Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:52 PM GMT

PDB ID	:	4JI4
Title	:	Crystal Structure of 30S ribosomal subunit from Thermus thermophilus
Authors	:	Demirci, H.; Wang, L.; Murphy IV, F.; Murphy, E.; Carr, J.; Blanchard, S.; Jogl, G.; Dahlberg, A.E.; Gregory, S.T.
Deposited on	:	2013-03-05
Resolution	:	3.69 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

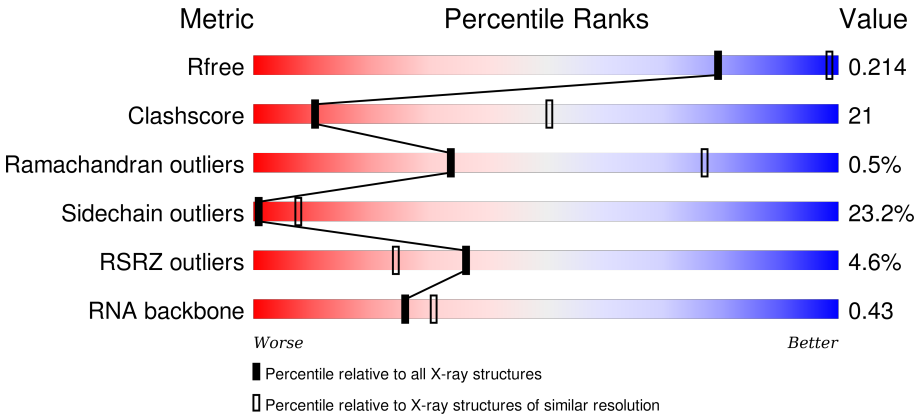
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.69 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1101 (3.90-3.50)
Clashscore	102246	1224 (3.90-3.50)
Ramachandran outliers	100387	1172 (3.90-3.50)
Sidechain outliers	100360	1170 (3.90-3.50)
RSRZ outliers	91569	1108 (3.90-3.50)
RNA backbone	2183	1067 (4.60-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	1522	3%, 19%, 43%, 30%, 7%, .
2	B	256	39%, 40%, 12%, 9%
3	C	239	8%, 36%, 40%, 10%, 14%
4	D	209	4%, 45%, 45%, 9%

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Mol	Chain	Length	Quality of chain
5	E	162	37% 42% 13% 7%
6	F	101	44% 43% 14%
7	G	156	3% 46% 40% 13%
8	H	138	38% 47% 14%
9	I	128	13% 37% 42% 20%
10	J	105	21% 31% 45% 16% 7%
11	K	129	2% 47% 36% 8% 10%
12	L	135	4% 41% 41% 8% 8%
13	M	126	17% 33% 48% 13% 6%
14	N	61	5% 36% 56% 7%
15	O	89	43% 40% 15%
16	P	88	2% 40% 44% 10% 6%
17	Q	105	% 39% 45% 9% 6%
18	R	88	% 30% 39% 11% 20%
19	S	93	16% 39% 35% 12% 14%
20	T	106	2% 36% 46% 11% 7%
21	U	27	15% 44% 26% 19% 11%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	5MC	A	967	-	-	X	-
12	0TD	L	92	-	-	X	-
22	MG	A	1605	-	-	-	X
22	MG	A	1656	-	-	-	X
22	MG	A	1661	-	-	-	X
22	MG	A	1670	-	-	-	X
22	MG	A	1706	-	-	-	X
22	MG	A	1711	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	MG	A	1728	-	-	-	X
22	MG	A	1738	-	-	-	X
22	MG	A	1747	-	-	-	X
22	MG	A	1755	-	-	-	X
22	MG	A	1767	-	-	-	X
22	MG	A	1776	-	-	-	X
22	MG	A	1786	-	-	-	X
22	MG	A	1789	-	-	-	X
22	MG	A	1792	-	-	-	X
22	MG	A	1809	-	-	-	X
22	MG	A	1816	-	-	-	X
22	MG	A	1817	-	-	-	X
22	MG	A	1828	-	-	-	X
22	MG	A	1833	-	-	-	X
22	MG	I	201	-	-	-	X
22	MG	J	201	-	-	-	X

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 52281 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	1512	32644	14540	6038	10548	1518	0	6	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1490	U	C	CONFLICT	GB M26923.1
A	1534	C	A	CONFLICT	GB M26923.1
A	1535	A	C	CONFLICT	GB M26923.1

- Molecule 2 is a protein called RIBOSOMAL PROTEIN S2.

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

- Molecule 3 is a protein called RIBOSOMAL PROTEIN S3.

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

- Molecule 4 is a protein called RIBOSOMAL PROTEIN S4.

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

- Molecule 5 is a protein called RIBOSOMAL PROTEIN S5.

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

- Molecule 6 is a protein called RIBOSOMAL PROTEIN S6.

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

- Molecule 7 is a protein called RIBOSOMAL PROTEIN S7.

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

- Molecule 8 is a protein called RIBOSOMAL PROTEIN S8.

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

- Molecule 9 is a protein called RIBOSOMAL PROTEIN S9.

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

- Molecule 10 is a protein called RIBOSOMAL PROTEIN S10.

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

- Molecule 11 is a protein called RIBOSOMAL PROTEIN S11.

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

- Molecule 12 is a protein called RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	124	Total	C	N	O	S	0	0	0
			973	613	195	163	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	94	LEU	PRO	CONFLICT	UNP F6DEQ7

- 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	151	142	2			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	P	1	Total	Mg	0	0
			1	1		
22	J	1	Total	Mg	0	0
			1	1		
22	Q	1	Total	Mg	0	0
			1	1		
22	D	3	Total	Mg	0	0
			3	3		
22	E	1	Total	Mg	0	0
			1	1		
22	H	1	Total	Mg	0	0
			1	1		
22	B	1	Total	Mg	0	0
			1	1		
22	I	1	Total	Mg	0	0
			1	1		
22	C	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	A	262	Total Mg 262 262	0	0
22	F	1	Total Mg 1 1	0	0

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

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

- Molecule 24 is water.

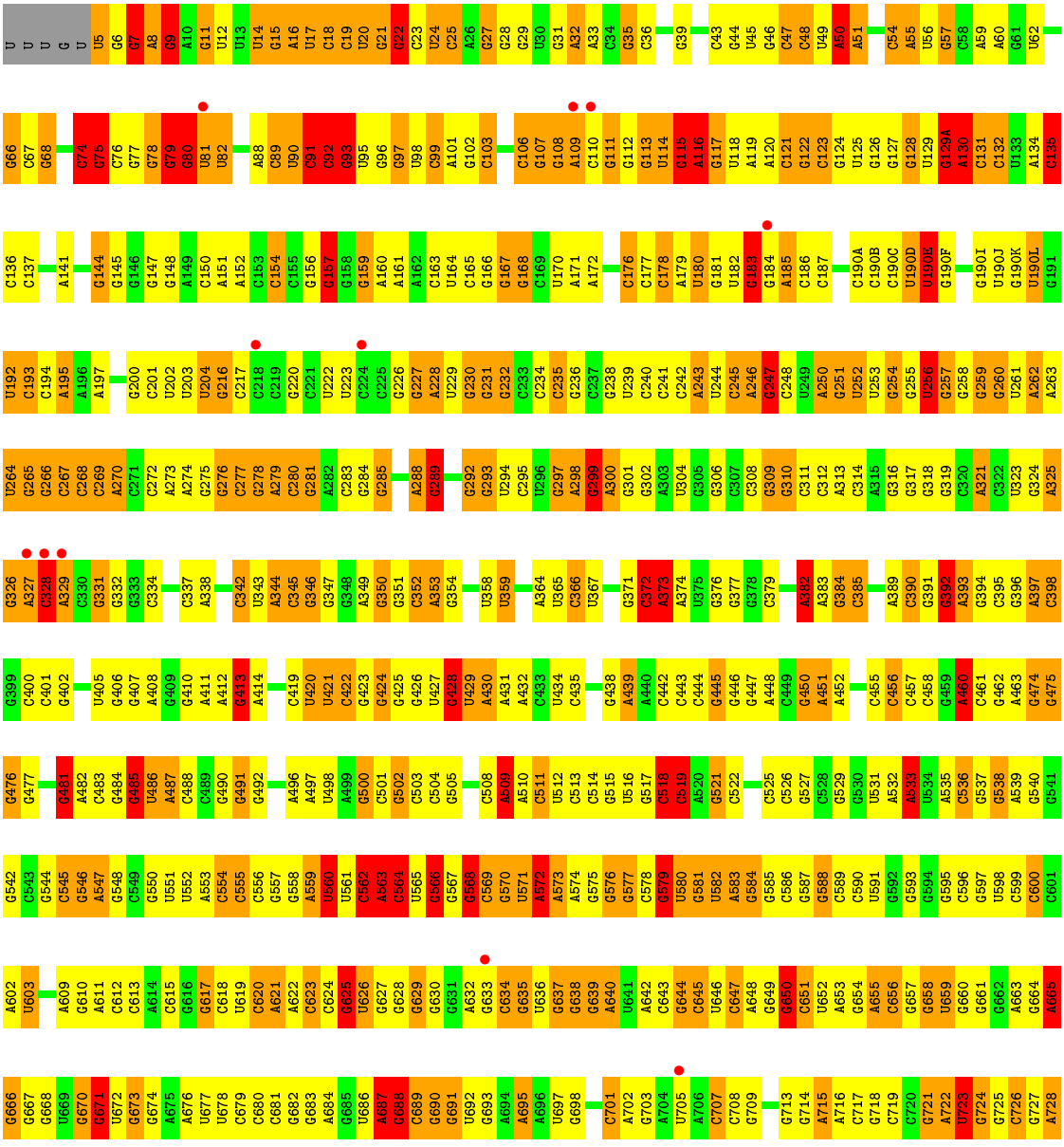
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	261	Total O 261 261	0	0
24	C	1	Total O 1 1	0	0
24	D	1	Total O 1 1	0	0
24	E	6	Total O 6 6	0	0
24	Q	2	Total O 2 2	0	0
24	T	1	Total O 1 1	0	0

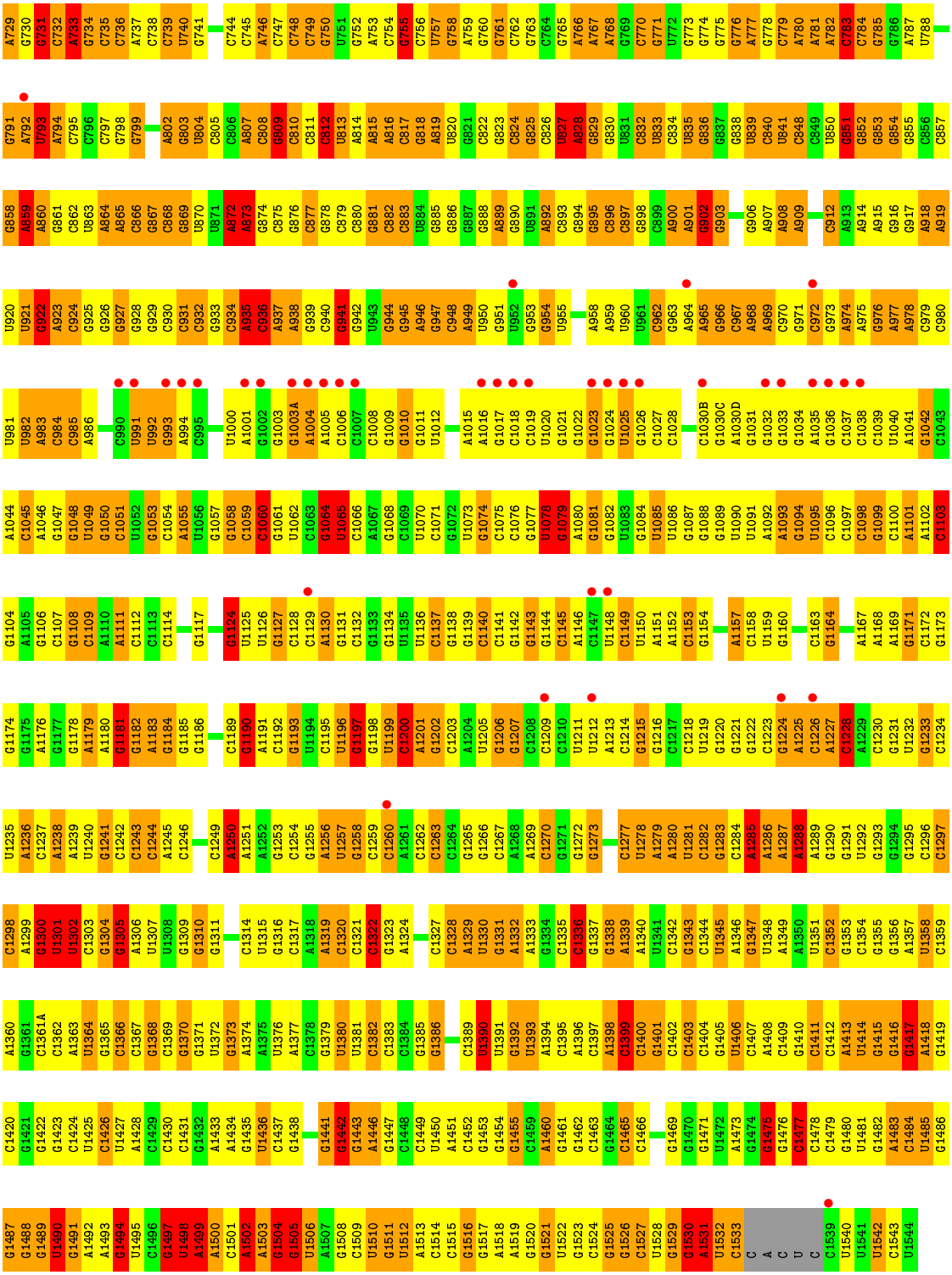
3 Residue-property plots (i)

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

- Molecule 1: 16S rRNA

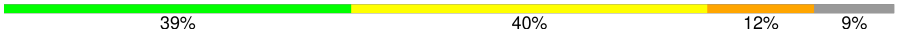
Chain A: 

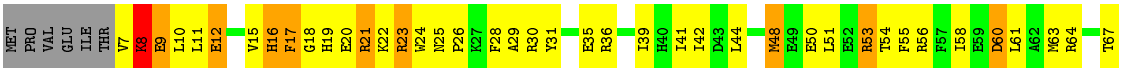


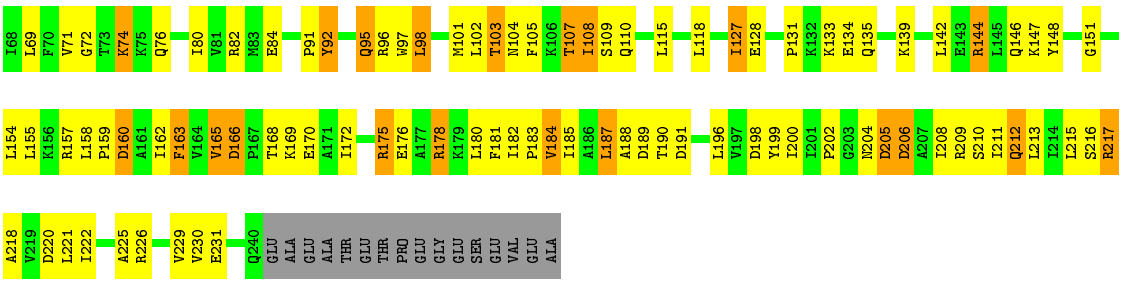


• Molecule 2: RIBOSOMAL PROTEIN S2

Chain B:

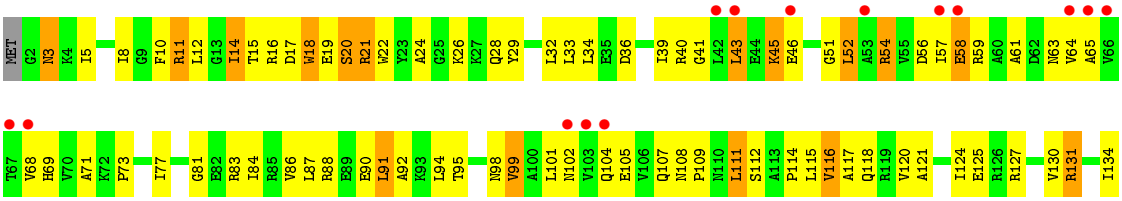


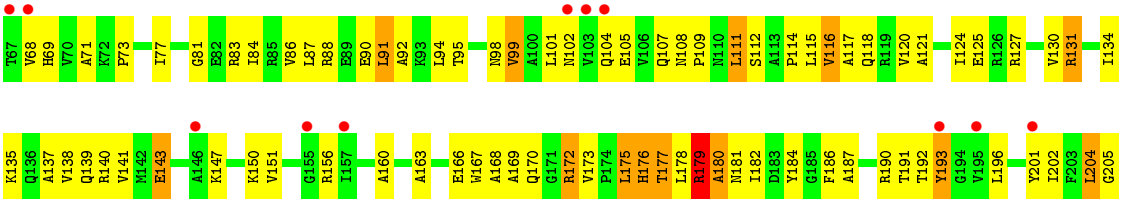


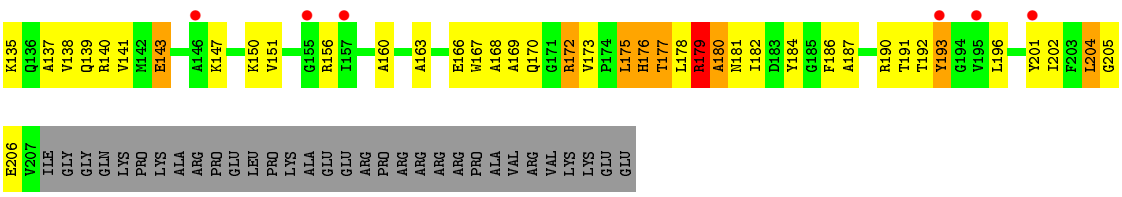


• Molecule 3: RIBOSOMAL PROTEIN S3

Chain C:

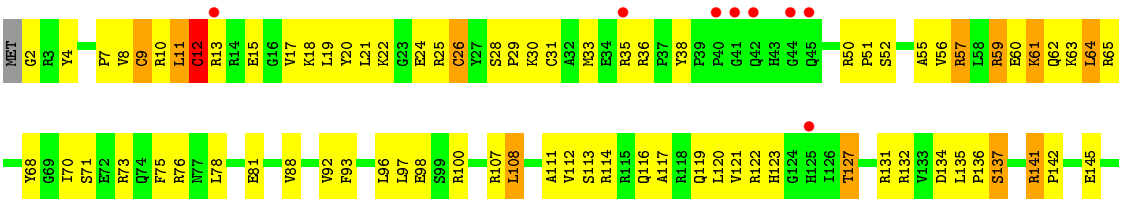


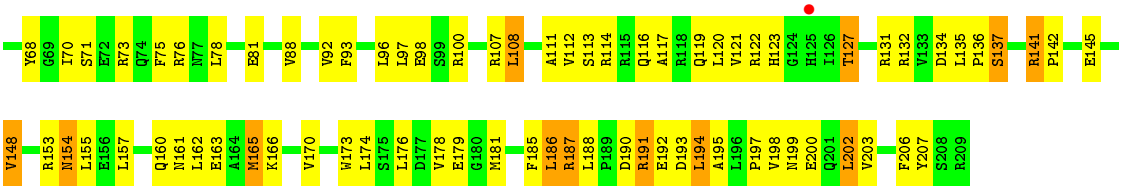




• Molecule 4: RIBOSOMAL PROTEIN S4

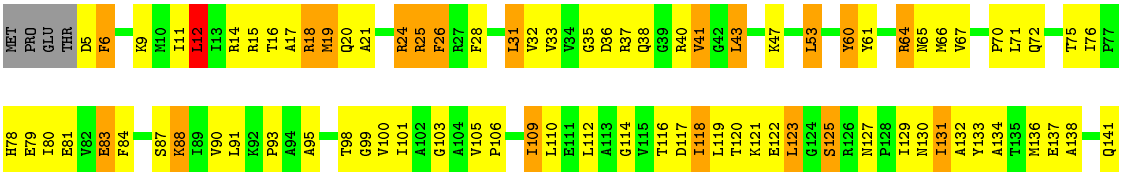
Chain D:

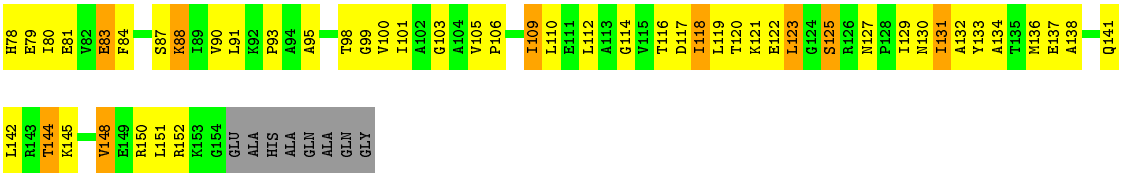




• Molecule 5: RIBOSOMAL PROTEIN S5

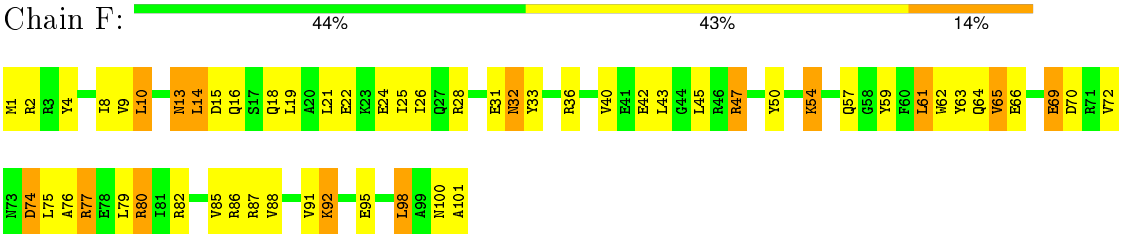
Chain E:





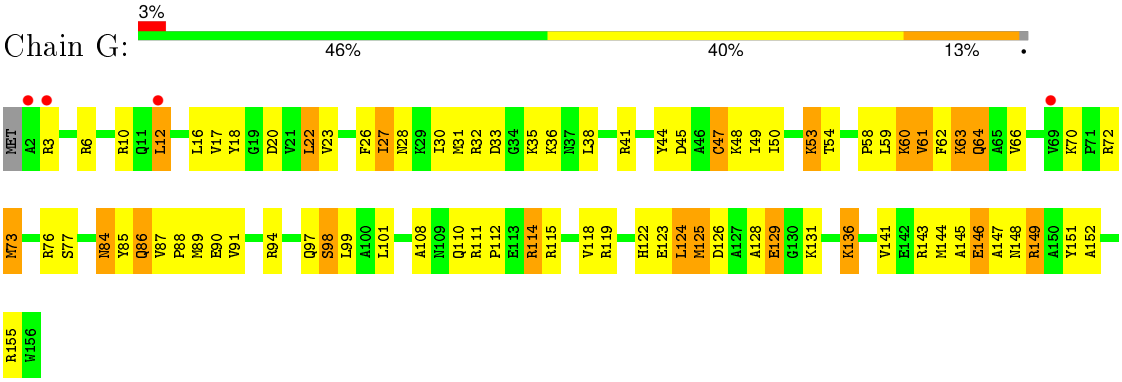
• Molecule 6: RIBOSOMAL PROTEIN S6

Chain F:



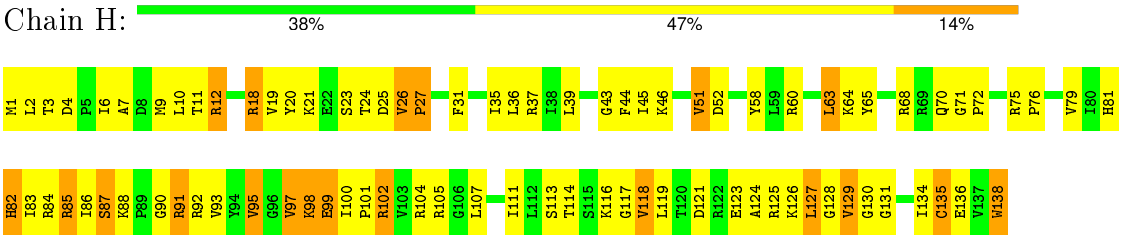
• Molecule 7: RIBOSOMAL PROTEIN S7

Chain G:



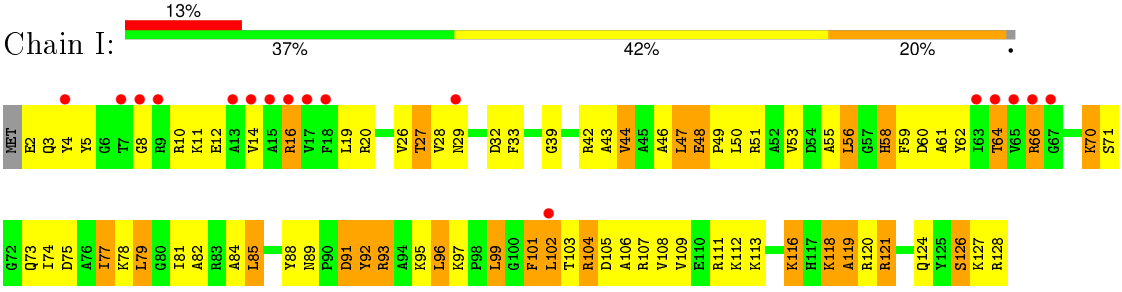
• Molecule 8: RIBOSOMAL PROTEIN S8

Chain H:



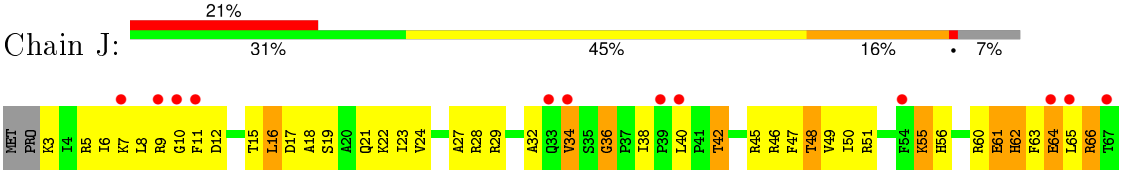
• Molecule 9: RIBOSOMAL PROTEIN S9

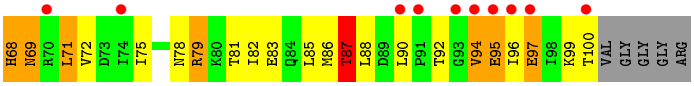
Chain I:



• Molecule 10: RIBOSOMAL PROTEIN S10

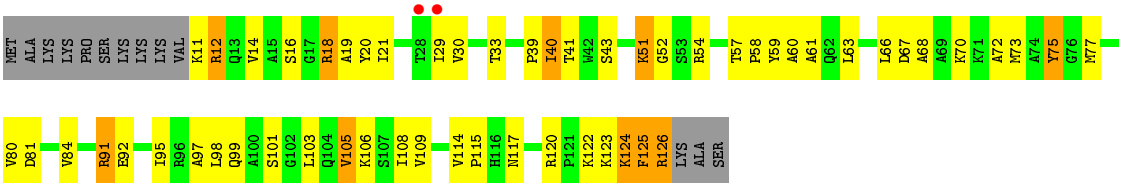
Chain J:





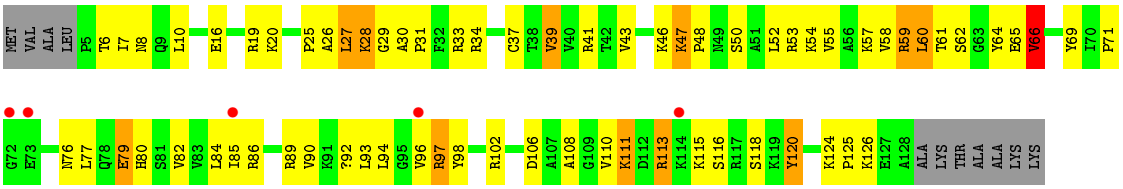
- Molecule 11: RIBOSOMAL PROTEIN S11

Chain K:



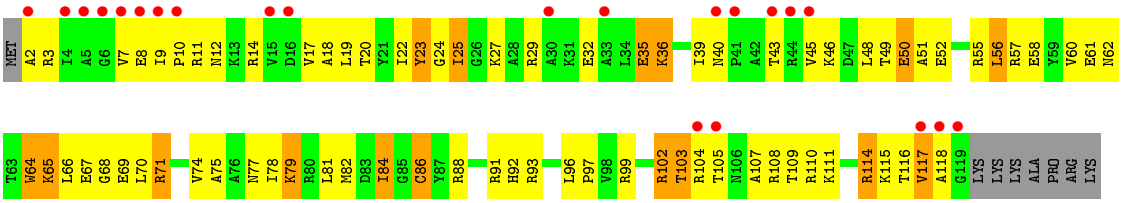
- Molecule 12: RIBOSOMAL PROTEIN S12

Chain L:



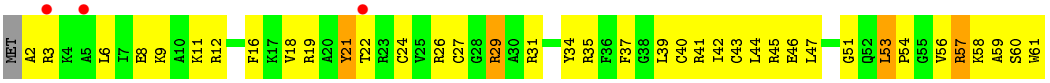
- Molecule 13: RIBOSOMAL PROTEIN S13

Chain M:



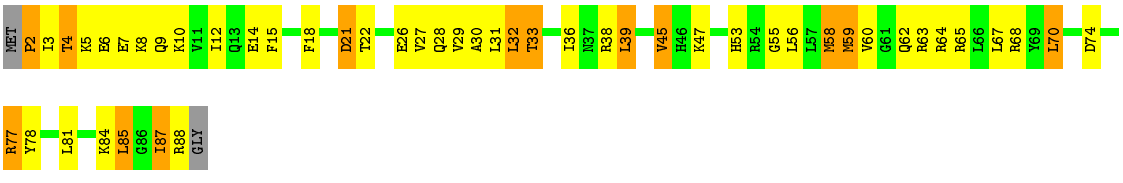
- Molecule 14: RIBOSOMAL PROTEIN S14

Chain N:



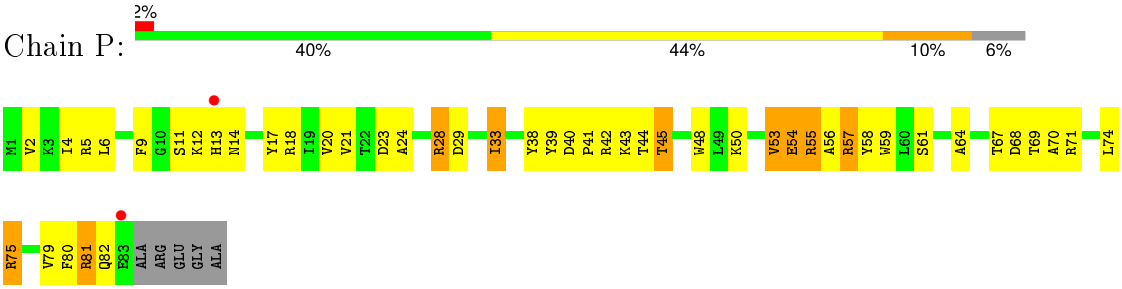
- Molecule 15: RIBOSOMAL PROTEIN S15

Chain O:



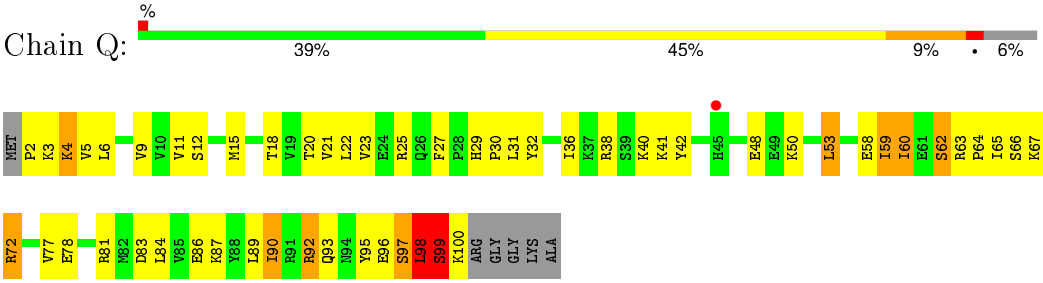
• Molecule 16: RIBOSOMAL PROTEIN S16

Chain P:



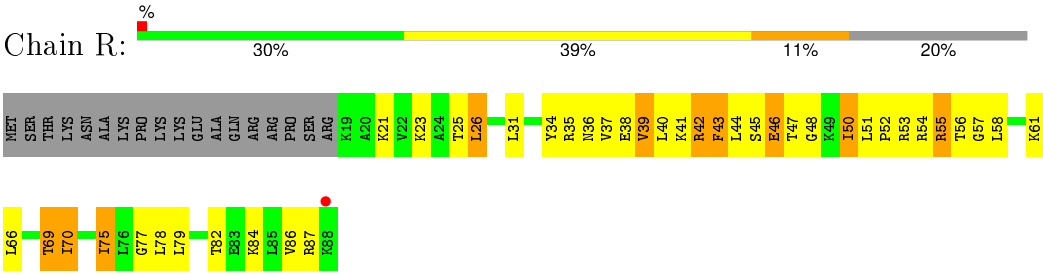
• Molecule 17: RIBOSOMAL PROTEIN S17

Chain Q:



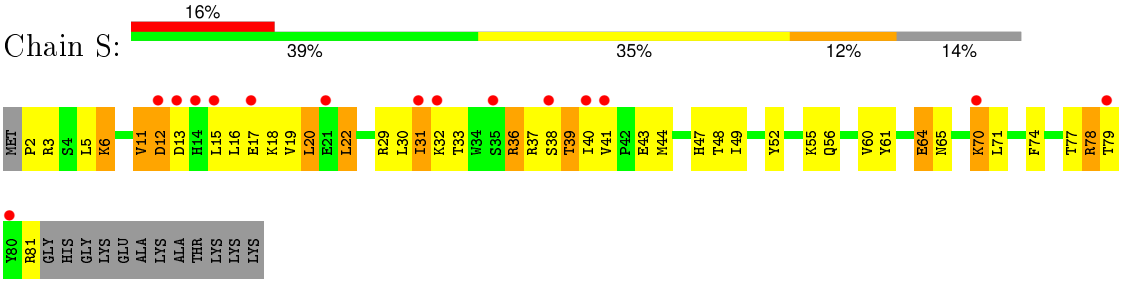
• Molecule 18: RIBOSOMAL PROTEIN S18

Chain R:



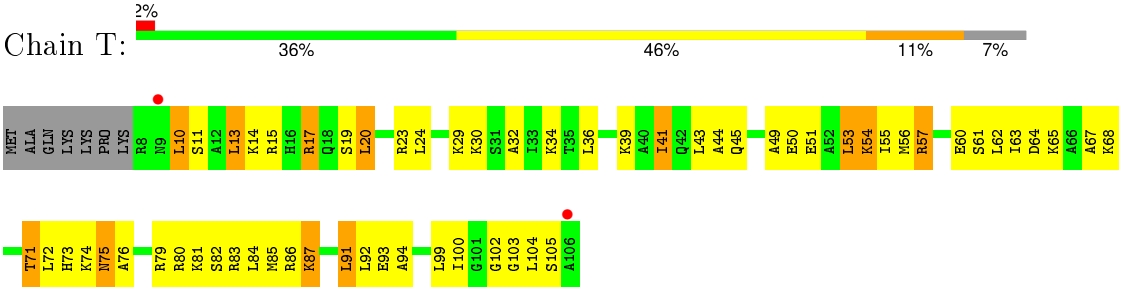
• Molecule 19: RIBOSOMAL PROTEIN S19

Chain S:



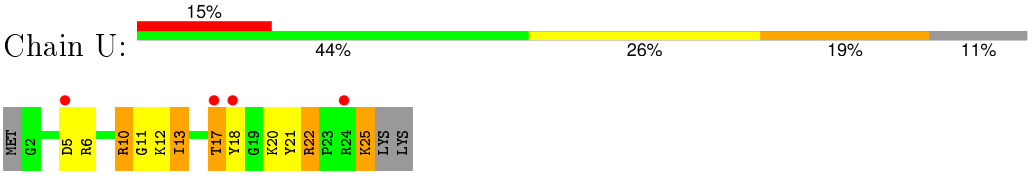
• Molecule 20: RIBOSOMAL PROTEIN S20

Chain T:



• Molecule 21: RIBOSOMAL PROTEIN THX

Chain U:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	402.08Å 402.08Å 174.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.30 – 3.69 49.60 – 3.69	Depositor EDS
% Data completeness (in resolution range)	98.5 (48.30-3.69) 98.5 (49.60-3.69)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.87 (at 3.67Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1119)	Depositor
R, R_{free}	0.156 , 0.214 0.162 , 0.214	Depositor DCC
R_{free} test set	7540 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	140.3	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 175.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Outliers	0 of 150281 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	52281	wwPDB-VP
Average B, all atoms (Å^2)	183.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.54% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	1.17	188/36139 (0.5%)	1.92	1603/56396 (2.8%)
2	B	0.72	0/1935	0.88	2/2609 (0.1%)
3	C	0.54	0/1636	0.76	2/2205 (0.1%)
4	D	0.71	1/1733 (0.1%)	0.88	1/2318 (0.0%)
5	E	0.92	0/1162	1.07	1/1564 (0.1%)
6	F	0.63	0/856	0.77	0/1154
7	G	0.57	0/1276	0.77	1/1709 (0.1%)
8	H	1.05	1/1136 (0.1%)	1.11	2/1527 (0.1%)
9	I	0.53	0/1029	0.77	0/1379
10	J	0.55	0/805	0.78	0/1082
11	K	0.71	0/879	0.88	0/1187
12	L	0.72	0/977	0.99	2/1305 (0.2%)
13	M	0.60	0/947	0.81	0/1270
14	N	0.48	0/501	0.75	0/664
15	O	0.77	0/740	0.92	1/987 (0.1%)
16	P	0.84	0/716	0.95	0/963
17	Q	0.93	0/836	1.10	2/1117 (0.2%)
18	R	0.77	1/579 (0.2%)	0.94	1/768 (0.1%)
19	S	0.46	0/661	0.76	1/890 (0.1%)
20	T	0.67	0/765	0.94	1/1007 (0.1%)
21	U	0.57	0/212	0.79	0/277
All	All	1.03	191/55520 (0.3%)	1.66	1620/82378 (2.0%)

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

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

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Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	2
7	G	0	1
8	H	0	2
10	J	0	4
12	L	0	1
15	O	0	1
20	T	0	2
All	All	0	17

All (191) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	817	C	N1-C6	-13.12	1.29	1.37
1	A	279	A	N9-C4	-11.47	1.30	1.37
1	A	279	A	N3-C4	-11.02	1.28	1.34
1	A	822	C	N1-C6	-10.98	1.30	1.37
1	A	279	A	N7-C5	-9.71	1.33	1.39
1	A	566	G	N7-C5	-9.03	1.33	1.39
1	A	288	A	N9-C4	-8.77	1.32	1.37
1	A	1500	A	N3-C4	-8.75	1.29	1.34
1	A	574	A	N9-C4	-8.51	1.32	1.37
1	A	266	G	N7-C5	-8.50	1.34	1.39
1	A	1500	A	C6-N1	-8.48	1.29	1.35
1	A	858	G	N1-C2	8.37	1.44	1.37
1	A	876	G	N3-C4	-8.29	1.29	1.35
4	D	12	CYS	CB-SG	8.29	1.96	1.82
1	A	569	C	N3-C4	-8.28	1.28	1.33
1	A	573	A	N7-C5	-8.01	1.34	1.39
1	A	858	G	N7-C5	-7.97	1.34	1.39
1	A	130	A	N3-C4	-7.81	1.30	1.34
1	A	130	A	N9-C4	-7.78	1.33	1.37
1	A	876	G	C5-C4	-7.72	1.32	1.38
1	A	858	G	C5-C6	-7.61	1.34	1.42
1	A	1064	G	N9-C4	-7.59	1.31	1.38
1	A	568	G	C6-N1	-7.55	1.34	1.39
1	A	828	A	N7-C5	-7.51	1.34	1.39
1	A	300	A	N7-C5	-7.46	1.34	1.39
1	A	1502	A	C5-C6	-7.42	1.34	1.41
1	A	860	A	N9-C4	-7.29	1.33	1.37
1	A	1499	A	N9-C4	-7.23	1.33	1.37
1	A	109	A	N3-C4	-7.02	1.30	1.34
1	A	793	U	C2-N3	7.02	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	570	G	C6-N1	-7.00	1.34	1.39
1	A	872	A	N7-C5	-6.97	1.35	1.39
1	A	722	A	C5-C6	-6.96	1.34	1.41
1	A	1502	A	N9-C4	-6.95	1.33	1.37
1	A	329	A	C5-C6	-6.93	1.34	1.41
1	A	860	A	N3-C4	-6.91	1.30	1.34
1	A	880	C	N1-C6	-6.90	1.33	1.37
1	A	586	C	N1-C6	-6.88	1.33	1.37
1	A	918	A	C5-C4	-6.87	1.33	1.38
1	A	665	A	C5-C4	-6.86	1.33	1.38
1	A	858	G	C5-C4	6.85	1.43	1.38
1	A	569	C	N1-C6	-6.82	1.33	1.37
1	A	1499	A	N3-C4	-6.78	1.30	1.34
1	A	863	U	C2-N3	-6.73	1.33	1.37
1	A	298	A	N3-C4	-6.70	1.30	1.34
1	A	753	A	N3-C4	-6.67	1.30	1.34
1	A	243	A	N3-C4	-6.63	1.30	1.34
1	A	570	G	N1-C2	-6.59	1.32	1.37
1	A	828	A	N9-C4	-6.56	1.33	1.37
1	A	574	A	C5-C4	-6.55	1.34	1.38
1	A	574	A	N3-C4	-6.53	1.30	1.34
1	A	568	G	N3-C4	-6.52	1.30	1.35
1	A	298	A	N9-C4	-6.50	1.33	1.37
1	A	382	A	N7-C5	-6.49	1.35	1.39
1	A	753	A	N9-C4	-6.48	1.33	1.37
8	H	135	CYS	CB-SG	-6.43	1.71	1.82
1	A	868	C	N3-C4	-6.34	1.29	1.33
1	A	1064	G	N3-C4	-6.34	1.31	1.35
1	A	665	A	N9-C4	-6.32	1.34	1.37
1	A	124	G	N3-C4	-6.29	1.31	1.35
1	A	946	A	N3-C4	-6.25	1.31	1.34
1	A	1401	G	N3-C4	-6.21	1.31	1.35
1	A	915	A	N3-C4	-6.20	1.31	1.34
1	A	722	A	N7-C5	-6.20	1.35	1.39
1	A	779	C	N1-C6	-6.16	1.33	1.37
1	A	872	A	C5-C6	-6.16	1.35	1.41
1	A	895	G	N7-C5	-6.11	1.35	1.39
1	A	236	G	C6-N1	-6.11	1.35	1.39
1	A	576	G	N3-C4	-6.09	1.31	1.35
1	A	869	G	C6-N1	6.08	1.43	1.39
1	A	824	C	N1-C6	-6.08	1.33	1.37
1	A	922	G	C6-N1	-6.07	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	584	G	C5-C4	-6.07	1.34	1.38
1	A	1077	G	N9-C8	-6.04	1.33	1.37
1	A	1509	C	N1-C6	-6.03	1.33	1.37
1	A	582	U	C2-N3	-6.03	1.33	1.37
1	A	274	A	N9-C4	-6.00	1.34	1.37
1	A	602	A	N9-C4	-5.98	1.34	1.37
1	A	869	G	C5-C6	-5.95	1.36	1.42
1	A	1514	C	N1-C6	-5.92	1.33	1.37
1	A	828	A	N3-C4	-5.91	1.31	1.34
1	A	881	G	C6-N1	-5.90	1.35	1.39
1	A	766	A	N9-C4	-5.89	1.34	1.37
1	A	1401	G	C6-N1	-5.89	1.35	1.39
1	A	566	G	N9-C8	-5.88	1.33	1.37
1	A	931	C	N1-C6	-5.88	1.33	1.37
1	A	266	G	C2-N3	5.87	1.37	1.32
1	A	665	A	N3-C4	-5.87	1.31	1.34
1	A	915	A	N9-C4	-5.86	1.34	1.37
1	A	1080	A	N3-C4	-5.86	1.31	1.34
1	A	325	A	N9-C4	-5.84	1.34	1.37
1	A	779	C	N3-C4	-5.82	1.29	1.33
1	A	21	G	N3-C4	-5.80	1.31	1.35
1	A	329	A	N9-C4	-5.80	1.34	1.37
1	A	946	A	N9-C4	-5.80	1.34	1.37
1	A	1504	G	C6-N1	-5.79	1.35	1.39
1	A	865	A	N7-C5	-5.77	1.35	1.39
1	A	757	U	N1-C2	-5.75	1.33	1.38
1	A	16	A	N3-C4	-5.75	1.31	1.34
1	A	715	A	N9-C4	-5.74	1.34	1.37
1	A	877	C	N1-C6	-5.72	1.33	1.37
1	A	125	U	C2-N3	-5.71	1.33	1.37
1	A	564	C	N1-C6	-5.71	1.33	1.37
1	A	918	A	N9-C8	-5.69	1.33	1.37
1	A	1401	G	C5-C4	-5.68	1.34	1.38
1	A	914	A	N9-C4	-5.67	1.34	1.37
1	A	1502	A	N3-C4	-5.65	1.31	1.34
1	A	589	C	N1-C6	-5.65	1.33	1.37
1	A	373	A	N9-C4	-5.62	1.34	1.37
1	A	1513	A	N9-C4	-5.62	1.34	1.37
1	A	666	G	N3-C4	-5.60	1.31	1.35
1	A	864	A	N3-C4	-5.59	1.31	1.34
1	A	918	A	N7-C5	-5.59	1.35	1.39
1	A	874	G	N9-C8	-5.58	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	635	G	C6-O6	5.58	1.29	1.24
1	A	1523	G	N3-C4	-5.57	1.31	1.35
1	A	109	A	N7-C5	-5.57	1.35	1.39
1	A	568	G	N1-C2	-5.56	1.33	1.37
1	A	787	A	N9-C4	-5.55	1.34	1.37
1	A	793	U	N3-C4	5.54	1.43	1.38
1	A	481	G	N9-C4	5.51	1.42	1.38
1	A	767	A	N3-C4	-5.51	1.31	1.34
1	A	559	A	N3-C4	-5.50	1.31	1.34
1	A	236	G	N7-C5	-5.50	1.35	1.39
1	A	1526	G	C5-C4	-5.50	1.34	1.38
1	A	109	A	N9-C4	-5.48	1.34	1.37
1	A	236	G	N9-C8	-5.47	1.34	1.37
1	A	263	A	N9-C4	-5.46	1.34	1.37
1	A	909	A	N9-C4	-5.45	1.34	1.37
1	A	236	G	C5-C4	-5.45	1.34	1.38
1	A	869	G	N9-C4	-5.43	1.33	1.38
1	A	572	A	C5-C4	-5.43	1.34	1.38
1	A	1377	A	N9-C4	-5.42	1.34	1.37
1	A	574	A	N9-C8	-5.41	1.33	1.37
1	A	243	A	N9-C4	-5.40	1.34	1.37
1	A	882	C	N3-C4	-5.39	1.30	1.33
1	A	917	G	N9-C4	-5.38	1.33	1.38
18	R	43	PHE	CB-CG	-5.38	1.42	1.51
1	A	295	C	N3-C4	-5.37	1.30	1.33
1	A	562	C	N1-C6	-5.37	1.33	1.37
1	A	879	C	N1-C6	-5.37	1.33	1.37
1	A	828	A	C5-C6	-5.37	1.36	1.41
1	A	917	G	N3-C4	-5.36	1.31	1.35
1	A	297	G	N7-C5	-5.35	1.36	1.39
1	A	882	C	N1-C6	-5.33	1.33	1.37
1	A	1529	G	N3-C4	-5.32	1.31	1.35
1	A	797	C	N3-C4	-5.30	1.30	1.33
1	A	836	G	C6-O6	5.29	1.28	1.24
1	A	868	C	N1-C6	-5.29	1.33	1.37
1	A	915	A	C5-C6	-5.29	1.36	1.41
1	A	1500	A	C5-C4	-5.29	1.35	1.38
1	A	1504	G	C5-C4	-5.28	1.34	1.38
1	A	755	G	N3-C4	-5.28	1.31	1.35
1	A	563	A	N3-C4	-5.27	1.31	1.34
1	A	1505	G	N7-C5	-5.25	1.36	1.39
1	A	1369	C	N3-C4	-5.23	1.30	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	862	C	C4-C5	-5.22	1.38	1.43
1	A	298	A	C5-C4	-5.21	1.35	1.38
1	A	116	A	N9-C4	-5.20	1.34	1.37
1	A	809	G	C6-N1	-5.19	1.35	1.39
1	A	1502	A	N7-C5	-5.18	1.36	1.39
1	A	572	A	C6-N6	-5.18	1.29	1.33
1	A	876	G	N1-C2	-5.18	1.33	1.37
1	A	793	U	C2-O2	5.17	1.27	1.22
1	A	695	A	N9-C4	-5.16	1.34	1.37
1	A	863	U	N3-C4	-5.16	1.33	1.38
1	A	782	A	C6-N1	-5.15	1.31	1.35
1	A	946	A	C6-N1	-5.14	1.31	1.35
1	A	574	A	N7-C5	-5.14	1.36	1.39
1	A	909	A	N7-C5	-5.13	1.36	1.39
1	A	862	C	C4-N4	-5.13	1.29	1.33
1	A	924	C	N1-C6	-5.12	1.34	1.37
1	A	673	G	N3-C4	-5.11	1.31	1.35
1	A	876	G	C2-N3	-5.09	1.28	1.32
1	A	107	G	N3-C4	-5.08	1.31	1.35
1	A	570	G	C5-C4	-5.08	1.34	1.38
1	A	1509	C	N3-C4	-5.07	1.30	1.33
1	A	68	G	C5-C4	-5.07	1.34	1.38
1	A	872	A	N9-C4	-5.06	1.34	1.37
1	A	21	G	N1-C2	-5.04	1.33	1.37
1	A	634	C	N1-C6	-5.04	1.34	1.37
1	A	809	G	C5-C6	-5.03	1.37	1.42
1	A	1074	G	N7-C5	-5.03	1.36	1.39
1	A	859	A	N9-C4	-5.03	1.34	1.37
1	A	1512	U	C4-O4	5.03	1.27	1.23
1	A	397	A	N7-C5	-5.02	1.36	1.39
1	A	898	G	N9-C4	-5.02	1.33	1.38
1	A	327	A	N9-C4	-5.01	1.34	1.37
1	A	728	A	N9-C4	-5.01	1.34	1.37
1	A	578	C	N3-C4	-5.01	1.30	1.33
1	A	946	A	N7-C5	-5.00	1.36	1.39

All (1620) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	858	G	N1-C6-O6	25.57	135.24	119.90
1	A	858	G	C6-C5-N7	-18.08	119.55	130.40
1	A	266	G	C6-C5-N7	-17.84	119.70	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	869	G	N1-C6-O6	17.27	130.26	119.90
1	A	869	G	C4-C5-N7	16.36	117.34	110.80
1	A	858	G	C2-N3-C4	-15.93	103.93	111.90
1	A	722	A	C2-N3-C4	-15.83	102.69	110.60
1	A	869	G	C5-C6-O6	-15.77	119.14	128.60
1	A	117	G	C6-C5-N7	-15.48	121.11	130.40
1	A	117	G	N1-C6-O6	15.22	129.03	119.90
1	A	266	G	N7-C8-N9	14.78	120.49	113.10
1	A	858	G	N7-C8-N9	14.62	120.41	113.10
1	A	858	G	C5-C6-O6	-14.55	119.87	128.60
1	A	858	G	C5-N7-C8	-14.37	97.12	104.30
1	A	1370	G	C8-N9-C4	-14.14	100.74	106.40
1	A	869	G	C5-N7-C8	-13.99	97.31	104.30
1	A	1395	C	C6-N1-C2	13.50	125.70	120.30
1	A	858	G	C5-C6-N1	-13.25	104.88	111.50
1	A	858	G	C4-C5-N7	12.99	115.99	110.80
1	A	1369	C	C6-N1-C2	-12.87	115.15	120.30
1	A	766	A	O5'-P-OP2	-12.74	94.23	105.70
1	A	266	G	C4-N9-C1'	12.71	143.02	126.50
1	A	824	C	C6-N1-C2	12.58	125.33	120.30
1	A	815	A	C8-N9-C4	12.27	110.71	105.80
1	A	858	G	N3-C2-N2	-12.21	111.35	119.90
1	A	1502	A	N1-C6-N6	12.17	125.90	118.60
1	A	266	G	C5-N7-C8	-12.07	98.27	104.30
1	A	600	C	C6-N1-C2	11.94	125.07	120.30
1	A	266	G	C8-N9-C4	-11.92	101.63	106.40
1	A	281	G	N1-C6-O6	11.87	127.02	119.90
1	A	570	G	N3-C4-C5	-11.82	122.69	128.60
1	A	1532	U	C5-C6-N1	11.77	128.58	122.70
1	A	562	C	C6-N1-C2	11.76	125.00	120.30
1	A	858	G	C8-N9-C4	-11.76	101.70	106.40
1	A	722	A	N1-C6-N6	11.58	125.55	118.60
1	A	481	G	N3-C4-N9	11.55	132.93	126.00
1	A	266	G	C4-C5-N7	11.54	115.41	110.80
1	A	731	G	N1-C6-O6	11.51	126.81	119.90
1	A	570	G	N1-C6-O6	-11.49	113.01	119.90
1	A	588	G	C8-N9-C4	11.34	110.93	106.40
1	A	635	G	C5-C6-N1	-11.32	105.84	111.50
1	A	555	C	C6-N1-C2	-11.18	115.83	120.30
1	A	896	C	N3-C4-C5	11.15	126.36	121.90
1	A	119	A	O5'-P-OP2	-11.14	95.68	105.70
1	A	15	G	N1-C6-O6	11.13	126.58	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	722	A	C6-C5-N7	-11.12	124.51	132.30
1	A	658	G	N9-C4-C5	-11.07	100.97	105.40
1	A	869	G	N3-C4-C5	10.89	134.04	128.60
1	A	740	U	O5'-P-OP2	-10.88	95.91	105.70
1	A	121	C	C6-N1-C2	10.83	124.63	120.30
1	A	1502	A	C2-N3-C4	-10.73	105.24	110.60
1	A	867	G	C5-C6-O6	-10.71	122.17	128.60
1	A	647	C	C6-N1-C2	10.69	124.57	120.30
1	A	756	C	C6-N1-C2	10.65	124.56	120.30
1	A	573	A	C8-N9-C4	-10.64	101.54	105.80
1	A	1505	G	C8-N9-C4	-10.63	102.15	106.40
1	A	1200	C	C2-N1-C1'	10.59	130.44	118.80
1	A	1238	A	C8-N9-C4	-10.57	101.57	105.80
1	A	481	G	N3-C4-C5	-10.56	123.32	128.60
1	A	731	G	C5-C6-O6	-10.47	122.32	128.60
1	A	658	G	C8-N9-C4	10.47	110.59	106.40
1	A	1502	A	C5-N7-C8	-10.40	98.70	103.90
1	A	600	C	C5-C6-N1	-10.34	115.83	121.00
1	A	862	C	N3-C4-C5	10.29	126.02	121.90
1	A	1331	G	N1-C6-O6	-10.26	113.75	119.90
1	A	279	A	C2-N3-C4	-10.25	105.48	110.60
1	A	1502	A	C6-C5-N7	-10.23	125.14	132.30
1	A	872	A	N1-C6-N6	10.18	124.70	118.60
1	A	1527	C	C6-N1-C2	-10.15	116.24	120.30
1	A	266	G	C4-C5-C6	10.14	124.88	118.80
1	A	1068	G	O5'-P-OP1	-10.14	96.58	105.70
1	A	579	G	C4-C5-N7	10.12	114.85	110.80
1	A	824	C	C5-C6-N1	-10.11	115.95	121.00
1	A	835	U	C5-C4-O4	10.10	131.96	125.90
1	A	873	A	C8-N9-C4	-10.10	101.76	105.80
1	A	922	G	C8-N9-C4	-10.08	102.37	106.40
1	A	117	G	C4-C5-C6	10.04	124.83	118.80
1	A	771	G	N1-C6-O6	9.97	125.88	119.90
1	A	579	G	N1-C6-O6	9.92	125.85	119.90
1	A	852	G	C5-C6-N1	-9.89	106.55	111.50
1	A	570	G	C6-N1-C2	-9.87	119.18	125.10
1	A	793	U	N1-C2-N3	-9.79	109.02	114.90
1	A	588	G	O5'-P-OP2	-9.78	96.90	105.70
1	A	1354	C	C6-N1-C2	-9.77	116.39	120.30
1	A	948	C	C6-N1-C2	9.75	124.20	120.30
1	A	1502	A	C4-C5-N7	9.75	115.58	110.70
1	A	1181	G	C8-N9-C4	9.74	110.30	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	569	C	C5-C6-N1	-9.71	116.14	121.00
1	A	279	A	C4-C5-C6	9.71	121.85	117.00
1	A	572	A	C5-C6-N1	9.70	122.55	117.70
1	A	908	A	C2-N3-C4	-9.63	105.78	110.60
1	A	812	C	N3-C4-C5	-9.62	118.05	121.90
1	A	1370	G	N7-C8-N9	9.60	117.90	113.10
1	A	931	C	C5-C6-N1	-9.55	116.22	121.00
1	A	722	A	C5-C6-N1	-9.54	112.93	117.70
1	A	144	G	N1-C6-O6	9.53	125.62	119.90
1	A	382	A	C8-N9-C4	-9.50	102.00	105.80
1	A	872	A	C2-N3-C4	-9.44	105.88	110.60
1	A	570	G	C5-C6-N1	9.43	116.22	111.50
1	A	731	G	C4-C5-N7	9.42	114.57	110.80
1	A	735	C	C6-N1-C2	9.40	124.06	120.30
1	A	1420	C	C6-N1-C2	-9.40	116.54	120.30
1	A	858	G	C4-C5-C6	9.38	124.42	118.80
1	A	1238	A	N9-C4-C5	9.33	109.53	105.80
1	A	117	G	C4-N9-C1'	9.32	138.62	126.50
1	A	1197	G	O5'-P-OP1	-9.31	97.32	105.70
1	A	779	C	N1-C2-N3	9.30	125.71	119.20
1	A	117	G	C2-N3-C4	-9.27	107.27	111.90
1	A	665	A	C5-C6-N1	9.25	122.32	117.70
1	A	579	G	C5-C6-O6	-9.21	123.07	128.60
1	A	235	C	C6-N1-C2	9.20	123.98	120.30
1	A	623	C	C6-N1-C2	9.12	123.95	120.30
1	A	117	G	C5-C6-N1	-9.11	106.94	111.50
1	A	250	A	N1-C6-N6	9.11	124.07	118.60
1	A	331	G	N1-C6-O6	9.07	125.34	119.90
1	A	854	G	O5'-P-OP1	-9.06	97.55	105.70
1	A	266	G	C8-N9-C1'	-9.03	115.26	127.00
1	A	279	A	C5-C6-N1	-9.02	113.19	117.70
1	A	1527	C	N3-C2-O2	-9.02	115.59	121.90
1	A	626	U	C6-N1-C2	-9.01	115.59	121.00
1	A	562	C	C5-C6-N1	-9.00	116.50	121.00
1	A	1373	G	N3-C4-N9	9.00	131.40	126.00
1	A	771	G	C5-C6-O6	-8.99	123.20	128.60
1	A	668	G	C8-N9-C4	8.98	109.99	106.40
1	A	125	U	C5-C6-N1	-8.98	118.21	122.70
1	A	863	U	N3-C4-O4	-8.98	113.12	119.40
1	A	869	G	N7-C8-N9	8.96	117.58	113.10
1	A	588	G	N7-C8-N9	-8.94	108.63	113.10
1	A	877	C	C2-N3-C4	-8.94	115.43	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	707	C	O5'-P-OP2	-8.93	97.66	105.70
1	A	624	C	C6-N1-C2	8.90	123.86	120.30
1	A	1098	C	C6-N1-C2	8.90	123.86	120.30
1	A	658	G	C8-N9-C1'	-8.89	115.44	127.00
1	A	867	G	N1-C6-O6	8.89	125.24	119.90
1	A	970	C	N1-C2-O2	8.89	124.23	118.90
1	A	1524	C	N1-C2-O2	-8.86	113.59	118.90
1	A	1516[A]	G	C8-N9-C4	-8.85	102.86	106.40
1	A	1516[B]	G	C8-N9-C4	-8.85	102.86	106.40
1	A	117	G	C8-N9-C1'	-8.85	115.50	127.00
1	A	885	G	C2-N3-C4	-8.84	107.48	111.90
1	A	279	A	N1-C2-N3	8.80	133.70	129.30
1	A	1490	U	C5-C6-N1	8.79	127.10	122.70
1	A	650	G	C8-N9-C4	-8.79	102.89	106.40
1	A	300	A	C8-N9-C4	-8.78	102.29	105.80
1	A	232	G	N9-C4-C5	-8.77	101.89	105.40
1	A	568	G	O5'-P-OP2	-8.77	97.81	105.70
1	A	1527	C	C2-N1-C1'	8.76	128.44	118.80
1	A	279	A	O4'-C1'-N9	-8.72	101.23	108.20
1	A	835	U	N1-C2-N3	8.71	120.12	114.90
1	A	281	G	C5-C6-O6	-8.69	123.39	128.60
1	A	309	G	C4-C5-N7	8.69	114.27	110.80
1	A	25	C	C6-N1-C2	8.68	123.77	120.30
1	A	650	G	N7-C8-N9	8.68	117.44	113.10
1	A	872	A	C6-C5-N7	-8.68	126.22	132.30
17	Q	98	LEU	CA-CB-CG	8.67	135.23	115.30
1	A	1512	U	N3-C4-C5	-8.65	109.41	114.60
1	A	666	G	C2-N3-C4	-8.65	107.58	111.90
1	A	936	C	C6-N1-C2	8.65	123.76	120.30
1	A	366	C	N1-C2-O2	8.64	124.09	118.90
1	A	569	C	N3-C4-N4	-8.62	111.97	118.00
1	A	1395	C	O5'-P-OP2	-8.61	97.95	105.70
1	A	835	U	N3-C4-C5	-8.61	109.43	114.60
1	A	762	C	O5'-P-OP2	8.57	120.99	110.70
1	A	941	G	C8-N9-C4	-8.57	102.97	106.40
1	A	559	A	C6-N1-C2	-8.56	113.46	118.60
1	A	745	C	N3-C4-C5	8.56	125.33	121.90
1	A	919	A	C8-N9-C4	8.53	109.21	105.80
1	A	277	C	C6-N1-C2	8.52	123.71	120.30
1	A	635	G	N1-C6-O6	8.51	125.00	119.90
1	A	579	G	C5-N7-C8	-8.50	100.05	104.30
1	A	266	G	N1-C6-O6	8.48	124.99	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	168	G	C6-C5-N7	-8.43	125.34	130.40
1	A	912	C	N3-C4-N4	8.40	123.88	118.00
1	A	1442	G	N3-C4-C5	-8.40	124.40	128.60
1	A	638	G	N1-C6-O6	8.38	124.93	119.90
1	A	366	C	N3-C2-O2	-8.38	116.04	121.90
1	A	279	A	C8-N9-C4	-8.37	102.45	105.80
1	A	281	G	C4-C5-N7	8.36	114.14	110.80
1	A	922	G	N1-C6-O6	-8.35	114.89	119.90
1	A	722	A	C4-C5-N7	8.34	114.87	110.70
1	A	1531	A	N1-C6-N6	8.33	123.60	118.60
1	A	451	A	C8-N9-C4	8.32	109.13	105.80
1	A	869	G	C6-C5-N7	-8.32	125.41	130.40
1	A	877	C	C5-C6-N1	-8.32	116.84	121.00
1	A	1200	C	N1-C2-O2	8.31	123.89	118.90
1	A	257	G	N1-C6-O6	8.30	124.88	119.90
1	A	1373	G	N3-C4-C5	-8.30	124.45	128.60
1	A	281	G	N9-C4-C5	-8.29	102.08	105.40
1	A	886	G	N1-C6-O6	8.28	124.87	119.90
1	A	550	G	C2-N3-C4	-8.23	107.78	111.90
1	A	252	U	C5-C6-N1	-8.22	118.59	122.70
1	A	650	G	C6-C5-N7	-8.22	125.47	130.40
1	A	658	G	N3-C4-N9	8.21	130.93	126.00
1	A	666	G	N1-C2-N3	8.21	128.83	123.90
1	A	715	A	C2-N3-C4	-8.20	106.50	110.60
1	A	667	G	C2-N3-C4	-8.19	107.80	111.90
1	A	812	C	C4-C5-C6	8.19	121.50	117.40
1	A	326	G	C4-C5-N7	-8.18	107.53	110.80
1	A	867	G	C6-C5-N7	-8.17	125.50	130.40
1	A	867	G	C4-C5-N7	8.16	114.06	110.80
1	A	117	G	C4-C5-N7	8.15	114.06	110.80
1	A	292	G	C5-C6-O6	-8.15	123.71	128.60
1	A	1060	C	N1-C2-O2	8.14	123.78	118.90
1	A	890	G	C4-C5-N7	-8.13	107.55	110.80
1	A	292	G	N1-C6-O6	8.13	124.78	119.90
1	A	615	C	O5'-P-OP1	-8.12	98.39	105.70
1	A	859	A	N1-C6-N6	8.11	123.47	118.60
1	A	511	C	C5-C6-N1	-8.10	116.95	121.00
1	A	266	G	N3-C4-N9	8.09	130.85	126.00
1	A	626	U	N1-C2-N3	8.09	119.75	114.90
1	A	835	U	C4-C5-C6	8.08	124.55	119.70
1	A	817	C	C4-C5-C6	8.07	121.44	117.40
1	A	835	U	N3-C2-O2	-8.06	116.56	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	875	C	C5-C6-N1	-8.05	116.97	121.00
1	A	858	G	N3-C4-C5	8.04	132.62	128.60
1	A	815	A	N7-C8-N9	-8.04	109.78	113.80
1	A	483	C	C4-C5-C6	8.02	121.41	117.40
1	A	824	C	C2-N3-C4	-8.02	115.89	119.90
1	A	1505	G	N7-C8-N9	8.00	117.10	113.10
1	A	658	G	N1-C2-N3	8.00	128.70	123.90
1	A	1490	U	N1-C2-N3	-8.00	110.10	114.90
1	A	919	A	O5'-P-OP2	-7.99	98.51	105.70
1	A	278	G	O5'-P-OP2	-7.98	98.52	105.70
1	A	1075	C	N3-C4-C5	7.98	125.09	121.90
1	A	659	U	C2-N3-C4	-7.97	122.22	127.00
1	A	232	G	C4-C5-N7	7.96	113.98	110.80
1	A	826	C	C5-C6-N1	-7.96	117.02	121.00
1	A	1307	U	N3-C2-O2	-7.96	116.62	122.20
1	A	1226	C	N1-C2-O2	7.95	123.67	118.90
1	A	650	G	C4-N9-C1'	7.93	136.81	126.50
1	A	658	G	N1-C2-N2	-7.92	109.07	116.20
1	A	835	U	C6-N1-C2	-7.91	116.25	121.00
1	A	817	C	C6-N1-C2	7.91	123.46	120.30
1	A	822	C	C4-C5-C6	7.91	121.35	117.40
1	A	342	C	C6-N1-C2	-7.90	117.14	120.30
1	A	731	G	N9-C4-C5	-7.90	102.24	105.40
1	A	1200	C	C5-C6-N1	7.89	124.94	121.00
1	A	8	A	N9-C4-C5	7.88	108.95	105.80
1	A	251	G	C4-C5-N7	7.88	113.95	110.80
1	A	805	C	C6-N1-C2	7.86	123.44	120.30
1	A	615	C	C6-N1-C2	-7.86	117.16	120.30
1	A	863	U	C5-C4-O4	7.85	130.61	125.90
1	A	916	G	C8-N9-C4	7.84	109.53	106.40
1	A	518	C	N1-C2-O2	7.84	123.60	118.90
1	A	1282	C	C6-N1-C2	-7.83	117.17	120.30
1	A	326	G	C5-C6-O6	7.83	133.30	128.60
1	A	122	G	N1-C6-O6	7.82	124.59	119.90
1	A	941	G	N7-C8-N9	7.82	117.01	113.10
1	A	1490	U	C5-C4-O4	-7.81	121.21	125.90
1	A	1200	C	C6-N1-C2	-7.81	117.17	120.30
1	A	600	C	C2-N3-C4	-7.80	116.00	119.90
1	A	1189	C	C6-N1-C2	7.79	123.42	120.30
1	A	1108	G	C8-N9-C4	-7.77	103.29	106.40
1	A	277	C	N3-C4-C5	7.76	125.00	121.90
1	A	825	G	C8-N9-C4	7.75	109.50	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1079	G	N3-C4-C5	-7.74	124.73	128.60
1	A	757	U	C2-N1-C1'	-7.73	108.42	117.70
1	A	116	A	C2-N3-C4	-7.72	106.74	110.60
1	A	281	G	C6-C5-N7	-7.72	125.77	130.40
1	A	691	G	C8-N9-C4	-7.71	103.31	106.40
1	A	18	C	C5-C6-N1	-7.71	117.14	121.00
1	A	190(E)	U	C2-N1-C1'	-7.70	108.46	117.70
1	A	1442	G	C4-N9-C1'	7.69	136.50	126.50
1	A	970	C	N3-C2-O2	-7.69	116.52	121.90
1	A	1505	G	C6-C5-N7	-7.68	125.79	130.40
1	A	569	C	C5-C4-N4	7.67	125.57	120.20
1	A	722	A	C5-N7-C8	-7.66	100.07	103.90
1	A	1158	C	C2-N1-C1'	7.65	127.21	118.80
1	A	643	C	N3-C4-C5	7.65	124.96	121.90
1	A	854	G	C4-N9-C1'	7.64	136.43	126.50
1	A	117	G	C5-C6-O6	-7.63	124.02	128.60
1	A	755	G	N1-C6-O6	7.63	124.48	119.90
1	A	922	G	N9-C4-C5	7.62	108.45	105.40
1	A	805	C	N3-C4-C5	7.62	124.95	121.90
1	A	833	U	C5-C4-O4	7.61	130.46	125.90
1	A	931	C	C2-N3-C4	-7.61	116.10	119.90
1	A	1078	U	N1-C2-O2	7.60	128.12	122.80
1	A	722	A	N1-C2-N3	7.59	133.10	129.30
1	A	599	C	C6-N1-C2	7.59	123.34	120.30
1	A	809	G	C4-C5-N7	7.58	113.83	110.80
1	A	331	G	C5-C6-N1	-7.58	107.71	111.50
1	A	18	C	C6-N1-C2	7.57	123.33	120.30
1	A	1452	C	C6-N1-C2	7.57	123.33	120.30
1	A	944	G	C5-C6-O6	7.57	133.14	128.60
1	A	665	A	C6-N1-C2	-7.56	114.06	118.60
1	A	836	G	C5-C6-N1	-7.56	107.72	111.50
1	A	877	C	O5'-P-OP2	-7.55	98.90	105.70
1	A	928	G	C4-C5-N7	7.55	113.82	110.80
1	A	273	A	C8-N9-C4	-7.55	102.78	105.80
1	A	558	G	O5'-P-OP1	7.55	119.75	110.70
1	A	250	A	N9-C4-C5	-7.54	102.78	105.80
1	A	130	A	N1-C2-N3	7.54	133.07	129.30
1	A	1051	C	C2-N1-C1'	7.54	127.09	118.80
1	A	309	G	C5-C6-O6	-7.54	124.08	128.60
1	A	768	A	N1-C6-N6	7.53	123.12	118.60
1	A	822	C	C2-N3-C4	-7.53	116.14	119.90
1	A	771	G	C6-C5-N7	-7.52	125.89	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	245	C	C5-C4-N4	-7.51	114.94	120.20
1	A	7	G	O4'-C1'-N9	7.51	114.21	108.20
1	A	817	C	C5-C6-N1	-7.51	117.25	121.00
1	A	483	C	C5-C6-N1	-7.50	117.25	121.00
1	A	715	A	N3-C4-C5	7.50	132.05	126.80
1	A	299	G	N1-C6-O6	7.49	124.39	119.90
1	A	1158	C	N1-C2-O2	7.49	123.39	118.90
1	A	695	A	C2-N3-C4	-7.49	106.86	110.60
1	A	815	A	O4'-C1'-N9	-7.48	102.22	108.20
1	A	602	A	C2-N3-C4	-7.48	106.86	110.60
1	A	867	G	N9-C4-C5	-7.47	102.41	105.40
1	A	872	A	C4-C5-N7	7.46	114.43	110.70
1	A	283	C	C5-C6-N1	7.46	124.73	121.00
1	A	814	A	C8-N9-C4	7.46	108.78	105.80
1	A	1371	G	O5'-P-OP1	-7.46	98.98	105.70
1	A	941	G	C5-N7-C8	-7.45	100.58	104.30
1	A	666	G	C5-C6-N1	-7.44	107.78	111.50
1	A	318	G	N1-C6-O6	7.44	124.36	119.90
1	A	578	C	N1-C2-O2	-7.43	114.44	118.90
1	A	1060	C	N3-C2-O2	-7.43	116.70	121.90
1	A	589	C	C4-C5-C6	7.42	121.11	117.40
1	A	123	C	N3-C4-C5	-7.42	118.93	121.90
1	A	111	G	N3-C4-N9	-7.41	121.55	126.00
1	A	1064	G	N3-C4-C5	7.40	132.30	128.60
1	A	314	C	C5-C6-N1	-7.39	117.31	121.00
1	A	331	G	C6-C5-N7	-7.39	125.97	130.40
1	A	8	A	N1-C6-N6	-7.38	114.17	118.60
1	A	826	C	C6-N1-C2	7.38	123.25	120.30
1	A	1094	G	C8-N9-C4	7.38	109.35	106.40
1	A	1087	G	C4-C5-N7	7.38	113.75	110.80
1	A	168	G	C4-N9-C1'	7.37	136.07	126.50
1	A	310	G	C5-C6-O6	-7.37	124.18	128.60
1	A	29	G	N1-C6-O6	7.36	124.32	119.90
1	A	264	U	N3-C2-O2	-7.36	117.05	122.20
1	A	21	G	C8-N9-C4	7.36	109.34	106.40
1	A	880	C	C2-N3-C4	-7.35	116.22	119.90
1	A	626	U	N3-C2-O2	-7.35	117.06	122.20
1	A	51	A	C8-N9-C4	-7.34	102.86	105.80
1	A	319	G	C5-C6-O6	-7.34	124.19	128.60
1	A	127	G	N1-C6-O6	7.34	124.30	119.90
1	A	279	A	N7-C8-N9	7.33	117.47	113.80
1	A	257	G	C6-C5-N7	-7.33	126.00	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	15	G	C6-C5-N7	-7.33	126.00	130.40
1	A	1339	A	N1-C6-N6	-7.32	114.21	118.60
1	A	585	G	C8-N9-C4	-7.32	103.47	106.40
1	A	240	C	N3-C4-C5	7.32	124.83	121.90
1	A	746	A	C8-N9-C4	7.31	108.73	105.80
1	A	600	C	N3-C4-C5	7.31	124.82	121.90
1	A	382	A	N7-C8-N9	7.31	117.45	113.80
1	A	864	A	C5-C6-N6	7.30	129.54	123.70
1	A	266	G	N3-C4-C5	-7.30	124.95	128.60
1	A	511	C	C6-N1-C2	7.29	123.22	120.30
1	A	491	G	N1-C6-O6	7.28	124.27	119.90
1	A	771	G	N9-C4-C5	-7.28	102.49	105.40
1	A	1442	G	N3-C4-N9	7.28	130.37	126.00
1	A	1084	G	N1-C2-N3	7.28	128.26	123.90
1	A	1500	A	N9-C4-C5	7.28	108.71	105.80
1	A	1490	U	C4-C5-C6	-7.27	115.34	119.70
1	A	648	A	C5-C6-N1	7.27	121.33	117.70
1	A	880	C	C5-C4-N4	-7.26	115.12	120.20
1	A	659	U	C5-C6-N1	-7.25	119.08	122.70
1	A	1524	C	C6-N1-C2	-7.25	117.40	120.30
1	A	121	C	N3-C2-O2	7.25	126.97	121.90
1	A	949	A	C2-N3-C4	-7.24	106.98	110.60
1	A	167	G	N3-C4-N9	7.24	130.34	126.00
1	A	129(A)	G	C6-C5-N7	-7.23	126.06	130.40
1	A	533	A	N1-C6-N6	-7.23	114.26	118.60
1	A	722	A	C4-C5-C6	7.23	120.62	117.00
1	A	254	G	C2-N3-C4	-7.23	108.29	111.90
1	A	379	C	C6-N1-C2	7.23	123.19	120.30
1	A	106	C	C6-N1-C2	-7.22	117.41	120.30
1	A	1361(A)	C	C5-C6-N1	7.22	124.61	121.00
1	A	126	G	C5-C6-N1	-7.21	107.89	111.50
1	A	266	G	O4'-C1'-N9	-7.21	102.43	108.20
1	A	907	A	N1-C2-N3	7.21	132.90	129.30
1	A	763	G	C5-C6-O6	-7.20	124.28	128.60
1	A	819	A	N1-C6-N6	7.20	122.92	118.60
1	A	1512	U	N3-C4-O4	7.19	124.44	119.40
1	A	875	C	C2-N3-C4	-7.19	116.31	119.90
1	A	919	A	N7-C8-N9	-7.18	110.21	113.80
1	A	1064	G	N3-C4-N9	-7.18	121.69	126.00
1	A	519	C	C6-N1-C2	7.18	123.17	120.30
1	A	1488	G	N3-C4-C5	-7.18	125.01	128.60
1	A	21	G	N9-C4-C5	-7.18	102.53	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1235	U	N1-C2-O2	-7.17	117.78	122.80
1	A	862	C	C5-C4-N4	-7.17	115.19	120.20
1	A	117	G	N9-C4-C5	-7.16	102.53	105.40
1	A	572	A	N1-C6-N6	-7.16	114.30	118.60
1	A	793	U	C5-C6-N1	7.16	126.28	122.70
1	A	576	G	O5'-P-OP2	-7.16	99.25	105.70
1	A	579	G	C6-C5-N7	-7.15	126.11	130.40
1	A	815	A	N9-C4-C5	-7.15	102.94	105.80
1	A	1190	G	O5'-P-OP2	-7.15	99.26	105.70
1	A	581	G	C2-N3-C4	-7.14	108.33	111.90
1	A	809	G	C5-C6-O6	-7.14	124.31	128.60
4	D	12	CYS	CA-CB-SG	7.14	126.85	114.00
1	A	309	G	N9-C4-C5	-7.14	102.55	105.40
1	A	292	G	C6-C5-N7	-7.14	126.12	130.40
1	A	256	U	N1-C2-N3	-7.13	110.62	114.90
1	A	557	G	N1-C6-O6	7.13	124.18	119.90
1	A	735	C	C5-C6-N1	-7.13	117.44	121.00
1	A	1200	C	C6-N1-C1'	-7.13	112.25	120.80
1	A	1354	C	C5-C6-N1	7.13	124.56	121.00
1	A	251	G	C5-C6-O6	-7.12	124.33	128.60
1	A	736	C	N3-C2-O2	-7.12	116.92	121.90
1	A	7	G	C8-N9-C4	-7.12	103.55	106.40
1	A	397	A	C6-C5-N7	-7.12	127.32	132.30
1	A	690	G	N3-C4-C5	7.11	132.16	128.60
1	A	1246	C	N3-C4-C5	7.11	124.75	121.90
12	L	66	VAL	CB-CA-C	-7.11	97.88	111.40
1	A	1441	G	C5-C6-N1	-7.11	107.94	111.50
1	A	779	C	C2-N3-C4	-7.11	116.35	119.90
1	A	413	G	O4'-C1'-N9	7.11	113.88	108.20
1	A	771	G	C4-C5-N7	7.10	113.64	110.80
1	A	867	G	N3-C4-N9	7.09	130.26	126.00
1	A	1485	U	C5-C4-O4	7.09	130.16	125.90
1	A	568	G	OP2-P-O3'	7.08	120.79	105.20
1	A	883	C	C6-N1-C2	7.08	123.13	120.30
1	A	1490	U	N1-C2-O2	7.08	127.76	122.80
1	A	1369	C	N3-C2-O2	-7.08	116.94	121.90
1	A	650	G	C4-C5-C6	7.08	123.05	118.80
1	A	379	C	O5'-P-OP2	-7.07	99.33	105.70
1	A	722	A	N9-C4-C5	-7.07	102.97	105.80
1	A	232	G	N1-C6-O6	7.06	124.14	119.90
1	A	254	G	O5'-P-OP1	-7.06	99.34	105.70
1	A	864	A	N1-C6-N6	-7.06	114.36	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	550	G	N1-C2-N3	7.06	128.13	123.90
1	A	1078	U	C2-N1-C1'	7.05	126.16	117.70
1	A	385	C	C6-N1-C2	-7.05	117.48	120.30
1	A	15	G	C2-N3-C4	-7.05	108.38	111.90
1	A	655	A	C5-C6-N1	7.05	121.22	117.70
1	A	1500	A	N1-C6-N6	-7.04	114.37	118.60
1	A	1502	A	C5-C6-N1	-7.04	114.18	117.70
1	A	823	G	N1-C2-N2	-7.04	109.87	116.20
1	A	569	C	O5'-P-OP2	-7.03	99.37	105.70
1	A	719	C	N1-C2-O2	7.03	123.12	118.90
1	A	661	G	C2-N3-C4	-7.03	108.39	111.90
1	A	920	U	C5-C4-O4	7.03	130.12	125.90
1	A	150	C	C6-N1-C2	-7.02	117.49	120.30
1	A	250	A	O5'-P-OP2	-7.01	99.39	105.70
1	A	329	A	N1-C6-N6	7.01	122.80	118.60
1	A	686	U	C5-C6-N1	-7.00	119.20	122.70
1	A	597	G	C5-C6-O6	-7.00	124.40	128.60
1	A	1455	G	C8-N9-C4	-7.00	103.60	106.40
1	A	1433	A	C8-N9-C4	-6.98	103.01	105.80
1	A	242	C	C6-N1-C2	6.98	123.09	120.30
1	A	329	A	C2-N3-C4	-6.98	107.11	110.60
1	A	809	G	C5-C6-N1	6.98	114.99	111.50
1	A	894	G	C2-N3-C4	-6.98	108.41	111.90
1	A	128	G	N1-C6-O6	6.98	124.08	119.90
1	A	895	G	C8-N9-C4	-6.97	103.61	106.40
1	A	1330	U	C5-C4-O4	-6.97	121.72	125.90
1	A	1074	G	C5-C6-N1	-6.97	108.01	111.50
1	A	397	A	N1-C6-N6	6.97	122.78	118.60
1	A	481	G	C8-N9-C1'	-6.96	117.95	127.00
1	A	552	U	C5-C6-N1	-6.96	119.22	122.70
1	A	319	G	N1-C6-O6	6.95	124.07	119.90
1	A	256	U	C5-C4-O4	-6.95	121.73	125.90
1	A	7	G	N9-C4-C5	6.95	108.18	105.40
1	A	280	C	OP1-P-OP2	6.95	130.02	119.60
1	A	1078	U	N3-C2-O2	-6.95	117.34	122.20
1	A	1530	G	C2-N3-C4	-6.94	108.43	111.90
1	A	147	G	N1-C6-O6	6.93	124.06	119.90
1	A	852	G	N1-C6-O6	6.92	124.05	119.90
1	A	1077	G	N1-C2-N2	-6.91	109.98	116.20
1	A	1087	G	C5-C6-O6	-6.91	124.45	128.60
1	A	66	G	C8-N9-C4	-6.90	103.64	106.40
1	A	1307	U	N1-C2-O2	6.90	127.63	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1373	G	C8-N9-C1'	-6.90	118.03	127.00
1	A	132	C	C6-N1-C2	-6.89	117.54	120.30
1	A	770	C	C2-N3-C4	-6.89	116.45	119.90
1	A	1149	C	C6-N1-C2	-6.89	117.54	120.30
1	A	793	U	C2-N3-C4	6.89	131.13	127.00
1	A	658	G	C2-N3-C4	-6.88	108.46	111.90
1	A	698	G	C4-N9-C1'	6.88	135.45	126.50
1	A	456	C	C6-N1-C2	6.88	123.05	120.30
1	A	1365	G	C8-N9-C4	-6.87	103.65	106.40
1	A	1417	G	C8-N9-C4	-6.87	103.65	106.40
1	A	525	C	C6-N1-C2	6.86	123.05	120.30
1	A	862	C	C6-N1-C2	6.86	123.05	120.30
1	A	300	A	N7-C8-N9	6.86	117.23	113.80
1	A	232	G	C6-C5-N7	-6.86	126.28	130.40
1	A	570	G	N3-C4-N9	6.86	130.12	126.00
1	A	15	G	C5-N7-C8	-6.85	100.88	104.30
1	A	721	G	C8-N9-C1'	-6.85	118.10	127.00
1	A	1305	G	P-O3'-C3'	6.83	127.90	119.70
1	A	185	A	O5'-P-OP2	-6.83	99.56	105.70
1	A	129(A)	G	C4-N9-C1'	6.82	135.37	126.50
1	A	268	C	N1-C2-O2	6.82	122.99	118.90
1	A	578	C	N1-C2-N3	6.82	123.98	119.20
1	A	299	G	C5-C6-N1	-6.82	108.09	111.50
1	A	310	G	C8-N9-C4	6.82	109.13	106.40
1	A	310	G	N1-C6-O6	6.82	123.99	119.90
1	A	35	G	N1-C6-O6	6.82	123.99	119.90
1	A	782	A	C2-N3-C4	-6.80	107.20	110.60
1	A	279	A	C6-C5-N7	-6.80	127.54	132.30
1	A	698	G	N3-C4-C5	-6.79	125.21	128.60
1	A	770	C	O5'-P-OP2	-6.79	99.59	105.70
1	A	15	G	C5-C6-N1	-6.78	108.11	111.50
1	A	892	A	N1-C2-N3	6.78	132.69	129.30
1	A	1514	C	N1-C2-O2	-6.77	114.84	118.90
1	A	773	G	N1-C6-O6	6.77	123.96	119.90
1	A	850	U	C5-C4-O4	6.76	129.96	125.90
1	A	649	G	C5-C6-N1	6.76	114.88	111.50
1	A	226	G	N1-C2-N2	-6.75	110.12	116.20
1	A	774	G	C5-C6-O6	-6.74	124.55	128.60
1	A	634	C	C6-N1-C2	-6.74	117.60	120.30
1	A	1502	A	N7-C8-N9	6.74	117.17	113.80
1	A	1505	G	C4-C5-C6	6.74	122.84	118.80
1	A	930	C	C2-N3-C4	-6.74	116.53	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	293	G	N3-C2-N2	-6.74	115.19	119.90
1	A	740	U	C5-C6-N1	-6.74	119.33	122.70
1	A	865	A	C6-N1-C2	-6.72	114.56	118.60
1	A	297	G	C4-C5-C6	6.72	122.83	118.80
1	A	1074	G	C6-C5-N7	-6.72	126.37	130.40
1	A	568	G	N1-C6-O6	-6.72	115.87	119.90
1	A	1331	G	C5-C6-O6	6.72	132.63	128.60
1	A	1525	G	N1-C2-N3	6.72	127.93	123.90
1	A	251	G	C5-N7-C8	-6.71	100.94	104.30
1	A	1477	C	C6-N1-C2	-6.71	117.62	120.30
1	A	352	C	C6-N1-C2	6.71	122.98	120.30
1	A	854	G	C6-C5-N7	-6.71	126.38	130.40
1	A	1346	A	N1-C6-N6	-6.70	114.58	118.60
1	A	854	G	C8-N9-C1'	-6.70	118.29	127.00
1	A	569	C	C4-C5-C6	6.70	120.75	117.40
1	A	8	A	C8-N9-C4	-6.70	103.12	105.80
1	A	1531	A	N7-C8-N9	6.69	117.15	113.80
1	A	1460	A	N1-C6-N6	6.69	122.61	118.60
1	A	1531	A	C5-C6-N1	-6.69	114.35	117.70
1	A	450	G	C8-N9-C4	6.69	109.08	106.40
1	A	570	G	C4-N9-C1'	6.69	135.19	126.50
1	A	859	A	C2-N3-C4	-6.69	107.26	110.60
1	A	1361(A)	C	C5-C4-N4	-6.68	115.52	120.20
1	A	724	G	C5-C6-N1	6.68	114.84	111.50
1	A	302	G	C5-C6-O6	-6.67	124.59	128.60
1	A	588	G	C5-N7-C8	6.67	107.64	104.30
1	A	947	G	C6-C5-N7	-6.67	126.40	130.40
1	A	560	U	N1-C2-O2	6.67	127.47	122.80
1	A	1347	G	N3-C4-N9	6.67	130.00	126.00
1	A	1193	G	N1-C6-O6	6.66	123.90	119.90
1	A	328	C	C2-N1-C1'	6.65	126.12	118.80
1	A	1527	C	N1-C2-O2	6.65	122.89	118.90
1	A	117	G	N1-C2-N3	6.65	127.89	123.90
1	A	615	C	C5-C6-N1	6.65	124.32	121.00
1	A	190(B)	C	C5-C6-N1	6.64	124.32	121.00
1	A	944	G	C8-N9-C4	-6.64	103.74	106.40
1	A	559	A	N1-C2-N3	6.64	132.62	129.30
20	T	94	ALA	N-CA-C	-6.64	93.08	111.00
1	A	485	G	P-O3'-C3'	6.63	127.66	119.70
1	A	941	G	C4-C5-N7	6.63	113.45	110.80
1	A	659	U	N1-C2-N3	6.63	118.88	114.90
1	A	698	G	C8-N9-C4	-6.62	103.75	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1082	G	C2-N3-C4	-6.62	108.59	111.90
1	A	103	C	N3-C4-C5	-6.62	119.25	121.90
8	H	12	ARG	NE-CZ-NH1	-6.62	116.99	120.30
1	A	595	G	C8-N9-C1'	-6.61	118.41	127.00
1	A	67	C	C6-N1-C2	-6.61	117.66	120.30
1	A	481	G	C2-N3-C4	6.60	115.20	111.90
1	A	906	G	N1-C6-O6	6.60	123.86	119.90
1	A	167	G	C8-N9-C1'	-6.60	118.42	127.00
1	A	23	C	C4-C5-C6	6.59	120.70	117.40
1	A	1087	G	N1-C6-O6	6.58	123.85	119.90
1	A	1395	C	C5-C6-N1	-6.58	117.71	121.00
1	A	262	A	C8-N9-C4	-6.58	103.17	105.80
1	A	1380	U	C5-C4-O4	6.58	129.85	125.90
1	A	168	G	C8-N9-C1'	-6.58	118.45	127.00
1	A	1073	U	C6-N1-C2	6.58	124.95	121.00
1	A	947	G	N1-C2-N2	-6.57	110.29	116.20
1	A	1124	G	N1-C6-O6	-6.56	115.96	119.90
1	A	863	U	N3-C2-O2	-6.55	117.61	122.20
1	A	874	G	C8-N9-C1'	-6.55	118.48	127.00
1	A	1505	G	P-O3'-C3'	6.55	127.56	119.70
1	A	718	G	N1-C6-O6	6.55	123.83	119.90
1	A	1073	U	C5-C6-N1	-6.55	119.43	122.70
1	A	372	C	C6-N1-C2	6.54	122.92	120.30
1	A	16	A	N7-C8-N9	-6.54	110.53	113.80
1	A	853	G	C5-C6-N1	-6.54	108.23	111.50
1	A	190(B)	C	C6-N1-C2	-6.53	117.69	120.30
1	A	529	G	N1-C6-O6	6.53	123.82	119.90
1	A	235	C	C5-C6-N1	-6.53	117.73	121.00
1	A	451	A	N9-C4-C5	-6.53	103.19	105.80
1	A	123	C	C6-N1-C2	-6.53	117.69	120.30
1	A	326	G	C5-C6-N1	-6.53	108.24	111.50
1	A	922	G	C5-C6-O6	6.53	132.52	128.60
1	A	529	G	C6-C5-N7	-6.52	126.49	130.40
1	A	656	C	N3-C4-N4	-6.52	113.44	118.00
1	A	651	C	C6-N1-C2	6.51	122.91	120.30
1	A	944	G	N1-C6-O6	-6.51	116.00	119.90
1	A	382	A	C6-C5-N7	-6.50	127.75	132.30
1	A	283	C	C2-N3-C4	6.50	123.15	119.90
1	A	858	G	N1-C2-N3	6.50	127.80	123.90
1	A	1442	G	C8-N9-C1'	-6.50	118.55	127.00
1	A	379	C	C5-C6-N1	-6.49	117.75	121.00
1	A	573	A	C4-C5-C6	6.49	120.25	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	579	G	C2-N3-C4	-6.49	108.65	111.90
1	A	557	G	C6-C5-N7	-6.49	126.51	130.40
1	A	257	G	C4-C5-N7	6.49	113.39	110.80
1	A	557	G	C2-N3-C4	-6.48	108.66	111.90
1	A	732	C	C2-N3-C4	-6.47	116.66	119.90
1	A	1510	U	N1-C2-O2	6.47	127.33	122.80
1	A	658	G	C6-C5-N7	-6.47	126.52	130.40
1	A	757	U	C6-N1-C2	6.47	124.88	121.00
1	A	933	G	N1-C6-O6	6.47	123.78	119.90
1	A	798	G	C6-N1-C2	-6.46	121.22	125.10
1	A	9	G	C2-N3-C4	-6.46	108.67	111.90
1	A	329	A	C4-C5-N7	6.46	113.93	110.70
1	A	564	C	N3-C2-O2	-6.45	117.38	121.90
1	A	168	G	C4-C5-C6	6.45	122.67	118.80
1	A	25	C	N3-C2-O2	6.45	126.41	121.90
1	A	74	C	C6-N1-C2	-6.45	117.72	120.30
1	A	638	G	C6-C5-N7	-6.45	126.53	130.40
1	A	109	A	C2-N3-C4	-6.44	107.38	110.60
1	A	456	C	N1-C2-O2	6.44	122.76	118.90
1	A	1076	C	C2-N1-C1'	6.44	125.88	118.80
1	A	314	C	C2-N3-C4	-6.43	116.68	119.90
1	A	829	G	N3-C4-N9	6.43	129.86	126.00
1	A	779	C	C4-C5-C6	6.43	120.61	117.40
1	A	1074	G	N1-C6-O6	6.43	123.76	119.90
1	A	144	G	C5-C6-N1	-6.42	108.29	111.50
1	A	626	U	C2-N1-C1'	6.42	125.40	117.70
1	A	569	C	C2-N3-C4	-6.41	116.69	119.90
1	A	251	G	N1-C6-O6	6.41	123.75	119.90
1	A	321	A	O5'-P-OP2	-6.41	99.93	105.70
1	A	89	C	C2-N1-C1'	6.41	125.84	118.80
1	A	1254	C	C6-N1-C2	-6.39	117.75	120.30
1	A	812	C	N1-C2-N3	6.38	123.67	119.20
1	A	1051	C	N1-C2-O2	6.38	122.73	118.90
1	A	59	A	O5'-P-OP2	-6.38	99.96	105.70
1	A	593	G	C5-C6-O6	6.37	132.42	128.60
1	A	611	A	N1-C6-N6	-6.36	114.78	118.60
1	A	650	G	N3-C4-C5	-6.36	125.42	128.60
1	A	311	C	C2-N3-C4	-6.35	116.72	119.90
1	A	1532	U	C4-C5-C6	-6.35	115.89	119.70
1	A	1079	G	N1-C6-O6	-6.35	116.09	119.90
1	A	1453	G	C4-C5-N7	6.35	113.34	110.80
1	A	533	A	N9-C4-C5	6.34	108.34	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	269	C	C5-C6-N1	-6.34	117.83	121.00
1	A	876	G	C5-C6-N1	6.34	114.67	111.50
1	A	288	A	C8-N9-C4	6.34	108.34	105.80
1	A	553	A	C8-N9-C4	6.34	108.33	105.80
1	A	903	G	C4-N9-C1'	6.34	134.74	126.50
1	A	903	G	C8-N9-C1'	-6.33	118.77	127.00
1	A	1386	G	N1-C2-N3	6.33	127.70	123.90
1	A	445	G	N1-C6-O6	6.33	123.70	119.90
1	A	758	G	C2-N3-C4	-6.33	108.73	111.90
1	A	1415	G	C8-N9-C4	-6.33	103.87	106.40
1	A	1502	A	N9-C4-C5	-6.33	103.27	105.80
1	A	882	C	C2-N3-C4	-6.33	116.74	119.90
1	A	919	A	C5-C6-N1	6.33	120.86	117.70
1	A	1079	G	C4-N9-C1'	6.33	134.72	126.50
1	A	1108	G	C4-C5-C6	6.33	122.59	118.80
1	A	929	G	C2-N3-C4	-6.32	108.74	111.90
1	A	634	C	N3-C4-C5	-6.32	119.37	121.90
1	A	326	G	N1-C2-N3	6.32	127.69	123.90
1	A	548	G	N1-C6-O6	6.32	123.69	119.90
1	A	918	A	C6-N1-C2	-6.31	114.81	118.60
1	A	481	G	C5-N7-C8	6.31	107.46	104.30
1	A	1362	C	C6-N1-C2	-6.30	117.78	120.30
1	A	1531	A	C6-C5-N7	-6.30	127.89	132.30
1	A	581	G	N3-C4-N9	-6.30	122.22	126.00
1	A	949	A	C8-N9-C4	6.30	108.32	105.80
1	A	719	C	N3-C2-O2	-6.30	117.49	121.90
1	A	141	A	C8-N9-C4	6.29	108.32	105.80
1	A	873	A	C5-C6-N1	6.29	120.85	117.70
1	A	27	G	N1-C6-O6	6.29	123.67	119.90
1	A	274	A	C8-N9-C4	6.29	108.31	105.80
1	A	1393	U	C5-C4-O4	-6.29	122.13	125.90
1	A	283	C	C6-N1-C2	-6.28	117.79	120.30
1	A	526	C	C6-N1-C2	6.28	122.81	120.30
1	A	715	A	C8-N9-C4	6.28	108.31	105.80
1	A	832	C	N3-C4-C5	6.28	124.41	121.90
1	A	89	C	C5-C6-N1	6.28	124.14	121.00
1	A	129(A)	G	N3-C4-N9	6.28	129.77	126.00
1	A	580	U	N3-C4-C5	-6.28	110.83	114.60
1	A	1181	G	N7-C8-N9	-6.28	109.96	113.10
1	A	1277	C	C6-N1-C2	-6.28	117.79	120.30
1	A	854	G	N1-C2-N3	6.28	127.67	123.90
1	A	589	C	C5-C6-N1	-6.28	117.86	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	546	G	N3-C4-N9	-6.27	122.24	126.00
1	A	912	C	C5-C4-N4	-6.27	115.81	120.20
1	A	1504	G	N1-C6-O6	-6.27	116.14	119.90
1	A	297	G	OP1-P-OP2	-6.27	110.20	119.60
1	A	695	A	C5-N7-C8	-6.27	100.77	103.90
1	A	254	G	N1-C2-N3	6.26	127.66	123.90
1	A	240	C	N3-C2-O2	6.25	126.28	121.90
1	A	122	G	C6-C5-N7	-6.25	126.65	130.40
1	A	1373	G	C4-N9-C1'	6.25	134.62	126.50
1	A	1441	G	C4-C5-N7	-6.25	108.30	110.80
1	A	279	A	N9-C4-C5	6.25	108.30	105.80
1	A	779	C	C6-N1-C2	-6.25	117.80	120.30
1	A	872	A	N9-C4-C5	-6.25	103.30	105.80
1	A	1231	G	OP1-P-O3'	6.25	118.94	105.20
1	A	518	C	N3-C2-O2	-6.25	117.53	121.90
1	A	773	G	C4-C5-N7	6.24	113.30	110.80
1	A	359	U	O5'-P-OP1	-6.24	100.08	105.70
1	A	302	G	N1-C6-O6	6.23	123.64	119.90
1	A	1511	G	OP1-P-OP2	-6.23	110.26	119.60
1	A	48	C	C6-N1-C2	6.23	122.79	120.30
1	A	881	G	N1-C2-N3	6.22	127.63	123.90
1	A	130	A	C2-N3-C4	-6.21	107.49	110.60
1	A	1377	A	N1-C6-N6	-6.21	114.87	118.60
1	A	21	G	N1-C2-N2	-6.21	110.61	116.20
1	A	1228	C	N1-C2-O2	6.21	122.63	118.90
1	A	570	G	N1-C2-N2	-6.21	110.61	116.20
1	A	106	C	OP2-P-O3'	6.20	118.84	105.20
1	A	558	G	C5-N7-C8	-6.20	101.20	104.30
1	A	731	G	C6-C5-N7	-6.20	126.68	130.40
1	A	836	G	C4-C5-C6	6.20	122.52	118.80
1	A	1230	C	C5-C6-N1	6.20	124.10	121.00
1	A	872	A	C5-N7-C8	-6.19	100.80	103.90
1	A	292	G	C4-C5-N7	6.19	113.28	110.80
1	A	1084	G	N3-C4-C5	-6.19	125.50	128.60
1	A	23	C	N1-C2-N3	6.19	123.53	119.20
1	A	1282	C	C2-N1-C1'	6.18	125.60	118.80
1	A	1523	G	N3-C2-N2	-6.18	115.57	119.90
1	A	670	G	N1-C6-O6	6.18	123.61	119.90
1	A	1300	G	OP2-P-O3'	6.18	118.79	105.20
1	A	584	G	N1-C2-N2	6.17	121.75	116.20
1	A	250	A	C8-N9-C4	6.17	108.27	105.80
1	A	812	C	P-O3'-C3'	6.17	127.10	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	823	G	N1-C2-N3	6.17	127.60	123.90
1	A	780	A	C6-N1-C2	-6.17	114.90	118.60
1	A	1108	G	N3-C4-C5	-6.16	125.52	128.60
1	A	573	A	N9-C4-C5	6.16	108.26	105.80
1	A	304	U	O5'-P-OP1	-6.16	100.16	105.70
1	A	529	G	C4-C5-C6	6.16	122.49	118.80
1	A	761	G	C6-C5-N7	-6.16	126.71	130.40
1	A	836	G	C8-N9-C1'	-6.15	119.00	127.00
1	A	860	A	N1-C2-N3	6.14	132.37	129.30
1	A	573	A	N7-C8-N9	6.14	116.87	113.80
1	A	264	U	C6-N1-C2	-6.14	117.32	121.00
1	A	1498	UR3	P-O3'-C3'	6.13	127.06	119.70
1	A	266	G	C5-C6-O6	-6.13	124.92	128.60
1	A	24	U	C5-C6-N1	-6.13	119.64	122.70
1	A	747	C	C5-C6-N1	-6.13	117.94	121.00
1	A	591	U	C5-C6-N1	-6.13	119.64	122.70
1	A	676	A	C2-N3-C4	-6.13	107.54	110.60
1	A	872	A	O5'-P-OP2	-6.13	100.19	105.70
1	A	882	C	C5-C6-N1	-6.13	117.94	121.00
1	A	962	C	N1-C2-O2	6.13	122.58	118.90
1	A	903	G	C6-C5-N7	-6.12	126.73	130.40
1	A	620	C	C6-N1-C2	6.12	122.75	120.30
1	A	565	U	N1-C2-N3	-6.12	111.23	114.90
1	A	334	C	C6-N1-C2	6.11	122.74	120.30
1	A	293	G	N3-C4-C5	6.11	131.65	128.60
1	A	852	G	C2-N3-C4	-6.11	108.85	111.90
1	A	1246	C	C6-N1-C2	6.10	122.74	120.30
1	A	1301	U	O5'-P-OP2	-6.10	100.21	105.70
1	A	117	G	N3-C4-N9	6.10	129.66	126.00
1	A	558	G	C4-C5-N7	6.09	113.24	110.80
1	A	667	G	N1-C2-N3	6.09	127.56	123.90
1	A	1301	U	P-O3'-C3'	6.09	127.01	119.70
1	A	1366	C	C5-C6-N1	6.09	124.04	121.00
1	A	880	C	C4-C5-C6	6.09	120.44	117.40
1	A	851	G	C6-C5-N7	-6.08	126.75	130.40
1	A	89	C	N1-C2-O2	6.08	122.55	118.90
1	A	557	G	N1-C2-N3	6.08	127.55	123.90
1	A	661	G	N3-C4-C5	6.08	131.64	128.60
1	A	342	C	C5-C6-N1	6.08	124.04	121.00
1	A	246	A	C5-C6-N1	6.07	120.74	117.70
1	A	254	G	C5-C6-N1	-6.07	108.46	111.50
1	A	635	G	C4-C5-C6	6.07	122.44	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	923	A	N9-C4-C5	-6.07	103.37	105.80
1	A	1529	G	N1-C6-O6	6.06	123.54	119.90
1	A	1238	A	C5-C6-N6	6.06	128.55	123.70
1	A	150	C	OP2-P-O3'	6.06	118.53	105.20
1	A	67	C	N3-C4-C5	-6.05	119.48	121.90
1	A	733	A	C2-N3-C4	-6.05	107.58	110.60
1	A	1079	G	C8-N9-C4	-6.05	103.98	106.40
1	A	836	G	C4-N9-C1'	6.05	134.36	126.50
1	A	342	C	N3-C4-C5	-6.04	119.48	121.90
1	A	797	C	N3-C2-O2	-6.04	117.67	121.90
1	A	890	G	N9-C4-C5	6.04	107.82	105.40
1	A	1500	A	C8-N9-C4	-6.04	103.38	105.80
1	A	643	C	C2-N3-C4	-6.04	116.88	119.90
1	A	1158	C	N3-C2-O2	-6.04	117.67	121.90
1	A	597	G	C4-C5-N7	6.04	113.22	110.80
1	A	309	G	C6-C5-N7	-6.04	126.78	130.40
1	A	310	G	N9-C4-C5	-6.04	102.98	105.40
1	A	245	C	C2-N3-C4	-6.03	116.88	119.90
1	A	372	C	C5-C6-N1	-6.03	117.98	121.00
1	A	1512	U	C6-N1-C2	-6.03	117.38	121.00
1	A	885	G	N1-C2-N3	6.03	127.52	123.90
1	A	596	C	C6-N1-C2	6.02	122.71	120.30
1	A	364	A	C4-C5-C6	6.02	120.01	117.00
1	A	703	G	C5-C6-N1	-6.01	108.49	111.50
1	A	1074	G	C2-N3-C4	-6.01	108.89	111.90
1	A	1509	C	C5-C6-N1	-6.01	117.99	121.00
1	A	130	A	C4-C5-C6	6.01	120.01	117.00
1	A	116	A	C5-C6-N1	-6.01	114.69	117.70
1	A	180	U	C2-N1-C1'	6.01	124.91	117.70
1	A	1060	C	C2-N1-C1'	6.01	125.41	118.80
1	A	740	U	C4-C5-C6	6.00	123.30	119.70
1	A	1062	U	C5-C4-O4	6.00	129.50	125.90
1	A	819	A	C6-C5-N7	-6.00	128.10	132.30
1	A	1394	A	N1-C6-N6	6.00	122.20	118.60
1	A	27	G	C5-C6-O6	-6.00	125.00	128.60
1	A	329	A	N3-C4-C5	6.00	131.00	126.80
1	A	903	G	C4-C5-C6	5.99	122.39	118.80
1	A	190(A)	C	C6-N1-C2	-5.99	117.90	120.30
1	A	1479	C	C6-N1-C2	-5.99	117.90	120.30
1	A	167	G	C4-N9-C1'	5.99	134.28	126.50
1	A	1490	U	C2-N1-C1'	5.99	124.89	117.70
1	A	732	C	N3-C4-C5	5.99	124.30	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	120	A	N1-C2-N3	5.99	132.29	129.30
1	A	230	G	C5-C6-N1	-5.99	108.51	111.50
1	A	860	A	C2-N3-C4	-5.99	107.61	110.60
1	A	782	A	N1-C2-N3	5.98	132.29	129.30
1	A	898	G	C2-N3-C4	-5.98	108.91	111.90
1	A	1510	U	N3-C2-O2	-5.98	118.01	122.20
2	B	44	LEU	CA-CB-CG	-5.98	101.55	115.30
1	A	168	G	C5-C6-N1	-5.98	108.51	111.50
1	A	1039	C	C6-N1-C2	-5.98	117.91	120.30
1	A	92	C	C2-N1-C1'	5.98	125.37	118.80
1	A	569	C	C2-N1-C1'	-5.97	112.23	118.80
1	A	398	C	N3-C4-C5	5.97	124.29	121.90
1	A	19	C	OP1-P-OP2	5.97	128.55	119.60
1	A	1508	G	C5-C6-O6	-5.96	125.02	128.60
1	A	44	G	N1-C6-O6	5.96	123.48	119.90
1	A	854	G	N1-C2-N2	-5.96	110.84	116.20
1	A	774	G	C4-C5-N7	5.96	113.18	110.80
1	A	933	G	C4-C5-N7	5.96	113.18	110.80
1	A	586	C	C5-C6-N1	-5.94	118.03	121.00
1	A	1414	U	C6-N1-C2	-5.94	117.44	121.00
1	A	5	U	P-O3'-C3'	5.93	126.82	119.70
1	A	1516[A]	G	N7-C8-N9	5.93	116.07	113.10
1	A	1516[B]	G	N7-C8-N9	5.93	116.07	113.10
1	A	168	G	N3-C4-N9	5.93	129.56	126.00
1	A	559	A	C4-C5-C6	5.93	119.97	117.00
1	A	1178	G	C8-N9-C4	-5.93	104.03	106.40
1	A	1532	U	C5-C4-O4	-5.93	122.34	125.90
1	A	752	G	C8-N9-C4	5.93	108.77	106.40
1	A	1527	C	C5-C4-N4	-5.93	116.05	120.20
1	A	691	G	C5-C6-O6	5.93	132.16	128.60
1	A	204	U	O4'-C1'-N1	-5.93	103.46	108.20
1	A	869	G	N9-C4-C5	-5.93	103.03	105.40
1	A	736	C	C5-C6-N1	-5.92	118.04	121.00
1	A	1238	A	N7-C8-N9	5.92	116.76	113.80
1	A	597	G	N3-C4-N9	5.92	129.55	126.00
1	A	755	G	C5-C6-O6	-5.92	125.05	128.60
1	A	1077	G	N3-C4-N9	5.92	129.55	126.00
1	A	869	G	C8-N9-C1'	5.92	134.70	127.00
1	A	1494	G	C8-N9-C4	-5.92	104.03	106.40
1	A	1495	U	N1-C2-N3	-5.92	111.35	114.90
1	A	19	C	N3-C4-C5	5.92	124.27	121.90
1	A	269	C	N3-C2-O2	-5.92	117.76	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	922	G	N7-C8-N9	5.92	116.06	113.10
1	A	1302	U	O4'-C1'-N1	-5.91	103.47	108.20
1	A	1361(A)	C	C4-C5-C6	-5.91	114.44	117.40
1	A	947	G	N1-C2-N3	5.91	127.45	123.90
1	A	729	A	N1-C6-N6	5.91	122.15	118.60
1	A	873	A	N9-C4-C5	5.91	108.16	105.80
1	A	80	G	N9-C4-C5	5.91	107.76	105.40
1	A	750	G	N1-C2-N3	5.91	127.44	123.90
1	A	638	G	N9-C4-C5	-5.91	103.04	105.40
1	A	721	G	C4-N9-C1'	5.90	134.17	126.50
1	A	168	G	N1-C6-O6	5.89	123.44	119.90
1	A	770	C	N3-C4-C5	5.89	124.26	121.90
1	A	251	G	C6-C5-N7	-5.89	126.87	130.40
1	A	585	G	OP1-P-OP2	5.89	128.43	119.60
1	A	1190	G	P-O3'-C3'	5.88	126.76	119.70
1	A	190(F)	G	N1-C6-O6	-5.88	116.37	119.90
1	A	522	C	N1-C2-O2	-5.88	115.37	118.90
1	A	750	G	N1-C6-O6	5.88	123.43	119.90
1	A	1346	A	N9-C4-C5	5.88	108.15	105.80
1	A	572	A	N9-C4-C5	5.88	108.15	105.80
1	A	1505	G	N3-C4-C5	-5.87	125.66	128.60
1	A	548	G	C5-C6-N1	-5.87	108.57	111.50
1	A	648	A	N7-C8-N9	-5.87	110.86	113.80
1	A	1332	A	C8-N9-C4	-5.87	103.45	105.80
1	A	635	G	N1-C2-N3	5.87	127.42	123.90
1	A	226	G	N1-C2-N3	5.86	127.42	123.90
1	A	297	G	C6-C5-N7	-5.86	126.88	130.40
1	A	1077	G	N3-C2-N2	5.86	124.00	119.90
1	A	1469	G	C5-C6-O6	-5.86	125.08	128.60
1	A	568	G	OP1-P-OP2	5.86	128.39	119.60
1	A	783	C	N3-C4-C5	5.86	124.24	121.90
1	A	1205	U	N3-C2-O2	-5.86	118.10	122.20
1	A	732	C	C5-C4-N4	-5.86	116.10	120.20
1	A	1415	G	N7-C8-N9	5.86	116.03	113.10
1	A	1431	C	N3-C4-C5	5.86	124.24	121.90
1	A	1331	G	C6-C5-N7	5.85	133.91	130.40
1	A	1143	G	N1-C6-O6	5.85	123.41	119.90
1	A	1343	G	C2-N3-C4	-5.85	108.97	111.90
1	A	729	A	C5-N7-C8	-5.84	100.98	103.90
1	A	135	C	N3-C2-O2	5.84	125.99	121.90
1	A	508	C	N3-C4-C5	5.84	124.23	121.90
7	G	124	LEU	CA-CB-CG	-5.84	101.87	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	689	C	N3-C4-C5	-5.84	119.56	121.90
1	A	581	G	N3-C4-C5	5.83	131.52	128.60
1	A	1542	U	C6-N1-C2	5.83	124.50	121.00
1	A	1501	C	C2-N3-C4	-5.83	116.98	119.90
1	A	552	U	C6-N1-C2	5.83	124.50	121.00
1	A	825	G	N9-C4-C5	-5.83	103.07	105.40
1	A	811	C	C6-N1-C2	5.83	122.63	120.30
1	A	902	G	C5-C6-O6	-5.83	125.11	128.60
1	A	1495	U	N1-C2-O2	5.83	126.88	122.80
1	A	864	A	N9-C4-C5	5.82	108.13	105.80
1	A	878	G	C5-C6-N1	5.82	114.41	111.50
1	A	892	A	C8-N9-C4	-5.82	103.47	105.80
1	A	21	G	C8-N9-C1'	-5.82	119.44	127.00
1	A	1281	U	N3-C4-O4	5.82	123.47	119.40
1	A	103	C	C4-C5-C6	5.82	120.31	117.40
1	A	289	G	N1-C6-O6	5.82	123.39	119.90
1	A	900	A	C8-N9-C4	-5.82	103.47	105.80
1	A	570	G	C2-N3-C4	5.81	114.81	111.90
1	A	603	U	C2-N1-C1'	-5.81	110.73	117.70
1	A	107	G	C5-N7-C8	-5.81	101.39	104.30
1	A	392	G	C6-C5-N7	-5.81	126.91	130.40
1	A	292	G	N9-C4-C5	-5.81	103.08	105.40
1	A	364	A	N1-C2-N3	5.81	132.20	129.30
1	A	502	G	C6-C5-N7	-5.81	126.92	130.40
1	A	885	G	C5-C6-N1	-5.81	108.60	111.50
3	C	5	ILE	CB-CA-C	-5.81	99.98	111.60
1	A	107	G	C4-C5-N7	5.80	113.12	110.80
1	A	814	A	N7-C8-N9	-5.80	110.90	113.80
1	A	1224	G	C4-C5-N7	-5.80	108.48	110.80
1	A	1380	U	N3-C4-O4	-5.80	115.34	119.40
1	A	1395	C	N3-C4-C5	5.80	124.22	121.90
1	A	80	G	N3-C2-N2	-5.80	115.84	119.90
1	A	311	C	N3-C4-C5	5.80	124.22	121.90
1	A	746	A	N1-C2-N3	5.80	132.20	129.30
1	A	128	G	C2-N3-C4	-5.80	109.00	111.90
1	A	600	C	N3-C4-N4	-5.80	113.94	118.00
1	A	1390	U	N3-C4-C5	-5.79	111.12	114.60
1	A	686	U	C5-C4-O4	5.79	129.38	125.90
1	A	908	A	N3-C4-C5	5.79	130.85	126.80
1	A	1058	G	C4-C5-N7	-5.79	108.48	110.80
1	A	1393	U	C6-N1-C2	5.79	124.47	121.00
1	A	485	G	OP2-P-O3'	5.79	117.94	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	779	C	N3-C2-O2	-5.79	117.85	121.90
1	A	1394	A	C8-N9-C4	5.79	108.12	105.80
1	A	1082	G	N1-C2-N3	5.79	127.37	123.90
1	A	176	C	C6-N1-C2	5.79	122.61	120.30
1	A	889	A	N1-C2-N3	5.78	132.19	129.30
1	A	931	C	C4-C5-C6	5.78	120.29	117.40
1	A	276	G	C8-N9-C4	5.78	108.71	106.40
1	A	804	U	N3-C2-O2	-5.78	118.15	122.20
1	A	1124	G	C6-C5-N7	5.78	133.87	130.40
1	A	651	C	N3-C4-C5	5.78	124.21	121.90
1	A	686	U	C4-C5-C6	5.78	123.17	119.70
1	A	638	G	C5-C6-N1	-5.78	108.61	111.50
1	A	1010	G	C8-N9-C4	-5.77	104.09	106.40
1	A	364	A	C2-N3-C4	-5.77	107.72	110.60
1	A	402	G	C8-N9-C4	-5.77	104.09	106.40
1	A	745	C	C2-N3-C4	-5.77	117.02	119.90
1	A	928	G	C5-N7-C8	-5.77	101.42	104.30
1	A	1310	G	C8-N9-C1'	-5.77	119.50	127.00
1	A	288	A	C2-N3-C4	-5.77	107.72	110.60
1	A	78	G	N1-C6-O6	5.76	123.36	119.90
1	A	1181	G	N9-C4-C5	-5.76	103.09	105.40
1	A	115	G	N3-C4-N9	5.76	129.46	126.00
1	A	698	G	C4-C5-C6	5.76	122.26	118.80
1	A	972	C	N3-C4-C5	-5.76	119.60	121.90
1	A	755	G	N3-C2-N2	-5.76	115.87	119.90
1	A	947	G	N3-C4-N9	5.76	129.46	126.00
1	A	739	C	C2-N3-C4	-5.76	117.02	119.90
1	A	1475	G	C8-N9-C4	-5.76	104.10	106.40
1	A	500	G	N1-C6-O6	5.75	123.35	119.90
1	A	1380	U	P-O3'-C3'	5.75	126.61	119.70
1	A	264	U	O5'-P-OP2	-5.75	100.52	105.70
1	A	932	C	N3-C2-O2	-5.75	117.87	121.90
1	A	1091	U	N3-C4-C5	-5.75	111.15	114.60
1	A	665	A	N1-C6-N6	-5.75	115.15	118.60
1	A	757	U	N3-C2-O2	5.75	126.22	122.20
1	A	928	G	C5-C6-O6	-5.75	125.15	128.60
1	A	103	C	C6-N1-C2	-5.75	118.00	120.30
1	A	827	U	N3-C4-C5	5.75	118.05	114.60
1	A	870	U	N1-C2-N3	-5.75	111.45	114.90
1	A	1090	U	C6-N1-C2	-5.75	117.55	121.00
1	A	667	G	N1-C6-O6	5.75	123.35	119.90
1	A	228	A	C2-N3-C4	-5.74	107.73	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1521	G	N3-C4-C5	-5.74	125.73	128.60
1	A	25	C	N1-C2-O2	-5.74	115.46	118.90
1	A	713	G	N9-C4-C5	5.73	107.69	105.40
1	A	730	G	N7-C8-N9	-5.73	110.23	113.10
1	A	730	G	C4-C5-N7	-5.73	108.51	110.80
1	A	1347	G	C6-C5-N7	-5.73	126.96	130.40
1	A	15	G	N7-C8-N9	5.73	115.97	113.10
1	A	240	C	C5-C4-N4	-5.73	116.19	120.20
1	A	289	G	C2-N3-C4	-5.73	109.04	111.90
1	A	822	C	N3-C4-N4	5.73	122.01	118.00
1	A	482	A	C8-N9-C4	-5.73	103.51	105.80
1	A	578	C	C2-N3-C4	-5.73	117.04	119.90
1	A	57	G	N1-C6-O6	-5.72	116.47	119.90
1	A	776	G	N3-C4-N9	-5.72	122.57	126.00
1	A	1051	C	C6-N1-C1'	-5.72	113.93	120.80
1	A	1179	A	C8-N9-C4	-5.72	103.51	105.80
1	A	1228	C	N3-C2-O2	-5.72	117.89	121.90
1	A	504	C	C6-N1-C2	-5.72	118.01	120.30
1	A	1434	A	C5-C6-N6	-5.72	119.12	123.70
1	A	948	C	N3-C2-O2	5.72	125.90	121.90
1	A	16	A	C8-N9-C4	5.71	108.09	105.80
1	A	144	G	C6-C5-N7	-5.71	126.97	130.40
1	A	1228	C	C2-N1-C1'	5.71	125.08	118.80
1	A	44	G	C6-C5-N7	-5.71	126.97	130.40
1	A	829	G	C4-N9-C1'	5.71	133.92	126.50
1	A	624	C	N3-C4-C5	5.71	124.18	121.90
1	A	90	U	C5-C6-N1	5.70	125.55	122.70
1	A	190(E)	U	N1-C2-O2	-5.70	118.81	122.80
1	A	965	A	C8-N9-C4	5.70	108.08	105.80
1	A	1532	U	C6-N1-C2	-5.70	117.58	121.00
1	A	1478	C	C6-N1-C2	-5.70	118.02	120.30
1	A	145	G	N1-C6-O6	5.70	123.32	119.90
1	A	609	A	N1-C2-N3	5.70	132.15	129.30
1	A	597	G	C6-C5-N7	-5.70	126.98	130.40
1	A	274	A	N7-C8-N9	-5.69	110.95	113.80
1	A	658	G	C4-N9-C1'	5.69	133.90	126.50
1	A	805	C	C2-N3-C4	-5.69	117.06	119.90
1	A	724	G	OP1-P-OP2	-5.68	111.07	119.60
1	A	66	G	N3-C2-N2	-5.68	115.92	119.90
1	A	942	G	N1-C6-O6	5.68	123.31	119.90
1	A	595	G	O4'-C1'-N9	-5.68	103.66	108.20
1	A	593	G	N1-C6-O6	-5.68	116.49	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	400	C	C5-C6-N1	-5.68	118.16	121.00
1	A	190(F)	G	C6-C5-N7	5.67	133.81	130.40
1	A	519	C	N1-C2-O2	5.67	122.30	118.90
1	A	1200	C	N3-C2-O2	-5.67	117.93	121.90
1	A	1370	G	N9-C4-C5	5.67	107.67	105.40
1	A	1078	U	O5'-P-OP2	-5.67	100.60	105.70
1	A	144	G	C5-N7-C8	-5.66	101.47	104.30
1	A	157	G	N1-C6-O6	5.66	123.30	119.90
1	A	392	G	N3-C4-N9	5.66	129.40	126.00
1	A	731	G	C5-N7-C8	-5.66	101.47	104.30
1	A	1392	G	N1-C2-N3	5.66	127.30	123.90
1	A	697	U	N3-C4-O4	-5.66	115.44	119.40
1	A	923	A	C4-C5-N7	5.66	113.53	110.70
1	A	1288	A	C8-N9-C4	-5.66	103.54	105.80
1	A	482	A	N7-C8-N9	5.66	116.63	113.80
5	E	12	LEU	CA-CB-CG	5.65	128.30	115.30
1	A	686	U	N1-C2-N3	5.65	118.29	114.90
1	A	773	G	C5-C6-O6	-5.65	125.21	128.60
1	A	867	G	C8-N9-C1'	-5.64	119.66	127.00
1	A	120	A	C2-N3-C4	-5.64	107.78	110.60
1	A	251	G	N7-C8-N9	5.64	115.92	113.10
1	A	113	G	C6-C5-N7	-5.64	127.02	130.40
1	A	400	C	N3-C4-N4	-5.64	114.05	118.00
1	A	687	A	P-O3'-C3'	5.64	126.47	119.70
1	A	642	A	C8-N9-C4	-5.64	103.55	105.80
1	A	859	A	C4-C5-C6	5.63	119.81	117.00
1	A	1307	U	C5-C4-O4	5.63	129.28	125.90
1	A	596	C	C5-C6-N1	-5.63	118.19	121.00
1	A	858	G	N3-C4-N9	-5.62	122.62	126.00
1	A	9	G	N1-C2-N3	5.62	127.27	123.90
1	A	20	U	OP1-P-OP2	5.62	128.03	119.60
1	A	776	G	N3-C4-C5	5.62	131.41	128.60
1	A	154	C	C5-C4-N4	-5.62	116.27	120.20
1	A	589	C	N3-C4-C5	-5.62	119.65	121.90
1	A	23	C	C2-N3-C4	-5.62	117.09	119.90
1	A	836	G	N1-C2-N3	5.62	127.27	123.90
1	A	617	G	C8-N9-C4	5.62	108.65	106.40
1	A	815	A	N1-C6-N6	5.62	121.97	118.60
1	A	590	C	N1-C2-O2	-5.61	115.53	118.90
1	A	885	G	N3-C4-C5	5.61	131.41	128.60
1	A	62	U	N3-C4-C5	-5.61	111.23	114.60
1	A	880	C	N3-C4-N4	5.61	121.93	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1064	G	C2-N3-C4	-5.61	109.10	111.90
1	A	122	G	C2-N3-C4	-5.60	109.10	111.90
1	A	279	A	C5-N7-C8	-5.60	101.10	103.90
1	A	1434	A	C4-C5-N7	5.60	113.50	110.70
1	A	80	G	C8-N9-C4	-5.60	104.16	106.40
1	A	595	G	N3-C4-N9	5.60	129.36	126.00
1	A	822	C	C2-N1-C1'	5.60	124.96	118.80
1	A	881	G	C6-N1-C2	-5.60	121.74	125.10
1	A	1530	G	N1-C6-O6	5.60	123.26	119.90
1	A	912	C	N1-C2-O2	-5.59	115.54	118.90
1	A	830	G	C4-C5-N7	-5.59	108.56	110.80
1	A	1469	G	N1-C6-O6	5.59	123.25	119.90
1	A	655	A	C6-N1-C2	-5.59	115.25	118.60
1	A	864	A	C4-C5-N7	-5.59	107.91	110.70
1	A	491	G	C5-C6-N1	-5.59	108.71	111.50
1	A	874	G	C8-N9-C4	5.59	108.64	106.40
1	A	9	G	N1-C6-O6	5.58	123.25	119.90
1	A	718	G	N3-C4-C5	5.58	131.39	128.60
1	A	1441	G	C5-C6-O6	5.58	131.95	128.60
1	A	243	A	N1-C2-N3	5.58	132.09	129.30
1	A	597	G	C6-N1-C2	-5.58	121.75	125.10
1	A	945	G	C5-C6-N1	5.58	114.29	111.50
1	A	691	G	N9-C4-C5	5.58	107.63	105.40
1	A	689	C	C6-N1-C2	-5.58	118.07	120.30
1	A	760	G	C5-C6-O6	5.58	131.94	128.60
1	A	941	G	C6-C5-N7	-5.58	127.05	130.40
1	A	293	G	N3-C4-N9	-5.57	122.66	126.00
1	A	572	A	C6-N1-C2	-5.57	115.26	118.60
1	A	635	G	N3-C2-N2	-5.57	116.00	119.90
1	A	876	G	C6-N1-C2	-5.57	121.76	125.10
12	L	26	ALA	N-CA-C	-5.57	95.96	111.00
1	A	190(E)	U	C6-N1-C2	5.57	124.34	121.00
1	A	238	G	C8-N9-C4	-5.57	104.17	106.40
1	A	723	U	C5-C6-N1	5.56	125.48	122.70
1	A	933	G	C6-C5-N7	-5.56	127.06	130.40
1	A	832	C	C2-N3-C4	-5.56	117.12	119.90
1	A	268	C	N3-C2-O2	-5.56	118.01	121.90
1	A	555	C	N1-C2-N3	5.56	123.09	119.20
1	A	568	G	N1-C2-N3	5.56	127.23	123.90
1	A	750	G	O5'-P-OP2	5.56	117.37	110.70
1	A	126	G	C2-N3-C4	-5.56	109.12	111.90
1	A	658	G	C5-C6-O6	-5.55	125.27	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1068	G	OP1-P-OP2	5.55	127.93	119.60
1	A	1370	G	OP1-P-O3'	5.55	117.42	105.20
1	A	721	G	C4-C5-C6	5.55	122.13	118.80
1	A	812	C	N1-C2-O2	-5.55	115.57	118.90
1	A	251	G	O4'-C1'-N9	-5.55	103.76	108.20
1	A	770	C	C5-C6-N1	-5.55	118.22	121.00
1	A	1300	G	C4-N9-C1'	-5.55	119.29	126.50
1	A	1281	U	C5-C6-N1	5.55	125.47	122.70
1	A	1485	U	N3-C2-O2	-5.55	118.32	122.20
1	A	125	U	C2-N3-C4	-5.55	123.67	127.00
1	A	777	A	C5'-C4'-O4'	5.55	115.76	109.10
1	A	885	G	N3-C4-N9	-5.55	122.67	126.00
1	A	27	G	C8-N9-C4	-5.54	104.18	106.40
1	A	365	U	C6-N1-C1'	-5.54	113.44	121.20
1	A	873	A	N1-C6-N6	-5.54	115.28	118.60
1	A	1414	U	N3-C2-O2	-5.54	118.32	122.20
1	A	509	A	N9-C1'-C2'	-5.54	105.91	112.00
1	A	329	A	N9-C4-C5	-5.54	103.58	105.80
1	A	823	G	C6-N1-C2	-5.54	121.78	125.10
1	A	167	G	N1-C2-N2	-5.53	111.22	116.20
1	A	1091	U	C6-N1-C2	-5.53	117.68	121.00
1	A	771	G	C8-N9-C4	5.53	108.61	106.40
1	A	640	A	OP2-P-O3'	5.53	117.36	105.20
1	A	921	U	N1-C2-O2	-5.53	118.93	122.80
1	A	309	G	C2-N3-C4	-5.52	109.14	111.90
1	A	553	A	C5-C6-N6	-5.52	119.28	123.70
1	A	919	A	C4-C5-C6	-5.52	114.24	117.00
1	A	1382	C	N1-C2-O2	5.52	122.21	118.90
1	A	256	U	N3-C2-O2	5.52	126.06	122.20
1	A	1394	A	N9-C4-C5	-5.52	103.59	105.80
1	A	635	G	C2-N3-C4	-5.51	109.14	111.90
1	A	666	G	O5'-P-OP1	-5.51	100.74	105.70
1	A	690	G	N3-C4-N9	-5.51	122.69	126.00
1	A	15	G	C4-C5-N7	5.51	113.00	110.80
1	A	1490	U	C6-N1-C1'	-5.51	113.48	121.20
1	A	22	G	C6-C5-N7	-5.51	127.09	130.40
1	A	610	G	N1-C6-O6	-5.51	116.59	119.90
1	A	813	U	C2-N1-C1'	5.51	124.31	117.70
1	A	882	C	N1-C2-N3	5.51	123.06	119.20
8	H	12	ARG	NE-CZ-NH2	5.51	123.06	120.30
1	A	1310	G	C6-C5-N7	-5.51	127.09	130.40
1	A	753	A	C2-N3-C4	-5.51	107.85	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	947	G	C8-N9-C1'	-5.51	119.84	127.00
1	A	1395	C	OP2-P-O3'	5.51	117.31	105.20
1	A	32	A	C6-N1-C2	-5.50	115.30	118.60
1	A	752	G	C5-C6-O6	5.50	131.90	128.60
18	R	78	LEU	CA-CB-CG	-5.50	102.64	115.30
1	A	793	U	O5'-P-OP2	-5.50	100.75	105.70
1	A	15	G	C5-C6-O6	-5.50	125.30	128.60
1	A	115	G	N3-C4-C5	-5.50	125.85	128.60
1	A	839	U	N1-C2-O2	5.50	126.65	122.80
1	A	750	G	C4-C5-C6	5.49	122.10	118.80
1	A	584	G	N1-C2-N3	-5.49	120.61	123.90
1	A	1477	C	C5-C6-N1	5.49	123.75	121.00
1	A	948	C	C2-N1-C1'	-5.49	112.76	118.80
1	A	1235	U	N1-C2-N3	5.49	118.19	114.90
1	A	1366	C	C6-N1-C2	-5.49	118.10	120.30
1	A	1075	C	C6-N1-C2	5.49	122.50	120.30
1	A	1099	G	N3-C4-N9	-5.49	122.71	126.00
1	A	1414	U	N3-C4-C5	-5.49	111.31	114.60
1	A	451	A	O4'-C1'-N9	-5.49	103.81	108.20
1	A	591	U	C2-N3-C4	-5.48	123.71	127.00
1	A	753	A	N1-C2-N3	5.48	132.04	129.30
1	A	392	G	C4-N9-C1'	5.48	133.63	126.50
1	A	879	C	C2-N3-C4	-5.48	117.16	119.90
1	A	22	G	OP2-P-O3'	5.48	117.25	105.20
1	A	487	A	C8-N9-C4	5.48	107.99	105.80
1	A	1283	G	C8-N9-C4	-5.48	104.21	106.40
1	A	111	G	N3-C4-C5	5.47	131.34	128.60
1	A	1060	C	N3-C4-C5	5.47	124.09	121.90
1	A	818	G	O5'-P-OP2	5.47	117.27	110.70
1	A	248	C	N3-C4-C5	5.47	124.09	121.90
1	A	621	A	N1-C6-N6	5.47	121.88	118.60
1	A	264	U	N1-C2-N3	5.47	118.18	114.90
1	A	761	G	C2-N3-C4	-5.47	109.17	111.90
1	A	109	A	C8-N9-C4	-5.47	103.61	105.80
1	A	623	C	N3-C4-C5	5.46	124.09	121.90
1	A	558	G	C8-N9-C4	-5.46	104.22	106.40
1	A	898	G	C8-N9-C4	5.46	108.58	106.40
1	A	933	G	C5-C6-O6	-5.46	125.32	128.60
1	A	1230	C	C6-N1-C2	-5.46	118.11	120.30
1	A	74	C	C5-C6-N1	5.46	123.73	121.00
1	A	1525	G	OP2-P-O3'	5.46	117.21	105.20
1	A	697	U	C6-N1-C2	5.46	124.28	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	625	G	N3-C4-N9	5.46	129.27	126.00
1	A	1183	A	C8-N9-C4	5.46	107.98	105.80
1	A	319	G	C4-C5-N7	5.46	112.98	110.80
1	A	17	U	C5-C6-N1	-5.45	119.97	122.70
1	A	1515[A]	C	N3-C2-O2	-5.45	118.08	121.90
1	A	1515[B]	C	N3-C2-O2	-5.45	118.08	121.90
1	A	869	G	N1-C2-N2	5.45	121.11	116.20
1	A	1526	G	O5'-P-OP2	-5.45	100.80	105.70
1	A	147	G	C5-C6-O6	-5.45	125.33	128.60
1	A	500	G	C5-C6-O6	-5.44	125.33	128.60
1	A	565	U	C5-C4-O4	-5.44	122.64	125.90
1	A	1344	C	N3-C4-N4	-5.44	114.19	118.00
1	A	1370	G	N1-C6-O6	-5.44	116.64	119.90
1	A	1393	U	N3-C2-O2	5.44	126.01	122.20
1	A	300	A	C5-N7-C8	-5.44	101.18	103.90
1	A	485	G	O4'-C1'-N9	5.44	112.55	108.20
1	A	570	G	C8-N9-C4	-5.44	104.22	106.40
1	A	836	G	N1-C6-O6	5.44	123.16	119.90
1	A	839	U	N3-C2-O2	-5.44	118.39	122.20
1	A	947	G	C4-N9-C1'	5.44	133.57	126.50
1	A	91	C	C5-C6-N1	5.44	123.72	121.00
1	A	828	A	C6-C5-N7	-5.43	128.50	132.30
1	A	668	G	N9-C4-C5	-5.43	103.23	105.40
1	A	11	G	N1-C2-N3	5.43	127.16	123.90
1	A	250	A	N3-C4-C5	5.43	130.60	126.80
1	A	129(A)	G	N3-C4-C5	-5.43	125.89	128.60
1	A	1529	G	C5-C6-O6	-5.43	125.34	128.60
1	A	106	C	O5'-P-OP1	-5.42	100.82	105.70
1	A	869	G	C2-N3-C4	-5.42	109.19	111.90
1	A	266	G	N1-C2-N2	-5.42	111.32	116.20
1	A	579	G	N7-C8-N9	5.42	115.81	113.10
1	A	25	C	C5-C6-N1	-5.42	118.29	121.00
1	A	648	A	C8-N9-C4	5.42	107.97	105.80
1	A	625	G	N3-C4-C5	-5.41	125.89	128.60
1	A	260	G	C5-C6-N1	-5.41	108.80	111.50
1	A	267	C	N3-C4-C5	5.41	124.06	121.90
1	A	47	C	C6-N1-C2	5.41	122.46	120.30
1	A	247	G	O5'-P-OP1	-5.41	100.83	105.70
1	A	890	G	O4'-C1'-N9	5.41	112.53	108.20
1	A	938	A	N1-C6-N6	-5.41	115.36	118.60
1	A	757	U	C5-C6-N1	-5.40	120.00	122.70
1	A	1434	A	N1-C6-N6	5.40	121.84	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	8	A	C4-C5-N7	-5.40	108.00	110.70
1	A	563	A	C8-N9-C4	-5.40	103.64	105.80
1	A	1380	U	C5-C6-N1	-5.40	120.00	122.70
1	A	761	G	N1-C6-O6	5.40	123.14	119.90
1	A	1354	C	N1-C2-O2	5.39	122.14	118.90
1	A	658	G	N1-C6-O6	5.39	123.14	119.90
1	A	808	C	N3-C4-C5	5.39	124.06	121.90
1	A	901	A	C2-N3-C4	-5.39	107.91	110.60
1	A	866	C	C2-N3-C4	-5.39	117.21	119.90
1	A	918	A	C5-C6-N1	5.39	120.39	117.70
1	A	923	A	C8-N9-C4	5.39	107.95	105.80
1	A	522	C	O5'-P-OP2	-5.39	100.85	105.70
1	A	1322	C	C2-N1-C1'	5.39	124.73	118.80
1	A	309	G	N1-C6-O6	5.38	123.13	119.90
1	A	886	G	C6-C5-N7	-5.38	127.17	130.40
1	A	1338	G	N1-C6-O6	-5.38	116.67	119.90
1	A	50	A	C8-N9-C4	5.38	107.95	105.80
1	A	590	C	C6-N1-C2	5.38	122.45	120.30
1	A	309	G	C5-N7-C8	-5.38	101.61	104.30
1	A	554	C	N1-C2-O2	-5.38	115.67	118.90
1	A	586	C	C4-C5-C6	5.38	120.09	117.40
1	A	1373	G	C4-C5-C6	5.38	122.03	118.80
1	A	1399	C	C6-N1-C2	-5.38	118.15	120.30
1	A	1426	C	C6-N1-C2	5.38	122.45	120.30
1	A	79	G	C2-N3-C4	5.38	114.59	111.90
1	A	502	G	N3-C4-N9	5.38	129.23	126.00
1	A	663	A	N1-C6-N6	-5.38	115.37	118.60
1	A	929	G	N3-C4-C5	5.38	131.29	128.60
1	A	485	G	C4-N9-C1'	-5.37	119.51	126.50
1	A	570	G	N1-C2-N3	5.37	127.12	123.90
1	A	621	A	C5-N7-C8	-5.37	101.22	103.90
1	A	752	G	N7-C8-N9	-5.37	110.41	113.10
1	A	667	G	C8-N9-C4	5.37	108.55	106.40
1	A	726	C	C4-C5-C6	5.37	120.08	117.40
1	A	851	G	C4-N9-C1'	5.37	133.48	126.50
1	A	317	G	C4-C5-N7	5.37	112.95	110.80
1	A	385	C	N3-C4-C5	5.37	124.05	121.90
1	A	267	C	C5-C6-N1	-5.36	118.32	121.00
1	A	1246	C	C2-N1-C1'	-5.36	112.90	118.80
17	Q	99	SER	N-CA-C	5.36	125.48	111.00
1	A	1186	G	N3-C4-C5	5.36	131.28	128.60
1	A	28	G	C6-N1-C2	-5.36	121.89	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	278	G	OP1-P-OP2	5.36	127.64	119.60
1	A	875	C	C6-N1-C2	5.36	122.44	120.30
1	A	1199	U	N3-C2-O2	-5.36	118.45	122.20
1	A	1368	G	C5-C6-N1	5.36	114.18	111.50
1	A	1487	G	N3-C4-C5	-5.36	125.92	128.60
1	A	14	U	N1-C2-N3	5.35	118.11	114.90
1	A	250	A	C4-C5-N7	5.35	113.38	110.70
1	A	267	C	C2-N3-C4	-5.35	117.22	119.90
1	A	825	G	C5-C6-O6	-5.35	125.39	128.60
1	A	1328	C	N3-C4-C5	5.35	124.04	121.90
1	A	565	U	C6-N1-C2	5.35	124.21	121.00
1	A	851	G	N1-C6-O6	5.35	123.11	119.90
1	A	747	C	C2-N3-C4	-5.35	117.23	119.90
1	A	1230	C	C5-C4-N4	-5.35	116.45	120.20
1	A	1509	C	C2-N3-C4	-5.35	117.22	119.90
1	A	1352	C	C6-N1-C2	-5.35	118.16	120.30
1	A	129(A)	G	C4-C5-N7	5.34	112.94	110.80
1	A	1521	G	N3-C4-N9	5.34	129.21	126.00
19	S	29	ARG	N-CA-C	5.34	125.43	111.00
1	A	125	U	N3-C2-O2	-5.34	118.46	122.20
1	A	1452	C	N1-C2-N3	-5.34	115.46	119.20
1	A	301	G	N1-C2-N3	5.34	127.10	123.90
1	A	553	A	N9-C4-C5	-5.34	103.67	105.80
1	A	722	A	N7-C8-N9	5.34	116.47	113.80
1	A	1186	G	N1-C6-O6	5.34	123.10	119.90
1	A	553	A	N1-C6-N6	5.33	121.80	118.60
1	A	873	A	N7-C8-N9	5.33	116.47	113.80
1	A	1108	G	C4-N9-C1'	5.33	133.43	126.50
1	A	243	A	C2-N3-C4	-5.33	107.93	110.60
1	A	1090	U	N3-C4-C5	-5.33	111.40	114.60
1	A	721	G	C6-C5-N7	-5.33	127.20	130.40
1	A	595	G	C4-N9-C1'	5.33	133.43	126.50
1	A	709	G	N1-C6-O6	5.32	123.09	119.90
1	A	876	G	N3-C4-N9	-5.32	122.81	126.00
1	A	1529	G	C6-C5-N7	-5.32	127.21	130.40
1	A	250	A	C6-N1-C2	5.32	121.79	118.60
1	A	306	G	C5-C6-N1	-5.32	108.84	111.50
1	A	768	A	OP2-P-O3'	5.32	116.90	105.20
1	A	1080	A	N9-C4-C5	5.32	107.93	105.80
1	A	1336	C	C6-N1-C2	5.32	122.43	120.30
1	A	931	C	N1-C2-N3	5.32	122.92	119.20
1	A	750	G	N3-C4-C5	-5.31	125.94	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	123	C	N1-C2-O2	-5.31	115.71	118.90
1	A	561	U	C5-C4-O4	-5.31	122.71	125.90
1	A	829	G	N3-C4-C5	-5.31	125.94	128.60
1	A	562	C	N1-C2-O2	5.31	122.09	118.90
1	A	829	G	C6-C5-N7	-5.31	127.21	130.40
1	A	115	G	P-O3'-C3'	5.31	126.07	119.70
1	A	366	C	C2-N1-C1'	5.31	124.64	118.80
1	A	598	U	C5-C6-N1	-5.31	120.05	122.70
1	A	28	G	C6-C5-N7	-5.30	127.22	130.40
1	A	397	A	C4-C5-N7	5.30	113.35	110.70
1	A	1506	U	N3-C2-O2	5.30	125.91	122.20
1	A	1344	C	C5-C6-N1	-5.30	118.35	121.00
1	A	428	G	P-O3'-C3'	5.30	126.06	119.70
1	A	620	C	N3-C4-C5	5.30	124.02	121.90
1	A	190(E)	U	C5-C6-N1	-5.30	120.05	122.70
1	A	756	C	N3-C4-C5	5.30	124.02	121.90
1	A	1253	G	N1-C6-O6	5.30	123.08	119.90
1	A	599	C	C5-C4-N4	-5.29	116.49	120.20
1	A	701	C	P-O3'-C3'	5.29	126.05	119.70
1	A	1103	C	N3-C2-O2	-5.29	118.19	121.90
1	A	402	G	N9-C4-C5	5.29	107.52	105.40
1	A	1158	C	C6-N1-C2	-5.29	118.18	120.30
1	A	1231	G	N1-C6-O6	5.29	123.08	119.90
1	A	740	U	N1-C2-N3	5.29	118.07	114.90
1	A	718	G	C2-N3-C4	-5.29	109.26	111.90
1	A	860	A	C5-N7-C8	-5.29	101.26	103.90
1	A	1310	G	C4-N9-C1'	5.28	133.37	126.50
1	A	227	G	N1-C6-O6	5.28	123.07	119.90
1	A	129(A)	G	C8-N9-C1'	-5.28	120.14	127.00
1	A	625	G	C5-C6-O6	-5.28	125.43	128.60
1	A	736	C	N1-C2-O2	5.27	122.06	118.90
1	A	1237	C	N3-C2-O2	-5.27	118.21	121.90
1	A	872	A	OP2-P-O3'	5.27	116.80	105.20
1	A	1106	G	C2-N3-C4	-5.27	109.26	111.90
1	A	726	C	O5'-P-OP1	-5.27	100.96	105.70
1	A	832	C	C5-C4-N4	-5.27	116.51	120.20
1	A	946	A	C8-N9-C4	-5.27	103.69	105.80
1	A	130	A	C6-C5-N7	-5.27	128.61	132.30
1	A	585	G	N7-C8-N9	5.27	115.73	113.10
1	A	1236	A	OP2-P-O3'	5.27	116.79	105.20
1	A	460	A	C2-N3-C4	5.27	113.23	110.60
1	A	802	A	C5-C6-N6	-5.27	119.49	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	829	G	N1-C2-N2	-5.27	111.46	116.20
1	A	1478	C	C5-C6-N1	5.27	123.63	121.00
1	A	1503	A	OP1-P-O3'	5.27	116.79	105.20
1	A	1530	G	C4-C5-N7	5.27	112.91	110.80
1	A	548	G	C2-N3-C4	-5.27	109.27	111.90
1	A	519	C	N1-C2-N3	-5.26	115.52	119.20
1	A	558	G	C6-C5-N7	-5.26	127.24	130.40
1	A	593	G	N1-C2-N2	-5.26	111.46	116.20
1	A	725	G	C8-N9-C4	5.26	108.51	106.40
1	A	774	G	N1-C6-O6	5.26	123.06	119.90
1	A	866	C	N1-C2-O2	-5.26	115.74	118.90
1	A	154	C	N3-C4-C5	5.26	124.00	121.90
1	A	767	A	N9-C4-C5	5.26	107.90	105.80
1	A	116	A	OP2-P-O3'	5.25	116.76	105.20
1	A	299	G	C6-C5-N7	-5.25	127.25	130.40
1	A	382	A	C5-N7-C8	-5.25	101.27	103.90
1	A	588	G	N9-C4-C5	-5.25	103.30	105.40
1	A	114	U	OP1-P-O3'	5.25	116.75	105.20
1	A	756	C	O5'-P-OP2	-5.25	100.98	105.70
1	A	809	G	C6-N1-C2	-5.25	121.95	125.10
1	A	474	G	N3-C4-C5	-5.25	125.98	128.60
1	A	51	A	C5-C6-N1	5.24	120.32	117.70
1	A	559	A	N3-C4-C5	-5.24	123.13	126.80
1	A	688	G	O5'-P-OP1	-5.24	100.98	105.70
1	A	475	G	C5-C6-N1	-5.24	108.88	111.50
1	A	668	G	N7-C8-N9	-5.24	110.48	113.10
1	A	865	A	C5-C6-N1	5.24	120.32	117.70
1	A	27	G	N7-C8-N9	5.24	115.72	113.10
1	A	257	G	N9-C4-C5	-5.24	103.31	105.40
1	A	382	A	C4-C5-C6	5.24	119.62	117.00
1	A	377	G	C5-C6-N1	-5.23	108.88	111.50
1	A	898	G	N7-C8-N9	-5.23	110.48	113.10
1	A	308	C	N1-C2-O2	5.23	122.04	118.90
1	A	1065	U	OP2-P-O3'	5.23	116.71	105.20
1	A	1406	U	N3-C4-O4	5.23	123.06	119.40
1	A	297	G	C4-N9-C1'	5.23	133.29	126.50
1	A	632	A	N1-C6-N6	5.23	121.74	118.60
1	A	1285	A	P-O3'-C3'	5.22	125.97	119.70
1	A	1393	U	C5-C6-N1	-5.22	120.09	122.70
1	A	288	A	N3-C4-C5	5.22	130.46	126.80
1	A	331	G	C4-C5-C6	5.22	121.93	118.80
1	A	1238	A	N1-C6-N6	-5.22	115.47	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1370	G	C5-N7-C8	-5.22	101.69	104.30
1	A	788	U	N3-C4-C5	-5.22	111.47	114.60
1	A	1344	C	N3-C4-C5	5.22	123.99	121.90
1	A	935	A	N1-C6-N6	-5.22	115.47	118.60
1	A	1528	U	O5'-P-OP2	-5.22	101.00	105.70
1	A	193	C	C6-N1-C2	5.22	122.39	120.30
1	A	392	G	C4-C5-C6	5.22	121.93	118.80
1	A	1117	G	N3-C4-C5	5.22	131.21	128.60
1	A	851	G	C8-N9-C4	-5.21	104.31	106.40
1	A	122	G	C5-C6-N1	-5.21	108.89	111.50
1	A	776	G	C2-N3-C4	-5.21	109.29	111.90
1	A	875	C	N3-C4-C5	5.21	123.98	121.90
1	A	109	A	N1-C2-N3	5.21	131.91	129.30
1	A	1087	G	C5-N7-C8	-5.21	101.69	104.30
1	A	397	A	N7-C8-N9	5.21	116.41	113.80
1	A	144	G	C4-C5-N7	5.21	112.88	110.80
1	A	932	C	C2-N1-C1'	5.21	124.53	118.80
1	A	1078	U	C5-C4-O4	-5.21	122.78	125.90
1	A	563	A	O4'-C1'-N9	5.21	112.36	108.20
1	A	328	C	O4'-C1'-N1	5.21	112.36	108.20
1	A	550	G	N1-C6-O6	5.21	123.02	119.90
1	A	727	G	C8-N9-C4	-5.20	104.32	106.40
1	A	1345	U	C5-C6-N1	-5.20	120.10	122.70
1	A	728	A	C2-N3-C4	-5.20	108.00	110.60
1	A	807	A	C8-N9-C4	5.20	107.88	105.80
1	A	54	C	N3-C4-C5	5.20	123.98	121.90
1	A	570	G	C8-N9-C1'	-5.20	120.24	127.00
1	A	568	G	C4-N9-C1'	5.20	133.25	126.50
1	A	1059	C	N3-C4-C5	-5.20	119.82	121.90
1	A	117	G	N7-C8-N9	5.19	115.70	113.10
1	A	235	C	N3-C4-C5	5.19	123.98	121.90
1	A	761	G	C5-N7-C8	-5.19	101.70	104.30
1	A	1109	C	N1-C2-O2	5.19	122.02	118.90
1	A	637	G	N1-C2-N3	5.19	127.01	123.90
1	A	1087	G	C6-C5-N7	-5.19	127.29	130.40
1	A	1420	C	C5-C6-N1	5.19	123.59	121.00
1	A	760	G	C2-N3-C4	-5.19	109.31	111.90
1	A	23	C	C5-C6-N1	-5.19	118.41	121.00
1	A	232	G	N3-C2-N2	5.18	123.53	119.90
1	A	129(A)	G	C5-C6-O6	-5.18	125.49	128.60
1	A	245	C	N3-C4-N4	5.18	121.63	118.00
1	A	854	G	C4-C5-C6	5.18	121.91	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	784	C	C2-N3-C4	-5.18	117.31	119.90
1	A	1403	C	C5-C6-N1	5.18	123.59	121.00
1	A	250	A	C5-C6-N1	-5.18	115.11	117.70
1	A	392	G	C8-N9-C1'	-5.18	120.27	127.00
1	A	259	G	C6-C5-N7	-5.18	127.29	130.40
1	A	373	A	N1-C2-N3	5.18	131.89	129.30
1	A	803	G	N9-C4-C5	5.18	107.47	105.40
1	A	824	C	N3-C4-C5	5.18	123.97	121.90
1	A	1158	C	C6-N1-C1'	-5.17	114.59	120.80
1	A	645	C	C6-N1-C2	5.17	122.37	120.30
1	A	167	G	C6-C5-N7	-5.17	127.30	130.40
1	A	192	U	C5-C6-N1	-5.17	120.11	122.70
1	A	713	G	C8-N9-C4	-5.17	104.33	106.40
1	A	82	U	C6-N1-C2	-5.17	117.90	121.00
1	A	317	G	N1-C6-O6	5.17	123.00	119.90
1	A	763	G	N3-C2-N2	-5.17	116.28	119.90
1	A	481	G	C4-N9-C1'	5.17	133.22	126.50
1	A	650	G	C8-N9-C1'	-5.17	120.28	127.00
1	A	816	A	O4'-C1'-N9	-5.17	104.07	108.20
1	A	877	C	N1-C2-N3	5.17	122.82	119.20
1	A	858	G	N1-C2-N2	5.16	120.85	116.20
1	A	115	G	C5-C6-O6	-5.16	125.50	128.60
1	A	377	G	C2-N3-C4	-5.16	109.32	111.90
1	A	717	C	N1-C2-O2	-5.16	115.80	118.90
1	A	245	C	N1-C2-O2	-5.16	115.81	118.90
1	A	405	U	C5-C6-N1	-5.16	120.12	122.70
1	A	703	G	C8-N9-C4	-5.16	104.34	106.40
1	A	1076	C	N3-C2-O2	-5.16	118.29	121.90
1	A	1453	G	C5-N7-C8	-5.16	101.72	104.30
1	A	1062	U	C6-N1-C2	-5.15	117.91	121.00
1	A	637	G	C8-N9-C4	5.15	108.46	106.40
1	A	878	G	C4-C5-N7	5.15	112.86	110.80
1	A	1228	C	OP2-P-O3'	5.15	116.53	105.20
1	A	1250	A	C8-N9-C4	-5.15	103.74	105.80
1	A	583	A	O5'-P-OP2	5.15	116.88	110.70
1	A	595	G	N1-C2-N2	-5.15	111.56	116.20
1	A	558	G	N7-C8-N9	5.15	115.67	113.10
1	A	560	U	C2-N1-C1'	5.15	123.88	117.70
1	A	822	C	N1-C2-N3	5.15	122.80	119.20
1	A	365	U	C2-N1-C1'	5.15	123.88	117.70
1	A	563	A	C4-C5-C6	5.15	119.57	117.00
1	A	597	G	C5-C6-N1	5.15	114.07	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	615	C	C5-C4-N4	-5.15	116.60	120.20
2	B	103	THR	CB-CA-C	-5.15	97.71	111.60
1	A	648	A	C6-N1-C2	-5.14	115.51	118.60
1	A	817	C	C6-N1-C1'	-5.14	114.63	120.80
1	A	247	G	OP1-P-OP2	5.14	127.31	119.60
1	A	392	G	N3-C4-C5	-5.14	126.03	128.60
1	A	865	A	C5-C6-N6	-5.14	119.59	123.70
1	A	872	A	C5-C6-N6	-5.14	119.59	123.70
1	A	1414	U	N1-C2-O2	5.14	126.40	122.80
1	A	661	G	N3-C4-N9	-5.14	122.92	126.00
1	A	1087	G	N9-C4-C5	-5.14	103.34	105.40
1	A	617	G	N9-C4-C5	-5.13	103.35	105.40
1	A	876	G	C6-C5-N7	5.13	133.48	130.40
1	A	947	G	C4-C5-C6	5.13	121.88	118.80
1	A	879	C	N1-C2-N3	5.13	122.79	119.20
1	A	275	G	C6-C5-N7	-5.13	127.32	130.40
1	A	919	A	C2-N3-C4	5.13	113.17	110.60
1	A	300	A	C6-C5-N7	-5.13	128.71	132.30
1	A	753	A	N9-C4-C5	5.13	107.85	105.80
1	A	877	C	C4-C5-C6	5.13	119.97	117.40
1	A	1078	U	C5-C6-N1	5.13	125.27	122.70
1	A	833	U	N3-C2-O2	-5.13	118.61	122.20
1	A	869	G	N3-C4-N9	-5.13	122.92	126.00
1	A	16	A	C4-C5-N7	-5.12	108.14	110.70
1	A	590	C	C5-C6-N1	-5.12	118.44	121.00
1	A	613	C	N3-C4-C5	5.12	123.95	121.90
1	A	144	G	N7-C8-N9	5.12	115.66	113.10
1	A	930	C	N1-C2-N3	5.12	122.78	119.20
1	A	1064	G	N3-C2-N2	-5.12	116.31	119.90
1	A	428	G	N1-C6-O6	-5.12	116.83	119.90
1	A	625	G	C5-C6-N1	5.12	114.06	111.50
1	A	739	C	N3-C4-C5	5.12	123.95	121.90
1	A	859	A	C6-C5-N7	-5.12	128.72	132.30
1	A	8	A	C5-C6-N6	5.12	127.79	123.70
1	A	28	G	N1-C2-N3	5.12	126.97	123.90
1	A	483	C	N1-C2-N3	5.12	122.78	119.20
1	A	615	C	N1-C2-O2	-5.12	115.83	118.90
1	A	125	U	N1-C2-N3	5.11	117.97	114.90
1	A	178	C	N1-C2-O2	5.11	121.97	118.90
1	A	945	G	C5-C6-O6	-5.11	125.53	128.60
1	A	1449	C	N3-C4-C5	5.11	123.95	121.90
1	A	93	G	OP1-P-OP2	-5.11	111.94	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	896	C	C4-C5-C6	-5.11	114.85	117.40
1	A	397	A	C5-N7-C8	-5.11	101.35	103.90
1	A	656	C	N3-C4-C5	5.10	123.94	121.90
1	A	559	A	C8-N9-C4	-5.10	103.76	105.80
1	A	634	C	N1-C2-N3	5.10	122.77	119.20
1	A	895	G	C6-C5-N7	-5.10	127.34	130.40
1	A	1433	A	N7-C8-N9	5.10	116.35	113.80
1	A	1390	U	C4-C5-C6	5.10	122.76	119.70
1	A	445	G	C5-C6-N1	-5.10	108.95	111.50
1	A	828	A	N1-C6-N6	5.10	121.66	118.60
1	A	43	C	C6-N1-C2	5.10	122.34	120.30
1	A	671	G	N1-C6-O6	5.10	122.96	119.90
1	A	829	G	C8-N9-C1'	-5.10	120.37	127.00
1	A	853	G	C4-C5-C6	5.10	121.86	118.80
1	A	266	G	N3-C2-N2	5.09	123.46	119.90
1	A	279	A	C4-N9-C1'	5.09	135.47	126.30
1	A	285	G	N3-C2-N2	-5.09	116.34	119.90
1	A	759	A	OP2-P-O3'	5.09	116.40	105.20
1	A	881	G	OP2-P-O3'	5.09	116.40	105.20
1	A	944	G	N9-C4-C5	5.09	107.44	105.40
1	A	1332	A	N1-C6-N6	-5.09	115.55	118.60
1	A	1368	G	N3-C4-C5	-5.09	126.06	128.60
1	A	16	A	C5-N7-C8	5.09	106.44	103.90
1	A	934	C	N3-C4-C5	5.09	123.93	121.90
1	A	240	C	C4-C5-C6	-5.08	114.86	117.40
1	A	577	G	OP1-P-O3'	5.08	116.37	105.20
1	A	1543	C	N1-C2-O2	5.08	121.95	118.90
1	A	460	A	C5-C6-N1	5.08	120.24	117.70
1	A	762	C	C5-C4-N4	-5.08	116.65	120.20
1	A	1329	A	N1-C6-N6	5.08	121.64	118.60
1	A	239	U	OP1-P-OP2	5.07	127.21	119.60
1	A	572	A	C2-N3-C4	5.07	113.14	110.60
1	A	75	G	C8-N9-C1'	-5.07	120.41	127.00
1	A	366	C	OP2-P-O3'	5.07	116.36	105.20
1	A	791	G	O5'-P-OP2	-5.07	101.14	105.70
1	A	863	U	O5'-P-OP1	-5.07	101.14	105.70
1	A	880	C	N1-C2-O2	-5.07	115.86	118.90
1	A	183	G	C4-C5-N7	5.07	112.83	110.80
1	A	502	G	C4-C5-N7	5.07	112.83	110.80
1	A	1465	C	N3-C4-C5	5.07	123.93	121.90
1	A	488	C	N3-C4-C5	5.07	123.93	121.90
1	A	649	G	C6-N1-C2	-5.07	122.06	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	750	G	C6-C5-N7	-5.06	127.36	130.40
1	A	721	G	N3-C4-N9	5.06	129.04	126.00
1	A	730	G	C6-N1-C2	-5.06	122.06	125.10
1	A	127	G	C2-N3-C4	-5.06	109.37	111.90
1	A	761	G	C4-C5-N7	5.06	112.82	110.80
1	A	293	G	N1-C6-O6	5.06	122.94	119.90
1	A	372	C	C4-C5-C6	5.05	119.93	117.40
1	A	1094	G	N7-C8-N9	-5.05	110.57	113.10
1	A	1499	A	C6-N1-C2	-5.05	115.57	118.60
1	A	1526	G	C5-C6-O6	-5.05	125.57	128.60
3	C	179	ARG	N-CA-C	-5.05	97.36	111.00
1	A	242	C	N3-C4-C5	5.05	123.92	121.90
1	A	568	G	C6-N1-C2	-5.05	122.07	125.10
1	A	766	A	OP1-P-OP2	5.05	127.18	119.60
1	A	962	C	N1-C2-N3	-5.05	115.66	119.20
1	A	1369	C	N1-C2-N3	5.05	122.74	119.20
1	A	306	G	N1-C6-O6	5.05	122.93	119.90
1	A	555	C	C2-N1-C1'	5.05	124.35	118.80
1	A	21	G	N1-C6-O6	5.05	122.93	119.90
1	A	227	G	C5-N7-C8	-5.05	101.78	104.30
1	A	725	G	C5-C6-N1	5.05	114.02	111.50
1	A	819	A	N7-C8-N9	5.05	116.32	113.80
1	A	827	U	C2-N3-C4	-5.05	123.97	127.00
1	A	1058	G	C5-C6-O6	5.05	131.63	128.60
1	A	1399	C	N1-C2-O2	-5.05	115.87	118.90
1	A	47	C	C6-N1-C1'	-5.04	114.75	120.80
1	A	392	G	O5'-P-OP2	-5.04	101.16	105.70
1	A	746	A	C6-N1-C2	-5.04	115.58	118.60
1	A	1336	C	O4'-C1'-N1	-5.04	104.17	108.20
1	A	819	A	C5-N7-C8	-5.04	101.38	103.90
1	A	1079	G	N1-C2-N2	-5.04	111.67	116.20
1	A	1497	G	N3-C4-C5	-5.04	126.08	128.60
15	O	85	LEU	CA-CB-CG	-5.04	103.71	115.30
1	A	609	A	C2-N3-C4	-5.04	108.08	110.60
1	A	1167	A	C8-N9-C4	-5.04	103.79	105.80
1	A	18	C	C4-C5-C6	5.03	119.92	117.40
1	A	639	G	N1-C2-N3	5.03	126.92	123.90
1	A	365	U	O4'-C1'-N1	5.03	112.22	108.20
1	A	393	A	C2-N3-C4	-5.03	108.09	110.60
1	A	1310	G	N3-C4-N9	5.03	129.02	126.00
1	A	558	G	N1-C6-O6	5.03	122.92	119.90
1	A	1338	G	C5-C6-O6	5.03	131.62	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	558	G	C5-C6-N1	-5.02	108.99	111.50
1	A	1331	G	C4-C5-N7	-5.02	108.79	110.80
1	A	722	A	N3-C4-C5	5.02	130.31	126.80
1	A	1512	U	N1-C2-O2	-5.02	119.29	122.80
1	A	11	G	C2-N3-C4	-5.02	109.39	111.90
1	A	267	C	N3-C4-N4	-5.02	114.49	118.00
1	A	1081	G	C5-N7-C8	-5.02	101.79	104.30
1	A	297	G	N1-C2-N3	5.01	126.91	123.90
1	A	873	A	C5-N7-C8	-5.01	101.39	103.90
1	A	1500	A	N1-C2-N3	5.01	131.81	129.30
1	A	331	G	N9-C4-C5	-5.01	103.40	105.40
1	A	822	C	C5-C4-N4	-5.01	116.69	120.20
1	A	826	C	C2-N3-C4	-5.01	117.39	119.90
1	A	584	G	C5-C6-O6	-5.01	125.59	128.60
1	A	697	U	C5-C6-N1	-5.01	120.19	122.70
1	A	256	U	C4-C5-C6	-5.01	116.69	119.70
1	A	270	A	N1-C6-N6	5.01	121.61	118.60
1	A	1239	A	O5'-P-OP2	-5.01	101.19	105.70
1	A	915	A	C2-N3-C4	-5.01	108.10	110.60
1	A	331	G	C8-N9-C1'	-5.00	120.50	127.00
1	A	747	C	C6-N1-C2	5.00	122.30	120.30

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	71	VAL	Peptide
2	B	8	LYS	Peptide
3	C	166	GLU	Peptide
3	C	179	ARG	Peptide
4	D	195	ALA	Peptide
4	D	29	PRO	Peptide
7	G	10	ARG	Peptide
8	H	27	PRO	Peptide
8	H	90	GLY	Peptide
10	J	36	GLY	Peptide
10	J	87	THR	Peptide
10	J	88	LEU	Peptide
10	J	90	LEU	Peptide
12	L	27	LEU	Peptide
15	O	2	PRO	Peptide
20	T	11	SER	Peptide

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Mol	Chain	Res	Type	Group
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	32644	0	16503	885	0
2	B	1900	0	1951	115	0
3	C	1612	0	1677	94	0
4	D	1703	0	1763	88	0
5	E	1146	0	1207	65	0
6	F	843	0	857	43	0
7	G	1257	0	1296	67	0
8	H	1116	0	1177	73	0
9	I	1010	0	1037	81	0
10	J	792	0	835	54	0
11	K	864	0	881	34	0
12	L	973	0	1062	62	0
13	M	937	0	995	62	0
14	N	492	0	529	40	0
15	O	729	0	768	38	0
16	P	700	0	720	38	0
17	Q	823	0	891	54	0
18	R	574	0	644	44	0
19	S	647	0	673	42	0
20	T	763	0	861	44	0
21	U	208	0	221	11	0
22	A	262	0	0	0	0
22	B	1	0	0	0	0
22	C	1	0	0	0	0
22	D	3	0	0	0	0
22	E	1	0	0	0	0
22	F	1	0	0	0	0
22	H	1	0	0	0	0
22	I	1	0	0	0	0
22	J	1	0	0	0	0
22	P	1	0	0	0	0
22	Q	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	D	1	0	0	0	0
23	N	1	0	0	0	0
24	A	261	0	0	11	0
24	C	1	0	0	1	0
24	D	1	0	0	0	0
24	E	6	0	0	0	0
24	Q	2	0	0	0	0
24	T	1	0	0	1	0
All	All	52281	0	36548	1858	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (1858) 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)
16:P:9:PHE:HD1	16:P:18:ARG:HG3	1.23	0.99
4:D:63:LYS:NZ	4:D:197:PRO:O	1.97	0.95
1:A:671:G:H4'	6:F:77:ARG:HE	1.32	0.95
1:A:1195:C:H3'	1:A:1196:U:H5"	1.49	0.94
8:H:95:VAL:HG12	8:H:99:GLU:HB2	1.51	0.93
1:A:1490:U:H2'	1:A:1491:G:H8	1.32	0.92
2:B:30:ARG:HD2	2:B:31:TYR:HE2	1.35	0.90
3:C:150:LYS:HA	3:C:169:ALA:HB3	1.54	0.90
5:E:17:ALA:HA	5:E:26:PHE:HB3	1.53	0.90
1:A:953:G:N7	13:M:104:ARG:NH2	2.20	0.89
12:L:25:PRO:HB3	12:L:27:LEU:HD22	1.52	0.89
1:A:419:C:H42	1:A:424:G:H1	1.12	0.89
6:F:14:LEU:HD13	6:F:18:GLN:HB3	1.52	0.88
1:A:443:C:H42	1:A:491:G:H1	1.21	0.88
9:I:8:GLY:HA3	9:I:79:LEU:HB3	1.56	0.87
1:A:144:G:H1	1:A:178:C:H42	1.20	0.86
13:M:49:THR:HB	13:M:52:GLU:H	1.39	0.85
2:B:24:TRP:CZ3	2:B:26:PRO:HA	2.11	0.85
1:A:600:C:H42	1:A:638:G:H1	1.21	0.85
21:U:10:ARG:HH11	21:U:10:ARG:HB2	1.42	0.85
1:A:262:A:H5'	20:T:74:LYS:HD3	1.57	0.84
19:S:41:VAL:HG22	19:S:44:MET:HG3	1.57	0.83
1:A:1034:G:H2'	1:A:1035:A:H8	1.44	0.83
1:A:103:C:OP1	20:T:17:ARG:NH1	2.11	0.82
1:A:1051:C:N4	1:A:1207:2MG:O6	2.13	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:581:G:O3'	15:O:64:ARG:NH2	2.13	0.81
1:A:1368:G:H5"	9:I:112:LYS:HB3	1.61	0.81
3:C:139:GLN:O	3:C:143:GLU:N	2.13	0.81
1:A:1300:G:OP2	1:A:1335:C:N4	2.14	0.81
1:A:1164:G:H1	1:A:1172:C:H42	1.28	0.81
1:A:1168:A:H2'	1:A:1169:A:C8	2.16	0.80
1:A:101:A:H2'	1:A:102:G:H8	1.45	0.80
18:R:51:LEU:HD22	18:R:55:ARG:HH12	1.45	0.80
20:T:54:LYS:HA	20:T:57:ARG:HD3	1.61	0.80
17:Q:48:GLU:HG3	17:Q:50:LYS:HB2	1.62	0.80
17:Q:81:ARG:HE	17:Q:84:LEU:HD11	1.47	0.79
1:A:1412:C:N4	1:A:1488:G:O6	2.13	0.79
5:E:15:ARG:HG2	5:E:28:PHE:HE2	1.47	0.79
6:F:22:GLU:OE1	6:F:82:ARG:NH1	2.15	0.79
5:E:95:ALA:O	5:E:98:THR:OG1	2.00	0.79
1:A:1064:G:N2	1:A:1190:G:H2'	1.97	0.79
10:J:48:THR:HA	10:J:62:HIS:HB3	1.63	0.78
1:A:1176:A:N6	1:A:1181:G:O6	2.16	0.78
2:B:60:ASP:OD2	2:B:64:ARG:NH1	2.14	0.78
18:R:37:VAL:O	18:R:40:LEU:N	2.17	0.78
1:A:89:C:H2'	1:A:90:U:C6	2.18	0.78
1:A:35:G:O2'	12:L:118:SER:O	2.01	0.78
2:B:97:TRP:HZ2	2:B:102:LEU:HD13	1.49	0.78
1:A:278:G:OP2	17:Q:41:LYS:NZ	2.15	0.78
1:A:673:G:H5"	6:F:87:ARG:HD3	1.63	0.78
1:A:1263:C:N4	1:A:1272:G:O6	2.17	0.77
1:A:298:A:N6	24:A:2049:HOH:O	2.06	0.77
1:A:413:G:H8	1:A:428:G:H21	1.32	0.77
10:J:48:THR:OG1	10:J:62:HIS:ND1	2.17	0.77
1:A:419:C:N3	1:A:424:G:N2	2.29	0.77
1:A:584:G:OP2	17:Q:87:LYS:NZ	2.13	0.77
8:H:116:LYS:HD2	8:H:129:VAL:HG11	1.65	0.77
3:C:108:ASN:HB3	3:C:111:LEU:HB2	1.67	0.77
12:L:102:ARG:NH2	12:L:108:ALA:O	2.17	0.77
2:B:10:LEU:HB2	2:B:11:LEU:HD12	1.68	0.76
4:D:154:ASN:N	4:D:154:ASN:OD1	2.18	0.76
10:J:50:ILE:HG13	10:J:60:ARG:HB3	1.68	0.76
1:A:1160:G:O6	1:A:1181:G:N1	2.14	0.76
14:N:8:GLU:HA	14:N:11:LYS:HB2	1.66	0.76
1:A:1309:G:OP2	13:M:99:ARG:NH1	2.18	0.76
1:A:958:A:O2'	1:A:985:C:O2'	1.99	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:27:LEU:C	12:L:29:GLY:H	1.86	0.76
1:A:1164:G:N2	1:A:1172:C:N3	2.30	0.76
1:A:869:G:N7	24:A:2098:HOH:O	2.18	0.75
3:C:176:HIS:ND1	24:C:401:HOH:O	2.19	0.75
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.67	0.75
1:A:966:M2G:HM13	1:A:967:5MC:H1'	1.67	0.75
1:A:1410:G:N2	1:A:1411:C:O2	2.19	0.75
1:A:1045:C:H2'	1:A:1046:A:H8	1.52	0.75
4:D:163:GLU:HG3	4:D:166:LYS:HE3	1.68	0.75
8:H:85:ARG:NE	8:H:87:SER:O	2.20	0.75
8:H:20:TYR:CE1	8:H:76:PRO:HD2	2.21	0.75
1:A:1497:G:H2'	1:A:1498:UR3:H5'	1.69	0.74
8:H:4:ASP:OD2	8:H:85:ARG:NH1	2.20	0.74
2:B:22:LYS:O	2:B:23:ARG:NH1	2.21	0.74
1:A:755:G:OP2	15:O:65:ARG:HD2	1.88	0.74
15:O:26:GLU:OE1	15:O:77:ARG:NH1	2.20	0.74
1:A:984:C:O2	1:A:1221:G:N2	2.18	0.73
17:Q:40:LYS:HD2	17:Q:42:TYR:CE1	2.23	0.73
1:A:132:C:O2	1:A:230:G:N2	2.20	0.73
1:A:184:G:H2'	1:A:185:A:H8	1.53	0.73
3:C:172:ARG:HH11	3:C:172:ARG:HB2	1.51	0.73
20:T:75:ASN:OD1	20:T:75:ASN:N	2.21	0.73
18:R:21:LYS:HD3	18:R:57:GLY:HA2	1.70	0.73
10:J:19:SER:HB2	10:J:94:VAL:HG21	1.70	0.73
1:A:79:G:N1	1:A:80:G:N7	2.37	0.73
1:A:241:C:H4'	12:L:19:ARG:HH22	1.53	0.73
1:A:1061:G:H1	1:A:1195:C:H42	1.36	0.73
1:A:130:A:H5'	17:Q:63:ARG:HE	1.54	0.73
1:A:1249:C:O2'	9:I:73:GLN:NE2	2.21	0.73
1:A:1226:C:OP2	13:M:91:ARG:NH1	2.22	0.73
1:A:1055:A:N7	1:A:1200:C:N4	2.37	0.72
13:M:84:ILE:HG13	13:M:86:CYS:H	1.52	0.72
1:A:103:C:P	20:T:17:ARG:HH12	2.12	0.72
1:A:1065:U:H5"	1:A:1190:G:N2	2.05	0.72
2:B:127:ILE:HG22	2:B:135:GLN:HG2	1.72	0.72
2:B:158:LEU:H	2:B:158:LEU:HD12	1.54	0.72
1:A:1316:G:N1	1:A:1319:A:OP2	2.23	0.72
1:A:1392:G:H21	1:A:1502:A:H8	1.34	0.72
3:C:86:VAL:HG12	3:C:87:LEU:HD23	1.72	0.72
1:A:1372:U:OP2	9:I:11:LYS:NZ	2.22	0.72
1:A:951:G:OP2	13:M:102:ARG:NH2	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:G:OP1	4:D:38:TYR:OH	2.09	0.71
2:B:23:ARG:NH1	2:B:23:ARG:HA	2.06	0.71
15:O:33:THR:OG1	15:O:63:ARG:NH1	2.22	0.71
1:A:258:G:H2'	1:A:259:G:H8	1.56	0.71
7:G:70:LYS:O	7:G:72:ARG:NH1	2.23	0.71
6:F:80:ARG:HD2	6:F:88:VAL:HB	1.72	0.71
1:A:992:U:H3	1:A:1044:A:H62	1.39	0.71
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.26	0.71
1:A:343:U:O2'	1:A:346:G:O6	2.08	0.71
5:E:15:ARG:HG2	5:E:28:PHE:CE2	2.24	0.70
13:M:3:ARG:HE	13:M:7:VAL:HA	1.55	0.70
17:Q:62:SER:HB3	17:Q:72:ARG:HD3	1.72	0.70
2:B:30:ARG:HD2	2:B:31:TYR:CE2	2.25	0.70
16:P:9:PHE:CD1	16:P:18:ARG:HG3	2.15	0.70
6:F:2:ARG:HE	6:F:69:GLU:HG2	1.57	0.70
1:A:902:G:H2'	1:A:903:G:H8	1.57	0.70
1:A:600:C:N3	1:A:638:G:N2	2.33	0.70
10:J:11:PHE:O	10:J:68:HIS:NE2	2.24	0.70
10:J:47:PHE:HB3	14:N:34:TYR:HE2	1.55	0.70
10:J:27:ALA:HB2	10:J:85:LEU:HD21	1.74	0.69
13:M:117:VAL:HG12	13:M:118:ALA:H	1.56	0.69
1:A:1309:G:O3'	13:M:77:ASN:ND2	2.24	0.69
1:A:1070:U:H2'	1:A:1071:C:H6	1.56	0.69
3:C:84:ILE:O	3:C:88:ARG:NH1	2.26	0.69
1:A:1244:C:H42	1:A:1293:G:H1	1.38	0.69
1:A:269:C:H2'	1:A:270:A:C8	2.27	0.69
12:L:52:LEU:O	12:L:54:LYS:NZ	2.24	0.69
1:A:384:G:H2'	1:A:385:C:C6	2.27	0.69
2:B:95:GLN:HG2	2:B:148:TYR:HD2	1.58	0.69
20:T:57:ARG:HE	20:T:102:GLY:HA3	1.58	0.68
4:D:119:GLN:HE21	4:D:123:HIS:HE1	1.41	0.68
15:O:6:GLU:OE1	15:O:6:GLU:N	2.21	0.68
1:A:18:C:H5"	5:E:127:ASN:HD21	1.58	0.68
1:A:1150:U:O4	1:A:1151:A:N6	2.27	0.68
9:I:4:TYR:HB2	9:I:88:TYR:HD1	1.59	0.68
14:N:40:CYS:O	14:N:44:LEU:N	2.24	0.68
2:B:23:ARG:HH11	2:B:23:ARG:HA	1.59	0.68
3:C:91:LEU:HD21	3:C:99:VAL:HG22	1.76	0.68
1:A:1255:G:H22	1:A:1283:G:H1'	1.57	0.68
1:A:1418:A:H2'	1:A:1419:G:O4'	1.93	0.68
1:A:656:C:H42	1:A:750:G:H1	1.41	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:113:ARG:HH11	12:L:116:SER:H	1.42	0.68
2:B:172:ILE:H	2:B:172:ILE:HD12	1.59	0.68
1:A:235:C:N4	24:A:1980:HOH:O	2.27	0.67
1:A:1345:U:OP1	9:I:120:ARG:NH1	2.27	0.67
1:A:1266:G:N2	1:A:1269:A:OP2	2.23	0.67
15:O:55:GLY:HA2	15:O:58:MET:HE2	1.76	0.67
6:F:74:ASP:OD2	6:F:74:ASP:N	2.23	0.67
2:B:21:ARG:HA	2:B:39:ILE:HG23	1.76	0.67
4:D:24:GLU:HG3	4:D:112:VAL:HG11	1.76	0.67
5:E:5:ASP:OD2	5:E:6:PHE:N	2.25	0.67
1:A:1262:C:H42	1:A:1273:G:H1	1.42	0.67
1:A:1417:G:O2'	1:A:1483:A:N6	2.26	0.67
7:G:18:TYR:HD2	7:G:59:LEU:HD13	1.59	0.67
2:B:160:ASP:N	2:B:160:ASP:OD2	2.27	0.67
6:F:42:GLU:HG3	6:F:61:LEU:HB3	1.75	0.67
3:C:14:ILE:HG12	3:C:15:THR:HG23	1.74	0.67
10:J:61:GLU:OE2	14:N:58:LYS:NZ	2.27	0.67
9:I:2:GLU:HG3	9:I:3:GLN:HG2	1.75	0.67
1:A:1141:C:H2'	1:A:1142:G:H8	1.57	0.67
1:A:858:G:N7	24:A:2098:HOH:O	2.27	0.67
3:C:131:ARG:HA	3:C:134:ILE:HD12	1.77	0.67
1:A:569:C:H42	1:A:881:G:H1	1.41	0.67
2:B:9:GLU:OE2	2:B:12:GLU:N	2.28	0.67
9:I:104:ARG:NH1	9:I:105:ASP:O	2.26	0.67
2:B:91:PRO:HG3	2:B:155:LEU:HD21	1.77	0.67
1:A:1100:C:OP2	2:B:96:ARG:NH1	2.27	0.67
6:F:47:ARG:HD2	6:F:47:ARG:H	1.59	0.67
1:A:1240:U:OP1	7:G:119:ARG:NH2	2.27	0.67
2:B:208:ILE:HD12	2:B:208:ILE:H	1.60	0.67
11:K:40:ILE:HG23	11:K:75:TYR:HD1	1.59	0.67
14:N:53:LEU:HD12	14:N:56:VAL:HG21	1.75	0.67
18:R:46:GLU:CD	18:R:46:GLU:H	1.99	0.66
13:M:23:TYR:CE2	13:M:70:LEU:HD12	2.29	0.66
1:A:1497:G:C2'	1:A:1498:UR3:H5'	2.25	0.66
12:L:27:LEU:C	12:L:29:GLY:N	2.48	0.66
1:A:1399:C:H4'	1:A:1400:5MC:H5"	1.76	0.66
7:G:114:ARG:O	7:G:119:ARG:NH1	2.28	0.66
1:A:921:U:O2'	5:E:19:MET:O	2.11	0.66
4:D:13:ARG:NH1	4:D:38:TYR:O	2.29	0.66
16:P:38:TYR:HE2	16:P:50:LYS:HE2	1.60	0.66
10:J:86:MET:SD	10:J:87:THR:N	2.69	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:4:ILE:HG12	16:P:21:VAL:HG22	1.78	0.66
1:A:1033:G:H2'	1:A:1034:G:C8	2.30	0.66
1:A:243:A:H4'	1:A:244:U:H5"	1.77	0.66
1:A:1249:C:H1'	9:I:70:LYS:HE2	1.78	0.66
18:R:55:ARG:HB3	18:R:55:ARG:NH1	2.11	0.66
12:L:66:VAL:HG11	12:L:98:TYR:CE1	2.31	0.66
1:A:384:G:H2'	1:A:385:C:H6	1.60	0.65
9:I:19:LEU:HD21	9:I:59:PHE:CG	2.32	0.65
20:T:87:LYS:O	20:T:91:LEU:HB2	1.96	0.65
14:N:16:PHE:HB2	14:N:19:ARG:HD2	1.77	0.65
1:A:166:G:H2'	1:A:167:G:C8	2.32	0.65
13:M:24:GLY:O	13:M:29:ARG:HD2	1.97	0.65
1:A:130:A:OP2	1:A:190(E):U:O2'	2.09	0.65
1:A:1435:G:H2'	1:A:1436:U:C6	2.32	0.65
20:T:30:LYS:HG2	20:T:34:LYS:HE2	1.78	0.65
1:A:985:C:H42	1:A:1220:G:H1	1.42	0.65
7:G:73:MET:HA	7:G:91:VAL:HG23	1.77	0.65
1:A:1151:A:H5"	10:J:42:THR:HG22	1.78	0.65
7:G:90:GLU:HG2	7:G:91:VAL:H	1.62	0.65
7:G:88:PRO:HG2	7:G:155:ARG:HH22	1.59	0.65
11:K:57:THR:HG23	11:K:60:ALA:H	1.62	0.64
19:S:64:GLU:OE2	19:S:65:ASN:ND2	2.30	0.64
1:A:184:G:H2'	1:A:185:A:C8	2.31	0.64
14:N:29:ARG:NH1	14:N:40:CYS:SG	2.70	0.64
1:A:547:A:OP2	4:D:2:GLY:N	2.29	0.64
4:D:155:LEU:HD13	4:D:157:LEU:H	1.61	0.64
19:S:77:THR:HG23	19:S:78:ARG:HG3	1.79	0.64
1:A:1257:U:H4'	1:A:1258:G:O5'	1.96	0.64
9:I:118:LYS:HG2	9:I:121:ARG:HB3	1.80	0.64
9:I:82:ALA:HB1	9:I:96:LEU:HD21	1.79	0.64
2:B:60:ASP:O	2:B:64:ARG:HG3	1.98	0.64
1:A:413:G:O6	4:D:36:ARG:NH1	2.31	0.64
1:A:633:G:H2'	1:A:634:C:C6	2.33	0.64
4:D:50:ARG:NH1	4:D:51:PRO:O	2.30	0.64
1:A:1338:G:H2'	1:A:1339:A:C8	2.31	0.64
9:I:89:ASN:O	9:I:92:TYR:HB2	1.97	0.64
1:A:1179:A:H2'	1:A:1180:A:O4'	1.98	0.64
6:F:1:MET:HB3	6:F:66:GLU:HG2	1.80	0.64
1:A:1004:A:H5"	1:A:1025:U:C2	2.33	0.63
1:A:1195:C:H3'	1:A:1196:U:C5'	2.26	0.63
10:J:79:ARG:O	10:J:82:ILE:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:127:ARG:HG2	3:C:193:TYR:OH	1.98	0.63
1:A:1095:U:OP1	1:A:1108:G:N2	2.27	0.63
1:A:783:C:H42	1:A:799:G:H1	1.46	0.63
1:A:1502:A:H2	1:A:1505:G:H1	1.47	0.63
9:I:47:LEU:HA	9:I:50:LEU:HD12	1.81	0.63
1:A:1320:C:H42	19:S:36:ARG:HD3	1.62	0.63
9:I:118:LYS:O	9:I:120:ARG:N	2.28	0.63
16:P:67:THR:HG22	16:P:68:ASP:H	1.64	0.63
4:D:59:ARG:HA	4:D:62:GLN:HB2	1.81	0.63
7:G:27:ILE:HA	7:G:30:ILE:HD12	1.80	0.63
1:A:1402:4OC:H2'	1:A:1403:C:O4'	1.98	0.63
10:J:7:LYS:HD3	10:J:9:ARG:NE	2.14	0.63
12:L:92:0TD:N	12:L:92:0TD:OD1	2.30	0.63
16:P:21:VAL:HG12	16:P:33:ILE:HG13	1.79	0.63
4:D:22:LYS:HB2	4:D:26:CYS:SG	2.38	0.63
1:A:79:G:C2	1:A:80:G:C8	2.86	0.62
1:A:1168:A:H2'	1:A:1169:A:H8	1.65	0.62
7:G:53:LYS:HB3	7:G:125:MET:HE1	1.81	0.62
1:A:986:A:N3	19:S:52:TYR:OH	2.24	0.62
1:A:9:G:OP2	5:E:121:LYS:NZ	2.28	0.62
2:B:50:GLU:O	2:B:53:ARG:HG3	1.99	0.62
9:I:43:ALA:HA	9:I:74:ILE:HD12	1.81	0.62
12:L:53:ARG:NH1	12:L:92:0TD:OD2	2.32	0.62
1:A:1301:U:O2'	1:A:1302:U:H3'	1.99	0.62
1:A:973:G:H3'	1:A:974:A:H5"	1.80	0.62
1:A:1336:C:H5"	1:A:1336:C:H6	1.64	0.62
2:B:74:LYS:HE3	2:B:206:ASP:HA	1.82	0.62
1:A:967:5MC:O3'	9:I:128:ARG:NH2	2.32	0.62
1:A:186:C:O2'	20:T:85:MET:SD	2.52	0.62
2:B:16:HIS:CB	2:B:210:SER:HB3	2.29	0.62
1:A:1412:C:N3	1:A:1488:G:N1	2.40	0.62
1:A:633:G:H2'	1:A:634:C:H6	1.65	0.62
1:A:1009:G:N2	1:A:1010:G:N3	2.46	0.62
1:A:101:A:H2'	1:A:102:G:C8	2.31	0.62
8:H:4:ASP:OD1	8:H:6:ILE:N	2.32	0.62
1:A:241:C:H4'	12:L:19:ARG:NH2	2.15	0.62
3:C:88:ARG:HG3	3:C:91:LEU:HD22	1.82	0.62
1:A:1112:C:O2'	3:C:179:ARG:NH1	2.32	0.62
1:A:1045:C:H2'	1:A:1046:A:C8	2.35	0.62
2:B:16:HIS:O	2:B:17:PHE:HD1	1.82	0.62
9:I:106:ALA:O	9:I:108:VAL:HG23	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1197:G:H5"	24:A:2057:HOH:O	2.00	0.62
1:A:1415:G:H2'	1:A:1416:G:H8	1.65	0.61
1:A:1034:G:H2'	1:A:1035:A:C8	2.31	0.61
1:A:80:G:H2'	1:A:81:U:H5'	1.82	0.61
6:F:2:ARG:O	6:F:66:GLU:HA	2.00	0.61
1:A:1347:G:N2	1:A:1373:G:H2'	2.15	0.61
3:C:124:ILE:HG12	3:C:130:VAL:HG12	1.82	0.61
2:B:82:ARG:HA	2:B:92:TYR:CE1	2.35	0.61
4:D:88:VAL:O	4:D:92:VAL:HG23	2.00	0.61
1:A:937:A:H5"	1:A:938:A:OP2	2.00	0.61
11:K:99:GLN:HG2	11:K:105:VAL:HG21	1.82	0.61
1:A:542:G:OP1	4:D:10:ARG:NH2	2.33	0.61
5:E:75:THR:OG1	5:E:76:ILE:N	2.24	0.61
1:A:1058:G:H2'	1:A:1059:C:O4'	2.00	0.61
12:L:59:ARG:HA	12:L:65:GLU:HG3	1.82	0.61
17:Q:97:SER:O	17:Q:98:LEU:HD12	2.01	0.61
8:H:6:ILE:HB	8:H:85:ARG:HH12	1.64	0.61
13:M:40:ASN:HD22	13:M:43:THR:HG23	1.65	0.61
6:F:47:ARG:HA	6:F:57:GLN:HG2	1.82	0.61
1:A:949:A:C2	1:A:1233:G:N3	2.69	0.61
1:A:618:C:N3	1:A:622:A:N6	2.47	0.61
12:L:126:LYS:HD2	12:L:126:LYS:H	1.65	0.61
1:A:1516[A]:G:H2'	1:A:1518[A]:MA6:OP2	2.01	0.61
1:A:691:G:H2'	1:A:692:U:C6	2.36	0.61
1:A:337:C:H2'	1:A:338:A:C8	2.36	0.61
1:A:353:A:H5'	1:A:353:A:H8	1.66	0.61
5:E:65:ASN:ND2	5:E:65:ASN:O	2.33	0.61
5:E:81:GLU:HG2	5:E:90:VAL:HG22	1.83	0.60
4:D:111:ALA:HB2	4:D:120:LEU:HD12	1.83	0.60
4:D:157:LEU:O	4:D:160:GLN:HB3	2.00	0.60
20:T:44:ALA:HB1	20:T:91:LEU:HB3	1.82	0.60
7:G:90:GLU:HG2	7:G:91:VAL:N	2.16	0.60
1:A:1046:A:H3'	1:A:1047:G:H8	1.67	0.60
1:A:978:A:O2'	1:A:1322:C:N3	2.35	0.60
20:T:49:ALA:HB3	20:T:99:LEU:HD12	1.84	0.60
1:A:1234:C:H1'	1:A:1364:U:O2	2.01	0.60
7:G:16:LEU:HD12	9:I:44:VAL:HG12	1.83	0.60
3:C:156:ARG:HG2	3:C:160:ALA:O	2.01	0.60
12:L:89:ARG:HG2	12:L:97:ARG:HA	1.84	0.60
1:A:358:U:H2'	1:A:359:U:H6	1.66	0.60
8:H:10:LEU:HD22	8:H:83:ILE:HD11	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:11:ARG:HB3	3:C:16:ARG:HB2	1.83	0.60
17:Q:97:SER:OG	17:Q:98:LEU:N	2.34	0.60
1:A:679:C:H2'	1:A:680:C:C6	2.37	0.60
1:A:235:C:H5'	17:Q:70:ARG:HG2	1.83	0.60
1:A:299:G:H2'	1:A:300:A:C8	2.37	0.60
1:A:625:G:H2'	1:A:626:U:C6	2.37	0.60
1:A:1356:G:H2'	1:A:1357:A:C8	2.37	0.60
5:E:20:GLN:NE2	5:E:25:ARG:HH21	2.00	0.60
1:A:1351:U:H4'	7:G:33:ASP:OD2	2.02	0.60
1:A:1074:G:O3'	2:B:103:THR:HG21	2.02	0.60
1:A:463:A:OP1	16:P:75:ARG:NH2	2.34	0.60
1:A:912:C:OP1	12:L:46:LYS:NZ	2.33	0.60
4:D:4:TYR:OH	4:D:7:PRO:O	2.17	0.60
2:B:191:ASP:N	2:B:191:ASP:OD1	2.28	0.60
1:A:1487:G:H2'	1:A:1488:G:O4'	2.02	0.59
1:A:1520[A]:G:H2'	1:A:1521:G:H8	1.66	0.59
3:C:21:ARG:HH21	3:C:58:GLU:HG3	1.67	0.59
11:K:66:LEU:HG	11:K:97:ALA:HB1	1.84	0.59
1:A:872:A:O2'	1:A:873:A:H5"	2.02	0.59
13:M:75:ALA:O	13:M:79:LYS:NZ	2.35	0.59
21:U:10:ARG:O	21:U:13:ILE:HG12	2.03	0.59
2:B:92:TYR:CD2	2:B:151:GLY:HA3	2.37	0.59
8:H:39:LEU:HB3	8:H:45:ILE:HG12	1.83	0.59
16:P:74:LEU:HB3	16:P:79:VAL:HG21	1.84	0.59
1:A:828:A:H5"	1:A:859:A:C2	2.38	0.59
6:F:2:ARG:NE	6:F:69:GLU:HG2	2.17	0.59
20:T:63:ILE:HG21	20:T:81:LYS:HG3	1.83	0.59
1:A:1093:A:N3	1:A:1109:C:O2'	2.34	0.59
2:B:54:THR:OG1	2:B:199:TYR:HB3	2.03	0.59
1:A:1510:U:H2'	1:A:1511:G:C8	2.37	0.59
1:A:900:A:H2'	1:A:901:A:O4'	2.03	0.59
4:D:75:PHE:O	4:D:78:LEU:HB3	2.02	0.59
15:O:14:GLU:HG3	15:O:15:PHE:HD1	1.67	0.59
5:E:127:ASN:HB3	5:E:130:ASN:HB2	1.84	0.59
1:A:485:G:O2'	1:A:486:U:OP2	2.14	0.59
10:J:10:GLY:HA3	10:J:16:LEU:HD21	1.85	0.59
10:J:17:ASP:O	10:J:21:GLN:HB2	2.01	0.59
1:A:1181:G:N2	1:A:1182:G:H22	2.01	0.59
1:A:268:C:H2'	1:A:269:C:H6	1.67	0.59
7:G:129:GLU:HB3	7:G:131:LYS:HG2	1.85	0.59
15:O:87:ILE:HG22	15:O:88:ARG:H	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:9:GLU:HB3	2:B:12:GLU:HG2	1.83	0.59
1:A:276:G:O3'	17:Q:68:ARG:NH1	2.35	0.59
11:K:72:ALA:HB1	11:K:77:MET:HG3	1.84	0.59
7:G:88:PRO:HG2	7:G:155:ARG:HH12	1.67	0.58
13:M:25:ILE:HD11	13:M:66:LEU:HD11	1.85	0.58
1:A:1437:C:H2'	1:A:1438:G:C8	2.39	0.58
4:D:98:GLU:OE2	4:D:107:ARG:NE	2.36	0.58
1:A:967:5MC:H5"	1:A:968:A:H2'	1.85	0.58
1:A:1427:U:H2'	1:A:1428:A:C8	2.38	0.58
1:A:79:G:N1	1:A:80:G:C5	2.72	0.58
1:A:858:G:C6	1:A:869:G:C8	2.91	0.58
1:A:1060:C:OP1	14:N:45:ARG:NH2	2.36	0.58
5:E:18:ARG:HG2	5:E:19:MET:N	2.16	0.58
1:A:793:U:H5'	24:A:2157:HOH:O	2.03	0.58
1:A:539:A:H2'	1:A:540:G:C8	2.37	0.58
6:F:4:TYR:HB2	6:F:65:VAL:HG22	1.84	0.58
1:A:628:G:H2'	1:A:629:G:C8	2.38	0.58
1:A:414:A:OP2	1:A:428:G:N2	2.30	0.58
17:Q:66:SER:OG	17:Q:69:LYS:HB3	2.03	0.58
17:Q:65:ILE:HB	17:Q:69:LYS:HG2	1.84	0.58
14:N:24:CYS:HB2	14:N:40:CYS:HB3	1.86	0.58
16:P:41:PRO:O	16:P:43:LYS:HE3	2.03	0.58
8:H:97:VAL:HG12	8:H:98:LYS:HG3	1.86	0.58
7:G:17:VAL:HG12	7:G:18:TYR:HD1	1.68	0.58
3:C:134:ILE:O	3:C:138:VAL:HG23	2.03	0.58
1:A:1111:A:N1	3:C:177:THR:HB	2.19	0.58
3:C:39:ILE:HD12	3:C:57:ILE:HD13	1.84	0.58
1:A:216:G:C2	1:A:217:C:C4	2.91	0.58
1:A:1049:U:H4'	1:A:1050:G:O5'	2.03	0.58
1:A:190(L):U:H3	20:T:105:SER:CB	2.17	0.58
1:A:864:A:H2'	1:A:865:A:C8	2.39	0.58
20:T:51:GLU:O	20:T:55:ILE:HG12	2.04	0.58
1:A:77:G:C6	1:A:93:G:N1	2.72	0.58
2:B:91:PRO:HB3	2:B:154:LEU:HB2	1.85	0.58
15:O:39:LEU:HD13	15:O:56:LEU:HB2	1.85	0.58
3:C:11:ARG:HH12	3:C:178:LEU:HA	1.68	0.58
1:A:1424:C:H2'	1:A:1425:U:C6	2.39	0.58
4:D:111:ALA:HB1	4:D:116:GLN:HG2	1.85	0.57
16:P:67:THR:HG22	16:P:68:ASP:N	2.19	0.57
3:C:12:LEU:HD21	14:N:51:GLY:HA2	1.85	0.57
2:B:9:GLU:O	2:B:10:LEU:HD23	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:67:THR:HB	16:P:70:ALA:H	1.69	0.57
3:C:88:ARG:HH21	3:C:101:LEU:HB2	1.69	0.57
1:A:401:C:O2'	1:A:621:A:N3	2.28	0.57
12:L:111:LYS:H	12:L:111:LYS:NZ	2.01	0.57
1:A:1517[A]:G:H2'	1:A:1518[A]:MA6:H8	1.86	0.57
18:R:47:THR:HG22	18:R:48:GLY:H	1.69	0.57
1:A:1530:G:H2'	1:A:1531:A:C8	2.39	0.57
18:R:34:TYR:CE1	18:R:35:ARG:HG3	2.40	0.57
2:B:175:ARG:HH11	2:B:175:ARG:HG3	1.68	0.57
19:S:11:VAL:HB	19:S:16:LEU:HD12	1.87	0.57
1:A:1401:G:N2	1:A:1402:4OC:H1'	2.19	0.57
1:A:1520[B]:G:H2'	1:A:1521:G:H8	1.69	0.57
1:A:1291:G:H5"	7:G:41:ARG:HH21	1.69	0.57
9:I:32:ASP:OD2	9:I:33:PHE:N	2.38	0.57
1:A:1437:C:H2'	1:A:1438:G:H8	1.70	0.57
1:A:617:G:H1	1:A:623:C:H42	1.52	0.57
6:F:13:ASN:N	6:F:13:ASN:OD1	2.30	0.57
17:Q:5:VAL:O	17:Q:6:LEU:HD23	2.04	0.57
17:Q:3:LYS:HB3	17:Q:60:ILE:HD11	1.84	0.57
7:G:45:ASP:O	7:G:49:ILE:HG12	2.05	0.57
19:S:18:LYS:NZ	19:S:32:LYS:HG2	2.20	0.57
6:F:50:TYR:OH	6:F:87:ARG:NH2	2.37	0.57
1:A:691:G:H2'	1:A:692:U:H6	1.68	0.57
5:E:84:PHE:HB3	5:E:134:ALA:HB2	1.84	0.57
16:P:23:ASP:OD1	16:P:24:ALA:N	2.37	0.57
1:A:442:C:H2'	1:A:443:C:H6	1.70	0.57
1:A:673:G:H2'	1:A:674:G:C8	2.39	0.57
1:A:258:G:H2'	1:A:259:G:C8	2.38	0.57
12:L:39:VAL:HG22	12:L:57:LYS:HB2	1.87	0.57
1:A:629:G:H2'	1:A:630:G:C8	2.39	0.57
8:H:6:ILE:HB	8:H:85:ARG:NH1	2.20	0.56
1:A:991:U:H3	1:A:1215:G:N2	2.03	0.56
7:G:18:TYR:CD2	7:G:59:LEU:HD22	2.40	0.56
3:C:179:ARG:NE	3:C:206:GLU:OE1	2.38	0.56
8:H:111:ILE:HG22	8:H:134:ILE:HD13	1.87	0.56
1:A:372:C:H4'	1:A:373:A:O5'	2.05	0.56
1:A:1415:G:H2'	1:A:1416:G:C8	2.40	0.56
13:M:48:LEU:HD12	13:M:52:GLU:HB3	1.87	0.56
1:A:1397:C:O2'	1:A:1398:A:OP1	2.19	0.56
1:A:1114:C:O2'	14:N:60:SER:O	2.09	0.56
1:A:444:C:H42	1:A:490:G:H1	1.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1026:G:O6	1:A:1036:G:N2	2.38	0.56
6:F:10:LEU:HB3	6:F:85:VAL:HA	1.87	0.56
6:F:82:ARG:HB3	6:F:85:VAL:HG23	1.87	0.56
1:A:517:G:H5'	1:A:519:C:C2	2.39	0.56
1:A:390:C:H2'	1:A:391:G:C8	2.41	0.56
3:C:184:TYR:HE2	3:C:186:PHE:HB2	1.70	0.56
12:L:25:PRO:HG3	12:L:27:LEU:HD13	1.87	0.56
18:R:25:THR:OG1	18:R:25:THR:O	2.23	0.56
1:A:264:U:H2'	1:A:265:G:O4'	2.05	0.56
18:R:56:THR:OG1	18:R:57:GLY:N	2.38	0.56
1:A:190(K):G:H2'	1:A:190(L):U:C6	2.41	0.56
13:M:17:VAL:O	13:M:20:THR:HG22	2.05	0.56
1:A:99:C:H2'	1:A:101:A:C8	2.41	0.56
1:A:411:A:OP1	4:D:30:LYS:NZ	2.38	0.56
1:A:1425:U:H2'	1:A:1426:C:C6	2.40	0.56
4:D:190:ASP:H	4:D:193:ASP:HB2	1.70	0.56
1:A:176:C:O2'	1:A:177:C:H5'	2.05	0.56
18:R:66:LEU:HD12	18:R:66:LEU:O	2.05	0.56
2:B:118:LEU:HB3	2:B:142:LEU:HD23	1.87	0.56
1:A:1004:A:O2'	1:A:1038:C:O2	2.22	0.56
18:R:61:LYS:HG2	18:R:65:ILE:HD11	1.87	0.56
12:L:57:LYS:HE3	12:L:65:GLU:HB3	1.88	0.56
4:D:174:LEU:O	4:D:186:LEU:HD11	2.06	0.56
9:I:16:ARG:HB2	9:I:64:THR:HG23	1.87	0.56
10:J:45:ARG:HB3	10:J:65:LEU:HB3	1.88	0.56
1:A:1004:A:H5"	1:A:1025:U:N3	2.20	0.56
1:A:411:A:N9	1:A:413:G:H1'	2.21	0.56
13:M:3:ARG:HA	13:M:8:GLU:O	2.06	0.56
1:A:664:G:H22	1:A:741:G:H1	1.54	0.56
13:M:96:LEU:O	13:M:110:ARG:NH1	2.38	0.56
7:G:94:ARG:O	7:G:97:GLN:HB3	2.06	0.56
18:R:45:SER:OG	18:R:47:THR:O	2.18	0.56
5:E:60:TYR:HD2	5:E:61:TYR:HD1	1.54	0.56
1:A:95:U:H2'	1:A:96:G:H8	1.71	0.56
1:A:1290:G:H2'	1:A:1291:G:C8	2.41	0.56
1:A:1009:G:H1	1:A:1020:U:H3	1.52	0.56
1:A:1201:A:H4'	1:A:1202:G:C5'	2.36	0.56
1:A:1004:A:N6	1:A:1036:G:O6	2.39	0.56
3:C:21:ARG:HA	14:N:54:PRO:HB3	1.88	0.56
1:A:1285:A:H4'	1:A:1286:A:O5'	2.06	0.56
1:A:939:G:H2'	1:A:940:C:C6	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:187:ARG:NE	4:D:188:LEU:H	2.03	0.56
1:A:1309:G:H2'	1:A:1310:G:C8	2.40	0.55
1:A:1442:G:C5	1:A:1446:A:C6	2.93	0.55
1:A:1003:G:H1	1:A:1038:C:H42	1.53	0.55
1:A:337:C:H2'	1:A:338:A:H8	1.71	0.55
1:A:1128:C:O2'	1:A:1130:A:N7	2.39	0.55
1:A:1413:A:H2'	1:A:1414:U:H6	1.71	0.55
1:A:166:G:H2'	1:A:167:G:H8	1.71	0.55
1:A:536:C:H2'	1:A:537:G:C8	2.41	0.55
12:L:66:VAL:HG11	12:L:98:TYR:HE1	1.68	0.55
1:A:277:C:P	17:Q:68:ARG:HH12	2.28	0.55
1:A:918:A:H2'	1:A:919:A:C8	2.41	0.55
18:R:44:LEU:HD13	18:R:48:GLY:O	2.06	0.55
11:K:109:VAL:HG11	18:R:84:LYS:HE2	1.88	0.55
11:K:120:ARG:HH22	11:K:126:ARG:HH12	1.54	0.55
1:A:1376:U:OP1	7:G:98:SER:OG	2.12	0.55
2:B:133:LYS:NZ	2:B:133:LYS:H	2.04	0.55
3:C:150:LYS:HB2	3:C:201:TYR:HB2	1.89	0.55
1:A:1366:C:H2'	1:A:1367:C:H6	1.71	0.55
1:A:1488:G:H2'	1:A:1489:G:C8	2.42	0.55
1:A:1258:G:H2'	1:A:1259:C:C6	2.42	0.55
9:I:104:ARG:HD3	9:I:105:ASP:H	1.72	0.55
1:A:186:C:H2'	1:A:187:C:C6	2.41	0.55
1:A:955:U:O2'	1:A:1227:A:N6	2.40	0.55
1:A:443:C:N4	1:A:491:G:H1	1.98	0.55
1:A:79:G:C2	1:A:80:G:N7	2.75	0.55
1:A:474:G:H4'	16:P:81:ARG:NH2	2.21	0.55
2:B:103:THR:HA	2:B:180:LEU:HD11	1.87	0.55
1:A:620:C:H2'	1:A:621:A:O4'	2.06	0.55
2:B:166:ASP:OD2	2:B:169:LYS:N	2.30	0.55
1:A:835:U:OP1	18:R:64:ARG:NH2	2.39	0.55
8:H:82:HIS:C	8:H:82:HIS:ND1	2.60	0.55
1:A:1504:G:H4'	1:A:1505:G:H5'	1.89	0.55
1:A:1232:U:H5"	9:I:124:GLN:O	2.07	0.55
1:A:560:U:H5'	1:A:566:G:C2	2.42	0.55
3:C:22:TRP:CH2	3:C:32:LEU:HB3	2.42	0.55
13:M:8:GLU:OE2	13:M:22:ILE:HA	2.07	0.55
2:B:80:ILE:HG22	2:B:215:LEU:HD12	1.89	0.55
3:C:64:VAL:HG12	3:C:65:ALA:H	1.71	0.55
4:D:60:GLU:OE2	4:D:199:ASN:N	2.32	0.55
1:A:103:C:OP2	20:T:14:LYS:HD2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1309:G:OP1	13:M:92:HIS:NE2	2.33	0.54
13:M:67:GLU:O	13:M:71:ARG:HG2	2.07	0.54
12:L:113:ARG:NH1	12:L:116:SER:H	2.04	0.54
17:Q:29:HIS:CE1	17:Q:31:LEU:H	2.24	0.54
2:B:28:PHE:CD2	2:B:190:THR:HA	2.41	0.54
1:A:204:U:H4'	1:A:216:G:O5'	2.08	0.54
9:I:46:ALA:HB1	9:I:77:ILE:HG21	1.89	0.54
1:A:344:A:H5'	1:A:345:C:C5	2.42	0.54
14:N:3:ARG:HB2	14:N:6:LEU:HB2	1.89	0.54
1:A:690:G:H2'	1:A:691:G:O4'	2.08	0.54
11:K:120:ARG:NH2	11:K:126:ARG:HH12	2.05	0.54
4:D:8:VAL:O	4:D:11:LEU:N	2.39	0.54
19:S:18:LYS:HD3	19:S:31:ILE:HG13	1.90	0.54
1:A:580:U:H2'	1:A:581:G:O4'	2.07	0.54
8:H:123:GLU:O	8:H:127:LEU:HB2	2.08	0.54
16:P:21:VAL:HG21	16:P:59:TRP:CD1	2.42	0.54
7:G:60:LYS:HZ3	7:G:64:GLN:HB2	1.72	0.54
9:I:51:ARG:HG2	9:I:56:LEU:HD11	1.89	0.54
17:Q:83:ASP:OD1	17:Q:84:LEU:N	2.39	0.54
9:I:19:LEU:HD12	9:I:61:ALA:HB2	1.88	0.54
1:A:116:A:H2'	1:A:117:G:H8	1.73	0.54
17:Q:11:VAL:O	17:Q:53:LEU:HD21	2.07	0.54
4:D:200:GLU:OE1	4:D:200:GLU:N	2.33	0.54
14:N:37:PHE:HB3	14:N:39:LEU:HD12	1.90	0.54
7:G:111:ARG:HG2	7:G:112:PRO:HD2	1.89	0.54
1:A:1047:G:C2'	1:A:1048:G:H5'	2.37	0.54
8:H:87:SER:HG	8:H:93:VAL:H	1.52	0.54
7:G:18:TYR:HB3	7:G:59:LEU:HD22	1.90	0.54
5:E:11:ILE:HB	5:E:31:LEU:HB3	1.88	0.54
1:A:309:G:H2'	1:A:310:G:H8	1.72	0.54
1:A:1000:U:C4	1:A:1042:G:C6	2.96	0.54
1:A:758:G:C8	24:A:1967:HOH:O	2.60	0.54
1:A:1028:C:H41	1:A:1033:G:H21	1.55	0.54
1:A:413:G:H8	1:A:428:G:N2	2.04	0.54
1:A:1520[A]:G:H2'	1:A:1521:G:C8	2.42	0.54
1:A:715:A:H2'	1:A:716:A:C8	2.43	0.54
1:A:866:C:H2'	1:A:867:G:O4'	2.08	0.54
10:J:19:SER:HA	10:J:22:LYS:HD2	1.89	0.54
17:Q:60:ILE:O	17:Q:62:SER:OG	2.26	0.54
10:J:79:ARG:O	10:J:83:GLU:N	2.39	0.54
1:A:612:C:H42	1:A:628:G:H1	1.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:80:ILE:HG22	8:H:104:ARG:NH2	2.22	0.54
1:A:1143:G:H2'	1:A:1144:G:C8	2.43	0.54
20:T:73:HIS:HB3	20:T:74:LYS:HG3	1.90	0.54
15:O:62:GLN:O	15:O:65:ARG:N	2.40	0.54
20:T:10:LEU:O	20:T:13:LEU:HB2	2.08	0.54
1:A:179:A:H2'	1:A:180:U:C6	2.42	0.54
1:A:443:C:N3	1:A:491:G:N2	2.51	0.54
1:A:966:M2G:C5	1:A:967:5MC:HM52	2.43	0.54
15:O:4:THR:OG1	15:O:7:GLU:OE2	2.25	0.54
1:A:923:A:OP1	5:E:21:ALA:HB2	2.08	0.53
18:R:65:ILE:O	18:R:69:THR:OG1	2.25	0.53
4:D:20:TYR:HB3	4:D:26:CYS:HB3	1.89	0.53
1:A:628:G:H2'	1:A:629:G:H8	1.71	0.53
1:A:1143:G:H2'	1:A:1144:G:H8	1.73	0.53
1:A:325:A:H2'	1:A:326:G:O4'	2.09	0.53
21:U:25:LYS:HA	21:U:25:LYS:HE3	1.90	0.53
2:B:208:ILE:HA	2:B:211:ILE:HD12	1.89	0.53
12:L:97:ARG:HB2	12:L:98:TYR:CE1	2.42	0.53
15:O:15:PHE:CD2	15:O:30:ALA:HB2	2.43	0.53
9:I:64:THR:OG1	9:I:66:ARG:NH2	2.41	0.53
10:J:49:VAL:HG12	14:N:41:ARG:HG3	1.91	0.53
4:D:108:LEU:HD12	4:D:176:LEU:HD13	1.89	0.53
1:A:60:A:P	1:A:331:G:H22	2.31	0.53
1:A:731:G:OP1	1:A:766:A:H1'	2.07	0.53
18:R:25:THR:O	18:R:26:LEU:HD13	2.08	0.53
1:A:1053:G:H4'	1:A:1054:C:H5'	1.90	0.53
2:B:91:PRO:HG3	2:B:155:LEU:CD2	2.38	0.53
1:A:456:C:H2'	1:A:457:C:C6	2.44	0.53
1:A:444:C:N4	1:A:490:G:H1	2.06	0.53
1:A:1461:G:H2'	1:A:1462:G:H8	1.73	0.53
1:A:170:U:O2'	1:A:171:A:H5'	2.08	0.53
19:S:22:LEU:HD13	19:S:47:HIS:CE1	2.44	0.53
12:L:46:LYS:HE2	12:L:47:LYS:HE3	1.91	0.53
1:A:1422:G:H2'	1:A:1423:G:H8	1.72	0.53
1:A:195:A:H4'	20:T:68:LYS:NZ	2.23	0.53
6:F:91:VAL:HG12	6:F:92:LYS:O	2.08	0.53
1:A:232:G:H1'	1:A:262:A:N1	2.23	0.53
1:A:1392:G:N2	1:A:1502:A:H8	2.03	0.53
1:A:1291:G:H4'	9:I:39:GLY:HA3	1.90	0.53
16:P:21:VAL:O	16:P:33:ILE:HG12	2.09	0.53
1:A:1366:C:H2'	1:A:1367:C:C6	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:13:HIS:O	16:P:42:ARG:NH1	2.41	0.53
1:A:1070:U:H2'	1:A:1071:C:C6	2.41	0.53
1:A:569:C:H5"	1:A:570:G:OP1	2.08	0.53
9:I:55:ALA:HA	9:I:58:HIS:HB2	1.90	0.53
1:A:279:A:H5"	1:A:281:G:O4'	2.09	0.53
1:A:407:G:C6	1:A:408:A:C6	2.96	0.53
1:A:1417:G:O3'	1:A:1418:A:H8	1.91	0.53
1:A:579:G:H2'	1:A:580:U:C6	2.43	0.53
1:A:1255:G:O2'	1:A:1258:G:H1'	2.09	0.53
7:G:59:LEU:HD12	7:G:62:PHE:HD1	1.71	0.53
1:A:567:G:H2'	1:A:568:G:O4'	2.08	0.53
1:A:908:A:C2	1:A:909:A:C4	2.96	0.53
1:A:1265:G:C6	1:A:1266:G:C6	2.97	0.53
1:A:758:G:N7	24:A:1967:HOH:O	2.34	0.53
1:A:1327:C:OP2	21:U:12:LYS:NZ	2.42	0.53
1:A:56:U:H2'	1:A:57:G:H8	1.73	0.53
2:B:178:ARG:O	8:H:71:GLY:HA2	2.08	0.53
1:A:268:C:H2'	1:A:269:C:C6	2.44	0.53
1:A:859:A:H2'	1:A:860:A:O4'	2.09	0.53
1:A:748:C:H4'	1:A:749:C:O5'	2.09	0.53
11:K:18:ARG:HB3	11:K:20:TYR:HE1	1.74	0.53
18:R:39:VAL:O	18:R:42:ARG:HB2	2.09	0.53
2:B:189:ASP:CG	2:B:205:ASP:HB3	2.29	0.53
1:A:358:U:H2'	1:A:359:U:C6	2.44	0.53
1:A:627:G:H2'	1:A:628:G:H8	1.74	0.53
1:A:554:C:H2'	1:A:555:C:C6	2.44	0.52
1:A:448:A:P	1:A:485:G:H22	2.31	0.52
1:A:1441:G:H4'	1:A:1442:G:C5	2.43	0.52
12:L:79:GLU:OE2	12:L:80:HIS:N	2.42	0.52
19:S:15:LEU:HD12	19:S:16:LEU:N	2.24	0.52
1:A:969:A:OP1	10:J:55:LYS:NZ	2.40	0.52
14:N:26:ARG:HD2	14:N:47:LEU:HD21	1.91	0.52
13:M:49:THR:HG22	13:M:51:ALA:H	1.74	0.52
1:A:600:C:N4	1:A:638:G:H1	1.97	0.52
15:O:14:GLU:HG3	15:O:15:PHE:CD1	2.44	0.52
8:H:114:THR:HG22	8:H:130:GLY:O	2.10	0.52
17:Q:92:ARG:HH11	17:Q:92:ARG:HB3	1.75	0.52
1:A:1047:G:H2'	1:A:1048:G:H5'	1.92	0.52
15:O:4:THR:H	15:O:7:GLU:CD	2.13	0.52
13:M:39:ILE:HG22	13:M:40:ASN:N	2.24	0.52
1:A:299:G:C6	1:A:300:A:C6	2.97	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:C:H2'	1:A:537:G:H8	1.75	0.52
1:A:757:U:H2'	1:A:758:G:O4'	2.08	0.52
5:E:35:GLY:HA3	5:E:112:LEU:HB3	1.91	0.52
5:E:41:VAL:HG23	5:E:67:VAL:CG1	2.39	0.52
16:P:6:LEU:HD23	16:P:17:TYR:CG	2.44	0.52
1:A:858:G:C6	1:A:869:G:N7	2.77	0.52
5:E:76:ILE:HB	5:E:93:PRO:HB3	1.91	0.52
1:A:793:U:H5"	1:A:794:A:H5"	1.91	0.52
8:H:81:HIS:N	8:H:138:TRP:O	2.40	0.52
1:A:1327:C:P	21:U:12:LYS:HZ1	2.32	0.52
5:E:145:LYS:HG3	8:H:107:LEU:HD21	1.92	0.52
4:D:28:SER:O	4:D:30:LYS:N	2.37	0.52
3:C:95:THR:HG21	3:C:99:VAL:HG13	1.92	0.52
3:C:135:LYS:O	3:C:138:VAL:HB	2.09	0.52
1:A:277:C:H5'	17:Q:68:ARG:NH1	2.25	0.52
1:A:841:U:H3'	1:A:848:C:O4'	2.10	0.52
8:H:1:MET:HG2	8:H:2:LEU:O	2.09	0.52
1:A:953:G:H2'	1:A:954:G:O4'	2.09	0.52
1:A:342:C:H2'	1:A:343:U:O4'	2.10	0.52
4:D:187:ARG:NH2	4:D:188:LEU:HD12	2.24	0.52
2:B:7:VAL:N	2:B:8:LYS:HZ2	2.08	0.52
8:H:87:SER:HA	8:H:93:VAL:HG13	1.92	0.52
17:Q:4:LYS:HG3	17:Q:5:VAL:N	2.24	0.52
14:N:40:CYS:SG	14:N:43:CYS:N	2.67	0.52
1:A:922:G:C2	1:A:1396:A:C6	2.98	0.52
4:D:68:TYR:OH	4:D:98:GLU:OE1	2.24	0.52
6:F:62:TRP:CD1	18:R:35:ARG:CZ	2.93	0.52
1:A:1465:C:H2'	1:A:1466:C:O4'	2.09	0.52
1:A:1181:G:O2'	1:A:1182:G:O5'	2.21	0.52
1:A:421:U:O4	3:C:127:ARG:NH2	2.43	0.52
1:A:986:A:O2'	19:S:55:LYS:O	2.27	0.52
4:D:121:VAL:O	4:D:134:ASP:HA	2.10	0.52
3:C:19:GLU:N	14:N:51:GLY:O	2.43	0.52
2:B:133:LYS:HZ3	2:B:133:LYS:H	1.56	0.52
1:A:344:A:H4'	1:A:345:C:OP2	2.09	0.52
1:A:502:G:H2'	1:A:503:C:O4'	2.09	0.52
1:A:159:G:H21	1:A:161:A:H8	1.57	0.52
1:A:284:G:H2'	1:A:285:G:H8	1.74	0.52
2:B:63:MET:HB3	2:B:225:ALA:HB1	1.91	0.52
4:D:31:CYS:C	4:D:33:MET:H	2.11	0.52
1:A:1399:C:C2	1:A:1401:G:C5	2.98	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1112:C:H42	3:C:178:LEU:H	1.58	0.52
20:T:39:LYS:HG2	20:T:55:ILE:HG21	1.92	0.52
4:D:190:ASP:HB3	4:D:193:ASP:HB2	1.91	0.52
1:A:1201:A:H4'	1:A:1202:G:H5"	1.92	0.52
2:B:15:VAL:HG11	2:B:213:LEU:HD22	1.92	0.52
3:C:116:VAL:HG21	3:C:202:ILE:HD11	1.92	0.52
1:A:1342:C:H2'	1:A:1343:G:C8	2.44	0.52
12:L:86:ARG:HH11	12:L:86:ARG:HG2	1.74	0.52
8:H:46:LYS:HG2	8:H:64:LYS:HG3	1.92	0.52
19:S:30:LEU:HD22	19:S:48:THR:HB	1.92	0.51
1:A:79:G:C6	1:A:80:G:N7	2.78	0.51
1:A:1053:G:HO2'	1:A:1199:U:H5	1.58	0.51
1:A:1141:C:H2'	1:A:1142:G:C8	2.43	0.51
20:T:81:LYS:O	20:T:85:MET:HG3	2.10	0.51
3:C:11:ARG:NH1	3:C:178:LEU:HA	2.24	0.51
1:A:1424:C:H2'	1:A:1425:U:H6	1.74	0.51
1:A:183:G:H21	1:A:223:U:HO2'	1.57	0.51
1:A:1078:U:H5"	1:A:1079:G:OP2	2.10	0.51
13:M:19:LEU:HD11	13:M:56:LEU:HD11	1.91	0.51
3:C:24:ALA:HB3	3:C:29:TYR:CD1	2.45	0.51
1:A:1484:C:H2'	1:A:1485:U:C6	2.45	0.51
2:B:31:TYR:HD2	2:B:31:TYR:N	2.08	0.51
1:A:438:G:H4'	4:D:123:HIS:CD2	2.46	0.51
5:E:12:LEU:HD13	5:E:31:LEU:HB2	1.91	0.51
6:F:28:ARG:O	6:F:32:ASN:HB2	2.10	0.51
1:A:689:C:O2'	1:A:705:U:O2'	2.24	0.51
6:F:98:LEU:HB2	6:F:101:ALA:HB2	1.92	0.51
12:L:111:LYS:H	12:L:111:LYS:HZ2	1.56	0.51
1:A:853:G:O2'	1:A:854:G:H5'	2.10	0.51
5:E:110:LEU:HD13	5:E:118:ILE:HD13	1.92	0.51
1:A:1382:C:H2'	1:A:1383:C:C6	2.45	0.51
1:A:677:U:H2'	1:A:678:U:H6	1.76	0.51
1:A:1415:G:H1	1:A:1485:U:H3	1.58	0.51
12:L:25:PRO:C	12:L:27:LEU:HB2	2.30	0.51
9:I:10:ARG:HE	9:I:11:LYS:HG3	1.76	0.51
1:A:1255:G:C6	1:A:1279:A:N7	2.78	0.51
7:G:17:VAL:HG12	7:G:18:TYR:CD1	2.44	0.51
21:U:5:ASP:O	21:U:11:GLY:HA3	2.09	0.51
4:D:148:VAL:HG12	4:D:153:ARG:NH1	2.24	0.51
1:A:1490:U:O2'	1:A:1491:G:H5'	2.10	0.51
1:A:1065:U:H5"	1:A:1190:G:H22	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:55:GLY:O	15:O:59:MET:HG2	2.10	0.51
4:D:8:VAL:HG11	4:D:21:LEU:HB3	1.91	0.51
3:C:202:ILE:HG22	3:C:204:LEU:HD23	1.93	0.51
1:A:1342:C:H2'	1:A:1343:G:H8	1.74	0.51
1:A:935:A:H2'	1:A:936:C:O4'	2.10	0.51
1:A:1181:G:N3	1:A:1182:G:N1	2.59	0.51
19:S:64:GLU:HG3	19:S:65:ASN:H	1.76	0.51
1:A:1411:C:H2'	1:A:1412:C:C6	2.46	0.51
18:R:21:LYS:HE3	18:R:54:ARG:O	2.11	0.51
12:L:46:LYS:HG3	12:L:92:0TD:O	2.10	0.51
1:A:183:G:N2	1:A:223:U:O2'	2.31	0.51
1:A:1181:G:C2	1:A:1182:G:N1	2.79	0.51
1:A:924:C:O2'	1:A:1502:A:N6	2.43	0.51
1:A:1265:G:H1	1:A:1270:C:H42	1.57	0.51
1:A:858:G:O6	1:A:869:G:C8	2.63	0.51
1:A:1498:UR3:O4'	1:A:1519[A]:MA6:H2	2.11	0.51
1:A:539:A:H2'	1:A:540:G:H8	1.75	0.51
8:H:43:GLY:O	8:H:64:LYS:NZ	2.41	0.51
1:A:736:C:H2'	1:A:737:A:C8	2.46	0.51
1:A:1242:C:H42	1:A:1295:G:H1	1.59	0.51
1:A:98:U:H2'	1:A:99:C:C6	2.46	0.51
6:F:62:TRP:CH2	6:F:64:GLN:HB2	2.46	0.51
19:S:74:PHE:N	19:S:74:PHE:CD1	2.79	0.51
1:A:1157:A:N7	1:A:1180:A:N6	2.59	0.50
2:B:157:ARG:HG3	2:B:158:LEU:O	2.11	0.50
3:C:180:ALA:HB3	3:C:182:ILE:HG13	1.92	0.50
1:A:1096:C:H2'	1:A:1097:C:H6	1.76	0.50
3:C:3:ASN:N	3:C:3:ASN:OD1	2.42	0.50
1:A:1101:A:H4'	1:A:1102:A:O5'	2.10	0.50
1:A:1171:G:H2'	1:A:1172:C:C6	2.46	0.50
2:B:21:ARG:HA	2:B:39:ILE:HA	1.94	0.50
10:J:92:THR:C	10:J:94:VAL:H	2.14	0.50
3:C:46:GLU:OE1	3:C:87:LEU:HD22	2.11	0.50
20:T:45:GLN:HG2	20:T:91:LEU:HD11	1.93	0.50
15:O:56:LEU:HD13	15:O:56:LEU:C	2.32	0.50
1:A:1152:A:H2'	1:A:1153:C:O4'	2.11	0.50
1:A:660:G:C2	1:A:746:A:C2	3.00	0.50
15:O:18:PHE:CE1	15:O:21:ASP:HB2	2.46	0.50
1:A:113:G:H2'	1:A:114:U:C6	2.47	0.50
1:A:1328:C:OP1	21:U:21:TYR:OH	2.17	0.50
1:A:131:C:H2'	1:A:132:C:C6	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:43:LEU:HD11	5:E:132:ALA:HB1	1.93	0.50
7:G:50:ILE:HG21	7:G:58:PRO:HA	1.93	0.50
1:A:1404:5MC:HN41	1:A:1497:G:H1	1.60	0.50
1:A:264:U:H4'	17:Q:63:ARG:HD3	1.94	0.50
1:A:448:A:C4	1:A:487:A:C2	3.00	0.50
1:A:566:G:H4'	1:A:567:G:OP1	2.11	0.50
9:I:113:LYS:H	9:I:119:ALA:HA	1.77	0.50
10:J:40:LEU:HB2	10:J:69:ASN:O	2.11	0.50
1:A:927:G:H1	1:A:1390:U:H3	1.59	0.50
1:A:744:C:H4'	1:A:852:G:O2'	2.11	0.50
1:A:926:G:N2	1:A:1542:U:OP1	2.45	0.50
1:A:243:A:C2	1:A:246:A:C8	2.99	0.50
6:F:4:TYR:CZ	6:F:72:VAL:HG21	2.47	0.50
1:A:1241:G:H2'	1:A:1242:C:H6	1.76	0.50
1:A:1330:U:H2'	1:A:1331:G:H5'	1.94	0.50
1:A:1525:G:H2'	1:A:1526:G:O4'	2.11	0.50
4:D:206:PHE:HD2	4:D:207:TYR:CE2	2.30	0.50
4:D:57:ARG:HA	4:D:202:LEU:HD12	1.93	0.50
20:T:53:LEU:HD12	20:T:102:GLY:H	1.76	0.50
1:A:1391:U:H2'	1:A:1392:G:C8	2.47	0.50
1:A:1240:U:C2	7:G:32:ARG:HD2	2.46	0.50
2:B:19:HIS:CE1	2:B:205:ASP:H	2.29	0.50
1:A:448:A:OP2	1:A:485:G:N2	2.42	0.50
8:H:134:ILE:HD12	8:H:134:ILE:H	1.77	0.50
1:A:1296:C:H3'	1:A:1297:C:H6	1.76	0.50
1:A:895:G:H2'	1:A:896:C:H6	1.76	0.50
20:T:71:THR:O	20:T:72:LEU:HD23	2.12	0.50
15:O:74:ASP:HB3	15:O:77:ARG:HG3	1.94	0.50
1:A:190(C):C:H2'	1:A:190(D):U:O4'	2.12	0.50
3:C:91:LEU:O	3:C:95:THR:HG22	2.11	0.50
9:I:48:GLU:N	9:I:49:PRO:HD2	2.27	0.50
4:D:22:LYS:HB2	4:D:26:CYS:HB2	1.94	0.50
12:L:59:ARG:NH2	12:L:65:GLU:HG2	2.26	0.50
1:A:619:U:N3	4:D:134:ASP:OD2	2.38	0.50
1:A:981:U:H3'	1:A:982:U:H6	1.77	0.50
1:A:190(L):U:H3	20:T:105:SER:HB3	1.77	0.50
19:S:49:ILE:HB	19:S:60:VAL:HG23	1.93	0.50
3:C:83:ARG:O	3:C:87:LEU:HG	2.12	0.50
10:J:42:THR:HB	10:J:68:HIS:HB3	1.94	0.50
2:B:16:HIS:HB2	2:B:210:SER:HB3	1.93	0.50
1:A:794:A:C5	1:A:795:C:C4	2.99	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:627:G:H2'	1:A:628:G:C8	2.47	0.50
1:A:1201:A:H4'	1:A:1202:G:O5'	2.11	0.50
1:A:1232:U:OP1	9:I:126:SER:HB2	2.12	0.50
1:A:784:C:H2'	1:A:785:G:O4'	2.11	0.50
11:K:59:TYR:CE2	11:K:63:LEU:HD11	2.47	0.50
18:R:50:ILE:HG12	18:R:70:ILE:HD13	1.93	0.50
5:E:122:GLU:OE1	5:E:131:ILE:HG13	2.12	0.50
9:I:8:GLY:HA2	9:I:79:LEU:HD12	1.93	0.50
10:J:62:HIS:O	14:N:59:ALA:HB3	2.12	0.50
1:A:812:C:OP1	1:A:903:G:H1'	2.12	0.50
1:A:279:A:OP1	1:A:280:C:O2'	2.23	0.50
1:A:665:A:C2	1:A:732:C:C2	3.00	0.50
2:B:24:TRP:HZ3	2:B:29:ALA:HB2	1.77	0.49
1:A:130:A:O2'	1:A:131:C:H5"	2.12	0.49
1:A:376:G:H5"	16:P:5:ARG:HD2	1.93	0.49
13:M:82:MET:CE	13:M:93:ARG:HH22	2.25	0.49
13:M:107:ALA:HB3	13:M:111:LYS:HE3	1.95	0.49
1:A:945:G:C2	1:A:1337:G:C2	3.00	0.49
9:I:93:ARG:HB3	9:I:93:ARG:HH11	1.76	0.49
1:A:1355:G:H2'	1:A:1356:G:H8	1.76	0.49
17:Q:81:ARG:HE	17:Q:84:LEU:CD1	2.22	0.49
1:A:1064:G:H1'	1:A:1190:G:N2	2.27	0.49
20:T:84:LEU:HA	20:T:87:LYS:HE2	1.94	0.49
4:D:107:ARG:HD2	4:D:173:TRP:HZ2	1.76	0.49
6:F:33:TYR:CG	6:F:75:LEU:HD23	2.47	0.49
11:K:98:LEU:O	11:K:101:SER:OG	2.17	0.49
1:A:672:U:O2'	1:A:673:G:H5'	2.12	0.49
13:M:23:TYR:HE2	13:M:70:LEU:HD12	1.73	0.49
17:Q:22:LEU:HD12	17:Q:40:LYS:O	2.13	0.49
10:J:7:LYS:HA	10:J:71:LEU:HD11	1.95	0.49
1:A:393:A:H2'	1:A:394:G:H8	1.78	0.49
13:M:97:PRO:HA	13:M:110:ARG:HH11	1.77	0.49
7:G:28:ASN:O	7:G:31:MET:HB3	2.12	0.49
1:A:1490:U:H2'	1:A:1491:G:C8	2.24	0.49
8:H:118:VAL:O	8:H:119:LEU:HD23	2.12	0.49
2:B:189:ASP:OD1	2:B:189:ASP:N	2.45	0.49
8:H:104:ARG:HD2	8:H:138:TRP:CG	2.48	0.49
12:L:90:VAL:HG21	12:L:93:LEU:HD12	1.93	0.49
1:A:1003:G:H2'	1:A:1003(A):G:H5"	1.95	0.49
1:A:1163:C:H2'	1:A:1164:G:C8	2.47	0.49
9:I:103:THR:HG22	9:I:104:ARG:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:16:HIS:HB3	2:B:210:SER:HB3	1.94	0.49
16:P:74:LEU:O	16:P:79:VAL:HG23	2.13	0.49
1:A:714:G:H2'	1:A:715:A:C8	2.48	0.49
17:Q:92:ARG:HB3	17:Q:92:ARG:NH1	2.28	0.49
1:A:410:G:N1	1:A:431:A:OP2	2.40	0.49
3:C:91:LEU:HD23	3:C:92:ALA:N	2.28	0.49
9:I:48:GLU:HB3	9:I:101:PHE:CZ	2.47	0.49
1:A:793:U:H4'	1:A:794:A:OP2	2.12	0.49
1:A:517:G:N1	1:A:533:A:OP2	2.34	0.49
1:A:1202:G:H1'	14:N:42:ILE:HD12	1.93	0.49
1:A:1443:G:H5'	1:A:1446:A:H5"	1.93	0.49
7:G:146:GLU:HA	7:G:149:ARG:HB2	1.95	0.49
16:P:53:VAL:O	16:P:55:ARG:N	2.46	0.49
2:B:131:PRO:HB2	2:B:134:GLU:HG3	1.95	0.49
1:A:767:A:H2'	1:A:768:A:O4'	2.13	0.49
16:P:28:ARG:HB3	16:P:29:ASP:OD2	2.12	0.49
1:A:1309:G:O2'	13:M:74:VAL:HG23	2.12	0.49
9:I:118:LYS:C	9:I:120:ARG:H	2.15	0.49
1:A:187:C:OP1	20:T:82:SER:OG	2.26	0.49
10:J:24:VAL:HG23	10:J:34:VAL:HG11	1.93	0.49
1:A:1228:C:H5'	13:M:115:LYS:O	2.13	0.49
1:A:564:C:O2'	8:H:91:ARG:NH2	2.42	0.49
11:K:43:SER:HB3	11:K:68:ALA:HB2	1.94	0.49
1:A:256:U:H2'	1:A:257:G:C8	2.48	0.49
17:Q:67:LYS:O	17:Q:69:LYS:N	2.46	0.49
1:A:1279:A:OP1	10:J:7:LYS:NZ	2.40	0.49
9:I:19:LEU:HD11	9:I:59:PHE:HB3	1.95	0.49
9:I:50:LEU:HB3	9:I:55:ALA:HB3	1.94	0.49
8:H:36:LEU:O	8:H:37:ARG:C	2.51	0.49
3:C:19:GLU:OE1	3:C:54:ARG:NH2	2.45	0.49
1:A:1124:G:H2'	1:A:1145:C:H41	1.77	0.49
5:E:145:LYS:O	5:E:148:VAL:HG23	2.13	0.49
1:A:420:U:H3'	1:A:422:C:N4	2.27	0.49
1:A:781:A:C5	1:A:802:A:C2	3.00	0.49
1:A:1136:U:H5"	1:A:1137:C:C4	2.48	0.49
1:A:1027:C:H2'	1:A:1034:G:H22	1.76	0.49
1:A:229:U:O2'	1:A:230:G:H5'	2.13	0.49
9:I:49:PRO:HD3	9:I:101:PHE:CE2	2.48	0.49
1:A:1425:U:H3	1:A:1475:G:H1	1.59	0.49
5:E:80:ILE:HD11	5:E:138:ALA:HB1	1.95	0.49
4:D:64:LEU:HG	4:D:198:VAL:HG11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:78:TYR:O	15:O:81:LEU:N	2.46	0.49
1:A:815:A:N3	1:A:1527:C:O2'	2.42	0.49
1:A:192:U:O4'	20:T:103:GLY:HA2	2.13	0.49
1:A:803:G:C6	1:A:804:U:C4	3.00	0.49
4:D:179:GLU:OE2	4:D:179:GLU:N	2.34	0.49
1:A:1486:G:C2	1:A:1487:G:C4	3.01	0.49
1:A:967:5MC:O2'	9:I:128:ARG:NH1	2.46	0.49
11:K:40:ILE:HG22	11:K:41:THR:HG22	1.94	0.49
2:B:175:ARG:NH1	2:B:175:ARG:HG3	2.27	0.49
1:A:538:G:H5"	12:L:115:LYS:HG3	1.94	0.49
1:A:113:G:H2'	1:A:114:U:H6	1.78	0.49
1:A:927:G:H4'	1:A:1503:A:C8	2.48	0.49
16:P:53:VAL:O	16:P:56:ALA:N	2.46	0.49
10:J:5:ARG:HB3	10:J:99:LYS:O	2.13	0.49
11:K:117:ASN:N	11:K:117:ASN:OD1	2.43	0.49
1:A:45:U:H2'	1:A:46:G:C8	2.47	0.49
10:J:12:ASP:O	10:J:15:THR:HB	2.13	0.49
9:I:11:LYS:HB3	9:I:11:LYS:HZ2	1.77	0.48
1:A:243:A:H2	1:A:245:C:H2'	1.78	0.48
1:A:279:A:C8	1:A:279:A:H5'	2.48	0.48
21:U:12:LYS:HG3	21:U:17:THR:OG1	2.12	0.48
12:L:41:ARG:NH2	12:L:43:VAL:HG12	2.28	0.48
1:A:518:C:H1'	12:L:50:SER:HB3	1.95	0.48
8:H:9:MET:HE1	8:H:35:ILE:HG21	1.94	0.48
1:A:1149:C:O2'	1:A:1280:A:N1	2.42	0.48
12:L:76:ASN:ND2	12:L:77:LEU:HD23	2.28	0.48
1:A:75:G:C6	1:A:76:C:C4	3.01	0.48
1:A:950:U:H2'	1:A:951:G:C8	2.48	0.48
1:A:97:G:H2'	1:A:98:U:O4'	2.14	0.48
18:R:55:ARG:HB3	18:R:55:ARG:HH11	1.77	0.48
1:A:429:U:P	4:D:36:ARG:HH12	2.36	0.48
2:B:135:GLN:O	2:B:139:LYS:HB2	2.13	0.48
10:J:42:THR:HB	10:J:68:HIS:HA	1.95	0.48
3:C:81:GLY:O	3:C:84:ILE:HG22	2.13	0.48
1:A:824:C:H2'	1:A:825:G:C8	2.48	0.48
1:A:794:A:H2'	1:A:795:C:C6	2.48	0.48
1:A:1227:A:N7	19:S:81:ARG:NH2	2.57	0.48
5:E:103:GLY:HA3	5:E:106:PRO:HD2	1.95	0.48
1:A:603:U:H3	1:A:635:G:H1	1.61	0.48
1:A:1358:U:O3'	14:N:35:ARG:HD2	2.13	0.48
15:O:85:LEU:HD23	15:O:85:LEU:HA	1.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:765:G:C6	1:A:812:C:C2	3.01	0.48
11:K:33:THR:HA	11:K:39:PRO:HA	1.96	0.48
12:L:48:PRO:HD2	12:L:92:0TD:CSB	2.43	0.48
2:B:18:GLY:HA3	2:B:41:ILE:HA	1.95	0.48
1:A:860:A:N6	1:A:861:G:C2	2.82	0.48
15:O:70:LEU:HD13	15:O:78:TYR:HA	1.96	0.48
2:B:31:TYR:CD2	2:B:31:TYR:N	2.80	0.48
1:A:77:G:H2'	1:A:78:G:C8	2.48	0.48
1:A:950:U:H2'	1:A:951:G:H8	1.78	0.48
1:A:463:A:H2'	1:A:474:G:O4'	2.14	0.48
6:F:4:TYR:CE2	6:F:72:VAL:HG21	2.48	0.48
3:C:39:ILE:O	3:C:43:LEU:HB2	2.13	0.48
1:A:109:A:C6	1:A:326:G:C6	3.01	0.48
11:K:98:LEU:HD23	11:K:98:LEU:HA	1.56	0.48
1:A:1148:U:H4'	9:I:14:VAL:HG11	1.95	0.48
1:A:247:G:OP2	17:Q:99:SER:HB2	2.13	0.48
1:A:1026:G:H3'	1:A:1027:C:C6	2.48	0.48
1:A:90:U:O2'	1:A:91:C:O5'	2.24	0.48
1:A:1310:G:N2	1:A:1328:C:N3	2.61	0.48
1:A:984:C:H2'	1:A:985:C:C6	2.49	0.48
1:A:255:G:C2	1:A:272:C:C2	3.02	0.48
4:D:111:ALA:HB3	4:D:117:ALA:HB2	1.96	0.48
1:A:1010:G:H1	1:A:1019:C:H42	1.61	0.48
13:M:56:LEU:O	13:M:60:VAL:HG23	2.12	0.48
1:A:11:G:C5	1:A:12:U:C5	3.02	0.48
5:E:83:GLU:HG3	5:E:88:LYS:HB2	1.94	0.48
1:A:1416:G:C2'	1:A:1417:G:H5'	2.43	0.48
1:A:1310:G:P	13:M:77:ASN:HD21	2.36	0.48
3:C:88:ARG:O	3:C:91:LEU:HB3	2.14	0.48
1:A:1086:U:H3	1:A:1099:G:H22	1.61	0.48
1:A:1493:A:O3'	1:A:1494:G:H8	1.97	0.48
1:A:255:G:P	17:Q:69:LYS:HZ1	2.37	0.48
12:L:113:ARG:NH2	12:L:120:TYR:HE1	2.12	0.48
1:A:571:U:H5"	1:A:572:A:OP2	2.14	0.48
9:I:97:LYS:HD2	9:I:102:LEU:HD11	1.95	0.48
18:R:38:GLU:HA	18:R:41:LYS:HE3	1.96	0.48
7:G:84:ASN:O	7:G:85:TYR:HD2	1.97	0.48
1:A:671:G:H5'	6:F:77:ARG:HH21	1.78	0.48
1:A:985:C:N4	1:A:1220:G:H1	2.11	0.48
8:H:6:ILE:HG13	8:H:31:PHE:CE2	2.49	0.48
9:I:104:ARG:CD	9:I:105:ASP:H	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:80:ILE:CD1	2:B:212:GLN:HG2	2.43	0.48
1:A:1373:G:H5"	7:G:36:LYS:HE2	1.95	0.48
1:A:828:A:H3'	1:A:828:A:C8	2.49	0.48
1:A:176:C:H2'	1:A:177:C:H6	1.79	0.48
1:A:1216:G:OP2	14:N:3:ARG:NH1	2.47	0.48
3:C:116:VAL:O	3:C:120:VAL:HG23	2.13	0.48
11:K:73:MET:CG	11:K:103:LEU:HD21	2.44	0.48
16:P:18:ARG:O	16:P:20:VAL:HG13	2.13	0.48
1:A:17:U:H2'	1:A:18:C:C6	2.48	0.48
1:A:1228:C:H4'	13:M:116:THR:HA	1.95	0.48
9:I:51:ARG:HD3	9:I:56:LEU:HD21	1.95	0.48
1:A:501:C:H2'	1:A:502:G:C8	2.49	0.48
1:A:190(D):U:O5'	1:A:190(D):U:H6	1.97	0.47
1:A:1226:C:OP2	13:M:103:THR:HG21	2.13	0.47
3:C:125:GLU:O	3:C:127:ARG:HG3	2.14	0.47
12:L:48:PRO:HD2	12:L:92:0TD:H8	1.94	0.47
1:A:1438:G:H1	1:A:1463:C:H42	1.62	0.47
1:A:164:U:H2'	1:A:165:C:C6	2.49	0.47
10:J:6:ILE:HB	10:J:72:VAL:HB	1.96	0.47
8:H:25:ASP:OD1	8:H:25:ASP:N	2.47	0.47
1:A:77:G:C4	1:A:93:G:N2	2.83	0.47
1:A:95:U:O2'	1:A:96:G:H5'	2.15	0.47
8:H:119:LEU:HD12	8:H:124:ALA:HB2	1.95	0.47
1:A:902:G:H2'	1:A:903:G:C8	2.44	0.47
2:B:180:LEU:HB2	2:B:182:ILE:HG13	1.96	0.47
1:A:983:A:O2'	1:A:1050:G:OP2	2.32	0.47
17:Q:15:MET:HB3	17:Q:18:THR:HB	1.95	0.47
1:A:1267:C:O2	21:U:20:LYS:HD2	2.14	0.47
1:A:1006:C:OP1	1:A:1037:C:O2'	2.32	0.47
1:A:1404:5MC:H1'	1:A:1499:A:C2	2.50	0.47
1:A:1372:U:H5"	9:I:71:SER:HB3	1.96	0.47
6:F:76:ALA:O	6:F:80:ARG:HD3	2.13	0.47
5:E:18:ARG:HE	5:E:18:ARG:HB3	1.40	0.47
1:A:190(J):U:H2'	1:A:190(K):G:C8	2.49	0.47
5:E:144:THR:O	5:E:148:VAL:HG22	2.14	0.47
1:A:809:G:C6	1:A:810:C:C5	3.03	0.47
1:A:349:A:H2'	1:A:350:G:H5"	1.97	0.47
13:M:55:ARG:O	13:M:58:GLU:HB2	2.14	0.47
3:C:130:VAL:O	3:C:134:ILE:HG13	2.13	0.47
7:G:16:LEU:HD11	9:I:42:ARG:HG3	1.96	0.47
1:A:1311:G:C2	1:A:1327:C:N3	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:43:LEU:HD23	5:E:43:LEU:HA	1.64	0.47
1:A:1389:C:H2'	1:A:1390:U:O4'	2.14	0.47
1:A:779:C:H2'	1:A:780:A:O4'	2.13	0.47
13:M:35:GLU:HG3	13:M:36:LYS:N	2.28	0.47
1:A:1454:G:O2'	1:A:1455:G:H5'	2.14	0.47
1:A:562:C:N3	12:L:16:GLU:HG2	2.29	0.47
7:G:115:ARG:HB3	7:G:118:VAL:HG23	1.96	0.47
1:A:35:G:H21	12:L:118:SER:HB3	1.80	0.47
1:A:1401:G:C2	1:A:1402:4OC:H1'	2.49	0.47
1:A:216:G:H2'	1:A:217:C:C6	2.49	0.47
1:A:1532:U:H2'	1:A:1533:C:H5"	1.96	0.47
11:K:124:LYS:HG3	11:K:125:PHE:N	2.29	0.47
1:A:451:A:N7	1:A:481:G:N1	2.62	0.47
7:G:76:ARG:HB2	7:G:89:MET:SD	2.55	0.47
1:A:1309:G:H5'	13:M:78:ILE:HD11	1.97	0.47
17:Q:21:VAL:HG23	17:Q:42:TYR:HB2	1.95	0.47
7:G:108:ALA:O	7:G:119:ARG:HB3	2.15	0.47
1:A:974:A:C8	14:N:31:ARG:HD2	2.49	0.47
16:P:40:ASP:HB3	16:P:48:TRP:HB2	1.96	0.47
1:A:345:C:OP2	1:A:345:C:H6	1.97	0.47
1:A:109:A:C4	1:A:327:A:C2	3.02	0.47
1:A:665:A:N3	1:A:732:C:H2'	2.29	0.47
2:B:131:PRO:HD2	2:B:134:GLU:OE2	2.15	0.47
1:A:509:A:H5'	4:D:55:ALA:HB2	1.96	0.47
2:B:105:PHE:O	2:B:108:ILE:N	2.47	0.47
1:A:1416:G:H2'	1:A:1417:G:H5'	1.96	0.47
1:A:1410:G:H1'	1:A:1491:G:H22	1.79	0.47
1:A:491:G:H2'	1:A:492:G:H8	1.78	0.47
1:A:74:C:C4	1:A:75:G:N7	2.82	0.47
8:H:124:ALA:O	8:H:128:GLY:N	2.27	0.47
1:A:1245:A:H61	1:A:1292:U:H3	1.63	0.47
9:I:89:ASN:HB2	9:I:92:TYR:CD1	2.50	0.47
1:A:116:A:H2'	1:A:117:G:C8	2.49	0.47
8:H:82:HIS:CE1	8:H:138:TRP:CZ2	3.03	0.47
9:I:46:ALA:HB1	9:I:77:ILE:CG2	2.45	0.47
20:T:83:ARG:NH2	24:T:201:HOH:O	2.48	0.47
1:A:434:U:H2'	1:A:435:C:C6	2.49	0.47
12:L:69:TYR:HE2	12:L:71:PRO:HA	1.80	0.47
17:Q:38:ARG:HA	17:Q:38:ARG:HD3	1.46	0.47
11:K:19:ALA:HB2	11:K:80:VAL:HG11	1.96	0.47
4:D:194:LEU:HD13	4:D:194:LEU:HA	1.66	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1499:A:H1'	1:A:1520[A]:G:H5'	1.97	0.47
17:Q:63:ARG:HG2	17:Q:64:PRO:HD2	1.96	0.47
12:L:47:LYS:HD2	12:L:48:PRO:HD3	1.96	0.47
2:B:72:GLY:HA3	2:B:165:VAL:HB	1.97	0.47
5:E:90:VAL:O	5:E:120:THR:HA	2.15	0.47
1:A:176:C:H2'	1:A:177:C:C6	2.49	0.47
1:A:1461:G:H2'	1:A:1462:G:C8	2.50	0.47
11:K:115:PRO:C	11:K:117:ASN:H	2.18	0.47
18:R:40:LEU:HB3	18:R:79:LEU:HD11	1.97	0.47
1:A:92:C:O2	1:A:93:G:C8	2.68	0.47
2:B:9:GLU:OE2	2:B:11:LEU:N	2.47	0.47
1:A:1107:C:OP1	3:C:172:ARG:NH1	2.47	0.47
1:A:1059:C:H2'	1:A:1060:C:C6	2.49	0.47
1:A:19:C:P	5:E:127:ASN:HD22	2.38	0.47
16:P:45:THR:O	16:P:48:TRP:HD1	1.98	0.47
14:N:37:PHE:C	14:N:39:LEU:H	2.17	0.47
1:A:833:U:H2'	1:A:834:C:C6	2.50	0.47
10:J:99:LYS:HD3	10:J:100:THR:H	1.79	0.47
13:M:11:ARG:HD2	13:M:12:ASN:H	1.79	0.47
1:A:227:G:H2'	1:A:228:A:O4'	2.15	0.47
1:A:897:C:H42	1:A:902:G:H1	1.63	0.47
4:D:119:GLN:HG3	4:D:123:HIS:CE1	2.50	0.47
4:D:174:LEU:C	4:D:186:LEU:HD21	2.35	0.47
7:G:143:ARG:O	7:G:147:ALA:HB2	2.14	0.47
1:A:1450:U:O2'	1:A:1451:A:H2'	2.14	0.47
12:L:25:PRO:HA	12:L:27:LEU:HD13	1.98	0.46
1:A:1505:G:H3'	1:A:1505:G:C8	2.49	0.46
1:A:926:G:H2'	1:A:1505:G:N3	2.29	0.46
1:A:259:G:C2	1:A:260:G:C4	3.03	0.46
1:A:457:C:H2'	1:A:458:C:H6	1.80	0.46
2:B:180:LEU:O	2:B:181:PHE:HB2	2.15	0.46
16:P:17:TYR:HB2	16:P:39:TYR:HB3	1.96	0.46
1:A:95:U:H2'	1:A:96:G:C8	2.49	0.46
1:A:7:G:H5'	1:A:298:A:O4'	2.14	0.46
3:C:83:ARG:HG2	3:C:87:LEU:HD21	1.98	0.46
2:B:74:LYS:HZ1	2:B:76:GLN:HG2	1.80	0.46
8:H:104:ARG:NH1	8:H:138:TRP:CE2	2.83	0.46
1:A:892:A:H2'	1:A:893:C:C6	2.50	0.46
9:I:5:TYR:O	9:I:84:ALA:HA	2.16	0.46
9:I:53:VAL:HG21	9:I:85:LEU:HG	1.98	0.46
3:C:175:LEU:HD11	3:C:201:TYR:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:G:H2'	1:A:231:G:O4'	2.15	0.46
1:A:1057:G:H2'	1:A:1058:G:O4'	2.16	0.46
7:G:18:TYR:CE2	7:G:59:LEU:HB2	2.50	0.46
9:I:2:GLU:HG3	9:I:3:GLN:N	2.31	0.46
1:A:1022:G:N2	1:A:1023:G:N7	2.55	0.46
1:A:1144:G:N2	1:A:1145:C:O2	2.48	0.46
20:T:10:LEU:HD22	20:T:10:LEU:HA	1.47	0.46
16:P:6:LEU:HD12	16:P:6:LEU:N	2.30	0.46
1:A:651:C:H2'	1:A:652:U:C6	2.49	0.46
1:A:1480:G:C2	1:A:1481:U:C2	3.03	0.46
10:J:36:GLY:O	10:J:38:ILE:HG13	2.15	0.46
6:F:14:LEU:HD22	6:F:14:LEU:HA	1.73	0.46
1:A:35:G:C6	1:A:36:C:N4	2.83	0.46
1:A:1398:A:H5"	1:A:1401:G:H4'	1.97	0.46
2:B:80:ILE:HG21	2:B:211:ILE:HG22	1.96	0.46
1:A:1223:C:P	19:S:78:ARG:HH21	2.38	0.46
7:G:53:LYS:HE3	7:G:125:MET:HE2	1.96	0.46
12:L:58:VAL:HG12	12:L:59:ARG:O	2.15	0.46
1:A:827:U:H5"	1:A:828:A:OP2	2.14	0.46
2:B:131:PRO:O	2:B:134:GLU:HB2	2.15	0.46
9:I:75:ASP:O	9:I:78:LYS:HG2	2.15	0.46
11:K:58:PRO:O	11:K:61:ALA:HB3	2.15	0.46
15:O:2:PRO:O	15:O:3:ILE:HG13	2.15	0.46
19:S:31:ILE:HG21	19:S:49:ILE:HG23	1.97	0.46
1:A:103:C:O2'	1:A:172:A:N1	2.45	0.46
1:A:1498:UR3:C4'	1:A:1519[A]:MA6:H2	2.45	0.46
13:M:91:ARG:HH22	13:M:103:THR:HG21	1.81	0.46
1:A:1008:C:H42	1:A:1021:G:H1	1.64	0.46
5:E:90:VAL:C	5:E:91:LEU:HD23	2.35	0.46
4:D:78:LEU:HD11	4:D:96:LEU:HB3	1.98	0.46
1:A:446:G:H3'	1:A:447:G:H8	1.80	0.46
8:H:71:GLY:HA3	8:H:72:PRO:HD2	1.67	0.46
3:C:167:TRP:CG	3:C:168:ALA:N	2.84	0.46
19:S:11:VAL:HG12	19:S:15:LEU:HD11	1.98	0.46
1:A:474:G:H2'	1:A:475:G:O4'	2.15	0.46
8:H:114:THR:N	8:H:117:GLY:O	2.42	0.46
1:A:284:G:H2'	1:A:285:G:C8	2.50	0.46
1:A:1304:G:C6	1:A:1305:G:N1	2.83	0.46
1:A:819:A:H4'	1:A:820:U:OP2	2.15	0.46
1:A:54:C:O2'	1:A:55:A:H5"	2.16	0.46
6:F:54:LYS:N	6:F:54:LYS:HD2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:G:C2	1:A:425:G:C5	3.03	0.46
8:H:75:ARG:HA	8:H:76:PRO:HD3	1.61	0.46
1:A:1502:A:H2'	1:A:1504:G:C8	2.50	0.46
1:A:977:A:H2'	1:A:978:A:H5'	1.97	0.46
1:A:216:G:H2'	1:A:217:C:H6	1.80	0.46
1:A:1297:C:O2'	1:A:1298:C:OP2	2.30	0.46
8:H:26:VAL:HG23	8:H:27:PRO:HD2	1.97	0.46
11:K:21:ILE:HD12	11:K:95:ILE:HG12	1.98	0.46
1:A:491:G:H2'	1:A:492:G:C8	2.50	0.46
1:A:1172:C:H2'	1:A:1173:G:H8	1.80	0.46
5:E:98:THR:O	5:E:101:ILE:HD11	2.15	0.46
1:A:1245:A:N1	1:A:1293:G:C2	2.84	0.46
1:A:921:U:H2'	1:A:922:G:O4'	2.16	0.46
1:A:15:G:H4'	5:E:24:ARG:NH2	2.30	0.46
20:T:91:LEU:HD22	20:T:91:LEU:HA	1.74	0.46
9:I:99:LEU:HD22	9:I:99:LEU:H	1.81	0.46
7:G:49:ILE:O	7:G:53:LYS:HB2	2.16	0.46
5:E:121:LYS:HG2	5:E:123:LEU:HD23	1.97	0.46
1:A:948:C:H42	1:A:1233:G:H1	1.64	0.46
1:A:276:G:O2'	17:Q:68:ARG:NH1	2.49	0.46
1:A:792:A:H1'	1:A:793:U:OP2	2.16	0.46
4:D:21:LEU:HA	4:D:21:LEU:HD12	1.70	0.46
10:J:99:LYS:CD	10:J:100:THR:H	2.29	0.46
1:A:1481:U:H2'	1:A:1482:G:O4'	2.15	0.46
1:A:636:U:H2'	1:A:637:G:C8	2.50	0.46
1:A:650:G:H8	1:A:650:G:C5'	2.29	0.46
1:A:583:A:H2'	1:A:584:G:O4'	2.16	0.46
1:A:1392:G:O2'	1:A:1393:U:H5'	2.16	0.46
2:B:144:ARG:NH1	2:B:148:TYR:OH	2.49	0.46
1:A:243:A:C2	1:A:245:C:H2'	2.51	0.46
1:A:1321:C:O2'	19:S:78:ARG:NH1	2.49	0.46
8:H:104:ARG:HD2	8:H:138:TRP:CD1	2.50	0.46
1:A:509:A:H3'	1:A:509:A:C8	2.51	0.46
1:A:14:U:O2	1:A:16:A:C8	2.69	0.46
13:M:2:ALA:N	13:M:9:ILE:HG23	2.31	0.46
1:A:1416:G:N2	1:A:1485:U:H1'	2.31	0.46
7:G:108:ALA:HB2	7:G:123:GLU:HG2	1.98	0.46
11:K:72:ALA:HB1	11:K:77:MET:CG	2.45	0.46
1:A:945:G:H2'	1:A:945:G:N3	2.31	0.46
8:H:102:ARG:HG3	8:H:102:ARG:O	2.16	0.46
1:A:134:A:C6	1:A:135:C:N3	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1418:A:OP2	1:A:1418:A:H3'	2.15	0.45
19:S:19:VAL:HA	19:S:22:LEU:HB2	1.98	0.45
14:N:24:CYS:CB	14:N:40:CYS:HB3	2.45	0.45
7:G:22:LEU:HD23	7:G:62:PHE:CZ	2.52	0.45
1:A:474:G:H4'	16:P:81:ARG:CZ	2.46	0.45
1:A:1020:U:H2'	1:A:1021:G:H8	1.82	0.45
2:B:24:TRP:CG	2:B:25:ASN:N	2.84	0.45
3:C:156:ARG:H	3:C:163:ALA:HA	1.81	0.45
4:D:111:ALA:HA	4:D:161:ASN:ND2	2.30	0.45
3:C:10:PHE:CZ	3:C:178:LEU:HD12	2.51	0.45
17:Q:95:TYR:HA	17:Q:98:LEU:HD11	1.97	0.45
3:C:40:ARG:HE	3:C:57:ILE:HD12	1.81	0.45
1:A:644:G:C5	1:A:645:C:C5	3.04	0.45
1:A:293:G:C6	1:A:294:U:C4	3.03	0.45
7:G:26:PHE:HD1	7:G:101:LEU:HD23	1.81	0.45
5:E:40:ARG:HH11	5:E:40:ARG:HG2	1.81	0.45
17:Q:58:GLU:O	17:Q:59:ILE:HD13	2.15	0.45
10:J:18:ALA:O	10:J:22:LYS:HG3	2.16	0.45
15:O:4:THR:H	15:O:4:THR:HG1	1.46	0.45
2:B:74:LYS:HZ2	2:B:76:GLN:H	1.64	0.45
16:P:53:VAL:O	16:P:54:GLU:C	2.53	0.45
8:H:102:ARG:HH11	8:H:105:ARG:HD3	1.82	0.45
16:P:58:TYR:O	16:P:61:SER:HB3	2.16	0.45
4:D:113:SER:OG	4:D:114:ARG:N	2.49	0.45
1:A:666:G:H5'	1:A:726:C:H1'	1.97	0.45
1:A:836:G:C6	1:A:851:G:C6	3.04	0.45
2:B:187:LEU:HD22	2:B:187:LEU:HA	1.40	0.45
3:C:51:GLY:O	3:C:71:ALA:N	2.39	0.45
1:A:136:C:H2'	1:A:137:C:H6	1.82	0.45
14:N:8:GLU:O	14:N:12:ARG:N	2.50	0.45
7:G:18:TYR:CD2	7:G:59:LEU:HD13	2.46	0.45
9:I:105:ASP:OD1	9:I:107:ARG:HG3	2.17	0.45
1:A:1406:U:O2'	1:A:1517[B]:G:N2	2.50	0.45
1:A:1074:G:C4'	2:B:104:ASN:HB2	2.47	0.45
8:H:100:ILE:HA	8:H:101:PRO:HD3	1.50	0.45
7:G:28:ASN:HA	7:G:31:MET:HE2	1.97	0.45
1:A:1148:U:H2'	1:A:1149:C:O4'	2.17	0.45
1:A:11:G:H2'	1:A:12:U:H6	1.80	0.45
1:A:882:C:O2'	1:A:883:C:H5'	2.17	0.45
1:A:27:G:H1	1:A:556:C:N4	2.15	0.45
20:T:41:ILE:HA	20:T:41:ILE:HD12	1.73	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1368:G:OP2	9:I:112:LYS:NZ	2.33	0.45
1:A:228:A:H2'	1:A:229:U:C6	2.51	0.45
12:L:120:TYR:CD2	12:L:120:TYR:N	2.84	0.45
14:N:54:PRO:O	14:N:56:VAL:HG23	2.16	0.45
2:B:74:LYS:NZ	2:B:76:GLN:H	2.15	0.45
1:A:447:G:H2'	1:A:485:G:N2	2.31	0.45
1:A:485:G:O2'	1:A:486:U:P	2.75	0.45
15:O:53:HIS:O	15:O:56:LEU:HB3	2.16	0.45
1:A:1130:A:H4'	9:I:20:ARG:HH21	1.81	0.45
17:Q:29:HIS:CE1	17:Q:32:TYR:H	2.33	0.45
1:A:1096:C:H2'	1:A:1097:C:C6	2.51	0.45
1:A:376:G:N3	1:A:389:A:C2	2.85	0.45
1:A:1088:G:C6	1:A:1089:G:C5	3.05	0.45
1:A:1001:A:N6	1:A:1041:A:H61	2.14	0.45
1:A:1181:G:HO2'	1:A:1182:G:P	2.36	0.45
18:R:25:THR:OG1	18:R:42:ARG:NH1	2.49	0.45
1:A:1400:5MC:H3'	1:A:1401:G:H5'	1.99	0.45
2:B:95:GLN:NE2	2:B:147:LYS:HE3	2.31	0.45
9:I:89:ASN:HB3	9:I:91:ASP:OD1	2.16	0.45
1:A:563:A:H2'	1:A:567:G:C8	2.51	0.45
11:K:18:ARG:HB3	11:K:20:TYR:CE1	2.51	0.45
19:S:17:GLU:HA	19:S:20:LEU:HD23	1.98	0.45
2:B:48:MET:HA	2:B:51:LEU:HB2	1.97	0.45
3:C:150:LYS:HG3	3:C:173:VAL:HG21	1.98	0.45
17:Q:62:SER:OG	17:Q:72:ARG:HG2	2.16	0.45
7:G:152:ALA:HA	7:G:155:ARG:CZ	2.46	0.45
1:A:1347:G:H1'	1:A:1348:U:H5	1.81	0.45
13:M:79:LYS:HB2	13:M:79:LYS:NZ	2.32	0.45
18:R:43:PHE:C	18:R:44:LEU:HD23	2.37	0.45
1:A:391:G:C6	1:A:392:G:C5	3.05	0.45
1:A:420:U:H3'	1:A:422:C:H41	1.81	0.45
7:G:86:GLN:HB2	7:G:148:ASN:HD22	1.81	0.45
1:A:118:U:H3'	1:A:288:A:H61	1.82	0.45
15:O:5:LYS:HE2	15:O:5:LYS:HB2	1.76	0.45
7:G:12:LEU:HG	7:G:12:LEU:H	1.60	0.45
13:M:45:VAL:O	13:M:48:LEU:HD23	2.17	0.45
1:A:1171:G:H2'	1:A:1172:C:H6	1.81	0.45
2:B:97:TRP:CZ2	2:B:102:LEU:HD13	2.40	0.45
1:A:739:C:OP2	6:F:2:ARG:NH2	2.49	0.45
1:A:521:G:P	12:L:54:LYS:HE2	2.57	0.45
3:C:121:ALA:O	3:C:124:ILE:HB	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:40:ILE:HG23	11:K:75:TYR:CD1	2.44	0.45
15:O:56:LEU:O	15:O:60:VAL:HG12	2.17	0.45
5:E:109:ILE:HG22	5:E:110:LEU:N	2.31	0.45
1:A:1184:G:H2'	1:A:1185:G:H8	1.80	0.45
10:J:3:LYS:NZ	10:J:3:LYS:HB2	2.32	0.45
1:A:1028:C:N4	1:A:1033:G:H21	2.14	0.45
1:A:1064:G:H22	1:A:1190:G:H2'	1.79	0.45
13:M:99:ARG:NH1	19:S:2:PRO:HG3	2.32	0.45
15:O:29:VAL:O	15:O:33:THR:HB	2.17	0.45
3:C:77:ILE:HG12	3:C:84:ILE:HD12	1.99	0.45
1:A:115:G:O2'	1:A:116:A:OP2	2.26	0.45
4:D:187:ARG:HD2	4:D:187:ARG:HA	1.33	0.45
14:N:57:ARG:HB2	14:N:57:ARG:NH1	2.32	0.45
2:B:217:ARG:HA	2:B:217:ARG:HD3	1.52	0.45
5:E:142:LEU:HA	5:E:142:LEU:HD23	1.70	0.45
1:A:1412:C:H2'	1:A:1413:A:H8	1.82	0.45
1:A:959:A:O2'	1:A:984:C:O2'	2.32	0.45
4:D:119:GLN:NE2	4:D:123:HIS:HE1	2.11	0.45
10:J:71:LEU:HA	10:J:71:LEU:HD12	1.80	0.45
2:B:84:GLU:OE1	2:B:216:SER:HA	2.17	0.45
1:A:222:U:H2'	1:A:223:U:C6	2.51	0.45
19:S:30:LEU:HD13	19:S:48:THR:O	2.16	0.44
1:A:76:C:N4	1:A:93:G:H1	2.16	0.44
1:A:411:A:C8	1:A:413:G:H1'	2.52	0.44
1:A:1278:U:H5"	1:A:1279:A:H5'	1.99	0.44
1:A:569:C:N4	1:A:881:G:H1	2.12	0.44
5:E:19:MET:SD	5:E:24:ARG:HB3	2.57	0.44
8:H:2:LEU:HD23	8:H:2:LEU:HA	1.46	0.44
1:A:1236:A:H4'	1:A:1304:G:H4'	1.99	0.44
1:A:122:G:C2	1:A:123:C:C2	3.04	0.44
15:O:12:ILE:HG23	15:O:27:VAL:HG11	1.99	0.44
8:H:95:VAL:HG23	8:H:131:GLY:O	2.17	0.44
19:S:30:LEU:HB3	19:S:31:ILE:H	1.53	0.44
6:F:22:GLU:OE2	6:F:82:ARG:HG2	2.17	0.44
1:A:429:U:H1'	1:A:430:A:H5"	1.99	0.44
8:H:6:ILE:HG13	8:H:31:PHE:HE2	1.82	0.44
1:A:1198:G:H2'	1:A:1199:U:C6	2.52	0.44
10:J:81:THR:O	10:J:85:LEU:HD13	2.17	0.44
1:A:1111:A:H2'	1:A:1112:C:O4'	2.16	0.44
18:R:47:THR:HG22	18:R:48:GLY:N	2.32	0.44
1:A:646:U:H2'	1:A:647:C:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1260:C:O5'	1:A:1284:C:H4'	2.17	0.44
8:H:63:LEU:HD13	8:H:63:LEU:N	2.32	0.44
1:A:1003(A):G:N2	1:A:1006:C:H41	2.16	0.44
5:E:98:THR:HB	5:E:117:ASP:HB3	1.99	0.44
8:H:127:LEU:HA	8:H:127:LEU:HD22	1.77	0.44
1:A:858:G:O6	1:A:869:G:N7	2.50	0.44
1:A:1057:G:C4	1:A:1058:G:C8	3.05	0.44
1:A:991:U:O2	1:A:993:G:H8	2.00	0.44
1:A:684:A:N3	11:K:39:PRO:HD2	2.32	0.44
4:D:15:GLU:OE1	4:D:62:GLN:HB3	2.17	0.44
13:M:39:ILE:CG2	13:M:40:ASN:N	2.80	0.44
3:C:20:SER:OG	3:C:40:ARG:NH2	2.50	0.44
1:A:112:G:O2'	1:A:113:G:H5'	2.17	0.44
1:A:382:A:H2'	1:A:383:A:C8	2.52	0.44
7:G:145:ALA:C	7:G:147:ALA:H	2.20	0.44
3:C:52:LEU:HD23	3:C:69:HIS:O	2.18	0.44
1:A:78:G:N1	1:A:92:C:N4	2.65	0.44
1:A:1225:A:H5"	13:M:103:THR:HG23	1.99	0.44
3:C:88:ARG:HA	3:C:91:LEU:HB3	1.98	0.44
8:H:97:VAL:HG12	8:H:98:LYS:HZ2	1.81	0.44
10:J:63:PHE:HD2	14:N:57:ARG:O	2.01	0.44
1:A:20:U:H2'	1:A:21:G:H5'	1.99	0.44
1:A:1476:G:H2'	1:A:1477:C:C6	2.53	0.44
1:A:455:C:H6	1:A:455:C:O5'	2.01	0.44
5:E:17:ALA:CA	5:E:26:PHE:HB3	2.35	0.44
18:R:40:LEU:HD23	18:R:40:LEU:HA	1.64	0.44
16:P:33:ILE:H	16:P:33:ILE:HG12	1.39	0.44
10:J:79:ARG:NH1	10:J:82:ILE:HG13	2.32	0.44
1:A:1010:G:N2	1:A:1019:C:N3	2.64	0.44
1:A:152:A:N6	1:A:170:U:C2	2.85	0.44
5:E:36:ASP:OD2	5:E:38:GLN:HB2	2.18	0.44
3:C:137:ALA:HA	3:C:140:ARG:HE	1.83	0.44
1:A:1035:A:H2'	1:A:1036:G:C8	2.53	0.44
1:A:346:G:H2'	1:A:347:G:O4'	2.18	0.44
4:D:120:LEU:HD23	4:D:120:LEU:HA	1.68	0.44
12:L:85:ILE:HG23	12:L:98:TYR:HB3	2.00	0.44
4:D:107:ARG:HD2	4:D:173:TRP:CZ2	2.52	0.44
1:A:650:G:H8	1:A:650:G:H5"	1.83	0.44
3:C:73:PRO:HD3	3:C:105:GLU:OE2	2.17	0.44
13:M:108:ARG:HG3	13:M:114:ARG:HH12	1.82	0.44
13:M:108:ARG:HG3	13:M:114:ARG:NH1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1316:G:H4'	14:N:18:VAL:HG11	1.99	0.44
2:B:84:GLU:HG3	2:B:215:LEU:HB3	2.00	0.44
2:B:165:VAL:HG12	2:B:166:ASP:N	2.32	0.44
3:C:43:LEU:HD11	3:C:68:VAL:HG21	2.00	0.44
1:A:1227:A:H2	1:A:1228:C:H1'	1.83	0.44
9:I:51:ARG:HG2	9:I:56:LEU:HD21	2.00	0.44
9:I:111:ARG:O	9:I:119:ALA:HB2	2.17	0.44
1:A:895:G:H2'	1:A:896:C:C6	2.52	0.44
1:A:546:G:OP1	4:D:73:ARG:HG2	2.18	0.44
1:A:1031:G:H2'	1:A:1032:G:H8	1.83	0.44
7:G:48:LYS:HD3	7:G:48:LYS:HA	1.89	0.44
1:A:775:G:H2'	1:A:776:G:O4'	2.16	0.44
1:A:88:A:H2'	1:A:89:C:O4'	2.17	0.44
1:A:130:A:H5'	17:Q:63:ARG:NE	2.29	0.44
10:J:7:LYS:HD3	10:J:9:ARG:HE	1.80	0.44
15:O:39:LEU:HB3	15:O:56:LEU:HD23	1.99	0.44
4:D:31:CYS:SG	4:D:31:CYS:O	2.75	0.44
1:A:1191:A:P	3:C:3:ASN:HD22	2.41	0.44
6:F:75:LEU:O	6:F:79:LEU:HD13	2.17	0.44
1:A:21:G:H2'	1:A:22:G:C8	2.52	0.44
3:C:112:SER:O	3:C:115:LEU:HB2	2.18	0.44
1:A:659:U:OP1	15:O:8:LYS:HD3	2.17	0.44
12:L:124:LYS:HD2	12:L:125:PRO:HD2	1.99	0.44
4:D:112:VAL:HG23	4:D:116:GLN:OE1	2.18	0.44
1:A:824:C:H2'	1:A:825:G:H8	1.81	0.44
1:A:476:G:C5	1:A:477:G:C8	3.06	0.44
4:D:78:LEU:O	4:D:81:GLU:HB3	2.16	0.44
10:J:28:ARG:HG2	10:J:29:ARG:HG2	2.00	0.44
17:Q:29:HIS:HA	17:Q:30:PRO:HD3	1.72	0.44
1:A:1295:G:C6	1:A:1296:C:C4	3.05	0.44
1:A:1454:G:H2'	1:A:1455:G:H8	1.81	0.44
1:A:514:C:H2'	1:A:515:G:H8	1.82	0.44
16:P:71:ARG:HG3	16:P:80:PHE:HE1	1.83	0.44
20:T:50:GLU:HA	20:T:100:ILE:HG13	2.00	0.44
1:A:1355:G:C6	1:A:1368:G:C6	3.06	0.43
1:A:91:C:H5'	1:A:92:C:OP2	2.17	0.43
18:R:53:ARG:HD2	18:R:58:LEU:O	2.17	0.43
3:C:131:ARG:HD2	3:C:131:ARG:H	1.83	0.43
2:B:92:TYR:CE2	2:B:151:GLY:HA3	2.53	0.43
3:C:184:TYR:CE2	3:C:186:PHE:HB2	2.51	0.43
1:A:117:G:P	24:A:1912:HOH:O	2.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:220:ASP:HA	2:B:230:VAL:HG21	2.00	0.43
12:L:7:ILE:O	12:L:8:ASN:C	2.55	0.43
1:A:1385:G:H2'	1:A:1386:G:O4'	2.17	0.43
1:A:144:G:N2	1:A:178:C:N3	2.42	0.43
1:A:581:G:C8	24:A:1966:HOH:O	2.71	0.43
20:T:53:LEU:HD22	20:T:53:LEU:HA	1.71	0.43
1:A:1055:A:H1'	3:C:156:ARG:HH21	1.83	0.43
3:C:18:TRP:CD1	14:N:54:PRO:HA	2.53	0.43
1:A:456:C:N4	1:A:457:C:H41	2.16	0.43
1:A:1085:U:C6	1:A:1094:G:N1	2.86	0.43
8:H:18:ARG:NH2	8:H:81:HIS:O	2.51	0.43
1:A:431:A:H2'	1:A:432:A:H8	1.82	0.43
1:A:1134:G:H1	1:A:1140:C:H42	1.66	0.43
5:E:9:LYS:N	5:E:33:VAL:O	2.50	0.43
12:L:34:ARG:O	12:L:61:THR:HG23	2.18	0.43
5:E:137:GLU:O	5:E:141:GLN:HG2	2.18	0.43
13:M:32:GLU:HG2	13:M:64:TRP:HZ2	1.83	0.43
16:P:12:LYS:C	16:P:14:ASN:H	2.21	0.43
4:D:162:LEU:HA	4:D:165:MET:HB2	2.00	0.43
4:D:17:VAL:HG22	4:D:18:LYS:H	1.83	0.43
1:A:1065:U:C5	1:A:1190:G:H1'	2.54	0.43
2:B:166:ASP:HB2	2:B:205:ASP:OD2	2.18	0.43
1:A:617:G:H1	1:A:623:C:N4	2.15	0.43
2:B:118:LEU:HA	2:B:118:LEU:HD23	1.79	0.43
20:T:20:LEU:O	20:T:23:ARG:HB3	2.18	0.43
1:A:687:A:H4'	1:A:688:G:O5'	2.18	0.43
2:B:107:THR:O	2:B:110:GLN:HB2	2.18	0.43
1:A:1412:C:H2'	1:A:1413:A:C8	2.53	0.43
9:I:79:LEU:HA	9:I:79:LEU:HD22	1.69	0.43
1:A:1505:G:H8	1:A:1505:G:H3'	1.82	0.43
1:A:1199:U:O5'	1:A:1199:U:H6	2.02	0.43
1:A:683:G:H2'	1:A:684:A:C8	2.52	0.43
13:M:65:LYS:H	13:M:65:LYS:HD3	1.84	0.43
1:A:1242:C:N4	1:A:1295:G:H1	2.16	0.43
1:A:75:G:C2	1:A:96:G:C2	3.06	0.43
17:Q:40:LYS:HB3	17:Q:42:TYR:HE1	1.84	0.43
10:J:51:ARG:HA	14:N:45:ARG:HD2	2.00	0.43
1:A:1094:G:H5"	1:A:1095:U:H5	1.83	0.43
16:P:43:LYS:HG2	16:P:48:TRP:CD2	2.53	0.43
1:A:505:G:C6	1:A:535:A:C2	3.06	0.43
3:C:114:PRO:HB2	3:C:118:GLN:NE2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1355:G:H2'	1:A:1356:G:C8	2.54	0.43
1:A:78:G:N2	1:A:92:C:C4	2.86	0.43
1:A:18:C:H5"	5:E:127:ASN:ND2	2.28	0.43
16:P:74:LEU:HB3	16:P:79:VAL:CG2	2.49	0.43
1:A:664:G:OP1	18:R:64:ARG:HD2	2.19	0.43
1:A:1441:G:O2'	1:A:1460:A:N6	2.51	0.43
1:A:564:C:C6	17:Q:31:LEU:HD11	2.53	0.43
1:A:56:U:H2'	1:A:57:G:C8	2.52	0.43
2:B:213:LEU:HA	2:B:213:LEU:HD12	1.73	0.43
1:A:737:A:H2'	1:A:738:C:C6	2.54	0.43
13:M:11:ARG:HD2	13:M:12:ASN:N	2.34	0.43
2:B:51:LEU:O	2:B:55:PHE:HB2	2.18	0.43
15:O:12:ILE:HG12	15:O:31:LEU:HD11	1.99	0.43
1:A:953:G:C5'	1:A:965:A:H61	2.32	0.43
2:B:97:TRP:CZ2	2:B:101:MET:HB2	2.53	0.43
13:M:71:ARG:O	13:M:74:VAL:HG12	2.19	0.43
19:S:2:PRO:HD2	19:S:3:ARG:HH21	1.84	0.43
19:S:3:ARG:NH1	19:S:3:ARG:HB3	2.33	0.43
9:I:19:LEU:HG	9:I:60:ASP:O	2.19	0.43
8:H:97:VAL:HA	8:H:100:ILE:HD11	2.01	0.43
1:A:190(I):G:H2'	1:A:190(J):U:O4'	2.19	0.43
1:A:392:G:H2'	1:A:393:A:C8	2.54	0.43
1:A:1228:C:O3'	13:M:116:THR:HG23	2.19	0.43
3:C:28:GLN:HG3	3:C:32:LEU:HD22	1.99	0.43
1:A:1098:C:H2'	1:A:1099:G:O4'	2.18	0.43
1:A:1031:G:H2'	1:A:1032:G:C8	2.54	0.43
1:A:24:U:H2'	1:A:25:C:C6	2.54	0.43
7:G:35:LYS:HD3	7:G:38:LEU:HD13	2.01	0.43
7:G:44:TYR:HA	7:G:44:TYR:HD2	1.61	0.43
1:A:1486:G:H2'	1:A:1487:G:O4'	2.19	0.43
15:O:59:MET:HG2	15:O:59:MET:H	1.56	0.43
9:I:33:PHE:CZ	9:I:47:LEU:HD21	2.53	0.43
2:B:17:PHE:CD1	2:B:18:GLY:N	2.87	0.43
3:C:54:ARG:HH12	3:C:56:ASP:HB2	1.83	0.43
1:A:179:A:H2'	1:A:180:U:H6	1.83	0.43
5:E:152:ARG:HA	8:H:64:LYS:HZ1	1.83	0.43
2:B:218:ALA:O	2:B:222:ILE:HG13	2.19	0.43
1:A:1281:U:OP2	1:A:1282:C:N4	2.43	0.43
13:M:57:ARG:O	13:M:61:GLU:HB2	2.18	0.43
7:G:124:LEU:HD23	7:G:124:LEU:HA	1.71	0.43
19:S:18:LYS:O	19:S:22:LEU:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:119:LEU:HB3	8:H:123:GLU:HB3	2.00	0.43
1:A:190(D):U:O2'	1:A:190(E):U:H5'	2.18	0.43
18:R:56:THR:OG1	18:R:58:LEU:HG	2.19	0.43
10:J:19:SER:O	10:J:22:LYS:HB2	2.18	0.43
9:I:2:GLU:HG3	9:I:3:GLN:H	1.84	0.43
1:A:300:A:H8	1:A:300:A:O5'	2.02	0.43
2:B:185:ILE:HA	2:B:199:TYR:O	2.19	0.43
1:A:517:G:H5'	1:A:519:C:N3	2.34	0.43
1:A:976:G:OP2	1:A:1358:U:O2'	2.31	0.43
12:L:30:ALA:HB1	12:L:31:PRO:HD2	1.99	0.43
1:A:728:A:H2'	1:A:729:A:O4'	2.19	0.43
1:A:923:A:O2'	1:A:1398:A:H2'	2.19	0.43
9:I:99:LEU:HB3	9:I:101:PHE:HD1	1.84	0.43
3:C:180:ALA:O	3:C:181:ASN:HB3	2.18	0.43
1:A:297:G:N2	1:A:300:A:OP2	2.46	0.43
1:A:940:C:H2'	1:A:941:G:O4'	2.19	0.43
1:A:1277:C:H1'	1:A:1282:C:H1'	2.01	0.43
1:A:1323:G:H2'	1:A:1324:A:C8	2.54	0.43
1:A:328:C:H4'	1:A:329:A:H5'	2.01	0.43
4:D:127:THR:HA	4:D:132:ARG:HA	2.01	0.43
1:A:1250:A:C6	1:A:1287:A:C2	3.06	0.43
15:O:28:GLN:O	15:O:32:LEU:HB2	2.19	0.43
7:G:99:LEU:HD23	7:G:99:LEU:HA	1.51	0.43
1:A:582:U:P	15:O:64:ARG:NH2	2.92	0.42
1:A:1256:A:H5"	1:A:1258:G:N9	2.34	0.42
10:J:7:LYS:HD2	10:J:97:GLU:HB2	2.01	0.42
2:B:61:LEU:HD21	2:B:160:ASP:HB2	2.01	0.42
2:B:80:ILE:HD11	2:B:212:GLN:HG2	2.01	0.42
7:G:88:PRO:HG2	7:G:155:ARG:NH2	2.29	0.42
5:E:152:ARG:CZ	8:H:44:PHE:HE1	2.32	0.42
1:A:689:C:HO2'	1:A:705:U:HO2'	1.52	0.42
11:K:84:VAL:HG11	11:K:91:ARG:HD3	2.01	0.42
1:A:1476:G:H2'	1:A:1477:C:H6	1.84	0.42
1:A:500:G:C6	1:A:546:G:C2	3.06	0.42
8:H:84:ARG:O	8:H:135:CYS:HB2	2.19	0.42
6:F:26:ILE:HG21	6:F:63:TYR:HE2	1.84	0.42
1:A:129:U:O3'	1:A:129(A):G:H3'	2.18	0.42
2:B:42:ILE:N	2:B:42:ILE:HD12	2.33	0.42
13:M:50:GLU:HG3	13:M:51:ALA:N	2.34	0.42
1:A:102:G:H2'	1:A:103:C:H6	1.83	0.42
1:A:1199:U:H5"	1:A:1200:C:OP2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:9:ARG:HB2	10:J:95:GLU:HB3	2.01	0.42
3:C:21:ARG:NH2	3:C:58:GLU:HG3	2.34	0.42
1:A:1018:C:H2'	1:A:1019:C:O4'	2.18	0.42
3:C:10:PHE:O	3:C:178:LEU:HD11	2.19	0.42
2:B:182:ILE:HA	2:B:183:PRO:HD3	1.92	0.42
1:A:1127:G:O2'	9:I:16:ARG:NH2	2.51	0.42
5:E:152:ARG:HB3	8:H:43:GLY:HA3	2.01	0.42
2:B:42:ILE:H	2:B:42:ILE:HD12	1.84	0.42
1:A:707:C:H2'	1:A:708:C:H6	1.84	0.42
5:E:53:LEU:HA	5:E:53:LEU:HD22	1.62	0.42
1:A:1418:A:C8	1:A:1483:A:N6	2.88	0.42
1:A:1489:G:H2'	1:A:1490:U:C6	2.54	0.42
1:A:1206:G:H22	1:A:1207:2MG:HM22	1.84	0.42
18:R:36:ASN:OD1	18:R:39:VAL:HG12	2.19	0.42
1:A:1404:5MC:N4	1:A:1498:UR3:H3U2	2.34	0.42
9:I:81:ILE:HD13	9:I:81:ILE:HA	1.89	0.42
1:A:986:A:H1'	19:S:55:LYS:HA	2.01	0.42
1:A:791:G:C6	1:A:792:A:N6	2.86	0.42
1:A:865:A:O5'	1:A:865:A:H8	2.03	0.42
1:A:1441:G:H4'	1:A:1442:G:C6	2.55	0.42
11:K:84:VAL:HG21	11:K:95:ILE:HD11	2.02	0.42
1:A:515:G:H2'	1:A:516:PSU:H6	1.84	0.42
3:C:114:PRO:O	3:C:117:ALA:HB3	2.20	0.42
1:A:1250:A:H3'	1:A:1251:A:C8	2.53	0.42
17:Q:27:PHE:CE2	17:Q:36:ILE:HG13	2.55	0.42
19:S:33:THR:HG21	19:S:71:LEU:HD21	2.02	0.42
20:T:29:LYS:O	20:T:32:ALA:HB3	2.18	0.42
11:K:51:LYS:HE3	11:K:51:LYS:HA	2.00	0.42
1:A:575:G:OP1	1:A:575:G:H4'	2.20	0.42
7:G:63:LYS:HD3	7:G:63:LYS:N	2.33	0.42
1:A:1163:C:N3	1:A:1174:G:C2	2.87	0.42
1:A:78:G:C6	1:A:79:G:C8	3.07	0.42
8:H:116:LYS:HD3	8:H:127:LEU:HD11	2.00	0.42
8:H:7:ALA:HB2	8:H:85:ARG:HD2	2.01	0.42
17:Q:21:VAL:HG21	17:Q:59:ILE:HG13	2.02	0.42
2:B:158:LEU:HB3	2:B:159:PRO:HD2	2.01	0.42
14:N:24:CYS:SG	14:N:40:CYS:HB3	2.59	0.42
9:I:50:LEU:HG	9:I:81:ILE:HG21	2.01	0.42
1:A:1425:U:H2'	1:A:1426:C:H6	1.85	0.42
12:L:110:VAL:HG12	12:L:111:LYS:O	2.19	0.42
4:D:108:LEU:HA	4:D:108:LEU:HD13	1.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:20:ASP:HB3	7:G:23:VAL:HG23	2.00	0.42
12:L:82:VAL:HG12	12:L:106:ASP:OD1	2.19	0.42
1:A:587:G:N2	1:A:754:C:OP2	2.48	0.42
18:R:37:VAL:HG13	18:R:79:LEU:HD21	2.00	0.42
8:H:116:LYS:HD3	8:H:127:LEU:CD1	2.49	0.42
8:H:86:ILE:HG22	8:H:87:SER:N	2.32	0.42
18:R:61:LYS:O	18:R:62:GLU:C	2.58	0.42
1:A:1291:G:H2'	1:A:1292:U:H6	1.84	0.42
15:O:4:THR:HB	15:O:6:GLU:OE1	2.19	0.42
1:A:625:G:H2'	1:A:626:U:H6	1.82	0.42
2:B:163:PHE:HA	2:B:185:ILE:HB	2.01	0.42
1:A:794:A:C6	1:A:795:C:N4	2.88	0.42
1:A:445:G:C2	1:A:490:G:N1	2.88	0.42
8:H:114:THR:OG1	8:H:117:GLY:O	2.21	0.42
1:A:636:U:H5'	17:Q:2:PRO:HG3	2.00	0.42
1:A:1184:G:H2'	1:A:1185:G:C8	2.54	0.42
4:D:70:ILE:HG22	4:D:71:SER:O	2.19	0.42
21:U:18:TYR:HD2	21:U:22:ARG:HD3	1.84	0.42
19:S:15:LEU:HD21	19:S:38:SER:OG	2.20	0.42
1:A:1181:G:N3	1:A:1182:G:C2	2.87	0.42
1:A:411:A:C4	1:A:413:G:H1'	2.55	0.42
17:Q:40:LYS:HD2	17:Q:42:TYR:CZ	2.55	0.42
18:R:61:LYS:O	18:R:65:ILE:HG13	2.19	0.42
7:G:151:TYR:O	7:G:155:ARG:NH2	2.53	0.42
1:A:807:A:C6	1:A:808:C:C4	3.08	0.42
1:A:639:G:O2'	1:A:640:A:H5'	2.20	0.42
1:A:657:G:H2'	1:A:658:G:H8	1.84	0.42
9:I:27:THR:OG1	9:I:28:VAL:N	2.53	0.42
1:A:1407:5MC:H2'	1:A:1408:A:H8	1.85	0.42
19:S:39:THR:HG22	19:S:40:ILE:H	1.84	0.42
1:A:1051:C:N4	1:A:1207:2MG:C6	2.85	0.42
5:E:99:GLY:H	5:E:117:ASP:CG	2.23	0.42
13:M:68:GLY:O	13:M:71:ARG:HG3	2.20	0.42
1:A:1520[B]:G:O2'	1:A:1521:G:H5'	2.19	0.42
17:Q:63:ARG:O	17:Q:65:ILE:HD12	2.20	0.42
14:N:2:ALA:HB2	14:N:29:ARG:HA	2.01	0.42
1:A:570:G:O6	1:A:873:A:C2	2.72	0.42
2:B:208:ILE:H	2:B:208:ILE:CD1	2.26	0.42
3:C:179:ARG:O	3:C:181:ASN:N	2.53	0.42
7:G:16:LEU:HG	9:I:42:ARG:HA	2.01	0.42
10:J:24:VAL:HG13	10:J:28:ARG:NH2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1427:U:H2'	1:A:1428:A:H8	1.84	0.42
1:A:204:U:H4'	1:A:216:G:O4'	2.20	0.42
5:E:84:PHE:CE2	5:E:133:TYR:HB2	2.55	0.42
5:E:118:ILE:C	5:E:119:LEU:HD23	2.39	0.42
1:A:376:G:C4	1:A:389:A:C2	3.07	0.42
1:A:451:A:H8	1:A:451:A:O5'	2.01	0.42
1:A:21:G:C2	1:A:22:G:C6	3.08	0.42
3:C:137:ALA:O	3:C:141:VAL:HG23	2.20	0.42
7:G:141:VAL:HA	7:G:144:MET:SD	2.60	0.42
11:K:52:GLY:C	11:K:54:ARG:N	2.72	0.42
1:A:544:G:C5	1:A:545:C:C5	3.08	0.42
14:N:9:LYS:HG3	14:N:21:TYR:O	2.20	0.42
1:A:110:C:H2'	1:A:111:G:O4'	2.19	0.42
9:I:127:LYS:HA	9:I:127:LYS:HD2	1.91	0.42
4:D:142:PRO:HA	4:D:185:PHE:HD2	1.83	0.42
18:R:26:LEU:HA	18:R:26:LEU:HD12	1.87	0.42
1:A:992:U:H4'	1:A:993:G:O5'	2.20	0.42
2:B:55:PHE:HA	2:B:58:ILE:HD12	2.02	0.42
8:H:65:TYR:HA	8:H:79:VAL:HG23	2.01	0.42
1:A:1332:A:H2'	1:A:1333:A:H8	1.84	0.42
1:A:734:G:N2	18:R:75:ILE:HD11	2.35	0.42
20:T:61:SER:O	20:T:62:LEU:C	2.58	0.42
1:A:1430:C:O2	1:A:1471:G:N2	2.53	0.42
1:A:1015:A:H2'	1:A:1016:A:O4'	2.20	0.42
1:A:946:A:H2'	1:A:947:G:C8	2.53	0.42
14:N:61:TRP:OXT	14:N:61:TRP:CG	2.73	0.42
3:C:175:LEU:HD11	3:C:201:TYR:CD2	2.54	0.42
19:S:15:LEU:HD13	19:S:44:MET:HE1	2.02	0.42
1:A:1163:C:N3	1:A:1174:G:N2	2.67	0.42
1:A:868:C:H2'	1:A:869:G:O4'	2.20	0.42
1:A:1255:G:N2	1:A:1283:G:H1'	2.30	0.42
10:J:32:ALA:O	10:J:34:VAL:HG23	2.19	0.42
4:D:190:ASP:CG	4:D:191:ARG:N	2.73	0.42
4:D:9:CYS:O	4:D:12:CYS:HB2	2.20	0.42
2:B:162:ILE:HB	2:B:184:VAL:HG23	2.01	0.42
1:A:681:C:H2'	1:A:682:G:O4'	2.20	0.42
1:A:200:G:C6	1:A:201:C:C4	3.07	0.42
11:K:12:ARG:HA	11:K:12:ARG:HE	1.85	0.42
17:Q:9:VAL:O	17:Q:9:VAL:HG13	2.20	0.42
1:A:1399:C:C2	1:A:1502:A:N6	2.88	0.42
2:B:36:ARG:O	2:B:39:ILE:HD12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:G:C2	1:A:475:G:C4	3.07	0.42
20:T:84:LEU:HD23	20:T:84:LEU:HA	1.80	0.42
9:I:92:TYR:O	9:I:96:LEU:HB2	2.20	0.42
1:A:979:C:H3'	1:A:980:C:C6	2.55	0.42
4:D:200:GLU:O	4:D:203:VAL:N	2.53	0.42
1:A:767:A:H2'	1:A:768:A:C8	2.55	0.42
10:J:66:ARG:HG3	14:N:57:ARG:HD2	2.02	0.42
1:A:106:C:H2'	1:A:107:G:O4'	2.19	0.42
8:H:60:ARG:HG3	8:H:60:ARG:HH11	1.83	0.42
15:O:67:LEU:HA	15:O:67:LEU:HD23	1.46	0.42
5:E:129:ILE:HG12	5:E:129:ILE:H	1.60	0.42
1:A:1061:G:H1'	10:J:56:HIS:CE1	2.54	0.41
13:M:49:THR:CG2	13:M:51:ALA:H	2.33	0.41
1:A:413:G:H2'	1:A:428:G:N2	2.35	0.41
1:A:1008:C:N4	1:A:1021:G:H1	2.19	0.41
1:A:853:G:C2	1:A:854:G:C8	3.07	0.41
1:A:68:G:H5'	1:A:171:A:O2'	2.20	0.41
5:E:41:VAL:HG23	5:E:67:VAL:HG13	2.02	0.41
20:T:67:ALA:HA	20:T:72:LEU:HB2	2.02	0.41
1:A:451:A:N6	1:A:481:G:C4	2.88	0.41
7:G:47:CYS:HB3	7:G:48:LYS:NZ	2.35	0.41
3:C:61:ALA:C	3:C:63:ASN:H	2.24	0.41
1:A:156:G:N1	1:A:157:G:C5	2.87	0.41
16:P:2:VAL:O	16:P:64:ALA:HA	2.19	0.41
1:A:1218:C:H2'	1:A:1219:U:C6	2.54	0.41
19:S:12:ASP:OD2	19:S:37:ARG:NH1	2.34	0.41
6:F:100:ASN:HB2	18:R:23:LYS:HE2	2.02	0.41
7:G:61:VAL:HG22	7:G:128:ALA:HB1	2.01	0.41
1:A:877:C:O2	8:H:3:THR:HG21	2.20	0.41
2:B:188:ALA:O	2:B:202:PRO:HA	2.20	0.41
12:L:60:LEU:HA	12:L:60:LEU:HD13	1.67	0.41
2:B:24:TRP:HA	2:B:190:THR:O	2.20	0.41
1:A:1249:C:HO2'	9:I:73:GLN:NE2	2.18	0.41
9:I:116:LYS:HB3	9:I:121:ARG:O	2.20	0.41
6:F:8:ILE:HB	6:F:61:LEU:HD12	2.02	0.41
3:C:138:VAL:HG11	3:C:170:GLN:H	1.85	0.41
11:K:33:THR:HA	11:K:40:ILE:H	1.85	0.41
1:A:977:A:O2'	1:A:980:C:N4	2.53	0.41
1:A:828:A:C3'	1:A:828:A:C8	3.03	0.41
4:D:206:PHE:CD2	4:D:207:TYR:CE2	3.08	0.41
4:D:57:ARG:HG3	4:D:202:LEU:HD13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:136:LYS:HB3	7:G:136:LYS:HE3	1.86	0.41
8:H:70:GLN:OE1	8:H:70:GLN:HA	2.19	0.41
1:A:1414:U:H2'	1:A:1415:G:C8	2.56	0.41
18:R:55:ARG:HB3	18:R:55:ARG:CZ	2.49	0.41
1:A:1181:G:C4	1:A:1182:G:C6	3.09	0.41
1:A:1521:G:C2	1:A:1522:U:C2	3.08	0.41
6:F:2:ARG:HG3	6:F:69:GLU:HG2	2.02	0.41
12:L:98:TYR:N	12:L:98:TYR:CD1	2.88	0.41
1:A:1008:C:H1'	1:A:1023:G:H1	1.85	0.41
1:A:979:C:N4	24:A:2063:HOH:O	2.54	0.41
1:A:261:U:OP2	20:T:79:ARG:NH2	2.53	0.41
3:C:147:LYS:HD3	3:C:205:GLY:H	1.86	0.41
1:A:1349:A:C2	1:A:1374:A:C4	3.09	0.41
16:P:57:ARG:HB3	16:P:57:ARG:HH11	1.85	0.41
1:A:78:G:H2'	1:A:79:G:C5'	2.50	0.41
13:M:23:TYR:HB2	13:M:67:GLU:OE2	2.20	0.41
1:A:1402:4OC:H2'	1:A:1403:C:H6	1.85	0.41
1:A:1372:U:H5"	9:I:71:SER:CB	2.49	0.41
1:A:1094:G:H5"	1:A:1095:U:C5	2.54	0.41
1:A:981:U:H3'	1:A:982:U:C6	2.56	0.41
15:O:10:LYS:O	15:O:14:GLU:HB3	2.21	0.41
1:A:312:C:H2'	1:A:313:A:O4'	2.20	0.41
7:G:60:LYS:NZ	7:G:64:GLN:HB2	2.36	0.41
1:A:840:C:H5"	1:A:841:U:OP1	2.20	0.41
1:A:1016:A:H2'	1:A:1017:G:O4'	2.20	0.41
6:F:9:VAL:HA	6:F:59:TYR:O	2.20	0.41
1:A:721:G:C6	1:A:733:A:C2	3.08	0.41
13:M:62:ASN:N	13:M:62:ASN:OD1	2.53	0.41
1:A:428:G:C5	1:A:430:A:C6	3.08	0.41
3:C:108:ASN:N	3:C:109:PRO:HD3	2.35	0.41
1:A:967:5MC:H4'	9:I:128:ARG:CZ	2.50	0.41
18:R:52:PRO:O	18:R:56:THR:HG23	2.20	0.41
1:A:1233:G:H2'	1:A:1234:C:C6	2.55	0.41
5:E:91:LEU:N	5:E:91:LEU:HD23	2.35	0.41
4:D:93:PHE:O	4:D:96:LEU:N	2.54	0.41
1:A:629:G:H2'	1:A:630:G:H8	1.83	0.41
1:A:865:A:H1'	1:A:918:A:O2'	2.21	0.41
19:S:12:ASP:CG	19:S:37:ARG:HH12	2.22	0.41
1:A:1262:C:N4	1:A:1273:G:H1	2.14	0.41
9:I:19:LEU:HD21	9:I:59:PHE:CD2	2.56	0.41
1:A:1222:G:P	19:S:77:THR:HG1	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:49:PRO:HG2	9:I:81:ILE:HG21	2.02	0.41
1:A:395:C:H2'	1:A:396:G:C8	2.56	0.41
1:A:939:G:H2'	1:A:940:C:H6	1.83	0.41
1:A:1422:G:C2	1:A:1423:G:N7	2.88	0.41
1:A:964:A:O2'	10:J:55:LYS:HD3	2.20	0.41
1:A:665:A:H2'	1:A:732:C:O2	2.21	0.41
1:A:815:A:O2'	1:A:816:A:OP1	2.30	0.41
1:A:46:G:H2'	1:A:366:C:H5	1.85	0.41
1:A:722:A:O3'	1:A:723:U:H6	2.03	0.41
19:S:5:LEU:O	19:S:6:LYS:HD3	2.20	0.41
1:A:671:G:H5'	6:F:77:ARG:NH2	2.36	0.41
1:A:1486:G:C6	1:A:1487:G:C6	3.09	0.41
20:T:73:HIS:O	20:T:76:ALA:HB3	2.21	0.41
1:A:1405:G:O2'	1:A:1406:U:H5'	2.20	0.41
8:H:36:LEU:HD23	8:H:39:LEU:HD12	2.02	0.41
15:O:15:PHE:CE1	15:O:84:LYS:HE2	2.56	0.41
1:A:1426:C:H2'	1:A:1427:U:H6	1.86	0.41
3:C:22:TRP:CD2	3:C:59:ARG:HD2	2.56	0.41
14:N:37:PHE:C	14:N:39:LEU:N	2.74	0.41
20:T:65:LYS:O	20:T:68:LYS:HB3	2.21	0.41
4:D:57:ARG:HB3	4:D:206:PHE:HD1	1.86	0.41
5:E:53:LEU:HD13	5:E:53:LEU:O	2.21	0.41
1:A:128:G:C2	1:A:234:C:C2	3.09	0.41
1:A:654:G:H2'	1:A:655:A:H8	1.84	0.41
1:A:1192:C:H2'	1:A:1193:G:O4'	2.19	0.41
12:L:102:ARG:HE	12:L:102:ARG:HB3	1.52	0.41
7:G:22:LEU:HD12	7:G:97:GLN:HE22	1.84	0.41
3:C:130:VAL:HG23	3:C:131:ARG:N	2.36	0.41
16:P:38:TYR:CE2	16:P:50:LYS:HE2	2.49	0.41
13:M:65:LYS:O	13:M:66:LEU:HD23	2.20	0.41
18:R:43:PHE:O	18:R:44:LEU:HD23	2.21	0.41
1:A:1227:A:C2	1:A:1228:C:H1'	2.55	0.41
1:A:832:C:H2'	1:A:833:U:O4'	2.21	0.41
12:L:41:ARG:CZ	12:L:43:VAL:HG12	2.51	0.41
10:J:8:LEU:HD21	10:J:72:VAL:HG23	2.02	0.41
14:N:57:ARG:HB2	14:N:57:ARG:CZ	2.50	0.41
4:D:100:ARG:NH1	4:D:137:SER:HA	2.35	0.41
8:H:51:VAL:HG23	8:H:52:ASP:N	2.35	0.41
17:Q:90:ILE:HD13	17:Q:90:ILE:O	2.21	0.41
12:L:94:LEU:HD22	12:L:94:LEU:HA	1.72	0.41
1:A:1164:G:H1	1:A:1172:C:N4	2.06	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1157:A:N1	1:A:1181:G:N3	2.69	0.41
1:A:75:G:C6	1:A:76:C:N4	2.88	0.41
2:B:97:TRP:HH2	2:B:176:GLU:CD	2.24	0.41
1:A:1328:C:H2'	1:A:1329:A:O4'	2.20	0.41
19:S:2:PRO:HD2	19:S:3:ARG:NH2	2.36	0.41
1:A:1498:UR3:H1'	1:A:1499:A:N7	2.36	0.41
17:Q:62:SER:CB	17:Q:72:ARG:HD3	2.46	0.41
1:A:439:A:OP1	4:D:123:HIS:HD2	2.04	0.41
5:E:125:SER:OG	5:E:127:ASN:HB2	2.21	0.41
1:A:1278:U:H2'	1:A:1278:U:H6	1.67	0.41
1:A:1320:C:OP1	19:S:70:LYS:HG2	2.20	0.41
1:A:979:C:H3'	1:A:980:C:H6	1.86	0.41
1:A:981:U:H2'	1:A:982:U:H5	1.85	0.41
10:J:21:GLN:HA	10:J:24:VAL:HG12	2.03	0.41
4:D:173:TRP:HE3	4:D:173:TRP:H	1.67	0.41
1:A:1103:C:H4'	2:B:98:LEU:HD21	2.01	0.41
1:A:677:U:H2'	1:A:678:U:C6	2.55	0.41
8:H:9:MET:HG3	8:H:26:VAL:HG21	2.03	0.41
8:H:27:PRO:HA	8:H:58:TYR:CD2	2.56	0.41
9:I:27:THR:HG23	9:I:62:TYR:HA	2.01	0.41
3:C:41:GLY:O	3:C:45:LYS:HB2	2.21	0.41
1:A:49:U:O2'	1:A:50:A:H2'	2.21	0.41
20:T:56:MET:CE	20:T:104:LEU:HD21	2.51	0.41
4:D:141:ARG:CZ	4:D:141:ARG:HB2	2.51	0.41
4:D:52:SER:O	4:D:56:VAL:HG23	2.19	0.41
10:J:46:ARG:CG	10:J:64:GLU:HB3	2.51	0.41
1:A:1409:C:H2'	1:A:1410:G:H8	1.85	0.41
1:A:491:G:C2	1:A:492:G:C5	3.08	0.41
18:R:37:VAL:O	18:R:39:VAL:N	2.55	0.41
17:Q:5:VAL:HA	17:Q:59:ILE:O	2.21	0.41
20:T:87:LYS:HE2	20:T:87:LYS:HB2	1.63	0.41
12:L:46:LYS:HB2	12:L:92:0TD:H8	2.03	0.41
1:A:513:C:H42	1:A:538:G:H1	1.68	0.41
1:A:803:G:C5	1:A:804:U:C4	3.09	0.41
1:A:836:G:H5"	1:A:836:G:H8	1.84	0.41
1:A:193:C:H2'	1:A:194:C:H6	1.86	0.41
1:A:1203:C:O5'	1:A:1203:C:H6	2.04	0.41
1:A:1314:C:H2'	1:A:1315:U:C6	2.56	0.41
1:A:1414:U:H3'	1:A:1415:G:H8	1.86	0.40
6:F:15:ASP:HB3	6:F:18:GLN:CG	2.51	0.40
19:S:44:MET:O	19:S:47:HIS:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:966:M2G:H2'	1:A:967:5MC:H6	1.85	0.40
1:A:1400:5MC:H3'	1:A:1401:G:C5'	2.52	0.40
1:A:254:G:OP1	17:Q:67:LYS:O	2.39	0.40
4:D:61:LYS:HZ3	4:D:62:GLN:N	2.18	0.40
2:B:74:LYS:HB2	2:B:165:VAL:HG11	2.03	0.40
1:A:860:A:H2'	1:A:861:G:O4'	2.21	0.40
8:H:113:SER:HB2	8:H:134:ILE:HD11	2.03	0.40
3:C:186:PHE:CG	3:C:187:ALA:N	2.88	0.40
1:A:108:G:H5'	1:A:109:A:H2	1.85	0.40
1:A:778:G:H2'	1:A:779:C:O4'	2.20	0.40
12:L:84:LEU:HA	12:L:84:LEU:HD12	1.69	0.40
1:A:673:G:O3'	6:F:87:ARG:NH1	2.54	0.40
1:A:1255:G:C2	1:A:1283:G:N3	2.89	0.40
7:G:88:PRO:HG2	7:G:155:ARG:NH1	2.34	0.40
1:A:980:C:H2'	1:A:981:U:O4'	2.21	0.40
1:A:1511:G:H2'	1:A:1512:U:O4'	2.22	0.40
1:A:394:G:H2'	1:A:395:C:H6	1.85	0.40
1:A:500:G:C5	1:A:546:G:N2	2.89	0.40
20:T:61:SER:O	20:T:64:ASP:N	2.54	0.40
5:E:37:ARG:O	5:E:114:GLY:HA3	2.22	0.40
1:A:770:C:O2'	1:A:771:G:H5'	2.20	0.40
17:Q:93:GLN:HG2	17:Q:96:GLU:OE2	2.20	0.40
2:B:196:LEU:HA	2:B:196:LEU:HD23	1.86	0.40
1:A:92:C:H2'	1:A:92:C:O2	2.21	0.40
2:B:23:ARG:CZ	2:B:23:ARG:HA	2.50	0.40
18:R:58:LEU:HB3	18:R:62:GLU:HB3	2.04	0.40
13:M:8:GLU:CD	13:M:22:ILE:HA	2.42	0.40
1:A:475:G:H2'	1:A:476:G:O4'	2.21	0.40
4:D:22:LYS:HB2	4:D:26:CYS:CB	2.50	0.40
7:G:53:LYS:HB3	7:G:53:LYS:HE3	1.88	0.40
2:B:16:HIS:CG	2:B:17:PHE:N	2.89	0.40
4:D:121:VAL:HG11	4:D:136:PRO:HA	2.03	0.40
1:A:460:A:C6	1:A:462:G:C5	3.09	0.40
1:A:551:U:O2'	12:L:86:ARG:HD2	2.21	0.40
1:A:1287:A:N7	1:A:1288:A:N6	2.70	0.40
2:B:184:VAL:HG12	2:B:198:ASP:H	1.86	0.40
1:A:323:U:H2'	1:A:324:G:O4'	2.20	0.40
5:E:64:ARG:H	5:E:64:ARG:HG2	1.45	0.40
6:F:15:ASP:CG	6:F:16:GLN:H	2.25	0.40
19:S:40:ILE:HA	19:S:44:MET:SD	2.61	0.40
10:J:50:ILE:N	10:J:50:ILE:HD12	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:88:ARG:NH1	19:S:3:ARG:HH22	2.20	0.40
14:N:45:ARG:HH11	14:N:45:ARG:HG2	1.85	0.40
1:A:1316:G:C2	1:A:1319:A:OP2	2.75	0.40
3:C:127:ARG:HB2	3:C:127:ARG:CZ	2.51	0.40
1:A:618:C:H3'	1:A:619:U:H5"	2.03	0.40
1:A:1531:A:C8	1:A:1531:A:OP2	2.74	0.40
1:A:1295:G:C5	1:A:1296:C:C5	3.09	0.40
1:A:809:G:HO2'	1:A:810:C:P	2.44	0.40
11:K:16:SER:CB	11:K:106:LYS:HZ1	2.35	0.40
12:L:28:LYS:HD3	12:L:28:LYS:HA	1.93	0.40
11:K:122:LYS:HB3	11:K:122:LYS:HE2	1.79	0.40
1:A:1243:C:OP1	21:U:10:ARG:NH1	2.55	0.40
8:H:124:ALA:O	8:H:125:ARG:C	2.60	0.40
2:B:21:ARG:HE	2:B:22:LYS:H	1.67	0.40
1:A:253:U:H2'	1:A:254:G:C8	2.56	0.40
1:A:427:U:OP1	4:D:13:ARG:NH2	2.54	0.40
1:A:1244:C:H5"	1:A:1245:A:OP2	2.22	0.40
3:C:134:ILE:HG23	3:C:151:VAL:CG1	2.52	0.40
1:A:570:G:C2	1:A:571:U:C4	3.09	0.40
1:A:115:G:O2'	1:A:289:G:H5"	2.22	0.40
5:E:80:ILE:O	5:E:80:ILE:HG13	2.21	0.40
8:H:82:HIS:C	8:H:82:HIS:HD1	2.25	0.40
1:A:735:C:O2'	1:A:736:C:H5'	2.22	0.40
1:A:945:G:N2	1:A:1337:G:N2	2.69	0.40
1:A:451:A:N6	1:A:481:G:C5	2.90	0.40
1:A:27:G:H1	1:A:556:C:H42	1.70	0.40
4:D:9:CYS:HA	4:D:12:CYS:HB2	2.03	0.40
1:A:154:C:C2	1:A:168:G:N2	2.90	0.40
7:G:3:ARG:HH11	7:G:3:ARG:HG2	1.84	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%)	206 (89%)	23 (10%)	3 (1%)	15 62
3	C	204/239 (85%)	179 (88%)	24 (12%)	1 (0%)	34 77
4	D	206/209 (99%)	190 (92%)	16 (8%)	0	100 100
5	E	148/162 (91%)	139 (94%)	8 (5%)	1 (1%)	26 72
6	F	99/101 (98%)	95 (96%)	4 (4%)	0	100 100
7	G	153/156 (98%)	137 (90%)	16 (10%)	0	100 100
8	H	136/138 (99%)	131 (96%)	5 (4%)	0	100 100
9	I	125/128 (98%)	113 (90%)	11 (9%)	1 (1%)	24 70
10	J	96/105 (91%)	78 (81%)	17 (18%)	1 (1%)	19 66
11	K	114/129 (88%)	101 (89%)	13 (11%)	0	100 100
12	L	121/135 (90%)	109 (90%)	11 (9%)	1 (1%)	24 70
13	M	116/126 (92%)	102 (88%)	12 (10%)	2 (2%)	11 57
14	N	58/61 (95%)	48 (83%)	10 (17%)	0	100 100
15	O	85/89 (96%)	74 (87%)	10 (12%)	1 (1%)	16 63
16	P	81/88 (92%)	72 (89%)	9 (11%)	0	100 100
17	Q	97/105 (92%)	89 (92%)	8 (8%)	0	100 100
18	R	68/88 (77%)	58 (85%)	10 (15%)	0	100 100
19	S	78/93 (84%)	71 (91%)	6 (8%)	1 (1%)	15 62
20	T	97/106 (92%)	83 (86%)	14 (14%)	0	100 100
21	U	22/27 (82%)	21 (96%)	1 (4%)	0	100 100
All	All	2336/2541 (92%)	2096 (90%)	228 (10%)	12 (0%)	34 77

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	21	ARG
12	L	28	LYS
19	S	31	ILE
2	B	95	GLN
9	I	119	ALA
3	C	180	ALA
13	M	23	TYR
5	E	70	PRO
2	B	229	VAL
10	J	34	VAL
13	M	84	ILE

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Mol	Chain	Res	Type
15	O	45	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	202/220 (92%)	157 (78%)	45 (22%)	1 8
3	C	160/188 (85%)	121 (76%)	39 (24%)	1 7
4	D	180/181 (99%)	146 (81%)	34 (19%)	2 13
5	E	115/123 (94%)	77 (67%)	38 (33%)	0 2
6	F	90/90 (100%)	64 (71%)	26 (29%)	0 4
7	G	126/127 (99%)	99 (79%)	27 (21%)	1 9
8	H	119/119 (100%)	90 (76%)	29 (24%)	1 7
9	I	98/99 (99%)	68 (69%)	30 (31%)	0 3
10	J	87/92 (95%)	67 (77%)	20 (23%)	1 8
11	K	88/99 (89%)	67 (76%)	21 (24%)	1 7
12	L	103/110 (94%)	84 (82%)	19 (18%)	2 14
13	M	94/101 (93%)	73 (78%)	21 (22%)	1 8
14	N	49/50 (98%)	42 (86%)	7 (14%)	4 28
15	O	79/80 (99%)	62 (78%)	17 (22%)	1 9
16	P	72/74 (97%)	59 (82%)	13 (18%)	2 15
17	Q	94/97 (97%)	74 (79%)	20 (21%)	1 9
18	R	61/77 (79%)	48 (79%)	13 (21%)	1 9
19	S	71/80 (89%)	56 (79%)	15 (21%)	1 10
20	T	76/82 (93%)	55 (72%)	21 (28%)	0 4
21	U	19/22 (86%)	13 (68%)	6 (32%)	0 3
All	All	1983/2111 (94%)	1522 (77%)	461 (23%)	1 8

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

Mol	Chain	Res	Type
2	B	8	LYS
2	B	9	GLU
2	B	12	GLU
2	B	16	HIS
2	B	17	PHE
2	B	20	GLU
2	B	23	ARG
2	B	35	GLU
2	B	48	MET
2	B	53	ARG
2	B	56	ARG
2	B	60	ASP
2	B	67	THR
2	B	69	LEU
2	B	74	LYS
2	B	92	TYR
2	B	98	LEU
2	B	107	THR
2	B	108	ILE
2	B	109	SER
2	B	115	LEU
2	B	127	ILE
2	B	128	GLU
2	B	144	ARG
2	B	146	GLN
2	B	160	ASP
2	B	163	PHE
2	B	165	VAL
2	B	166	ASP
2	B	168	THR
2	B	170	GLU
2	B	175	ARG
2	B	178	ARG
2	B	184	VAL
2	B	187	LEU
2	B	200	ILE
2	B	204	ASN
2	B	205	ASP
2	B	206	ASP
2	B	209	ARG
2	B	212	GLN
2	B	217	ARG
2	B	221	LEU

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Mol	Chain	Res	Type
2	B	226	ARG
2	B	231	GLU
3	C	3	ASN
3	C	8	ILE
3	C	11	ARG
3	C	14	ILE
3	C	17	ASP
3	C	18	TRP
3	C	20	SER
3	C	21	ARG
3	C	26	LYS
3	C	33	LEU
3	C	34	LEU
3	C	36	ASP
3	C	43	LEU
3	C	45	LYS
3	C	52	LEU
3	C	54	ARG
3	C	58	GLU
3	C	90	GLU
3	C	91	LEU
3	C	94	LEU
3	C	98	ASN
3	C	99	VAL
3	C	102	ASN
3	C	104	GLN
3	C	107	GLN
3	C	111	LEU
3	C	116	VAL
3	C	131	ARG
3	C	143	GLU
3	C	172	ARG
3	C	175	LEU
3	C	176	HIS
3	C	177	THR
3	C	190	ARG
3	C	191	THR
3	C	192	THR
3	C	193	TYR
3	C	196	LEU
3	C	204	LEU
4	D	9	CYS

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Mol	Chain	Res	Type
4	D	11	LEU
4	D	12	CYS
4	D	19	LEU
4	D	25	ARG
4	D	26	CYS
4	D	35	ARG
4	D	57	ARG
4	D	59	ARG
4	D	61	LYS
4	D	64	LEU
4	D	65	ARG
4	D	76	ARG
4	D	97	LEU
4	D	108	LEU
4	D	122	ARG
4	D	127	THR
4	D	131	ARG
4	D	135	LEU
4	D	137	SER
4	D	141	ARG
4	D	145	GLU
4	D	148	VAL
4	D	154	ASN
4	D	165	MET
4	D	170	VAL
4	D	178	VAL
4	D	181	MET
4	D	186	LEU
4	D	187	ARG
4	D	191	ARG
4	D	192	GLU
4	D	194	LEU
4	D	202	LEU
5	E	6	PHE
5	E	12	LEU
5	E	14	ARG
5	E	16	THR
5	E	18	ARG
5	E	19	MET
5	E	24	ARG
5	E	25	ARG
5	E	26	PHE

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Mol	Chain	Res	Type
5	E	31	LEU
5	E	32	VAL
5	E	41	VAL
5	E	43	LEU
5	E	47	LYS
5	E	53	LEU
5	E	60	TYR
5	E	64	ARG
5	E	66	MET
5	E	71	LEU
5	E	72	GLN
5	E	78	HIS
5	E	79	GLU
5	E	83	GLU
5	E	87	SER
5	E	88	LYS
5	E	100	VAL
5	E	105	VAL
5	E	109	ILE
5	E	116	THR
5	E	118	ILE
5	E	123	LEU
5	E	125	SER
5	E	131	ILE
5	E	136	MET
5	E	144	THR
5	E	148	VAL
5	E	150	ARG
5	E	151	LEU
6	F	10	LEU
6	F	13	ASN
6	F	14	LEU
6	F	19	LEU
6	F	21	LEU
6	F	24	GLU
6	F	25	ILE
6	F	31	GLU
6	F	32	ASN
6	F	36	ARG
6	F	40	VAL
6	F	43	LEU
6	F	45	LEU

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Mol	Chain	Res	Type
6	F	47	ARG
6	F	54	LYS
6	F	61	LEU
6	F	65	VAL
6	F	69	GLU
6	F	70	ASP
6	F	74	ASP
6	F	77	ARG
6	F	80	ARG
6	F	86	ARG
6	F	92	LYS
6	F	95	GLU
6	F	98	LEU
7	G	6	ARG
7	G	12	LEU
7	G	22	LEU
7	G	27	ILE
7	G	47	CYS
7	G	53	LYS
7	G	54	THR
7	G	60	LYS
7	G	61	VAL
7	G	63	LYS
7	G	64	GLN
7	G	66	VAL
7	G	73	MET
7	G	77	SER
7	G	84	ASN
7	G	86	GLN
7	G	87	VAL
7	G	98	SER
7	G	110	GLN
7	G	114	ARG
7	G	122	HIS
7	G	125	MET
7	G	126	ASP
7	G	129	GLU
7	G	136	LYS
7	G	146	GLU
7	G	149	ARG
8	H	11	THR
8	H	12	ARG

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Mol	Chain	Res	Type
8	H	18	ARG
8	H	19	VAL
8	H	21	LYS
8	H	23	SER
8	H	24	THR
8	H	26	VAL
8	H	51	VAL
8	H	63	LEU
8	H	68	ARG
8	H	82	HIS
8	H	85	ARG
8	H	87	SER
8	H	88	LYS
8	H	91	ARG
8	H	92	ARG
8	H	95	VAL
8	H	97	VAL
8	H	98	LYS
8	H	99	GLU
8	H	102	ARG
8	H	118	VAL
8	H	121	ASP
8	H	126	LYS
8	H	127	LEU
8	H	129	VAL
8	H	136	GLU
8	H	138	TRP
9	I	12	GLU
9	I	16	ARG
9	I	26	VAL
9	I	27	THR
9	I	29	ASN
9	I	44	VAL
9	I	47	LEU
9	I	48	GLU
9	I	56	LEU
9	I	58	HIS
9	I	64	THR
9	I	66	ARG
9	I	70	LYS
9	I	77	ILE
9	I	79	LEU

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Mol	Chain	Res	Type
9	I	85	LEU
9	I	91	ASP
9	I	92	TYR
9	I	93	ARG
9	I	95	LYS
9	I	96	LEU
9	I	99	LEU
9	I	101	PHE
9	I	102	LEU
9	I	104	ARG
9	I	109	VAL
9	I	116	LYS
9	I	118	LYS
9	I	121	ARG
9	I	126	SER
10	J	16	LEU
10	J	23	ILE
10	J	42	THR
10	J	48	THR
10	J	55	LYS
10	J	61	GLU
10	J	62	HIS
10	J	64	GLU
10	J	66	ARG
10	J	68	HIS
10	J	69	ASN
10	J	71	LEU
10	J	75	ILE
10	J	78	ASN
10	J	79	ARG
10	J	87	THR
10	J	94	VAL
10	J	95	GLU
10	J	96	ILE
10	J	97	GLU
11	K	11	LYS
11	K	12	ARG
11	K	14	VAL
11	K	18	ARG
11	K	29	ILE
11	K	30	VAL
11	K	40	ILE

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Mol	Chain	Res	Type
11	K	51	LYS
11	K	67	ASP
11	K	70	LYS
11	K	75	TYR
11	K	81	ASP
11	K	91	ARG
11	K	92	GLU
11	K	105	VAL
11	K	108	ILE
11	K	114	VAL
11	K	123	LYS
11	K	124	LYS
11	K	125	PHE
11	K	126	ARG
12	L	6	THR
12	L	10	LEU
12	L	20	LYS
12	L	33	ARG
12	L	37	CYS
12	L	39	VAL
12	L	47	LYS
12	L	55	VAL
12	L	59	ARG
12	L	60	LEU
12	L	62	SER
12	L	64	TYR
12	L	66	VAL
12	L	79	GLU
12	L	96	VAL
12	L	97	ARG
12	L	111	LYS
12	L	113	ARG
12	L	120	TYR
13	M	14	ARG
13	M	25	ILE
13	M	27	LYS
13	M	35	GLU
13	M	36	LYS
13	M	46	LYS
13	M	50	GLU
13	M	56	LEU
13	M	64	TRP

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Mol	Chain	Res	Type
13	M	65	LYS
13	M	69	GLU
13	M	71	ARG
13	M	79	LYS
13	M	81	LEU
13	M	86	CYS
13	M	102	ARG
13	M	103	THR
13	M	105	THR
13	M	109	THR
13	M	114	ARG
13	M	117	VAL
14	N	21	TYR
14	N	22	THR
14	N	27	CYS
14	N	29	ARG
14	N	46	GLU
14	N	53	LEU
14	N	57	ARG
15	O	4	THR
15	O	9	GLN
15	O	21	ASP
15	O	22	THR
15	O	32	LEU
15	O	33	THR
15	O	36	ILE
15	O	38	ARG
15	O	39	LEU
15	O	45	VAL
15	O	47	LYS
15	O	58	MET
15	O	59	MET
15	O	68	ARG
15	O	70	LEU
15	O	77	ARG
15	O	87	ILE
16	P	11	SER
16	P	28	ARG
16	P	33	ILE
16	P	44	THR
16	P	45	THR
16	P	53	VAL

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Mol	Chain	Res	Type
16	P	54	GLU
16	P	55	ARG
16	P	57	ARG
16	P	69	THR
16	P	75	ARG
16	P	81	ARG
16	P	82	GLN
17	Q	4	LYS
17	Q	12	SER
17	Q	20	THR
17	Q	23	VAL
17	Q	25	ARG
17	Q	53	LEU
17	Q	59	ILE
17	Q	60	ILE
17	Q	62	SER
17	Q	72	ARG
17	Q	77	VAL
17	Q	78	GLU
17	Q	86	GLU
17	Q	89	LEU
17	Q	90	ILE
17	Q	92	ARG
17	Q	97	SER
17	Q	98	LEU
17	Q	99	SER
17	Q	100	LYS
18	R	26	LEU
18	R	31	LEU
18	R	39	VAL
18	R	42	ARG
18	R	46	GLU
18	R	50	ILE
18	R	55	ARG
18	R	69	THR
18	R	70	ILE
18	R	75	ILE
18	R	82	THR
18	R	86	VAL
18	R	87	ARG
19	S	6	LYS
19	S	11	VAL

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Mol	Chain	Res	Type
19	S	12	ASP
19	S	13	ASP
19	S	20	LEU
19	S	22	LEU
19	S	36	ARG
19	S	39	THR
19	S	43	GLU
19	S	56	GLN
19	S	61	TYR
19	S	64	GLU
19	S	70	LYS
19	S	78	ARG
19	S	79	THR
20	T	10	LEU
20	T	13	LEU
20	T	15	ARG
20	T	17	ARG
20	T	19	SER
20	T	20	LEU
20	T	24	LEU
20	T	36	LEU
20	T	41	ILE
20	T	43	LEU
20	T	53	LEU
20	T	54	LYS
20	T	57	ARG
20	T	60	GLU
20	T	71	THR
20	T	75	ASN
20	T	80	ARG
20	T	86	ARG
20	T	87	LYS
20	T	91	LEU
20	T	92	LEU
21	U	6	ARG
21	U	10	ARG
21	U	13	ILE
21	U	17	THR
21	U	22	ARG
21	U	25	LYS

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

Mol	Chain	Res	Type
4	D	42	GLN
4	D	43	HIS
4	D	123	HIS
5	E	127	ASN
6	F	7	ASN
9	I	73	GLN
13	M	77	ASN
19	S	47	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1504/1522 (98%)	379 (25%)	43 (2%)

All (379) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	7	G
1	A	8	A
1	A	9	G
1	A	22	G
1	A	31	G
1	A	32	A
1	A	33	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	50	A
1	A	51	A
1	A	55	A
1	A	66	G
1	A	74	C
1	A	75	G
1	A	79	G
1	A	80	G
1	A	81	U
1	A	82	U
1	A	92	C
1	A	93	G
1	A	97	G
1	A	99	C

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Mol	Chain	Res	Type
1	A	108	G
1	A	115	G
1	A	116	A
1	A	121	C
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	135	C
1	A	148	G
1	A	151	A
1	A	157	G
1	A	159	G
1	A	160	A
1	A	163	C
1	A	181	G
1	A	182	U
1	A	183	G
1	A	190(D)	U
1	A	190(E)	U
1	A	190(L)	U
1	A	195	A
1	A	197	A
1	A	202	U
1	A	203	U
1	A	216	G
1	A	220	G
1	A	231	G
1	A	247	G
1	A	251	G
1	A	252	U
1	A	256	U
1	A	265	G
1	A	266	G
1	A	267	C
1	A	289	G
1	A	292	G
1	A	299	G
1	A	316	G
1	A	321	A
1	A	328	C
1	A	332	G
1	A	344	A

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Mol	Chain	Res	Type
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	367	U
1	A	371	G
1	A	372	C
1	A	373	A
1	A	374	A
1	A	382	A
1	A	384	G
1	A	390	C
1	A	392	G
1	A	397	A
1	A	398	C
1	A	406	G
1	A	412	A
1	A	413	G
1	A	420	U
1	A	421	U
1	A	422	C
1	A	423	G
1	A	424	G
1	A	429	U
1	A	430	A
1	A	439	A
1	A	450	G
1	A	452	A
1	A	460	A
1	A	461	C
1	A	476	G
1	A	481	G
1	A	485	G
1	A	486	U
1	A	496	A
1	A	497	A
1	A	498	U
1	A	509	A
1	A	510	A

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Mol	Chain	Res	Type
1	A	511	C
1	A	512	U
1	A	518	C
1	A	519	C
1	A	521	G
1	A	527	7MG
1	A	531	U
1	A	532	A
1	A	533	A
1	A	536	C
1	A	538	G
1	A	545	C
1	A	547	A
1	A	559	A
1	A	560	U
1	A	562	C
1	A	563	A
1	A	564	C
1	A	566	G
1	A	568	G
1	A	571	U
1	A	572	A
1	A	573	A
1	A	576	G
1	A	577	G
1	A	579	G
1	A	588	G
1	A	625	G
1	A	629	G
1	A	644	G
1	A	650	G
1	A	653	A
1	A	665	A
1	A	670	G
1	A	671	G
1	A	687	A
1	A	688	G
1	A	693	G
1	A	695	A
1	A	701	C
1	A	702	A
1	A	723	U

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Mol	Chain	Res	Type
1	A	724	G
1	A	731	G
1	A	733	A
1	A	734	G
1	A	740	U
1	A	749	C
1	A	755	G
1	A	761	G
1	A	777	A
1	A	781	A
1	A	782	A
1	A	783	C
1	A	785	G
1	A	792	A
1	A	793	U
1	A	794	A
1	A	799	G
1	A	810	C
1	A	812	C
1	A	813	U
1	A	817	C
1	A	818	G
1	A	827	U
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	851	G
1	A	855	G
1	A	857	C
1	A	859	A
1	A	872	A
1	A	873	A
1	A	888	G
1	A	889	A
1	A	897	C
1	A	902	G
1	A	922	G
1	A	925	G

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Mol	Chain	Res	Type
1	A	927	G
1	A	931	C
1	A	932	C
1	A	934	C
1	A	935	A
1	A	936	C
1	A	937	A
1	A	941	G
1	A	944	G
1	A	954	G
1	A	960	U
1	A	962	C
1	A	963	G
1	A	966	M2G
1	A	967	5MC
1	A	968	A
1	A	969	A
1	A	971	G
1	A	972	C
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	978	A
1	A	982	U
1	A	983	A
1	A	984	C
1	A	985	C
1	A	991	U
1	A	992	U
1	A	993	G
1	A	994	A
1	A	1003(A)	G
1	A	1004	A
1	A	1005	A
1	A	1011	G
1	A	1012	U
1	A	1023	G
1	A	1024	G
1	A	1025	U
1	A	1030(B)	C
1	A	1030(C)	G

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Mol	Chain	Res	Type
1	A	1030(D)	A
1	A	1040	U
1	A	1042	G
1	A	1045	C
1	A	1048	G
1	A	1050	G
1	A	1053	G
1	A	1055	A
1	A	1060	C
1	A	1064	G
1	A	1065	U
1	A	1066	C
1	A	1078	U
1	A	1079	G
1	A	1081	G
1	A	1085	U
1	A	1092	A
1	A	1093	A
1	A	1095	U
1	A	1101	A
1	A	1103	C
1	A	1104	G
1	A	1111	A
1	A	1124	G
1	A	1125	U
1	A	1126	U
1	A	1127	G
1	A	1129	C
1	A	1130	A
1	A	1131	G
1	A	1132	C
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1140	C
1	A	1146	A
1	A	1153	C
1	A	1154	G
1	A	1157	A
1	A	1159	U
1	A	1164	G
1	A	1171	G

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Mol	Chain	Res	Type
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	1200	C
1	A	1201	A
1	A	1202	G
1	A	1206	G
1	A	1207	2MG
1	A	1209	C
1	A	1211	U
1	A	1212	U
1	A	1213	A
1	A	1214	C
1	A	1215	G
1	A	1224	G
1	A	1225	A
1	A	1227	A
1	A	1228	C
1	A	1233	G
1	A	1238	A
1	A	1241	G
1	A	1243	C
1	A	1244	C
1	A	1250	A
1	A	1256	A
1	A	1257	U
1	A	1258	G
1	A	1260	C
1	A	1263	C
1	A	1270	C
1	A	1273	G
1	A	1278	U
1	A	1279	A
1	A	1280	A
1	A	1286	A
1	A	1287	A
1	A	1288	A
1	A	1289	A
1	A	1297	C

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Mol	Chain	Res	Type
1	A	1298	C
1	A	1299	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1303	C
1	A	1304	G
1	A	1306	A
1	A	1317	C
1	A	1319	A
1	A	1320	C
1	A	1322	C
1	A	1336	C
1	A	1340	A
1	A	1352	C
1	A	1353	G
1	A	1359	C
1	A	1360	A
1	A	1363	A
1	A	1364	U
1	A	1370	G
1	A	1379	G
1	A	1381	U
1	A	1390	U
1	A	1398	A
1	A	1399	C
1	A	1400	5MC
1	A	1411	C
1	A	1413	A
1	A	1416	G
1	A	1417	G
1	A	1418	A
1	A	1436	U
1	A	1442	G
1	A	1443	G
1	A	1446	A
1	A	1447	G
1	A	1473	A
1	A	1475	G
1	A	1477	C
1	A	1483	A
1	A	1484	C

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Mol	Chain	Res	Type
1	A	1489	G
1	A	1490	U
1	A	1491	G
1	A	1492	A
1	A	1494	G
1	A	1497	G
1	A	1498	UR3
1	A	1499	A
1	A	1500	A
1	A	1502	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1529	G
1	A	1530	G
1	A	1531	A
1	A	1533	C
1	A	1540	PSU

All (43) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U
1	A	91	C
1	A	115	G
1	A	129(A)	G
1	A	181	G
1	A	250	A
1	A	251	G
1	A	344	A
1	A	350	G
1	A	372	C
1	A	422	C
1	A	428	G
1	A	429	U
1	A	484	G
1	A	485	G
1	A	509	A
1	A	518	C
1	A	559	A
1	A	687	A
1	A	701	C

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Mol	Chain	Res	Type
1	A	748	C
1	A	777	A
1	A	792	A
1	A	809	G
1	A	812	C
1	A	828	A
1	A	992	U
1	A	1049	U
1	A	1065	U
1	A	1139	G
1	A	1145	C
1	A	1181	G
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	1301	U
1	A	1305	G
1	A	1358	U
1	A	1380	U
1	A	1505	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	2MG	A	1207	1	17,26,27	2.12	4 (23%)	21,38,41	2.28	5 (23%)
1	5MC	A	1400	1	13,22,23	1.35	3 (23%)	15,32,35	1.11	1 (6%)
1	4OC	A	1402	1	13,23,24	1.61	2 (15%)	18,32,35	0.65	0
1	5MC	A	1404	1	13,22,23	1.52	2 (15%)	15,32,35	1.42	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	5MC	A	1407	1	13,22,23	1.54	2 (15%)	15,32,35	1.13	1 (6%)
1	UR3	A	1498	1	12,22,23	1.23	2 (16%)	16,32,35	1.69	2 (12%)
1	MA6	A	1518[A]	1	16,26,27	0.71	0	18,38,41	0.96	1 (5%)
1	MA6	A	1518[B]	1	16,26,27	1.18	3 (18%)	18,38,41	1.21	2 (11%)
1	MA6	A	1519[A]	1	16,26,27	0.96	1 (6%)	18,38,41	1.17	3 (16%)
1	MA6	A	1519[B]	1	16,26,27	1.49	4 (25%)	18,38,41	0.97	2 (11%)
1	PSU	A	1540	1	13,21,22	1.05	1 (7%)	18,30,33	3.63	5 (27%)
1	PSU	A	1541	1	13,21,22	1.10	1 (7%)	18,30,33	3.54	6 (33%)
1	PSU	A	516	1	13,21,22	1.05	1 (7%)	18,30,33	3.65	4 (22%)
1	7MG	A	527	1,22	19,26,27	2.36	5 (26%)	24,39,42	1.79	4 (16%)
1	M2G	A	966	1	17,27,28	1.63	3 (17%)	22,40,43	2.19	4 (18%)
1	5MC	A	967	1	13,22,23	0.86	1 (7%)	15,32,35	1.12	1 (6%)
12	0TD	L	92	12	4,9,10	0.90	0	4,11,13	3.00	3 (75%)

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

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

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	7MG	C8-N9	-6.82	1.35	1.45
1	A	527	7MG	C2-N3	-3.49	1.29	1.35
1	A	527	7MG	O6-C6	-2.87	1.17	1.24
1	A	1498	UR3	C6-N1	-2.79	1.31	1.35
1	A	1404	5MC	C4-N3	-2.29	1.31	1.35
1	A	1498	UR3	C4-N3	-2.17	1.35	1.38
1	A	1518[B]	MA6	C2-N1	2.01	1.37	1.33
1	A	967	5MC	C6-N1	2.01	1.38	1.35
1	A	1207	2MG	C2-N1	2.02	1.41	1.34
1	A	1518[B]	MA6	C5-C4	2.04	1.45	1.40
1	A	1407	5MC	C4-N4	2.07	1.39	1.34
1	A	1519[A]	MA6	C6-N1	2.21	1.37	1.34
1	A	1400	5MC	C4-N4	2.49	1.40	1.34
1	A	1400	5MC	C6-N1	2.58	1.38	1.35
1	A	1518[B]	MA6	C6-N1	2.59	1.37	1.34
1	A	1519[B]	MA6	C6-N1	2.60	1.37	1.34
1	A	1519[B]	MA6	C2-N3	2.63	1.36	1.32
1	A	1519[B]	MA6	C2-N1	2.65	1.38	1.33
1	A	1402	4OC	C5-C4	2.71	1.45	1.39
1	A	1207	2MG	C4-N3	2.71	1.40	1.35
1	A	527	7MG	C4-N3	2.77	1.37	1.34
1	A	1400	5MC	C5-C4	2.81	1.45	1.41
1	A	516	PSU	C4-N3	2.90	1.38	1.33
1	A	1540	PSU	C4-N3	2.90	1.38	1.33
1	A	1541	PSU	C4-N3	3.06	1.38	1.33
1	A	1519[B]	MA6	C4-N3	3.11	1.40	1.35
1	A	966	M2G	C2-N2	3.14	1.40	1.34
1	A	966	M2G	C6-N1	3.35	1.39	1.33
1	A	966	M2G	C4-N3	3.69	1.41	1.35
1	A	527	7MG	C2-N2	3.92	1.42	1.34
1	A	1402	4OC	CM4-N4	4.26	1.53	1.45
1	A	1404	5MC	C5-C4	4.32	1.48	1.41
1	A	1407	5MC	C5-C4	4.49	1.48	1.41
1	A	1207	2MG	C2-N2	4.49	1.39	1.34
1	A	1207	2MG	C6-N1	6.34	1.44	1.33

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	516	PSU	N1-C2-N3	-13.30	119.84	128.33
1	A	1540	PSU	N1-C2-N3	-13.20	119.91	128.33
1	A	1541	PSU	N1-C2-N3	-12.61	120.29	128.33
1	A	1207	2MG	C5-C6-N1	-7.69	113.08	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	966	M2G	C5-C6-N1	-7.39	113.49	123.59
1	A	527	7MG	C5-C4-N3	-5.28	121.68	126.82
1	A	966	M2G	N1-C2-N2	-4.41	112.19	117.16
1	A	1404	5MC	N4-C4-N3	-4.26	110.78	116.95
12	L	92	0TD	CB-CA-N	-4.21	100.55	109.66
12	L	92	0TD	CSB-SB-CB	-3.62	94.71	101.54
1	A	527	7MG	C4-N9-C1'	-3.56	118.12	126.70
1	A	1407	5MC	N4-C4-N3	-3.31	112.15	116.95
1	A	1540	PSU	C5-C6-N1	-2.86	120.36	124.39
1	A	1207	2MG	C1'-N9-C4	-2.63	122.97	126.94
1	A	1541	PSU	C5-C1'-C2'	-2.62	110.87	115.52
1	A	1541	PSU	C5-C6-N1	-2.54	120.81	124.39
1	A	1207	2MG	C2'-C1'-N9	-2.47	110.52	114.29
1	A	1519[A]	MA6	C2'-C1'-N9	-2.33	110.74	114.29
12	L	92	0TD	O-C-CA	-2.27	119.45	125.44
1	A	1400	5MC	N4-C4-N3	-2.06	113.96	116.95
1	A	527	7MG	N1-C2-N3	-2.03	122.21	125.53
1	A	1519[B]	MA6	N3-C2-N1	2.17	130.56	128.89
1	A	1519[A]	MA6	N3-C2-N1	2.24	130.61	128.89
1	A	1519[B]	MA6	C2-N1-C6	2.25	116.21	111.43
1	A	1404	5MC	C5-C4-N3	2.26	125.06	121.27
1	A	966	M2G	C1'-N9-C4	2.28	130.38	126.94
1	A	1518[B]	MA6	N3-C2-N1	2.49	130.80	128.89
1	A	1518[A]	MA6	C2-N1-C6	2.55	116.85	111.43
1	A	516	PSU	C6-N1-C2	2.55	119.57	115.47
1	A	1519[A]	MA6	C2-N1-C6	2.65	117.07	111.43
1	A	1498	UR3	O3'-C3'-C2'	2.66	120.47	111.83
1	A	1518[B]	MA6	C2-N1-C6	2.67	117.10	111.43
1	A	967	5MC	CM5-C5-C6	2.73	124.12	118.62
1	A	516	PSU	O4'-C1'-C2'	2.73	107.51	104.73
1	A	1207	2MG	C4-C5-N7	2.77	112.03	109.48
1	A	527	7MG	C6-N1-C2	2.79	119.81	115.94
1	A	1541	PSU	O4'-C1'-C2'	2.86	107.64	104.73
1	A	1541	PSU	C6-N1-C2	3.07	120.41	115.47
1	A	1540	PSU	C6-N1-C2	3.27	120.73	115.47
1	A	1540	PSU	O4'-C1'-C2'	3.43	108.22	104.73
1	A	1498	UR3	C6-C5-C4	3.75	124.29	117.28
1	A	966	M2G	N3-C2-N2	4.15	121.86	117.16
1	A	1207	2MG	C6-N1-C2	4.89	122.42	115.31
1	A	1540	PSU	C4-N3-C2	5.13	119.68	115.25
1	A	1541	PSU	C4-N3-C2	5.48	119.99	115.25
1	A	516	PSU	C4-N3-C2	6.18	120.59	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1207	2MG	3	0
1	A	1400	5MC	3	0
1	A	1402	4OC	4	0
1	A	1404	5MC	3	0
1	A	1407	5MC	1	0
1	A	1498	UR3	6	0
1	A	1518[A]	MA6	2	0
1	A	1519[A]	MA6	2	0
1	A	516	PSU	1	0
1	A	966	M2G	3	0
1	A	967	5MC	7	0
12	L	92	0TD	6	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 276 ligands modelled in this entry, 276 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	-0.09	51 (3%) 49 34	93, 162, 316, 389	0
2	B	234/256 (91%)	-0.20	0 100 100	133, 184, 270, 282	0
3	C	206/239 (86%)	0.14	20 (9%) 10 6	206, 252, 287, 299	0
4	D	208/209 (99%)	-0.11	8 (3%) 44 30	111, 168, 217, 268	0
5	E	150/162 (92%)	-0.22	0 100 100	94, 134, 188, 231	0
6	F	101/101 (100%)	-0.37	0 100 100	133, 181, 218, 291	0
7	G	155/156 (99%)	0.06	4 (2%) 59 43	158, 220, 277, 309	0
8	H	138/138 (100%)	-0.48	0 100 100	95, 124, 178, 206	0
9	I	127/128 (99%)	0.70	17 (13%) 4 4	171, 232, 283, 313	0
10	J	98/105 (93%)	0.91	22 (22%) 1 1	209, 279, 336, 389	0
11	K	116/129 (89%)	-0.03	2 (1%) 73 58	115, 162, 201, 226	0
12	L	123/135 (91%)	0.19	5 (4%) 41 27	107, 168, 206, 263	0
13	M	118/126 (93%)	0.56	22 (18%) 2 1	154, 195, 252, 307	0
14	N	60/61 (98%)	0.01	3 (5%) 32 21	202, 244, 301, 320	0
15	O	87/89 (97%)	-0.15	0 100 100	118, 158, 219, 250	0
16	P	83/88 (94%)	0.16	2 (2%) 62 46	111, 173, 212, 270	0
17	Q	99/105 (94%)	-0.08	1 (1%) 84 72	103, 137, 184, 194	0
18	R	70/88 (79%)	-0.46	1 (1%) 78 64	118, 173, 224, 263	0
19	S	80/93 (86%)	0.63	15 (18%) 2 1	207, 262, 310, 335	0
20	T	99/106 (93%)	-0.13	2 (2%) 68 53	127, 166, 233, 261	0
21	U	24/27 (88%)	0.66	4 (16%) 2 2	150, 219, 232, 233	0
All	All	3874/4063 (95%)	-0.00	179 (4%) 36 24	93, 177, 288, 389	0

All (179) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	I	15	ALA	10.3
1	A	1018	C	7.9
1	A	1003(A)	G	7.8
1	A	1017	G	7.6
9	I	8	GLY	6.6
13	M	7	VAL	6.1
3	C	66	VAL	6.1
9	I	64	THR	5.8
13	M	43	THR	5.8
19	S	12	ASP	5.8
9	I	9	ARG	5.5
9	I	16	ARG	5.4
9	I	13	ALA	5.2
9	I	14	VAL	5.1
10	J	93	GLY	5.1
9	I	7	THR	5.1
1	A	1006	C	4.8
9	I	65	VAL	4.7
4	D	40	PRO	4.6
1	A	1005	A	4.6
14	N	3	ARG	4.5
3	C	103	VAL	4.5
1	A	1037	C	4.5
4	D	41	GLY	4.4
1	A	1036	G	4.4
13	M	117	VAL	4.4
10	J	90	LEU	4.4
10	J	34	VAL	4.3
3	C	65	ALA	4.3
1	A	1002	G	4.3
3	C	67	THR	4.3
13	M	119	GLY	4.3
1	A	1019	C	4.2
1	A	1539	C	4.1
19	S	31	ILE	4.0
13	M	10	PRO	4.0
10	J	10	GLY	3.9
13	M	15	VAL	3.9
4	D	42	GLN	3.9
1	A	990	C	3.9
13	M	8	GLU	3.8
14	N	5	ALA	3.8
3	C	64	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
19	S	38	SER	3.8
13	M	45	VAL	3.7
1	A	1004	A	3.7
1	A	1024	G	3.7
1	A	993	G	3.6
21	U	17	THR	3.6
7	G	2	ALA	3.6
9	I	17	VAL	3.5
9	I	66	ARG	3.5
1	A	1033	G	3.5
13	M	118	ALA	3.5
10	J	39	PRO	3.5
10	J	94	VAL	3.5
1	A	1148	U	3.4
3	C	193	TYR	3.4
1	A	1032	G	3.3
13	M	6	GLY	3.3
10	J	96	ILE	3.3
21	U	18	TYR	3.3
19	S	41	VAL	3.3
1	A	1025	U	3.3
3	C	104	GLN	3.2
1	A	1023	G	3.2
3	C	102	ASN	3.2
1	A	1224	G	3.2
13	M	44	ARG	3.2
13	M	104	ARG	3.1
10	J	65	LEU	3.1
1	A	994	A	3.1
13	M	9	ILE	3.0
1	A	1016	A	3.0
7	G	69	VAL	3.0
10	J	7	LYS	3.0
10	J	95	GLU	3.0
3	C	201	TYR	2.9
4	D	35	ARG	2.9
13	M	30	ALA	2.9
4	D	125	HIS	2.9
10	J	70	ARG	2.9
3	C	155	GLY	2.9
20	T	106	ALA	2.9
1	A	218	C	2.8

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Mol	Chain	Res	Type	RSRZ
13	M	16	ASP	2.8
19	S	40	ILE	2.8
9	I	67	GLY	2.7
10	J	91	PRO	2.7
1	A	328	C	2.7
13	M	4	ILE	2.7
10	J	9	ARG	2.7
11	K	28	THR	2.6
10	J	74	ILE	2.6
1	A	1129	C	2.6
10	J	67	THR	2.6
20	T	9	ASN	2.6
10	J	97	GLU	2.6
17	Q	45	HIS	2.6
13	M	33	ALA	2.5
19	S	14	HIS	2.5
12	L	73	GLU	2.5
12	L	72	GLY	2.5
9	I	18	PHE	2.5
3	C	68	VAL	2.5
1	A	1212	U	2.5
19	S	13	ASP	2.5
4	D	13	ARG	2.5
13	M	5	ALA	2.5
10	J	40	LEU	2.4
3	C	146	ALA	2.4
21	U	24	ARG	2.4
3	C	53	ALA	2.4
1	A	964	A	2.4
13	M	2	ALA	2.4
1	A	991	U	2.4
1	A	1035	A	2.4
4	D	45	GLN	2.4
1	A	1001	A	2.4
3	C	42	LEU	2.4
1	A	184	G	2.4
9	I	63	ILE	2.4
1	A	1007	C	2.3
1	A	1260	C	2.3
21	U	5	ASP	2.3
1	A	633	G	2.3
3	C	43	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
3	C	157	ILE	2.3
3	C	195	VAL	2.3
12	L	96	VAL	2.3
10	J	11	PHE	2.3
1	A	1209	C	2.3
1	A	1226	C	2.3
1	A	995	C	2.3
1	A	1030(B)	C	2.3
19	S	79	THR	2.3
3	C	46	GLU	2.3
19	S	70	LYS	2.3
4	D	44	GLY	2.3
13	M	41	PRO	2.3
1	A	81	U	2.3
9	I	102	LEU	2.2
19	S	21	GLU	2.2
19	S	17	GLU	2.2
1	A	327	A	2.2
1	A	110	C	2.2
19	S	32	LYS	2.2
11	K	29	ILE	2.2
9	I	29	ASN	2.2
9	I	4	TYR	2.2
1	A	1038	C	2.2
16	P	13	HIS	2.2
1	A	109	A	2.2
18	R	88	LYS	2.2
7	G	3	ARG	2.1
1	A	705	U	2.1
1	A	792	A	2.1
13	M	40	ASN	2.1
1	A	952	U	2.1
13	M	105	THR	2.1
19	S	15	LEU	2.1
1	A	1147	C	2.1
12	L	85	ILE	2.1
1	A	329	A	2.1
19	S	35	SER	2.1
1	A	1026	G	2.1
10	J	33	GLN	2.1
12	L	114	LYS	2.1
3	C	58	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
16	P	83	GLU	2.1
7	G	12	LEU	2.0
1	A	972	C	2.0
10	J	64	GLU	2.0
3	C	57	ILE	2.0
1	A	224	C	2.0
10	J	54	PHE	2.0
14	N	22	THR	2.0
10	J	100	THR	2.0
19	S	80	TYR	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	PSU	A	1541	20/21	0.89	0.60	-	303,317,323,326	0
1	5MC	A	1407	21/22	0.95	0.12	-	180,203,212,220	0
1	MA6	A	1518[B]	24/25	0.88	0.31	-	132,148,153,153	24
1	MA6	A	1519[B]	24/25	0.94	0.44	-	123,131,165,167	24
1	PSU	A	516	20/21	0.91	0.10	-	169,189,225,229	0
1	4OC	A	1402	22/23	0.93	0.20	-	130,142,160,168	0
1	2MG	A	1207	24/25	0.95	0.15	-	239,249,316,321	0
1	7MG	A	527	24/25	0.91	0.22	-	142,153,170,174	0
1	5MC	A	1400	21/22	0.95	0.17	-	125,139,150,167	0
1	MA6	A	1518[A]	24/25	0.88	0.31	-	133,147,161,163	24
1	PSU	A	1540	20/21	0.53	0.95	-	318,324,373,375	0
1	UR3	A	1498	21/22	0.97	0.38	-	131,139,164,169	0
1	5MC	A	1404	21/22	0.92	0.22	-	132,144,188,193	0
1	5MC	A	967	21/22	0.96	0.13	-	154,169,181,182	0
1	M2G	A	966	25/26	0.96	0.15	-	168,177,186,189	0
12	0TD	L	92	10/11	0.95	0.58	-	161,185,287,345	0
1	MA6	A	1519[A]	24/25	0.94	0.44	-	118,127,134,135	24

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
22	MG	A	1605	1/1	0.90	0.99	47.46	103,103,103,103	0
22	MG	A	1786	1/1	0.95	0.35	16.45	131,131,131,131	0
22	MG	A	1755	1/1	0.88	0.41	15.90	150,150,150,150	0
22	MG	A	1828	1/1	0.90	0.41	14.73	114,114,114,114	0
22	MG	A	1747	1/1	0.52	0.63	13.95	132,132,132,132	0
22	MG	A	1816	1/1	0.72	0.29	10.78	181,181,181,181	0
22	MG	A	1792	1/1	0.96	0.32	10.05	313,313,313,313	0
22	MG	A	1711	1/1	0.91	0.45	10.04	185,185,185,185	0
22	MG	I	201	1/1	0.99	0.73	9.82	138,138,138,138	0
22	MG	A	1670	1/1	0.87	0.25	7.26	199,199,199,199	0
22	MG	A	1817	1/1	0.93	0.28	6.65	148,148,148,148	0
22	MG	A	1789	1/1	0.95	0.38	5.58	157,157,157,157	0
22	MG	A	1833	1/1	0.86	0.35	5.17	182,182,182,182	0
22	MG	A	1809	1/1	0.93	0.26	4.91	114,114,114,114	0
22	MG	A	1728	1/1	0.87	0.41	4.71	138,138,138,138	0
22	MG	J	201	1/1	0.92	0.57	4.66	128,128,128,128	0
22	MG	A	1706	1/1	0.97	0.37	4.21	105,105,105,105	0
22	MG	A	1738	1/1	0.94	0.27	3.65	113,113,113,113	0
22	MG	A	1656	1/1	0.94	0.30	2.66	106,106,106,106	0
22	MG	A	1776	1/1	0.71	0.26	2.57	139,139,139,139	0
22	MG	A	1661	1/1	0.90	0.24	2.23	120,120,120,120	0
22	MG	A	1740	1/1	0.98	0.18	1.57	119,119,119,119	0
22	MG	A	1662	1/1	0.71	0.33	1.54	108,108,108,108	0
22	MG	A	1616	1/1	0.98	0.32	1.39	85,85,85,85	0
22	MG	A	1751	1/1	0.99	0.23	1.39	104,104,104,104	0
22	MG	A	1823	1/1	0.92	0.25	1.34	128,128,128,128	0
22	MG	A	1847	1/1	0.69	0.14	1.29	145,145,145,145	0
22	MG	A	1767	1/1	0.99	0.48	1.15	130,130,130,130	0
22	MG	A	1790	1/1	0.89	0.17	1.12	217,217,217,217	0
22	MG	A	1667	1/1	0.34	0.37	1.06	157,157,157,157	0
22	MG	A	1630	1/1	0.93	0.27	0.99	124,124,124,124	0
22	MG	A	1651	1/1	0.96	0.21	0.79	113,113,113,113	0
22	MG	A	1621	1/1	0.88	0.20	0.78	149,149,149,149	0
22	MG	A	1757	1/1	0.96	0.22	0.76	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
22	MG	A	1648	1/1	0.95	0.27	0.56	149,149,149,149	0
22	MG	D	303	1/1	0.86	0.20	0.41	137,137,137,137	0
22	MG	A	1641	1/1	0.84	0.24	0.28	130,130,130,130	0
22	MG	A	1713	1/1	0.96	0.16	0.17	229,229,229,229	0
22	MG	A	1615	1/1	0.98	0.19	0.16	81,81,81,81	0
22	MG	A	1793	1/1	0.91	0.24	0.14	444,444,444,444	0
22	MG	A	1801	1/1	0.89	0.20	0.13	129,129,129,129	0
22	MG	A	1707	1/1	0.99	0.16	0.11	208,208,208,208	0
22	MG	A	1737	1/1	0.93	0.24	0.10	119,119,119,119	0
22	MG	A	1693	1/1	0.99	0.15	0.02	160,160,160,160	0
22	MG	A	1708	1/1	0.96	0.24	0.00	155,155,155,155	0
22	MG	D	302	1/1	0.95	0.17	-0.02	137,137,137,137	0
23	ZN	D	301	1/1	1.00	0.29	-0.07	154,154,154,154	0
22	MG	A	1814	1/1	0.93	0.16	-0.22	70,70,70,70	0
22	MG	A	1647	1/1	0.97	0.17	-0.28	175,175,175,175	0
22	MG	A	1760	1/1	0.84	0.24	-0.48	140,140,140,140	0
23	ZN	N	101	1/1	0.94	0.18	-0.48	223,223,223,223	0
22	MG	C	301	1/1	0.79	0.21	-0.50	143,143,143,143	0
22	MG	A	1736	1/1	0.96	0.18	-0.54	99,99,99,99	0
22	MG	A	1851	1/1	0.95	0.10	-0.64	366,366,366,366	0
22	MG	A	1778	1/1	0.97	0.15	-0.71	127,127,127,127	0
22	MG	A	1788	1/1	0.97	0.29	-0.76	151,151,151,151	0
22	MG	B	301	1/1	0.77	0.10	-0.86	132,132,132,132	0
22	MG	F	201	1/1	0.92	0.13	-1.07	127,127,127,127	0
22	MG	A	1631	1/1	1.00	0.14	-1.10	154,154,154,154	0
22	MG	A	1720	1/1	0.95	0.14	-1.12	196,196,196,196	0
22	MG	A	1610	1/1	0.99	0.11	-1.59	112,112,112,112	0
22	MG	A	1607	1/1	0.99	0.14	-1.63	105,105,105,105	0
22	MG	A	1717	1/1	0.99	0.08	-1.88	157,157,157,157	0
22	MG	A	1710	1/1	0.98	0.14	-1.98	94,94,94,94	0
22	MG	A	1663	1/1	0.99	0.07	-2.47	162,162,162,162	0
22	MG	A	1634	1/1	0.97	0.07	-2.53	161,161,161,161	0
22	MG	A	1644	1/1	0.98	0.05	-5.54	111,111,111,111	0
22	MG	A	1660	1/1	0.84	0.29	-	155,155,155,155	0
22	MG	A	1727	1/1	0.95	0.18	-	106,106,106,106	0
22	MG	A	1649	1/1	0.99	0.24	-	150,150,150,150	0
22	MG	A	1624	1/1	0.68	0.30	-	134,134,134,134	0
22	MG	A	1723	1/1	0.83	0.81	-	120,120,120,120	0
22	MG	A	1818	1/1	0.92	0.53	-	109,109,109,109	0
22	MG	A	1748	1/1	0.73	0.11	-	177,177,177,177	0
22	MG	A	1777	1/1	0.99	0.36	-	111,111,111,111	0
22	MG	A	1787	1/1	0.92	0.08	-	147,147,147,147	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
22	MG	A	1843	1/1	0.90	0.51	-	132,132,132,132	0
22	MG	A	1672	1/1	0.87	0.32	-	146,146,146,146	0
22	MG	A	1825	1/1	0.94	0.16	-	139,139,139,139	0
22	MG	A	1815	1/1	0.70	0.99	-	124,124,124,124	0
22	MG	A	1629	1/1	0.98	0.15	-	131,131,131,131	0
22	MG	A	1837	1/1	0.97	0.16	-	87,87,87,87	0
22	MG	A	1820	1/1	0.74	0.62	-	144,144,144,144	0
22	MG	A	1835	1/1	0.83	0.73	-	139,139,139,139	0
22	MG	A	1709	1/1	0.99	0.15	-	169,169,169,169	0
22	MG	A	1842	1/1	0.65	0.30	-	152,152,152,152	0
22	MG	A	1698	1/1	0.99	0.33	-	186,186,186,186	0
22	MG	A	1797	1/1	0.70	0.45	-	146,146,146,146	0
22	MG	A	1676	1/1	0.92	0.20	-	136,136,136,136	0
22	MG	A	1726	1/1	0.96	0.09	-	349,349,349,349	0
22	MG	A	1741	1/1	0.94	0.16	-	128,128,128,128	0
22	MG	A	1768	1/1	0.86	0.25	-	166,166,166,166	0
22	MG	A	1620	1/1	0.94	0.25	-	162,162,162,162	0
22	MG	A	1653	1/1	0.98	0.12	-	76,76,76,76	0
22	MG	A	1819	1/1	0.83	0.67	-	137,137,137,137	0
22	MG	A	1802	1/1	0.95	0.74	-	180,180,180,180	0
22	MG	A	1732	1/1	0.84	0.65	-	94,94,94,94	0
22	MG	A	1791	1/1	0.94	0.09	-	294,294,294,294	0
22	MG	A	1627	1/1	0.90	1.47	-	101,101,101,101	0
22	MG	P	101	1/1	0.91	0.26	-	106,106,106,106	0
22	MG	A	1673	1/1	0.76	0.30	-	211,211,211,211	0
22	MG	A	1700	1/1	0.74	0.16	-	204,204,204,204	0
22	MG	A	1679	1/1	0.99	0.37	-	124,124,124,124	0
22	MG	A	1761	1/1	0.91	0.22	-	147,147,147,147	0
22	MG	A	1612	1/1	0.96	0.34	-	178,178,178,178	0
22	MG	A	1849	1/1	0.83	0.20	-	550,550,550,550	0
22	MG	A	1637	1/1	0.87	0.28	-	116,116,116,116	0
22	MG	A	1643	1/1	0.93	0.25	-	102,102,102,102	0
22	MG	A	1805	1/1	0.98	0.09	-	119,119,119,119	0
22	MG	A	1804	1/1	0.94	0.11	-	120,120,120,120	0
22	MG	A	1766	1/1	0.97	0.09	-	126,126,126,126	0
22	MG	A	1701	1/1	0.91	0.33	-	161,161,161,161	0
22	MG	A	1838	1/1	0.80	0.40	-	150,150,150,150	0
22	MG	A	1691	1/1	0.98	0.48	-	155,155,155,155	0
22	MG	A	1721	1/1	0.95	0.17	-	149,149,149,149	0
22	MG	A	1734	1/1	0.88	0.58	-	139,139,139,139	0
22	MG	A	1705	1/1	0.97	0.34	-	319,319,319,319	0
22	MG	A	1742	1/1	0.78	0.55	-	152,152,152,152	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
22	MG	A	1697	1/1	0.95	0.34	-	133,133,133,133	0
22	MG	A	1665	1/1	0.55	0.31	-	111,111,111,111	0
22	MG	A	1671	1/1	0.99	0.09	-	170,170,170,170	0
22	MG	A	1636	1/1	1.00	0.45	-	90,90,90,90	0
22	MG	A	1633	1/1	0.99	0.20	-	198,198,198,198	0
22	MG	A	1666	1/1	0.94	0.20	-	141,141,141,141	0
22	MG	A	1844	1/1	0.55	0.47	-	132,132,132,132	0
22	MG	A	1685	1/1	0.83	0.35	-	159,159,159,159	0
22	MG	A	1811	1/1	0.95	1.03	-	156,156,156,156	0
22	MG	A	1795	1/1	0.44	0.39	-	182,182,182,182	0
22	MG	A	1602	1/1	0.98	0.40	-	168,168,168,168	0
22	MG	A	1848	1/1	0.75	0.26	-	527,527,527,527	0
22	MG	A	1782	1/1	0.86	0.63	-	159,159,159,159	0
22	MG	A	1689	1/1	0.91	1.29	-	214,214,214,214	0
22	MG	A	1687	1/1	0.91	0.12	-	234,234,234,234	0
22	MG	A	1754	1/1	0.98	0.32	-	137,137,137,137	0
22	MG	A	1696	1/1	0.97	0.27	-	160,160,160,160	0
22	MG	A	1765	1/1	0.89	0.12	-	126,126,126,126	0
22	MG	A	1775	1/1	0.85	0.30	-	146,146,146,146	0
22	MG	A	1684	1/1	0.81	0.97	-	135,135,135,135	0
22	MG	A	1796	1/1	0.79	0.30	-	121,121,121,121	0
22	MG	A	1821	1/1	0.94	0.38	-	138,138,138,138	0
22	MG	H	201	1/1	0.48	0.62	-	167,167,167,167	0
22	MG	A	1642	1/1	0.97	0.30	-	98,98,98,98	0
22	MG	A	1722	1/1	0.98	0.29	-	122,122,122,122	0
22	MG	A	1690	1/1	0.91	0.13	-	169,169,169,169	0
22	MG	A	1808	1/1	0.79	0.15	-	164,164,164,164	0
22	MG	A	1803	1/1	0.94	1.15	-	115,115,115,115	0
22	MG	A	1856	1/1	0.92	0.65	-	143,143,143,143	0
22	MG	A	1845	1/1	0.97	0.19	-	113,113,113,113	0
22	MG	A	1655	1/1	0.99	0.12	-	156,156,156,156	0
22	MG	A	1724	1/1	0.97	0.47	-	169,169,169,169	0
22	MG	A	1668	1/1	0.93	0.37	-	134,134,134,134	0
22	MG	A	1645	1/1	0.87	0.90	-	141,141,141,141	0
22	MG	A	1604	1/1	0.98	0.12	-	123,123,123,123	0
22	MG	A	1664	1/1	0.83	0.31	-	121,121,121,121	0
22	MG	A	1683	1/1	0.38	0.41	-	118,118,118,118	0
22	MG	A	1730	1/1	0.82	0.39	-	138,138,138,138	0
22	MG	A	1853	1/1	0.92	0.96	-	150,150,150,150	0
22	MG	A	1758	1/1	0.88	0.52	-	103,103,103,103	0
22	MG	A	1601	1/1	0.83	0.28	-	152,152,152,152	0
22	MG	A	1779	1/1	0.96	0.42	-	112,112,112,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
22	MG	A	1646	1/1	0.95	0.72	-	236,236,236,236	0
22	MG	A	1619	1/1	0.98	0.16	-	106,106,106,106	0
22	MG	A	1675	1/1	0.91	0.89	-	143,143,143,143	0
22	MG	A	1606	1/1	0.99	0.12	-	107,107,107,107	0
22	MG	A	1626	1/1	0.98	1.13	-	105,105,105,105	0
22	MG	A	1692	1/1	0.92	0.25	-	165,165,165,165	0
22	MG	A	1718	1/1	0.93	0.34	-	134,134,134,134	0
22	MG	A	1702	1/1	0.71	0.66	-	166,166,166,166	0
22	MG	A	1794	1/1	0.96	0.16	-	278,278,278,278	0
22	MG	A	1832	1/1	0.91	0.24	-	149,149,149,149	0
22	MG	A	1652	1/1	0.99	0.18	-	132,132,132,132	0
22	MG	A	1800	1/1	0.95	0.19	-	158,158,158,158	0
22	MG	A	1682	1/1	0.71	0.36	-	180,180,180,180	0
22	MG	A	1753	1/1	0.70	0.28	-	136,136,136,136	0
22	MG	A	1719	1/1	0.99	0.29	-	514,514,514,514	0
22	MG	A	1699	1/1	0.96	0.25	-	124,124,124,124	0
22	MG	A	1609	1/1	0.98	0.15	-	120,120,120,120	0
22	MG	A	1613	1/1	0.96	0.23	-	153,153,153,153	0
22	MG	A	1829	1/1	0.53	0.43	-	156,156,156,156	0
22	MG	A	1735	1/1	0.77	0.43	-	93,93,93,93	0
22	MG	A	1860	1/1	0.89	0.53	-	133,133,133,133	0
22	MG	A	1830	1/1	0.94	0.17	-	130,130,130,130	0
22	MG	A	1714	1/1	0.84	0.61	-	162,162,162,162	0
22	MG	A	1798	1/1	0.74	0.21	-	163,163,163,163	0
22	MG	A	1862	1/1	0.84	0.38	-	161,161,161,161	0
22	MG	Q	201	1/1	0.63	0.18	-	142,142,142,142	0
22	MG	A	1774	1/1	0.96	0.40	-	157,157,157,157	0
22	MG	A	1694	1/1	0.80	0.28	-	105,105,105,105	0
22	MG	A	1608	1/1	0.84	0.14	-	169,169,169,169	0
22	MG	A	1614	1/1	0.94	0.19	-	141,141,141,141	0
22	MG	A	1855	1/1	0.81	1.26	-	143,143,143,143	0
22	MG	A	1617	1/1	0.97	0.43	-	175,175,175,175	0
22	MG	A	1658	1/1	0.98	0.23	-	156,156,156,156	0
22	MG	A	1731	1/1	0.83	0.26	-	145,145,145,145	0
22	MG	A	1603	1/1	0.85	0.18	-	137,137,137,137	0
22	MG	A	1764	1/1	0.78	1.50	-	137,137,137,137	0
22	MG	A	1752	1/1	0.82	0.45	-	142,142,142,142	0
22	MG	A	1715	1/1	0.99	0.44	-	112,112,112,112	0
22	MG	A	1846	1/1	0.94	0.20	-	126,126,126,126	0
22	MG	A	1750	1/1	0.91	0.25	-	157,157,157,157	0
22	MG	A	1688	1/1	0.80	0.26	-	164,164,164,164	0
22	MG	A	1834	1/1	0.67	0.42	-	138,138,138,138	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
22	MG	A	1857	1/1	0.77	1.23	-	128,128,128,128	0
22	MG	A	1763	1/1	0.95	0.26	-	111,111,111,111	0
22	MG	A	1635	1/1	0.99	0.12	-	99,99,99,99	0
22	MG	A	1807	1/1	0.63	0.15	-	141,141,141,141	0
22	MG	A	1628	1/1	0.92	0.40	-	141,141,141,141	0
22	MG	A	1831	1/1	0.64	1.11	-	160,160,160,160	0
22	MG	A	1827	1/1	0.90	0.13	-	151,151,151,151	0
22	MG	A	1744	1/1	0.98	0.26	-	127,127,127,127	0
22	MG	A	1785	1/1	0.75	0.19	-	184,184,184,184	0
22	MG	A	1695	1/1	0.99	0.13	-	113,113,113,113	0
22	MG	A	1850	1/1	0.62	0.06	-	450,450,450,450	0
22	MG	A	1743	1/1	0.37	0.62	-	147,147,147,147	0
22	MG	A	1657	1/1	0.96	0.26	-	146,146,146,146	0
22	MG	A	1749	1/1	0.91	0.30	-	157,157,157,157	0
22	MG	A	1677	1/1	0.94	0.23	-	128,128,128,128	0
22	MG	A	1618	1/1	0.90	0.56	-	141,141,141,141	0
22	MG	A	1799	1/1	0.98	0.21	-	125,125,125,125	0
22	MG	A	1780	1/1	0.99	0.21	-	143,143,143,143	0
22	MG	A	1632	1/1	0.62	0.73	-	131,131,131,131	0
22	MG	A	1861	1/1	0.61	1.44	-	178,178,178,178	0
22	MG	A	1812	1/1	0.96	0.33	-	417,417,417,417	0
22	MG	A	1712	1/1	0.96	0.27	-	324,324,324,324	0
22	MG	A	1822	1/1	0.87	0.82	-	148,148,148,148	0
22	MG	A	1686	1/1	0.96	0.11	-	241,241,241,241	0
22	MG	A	1813	1/1	0.88	0.53	-	520,520,520,520	0
22	MG	A	1824	1/1	0.72	0.68	-	139,139,139,139	0
22	MG	A	1654	1/1	0.99	0.11	-	156,156,156,156	0
22	MG	A	1840	1/1	0.88	0.29	-	143,143,143,143	0
22	MG	A	1680	1/1	0.86	0.24	-	175,175,175,175	0
22	MG	A	1650	1/1	0.98	0.12	-	104,104,104,104	0
22	MG	A	1611	1/1	0.93	0.09	-	184,184,184,184	0
22	MG	A	1625	1/1	0.79	0.48	-	101,101,101,101	0
22	MG	A	1703	1/1	0.91	0.17	-	291,291,291,291	0
22	MG	A	1756	1/1	0.97	0.27	-	112,112,112,112	0
22	MG	A	1640	1/1	0.98	0.10	-	186,186,186,186	0
22	MG	A	1839	1/1	0.95	0.13	-	144,144,144,144	0
22	MG	A	1674	1/1	0.96	0.16	-	136,136,136,136	0
22	MG	A	1704	1/1	0.81	0.11	-	211,211,211,211	0
22	MG	A	1858	1/1	0.61	0.97	-	147,147,147,147	0
22	MG	A	1623	1/1	0.91	0.50	-	129,129,129,129	0
22	MG	A	1762	1/1	0.80	0.61	-	124,124,124,124	0
22	MG	A	1854	1/1	0.94	0.77	-	149,149,149,149	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
22	MG	A	1772	1/1	0.79	0.47	-	120,120,120,120	0
22	MG	A	1769	1/1	0.73	0.68	-	151,151,151,151	0
22	MG	A	1678	1/1	0.88	0.24	-	350,350,350,350	0
22	MG	A	1770	1/1	0.82	0.40	-	103,103,103,103	0
22	MG	A	1681	1/1	0.98	0.30	-	167,167,167,167	0
22	MG	A	1859	1/1	0.82	0.13	-	147,147,147,147	0
22	MG	A	1826	1/1	0.98	0.53	-	121,121,121,121	0
22	MG	A	1783	1/1	0.82	0.32	-	119,119,119,119	0
22	MG	A	1622	1/1	0.99	0.09	-	106,106,106,106	0
22	MG	A	1733	1/1	0.88	0.28	-	147,147,147,147	0
22	MG	A	1841	1/1	0.86	0.16	-	147,147,147,147	0
22	MG	A	1729	1/1	0.86	0.26	-	119,119,119,119	0
22	MG	A	1836	1/1	0.97	0.54	-	143,143,143,143	0
22	MG	A	1759	1/1	0.68	0.51	-	126,126,126,126	0
22	MG	A	1639	1/1	0.98	0.16	-	82,82,82,82	0
22	MG	A	1669	1/1	0.95	0.18	-	149,149,149,149	0
22	MG	A	1784	1/1	0.74	0.41	-	175,175,175,175	0
22	MG	D	304	1/1	0.88	0.88	-	147,147,147,147	0
22	MG	A	1746	1/1	0.80	0.71	-	111,111,111,111	0
22	MG	A	1638	1/1	0.96	0.58	-	189,189,189,189	0
22	MG	A	1773	1/1	0.84	0.34	-	156,156,156,156	0
22	MG	A	1659	1/1	0.94	0.21	-	128,128,128,128	0
22	MG	A	1745	1/1	0.73	0.69	-	169,169,169,169	0
22	MG	E	201	1/1	0.78	0.19	-	177,177,177,177	0
22	MG	A	1806	1/1	0.68	0.82	-	127,127,127,127	0
22	MG	A	1716	1/1	0.87	0.27	-	118,118,118,118	0
22	MG	A	1739	1/1	0.93	0.14	-	139,139,139,139	0
22	MG	A	1725	1/1	0.96	0.50	-	156,156,156,156	0
22	MG	A	1852	1/1	0.97	0.51	-	530,530,530,530	0
22	MG	A	1810	1/1	0.61	1.06	-	143,143,143,143	0
22	MG	A	1771	1/1	0.72	0.71	-	127,127,127,127	0
22	MG	A	1781	1/1	0.95	0.90	-	158,158,158,158	0

6.5 Other polymers (i)

There are no such residues in this entry.