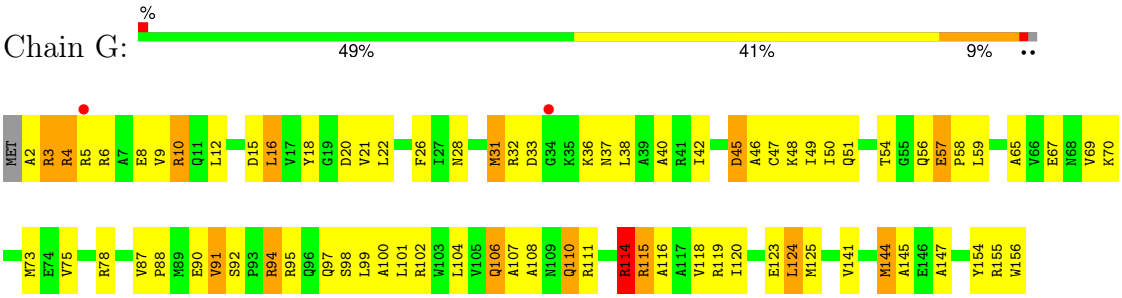
• Molecule 6: ribosomal protein S6

Chain F:



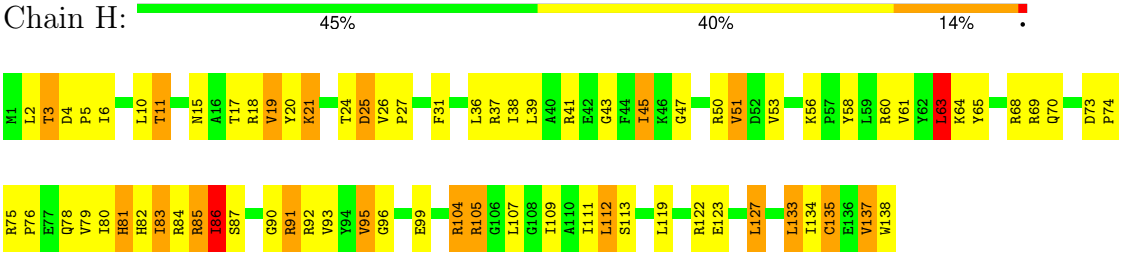
• Molecule 7: ribosomal protein S7

Chain G:



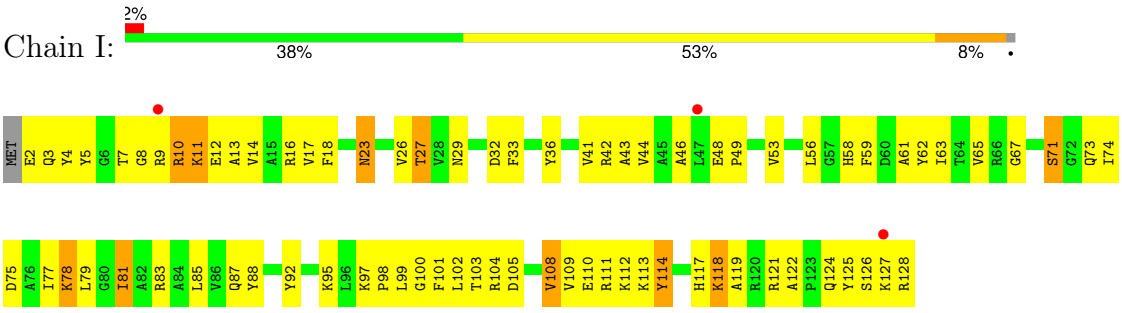
• Molecule 8: ribosomal protein S8

Chain H:



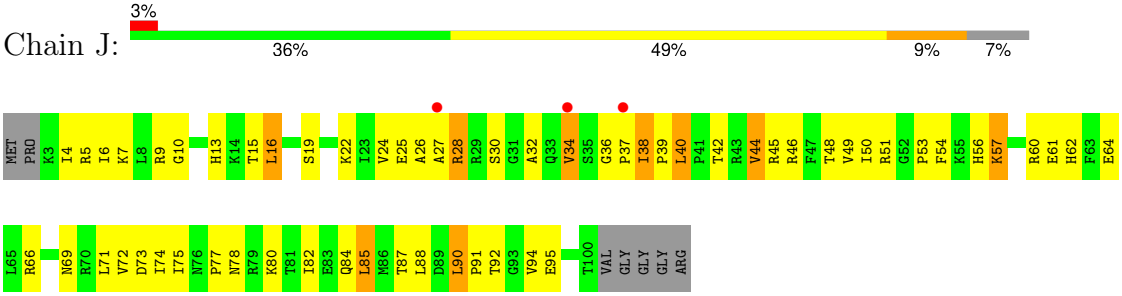
• Molecule 9: ribosomal protein S9

Chain I:



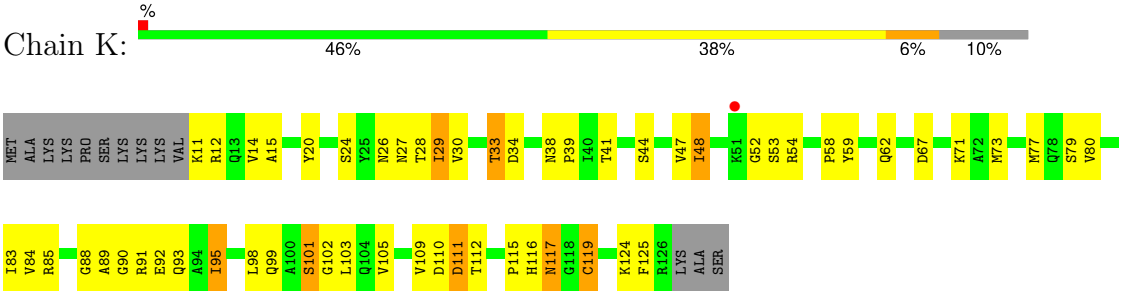
• Molecule 10: ribosomal protein S10

Chain J:



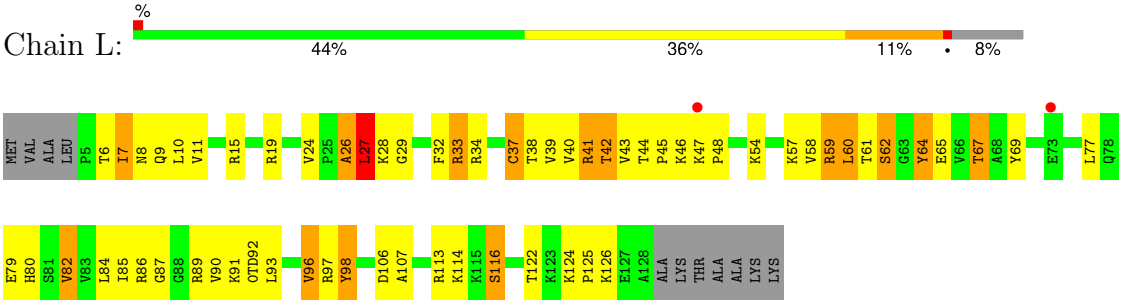
• Molecule 11: ribosomal protein S11

Chain K:



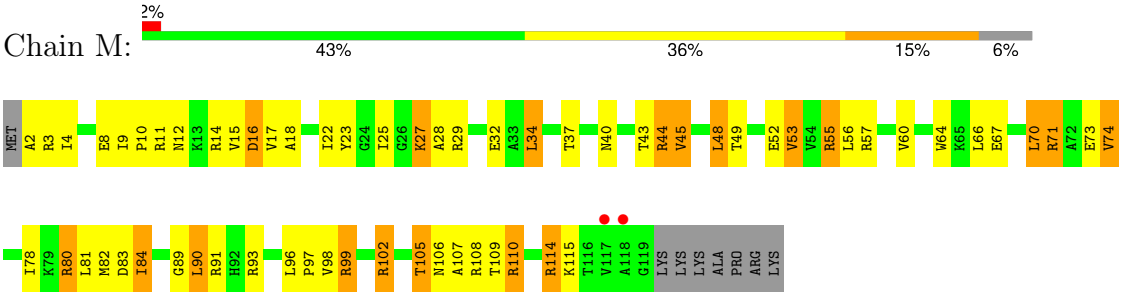
• Molecule 12: ribosomal protein S12

Chain L:



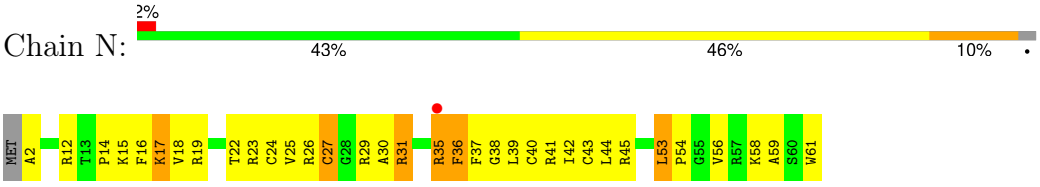
• Molecule 13: ribosomal protein S13

Chain M:



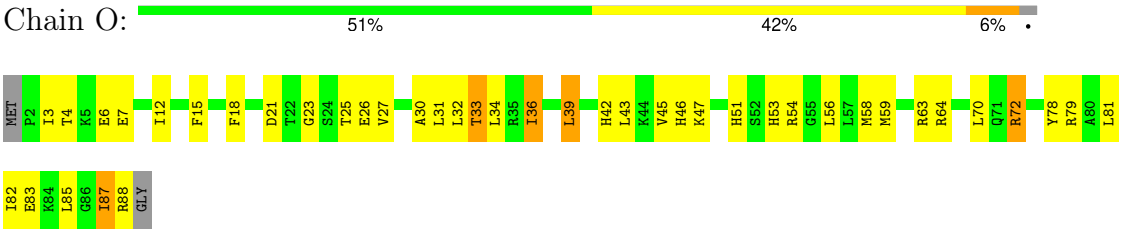
• Molecule 14: ribosomal protein S14

Chain N:



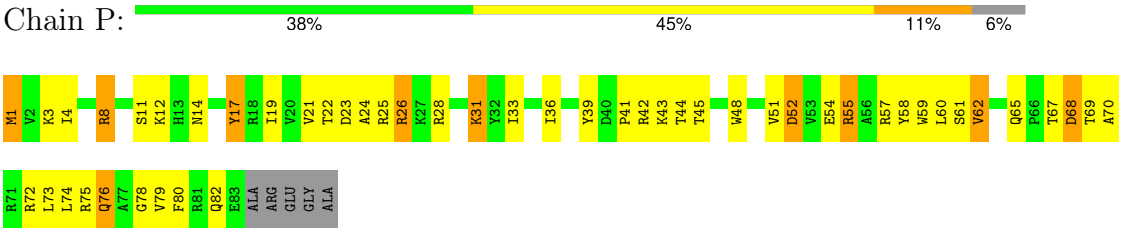
• Molecule 15: ribosomal protein S15

Chain O:



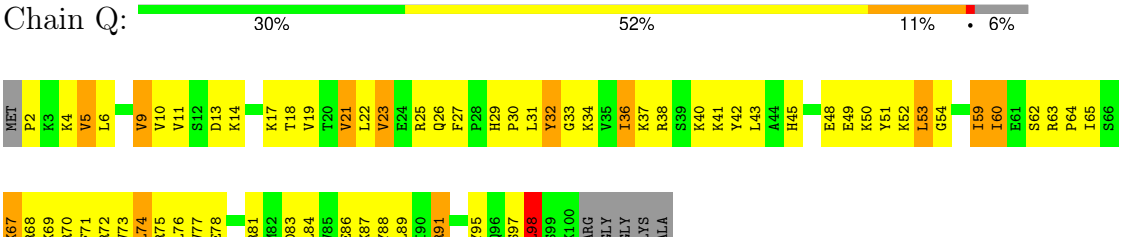
• Molecule 16: ribosomal protein S16

Chain P:



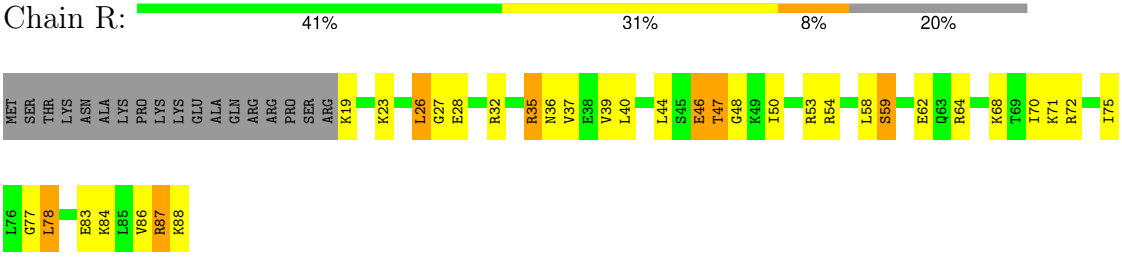
• Molecule 17: ribosomal protein S17

Chain Q:



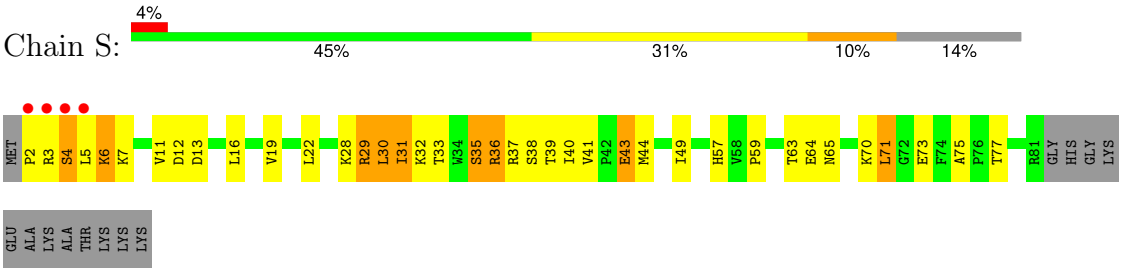
• Molecule 18: ribosomal protein S18

Chain R:

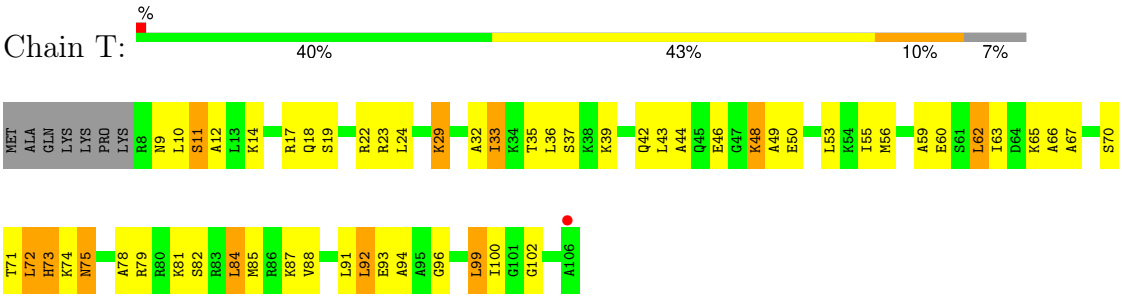


• Molecule 19: ribosomal protein S19

Chain S:



• Molecule 20: ribosomal protein S20



• 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	402.98Å 402.98Å 172.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.75 – 3.55 29.75 – 3.55	Depositor EDS
% Data completeness (in resolution range)	96.5 (29.75-3.55) 96.1 (29.75-3.55)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.17 (at 3.55Å)	Xtriage
Refinement program	PHENIX dev_978	Depositor
R, R_{free}	0.166 , 0.220 0.166 , 0.219	Depositor DCC
R_{free} test set	8261 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	118.0	Xtriage
Anisotropy	0.504	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 112.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	52302	wwPDB-VP
Average B, all atoms (Å^2)	152.0	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	1.20	169/36043 (0.5%)	1.90	1783/56248 (3.2%)
2	B	0.80	1/1935 (0.1%)	0.95	1/2609 (0.0%)
3	C	0.62	0/1636	0.82	2/2205 (0.1%)
4	D	0.73	1/1733 (0.1%)	0.93	6/2318 (0.3%)
5	E	0.93	0/1162	1.13	5/1564 (0.3%)
6	F	0.63	0/856	0.81	0/1154
7	G	0.62	0/1276	0.83	2/1709 (0.1%)
8	H	1.04	2/1136 (0.2%)	1.13	4/1527 (0.3%)
9	I	0.69	0/1029	0.88	0/1379
10	J	0.64	0/805	0.88	1/1082 (0.1%)
11	K	0.74	1/879 (0.1%)	0.92	0/1187
12	L	0.89	0/977	1.05	1/1306 (0.1%)
13	M	0.65	0/947	0.86	0/1270
14	N	0.65	1/501 (0.2%)	0.76	0/664
15	O	0.78	0/740	0.89	0/987
16	P	0.82	0/716	0.95	0/963
17	Q	1.07	2/836 (0.2%)	1.24	6/1117 (0.5%)
18	R	0.68	0/579	0.89	1/768 (0.1%)
19	S	0.54	0/661	0.75	0/890
20	T	0.77	0/765	1.10	1/1007 (0.1%)
21	U	0.62	0/212	0.80	0/277
All	All	1.07	177/55424 (0.3%)	1.66	1813/82231 (2.2%)

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	1
3	C	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
7	G	0	1
8	H	0	1
10	J	0	1
12	L	0	1
13	M	0	1
17	Q	0	1
20	T	0	1
All	All	0	11

All (177) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	279	A	N3-C4	-11.12	1.28	1.34
1	A	1509	C	N1-C6	-10.10	1.31	1.37
1	A	1502	A	N9-C4	-10.09	1.31	1.37
1	A	266	G	N9-C4	-9.73	1.30	1.38
1	A	1377	A	N3-C4	-9.22	1.29	1.34
1	A	279	A	N9-C4	-9.04	1.32	1.37
1	A	780	A	N9-C4	-8.83	1.32	1.37
1	A	860	A	N3-C4	-8.54	1.29	1.34
1	A	1227	A	N9-C4	-8.48	1.32	1.37
1	A	1513	A	N9-C4	-8.43	1.32	1.37
1	A	1334	G	N9-C8	-8.31	1.32	1.37
1	A	279	A	N7-C5	-8.07	1.34	1.39
1	A	1080	A	N3-C4	-7.83	1.30	1.34
1	A	1502	A	C5-C6	-7.66	1.34	1.41
1	A	298	A	N9-C4	-7.64	1.33	1.37
1	A	564	C	N1-C6	-7.62	1.32	1.37
1	A	1509	C	N3-C4	-7.58	1.28	1.33
1	A	130	A	N3-C4	-7.50	1.30	1.34
1	A	372	C	C2-O2	7.36	1.31	1.24
1	A	1333	A	N7-C5	-7.28	1.34	1.39
1	A	918	A	C6-N1	-7.28	1.30	1.35
1	A	326	G	C6-O6	7.17	1.30	1.24
1	A	1334	G	N9-C4	-7.14	1.32	1.38
1	A	16	A	N9-C4	-7.12	1.33	1.37
1	A	569	C	N3-C4	-7.10	1.28	1.33
1	A	801	U	C2-N3	-7.08	1.32	1.37
1	A	481	G	N9-C4	7.05	1.43	1.38
1	A	1377	A	N9-C4	-7.00	1.33	1.37
1	A	298	A	N3-C4	-6.98	1.30	1.34
1	A	300	A	N9-C4	-6.96	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	889	A	N7-C5	-6.90	1.35	1.39
1	A	730	G	N3-C4	-6.89	1.30	1.35
1	A	912	A	N9-C4	-6.87	1.33	1.37
1	A	564	C	C2-O2	6.85	1.30	1.24
1	A	570	G	N3-C4	-6.85	1.30	1.35
1	A	245	C	N1-C6	-6.84	1.33	1.37
1	A	266	G	N7-C5	-6.82	1.35	1.39
1	A	300	A	N3-C4	-6.80	1.30	1.34
1	A	817	C	C4-C5	-6.73	1.37	1.43
1	A	602	A	N9-C4	-6.72	1.33	1.37
1	A	882	C	N3-C4	-6.68	1.29	1.33
1	A	328	C	N3-C4	-6.58	1.29	1.33
8	H	135	CYS	CB-SG	-6.58	1.71	1.82
1	A	1334	G	C8-N7	-6.56	1.27	1.30
1	A	1401	G	N7-C5	-6.50	1.35	1.39
4	D	12	CYS	CB-SG	6.49	1.93	1.82
1	A	553	A	N3-C4	-6.48	1.30	1.34
1	A	320	C	N1-C6	-6.46	1.33	1.37
1	A	586	C	N1-C6	-6.41	1.33	1.37
1	A	889	A	C5-C6	-6.39	1.35	1.41
1	A	1401	G	N9-C8	-6.38	1.33	1.37
1	A	1080	A	C6-N1	-6.35	1.31	1.35
11	K	119	CYS	CB-SG	-6.33	1.71	1.82
1	A	88	A	N9-C4	6.31	1.41	1.37
1	A	284	G	N7-C5	-6.31	1.35	1.39
1	A	644	G	C6-N1	-6.27	1.35	1.39
1	A	644	G	N1-C2	-6.26	1.32	1.37
1	A	697	U	N1-C2	-6.25	1.32	1.38
1	A	788	U	C2-N3	6.23	1.42	1.37
1	A	567	G	N3-C4	-6.14	1.31	1.35
1	A	108	G	N9-C8	6.13	1.42	1.37
1	A	635	G	N3-C4	-6.13	1.31	1.35
1	A	947	G	N7-C5	-6.12	1.35	1.39
1	A	802	A	C5-C4	-6.11	1.34	1.38
1	A	862	C	C4-C5	-6.11	1.38	1.43
1	A	372	C	N1-C2	6.11	1.46	1.40
1	A	481	G	N3-C4	6.10	1.39	1.35
1	A	325	A	N3-C4	-6.05	1.31	1.34
1	A	779	C	N1-C6	-6.05	1.33	1.37
1	A	1079	G	N7-C5	-6.00	1.35	1.39
1	A	326	G	C5-C6	6.00	1.48	1.42
1	A	1079	G	N3-C4	-6.00	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	279	A	C5-C6	-5.99	1.35	1.41
1	A	1336	C	N1-C6	-5.97	1.33	1.37
1	A	1520	G	C5-C4	-5.93	1.34	1.38
1	A	807	A	N9-C4	-5.92	1.34	1.37
1	A	815	A	C5-C6	-5.92	1.35	1.41
1	A	767	A	C5-C4	-5.91	1.34	1.38
1	A	1500	A	N3-C4	-5.91	1.31	1.34
1	A	1514	C	N1-C6	-5.91	1.33	1.37
1	A	599	C	N1-C6	-5.91	1.33	1.37
1	A	746	A	N9-C4	-5.91	1.34	1.37
1	A	918	A	N9-C4	-5.90	1.34	1.37
1	A	908	A	N7-C5	-5.89	1.35	1.39
1	A	1334	G	C5-C4	-5.87	1.34	1.38
1	A	1102	A	N9-C4	-5.87	1.34	1.37
1	A	880	C	C2-O2	5.86	1.29	1.24
1	A	1488	G	C5-C4	-5.85	1.34	1.38
1	A	901	A	N3-C4	-5.85	1.31	1.34
1	A	876	G	C5-C4	-5.80	1.34	1.38
1	A	1394	A	N9-C4	-5.75	1.34	1.37
1	A	873	A	N1-C2	-5.74	1.29	1.34
1	A	909	A	N9-C4	-5.73	1.34	1.37
1	A	245	C	C4-C5	-5.73	1.38	1.43
1	A	912	A	C5-C6	-5.70	1.35	1.41
1	A	1306	A	N9-C8	-5.70	1.33	1.37
1	A	1338	G	C6-N1	-5.67	1.35	1.39
1	A	55	A	N9-C4	5.67	1.41	1.37
1	A	764	C	N1-C6	-5.66	1.33	1.37
1	A	822	C	N1-C6	-5.65	1.33	1.37
1	A	753	A	N3-C4	-5.65	1.31	1.34
17	Q	91	ARG	CG-CD	5.64	1.66	1.51
1	A	1499	A	N3-C4	-5.64	1.31	1.34
1	A	915	A	N9-C4	-5.62	1.34	1.37
1	A	733	A	N9-C4	-5.58	1.34	1.37
1	A	729	A	N7-C5	-5.57	1.35	1.39
1	A	11	G	N9-C4	-5.55	1.33	1.38
1	A	117	G	N7-C5	-5.54	1.35	1.39
1	A	970	C	N1-C2	5.50	1.45	1.40
1	A	1502	A	N7-C5	-5.49	1.35	1.39
1	A	250	A	C5-C4	5.48	1.42	1.38
1	A	813	U	P-O5'	-5.46	1.54	1.59
1	A	564	C	N3-C4	-5.43	1.30	1.33
1	A	782	A	N7-C5	-5.42	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	862	C	C2-O2	5.42	1.29	1.24
1	A	780	A	N3-C4	-5.42	1.31	1.34
1	A	274	A	C5-C4	-5.42	1.34	1.38
1	A	913	A	C3'-O3'	5.41	1.49	1.42
1	A	1334	G	N3-C4	-5.38	1.31	1.35
2	B	24	TRP	CB-CG	5.37	1.59	1.50
1	A	825	G	N9-C8	-5.34	1.34	1.37
1	A	372	C	N3-C4	5.34	1.37	1.33
1	A	1229	A	N9-C4	-5.34	1.34	1.37
1	A	865	A	C6-N6	-5.31	1.29	1.33
1	A	131	C	N3-C4	-5.30	1.30	1.33
1	A	634	C	N1-C6	-5.29	1.33	1.37
1	A	1346	A	C3'-O3'	5.27	1.49	1.42
1	A	35	G	N7-C5	-5.27	1.36	1.39
1	A	889	A	N9-C4	-5.27	1.34	1.37
1	A	926	G	N9-C4	5.27	1.42	1.38
1	A	535	A	N9-C8	-5.26	1.33	1.37
1	A	814	A	N7-C5	-5.26	1.36	1.39
1	A	622	A	C5-C6	-5.26	1.36	1.41
1	A	727	G	N9-C8	-5.26	1.34	1.37
1	A	522	C	N3-C4	-5.25	1.30	1.33
1	A	322	C	N1-C6	-5.25	1.34	1.37
1	A	778	G	N3-C4	-5.24	1.31	1.35
1	A	1287	A	N9-C4	5.23	1.41	1.37
1	A	1502	A	N3-C4	-5.22	1.31	1.34
1	A	802	A	C5-C6	-5.20	1.36	1.41
1	A	357	G	N3-C4	-5.20	1.31	1.35
1	A	384	G	C6-N1	-5.20	1.35	1.39
1	A	792	A	N9-C4	5.20	1.41	1.37
1	A	1339	A	C5-C4	-5.19	1.35	1.38
1	A	758	G	N3-C4	-5.18	1.31	1.35
8	H	137	VAL	CB-CG1	-5.17	1.42	1.52
1	A	807	A	N3-C4	-5.16	1.31	1.34
1	A	228	A	N9-C4	-5.14	1.34	1.37
1	A	781	A	N7-C5	-5.14	1.36	1.39
1	A	328	C	C2-N3	-5.14	1.31	1.35
1	A	1521	G	N1-C2	-5.13	1.33	1.37
1	A	131	C	C2-N3	-5.13	1.31	1.35
1	A	181	G	N9-C4	5.13	1.42	1.38
1	A	1460	A	N3-C4	-5.12	1.31	1.34
1	A	817	C	C2-O2	5.11	1.29	1.24
1	A	1514	C	N3-C4	-5.09	1.30	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1499	A	N9-C4	-5.09	1.34	1.37
1	A	1524	C	N1-C6	-5.08	1.34	1.37
14	N	27	CYS	CB-SG	-5.08	1.73	1.81
1	A	1526	G	N3-C4	-5.07	1.31	1.35
1	A	918	A	C5-C4	-5.07	1.35	1.38
1	A	746	A	N3-C4	-5.07	1.31	1.34
1	A	728	A	C5-C6	-5.05	1.36	1.41
1	A	1180	A	N9-C4	5.05	1.40	1.37
17	Q	9	VAL	CA-CB	-5.04	1.44	1.54
1	A	1306	A	N7-C5	-5.03	1.36	1.39
1	A	876	G	N9-C4	-5.03	1.33	1.38
1	A	1504	G	P-O5'	-5.03	1.54	1.59
1	A	1103	C	N1-C6	-5.03	1.34	1.37
1	A	1347	G	N9-C8	-5.03	1.34	1.37
1	A	321	A	N9-C4	-5.02	1.34	1.37
1	A	759	A	C5-C6	-5.02	1.36	1.41
1	A	938	A	N3-C4	-5.02	1.31	1.34
1	A	941	G	N9-C4	-5.02	1.33	1.38
1	A	327	A	C6-N6	-5.01	1.29	1.33
1	A	1504	G	N9-C8	-5.00	1.34	1.37
1	A	1520	G	C6-N1	-5.00	1.36	1.39

All (1813) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	117	G	N1-C6-O6	17.30	130.28	119.90
1	A	117	G	C5-C6-N1	-16.49	103.26	111.50
1	A	1502	A	N1-C6-N6	16.22	128.33	118.60
1	A	284	G	N1-C6-O6	15.41	129.15	119.90
1	A	912	A	C2-N3-C4	-15.22	102.99	110.60
1	A	117	G	C6-C5-N7	-15.15	121.31	130.40
1	A	117	G	C2-N3-C4	-14.88	104.46	111.90
1	A	266	G	C5-N7-C8	-14.76	96.92	104.30
1	A	1505	G	C8-N9-C4	-14.71	100.52	106.40
1	A	279	A	C6-C5-N7	-14.59	122.08	132.30
1	A	825	G	C8-N9-C4	14.51	112.20	106.40
1	A	279	A	C4-C5-C6	14.44	124.22	117.00
1	A	372	C	C6-N1-C2	14.41	126.06	120.30
1	A	1502	A	C5-N7-C8	-14.36	96.72	103.90
1	A	1502	A	C4-C5-N7	14.00	117.70	110.70
1	A	266	G	C4-C5-N7	13.85	116.34	110.80
1	A	1080	A	N1-C6-N6	-13.78	110.33	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	328	C	N3-C4-N4	-13.55	108.52	118.00
1	A	729	A	N1-C6-N6	13.33	126.60	118.60
1	A	279	A	N1-C6-N6	13.07	126.44	118.60
1	A	144	G	N1-C6-O6	13.00	127.70	119.90
1	A	912	A	N1-C6-N6	12.84	126.31	118.60
1	A	1502	A	C6-C5-N7	-12.83	123.32	132.30
1	A	825	G	N7-C8-N9	-12.53	106.84	113.10
1	A	252	U	C5-C6-N1	-12.52	116.44	122.70
1	A	1517	G	C8-N9-C4	-12.45	101.42	106.40
1	A	1531	A	N1-C6-N6	12.37	126.02	118.60
1	A	481	G	N3-C4-N9	12.36	133.42	126.00
1	A	232	G	N9-C4-C5	-12.32	100.47	105.40
1	A	928	G	C4-C5-N7	12.24	115.70	110.80
1	A	928	G	N1-C6-O6	12.21	127.22	119.90
1	A	285	G	N1-C6-O6	12.17	127.20	119.90
1	A	326	G	C5-C6-O6	12.10	135.86	128.60
1	A	864	A	C8-N9-C4	-11.89	101.05	105.80
1	A	1505	G	N7-C8-N9	11.71	118.96	113.10
1	A	1370	G	C8-N9-C4	-11.64	101.74	106.40
1	A	117	G	C4-C5-C6	11.44	125.67	118.80
1	A	1334	G	C8-N9-C4	11.41	110.97	106.40
1	A	873	A	C8-N9-C4	-11.32	101.27	105.80
1	A	328	C	N3-C2-O2	-11.29	114.00	121.90
1	A	279	A	N1-C2-N3	11.21	134.91	129.30
1	A	564	C	C6-N1-C2	11.18	124.77	120.30
1	A	797	C	C6-N1-C2	11.12	124.75	120.30
1	A	1502	A	C2-N3-C4	-11.10	105.05	110.60
1	A	1347	G	C8-N9-C4	11.07	110.83	106.40
1	A	481	G	N3-C4-C5	-11.01	123.09	128.60
1	A	941	G	N1-C6-O6	11.01	126.50	119.90
1	A	255	G	N1-C6-O6	10.88	126.42	119.90
1	A	131	C	C5-C6-N1	-10.82	115.59	121.00
1	A	1235	U	C5-C4-O4	-10.81	119.42	125.90
1	A	912	A	C5-C6-N1	-10.67	112.36	117.70
1	A	928	G	C5-C6-O6	-10.67	122.20	128.60
1	A	1490	C	C5-C6-N1	10.67	126.33	121.00
1	A	1490	C	C6-N1-C2	-10.66	116.03	120.30
1	A	919	A	C8-N9-C4	10.66	110.06	105.80
1	A	255	G	C6-C5-N7	-10.61	124.03	130.40
1	A	1080	A	C5-C6-N6	10.61	132.19	123.70
1	A	928	G	C6-C5-N7	-10.57	124.06	130.40
1	A	266	G	N7-C8-N9	10.45	118.32	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	929	G	N1-C6-O6	10.45	126.17	119.90
1	A	279	A	C4-N9-C1'	10.44	145.08	126.30
1	A	327	A	C5-C6-N1	10.39	122.89	117.70
1	A	284	G	C5-C6-O6	-10.38	122.37	128.60
1	A	1388	C	C6-N1-C2	10.31	124.42	120.30
1	A	529	G	N1-C6-O6	10.30	126.08	119.90
1	A	188	C	N3-C4-C5	-10.29	117.78	121.90
1	A	328	C	N1-C2-O2	10.28	125.07	118.90
1	A	1329	A	C8-N9-C4	-10.21	101.72	105.80
1	A	872	A	N9-C4-C5	-10.20	101.72	105.80
1	A	970	C	N1-C2-O2	10.18	125.01	118.90
1	A	1080	A	N9-C4-C5	10.18	109.87	105.80
1	A	928	G	N9-C4-C5	-10.16	101.33	105.40
1	A	1502	A	N9-C4-C5	-10.13	101.75	105.80
1	A	107	G	C4-C5-N7	10.13	114.85	110.80
1	A	820	U	N1-C2-N3	10.10	120.96	114.90
1	A	873	A	C2-N3-C4	10.09	115.64	110.60
1	A	628	G	N3-C4-C5	-10.08	123.56	128.60
1	A	745	C	C6-N1-C2	10.08	124.33	120.30
1	A	296	U	C5-C6-N1	-10.03	117.69	122.70
1	A	1388	C	C5-C6-N1	-10.02	115.99	121.00
1	A	864	A	N9-C4-C5	9.99	109.80	105.80
1	A	1080	A	C4-C5-N7	-9.99	105.71	110.70
1	A	474	G	N1-C6-O6	9.97	125.88	119.90
1	A	326	G	C4-C5-N7	-9.97	106.81	110.80
1	A	279	A	C8-N9-C1'	-9.92	109.85	127.70
1	A	20	U	C5-C4-O4	-9.91	119.95	125.90
1	A	570	G	C4-N9-C1'	9.90	139.37	126.50
1	A	328	C	N3-C4-C5	9.89	125.86	121.90
1	A	559	A	C6-N1-C2	-9.89	112.67	118.60
1	A	255	G	C5-C6-O6	-9.85	122.69	128.60
1	A	232	G	C4-C5-N7	9.84	114.74	110.80
1	A	1306	A	N1-C6-N6	9.83	124.50	118.60
1	A	862	C	N3-C4-C5	9.83	125.83	121.90
1	A	1079	G	C6-C5-N7	-9.83	124.50	130.40
1	A	598	U	C5-C6-N1	-9.79	117.81	122.70
1	A	232	G	C8-N9-C4	9.78	110.31	106.40
1	A	1181	G	C8-N9-C4	9.76	110.31	106.40
1	A	1369	C	C6-N1-C2	-9.75	116.40	120.30
1	A	266	G	N3-C4-C5	9.75	133.47	128.60
1	A	284	G	C6-C5-N7	-9.74	124.56	130.40
1	A	589	C	C6-N1-C2	9.73	124.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	327	A	C6-N1-C2	-9.72	112.77	118.60
1	A	372	C	N1-C2-N3	-9.67	112.43	119.20
1	A	798	G	C2-N3-C4	-9.64	107.08	111.90
1	A	1082	G	C8-N9-C4	9.64	110.26	106.40
1	A	107	G	C6-C5-N7	-9.62	124.63	130.40
1	A	88	A	C8-N9-C4	-9.59	101.97	105.80
1	A	753	A	N1-C2-N3	9.58	134.09	129.30
1	A	586	C	C6-N1-C2	9.58	124.13	120.30
1	A	941	G	N3-C4-C5	9.58	133.39	128.60
1	A	1235	U	N3-C4-O4	9.58	126.11	119.40
1	A	524	G	N3-C4-C5	-9.57	123.82	128.60
1	A	481	G	C2-N3-C4	9.55	116.67	111.90
1	A	589	C	C5-C6-N1	-9.50	116.25	121.00
1	A	108	G	C8-N9-C4	-9.49	102.61	106.40
1	A	9	G	N1-C6-O6	9.47	125.58	119.90
1	A	1526	G	N1-C6-O6	9.44	125.56	119.90
1	A	859	A	C4-C5-C6	9.43	121.71	117.00
1	A	130	A	N1-C2-N3	9.42	134.01	129.30
1	A	769	G	N1-C6-O6	9.41	125.54	119.90
1	A	559	A	N3-C4-C5	-9.40	120.22	126.80
1	A	971	G	C8-N9-C4	9.33	110.13	106.40
1	A	562	C	C6-N1-C2	9.32	124.03	120.30
1	A	1071	C	C5-C4-N4	-9.32	113.68	120.20
1	A	945	G	C4-C5-N7	9.31	114.52	110.80
1	A	872	A	C4-C5-N7	9.30	115.35	110.70
1	A	862	C	C6-N1-C2	9.27	124.01	120.30
1	A	873	A	N1-C6-N6	-9.25	113.05	118.60
1	A	541	G	N1-C6-O6	9.21	125.43	119.90
1	A	778	G	C5-C6-N1	-9.21	106.90	111.50
1	A	1300	G	N1-C6-O6	-9.20	114.38	119.90
1	A	1531	A	C6-C5-N7	-9.20	125.86	132.30
1	A	1149	C	C6-N1-C2	-9.20	116.62	120.30
1	A	926	G	C6-C5-N7	-9.19	124.89	130.40
1	A	647	C	C6-N1-C2	9.19	123.97	120.30
1	A	830	G	C5-C6-N1	-9.18	106.91	111.50
1	A	774	G	N1-C6-O6	9.16	125.40	119.90
1	A	805	C	N3-C4-C5	9.12	125.55	121.90
1	A	1496	C	C5-C6-N1	9.11	125.55	121.00
1	A	814	A	N1-C2-N3	9.10	133.85	129.30
1	A	1339	A	C5-C6-N1	9.10	122.25	117.70
1	A	774	G	N9-C4-C5	-9.09	101.77	105.40
1	A	372	C	N1-C2-O2	9.03	124.32	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	529	G	C6-C5-N7	-9.02	124.99	130.40
1	A	927	G	N1-C6-O6	9.01	125.30	119.90
1	A	241	C	N3-C4-C5	8.99	125.49	121.90
1	A	912	A	C5-N7-C8	-8.98	99.41	103.90
1	A	731	G	N1-C6-O6	8.93	125.26	119.90
1	A	524	G	C5-C6-O6	-8.91	123.25	128.60
1	A	862	C	C5-C4-N4	-8.90	113.97	120.20
1	A	729	A	C6-C5-N7	-8.87	126.09	132.30
1	A	826	C	N3-C4-C5	8.86	125.44	121.90
1	A	774	G	C4-C5-N7	8.85	114.34	110.80
1	A	16	A	C8-N9-C4	8.85	109.34	105.80
1	A	285	G	C5-C6-N1	-8.82	107.09	111.50
1	A	384	G	N3-C4-C5	-8.82	124.19	128.60
1	A	912	A	C6-C5-N7	-8.79	126.15	132.30
1	A	117	G	N9-C4-C5	-8.78	101.89	105.40
1	A	767	A	C5-C6-N1	8.77	122.08	117.70
1	A	117	G	C8-N9-C1'	-8.75	115.62	127.00
1	A	825	G	C5-N7-C8	8.75	108.67	104.30
1	A	279	A	C5-N7-C8	-8.74	99.53	103.90
1	A	721	G	C6-C5-N7	-8.74	125.16	130.40
1	A	1467	G	C8-N9-C4	-8.73	102.91	106.40
1	A	912	A	C4-C5-N7	8.73	115.06	110.70
1	A	725	G	N1-C6-O6	8.71	125.13	119.90
1	A	944	G	C8-N9-C4	-8.71	102.92	106.40
1	A	326	G	N3-C4-C5	-8.70	124.25	128.60
1	A	1181	G	C4-N9-C1'	-8.68	115.22	126.50
1	A	878	G	C5-C6-O6	-8.67	123.40	128.60
1	A	1074	G	C8-N9-C4	-8.67	102.93	106.40
1	A	805	C	C5-C4-N4	-8.67	114.13	120.20
1	A	1249	C	C6-N1-C2	-8.66	116.83	120.30
1	A	181	G	N3-C4-N9	8.66	131.20	126.00
1	A	310	G	C5-C6-O6	-8.65	123.41	128.60
1	A	9	G	C6-C5-N7	-8.65	125.21	130.40
1	A	79	G	C8-N9-C4	-8.64	102.94	106.40
1	A	944	G	N1-C6-O6	-8.63	114.72	119.90
1	A	372	C	C5-C4-N4	-8.62	114.16	120.20
1	A	735	C	C6-N1-C2	8.62	123.75	120.30
1	A	1353	G	C8-N9-C4	-8.59	102.96	106.40
1	A	931	C	C5-C6-N1	-8.58	116.71	121.00
1	A	703	G	C4-C5-N7	-8.57	107.37	110.80
1	A	1287	A	C8-N9-C4	-8.56	102.38	105.80
1	A	779	C	C4-C5-C6	8.56	121.68	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	372	C	C6-N1-C1'	-8.56	110.53	120.80
1	A	266	G	C6-C5-N7	-8.55	125.27	130.40
1	A	945	G	C5-C6-O6	-8.55	123.47	128.60
1	A	1367	C	C6-N1-C2	-8.54	116.88	120.30
1	A	1512	U	N1-C2-O2	-8.53	116.83	122.80
1	A	252	U	C6-N1-C2	8.52	126.11	121.00
1	A	1087	G	C4-C5-N7	8.51	114.20	110.80
1	A	1524	C	N1-C2-O2	-8.51	113.80	118.90
1	A	1377	A	N1-C6-N6	-8.49	113.50	118.60
1	A	19	C	N1-C2-O2	-8.49	113.81	118.90
1	A	814	A	C2-N3-C4	-8.49	106.36	110.60
1	A	580	U	N3-C4-C5	-8.49	109.51	114.60
1	A	324	G	C8-N9-C4	-8.48	103.01	106.40
1	A	1370	G	N1-C6-O6	-8.48	114.81	119.90
1	A	797	C	N3-C4-C5	8.46	125.28	121.90
1	A	628	G	N3-C4-N9	8.46	131.07	126.00
1	A	310	G	N1-C6-O6	8.45	124.97	119.90
1	A	90	U	C6-N1-C2	-8.45	115.93	121.00
1	A	1327	C	C5-C6-N1	-8.45	116.78	121.00
1	A	181	G	N3-C4-C5	-8.44	124.38	128.60
1	A	605	U	N1-C2-N3	8.44	119.96	114.90
1	A	541	G	C5-C6-O6	-8.44	123.54	128.60
1	A	21	G	C5-N7-C8	8.43	108.52	104.30
1	A	778	G	C2-N3-C4	-8.42	107.69	111.90
1	A	877	C	C5-C6-N1	-8.40	116.80	121.00
1	A	722	A	C2-N3-C4	-8.40	106.40	110.60
1	A	729	A	C5-C6-N6	-8.39	116.98	123.70
1	A	798	G	C8-N9-C4	8.39	109.76	106.40
1	A	1524	C	N3-C4-C5	-8.36	118.56	121.90
1	A	919	A	N1-C2-N3	-8.35	125.12	129.30
1	A	1517	G	N9-C4-C5	8.35	108.74	105.40
1	A	326	G	N1-C2-N2	-8.34	108.69	116.20
1	A	572	A	N1-C6-N6	-8.34	113.60	118.60
1	A	396	G	C8-N9-C4	-8.33	103.07	106.40
1	A	1496	C	C6-N1-C2	-8.32	116.97	120.30
1	A	1347	G	N7-C8-N9	-8.31	108.94	113.10
1	A	1079	G	C8-N9-C1'	-8.31	116.19	127.00
1	A	1342	C	N1-C2-O2	-8.30	113.92	118.90
1	A	132	C	C4-C5-C6	8.30	121.55	117.40
1	A	190(G)	G	C5-C6-N1	-8.29	107.35	111.50
1	A	728	A	N1-C6-N6	8.28	123.57	118.60
1	A	774	G	C5-C6-O6	-8.27	123.64	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1087	G	N1-C6-O6	8.27	124.86	119.90
1	A	326	G	C5-C6-N1	-8.27	107.37	111.50
1	A	1074	G	N7-C8-N9	8.26	117.23	113.10
1	A	279	A	C6-N1-C2	-8.26	113.64	118.60
1	A	295	C	C6-N1-C2	8.25	123.60	120.30
1	A	107	G	N1-C6-O6	8.23	124.84	119.90
1	A	910	C	C5-C6-N1	-8.22	116.89	121.00
1	A	1531	A	N7-C8-N9	8.22	117.91	113.80
1	A	793	U	C6-N1-C2	-8.21	116.08	121.00
1	A	524	G	N3-C4-N9	8.21	130.92	126.00
1	A	144	G	C5-C6-N1	-8.20	107.40	111.50
1	A	16	A	N7-C8-N9	-8.20	109.70	113.80
1	A	43	C	C5-C6-N1	-8.20	116.90	121.00
1	A	685	G	C2-N3-C4	-8.18	107.81	111.90
1	A	285	G	C2-N3-C4	-8.18	107.81	111.90
1	A	701	C	N3-C2-O2	-8.16	116.19	121.90
1	A	873	A	C5-C6-N1	8.15	121.78	117.70
1	A	1502	A	N7-C8-N9	8.14	117.87	113.80
1	A	1351	U	C2-N1-C1'	8.14	127.47	117.70
1	A	701	C	N1-C2-O2	8.13	123.78	118.90
1	A	774	G	C6-C5-N7	-8.13	125.52	130.40
1	A	318	G	N1-C6-O6	8.12	124.77	119.90
1	A	481	G	C5-N7-C8	8.11	108.35	104.30
1	A	522	C	C5-C4-N4	8.11	125.87	120.20
1	A	864	A	C5-C6-N6	8.09	130.17	123.70
1	A	487	A	C8-N9-C4	8.07	109.03	105.80
1	A	93	G	C8-N9-C4	8.06	109.62	106.40
1	A	929	G	C5-C6-N1	-8.06	107.47	111.50
1	A	815	A	N1-C6-N6	8.06	123.43	118.60
1	A	761	G	C4-C5-N7	8.05	114.02	110.80
1	A	1354	C	C6-N1-C2	-8.04	117.08	120.30
1	A	314	C	N3-C4-N4	-8.04	112.38	118.00
1	A	1517	G	N7-C8-N9	8.02	117.11	113.10
1	A	625	G	C8-N9-C4	-8.01	103.20	106.40
1	A	1338	G	N1-C2-N2	-8.01	108.99	116.20
1	A	817	C	N1-C2-N3	-8.01	113.59	119.20
1	A	881	G	C6-C5-N7	-8.01	125.60	130.40
1	A	1346	A	C5-C6-N1	8.01	121.70	117.70
1	A	930	C	N3-C4-C5	8.00	125.10	121.90
1	A	971	G	N1-C6-O6	8.00	124.70	119.90
1	A	865	A	N1-C6-N6	-7.98	113.81	118.60
1	A	570	G	C8-N9-C1'	-7.97	116.64	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1238	A	N9-C4-C5	7.97	108.99	105.80
1	A	600	C	N3-C4-C5	7.97	125.09	121.90
1	A	926	G	N3-C4-N9	7.96	130.78	126.00
1	A	1452	C	N1-C2-O2	7.96	123.67	118.90
1	A	279	A	N7-C8-N9	7.95	117.78	113.80
1	A	1084	G	N1-C6-O6	-7.95	115.13	119.90
1	A	108	G	N3-C2-N2	-7.95	114.34	119.90
1	A	578	C	N3-C4-C5	-7.95	118.72	121.90
1	A	232	G	N1-C6-O6	7.93	124.66	119.90
1	A	703	G	N3-C4-C5	-7.93	124.63	128.60
1	A	881	G	N1-C6-O6	7.93	124.66	119.90
3	C	179	ARG	N-CA-C	-7.93	89.59	111.00
1	A	927	G	N3-C4-C5	7.93	132.56	128.60
1	A	229	U	N1-C2-O2	-7.92	117.25	122.80
1	A	831	U	N3-C4-C5	-7.92	109.85	114.60
1	A	930	C	N3-C4-N4	-7.92	112.46	118.00
1	A	1157	A	C4-C5-C6	7.91	120.95	117.00
1	A	1351	U	C6-N1-C2	-7.89	116.27	121.00
1	A	1401	G	C6-C5-N7	-7.88	125.67	130.40
1	A	1483	A	N1-C6-N6	-7.88	113.87	118.60
1	A	941	G	C5-C6-O6	-7.87	123.88	128.60
1	A	1401	G	N1-C6-O6	7.87	124.62	119.90
1	A	916	G	C5-C6-O6	-7.87	123.88	128.60
1	A	1165	C	C6-N1-C2	-7.86	117.16	120.30
1	A	881	G	C5-C6-O6	-7.86	123.89	128.60
1	A	947	G	N1-C6-O6	7.86	124.61	119.90
1	A	945	G	C5-N7-C8	-7.85	100.38	104.30
1	A	1099	G	C2-N3-C4	-7.84	107.98	111.90
1	A	880	C	C6-N1-C2	7.84	123.44	120.30
1	A	941	G	C2-N3-C4	-7.84	107.98	111.90
1	A	731	G	C5-C6-O6	-7.83	123.90	128.60
1	A	283	C	N1-C2-O2	7.82	123.59	118.90
1	A	733	A	C2-N3-C4	-7.82	106.69	110.60
1	A	1099	G	N3-C4-C5	7.82	132.51	128.60
1	A	907	A	N1-C2-N3	7.82	133.21	129.30
1	A	522	C	N3-C4-N4	-7.82	112.53	118.00
1	A	125	U	C5-C6-N1	-7.82	118.79	122.70
1	A	865	A	C5-C6-N1	7.82	121.61	117.70
1	A	912	A	N3-C4-C5	7.81	132.27	126.80
1	A	229	U	N1-C2-N3	7.81	119.58	114.90
1	A	780	A	N1-C2-N3	7.81	133.20	129.30
1	A	771	G	C2-N3-C4	-7.80	108.00	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	932	C	C6-N1-C2	-7.79	117.18	120.30
1	A	860	A	C8-N9-C4	-7.78	102.69	105.80
1	A	306	G	N3-C2-N2	-7.78	114.46	119.90
1	A	252	U	C2-N3-C4	-7.77	122.34	127.00
1	A	1304	G	N1-C6-O6	-7.77	115.24	119.90
1	A	326	G	C4-N9-C1'	7.76	136.59	126.50
1	A	328	C	C5-C4-N4	7.75	125.62	120.20
1	A	1467	G	N9-C4-C5	7.75	108.50	105.40
1	A	1502	A	C5-C6-N6	-7.75	117.50	123.70
1	A	1180	A	C8-N9-C4	-7.74	102.70	105.80
1	A	109	A	N1-C6-N6	7.74	123.25	118.60
1	A	1267	C	C6-N1-C2	-7.74	117.20	120.30
1	A	285	G	C8-N9-C4	7.72	109.49	106.40
1	A	28	G	N1-C6-O6	7.72	124.53	119.90
1	A	569	C	C2-N3-C4	-7.72	116.04	119.90
1	A	933	G	C5-C6-O6	-7.71	123.97	128.60
1	A	97	G	C8-N9-C4	-7.70	103.32	106.40
1	A	1339	A	N1-C6-N6	-7.70	113.98	118.60
1	A	124	G	C2-N3-C4	-7.70	108.05	111.90
1	A	59	A	C4-C5-C6	-7.69	113.16	117.00
1	A	830	G	N1-C6-O6	7.68	124.51	119.90
1	A	131	C	C6-N1-C2	7.68	123.37	120.30
1	A	483	C	C5-C4-N4	7.68	125.58	120.20
1	A	884	U	C5-C6-N1	-7.67	118.86	122.70
1	A	899	C	N3-C4-C5	-7.67	118.83	121.90
1	A	1531	A	C4-C5-N7	7.66	114.53	110.70
1	A	135	C	N3-C4-C5	-7.65	118.84	121.90
1	A	1080	A	C5-N7-C8	7.65	107.73	103.90
1	A	559	A	N1-C2-N3	7.65	133.12	129.30
1	A	595	G	N1-C6-O6	7.64	124.49	119.90
1	A	1531	A	C5-N7-C8	-7.64	100.08	103.90
1	A	1342	C	N3-C2-O2	7.64	127.25	121.90
1	A	928	G	C5-N7-C8	-7.64	100.48	104.30
1	A	1442	G	C4-N9-C1'	7.63	136.42	126.50
1	A	357	G	C8-N9-C4	7.63	109.45	106.40
1	A	260	G	N1-C6-O6	7.62	124.47	119.90
1	A	761	G	C6-C5-N7	-7.61	125.84	130.40
1	A	1359	C	C2-N1-C1'	7.61	127.17	118.80
1	A	1359	C	N1-C2-O2	7.60	123.46	118.90
1	A	1539	C	C5-C6-N1	7.60	124.80	121.00
1	A	1181	G	N7-C8-N9	-7.59	109.31	113.10
1	A	1390	U	C5-C4-O4	7.58	130.45	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1079	G	N3-C4-N9	7.57	130.54	126.00
1	A	579	G	N1-C6-O6	7.57	124.44	119.90
1	A	586	C	C5-C6-N1	-7.57	117.22	121.00
1	A	855	G	C8-N9-C4	7.57	109.43	106.40
1	A	474	G	C5-C6-O6	-7.56	124.07	128.60
1	A	753	A	C6-N1-C2	-7.56	114.06	118.60
1	A	1349	A	N1-C6-N6	-7.56	114.07	118.60
1	A	279	A	C5-C6-N6	-7.55	117.66	123.70
1	A	856	C	C6-N1-C2	-7.55	117.28	120.30
1	A	1370	G	N7-C8-N9	7.55	116.88	113.10
1	A	765	G	C2-N3-C4	-7.55	108.13	111.90
1	A	1071	C	C6-N1-C2	7.54	123.32	120.30
1	A	255	G	N3-C4-N9	7.54	130.52	126.00
1	A	1139	G	N3-C4-C5	-7.53	124.83	128.60
1	A	1515	C	N3-C4-C5	7.53	124.91	121.90
1	A	269	C	C4-C5-C6	7.53	121.17	117.40
1	A	654	G	C2-N3-C4	-7.53	108.14	111.90
1	A	300	A	C2-N3-C4	-7.52	106.84	110.60
1	A	864	A	N1-C6-N6	-7.52	114.09	118.60
1	A	1344	C	C5-C6-N1	-7.51	117.24	121.00
1	A	559	A	C4-C5-C6	7.51	120.75	117.00
1	A	759	A	N1-C6-N6	7.51	123.11	118.60
1	A	106	C	C4-C5-C6	7.50	121.15	117.40
1	A	483	C	N3-C4-C5	-7.50	118.90	121.90
1	A	1099	G	C5-C6-N1	-7.50	107.75	111.50
1	A	279	A	C2-N3-C4	-7.49	106.86	110.60
1	A	930	C	C2-N3-C4	-7.49	116.16	119.90
1	A	454	C	C5-C6-N1	7.49	124.74	121.00
1	A	870	U	N3-C2-O2	-7.49	116.96	122.20
1	A	17	U	C5-C6-N1	-7.48	118.96	122.70
1	A	201	C	C6-N1-C2	-7.47	117.31	120.30
1	A	807	A	C2-N3-C4	-7.47	106.86	110.60
1	A	1376	U	N3-C2-O2	-7.46	116.98	122.20
1	A	919	A	N7-C8-N9	-7.46	110.07	113.80
1	A	707	C	C5-C6-N1	-7.45	117.27	121.00
1	A	941	G	C4-C5-N7	7.45	113.78	110.80
1	A	594	G	N3-C4-C5	-7.45	124.88	128.60
1	A	771	G	N1-C6-O6	7.43	124.36	119.90
1	A	826	C	C6-N1-C2	7.42	123.27	120.30
1	A	1516	G	C4-C5-N7	7.41	113.77	110.80
1	A	1526	G	C5-C6-O6	-7.41	124.15	128.60
1	A	564	C	N1-C2-N3	-7.40	114.02	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	873	A	N9-C4-C5	7.40	108.76	105.80
1	A	1339	A	C2-N3-C4	7.40	114.30	110.60
1	A	1356	G	C8-N9-C4	-7.40	103.44	106.40
1	A	1200	C	C2-N1-C1'	7.39	126.93	118.80
1	A	570	G	C8-N9-C4	-7.39	103.44	106.40
1	A	918	A	N1-C2-N3	7.38	132.99	129.30
1	A	301	G	N1-C2-N3	7.38	128.33	123.90
1	A	1362	C	C6-N1-C2	-7.38	117.35	120.30
1	A	799	G	C6-C5-N7	-7.38	125.97	130.40
1	A	1087	G	C5-C6-O6	-7.38	124.17	128.60
1	A	327	A	C5-C6-N6	-7.37	117.81	123.70
1	A	703	G	C5-C6-O6	7.36	133.02	128.60
1	A	595	G	C6-C5-N7	-7.36	125.98	130.40
1	A	877	C	C4-C5-C6	7.36	121.08	117.40
1	A	1417	G	N3-C4-N9	7.36	130.41	126.00
1	A	880	C	N1-C2-N3	-7.35	114.05	119.20
1	A	1351	U	N3-C2-O2	-7.35	117.06	122.20
1	A	933	G	C4-C5-N7	7.35	113.74	110.80
1	A	242	C	C5-C6-N1	-7.34	117.33	121.00
1	A	819	A	N1-C2-N3	7.34	132.97	129.30
1	A	799	G	C4-C5-N7	7.34	113.74	110.80
1	A	779	C	C5-C6-N1	-7.34	117.33	121.00
1	A	20	U	N3-C4-O4	7.33	124.53	119.40
1	A	245	C	N3-C4-N4	7.33	123.13	118.00
1	A	108	G	N7-C8-N9	7.33	116.76	113.10
1	A	572	A	N9-C4-C5	7.33	108.73	105.80
1	A	881	G	N1-C2-N3	7.33	128.30	123.90
1	A	262	A	N1-C6-N6	-7.32	114.21	118.60
1	A	809	G	C8-N9-C4	-7.32	103.47	106.40
1	A	317	G	C8-N9-C4	7.32	109.33	106.40
1	A	926	G	N3-C4-C5	-7.32	124.94	128.60
1	A	1455	G	N1-C6-O6	7.32	124.29	119.90
1	A	929	G	C2-N3-C4	-7.31	108.24	111.90
1	A	1238	A	C5-C6-N6	7.31	129.55	123.70
1	A	283	C	C6-N1-C2	-7.31	117.38	120.30
1	A	522	C	C5-C6-N1	-7.30	117.35	121.00
1	A	571	U	C5-C6-N1	-7.30	119.05	122.70
1	A	578	C	N1-C2-O2	-7.30	114.52	118.90
1	A	123	C	C6-N1-C2	-7.30	117.38	120.30
1	A	785	G	N1-C6-O6	7.29	124.27	119.90
1	A	730	G	C4-C5-N7	-7.28	107.89	110.80
1	A	1361(A)	C	N1-C2-O2	7.28	123.27	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1447	G	N7-C8-N9	7.28	116.74	113.10
1	A	89	C	C5-C6-N1	7.27	124.64	121.00
1	A	728	A	C6-C5-N7	-7.27	127.21	132.30
1	A	232	G	C5-C6-O6	-7.27	124.24	128.60
1	A	628	G	N1-C2-N2	-7.27	109.66	116.20
1	A	913	A	C5-N7-C8	7.26	107.53	103.90
1	A	130	A	C4-C5-C6	7.26	120.63	117.00
1	A	1079	G	C4-N9-C1'	7.25	135.93	126.50
1	A	545	C	N3-C4-C5	-7.25	119.00	121.90
1	A	1351	U	N3-C4-C5	-7.25	110.25	114.60
1	A	109	A	C2-N3-C4	-7.25	106.98	110.60
1	A	605	U	C6-N1-C2	-7.25	116.65	121.00
1	A	16	A	N1-C2-N3	7.24	132.92	129.30
1	A	819	A	C4-C5-C6	7.24	120.62	117.00
1	A	264	U	N3-C2-O2	-7.24	117.13	122.20
1	A	615	C	N3-C4-C5	7.24	124.80	121.90
1	A	1200	C	N1-C2-O2	7.24	123.24	118.90
1	A	725	G	C5-C6-O6	-7.23	124.26	128.60
1	A	859	A	N1-C6-N6	7.22	122.93	118.60
1	A	394	G	C5-C6-O6	7.22	132.93	128.60
1	A	785	G	C5-C6-O6	-7.21	124.27	128.60
1	A	928	G	C2-N3-C4	-7.21	108.29	111.90
1	A	384	G	N1-C6-O6	-7.21	115.58	119.90
1	A	299	G	C4-C5-N7	7.20	113.68	110.80
1	A	266	G	N1-C6-O6	7.20	124.22	119.90
1	A	625	G	N3-C4-C5	-7.20	125.00	128.60
1	A	799	G	N9-C4-C5	-7.20	102.52	105.40
1	A	53	A	N1-C6-N6	-7.19	114.28	118.60
1	A	875	C	C5-C6-N1	-7.19	117.41	121.00
1	A	1516	G	N1-C6-O6	7.19	124.21	119.90
1	A	260	G	C8-N9-C4	-7.17	103.53	106.40
1	A	487	A	N7-C8-N9	-7.17	110.22	113.80
1	A	1344	C	C2-N3-C4	-7.17	116.32	119.90
1	A	930	C	C5-C6-N1	-7.16	117.42	121.00
1	A	117	G	N1-C2-N3	7.16	128.19	123.90
1	A	1488	G	N3-C4-C5	-7.16	125.02	128.60
1	A	723	U	C6-N1-C2	-7.14	116.71	121.00
1	A	1508	G	N9-C4-C5	7.14	108.25	105.40
1	A	594	G	C8-N9-C4	-7.13	103.55	106.40
1	A	484	G	C8-N9-C1'	-7.12	117.75	127.00
1	A	1162	C	N1-C2-O2	7.11	123.17	118.90
1	A	79	G	N1-C6-O6	7.11	124.17	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	602	A	C2-N3-C4	-7.11	107.05	110.60
1	A	1074	G	C6-C5-N7	-7.11	126.13	130.40
1	A	1202	G	N1-C6-O6	-7.11	115.64	119.90
1	A	1346	A	C2-N3-C4	7.10	114.15	110.60
1	A	1486	G	N1-C6-O6	7.10	124.16	119.90
1	A	518	C	C2-N1-C1'	7.09	126.60	118.80
1	A	35	G	N1-C6-O6	7.09	124.16	119.90
1	A	324	G	N7-C8-N9	7.09	116.64	113.10
1	A	1381	U	N3-C2-O2	-7.09	117.24	122.20
1	A	1329	A	N7-C8-N9	7.09	117.34	113.80
1	A	117	G	C4-N9-C1'	7.08	135.70	126.50
20	T	94	ALA	N-CA-C	-7.08	91.89	111.00
1	A	1382	C	C6-N1-C2	-7.08	117.47	120.30
1	A	1370	G	C5-C6-O6	7.07	132.84	128.60
1	A	524	G	C2-N3-C4	7.07	115.44	111.90
1	A	1227	A	C2-N3-C4	-7.07	107.07	110.60
1	A	1502	A	C5-C6-N1	-7.06	114.17	117.70
1	A	6	G	C4-N9-C1'	7.06	135.68	126.50
1	A	477	G	N1-C6-O6	7.06	124.13	119.90
1	A	605	U	N3-C2-O2	-7.05	117.26	122.20
1	A	1125	U	C5-C6-N1	7.05	126.23	122.70
1	A	18	C	C5-C6-N1	-7.05	117.47	121.00
1	A	823	G	C2-N3-C4	-7.05	108.38	111.90
1	A	309	G	C8-N9-C4	7.05	109.22	106.40
1	A	281	G	N1-C6-O6	7.05	124.13	119.90
1	A	127	G	N1-C6-O6	7.04	124.12	119.90
1	A	524	G	C4-N9-C1'	7.04	135.66	126.50
1	A	1377	A	C6-N1-C2	-7.04	114.38	118.60
1	A	782	A	C5-C6-N6	-7.04	118.07	123.70
1	A	707	C	C2-N3-C4	-7.03	116.38	119.90
1	A	1401	G	C4-N9-C1'	7.03	135.64	126.50
1	A	275	G	C8-N9-C4	7.02	109.21	106.40
1	A	947	G	C6-C5-N7	-7.02	126.19	130.40
1	A	1231	G	N1-C6-O6	7.02	124.11	119.90
1	A	839	U	N1-C2-O2	7.02	127.72	122.80
1	A	1238	A	C4-C5-N7	-7.02	107.19	110.70
1	A	1401	G	C5-C6-O6	-7.02	124.39	128.60
1	A	166	G	N9-C4-C5	-7.02	102.59	105.40
1	A	454	C	N1-C2-O2	7.01	123.11	118.90
1	A	66	G	C8-N9-C4	-7.01	103.60	106.40
1	A	385	C	N3-C2-O2	-7.01	117.00	121.90
1	A	241	C	C5-C4-N4	-7.00	115.30	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1447	G	C8-N9-C4	-7.00	103.60	106.40
1	A	862	C	N1-C2-N3	-6.99	114.30	119.20
1	A	1335	C	N1-C2-O2	6.99	123.09	118.90
1	A	1417	G	C8-N9-C1'	-6.99	117.91	127.00
1	A	1447	G	C4-C5-N7	6.99	113.59	110.80
1	A	1334	G	N7-C8-N9	-6.98	109.61	113.10
1	A	1447	G	C5-C6-O6	-6.98	124.41	128.60
1	A	927	G	C5-C6-N1	-6.98	108.01	111.50
1	A	872	A	N1-C6-N6	6.97	122.78	118.60
1	A	628	G	C4-C5-C6	6.97	122.98	118.80
1	A	1235	U	N1-C2-O2	-6.97	117.92	122.80
1	A	856	C	N3-C4-C5	-6.96	119.12	121.90
1	A	484	G	C4-N9-C1'	6.96	135.54	126.50
1	A	881	G	N9-C4-C5	-6.95	102.62	105.40
1	A	786	G	N1-C6-O6	6.95	124.07	119.90
1	A	10	A	C8-N9-C4	6.94	108.58	105.80
1	A	137	C	N3-C4-C5	6.94	124.68	121.90
1	A	474	G	C6-C5-N7	-6.94	126.24	130.40
1	A	580	U	C5-C4-O4	6.94	130.06	125.90
1	A	805	C	C4-C5-C6	-6.94	113.93	117.40
1	A	737	A	N1-C6-N6	6.93	122.76	118.60
1	A	759	A	C5-N7-C8	-6.92	100.44	103.90
1	A	1304	G	C8-N9-C4	-6.92	103.63	106.40
4	D	202	LEU	CA-CB-CG	-6.91	99.40	115.30
1	A	761	G	N3-C2-N2	6.91	124.74	119.90
1	A	1496	C	C2-N1-C1'	6.91	126.40	118.80
1	A	689	C	C6-N1-C2	-6.91	117.54	120.30
1	A	880	C	C5-C4-N4	-6.90	115.37	120.20
1	A	522	C	C2-N1-C1'	-6.90	111.22	118.80
1	A	909	A	C5-C6-N1	6.89	121.15	117.70
1	A	1335	C	N3-C2-O2	-6.89	117.08	121.90
1	A	1417	G	C4-N9-C1'	6.88	135.45	126.50
1	A	942	G	C5-C6-N1	-6.88	108.06	111.50
1	A	1464	G	C5-C6-O6	-6.88	124.47	128.60
1	A	797	C	C5-C6-N1	-6.87	117.56	121.00
1	A	1306	A	C6-C5-N7	-6.87	127.49	132.30
1	A	481	G	C5-C6-N1	6.86	114.93	111.50
1	A	556	C	C2-N3-C4	-6.86	116.47	119.90
1	A	723	U	C5-C6-N1	6.86	126.13	122.70
1	A	483	C	C4-C5-C6	6.86	120.83	117.40
1	A	1516	G	C5-C6-O6	-6.86	124.49	128.60
1	A	10	A	N9-C4-C5	-6.85	103.06	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	769	G	C5-C6-O6	-6.85	124.49	128.60
1	A	529	G	C4-C5-C6	6.85	122.91	118.80
1	A	1158	C	N1-C2-O2	6.84	123.01	118.90
1	A	1544	U	N3-C2-O2	6.84	126.99	122.20
1	A	692	U	N3-C2-O2	-6.84	117.41	122.20
1	A	759	A	C4-C5-N7	6.83	114.12	110.70
1	A	474	G	C4-C5-N7	6.83	113.53	110.80
1	A	1489	G	C5-C6-N1	-6.83	108.08	111.50
1	A	106	C	N1-C2-N3	6.83	123.98	119.20
1	A	79	G	N7-C8-N9	6.83	116.51	113.10
1	A	285	G	N3-C2-N2	-6.83	115.12	119.90
1	A	1094	G	N1-C6-O6	-6.82	115.81	119.90
1	A	771	G	C4-C5-N7	6.82	113.53	110.80
1	A	765	G	N3-C4-C5	6.81	132.01	128.60
1	A	484	G	N3-C4-N9	6.80	130.08	126.00
1	A	1411	C	C6-N1-C2	-6.80	117.58	120.30
1	A	16	A	C2-N3-C4	-6.80	107.20	110.60
1	A	665	A	N1-C6-N6	-6.80	114.52	118.60
1	A	933	G	C6-C5-N7	-6.80	126.32	130.40
1	A	1494	G	N3-C4-N9	6.80	130.08	126.00
1	A	1359	C	N3-C2-O2	-6.80	117.14	121.90
1	A	1084	G	N9-C4-C5	6.79	108.12	105.40
1	A	241	C	C6-N1-C2	6.79	123.02	120.30
1	A	778	G	N1-C6-O6	6.79	123.97	119.90
1	A	1469	G	N1-C6-O6	6.78	123.97	119.90
1	A	35	G	C5-C6-O6	-6.78	124.53	128.60
1	A	1401	G	C8-N9-C1'	-6.77	118.19	127.00
1	A	255	G	C4-C5-N7	6.77	113.51	110.80
1	A	301	G	C8-N9-C4	-6.77	103.69	106.40
1	A	820	U	C2-N3-C4	-6.77	122.94	127.00
1	A	914	A	N1-C6-N6	6.76	122.66	118.60
1	A	144	G	C6-C5-N7	-6.75	126.35	130.40
1	A	317	G	C5-C6-O6	-6.75	124.55	128.60
1	A	559	A	C8-N9-C4	-6.75	103.10	105.80
1	A	1074	G	C5-C6-N1	-6.75	108.13	111.50
1	A	523	A	N1-C6-N6	6.75	122.65	118.60
1	A	755	G	C5-C6-O6	-6.75	124.55	128.60
1	A	815	A	C5-C6-N6	-6.74	118.31	123.70
1	A	823	G	N1-C2-N3	6.74	127.94	123.90
1	A	1264	C	C6-N1-C2	-6.73	117.61	120.30
1	A	723	U	C2-N1-C1'	6.73	125.78	117.70
4	D	65	ARG	NE-CZ-NH1	6.73	123.67	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	580	U	C4-C5-C6	6.73	123.74	119.70
1	A	617	G	N3-C4-N9	6.73	130.04	126.00
1	A	882	C	C5-C6-N1	-6.73	117.64	121.00
1	A	1108	G	N3-C4-C5	-6.72	125.24	128.60
1	A	1338	G	N1-C2-N3	6.72	127.94	123.90
1	A	1416	G	C6-C5-N7	-6.72	126.37	130.40
1	A	759	A	C5-C6-N6	-6.72	118.32	123.70
1	A	872	A	C5-N7-C8	-6.72	100.54	103.90
1	A	1157	A	C8-N9-C4	-6.72	103.11	105.80
1	A	44	G	C6-C5-N7	-6.72	126.37	130.40
1	A	123	C	N1-C2-O2	-6.72	114.87	118.90
1	A	798	G	N3-C4-C5	6.71	131.96	128.60
1	A	54	C	N3-C4-C5	6.71	124.58	121.90
1	A	1054	C	C5-C6-N1	6.71	124.35	121.00
1	A	1528	U	N3-C2-O2	6.71	126.90	122.20
1	A	1442	G	C6-C5-N7	-6.69	126.38	130.40
1	A	314	C	C5-C6-N1	-6.69	117.65	121.00
1	A	732	C	N3-C4-C5	6.69	124.58	121.90
1	A	812	C	C5-C4-N4	6.69	124.88	120.20
1	A	836	G	C4-C5-N7	6.69	113.48	110.80
1	A	530	G	C4-N9-C1'	6.69	135.20	126.50
1	A	628	G	N1-C2-N3	6.69	127.91	123.90
1	A	128	G	C5-C6-O6	-6.68	124.59	128.60
1	A	507	C	N3-C4-C5	6.68	124.57	121.90
1	A	326	G	C4-C5-C6	6.68	122.81	118.80
1	A	325	A	N9-C4-C5	6.68	108.47	105.80
1	A	93	G	N9-C4-C5	-6.68	102.73	105.40
1	A	297	G	N1-C6-O6	6.68	123.91	119.90
1	A	1158	C	C2-N1-C1'	6.68	126.14	118.80
1	A	1512	U	N3-C4-O4	6.68	124.07	119.40
1	A	735	C	C5-C6-N1	-6.67	117.66	121.00
1	A	818	G	N1-C6-O6	6.67	123.90	119.90
1	A	244	U	N1-C2-O2	6.67	127.47	122.80
1	A	800	G	C4-N9-C1'	6.67	135.17	126.50
1	A	918	A	C6-N1-C2	-6.66	114.60	118.60
1	A	1505	G	N3-C4-C5	-6.66	125.27	128.60
1	A	98	U	C5-C6-N1	6.66	126.03	122.70
1	A	614	A	N1-C2-N3	6.66	132.63	129.30
1	A	190(F)	G	C4-N9-C1'	-6.65	117.85	126.50
1	A	634	C	N3-C2-O2	-6.65	117.24	121.90
17	Q	98	LEU	CA-CB-CG	6.65	130.59	115.30
1	A	283	C	C5-C6-N1	6.65	124.32	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	795	C	C2-N3-C4	6.64	123.22	119.90
1	A	651	C	C6-N1-C2	6.64	122.96	120.30
1	A	1412	C	N3-C4-C5	6.64	124.56	121.90
1	A	947	G	C4-C5-N7	6.64	113.45	110.80
1	A	703	G	C5-N7-C8	6.63	107.62	104.30
1	A	462	G	C8-N9-C4	-6.63	103.75	106.40
1	A	800	G	C8-N9-C1'	-6.63	118.39	127.00
1	A	911	U	C5-C6-N1	-6.62	119.39	122.70
1	A	366	C	N1-C2-O2	6.62	122.87	118.90
1	A	1104	G	N7-C8-N9	6.62	116.41	113.10
1	A	107	G	C5-N7-C8	-6.62	100.99	104.30
1	A	1417	G	C6-C5-N7	-6.62	126.43	130.40
1	A	93	G	N3-C4-N9	6.61	129.97	126.00
1	A	144	G	N3-C2-N2	-6.61	115.27	119.90
1	A	1346	A	N1-C6-N6	-6.61	114.63	118.60
1	A	518	C	C6-N1-C1'	-6.61	112.87	120.80
1	A	817	C	C5-C4-N4	-6.61	115.58	120.20
1	A	927	G	C2-N3-C4	-6.61	108.60	111.90
1	A	1299	A	C5-N7-C8	-6.61	100.60	103.90
1	A	301	G	C4-N9-C1'	6.60	135.09	126.50
1	A	316	G	C5-C6-O6	-6.60	124.64	128.60
1	A	610	G	N1-C6-O6	-6.60	115.94	119.90
1	A	944	G	C5-C6-O6	6.60	132.56	128.60
1	A	1079	G	N1-C2-N2	-6.59	110.27	116.20
1	A	730	G	N1-C2-N3	6.59	127.85	123.90
1	A	707	C	C2-N1-C1'	-6.58	111.56	118.80
1	A	474	G	C5-N7-C8	-6.58	101.01	104.30
1	A	277	C	C6-N1-C2	6.58	122.93	120.30
1	A	863	U	C5-C4-O4	-6.58	121.95	125.90
1	A	1243	C	C6-N1-C2	6.58	122.93	120.30
1	A	721	G	C4-C5-C6	6.58	122.75	118.80
1	A	793	U	C5-C6-N1	6.58	125.99	122.70
1	A	317	G	N9-C4-C5	-6.57	102.77	105.40
1	A	822	C	C4-C5-C6	6.57	120.69	117.40
1	A	285	G	N3-C4-C5	6.57	131.88	128.60
1	A	569	C	N3-C4-N4	-6.56	113.41	118.00
1	A	298	A	C2-N3-C4	-6.56	107.32	110.60
1	A	6	G	C8-N9-C1'	-6.55	118.49	127.00
1	A	135	C	C5-C4-N4	6.54	124.78	120.20
1	A	283	C	C2-N1-C1'	6.54	125.99	118.80
1	A	1387	G	C2-N3-C4	-6.54	108.63	111.90
1	A	251	G	N7-C8-N9	6.53	116.37	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	310	G	N1-C2-N2	6.53	122.08	116.20
1	A	535	A	C5-N7-C8	6.53	107.17	103.90
1	A	122	G	N1-C6-O6	6.53	123.81	119.90
1	A	324	G	C5-C6-N1	-6.53	108.24	111.50
1	A	319	G	C5-C6-O6	-6.52	124.69	128.60
1	A	1187	G	C4-N9-C1'	6.52	134.98	126.50
1	A	878	G	N1-C6-O6	6.52	123.81	119.90
1	A	1365	G	C8-N9-C4	-6.52	103.79	106.40
1	A	200	G	C5-C6-N1	-6.52	108.24	111.50
1	A	1342	C	C2-N1-C1'	-6.52	111.63	118.80
1	A	662	G	C2-N3-C4	-6.51	108.64	111.90
1	A	454	C	C6-N1-C2	-6.51	117.69	120.30
1	A	618	C	C6-N1-C2	6.51	122.91	120.30
1	A	820	U	C6-N1-C2	-6.51	117.09	121.00
1	A	1078	U	N1-C2-O2	-6.51	118.24	122.80
1	A	245	C	C5-C4-N4	-6.51	115.65	120.20
1	A	553	A	N1-C2-N3	6.51	132.55	129.30
1	A	973	G	N3-C4-N9	6.50	129.90	126.00
1	A	137	C	C5-C6-N1	-6.50	117.75	121.00
1	A	226	G	C5-C6-N1	6.50	114.75	111.50
1	A	1442	G	C8-N9-C1'	-6.49	118.56	127.00
1	A	78	G	C5-C6-N1	6.49	114.75	111.50
1	A	299	G	C5-C6-O6	-6.49	124.71	128.60
1	A	1539	C	N1-C2-N3	-6.49	114.66	119.20
1	A	1338	G	N1-C6-O6	-6.49	116.01	119.90
1	A	170	U	N1-C2-O2	-6.48	118.26	122.80
1	A	933	G	N1-C6-O6	6.48	123.79	119.90
1	A	872	A	C8-N9-C4	6.48	108.39	105.80
1	A	190(C)	C	C6-N1-C2	-6.47	117.71	120.30
1	A	199	G	N1-C6-O6	6.47	123.78	119.90
1	A	219	C	N1-C2-O2	-6.47	115.02	118.90
1	A	260	G	C6-C5-N7	-6.47	126.52	130.40
1	A	326	G	C8-N9-C1'	-6.47	118.59	127.00
1	A	612	C	N3-C4-N4	6.47	122.53	118.00
1	A	884	U	C4-C5-C6	6.47	123.58	119.70
1	A	609	A	C2-N3-C4	-6.47	107.37	110.60
1	A	266	G	C2-N3-C4	-6.46	108.67	111.90
1	A	1505	G	N9-C4-C5	6.46	107.98	105.40
1	A	43	C	C2-N3-C4	-6.46	116.67	119.90
1	A	582	U	C2-N3-C4	-6.46	123.13	127.00
1	A	1377	A	N1-C2-N3	6.46	132.53	129.30
1	A	7	G	C8-N9-C4	6.45	108.98	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	635	G	N1-C2-N3	6.45	127.77	123.90
1	A	21	G	N1-C2-N2	-6.45	110.40	116.20
1	A	1231	G	C5-C6-O6	-6.44	124.73	128.60
1	A	166	G	C8-N9-C4	6.44	108.98	106.40
7	G	124	LEU	CA-CB-CG	-6.44	100.49	115.30
1	A	524	G	C8-N9-C4	-6.43	103.83	106.40
1	A	1079	G	C4-C5-C6	6.43	122.66	118.80
1	A	1103	C	C2-N3-C4	-6.43	116.69	119.90
1	A	1409	C	C5-C6-N1	6.43	124.22	121.00
1	A	399	G	C2-N3-C4	-6.42	108.69	111.90
1	A	609	A	N1-C2-N3	6.42	132.51	129.30
1	A	201	C	C2-N1-C1'	6.42	125.86	118.80
1	A	1305	G	N1-C6-O6	6.42	123.75	119.90
1	A	913	A	C4-C5-N7	-6.41	107.49	110.70
1	A	1323	G	C2-N3-C4	-6.41	108.69	111.90
1	A	291	C	N3-C4-C5	6.41	124.47	121.90
1	A	283	C	N3-C4-C5	-6.41	119.34	121.90
1	A	916	G	C6-C5-N7	-6.40	126.56	130.40
1	A	926	G	C4-N9-C1'	6.40	134.83	126.50
1	A	21	G	N7-C8-N9	-6.40	109.90	113.10
1	A	721	G	C4-N9-C1'	6.40	134.82	126.50
1	A	131	C	C2-N3-C4	-6.39	116.70	119.90
1	A	108	G	N3-C4-N9	-6.39	122.17	126.00
1	A	857	C	C6-N1-C2	-6.39	117.75	120.30
1	A	817	C	C6-N1-C2	6.38	122.85	120.30
1	A	1077	G	N1-C6-O6	6.38	123.73	119.90
1	A	188	C	C4-C5-C6	6.38	120.59	117.40
1	A	628	G	C4-N9-C1'	6.38	134.79	126.50
1	A	636	U	C4-C5-C6	6.38	123.53	119.70
1	A	822	C	N3-C4-C5	-6.38	119.35	121.90
1	A	1106	G	N3-C4-N9	-6.37	122.18	126.00
1	A	617	G	C8-N9-C1'	-6.37	118.72	127.00
1	A	916	G	N1-C6-O6	6.37	123.72	119.90
1	A	1231	G	C6-C5-N7	-6.37	126.58	130.40
1	A	1505	G	C5-N7-C8	-6.37	101.12	104.30
1	A	559	A	N3-C4-N9	6.36	132.49	127.40
1	A	1099	G	N3-C4-N9	-6.36	122.18	126.00
1	A	518	C	N1-C2-O2	6.36	122.72	118.90
1	A	659	U	C5-C6-N1	-6.36	119.52	122.70
1	A	703	G	N1-C6-O6	-6.36	116.08	119.90
1	A	284	G	C4-C5-C6	6.36	122.61	118.80
1	A	872	A	N3-C4-C5	6.36	131.25	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	582	U	C5-C4-O4	-6.36	122.09	125.90
1	A	725	G	C5-N7-C8	-6.35	101.12	104.30
1	A	945	G	N7-C8-N9	6.35	116.28	113.10
1	A	1095	U	C5-C4-O4	-6.35	122.09	125.90
1	A	1240	U	C5-C4-O4	6.35	129.71	125.90
1	A	599	C	N3-C4-N4	6.34	122.44	118.00
1	A	1464	G	N1-C6-O6	6.34	123.71	119.90
1	A	229	U	N3-C4-C5	-6.34	110.80	114.60
1	A	765	G	N1-C6-O6	6.34	123.70	119.90
1	A	625	G	C5-C6-N1	6.34	114.67	111.50
1	A	1246	C	C6-N1-C2	-6.34	117.77	120.30
1	A	88	A	N9-C4-C5	6.33	108.33	105.80
1	A	621	A	N1-C6-N6	6.33	122.40	118.60
1	A	1513	A	C8-N9-C4	6.33	108.33	105.80
1	A	318	G	C5-C6-O6	-6.33	124.80	128.60
1	A	729	A	C4-C5-N7	6.33	113.86	110.70
1	A	317	G	N1-C6-O6	6.32	123.69	119.90
1	A	573	A	C4-C5-C6	6.32	120.16	117.00
1	A	570	G	N7-C8-N9	6.32	116.26	113.10
1	A	144	G	N7-C8-N9	6.32	116.26	113.10
1	A	585	G	N1-C6-O6	6.31	123.69	119.90
1	A	855	G	N7-C8-N9	-6.31	109.94	113.10
1	A	110	C	N1-C2-O2	-6.31	115.11	118.90
1	A	1071	C	N3-C2-O2	6.31	126.32	121.90
1	A	308	C	N3-C4-C5	6.31	124.42	121.90
1	A	314	C	N3-C4-C5	6.31	124.42	121.90
1	A	333	G	C8-N9-C4	6.30	108.92	106.40
1	A	369	C	N3-C4-C5	6.30	124.42	121.90
1	A	647	C	C5-C6-N1	-6.30	117.85	121.00
1	A	670	G	C5-C6-O6	-6.30	124.82	128.60
1	A	1304	G	C5-C6-O6	6.30	132.38	128.60
1	A	20	U	N3-C2-O2	6.30	126.61	122.20
1	A	546	G	N3-C4-C5	-6.30	125.45	128.60
1	A	1138	G	C2-N3-C4	6.30	115.05	111.90
1	A	916	G	C6-N1-C2	-6.30	121.32	125.10
1	A	1425	U	C5-C4-O4	6.30	129.68	125.90
1	A	1087	G	C5-N7-C8	-6.30	101.15	104.30
1	A	1103	C	N3-C4-C5	6.29	124.42	121.90
1	A	727	G	N1-C2-N2	-6.29	110.53	116.20
1	A	190(G)	G	N1-C6-O6	6.29	123.67	119.90
1	A	28	G	C6-C5-N7	-6.29	126.63	130.40
1	A	326	G	C5-N7-C8	6.29	107.44	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	595	G	C5-C6-N1	-6.29	108.36	111.50
1	A	1227	A	N3-C4-C5	6.29	131.20	126.80
1	A	262	A	C4-C5-C6	-6.28	113.86	117.00
1	A	574	A	N1-C6-N6	-6.28	114.83	118.60
1	A	454	C	N3-C4-N4	6.28	122.39	118.00
1	A	912	A	N9-C4-C5	-6.28	103.29	105.80
1	A	913	A	N1-C6-N6	-6.28	114.83	118.60
1	A	53	A	C6-N1-C2	-6.27	114.84	118.60
1	A	241	C	N3-C2-O2	6.27	126.29	121.90
1	A	605	U	N3-C4-C5	-6.27	110.84	114.60
1	A	107	G	N9-C4-C5	-6.27	102.89	105.40
1	A	139	G	N1-C6-O6	6.27	123.66	119.90
1	A	944	G	N3-C4-C5	-6.27	125.47	128.60
1	A	1238	A	N1-C6-N6	-6.26	114.84	118.60
1	A	1447	G	C5-N7-C8	-6.26	101.17	104.30
1	A	373	A	C2-N3-C4	-6.26	107.47	110.60
1	A	1331	G	C4-C5-N7	-6.26	108.30	110.80
1	A	676	A	C8-N9-C4	6.26	108.30	105.80
1	A	1313	U	C6-N1-C2	6.26	124.75	121.00
1	A	901	A	N9-C4-C5	6.25	108.30	105.80
1	A	112	G	N1-C6-O6	6.25	123.65	119.90
1	A	910	C	C6-N1-C2	6.25	122.80	120.30
1	A	1306	A	C4-C5-C6	6.25	120.12	117.00
1	A	1081	G	C8-N9-C4	-6.25	103.90	106.40
1	A	1367	C	C5-C6-N1	6.25	124.12	121.00
1	A	1488	G	C6-N1-C2	-6.25	121.35	125.10
1	A	617	G	N9-C4-C5	-6.25	102.90	105.40
1	A	1153	C	N3-C4-C5	6.25	124.40	121.90
1	A	1108	G	N3-C4-N9	6.24	129.75	126.00
1	A	1229	A	C8-N9-C4	6.24	108.30	105.80
1	A	460	A	C8-N9-C4	-6.24	103.30	105.80
1	A	825	G	C8-N9-C1'	-6.24	118.89	127.00
1	A	931	C	C2-N3-C4	-6.24	116.78	119.90
1	A	1297	C	N3-C4-N4	-6.24	113.63	118.00
1	A	641	U	N1-C2-N3	6.24	118.64	114.90
1	A	462	G	C4-N9-C1'	6.24	134.61	126.50
1	A	896	C	C6-N1-C2	-6.23	117.81	120.30
1	A	881	G	C2-N3-C4	-6.23	108.79	111.90
1	A	901	A	N1-C2-N3	6.23	132.41	129.30
1	A	815	A	C6-C5-N7	-6.22	127.94	132.30
1	A	1295	G	C8-N9-C4	-6.22	103.91	106.40
1	A	190(I)	G	C8-N9-C4	6.22	108.89	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	201	C	N3-C2-O2	-6.22	117.55	121.90
1	A	921	U	N1-C2-N3	6.22	118.63	114.90
1	A	19	C	N3-C2-O2	6.22	126.25	121.90
1	A	306	G	N1-C2-N2	6.22	121.80	116.20
1	A	326	G	N1-C2-N3	6.22	127.63	123.90
1	A	405	U	C2-N1-C1'	6.22	125.16	117.70
1	A	779	C	C2-N3-C4	-6.22	116.79	119.90
1	A	909	A	C6-N1-C2	-6.22	114.87	118.60
1	A	812	C	C4-C5-C6	6.22	120.51	117.40
1	A	971	G	C5-C6-N1	-6.21	108.39	111.50
1	A	1084	G	C5-C6-O6	6.21	132.33	128.60
1	A	227	G	N3-C2-N2	-6.21	115.55	119.90
1	A	28	G	C5-C6-O6	-6.21	124.87	128.60
1	A	295	C	C5-C6-N1	-6.21	117.90	121.00
1	A	1178	G	N9-C4-C5	6.21	107.88	105.40
1	A	1106	G	N3-C4-C5	6.21	131.70	128.60
1	A	405	U	C6-N1-C1'	-6.20	112.52	121.20
1	A	1390	U	N3-C4-C5	-6.20	110.88	114.60
1	A	229	U	C4-C5-C6	6.20	123.42	119.70
1	A	940	C	N3-C4-C5	6.19	124.38	121.90
1	A	1063	C	C6-N1-C2	-6.19	117.82	120.30
1	A	873	A	N1-C2-N3	-6.19	126.20	129.30
1	A	283	C	N3-C2-O2	-6.19	117.57	121.90
1	A	1268	A	C8-N9-C4	-6.18	103.33	105.80
1	A	257	G	N1-C6-O6	-6.18	116.19	119.90
1	A	1348	U	C2-N1-C1'	6.18	125.12	117.70
5	E	41	VAL	CB-CA-C	-6.18	99.65	111.40
1	A	9	G	C5-C6-O6	-6.18	124.89	128.60
1	A	947	G	C5-C6-O6	-6.18	124.89	128.60
1	A	232	G	N3-C2-N2	6.17	124.22	119.90
1	A	641	U	N1-C2-O2	-6.17	118.48	122.80
1	A	1231	G	C4-C5-N7	6.17	113.27	110.80
1	A	144	G	C5-C6-O6	-6.16	124.90	128.60
1	A	685	G	N3-C4-C5	6.15	131.68	128.60
1	A	1299	A	C4-C5-N7	6.15	113.78	110.70
1	A	839	U	C2-N1-C1'	6.15	125.08	117.70
1	A	1187	G	C6-C5-N7	-6.15	126.71	130.40
1	A	242	C	C6-N1-C2	6.15	122.76	120.30
1	A	1071	C	N3-C4-N4	6.15	122.30	118.00
1	A	1254	C	N3-C4-C5	-6.15	119.44	121.90
1	A	190(F)	G	N3-C4-N9	-6.14	122.31	126.00
1	A	1200	C	C6-N1-C1'	-6.14	113.43	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	585	G	C5-C6-O6	-6.14	124.92	128.60
1	A	614	A	C2-N3-C4	-6.14	107.53	110.60
1	A	877	C	C2-N3-C4	-6.14	116.83	119.90
1	A	768	A	N1-C2-N3	6.14	132.37	129.30
1	A	798	G	N1-C2-N3	6.14	127.58	123.90
1	A	1191	A	C2-N3-C4	6.13	113.67	110.60
1	A	172	A	N1-C2-N3	6.13	132.37	129.30
1	A	252	U	C2-N1-C1'	-6.13	110.34	117.70
1	A	1060	C	C2-N1-C1'	6.13	125.54	118.80
1	A	797	C	C2-N3-C4	-6.12	116.84	119.90
1	A	109	A	C6-C5-N7	-6.12	128.02	132.30
1	A	220	G	C5-C6-O6	-6.12	124.93	128.60
1	A	599	C	C6-N1-C2	6.12	122.75	120.30
1	A	255	G	N9-C4-C5	-6.11	102.95	105.40
1	A	1496	C	C2-N3-C4	6.11	122.95	119.90
1	A	1087	G	C6-C5-N7	-6.11	126.73	130.40
1	A	577	G	C5-C6-O6	-6.11	124.94	128.60
1	A	577	G	C8-N9-C4	6.11	108.84	106.40
1	A	600	C	C6-N1-C2	6.11	122.74	120.30
1	A	368	U	N3-C4-O4	-6.10	115.13	119.40
1	A	1508	G	N1-C6-O6	-6.10	116.24	119.90
1	A	251	G	C5-N7-C8	-6.10	101.25	104.30
1	A	529	G	C5-C6-N1	-6.10	108.45	111.50
1	A	870	U	C5-C4-O4	6.10	129.56	125.90
1	A	255	G	C4-C5-C6	6.10	122.46	118.80
1	A	920	U	N3-C4-C5	-6.10	110.94	114.60
1	A	918	A	C2-N3-C4	-6.09	107.55	110.60
1	A	1334	G	C5-C6-N1	-6.09	108.45	111.50
1	A	445	G	C8-N9-C4	-6.09	103.97	106.40
1	A	1067	A	C8-N9-C4	-6.09	103.36	105.80
1	A	1494	G	C8-N9-C1'	-6.08	119.10	127.00
1	A	292	G	C5-C6-O6	-6.08	124.95	128.60
4	D	58	LEU	CA-CB-CG	6.08	129.27	115.30
1	A	729	A	C4-C5-C6	6.07	120.04	117.00
1	A	899	C	C6-N1-C2	-6.07	117.87	120.30
1	A	876	G	C5-C6-N1	6.07	114.53	111.50
1	A	1511	G	C8-N9-C4	-6.06	103.97	106.40
1	A	18	C	C6-N1-C2	6.06	122.72	120.30
1	A	701	C	C2-N1-C1'	6.06	125.47	118.80
1	A	1492	A	N1-C6-N6	-6.06	114.97	118.60
1	A	90	U	N3-C4-C5	-6.05	110.97	114.60
1	A	1077	G	C4-C5-N7	6.05	113.22	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	196	LEU	CA-CB-CG	-6.05	101.39	115.30
1	A	137	C	C2-N3-C4	-6.04	116.88	119.90
1	A	926	G	C4-C5-C6	6.04	122.42	118.80
1	A	1294	G	C8-N9-C4	-6.04	103.98	106.40
1	A	1494	G	C4-N9-C1'	6.04	134.35	126.50
1	A	284	G	C5-C6-N1	-6.04	108.48	111.50
1	A	767	A	C6-N1-C2	-6.04	114.98	118.60
1	A	945	G	C8-N9-C4	-6.04	103.99	106.40
1	A	1079	G	N3-C2-N2	6.03	124.12	119.90
1	A	1512	U	N3-C2-O2	6.03	126.42	122.20
1	A	1513	A	C2-N3-C4	-6.03	107.58	110.60
1	A	448	A	N1-C6-N6	-6.03	114.98	118.60
1	A	1401	G	C4-C5-C6	6.03	122.42	118.80
1	A	824	C	C6-N1-C2	6.03	122.71	120.30
1	A	1520	G	C5-C6-N1	6.03	114.51	111.50
1	A	149	A	C2-N3-C4	-6.03	107.59	110.60
1	A	931	C	C6-N1-C2	6.03	122.71	120.30
1	A	1516	G	C6-C5-N7	-6.03	126.78	130.40
1	A	15	G	C4-N9-C1'	6.02	134.33	126.50
1	A	665	A	C6-N1-C2	-6.02	114.99	118.60
1	A	78	G	C4-C5-N7	6.02	113.21	110.80
1	A	927	G	N3-C4-N9	-6.02	122.39	126.00
1	A	15	G	C8-N9-C1'	-6.02	119.18	127.00
1	A	129(A)	G	C4-C5-N7	6.02	113.21	110.80
1	A	301	G	N7-C8-N9	6.01	116.11	113.10
1	A	814	A	C4-C5-C6	6.01	120.01	117.00
1	A	963	G	C8-N9-C4	-6.01	104.00	106.40
1	A	1157	A	N1-C2-N3	6.01	132.31	129.30
1	A	1508	G	C8-N9-C4	-6.01	104.00	106.40
1	A	591	U	N1-C2-O2	-6.01	118.59	122.80
1	A	1539	C	C4-C5-C6	-6.01	114.39	117.40
1	A	499	A	N1-C6-N6	-6.01	115.00	118.60
1	A	758	G	C2-N3-C4	-6.01	108.90	111.90
1	A	903	G	N1-C2-N3	6.01	127.50	123.90
1	A	562	C	N1-C2-O2	6.00	122.50	118.90
1	A	1531	A	C5-C6-N6	-6.00	118.90	123.70
1	A	27	G	C6-C5-N7	-6.00	126.80	130.40
1	A	785	G	C4-C5-N7	6.00	113.20	110.80
1	A	264	U	C2-N1-C1'	6.00	124.90	117.70
1	A	482	A	N1-C6-N6	6.00	122.20	118.60
1	A	1376	U	C5-C6-N1	-6.00	119.70	122.70
1	A	1544	U	C5-C4-O4	-6.00	122.30	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	279	A	C4-C5-N7	5.99	113.69	110.70
1	A	297	G	C5-C6-N1	-5.99	108.50	111.50
1	A	1266	G	N3-C4-C5	5.99	131.59	128.60
1	A	132	C	N1-C2-N3	5.99	123.39	119.20
1	A	535	A	C4-C5-N7	-5.99	107.70	110.70
1	A	124	G	N1-C2-N3	5.99	127.49	123.90
1	A	127	G	N3-C4-C5	5.98	131.59	128.60
1	A	812	C	N3-C4-C5	-5.98	119.51	121.90
1	A	721	G	N3-C4-N9	5.98	129.59	126.00
1	A	920	U	C6-N1-C2	-5.98	117.41	121.00
1	A	830	G	C2-N3-C4	-5.98	108.91	111.90
1	A	1080	A	C6-C5-N7	5.98	136.49	132.30
1	A	1229	A	C4-C5-C6	-5.98	114.01	117.00
1	A	625	G	C2-N3-C4	5.97	114.89	111.90
1	A	670	G	N1-C6-O6	5.97	123.48	119.90
1	A	1061	G	C5-C6-N1	-5.97	108.51	111.50
1	A	771	G	N9-C4-C5	-5.97	103.01	105.40
1	A	800	G	C6-C5-N7	-5.97	126.82	130.40
1	A	1057	G	N1-C6-O6	5.97	123.48	119.90
1	A	396	G	N3-C4-C5	-5.97	125.62	128.60
1	A	1417	G	N3-C4-C5	-5.96	125.62	128.60
1	A	893	C	N3-C2-O2	-5.96	117.73	121.90
1	A	725	G	N7-C8-N9	5.96	116.08	113.10
1	A	258	G	C2-N3-C4	-5.96	108.92	111.90
1	A	728	A	C5-C6-N6	-5.96	118.94	123.70
1	A	1344	C	N3-C2-O2	-5.95	117.73	121.90
1	A	944	G	N7-C8-N9	5.95	116.08	113.10
1	A	1116	C	N3-C4-C5	5.95	124.28	121.90
1	A	1178	G	C8-N9-C4	-5.95	104.02	106.40
1	A	305	G	C4-C5-N7	5.94	113.18	110.80
1	A	1502	A	N3-C4-C5	5.94	130.96	126.80
1	A	266	G	N3-C4-N9	-5.94	122.44	126.00
1	A	301	G	C6-C5-N7	-5.94	126.84	130.40
1	A	132	C	C6-N1-C2	-5.93	117.93	120.30
1	A	126	G	N3-C4-N9	-5.93	122.44	126.00
1	A	925	G	C4-C5-N7	5.93	113.17	110.80
1	A	1081	G	N7-C8-N9	5.93	116.06	113.10
1	A	1104	G	C5-N7-C8	-5.93	101.33	104.30
1	A	228	A	C2-N3-C4	-5.93	107.64	110.60
1	A	882	C	N3-C4-C5	5.93	124.27	121.90
1	A	1060	C	N3-C2-O2	-5.92	117.75	121.90
1	A	754	C	C2-N1-C1'	5.92	125.31	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	860	A	N7-C8-N9	5.92	116.76	113.80
1	A	1080	A	N7-C8-N9	-5.92	110.84	113.80
1	A	394	G	C4-C5-N7	-5.91	108.44	110.80
1	A	942	G	C2-N3-C4	-5.91	108.94	111.90
1	A	108	G	C5-N7-C8	-5.91	101.34	104.30
1	A	1185	G	N3-C4-C5	-5.91	125.65	128.60
1	A	93	G	N3-C2-N2	5.91	124.03	119.90
1	A	221	C	N1-C2-O2	5.90	122.44	118.90
1	A	5	U	N1-C2-O2	5.90	126.93	122.80
1	A	190	C	N3-C2-O2	-5.90	117.77	121.90
1	A	579	G	C2-N3-C4	-5.90	108.95	111.90
1	A	971	G	N9-C4-C5	-5.90	103.04	105.40
1	A	243	A	C8-N9-C4	-5.90	103.44	105.80
1	A	878	G	C4-C5-N7	5.90	113.16	110.80
1	A	376	G	C8-N9-C4	5.89	108.76	106.40
1	A	580	U	C6-N1-C2	-5.89	117.46	121.00
1	A	27	G	N1-C6-O6	5.89	123.44	119.90
1	A	120	A	C4-C5-C6	5.89	119.95	117.00
1	A	190(A)	C	C6-N1-C2	-5.89	117.94	120.30
1	A	1417	G	C4-C5-C6	5.89	122.33	118.80
1	A	107	G	N3-C4-N9	5.89	129.53	126.00
1	A	1442	G	N3-C4-N9	5.89	129.53	126.00
1	A	776	G	N3-C4-C5	5.89	131.54	128.60
1	A	638	G	C5-C6-O6	-5.88	125.07	128.60
1	A	782	A	N1-C6-N6	5.88	122.13	118.60
1	A	1347	G	N1-C6-O6	5.88	123.43	119.90
1	A	97	G	N7-C8-N9	5.88	116.04	113.10
1	A	692	U	N1-C2-N3	5.87	118.42	114.90
1	A	945	G	N1-C6-O6	5.87	123.42	119.90
1	A	780	A	C6-N1-C2	-5.87	115.08	118.60
1	A	567	G	N1-C2-N3	5.87	127.42	123.90
1	A	1227	A	C5-N7-C8	-5.87	100.97	103.90
1	A	1526	G	C6-C5-N7	-5.87	126.88	130.40
1	A	524	G	C5-C6-N1	5.86	114.43	111.50
5	E	15	ARG	N-CA-C	5.86	126.81	111.00
1	A	1300	G	C5-C6-O6	5.86	132.11	128.60
4	D	188	LEU	CA-CB-CG	5.86	128.77	115.30
1	A	190(F)	G	C8-N9-C1'	5.85	134.61	127.00
1	A	389	A	C8-N9-C4	-5.85	103.46	105.80
1	A	946	A	C6-N1-C2	-5.85	115.09	118.60
1	A	1361(A)	C	N3-C2-O2	-5.85	117.81	121.90
1	A	310	G	N3-C2-N2	-5.84	115.81	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	553	A	C6-N1-C2	-5.84	115.09	118.60
1	A	29	G	C5-C6-N1	-5.84	108.58	111.50
1	A	800	G	N3-C4-N9	5.84	129.50	126.00
1	A	970	C	N3-C2-O2	-5.84	117.81	121.90
1	A	235	C	C6-N1-C2	5.84	122.64	120.30
1	A	104	G	C2-N3-C4	-5.84	108.98	111.90
1	A	675	A	C4-C5-N7	5.84	113.62	110.70
1	A	35	G	N3-C4-N9	5.83	129.50	126.00
17	Q	5	VAL	CB-CA-C	-5.83	100.31	111.40
1	A	524	G	C6-C5-N7	-5.83	126.90	130.40
1	A	635	G	C5-C6-N1	-5.83	108.58	111.50
1	A	912	A	N1-C2-N3	5.83	132.22	129.30
1	A	1077	G	N9-C4-C5	-5.83	103.07	105.40
1	A	1030(D)	A	C8-N9-C4	-5.83	103.47	105.80
1	A	10	A	C2-N3-C4	-5.83	107.69	110.60
1	A	705	U	N1-C2-O2	-5.82	118.72	122.80
1	A	589	C	C2-N1-C1'	-5.82	112.40	118.80
1	A	693	G	N9-C4-C5	-5.82	103.07	105.40
1	A	700	G	N1-C6-O6	5.82	123.39	119.90
1	A	974	A	C8-N9-C4	-5.82	103.47	105.80
1	A	109	A	C5-N7-C8	-5.82	100.99	103.90
1	A	277	C	N3-C4-C5	5.82	124.23	121.90
1	A	53	A	N9-C4-C5	5.81	108.12	105.80
1	A	822	C	C6-N1-C2	-5.81	117.97	120.30
1	A	864	A	N7-C8-N9	5.81	116.71	113.80
1	A	1346	A	P-O3'-C3'	5.81	126.67	119.70
1	A	1376	U	C5-C4-O4	5.81	129.39	125.90
1	A	291	C	C2-N3-C4	-5.81	117.00	119.90
1	A	612	C	C6-N1-C2	-5.81	117.98	120.30
1	A	600	C	C2-N3-C4	-5.80	117.00	119.90
1	A	918	A	N7-C8-N9	-5.80	110.90	113.80
8	H	86	ILE	CG1-CB-CG2	-5.80	98.63	111.40
1	A	46	G	C6-C5-N7	-5.80	126.92	130.40
1	A	777	A	C5-C6-N6	-5.80	119.06	123.70
1	A	106	C	C6-N1-C2	-5.80	117.98	120.30
1	A	725	G	C4-C5-N7	5.80	113.12	110.80
1	A	1251	A	C8-N9-C4	-5.80	103.48	105.80
1	A	654	G	N1-C2-N3	5.80	127.38	123.90
1	A	137	C	N3-C4-N4	-5.80	113.94	118.00
1	A	1194	U	C5-C6-N1	5.80	125.60	122.70
1	A	919	A	C2-N3-C4	5.79	113.50	110.60
1	A	1154	G	C5-C6-N1	5.79	114.39	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	727	G	N3-C2-N2	5.79	123.95	119.90
1	A	1182	G	N1-C6-O6	5.78	123.37	119.90
1	A	190(F)	G	N3-C4-C5	5.78	131.49	128.60
1	A	799	G	N3-C4-N9	5.77	129.46	126.00
1	A	79	G	C5-C6-N1	-5.77	108.61	111.50
1	A	703	G	N1-C2-N3	5.77	127.36	123.90
1	A	1295	G	N9-C4-C5	5.77	107.71	105.40
1	A	201	C	N1-C2-O2	5.76	122.36	118.90
1	A	459	G	N1-C6-O6	-5.76	116.44	119.90
1	A	831	U	C6-N1-C2	-5.76	117.54	121.00
1	A	873	A	N7-C8-N9	5.76	116.68	113.80
1	A	1381	U	N1-C2-O2	5.76	126.83	122.80
1	A	107	G	C5-C6-O6	-5.76	125.14	128.60
1	A	1483	A	C4-C5-N7	-5.76	107.82	110.70
1	A	565	U	C6-N1-C2	5.76	124.45	121.00
1	A	589	C	C2-N3-C4	-5.76	117.02	119.90
1	A	774	G	N3-C4-N9	5.76	129.45	126.00
1	A	79	G	N3-C2-N2	-5.75	115.87	119.90
1	A	320	C	C6-N1-C2	5.75	122.60	120.30
1	A	489	C	N3-C2-O2	5.75	125.93	121.90
1	A	823	G	C8-N9-C4	5.75	108.70	106.40
1	A	182	U	N3-C2-O2	5.75	126.22	122.20
1	A	599	C	C5-C4-N4	-5.75	116.18	120.20
1	A	391	G	N3-C4-C5	-5.75	125.73	128.60
1	A	629	G	C5-C6-N1	5.75	114.37	111.50
1	A	1524	C	C6-N1-C2	-5.75	118.00	120.30
1	A	859	A	N3-C4-C5	-5.75	122.78	126.80
1	A	376	G	N7-C8-N9	-5.74	110.23	113.10
1	A	748	C	C5-C6-N1	-5.74	118.13	121.00
1	A	1334	G	N1-C6-O6	5.74	123.35	119.90
1	A	707	C	N3-C4-N4	-5.74	113.98	118.00
1	A	1243	C	N3-C4-C5	5.74	124.20	121.90
1	A	649	G	N1-C6-O6	5.74	123.34	119.90
1	A	106	C	N3-C2-O2	-5.74	117.89	121.90
1	A	299	G	N1-C6-O6	5.74	123.34	119.90
1	A	569	C	C5-C6-N1	-5.74	118.13	121.00
1	A	837	G	C8-N9-C4	5.74	108.69	106.40
1	A	1060	C	N1-C2-O2	5.73	122.34	118.90
1	A	1524	C	C4-C5-C6	5.73	120.27	117.40
1	A	350	G	N7-C8-N9	5.73	115.97	113.10
1	A	491	G	C8-N9-C4	5.73	108.69	106.40
1	A	1373	G	C5-C6-O6	5.73	132.04	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	801	U	N3-C4-C5	5.73	118.04	114.60
1	A	1465	C	N1-C2-O2	5.73	122.34	118.90
1	A	1530	G	C8-N9-C4	5.73	108.69	106.40
1	A	1475	G	C5-C6-N1	-5.73	108.64	111.50
1	A	247	G	N1-C6-O6	5.72	123.33	119.90
1	A	873	A	C4-C5-C6	-5.72	114.14	117.00
1	A	514	C	C6-N1-C2	-5.72	118.01	120.30
1	A	697	U	C5-C6-N1	5.72	125.56	122.70
1	A	221	C	N3-C4-C5	5.72	124.19	121.90
1	A	753	A	N9-C4-C5	5.72	108.09	105.80
1	A	1181	G	C8-N9-C1'	5.72	134.44	127.00
1	A	1337	G	N3-C2-N2	-5.72	115.90	119.90
1	A	570	G	N3-C4-C5	-5.72	125.74	128.60
1	A	1305	G	C4-C5-C6	5.72	122.23	118.80
1	A	190(J)	U	C5-C6-N1	-5.72	119.84	122.70
1	A	1148	U	C5-C6-N1	5.72	125.56	122.70
1	A	1471	G	C8-N9-C4	5.71	108.69	106.40
1	A	1359	C	C6-N1-C1'	-5.70	113.95	120.80
1	A	21	G	N3-C4-N9	5.70	129.42	126.00
1	A	181	G	C4-N9-C1'	5.70	133.91	126.50
1	A	918	A	N1-C6-N6	-5.70	115.18	118.60
1	A	1266	G	C8-N9-C4	5.70	108.68	106.40
1	A	489	C	C6-N1-C2	5.70	122.58	120.30
1	A	623	C	N3-C4-C5	5.70	124.18	121.90
1	A	1539	C	C2-N3-C4	5.70	122.75	119.90
1	A	530	G	C8-N9-C1'	-5.69	119.60	127.00
1	A	146	G	C5-C6-N1	-5.69	108.65	111.50
1	A	350	G	C5-N7-C8	-5.69	101.45	104.30
1	A	147	G	N3-C2-N2	-5.69	115.92	119.90
1	A	298	A	N1-C2-N3	5.69	132.15	129.30
1	A	1187	G	C8-N9-C4	-5.69	104.12	106.40
1	A	1287	A	N7-C8-N9	5.69	116.64	113.80
1	A	1387	G	C8-N9-C4	5.69	108.67	106.40
1	A	1496	C	N1-C2-O2	5.69	122.31	118.90
1	A	120	A	N1-C2-N3	5.69	132.14	129.30
1	A	1251	A	N7-C8-N9	5.69	116.64	113.80
1	A	1349	A	N9-C4-C5	5.69	108.07	105.80
1	A	131	C	N3-C4-N4	-5.68	114.02	118.00
1	A	1332	A	N1-C6-N6	-5.68	115.19	118.60
1	A	921	U	N1-C2-O2	-5.68	118.82	122.80
1	A	1528	U	C5-C4-O4	-5.68	122.49	125.90
1	A	1401	G	N3-C4-N9	5.68	129.41	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	577	G	N9-C4-C5	-5.68	103.13	105.40
1	A	716	A	N1-C2-N3	5.67	132.14	129.30
1	A	559	A	C5-C6-N1	5.67	120.54	117.70
1	A	115	G	P-O3'-C3'	5.67	126.51	119.70
1	A	767	A	C2-N3-C4	5.67	113.43	110.60
1	A	941	G	N3-C2-N2	-5.67	115.94	119.90
1	A	1370	G	N9-C4-C5	5.67	107.67	105.40
1	A	731	G	C6-C5-N7	-5.66	127.00	130.40
1	A	556	C	N3-C4-C5	5.66	124.17	121.90
1	A	1254	C	C6-N1-C2	-5.66	118.04	120.30
1	A	598	U	C6-N1-C2	5.66	124.39	121.00
1	A	761	G	C5-N7-C8	-5.66	101.47	104.30
1	A	1473	A	N1-C6-N6	5.66	122.00	118.60
1	A	106	C	C2-N3-C4	-5.66	117.07	119.90
1	A	1367	C	C2-N1-C1'	5.66	125.02	118.80
1	A	1482	G	N3-C4-C5	-5.66	125.77	128.60
1	A	281	G	C5-N7-C8	-5.66	101.47	104.30
1	A	392	G	C6-C5-N7	-5.66	127.01	130.40
1	A	830	G	N3-C2-N2	-5.66	115.94	119.90
1	A	692	U	C4-C5-C6	5.65	123.09	119.70
1	A	875	C	C4-C5-C6	5.65	120.23	117.40
8	H	63	LEU	CA-CB-CG	5.65	128.30	115.30
1	A	384	G	C5-C6-N1	5.65	114.33	111.50
1	A	62	U	C5-C6-N1	-5.65	119.88	122.70
1	A	628	G	C8-N9-C1'	-5.65	119.66	127.00
1	A	27	G	C8-N9-C1'	-5.64	119.66	127.00
5	E	126	ARG	NE-CZ-NH1	-5.64	117.48	120.30
1	A	761	G	N9-C4-C5	-5.64	103.14	105.40
1	A	616	G	C2-N3-C4	-5.64	109.08	111.90
1	A	814	A	C6-N1-C2	-5.64	115.22	118.60
1	A	881	G	N1-C2-N2	-5.63	111.13	116.20
1	A	1084	G	C4-C5-N7	-5.63	108.55	110.80
1	A	462	G	N3-C4-C5	-5.63	125.78	128.60
1	A	227	G	N1-C2-N2	5.63	121.27	116.20
1	A	827	U	C4-C5-C6	5.63	123.08	119.70
1	A	938	A	N1-C6-N6	-5.63	115.22	118.60
1	A	190(H)	G	C8-N9-C4	5.63	108.65	106.40
1	A	671	G	N3-C4-C5	5.63	131.41	128.60
1	A	1253	G	C8-N9-C4	-5.62	104.15	106.40
1	A	255	G	C4-N9-C1'	5.62	133.81	126.50
1	A	675	A	N1-C6-N6	5.62	121.97	118.60
1	A	122	G	C6-C5-N7	-5.61	127.03	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	876	G	N3-C4-N9	-5.61	122.63	126.00
1	A	325	A	N1-C6-N6	-5.61	115.24	118.60
1	A	861	G	C5-C6-O6	-5.61	125.24	128.60
1	A	233	C	C6-N1-C2	5.60	122.54	120.30
1	A	1360	A	C8-N9-C4	-5.60	103.56	105.80
1	A	243	A	P-O3'-C3'	5.60	126.42	119.70
1	A	453	A	C2-N3-C4	-5.60	107.80	110.60
1	A	29	G	C2-N3-C4	-5.60	109.10	111.90
1	A	653	A	N1-C6-N6	5.60	121.96	118.60
1	A	1079	G	N3-C4-C5	-5.60	125.80	128.60
1	A	913	A	P-O3'-C3'	5.60	126.42	119.70
1	A	53	A	C8-N9-C4	-5.60	103.56	105.80
1	A	729	A	N9-C4-C5	-5.60	103.56	105.80
1	A	971	G	C2-N3-C4	-5.59	109.10	111.90
1	A	1327	C	C2-N3-C4	-5.59	117.10	119.90
1	A	1472	U	C5-C6-N1	-5.59	119.90	122.70
1	A	758	G	N3-C4-N9	-5.59	122.64	126.00
1	A	482	A	N7-C8-N9	5.59	116.59	113.80
1	A	535	A	C4-C5-C6	5.59	119.80	117.00
1	A	1437	C	C5-C6-N1	5.59	123.80	121.00
1	A	264	U	C6-N1-C2	-5.59	117.65	121.00
1	A	137	C	C6-N1-C2	5.59	122.53	120.30
1	A	314	C	C2-N3-C4	-5.59	117.11	119.90
1	A	307	C	N3-C4-C5	5.58	124.13	121.90
1	A	89	C	C4-C5-C6	-5.58	114.61	117.40
1	A	727	G	N3-C4-N9	5.58	129.34	126.00
1	A	1323	G	C8-N9-C4	5.58	108.63	106.40
1	A	1486	G	C5-C6-O6	-5.58	125.25	128.60
1	A	269	C	N3-C4-C5	-5.57	119.67	121.90
1	A	394	G	C5-C6-N1	-5.57	108.71	111.50
1	A	715	A	C2-N3-C4	-5.57	107.81	110.60
1	A	1447	G	C6-C5-N7	-5.57	127.06	130.40
1	A	283	C	C2-N3-C4	5.57	122.69	119.90
1	A	728	A	C4-C5-N7	5.57	113.48	110.70
1	A	1331	G	C5-N7-C8	5.57	107.08	104.30
1	A	337	C	C6-N1-C2	5.57	122.53	120.30
1	A	1349	A	N1-C2-N3	5.57	132.08	129.30
1	A	794	A	N9-C4-C5	5.56	108.02	105.80
1	A	1054	C	C4-C5-C6	-5.56	114.62	117.40
1	A	16	A	N1-C6-N6	-5.56	115.27	118.60
1	A	369	C	N1-C2-O2	5.56	122.23	118.90
1	A	481	G	C8-N9-C1'	-5.56	119.77	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	117	G	C4-C5-N7	5.55	113.02	110.80
1	A	552	U	C5-C4-O4	-5.55	122.57	125.90
1	A	926	G	C8-N9-C4	-5.55	104.18	106.40
1	A	1353	G	N7-C8-N9	5.55	115.88	113.10
1	A	318	G	C6-C5-N7	-5.55	127.07	130.40
1	A	862	C	N3-C2-O2	5.55	125.79	121.90
1	A	1179	A	C4-C5-N7	-5.55	107.92	110.70
1	A	229	U	C6-N1-C2	-5.54	117.67	121.00
1	A	623	C	C6-N1-C2	5.54	122.52	120.30
1	A	1085	U	C5-C6-N1	5.54	125.47	122.70
1	A	167	G	N1-C6-O6	-5.54	116.57	119.90
1	A	60	A	C5-C6-N1	5.54	120.47	117.70
1	A	1414	U	N3-C2-O2	-5.54	118.32	122.20
1	A	573	A	C4-C5-N7	-5.54	107.93	110.70
1	A	148	G	C5-C6-O6	-5.54	125.28	128.60
1	A	854	G	N1-C2-N3	5.54	127.22	123.90
1	A	1087	G	N9-C4-C5	-5.54	103.19	105.40
1	A	380	G	C5-C6-N1	-5.54	108.73	111.50
1	A	1082	G	N7-C8-N9	-5.54	110.33	113.10
1	A	1198	G	C8-N9-C4	5.54	108.61	106.40
1	A	521	G	C4-C5-N7	-5.53	108.59	110.80
1	A	754	C	C6-N1-C1'	-5.53	114.16	120.80
1	A	444	C	C6-N1-C2	-5.53	118.09	120.30
1	A	190(G)	G	C2-N3-C4	-5.53	109.14	111.90
1	A	917	G	C8-N9-C1'	-5.53	119.81	127.00
1	A	129(A)	G	N9-C4-C5	-5.53	103.19	105.40
1	A	1104	G	C8-N9-C4	-5.53	104.19	106.40
1	A	1184	G	C4-N9-C1'	-5.53	119.32	126.50
1	A	112	G	N3-C4-C5	5.52	131.36	128.60
1	A	1490	C	C4-C5-C6	-5.52	114.64	117.40
1	A	562	C	N3-C4-C5	5.52	124.11	121.90
1	A	567	G	C5-C6-O6	5.52	131.91	128.60
1	A	17	U	N3-C4-C5	5.52	117.91	114.60
1	A	183	G	C8-N9-C4	-5.52	104.19	106.40
1	A	1164	G	N1-C6-O6	5.52	123.21	119.90
1	A	1464	G	C6-C5-N7	-5.52	127.09	130.40
1	A	881	G	N3-C4-N9	5.52	129.31	126.00
1	A	913	A	N7-C8-N9	-5.52	111.04	113.80
1	A	852	G	C5-C6-N1	-5.51	108.74	111.50
1	A	595	G	C8-N9-C1'	-5.51	119.83	127.00
1	A	27	G	N1-C2-N3	5.51	127.21	123.90
1	A	771	G	C6-C5-N7	-5.51	127.09	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	676	A	N7-C8-N9	-5.51	111.05	113.80
1	A	706	A	C2-N3-C4	-5.51	107.85	110.60
1	A	381	C	N1-C2-O2	5.50	122.20	118.90
1	A	886	G	N1-C2-N3	5.50	127.20	123.90
1	A	1156	G	N1-C6-O6	-5.50	116.60	119.90
1	A	1387	G	N9-C4-C5	-5.50	103.20	105.40
1	A	269	C	N3-C2-O2	-5.50	118.05	121.90
1	A	276	G	N1-C6-O6	5.50	123.20	119.90
1	A	366	C	N3-C2-O2	-5.50	118.05	121.90
1	A	809	G	N9-C4-C5	5.50	107.60	105.40
1	A	812	C	P-O3'-C3'	5.50	126.30	119.70
1	A	17	U	C2-N3-C4	-5.50	123.70	127.00
1	A	562	C	C5-C6-N1	-5.50	118.25	121.00
1	A	836	G	C5-N7-C8	-5.50	101.55	104.30
1	A	1461	G	C8-N9-C4	5.50	108.60	106.40
1	A	914	A	N1-C2-N3	-5.50	126.55	129.30
1	A	926	G	N1-C6-O6	5.50	123.20	119.90
1	A	1101	A	C2-N3-C4	5.50	113.35	110.60
1	A	1475	G	N1-C6-O6	5.50	123.20	119.90
1	A	1357	A	C8-N9-C4	-5.49	103.60	105.80
1	A	260	G	C5-C6-N1	-5.49	108.75	111.50
1	A	831	U	C5-C4-O4	5.49	129.19	125.90
1	A	368	U	C2-N1-C1'	-5.49	111.11	117.70
1	A	830	G	N3-C4-N9	-5.49	122.71	126.00
1	A	1304	G	N9-C4-C5	5.49	107.60	105.40
1	A	307	C	C6-N1-C2	5.49	122.50	120.30
1	A	759	A	C6-C5-N7	-5.49	128.46	132.30
1	A	640	A	C8-N9-C4	-5.48	103.61	105.80
1	A	1078	U	N3-C2-O2	5.48	126.04	122.20
1	A	1074	G	C5-N7-C8	-5.48	101.56	104.30
1	A	16	A	C5-N7-C8	5.48	106.64	103.90
1	A	595	G	C4-C5-C6	5.48	122.09	118.80
1	A	827	U	N3-C4-O4	5.48	123.24	119.40
1	A	1412	C	C2-N3-C4	-5.48	117.16	119.90
1	A	665	A	N1-C2-N3	5.48	132.04	129.30
1	A	700	G	C6-C5-N7	-5.48	127.11	130.40
1	A	1521	G	C8-N9-C4	5.48	108.59	106.40
1	A	576	G	C6-N1-C2	-5.48	121.81	125.10
1	A	1056	U	N3-C2-O2	-5.48	118.37	122.20
1	A	1187	G	N1-C6-O6	5.48	123.19	119.90
1	A	1516	G	C5-N7-C8	-5.48	101.56	104.30
8	H	2	LEU	CA-CB-CG	-5.48	102.70	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	551	U	C6-N1-C2	-5.48	117.71	121.00
1	A	756	C	C5-C4-N4	-5.48	116.37	120.20
1	A	973	G	N3-C4-C5	-5.48	125.86	128.60
1	A	1351	U	C5-C6-N1	5.47	125.44	122.70
1	A	825	G	C4-C5-N7	-5.47	108.61	110.80
1	A	1392	G	C8-N9-C4	-5.47	104.21	106.40
1	A	481	G	N7-C8-N9	-5.47	110.37	113.10
1	A	1527	C	C5-C4-N4	-5.47	116.37	120.20
4	D	12	CYS	CA-CB-SG	5.47	123.84	114.00
1	A	776	G	C5-C6-N1	-5.47	108.77	111.50
1	A	9	G	C4-C5-C6	5.46	122.08	118.80
1	A	403	C	C5-C6-N1	-5.46	118.27	121.00
1	A	901	A	C5-C6-N6	5.46	128.07	123.70
1	A	748	C	C4-C5-C6	5.46	120.13	117.40
1	A	1084	G	C2-N3-C4	5.46	114.63	111.90
1	A	21	G	N3-C4-C5	-5.46	125.87	128.60
1	A	384	G	N3-C4-N9	5.46	129.27	126.00
1	A	875	C	C6-N1-C2	5.46	122.48	120.30
1	A	687	A	P-O3'-C3'	5.46	126.25	119.70
5	E	15	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	A	594	G	N9-C4-C5	5.45	107.58	105.40
1	A	255	G	C8-N9-C1'	-5.45	119.92	127.00
1	A	1061	G	N1-C6-O6	5.45	123.17	119.90
1	A	1529	G	C8-N9-C4	-5.45	104.22	106.40
1	A	1459	C	C5-C4-N4	-5.44	116.39	120.20
1	A	1416	G	C4-C5-C6	5.44	122.07	118.80
1	A	132	C	N3-C4-C5	-5.44	119.72	121.90
1	A	372	C	N3-C4-N4	5.44	121.81	118.00
1	A	817	C	N3-C2-O2	5.44	125.71	121.90
1	A	1081	G	C5-N7-C8	-5.44	101.58	104.30
1	A	1376	U	N3-C4-O4	-5.44	115.59	119.40
1	A	721	G	N1-C6-O6	5.43	123.16	119.90
1	A	721	G	N3-C4-C5	-5.43	125.88	128.60
1	A	863	U	C6-N1-C2	5.43	124.26	121.00
1	A	618	C	N1-C2-N3	-5.43	115.40	119.20
1	A	1452	C	C5-C6-N1	5.43	123.72	121.00
1	A	9	G	N1-C2-N3	5.43	127.16	123.90
1	A	643	C	N3-C4-C5	5.42	124.07	121.90
1	A	400	C	N3-C4-N4	-5.42	114.20	118.00
1	A	546	G	C8-N9-C4	-5.42	104.23	106.40
1	A	1138	G	N3-C4-C5	-5.42	125.89	128.60
1	A	1529	G	N7-C8-N9	5.42	115.81	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	126	G	N3-C2-N2	-5.42	116.11	119.90
1	A	1071	C	C4-C5-C6	-5.42	114.69	117.40
1	A	1108	G	C4-N9-C1'	5.42	133.54	126.50
1	A	1186	G	C8-N9-C4	5.42	108.57	106.40
1	A	125	U	N1-C2-N3	5.41	118.15	114.90
1	A	573	A	C5-C6-N1	-5.41	114.99	117.70
1	A	926	G	C5-C6-O6	-5.41	125.35	128.60
1	A	1494	G	N3-C4-C5	-5.41	125.89	128.60
1	A	1531	A	N9-C4-C5	-5.41	103.64	105.80
1	A	547	A	N1-C6-N6	5.41	121.84	118.60
1	A	761	G	N1-C2-N2	-5.40	111.34	116.20
1	A	326	G	N9-C4-C5	5.40	107.56	105.40
1	A	1508	G	C4-C5-N7	-5.40	108.64	110.80
1	A	610	G	N3-C4-C5	-5.40	125.90	128.60
1	A	839	U	C6-N1-C1'	-5.40	113.64	121.20
12	L	26	ALA	N-CA-C	-5.40	96.42	111.00
1	A	1333	A	C4-C5-C6	5.40	119.70	117.00
1	A	729	A	C5-N7-C8	-5.39	101.20	103.90
1	A	771	G	N3-C4-C5	5.39	131.30	128.60
1	A	1368	G	N3-C4-C5	-5.39	125.90	128.60
1	A	1416	G	C8-N9-C4	-5.39	104.24	106.40
1	A	863	U	C5-C6-N1	-5.39	120.00	122.70
1	A	1156	G	C5-C6-O6	5.39	131.84	128.60
1	A	1238	A	N1-C2-N3	5.39	132.00	129.30
1	A	1543	C	N1-C2-O2	5.39	122.14	118.90
1	A	6	G	C4-C5-C6	5.39	122.03	118.80
1	A	174	C	N3-C4-C5	5.39	124.06	121.90
1	A	232	G	N3-C4-N9	5.39	129.23	126.00
1	A	753	A	C8-N9-C4	-5.39	103.64	105.80
1	A	365	U	C2-N1-C1'	5.39	124.17	117.70
1	A	474	G	N7-C8-N9	5.39	115.79	113.10
1	A	881	G	C8-N9-C4	5.39	108.56	106.40
1	A	326	G	N3-C2-N2	5.38	123.67	119.90
1	A	573	A	N9-C4-C5	5.38	107.95	105.80
1	A	1512	U	N3-C4-C5	-5.38	111.37	114.60
17	Q	21	VAL	CB-CA-C	-5.38	101.17	111.40
1	A	88	A	N3-C4-C5	-5.38	123.03	126.80
1	A	863	U	C2-N3-C4	-5.38	123.77	127.00
17	Q	74	LEU	CB-CG-CD1	-5.38	101.85	111.00
1	A	764	C	C6-N1-C2	5.38	122.45	120.30
1	A	1477	C	C6-N1-C2	-5.38	118.15	120.30
1	A	220	G	C2-N3-C4	5.38	114.59	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	581	G	N3-C4-N9	-5.37	122.78	126.00
1	A	524	G	C8-N9-C1'	-5.37	120.02	127.00
3	C	138	VAL	CB-CA-C	-5.37	101.20	111.40
1	A	131	C	N3-C2-O2	-5.37	118.14	121.90
1	A	778	G	C6-C5-N7	-5.37	127.18	130.40
1	A	999	C	C6-N1-C2	-5.37	118.15	120.30
1	A	620	C	C6-N1-C2	5.37	122.45	120.30
1	A	801	U	C2-N3-C4	-5.37	123.78	127.00
1	A	901	A	C2-N3-C4	-5.37	107.92	110.60
1	A	772	U	N1-C2-O2	-5.36	119.05	122.80
1	A	1219	U	C6-N1-C2	-5.36	117.78	121.00
1	A	82	U	C6-N1-C2	-5.36	117.78	121.00
1	A	1348	U	C6-N1-C1'	-5.36	113.69	121.20
1	A	1462	G	N1-C6-O6	5.36	123.12	119.90
1	A	181	G	N3-C2-N2	5.36	123.65	119.90
1	A	800	G	N1-C6-O6	5.36	123.11	119.90
1	A	867	G	N1-C6-O6	5.36	123.11	119.90
1	A	717	C	C6-N1-C1'	-5.36	114.37	120.80
1	A	826	C	C5-C4-N4	-5.36	116.45	120.20
1	A	941	G	C5-N7-C8	-5.36	101.62	104.30
1	A	1249	C	C5-C6-N1	5.36	123.68	121.00
1	A	1368	G	C5-C6-N1	5.36	114.18	111.50
1	A	788	U	N3-C4-O4	5.35	123.15	119.40
1	A	1368	G	N3-C4-N9	5.35	129.21	126.00
1	A	44	G	N1-C6-O6	5.35	123.11	119.90
1	A	257	G	N3-C2-N2	5.35	123.64	119.90
1	A	54	C	C2-N3-C4	-5.35	117.23	119.90
1	A	1340	A	C8-N9-C4	5.35	107.94	105.80
1	A	584	G	C5-C6-O6	-5.35	125.39	128.60
1	A	1471	G	C5-N7-C8	5.35	106.97	104.30
1	A	499	A	N9-C4-C5	5.34	107.94	105.80
1	A	628	G	C6-N1-C2	-5.34	121.89	125.10
1	A	881	G	C4-C5-N7	5.34	112.94	110.80
1	A	66	G	N3-C2-N2	-5.34	116.16	119.90
1	A	882	C	C2-N3-C4	-5.34	117.23	119.90
1	A	190(K)	G	N1-C6-O6	5.34	123.10	119.90
1	A	275	G	N7-C8-N9	-5.34	110.43	113.10
1	A	322	C	C4-C5-C6	5.34	120.07	117.40
1	A	389	A	N7-C8-N9	5.34	116.47	113.80
1	A	572	A	C8-N9-C1'	5.34	137.31	127.70
1	A	927	G	N3-C2-N2	-5.34	116.16	119.90
1	A	218	C	N3-C4-C5	5.34	124.03	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	733	A	N3-C4-C5	5.34	130.54	126.80
1	A	787	A	N1-C6-N6	-5.34	115.40	118.60
1	A	1108	G	C4-C5-C6	5.34	122.00	118.80
1	A	716	A	C6-N1-C2	-5.33	115.40	118.60
1	A	35	G	C6-C5-N7	-5.33	127.20	130.40
1	A	569	C	N1-C2-N3	5.33	122.93	119.20
1	A	384	G	C6-N1-C2	-5.33	121.90	125.10
1	A	305	G	C2-N3-C4	-5.33	109.24	111.90
1	A	454	C	C2-N1-C1'	5.33	124.66	118.80
1	A	765	G	C5-C6-N1	-5.33	108.84	111.50
1	A	147	G	N1-C6-O6	5.33	123.10	119.90
1	A	612	C	C2-N1-C1'	5.33	124.66	118.80
1	A	1443	G	N9-C4-C5	-5.33	103.27	105.40
1	A	372	C	N3-C4-C5	5.32	124.03	121.90
1	A	1514	C	N1-C2-O2	-5.32	115.71	118.90
1	A	174	C	N1-C2-O2	5.32	122.09	118.90
1	A	570	G	C6-C5-N7	-5.32	127.21	130.40
1	A	1071	C	N1-C2-N3	-5.32	115.48	119.20
1	A	1077	G	C6-C5-N7	-5.32	127.21	130.40
1	A	638	G	N1-C6-O6	5.32	123.09	119.90
1	A	21	G	C4-C5-N7	-5.32	108.67	110.80
1	A	80	G	C8-N9-C4	-5.32	104.27	106.40
1	A	167	G	N3-C4-C5	-5.32	125.94	128.60
1	A	373	A	N1-C2-N3	5.32	131.96	129.30
1	A	769	G	C6-C5-N7	-5.32	127.21	130.40
1	A	1306	A	C5-C6-N6	-5.32	119.45	123.70
1	A	1517	G	C5-C6-O6	5.32	131.79	128.60
1	A	602	A	N1-C2-N3	5.32	131.96	129.30
1	A	703	G	C4-C5-C6	5.32	121.99	118.80
1	A	1442	G	N3-C4-C5	-5.32	125.94	128.60
1	A	266	G	C5-C6-O6	-5.31	125.41	128.60
1	A	719	C	N3-C4-C5	5.31	124.03	121.90
1	A	609	A	C5-C6-N1	-5.31	115.04	117.70
1	A	152	A	C4-N9-C1'	-5.31	116.74	126.30
1	A	376	G	N1-C6-O6	5.31	123.08	119.90
1	A	703	G	N1-C2-N2	-5.31	111.42	116.20
1	A	925	G	N9-C4-C5	-5.31	103.28	105.40
1	A	1327	C	N3-C4-N4	-5.31	114.28	118.00
1	A	774	G	C5-N7-C8	-5.31	101.65	104.30
1	A	886	G	C2-N3-C4	-5.31	109.25	111.90
1	A	1234	C	C5-C6-N1	5.31	123.65	121.00
1	A	279	A	O4'-C1'-N9	-5.30	103.96	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1378	C	C6-N1-C2	-5.30	118.18	120.30
1	A	698	G	C6-N1-C2	-5.30	121.92	125.10
1	A	1165	C	C5-C6-N1	5.30	123.65	121.00
1	A	1179	A	N1-C6-N6	-5.30	115.42	118.60
1	A	195	A	C2-N3-C4	-5.30	107.95	110.60
1	A	322	C	C5-C6-N1	-5.30	118.35	121.00
1	A	721	G	C8-N9-C1'	-5.30	120.11	127.00
1	A	462	G	N7-C8-N9	5.30	115.75	113.10
1	A	1333	A	C8-N9-C4	-5.30	103.68	105.80
1	A	522	C	C6-N1-C1'	5.29	127.15	120.80
1	A	1306	A	N9-C4-C5	-5.29	103.68	105.80
1	A	1499	A	N1-C2-N3	5.29	131.95	129.30
1	A	801	U	N3-C4-O4	-5.29	115.70	119.40
1	A	1180	A	N9-C4-C5	5.29	107.92	105.80
1	A	573	A	C5-C6-N6	5.29	127.93	123.70
1	A	7	G	N7-C8-N9	-5.29	110.46	113.10
1	A	190(J)	U	N3-C2-O2	-5.29	118.50	122.20
1	A	733	A	C5-N7-C8	-5.29	101.26	103.90
1	A	1071	C	N3-C4-C5	5.29	124.01	121.90
1	A	108	G	N9-C4-C5	5.28	107.51	105.40
1	A	859	A	N1-C2-N3	5.28	131.94	129.30
18	R	78	LEU	CA-CB-CG	-5.28	103.15	115.30
1	A	219	C	C6-N1-C2	-5.28	118.19	120.30
1	A	1524	C	N3-C4-N4	5.28	121.70	118.00
1	A	1455	G	N3-C2-N2	-5.28	116.20	119.90
1	A	1482	G	N3-C4-N9	5.28	129.17	126.00
1	A	771	G	C5-C6-O6	-5.28	125.43	128.60
1	A	785	G	C6-C5-N7	-5.28	127.23	130.40
1	A	798	G	C5-C6-N1	-5.28	108.86	111.50
1	A	541	G	N3-C2-N2	-5.28	116.21	119.90
1	A	722	A	N1-C6-N6	5.28	121.77	118.60
1	A	698	G	N3-C4-C5	-5.27	125.96	128.60
1	A	1281	U	C5-C6-N1	5.27	125.34	122.70
1	A	204	U	N3-C2-O2	-5.27	118.51	122.20
1	A	336	C	N3-C2-O2	5.27	125.59	121.90
1	A	881	G	C6-N1-C2	-5.27	121.94	125.10
1	A	1416	G	N7-C8-N9	5.27	115.74	113.10
1	A	115	G	C8-N9-C4	5.27	108.51	106.40
1	A	878	G	C6-C5-N7	-5.27	127.24	130.40
17	Q	32	TYR	CB-CG-CD2	-5.27	117.84	121.00
1	A	572	A	C6-C5-N7	5.27	135.99	132.30
1	A	879	C	C5-C4-N4	-5.27	116.51	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	812	C	N3-C2-O2	-5.26	118.22	121.90
1	A	1520	G	N1-C6-O6	-5.26	116.74	119.90
1	A	262	A	C8-N9-C4	-5.26	103.70	105.80
1	A	724	G	N7-C8-N9	5.26	115.73	113.10
1	A	650	G	C8-N9-C4	5.26	108.50	106.40
1	A	107	G	N7-C8-N9	5.25	115.73	113.10
1	A	262	A	N9-C4-C5	5.25	107.90	105.80
1	A	113	G	N9-C4-C5	-5.25	103.30	105.40
1	A	1352	C	C6-N1-C2	-5.25	118.20	120.30
1	A	576	G	N3-C2-N2	-5.25	116.23	119.90
1	A	734	G	C5-C6-O6	-5.25	125.45	128.60
1	A	947	G	N9-C4-C5	-5.25	103.30	105.40
1	A	1509	C	C4-C5-C6	5.25	120.02	117.40
7	G	33	ASP	CB-CG-OD1	-5.25	113.58	118.30
1	A	1106	G	C4-N9-C1'	-5.25	119.68	126.50
1	A	1393	U	C5-C6-N1	-5.25	120.08	122.70
1	A	1455	G	C6-C5-N7	-5.25	127.25	130.40
1	A	1076	C	N3-C4-N4	5.24	121.67	118.00
1	A	1531	A	C5-C6-N1	-5.24	115.08	117.70
1	A	391	G	C2-N3-C4	5.24	114.52	111.90
1	A	454	C	C5-C4-N4	-5.24	116.53	120.20
1	A	1471	G	N7-C8-N9	-5.24	110.48	113.10
1	A	274	A	C5-C6-N1	5.24	120.32	117.70
1	A	859	A	C6-C5-N7	-5.23	128.64	132.30
1	A	1478	C	C6-N1-C2	-5.23	118.21	120.30
1	A	728	A	N9-C4-C5	-5.23	103.71	105.80
1	A	1461	G	N9-C4-C5	-5.23	103.31	105.40
1	A	1107	C	N3-C4-C5	-5.23	119.81	121.90
1	A	1331	G	C5-C6-O6	5.23	131.74	128.60
1	A	776	G	N3-C4-N9	-5.23	122.86	126.00
1	A	530	G	C6-C5-N7	-5.22	127.27	130.40
1	A	698	G	N1-C2-N3	5.22	127.03	123.90
1	A	529	G	C5-C6-O6	-5.22	125.47	128.60
1	A	1401	G	N3-C4-C5	-5.22	125.99	128.60
1	A	311	C	C2-N3-C4	-5.22	117.29	119.90
1	A	326	G	N1-C6-O6	-5.22	116.77	119.90
1	A	1187	G	N7-C8-N9	5.22	115.71	113.10
1	A	1531	A	C4-C5-C6	5.22	119.61	117.00
1	A	59	A	C5-C6-N1	5.21	120.31	117.70
1	A	746	A	C8-N9-C4	5.21	107.89	105.80
1	A	929	G	C6-C5-N7	-5.21	127.27	130.40
1	A	1067	A	N7-C8-N9	5.21	116.41	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1181	G	N3-C4-C5	5.21	131.21	128.60
1	A	617	G	C6-C5-N7	-5.21	127.28	130.40
1	A	726	C	N3-C4-C5	5.21	123.98	121.90
1	A	833	U	C4-C5-C6	5.21	122.82	119.70
1	A	1194	U	C6-N1-C2	-5.21	117.88	121.00
1	A	616	G	C6-C5-N7	-5.21	127.28	130.40
1	A	300	A	N1-C2-N3	5.20	131.90	129.30
1	A	1521	G	N3-C4-N9	5.20	129.12	126.00
1	A	178	C	N1-C2-O2	5.20	122.02	118.90
1	A	266	G	C8-N9-C4	-5.20	104.32	106.40
1	A	577	G	C4-C5-N7	5.20	112.88	110.80
1	A	1334	G	N3-C4-C5	5.20	131.20	128.60
1	A	117	G	N3-C4-C5	5.20	131.20	128.60
1	A	323	U	N3-C4-O4	5.20	123.04	119.40
1	A	1149	C	N3-C2-O2	-5.20	118.26	121.90
1	A	1490	C	C2-N1-C1'	5.20	124.52	118.80
1	A	642	A	C6-N1-C2	-5.19	115.48	118.60
1	A	110	C	N3-C2-O2	5.19	125.53	121.90
1	A	1394	A	N3-C4-C5	5.19	130.43	126.80
1	A	558	G	C8-N9-C4	-5.19	104.32	106.40
1	A	540	G	C8-N9-C4	5.19	108.47	106.40
1	A	1409	C	C6-N1-C2	-5.19	118.22	120.30
1	A	663	A	C8-N9-C4	5.19	107.88	105.80
1	A	730	G	N9-C4-C5	5.19	107.47	105.40
1	A	1382	C	C5-C6-N1	5.19	123.59	121.00
10	J	90	LEU	N-CA-C	5.19	125.00	111.00
1	A	1398	A	N1-C6-N6	-5.18	115.49	118.60
1	A	1197	G	C4-N9-C1'	5.18	133.24	126.50
1	A	1469	G	C6-C5-N7	-5.18	127.29	130.40
1	A	572	A	C5-C6-N1	5.18	120.29	117.70
1	A	799	G	C8-N9-C1'	-5.17	120.28	127.00
1	A	1202	G	C5-C6-O6	5.17	131.70	128.60
1	A	925	G	N3-C2-N2	5.17	123.52	119.90
1	A	1108	G	C6-C5-N7	-5.17	127.30	130.40
1	A	125	U	C5-C4-O4	5.17	129.00	125.90
1	A	802	A	C8-N9-C4	5.17	107.87	105.80
1	A	107	G	N3-C2-N2	5.17	123.52	119.90
1	A	227	G	C8-N9-C1'	5.16	133.71	127.00
1	A	815	A	C4-C5-C6	5.16	119.58	117.00
1	A	788	U	N3-C2-O2	5.16	125.81	122.20
1	A	1327	C	C4-C5-C6	5.16	119.98	117.40
1	A	1483	A	N9-C4-C5	5.16	107.86	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1363	A	C8-N9-C4	-5.16	103.74	105.80
1	A	316	G	N3-C4-N9	5.16	129.09	126.00
1	A	954	G	N1-C6-O6	5.16	122.99	119.90
1	A	79	G	C6-C5-N7	-5.15	127.31	130.40
1	A	1248	A	C2-N3-C4	5.15	113.18	110.60
1	A	798	G	N7-C8-N9	-5.15	110.52	113.10
1	A	933	G	C5-N7-C8	-5.15	101.72	104.30
1	A	286	G	C5-C6-O6	-5.15	125.51	128.60
4	D	185	PHE	N-CA-C	-5.14	97.11	111.00
1	A	155	C	N1-C2-O2	5.14	121.98	118.90
1	A	485	G	P-O3'-C3'	5.14	125.87	119.70
1	A	750	G	N3-C4-N9	5.14	129.08	126.00
1	A	807	A	N1-C2-N3	5.14	131.87	129.30
1	A	1065	U	C6-N1-C2	5.14	124.08	121.00
1	A	595	G	C4-N9-C1'	5.14	133.18	126.50
1	A	1435	G	N1-C6-O6	-5.14	116.82	119.90
1	A	143	A	N1-C6-N6	5.13	121.68	118.60
1	A	734	G	C4-C5-N7	5.13	112.85	110.80
1	A	325	A	C6-N1-C2	-5.13	115.52	118.60
1	A	1323	G	N3-C4-C5	5.13	131.17	128.60
1	A	402	G	N3-C4-C5	-5.13	126.03	128.60
1	A	1340	A	N7-C8-N9	-5.13	111.23	113.80
1	A	265	G	C5-C6-N1	-5.13	108.94	111.50
1	A	484	G	N3-C4-C5	-5.13	126.04	128.60
1	A	719	C	C2-N3-C4	-5.13	117.34	119.90
1	A	781	A	C5-C6-N6	-5.13	119.60	123.70
1	A	894	G	N1-C2-N3	5.13	126.98	123.90
1	A	328	C	P-O3'-C3'	5.12	125.85	119.70
1	A	366	C	C2-N1-C1'	5.12	124.44	118.80
1	A	131	C	C4-C5-C6	5.12	119.96	117.40
1	A	603	U	C5-C6-N1	-5.12	120.14	122.70
1	A	453	A	C8-N9-C4	5.12	107.85	105.80
1	A	892	A	C2-N3-C4	-5.12	108.04	110.60
1	A	357	G	N7-C8-N9	-5.12	110.54	113.10
5	E	15	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	281	G	C5-C6-N1	-5.11	108.94	111.50
1	A	393	A	C8-N9-C4	5.11	107.84	105.80
1	A	564	C	N1-C2-O2	5.11	121.97	118.90
1	A	571	U	N3-C4-O4	-5.11	115.82	119.40
1	A	1339	A	C6-N1-C2	-5.11	115.53	118.60
1	A	1286	A	N7-C8-N9	5.11	116.36	113.80
1	A	127	G	C2-N3-C4	-5.11	109.35	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	221	C	N3-C2-O2	-5.11	118.33	121.90
1	A	676	A	C2-N3-C4	-5.11	108.05	110.60
1	A	1294	G	N7-C8-N9	5.11	115.65	113.10
1	A	1080	A	N1-C2-N3	5.10	131.85	129.30
1	A	43	C	C4-C5-C6	5.10	119.95	117.40
1	A	169	C	N3-C4-C5	-5.10	119.86	121.90
1	A	1481	U	N3-C4-C5	-5.10	111.54	114.60
1	A	671	G	N1-C6-O6	5.10	122.96	119.90
1	A	238	G	C8-N9-C4	-5.10	104.36	106.40
1	A	830	G	N3-C4-C5	5.10	131.15	128.60
8	H	112	LEU	CB-CG-CD2	-5.10	102.33	111.00
1	A	632	A	C5-N7-C8	-5.10	101.35	103.90
1	A	551	U	N3-C4-C5	-5.10	111.54	114.60
1	A	348	G	N1-C6-O6	5.09	122.96	119.90
1	A	536	C	C6-N1-C2	-5.09	118.26	120.30
1	A	968	A	N1-C6-N6	5.09	121.66	118.60
1	A	1106	G	C5-C6-O6	5.09	131.66	128.60
1	A	1454	G	C4-C5-N7	5.09	112.84	110.80
1	A	309	G	N7-C8-N9	-5.09	110.55	113.10
1	A	1124	G	C6-C5-N7	5.09	133.46	130.40
1	A	258	G	N1-C2-N3	5.09	126.95	123.90
1	A	260	G	N3-C2-N2	-5.09	116.34	119.90
1	A	578	C	C4-C5-C6	5.09	119.95	117.40
1	A	90	U	C5-C6-N1	5.09	125.25	122.70
1	A	92	C	C4-C5-C6	5.09	119.94	117.40
1	A	860	A	C5-N7-C8	-5.09	101.36	103.90
1	A	1470	G	N3-C2-N2	-5.09	116.34	119.90
1	A	912	A	N7-C8-N9	5.09	116.34	113.80
1	A	311	C	N1-C2-O2	-5.08	115.85	118.90
1	A	777	A	N1-C6-N6	5.08	121.65	118.60
1	A	368	U	C5-C4-O4	5.08	128.95	125.90
1	A	190(G)	G	C4-C5-C6	5.08	121.85	118.80
1	A	204	U	N1-C2-O2	5.08	126.36	122.80
1	A	827	U	N1-C2-N3	5.08	117.95	114.90
1	A	1079	G	C4-C5-N7	5.08	112.83	110.80
1	A	861	G	N1-C6-O6	5.07	122.94	119.90
1	A	1300	G	C4-C5-N7	-5.07	108.77	110.80
1	A	1416	G	C4-N9-C1'	5.07	133.09	126.50
1	A	183	G	C4-N9-C1'	5.07	133.09	126.50
1	A	461	C	C6-N1-C2	-5.07	118.27	120.30
1	A	251	G	C4-C5-N7	5.07	112.83	110.80
1	A	481	G	N3-C2-N2	5.07	123.45	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1173	G	C8-N9-C4	5.07	108.43	106.40
1	A	1185	G	N3-C4-N9	5.07	129.04	126.00
1	A	129	U	C4-C5-C6	5.07	122.74	119.70
1	A	732	C	C2-N3-C4	-5.07	117.36	119.90
1	A	971	G	N7-C8-N9	-5.07	110.56	113.10
1	A	66	G	N7-C8-N9	5.07	115.63	113.10
1	A	274	A	N7-C8-N9	-5.07	111.27	113.80
1	A	936	C	C6-N1-C2	5.07	122.33	120.30
1	A	1286	A	C8-N9-C4	-5.07	103.77	105.80
1	A	863	U	N3-C2-O2	5.06	125.75	122.20
1	A	944	G	N9-C4-C5	5.06	107.42	105.40
1	A	1323	G	N1-C6-O6	5.06	122.94	119.90
1	A	53	A	N1-C2-N3	5.06	131.83	129.30
1	A	1200	C	C5-C6-N1	5.06	123.53	121.00
1	A	1416	G	C5-C6-N1	-5.06	108.97	111.50
1	A	254	G	C2-N3-C4	-5.06	109.37	111.90
1	A	284	G	C4-C5-N7	5.06	112.82	110.80
1	A	1484	C	C6-N1-C2	-5.06	118.28	120.30
1	A	399	G	N1-C2-N3	5.05	126.93	123.90
1	A	316	G	C6-C5-N7	-5.05	127.37	130.40
1	A	720	C	N3-C2-O2	-5.05	118.36	121.90
1	A	74	C	N3-C4-N4	5.05	121.54	118.00
1	A	571	U	C6-N1-C2	5.05	124.03	121.00
1	A	693	G	N1-C2-N2	-5.05	111.66	116.20
1	A	222	U	N1-C2-O2	-5.05	119.27	122.80
1	A	872	A	C4-C5-C6	-5.05	114.48	117.00
1	A	1181	G	C6-C5-N7	5.05	133.43	130.40
1	A	244	U	N3-C2-O2	-5.05	118.67	122.20
1	A	1310	G	C6-C5-N7	-5.04	127.37	130.40
1	A	1509	C	C5-C6-N1	-5.04	118.48	121.00
1	A	242	C	C2-N3-C4	-5.04	117.38	119.90
1	A	703	G	C4-N9-C1'	5.04	133.06	126.50
1	A	1357	A	N7-C8-N9	5.04	116.32	113.80
1	A	404	U	N1-C2-O2	-5.04	119.27	122.80
1	A	611	A	N1-C6-N6	-5.04	115.58	118.60
1	A	889	A	C5-N7-C8	-5.04	101.38	103.90
1	A	131	C	N3-C4-C5	5.04	123.92	121.90
1	A	942	G	N1-C6-O6	5.04	122.92	119.90
1	A	17	U	C6-N1-C2	5.04	124.02	121.00
1	A	21	G	N1-C2-N3	5.04	126.92	123.90
1	A	261	U	N3-C4-C5	-5.04	111.58	114.60
1	A	477	G	C5-C6-N1	-5.04	108.98	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	614	A	C8-N9-C4	-5.03	103.79	105.80
1	A	717	C	C2-N1-C1'	5.03	124.34	118.80
1	A	1421	G	C5-C6-O6	-5.03	125.58	128.60
1	A	644	G	N1-C6-O6	-5.03	116.88	119.90
1	A	771	G	C8-N9-C4	5.03	108.41	106.40
1	A	16	A	C4-C5-N7	-5.03	108.19	110.70
1	A	1198	G	N3-C4-C5	5.03	131.12	128.60
1	A	122	G	C5-C6-N1	-5.03	108.98	111.50
1	A	130	A	C6-C5-N7	-5.03	128.78	132.30
1	A	1064	G	N1-C2-N3	5.03	126.92	123.90
1	A	677	U	C5-C6-N1	-5.03	120.19	122.70
1	A	725	G	C6-C5-N7	-5.03	127.39	130.40
1	A	922	G	C8-N9-C4	-5.03	104.39	106.40
1	A	1227	A	N3-C4-N9	-5.02	123.38	127.40
1	A	521	G	C6-C5-N7	5.02	133.41	130.40
1	A	188	C	C5-C4-N4	5.02	123.71	120.20
1	A	860	A	C6-N1-C2	-5.02	115.59	118.60
1	A	1158	C	C6-N1-C1'	-5.02	114.78	120.80
17	Q	67	LYS	N-CA-C	-5.02	97.45	111.00
1	A	260	G	C4-C5-C6	5.02	121.81	118.80
1	A	307	C	C4-C5-C6	-5.02	114.89	117.40
1	A	594	G	C2-N3-C4	5.02	114.41	111.90
1	A	111	G	N3-C4-N9	-5.02	122.99	126.00
1	A	564	C	N3-C4-C5	5.01	123.91	121.90
1	A	883	C	N3-C2-O2	-5.01	118.39	121.90
1	A	675	A	C5-N7-C8	-5.01	101.39	103.90
1	A	637	G	C8-N9-C1'	-5.01	120.49	127.00
1	A	1350	A	C2-N3-C4	-5.01	108.10	110.60
1	A	386	C	C5-C4-N4	-5.01	116.70	120.20
1	A	1459	C	N3-C4-N4	5.01	121.50	118.00
1	A	1075	C	C6-N1-C2	5.00	122.30	120.30
1	A	292	G	N1-C6-O6	5.00	122.90	119.90

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	8	LYS	Peptide
3	C	166	GLU	Peptide
3	C	179	ARG	Peptide
3	C	24	ALA	Peptide
7	G	154	TYR	Peptide

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Mol	Chain	Res	Type	Group
8	H	90	GLY	Peptide
10	J	87	THR	Peptide
12	L	27	LEU	Peptide
13	M	105	THR	Peptide
17	Q	13	ASP	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	32509	0	16433	726	0
2	B	1900	0	1951	97	0
3	C	1612	0	1677	88	0
4	D	1703	0	1763	72	0
5	E	1146	0	1207	73	0
6	F	843	0	857	54	0
7	G	1257	0	1296	56	0
8	H	1116	0	1177	68	0
9	I	1010	0	1037	75	0
10	J	792	0	835	47	0
11	K	864	0	881	35	0
12	L	972	0	1058	51	0
13	M	937	0	995	47	0
14	N	492	0	529	36	0
15	O	729	0	768	25	0
16	P	700	0	720	44	0
17	Q	823	0	893	52	0
18	R	574	0	644	33	0
19	S	647	0	673	31	0
20	T	763	0	861	42	0
21	U	208	0	221	15	0
22	A	40	0	37	7	0
23	A	259	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	J	2	0	0	0	0
23	K	1	0	0	0	0
23	M	3	0	0	0	0
23	N	1	0	0	0	0
23	P	3	0	0	0	0
23	Q	2	0	0	0	0
23	S	1	0	0	0	0
23	T	1	0	0	0	0
24	D	1	0	0	0	0
24	N	1	0	0	0	0
25	A	369	0	0	11	0
25	D	1	0	0	0	0
25	E	6	0	0	0	0
25	J	1	0	0	0	0
25	L	1	0	0	0	0
25	Q	1	0	0	0	0
25	T	2	0	0	1	0
25	U	1	0	0	1	0
All	All	52302	0	36513	1594	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 18.

All (1594) 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:1249:C:O2'	9:I:73:GLN:NE2	2.00	0.93
1:A:1125:U:OP2	1:A:1145:C:N4	2.03	0.91
7:G:69:VAL:HG21	7:G:104:LEU:HD21	1.53	0.91
1:A:1182:G:H4'	1:A:1183:A:H5'	1.53	0.90
6:F:4:TYR:HE1	6:F:92:LYS:HG2	1.38	0.89
9:I:114:TYR:HD1	10:J:60:ARG:HB2	1.37	0.89
1:A:990:C:H42	1:A:1215:G:H1	1.22	0.88
1:A:1347:G:H3'	9:I:108:VAL:O	1.73	0.88
1:A:1290:G:H2'	1:A:1291:G:C8	2.10	0.87
3:C:25:GLY:HA2	3:C:29:TYR:HB2	1.56	0.86
14:N:12:ARG:HG2	14:N:14:PRO:HD3	1.57	0.86
1:A:18:C:H5"	5:E:127:ASN:HD21	1.39	0.85
1:A:235:C:N4	25:A:1971:HOH:O	2.10	0.85
6:F:11:ASN:HD22	6:F:86:ARG:HH21	1.24	0.84
3:C:22:TRP:HB3	3:C:59:ARG:HB3	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:37:PRO:HA	10:J:72:VAL:H	1.41	0.84
4:D:103:ASN:OD1	4:D:114:ARG:NH1	2.11	0.83
1:A:1280:A:O2'	25:A:2110:HOH:O	1.95	0.83
1:A:1290:G:H2'	1:A:1291:G:H8	1.44	0.83
1:A:451:A:O2'	25:A:2128:HOH:O	1.95	0.83
1:A:130:A:H5'	17:Q:63:ARG:HE	1.43	0.82
1:A:1126:U:O4	1:A:1148:U:N3	2.12	0.82
1:A:1240:U:OP1	7:G:119:ARG:NH2	2.13	0.82
1:A:967:5MC:H4'	9:I:128:ARG:HG3	1.62	0.82
13:M:11:ARG:HA	13:M:45:VAL:HG11	1.62	0.82
1:A:130:A:OP2	1:A:190(E):U:O2'	1.96	0.81
15:O:33:THR:OG1	15:O:63:ARG:NH1	2.14	0.81
5:E:64:ARG:O	5:E:65:ASN:ND2	2.14	0.81
1:A:1373:G:H5"	7:G:36:LYS:HD2	1.62	0.81
4:D:65:ARG:HG2	4:D:65:ARG:HH11	1.45	0.80
19:S:11:VAL:HG22	19:S:39:THR:HB	1.62	0.80
1:A:1237:C:H4'	1:A:1300:G:H22	1.47	0.80
16:P:3:LYS:HG3	16:P:24:ALA:HB2	1.64	0.79
1:A:633:G:H2'	1:A:634:C:C6	2.19	0.78
1:A:501:C:H2'	1:A:502:G:C8	2.18	0.78
9:I:26:VAL:HG22	9:I:61:ALA:H	1.49	0.78
1:A:1347:G:N2	1:A:1374:A:OP2	2.15	0.77
16:P:14:ASN:HA	16:P:42:ARG:HH21	1.49	0.77
1:A:1004:A:H8	1:A:1025:U:H3	1.30	0.77
1:A:792:A:H1'	1:A:793:U:H2'	1.65	0.77
3:C:44:GLU:HA	3:C:52:LEU:HD11	1.67	0.77
2:B:114:ARG:NH1	2:B:141:GLU:OE2	2.18	0.76
1:A:1089:G:H1	1:A:1096:C:H42	1.32	0.76
6:F:4:TYR:CE1	6:F:92:LYS:HG2	2.21	0.75
8:H:86:ILE:HG21	8:H:133:LEU:HD13	1.68	0.75
1:A:1200:C:O2	1:A:1205:U:N3	2.17	0.75
1:A:1358:U:H5"	14:N:35:ARG:HG3	1.69	0.75
20:T:75:ASN:OD1	20:T:75:ASN:N	2.19	0.75
1:A:633:G:H2'	1:A:634:C:H6	1.52	0.74
1:A:427:U:OP1	4:D:13:ARG:NH2	2.20	0.74
1:A:664:G:H22	1:A:741:G:H1	1.36	0.74
1:A:976:G:OP2	1:A:1358:U:H1'	1.86	0.74
1:A:1510:U:H2'	1:A:1511:G:C8	2.22	0.74
1:A:1249:C:HO2'	9:I:73:GLN:NE2	1.84	0.74
1:A:1133:G:H1	1:A:1141:C:H42	1.36	0.74
13:M:96:LEU:O	13:M:110:ARG:NH1	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1435:G:H2'	1:A:1436:U:C6	2.23	0.74
1:A:1073:U:OP2	5:E:57:LYS:NZ	2.14	0.73
10:J:6:ILE:HB	10:J:72:VAL:HB	1.69	0.73
3:C:156:ARG:H	3:C:163:ALA:HA	1.53	0.73
20:T:12:ALA:HA	25:T:302:HOH:O	1.88	0.73
1:A:279:A:OP1	1:A:280:C:O2'	2.03	0.73
8:H:51:VAL:HG11	8:H:60:ARG:HG2	1.71	0.73
4:D:13:ARG:NH1	4:D:38:TYR:O	2.22	0.73
3:C:188:LEU:HD11	3:C:195:VAL:HG13	1.69	0.73
19:S:19:VAL:HA	19:S:22:LEU:HG	1.71	0.72
6:F:11:ASN:HB2	6:F:86:ARG:HE	1.53	0.72
9:I:111:ARG:HG3	14:N:61:TRP:HE1	1.55	0.72
1:A:1163:C:H2'	1:A:1164:G:H8	1.55	0.72
6:F:4:TYR:HD1	6:F:92:LYS:HA	1.54	0.72
20:T:71:THR:HG22	20:T:72:LEU:HD23	1.71	0.72
1:A:1407:5MC:H2'	1:A:1408:A:H5'	1.70	0.71
3:C:156:ARG:NH1	3:C:160:ALA:O	2.23	0.71
5:E:144:THR:O	5:E:148:VAL:HG23	1.89	0.71
10:J:38:ILE:HG23	10:J:71:LEU:HD12	1.72	0.71
1:A:1239:A:H62	1:A:1299:A:H62	1.38	0.71
17:Q:74:LEU:HD23	17:Q:75:ARG:HG2	1.70	0.71
1:A:1518:MA6:H102	1:A:1519:MA6:H103	1.72	0.71
1:A:177:C:H2'	1:A:178:C:H6	1.56	0.71
1:A:279:A:H5"	1:A:281:G:H5'	1.73	0.71
1:A:1399:C:H4'	1:A:1400:5MC:H5"	1.73	0.71
1:A:1426:C:H42	1:A:1474:G:H1	1.37	0.71
1:A:1498:UR3:O2'	1:A:1499:A:OP2	2.08	0.71
1:A:18:C:H5"	5:E:127:ASN:ND2	2.06	0.70
4:D:102:ASP:OD1	4:D:103:ASN:N	2.23	0.70
1:A:1316:G:H4'	14:N:18:VAL:HG11	1.72	0.70
1:A:992:U:H3	1:A:1044:A:N6	1.88	0.70
9:I:27:THR:HG22	9:I:32:ASP:HA	1.72	0.70
1:A:393:A:OP2	16:P:12:LYS:NZ	2.18	0.70
1:A:279:A:OP2	17:Q:95:TYR:OH	2.08	0.70
1:A:344:A:H5'	1:A:345:C:C5	2.26	0.70
1:A:1355:G:H2'	1:A:1356:G:H8	1.56	0.70
3:C:91:LEU:HD21	3:C:99:VAL:HG22	1.73	0.70
1:A:1065:U:H5"	1:A:1190:G:N2	2.06	0.70
1:A:517:G:N1	1:A:533:A:OP2	2.13	0.70
18:R:86:VAL:HG12	18:R:87:ARG:H	1.56	0.70
1:A:1496:C:O2'	1:A:1497:G:O5'	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:95:VAL:HG12	8:H:99:GLU:HB2	1.74	0.69
13:M:25:ILE:HD11	13:M:66:LEU:HD21	1.73	0.69
1:A:1338:G:H2'	1:A:1339:A:C8	2.27	0.69
3:C:134:ILE:HD11	3:C:153:VAL:HG23	1.73	0.69
7:G:75:VAL:HA	7:G:88:PRO:HA	1.74	0.69
1:A:1148:U:H5"	9:I:7:THR:HG23	1.74	0.69
1:A:1412:C:H2'	1:A:1413:A:C8	2.27	0.69
17:Q:97:SER:HB2	17:Q:98:LEU:HD23	1.74	0.69
1:A:384:G:H2'	1:A:385:C:H6	1.56	0.69
1:A:579:G:H4'	15:O:54:ARG:HH21	1.58	0.69
11:K:27:ASN:OD1	11:K:28:THR:N	2.25	0.69
2:B:73:THR:HG21	2:B:96:ARG:HD2	1.74	0.69
1:A:328:C:H2'	1:A:328:C:O2	1.91	0.69
2:B:82:ARG:NH1	2:B:92:TYR:OH	2.26	0.69
9:I:17:VAL:HG22	9:I:63:ILE:HG23	1.74	0.69
5:E:137:GLU:O	5:E:141:GLN:HG3	1.93	0.69
21:U:18:TYR:CD2	21:U:24:ARG:HG2	2.28	0.69
1:A:914:A:OP1	22:A:1601:SRY:HI33	1.93	0.68
15:O:39:LEU:HD12	15:O:56:LEU:HD13	1.75	0.68
20:T:46:GLU:OE1	20:T:48:LYS:NZ	2.27	0.68
1:A:258:G:H2'	1:A:259:G:H8	1.59	0.68
1:A:933:G:OP2	7:G:3:ARG:HB3	1.92	0.68
12:L:24:VAL:HG13	12:L:98:TYR:CE2	2.27	0.68
2:B:178:ARG:HD3	2:B:196:LEU:HD23	1.74	0.68
1:A:973:G:H3'	1:A:974:A:H5"	1.76	0.68
1:A:1168:A:H2'	1:A:1169:A:C8	2.29	0.68
1:A:501:C:H2'	1:A:502:G:H8	1.57	0.68
9:I:79:LEU:HD13	9:I:83:ARG:HG3	1.73	0.68
1:A:768:A:N6	25:A:2194:HOH:O	2.26	0.67
7:G:21:VAL:HG23	7:G:22:LEU:HD23	1.76	0.67
9:I:10:ARG:NH1	9:I:105:ASP:OD1	2.27	0.67
9:I:114:TYR:CD1	10:J:60:ARG:HB2	2.24	0.67
8:H:41:ARG:NH2	8:H:123:GLU:OE2	2.27	0.67
3:C:167:TRP:HE3	3:C:168:ALA:H	1.41	0.67
1:A:1356:G:H2'	1:A:1357:A:C8	2.28	0.67
1:A:1376:U:OP1	7:G:98:SER:OG	2.07	0.67
1:A:1316:G:N2	1:A:1319:A:OP2	2.27	0.67
8:H:84:ARG:HG3	8:H:84:ARG:HH11	1.59	0.67
10:J:49:VAL:HG12	10:J:50:ILE:O	1.95	0.67
6:F:3:ARG:HG3	6:F:66:GLU:HG3	1.77	0.67
1:A:1241:G:H2'	1:A:1242:C:H6	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:1601:SRY:H41	12:L:47:LYS:HD3	1.77	0.67
12:L:24:VAL:HG13	12:L:98:TYR:HE2	1.59	0.67
16:P:21:VAL:HG12	16:P:33:ILE:HD12	1.77	0.67
1:A:1203:C:OP1	14:N:2:ALA:N	2.28	0.67
1:A:1321:C:H42	19:S:37:ARG:HH12	1.43	0.67
1:A:928:G:O2'	1:A:1533:C:OP1	2.14	0.66
10:J:82:ILE:HA	10:J:85:LEU:HB2	1.75	0.66
14:N:37:PHE:HD1	14:N:44:LEU:HD11	1.59	0.66
16:P:52:ASP:OD2	16:P:55:ARG:HB2	1.95	0.66
3:C:77:ILE:HG22	3:C:81:GLY:HA2	1.78	0.66
18:R:46:GLU:OE1	18:R:46:GLU:N	2.26	0.66
13:M:37:THR:HG21	13:M:56:LEU:HA	1.76	0.66
15:O:36:ILE:HG13	15:O:59:MET:HE2	1.77	0.66
1:A:1392:G:H21	1:A:1502:A:H8	1.43	0.66
10:J:27:ALA:HB2	10:J:85:LEU:HD11	1.76	0.66
1:A:1366:C:H2'	1:A:1367:C:C6	2.30	0.66
1:A:1163:C:H2'	1:A:1164:G:C8	2.30	0.66
11:K:48:ILE:HD11	11:K:67:ASP:HB2	1.78	0.66
12:L:39:VAL:HB	12:L:57:LYS:HB2	1.78	0.66
1:A:1095:U:OP1	1:A:1108:G:N2	2.27	0.66
13:M:16:ASP:OD1	13:M:16:ASP:N	2.26	0.66
1:A:1347:G:N2	1:A:1373:G:H2'	2.11	0.65
5:E:71:LEU:HD21	5:E:115:VAL:HG22	1.77	0.65
6:F:10:LEU:HB2	6:F:59:TYR:HB3	1.78	0.65
6:F:43:LEU:HD21	18:R:35:ARG:HH22	1.60	0.65
1:A:1035:A:H2'	1:A:1036:G:C8	2.31	0.65
1:A:17:U:H2'	1:A:18:C:C6	2.32	0.65
1:A:411:A:N7	1:A:413:G:H1'	2.11	0.65
1:A:372:C:H4'	1:A:373:A:O5'	1.95	0.65
1:A:95:U:H2'	1:A:96:G:H8	1.62	0.65
1:A:1026:G:N7	1:A:1027:C:N4	2.44	0.65
2:B:96:ARG:NH1	2:B:97:TRP:H	1.95	0.65
1:A:612:C:O2	1:A:628:G:N2	2.23	0.65
10:J:26:ALA:O	10:J:84:GLN:NE2	2.27	0.65
2:B:240:GLN:N	2:B:240:GLN:OE1	2.30	0.65
1:A:895:G:H2'	1:A:896:C:H6	1.62	0.65
1:A:953:G:H5'	1:A:965:A:H61	1.60	0.65
1:A:1236:A:H4'	1:A:1304:G:H4'	1.78	0.64
1:A:390:C:H4'	16:P:28:ARG:HH21	1.62	0.64
1:A:1006:C:H42	1:A:1022:G:N2	1.95	0.64
4:D:55:ALA:O	4:D:59:ARG:HG2	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1279:A:OP1	10:J:7:LYS:NZ	2.28	0.64
15:O:25:THR:HG21	15:O:70:LEU:HB2	1.79	0.64
1:A:95:U:H2'	1:A:96:G:C8	2.33	0.64
1:A:384:G:H2'	1:A:385:C:C6	2.32	0.64
1:A:686:U:O2'	1:A:687:A:H8	1.80	0.64
1:A:1022:G:N2	1:A:1023:G:O6	2.29	0.64
1:A:1334:G:O5'	1:A:1334:G:H8	1.79	0.64
1:A:78:G:O6	1:A:91:C:N4	2.30	0.64
1:A:1238:A:H5'	1:A:1336:C:H41	1.60	0.64
1:A:503:C:OP2	12:L:116:SER:HB3	1.98	0.64
1:A:958:A:N6	19:S:77:THR:O	2.31	0.64
1:A:992:U:H3	1:A:1044:A:H62	1.44	0.64
10:J:50:ILE:HD13	14:N:41:ARG:HH11	1.62	0.64
1:A:967:5MC:C4'	9:I:128:ARG:HG3	2.27	0.64
10:J:7:LYS:HD3	10:J:9:ARG:HE	1.63	0.64
1:A:241:C:H42	1:A:285:G:H1	1.43	0.63
14:N:53:LEU:HD12	14:N:56:VAL:HG21	1.79	0.63
1:A:1350:A:OP2	9:I:118:LYS:NZ	2.22	0.63
1:A:1518:MA6:H93	1:A:1519:MA6:N1	2.13	0.63
16:P:67:THR:HB	16:P:70:ALA:H	1.63	0.63
1:A:1320:C:H1'	19:S:73:GLU:HG2	1.80	0.63
1:A:1436:U:H2'	1:A:1437:C:H6	1.63	0.63
2:B:129:GLU:HG2	2:B:130:ARG:HG2	1.80	0.63
1:A:1035:A:H2'	1:A:1036:G:H8	1.63	0.63
1:A:1407:5MC:H2'	1:A:1408:A:C5'	2.29	0.63
9:I:112:LYS:HE3	9:I:117:HIS:O	1.99	0.63
5:E:101:ILE:O	5:E:120:THR:HB	1.97	0.63
2:B:200:ILE:O	2:B:200:ILE:HG13	1.97	0.63
1:A:1141:C:H2'	1:A:1142:G:C8	2.33	0.63
5:E:15:ARG:HD3	5:E:28:PHE:CE2	2.33	0.63
7:G:26:PHE:CD1	7:G:101:LEU:HD22	2.33	0.63
1:A:62:U:O2'	1:A:379:C:O2	2.16	0.63
4:D:8:VAL:HG11	4:D:21:LEU:HB2	1.81	0.63
9:I:111:ARG:HH12	9:I:113:LYS:HA	1.63	0.63
10:J:45:ARG:HD3	14:N:36:PHE:HE2	1.62	0.63
1:A:518:C:H2'	1:A:530:G:C8	2.34	0.63
1:A:880:C:OP1	12:L:8:ASN:ND2	2.26	0.63
2:B:96:ARG:HH11	2:B:97:TRP:H	1.45	0.63
16:P:4:ILE:HG12	16:P:21:VAL:HG22	1.81	0.62
1:A:1181:G:O2'	1:A:1182:G:O5'	2.17	0.62
4:D:119:GLN:HG3	4:D:123:HIS:HD2	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:121:ARG:NH1	9:I:122:ALA:O	2.32	0.62
9:I:29:ASN:O	9:I:29:ASN:ND2	2.32	0.62
13:M:64:TRP:HE3	13:M:66:LEU:HD11	1.65	0.62
11:K:90:GLY:HA2	11:K:93:GLN:HB2	1.82	0.62
9:I:97:LYS:O	9:I:100:GLY:N	2.28	0.62
1:A:421:U:H5"	1:A:422:C:H5	1.64	0.62
1:A:1436:U:H2'	1:A:1437:C:C6	2.35	0.62
3:C:155:GLY:HA2	3:C:164:ARG:O	2.00	0.62
1:A:1126:U:O4	1:A:1149:C:H1'	1.99	0.62
2:B:115:LEU:HD13	2:B:145:LEU:HB2	1.80	0.62
12:L:124:LYS:HD2	12:L:125:PRO:HD2	1.82	0.62
1:A:177:C:H2'	1:A:178:C:C6	2.34	0.62
5:E:8:GLU:HG2	5:E:34:VAL:HG22	1.80	0.62
6:F:4:TYR:CD1	6:F:92:LYS:HA	2.34	0.62
12:L:27:LEU:C	12:L:29:GLY:H	2.01	0.62
14:N:27:CYS:SG	14:N:29:ARG:HB2	2.39	0.62
20:T:100:ILE:HB	20:T:102:GLY:H	1.65	0.62
1:A:1054:C:H3'	1:A:1054:C:H6	1.63	0.61
1:A:1160:G:H1	1:A:1177:G:N2	1.98	0.61
2:B:147:LYS:HD2	2:B:148:TYR:CE2	2.35	0.61
9:I:8:GLY:HA2	9:I:79:LEU:HD12	1.81	0.61
9:I:42:ARG:HH21	9:I:71:SER:HB2	1.65	0.61
13:M:108:ARG:HD3	13:M:114:ARG:HH21	1.64	0.61
3:C:19:GLU:O	3:C:56:ASP:HA	1.99	0.61
1:A:532:A:N6	3:C:158:GLY:O	2.33	0.61
1:A:1049:U:H4'	1:A:1050:G:O5'	1.99	0.61
9:I:111:ARG:NH1	9:I:112:LYS:O	2.33	0.61
1:A:932:C:H5'	7:G:4:ARG:HG2	1.82	0.61
1:A:1139:G:O2'	1:A:1140:C:OP2	2.14	0.61
1:A:1255:G:C6	1:A:1279:A:N7	2.68	0.61
3:C:6:HIS:CD2	3:C:8:ILE:HB	2.36	0.61
1:A:1195:C:H3'	1:A:1196:U:H5"	1.81	0.61
1:A:1309:G:H1'	13:M:74:VAL:HG22	1.83	0.61
1:A:35:G:H2'	1:A:36:C:C6	2.36	0.61
1:A:790:A:C8	1:A:791:G:N7	2.69	0.61
1:A:1442:G:N7	1:A:1446:A:N6	2.49	0.61
1:A:1532:U:H2'	1:A:1533:C:H3'	1.83	0.61
4:D:15:GLU:OE1	4:D:59:ARG:NH2	2.34	0.61
5:E:17:ALA:HB2	5:E:26:PHE:CD2	2.35	0.61
13:M:4:ILE:HD12	13:M:56:LEU:HD22	1.83	0.61
1:A:258:G:H2'	1:A:259:G:C8	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:579:G:H5'	1:A:728:A:H1'	1.82	0.61
2:B:197:VAL:HB	2:B:200:ILE:HG22	1.83	0.61
6:F:22:GLU:HA	6:F:25:ILE:HD12	1.81	0.61
9:I:108:VAL:HG12	9:I:109:VAL:H	1.66	0.61
15:O:87:ILE:HG22	15:O:88:ARG:H	1.65	0.61
1:A:1189:C:H4'	3:C:10:PHE:CE1	2.36	0.61
1:A:922:G:H8	1:A:922:G:H5"	1.66	0.60
1:A:1118:C:H5'	9:I:104:ARG:HG3	1.83	0.60
3:C:150:LYS:HB3	3:C:201:TYR:HB2	1.83	0.60
5:E:122:GLU:OE1	5:E:131:ILE:HG13	2.01	0.60
7:G:40:ALA:HB3	9:I:41:VAL:HG21	1.82	0.60
4:D:36:ARG:HA	4:D:38:TYR:CE2	2.35	0.60
4:D:176:LEU:HD21	4:D:178:VAL:HB	1.81	0.60
17:Q:64:PRO:HB3	17:Q:70:ARG:NE	2.16	0.60
20:T:50:GLU:H	20:T:99:LEU:HD13	1.66	0.60
1:A:427:U:OP2	4:D:36:ARG:NH2	2.35	0.60
1:A:1150:U:H2'	1:A:1151:A:H5'	1.83	0.60
1:A:631:G:H2'	1:A:632:A:C8	2.36	0.60
1:A:1279:A:OP2	10:J:9:ARG:NH2	2.30	0.60
7:G:115:ARG:HB2	7:G:118:VAL:HG23	1.82	0.60
1:A:324:G:H8	1:A:324:G:H5"	1.66	0.60
1:A:1089:G:H1	1:A:1096:C:N4	1.98	0.60
6:F:28:ARG:NH1	6:F:28:ARG:HB2	2.16	0.60
7:G:5:ARG:HG2	7:G:6:ARG:H	1.67	0.60
3:C:156:ARG:HB3	3:C:196:LEU:HD21	1.82	0.60
5:E:11:ILE:HB	5:E:31:LEU:HB3	1.84	0.60
8:H:82:HIS:ND1	8:H:138:TRP:NE1	2.40	0.60
1:A:539:A:H2'	1:A:540:G:C8	2.35	0.60
1:A:992:U:O2'	1:A:993:G:OP2	2.15	0.60
1:A:1241:G:H2'	1:A:1242:C:C6	2.37	0.60
3:C:35:GLU:OE2	3:C:59:ARG:NH2	2.34	0.60
13:M:40:ASN:HD22	13:M:43:THR:HG23	1.67	0.60
22:A:1601:SRY:O21	22:A:1601:SRY:NE1	2.35	0.60
6:F:91:VAL:HG11	18:R:72:ARG:HH12	1.67	0.60
1:A:1147:C:HO2'	9:I:5:TYR:HH	1.49	0.60
18:R:59:SER:H	18:R:62:GLU:HB2	1.67	0.59
1:A:1184:G:H2'	1:A:1185:G:H8	1.66	0.59
1:A:1497:G:H2'	1:A:1498:UR3:H5'	1.83	0.59
1:A:922:G:C6	1:A:923:A:C6	2.91	0.59
1:A:1407:5MC:C2'	1:A:1408:A:H5'	2.32	0.59
5:E:90:VAL:C	5:E:91:LEU:HD23	2.22	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:152:ARG:NH2	8:H:107:LEU:O	2.32	0.59
17:Q:40:LYS:HE3	17:Q:42:TYR:CZ	2.36	0.59
1:A:1009:G:N2	1:A:1020:U:O2	2.30	0.59
1:A:1133:G:N2	1:A:1141:C:N3	2.43	0.59
5:E:80:ILE:HA	8:H:104:ARG:NH2	2.17	0.59
12:L:113:ARG:HH12	12:L:116:SER:H	1.50	0.59
2:B:178:ARG:HH21	8:H:74:PRO:HB3	1.67	0.59
21:U:10:ARG:O	21:U:13:ILE:HG22	2.03	0.59
2:B:186:ALA:HB3	2:B:197:VAL:HG11	1.85	0.59
5:E:15:ARG:HH11	5:E:15:ARG:HB3	1.67	0.59
19:S:31:ILE:HG22	19:S:49:ILE:HA	1.85	0.59
20:T:10:LEU:HD13	20:T:12:ALA:H	1.67	0.59
1:A:345:C:OP2	1:A:345:C:H6	1.85	0.59
1:A:730:G:C5	1:A:731:G:H1'	2.37	0.59
1:A:184:G:H2'	1:A:185:A:H8	1.68	0.59
2:B:17:PHE:HA	2:B:44:LEU:HD11	1.84	0.59
12:L:46:LYS:HG2	12:L:47:LYS:H	1.68	0.59
17:Q:26:GLN:HE21	17:Q:37:LYS:HE2	1.68	0.59
1:A:250:A:H4'	1:A:251:G:O5'	2.01	0.59
3:C:34:LEU:HD13	3:C:38:ARG:HH21	1.68	0.59
17:Q:4:LYS:HG2	17:Q:6:LEU:HD21	1.84	0.59
1:A:413:G:O6	4:D:36:ARG:NE	2.36	0.59
1:A:1020:U:H2'	1:A:1021:G:H8	1.68	0.59
6:F:2:ARG:HE	6:F:69:GLU:HG2	1.67	0.59
12:L:97:ARG:HB2	12:L:98:TYR:CE1	2.38	0.59
2:B:107:THR:O	2:B:110:GLN:HG3	2.03	0.58
3:C:152:ILE:HB	3:C:199:LYS:HB2	1.84	0.58
9:I:33:PHE:HE2	9:I:43:ALA:HB1	1.68	0.58
9:I:75:ASP:OD1	9:I:78:LYS:NZ	2.30	0.58
20:T:39:LYS:HB3	20:T:55:ILE:HG21	1.85	0.58
1:A:617:G:H1	1:A:623:C:H42	1.50	0.58
1:A:1197:G:H5"	25:A:2043:HOH:O	2.02	0.58
1:A:35:G:H2'	1:A:36:C:H6	1.66	0.58
1:A:835:U:OP1	18:R:64:ARG:NH2	2.36	0.58
2:B:9:GLU:HG2	2:B:10:LEU:H	1.67	0.58
2:B:16:HIS:NE2	2:B:204:ASN:N	2.49	0.58
17:Q:27:PHE:CE1	17:Q:36:ILE:HD11	2.39	0.58
1:A:833:U:H2'	1:A:834:C:C6	2.38	0.58
1:A:1355:G:H2'	1:A:1356:G:C8	2.38	0.58
1:A:90:U:H2'	1:A:91:C:C6	2.39	0.58
17:Q:29:HIS:CG	17:Q:30:PRO:HD2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:G:H1'	1:A:354:G:H5'	1.86	0.58
1:A:1125:U:H3	10:J:5:ARG:HH21	1.52	0.58
1:A:1366:C:H2'	1:A:1367:C:H6	1.67	0.58
9:I:46:ALA:HB2	9:I:74:ILE:HG23	1.86	0.58
12:L:82:VAL:HG23	12:L:106:ASP:OD1	2.04	0.58
1:A:619:U:N3	4:D:134:ASP:OD1	2.28	0.58
3:C:155:GLY:HA3	3:C:163:ALA:HB1	1.85	0.58
11:K:84:VAL:HG11	11:K:91:ARG:HD2	1.85	0.58
1:A:174:C:H2'	1:A:175:C:C6	2.39	0.58
1:A:989:C:O2	1:A:1216:G:N2	2.36	0.58
1:A:1030(D):A:C5	1:A:1031:G:H1'	2.39	0.58
4:D:65:ARG:HG3	4:D:70:ILE:HG22	1.85	0.58
3:C:88:ARG:HE	3:C:101:LEU:HB2	1.69	0.58
16:P:74:LEU:HD22	16:P:79:VAL:HG21	1.86	0.58
1:A:1291:G:OP1	7:G:37:ASN:ND2	2.37	0.57
8:H:109:ILE:O	8:H:109:ILE:HG13	2.03	0.57
10:J:74:ILE:O	10:J:77:PRO:HD3	2.04	0.57
18:R:26:LEU:HD12	18:R:27:GLY:H	1.68	0.57
1:A:184:G:H2'	1:A:185:A:C8	2.39	0.57
1:A:922:G:H4'	5:E:20:GLN:HA	1.85	0.57
1:A:975:A:H4'	1:A:976:G:O5'	2.03	0.57
2:B:16:HIS:CE1	2:B:210:SER:HB2	2.39	0.57
13:M:14:ARG:HG3	13:M:44:ARG:HH21	1.69	0.57
1:A:1027:C:H2'	1:A:1028:C:C6	2.39	0.57
1:A:1162:C:H42	1:A:1174:G:H1	1.52	0.57
2:B:54:THR:O	2:B:58:ILE:HG12	2.04	0.57
3:C:5:ILE:HD13	3:C:10:PHE:HB2	1.86	0.57
5:E:51:VAL:HB	5:E:52:PRO:HD3	1.86	0.57
7:G:91:VAL:HG12	7:G:92:SER:H	1.70	0.57
8:H:53:VAL:HB	8:H:58:TYR:HD1	1.68	0.57
12:L:27:LEU:C	12:L:29:GLY:N	2.58	0.57
15:O:42:HIS:CD2	15:O:43:LEU:HD23	2.40	0.57
1:A:1357:A:H2'	1:A:1358:U:C6	2.39	0.57
1:A:1378:C:H5"	1:A:1379:G:OP2	2.04	0.57
5:E:105:VAL:HG11	5:E:131:ILE:HG22	1.87	0.57
8:H:10:LEU:HD22	8:H:83:ILE:HG23	1.87	0.57
9:I:111:ARG:HG3	14:N:61:TRP:NE1	2.19	0.57
20:T:50:GLU:HB2	20:T:99:LEU:HD22	1.86	0.57
1:A:9:G:OP1	5:E:122:GLU:HG3	2.05	0.57
6:F:11:ASN:HB2	6:F:86:ARG:NE	2.20	0.57
8:H:83:ILE:HD13	8:H:137:VAL:HG22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:155:GLY:HA2	3:C:164:ARG:H	1.70	0.57
19:S:19:VAL:HG11	19:S:44:MET:HG2	1.87	0.57
1:A:269:C:H2'	1:A:270:A:C8	2.40	0.57
1:A:1243:C:OP1	21:U:10:ARG:HD2	2.04	0.57
1:A:113:G:H2'	1:A:114:U:C6	2.39	0.57
3:C:54:ARG:HB3	3:C:69:HIS:HB2	1.86	0.57
6:F:2:ARG:HG3	6:F:69:GLU:HG2	1.85	0.56
7:G:115:ARG:H	7:G:115:ARG:HD3	1.70	0.56
1:A:1053:G:H4'	1:A:1054:C:H5'	1.86	0.56
1:A:1190:G:OP1	3:C:4:LYS:HA	2.05	0.56
1:A:1505:G:C8	1:A:1505:G:H3'	2.40	0.56
2:B:23:ARG:O	2:B:24:TRP:CD1	2.57	0.56
2:B:158:LEU:HD12	2:B:158:LEU:H	1.70	0.56
4:D:119:GLN:HG3	4:D:123:HIS:CD2	2.39	0.56
1:A:1130:A:O2'	9:I:3:GLN:NE2	2.30	0.56
1:A:1148:U:H2'	1:A:1149:C:O4'	2.06	0.56
2:B:23:ARG:NH1	2:B:23:ARG:HB2	2.20	0.56
2:B:181:PHE:CD2	8:H:70:GLN:HB3	2.40	0.56
3:C:195:VAL:O	3:C:196:LEU:HD23	2.06	0.56
5:E:15:ARG:HD3	5:E:28:PHE:HE2	1.70	0.56
7:G:108:ALA:HB2	7:G:123:GLU:HG2	1.88	0.56
1:A:174:C:H2'	1:A:175:C:H6	1.71	0.56
1:A:381:C:H2'	1:A:382:A:O4'	2.05	0.56
1:A:895:G:H2'	1:A:896:C:C6	2.39	0.56
1:A:1285:A:H4'	1:A:1286:A:O5'	2.06	0.56
3:C:21:ARG:HH21	10:J:92:THR:HG21	1.71	0.56
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.87	0.56
15:O:79:ARG:O	15:O:83:GLU:HG2	2.04	0.56
1:A:789:U:N3	1:A:792:A:OP2	2.38	0.56
1:A:1006:C:H42	1:A:1022:G:H22	1.52	0.56
2:B:89:GLY:H	2:B:226:ARG:HH22	1.53	0.56
2:B:97:TRP:CH2	2:B:101:MET:HB2	2.40	0.56
8:H:21:LYS:O	8:H:65:TYR:OH	2.11	0.56
17:Q:64:PRO:HB3	17:Q:70:ARG:HE	1.70	0.56
1:A:447:G:H2'	1:A:485:G:N2	2.20	0.56
1:A:980:C:H5'	1:A:981:U:OP2	2.06	0.56
1:A:1531:A:O5'	1:A:1531:A:H8	1.88	0.56
12:L:67:THR:HB	12:L:96:VAL:HG13	1.88	0.56
1:A:580:U:H2'	1:A:581:G:O4'	2.06	0.56
1:A:677:U:H3	1:A:713:G:H22	1.54	0.56
1:A:1356:G:H2'	1:A:1357:A:H8	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:91:VAL:HG12	7:G:95:ARG:HB3	1.88	0.56
1:A:103:C:OP1	20:T:17:ARG:NH1	2.38	0.56
1:A:1497:G:O6	1:A:1498:UR3:H3U2	2.06	0.56
3:C:14:ILE:O	3:C:16:ARG:N	2.38	0.56
1:A:1289:A:H5"	1:A:1290:G:OP2	2.06	0.56
3:C:48:TYR:HA	3:C:52:LEU:HD22	1.88	0.56
10:J:32:ALA:O	10:J:34:VAL:HG23	2.05	0.56
10:J:57:LYS:HB2	10:J:60:ARG:NH2	2.20	0.56
1:A:1126:U:OP1	1:A:1127:G:N2	2.39	0.56
2:B:84:GLU:OE2	2:B:235:SER:OG	2.20	0.56
4:D:61:LYS:HD3	4:D:206:PHE:CE2	2.40	0.56
8:H:91:ARG:NH1	17:Q:33:GLY:HA3	2.21	0.56
11:K:101:SER:OG	11:K:102:GLY:N	2.38	0.56
20:T:67:ALA:O	20:T:73:HIS:ND1	2.38	0.56
21:U:6:ARG:O	21:U:12:LYS:HD3	2.06	0.56
1:A:83:U:O2'	1:A:84:U:H5'	2.06	0.55
4:D:78:LEU:HD21	4:D:96:LEU:HB3	1.89	0.55
1:A:1316:G:H22	1:A:1319:A:H5'	1.72	0.55
12:L:32:PHE:HB3	12:L:84:LEU:HD11	1.87	0.55
1:A:1121:U:H2'	1:A:1122:U:C6	2.40	0.55
1:A:1323:G:OP2	19:S:3:ARG:NH1	2.39	0.55
10:J:44:VAL:HG13	10:J:66:ARG:HG2	1.87	0.55
20:T:14:LYS:O	20:T:18:GLN:HG3	2.07	0.55
1:A:411:A:C5	1:A:413:G:H1'	2.41	0.55
1:A:838:G:O6	1:A:848:C:N4	2.34	0.55
3:C:157:ILE:HG21	3:C:164:ARG:HH12	1.70	0.55
1:A:731:G:OP1	1:A:766:A:H1'	2.06	0.55
1:A:1057:G:H5"	3:C:154:SER:HB2	1.89	0.55
1:A:1337:G:H5"	1:A:1338:G:OP1	2.06	0.55
21:U:5:ASP:HB3	21:U:8:THR:OG1	2.06	0.55
1:A:1275:A:H2'	1:A:1276:G:O4'	2.07	0.55
4:D:127:THR:HG23	4:D:130:GLY:H	1.72	0.55
6:F:60:PHE:CE2	18:R:78:LEU:HD21	2.41	0.55
17:Q:5:VAL:HG22	17:Q:60:ILE:HG12	1.89	0.55
1:A:320:C:O2'	1:A:1435:G:H1'	2.06	0.55
1:A:526:C:O3'	22:A:1601:SRY:HI31	2.06	0.55
1:A:547:A:OP2	4:D:2:GLY:N	2.40	0.55
3:C:27:LYS:HA	3:C:30:ARG:HH12	1.71	0.55
15:O:15:PHE:CD2	15:O:30:ALA:HB2	2.41	0.55
1:A:757:U:H2'	1:A:758:G:O4'	2.05	0.55
1:A:1237:C:H4'	1:A:1300:G:N2	2.18	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1392:G:N2	1:A:1502:A:H8	2.05	0.55
8:H:113:SER:HB2	8:H:134:ILE:HD11	1.89	0.55
16:P:68:ASP:OD1	16:P:68:ASP:N	2.38	0.55
21:U:2:GLY:N	25:U:101:HOH:O	2.40	0.55
1:A:1053:G:HO2'	1:A:1199:U:H5	1.54	0.55
11:K:92:GLU:HA	11:K:95:ILE:HG13	1.89	0.55
1:A:186:C:H2'	1:A:187:C:C6	2.42	0.55
1:A:818:G:C3'	1:A:819:A:H5"	2.37	0.55
17:Q:62:SER:OG	17:Q:72:ARG:HG3	2.07	0.55
1:A:1305:G:O2'	1:A:1306:A:H8	1.90	0.54
1:A:1305:G:O2'	1:A:1306:A:O5'	2.24	0.54
1:A:646:U:H2'	1:A:647:C:C6	2.42	0.54
1:A:1005:A:C4	1:A:1026:G:N2	2.75	0.54
2:B:163:PHE:HD2	2:B:164:VAL:N	2.06	0.54
6:F:11:ASN:HD21	6:F:13:ASN:ND2	2.06	0.54
1:A:715:A:H2'	1:A:716:A:C8	2.41	0.54
1:A:988:G:C2	1:A:989:C:H1'	2.42	0.54
1:A:1359:C:O2'	1:A:1361:G:N7	2.40	0.54
1:A:1305:G:C8	1:A:1305:G:OP2	2.60	0.54
1:A:1305:G:HO2'	1:A:1306:A:H8	1.54	0.54
16:P:21:VAL:HG21	16:P:59:TRP:CD1	2.42	0.54
1:A:129:U:O3'	1:A:129(A):G:H3'	2.07	0.54
1:A:1195:C:H3'	1:A:1196:U:C5'	2.38	0.54
3:C:167:TRP:HE3	3:C:168:ALA:N	2.06	0.54
4:D:70:ILE:HG23	4:D:71:SER:N	2.21	0.54
4:D:187:ARG:NH2	4:D:188:LEU:HB2	2.22	0.54
4:D:187:ARG:NE	4:D:188:LEU:H	2.05	0.54
1:A:565:U:H3'	1:A:566:G:H2'	1.89	0.54
1:A:951:G:OP2	13:M:102:ARG:NH2	2.40	0.54
5:E:84:PHE:HB2	5:E:134:ALA:HB2	1.89	0.54
12:L:60:LEU:HB2	12:L:64:TYR:O	2.08	0.54
16:P:51:VAL:O	16:P:52:ASP:HB3	2.08	0.54
18:R:87:ARG:HH11	18:R:87:ARG:HB2	1.71	0.54
1:A:522:C:H42	1:A:527:7MG:HN1	1.56	0.54
1:A:1323:G:H2'	1:A:1324:A:C8	2.43	0.54
1:A:1342:C:O2'	9:I:124:GLN:HB2	2.08	0.54
12:L:38:THR:HG22	12:L:39:VAL:HG23	1.89	0.54
20:T:81:LYS:O	20:T:85:MET:HG3	2.08	0.54
1:A:574:A:N3	1:A:883:C:H1'	2.22	0.53
1:A:953:G:C6	1:A:954:G:C4	2.96	0.53
1:A:1174:G:H2'	1:A:1175:G:H8	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1392:G:C5	1:A:1393:U:C5	2.96	0.53
2:B:219:VAL:O	2:B:223:ILE:HG12	2.08	0.53
7:G:107:ALA:O	7:G:110:GLN:HB2	2.08	0.53
21:U:5:ASP:O	21:U:8:THR:OG1	2.26	0.53
1:A:1328:C:H2'	1:A:1329:A:H8	1.73	0.53
12:L:47:LYS:HG3	12:L:48:PRO:HD3	1.89	0.53
1:A:1181:G:C2	1:A:1182:G:N2	2.77	0.53
2:B:76:GLN:HG3	2:B:206:ASP:OD1	2.08	0.53
3:C:137:ALA:HA	3:C:140:ARG:CZ	2.39	0.53
4:D:7:PRO:HG2	4:D:10:ARG:HD2	1.90	0.53
5:E:13:ILE:HG21	5:E:51:VAL:HG13	1.91	0.53
10:J:7:LYS:HD3	10:J:9:ARG:HH21	1.73	0.53
1:A:1502:A:H2	1:A:1505:G:H1	1.56	0.53
6:F:42:GLU:HG2	6:F:61:LEU:HB3	1.91	0.53
7:G:26:PHE:HD1	7:G:101:LEU:HD22	1.73	0.53
1:A:299:G:H2'	1:A:300:A:C8	2.44	0.53
5:E:76:ILE:HB	5:E:77:PRO:HD2	1.91	0.53
7:G:120:ILE:HD12	7:G:120:ILE:H	1.74	0.53
10:J:57:LYS:HE2	10:J:60:ARG:HH22	1.74	0.53
1:A:481:G:O2'	1:A:482:A:H8	1.91	0.53
1:A:527:7MG:O2'	1:A:535:A:N1	2.38	0.53
9:I:4:TYR:CD1	9:I:88:TYR:HB2	2.44	0.53
1:A:115:G:O2'	1:A:116:A:OP2	2.10	0.53
1:A:177:C:OP1	20:T:65:LYS:NZ	2.27	0.53
4:D:68:TYR:CD1	4:D:97:LEU:HD22	2.44	0.53
6:F:67:MET:SD	6:F:72:VAL:HG22	2.48	0.53
16:P:22:THR:HA	16:P:33:ILE:HG13	1.91	0.53
1:A:644:G:C5	1:A:645:C:C5	2.96	0.53
1:A:1005:A:H1'	1:A:1026:G:H22	1.74	0.53
1:A:1305:G:O2'	1:A:1306:A:P	2.67	0.53
7:G:102:ARG:HG2	7:G:106:GLN:OE1	2.09	0.53
10:J:25:GLU:HA	10:J:28:ARG:HB2	1.91	0.53
11:K:58:PRO:HA	11:K:90:GLY:HA3	1.91	0.53
14:N:25:VAL:HG12	14:N:38:GLY:O	2.09	0.53
1:A:927:G:H4'	1:A:1503:A:N7	2.24	0.53
3:C:24:ALA:HB2	3:C:32:LEU:HD12	1.91	0.53
10:J:36:GLY:N	10:J:73:ASP:O	2.34	0.53
13:M:49:THR:HB	13:M:52:GLU:HB2	1.90	0.53
2:B:118:LEU:HB3	2:B:142:LEU:HG	1.91	0.53
4:D:70:ILE:HG21	4:D:75:PHE:HD1	1.73	0.53
11:K:15:ALA:HA	11:K:77:MET:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1489:G:H2'	1:A:1490:C:H6	1.73	0.52
2:B:181:PHE:HD2	8:H:70:GLN:HB3	1.73	0.52
2:B:194:PRO:O	2:B:197:VAL:HG23	2.09	0.52
5:E:43:LEU:HD23	5:E:43:LEU:O	2.09	0.52
5:E:129:ILE:HG22	5:E:130:ASN:N	2.24	0.52
6:F:19:LEU:HG	6:F:23:LYS:HE3	1.91	0.52
1:A:1306:A:C2	1:A:1307:U:H1'	2.45	0.52
1:A:98:U:H2'	1:A:99:C:C6	2.45	0.52
1:A:372:C:H1'	1:A:373:A:OP2	2.09	0.52
1:A:1067:A:H4'	1:A:1068:G:OP1	2.09	0.52
4:D:141:ARG:HB2	4:D:141:ARG:CZ	2.38	0.52
8:H:53:VAL:HB	8:H:58:TYR:CD1	2.44	0.52
1:A:106:C:O2	1:A:379:C:H4'	2.09	0.52
1:A:1243:C:H2'	1:A:1244:C:C6	2.43	0.52
12:L:82:VAL:O	12:L:106:ASP:HB2	2.10	0.52
1:A:697:U:H5"	1:A:698:G:OP2	2.09	0.52
1:A:923:A:OP1	5:E:21:ALA:HB2	2.10	0.52
2:B:16:HIS:CD2	2:B:204:ASN:H	2.28	0.52
1:A:359:U:H2'	1:A:360:A:C8	2.45	0.52
1:A:539:A:H2'	1:A:540:G:H8	1.75	0.52
1:A:620:C:N1	4:D:135:LEU:HD13	2.25	0.52
1:A:747:C:H2'	1:A:748:C:H5'	1.92	0.52
1:A:766:A:C8	1:A:814:A:N6	2.78	0.52
1:A:1281:U:H5"	25:A:2110:HOH:O	2.09	0.52
1:A:279:A:C4	17:Q:98:LEU:HD12	2.45	0.52
1:A:1126:U:H4'	25:A:2111:HOH:O	2.09	0.52
1:A:1358:U:O2'	1:A:1359:C:OP1	2.25	0.52
1:A:1421:G:H1	1:A:1479:C:H42	1.56	0.52
1:A:691:G:H3'	11:K:26:ASN:HD21	1.74	0.52
1:A:1321:C:H42	19:S:37:ARG:NH1	2.06	0.52
2:B:92:TYR:CD2	2:B:151:GLY:HA3	2.45	0.52
4:D:9:CYS:O	4:D:12:CYS:HB2	2.09	0.52
8:H:111:ILE:HG22	8:H:134:ILE:HD12	1.90	0.52
1:A:33:A:H2'	1:A:34:C:H6	1.74	0.52
1:A:451:A:N6	1:A:481:G:C4	2.78	0.52
1:A:232:G:H1'	1:A:262:A:N1	2.24	0.52
1:A:1138:G:H3'	1:A:1138:G:N3	2.24	0.52
7:G:46:ALA:O	7:G:50:ILE:HG13	2.10	0.52
8:H:4:ASP:CG	8:H:85:ARG:HH21	2.12	0.52
8:H:85:ARG:NH1	8:H:87:SER:O	2.42	0.52
11:K:115:PRO:C	11:K:117:ASN:H	2.13	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:U:H4'	1:A:6:G:O5'	2.09	0.51
1:A:1128:C:O2'	1:A:1130:A:OP2	2.17	0.51
2:B:71:VAL:HG22	2:B:93:VAL:HB	1.91	0.51
4:D:31:CYS:C	4:D:33:MET:H	2.13	0.51
5:E:82:VAL:HG12	5:E:134:ALA:HB1	1.93	0.51
1:A:560:U:H5'	1:A:566:G:N2	2.25	0.51
1:A:562:C:H1'	12:L:15:ARG:HB3	1.92	0.51
1:A:1316:G:H5"	14:N:17:LYS:HE3	1.92	0.51
3:C:125:GLU:HG3	3:C:189:ALA:HB1	1.93	0.51
13:M:60:VAL:HG13	13:M:64:TRP:HZ3	1.74	0.51
1:A:1054:C:H3'	1:A:1054:C:C6	2.45	0.51
1:A:1497:G:C2'	1:A:1498:UR3:H5'	2.40	0.51
2:B:218:ALA:O	2:B:222:ILE:HG13	2.10	0.51
5:E:87:SER:HB3	5:E:131:ILE:HD13	1.91	0.51
9:I:48:GLU:N	9:I:49:PRO:HD2	2.26	0.51
10:J:42:THR:HG21	10:J:66:ARG:HH12	1.75	0.51
1:A:1425:U:H2'	1:A:1426:C:C6	2.46	0.51
1:A:1435:G:H2'	1:A:1436:U:H6	1.74	0.51
3:C:130:VAL:HG21	3:C:157:ILE:HD12	1.92	0.51
5:E:15:ARG:HH11	5:E:15:ARG:CB	2.23	0.51
5:E:47:LYS:O	5:E:57:LYS:HE2	2.08	0.51
8:H:20:TYR:CE1	8:H:76:PRO:HG2	2.46	0.51
17:Q:78:GLU:OE2	17:Q:81:ARG:HD2	2.09	0.51
1:A:279:A:C5	17:Q:98:LEU:HD12	2.45	0.51
1:A:620:C:H2'	1:A:621:A:C8	2.45	0.51
1:A:1141:C:H2'	1:A:1142:G:H8	1.74	0.51
2:B:21:ARG:HA	2:B:39:ILE:HG23	1.90	0.51
4:D:61:LYS:HD2	4:D:207:TYR:OH	2.10	0.51
6:F:3:ARG:O	6:F:93:SER:HB2	2.11	0.51
1:A:1060:C:OP1	14:N:45:ARG:NH2	2.44	0.51
1:A:1225:A:H2'	1:A:1225:A:N3	2.24	0.51
13:M:60:VAL:HG13	13:M:64:TRP:CZ3	2.46	0.51
1:A:1106:G:H5"	3:C:172:ARG:HB3	1.91	0.51
8:H:43:GLY:O	8:H:64:LYS:HE2	2.11	0.51
10:J:9:ARG:HG3	10:J:95:GLU:HB3	1.91	0.51
1:A:551:U:O2'	12:L:86:ARG:HD2	2.10	0.51
1:A:1201:A:H4'	1:A:1202:G:O5'	2.11	0.51
1:A:1510:U:H2'	1:A:1511:G:H8	1.74	0.51
2:B:74:LYS:HD2	2:B:166:ASP:HB2	1.92	0.51
5:E:28:PHE:O	5:E:47:LYS:HA	2.11	0.51
12:L:6:THR:OG1	12:L:9:GLN:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:15:VAL:HB	13:M:34:LEU:HD11	1.92	0.51
19:S:12:ASP:OD2	19:S:35:SER:OG	2.28	0.51
1:A:1149:C:OP2	9:I:9:ARG:NH1	2.43	0.51
1:A:1374:A:H2'	1:A:1375:A:O4'	2.11	0.51
12:L:87:GLY:HA2	12:L:98:TYR:HA	1.93	0.51
18:R:47:THR:HA	18:R:83:GLU:HB2	1.92	0.51
20:T:10:LEU:HD22	20:T:11:SER:H	1.76	0.51
1:A:45:U:H2'	1:A:46:G:C8	2.46	0.51
1:A:254:G:OP1	17:Q:67:LYS:O	2.28	0.51
1:A:277:C:OP1	17:Q:41:LYS:HE3	2.11	0.51
1:A:663:A:H2'	1:A:664:G:O4'	2.11	0.51
1:A:690:G:C6	1:A:691:G:C6	2.99	0.51
13:M:2:ALA:O	13:M:10:PRO:HD2	2.11	0.51
1:A:448:A:C4	1:A:487:A:C2	2.98	0.50
1:A:975:A:H5'	1:A:975:A:H8	1.75	0.50
1:A:1094:G:O2'	1:A:1108:G:N2	2.44	0.50
8:H:20:TYR:HE1	8:H:76:PRO:HG2	1.76	0.50
8:H:25:ASP:N	8:H:25:ASP:OD1	2.43	0.50
8:H:119:LEU:HB3	8:H:123:GLU:HB2	1.93	0.50
9:I:17:VAL:HG13	9:I:63:ILE:HG12	1.93	0.50
1:A:1184:G:H2'	1:A:1185:G:C8	2.46	0.50
1:A:1504:G:H4'	1:A:1505:G:H5'	1.92	0.50
1:A:1542:U:H2'	1:A:1543:C:C6	2.46	0.50
1:A:350:G:H8	1:A:350:G:C5'	2.24	0.50
1:A:438:G:H4'	4:D:123:HIS:ND1	2.26	0.50
1:A:833:U:H2'	1:A:834:C:H6	1.73	0.50
1:A:192:U:H2'	1:A:193:C:H6	1.77	0.50
1:A:666:G:H5'	1:A:726:C:H1'	1.93	0.50
1:A:791:G:O2'	1:A:793:U:O4	2.22	0.50
1:A:946:A:N3	1:A:1333:A:H2	2.10	0.50
5:E:41:VAL:HG13	5:E:113:ALA:HB2	1.94	0.50
10:J:16:LEU:HD22	10:J:94:VAL:HG22	1.94	0.50
11:K:124:LYS:HG2	11:K:125:PHE:CE2	2.47	0.50
1:A:130:A:O2'	1:A:131:C:H5"	2.11	0.50
1:A:344:A:H4'	1:A:345:C:OP2	2.11	0.50
1:A:738:C:OP1	6:F:92:LYS:HD3	2.11	0.50
1:A:1101:A:H4'	1:A:1102:A:O5'	2.10	0.50
1:A:1148:U:O3'	9:I:14:VAL:HG11	2.12	0.50
2:B:24:TRP:HB3	2:B:40:HIS:CE1	2.46	0.50
3:C:134:ILE:HG22	3:C:135:LYS:N	2.24	0.50
3:C:150:LYS:HA	3:C:169:ALA:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:16:LEU:HG	9:I:44:VAL:HB	1.93	0.50
7:G:26:PHE:HA	7:G:101:LEU:HD13	1.93	0.50
7:G:47:CYS:HA	7:G:50:ILE:HD12	1.93	0.50
15:O:45:VAL:HG23	15:O:46:HIS:ND1	2.26	0.50
1:A:1374:A:C4	1:A:1375:A:C8	2.99	0.50
1:A:1518:MA6:H93	1:A:1519:MA6:C2	2.41	0.50
3:C:148:GLY:HA3	3:C:172:ARG:O	2.11	0.50
4:D:173:TRP:CE2	4:D:189:PRO:HB3	2.46	0.50
8:H:83:ILE:CD1	8:H:137:VAL:HG22	2.42	0.50
10:J:10:GLY:HA3	10:J:16:LEU:HD21	1.94	0.50
17:Q:83:ASP:OD2	17:Q:84:LEU:N	2.44	0.50
1:A:765:G:C6	1:A:812:C:C2	3.00	0.50
7:G:20:ASP:OD1	7:G:22:LEU:N	2.43	0.50
7:G:78:ARG:HD2	7:G:156:TRP:HB2	1.94	0.50
9:I:85:LEU:HG	9:I:92:TYR:HD1	1.76	0.50
1:A:544:G:OP2	4:D:66:ARG:NH2	2.45	0.50
2:B:89:GLY:H	2:B:226:ARG:NH2	2.10	0.50
2:B:185:ILE:HA	2:B:199:TYR:O	2.11	0.50
4:D:116:GLN:O	4:D:119:GLN:HB3	2.11	0.50
7:G:94:ARG:O	7:G:97:GLN:HB3	2.12	0.50
1:A:575:G:H4’	1:A:575:G:OP1	2.12	0.50
1:A:1373:G:O2’	1:A:1374:A:O5’	2.20	0.50
4:D:54:TYR:CE2	4:D:58:LEU:HD23	2.47	0.50
17:Q:81:ARG:HE	17:Q:84:LEU:HD12	1.76	0.50
1:A:350:G:H8	1:A:350:G:H5”	1.77	0.49
2:B:69:LEU:HB3	2:B:162:ILE:HD12	1.93	0.49
7:G:47:CYS:HB3	7:G:58:PRO:HB3	1.93	0.49
9:I:10:ARG:HG3	9:I:11:LYS:N	2.25	0.49
1:A:563:A:H5”	1:A:564:C:OP1	2.12	0.49
1:A:652:U:O4	1:A:752:G:O2’	2.28	0.49
1:A:837:G:H1	1:A:849:C:H42	1.59	0.49
1:A:1009:G:H1	1:A:1020:U:H3	1.59	0.49
1:A:1316:G:N2	1:A:1319:A:H5’	2.28	0.49
1:A:1425:U:H2’	1:A:1426:C:H6	1.77	0.49
5:E:92:LYS:HB2	5:E:119:LEU:HB2	1.93	0.49
7:G:12:LEU:HD12	7:G:12:LEU:H	1.78	0.49
1:A:505:G:C6	1:A:535:A:C2	3.00	0.49
1:A:1113:C:H42	1:A:1187:G:H1	1.61	0.49
6:F:80:ARG:HG2	6:F:88:VAL:HB	1.94	0.49
9:I:126:SER:HB2	9:I:127:LYS:HE2	1.94	0.49
10:J:34:VAL:HA	10:J:74:ILE:HG23	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:78:GLY:C	16:P:80:PHE:N	2.66	0.49
1:A:1004:A:O2'	1:A:1005:A:OP1	2.30	0.49
1:A:1068:G:OP1	1:A:1387:G:O2'	2.30	0.49
1:A:1305:G:H5"	21:U:4:GLY:HA3	1.94	0.49
1:A:1427:U:H2'	1:A:1428:A:C8	2.48	0.49
2:B:223:ILE:HG21	2:B:230:VAL:HB	1.95	0.49
6:F:9:VAL:HG22	6:F:60:PHE:CE1	2.48	0.49
7:G:73:MET:SD	7:G:90:GLU:HA	2.52	0.49
8:H:127:LEU:N	8:H:127:LEU:HD23	2.28	0.49
12:L:24:VAL:HG12	12:L:26:ALA:H	1.78	0.49
15:O:82:ILE:HD12	15:O:88:ARG:HB2	1.94	0.49
1:A:583:A:H2'	1:A:584:G:O4'	2.12	0.49
1:A:667:G:H4'	15:O:51:HIS:CE1	2.47	0.49
1:A:923:A:O5'	1:A:923:A:H8	1.96	0.49
1:A:929:G:H1	1:A:1388:C:H42	1.61	0.49
3:C:40:ARG:NH2	3:C:55:VAL:O	2.46	0.49
5:E:147:ASP:O	5:E:151:LEU:HB2	2.11	0.49
11:K:34:ASP:OD2	11:K:38:ASN:HB2	2.11	0.49
1:A:33:A:N3	12:L:32:PHE:HE2	2.11	0.49
1:A:128:G:H5'	17:Q:2:PRO:N	2.27	0.49
1:A:1085:U:C6	1:A:1094:G:N1	2.81	0.49
1:A:1103:C:H5'	2:B:98:LEU:HD13	1.93	0.49
1:A:1404:5MC:H1'	1:A:1499:A:C2	2.47	0.49
6:F:77:ARG:O	6:F:81:ILE:HG12	2.12	0.49
8:H:104:ARG:NE	8:H:138:TRP:CZ2	2.81	0.49
13:M:82:MET:HA	13:M:89:GLY:HA3	1.94	0.49
17:Q:21:VAL:HG21	17:Q:59:ILE:HD11	1.95	0.49
19:S:30:LEU:O	19:S:31:ILE:HB	2.13	0.49
1:A:19:C:P	5:E:127:ASN:HD22	2.35	0.49
1:A:1342:C:H2'	1:A:1343:G:H8	1.77	0.49
1:A:1379:G:N7	7:G:2:ALA:HB3	2.27	0.49
2:B:88:ALA:HB2	2:B:219:VAL:HG13	1.95	0.49
9:I:99:LEU:HB2	9:I:101:PHE:HD1	1.77	0.49
10:J:40:LEU:HB2	10:J:69:ASN:O	2.13	0.49
1:A:651:C:C2'	1:A:652:U:H5'	2.43	0.49
1:A:1343:G:H4'	9:I:122:ALA:HB3	1.93	0.49
4:D:152:SER:HA	4:D:155:LEU:HD23	1.95	0.49
5:E:95:ALA:O	5:E:98:THR:OG1	2.15	0.49
9:I:13:ALA:HA	9:I:67:GLY:O	2.13	0.49
1:A:320:C:H2'	1:A:321:A:O4'	2.13	0.49
1:A:780:A:N6	1:A:801:U:OP2	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1139:G:O6	1:A:1143:G:N2	2.38	0.49
16:P:19:ILE:HD11	16:P:39:TYR:HB2	1.94	0.49
19:S:22:LEU:HD13	19:S:28:LYS:HD2	1.95	0.49
1:A:986:A:H2'	1:A:987:G:O4'	2.13	0.49
1:A:1221:G:N2	1:A:1222:G:H1'	2.28	0.49
1:A:1311:G:N7	19:S:2:PRO:HB2	2.28	0.49
2:B:28:PHE:HD1	2:B:194:PRO:HG3	1.78	0.49
2:B:189:ASP:HB3	2:B:203:GLY:O	2.12	0.49
9:I:63:ILE:HG21	9:I:77:ILE:HG12	1.95	0.49
1:A:434:U:H2'	1:A:435:C:C6	2.48	0.48
1:A:979:C:N4	14:N:18:VAL:O	2.43	0.48
12:L:60:LEU:HD21	12:L:85:ILE:HD12	1.95	0.48
17:Q:17:LYS:H	17:Q:49:GLU:CD	2.17	0.48
1:A:349:A:H2'	1:A:350:G:H5"	1.94	0.48
1:A:894:G:H2'	1:A:895:G:H8	1.78	0.48
1:A:1243:C:H2'	1:A:1244:C:H6	1.78	0.48
5:E:12:LEU:HD22	5:E:12:LEU:O	2.13	0.48
7:G:28:ASN:HA	7:G:31:MET:HE3	1.95	0.48
17:Q:45:HIS:ND1	17:Q:65:ILE:HD13	2.29	0.48
1:A:556:C:H2'	1:A:557:G:O4'	2.12	0.48
1:A:1329:A:H5'	13:M:29:ARG:HD2	1.95	0.48
2:B:107:THR:HA	2:B:110:GLN:HG3	1.94	0.48
12:L:90:VAL:HG11	12:L:93:LEU:HG	1.95	0.48
1:A:374:A:H2'	1:A:375:U:C6	2.48	0.48
1:A:1058:G:H5'	3:C:186:PHE:CZ	2.49	0.48
1:A:1196:U:H3	3:C:162:GLN:NE2	2.11	0.48
1:A:1261:A:H1'	1:A:1283:G:H5"	1.95	0.48
6:F:53:ALA:HB3	6:F:86:ARG:NH1	2.28	0.48
7:G:9:VAL:HG12	7:G:10:ARG:O	2.13	0.48
8:H:17:THR:O	8:H:78:GLN:NE2	2.46	0.48
8:H:27:PRO:HA	8:H:58:TYR:CD2	2.48	0.48
1:A:49:U:O2'	1:A:50:A:H2'	2.13	0.48
1:A:1255:G:H1	1:A:1282:C:H42	1.59	0.48
4:D:19:LEU:HD12	4:D:19:LEU:O	2.13	0.48
11:K:20:TYR:CE2	11:K:83:ILE:HD13	2.48	0.48
11:K:29:ILE:HD12	11:K:30:VAL:N	2.28	0.48
1:A:353:A:H5'	1:A:353:A:H8	1.78	0.48
1:A:475:G:H2'	1:A:476:G:O4'	2.13	0.48
1:A:555:C:H2'	1:A:556:C:C6	2.48	0.48
1:A:1403:C:C5	1:A:1404:5MC:HM52	2.48	0.48
4:D:8:VAL:O	4:D:11:LEU:N	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:80:ILE:CG2	8:H:83:ILE:HG12	2.44	0.48
9:I:23:ASN:O	9:I:23:ASN:ND2	2.46	0.48
12:L:86:ARG:HH11	12:L:86:ARG:HG2	1.78	0.48
1:A:518:C:H4'	1:A:519:C:O5'	2.13	0.48
1:A:677:U:H2'	1:A:678:U:O4'	2.13	0.48
8:H:27:PRO:HG3	8:H:58:TYR:HE2	1.78	0.48
12:L:27:LEU:CA	12:L:29:GLY:H	2.26	0.48
12:L:27:LEU:HA	12:L:29:GLY:H	1.78	0.48
13:M:91:ARG:HB2	13:M:98:VAL:HG22	1.95	0.48
17:Q:9:VAL:HG21	17:Q:84:LEU:HD13	1.94	0.48
17:Q:40:LYS:HG3	17:Q:41:LYS:N	2.28	0.48
1:A:509:A:H3'	25:A:2202:HOH:O	2.12	0.48
1:A:1065:U:C4	1:A:1190:G:H1'	2.49	0.48
1:A:1191:A:H2'	1:A:1192:C:C6	2.49	0.48
1:A:1511:G:H2'	1:A:1512:U:O4'	2.13	0.48
4:D:64:LEU:O	4:D:67:ILE:HB	2.14	0.48
4:D:104:VAL:O	4:D:108:LEU:HB2	2.13	0.48
10:J:64:GLU:HG2	14:N:59:ALA:HB2	1.95	0.48
12:L:93:LEU:O	12:L:96:VAL:HG23	2.13	0.48
20:T:33:ILE:HG12	20:T:62:LEU:HD12	1.95	0.48
1:A:818:G:H3'	1:A:819:A:C5'	2.44	0.48
1:A:818:G:H3'	1:A:819:A:H5"	1.94	0.48
2:B:131:PRO:HD2	2:B:134:GLU:HG3	1.96	0.48
5:E:139:LEU:HD23	5:E:139:LEU:HA	1.60	0.48
6:F:91:VAL:HG12	6:F:92:LYS:N	2.29	0.48
14:N:26:ARG:HB3	14:N:43:CYS:SG	2.54	0.48
17:Q:27:PHE:CZ	17:Q:36:ILE:HD11	2.48	0.48
20:T:49:ALA:HB3	20:T:99:LEU:HD12	1.95	0.48
1:A:828:A:H4'	1:A:828:A:OP1	2.13	0.48
1:A:943:U:C2'	1:A:944:G:H5'	2.43	0.48
1:A:966:M2G:HM13	9:I:128:ARG:OXT	2.13	0.48
1:A:1210:C:H5'	1:A:1214:C:N4	2.29	0.48
6:F:28:ARG:HB2	6:F:28:ARG:CZ	2.44	0.48
17:Q:22:LEU:HD12	17:Q:23:VAL:N	2.28	0.48
18:R:37:VAL:HG21	18:R:78:LEU:HB3	1.95	0.48
19:S:13:ASP:HA	19:S:16:LEU:HB3	1.95	0.48
1:A:117:G:O5'	1:A:117:G:H8	1.97	0.47
1:A:411:A:C8	1:A:413:G:H1'	2.48	0.47
3:C:44:GLU:HA	3:C:52:LEU:CD1	2.42	0.47
17:Q:10:VAL:HG23	17:Q:54:GLY:H	1.79	0.47
20:T:92:LEU:O	20:T:96:GLY:HA2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:A:H2'	1:A:180:U:C6	2.48	0.47
7:G:31:MET:HE1	7:G:36:LYS:HG3	1.96	0.47
11:K:101:SER:HG	11:K:103:LEU:H	1.58	0.47
16:P:73:LEU:O	16:P:76:GLN:HB3	2.14	0.47
16:P:74:LEU:HB3	16:P:79:VAL:CG2	2.43	0.47
1:A:1252:A:H2'	1:A:1253:G:O4'	2.14	0.47
2:B:31:TYR:N	2:B:31:TYR:CD2	2.82	0.47
3:C:88:ARG:NE	3:C:101:LEU:HB2	2.29	0.47
1:A:35:G:C6	1:A:36:C:N4	2.82	0.47
1:A:93:G:C2	1:A:95:U:C2	3.02	0.47
1:A:113:G:H2'	1:A:114:U:H6	1.79	0.47
1:A:146:G:C2	1:A:147:G:C4	3.02	0.47
1:A:695:A:OP1	11:K:52:GLY:HA3	2.15	0.47
1:A:778:G:H2'	1:A:779:C:O4'	2.14	0.47
2:B:12:GLU:OE2	2:B:12:GLU:HA	2.14	0.47
8:H:81:HIS:ND1	8:H:81:HIS:N	2.63	0.47
9:I:10:ARG:HD2	9:I:105:ASP:HB3	1.96	0.47
10:J:24:VAL:HG21	10:J:37:PRO:HD3	1.96	0.47
18:R:53:ARG:NH1	18:R:58:LEU:O	2.47	0.47
1:A:448:A:H2'	1:A:449:C:C6	2.50	0.47
1:A:651:C:O2'	1:A:652:U:H5'	2.15	0.47
1:A:953:G:H2'	1:A:954:G:O4'	2.14	0.47
1:A:991:U:O4	1:A:1212:U:H1'	2.14	0.47
1:A:1373:G:OP2	9:I:71:SER:OG	2.13	0.47
19:S:31:ILE:HG21	19:S:49:ILE:HG12	1.95	0.47
1:A:59:A:C2	1:A:354:G:C4	3.02	0.47
1:A:241:C:N4	1:A:285:G:H1	2.11	0.47
1:A:321:A:H2'	1:A:322:C:C6	2.50	0.47
1:A:792:A:N6	1:A:794:A:N1	2.63	0.47
1:A:1256:A:H4'	1:A:1257:U:O5'	2.14	0.47
6:F:100:ASN:OD1	18:R:23:LYS:HD3	2.14	0.47
9:I:112:LYS:HE2	9:I:113:LYS:O	2.14	0.47
15:O:33:THR:OG1	15:O:63:ARG:HD2	2.15	0.47
1:A:110:C:H2'	1:A:111:G:O4'	2.15	0.47
1:A:485:G:H1'	1:A:486:U:OP2	2.14	0.47
1:A:620:C:C2	4:D:135:LEU:HD13	2.49	0.47
1:A:943:U:H2'	1:A:944:G:H5'	1.96	0.47
1:A:1314:C:C5	19:S:6:LYS:HG2	2.50	0.47
1:A:1443:G:H4'	1:A:1446:A:H5"	1.96	0.47
4:D:7:PRO:HB2	4:D:10:ARG:HG2	1.97	0.47
4:D:108:LEU:HD11	4:D:183:GLY:HA3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.49	0.47
6:F:60:PHE:HE2	18:R:78:LEU:HD11	1.79	0.47
8:H:19:VAL:O	8:H:19:VAL:HG23	2.14	0.47
8:H:80:ILE:HG21	8:H:83:ILE:HG12	1.96	0.47
13:M:12:ASN:H	13:M:45:VAL:CG1	2.27	0.47
16:P:17:TYR:HE1	16:P:41:PRO:HG3	1.80	0.47
18:R:50:ILE:HG12	18:R:70:ILE:CD1	2.44	0.47
20:T:39:LYS:O	20:T:43:LEU:HD23	2.14	0.47
20:T:92:LEU:HD13	20:T:92:LEU:HA	1.59	0.47
1:A:353:A:O2'	1:A:354:G:OP2	2.26	0.47
1:A:724:G:C2'	1:A:725:G:H5'	2.44	0.47
1:A:1121:U:H2'	1:A:1122:U:H6	1.80	0.47
1:A:1482:G:HO2'	1:A:1483:A:H8	1.61	0.47
5:E:151:LEU:HD22	8:H:79:VAL:HG22	1.96	0.47
7:G:47:CYS:O	7:G:50:ILE:HB	2.14	0.47
8:H:6:ILE:HG12	8:H:31:PHE:HE2	1.80	0.47
21:U:6:ARG:HG3	21:U:12:LYS:HE3	1.97	0.47
1:A:1054:C:OP1	1:A:1197:G:OP1	2.33	0.47
1:A:1123:A:H2'	1:A:1124:G:C8	2.50	0.47
5:E:109:ILE:HG22	5:E:110:LEU:N	2.28	0.47
7:G:45:ASP:HA	7:G:48:LYS:HD2	1.97	0.47
1:A:358:U:H2'	1:A:359:U:O4'	2.15	0.47
1:A:975:A:H5'	1:A:975:A:C8	2.50	0.47
1:A:1242:C:H42	1:A:1295:G:H1	1.63	0.47
4:D:107:ARG:HD2	4:D:107:ARG:HA	1.80	0.47
4:D:200:GLU:CD	4:D:200:GLU:H	2.18	0.47
5:E:129:ILE:HD12	5:E:129:ILE:HA	1.69	0.47
18:R:46:GLU:H	18:R:46:GLU:CD	2.17	0.47
1:A:580:U:H5"	15:O:58:MET:HG2	1.97	0.46
1:A:724:G:O2'	1:A:725:G:H5'	2.15	0.46
1:A:1196:U:H3	3:C:162:GLN:HE21	1.62	0.46
2:B:122:PHE:HA	2:B:127:ILE:HD11	1.98	0.46
3:C:88:ARG:HD3	3:C:100:ALA:HA	1.97	0.46
3:C:172:ARG:NH1	3:C:172:ARG:HB2	2.31	0.46
7:G:99:LEU:HD23	7:G:99:LEU:HA	1.61	0.46
11:K:58:PRO:HB3	11:K:93:GLN:HG3	1.97	0.46
17:Q:29:HIS:CE1	17:Q:32:TYR:H	2.33	0.46
1:A:216:G:H2'	1:A:217:C:C6	2.50	0.46
1:A:393:A:O2'	1:A:394:G:H5'	2.16	0.46
1:A:877:C:O2'	8:H:3:THR:HG23	2.16	0.46
1:A:1126:U:H6	1:A:1126:U:O5'	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1244:C:H42	1:A:1293:G:H1	1.63	0.46
1:A:1313:U:O4	19:S:4:SER:OG	2.27	0.46
2:B:24:TRP:CD1	2:B:25:ASN:N	2.83	0.46
1:A:56:U:H2'	1:A:57:G:H8	1.81	0.46
1:A:370:C:C2'	1:A:371:G:H5'	2.45	0.46
1:A:877:C:O2'	1:A:878:G:H5'	2.15	0.46
1:A:1255:G:N1	1:A:1279:A:N7	2.63	0.46
5:E:131:ILE:HD13	5:E:131:ILE:HA	1.67	0.46
9:I:4:TYR:CD2	9:I:88:TYR:HA	2.50	0.46
11:K:41:THR:HG21	11:K:71:LYS:HB3	1.98	0.46
13:M:108:ARG:HD3	13:M:114:ARG:NH2	2.30	0.46
19:S:40:ILE:HG13	19:S:70:LYS:O	2.15	0.46
1:A:152:A:N6	1:A:170:U:O2	2.49	0.46
1:A:396:G:N2	1:A:398:C:C2	2.84	0.46
1:A:411:A:N7	1:A:413:G:N3	2.63	0.46
1:A:1342:C:H2'	1:A:1343:G:C8	2.49	0.46
2:B:62:ALA:HB2	2:B:222:ILE:HG23	1.97	0.46
2:B:82:ARG:NH1	2:B:82:ARG:HG3	2.30	0.46
3:C:190:ARG:HG2	3:C:195:VAL:HG22	1.96	0.46
13:M:90:LEU:HD23	13:M:93:ARG:HH12	1.80	0.46
1:A:500:G:C6	1:A:501:C:N4	2.83	0.46
1:A:1005:A:C8	1:A:1006:C:H1'	2.50	0.46
2:B:82:ARG:HG3	2:B:92:TYR:OH	2.15	0.46
8:H:20:TYR:CZ	8:H:76:PRO:HD2	2.50	0.46
8:H:45:ILE:HG13	8:H:47:GLY:N	2.30	0.46
8:H:63:LEU:H	8:H:63:LEU:HD22	1.80	0.46
15:O:43:LEU:HD13	15:O:53:HIS:HB2	1.97	0.46
19:S:28:LYS:HG2	19:S:29:ARG:HD2	1.98	0.46
1:A:91:C:H5"	1:A:91:C:H6	1.81	0.46
1:A:328:C:O2'	1:A:329:A:OP2	2.26	0.46
1:A:1400:5MC:H3'	1:A:1401:G:H5'	1.98	0.46
9:I:95:LYS:HA	9:I:95:LYS:HD3	1.56	0.46
18:R:71:LYS:O	18:R:75:ILE:HG12	2.15	0.46
1:A:93:G:C2	1:A:95:U:O2	2.69	0.46
1:A:216:G:H2'	1:A:217:C:H6	1.80	0.46
1:A:1011:G:H2'	1:A:1012:U:C6	2.50	0.46
1:A:1117:G:H5"	9:I:104:ARG:NH2	2.31	0.46
1:A:1257:U:H1'	1:A:1258:G:OP2	2.15	0.46
1:A:1316:G:O6	19:S:6:LYS:NZ	2.40	0.46
1:A:1462:G:H2'	1:A:1463:C:C6	2.51	0.46
1:A:1502:A:H2	1:A:1505:G:N1	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:599:C:C2	1:A:640:A:C2	3.04	0.46
1:A:826:C:O2	8:H:15:ASN:ND2	2.48	0.46
1:A:892:A:C2	1:A:907:A:C4	3.04	0.46
5:E:149:GLU:O	5:E:153:LYS:HB2	2.16	0.46
12:L:59:ARG:HD3	12:L:65:GLU:HG3	1.98	0.46
20:T:60:GLU:HG3	20:T:81:LYS:HD2	1.98	0.46
1:A:182:U:HO2'	1:A:183:G:P	2.39	0.46
1:A:792:A:C6	1:A:794:A:C2	3.04	0.46
1:A:1004:A:OP1	1:A:1024:G:N1	2.48	0.46
1:A:1428:A:H2'	1:A:1429:C:O4'	2.16	0.46
1:A:1539:C:H6	1:A:1539:C:O5'	1.99	0.46
2:B:178:ARG:HE	8:H:74:PRO:HG3	1.81	0.46
8:H:137:VAL:HG12	8:H:138:TRP:N	2.30	0.46
10:J:22:LYS:NZ	10:J:90:LEU:HD12	2.30	0.46
10:J:44:VAL:CG1	10:J:66:ARG:HG2	2.46	0.46
10:J:48:THR:OG1	10:J:62:HIS:HD2	1.99	0.46
1:A:544:G:C6	1:A:545:C:C4	3.04	0.46
1:A:1005:A:N3	1:A:1026:G:N2	2.64	0.46
1:A:1098:C:H2'	1:A:1099:G:O4'	2.16	0.46
1:A:1103:C:H2'	1:A:1104:G:O4'	2.16	0.46
1:A:1405:G:H1	1:A:1496:C:N4	2.14	0.46
1:A:1505:G:H3'	1:A:1505:G:H8	1.81	0.46
4:D:175:SER:HB3	4:D:186:LEU:HD11	1.98	0.46
5:E:7:GLU:OE1	5:E:112:LEU:HD21	2.17	0.46
6:F:4:TYR:HB2	6:F:65:VAL:HG22	1.98	0.46
1:A:243:A:C2	1:A:245:C:C2	3.04	0.45
1:A:608:A:P	25:A:2086:HOH:O	2.74	0.45
1:A:940:C:H2'	1:A:941:G:O4'	2.16	0.45
1:A:1308:U:OP2	13:M:99:ARG:HG3	2.16	0.45
1:A:1371:G:C5	1:A:1372:U:C5	3.04	0.45
2:B:139:LYS:HA	2:B:139:LYS:HD2	1.70	0.45
4:D:57:ARG:NH2	5:E:107:ARG:HD3	2.31	0.45
4:D:65:ARG:HG2	4:D:65:ARG:NH1	2.15	0.45
7:G:50:ILE:HG21	7:G:58:PRO:HA	1.98	0.45
7:G:116:ALA:O	7:G:119:ARG:N	2.49	0.45
9:I:63:ILE:CG2	9:I:77:ILE:HG12	2.45	0.45
9:I:126:SER:OG	9:I:127:LYS:N	2.49	0.45
16:P:39:TYR:CE2	16:P:41:PRO:HB3	2.50	0.45
20:T:63:ILE:O	20:T:66:ALA:HB3	2.16	0.45
1:A:6:G:O2'	1:A:7:G:H5'	2.16	0.45
1:A:706:A:O2'	11:K:29:ILE:HD11	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:918:A:H2'	1:A:919:A:C8	2.51	0.45
1:A:1285:A:H5'	1:A:1286:A:C5	2.51	0.45
22:A:1601:SRY:O61	12:L:46:LYS:HD3	2.16	0.45
5:E:64:ARG:HH11	5:E:64:ARG:HB3	1.81	0.45
6:F:43:LEU:HD21	18:R:35:ARG:HH12	1.81	0.45
11:K:99:GLN:HG2	11:K:105:VAL:HG21	1.98	0.45
13:M:27:LYS:HD2	13:M:27:LYS:HA	1.57	0.45
14:N:31:ARG:NH1	14:N:31:ARG:HB2	2.30	0.45
4:D:20:TYR:N	4:D:20:TYR:CD2	2.82	0.45
5:E:31:LEU:HD23	5:E:45:PHE:HD1	1.82	0.45
6:F:48:LEU:CD1	6:F:52:ILE:HB	2.46	0.45
11:K:59:TYR:O	11:K:62:GLN:HB3	2.16	0.45
13:M:3:ARG:HG2	13:M:9:ILE:HG12	1.97	0.45
20:T:48:LYS:H	20:T:48:LYS:HG2	1.47	0.45
1:A:980:C:H5"	1:A:981:U:C5	2.51	0.45
1:A:1468:A:O5'	1:A:1468:A:H8	2.00	0.45
3:C:29:TYR:OH	14:N:54:PRO:HG2	2.17	0.45
6:F:4:TYR:HB2	6:F:65:VAL:CG2	2.47	0.45
6:F:8:ILE:HD13	6:F:26:ILE:HG12	1.97	0.45
6:F:55:ASP:CG	6:F:86:ARG:HH22	2.18	0.45
9:I:99:LEU:HB2	9:I:101:PHE:CD1	2.51	0.45
11:K:80:VAL:HG21	11:K:103:LEU:HD13	1.97	0.45
11:K:88:GLY:O	11:K:91:ARG:N	2.49	0.45
1:A:324:G:H2'	1:A:326:G:N7	2.31	0.45
1:A:373:A:H1'	1:A:481:G:N3	2.32	0.45
1:A:526:C:OP1	12:L:91:LYS:NZ	2.44	0.45
1:A:652:U:C2	1:A:752:G:N2	2.85	0.45
9:I:5:TYR:CE1	9:I:18:PHE:HE2	2.34	0.45
14:N:39:LEU:HB3	14:N:43:CYS:HB3	1.98	0.45
17:Q:18:THR:HG23	17:Q:69:LYS:HE3	1.98	0.45
1:A:394:G:H2'	1:A:395:C:H6	1.82	0.45
1:A:551:U:C2	1:A:552:U:C5	3.04	0.45
1:A:631:G:C2'	1:A:632:A:C8	2.99	0.45
1:A:1133:G:C2	1:A:1142:G:C2	3.05	0.45
1:A:1185:G:O2'	1:A:1186:G:H5'	2.17	0.45
2:B:15:VAL:HG13	2:B:209:ARG:HB3	1.99	0.45
2:B:197:VAL:HB	2:B:200:ILE:CG2	2.47	0.45
4:D:187:ARG:CZ	4:D:188:LEU:H	2.30	0.45
6:F:3:ARG:HA	6:F:65:VAL:O	2.17	0.45
16:P:67:THR:HG22	16:P:69:THR:H	1.81	0.45
17:Q:48:GLU:HB2	17:Q:50:LYS:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:88:TYR:CD2	17:Q:89:LEU:HD23	2.52	0.45
1:A:78:G:N1	1:A:92:C:C4	2.85	0.45
1:A:527:7MG:OP2	22:A:1601:SRY:O32	2.21	0.45
1:A:1278:U:H5'	1:A:1279:A:O4'	2.16	0.45
1:A:1411:C:H42	1:A:1489:G:H1	1.64	0.45
2:B:16:HIS:HD2	2:B:17:PHE:O	1.99	0.45
2:B:41:ILE:HD13	2:B:41:ILE:HA	1.78	0.45
4:D:20:TYR:CD1	4:D:27:TYR:HE1	2.35	0.45
4:D:64:LEU:HG	4:D:198:VAL:HG11	1.99	0.45
7:G:40:ALA:CB	9:I:41:VAL:HG21	2.47	0.45
12:L:98:TYR:N	12:L:98:TYR:CD1	2.85	0.45
21:U:6:ARG:HD3	21:U:15:ARG:HH12	1.82	0.45
1:A:97:G:C6	1:A:98:U:C4	3.05	0.45
1:A:617:G:H1	1:A:623:C:N4	2.15	0.45
2:B:71:VAL:O	2:B:165:VAL:HG23	2.16	0.45
3:C:46:GLU:HB3	3:C:47:LEU:HD12	1.99	0.45
3:C:47:LEU:HB2	3:C:52:LEU:HD13	1.98	0.45
3:C:84:ILE:O	3:C:88:ARG:HB2	2.17	0.45
3:C:154:SER:OG	3:C:196:LEU:HD22	2.17	0.45
12:L:60:LEU:HD12	12:L:60:LEU:HA	1.52	0.45
17:Q:75:ARG:NH1	17:Q:76:LEU:O	2.50	0.45
1:A:131:C:H2'	1:A:132:C:C6	2.52	0.45
1:A:1434:A:H2'	1:A:1435:G:O4'	2.16	0.45
1:A:357:G:C2	1:A:358:U:C5	3.05	0.45
1:A:532:A:C2'	1:A:533:A:OP1	2.65	0.45
1:A:569:C:H42	1:A:881:G:H1	1.64	0.45
1:A:1181:G:C5	1:A:1182:G:N1	2.85	0.45
1:A:1320:C:H5"	19:S:3:ARG:HH21	1.81	0.45
1:A:1358:U:HO2'	1:A:1359:C:P	2.40	0.45
8:H:73:ASP:OD1	8:H:75:ARG:NH2	2.43	0.45
17:Q:5:VAL:HA	17:Q:59:ILE:O	2.17	0.45
1:A:421:U:O2	3:C:126:ARG:NE	2.50	0.44
1:A:886:G:C6	1:A:912:A:H2	2.35	0.44
1:A:912:A:H3'	1:A:912:A:C8	2.53	0.44
1:A:1065:U:H1'	1:A:1066:C:OP2	2.17	0.44
1:A:1299:A:C5	1:A:1301:U:O2	2.70	0.44
8:H:6:ILE:HG12	8:H:31:PHE:CE2	2.52	0.44
18:R:87:ARG:HB3	18:R:88:LYS:H	1.59	0.44
19:S:57:HIS:O	19:S:59:PRO:HD3	2.17	0.44
1:A:42:G:H1	1:A:400:C:H42	1.65	0.44
1:A:1071:C:H5"	5:E:49:PRO:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1283:G:H2'	1:A:1284:C:H6	1.82	0.44
2:B:7:VAL:HG21	2:B:221:LEU:HD23	1.98	0.44
2:B:116:GLU:CG	2:B:153:ARG:HH12	2.30	0.44
6:F:91:VAL:HG11	18:R:72:ARG:NH1	2.30	0.44
8:H:82:HIS:HD1	8:H:138:TRP:HE1	1.53	0.44
16:P:39:TYR:OH	16:P:72:ARG:NH2	2.50	0.44
16:P:78:GLY:C	16:P:80:PHE:H	2.19	0.44
20:T:56:MET:HG3	20:T:88:VAL:HG21	1.98	0.44
1:A:602:A:H2'	1:A:603:U:O4'	2.18	0.44
1:A:860:A:H2'	1:A:861:G:O4'	2.18	0.44
1:A:1357:A:H2'	1:A:1358:U:C5	2.53	0.44
4:D:152:SER:O	4:D:155:LEU:HB2	2.16	0.44
6:F:30:LEU:HD23	6:F:75:LEU:HD21	1.99	0.44
7:G:65:ALA:O	7:G:69:VAL:HG23	2.17	0.44
10:J:53:PRO:HB3	14:N:42:ILE:CD1	2.47	0.44
13:M:22:ILE:HG22	13:M:23:TYR:N	2.33	0.44
1:A:92:C:O2'	1:A:93:G:H5'	2.17	0.44
1:A:1343:G:H2'	1:A:1344:C:C6	2.51	0.44
1:A:1352:C:H2'	1:A:1353:G:C8	2.53	0.44
1:A:1521:G:H2'	1:A:1522:U:C6	2.53	0.44
5:E:147:ASP:OD1	5:E:147:ASP:N	2.34	0.44
9:I:111:ARG:NH1	9:I:113:LYS:HA	2.31	0.44
12:L:40:VAL:HG23	12:L:79:GLU:HA	1.99	0.44
16:P:58:TYR:O	16:P:61:SER:OG	2.17	0.44
17:Q:63:ARG:HG2	17:Q:64:PRO:CD	2.48	0.44
20:T:53:LEU:HB2	20:T:100:ILE:HD12	2.00	0.44
1:A:11:G:C5	1:A:12:U:C5	3.05	0.44
1:A:954:G:C6	1:A:955:U:C4	3.06	0.44
1:A:1251:A:H2'	1:A:1252:A:O4'	2.18	0.44
1:A:1371:G:OP1	9:I:11:LYS:HD3	2.16	0.44
2:B:82:ARG:HG3	2:B:82:ARG:HH11	1.81	0.44
2:B:114:ARG:HD2	2:B:114:ARG:HA	1.85	0.44
3:C:67:THR:HA	3:C:102:ASN:HB3	2.00	0.44
4:D:135:LEU:HA	4:D:136:PRO:HD3	1.66	0.44
1:A:117:G:H2'	1:A:118:U:O4'	2.18	0.44
1:A:299:G:C6	1:A:300:A:C6	3.05	0.44
1:A:401:C:H1'	1:A:622:A:H1'	2.00	0.44
1:A:636:U:H2'	1:A:637:G:C8	2.52	0.44
1:A:782:A:H4'	1:A:1514:C:O2'	2.17	0.44
1:A:946:A:H2'	1:A:947:G:H8	1.82	0.44
1:A:1074:G:C6	1:A:1075:C:C4	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1205:U:H4'	3:C:195:VAL:HG21	1.99	0.44
1:A:1283:G:O2'	1:A:1284:C:H5'	2.18	0.44
1:A:1397:C:O2'	1:A:1398:A:OP1	2.33	0.44
2:B:117:GLU:O	2:B:120:ALA:HB3	2.18	0.44
2:B:188:ALA:O	2:B:202:PRO:HA	2.17	0.44
3:C:166:GLU:OE2	3:C:166:GLU:HA	2.16	0.44
4:D:155:LEU:HD13	4:D:155:LEU:HA	1.72	0.44
10:J:51:ARG:CZ	10:J:61:GLU:HB2	2.46	0.44
11:K:103:LEU:HD23	11:K:103:LEU:HA	1.84	0.44
13:M:105:THR:O	13:M:107:ALA:N	2.50	0.44
17:Q:59:ILE:HG23	17:Q:71:PHE:HB3	1.99	0.44
18:R:37:VAL:O	18:R:40:LEU:N	2.50	0.44
1:A:1150:U:C2'	1:A:1151:A:H5'	2.47	0.44
1:A:1183:A:H2'	25:A:2132:HOH:O	2.18	0.44
1:A:1326:C:OP2	21:U:6:ARG:HD2	2.18	0.44
2:B:83:MET:HB2	2:B:235:SER:HB3	2.00	0.44
7:G:108:ALA:O	7:G:119:ARG:HD2	2.18	0.44
7:G:124:LEU:HA	7:G:124:LEU:HD23	1.55	0.44
14:N:23:ARG:NH1	14:N:30:ALA:HB2	2.33	0.44
19:S:31:ILE:CG2	19:S:49:ILE:HG12	2.47	0.44
1:A:95:U:O2'	1:A:96:G:H5'	2.18	0.44
1:A:122:G:H2'	1:A:123:C:O4'	2.18	0.44
1:A:321:A:C2	1:A:333:G:C2	3.05	0.44
1:A:750:G:H1'	15:O:23:GLY:H	1.82	0.44
1:A:1332:A:H2'	1:A:1333:A:C8	2.53	0.44
1:A:1541:PSU:H2'	1:A:1541:PSU:O4	2.17	0.44
4:D:23:GLY:HA3	4:D:112:VAL:HG12	2.00	0.44
5:E:11:ILE:HG21	5:E:105:VAL:HG22	1.99	0.44
5:E:96:PRO:HA	5:E:117:ASP:OD2	2.17	0.44
5:E:130:ASN:N	5:E:130:ASN:OD1	2.50	0.44
14:N:14:PRO:HB2	14:N:16:PHE:O	2.18	0.44
14:N:61:TRP:CD1	14:N:61:TRP:C	2.91	0.44
16:P:26:ARG:HD3	16:P:31:LYS:O	2.17	0.44
17:Q:11:VAL:HA	17:Q:53:LEU:HD11	2.00	0.44
19:S:19:VAL:HA	19:S:22:LEU:CG	2.45	0.44
1:A:1007:C:O2	1:A:1023:G:N1	2.51	0.44
3:C:131:ARG:HH11	3:C:131:ARG:HG2	1.82	0.44
5:E:112:LEU:HD23	5:E:112:LEU:HA	1.56	0.44
12:L:69:TYR:CD1	12:L:90:VAL:HG21	2.53	0.44
18:R:36:ASN:OD1	18:R:39:VAL:HG12	2.17	0.44
1:A:567:G:H2'	1:A:568:G:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:723:U:O2	1:A:723:U:H2'	2.18	0.43
1:A:977:A:H2'	1:A:978:A:H5"	2.00	0.43
1:A:1028:C:N4	1:A:1033:G:H22	2.16	0.43
1:A:1260:C:OP1	1:A:1284:C:O2'	2.33	0.43
2:B:157:ARG:HG2	2:B:158:LEU:N	2.33	0.43
3:C:113:ALA:N	3:C:114:PRO:HD2	2.33	0.43
3:C:200:ALA:C	3:C:201:TYR:HD1	2.22	0.43
5:E:92:LYS:O	5:E:118:ILE:HG12	2.18	0.43
12:L:62:SER:HB2	12:L:64:TYR:HB2	1.99	0.43
1:A:407:G:N2	1:A:436:C:C2	2.86	0.43
1:A:450:G:H5'	16:P:41:PRO:O	2.18	0.43
1:A:1180:A:OP1	9:I:103:THR:HG23	2.18	0.43
1:A:1489:G:H2'	1:A:1490:C:C6	2.52	0.43
2:B:23:ARG:HB2	2:B:23:ARG:CZ	2.48	0.43
2:B:80:ILE:HD12	2:B:208:ILE:HG12	2.00	0.43
2:B:87:ARG:HE	2:B:87:ARG:HB3	1.49	0.43
2:B:152:PHE:CE1	2:B:155:LEU:HD12	2.53	0.43
2:B:174:VAL:HG13	2:B:184:VAL:HG11	2.00	0.43
8:H:84:ARG:O	8:H:135:CYS:HB2	2.18	0.43
9:I:63:ILE:HD13	9:I:77:ILE:HG23	2.00	0.43
20:T:43:LEU:HD13	20:T:43:LEU:HA	1.68	0.43
1:A:419:C:H5"	1:A:420:U:OP2	2.18	0.43
1:A:599:C:H5"	8:H:96:GLY:HA2	1.99	0.43
1:A:653:A:P	8:H:56:LYS:HZ1	2.42	0.43
2:B:49:GLU:O	2:B:52:GLU:HB3	2.19	0.43
3:C:115:LEU:HD23	3:C:115:LEU:HA	1.58	0.43
5:E:118:ILE:HG12	5:E:119:LEU:H	1.84	0.43
5:E:122:GLU:O	5:E:123:LEU:HD23	2.18	0.43
9:I:17:VAL:HG11	9:I:81:ILE:HG13	2.01	0.43
9:I:65:VAL:HG11	9:I:77:ILE:HD11	2.00	0.43
16:P:74:LEU:O	16:P:78:GLY:N	2.51	0.43
17:Q:10:VAL:HG21	17:Q:52:LYS:O	2.18	0.43
18:R:47:THR:HG22	18:R:83:GLU:H	1.83	0.43
1:A:415:A:H2'	1:A:416:G:C8	2.53	0.43
4:D:61:LYS:HE2	4:D:62:GLN:HG2	2.00	0.43
10:J:46:ARG:NH1	10:J:64:GLU:OE2	2.51	0.43
11:K:85:ARG:HE	11:K:111:ASP:HB3	1.83	0.43
13:M:23:TYR:CZ	13:M:71:ARG:HD3	2.53	0.43
17:Q:67:LYS:O	17:Q:68:ARG:HB2	2.18	0.43
19:S:41:VAL:HG23	19:S:43:GLU:HG2	2.00	0.43
20:T:62:LEU:HD22	20:T:62:LEU:HA	1.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:72:LEU:HD22	20:T:72:LEU:HA	1.79	0.43
1:A:532:A:O2'	1:A:533:A:OP1	2.29	0.43
1:A:618:C:H5"	1:A:619:U:H5"	2.00	0.43
1:A:1174:G:C2	1:A:1175:G:C5	3.07	0.43
1:A:1532:U:H6	1:A:1532:U:O5'	2.01	0.43
2:B:183:PRO:HA	2:B:198:ASP:OD2	2.17	0.43
3:C:6:HIS:HA	3:C:7:PRO:HD2	1.81	0.43
5:E:17:ALA:HB2	5:E:26:PHE:HD2	1.80	0.43
8:H:45:ILE:HD12	8:H:61:VAL:HG13	2.01	0.43
11:K:33:THR:HB	11:K:39:PRO:HA	2.01	0.43
12:L:44:THR:HA	12:L:45:PRO:HD2	1.83	0.43
13:M:74:VAL:O	13:M:78:ILE:HD12	2.18	0.43
13:M:96:LEU:HD23	13:M:96:LEU:HA	1.77	0.43
1:A:504:C:C2	1:A:542:G:N2	2.86	0.43
1:A:607:A:C4	1:A:608:A:C8	3.07	0.43
1:A:664:G:OP1	18:R:64:ARG:NH1	2.52	0.43
1:A:737:A:H2'	1:A:738:C:C6	2.53	0.43
1:A:778:G:O5'	1:A:778:G:H8	2.02	0.43
1:A:1003:G:N2	1:A:1003(A):G:C6	2.87	0.43
1:A:1349:A:C2	1:A:1374:A:C8	3.07	0.43
1:A:1405:G:N3	1:A:1497:G:C2	2.87	0.43
2:B:28:PHE:CD2	2:B:190:THR:HA	2.53	0.43
9:I:26:VAL:O	9:I:33:PHE:HB2	2.19	0.43
1:A:7:G:H5"	1:A:298:A:O4'	2.18	0.43
1:A:263:A:OP2	20:T:79:ARG:NH1	2.52	0.43
1:A:836:G:C6	1:A:851:G:C6	3.06	0.43
1:A:1095:U:H5"	1:A:1109:C:O2	2.18	0.43
1:A:1399:C:C2	1:A:1502:A:N6	2.87	0.43
5:E:106:PRO:O	5:E:107:ARG:C	2.56	0.43
10:J:16:LEU:HD22	10:J:16:LEU:HA	1.81	0.43
10:J:49:VAL:O	10:J:60:ARG:HA	2.18	0.43
11:K:44:SER:OG	11:K:47:VAL:HG23	2.19	0.43
20:T:50:GLU:CB	20:T:99:LEU:HD13	2.48	0.43
20:T:60:GLU:O	20:T:63:ILE:HB	2.18	0.43
1:A:76:C:O2'	1:A:77:G:H5'	2.19	0.43
1:A:778:G:H2'	1:A:779:C:H6	1.83	0.43
1:A:782:A:H2'	1:A:783:C:O4'	2.18	0.43
4:D:42:GLN:HG3	4:D:43:HIS:CE1	2.53	0.43
8:H:86:ILE:HG22	8:H:133:LEU:O	2.19	0.43
8:H:104:ARG:HG2	8:H:138:TRP:CE3	2.54	0.43
8:H:112:LEU:HA	8:H:112:LEU:HD23	1.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:59:TRP:O	16:P:60:LEU:C	2.56	0.43
17:Q:62:SER:CB	17:Q:72:ARG:HG3	2.49	0.43
18:R:44:LEU:HD21	18:R:70:ILE:HD13	2.01	0.43
1:A:56:U:H2'	1:A:57:G:C8	2.54	0.43
1:A:57:G:H2'	1:A:58:C:C6	2.54	0.43
1:A:406:G:H21	4:D:119:GLN:HE22	1.67	0.43
1:A:825:G:H21	8:H:11:THR:HG21	1.84	0.43
1:A:854:G:C6	1:A:855:G:N7	2.86	0.43
1:A:1054:C:C6	1:A:1054:C:C3'	3.01	0.43
1:A:1495:U:H2'	1:A:1496:C:O2	2.19	0.43
2:B:80:ILE:HD13	2:B:212:GLN:HB2	2.01	0.43
3:C:120:VAL:O	3:C:124:ILE:HG12	2.19	0.43
4:D:10:ARG:HA	4:D:13:ARG:HG2	2.00	0.43
5:E:91:LEU:HD23	5:E:91:LEU:N	2.33	0.43
6:F:5:GLU:HB3	6:F:62:TRP:HE1	1.83	0.43
6:F:21:LEU:HG	6:F:25:ILE:HD11	2.00	0.43
6:F:39:LYS:HB2	6:F:39:LYS:HE3	1.49	0.43
6:F:43:LEU:HD22	6:F:43:LEU:H	1.84	0.43
21:U:18:TYR:CE2	21:U:24:ARG:HG2	2.53	0.43
1:A:83:U:C2'	1:A:84:U:H5'	2.49	0.43
1:A:785:G:N2	1:A:798:G:C4	2.87	0.43
10:J:57:LYS:HE2	10:J:60:ARG:NH2	2.32	0.43
11:K:20:TYR:HE1	11:K:33:THR:HG21	1.84	0.43
13:M:4:ILE:HD11	13:M:53:VAL:HG22	2.00	0.43
17:Q:63:ARG:HG2	17:Q:64:PRO:HD2	2.01	0.43
19:S:36:ARG:NH2	19:S:75:ALA:O	2.52	0.43
20:T:24:LEU:HD12	20:T:24:LEU:HA	1.69	0.43
1:A:243:A:C2	1:A:246:A:C8	3.06	0.42
1:A:765:G:H5"	1:A:766:A:OP1	2.19	0.42
1:A:1329:A:P	13:M:28:ALA:HB3	2.59	0.42
1:A:1347:G:H2'	1:A:1373:G:H1	1.84	0.42
1:A:1418:A:C2	1:A:1483:A:C4	3.07	0.42
2:B:215:LEU:HA	2:B:215:LEU:HD23	1.48	0.42
3:C:35:GLU:O	3:C:39:ILE:HG13	2.19	0.42
7:G:87:VAL:HG13	7:G:88:PRO:HD2	2.01	0.42
8:H:38:ILE:HD13	8:H:41:ARG:HH21	1.83	0.42
18:R:78:LEU:HD23	18:R:78:LEU:HA	1.71	0.42
1:A:779:C:H2'	1:A:780:A:O4'	2.19	0.42
1:A:827:U:H3'	1:A:870:U:O4	2.19	0.42
1:A:938:A:C6	1:A:939:G:C5	3.08	0.42
5:E:11:ILE:HD12	5:E:11:ILE:HG23	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:129:ILE:N	5:E:129:ILE:HD13	2.33	0.42
8:H:87:SER:HB2	8:H:93:VAL:H	1.84	0.42
14:N:44:LEU:HD12	14:N:44:LEU:HA	1.79	0.42
1:A:269:C:H2'	1:A:270:A:H8	1.84	0.42
1:A:391:G:C5	1:A:392:G:C8	3.07	0.42
1:A:914:A:P	22:A:1601:SRY:HI33	2.59	0.42
5:E:80:ILE:HD13	5:E:138:ALA:HB1	2.01	0.42
7:G:144:MET:O	7:G:147:ALA:HB3	2.19	0.42
8:H:36:LEU:HD23	8:H:36:LEU:HA	1.80	0.42
10:J:37:PRO:HA	10:J:72:VAL:N	2.23	0.42
14:N:14:PRO:O	14:N:15:LYS:HB3	2.19	0.42
14:N:40:CYS:H	14:N:43:CYS:HB2	1.83	0.42
18:R:40:LEU:HA	18:R:40:LEU:HD23	1.69	0.42
20:T:22:ARG:O	20:T:23:ARG:C	2.58	0.42
1:A:35:G:C4	1:A:36:C:C5	3.07	0.42
1:A:802:A:H2'	1:A:803:G:O4'	2.19	0.42
1:A:1061:G:H1'	10:J:56:HIS:CE1	2.54	0.42
6:F:69:GLU:HA	6:F:72:VAL:HG23	2.01	0.42
7:G:38:LEU:O	7:G:42:ILE:HG13	2.20	0.42
8:H:83:ILE:HD13	8:H:83:ILE:HA	1.85	0.42
11:K:98:LEU:HD23	11:K:98:LEU:HA	1.78	0.42
12:L:7:ILE:CG2	12:L:8:ASN:N	2.82	0.42
14:N:37:PHE:CD1	14:N:44:LEU:HD11	2.47	0.42
20:T:44:ALA:HB1	20:T:91:LEU:HB2	2.00	0.42
1:A:449:C:H3'	1:A:450:G:H8	1.84	0.42
1:A:689:C:H2'	1:A:690:G:O4'	2.19	0.42
1:A:803:G:C6	1:A:804:U:C4	3.08	0.42
1:A:1181:G:HO2'	1:A:1182:G:P	2.40	0.42
1:A:1239:A:C4	1:A:1298:C:N4	2.87	0.42
1:A:1406:U:H3	1:A:1495:U:H3	1.65	0.42
6:F:48:LEU:HD13	6:F:52:ILE:HB	2.02	0.42
8:H:73:ASP:OD2	8:H:75:ARG:HB2	2.20	0.42
11:K:88:GLY:O	11:K:89:ALA:C	2.58	0.42
12:L:85:ILE:HG21	12:L:85:ILE:HD13	1.77	0.42
14:N:61:TRP:CD1	14:N:61:TRP:O	2.72	0.42
1:A:162:A:H1'	1:A:348:G:O2'	2.19	0.42
1:A:335:C:O2'	1:A:336:C:H5'	2.19	0.42
1:A:392:G:C2	1:A:393:A:C4	3.07	0.42
1:A:665:A:H5'	1:A:666:G:OP2	2.19	0.42
1:A:943:U:H1'	9:I:124:GLN:HE22	1.85	0.42
1:A:1324:A:H2'	1:A:1325:C:O4'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:92:TYR:CE2	2:B:151:GLY:HA3	2.55	0.42
3:C:39:ILE:HG22	3:C:43:LEU:HD12	2.01	0.42
3:C:110:ASN:O	3:C:141:VAL:HG22	2.19	0.42
7:G:12:LEU:HD12	7:G:12:LEU:N	2.35	0.42
7:G:70:LYS:HG2	7:G:100:ALA:HB2	2.01	0.42
16:P:43:LYS:HG2	16:P:48:TRP:CG	2.54	0.42
16:P:67:THR:HG22	16:P:68:ASP:N	2.34	0.42
17:Q:83:ASP:O	17:Q:86:GLU:HB2	2.19	0.42
20:T:29:LYS:O	20:T:32:ALA:HB3	2.19	0.42
1:A:127:G:O3'	17:Q:2:PRO:HD2	2.19	0.42
1:A:134:A:H2'	1:A:135:C:O4'	2.19	0.42
1:A:321:A:H2'	1:A:322:C:H6	1.85	0.42
1:A:374:A:C6	1:A:375:U:C4	3.07	0.42
1:A:453:A:H4'	16:P:72:ARG:HG3	2.02	0.42
1:A:1041:A:H2'	1:A:1042:G:O4'	2.18	0.42
1:A:1242:C:H5'	21:U:10:ARG:HH11	1.85	0.42
1:A:1441:G:H5"	1:A:1442:G:OP1	2.20	0.42
3:C:6:HIS:HD2	3:C:8:ILE:H	1.66	0.42
8:H:86:ILE:HG23	8:H:86:ILE:HD12	1.54	0.42
9:I:32:ASP:OD1	9:I:33:PHE:N	2.49	0.42
10:J:19:SER:OG	10:J:91:PRO:HB3	2.20	0.42
11:K:95:ILE:O	11:K:99:GLN:HG3	2.20	0.42
12:L:34:ARG:O	12:L:60:LEU:HD12	2.19	0.42
14:N:36:PHE:HD1	14:N:36:PHE:O	2.03	0.42
16:P:75:ARG:HB2	16:P:80:PHE:HD1	1.85	0.42
17:Q:60:ILE:HG13	17:Q:74:LEU:HD13	2.01	0.42
17:Q:76:LEU:HD23	17:Q:77:VAL:N	2.34	0.42
1:A:289:G:P	25:A:1908:HOH:O	2.77	0.42
1:A:818:G:C2'	1:A:819:A:H5"	2.49	0.42
3:C:50:ALA:HB2	3:C:75:VAL:HB	2.01	0.42
4:D:78:LEU:HD23	4:D:78:LEU:O	2.19	0.42
5:E:118:ILE:HG12	5:E:119:LEU:N	2.35	0.42
6:F:4:TYR:CE2	6:F:72:VAL:HG21	2.54	0.42
13:M:106:ASN:C	13:M:108:ARG:H	2.23	0.42
1:A:363:A:N6	1:A:364:A:C6	2.88	0.42
1:A:404:U:H2'	1:A:405:U:H6	1.85	0.42
1:A:1254:C:H2'	1:A:1255:G:C8	2.55	0.42
1:A:1317:C:OP2	14:N:17:LYS:HE2	2.20	0.42
1:A:1462:G:H2'	1:A:1463:C:H6	1.85	0.42
1:A:1502:A:H2'	1:A:1504:G:C8	2.54	0.42
3:C:83:ARG:HH22	3:C:87:LEU:HD11	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:9:VAL:HG22	6:F:60:PHE:CD1	2.55	0.42
7:G:5:ARG:HG2	7:G:6:ARG:N	2.32	0.42
13:M:16:ASP:HB2	13:M:27:LYS:HE3	2.01	0.42
16:P:23:ASP:OD1	16:P:25:ARG:HG2	2.19	0.42
18:R:50:ILE:HG12	18:R:70:ILE:HD12	2.02	0.42
19:S:38:SER:OG	19:S:71:LEU:HD12	2.20	0.42
20:T:50:GLU:H	20:T:99:LEU:CD1	2.32	0.42
1:A:945:G:C2	1:A:946:A:C8	3.08	0.42
1:A:1174:G:H2'	1:A:1175:G:C8	2.52	0.42
1:A:1193:G:OP1	3:C:167:TRP:NE1	2.52	0.42
1:A:1221:G:H2'	1:A:1222:G:O4'	2.20	0.42
1:A:1265:G:C6	1:A:1266:G:C6	3.08	0.42
2:B:50:GLU:HB3	2:B:200:ILE:O	2.20	0.42
4:D:162:LEU:HD23	4:D:162:LEU:HA	1.76	0.42
6:F:26:ILE:HG21	6:F:63:TYR:HE2	1.84	0.42
12:L:37:CYS:HB2	12:L:79:GLU:O	2.20	0.42
14:N:39:LEU:HB3	14:N:43:CYS:CB	2.50	0.42
15:O:15:PHE:CZ	15:O:85:LEU:HD21	2.55	0.42
16:P:8:ARG:HB3	16:P:28:ARG:NH1	2.35	0.42
1:A:245:C:O2	1:A:283:C:N3	2.52	0.41
1:A:502:G:H2'	1:A:503:C:O4'	2.20	0.41
1:A:540:G:H2'	1:A:541:G:O4'	2.20	0.41
1:A:907:A:C2	1:A:908:A:C8	3.08	0.41
1:A:1133:G:C2	1:A:1134:G:N7	2.88	0.41
1:A:1347:G:H2'	1:A:1373:G:N1	2.36	0.41
1:A:1465:C:H2'	1:A:1466:C:O4'	2.20	0.41
1:A:1499:A:H1'	1:A:1520:G:H5'	2.02	0.41
1:A:1501:C:N4	1:A:1504:G:C2	2.88	0.41
2:B:144:ARG:HD3	2:B:145:LEU:N	2.35	0.41
3:C:130:VAL:HG11	3:C:157:ILE:HD12	2.02	0.41
3:C:175:LEU:HD21	3:C:201:TYR:CD2	2.55	0.41
7:G:46:ALA:HA	7:G:49:ILE:HD12	2.02	0.41
7:G:57:GLU:H	7:G:57:GLU:HG3	1.60	0.41
9:I:17:VAL:HG11	9:I:81:ILE:HA	2.00	0.41
10:J:38:ILE:HA	10:J:39:PRO:HD3	1.81	0.41
13:M:8:GLU:OE2	13:M:22:ILE:HA	2.20	0.41
13:M:96:LEU:HA	13:M:97:PRO:HD3	1.82	0.41
15:O:72:ARG:HE	15:O:72:ARG:HB3	1.53	0.41
16:P:82:GLN:H	16:P:82:GLN:HG2	1.70	0.41
1:A:113:G:C1'	1:A:354:G:H5'	2.49	0.41
1:A:572:A:N3	1:A:917:G:H1'	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1174:G:C2	1:A:1175:G:N7	2.88	0.41
1:A:1200:C:H5'	1:A:1201:A:H3'	2.02	0.41
1:A:1223:C:H3'	1:A:1224:G:C5'	2.49	0.41
1:A:1279:A:H8	1:A:1282:C:N4	2.18	0.41
3:C:130:VAL:HG11	3:C:166:GLU:HG3	2.01	0.41
6:F:79:LEU:HB3	6:F:88:VAL:HG21	2.03	0.41
7:G:114:ARG:H	7:G:114:ARG:HG2	1.32	0.41
16:P:11:SER:OG	16:P:14:ASN:HB3	2.19	0.41
1:A:416:G:C5	1:A:417:C:C4	3.09	0.41
1:A:872:A:H2'	1:A:872:A:N3	2.35	0.41
1:A:1093:A:N3	1:A:1095:U:H5'	2.35	0.41
1:A:1278:U:H4'	1:A:1279:A:N3	2.35	0.41
1:A:1342:C:H4'	9:I:125:TYR:O	2.20	0.41
1:A:1381:U:O2	1:A:1381:U:H2'	2.20	0.41
4:D:25:ARG:O	4:D:25:ARG:HG2	2.20	0.41
7:G:145:ALA:C	7:G:147:ALA:H	2.24	0.41
11:K:53:SER:OG	11:K:54:ARG:N	2.54	0.41
15:O:18:PHE:CE2	15:O:21:ASP:HB2	2.55	0.41
1:A:146:G:N1	1:A:147:G:C5	2.89	0.41
1:A:324:G:H5"	1:A:324:G:C8	2.52	0.41
1:A:1236:A:O3'	1:A:1304:G:H5'	2.21	0.41
1:A:1240:U:C2	7:G:32:ARG:HD2	2.55	0.41
1:A:1363:A:H4'	1:A:1364:U:H2'	2.02	0.41
4:D:11:LEU:HD13	4:D:66:ARG:CD	2.51	0.41
8:H:95:VAL:HG21	8:H:133:LEU:HG	2.02	0.41
9:I:10:ARG:HG3	9:I:11:LYS:HB2	2.02	0.41
13:M:84:ILE:H	13:M:84:ILE:HG12	1.57	0.41
1:A:229:U:H2'	1:A:230:G:C8	2.56	0.41
1:A:1248:A:O2'	9:I:36:TYR:HE1	2.03	0.41
1:A:1286:A:H2'	1:A:1287:A:H4'	2.03	0.41
6:F:72:VAL:O	6:F:75:LEU:HB3	2.21	0.41
8:H:83:ILE:HG23	8:H:83:ILE:HD12	1.78	0.41
15:O:12:ILE:HG23	15:O:27:VAL:HG11	2.02	0.41
17:Q:43:LEU:HD23	17:Q:43:LEU:HA	1.70	0.41
1:A:132:C:H2'	1:A:133:U:H6	1.85	0.41
1:A:512:U:P	4:D:46:LYS:HZ2	2.44	0.41
2:B:144:ARG:HH11	2:B:145:LEU:HD23	1.85	0.41
4:D:196:LEU:HA	4:D:197:PRO:HD2	1.82	0.41
5:E:9:LYS:HE3	5:E:108:ALA:HB1	2.01	0.41
5:E:76:ILE:HD13	5:E:118:ILE:HD11	2.03	0.41
7:G:111:ARG:HB2	7:G:119:ARG:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:3:LYS:HD3	16:P:65:GLN:O	2.21	0.41
1:A:778:G:H2'	1:A:779:C:C6	2.55	0.41
1:A:927:G:H1	1:A:1390:U:H3	1.68	0.41
1:A:950:U:H2'	1:A:951:G:H8	1.86	0.41
1:A:1245:A:OP2	21:U:9:ARG:NH1	2.54	0.41
1:A:1408:A:H2'	1:A:1409:C:H6	1.85	0.41
2:B:118:LEU:HA	2:B:118:LEU:HD23	1.78	0.41
3:C:67:THR:HG22	3:C:69:HIS:CE1	2.56	0.41
12:L:41:ARG:HD3	12:L:42:THR:N	2.35	0.41
12:L:77:LEU:HD21	12:L:107:ALA:CB	2.51	0.41
12:L:85:ILE:HG23	12:L:98:TYR:HB3	2.03	0.41
13:M:80:ARG:HB3	13:M:80:ARG:NH1	2.36	0.41
17:Q:60:ILE:HG13	17:Q:74:LEU:CD1	2.51	0.41
19:S:71:LEU:C	19:S:73:GLU:H	2.24	0.41
20:T:70:SER:HA	20:T:73:HIS:CD2	2.55	0.41
1:A:379:C:C2'	1:A:380:G:H5'	2.50	0.41
1:A:416:G:H2'	1:A:417:C:C6	2.56	0.41
1:A:491:G:C4	1:A:492:G:C8	3.09	0.41
1:A:950:U:H2'	1:A:951:G:C8	2.55	0.41
1:A:1287:A:H2'	1:A:1288:A:C8	2.55	0.41
2:B:74:LYS:HE2	2:B:74:LYS:HB3	1.88	0.41
4:D:205:GLU:OE1	5:E:100:VAL:HG23	2.20	0.41
5:E:84:PHE:CB	5:E:134:ALA:HB2	2.51	0.41
11:K:110:ASP:OD2	18:R:88:LYS:HE2	2.21	0.41
12:L:7:ILE:HA	12:L:7:ILE:HD12	1.39	0.41
13:M:108:ARG:CD	13:M:114:ARG:HE	2.34	0.41
15:O:18:PHE:CD2	15:O:18:PHE:N	2.88	0.41
17:Q:51:TYR:CE1	17:Q:73:VAL:HG11	2.55	0.41
1:A:232:G:H2'	1:A:233:C:C6	2.56	0.41
1:A:322:C:O2'	1:A:323:U:H5'	2.21	0.41
1:A:407:G:O5'	1:A:407:G:H8	2.04	0.41
1:A:451:A:H2	1:A:480:U:C5	2.39	0.41
1:A:500:G:H2'	1:A:501:C:C6	2.56	0.41
1:A:560:U:H5'	1:A:566:G:C2	2.56	0.41
1:A:803:G:C5	1:A:804:U:C4	3.09	0.41
1:A:907:A:N3	1:A:907:A:H2'	2.35	0.41
1:A:909:A:H2'	1:A:910:C:O4'	2.21	0.41
1:A:922:G:H2'	1:A:923:A:C8	2.56	0.41
1:A:946:A:H2'	1:A:947:G:C8	2.56	0.41
1:A:1077:G:N2	1:A:1080:A:OP2	2.48	0.41
1:A:1152:A:H5'	10:J:13:HIS:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1188:A:O3'	14:N:58:LYS:NZ	2.36	0.41
1:A:1196:U:OP1	1:A:1197:G:H5'	2.20	0.41
1:A:1250:A:H2'	1:A:1251:A:C8	2.56	0.41
1:A:1287:A:H2	1:A:1353:G:N3	2.18	0.41
1:A:1393:U:O4'	1:A:1502:A:H5'	2.21	0.41
2:B:24:TRP:HB3	2:B:40:HIS:HE1	1.85	0.41
2:B:62:ALA:CB	2:B:222:ILE:HG23	2.51	0.41
3:C:21:ARG:O	3:C:58:GLU:HA	2.21	0.41
3:C:155:GLY:CA	3:C:164:ARG:H	2.31	0.41
3:C:182:ILE:HA	3:C:202:ILE:O	2.21	0.41
4:D:76:ARG:O	4:D:80:GLU:HG2	2.21	0.41
6:F:94:GLN:HG3	18:R:32:ARG:HD3	2.02	0.41
8:H:86:ILE:HD13	8:H:86:ILE:HA	1.81	0.41
11:K:111:ASP:O	11:K:112:THR:C	2.59	0.41
13:M:105:THR:OG1	13:M:106:ASN:HB2	2.21	0.41
15:O:85:LEU:HD23	15:O:85:LEU:HA	1.76	0.41
18:R:47:THR:HG22	18:R:48:GLY:H	1.86	0.41
20:T:79:ARG:O	20:T:82:SER:HB3	2.21	0.41
21:U:13:ILE:HG13	21:U:22:ARG:NH2	2.36	0.41
1:A:11:G:H2'	1:A:12:U:H6	1.86	0.41
1:A:376:G:OP2	16:P:67:THR:HG21	2.21	0.41
1:A:390:C:H4'	16:P:28:ARG:NH2	2.31	0.41
1:A:1005:A:C1'	1:A:1026:G:H22	2.32	0.41
1:A:1145:C:O2'	1:A:1146:A:P	2.79	0.41
1:A:1306:A:H2'	1:A:1307:U:O4'	2.22	0.41
2:B:84:GLU:HB3	2:B:219:VAL:HG21	2.03	0.41
2:B:217:ARG:O	2:B:220:ASP:HB2	2.21	0.41
3:C:22:TRP:CB	3:C:59:ARG:HB3	2.41	0.41
15:O:70:LEU:HD13	15:O:78:TYR:HB2	2.04	0.41
17:Q:40:LYS:HE3	17:Q:42:TYR:OH	2.19	0.41
1:A:6:G:N2	5:E:98:THR:HG23	2.36	0.40
1:A:359:U:H2'	1:A:360:A:H8	1.86	0.40
1:A:410:G:H2'	1:A:429:U:C4	2.55	0.40
1:A:460:A:C6	1:A:462:G:C5	3.09	0.40
1:A:581:G:O3'	15:O:64:ARG:NH2	2.54	0.40
1:A:945:G:H21	1:A:1334:G:H4'	1.86	0.40
1:A:1447:G:C2	1:A:1448:C:C6	3.09	0.40
2:B:20:GLU:HB2	2:B:190:THR:HB	2.03	0.40
3:C:39:ILE:HG21	3:C:57:ILE:HD11	2.02	0.40
3:C:180:ALA:O	3:C:181:ASN:HB3	2.21	0.40
4:D:36:ARG:N	4:D:37:PRO:HD3	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:133:LEU:HA	8:H:133:LEU:HD23	1.77	0.40
10:J:38:ILE:HG12	10:J:71:LEU:HG	2.02	0.40
12:L:8:ASN:O	12:L:11:VAL:HG22	2.21	0.40
12:L:33:ARG:O	12:L:84:LEU:HD12	2.21	0.40
13:M:23:TYR:HD2	13:M:70:LEU:HB3	1.86	0.40
13:M:108:ARG:HD3	13:M:114:ARG:HE	1.86	0.40
15:O:43:LEU:HD11	15:O:53:HIS:HA	2.02	0.40
16:P:14:ASN:CA	16:P:42:ARG:HH21	2.28	0.40
1:A:186:C:H5'	20:T:78:ALA:HB1	2.04	0.40
1:A:232:G:H2'	1:A:233:C:H6	1.87	0.40
1:A:394:G:H2'	1:A:395:C:C6	2.56	0.40
1:A:695:A:C2	1:A:696:A:C4	3.10	0.40
1:A:1036:G:H2'	1:A:1037:C:O4'	2.21	0.40
2:B:24:TRP:CG	2:B:25:ASN:N	2.90	0.40
3:C:95:THR:HG23	3:C:99:VAL:HG11	2.03	0.40
4:D:12:CYS:SG	4:D:19:LEU:O	2.79	0.40
5:E:5:ASP:CG	5:E:6:PHE:H	2.24	0.40
5:E:10:MET:O	5:E:11:ILE:HD13	2.22	0.40
16:P:19:ILE:HG22	16:P:36:ILE:HG13	2.03	0.40
17:Q:31:LEU:HA	17:Q:31:LEU:HD12	1.70	0.40
1:A:15:G:O2'	5:E:24:ARG:HD3	2.21	0.40
1:A:227:G:N2	16:P:62:VAL:O	2.54	0.40
1:A:918:A:H2'	1:A:919:A:O4'	2.20	0.40
1:A:922:G:C2	1:A:1396:A:C6	3.10	0.40
3:C:21:ARG:HA	14:N:54:PRO:HB3	2.02	0.40
4:D:203:VAL:H	4:D:203:VAL:HG23	1.69	0.40
6:F:18:GLN:O	6:F:22:GLU:HG2	2.20	0.40
9:I:53:VAL:HG21	9:I:85:LEU:CD2	2.50	0.40
9:I:97:LYS:HB3	9:I:98:PRO:HD3	2.03	0.40
13:M:48:LEU:HD22	13:M:53:VAL:HG23	2.03	0.40
16:P:74:LEU:HB3	16:P:79:VAL:HG23	2.03	0.40
1:A:620:C:H2'	1:A:621:A:O4'	2.21	0.40
1:A:872:A:C8	1:A:874:G:C8	3.10	0.40
1:A:1117:G:O3'	9:I:104:ARG:NE	2.54	0.40
1:A:1202:G:H1'	14:N:29:ARG:HD2	2.03	0.40
3:C:167:TRP:CE3	3:C:168:ALA:N	2.86	0.40
3:C:186:PHE:HE2	3:C:188:LEU:HD23	1.86	0.40
6:F:67:MET:HB2	6:F:68:PRO:HD2	2.04	0.40
8:H:105:ARG:HD3	8:H:105:ARG:HA	1.92	0.40
11:K:58:PRO:HG3	11:K:90:GLY:N	2.37	0.40
13:M:14:ARG:HG3	13:M:14:ARG:H	1.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:52:GLU:HG2	13:M:55:ARG:HH21	1.86	0.40
14:N:31:ARG:HB2	14:N:31:ARG:HH11	1.87	0.40
16:P:79:VAL:HG23	16:P:79:VAL:H	1.66	0.40
19:S:30:LEU:HB3	19:S:31:ILE:H	1.63	0.40
19:S:70:LYS:N	19:S:73:GLU:OE2	2.39	0.40
20:T:42:GLN:HA	20:T:42:GLN:OE1	2.22	0.40
20:T:59:ALA:O	20:T:60:GLU:C	2.58	0.40
1:A:136:C:H1'	16:P:1:MET:HG3	2.03	0.40
1:A:273:A:C2'	1:A:274:A:H5'	2.51	0.40
1:A:357:G:N1	1:A:358:U:C4	2.90	0.40
1:A:633:G:C5	1:A:634:C:C5	3.09	0.40
1:A:1338:G:C6	1:A:1339:A:C6	3.09	0.40
1:A:1349:A:C2	1:A:1374:A:C4	3.09	0.40
2:B:16:HIS:HB3	2:B:17:PHE:H	1.76	0.40
2:B:116:GLU:HG2	2:B:153:ARG:HH12	1.85	0.40
2:B:214:ILE:HD13	2:B:214:ILE:HA	1.94	0.40
3:C:26:LYS:HB2	3:C:27:LYS:H	1.67	0.40
12:L:24:VAL:HG12	12:L:24:VAL:O	2.22	0.40
18:R:88:LYS:HE3	18:R:88:LYS:HB3	1.61	0.40
19:S:11:VAL:HG13	19:S:38:SER:HB2	2.03	0.40
20:T:49:ALA:HB3	20:T:99:LEU:HB2	2.03	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%)	199 (86%)	30 (13%)	3 (1%)	10 42
3	C	204/239 (85%)	171 (84%)	32 (16%)	1 (0%)	25 59
4	D	206/209 (99%)	187 (91%)	19 (9%)	0	100 100
5	E	148/162 (91%)	131 (88%)	16 (11%)	1 (1%)	19 54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
6	F	99/101 (98%)	90 (91%)	9 (9%)	0	100 100
7	G	153/156 (98%)	138 (90%)	14 (9%)	1 (1%)	19 54
8	H	136/138 (99%)	129 (95%)	7 (5%)	0	100 100
9	I	125/128 (98%)	113 (90%)	11 (9%)	1 (1%)	16 51
10	J	96/105 (91%)	78 (81%)	16 (17%)	2 (2%)	5 33
11	K	114/129 (88%)	100 (88%)	13 (11%)	1 (1%)	14 49
12	L	121/135 (90%)	113 (93%)	7 (6%)	1 (1%)	16 51
13	M	116/126 (92%)	102 (88%)	14 (12%)	0	100 100
14	N	58/61 (95%)	50 (86%)	8 (14%)	0	100 100
15	O	85/89 (96%)	76 (89%)	9 (11%)	0	100 100
16	P	81/88 (92%)	78 (96%)	3 (4%)	0	100 100
17	Q	97/105 (92%)	87 (90%)	10 (10%)	0	100 100
18	R	68/88 (77%)	61 (90%)	7 (10%)	0	100 100
19	S	78/93 (84%)	70 (90%)	7 (9%)	1 (1%)	10 42
20	T	97/106 (92%)	80 (82%)	15 (16%)	2 (2%)	5 33
21	U	22/27 (82%)	21 (96%)	1 (4%)	0	100 100
All	All	2336/2541 (92%)	2074 (89%)	248 (11%)	14 (1%)	22 56

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	21	ARG
19	S	31	ILE
12	L	28	LYS
3	C	15	THR
20	T	73	HIS
2	B	95	GLN
9	I	119	ALA
10	J	54	PHE
11	K	117	ASN
20	T	84	LEU
7	G	114	ARG
5	E	55	VAL
10	J	34	VAL
2	B	229	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%)	157 (78%)	45 (22%)	1	4
3	C	160/188 (85%)	124 (78%)	36 (22%)	1	4
4	D	180/181 (99%)	150 (83%)	30 (17%)	2	10
5	E	115/123 (94%)	89 (77%)	26 (23%)	1	4
6	F	90/90 (100%)	75 (83%)	15 (17%)	2	10
7	G	126/127 (99%)	101 (80%)	25 (20%)	1	6
8	H	119/119 (100%)	90 (76%)	29 (24%)	0	3
9	I	98/99 (99%)	78 (80%)	20 (20%)	1	6
10	J	87/92 (95%)	73 (84%)	14 (16%)	2	12
11	K	88/99 (89%)	73 (83%)	15 (17%)	1	10
12	L	103/110 (94%)	77 (75%)	26 (25%)	0	3
13	M	94/101 (93%)	67 (71%)	27 (29%)	0	2
14	N	49/50 (98%)	41 (84%)	8 (16%)	2	11
15	O	79/80 (99%)	64 (81%)	15 (19%)	1	7
16	P	72/74 (97%)	58 (81%)	14 (19%)	1	6
17	Q	94/97 (97%)	81 (86%)	13 (14%)	3	17
18	R	61/77 (79%)	50 (82%)	11 (18%)	1	8
19	S	71/80 (89%)	56 (79%)	15 (21%)	1	5
20	T	76/82 (93%)	59 (78%)	17 (22%)	1	4
21	U	19/22 (86%)	15 (79%)	4 (21%)	1	5
All	All	1983/2111 (94%)	1578 (80%)	405 (20%)	1	6

All (405) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	8	LYS
2	B	10	LEU
2	B	16	HIS

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Mol	Chain	Res	Type
2	B	21	ARG
2	B	23	ARG
2	B	24	TRP
2	B	33	TYR
2	B	45	GLN
2	B	56	ARG
2	B	67	THR
2	B	81	VAL
2	B	82	ARG
2	B	97	TRP
2	B	98	LEU
2	B	103	THR
2	B	107	THR
2	B	110	GLN
2	B	111	ARG
2	B	121	LEU
2	B	129	GLU
2	B	142	LEU
2	B	144	ARG
2	B	153	ARG
2	B	157	ARG
2	B	158	LEU
2	B	162	ILE
2	B	163	PHE
2	B	164	VAL
2	B	165	VAL
2	B	175	ARG
2	B	178	ARG
2	B	180	LEU
2	B	187	LEU
2	B	190	THR
2	B	191	ASP
2	B	196	LEU
2	B	197	VAL
2	B	200	ILE
2	B	204	ASN
2	B	206	ASP
2	B	208	ILE
2	B	209	ARG
2	B	213	LEU
2	B	221	LEU
2	B	231	GLU

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Mol	Chain	Res	Type
3	C	3	ASN
3	C	11	ARG
3	C	14	ILE
3	C	15	THR
3	C	22	TRP
3	C	27	LYS
3	C	28	GLN
3	C	33	LEU
3	C	34	LEU
3	C	42	LEU
3	C	46	GLU
3	C	52	LEU
3	C	58	GLU
3	C	63	ASN
3	C	69	HIS
3	C	79	ARG
3	C	89	GLU
3	C	90	GLU
3	C	91	LEU
3	C	95	THR
3	C	102	ASN
3	C	108	ASN
3	C	111	LEU
3	C	112	SER
3	C	116	VAL
3	C	120	VAL
3	C	124	ILE
3	C	135	LYS
3	C	139	GLN
3	C	162	GLN
3	C	167	TRP
3	C	172	ARG
3	C	178	LEU
3	C	188	LEU
3	C	195	VAL
3	C	202	ILE
4	D	5	ILE
4	D	9	CYS
4	D	10	ARG
4	D	15	GLU
4	D	19	LEU
4	D	20	TYR

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Mol	Chain	Res	Type
4	D	24	GLU
4	D	25	ARG
4	D	34	GLU
4	D	35	ARG
4	D	58	LEU
4	D	64	LEU
4	D	65	ARG
4	D	70	ILE
4	D	73	ARG
4	D	76	ARG
4	D	83	SER
4	D	107	ARG
4	D	108	LEU
4	D	122	ARG
4	D	127	THR
4	D	135	LEU
4	D	141	ARG
4	D	145	GLU
4	D	165	MET
4	D	170	VAL
4	D	174	LEU
4	D	176	LEU
4	D	187	ARG
4	D	194	LEU
5	E	12	LEU
5	E	13	ILE
5	E	15	ARG
5	E	19	MET
5	E	31	LEU
5	E	38	GLN
5	E	41	VAL
5	E	43	LEU
5	E	53	LEU
5	E	57	LYS
5	E	64	ARG
5	E	65	ASN
5	E	76	ILE
5	E	79	GLU
5	E	80	ILE
5	E	100	VAL
5	E	120	THR
5	E	123	LEU

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Mol	Chain	Res	Type
5	E	125	SER
5	E	129	ILE
5	E	130	ASN
5	E	136	MET
5	E	144	THR
5	E	147	ASP
5	E	150	ARG
5	E	151	LEU
6	F	11	ASN
6	F	16	GLN
6	F	19	LEU
6	F	27	GLN
6	F	43	LEU
6	F	47	ARG
6	F	52	ILE
6	F	69	GLU
6	F	77	ARG
6	F	79	LEU
6	F	83	ASP
6	F	84	ASN
6	F	87	ARG
6	F	93	SER
6	F	94	GLN
7	G	3	ARG
7	G	4	ARG
7	G	8	GLU
7	G	10	ARG
7	G	15	ASP
7	G	16	LEU
7	G	18	TYR
7	G	31	MET
7	G	45	ASP
7	G	51	GLN
7	G	54	THR
7	G	56	GLN
7	G	57	GLU
7	G	59	LEU
7	G	67	GLU
7	G	91	VAL
7	G	94	ARG
7	G	106	GLN
7	G	110	GLN

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Mol	Chain	Res	Type
7	G	114	ARG
7	G	115	ARG
7	G	125	MET
7	G	141	VAL
7	G	144	MET
7	G	155	ARG
8	H	3	THR
8	H	5	PRO
8	H	11	THR
8	H	18	ARG
8	H	19	VAL
8	H	21	LYS
8	H	24	THR
8	H	25	ASP
8	H	26	VAL
8	H	37	ARG
8	H	39	LEU
8	H	45	ILE
8	H	50	ARG
8	H	51	VAL
8	H	63	LEU
8	H	68	ARG
8	H	69	ARG
8	H	81	HIS
8	H	83	ILE
8	H	85	ARG
8	H	86	ILE
8	H	91	ARG
8	H	92	ARG
8	H	95	VAL
8	H	104	ARG
8	H	105	ARG
8	H	122	ARG
8	H	127	LEU
8	H	133	LEU
9	I	2	GLU
9	I	10	ARG
9	I	11	LYS
9	I	12	GLU
9	I	16	ARG
9	I	23	ASN
9	I	27	THR

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Mol	Chain	Res	Type
9	I	56	LEU
9	I	58	HIS
9	I	59	PHE
9	I	62	TYR
9	I	71	SER
9	I	78	LYS
9	I	81	ILE
9	I	87	GLN
9	I	102	LEU
9	I	108	VAL
9	I	110	GLU
9	I	114	TYR
9	I	118	LYS
10	J	4	ILE
10	J	15	THR
10	J	16	LEU
10	J	28	ARG
10	J	30	SER
10	J	38	ILE
10	J	40	LEU
10	J	44	VAL
10	J	57	LYS
10	J	75	ILE
10	J	78	ASN
10	J	80	LYS
10	J	85	LEU
10	J	88	LEU
11	K	11	LYS
11	K	12	ARG
11	K	14	VAL
11	K	24	SER
11	K	29	ILE
11	K	33	THR
11	K	48	ILE
11	K	73	MET
11	K	79	SER
11	K	95	ILE
11	K	101	SER
11	K	109	VAL
11	K	111	ASP
11	K	116	HIS
11	K	119	CYS

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Mol	Chain	Res	Type
12	L	7	ILE
12	L	10	LEU
12	L	19	ARG
12	L	27	LEU
12	L	33	ARG
12	L	37	CYS
12	L	41	ARG
12	L	42	THR
12	L	43	VAL
12	L	54	LYS
12	L	58	VAL
12	L	59	ARG
12	L	60	LEU
12	L	61	THR
12	L	62	SER
12	L	64	TYR
12	L	67	THR
12	L	80	HIS
12	L	82	VAL
12	L	89	ARG
12	L	96	VAL
12	L	98	TYR
12	L	114	LYS
12	L	116	SER
12	L	122	THR
12	L	126	LYS
13	M	16	ASP
13	M	17	VAL
13	M	27	LYS
13	M	32	GLU
13	M	34	LEU
13	M	44	ARG
13	M	45	VAL
13	M	48	LEU
13	M	53	VAL
13	M	55	ARG
13	M	57	ARG
13	M	67	GLU
13	M	70	LEU
13	M	71	ARG
13	M	73	GLU
13	M	74	VAL

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Mol	Chain	Res	Type
13	M	80	ARG
13	M	81	LEU
13	M	83	ASP
13	M	84	ILE
13	M	90	LEU
13	M	99	ARG
13	M	102	ARG
13	M	109	THR
13	M	110	ARG
13	M	114	ARG
13	M	115	LYS
14	N	17	LYS
14	N	19	ARG
14	N	22	THR
14	N	24	CYS
14	N	31	ARG
14	N	35	ARG
14	N	36	PHE
14	N	53	LEU
15	O	3	ILE
15	O	4	THR
15	O	6	GLU
15	O	7	GLU
15	O	26	GLU
15	O	31	LEU
15	O	32	LEU
15	O	33	THR
15	O	34	LEU
15	O	36	ILE
15	O	39	LEU
15	O	47	LYS
15	O	72	ARG
15	O	81	LEU
15	O	87	ILE
16	P	1	MET
16	P	8	ARG
16	P	17	TYR
16	P	26	ARG
16	P	31	LYS
16	P	44	THR
16	P	45	THR
16	P	52	ASP

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Mol	Chain	Res	Type
16	P	54	GLU
16	P	55	ARG
16	P	57	ARG
16	P	62	VAL
16	P	68	ASP
16	P	76	GLN
17	Q	14	LYS
17	Q	19	VAL
17	Q	23	VAL
17	Q	25	ARG
17	Q	34	LYS
17	Q	36	ILE
17	Q	38	ARG
17	Q	53	LEU
17	Q	59	ILE
17	Q	60	ILE
17	Q	87	LYS
17	Q	91	ARG
17	Q	98	LEU
18	R	19	LYS
18	R	26	LEU
18	R	28	GLU
18	R	35	ARG
18	R	46	GLU
18	R	47	THR
18	R	54	ARG
18	R	59	SER
18	R	68	LYS
18	R	84	LYS
18	R	87	ARG
19	S	4	SER
19	S	5	LEU
19	S	6	LYS
19	S	7	LYS
19	S	29	ARG
19	S	30	LEU
19	S	32	LYS
19	S	33	THR
19	S	35	SER
19	S	36	ARG
19	S	43	GLU
19	S	63	THR

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Mol	Chain	Res	Type
19	S	64	GLU
19	S	65	ASN
19	S	71	LEU
20	T	9	ASN
20	T	11	SER
20	T	19	SER
20	T	29	LYS
20	T	33	ILE
20	T	35	THR
20	T	36	LEU
20	T	37	SER
20	T	48	LYS
20	T	62	LEU
20	T	72	LEU
20	T	74	LYS
20	T	75	ASN
20	T	84	LEU
20	T	87	LYS
20	T	92	LEU
20	T	99	LEU
21	U	10	ARG
21	U	12	LYS
21	U	13	ILE
21	U	15	ARG

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

Mol	Chain	Res	Type
2	B	204	ASN
3	C	6	HIS
4	D	119	GLN
6	F	11	ASN
9	I	73	GLN
10	J	62	HIS
17	Q	26	GLN
20	T	18	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1508/1522 (99%)	369 (24%)	48 (3%)

All (369) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	7	G
1	A	9	G
1	A	31	G
1	A	32	A
1	A	33	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	49	U
1	A	50	A
1	A	51	A
1	A	54	C
1	A	67	C
1	A	69	G
1	A	81	U
1	A	82	U
1	A	91	C
1	A	101	A
1	A	106	C
1	A	108	G
1	A	109	A
1	A	116	A
1	A	117	G
1	A	121	C
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	144	G
1	A	151	A
1	A	161	A
1	A	163	C
1	A	176	C
1	A	180	U
1	A	182	U
1	A	183	G
1	A	190(E)	U
1	A	195	A

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Mol	Chain	Res	Type
1	A	197	A
1	A	201	C
1	A	202	U
1	A	203	U
1	A	204	U
1	A	216	G
1	A	217	C
1	A	220	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	266	G
1	A	267	C
1	A	279	A
1	A	289	G
1	A	299	G
1	A	301	G
1	A	321	A
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	346	G
1	A	350	G
1	A	351	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	356	A
1	A	367	U
1	A	372	C
1	A	373	A
1	A	374	A
1	A	382	A
1	A	390	C
1	A	392	G

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Mol	Chain	Res	Type
1	A	397	A
1	A	398	C
1	A	406	G
1	A	409	G
1	A	411	A
1	A	412	A
1	A	419	C
1	A	421	U
1	A	424	G
1	A	429	U
1	A	445	G
1	A	450	G
1	A	452	A
1	A	460	A
1	A	461	C
1	A	476	G
1	A	478	A
1	A	481	G
1	A	485	G
1	A	486	U
1	A	488	C
1	A	497	A
1	A	498	U
1	A	509	A
1	A	510	A
1	A	511	C
1	A	517	G
1	A	518	C
1	A	519	C
1	A	522	C
1	A	527	7MG
1	A	532	A
1	A	533	A
1	A	536	C
1	A	547	A
1	A	559	A
1	A	560	U
1	A	562	C
1	A	563	A
1	A	564	C
1	A	568	G
1	A	572	A

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Mol	Chain	Res	Type
1	A	573	A
1	A	575	G
1	A	576	G
1	A	577	G
1	A	579	G
1	A	587	G
1	A	588	G
1	A	616	G
1	A	617	G
1	A	620	C
1	A	631	G
1	A	641	U
1	A	644	G
1	A	652	U
1	A	653	A
1	A	656	C
1	A	662	G
1	A	665	A
1	A	670	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	703	G
1	A	722	A
1	A	723	U
1	A	724	G
1	A	731	G
1	A	733	A
1	A	734	G
1	A	749	C
1	A	755	G
1	A	777	A
1	A	781	A
1	A	782	A
1	A	792	A
1	A	793	U
1	A	794	A
1	A	799	G
1	A	812	C

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Mol	Chain	Res	Type
1	A	813	U
1	A	815	A
1	A	817	C
1	A	819	A
1	A	828	A
1	A	829	G
1	A	838	G
1	A	839	U
1	A	840	C
1	A	841	U
1	A	848	C
1	A	867	G
1	A	869	G
1	A	871	U
1	A	872	A
1	A	876	G
1	A	887	G
1	A	889	A
1	A	902	G
1	A	910	C
1	A	914	A
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	940	C
1	A	947	G
1	A	960	U
1	A	966	M2G
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	986	A
1	A	987	G
1	A	989	C
1	A	990	C
1	A	991	U

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Mol	Chain	Res	Type
1	A	992	U
1	A	993	G
1	A	1002	G
1	A	1004	A
1	A	1005	A
1	A	1006	C
1	A	1007	C
1	A	1010	G
1	A	1011	G
1	A	1018	C
1	A	1023	G
1	A	1024	G
1	A	1025	U
1	A	1026	G
1	A	1030(C)	G
1	A	1031	G
1	A	1045	C
1	A	1050	G
1	A	1051	C
1	A	1057	G
1	A	1064	G
1	A	1065	U
1	A	1066	C
1	A	1068	G
1	A	1085	U
1	A	1086	U
1	A	1092	A
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1107	C
1	A	1108	G
1	A	1110	A
1	A	1124	G
1	A	1126	U
1	A	1127	G
1	A	1128	C
1	A	1129	C
1	A	1130	A
1	A	1131	G
1	A	1132	C
1	A	1137	C

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Mol	Chain	Res	Type
1	A	1138	G
1	A	1139	G
1	A	1140	C
1	A	1141	C
1	A	1146	A
1	A	1148	U
1	A	1149	C
1	A	1152	A
1	A	1159	U
1	A	1160	G
1	A	1161	C
1	A	1164	G
1	A	1165	C
1	A	1171	G
1	A	1174	G
1	A	1175	G
1	A	1182	G
1	A	1183	A
1	A	1184	G
1	A	1190	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	1212	U
1	A	1214	C
1	A	1222	G
1	A	1224	G
1	A	1225	A
1	A	1227	A
1	A	1238	A
1	A	1241	G
1	A	1243	C
1	A	1253	G
1	A	1257	U
1	A	1258	G
1	A	1260	C
1	A	1261	A
1	A	1262	C
1	A	1268	A

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Mol	Chain	Res	Type
1	A	1270	C
1	A	1278	U
1	A	1279	A
1	A	1280	A
1	A	1281	U
1	A	1282	C
1	A	1286	A
1	A	1287	A
1	A	1289	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	1311	G
1	A	1312	G
1	A	1320	C
1	A	1322	C
1	A	1334	G
1	A	1335	C
1	A	1336	C
1	A	1338	G
1	A	1346	A
1	A	1347	G
1	A	1348	U
1	A	1351	U
1	A	1352	C
1	A	1353	G
1	A	1357	A
1	A	1359	C
1	A	1363	A
1	A	1368	G
1	A	1370	G
1	A	1377	A
1	A	1378	C
1	A	1379	G
1	A	1381	U
1	A	1397	C

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Mol	Chain	Res	Type
1	A	1398	A
1	A	1399	C
1	A	1400	5MC
1	A	1411	C
1	A	1414	U
1	A	1437	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	1474	G
1	A	1483	A
1	A	1487	G
1	A	1491	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	1502	A
1	A	1503	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1507	A
1	A	1520	G
1	A	1529	G
1	A	1530	G
1	A	1531	A
1	A	1533	C
1	A	1541	PSU

All (48) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U

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Mol	Chain	Res	Type
1	A	115	G
1	A	129(A)	G
1	A	181	G
1	A	182	U
1	A	243	A
1	A	250	A
1	A	251	G
1	A	328	C
1	A	350	G
1	A	372	C
1	A	428	G
1	A	484	G
1	A	485	G
1	A	509	A
1	A	518	C
1	A	532	A
1	A	559	A
1	A	587	G
1	A	686	U
1	A	687	A
1	A	701	C
1	A	748	C
1	A	812	C
1	A	870	U
1	A	913	A
1	A	975	A
1	A	991	U
1	A	992	U
1	A	1004	A
1	A	1049	U
1	A	1065	U
1	A	1139	G
1	A	1145	C
1	A	1182	G
1	A	1183	A
1	A	1196	U
1	A	1201	A
1	A	1256	A
1	A	1257	U
1	A	1285	A
1	A	1300	G
1	A	1305	G

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Mol	Chain	Res	Type
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	M2G	A	966	1	20,27,28	2.03	4 (20%)	19,40,43	1.32	2 (10%)
1	2MG	A	1207	1	18,26,27	1.78	4 (22%)	16,38,41	1.36	3 (18%)
1	4OC	A	1402	1	20,23,24	1.36	2 (10%)	25,32,35	1.03	2 (8%)
1	5MC	A	1400	1	19,22,23	1.93	5 (26%)	26,32,35	0.94	1 (3%)
1	PSU	A	516	1,23	18,21,22	1.09	2 (11%)	21,30,33	2.28	6 (28%)
12	0TD	L	92	12	8,9,10	2.31	2 (25%)	6,11,13	2.12	2 (33%)
1	UR3	A	1498	1	19,22,23	1.42	3 (15%)	26,32,35	1.59	3 (11%)
1	MA6	A	1519	1	19,26,27	2.13	5 (26%)	18,38,41	0.72	0
1	5MC	A	1404	1	19,22,23	1.71	4 (21%)	26,32,35	1.11	2 (7%)
1	PSU	A	1540	1,23	18,21,22	1.26	1 (5%)	21,30,33	1.71	4 (19%)
1	MA6	A	1518	1	19,26,27	1.13	2 (10%)	18,38,41	1.47	2 (11%)
1	5MC	A	1407	1	19,22,23	2.04	4 (21%)	26,32,35	1.28	4 (15%)
1	7MG	A	527	1	23,26,27	3.74	3 (13%)	27,39,42	2.39	10 (37%)
1	5MC	A	967	1	19,22,23	1.39	2 (10%)	26,32,35	0.94	1 (3%)
1	PSU	A	1541	1	18,21,22	1.31	2 (11%)	21,30,33	1.90	6 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	M2G	A	966	1	-	6/7/29/30	0/3/3/3
1	2MG	A	1207	1	-	1/5/27/28	0/3/3/3
1	4OC	A	1402	1	-	4/9/29/30	0/2/2/2
1	5MC	A	1400	1	-	2/7/25/26	0/2/2/2
1	PSU	A	516	1,23	-	0/7/25/26	0/2/2/2
12	0TD	L	92	12	-	2/7/12/14	-
1	UR3	A	1498	1	-	4/7/25/26	0/2/2/2
1	MA6	A	1519	1	-	2/7/29/30	0/3/3/3
1	5MC	A	1404	1	-	0/7/25/26	0/2/2/2
1	PSU	A	1540	1,23	-	0/7/25/26	0/2/2/2
1	MA6	A	1518	1	-	2/7/29/30	0/3/3/3
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
1	7MG	A	527	1	-	2/7/37/38	0/3/3/3
1	5MC	A	967	1	-	0/7/25/26	0/2/2/2
1	PSU	A	1541	1	-	3/7/25/26	0/2/2/2

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	7MG	C8-N9	-14.51	1.36	1.45
1	A	527	7MG	C5-N7	8.89	1.46	1.35
1	A	1407	5MC	C5-C4	6.43	1.49	1.44
1	A	966	M2G	C2-N3	5.06	1.37	1.30
1	A	966	M2G	C2-N2	5.04	1.44	1.35
1	A	1519	MA6	C6-N1	4.97	1.39	1.32
1	A	967	5MC	C5-C4	-4.79	1.40	1.44
1	A	1541	PSU	C6-C5	4.66	1.40	1.35
1	A	1519	MA6	C4-N3	4.66	1.41	1.35
12	L	92	0TD	CB-CA	4.57	1.56	1.54
1	A	1540	PSU	C6-C5	4.48	1.40	1.35
1	A	1404	5MC	C2-N1	4.21	1.48	1.40
1	A	1400	5MC	C2-N1	4.14	1.48	1.40
1	A	1207	2MG	C6-N1	4.13	1.44	1.37
1	A	966	M2G	C6-N1	4.12	1.44	1.37
1	A	1400	5MC	C2-N3	3.99	1.44	1.36
1	A	1402	4OC	C2-N3	3.95	1.44	1.36
1	A	1400	5MC	C6-C5	3.93	1.41	1.34
1	A	1404	5MC	C2-N3	3.92	1.44	1.36
1	A	1207	2MG	C2-N1	3.88	1.42	1.36
1	A	527	7MG	C2-N2	3.75	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1519	MA6	C2-N1	3.73	1.40	1.33
1	A	1498	UR3	C4-N3	-3.68	1.33	1.40
1	A	1519	MA6	C2-N3	3.48	1.37	1.32
12	L	92	0TD	CB-CG	3.44	1.57	1.52
1	A	1207	2MG	C2-N2	3.30	1.40	1.33
1	A	1207	2MG	C5-C6	-3.18	1.41	1.47
1	A	1407	5MC	C2-N3	3.15	1.42	1.36
1	A	516	PSU	C6-C5	3.15	1.38	1.35
1	A	1407	5MC	C2-N1	3.04	1.46	1.40
1	A	1404	5MC	O2-C2	2.81	1.28	1.23
1	A	1498	UR3	C1'-N1	2.76	1.55	1.47
1	A	1400	5MC	C4-N4	2.70	1.41	1.34
1	A	1404	5MC	C4-N3	2.68	1.38	1.34
1	A	1407	5MC	C4-N4	2.50	1.40	1.34
1	A	1402	4OC	C4-N4	-2.38	1.31	1.36
1	A	966	M2G	C2-N1	2.38	1.42	1.36
1	A	1400	5MC	C1'-N1	2.34	1.54	1.47
1	A	967	5MC	C2-N3	2.33	1.41	1.36
1	A	1519	MA6	C9-N6	2.30	1.50	1.45
1	A	1518	MA6	C6-N1	2.28	1.35	1.32
1	A	1518	MA6	C10-N6	2.27	1.50	1.45
1	A	1498	UR3	C2-N1	2.10	1.41	1.38
1	A	1541	PSU	C1'-C5	2.04	1.54	1.50
1	A	516	PSU	O4'-C1'	-2.00	1.41	1.43

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1498	UR3	C6-N1-C2	-5.78	117.07	121.80
1	A	516	PSU	N1-C2-N3	5.54	121.01	115.17
1	A	516	PSU	C4-N3-C2	-5.29	119.09	126.37
1	A	527	7MG	C5-C6-N1	5.23	120.14	110.94
1	A	527	7MG	C6-C5-N7	5.02	139.72	131.93
1	A	527	7MG	C2-N3-C4	4.88	120.70	112.30
1	A	1518	MA6	N1-C6-N6	-4.33	111.83	116.83
1	A	516	PSU	C6-C5-C4	4.25	121.04	118.17
1	A	527	7MG	C6-C5-C4	-4.14	115.12	122.40
1	A	1541	PSU	C4-N3-C2	-3.91	120.99	126.37
1	A	1541	PSU	O4-C4-N3	-3.85	112.88	120.11
12	L	92	0TD	CSB-SB-CB	-3.80	95.54	102.36
1	A	1540	PSU	N1-C2-N3	3.75	119.12	115.17
1	A	1541	PSU	C6-C5-C4	-3.65	115.71	118.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1540	PSU	C4-N3-C2	-3.61	121.40	126.37
1	A	527	7MG	C5-C4-N3	-3.56	121.44	128.13
1	A	1518	MA6	C1'-N9-C4	-3.46	120.55	126.64
1	A	1541	PSU	N1-C2-N3	3.36	118.72	115.17
1	A	1540	PSU	C6-N1-C2	-3.36	119.57	122.69
1	A	1540	PSU	O2-C2-N1	-3.34	119.34	122.79
1	A	966	M2G	O6-C6-N1	-3.34	116.66	120.62
1	A	966	M2G	O6-C6-C5	3.31	130.89	124.32
1	A	1207	2MG	O6-C6-C5	3.27	130.80	124.32
1	A	527	7MG	C2-N1-C6	-3.25	119.22	125.11
1	A	1207	2MG	O6-C6-N1	-3.03	117.02	120.62
1	A	527	7MG	N9-C4-N3	2.93	129.76	125.46
1	A	527	7MG	N9-C8-N7	2.86	107.43	103.37
12	L	92	0TD	CB-CA-N	-2.84	103.34	109.10
1	A	516	PSU	O2-C2-N1	-2.82	119.88	122.79
1	A	516	PSU	C6-N1-C2	-2.56	120.31	122.69
1	A	1404	5MC	C1'-N1-C6	-2.55	116.96	121.15
1	A	1407	5MC	C4-N3-C2	-2.51	117.33	120.81
1	A	1407	5MC	N4-C4-N3	-2.51	113.97	118.51
1	A	1498	UR3	C1'-N1-C2	2.43	121.01	117.04
1	A	967	5MC	C5-C4-N3	2.42	124.23	121.75
1	A	1207	2MG	N2-C2-N3	-2.40	117.46	120.51
1	A	516	PSU	O4'-C1'-C2'	2.35	108.41	105.15
1	A	1402	4OC	C5-C4-N4	-2.32	117.30	122.40
1	A	1402	4OC	CM4-N4-C4	-2.20	118.16	122.45
1	A	1407	5MC	CM5-C5-C6	-2.14	119.96	122.85
1	A	1404	5MC	N1-C2-N3	-2.11	115.15	118.80
1	A	1541	PSU	C5-C4-N3	2.10	121.18	116.55
1	A	1407	5MC	O2-C2-N3	-2.10	119.03	122.33
1	A	527	7MG	N2-C2-N3	-2.08	115.61	119.67
1	A	1400	5MC	C6-N1-C2	-2.07	118.20	120.95
1	A	1541	PSU	C3'-C2'-C1'	-2.06	99.25	101.69
1	A	1498	UR3	O2-C2-N3	-2.05	118.50	121.33
1	A	527	7MG	N2-C2-N1	2.01	121.01	116.76

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	527	7MG	O4'-C4'-C5'-O5'
1	A	527	7MG	C3'-C4'-C5'-O5'
1	A	966	M2G	N1-C2-N2-CM1

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Mol	Chain	Res	Type	Atoms
1	A	966	M2G	N3-C2-N2-CM1
1	A	966	M2G	N3-C2-N2-CM2
1	A	1207	2MG	N3-C2-N2-CM2
1	A	1400	5MC	O4'-C4'-C5'-O5'
1	A	1402	4OC	O4'-C4'-C5'-O5'
1	A	1518	MA6	O4'-C4'-C5'-O5'
1	A	1519	MA6	N1-C6-N6-C9
1	A	1541	PSU	C2'-C1'-C5-C4
1	A	1541	PSU	C2'-C1'-C5-C6
1	A	966	M2G	O4'-C4'-C5'-O5'
1	A	1402	4OC	C3'-C4'-C5'-O5'
1	A	1518	MA6	C3'-C4'-C5'-O5'
1	A	1400	5MC	C3'-C4'-C5'-O5'
1	A	966	M2G	C3'-C4'-C5'-O5'
1	A	1498	UR3	O4'-C4'-C5'-O5'
1	A	1498	UR3	C3'-C4'-C5'-O5'
1	A	966	M2G	N1-C2-N2-CM2
12	L	92	0TD	CG-CB-SB-CSB
1	A	1519	MA6	C5-C6-N6-C9
12	L	92	0TD	SB-CB-CG-OD1
1	A	1541	PSU	O4'-C1'-C5-C4
1	A	1498	UR3	O4'-C1'-N1-C6
1	A	1402	4OC	C3'-C2'-O2'-CM2
1	A	1498	UR3	C2'-C1'-N1-C6
1	A	1402	4OC	C2'-C1'-N1-C2

There are no ring outliers.

10 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	966	M2G	1	0
1	A	1400	5MC	2	0
1	A	1498	UR3	4	0
1	A	1519	MA6	3	0
1	A	1404	5MC	2	0
1	A	1518	MA6	3	0
1	A	1407	5MC	3	0
1	A	527	7MG	3	0
1	A	967	5MC	2	0
1	A	1541	PSU	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 284 ligands modelled in this entry, 283 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	SRY	A	1601	-	40,42,42	2.37	11 (27%)	49,63,63	2.39	15 (30%)

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	-	-	3/20/87/87	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	1601	SRY	CD1-N31	9.67	1.49	1.33
22	A	1601	SRY	CA1-N11	6.27	1.44	1.33
22	A	1601	SRY	O53-C53	-3.74	1.35	1.44
22	A	1601	SRY	CA1-NB1	2.92	1.45	1.34
22	A	1601	SRY	CD1-NE1	2.78	1.44	1.34
22	A	1601	SRY	C23-N23	-2.60	1.43	1.47
22	A	1601	SRY	C11-N11	-2.44	1.42	1.45
22	A	1601	SRY	O51-C51	-2.40	1.37	1.43
22	A	1601	SRY	C41-C31	-2.24	1.49	1.53
22	A	1601	SRY	O32-C32	-2.14	1.40	1.44
22	A	1601	SRY	O43-C43	-2.08	1.37	1.43

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	1601	SRY	C13-O13-C22	-6.06	105.96	116.26
22	A	1601	SRY	CI3-N23-C23	-5.61	106.98	114.23
22	A	1601	SRY	O13-C13-C23	5.42	116.87	108.07
22	A	1601	SRY	O41-C12-O42	-4.47	106.81	111.37
22	A	1601	SRY	C61-C11-N11	-4.46	102.40	110.62
22	A	1601	SRY	O61-C61-C11	4.04	117.62	109.58
22	A	1601	SRY	C21-C31-N31	3.93	117.86	110.62
22	A	1601	SRY	C12-O42-C42	-3.86	102.24	108.48
22	A	1601	SRY	O51-C51-C61	-3.49	102.14	110.38
22	A	1601	SRY	O42-C12-C22	-3.02	104.08	107.31
22	A	1601	SRY	O13-C22-C32	2.91	118.22	111.79
22	A	1601	SRY	C21-C11-N11	-2.90	105.27	110.62
22	A	1601	SRY	O21-C21-C31	2.58	114.71	109.58
22	A	1601	SRY	C43-C33-C23	-2.28	107.08	110.40
22	A	1601	SRY	C13-C23-N23	2.17	114.71	110.92

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

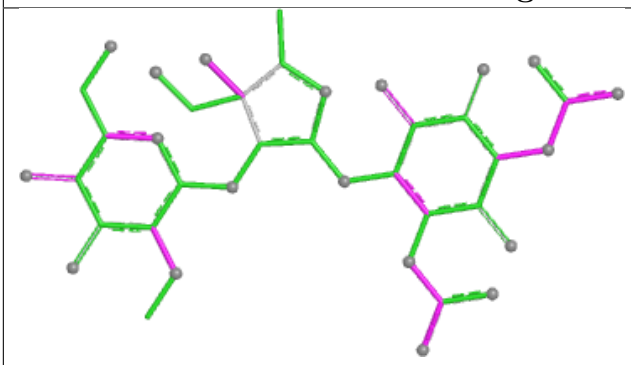
There are no ring outliers.

1 monomer is involved in 7 short contacts:

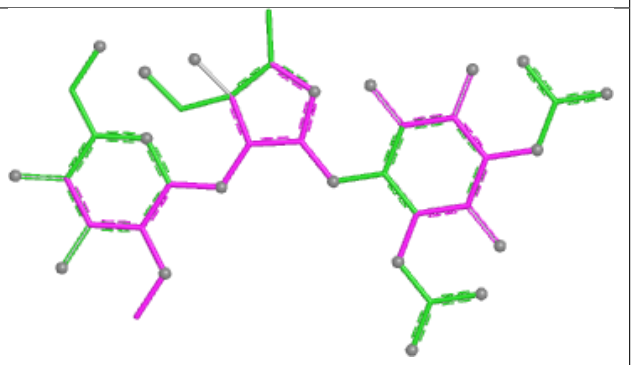
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	1601	SRY	7	0

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

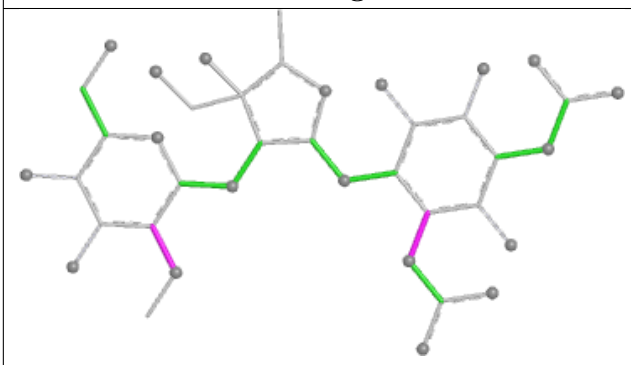
Ligand SRY A 1601



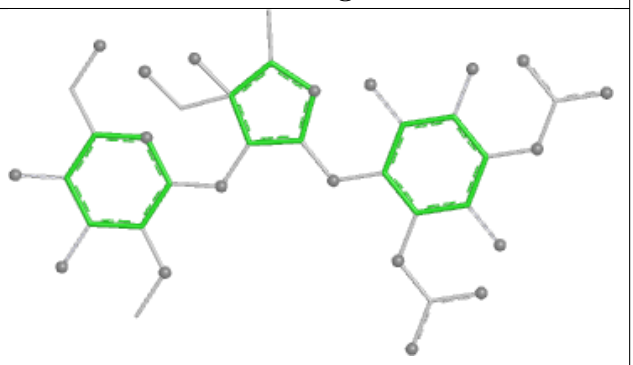
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1498/1522 (98%)	-0.47	11 (0%) 84 66	77, 136, 263, 391	0
2	B	234/256 (91%)	-0.56	1 (0%) 89 77	102, 148, 207, 245	0
3	C	206/239 (86%)	-0.35	2 (0%) 79 59	129, 192, 249, 279	0
4	D	208/209 (99%)	-0.34	8 (3%) 44 28	85, 139, 187, 218	0
5	E	150/162 (92%)	-0.70	0 100 100	74, 111, 149, 166	0
6	F	101/101 (100%)	-0.64	0 100 100	115, 160, 188, 229	0
7	G	155/156 (99%)	-0.47	2 (1%) 74 53	138, 187, 250, 276	0
8	H	138/138 (100%)	-0.84	0 100 100	63, 98, 143, 166	0
9	I	127/128 (99%)	-0.16	3 (2%) 59 39	141, 207, 248, 258	0
10	J	98/105 (93%)	0.12	3 (3%) 51 33	171, 230, 284, 340	0
11	K	116/129 (89%)	-0.56	1 (0%) 81 61	104, 130, 179, 211	0
12	L	123/135 (91%)	-0.45	2 (1%) 70 49	75, 131, 171, 211	0
13	M	118/126 (93%)	-0.24	2 (1%) 69 47	123, 166, 204, 229	0
14	N	60/61 (98%)	-0.00	1 (1%) 69 47	136, 206, 243, 259	0
15	O	87/89 (97%)	-0.69	0 100 100	79, 120, 171, 185	0
16	P	83/88 (94%)	-0.44	0 100 100	93, 128, 165, 189	0
17	Q	99/105 (94%)	-0.57	0 100 100	81, 109, 146, 174	0
18	R	70/88 (79%)	-0.67	0 100 100	92, 136, 177, 203	0
19	S	80/93 (86%)	-0.03	4 (5%) 35 23	164, 214, 256, 290	0
20	T	99/106 (93%)	-0.48	1 (1%) 79 59	94, 132, 176, 217	0
21	U	24/27 (88%)	0.24	1 (4%) 41 26	139, 191, 208, 221	0
All	All	3874/4063 (95%)	-0.45	42 (1%) 77 56	63, 145, 243, 391	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	2	GLY	6.5
1	A	1129	C	6.4
12	L	73	GLU	4.2
19	S	3	ARG	4.0
10	J	37	PRO	4.0
4	D	31	CYS	3.5
19	S	4	SER	3.4
4	D	3	ARG	3.2
10	J	34	VAL	3.1
13	M	117	VAL	3.1
4	D	9	CYS	3.1
1	A	1124	G	3.0
14	N	35	ARG	3.0
1	A	984	C	2.9
1	A	985	C	2.8
21	U	6	ARG	2.8
4	D	5	ILE	2.7
9	I	9	ARG	2.7
20	T	106	ALA	2.7
7	G	34	GLY	2.7
3	C	103	VAL	2.6
1	A	1219	U	2.6
3	C	193	TYR	2.6
1	A	1005	A	2.6
4	D	22	LYS	2.5
12	L	47	LYS	2.4
9	I	127	LYS	2.4
19	S	5	LEU	2.4
4	D	26	CYS	2.4
1	A	793	U	2.4
7	G	5	ARG	2.3
10	J	27	ALA	2.3
19	S	2	PRO	2.2
11	K	51	LYS	2.2
1	A	1255	G	2.2
1	A	78	G	2.1
2	B	193	ASP	2.1
1	A	6	G	2.1
9	I	47	LEU	2.1
4	D	35	ARG	2.1
13	M	118	ALA	2.1
1	A	1532	U	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	PSU	A	1540	20/21	0.80	0.13	284,295,304,304	0
1	PSU	A	1541	20/21	0.83	0.15	194,232,275,275	0
1	2MG	A	1207	24/25	0.93	0.10	171,214,228,232	0
1	5MC	A	1407	21/22	0.94	0.10	137,157,169,173	0
1	MA6	A	1518	24/25	0.94	0.07	109,126,150,152	0
1	UR3	A	1498	21/22	0.95	0.13	119,127,136,154	0
1	5MC	A	1404	21/22	0.96	0.09	105,128,135,142	0
1	MA6	A	1519	24/25	0.96	0.08	106,122,139,141	0
1	5MC	A	967	21/22	0.96	0.06	122,133,140,142	0
1	M2G	A	966	25/26	0.96	0.05	111,131,155,159	0
1	4OC	A	1402	22/23	0.97	0.09	111,116,133,174	0
1	7MG	A	527	24/25	0.97	0.07	95,109,116,120	0
1	PSU	A	516	20/21	0.97	0.09	143,147,160,163	0
1	5MC	A	1400	21/22	0.97	0.06	97,136,144,154	0
12	0TD	L	92	10/11	0.98	0.09	99,116,135,216	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	MG	A	1625	1/1	0.46	0.37	178,178,178,178	0
23	MG	A	1756	1/1	0.48	0.14	154,154,154,154	0
23	MG	A	1670	1/1	0.65	0.52	181,181,181,181	0
23	MG	A	1626	1/1	0.67	0.34	124,124,124,124	0
23	MG	A	1781	1/1	0.68	0.10	490,490,490,490	0
23	MG	M	203	1/1	0.68	0.72	135,135,135,135	0
23	MG	A	1720	1/1	0.70	0.22	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	MG	A	1735	1/1	0.74	0.28	98,98,98,98	0
23	MG	A	1858	1/1	0.74	0.11	279,279,279,279	0
23	MG	A	1662	1/1	0.74	0.17	161,161,161,161	0
23	MG	A	1768	1/1	0.75	0.38	152,152,152,152	0
23	MG	A	1684	1/1	0.75	0.30	172,172,172,172	0
23	MG	A	1750	1/1	0.76	0.42	106,106,106,106	0
23	MG	A	1800	1/1	0.76	0.27	124,124,124,124	0
23	MG	S	101	1/1	0.76	0.40	107,107,107,107	0
23	MG	A	1742	1/1	0.77	0.56	151,151,151,151	0
23	MG	A	1770	1/1	0.77	0.23	107,107,107,107	0
23	MG	A	1806	1/1	0.77	0.25	109,109,109,109	0
23	MG	A	1696	1/1	0.78	0.12	125,125,125,125	0
23	MG	A	1655	1/1	0.78	0.24	129,129,129,129	0
23	MG	A	1773	1/1	0.78	0.13	116,116,116,116	0
23	MG	A	1839	1/1	0.79	0.40	118,118,118,118	0
23	MG	A	1663	1/1	0.79	0.34	121,121,121,121	0
23	MG	A	1749	1/1	0.79	0.35	102,102,102,102	0
23	MG	A	1763	1/1	0.79	0.18	94,94,94,94	0
23	MG	A	1701	1/1	0.80	0.12	205,205,205,205	0
23	MG	A	1668	1/1	0.80	0.11	167,167,167,167	0
23	MG	P	102	1/1	0.80	0.15	123,123,123,123	0
23	MG	A	1783	1/1	0.80	0.21	126,126,126,126	0
23	MG	A	1791	1/1	0.81	0.36	116,116,116,116	0
23	MG	K	201	1/1	0.81	0.14	154,154,154,154	0
23	MG	A	1698	1/1	0.81	0.14	128,128,128,128	0
23	MG	A	1751	1/1	0.81	0.33	100,100,100,100	0
23	MG	A	1706	1/1	0.81	0.36	129,129,129,129	0
23	MG	A	1843	1/1	0.82	0.31	101,101,101,101	0
23	MG	A	1798	1/1	0.82	0.25	126,126,126,126	0
23	MG	A	1743	1/1	0.82	0.46	108,108,108,108	0
23	MG	A	1790	1/1	0.83	0.23	98,98,98,98	0
23	MG	A	1699	1/1	0.83	0.17	128,128,128,128	0
23	MG	A	1709	1/1	0.83	0.11	107,107,107,107	0
23	MG	A	1758	1/1	0.83	0.12	305,305,305,305	0
23	MG	A	1803	1/1	0.84	0.11	109,109,109,109	0
23	MG	A	1740	1/1	0.84	0.13	141,141,141,141	0
23	MG	A	1792	1/1	0.84	0.24	106,106,106,106	0
23	MG	A	1730	1/1	0.85	0.32	112,112,112,112	0
23	MG	A	1853	1/1	0.85	0.23	208,208,208,208	0
23	MG	A	1745	1/1	0.85	0.10	128,128,128,128	0
23	MG	A	1776	1/1	0.85	0.22	133,133,133,133	0
23	MG	A	1715	1/1	0.85	0.68	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	MG	A	1820	1/1	0.85	0.19	376,376,376,376	0
23	MG	A	1793	1/1	0.85	0.18	125,125,125,125	0
23	MG	A	1786	1/1	0.86	0.09	114,114,114,114	0
23	MG	A	1619	1/1	0.86	0.17	113,113,113,113	0
23	MG	A	1767	1/1	0.86	0.16	152,152,152,152	0
23	MG	A	1673	1/1	0.87	0.23	126,126,126,126	0
23	MG	A	1739	1/1	0.87	0.43	107,107,107,107	0
23	MG	A	1787	1/1	0.87	0.27	140,140,140,140	0
23	MG	A	1697	1/1	0.87	0.33	147,147,147,147	0
23	MG	A	1845	1/1	0.88	0.12	154,154,154,154	0
23	MG	A	1607	1/1	0.88	0.19	252,252,252,252	0
23	MG	A	1748	1/1	0.88	0.18	103,103,103,103	0
23	MG	D	302	1/1	0.88	0.12	121,121,121,121	0
23	MG	A	1810	1/1	0.88	0.10	131,131,131,131	0
23	MG	M	201	1/1	0.88	0.29	126,126,126,126	0
23	MG	A	1772	1/1	0.88	0.15	118,118,118,118	0
23	MG	A	1764	1/1	0.88	0.60	108,108,108,108	0
23	MG	A	1722	1/1	0.88	0.11	101,101,101,101	0
23	MG	A	1736	1/1	0.89	0.30	108,108,108,108	0
23	MG	A	1855	1/1	0.89	0.11	295,295,295,295	0
23	MG	A	1602	1/1	0.89	0.10	155,155,155,155	0
23	MG	A	1859	1/1	0.89	0.23	102,102,102,102	0
23	MG	A	1807	1/1	0.89	0.12	114,114,114,114	0
23	MG	A	1659	1/1	0.89	0.07	142,142,142,142	0
23	MG	A	1741	1/1	0.89	0.18	87,87,87,87	0
23	MG	A	1712	1/1	0.89	0.25	89,89,89,89	0
23	MG	A	1784	1/1	0.89	0.14	110,110,110,110	0
23	MG	Q	201	1/1	0.89	0.12	101,101,101,101	0
23	MG	A	1666	1/1	0.89	0.17	112,112,112,112	0
23	MG	A	1762	1/1	0.90	0.12	97,97,97,97	0
23	MG	H	203	1/1	0.90	0.06	103,103,103,103	0
23	MG	A	1679	1/1	0.90	0.16	94,94,94,94	0
23	MG	A	1794	1/1	0.90	0.21	115,115,115,115	0
23	MG	A	1797	1/1	0.90	0.12	110,110,110,110	0
23	MG	N	102	1/1	0.90	0.05	118,118,118,118	0
23	MG	A	1717	1/1	0.90	0.45	134,134,134,134	0
23	MG	A	1727	1/1	0.90	0.11	97,97,97,97	0
23	MG	A	1860	1/1	0.90	0.25	113,113,113,113	0
23	MG	A	1785	1/1	0.91	0.50	116,116,116,116	0
23	MG	A	1616	1/1	0.91	0.08	84,84,84,84	0
23	MG	A	1704	1/1	0.91	0.18	108,108,108,108	0
23	MG	A	1789	1/1	0.91	0.16	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	MG	A	1671	1/1	0.91	0.21	124,124,124,124	0
23	MG	A	1624	1/1	0.91	0.11	98,98,98,98	0
23	MG	A	1818	1/1	0.91	0.10	209,209,209,209	0
23	MG	A	1729	1/1	0.91	0.29	102,102,102,102	0
23	MG	A	1675	1/1	0.91	0.29	83,83,83,83	0
23	MG	A	1840	1/1	0.91	0.26	127,127,127,127	0
23	MG	A	1713	1/1	0.91	0.15	72,72,72,72	0
23	MG	A	1796	1/1	0.91	0.17	100,100,100,100	0
23	MG	A	1635	1/1	0.91	0.11	75,75,75,75	0
23	MG	A	1841	1/1	0.92	0.14	96,96,96,96	0
23	MG	A	1687	1/1	0.92	0.07	277,277,277,277	0
23	MG	A	1774	1/1	0.92	0.17	126,126,126,126	0
23	MG	A	1846	1/1	0.92	0.20	396,396,396,396	0
23	MG	A	1775	1/1	0.92	0.07	87,87,87,87	0
23	MG	A	1642	1/1	0.92	0.17	91,91,91,91	0
23	MG	A	1646	1/1	0.92	0.15	102,102,102,102	0
23	MG	A	1649	1/1	0.92	0.15	117,117,117,117	0
23	MG	A	1801	1/1	0.92	0.63	130,130,130,130	0
23	MG	B	301	1/1	0.92	0.11	118,118,118,118	0
23	MG	B	302	1/1	0.92	0.13	97,97,97,97	0
23	MG	A	1634	1/1	0.92	0.52	125,125,125,125	0
23	MG	A	1805	1/1	0.92	0.09	117,117,117,117	0
23	MG	H	204	1/1	0.92	0.25	106,106,106,106	0
23	MG	A	1718	1/1	0.92	0.22	147,147,147,147	0
23	MG	A	1640	1/1	0.92	0.28	118,118,118,118	0
23	MG	A	1685	1/1	0.92	0.18	129,129,129,129	0
23	MG	A	1725	1/1	0.92	0.18	91,91,91,91	0
23	MG	A	1705	1/1	0.92	0.09	135,135,135,135	0
23	MG	P	103	1/1	0.92	0.08	98,98,98,98	0
23	MG	A	1771	1/1	0.92	0.15	113,113,113,113	0
23	MG	A	1686	1/1	0.92	0.07	264,264,264,264	0
23	MG	A	1761	1/1	0.93	0.06	100,100,100,100	0
23	MG	A	1782	1/1	0.93	0.07	94,94,94,94	0
23	MG	A	1608	1/1	0.93	0.16	93,93,93,93	0
23	MG	A	1620	1/1	0.93	0.23	143,143,143,143	0
23	MG	A	1804	1/1	0.93	0.22	107,107,107,107	0
23	MG	A	1707	1/1	0.93	0.12	99,99,99,99	0
23	MG	A	1765	1/1	0.93	0.24	128,128,128,128	0
23	MG	A	1724	1/1	0.93	0.32	133,133,133,133	0
23	MG	A	1808	1/1	0.93	0.35	105,105,105,105	0
23	MG	H	202	1/1	0.93	0.04	73,73,73,73	0
23	MG	A	1648	1/1	0.93	0.18	122,122,122,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	MG	A	1683	1/1	0.93	0.16	256,256,256,256	0
23	MG	A	1819	1/1	0.93	0.10	175,175,175,175	0
23	MG	A	1612	1/1	0.93	0.07	115,115,115,115	0
23	MG	A	1838	1/1	0.93	0.07	101,101,101,101	0
23	MG	A	1714	1/1	0.93	0.46	107,107,107,107	0
23	MG	A	1731	1/1	0.93	0.14	82,82,82,82	0
23	MG	A	1734	1/1	0.93	0.13	102,102,102,102	0
23	MG	A	1636	1/1	0.93	0.14	85,85,85,85	0
23	MG	Q	202	1/1	0.93	0.14	72,72,72,72	0
23	MG	A	1604	1/1	0.93	0.22	114,114,114,114	0
23	MG	A	1711	1/1	0.94	0.37	130,130,130,130	0
23	MG	A	1667	1/1	0.94	0.08	135,135,135,135	0
23	MG	A	1678	1/1	0.94	0.34	96,96,96,96	0
23	MG	A	1606	1/1	0.94	0.26	100,100,100,100	0
23	MG	A	1681	1/1	0.94	0.06	93,93,93,93	0
23	MG	A	1700	1/1	0.94	0.10	174,174,174,174	0
23	MG	A	1822	1/1	0.94	0.09	300,300,300,300	0
23	MG	A	1824	1/1	0.94	0.12	200,200,200,200	0
23	MG	A	1828	1/1	0.94	0.15	400,400,400,400	0
23	MG	A	1832	1/1	0.94	0.41	218,218,218,218	0
23	MG	J	201	1/1	0.94	0.22	113,113,113,113	0
23	MG	A	1737	1/1	0.94	0.16	131,131,131,131	0
23	MG	A	1669	1/1	0.94	0.18	138,138,138,138	0
23	MG	A	1638	1/1	0.94	0.11	192,192,192,192	0
23	MG	A	1665	1/1	0.94	0.10	121,121,121,121	0
23	MG	A	1672	1/1	0.94	0.22	140,140,140,140	0
23	MG	A	1603	1/1	0.94	0.15	106,106,106,106	0
23	MG	A	1744	1/1	0.94	0.10	124,124,124,124	0
23	MG	A	1847	1/1	0.94	0.18	328,328,328,328	0
23	MG	A	1688	1/1	0.94	0.18	112,112,112,112	0
23	MG	A	1723	1/1	0.95	0.31	120,120,120,120	0
23	MG	A	1830	1/1	0.95	0.20	312,312,312,312	0
23	MG	A	1738	1/1	0.95	0.19	114,114,114,114	0
23	MG	A	1682	1/1	0.95	0.25	134,134,134,134	0
23	MG	A	1695	1/1	0.95	0.17	118,118,118,118	0
23	MG	A	1654	1/1	0.95	0.34	115,115,115,115	0
23	MG	A	1639	1/1	0.95	0.08	120,120,120,120	0
23	MG	A	1842	1/1	0.95	0.06	187,187,187,187	0
23	MG	J	202	1/1	0.95	0.10	133,133,133,133	0
23	MG	A	1716	1/1	0.95	0.14	112,112,112,112	0
23	MG	A	1815	1/1	0.95	0.06	98,98,98,98	0
23	MG	A	1609	1/1	0.95	0.09	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	MG	A	1660	1/1	0.95	0.30	118,118,118,118	0
23	MG	A	1747	1/1	0.95	0.10	116,116,116,116	0
23	MG	A	1821	1/1	0.95	0.10	278,278,278,278	0
23	MG	A	1857	1/1	0.95	0.07	287,287,287,287	0
23	MG	A	1710	1/1	0.95	0.15	104,104,104,104	0
23	MG	A	1661	1/1	0.95	0.17	98,98,98,98	0
23	MG	A	1795	1/1	0.96	0.11	115,115,115,115	0
23	MG	A	1732	1/1	0.96	0.09	89,89,89,89	0
23	MG	A	1856	1/1	0.96	0.15	231,231,231,231	0
23	MG	A	1766	1/1	0.96	0.19	124,124,124,124	0
23	MG	A	1611	1/1	0.96	0.10	105,105,105,105	0
23	MG	A	1752	1/1	0.96	0.10	142,142,142,142	0
23	MG	A	1825	1/1	0.96	0.15	199,199,199,199	0
23	MG	A	1826	1/1	0.96	0.27	196,196,196,196	0
23	MG	A	1827	1/1	0.96	0.06	162,162,162,162	0
23	MG	A	1769	1/1	0.96	0.12	131,131,131,131	0
23	MG	A	1755	1/1	0.96	0.14	114,114,114,114	0
23	MG	A	1680	1/1	0.96	0.12	121,121,121,121	0
23	MG	A	1788	1/1	0.96	0.41	103,103,103,103	0
23	MG	A	1628	1/1	0.96	0.17	84,84,84,84	0
23	MG	A	1621	1/1	0.96	0.05	128,128,128,128	0
23	MG	A	1689	1/1	0.96	0.14	230,230,230,230	0
23	MG	A	1809	1/1	0.96	0.18	80,80,80,80	0
23	MG	M	202	1/1	0.96	0.22	130,130,130,130	0
23	MG	A	1617	1/1	0.96	0.29	103,103,103,103	0
23	MG	A	1844	1/1	0.96	0.17	116,116,116,116	0
23	MG	P	101	1/1	0.96	0.15	82,82,82,82	0
22	SRY	A	1601	40/40	0.96	0.09	88,116,133,137	0
23	MG	A	1816	1/1	0.96	0.21	120,120,120,120	0
23	MG	A	1779	1/1	0.96	0.07	213,213,213,213	0
23	MG	A	1849	1/1	0.96	0.26	235,235,235,235	0
23	MG	A	1850	1/1	0.96	0.21	350,350,350,350	0
24	ZN	D	301	1/1	0.96	0.20	106,106,106,106	0
23	MG	A	1848	1/1	0.97	0.10	235,235,235,235	0
23	MG	A	1812	1/1	0.97	0.12	68,68,68,68	0
23	MG	A	1813	1/1	0.97	0.11	103,103,103,103	0
23	MG	A	1852	1/1	0.97	0.18	353,353,353,353	0
23	MG	A	1644	1/1	0.97	0.10	83,83,83,83	0
23	MG	A	1702	1/1	0.97	0.07	84,84,84,84	0
23	MG	A	1817	1/1	0.97	0.14	97,97,97,97	0
23	MG	A	1721	1/1	0.97	0.12	101,101,101,101	0
23	MG	A	1703	1/1	0.97	0.31	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	MG	A	1613	1/1	0.97	0.05	84,84,84,84	0
23	MG	A	1647	1/1	0.97	0.09	133,133,133,133	0
23	MG	A	1622	1/1	0.97	0.10	106,106,106,106	0
23	MG	A	1726	1/1	0.97	0.06	84,84,84,84	0
23	MG	A	1674	1/1	0.97	0.13	186,186,186,186	0
23	MG	E	201	1/1	0.97	0.04	232,232,232,232	0
23	MG	H	201	1/1	0.97	0.09	77,77,77,77	0
23	MG	A	1629	1/1	0.97	0.25	87,87,87,87	0
23	MG	A	1676	1/1	0.97	0.10	96,96,96,96	0
23	MG	A	1691	1/1	0.97	0.07	102,102,102,102	0
23	MG	A	1829	1/1	0.97	0.14	244,244,244,244	0
23	MG	A	1799	1/1	0.97	0.13	114,114,114,114	0
23	MG	A	1677	1/1	0.97	0.12	128,128,128,128	0
23	MG	A	1836	1/1	0.97	0.16	341,341,341,341	0
23	MG	A	1778	1/1	0.97	0.04	314,314,314,314	0
23	MG	A	1802	1/1	0.97	0.07	150,150,150,150	0
23	MG	A	1753	1/1	0.97	0.24	89,89,89,89	0
23	MG	A	1780	1/1	0.97	0.09	211,211,211,211	0
23	MG	A	1733	1/1	0.97	0.37	107,107,107,107	0
23	MG	A	1650	1/1	0.97	0.05	107,107,107,107	0
23	MG	A	1651	1/1	0.97	0.08	239,239,239,239	0
23	MG	A	1614	1/1	0.97	0.07	80,80,80,80	0
23	MG	A	1610	1/1	0.97	0.09	83,83,83,83	0
23	MG	T	201	1/1	0.97	0.18	135,135,135,135	0
23	MG	A	1656	1/1	0.97	0.09	149,149,149,149	0
23	MG	A	1641	1/1	0.98	0.08	119,119,119,119	0
23	MG	A	1814	1/1	0.98	0.12	103,103,103,103	0
23	MG	A	1746	1/1	0.98	0.06	91,91,91,91	0
23	MG	A	1605	1/1	0.98	0.05	114,114,114,114	0
23	MG	A	1664	1/1	0.98	0.12	120,120,120,120	0
23	MG	A	1631	1/1	0.98	0.10	95,95,95,95	0
23	MG	A	1708	1/1	0.98	0.05	93,93,93,93	0
23	MG	A	1728	1/1	0.98	0.10	84,84,84,84	0
23	MG	A	1627	1/1	0.98	0.09	168,168,168,168	0
23	MG	A	1719	1/1	0.98	0.15	118,118,118,118	0
23	MG	A	1823	1/1	0.98	0.19	365,365,365,365	0
23	MG	A	1754	1/1	0.98	0.09	120,120,120,120	0
23	MG	A	1692	1/1	0.98	0.18	331,331,331,331	0
23	MG	A	1851	1/1	0.98	0.11	246,246,246,246	0
23	MG	A	1694	1/1	0.98	0.10	142,142,142,142	0
23	MG	A	1757	1/1	0.98	0.11	190,190,190,190	0
23	MG	A	1854	1/1	0.98	0.20	359,359,359,359	0

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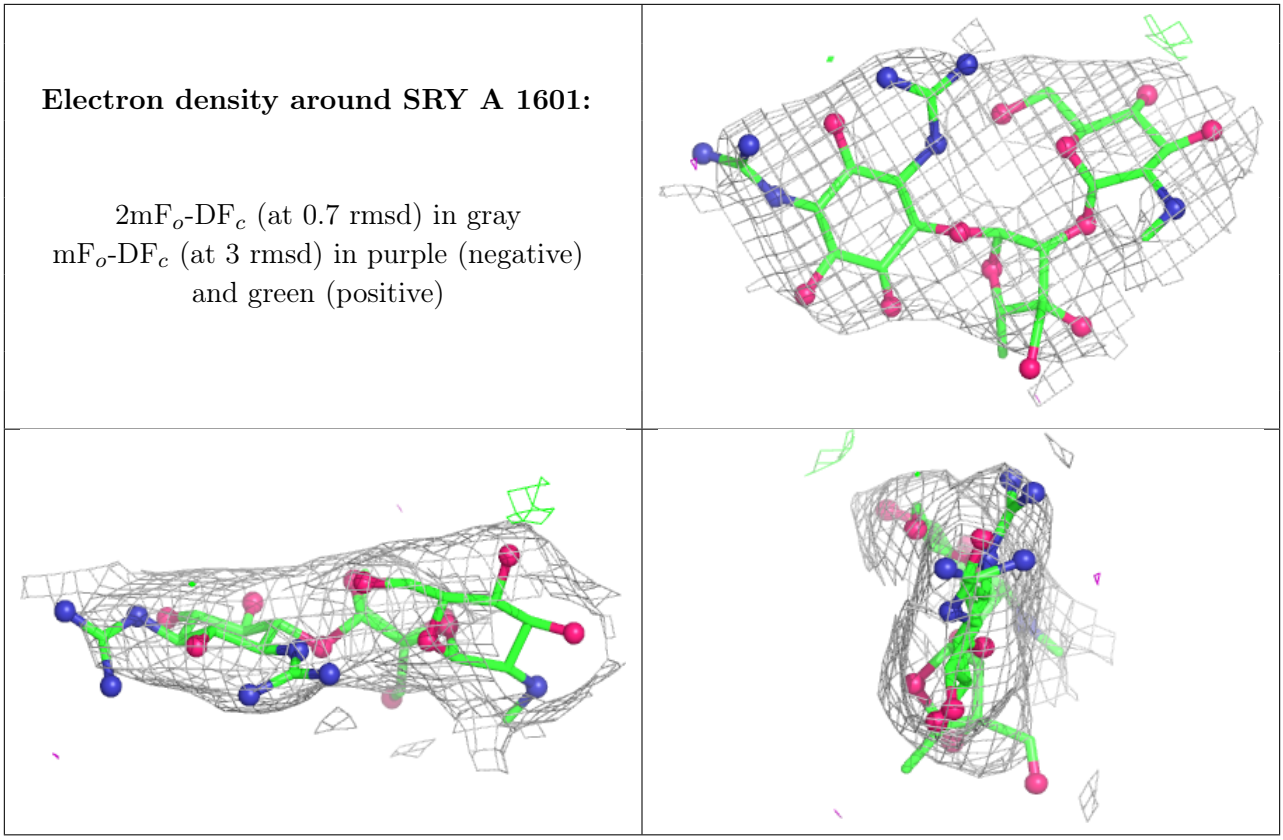
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	MG	A	1615	1/1	0.98	0.12	75,75,75,75	0
23	MG	A	1759	1/1	0.98	0.09	197,197,197,197	0
23	MG	A	1760	1/1	0.98	0.15	194,194,194,194	0
23	MG	A	1811	1/1	0.98	0.09	102,102,102,102	0
23	MG	A	1834	1/1	0.98	0.21	335,335,335,335	0
23	MG	A	1777	1/1	0.98	0.09	219,219,219,219	0
23	MG	A	1643	1/1	0.99	0.09	110,110,110,110	0
23	MG	A	1693	1/1	0.99	0.16	144,144,144,144	0
23	MG	A	1618	1/1	0.99	0.07	69,69,69,69	0
23	MG	A	1657	1/1	0.99	0.09	97,97,97,97	0
23	MG	A	1658	1/1	0.99	0.17	202,202,202,202	0
23	MG	A	1645	1/1	0.99	0.13	91,91,91,91	0
23	MG	A	1623	1/1	0.99	0.12	159,159,159,159	0
23	MG	A	1831	1/1	0.99	0.19	231,231,231,231	0
23	MG	A	1652	1/1	0.99	0.06	137,137,137,137	0
23	MG	A	1833	1/1	0.99	0.05	180,180,180,180	0
23	MG	A	1653	1/1	0.99	0.25	154,154,154,154	0
23	MG	A	1835	1/1	0.99	0.04	103,103,103,103	0
23	MG	A	1690	1/1	0.99	0.04	75,75,75,75	0
23	MG	A	1837	1/1	0.99	0.05	134,134,134,134	0
23	MG	A	1630	1/1	0.99	0.12	139,139,139,139	0
24	ZN	N	101	1/1	0.99	0.04	173,173,173,173	0
23	MG	A	1632	1/1	1.00	0.03	100,100,100,100	0
23	MG	A	1637	1/1	1.00	0.02	62,62,62,62	0
23	MG	A	1633	1/1	1.00	0.07	67,67,67,67	0

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

Electron density around SRY A 1601:

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



6.5 Other polymers (i)

There are no such residues in this entry.