



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 07:39 AM GMT

PDB ID : 4DHB
Title : Crystal structure of YAEJ bound to the 70S ribosome
Authors : Gagnon, M.G.; Seetharaman, S.V.; Bulkley, D.P.; Steitz, T.A.
Deposited on : 2012-01-27
Resolution : 3.20 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

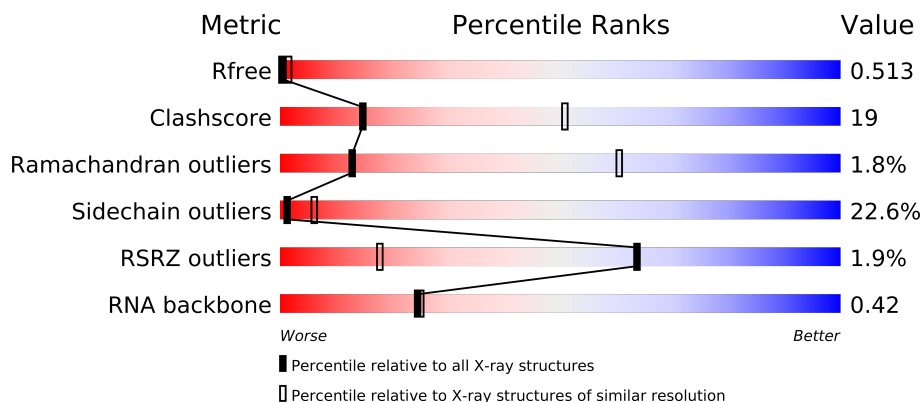
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.20 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.



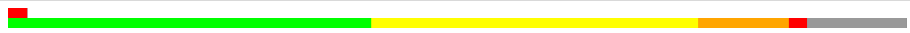
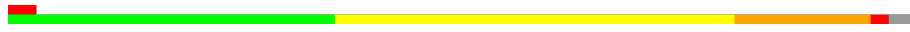


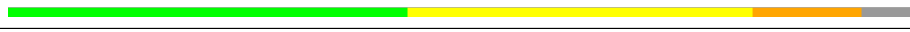

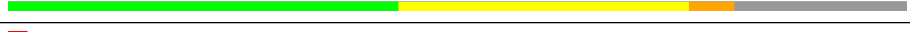


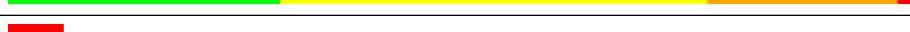
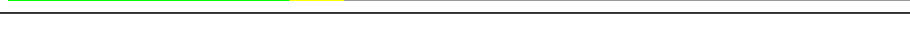
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)
RNA backbone	1838	1002 (3.72-2.68)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1522	
2	B	256	
3	C	239	
4	D	209	
5	E	162	
6	F	101	
7	G	156	
8	H	138	
9	I	128	
10	J	105	
11	K	129	
12	L	132	

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Mol	Chain	Length	Quality of chain
13	M	126	
14	N	61	
15	O	89	
16	P	88	
17	Q	105	
18	R	88	
19	S	93	
20	T	106	
21	U	27	
22	V	77	
23	X	16	

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 51411 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1461	Total	C	N	O	P	0	0	0
			31406	13979	5822	10145	1460			

- Molecule 2 is a protein called 30S Ribosomal Protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	235	Total	C	N	O	S	0	0	1
			1817	1160	325	327	5			

- Molecule 3 is a protein called 30S Ribosomal Protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	206	Total	C	N	O	S	0	0	0
			1453	908	280	264	1			

- Molecule 4 is a protein called 30S Ribosomal Protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	208	Total	C	N	O	S	0	0	0
			1537	968	287	276	6			

- Molecule 5 is a protein called 30S Ribosomal Protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	149	Total	C	N	O	S	0	0	0
			1115	706	206	199	4			

- Molecule 6 is a protein called 30S Ribosomal Protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	100	Total	C	N	O	S	0	0	0
			784	496	137	148	3			

- Molecule 7 is a protein called 30S Ribosomal Protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	154	Total	C	N	O	S	0	0	0
			1149	715	222	206	6			

- Molecule 8 is a protein called 30S Ribosomal Protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	138	Total	C	N	O	S	0	0	0
			1049	667	188	192	2			

- Molecule 9 is a protein called 30S Ribosomal Protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	125	Total	C	N	O	0	0	0
			849	531	161	157			

- Molecule 10 is a protein called 30S Ribosomal Protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	96	Total	C	N	O	0	0	0
			657	407	129	121			

- Molecule 11 is a protein called 30S Ribosomal Protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	114	Total	C	N	O	S	0	0	0
			828	516	155	154	3			

- Molecule 12 is a protein called 30S Ribosomal Protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	122	Total	C	N	O	S	0	0	0
			905	567	178	159	1			

- Molecule 13 is a protein called 30S Ribosomal Protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	112	Total	C	N	O	S	0	0	0
			784	486	159	138	1			

- Molecule 14 is a protein called 30S Ribosomal Protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	59	Total	C	N	O	S	0	0	0
			469	297	97	71	4			

- Molecule 15 is a protein called 30S Ribosomal Protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	88	Total	C	N	O	S	0	0	0
			724	453	143	126	2			

- Molecule 16 is a protein called 30S Ribosomal Protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	82	Total	C	N	O	S	0	0	0
			661	421	126	113	1			

- Molecule 17 is a protein called 30S Ribosomal Protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	99	Total	C	N	O	S	0	0	0
			819	525	150	142	2			

- Molecule 18 is a protein called 30S Ribosomal Protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	68	Total	C	N	O	0	0	0
			514	329	98	87			

- Molecule 19 is a protein called 30S Ribosomal Protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	75	Total	C	N	O	S	0	0	0
			529	332	102	93	2			

- Molecule 20 is a protein called 30S Ribosomal Protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	104	Total	C	N	O	S	0	0	0
			773	476	162	133	2			

- Molecule 21 is a protein called 30S Ribosomal Protein THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	23	Total	C	N	O	0	0	0
			180	112	41	27			

- Molecule 22 is a RNA chain called P-site fMet-tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	77	Total	C	N	O	P	0	0	0
			1644	732	297	538	77			

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	X	6	Total	C	N	O	P	0	0	0
			131	59	27	39	6			

- Molecule 24 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	D	1	Total	Mg	0	0
			1	1		
24	V	13	Total	Mg	0	0
			13	13		
24	A	230	Total	Mg	0	0
			230	230		
24	T	1	Total	Mg	0	0
			1	1		
24	X	1	Total	Mg	0	0
			1	1		
24	O	1	Total	Mg	0	0
			1	1		

- Molecule 25 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 26 is water.

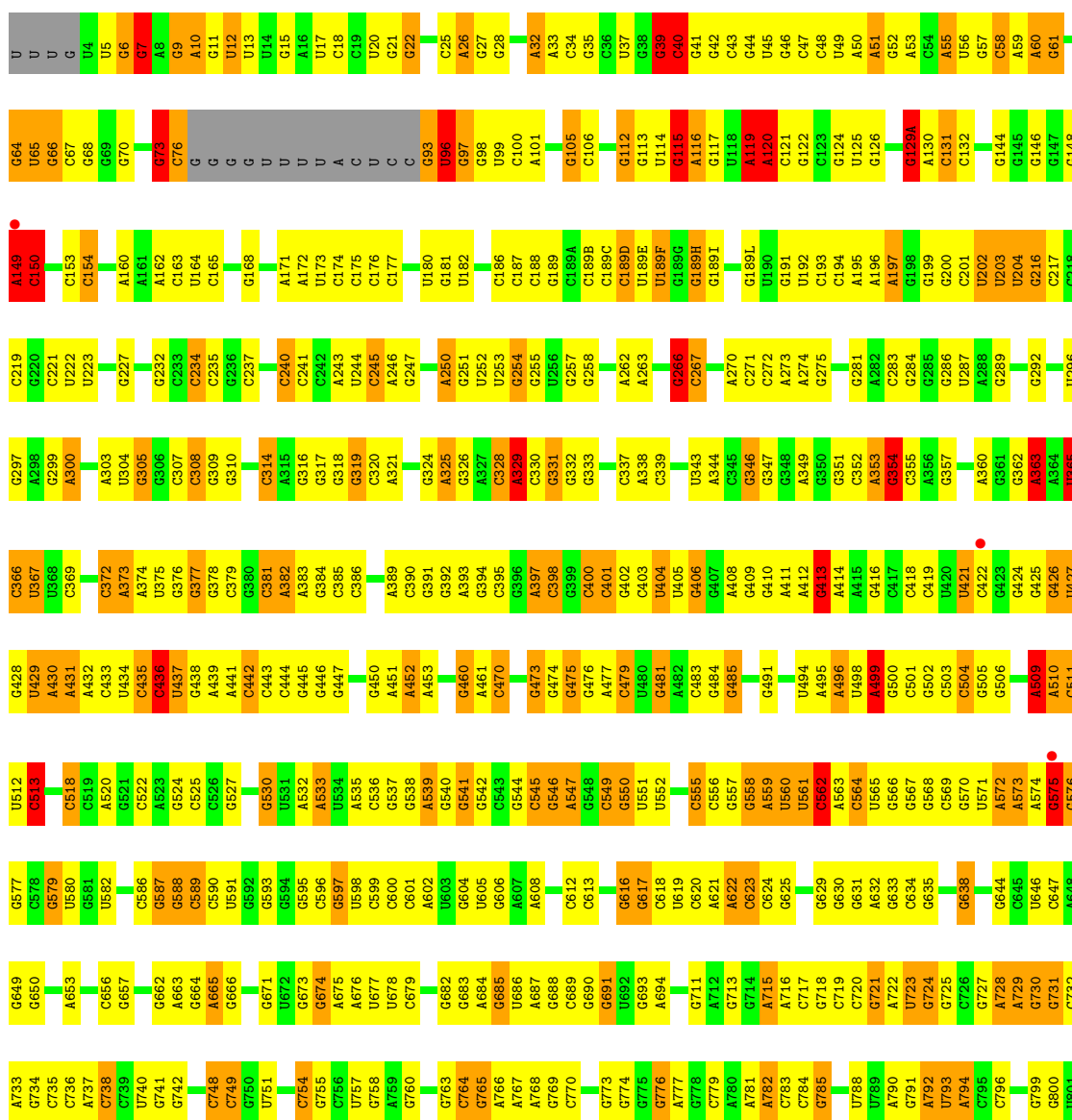
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	347	Total O 347 347	0	0
26	B	1	Total O 1 1	0	0
26	C	1	Total O 1 1	0	0
26	D	3	Total O 3 3	0	0
26	K	2	Total O 2 2	0	0
26	L	1	Total O 1 1	0	0
26	N	2	Total O 2 2	0	0
26	O	2	Total O 2 2	0	0
26	Q	1	Total O 1 1	0	0
26	T	2	Total O 2 2	0	0
26	V	22	Total O 22 22	0	0
26	X	1	Total O 1 1	0	0

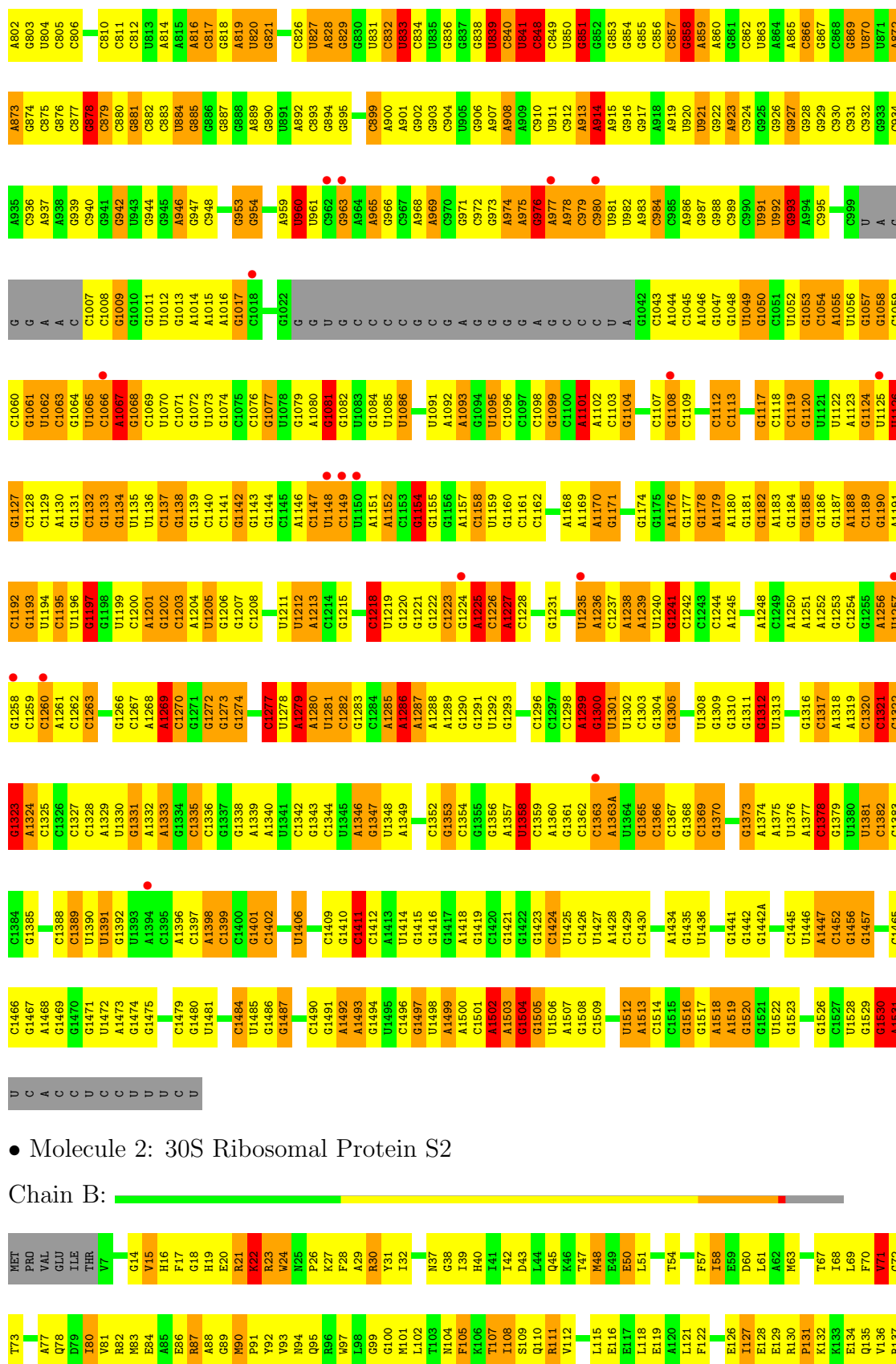
3 Residue-property plots

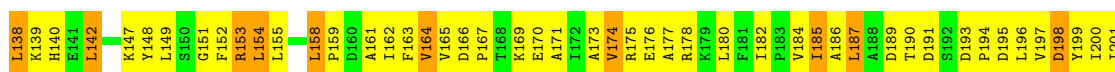
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 Ribosomal RNA

Chain A: 

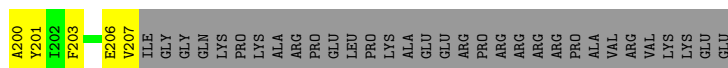
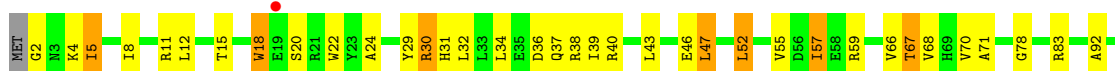






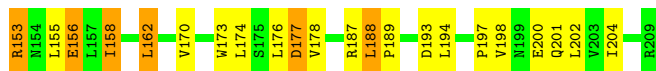
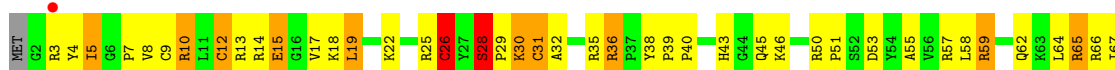
• Molecule 3: 30S Ribosomal Protein S3

Chain C:



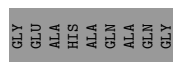
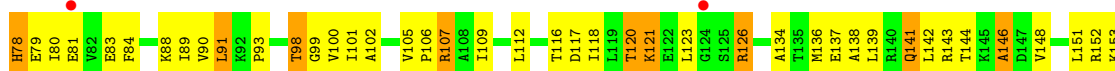
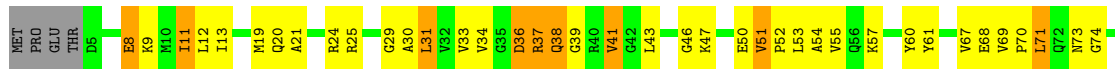
• Molecule 4: 30S Ribosomal Protein S4

Chain D:



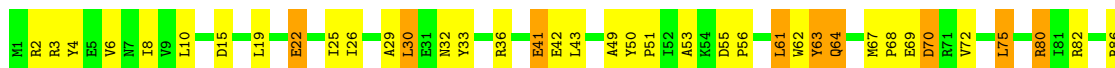
• Molecule 5: 30S Ribosomal Protein S5

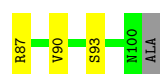
Chain E:



• Molecule 6: 30S Ribosomal Protein S6

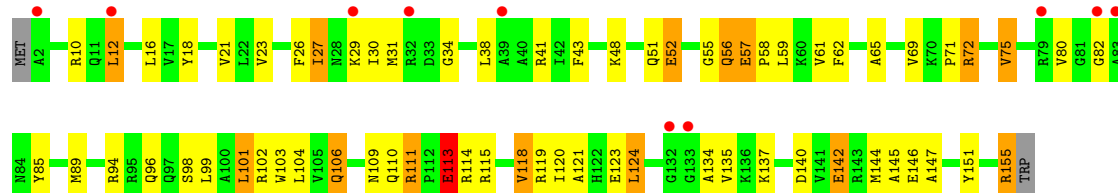
Chain F:





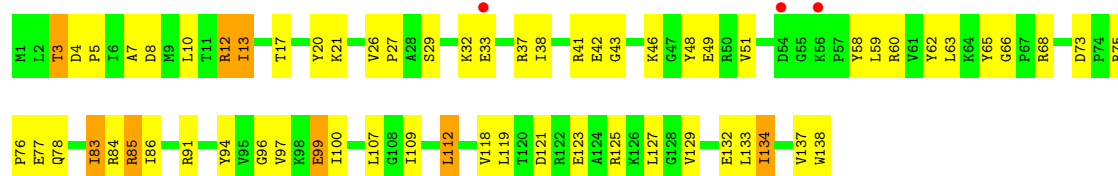
• Molecule 7: 30S Ribosomal Protein S7

Chain G:



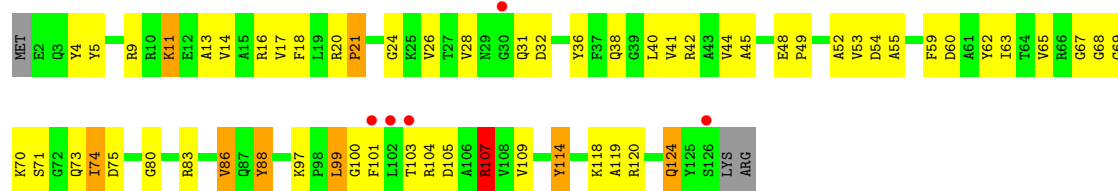
• Molecule 8: 30S Ribosomal Protein S8

Chain H:



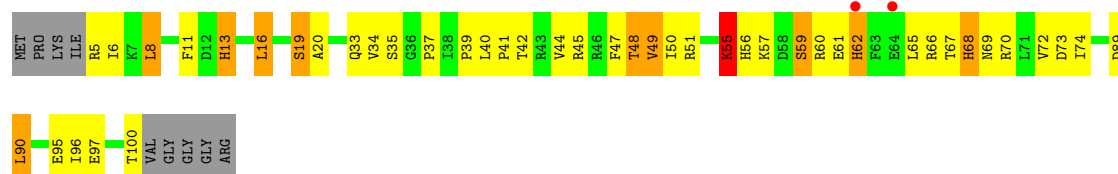
• Molecule 9: 30S Ribosomal Protein S9

Chain I:



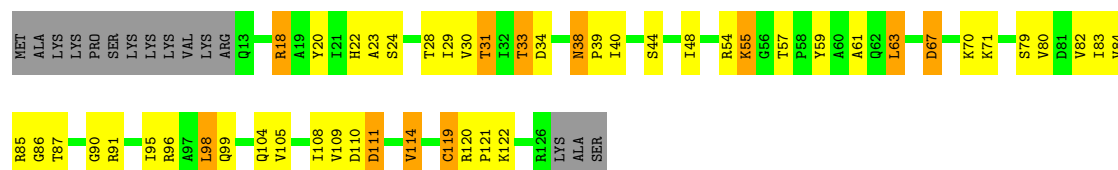
• Molecule 10: 30S Ribosomal Protein S10

Chain J:



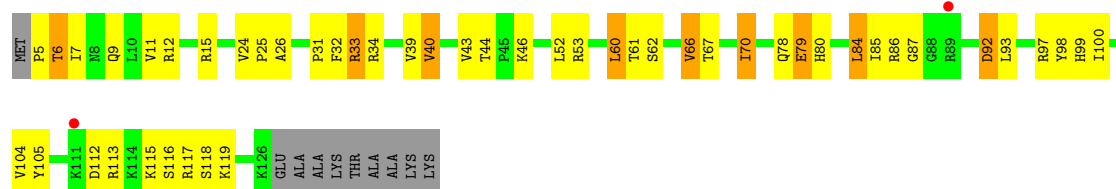
• Molecule 11: 30S Ribosomal Protein S11

Chain K:



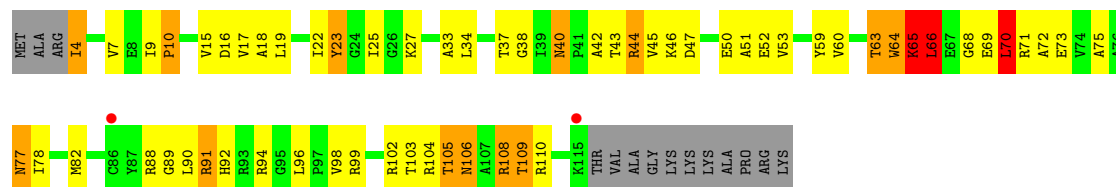
- Molecule 12: 30S Ribosomal Protein S12

Chain L:



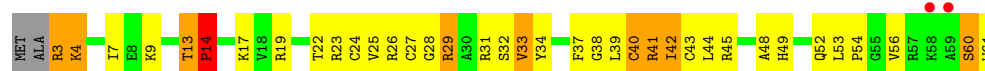
- Molecule 13: 30S Ribosomal Protein S13

Chain M:



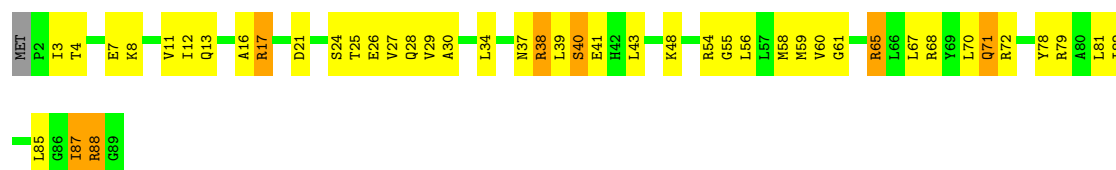
- Molecule 14: 30S Ribosomal Protein S14

Chain N:



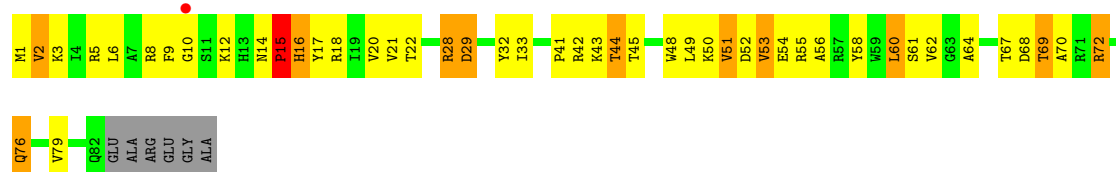
- Molecule 15: 30S Ribosomal Protein S15

Chain O:



- Molecule 16: 30S Ribosomal Protein S16

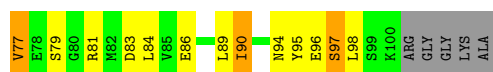
Chain P:



- Molecule 17: 30S Ribosomal Protein S17

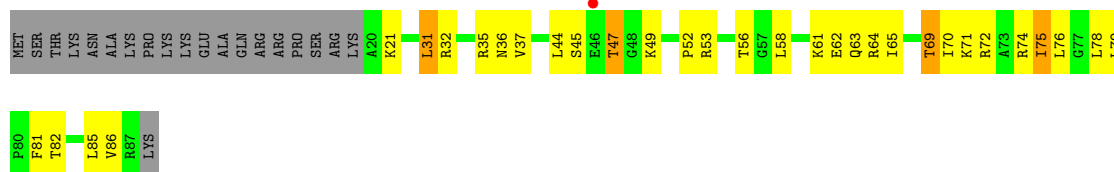
Chain Q:





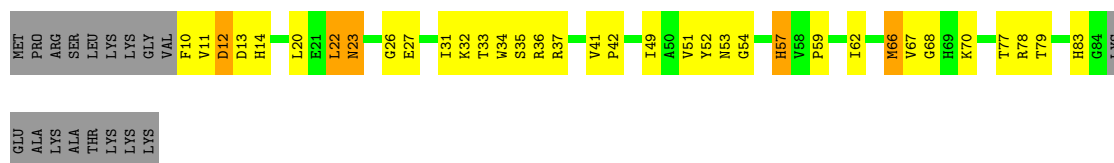
• Molecule 18: 30S Ribosomal Protein S18

Chain R:



• Molecule 19: 30S Ribosomal Protein S19

Chain S:



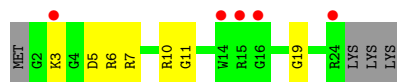
• Molecule 20: 30S Ribosomal Protein S20

Chain T:



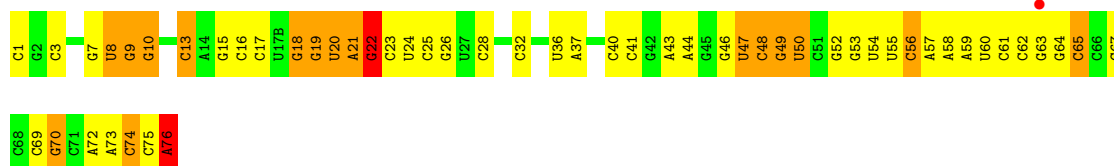
• Molecule 21: 30S Ribosomal Protein THX

Chain U:



• Molecule 22: P-site fMet-tRNA

Chain V:



• Molecule 23: mRNA

Chain X:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.96Å 448.86Å 624.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.91 – 3.20 34.91 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (34.91-3.20) 99.8 (34.91-3.20)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 3.18Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.188 , 0.245 0.512 , 0.513	Depositor DCC
R_{free} test set	48022 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	73.8	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 65.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 956750 reflections	Xtriage
F_o, F_c correlation	0.45	EDS
Total number of atoms	51411	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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	0.89	15/35152 (0.0%)	1.51	525/54858 (1.0%)
2	B	0.55	0/1852	0.79	1/2510 (0.0%)
3	C	0.53	0/1477	0.75	0/2006
4	D	0.70	3/1567 (0.2%)	0.95	4/2125 (0.2%)
5	E	0.68	0/1131	0.92	0/1529
6	F	0.60	0/797	0.81	0/1085
7	G	0.53	0/1166	0.77	0/1576
8	H	0.57	0/1069	0.80	0/1450
9	I	0.53	0/864	0.80	1/1177 (0.1%)
10	J	0.55	0/670	0.84	0/917
11	K	0.58	0/843	0.77	0/1144
12	L	0.64	0/921	0.88	0/1247
13	M	0.55	0/794	0.81	1/1081 (0.1%)
14	N	0.60	0/478	0.86	0/638
15	O	0.59	0/735	0.84	0/981
16	P	0.60	0/677	0.91	0/917
17	Q	0.63	0/832	0.84	1/1113 (0.1%)
18	R	0.59	0/519	0.79	0/699
19	S	0.46	0/543	0.73	1/740 (0.1%)
20	T	0.62	0/776	0.85	0/1026
21	U	0.60	0/184	0.78	0/244
22	V	0.78	1/1836 (0.1%)	1.29	11/2859 (0.4%)
23	X	0.85	0/147	1.11	0/227
All	All	0.80	19/55030 (0.0%)	1.34	545/82149 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	2
4	D	0	5
5	E	0	1
7	G	0	1
10	J	0	2
13	M	0	2
14	N	0	1
16	P	0	1
20	T	0	2
21	U	0	1
All	All	0	19

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	189(D)	C	N3-C4	-15.70	1.23	1.33
1	A	129(A)	G	N1-C2	-14.59	1.26	1.37
1	A	189(D)	C	C2-N3	-13.63	1.24	1.35
1	A	129(A)	G	C6-N1	-13.61	1.30	1.39
22	V	1	C	OP3-P	-10.44	1.48	1.61
4	D	12	CYS	CB-SG	8.07	1.96	1.82
1	A	129(A)	G	C6-O6	7.32	1.30	1.24
1	A	189(D)	C	N1-C6	7.01	1.41	1.37
1	A	189(D)	C	C4-N4	-6.73	1.27	1.33
1	A	115	G	N7-C5	-6.47	1.35	1.39
4	D	26	CYS	CB-SG	6.34	1.93	1.82
1	A	129(A)	G	C8-N7	6.24	1.34	1.30
1	A	189(D)	C	C2-O2	6.19	1.30	1.24
1	A	1279	A	N9-C4	6.05	1.41	1.37
1	A	969	A	N9-C4	5.95	1.41	1.37
1	A	129(A)	G	N3-C4	5.44	1.39	1.35
1	A	129(A)	G	C5-C4	5.29	1.42	1.38
4	D	31	CYS	CB-SG	5.13	1.91	1.82
1	A	1513	A	C5-C6	-5.07	1.36	1.41

All (545) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189(D)	C	N1-C2-O2	44.80	145.78	118.90
1	A	189(D)	C	N3-C4-N4	-44.60	86.78	118.00
1	A	129(A)	G	N3-C2-N2	37.08	145.85	119.90
1	A	129(A)	G	C5-C6-O6	36.54	150.53	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189(D)	C	C5-C4-N4	34.87	144.61	120.20
1	A	129(A)	G	N1-C6-O6	-31.33	101.10	119.90
1	A	129(A)	G	N1-C2-N2	-29.48	89.67	116.20
1	A	189(D)	C	N3-C2-O2	-25.39	104.13	121.90
1	A	189(D)	C	C4-C5-C6	-20.88	106.96	117.40
1	A	189(D)	C	C2-N3-C4	19.88	129.84	119.90
1	A	1363(A)	A	N1-C6-N6	-17.69	107.99	118.60
1	A	189(D)	C	N3-C4-C5	15.74	128.19	121.90
1	A	129(A)	G	C6-N1-C2	15.37	134.32	125.10
1	A	189(D)	C	N1-C2-N3	-13.03	110.08	119.20
1	A	1358	U	N3-C4-O4	-12.61	110.57	119.40
1	A	1149	C	C6-N1-C2	-10.89	115.94	120.30
1	A	728	A	C8-N9-C4	-10.69	101.52	105.80
1	A	266	G	C5-N7-C8	-10.37	99.12	104.30
1	A	1363(A)	A	C5-C6-N6	10.31	131.95	123.70
1	A	899	C	C6-N1-C2	10.25	124.40	120.30
1	A	299	G	N1-C6-O6	10.07	125.94	119.90
1	A	400	C	C6-N1-C2	10.02	124.31	120.30
1	A	893	C	C6-N1-C2	9.96	124.28	120.30
22	V	76	A	C8-N9-C4	9.84	109.74	105.80
1	A	1279	A	C8-N9-C4	-9.74	101.91	105.80
1	A	1279	A	N7-C8-N9	9.61	118.61	113.80
1	A	266	G	C4-C5-N7	9.35	114.54	110.80
1	A	194	C	C6-N1-C2	-9.19	116.62	120.30
1	A	1112	C	C6-N1-C2	-9.18	116.63	120.30
1	A	1519	A	C8-N9-C4	-9.05	102.18	105.80
1	A	1358	U	C2-N3-C4	-9.02	121.59	127.00
1	A	266	G	N7-C8-N9	8.91	117.55	113.10
1	A	802	A	C8-N9-C4	-8.81	102.27	105.80
4	D	188	LEU	CA-CB-CG	8.75	135.42	115.30
1	A	1381	U	N1-C2-O2	8.59	128.81	122.80
1	A	899	C	N3-C4-C5	8.59	125.33	121.90
1	A	1267	C	N1-C2-O2	8.56	124.04	118.90
1	A	1267	C	C2-N1-C1'	8.53	128.18	118.80
1	A	839	U	N1-C2-O2	8.51	128.76	122.80
1	A	1358	U	C5-C4-O4	8.48	130.99	125.90
1	A	129(A)	G	C6-C5-N7	8.46	135.47	130.40
1	A	1054	C	C6-N1-C2	-8.42	116.93	120.30
1	A	638	G	C8-N9-C4	8.38	109.75	106.40
1	A	1484	C	C6-N1-C2	8.36	123.64	120.30
1	A	317	G	C8-N9-C4	-8.31	103.08	106.40
1	A	839	U	N3-C2-O2	-8.27	116.41	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	841	U	C5-C6-N1	8.27	126.84	122.70
1	A	1381	U	N3-C2-O2	-8.22	116.44	122.20
1	A	960	U	C2-N1-C1'	8.22	127.56	117.70
1	A	1158	C	N1-C2-O2	8.21	123.82	118.90
1	A	40	C	N1-C2-O2	8.13	123.78	118.90
1	A	1499	A	C8-N9-C4	8.07	109.03	105.80
1	A	1366	C	C2-N3-C4	8.04	123.92	119.90
1	A	129(A)	G	C4-C5-N7	-8.01	107.60	110.80
1	A	1119	C	C6-N1-C2	-7.98	117.11	120.30
1	A	1197	G	N3-C4-N9	7.93	130.76	126.00
1	A	1133	G	N3-C4-N9	-7.93	121.24	126.00
1	A	398	C	N3-C4-N4	-7.89	112.47	118.00
1	A	1149	C	C5-C6-N1	7.83	124.91	121.00
1	A	960	U	N1-C2-O2	7.82	128.27	122.80
1	A	599	C	C6-N1-C2	7.76	123.41	120.30
1	A	1321	C	C6-N1-C2	-7.76	117.19	120.30
1	A	372	C	C6-N1-C2	7.72	123.39	120.30
1	A	1077	G	C8-N9-C4	7.71	109.48	106.40
1	A	513	C	N1-C2-O2	7.68	123.51	118.90
1	A	1441	G	C8-N9-C4	-7.63	103.35	106.40
1	A	28	G	C8-N9-C4	-7.54	103.38	106.40
1	A	1218	C	C6-N1-C2	-7.52	117.29	120.30
1	A	1197	G	N3-C4-C5	-7.50	124.85	128.60
1	A	893	C	N1-C2-O2	7.47	123.38	118.90
1	A	1366	C	C5-C4-N4	7.47	125.43	120.20
1	A	299	G	C6-C5-N7	-7.46	125.92	130.40
1	A	314	C	C6-N1-C2	-7.46	117.32	120.30
1	A	685	G	N3-C4-N9	-7.46	121.53	126.00
1	A	1279	A	C4-C5-C6	7.45	120.73	117.00
1	A	728	A	N7-C8-N9	7.45	117.53	113.80
1	A	893	C	N3-C4-C5	7.43	124.87	121.90
1	A	1358	U	C5-C6-N1	-7.38	119.01	122.70
1	A	363	A	N1-C6-N6	-7.35	114.19	118.60
1	A	853	G	C8-N9-C4	-7.30	103.48	106.40
1	A	816	A	N1-C6-N6	-7.29	114.22	118.60
1	A	1356	G	C8-N9-C4	-7.27	103.49	106.40
1	A	73	G	N1-C6-O6	-7.26	115.54	119.90
1	A	1158	C	N3-C2-O2	-7.21	116.85	121.90
1	A	1410	G	C8-N9-C4	7.21	109.29	106.40
1	A	1373	G	N3-C4-C5	-7.21	125.00	128.60
1	A	1518	A	C8-N9-C4	-7.21	102.92	105.80
1	A	1519	A	N7-C8-N9	7.20	117.40	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1373	G	N3-C4-N9	7.18	130.31	126.00
1	A	917	G	C8-N9-C4	-7.17	103.53	106.40
1	A	1187	G	N3-C2-N2	-7.13	114.91	119.90
1	A	1391	U	C5-C4-O4	7.10	130.16	125.90
1	A	129(A)	G	O4'-C1'-N9	7.09	113.88	108.20
1	A	892	A	N1-C6-N6	7.08	122.85	118.60
1	A	831	U	C6-N1-C2	-7.08	116.75	121.00
4	D	31	CYS	N-CA-CB	7.08	123.34	110.60
1	A	546	G	N1-C6-O6	-7.08	115.65	119.90
1	A	579	G	N3-C4-C5	-7.07	125.07	128.60
1	A	1277	C	N1-C2-O2	7.05	123.13	118.90
1	A	1523	G	N9-C4-C5	7.03	108.21	105.40
1	A	194	C	C5-C6-N1	7.01	124.50	121.00
1	A	333	G	N1-C6-O6	7.00	124.10	119.90
1	A	1502	A	C5-N7-C8	-6.95	100.43	103.90
1	A	1324	A	C8-N9-C4	-6.93	103.03	105.80
1	A	1267	C	N3-C2-O2	-6.90	117.07	121.90
1	A	1267	C	C6-N1-C2	-6.87	117.55	120.30
1	A	1260	C	C6-N1-C2	-6.87	117.55	120.30
1	A	1205	U	C6-N1-C2	-6.86	116.88	121.00
1	A	976	G	N3-C4-C5	-6.86	125.17	128.60
1	A	851	G	C4-N9-C1'	6.85	135.40	126.50
1	A	1279	A	C4-N9-C1'	6.84	138.62	126.30
1	A	354	G	C6-C5-N7	-6.84	126.30	130.40
1	A	908	A	C8-N9-C4	6.84	108.53	105.80
1	A	513	C	C2-N1-C1'	6.83	126.31	118.80
1	A	1281	U	C5-C6-N1	6.83	126.11	122.70
1	A	1129	C	C6-N1-C2	-6.83	117.57	120.30
1	A	691	G	C8-N9-C4	6.82	109.13	106.40
1	A	904	C	N3-C4-C5	6.75	124.60	121.90
1	A	629	G	N3-C4-N9	-6.74	121.95	126.00
1	A	622	A	C2-N3-C4	-6.74	107.23	110.60
22	V	76	A	C4-C5-C6	-6.74	113.63	117.00
1	A	976	G	N3-C4-N9	6.72	130.03	126.00
1	A	421	U	N1-C2-O2	6.72	127.50	122.80
1	A	100	C	C6-N1-C2	-6.71	117.62	120.30
1	A	832	C	C2-N1-C1'	6.71	126.17	118.80
1	A	266	G	C8-N9-C4	-6.68	103.73	106.40
1	A	1323	G	C8-N9-C4	-6.67	103.73	106.40
1	A	916	G	C8-N9-C4	-6.66	103.73	106.40
22	V	67	C	C6-N1-C2	-6.65	117.64	120.30
1	A	1378	C	N3-C4-C5	-6.64	119.24	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	848	C	C6-N1-C2	-6.64	117.64	120.30
1	A	442	C	C2-N1-C1'	6.63	126.09	118.80
4	D	12	CYS	CA-CB-SG	6.63	125.93	114.00
1	A	129(A)	G	C8-N9-C4	-6.62	103.75	106.40
1	A	470	C	N1-C2-O2	6.62	122.87	118.90
1	A	308	C	C6-N1-C2	6.62	122.95	120.30
1	A	266	G	C6-C5-N7	-6.61	126.43	130.40
1	A	685	G	N3-C4-C5	6.61	131.91	128.60
1	A	1278	U	C5-C6-N1	6.61	126.00	122.70
22	V	22	G	C8-N9-C4	-6.61	103.76	106.40
1	A	413	G	N3-C4-N9	6.60	129.96	126.00
1	A	839	U	C2-N1-C1'	6.60	125.62	117.70
1	A	1126	U	C5-C6-N1	6.60	126.00	122.70
1	A	1474	G	C8-N9-C4	6.60	109.04	106.40
22	V	76	A	N7-C8-N9	-6.60	110.50	113.80
1	A	1356	G	C6-N1-C2	6.58	129.05	125.10
1	A	129(A)	G	N9-C4-C5	6.57	108.03	105.40
1	A	1484	C	C2-N1-C1'	-6.56	111.58	118.80
1	A	204	U	C2-N1-C1'	6.56	125.57	117.70
1	A	858	G	C4-N9-C1'	6.56	135.03	126.50
1	A	1323	G	C6-C5-N7	-6.55	126.47	130.40
1	A	887	G	C5-C6-O6	-6.55	124.67	128.60
1	A	1373	G	C6-C5-N7	-6.55	126.47	130.40
1	A	421	U	N3-C2-O2	-6.54	117.62	122.20
1	A	365	U	C5-C4-O4	6.53	129.82	125.90
1	A	1321	C	C5-C6-N1	6.52	124.26	121.00
1	A	1363(A)	A	N9-C4-C5	6.52	108.41	105.80
1	A	616	G	C4-N9-C1'	6.50	134.94	126.50
1	A	546	G	N3-C4-C5	-6.50	125.35	128.60
1	A	960	U	C6-N1-C1'	-6.49	112.11	121.20
1	A	963	G	C8-N9-C4	-6.49	103.80	106.40
1	A	832	C	C6-N1-C1'	-6.47	113.03	120.80
1	A	495	A	N1-C6-N6	-6.47	114.72	118.60
1	A	1269	A	N1-C6-N6	-6.47	114.72	118.60
1	A	895	G	C5-C6-O6	-6.45	124.73	128.60
1	A	1290	G	N3-C4-N9	6.45	129.87	126.00
1	A	629	G	N3-C4-C5	6.45	131.82	128.60
1	A	398	C	C5-C4-N4	6.42	124.70	120.20
1	A	499	A	C8-N9-C4	6.42	108.37	105.80
1	A	1414	U	N3-C2-O2	-6.42	117.71	122.20
1	A	638	G	C4-N9-C1'	-6.41	118.17	126.50
1	A	1259	C	C5-C6-N1	6.40	124.20	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1358	U	N3-C4-C5	6.39	118.44	114.60
1	A	1274	G	C6-C5-N7	-6.39	126.57	130.40
1	A	1502	A	C4-C5-N7	6.38	113.89	110.70
1	A	979	C	C6-N1-C2	-6.38	117.75	120.30
4	D	31	CYS	CB-CA-C	6.37	123.15	110.40
1	A	904	C	C5-C4-N4	-6.36	115.75	120.20
1	A	1290	G	N3-C4-C5	-6.35	125.43	128.60
1	A	740	U	C5-C6-N1	-6.34	119.53	122.70
1	A	416	G	C5-C6-O6	-6.34	124.80	128.60
1	A	546	G	C8-N9-C4	-6.34	103.87	106.40
1	A	525	C	C5-C6-N1	6.33	124.17	121.00
1	A	297	G	C8-N9-C4	6.33	108.93	106.40
1	A	917	G	N7-C8-N9	6.33	116.26	113.10
1	A	219	C	C6-N1-C2	-6.32	117.77	120.30
1	A	20	U	C5-C6-N1	-6.31	119.55	122.70
1	A	395	C	C6-N1-C2	-6.28	117.79	120.30
1	A	254	G	C8-N9-C4	-6.26	103.89	106.40
1	A	129(A)	G	C5-C6-N1	-6.26	108.37	111.50
1	A	831	U	C5-C6-N1	6.25	125.83	122.70
1	A	1516	G	C8-N9-C4	6.22	108.89	106.40
1	A	363	A	N7-C8-N9	-6.22	110.69	113.80
1	A	473	G	N9-C4-C5	6.20	107.88	105.40
1	A	1192	C	C6-N1-C2	-6.20	117.82	120.30
1	A	299	G	C8-N9-C1'	-6.19	118.95	127.00
1	A	416	G	N1-C6-O6	6.19	123.61	119.90
1	A	858	G	N3-C4-N9	6.19	129.71	126.00
1	A	662	G	N3-C4-C5	-6.18	125.51	128.60
1	A	1356	G	N7-C8-N9	6.18	116.19	113.10
1	A	300	A	N1-C6-N6	-6.17	114.89	118.60
1	A	857	C	C6-N1-C2	6.17	122.77	120.30
1	A	833	U	C5-C4-O4	6.17	129.60	125.90
1	A	266	G	C2-N3-C4	-6.15	108.83	111.90
1	A	1401	G	N1-C6-O6	6.15	123.59	119.90
1	A	907	A	C2-N3-C4	-6.14	107.53	110.60
1	A	1299	A	C8-N9-C4	-6.14	103.34	105.80
1	A	509	A	C8-N9-C4	-6.14	103.34	105.80
1	A	912	C	C6-N1-C2	6.12	122.75	120.30
1	A	865	A	C6-C5-N7	-6.12	128.01	132.30
1	A	721	G	N1-C6-O6	6.11	123.57	119.90
1	A	1512	U	N1-C2-O2	-6.11	118.52	122.80
1	A	1274	G	N3-C4-N9	6.11	129.67	126.00
1	A	360	A	N1-C6-N6	-6.11	114.94	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1502	A	C2-N3-C4	-6.09	107.55	110.60
1	A	530	G	C4-N9-C1'	6.09	134.42	126.50
1	A	718	G	C4-N9-C1'	6.09	134.42	126.50
1	A	865	A	C2-N3-C4	-6.09	107.56	110.60
1	A	317	G	N7-C8-N9	6.08	116.14	113.10
1	A	1225	A	C8-N9-C4	-6.08	103.37	105.80
1	A	1312	G	C8-N9-C4	-6.08	103.97	106.40
1	A	1063	C	C6-N1-C2	-6.07	117.87	120.30
1	A	865	A	N7-C8-N9	6.07	116.83	113.80
1	A	1176	A	C8-N9-C4	-6.06	103.38	105.80
1	A	1300	G	C6-C5-N7	6.06	134.04	130.40
1	A	1414	U	N1-C2-O2	6.06	127.04	122.80
22	V	13	C	C6-N1-C2	-6.06	117.88	120.30
1	A	1502	A	C6-C5-N7	-6.06	128.06	132.30
1	A	40	C	N3-C2-O2	-6.05	117.66	121.90
1	A	365	U	C5-C6-N1	-6.05	119.67	122.70
1	A	881	G	N1-C6-O6	6.05	123.53	119.90
1	A	504	C	C5-C6-N1	6.05	124.02	121.00
1	A	522	C	N1-C2-O2	6.04	122.53	118.90
1	A	343	U	N3-C2-O2	-6.04	117.97	122.20
1	A	565	U	N3-C4-O4	6.04	123.62	119.40
1	A	1241	G	C8-N9-C4	6.03	108.81	106.40
1	A	292	G	C6-C5-N7	-6.03	126.78	130.40
1	A	865	A	C5-N7-C8	-6.00	100.90	103.90
1	A	589	C	C6-N1-C2	-6.00	117.90	120.30
1	A	1081	G	N9-C4-C5	-5.99	103.00	105.40
1	A	963	G	N3-C4-C5	-5.97	125.61	128.60
1	A	915	A	N7-C8-N9	-5.96	110.82	113.80
1	A	940	C	C5-C6-N1	5.96	123.98	121.00
1	A	851	G	N3-C4-C5	-5.96	125.62	128.60
1	A	545	C	C5-C6-N1	-5.96	118.02	121.00
1	A	189(D)	C	C5-C6-N1	5.95	123.97	121.00
1	A	1108	G	C4-C5-N7	-5.94	108.42	110.80
1	A	562	C	N3-C4-C5	5.93	124.27	121.90
1	A	1197	G	C4-N9-C1'	5.93	134.21	126.50
1	A	1418	A	C8-N9-C4	5.92	108.17	105.80
1	A	848	C	C5-C6-N1	5.92	123.96	121.00
1	A	1378	C	C4-C5-C6	5.92	120.36	117.40
1	A	879	C	C5-C6-N1	-5.91	118.04	121.00
1	A	600	C	C6-N1-C2	5.91	122.67	120.30
1	A	43	C	C6-N1-C2	5.91	122.66	120.30
1	A	606	G	N3-C4-C5	-5.90	125.65	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	774	G	C8-N9-C4	-5.90	104.04	106.40
1	A	912	C	C5-C6-N1	-5.90	118.05	121.00
1	A	27	G	C8-N9-C4	-5.89	104.05	106.40
1	A	1197	G	C8-N9-C1'	-5.88	119.35	127.00
22	V	1	C	C6-N1-C2	-5.88	117.95	120.30
1	A	1516	G	N3-C4-C5	5.88	131.54	128.60
1	A	120	A	N1-C2-N3	5.87	132.24	129.30
1	A	413	G	N3-C4-C5	-5.87	125.66	128.60
1	A	1274	G	N7-C8-N9	5.87	116.04	113.10
1	A	1381	U	C2-N1-C1'	5.87	124.75	117.70
1	A	346	G	C4-N9-C1'	5.87	134.13	126.50
1	A	1099	G	N9-C4-C5	5.87	107.75	105.40
1	A	1101	A	C8-N9-C4	5.86	108.14	105.80
1	A	1272	G	C4-N9-C1'	5.85	134.10	126.50
1	A	1290	G	C4-N9-C1'	5.85	134.10	126.50
1	A	1124	G	C8-N9-C4	-5.84	104.06	106.40
1	A	1158	C	C6-N1-C2	-5.84	117.97	120.30
1	A	1149	C	N1-C2-O2	5.82	122.39	118.90
1	A	662	G	C8-N9-C4	-5.82	104.07	106.40
1	A	1048	G	C8-N9-C4	-5.82	104.07	106.40
1	A	310	G	N1-C6-O6	5.82	123.39	119.90
1	A	720	C	C2-N1-C1'	5.82	125.20	118.80
1	A	1504	G	C8-N9-C4	-5.82	104.07	106.40
1	A	1274	G	C8-N9-C4	-5.82	104.07	106.40
1	A	20	U	C6-N1-C2	5.81	124.49	121.00
1	A	1108	G	C5-C6-O6	5.81	132.09	128.60
1	A	1512	U	N1-C2-N3	5.81	118.39	114.90
1	A	506	G	N3-C4-C5	-5.81	125.69	128.60
1	A	1312	G	N9-C4-C5	5.80	107.72	105.40
1	A	1300	G	C4-N9-C1'	-5.78	118.99	126.50
1	A	305	G	C4-C5-N7	-5.78	108.49	110.80
1	A	851	G	C4-C5-C6	5.78	122.27	118.80
1	A	942	G	N3-C4-N9	5.77	129.46	126.00
1	A	299	G	C5-C6-O6	-5.76	125.14	128.60
1	A	674	G	N1-C6-O6	5.76	123.36	119.90
1	A	401	C	N1-C2-O2	-5.75	115.45	118.90
1	A	851	G	C8-N9-C1'	-5.75	119.52	127.00
1	A	1502	A	N1-C6-N6	5.74	122.05	118.60
1	A	1497	G	N3-C4-N9	-5.73	122.56	126.00
1	A	555	C	N3-C4-C5	-5.72	119.61	121.90
1	A	638	G	N7-C8-N9	-5.72	110.24	113.10
1	A	481	G	C4-N9-C1'	5.72	133.93	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	162	A	N1-C6-N6	-5.71	115.17	118.60
1	A	817	C	N1-C2-O2	5.71	122.32	118.90
1	A	803	G	N1-C6-O6	5.70	123.32	119.90
1	A	914	A	N1-C6-N6	-5.70	115.18	118.60
1	A	858	G	C8-N9-C1'	-5.70	119.59	127.00
1	A	575	G	N1-C6-O6	5.70	123.32	119.90
1	A	1108	G	C5-C6-N1	-5.70	108.65	111.50
1	A	1274	G	C4-N9-C1'	5.70	133.91	126.50
1	A	1272	G	C8-N9-C1'	-5.69	119.60	127.00
1	A	616	G	N3-C4-C5	-5.69	125.76	128.60
1	A	1154	G	N3-C4-N9	5.68	129.41	126.00
1	A	1158	C	C2-N1-C1'	5.67	125.03	118.80
1	A	506	G	N1-C6-O6	-5.66	116.50	119.90
1	A	774	G	N7-C8-N9	5.65	115.92	113.10
1	A	993	G	N3-C4-N9	5.64	129.39	126.00
1	A	892	A	C5-C6-N6	-5.64	119.19	123.70
1	A	1528	U	C5-C6-N1	-5.64	119.88	122.70
1	A	1366	C	N3-C4-C5	-5.62	119.65	121.90
22	V	60	U	N3-C2-O2	-5.62	118.27	122.20
1	A	953	G	N3-C4-N9	5.62	129.37	126.00
1	A	1205	U	N3-C4-C5	-5.61	111.23	114.60
1	A	1323	G	C4-C5-C6	5.60	122.16	118.80
1	A	1473	A	C8-N9-C4	5.60	108.04	105.80
1	A	150	C	C5-C6-N1	5.59	123.80	121.00
1	A	1499	A	N7-C8-N9	-5.58	111.01	113.80
1	A	572	A	N7-C8-N9	-5.58	111.01	113.80
1	A	96	U	C5-C6-N1	5.58	125.49	122.70
1	A	333	G	C5-C6-O6	-5.58	125.25	128.60
1	A	892	A	N9-C4-C5	-5.58	103.57	105.80
2	B	238	LEU	CA-CB-CG	5.58	128.12	115.30
1	A	942	G	N3-C4-C5	-5.57	125.82	128.60
1	A	522	C	N3-C2-O2	-5.57	118.00	121.90
1	A	921	U	C2-N3-C4	5.57	130.34	127.00
1	A	234	C	C6-N1-C2	5.56	122.53	120.30
1	A	1530	G	N1-C6-O6	5.56	123.24	119.90
1	A	730	G	N1-C6-O6	-5.56	116.56	119.90
1	A	1227	A	C8-N9-C4	-5.55	103.58	105.80
1	A	720	C	C6-N1-C2	-5.55	118.08	120.30
1	A	878	G	C4-N9-C1'	5.54	133.71	126.50
1	A	629	G	C2-N3-C4	-5.54	109.13	111.90
1	A	1502	A	N7-C8-N9	5.54	116.57	113.80
1	A	427	U	N1-C2-O2	5.53	126.67	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	856	C	N3-C4-C5	-5.53	119.69	121.90
1	A	1325	C	C2-N1-C1'	-5.53	112.72	118.80
1	A	299	G	N9-C4-C5	-5.53	103.19	105.40
22	V	32	C	N1-C2-O2	5.53	122.22	118.90
1	A	1077	G	N3-C4-C5	5.52	131.36	128.60
1	A	76	C	C6-N1-C2	-5.52	118.09	120.30
1	A	113	G	N1-C6-O6	5.52	123.21	119.90
1	A	740	U	C2-N1-C1'	-5.52	111.08	117.70
1	A	866	C	C6-N1-C2	-5.52	118.09	120.30
1	A	1274	G	N3-C4-C5	-5.51	125.84	128.60
1	A	1227	A	N7-C8-N9	5.51	116.56	113.80
1	A	1497	G	N3-C2-N2	-5.51	116.05	119.90
1	A	644	G	C8-N9-C4	5.50	108.60	106.40
1	A	1279	A	N3-C4-C5	-5.50	122.95	126.80
19	S	26	GLY	N-CA-C	5.50	126.84	113.10
1	A	363	A	C8-N9-C4	5.49	108.00	105.80
1	A	363	A	C6-C5-N7	5.49	136.14	132.30
1	A	597	G	N1-C6-O6	-5.48	116.61	119.90
1	A	473	G	N3-C2-N2	-5.48	116.06	119.90
1	A	764	C	C6-N1-C2	-5.48	118.11	120.30
1	A	149	A	C3'-C2'-C1'	5.48	105.88	101.50
1	A	73	G	C6-C5-N7	5.47	133.69	130.40
1	A	1424	C	C6-N1-C2	-5.46	118.11	120.30
1	A	1290	G	C5-C6-O6	-5.46	125.32	128.60
1	A	354	G	C4-C5-N7	5.46	112.98	110.80
1	A	460	G	C5-C6-N1	-5.46	108.77	111.50
1	A	827	U	N1-C2-O2	5.45	126.62	122.80
1	A	1277	C	N3-C2-O2	-5.45	118.08	121.90
1	A	1267	C	C6-N1-C1'	-5.45	114.26	120.80
1	A	76	C	N1-C2-O2	5.45	122.17	118.90
1	A	481	G	N3-C4-N9	5.44	129.27	126.00
1	A	1141	C	C6-N1-C1'	5.44	127.33	120.80
1	A	1195	C	C6-N1-C2	-5.44	118.12	120.30
1	A	446	G	C8-N9-C4	-5.43	104.23	106.40
1	A	496	A	N1-C6-N6	5.43	121.86	118.60
1	A	806	C	N1-C2-O2	5.43	122.16	118.90
1	A	1523	G	N1-C6-O6	-5.43	116.64	119.90
1	A	946	A	C4-C5-C6	5.43	119.71	117.00
1	A	435	C	N1-C2-O2	5.43	122.16	118.90
1	A	976	G	C4-N9-C1'	5.42	133.55	126.50
1	A	863	U	C5-C4-O4	5.42	129.15	125.90
1	A	1225	A	N7-C8-N9	5.42	116.51	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1286	A	C8-N9-C4	-5.42	103.63	105.80
1	A	1526	G	C8-N9-C4	5.42	108.57	106.40
1	A	481	G	C6-C5-N7	-5.42	127.15	130.40
1	A	129(A)	G	C2-N3-C4	-5.42	109.19	111.90
1	A	953	G	N3-C4-C5	-5.41	125.89	128.60
1	A	1518	A	C4-C5-C6	5.41	119.70	117.00
1	A	1378	C	C6-N1-C2	-5.41	118.14	120.30
1	A	1401	G	C5-N7-C8	-5.41	101.60	104.30
1	A	299	G	C4-C5-C6	5.40	122.04	118.80
1	A	129(A)	G	C8-N9-C1'	-5.40	119.99	127.00
1	A	728	A	N1-C2-N3	5.39	132.00	129.30
1	A	1391	U	N3-C2-O2	-5.39	118.42	122.20
1	A	325	A	N1-C6-N6	-5.39	115.37	118.60
1	A	915	A	N1-C6-N6	-5.38	115.37	118.60
1	A	1223	C	N1-C2-O2	5.38	122.13	118.90
1	A	1133	G	C5-C6-O6	5.38	131.83	128.60
1	A	728	A	C4-C5-C6	5.38	119.69	117.00
1	A	320	C	C2-N1-C1'	-5.37	112.89	118.80
1	A	865	A	C8-N9-C4	-5.37	103.65	105.80
1	A	865	A	C4-C5-N7	5.36	113.38	110.70
1	A	1467	G	N3-C4-N9	-5.36	122.78	126.00
1	A	119	A	P-O3'-C3'	5.36	126.14	119.70
1	A	372	C	N3-C4-C5	5.36	124.05	121.90
1	A	682	G	C8-N9-C4	-5.36	104.26	106.40
1	A	1441	G	N3-C4-C5	-5.36	125.92	128.60
1	A	240	C	N3-C4-N4	-5.35	114.25	118.00
1	A	305	G	C5-C6-O6	5.35	131.81	128.60
1	A	1133	G	N3-C4-C5	5.34	131.27	128.60
1	A	728	A	N9-C4-C5	5.34	107.94	105.80
1	A	483	C	C6-N1-C2	5.34	122.44	120.30
1	A	776	G	N9-C4-C5	5.33	107.53	105.40
1	A	894	G	C8-N9-C4	5.33	108.53	106.40
1	A	299	G	C2-N3-C4	-5.33	109.23	111.90
1	A	965	A	C8-N9-C4	5.33	107.93	105.80
1	A	305	G	N1-C2-N3	5.33	127.10	123.90
22	V	28	C	C5-C6-N1	5.33	123.66	121.00
1	A	1120	G	C8-N9-C4	-5.32	104.27	106.40
1	A	802	A	N7-C8-N9	5.32	116.46	113.80
1	A	884	U	N3-C4-O4	5.32	123.13	119.40
1	A	863	U	C2-N1-C1'	-5.32	111.32	117.70
1	A	915	A	C5-N7-C8	5.31	106.56	103.90
1	A	893	C	N1-C2-N3	-5.30	115.49	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	887	G	N1-C6-O6	5.30	123.08	119.90
1	A	1300	G	C8-N9-C1'	5.30	133.89	127.00
1	A	1132	C	C6-N1-C2	-5.29	118.18	120.30
1	A	479	C	C6-N1-C2	-5.29	118.19	120.30
1	A	513	C	C6-N1-C1'	-5.29	114.45	120.80
1	A	1267	C	C5-C6-N1	5.29	123.64	121.00
1	A	785	G	C8-N9-C4	5.28	108.51	106.40
1	A	1402	C	C6-N1-C2	-5.28	118.19	120.30
1	A	638	G	N3-C4-C5	5.28	131.24	128.60
1	A	1081	G	C8-N9-C4	5.27	108.51	106.40
1	A	1518	A	N7-C8-N9	5.27	116.44	113.80
1	A	442	C	C5-C6-N1	5.27	123.63	121.00
1	A	565	U	C6-N1-C2	-5.27	117.84	121.00
1	A	1356	G	C5-C6-N1	-5.27	108.87	111.50
1	A	1363(A)	A	C4-C5-N7	-5.27	108.07	110.70
1	A	1385	G	N3-C2-N2	-5.26	116.22	119.90
1	A	1414	U	C2-N1-C1'	5.26	124.02	117.70
1	A	481	G	C8-N9-C1'	-5.26	120.16	127.00
1	A	1500	A	N1-C6-N6	5.26	121.75	118.60
1	A	64	G	N1-C6-O6	5.26	123.05	119.90
22	V	22	G	N7-C8-N9	5.25	115.73	113.10
1	A	318	G	N3-C2-N2	-5.25	116.22	119.90
1	A	416	G	C6-C5-N7	-5.25	127.25	130.40
13	M	70	LEU	CA-CB-CG	5.25	127.38	115.30
1	A	1149	C	N3-C2-O2	-5.25	118.22	121.90
1	A	506	G	C8-N9-C4	-5.25	104.30	106.40
1	A	314	C	C2-N1-C1'	5.24	124.57	118.80
1	A	319	G	C2-N3-C4	-5.24	109.28	111.90
1	A	1119	C	C5-C6-N1	5.24	123.62	121.00
1	A	1399	C	N3-C4-C5	-5.24	119.81	121.90
1	A	816	A	N9-C4-C5	5.23	107.89	105.80
1	A	1406	U	N3-C2-O2	-5.22	118.55	122.20
1	A	1523	G	C5-C6-O6	5.22	131.73	128.60
1	A	1197	G	C5-C6-N1	5.22	114.11	111.50
1	A	1149	C	C2-N1-C1'	5.21	124.53	118.80
1	A	504	C	C2-N1-C1'	5.21	124.53	118.80
1	A	1411	C	N3-C4-C5	5.21	123.98	121.90
1	A	1323	G	N7-C8-N9	5.21	115.70	113.10
1	A	616	G	C6-C5-N7	-5.20	127.28	130.40
1	A	1281	U	N1-C2-O2	5.20	126.44	122.80
1	A	1112	C	N1-C2-N3	5.20	122.84	119.20
1	A	1363(A)	A	C6-N1-C2	-5.20	115.48	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	G	C6-C5-N7	-5.19	127.28	130.40
1	A	913	A	P-O3'-C3'	5.19	125.92	119.70
1	A	1133	G	N9-C4-C5	5.19	107.47	105.40
1	A	530	G	C8-N9-C1'	-5.18	120.26	127.00
1	A	1333	A	N1-C6-N6	-5.18	115.49	118.60
1	A	685	G	C8-N9-C1'	5.17	133.73	127.00
1	A	932	C	N3-C2-O2	-5.17	118.28	121.90
1	A	530	G	N7-C8-N9	5.17	115.69	113.10
1	A	115	G	P-O3'-C3'	5.17	125.90	119.70
1	A	299	G	C5-C6-N1	-5.17	108.92	111.50
1	A	576	G	C5-C6-O6	-5.17	125.50	128.60
1	A	1272	G	C6-C5-N7	-5.17	127.30	130.40
1	A	853	G	N9-C4-C5	5.16	107.47	105.40
1	A	783	C	N3-C4-C5	5.16	123.96	121.90
1	A	55	A	C8-N9-C4	-5.15	103.74	105.80
1	A	738	C	C5-C6-N1	5.15	123.57	121.00
1	A	539	A	C2-N3-C4	5.14	113.17	110.60
1	A	39	G	N1-C6-O6	-5.14	116.82	119.90
1	A	593	G	N1-C6-O6	5.14	122.98	119.90
1	A	44	G	C8-N9-C1'	-5.14	120.32	127.00
1	A	1235	U	C5-C6-N1	5.14	125.27	122.70
1	A	129(A)	G	C4-N9-C1'	5.14	133.18	126.50
1	A	1325	C	C6-N1-C1'	5.13	126.96	120.80
1	A	572	A	C8-N9-C4	5.13	107.85	105.80
1	A	337	C	C6-N1-C2	-5.13	118.25	120.30
1	A	1259	C	C6-N1-C2	-5.13	118.25	120.30
1	A	495	A	N9-C4-C5	5.13	107.85	105.80
1	A	691	G	N9-C4-C5	-5.12	103.35	105.40
1	A	733	A	C8-N9-C4	5.12	107.85	105.80
1	A	1516	G	C2-N3-C4	-5.12	109.34	111.90
1	A	168	G	C8-N9-C4	5.12	108.45	106.40
1	A	525	C	N3-C4-N4	5.12	121.58	118.00
1	A	426	G	C8-N9-C4	-5.11	104.36	106.40
1	A	1272	G	N3-C4-N9	5.11	129.06	126.00
1	A	730	G	C2-N3-C4	5.10	114.45	111.90
1	A	993	G	C4-N9-C1'	5.10	133.13	126.50
1	A	1142	G	C8-N9-C4	5.10	108.44	106.40
1	A	357	G	C8-N9-C4	-5.10	104.36	106.40
1	A	546	G	C2-N3-C4	5.10	114.45	111.90
1	A	715	A	C5-C6-N1	-5.09	115.16	117.70
1	A	1430	C	C6-N1-C2	-5.08	118.27	120.30
1	A	878	G	C8-N9-C1'	-5.08	120.40	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	377	G	N1-C6-O6	5.07	122.94	119.90
1	A	833	U	N1-C2-N3	5.06	117.94	114.90
1	A	895	G	N1-C6-O6	5.06	122.94	119.90
1	A	1189	C	C6-N1-C2	5.06	122.32	120.30
1	A	304	U	C4-C5-C6	5.06	122.73	119.70
1	A	1335	C	C6-N1-C2	5.06	122.32	120.30
1	A	879	C	C6-N1-C2	5.06	122.32	120.30
1	A	1067	A	C8-N9-C4	-5.05	103.78	105.80
1	A	773	G	N1-C2-N3	-5.05	120.87	123.90
1	A	894	G	C2-N3-C4	-5.05	109.37	111.90
1	A	1523	G	C8-N9-C4	-5.04	104.38	106.40
1	A	413	G	C8-N9-C1'	-5.04	120.44	127.00
1	A	662	G	N3-C4-N9	5.04	129.03	126.00
1	A	1081	G	N3-C4-N9	5.04	129.03	126.00
1	A	1528	U	C6-N1-C2	5.04	124.03	121.00
1	A	7	G	N1-C6-O6	5.04	122.92	119.90
1	A	597	G	C5-C6-N1	5.04	114.02	111.50
1	A	1429	C	N3-C2-O2	-5.04	118.37	121.90
1	A	1520	G	C6-C5-N7	5.04	133.42	130.40
1	A	12	U	N3-C4-C5	-5.03	111.58	114.60
1	A	329	A	C8-N9-C4	-5.03	103.79	105.80
1	A	1531	A	N1-C6-N6	5.03	121.62	118.60
1	A	616	G	N3-C4-N9	5.03	129.02	126.00
1	A	851	G	C6-C5-N7	-5.03	127.38	130.40
1	A	869	G	C5-C6-N1	-5.03	108.98	111.50
1	A	644	G	N7-C8-N9	-5.03	110.59	113.10
1	A	377	G	C6-C5-N7	-5.03	127.39	130.40
1	A	1484	C	N3-C4-C5	5.02	123.91	121.90
1	A	1338	G	N1-C6-O6	-5.02	116.89	119.90
1	A	93	G	N3-C4-C5	-5.02	126.09	128.60
1	A	436	C	C5-C6-N1	5.01	123.50	121.00
9	I	107	ARG	CG-CD-NE	5.01	122.32	111.80
1	A	1373	G	C8-N9-C4	-5.01	104.40	106.40
1	A	509	A	N7-C8-N9	5.00	116.30	113.80
1	A	923	A	N1-C2-N3	5.00	131.80	129.30
17	Q	6	LEU	CA-CB-CG	5.00	126.81	115.30
1	A	865	A	N1-C6-N6	5.00	121.60	118.60

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	129(A)	G	Sidechain
2	B	22	LYS	Peptide
2	B	71	VAL	Peptide
4	D	147	ALA	Peptide
4	D	28	SER	Peptide
4	D	29	PRO	Peptide
4	D	3	ARG	Peptide
4	D	30	LYS	Peptide
5	E	36	ASP	Peptide
7	G	113	GLU	Peptide
10	J	55	LYS	Peptide
10	J	90	LEU	Peptide
13	M	44	ARG	Peptide
13	M	65	LYS	Peptide
14	N	14	PRO	Peptide
16	P	15	PRO	Peptide
20	T	11	SER	Peptide
20	T	45	GLN	Peptide
21	U	6	ARG	Peptide

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	31406	0	15852	819	0
2	B	1817	0	1785	126	0
3	C	1453	0	1320	64	0
4	D	1537	0	1430	81	0
5	E	1115	0	1145	55	0
6	F	784	0	739	29	0
7	G	1149	0	1096	52	0
8	H	1049	0	1037	52	0
9	I	849	0	735	54	0
10	J	657	0	547	40	0
11	K	828	0	822	31	0
12	L	905	0	916	30	0
13	M	784	0	730	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	N	469	0	482	37	0
15	O	724	0	749	30	0
16	P	661	0	653	45	0
17	Q	819	0	880	38	0
18	R	514	0	530	21	0
19	S	529	0	443	22	0
20	T	773	0	836	32	0
21	U	180	0	173	4	0
22	V	1644	0	836	36	0
23	X	131	0	66	2	0
24	A	230	0	0	0	0
24	D	1	0	0	0	0
24	O	1	0	0	0	0
24	T	1	0	0	0	0
24	V	13	0	0	0	0
24	X	1	0	0	0	0
25	D	1	0	0	0	0
25	N	1	0	0	0	0
26	A	347	0	0	17	0
26	B	1	0	0	1	0
26	C	1	0	0	0	0
26	D	3	0	0	0	0
26	K	2	0	0	0	0
26	L	1	0	0	1	0
26	N	2	0	0	0	0
26	O	2	0	0	1	0
26	Q	1	0	0	1	0
26	T	2	0	0	0	0
26	V	22	0	0	0	0
26	X	1	0	0	0	0
All	All	51411	0	33802	1587	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 19.

All (1587) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1358:U:H3	1:A:1363(A):A:N6	1.35	1.22
1:A:1162:C:N4	1:A:1174:G:H1	1.58	1.01
1:A:1358:U:O4	1:A:1363(A):A:N1	1.94	0.99
1:A:1502:A:H2	1:A:1505:G:H1	1.16	0.94
1:A:377:G:H1	1:A:386:C:H42	1.12	0.94

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1352:C:OP1	21:U:3:LYS:NZ	2.03	0.91
1:A:1277:C:HO2'	1:A:1279:A:H8	0.96	0.90
1:A:1158:C:N3	1:A:1181:G:N2	2.24	0.86
1:A:1321:C:H5'	1:A:1322:C:H5''	1.58	0.85
1:A:953:G:H5'	1:A:965:A:H61	1.39	0.85
18:R:53:ARG:HG3	18:R:63:GLN:HE21	1.42	0.85
1:A:922:G:H4'	5:E:20:GLN:HA	1.59	0.85
5:E:31:LEU:HD22	5:E:43:LEU:HD11	1.59	0.84
1:A:1162:C:H42	1:A:1174:G:H1	0.84	0.83
9:I:28:VAL:HG22	9:I:63:ILE:HB	1.61	0.83
3:C:24:ALA:HB3	3:C:29:TYR:HB2	1.59	0.83
1:A:673:G:H2'	1:A:674:G:C8	2.13	0.83
1:A:976:G:N2	1:A:1363:C:OP2	2.12	0.82
7:G:23:VAL:HG13	7:G:43:PHE:HE2	1.42	0.82
5:E:36:ASP:HB3	5:E:38:GLN:H	1.45	0.82
5:E:36:ASP:CB	5:E:38:GLN:H	1.92	0.81
16:P:43:LYS:HA	16:P:48:TRP:HB3	1.60	0.81
8:H:10:LEU:HD22	8:H:83:ILE:HD11	1.63	0.81
10:J:44:VAL:HG22	10:J:66:ARG:HG2	1.63	0.80
2:B:68:ILE:HG22	2:B:90:MET:HG2	1.63	0.80
8:H:12:ARG:NH2	8:H:27:PRO:HD3	1.97	0.79
20:T:47:GLY:HA2	20:T:48:LYS:HB2	1.63	0.79
16:P:22:THR:HA	16:P:33:ILE:HG12	1.64	0.79
1:A:562:C:H1'	12:L:15:ARG:HB3	1.65	0.78
4:D:189:PRO:HB3	4:D:194:LEU:HD21	1.64	0.78
5:E:51:VAL:HG23	5:E:52:PRO:HD3	1.64	0.78
10:J:35:SER:HB3	10:J:73:ASP:HB2	1.65	0.78
6:F:8:ILE:HD13	6:F:26:ILE:HD13	1.64	0.78
1:A:1147:C:O2	9:I:16:ARG:NH1	2.17	0.78
16:P:72:ARG:HG3	16:P:72:ARG:HH11	1.45	0.78
13:M:64:TRP:H	13:M:64:TRP:HE3	1.29	0.77
10:J:50:ILE:HB	14:N:41:ARG:HD2	1.66	0.77
18:R:56:THR:HB	18:R:58:LEU:HD13	1.67	0.77
1:A:1358:U:N3	1:A:1363(A):A:N6	2.10	0.77
2:B:161:ALA:HB1	2:B:185:ILE:HD11	1.67	0.76
8:H:21:LYS:O	8:H:65:TYR:OH	2.00	0.76
1:A:404:U:H2'	1:A:405:U:H6	1.50	0.76
1:A:1347:G:C8	9:I:107:ARG:HB3	2.20	0.76
1:A:586:C:H2'	1:A:587:G:H5'	1.68	0.76
1:A:826:C:O2	1:A:874:G:N2	2.18	0.76
22:V:3:C:H42	22:V:70:G:H1	1.34	0.75
10:J:48:THR:HA	10:J:62:HIS:HB3	1.67	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:T:49:ALA:HA	20:T:52:ALA:HB3	1.69	0.75
1:A:559:A:H4'	1:A:560:U:H5''	1.67	0.75
3:C:179:ARG:HD2	3:C:206:GLU:HB3	1.69	0.75
5:E:102:ALA:HB1	5:E:106:PRO:HG2	1.69	0.74
1:A:1162:C:N3	1:A:1174:G:N2	2.32	0.74
1:A:564:C:O2'	8:H:91:ARG:NH2	2.19	0.74
2:B:21:ARG:HB3	2:B:39:ILE:HA	1.70	0.74
16:P:28:ARG:HH11	16:P:28:ARG:HG2	1.50	0.74
1:A:130:A:H5'	17:Q:63:ARG:HE	1.52	0.74
9:I:107:ARG:HH11	9:I:107:ARG:HG2	1.53	0.74
10:J:39:PRO:HA	10:J:70:ARG:HD3	1.70	0.73
1:A:1152:A:H5'	10:J:13:HIS:CD2	2.24	0.73
2:B:84:GLU:HB3	2:B:219:VAL:HG21	1.71	0.73
1:A:316:G:OP2	1:A:351:G:O2'	2.05	0.73
17:Q:57:VAL:HG12	17:Q:76:LEU:HA	1.70	0.72
9:I:9:ARG:HG2	9:I:14:VAL:HG12	1.69	0.72
2:B:95:GLN:HG3	2:B:148:TYR:HA	1.72	0.72
1:A:1059:C:N4	26:A:2124:HOH:O	2.09	0.72
2:B:71:VAL:HB	2:B:164:VAL:HG13	1.72	0.72
1:A:572:A:OP2	26:A:1965:HOH:O	2.07	0.71
1:A:677:U:H3	1:A:713:G:H22	1.36	0.71
16:P:28:ARG:NH1	16:P:29:ASP:OD1	2.23	0.71
3:C:110:ASN:HB2	3:C:111:LEU:HD12	1.73	0.71
1:A:1308:U:H5''	13:M:98:VAL:HG22	1.71	0.71
6:F:6:VAL:HG22	6:F:90:VAL:HG22	1.72	0.71
1:A:568:G:N7	12:L:5:PRO:HD3	2.06	0.71
2:B:97:TRP:CH2	2:B:173:ALA:HA	2.26	0.71
1:A:129(A):G:O6	1:A:189(D):C:C2	2.44	0.71
9:I:103:THR:OG1	9:I:104:ARG:N	2.22	0.71
1:A:1239:A:H2'	1:A:1298:C:H42	1.55	0.71
22:V:40:C:H2'	22:V:41:C:H6	1.56	0.71
2:B:155:LEU:HD11	2:B:159:PRO:HD3	1.71	0.70
1:A:826:C:H4'	8:H:12:ARG:HD2	1.72	0.70
1:A:503:C:OP2	12:L:116:SER:HB3	1.91	0.70
16:P:29:ASP:OD2	16:P:29:ASP:N	2.22	0.70
1:A:404:U:H2'	1:A:405:U:C6	2.26	0.70
1:A:400:C:H5''	4:D:73:ARG:HH12	1.57	0.70
1:A:97:G:HO2'	1:A:98:G:H8	1.40	0.70
3:C:127:ARG:NH2	3:C:192:THR:OG1	2.24	0.70
1:A:1244:C:H42	1:A:1293:G:H1	1.39	0.70
1:A:736:C:H2'	1:A:737:A:C8	2.26	0.70
1:A:518:C:H2'	1:A:530:G:C8	2.26	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1012:U:H3	1:A:1017:G:H1	1.37	0.69
19:S:22:LEU:HD22	19:S:27:GLU:HA	1.75	0.69
1:A:954:G:H21	1:A:1227:A:N6	1.89	0.69
1:A:736:C:H2'	1:A:737:A:H8	1.58	0.69
6:F:70:ASP:N	6:F:70:ASP:OD1	2.26	0.69
1:A:243:A:H4'	1:A:244:U:H5''	1.74	0.69
1:A:920:U:H2'	1:A:921:U:C6	2.27	0.69
7:G:18:TYR:CE2	7:G:59:LEU:HB2	2.27	0.69
4:D:204:ILE:HG21	5:E:98:THR:O	1.91	0.69
1:A:1292:U:H5'	9:I:38:GLN:HG2	1.75	0.69
2:B:27:LYS:HB2	2:B:194:PRO:HD2	1.75	0.69
2:B:88:ALA:HB2	2:B:219:VAL:HG13	1.73	0.68
1:A:582:U:OP1	15:O:68:ARG:NH2	2.27	0.68
7:G:151:TYR:OH	11:K:54:ARG:NH1	2.27	0.68
1:A:1457:G:OP1	20:T:39:LYS:NZ	2.26	0.68
3:C:18:TRP:HE3	3:C:18:TRP:H	1.39	0.68
1:A:9:G:H2'	1:A:10:A:C8	2.28	0.68
1:A:924:C:O2'	1:A:1502:A:N6	2.27	0.68
1:A:728:A:H2'	1:A:729:A:C8	2.28	0.68
1:A:748:C:H4'	1:A:749:C:O5'	1.92	0.68
1:A:460:G:C6	1:A:470:C:H5''	2.27	0.68
3:C:36:ASP:HA	3:C:39:ILE:HD12	1.76	0.67
12:L:70:ILE:HG23	12:L:100:ILE:HD12	1.75	0.67
1:A:148:G:H2'	1:A:149:A:H8	1.58	0.67
1:A:1158:C:H42	1:A:1181:G:H1	1.43	0.67
7:G:120:ILE:O	7:G:124:LEU:HB2	1.95	0.67
9:I:13:ALA:HB2	9:I:68:GLY:HA3	1.76	0.67
1:A:1261:A:H61	1:A:1274:G:H1'	1.58	0.67
1:A:509:A:H3'	1:A:509:A:C8	2.29	0.67
1:A:1270:C:HO2'	1:A:1313:U:HO2'	1.34	0.67
1:A:353:A:H5'	1:A:353:A:H8	1.60	0.67
4:D:162:LEU:HD22	4:D:178:VAL:HG13	1.75	0.67
6:F:69:GLU:O	6:F:72:VAL:HG12	1.96	0.66
1:A:1143:G:H2'	1:A:1144:G:H8	1.60	0.66
1:A:9:G:H2'	1:A:10:A:H8	1.59	0.66
5:E:91:LEU:HD12	5:E:120:THR:HB	1.77	0.66
1:A:509:A:H3'	1:A:509:A:H8	1.61	0.66
1:A:980:C:H5'	1:A:981:U:OP2	1.96	0.66
2:B:178:ARG:HH12	8:H:68:ARG:NH2	1.93	0.66
3:C:18:TRP:CD1	14:N:54:PRO:HA	2.31	0.66
1:A:1513:A:H2'	1:A:1514:C:C6	2.30	0.66
5:E:71:LEU:HD13	5:E:74:GLY:HA2	1.75	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:14:ARG:HA	4:D:39:PRO:HG3	1.77	0.66
1:A:1347:G:H8	9:I:107:ARG:HB3	1.60	0.66
1:A:1074:G:O2'	1:A:1101:A:N1	2.25	0.66
1:A:975:A:H4'	1:A:976:G:H5''	1.77	0.66
16:P:56:ALA:O	16:P:60:LEU:HB2	1.95	0.66
5:E:102:ALA:O	5:E:107:ARG:NH1	2.29	0.66
3:C:47:LEU:HB3	3:C:52:LEU:HD12	1.77	0.66
20:T:90:GLN:HA	20:T:93:GLU:HB2	1.78	0.66
6:F:61:LEU:HB3	6:F:63:TYR:HE2	1.61	0.65
1:A:1128:C:O2'	1:A:1130:A:N7	2.28	0.65
2:B:47:THR:O	2:B:51:LEU:N	2.28	0.65
17:Q:24:GLU:HA	17:Q:39:SER:HB3	1.77	0.65
1:A:619:U:N3	4:D:134:ASP:OD2	2.30	0.65
11:K:87:THR:HA	11:K:91:ARG:HH21	1.59	0.65
1:A:971:G:OP2	1:A:1231:G:N2	2.20	0.65
1:A:376:G:H4'	16:P:5:ARG:NH1	2.12	0.65
1:A:60:A:H4'	1:A:61:G:O5'	1.96	0.65
1:A:222:U:H2'	1:A:223:U:C6	2.32	0.65
1:A:766:A:OP2	26:A:2040:HOH:O	2.13	0.65
1:A:1490:C:H2'	1:A:1491:G:O4'	1.97	0.65
3:C:134:ILE:HD11	3:C:153:VAL:HG21	1.79	0.65
2:B:178:ARG:HH12	8:H:68:ARG:HH22	1.45	0.65
2:B:86:GLU:O	2:B:89:GLY:N	2.30	0.65
1:A:1320:C:H5'	19:S:70:LYS:HD3	1.78	0.65
1:A:1492:A:H4'	1:A:1493:A:OP1	1.95	0.65
2:B:134:GLU:HA	2:B:137:ARG:HE	1.61	0.65
14:N:24:CYS:SG	14:N:25:VAL:N	2.70	0.65
15:O:56:LEU:O	15:O:60:VAL:HG23	1.96	0.64
2:B:163:PHE:HA	2:B:185:ILE:O	1.96	0.64
8:H:85:ARG:HH21	8:H:134:ILE:HG23	1.62	0.64
1:A:1072:G:H2'	1:A:1073:U:C6	2.32	0.64
1:A:552:U:O3'	12:L:87:GLY:HA3	1.98	0.64
1:A:1376:U:H2'	1:A:1377:A:C8	2.33	0.64
2:B:97:TRP:HZ2	2:B:102:LEU:HD13	1.62	0.64
15:O:82:ILE:HD12	15:O:88:ARG:HH22	1.62	0.64
1:A:1197:G:OP2	26:A:2066:HOH:O	2.15	0.64
1:A:45:U:H2'	1:A:46:G:C8	2.33	0.64
15:O:25:THR:HG21	15:O:70:LEU:HB2	1.79	0.64
22:V:19:G:N2	22:V:56:C:O2	2.29	0.64
1:A:1423:G:H2'	1:A:1424:C:C6	2.33	0.64
1:A:758:G:N7	26:A:1983:HOH:O	2.30	0.64
7:G:111:ARG:NH1	7:G:113:GLU:OE2	2.30	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1117:G:H5'	1:A:1118:C:OP2	1.96	0.64
1:A:501:C:H2'	1:A:502:G:H8	1.63	0.64
3:C:164:ARG:NH1	3:C:166:GLU:OE1	2.31	0.64
2:B:163:PHE:CD2	2:B:185:ILE:HB	2.32	0.64
10:J:37:PRO:HA	10:J:72:VAL:HG12	1.80	0.64
17:Q:57:VAL:HA	17:Q:77:VAL:HG23	1.80	0.64
4:D:22:LYS:HG3	4:D:31:CYS:SG	2.38	0.64
1:A:129(A):G:N2	1:A:189(H):G:N7	2.45	0.64
1:A:473:G:H2'	1:A:474:G:H8	1.63	0.64
1:A:646:U:H2'	1:A:647:C:C6	2.33	0.64
2:B:78:GLN:O	2:B:94:ASN:ND2	2.31	0.64
1:A:1126:U:O2'	1:A:1127:G:O5'	2.10	0.64
1:A:1143:G:H2'	1:A:1144:G:C8	2.33	0.64
12:L:113:ARG:NH2	26:L:201:HOH:O	2.31	0.63
1:A:1358:U:H5''	14:N:34:TYR:HA	1.79	0.63
13:M:94:ARG:HB3	13:M:96:LEU:HG	1.79	0.63
1:A:6:G:O2'	1:A:7:G:H5''	1.97	0.63
1:A:1323:G:H2'	1:A:1324:A:C8	2.34	0.63
8:H:97:VAL:O	8:H:100:ILE:HG13	1.99	0.63
1:A:586:C:C2'	1:A:587:G:H5'	2.29	0.63
6:F:62:TRP:C	6:F:63:TYR:HD2	2.02	0.63
1:A:993:G:N7	1:A:1213:A:N6	2.47	0.63
13:M:16:ASP:HB3	13:M:34:LEU:HD11	1.79	0.63
1:A:1497:G:H8	26:A:2234:HOH:O	1.81	0.63
1:A:728:A:N7	15:O:54:ARG:HD2	2.13	0.63
13:M:44:ARG:O	13:M:46:LYS:N	2.26	0.63
1:A:953:G:H5'	1:A:965:A:N6	2.13	0.63
1:A:1292:U:OP2	7:G:41:ARG:NH2	2.32	0.63
3:C:67:THR:HB	3:C:102:ASN:HB3	1.81	0.63
1:A:1262:C:H2'	1:A:1263:C:C6	2.33	0.63
1:A:870:U:H5'	1:A:870:U:H6	1.63	0.63
13:M:90:LEU:O	13:M:91:ARG:HG2	1.99	0.62
11:K:29:ILE:HG23	11:K:44:SER:HB3	1.81	0.62
16:P:43:LYS:O	16:P:45:THR:N	2.31	0.62
1:A:559:A:H4'	1:A:560:U:C5'	2.29	0.62
20:T:18:GLN:O	20:T:22:ARG:HG3	1.99	0.62
5:E:126:ARG:HH11	5:E:126:ARG:CG	2.12	0.62
1:A:129(A):G:O6	1:A:189(D):C:N3	2.31	0.62
2:B:163:PHE:HD2	2:B:185:ILE:HB	1.64	0.62
1:A:811:C:O2'	1:A:901:A:N1	2.32	0.62
1:A:1369:C:OP1	14:N:61:TRP:NE1	2.29	0.62
7:G:89:MET:HG3	7:G:155:ARG:HG3	1.80	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:520:A:N1	1:A:536:C:H1'	2.15	0.62
2:B:185:ILE:HG23	2:B:199:TYR:HB2	1.82	0.62
4:D:59:ARG:O	4:D:62:GLN:N	2.33	0.62
11:K:82:VAL:HB	11:K:108:ILE:HG12	1.82	0.62
10:J:40:LEU:HB3	10:J:41:PRO:HD2	1.81	0.62
13:M:73:GLU:O	13:M:77:ASN:HB2	1.99	0.62
2:B:100:GLY:HA2	2:B:104:ASN:H	1.64	0.61
1:A:573:A:N3	1:A:883:C:O2'	2.33	0.61
1:A:17:U:H2'	1:A:18:C:C6	2.36	0.61
1:A:1348:U:H2'	1:A:1349:A:H8	1.66	0.61
4:D:19:LEU:HD22	4:D:19:LEU:H	1.66	0.61
17:Q:13:ASP:HB2	26:Q:201:HOH:O	2.00	0.61
17:Q:96:GLU:O	17:Q:97:SER:HB3	2.00	0.61
11:K:20:TYR:HB2	11:K:31:THR:HG22	1.83	0.61
3:C:131:ARG:H	3:C:134:ILE:HD12	1.64	0.61
1:A:1049:U:H4'	1:A:1050:G:C5'	2.31	0.61
1:A:192:U:H2'	1:A:193:C:H6	1.65	0.61
14:N:37:PHE:HB3	14:N:39:LEU:HD12	1.81	0.61
16:P:15:PRO:O	16:P:16:HIS:ND1	2.33	0.61
2:B:102:LEU:HD23	2:B:182:ILE:HD12	1.82	0.61
1:A:1445:C:O2'	1:A:1447:A:N6	2.34	0.61
1:A:390:C:O3'	16:P:28:ARG:NH2	2.33	0.61
1:A:590:C:O2	1:A:649:G:N2	2.21	0.61
1:A:1107:C:C4	1:A:1108:G:C8	2.88	0.61
2:B:187:LEU:HA	2:B:201:ILE:HB	1.82	0.61
1:A:954:G:H21	1:A:1227:A:H62	1.49	0.61
1:A:765:G:H5''	1:A:766:A:OP1	2.01	0.61
1:A:922:G:H2'	1:A:923:A:C8	2.36	0.61
11:K:18:ARG:HB2	11:K:33:THR:HG23	1.81	0.61
1:A:64:G:H4'	1:A:65:U:H3'	1.83	0.61
1:A:1281:U:H3'	1:A:1281:U:H6	1.65	0.60
1:A:501:C:H2'	1:A:502:G:C8	2.36	0.60
1:A:939:G:H1	1:A:1344:C:H42	1.49	0.60
4:D:43:HIS:HA	4:D:46:LYS:HD2	1.83	0.60
1:A:1170:A:C2	1:A:1171:G:H1'	2.36	0.60
1:A:437:U:H5''	4:D:155:LEU:HD11	1.81	0.60
2:B:80:ILE:HD13	2:B:212:GLN:HG2	1.83	0.60
1:A:1170:A:N6	1:A:1171:G:N3	2.50	0.60
1:A:450:G:H4'	16:P:41:PRO:HB2	1.82	0.60
2:B:19:HIS:NE2	2:B:206:ASP:HB2	2.15	0.60
6:F:62:TRP:CH2	6:F:64:GLN:HB2	2.37	0.60
1:A:1227:A:H3'	1:A:1227:A:C8	2.37	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:869:G:N7	26:A:1969:HOH:O	2.32	0.60
20:T:38:LYS:HG3	20:T:41:ILE:HD11	1.83	0.60
1:A:1201:A:H4'	1:A:1202:G:O5'	2.02	0.60
5:E:36:ASP:HB2	5:E:38:GLN:H	1.67	0.60
22:V:40:C:H2'	22:V:41:C:C6	2.36	0.60
1:A:1344:C:H4'	9:I:120:ARG:HB3	1.84	0.60
4:D:79:PHE:O	4:D:82:ALA:HB3	2.02	0.60
1:A:1205:U:H4'	3:C:195:VAL:HG21	1.83	0.60
10:J:11:PHE:CE2	10:J:67:THR:HG22	2.36	0.60
16:P:76:GLN:O	16:P:76:GLN:NE2	2.31	0.60
7:G:18:TYR:HD2	7:G:59:LEU:HD22	1.65	0.59
7:G:111:ARG:HB2	7:G:113:GLU:OE1	2.02	0.59
1:A:715:A:H2'	1:A:716:A:C8	2.37	0.59
9:I:17:VAL:HG12	9:I:63:ILE:HG12	1.84	0.59
1:A:1279:A:O2'	1:A:1281:U:OP2	2.12	0.59
18:R:44:LEU:HD21	18:R:70:ILE:HG21	1.85	0.59
5:E:8:GLU:HB3	5:E:34:VAL:HG23	1.84	0.59
11:K:85:ARG:HE	11:K:111:ASP:HB3	1.68	0.59
1:A:986:A:H1'	19:S:54:GLY:O	2.02	0.59
20:T:69:GLY:O	20:T:73:HIS:CD2	2.55	0.59
1:A:1320:C:H2'	1:A:1321:C:O4'	2.03	0.59
4:D:26:CYS:HA	4:D:31:CYS:HB3	1.85	0.59
1:A:40:C:H42	1:A:402:G:H1	1.50	0.59
1:A:384:G:H2'	1:A:385:C:C6	2.38	0.59
1:A:129(A):G:N2	1:A:189(H):G:C5	2.71	0.59
4:D:105:VAL:HG21	4:D:126:ILE:HD12	1.85	0.59
12:L:6:THR:HG23	12:L:9:GLN:HB2	1.84	0.59
7:G:82:GLY:HA2	23:X:1:A:C8	2.37	0.59
4:D:22:LYS:HB2	4:D:26:CYS:SG	2.43	0.58
2:B:165:VAL:HG23	2:B:166:ASP:H	1.67	0.58
1:A:1060:C:O2'	1:A:1061:G:H5'	2.03	0.58
8:H:38:ILE:HD12	8:H:118:VAL:HG12	1.85	0.58
1:A:857:C:H2'	1:A:858:G:O4'	2.03	0.58
11:K:22:HIS:O	11:K:28:THR:HA	2.03	0.58
2:B:178:ARG:HH22	8:H:68:ARG:HH12	1.51	0.58
1:A:1095:U:OP1	1:A:1108:G:N2	2.29	0.58
1:A:989:C:H1'	1:A:1016:A:H2	1.68	0.58
1:A:980:C:OP1	26:A:2056:HOH:O	2.17	0.58
4:D:155:LEU:HD23	4:D:156:GLU:N	2.18	0.58
2:B:127:ILE:HG12	2:B:128:GLU:H	1.67	0.58
4:D:71:SER:O	4:D:75:PHE:N	2.27	0.58
4:D:38:TYR:OH	4:D:45:GLN:NE2	2.34	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
18:R:74:ARG:HE	18:R:81:PHE:HA	1.69	0.58
1:A:1272:G:H5''	1:A:1272:G:H8	1.69	0.58
1:A:401:C:O2'	1:A:621:A:N3	2.33	0.58
13:M:16:ASP:OD2	13:M:16:ASP:N	2.33	0.58
4:D:127:THR:HG23	4:D:147:ALA:HB3	1.84	0.58
4:D:28:SER:OG	4:D:30:LYS:N	2.31	0.58
1:A:828:A:H2'	1:A:829:G:O4'	2.02	0.58
2:B:28:PHE:CZ	2:B:189:ASP:HA	2.38	0.58
3:C:70:VAL:HG12	3:C:71:ALA:H	1.69	0.58
1:A:828:A:H5''	1:A:859:A:C2	2.39	0.58
1:A:671:G:N2	1:A:735:C:O2	2.36	0.58
13:M:105:THR:OG1	13:M:106:ASN:OD1	2.19	0.58
1:A:460:G:N1	1:A:470:C:H5''	2.19	0.58
5:E:11:ILE:HG21	5:E:105:VAL:HA	1.84	0.58
19:S:31:ILE:HD11	19:S:49:ILE:HG12	1.85	0.58
1:A:728:A:H2'	1:A:729:A:H8	1.69	0.58
1:A:598:U:H4'	8:H:94:TYR:CG	2.39	0.58
17:Q:95:TYR:O	17:Q:98:LEU:N	2.36	0.58
17:Q:58:GLU:OE1	17:Q:75:ARG:NH2	2.37	0.57
1:A:32:A:C2	1:A:33:A:C4	2.92	0.57
1:A:116:A:OP2	26:A:1979:HOH:O	2.17	0.57
1:A:1360:A:H8	1:A:1360:A:OP1	1.87	0.57
1:A:1119:C:H2'	1:A:1120:G:C8	2.38	0.57
1:A:67:C:H2'	1:A:68:G:C8	2.39	0.57
1:A:983:A:H3'	1:A:983:A:N3	2.19	0.57
1:A:365:U:H5''	1:A:366:C:OP1	2.04	0.57
1:A:833:U:H2'	1:A:834:C:C6	2.39	0.57
1:A:560:U:H4'	1:A:561:U:O5'	2.04	0.57
1:A:1060:C:C5	3:C:2:GLY:HA3	2.40	0.57
12:L:33:ARG:HD3	12:L:62:SER:HB3	1.86	0.57
7:G:26:PHE:O	7:G:30:ILE:HG13	2.04	0.57
1:A:656:C:O2'	15:O:28:GLN:NE2	2.30	0.57
8:H:26:VAL:O	8:H:59:LEU:N	2.37	0.57
2:B:162:ILE:O	2:B:185:ILE:HG12	2.05	0.57
8:H:86:ILE:HG21	8:H:133:LEU:HD13	1.85	0.57
1:A:947:G:O3'	13:M:109:THR:OG1	2.23	0.57
13:M:91:ARG:HB3	13:M:96:LEU:HB2	1.87	0.57
1:A:800:G:O6	26:A:2119:HOH:O	2.15	0.57
8:H:41:ARG:HG2	8:H:41:ARG:O	2.05	0.57
1:A:1367:C:H5'	10:J:60:ARG:NH1	2.20	0.57
10:J:49:VAL:HG22	14:N:41:ARG:HG3	1.87	0.57
14:N:32:SER:HB3	14:N:41:ARG:HB3	1.87	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:97:G:O2'	1:A:98:G:H8	1.87	0.56
4:D:100:ARG:HH12	4:D:137:SER:HB3	1.69	0.56
1:A:174:C:H2'	1:A:175:C:C6	2.40	0.56
1:A:820:U:H4'	1:A:821:G:OP2	2.05	0.56
15:O:55:GLY:HA2	15:O:58:MET:HE3	1.85	0.56
1:A:953:G:C2	1:A:954:G:H1'	2.39	0.56
1:A:1186:G:N2	14:N:61:TRP:OXT	2.37	0.56
10:J:68:HIS:N	10:J:68:HIS:ND1	2.53	0.56
8:H:20:TYR:HA	8:H:65:TYR:CE2	2.40	0.56
1:A:1292:U:H2'	1:A:1293:G:H8	1.68	0.56
1:A:1270:C:O2'	1:A:1313:U:O2'	2.11	0.56
1:A:1376:U:P	7:G:94:ARG:HH22	2.27	0.56
1:A:1226:C:H42	13:M:104:ARG:HD2	1.70	0.56
1:A:1220:G:H5'	19:S:34:TRP:O	2.05	0.56
1:A:1251:A:H2'	1:A:1252:A:C8	2.39	0.56
1:A:1252:A:H2'	1:A:1253:G:O4'	2.05	0.56
1:A:70:G:H1	1:A:99:U:H3	1.50	0.56
2:B:69:LEU:HB3	2:B:162:ILE:HG22	1.87	0.56
1:A:10:A:H2'	1:A:11:G:H8	1.70	0.56
1:A:126:G:OP1	1:A:605:U:O2'	2.23	0.56
2:B:134:GLU:O	2:B:138:LEU:HD11	2.05	0.56
16:P:58:TYR:O	16:P:61:SER:OG	2.12	0.56
7:G:58:PRO:HA	7:G:61:VAL:HG12	1.87	0.56
9:I:114:TYR:H	9:I:114:TYR:HD2	1.52	0.56
7:G:102:ARG:O	7:G:106:GLN:HB2	2.05	0.56
9:I:20:ARG:O	9:I:60:ASP:HB2	2.05	0.56
1:A:826:C:H2'	1:A:827:U:H6	1.70	0.56
1:A:1347:G:N2	1:A:1373:G:H2'	2.21	0.56
11:K:80:VAL:H	11:K:104:GLN:HB2	1.71	0.56
4:D:88:VAL:O	4:D:92:VAL:HG23	2.05	0.56
1:A:202:U:H3'	1:A:203:U:H6	1.70	0.56
1:A:1323:G:H2'	1:A:1324:A:H8	1.69	0.56
2:B:100:GLY:CA	2:B:104:ASN:H	2.18	0.56
1:A:189(C):C:H2'	1:A:189(D):C:O4'	2.05	0.56
13:M:15:VAL:O	13:M:19:LEU:HD23	2.05	0.56
1:A:1095:U:H5''	1:A:1109:C:O2	2.05	0.56
1:A:1317:C:N4	14:N:19:ARG:HH21	2.04	0.56
1:A:1310:G:H1	1:A:1327:C:H42	1.54	0.56
1:A:1014:A:H1'	19:S:34:TRP:HB2	1.88	0.56
11:K:99:GLN:HE21	11:K:105:VAL:HG21	1.70	0.56
13:M:33:ALA:HA	13:M:59:TYR:CE1	2.41	0.56
1:A:1067:A:O5'	1:A:1067:A:H8	1.88	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:I:118:LYS:O	9:I:120:ARG:N	2.35	0.56
1:A:1530:G:O2'	1:A:1531:A:OP1	2.17	0.56
1:A:1353:G:H2'	1:A:1354:C:C6	2.41	0.55
4:D:19:LEU:HB3	4:D:67:ILE:HG12	1.87	0.55
2:B:97:TRP:HH2	2:B:176:GLU:HB2	1.72	0.55
5:E:8:GLU:HA	5:E:34:VAL:HA	1.88	0.55
7:G:69:VAL:HG22	7:G:135:VAL:HG22	1.89	0.55
5:E:36:ASP:HB3	5:E:38:GLN:N	2.20	0.55
14:N:24:CYS:CB	14:N:28:GLY:HA2	2.36	0.55
7:G:111:ARG:HE	7:G:123:GLU:HB2	1.71	0.55
4:D:30:LYS:CB	4:D:35:ARG:HD2	2.37	0.55
1:A:1188:A:H2'	1:A:1189:C:O4'	2.06	0.55
14:N:29:ARG:HG2	14:N:40:CYS:HB3	1.87	0.55
13:M:10:PRO:HG2	13:M:18:ALA:HB1	1.88	0.55
1:A:804:U:H5''	1:A:805:C:OP2	2.06	0.55
5:E:83:GLU:HG2	5:E:88:LYS:HD2	1.87	0.55
22:V:10:G:N2	22:V:26:G:H1'	2.21	0.55
1:A:1321:C:H6	1:A:1321:C:H5''	1.71	0.55
1:A:1205:U:H4'	3:C:195:VAL:CG2	2.36	0.55
1:A:1014:A:C2	1:A:1219:U:H1'	2.42	0.55
11:K:38:ASN:OD1	11:K:38:ASN:N	2.40	0.55
9:I:99:LEU:HB3	9:I:101:PHE:CE1	2.42	0.55
5:E:24:ARG:O	5:E:25:ARG:HG3	2.07	0.55
1:A:1236:A:H4'	1:A:1304:G:H4'	1.89	0.55
10:J:55:LYS:H	10:J:56:HIS:HD2	1.54	0.55
4:D:149:ALA:HB3	4:D:152:SER:HB2	1.89	0.55
1:A:1118:C:H1'	1:A:1179:A:C4	2.41	0.55
2:B:47:THR:HA	2:B:202:PRO:HG2	1.88	0.55
4:D:10:ARG:HB3	4:D:40:PRO:HG3	1.88	0.55
1:A:1227:A:H3'	1:A:1227:A:H8	1.71	0.55
5:E:80:ILE:HD13	5:E:138:ALA:HB1	1.89	0.55
1:A:974:A:H8	1:A:974:A:OP1	1.90	0.55
4:D:53:ASP:O	4:D:57:ARG:NH1	2.40	0.55
1:A:826:C:H5'	8:H:12:ARG:HH11	1.72	0.55
1:A:11:G:C5	1:A:12:U:C5	2.95	0.55
1:A:216:G:H2'	1:A:217:C:C6	2.41	0.55
18:R:45:SER:OG	18:R:47:THR:HG22	2.07	0.55
2:B:166:ASP:HB3	2:B:169:LYS:HB3	1.90	0.54
1:A:736:C:OP1	18:R:72:ARG:NH1	2.41	0.54
2:B:149:LEU:HD23	2:B:152:PHE:HB3	1.87	0.54
5:E:148:VAL:HG21	8:H:107:LEU:HD12	1.89	0.54
1:A:1189:C:OP1	10:J:51:ARG:NH2	2.40	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
17:Q:13:ASP:O	17:Q:15:MET:N	2.40	0.54
1:A:1220:G:H2'	1:A:1221:G:O4'	2.08	0.54
20:T:36:LEU:HD12	20:T:55:ILE:HG23	1.90	0.54
9:I:40:LEU:HD11	9:I:70:LYS:HB3	1.88	0.54
8:H:97:VAL:HA	8:H:100:ILE:HD11	1.89	0.54
8:H:49:GLU:OE2	8:H:62:TYR:OH	2.24	0.54
1:A:443:C:H2'	1:A:444:C:H6	1.73	0.54
14:N:48:ALA:HB2	14:N:53:LEU:HD12	1.90	0.54
13:M:15:VAL:HG13	13:M:44:ARG:HA	1.90	0.54
1:A:1170:A:N1	1:A:1171:G:H1'	2.23	0.54
1:A:376:G:H4'	16:P:5:ARG:HH11	1.73	0.54
3:C:29:TYR:H	3:C:32:LEU:HG	1.72	0.54
1:A:59:A:H3'	1:A:331:G:H22	1.72	0.54
1:A:443:C:H2'	1:A:444:C:C6	2.42	0.54
1:A:1148:U:H2'	1:A:1149:C:O4'	2.07	0.54
6:F:33:TYR:CG	6:F:75:LEU:HD23	2.43	0.54
22:V:15:G:H2'	22:V:59:A:N1	2.22	0.54
2:B:50:GLU:O	2:B:54:THR:OG1	2.24	0.54
1:A:878:G:H1'	8:H:3:THR:HG21	1.90	0.54
15:O:59:MET:HE1	26:O:201:HOH:O	2.07	0.54
1:A:438:G:H4'	4:D:123:HIS:CD2	2.43	0.54
1:A:988:G:H2'	1:A:989:C:O4'	2.07	0.54
1:A:1261:A:N6	1:A:1274:G:H1'	2.22	0.54
1:A:1062:U:H2'	1:A:1063:C:C5	2.43	0.54
1:A:1062:U:H2'	1:A:1063:C:C6	2.43	0.54
3:C:113:ALA:HB3	3:C:114:PRO:HD3	1.88	0.54
1:A:1268:A:H2'	1:A:1269:A:C8	2.43	0.54
4:D:173:TRP:HZ3	4:D:193:ASP:HB3	1.73	0.54
1:A:769:G:H4'	1:A:1513:A:H4'	1.90	0.54
1:A:604:G:H2'	1:A:605:U:O4'	2.08	0.54
1:A:1300:G:HO2'	1:A:1301:U:P	2.29	0.54
3:C:117:ALA:HB2	3:C:200:ALA:HB2	1.89	0.54
17:Q:86:GLU:HG3	17:Q:90:ILE:HG13	1.89	0.54
1:A:1103:C:H2'	1:A:1104:G:O4'	2.08	0.54
13:M:22:ILE:HB	13:M:25:ILE:HD13	1.90	0.54
1:A:1065:U:H4'	1:A:1066:C:O5'	2.08	0.53
2:B:22:LYS:NZ	26:B:301:HOH:O	2.29	0.53
6:F:67:MET:HG3	6:F:68:PRO:HD2	1.90	0.53
15:O:70:LEU:HD12	15:O:70:LEU:O	2.08	0.53
11:K:59:TYR:CE2	11:K:63:LEU:HD12	2.43	0.53
20:T:61:SER:OG	20:T:65:LYS:HE3	2.08	0.53
15:O:34:LEU:HD11	15:O:38:ARG:HH11	1.72	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1358:U:H3	1:A:1363(A):A:H61	0.61	0.53
1:A:1157:A:O4'	1:A:1181:G:N2	2.42	0.53
1:A:171:A:H2'	1:A:172:A:C8	2.42	0.53
1:A:1292:U:H2'	1:A:1293:G:C8	2.43	0.53
22:V:18:G:O2'	22:V:19:G:O5'	2.26	0.53
2:B:92:TYR:CD2	2:B:151:GLY:HA3	2.43	0.53
13:M:50:GLU:HA	13:M:53:VAL:HB	1.89	0.53
13:M:63:THR:HB	13:M:64:TRP:CE3	2.43	0.53
1:A:1298:C:H4'	1:A:1299:A:C4	2.43	0.53
22:V:47:U:H3'	22:V:48:C:H5'	1.90	0.53
9:I:53:VAL:O	9:I:55:ALA:N	2.42	0.53
1:A:1239:A:C2'	1:A:1298:C:H42	2.21	0.53
1:A:1207:G:H2'	1:A:1208:C:C6	2.43	0.53
1:A:1169:A:H2'	1:A:1170:A:H8	1.74	0.53
1:A:859:A:H2'	1:A:860:A:O4'	2.09	0.53
1:A:187:C:H2'	1:A:188:C:C6	2.43	0.53
1:A:675:A:O2'	11:K:114:VAL:O	2.26	0.53
1:A:881:G:P	12:L:12:ARG:HH22	2.31	0.53
3:C:43:LEU:HB3	3:C:47:LEU:HD12	1.90	0.53
1:A:436:C:O2'	1:A:437:U:H6	1.91	0.53
20:T:73:HIS:HB3	20:T:74:LYS:HG2	1.90	0.53
1:A:1235:U:O2'	1:A:1305:G:O5'	2.27	0.53
1:A:623:C:O5'	1:A:623:C:H6	1.92	0.53
1:A:922:G:N3	1:A:1398:A:H2	2.07	0.53
6:F:61:LEU:HB3	6:F:63:TYR:CE2	2.41	0.53
1:A:1409:C:H42	1:A:1491:G:H1	1.57	0.53
1:A:1250:A:H4'	9:I:67:GLY:HA2	1.90	0.53
5:E:29:GLY:HA2	5:E:46:GLY:O	2.09	0.53
1:A:1070:U:H2'	1:A:1071:C:H6	1.73	0.53
4:D:25:ARG:HG2	4:D:30:LYS:O	2.08	0.53
1:A:946:A:H2'	1:A:947:G:C8	2.44	0.53
1:A:188:C:H1'	20:T:104:LEU:CB	2.38	0.53
1:A:1053:G:N7	1:A:1200:C:H5''	2.24	0.53
14:N:25:VAL:HG22	14:N:38:GLY:O	2.09	0.53
1:A:192:U:H2'	1:A:193:C:C6	2.44	0.53
1:A:115:G:H1'	1:A:116:A:N7	2.23	0.53
1:A:202:U:H3'	1:A:203:U:C6	2.44	0.53
2:B:42:ILE:HG22	2:B:43:ASP:H	1.73	0.53
1:A:1151:A:O2'	1:A:1152:A:O5'	2.21	0.52
2:B:186:ALA:HB3	2:B:197:VAL:HG11	1.89	0.52
1:A:928:G:H1	1:A:1389:C:H42	1.57	0.52
1:A:1241:G:H1	1:A:1296:C:H42	1.55	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:296:U:O2'	1:A:556:C:O2	2.25	0.52
1:A:663:A:O3'	18:R:64:ARG:NH2	2.42	0.52
2:B:57:PHE:O	2:B:61:LEU:N	2.42	0.52
9:I:17:VAL:HG21	9:I:80:GLY:C	2.29	0.52
1:A:1052:U:H2'	1:A:1055:A:OP1	2.09	0.52
1:A:1144:G:N2	1:A:1146:A:H62	2.08	0.52
1:A:512:U:H2'	1:A:513:C:H6	1.74	0.52
1:A:939:G:H5''	7:G:102:ARG:HH12	1.73	0.52
19:S:49:ILE:HG13	19:S:62:ILE:HD11	1.90	0.52
1:A:1057:G:H2'	1:A:1058:G:O4'	2.09	0.52
12:L:53:ARG:NH1	12:L:92:ASP:OD2	2.42	0.52
1:A:397:A:N3	1:A:397:A:H3'	2.24	0.52
1:A:1135:U:H2'	1:A:1137:C:O2	2.10	0.52
20:T:49:ALA:HB2	20:T:92:LEU:HD22	1.91	0.52
2:B:48:MET:HA	2:B:51:LEU:HB2	1.91	0.52
13:M:34:LEU:O	13:M:38:GLY:N	2.42	0.52
5:E:126:ARG:HH11	5:E:126:ARG:HG2	1.75	0.52
1:A:833:U:H2'	1:A:834:C:H6	1.74	0.52
1:A:438:G:O2'	1:A:494:U:O4	2.23	0.52
10:J:8:LEU:HD11	10:J:20:ALA:HB2	1.91	0.52
6:F:80:ARG:HG3	6:F:80:ARG:HH21	1.73	0.52
1:A:1502:A:H4'	1:A:1503:A:OP2	2.09	0.52
1:A:148:G:H2'	1:A:149:A:C8	2.43	0.52
1:A:131:C:H2'	1:A:132:C:C6	2.45	0.52
1:A:433:C:H2'	1:A:434:U:H6	1.75	0.52
1:A:1411:C:H2'	1:A:1412:C:C6	2.45	0.52
1:A:1098:C:H2'	1:A:1099:G:O4'	2.09	0.52
5:E:100:VAL:HA	5:E:118:ILE:HG22	1.92	0.52
1:A:737:A:H2'	1:A:738:C:H6	1.74	0.52
1:A:243:A:H4'	1:A:244:U:C5'	2.39	0.52
1:A:664:G:P	18:R:64:ARG:HH21	2.32	0.52
22:V:36:U:H2'	22:V:37:A:O4'	2.10	0.52
1:A:874:G:H2'	1:A:875:C:C6	2.44	0.52
1:A:401:C:H2'	1:A:402:G:C8	2.44	0.52
1:A:737:A:H2'	1:A:738:C:C6	2.44	0.52
1:A:1131:G:H2'	1:A:1132:C:C6	2.45	0.52
14:N:27:CYS:SG	14:N:43:CYS:SG	3.05	0.52
1:A:1170:A:C6	1:A:1171:G:H1'	2.45	0.52
1:A:973:G:H3'	1:A:974:A:H5''	1.90	0.52
4:D:64:LEU:HD22	4:D:198:VAL:HG11	1.92	0.52
1:A:538:G:OP2	12:L:115:LYS:HB2	2.09	0.52
4:D:17:VAL:HG22	4:D:18:LYS:H	1.75	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:872:A:C4	1:A:874:G:N7	2.78	0.52
4:D:189:PRO:CB	4:D:194:LEU:HD21	2.38	0.52
15:O:67:LEU:O	15:O:71:GLN:HB2	2.10	0.52
1:A:500:G:N2	1:A:546:G:H1'	2.25	0.52
1:A:1281:U:C6	1:A:1281:U:H3'	2.45	0.52
8:H:20:TYR:HD1	8:H:65:TYR:CD2	2.27	0.52
2:B:171:ALA:HA	2:B:174:VAL:HG23	1.92	0.52
1:A:751:U:H1'	15:O:24:SER:H	1.75	0.52
1:A:1218:C:H2'	1:A:1219:U:C6	2.45	0.52
1:A:1416:G:H1	1:A:1484:C:H42	1.58	0.52
5:E:33:VAL:HG21	5:E:109:ILE:HA	1.92	0.52
8:H:77:GLU:HG3	8:H:78:GLN:N	2.25	0.52
10:J:11:PHE:HE2	10:J:67:THR:HG22	1.75	0.52
3:C:132:ARG:O	3:C:136:GLN:HB2	2.10	0.52
1:A:545:C:O2'	1:A:549:C:OP1	2.28	0.52
1:A:1381:U:H2'	1:A:1381:U:O2	2.09	0.52
9:I:28:VAL:HA	9:I:63:ILE:O	2.10	0.51
1:A:793:U:O2	1:A:1516:G:H4'	2.10	0.51
19:S:67:VAL:HG23	19:S:68:GLY:H	1.75	0.51
16:P:43:LYS:C	16:P:45:THR:H	2.13	0.51
1:A:189(D):C:N4	1:A:189(E):U:C2	2.78	0.51
1:A:1142:G:H3'	1:A:1143:G:C8	2.45	0.51
14:N:24:CYS:HB3	14:N:28:GLY:HA2	1.91	0.51
15:O:78:TYR:O	15:O:82:ILE:HG12	2.10	0.51
1:A:1119:C:OP1	9:I:83:ARG:NH1	2.38	0.51
12:L:79:GLU:O	12:L:80:HIS:HB2	2.10	0.51
4:D:15:GLU:OE2	4:D:66:ARG:NH1	2.43	0.51
4:D:4:TYR:C	4:D:4:TYR:CD2	2.83	0.51
2:B:100:GLY:O	2:B:108:ILE:HG13	2.09	0.51
1:A:164:U:H2'	1:A:165:C:C6	2.45	0.51
1:A:724:G:C2	1:A:725:G:C8	2.99	0.51
9:I:114:TYR:HE1	10:J:60:ARG:H	1.55	0.51
1:A:1151:A:H5'	10:J:40:LEU:O	2.11	0.51
1:A:97:G:O2'	1:A:98:G:H5''	2.11	0.51
1:A:589:C:H2'	1:A:590:C:H6	1.76	0.51
22:V:16:C:H5'	22:V:59:A:N1	2.25	0.51
3:C:20:SER:OG	3:C:40:ARG:NH2	2.37	0.51
1:A:978:A:O2'	1:A:1322:C:N3	2.35	0.51
2:B:102:LEU:HB3	2:B:180:LEU:CD1	2.40	0.51
4:D:100:ARG:NH1	4:D:137:SER:HA	2.25	0.51
22:V:47:U:H3'	22:V:48:C:C5'	2.40	0.51
15:O:8:LYS:O	15:O:12:ILE:HG13	2.10	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
18:R:53:ARG:HA	18:R:56:THR:OG1	2.10	0.51
1:A:1126:U:H6	1:A:1126:U:P	2.34	0.51
9:I:105:ASP:HB2	9:I:107:ARG:HD3	1.93	0.51
1:A:1206:G:C6	1:A:1207:G:C5	2.98	0.51
1:A:889:A:H4'	1:A:890:G:OP1	2.10	0.51
1:A:693:G:H2'	1:A:694:A:C8	2.46	0.51
8:H:4:ASP:OD1	8:H:85:ARG:HD2	2.10	0.51
1:A:1370:G:C8	9:I:109:VAL:HG11	2.46	0.51
1:A:1365:G:H2'	1:A:1366:C:O4'	2.11	0.51
1:A:939:G:H5''	7:G:102:ARG:HH22	1.75	0.51
1:A:1222:G:C6	1:A:1223:C:C4	2.99	0.51
17:Q:67:LYS:HA	17:Q:70:ARG:HH12	1.75	0.51
1:A:963:G:H4'	26:A:2218:HOH:O	2.11	0.51
1:A:232:G:H1'	1:A:262:A:N1	2.25	0.51
5:E:41:VAL:HG23	5:E:67:VAL:HG13	1.93	0.51
1:A:1225:A:N3	1:A:1225:A:H2'	2.26	0.51
1:A:418:C:H1'	1:A:540:G:O2'	2.11	0.51
2:B:134:GLU:HA	2:B:137:ARG:NE	2.26	0.51
14:N:40:CYS:O	14:N:43:CYS:HB3	2.11	0.51
1:A:734:G:H21	18:R:75:ILE:HD11	1.75	0.51
1:A:202:U:H5''	1:A:203:U:H5	1.75	0.51
1:A:475:G:H2'	1:A:476:G:H8	1.75	0.51
1:A:191:G:N3	20:T:103:GLY:HA2	2.26	0.51
1:A:678:U:H2'	1:A:679:C:C6	2.46	0.51
1:A:130:A:O2'	1:A:131:C:O5'	2.26	0.50
14:N:23:ARG:HD3	14:N:29:ARG:O	2.11	0.50
1:A:811:C:H4'	1:A:900:A:N6	2.25	0.50
13:M:68:GLY:H	13:M:71:ARG:NH2	2.09	0.50
1:A:991:U:O4	1:A:1212:U:O2'	2.29	0.50
2:B:236:TYR:HA	2:B:239:VAL:CG2	2.42	0.50
1:A:382:A:H2'	1:A:383:A:C8	2.46	0.50
1:A:1321:C:C5'	1:A:1322:C:H5''	2.38	0.50
1:A:1513:A:H2'	1:A:1514:C:H6	1.74	0.50
1:A:1375:A:H4'	7:G:29:LYS:NZ	2.26	0.50
22:V:55:U:N3	22:V:58:A:OP2	2.27	0.50
1:A:1496:C:H2'	1:A:1497:G:O4'	2.10	0.50
1:A:1256:A:H4'	1:A:1257:U:OP1	2.10	0.50
2:B:24:TRP:CZ3	2:B:29:ALA:HB2	2.46	0.50
1:A:767:A:H2'	1:A:768:A:O4'	2.11	0.50
2:B:166:ASP:O	2:B:170:GLU:N	2.44	0.50
1:A:437:U:H5''	4:D:155:LEU:HD21	1.93	0.50
1:A:1061:G:O2'	1:A:1062:U:OP1	2.25	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:I:45:ALA:HB3	9:I:48:GLU:HB2	1.93	0.50
18:R:61:LYS:O	18:R:65:ILE:HG12	2.12	0.50
9:I:21:PRO:HA	9:I:59:PHE:HA	1.93	0.50
1:A:622:A:C8	1:A:623:C:C6	2.99	0.50
15:O:29:VAL:HG12	15:O:85:LEU:HD13	1.94	0.50
22:V:75:C:H5'	22:V:76:A:OP2	2.10	0.50
3:C:11:ARG:HB3	3:C:15:THR:H	1.76	0.50
22:V:23:C:H2'	22:V:24:U:C6	2.46	0.50
5:E:12:LEU:HB3	5:E:31:LEU:HB2	1.92	0.50
1:A:308:C:OP1	26:A:2120:HOH:O	2.20	0.50
1:A:49:U:O2	1:A:362:G:H1'	2.11	0.50
18:R:31:LEU:HD11	18:R:62:GLU:HB3	1.93	0.50
7:G:10:ARG:HH11	7:G:10:ARG:HG2	1.76	0.50
1:A:1279:A:H4'	1:A:1280:A:OP1	2.12	0.50
1:A:176:C:H2'	1:A:177:C:H6	1.77	0.50
1:A:186:C:H2'	1:A:187:C:C6	2.47	0.50
16:P:49:LEU:HD12	16:P:50:LYS:H	1.75	0.50
1:A:1286:A:H2'	1:A:1287:A:H4'	1.94	0.50
1:A:57:G:C6	1:A:58:C:C4	3.00	0.50
1:A:690:G:H2'	1:A:691:G:O4'	2.10	0.50
1:A:1244:C:N4	1:A:1293:G:H1	2.07	0.50
1:A:1184:G:H2'	1:A:1185:G:H5'	1.93	0.50
1:A:685:G:C2	1:A:686:U:C4	3.00	0.50
7:G:12:LEU:H	7:G:12:LEU:HD12	1.76	0.50
3:C:43:LEU:O	3:C:47:LEU:HB2	2.12	0.50
1:A:757:U:H2'	1:A:758:G:O4'	2.12	0.50
1:A:900:A:H2'	1:A:901:A:O4'	2.12	0.50
1:A:411:A:O2'	1:A:413:G:H5'	2.10	0.50
1:A:790:A:H61	1:A:1498:U:P	2.35	0.50
12:L:40:VAL:HG21	12:L:78:GLN:HA	1.93	0.50
1:A:1452:C:O2'	1:A:1456:G:P	2.70	0.50
1:A:840:C:H4'	1:A:841:U:OP1	2.10	0.50
1:A:1279:A:O2'	1:A:1280:A:O5'	2.30	0.50
11:K:33:THR:OG1	11:K:34:ASP:O	2.30	0.50
1:A:187:C:H2'	1:A:188:C:H6	1.76	0.50
1:A:1137:C:H4'	1:A:1138:G:C2	2.47	0.50
1:A:903:G:OP1	26:A:2060:HOH:O	2.20	0.50
3:C:150:LYS:HG3	3:C:169:ALA:HB2	1.94	0.50
12:L:32:PHE:HE1	12:L:86:ARG:HG3	1.76	0.50
1:A:944:G:C2	1:A:1340:A:C6	2.99	0.49
1:A:1308:U:OP2	13:M:99:ARG:HG3	2.12	0.49
2:B:97:TRP:CZ2	2:B:102:LEU:HD13	2.45	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:437:U:C5'	4:D:155:LEU:HD21	2.42	0.49
7:G:140:ASP:O	7:G:144:MET:N	2.45	0.49
10:J:45:ARG:HD3	10:J:65:LEU:HD23	1.94	0.49
1:A:21:G:H2'	1:A:22:G:C8	2.46	0.49
1:A:52:G:O2'	1:A:53:A:H5'	2.12	0.49
2:B:198:ASP:N	2:B:198:ASP:OD2	2.45	0.49
7:G:27:ILE:HD11	7:G:43:PHE:HD2	1.77	0.49
2:B:69:LEU:HD13	2:B:91:PRO:HB2	1.94	0.49
1:A:872:A:O2'	1:A:873:A:H5''	2.11	0.49
13:M:69:GLU:C	13:M:71:ARG:H	2.16	0.49
1:A:1095:U:H2'	1:A:1096:C:O4'	2.11	0.49
1:A:959:A:O2'	1:A:984:C:O2'	2.30	0.49
9:I:26:VAL:O	9:I:32:ASP:HA	2.12	0.49
1:A:1352:C:H42	1:A:1370:G:H1	1.61	0.49
8:H:12:ARG:HH21	8:H:26:VAL:HA	1.78	0.49
3:C:18:TRP:HD1	14:N:54:PRO:HA	1.74	0.49
3:C:52:LEU:HD21	3:C:55:VAL:HG22	1.94	0.49
1:A:1268:A:O2'	1:A:1269:A:O5'	2.30	0.49
1:A:991:U:H4'	1:A:992:U:O5'	2.12	0.49
1:A:1190:G:OP1	3:C:5:ILE:N	2.30	0.49
1:A:376:G:O3'	16:P:5:ARG:HD2	2.13	0.49
1:A:920:U:H2'	1:A:921:U:H6	1.72	0.49
11:K:105:VAL:O	11:K:105:VAL:HG23	2.13	0.49
17:Q:66:SER:OG	17:Q:67:LYS:O	2.28	0.49
20:T:10:LEU:HG	20:T:12:ALA:H	1.76	0.49
1:A:180:U:H2'	1:A:181:G:H5'	1.94	0.49
8:H:12:ARG:HH21	8:H:27:PRO:HD3	1.73	0.49
3:C:30:ARG:HH21	14:N:38:GLY:HA2	1.76	0.49
1:A:1423:G:H2'	1:A:1424:C:H6	1.76	0.49
9:I:83:ARG:O	9:I:86:VAL:HG22	2.12	0.49
10:J:55:LYS:H	10:J:56:HIS:CD2	2.30	0.49
2:B:82:ARG:HG3	2:B:92:TYR:CZ	2.48	0.49
1:A:551:U:H5'	12:L:119:LYS:HE2	1.95	0.49
16:P:28:ARG:HG2	16:P:28:ARG:NH1	2.25	0.49
14:N:27:CYS:HG	14:N:43:CYS:HG	1.55	0.49
19:S:62:ILE:HG23	19:S:66:MET:HG3	1.94	0.49
22:V:53:G:H2'	22:V:54:U:C6	2.47	0.49
8:H:13:ILE:O	8:H:17:THR:HG23	2.12	0.49
1:A:1157:A:H62	1:A:1177:G:N2	2.10	0.49
2:B:80:ILE:HG12	2:B:211:ILE:HG22	1.93	0.49
2:B:20:GLU:O	2:B:40:HIS:HB2	2.11	0.49
2:B:189:ASP:OD1	2:B:189:ASP:N	2.45	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:977:A:O2'	1:A:981:U:N3	2.45	0.49
2:B:174:VAL:O	2:B:178:ARG:HG3	2.13	0.49
1:A:722:A:H5'	1:A:723:U:OP2	2.13	0.49
2:B:83:MET:SD	2:B:234:PRO:HB2	2.52	0.49
5:E:100:VAL:O	5:E:107:ARG:NH2	2.45	0.49
1:A:1245:A:H61	1:A:1292:U:H3	1.61	0.49
12:L:33:ARG:HG2	12:L:60:LEU:HG	1.93	0.49
3:C:78:GLY:HA3	3:C:83:ARG:H	1.76	0.49
2:B:153:ARG:HG3	2:B:154:LEU:N	2.28	0.49
1:A:1378:C:H5	1:A:1379:G:N9	2.10	0.49
1:A:1112:C:H2'	1:A:1113:C:H5'	1.94	0.49
1:A:1281:U:H5''	1:A:1282:C:OP2	2.13	0.49
1:A:1182:G:H4'	1:A:1183:A:H3'	1.95	0.49
1:A:1360:A:H2'	1:A:1361:G:O4'	2.13	0.49
14:N:23:ARG:HG3	14:N:24:CYS:N	2.26	0.49
1:A:434:U:H2'	1:A:435:C:H6	1.77	0.49
8:H:51:VAL:HG11	8:H:60:ARG:NH1	2.28	0.49
18:R:65:ILE:O	18:R:69:THR:HG23	2.13	0.49
11:K:23:ALA:O	11:K:86:GLY:HA3	2.12	0.49
1:A:376:G:H5''	16:P:5:ARG:HB2	1.94	0.49
2:B:84:GLU:OE1	2:B:87:ARG:NH1	2.46	0.49
3:C:70:VAL:O	3:C:106:VAL:N	2.40	0.49
1:A:1169:A:H2'	1:A:1170:A:C8	2.48	0.49
22:V:9:G:O2'	22:V:10:G:N7	2.35	0.49
1:A:588:G:N3	1:A:588:G:H2'	2.27	0.49
1:A:1161:C:H2'	1:A:1162:C:C6	2.48	0.48
1:A:377:G:H1	1:A:386:C:N4	1.96	0.48
4:D:38:TYR:CE1	4:D:45:GLN:HG3	2.48	0.48
12:L:6:THR:O	12:L:9:GLN:HB2	2.13	0.48
1:A:927:G:N2	1:A:1391:U:H1'	2.27	0.48
1:A:1362:C:H2'	1:A:1363:C:H5''	1.95	0.48
1:A:1227:A:C8	1:A:1227:A:C3'	2.95	0.48
17:Q:7:THR:HG23	17:Q:58:GLU:HG3	1.96	0.48
1:A:1378:C:C5	1:A:1379:G:C8	3.01	0.48
17:Q:6:LEU:HB3	17:Q:23:VAL:HG11	1.95	0.48
5:E:50:GLU:HB2	5:E:53:LEU:HD13	1.95	0.48
7:G:109:ASN:O	7:G:110:GLN:NE2	2.46	0.48
1:A:978:A:H5''	1:A:979:C:OP2	2.12	0.48
5:E:36:ASP:O	5:E:37:ARG:HB2	2.12	0.48
1:A:1142:G:H3'	1:A:1143:G:H8	1.77	0.48
4:D:117:ALA:O	4:D:121:VAL:HG23	2.12	0.48
1:A:1343:G:H2'	1:A:1344:C:C6	2.48	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
22:V:49:G:C2'	22:V:50:U:H5'	2.44	0.48
17:Q:68:ARG:H	17:Q:70:ARG:NH1	2.11	0.48
4:D:107:ARG:HB3	4:D:174:LEU:HD11	1.95	0.48
2:B:212:GLN:O	2:B:216:SER:OG	2.26	0.48
5:E:80:ILE:CD1	5:E:91:LEU:HB2	2.43	0.48
1:A:1226:C:OP2	13:M:103:THR:OG1	2.21	0.48
13:M:65:LYS:HA	13:M:66:LEU:CB	2.44	0.48
13:M:65:LYS:HA	13:M:66:LEU:CG	2.44	0.48
8:H:51:VAL:HG11	8:H:60:ARG:HH11	1.77	0.48
22:V:21:A:H2'	22:V:46:G:O6	2.14	0.48
1:A:363:A:C2	12:L:31:PRO:HG2	2.48	0.48
1:A:271:C:H2'	1:A:272:C:H6	1.78	0.48
1:A:1192:C:OP2	3:C:4:LYS:NZ	2.38	0.48
1:A:502:G:C2	1:A:503:C:C2	3.01	0.48
1:A:539:A:H2'	1:A:540:G:C8	2.49	0.48
1:A:411:A:OP2	4:D:25:ARG:NH2	2.46	0.48
1:A:946:A:O2'	1:A:1333:A:N3	2.41	0.48
1:A:1065:U:H1'	1:A:1066:C:OP2	2.14	0.48
1:A:1135:U:H2'	1:A:1137:C:C2	2.48	0.48
1:A:266:G:H5''	1:A:267:C:C5	2.48	0.48
20:T:92:LEU:O	20:T:96:GLY:HA2	2.12	0.48
1:A:677:U:H3	1:A:713:G:N2	2.08	0.48
9:I:11:LYS:H	9:I:104:ARG:NH1	2.11	0.48
1:A:73:G:C6	1:A:97:G:C6	3.01	0.48
14:N:29:ARG:HH21	14:N:42:ILE:HD11	1.78	0.48
2:B:58:ILE:HG13	2:B:58:ILE:H	1.42	0.48
20:T:54:LYS:HA	20:T:57:ARG:NH2	2.29	0.48
1:A:1123:A:H4'	10:J:37:PRO:HD2	1.96	0.48
1:A:541:G:C6	1:A:542:G:C5	3.02	0.48
1:A:509:A:C3'	1:A:509:A:C8	2.96	0.48
5:E:80:ILE:HD12	5:E:91:LEU:HB2	1.94	0.48
1:A:764:C:C2	1:A:765:G:C8	3.02	0.48
1:A:406:G:H21	4:D:119:GLN:HE22	1.59	0.48
10:J:8:LEU:HB2	10:J:16:LEU:HD21	1.94	0.48
1:A:1056:U:O3'	3:C:155:GLY:HA2	2.14	0.48
2:B:30:ARG:HG3	2:B:31:TYR:N	2.29	0.48
1:A:537:G:H5''	12:L:113:ARG:NH1	2.29	0.48
1:A:1253:G:H2'	1:A:1254:C:C6	2.49	0.48
1:A:848:C:H2'	1:A:849:C:O4'	2.14	0.48
1:A:560:U:H5'	1:A:566:G:N2	2.29	0.48
1:A:189(H):G:C6	1:A:189(I):G:C5	3.01	0.48
1:A:1273:G:H5'	1:A:1274:G:OP2	2.14	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1493:A:OP2	1:A:1493:A:C8	2.67	0.48
2:B:187:LEU:HD23	2:B:201:ILE:HG22	1.95	0.48
1:A:433:C:H2'	1:A:434:U:C6	2.49	0.48
18:R:70:ILE:O	18:R:74:ARG:HG3	2.13	0.48
13:M:65:LYS:HA	13:M:66:LEU:HG	1.95	0.48
1:A:1203:C:OP1	14:N:3:ARG:HD3	2.14	0.48
1:A:561:U:O2'	1:A:562:C:OP1	2.27	0.47
1:A:562:C:H4'	1:A:563:A:O5'	2.14	0.47
1:A:1268:A:H4'	21:U:19:GLY:HA2	1.95	0.47
1:A:240:C:H2'	1:A:241:C:C6	2.49	0.47
1:A:477:A:H2'	1:A:479:C:H6	1.79	0.47
2:B:109:SER:O	2:B:112:VAL:N	2.47	0.47
2:B:69:LEU:HD12	2:B:70:PHE:N	2.29	0.47
1:A:574:A:H5''	1:A:575:G:OP2	2.14	0.47
1:A:881:G:H2'	1:A:882:C:O4'	2.14	0.47
3:C:39:ILE:O	3:C:43:LEU:HG	2.14	0.47
1:A:619:U:C2	4:D:135:LEU:HD21	2.49	0.47
1:A:257:G:C4	1:A:258:G:C8	3.02	0.47
1:A:1411:C:H2'	1:A:1412:C:H6	1.80	0.47
22:V:72:A:H2'	22:V:73:A:O4'	2.14	0.47
1:A:1353:G:H2'	1:A:1354:C:H6	1.78	0.47
1:A:1308:U:H5''	13:M:98:VAL:CG2	2.42	0.47
6:F:2:ARG:CZ	6:F:69:GLU:HG2	2.44	0.47
1:A:1512:U:H2'	1:A:1513:A:H8	1.78	0.47
1:A:544:G:OP1	4:D:62:GLN:NE2	2.30	0.47
1:A:114:U:H2'	1:A:115:G:C8	2.48	0.47
1:A:1389:C:H5''	1:A:1390:U:OP2	2.14	0.47
9:I:24:GLY:HA2	9:I:59:PHE:O	2.15	0.47
20:T:26:ASN:OD1	20:T:71:THR:HG23	2.14	0.47
6:F:50:TYR:HB2	6:F:51:PRO:HD2	1.96	0.47
2:B:185:ILE:HA	2:B:199:TYR:O	2.14	0.47
1:A:189(D):C:O2	1:A:189(H):G:C2	2.67	0.47
4:D:162:LEU:HD23	4:D:162:LEU:HA	1.65	0.47
1:A:832:C:O2'	1:A:833:U:P	2.73	0.47
1:A:270:A:C5	1:A:271:C:C4	3.02	0.47
1:A:234:C:H2'	1:A:235:C:H6	1.79	0.47
22:V:61:C:O2'	22:V:62:C:H5'	2.14	0.47
4:D:103:ASN:O	4:D:106:TYR:N	2.48	0.47
1:A:836:G:C6	1:A:851:G:C6	3.03	0.47
4:D:110:PHE:CD1	4:D:110:PHE:N	2.82	0.47
19:S:35:SER:HB3	19:S:37:ARG:HD3	1.96	0.47
1:A:1181:G:H2'	1:A:1182:G:C4	2.50	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:19:HIS:ND1	2:B:20:GLU:HG2	2.29	0.47
8:H:4:ASP:OD1	8:H:85:ARG:NH1	2.41	0.47
1:A:832:C:N4	1:A:855:G:C6	2.82	0.47
13:M:9:ILE:HA	13:M:10:PRO:HD3	1.53	0.47
10:J:55:LYS:O	10:J:57:LYS:N	2.48	0.47
1:A:664:G:H22	1:A:741:G:H1	1.61	0.47
9:I:44:VAL:HA	9:I:45:ALA:HA	1.54	0.47
2:B:136:VAL:O	2:B:139:LYS:HB3	2.14	0.47
1:A:1168:A:H8	1:A:1168:A:OP1	1.97	0.47
8:H:73:ASP:OD2	8:H:75:ARG:HD3	2.15	0.47
2:B:32:ILE:HD11	2:B:190:THR:HG22	1.96	0.47
1:A:983:A:N1	1:A:1222:G:N2	2.52	0.47
11:K:34:ASP:HB3	11:K:40:ILE:HD11	1.96	0.47
1:A:378:G:C6	1:A:379:C:C4	3.01	0.47
1:A:1007:C:H2'	1:A:1008:C:H6	1.79	0.47
1:A:55:A:C5	1:A:56:U:C5	3.02	0.47
1:A:1392:G:N2	1:A:1502:A:H8	2.12	0.47
1:A:1127:G:C2'	1:A:1147:C:H42	2.28	0.47
1:A:1347:G:HO2'	1:A:1373:G:H1	1.63	0.47
1:A:129(A):G:N7	1:A:189(E):U:O3'	2.48	0.47
6:F:2:ARG:HB2	6:F:4:TYR:CE2	2.49	0.47
1:A:1016:A:C5	1:A:1017:G:H1'	2.50	0.47
1:A:920:U:O4'	1:A:1080:A:C2	2.68	0.47
4:D:118:ARG:O	4:D:121:VAL:N	2.48	0.47
1:A:1226:C:H2'	13:M:103:THR:HB	1.96	0.47
11:K:104:GLN:O	11:K:105:VAL:HG22	2.14	0.47
1:A:452:A:H1'	1:A:453:A:C8	2.49	0.47
3:C:152:ILE:HD12	3:C:199:LYS:HD2	1.97	0.47
20:T:67:ALA:HB2	20:T:77:ALA:HB2	1.96	0.47
8:H:20:TYR:HD1	8:H:65:TYR:CE2	2.32	0.47
16:P:51:VAL:CG1	16:P:53:VAL:H	2.28	0.47
1:A:436:C:HO2'	1:A:437:U:H6	1.57	0.47
1:A:947:G:H2'	1:A:948:C:C6	2.50	0.47
20:T:56:MET:HE1	20:T:85:MET:HA	1.96	0.47
7:G:134:ALA:O	7:G:137:LYS:HB3	2.15	0.47
1:A:781:A:H4'	1:A:1522:U:O2'	2.15	0.47
1:A:377:G:OP1	16:P:3:LYS:HD2	2.15	0.47
1:A:450:G:OP1	16:P:43:LYS:NZ	2.47	0.47
2:B:68:ILE:HG13	2:B:161:ALA:HB3	1.97	0.47
9:I:114:TYR:CD1	10:J:60:ARG:HB2	2.50	0.47
1:A:426:G:OP1	4:D:36:ARG:NH1	2.47	0.47
2:B:28:PHE:CD2	2:B:194:PRO:HG3	2.50	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
22:V:8:U:O2'	22:V:21:A:N1	2.34	0.47
17:Q:5:VAL:HG23	17:Q:60:ILE:HD12	1.97	0.47
1:A:124:G:H2'	1:A:125:U:H6	1.79	0.47
12:L:34:ARG:O	12:L:61:THR:HG23	2.14	0.47
1:A:862:C:H1'	1:A:874:G:H5''	1.96	0.47
13:M:90:LEU:C	13:M:91:ARG:HG2	2.36	0.47
1:A:1095:U:P	1:A:1108:G:H1	2.38	0.47
4:D:32:ALA:HA	4:D:35:ARG:HG3	1.96	0.47
12:L:33:ARG:HH11	12:L:62:SER:HB3	1.78	0.47
1:A:741:G:H2'	1:A:742:G:O4'	2.14	0.47
1:A:885:G:O2'	1:A:914:A:N1	2.36	0.47
15:O:7:GLU:O	15:O:11:VAL:HG23	2.15	0.47
1:A:1151:A:O2'	1:A:1152:A:H8	1.98	0.46
1:A:572:A:H5'	1:A:573:A:OP2	2.15	0.46
1:A:818:G:O2'	1:A:819:A:H5'	2.15	0.46
1:A:216:G:H2'	1:A:217:C:H6	1.79	0.46
1:A:790:A:C6	1:A:791:G:C6	3.03	0.46
2:B:112:VAL:O	2:B:115:LEU:HB3	2.15	0.46
15:O:61:GLY:O	15:O:65:ARG:HD3	2.16	0.46
15:O:48:LYS:HA	15:O:48:LYS:HD2	1.78	0.46
2:B:162:ILE:HG13	2:B:184:VAL:HG13	1.97	0.46
2:B:178:ARG:HH22	8:H:68:ARG:NH1	2.14	0.46
2:B:135:GLN:O	2:B:138:LEU:HD12	2.15	0.46
1:A:328:C:H4'	1:A:329:A:O5'	2.15	0.46
7:G:31:MET:SD	7:G:34:GLY:HA2	2.55	0.46
1:A:385:C:O2'	1:A:386:C:H5'	2.16	0.46
1:A:377:G:N2	1:A:386:C:N3	2.41	0.46
4:D:158:ILE:O	4:D:162:LEU:HB2	2.16	0.46
4:D:121:VAL:O	4:D:134:ASP:HA	2.15	0.46
4:D:68:TYR:CD2	4:D:97:LEU:HD22	2.50	0.46
2:B:129:GLU:C	2:B:130:ARG:HD2	2.36	0.46
1:A:878:G:H5''	1:A:879:C:OP2	2.16	0.46
1:A:406:G:H21	4:D:119:GLN:NE2	2.14	0.46
1:A:325:A:H2'	1:A:326:G:O4'	2.15	0.46
9:I:42:ARG:O	9:I:74:ILE:HG21	2.15	0.46
3:C:125:GLU:HA	3:C:191:THR:HG22	1.98	0.46
1:A:1085:U:H3'	1:A:1086:U:H5	1.80	0.46
4:D:101:LEU:HD23	4:D:138:TYR:HB3	1.96	0.46
1:A:197:A:N6	1:A:221:C:H5'	2.30	0.46
1:A:1352:C:H2'	1:A:1353:G:C8	2.50	0.46
1:A:1366:C:H2'	1:A:1367:C:C6	2.50	0.46
1:A:880:C:H2'	1:A:881:G:C8	2.50	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:665:A:N3	1:A:732:C:H2'	2.30	0.46
1:A:839:U:H5'	1:A:840:C:H5	1.80	0.46
20:T:58:LYS:HE3	20:T:62:LEU:HD11	1.97	0.46
11:K:122:LYS:HB3	11:K:122:LYS:HE2	1.70	0.46
4:D:150:GLU:HA	4:D:153:ARG:HE	1.80	0.46
3:C:24:ALA:CB	3:C:29:TYR:HB2	2.40	0.46
1:A:968:A:C8	1:A:1062:U:H4'	2.51	0.46
1:A:1007:C:H2'	1:A:1008:C:C6	2.50	0.46
1:A:570:G:H2'	1:A:571:U:C6	2.50	0.46
1:A:784:C:H2'	1:A:785:G:C8	2.50	0.46
1:A:149:A:O2'	1:A:150:C:H5'	2.15	0.46
1:A:1133:G:N2	1:A:1142:G:C4	2.83	0.46
1:A:509:A:H5''	4:D:55:ALA:HB2	1.98	0.46
1:A:1316:G:H2'	1:A:1317:C:H5''	1.97	0.46
1:A:262:A:C6	1:A:263:A:C6	3.03	0.46
10:J:6:ILE:HA	10:J:97:GLU:O	2.15	0.46
11:K:84:VAL:HG12	11:K:110:ASP:OD1	2.15	0.46
1:A:1399:C:C2	1:A:1502:A:N6	2.84	0.46
18:R:52:PRO:O	18:R:56:THR:HG23	2.15	0.46
1:A:781:A:H5'	1:A:782:A:OP2	2.16	0.46
1:A:124:G:H2'	1:A:125:U:C6	2.51	0.46
20:T:82:SER:O	20:T:86:ARG:HG3	2.16	0.46
1:A:408:A:C6	1:A:409:G:C5	3.04	0.46
1:A:734:G:H2'	1:A:735:C:H6	1.81	0.46
1:A:330:C:H2'	1:A:331:G:H5'	1.98	0.46
1:A:124:G:H1	1:A:237:C:H42	1.62	0.46
9:I:71:SER:HA	9:I:74:ILE:HB	1.97	0.46
1:A:1427:U:H2'	1:A:1428:A:C8	2.51	0.46
1:A:1157:A:H4'	1:A:1158:C:O5'	2.15	0.46
1:A:518:C:H2'	1:A:530:G:H8	1.77	0.46
1:A:10:A:H2'	1:A:11:G:C8	2.50	0.46
2:B:47:THR:HG23	2:B:202:PRO:HG2	1.98	0.46
1:A:1343:G:C6	1:A:1344:C:N4	2.84	0.46
14:N:33:VAL:HA	14:N:39:LEU:O	2.16	0.46
19:S:51:VAL:O	19:S:57:HIS:HA	2.16	0.46
1:A:604:G:C6	1:A:605:U:N3	2.84	0.46
1:A:273:A:N6	1:A:274:A:C6	2.84	0.46
1:A:976:G:H5''	1:A:1358:U:O2	2.15	0.46
2:B:165:VAL:HG23	2:B:166:ASP:N	2.30	0.46
10:J:55:LYS:HE2	10:J:55:LYS:HB3	1.45	0.46
1:A:382:A:H2'	1:A:383:A:H8	1.80	0.46
16:P:68:ASP:C	16:P:70:ALA:N	2.68	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:189:ALA:HB3	3:C:196:LEU:HB2	1.98	0.46
1:A:1501:C:OP2	1:A:1504:G:H2'	2.15	0.45
1:A:922:G:C2	1:A:923:A:C4	3.04	0.45
1:A:1189:C:O2	26:A:2104:HOH:O	2.20	0.45
1:A:1291:G:H2'	1:A:1292:U:C6	2.51	0.45
16:P:53:VAL:HG13	16:P:79:VAL:HG23	1.98	0.45
3:C:30:ARG:NH2	14:N:38:GLY:HA2	2.30	0.45
2:B:130:ARG:HB3	2:B:131:PRO:HD2	1.98	0.45
2:B:111:ARG:HD3	2:B:111:ARG:HA	1.58	0.45
15:O:16:ALA:HB1	15:O:21:ASP:HB3	1.98	0.45
1:A:975:A:H4'	1:A:1358:U:O2	2.16	0.45
1:A:1347:G:H22	1:A:1374:A:P	2.38	0.45
1:A:501:C:OP1	12:L:117:ARG:NH2	2.49	0.45
1:A:986:A:N3	19:S:52:TYR:OH	2.41	0.45
16:P:55:ARG:O	16:P:58:TYR:N	2.45	0.45
4:D:57:ARG:HG2	4:D:202:LEU:O	2.17	0.45
1:A:234:C:H2'	1:A:235:C:C6	2.51	0.45
19:S:12:ASP:HB3	19:S:13:ASP:H	1.48	0.45
3:C:137:ALA:HA	3:C:140:ARG:HE	1.81	0.45
15:O:17:ARG:HH11	15:O:17:ARG:HG3	1.82	0.45
1:A:923:A:H2'	1:A:924:C:H6	1.81	0.45
1:A:1176:A:H2'	1:A:1177:G:O4'	2.16	0.45
1:A:1015:A:H2'	1:A:1016:A:C8	2.51	0.45
2:B:178:ARG:HD2	2:B:196:LEU:O	2.17	0.45
22:V:19:G:C4	22:V:57:A:C2	3.05	0.45
6:F:29:ALA:O	6:F:32:ASN:HB2	2.15	0.45
1:A:1091:U:O2	1:A:1093:A:C8	2.69	0.45
1:A:910:C:H2'	1:A:911:U:O4'	2.16	0.45
20:T:33:ILE:O	20:T:37:SER:OG	2.27	0.45
2:B:107:THR:HA	2:B:110:GLN:HG3	1.99	0.45
13:M:72:ALA:O	13:M:75:ALA:HB3	2.16	0.45
17:Q:83:ASP:N	17:Q:83:ASP:OD1	2.48	0.45
1:A:376:G:H2'	1:A:377:G:H8	1.81	0.45
1:A:1122:U:H2'	1:A:1123:A:O4'	2.17	0.45
1:A:129(A):G:O6	1:A:189(E):U:O4'	2.34	0.45
1:A:770:C:O2'	1:A:899:C:N3	2.39	0.45
1:A:1206:G:H4'	3:C:192:THR:O	2.15	0.45
3:C:18:TRP:CD1	14:N:53:LEU:O	2.70	0.45
1:A:460:G:O6	1:A:470:C:H5''	2.15	0.45
1:A:624:C:O3'	16:P:10:GLY:HA2	2.17	0.45
7:G:26:PHE:CG	7:G:62:PHE:HE1	2.34	0.45
10:J:8:LEU:O	10:J:16:LEU:HD11	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:373:A:C2	1:A:374:A:C8	3.04	0.45
1:A:1318:A:H4'	19:S:10:PHE:CE2	2.51	0.45
17:Q:45:HIS:HB3	17:Q:72:ARG:HB3	1.98	0.45
4:D:89:THR:O	4:D:93:PHE:N	2.39	0.45
2:B:37:ASN:O	2:B:39:ILE:HG13	2.16	0.45
1:A:503:C:H2'	1:A:504:C:H6	1.82	0.45
1:A:622:A:C8	1:A:623:C:C5	3.04	0.45
5:E:12:LEU:O	5:E:30:ALA:HA	2.16	0.45
10:J:42:THR:OG1	10:J:68:HIS:HB3	2.16	0.45
1:A:872:A:C5	1:A:874:G:C8	3.05	0.45
1:A:563:A:N7	1:A:567:G:H1'	2.32	0.45
1:A:677:U:H1'	11:K:119:CYS:SG	2.56	0.45
2:B:167:PRO:O	2:B:171:ALA:N	2.49	0.45
1:A:939:G:H5''	7:G:102:ARG:NH1	2.31	0.45
1:A:1446:U:H4'	1:A:1447:A:C6	2.51	0.45
17:Q:45:HIS:NE2	17:Q:47:PRO:HG3	2.32	0.45
3:C:139:GLN:HA	3:C:139:GLN:OE1	2.17	0.45
8:H:66:GLY:O	8:H:76:PRO:HB3	2.17	0.45
1:A:1281:U:C6	1:A:1281:U:C3'	3.00	0.45
1:A:1157:A:H62	1:A:1177:G:H22	1.65	0.45
1:A:1227:A:N3	19:S:83:HIS:HB3	2.32	0.45
18:R:53:ARG:HG3	18:R:63:GLN:NE2	2.22	0.45
18:R:53:ARG:NE	18:R:58:LEU:O	2.50	0.45
1:A:1366:C:H2'	1:A:1367:C:H6	1.82	0.45
7:G:111:ARG:NE	7:G:123:GLU:HB2	2.31	0.45
18:R:74:ARG:HA	18:R:79:LEU:O	2.17	0.45
1:A:947:G:H2'	1:A:948:C:H6	1.82	0.45
7:G:16:LEU:HD12	9:I:41:VAL:HG12	1.98	0.45
1:A:250:A:H5'	1:A:252:U:H1'	1.99	0.45
1:A:120:A:C6	1:A:122:G:C2	3.05	0.45
2:B:16:HIS:CD2	2:B:209:ARG:HG3	2.52	0.45
3:C:8:ILE:O	3:C:12:LEU:HG	2.16	0.45
2:B:21:ARG:CB	2:B:39:ILE:HA	2.44	0.45
2:B:20:GLU:OE2	2:B:23:ARG:NH2	2.45	0.45
1:A:939:G:H5''	7:G:102:ARG:NH2	2.32	0.45
13:M:65:LYS:O	13:M:65:LYS:HE3	2.17	0.45
1:A:499:A:H4'	1:A:500:G:OP1	2.16	0.45
1:A:1285:A:H4'	1:A:1286:A:O5'	2.17	0.45
1:A:1421:G:H1	1:A:1479:C:H42	1.64	0.45
1:A:1415:G:N3	1:A:1486:G:C2	2.85	0.45
9:I:5:TYR:OH	9:I:16:ARG:HG2	2.16	0.45
2:B:87:ARG:CZ	2:B:233:SER:HB2	2.47	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:731:G:OP1	1:A:766:A:H1'	2.17	0.45
14:N:29:ARG:NH2	14:N:42:ILE:HD11	2.32	0.45
7:G:82:GLY:HA2	23:X:1:A:N7	2.32	0.45
1:A:1317:C:H42	14:N:19:ARG:HH21	1.63	0.45
14:N:13:THR:N	14:N:14:PRO:HD2	2.32	0.45
1:A:189:G:C2	1:A:189(L):G:C2	3.05	0.45
1:A:245:C:O2	1:A:283:C:N3	2.50	0.45
5:E:79:GLU:HG3	5:E:93:PRO:HD2	1.98	0.45
1:A:936:C:H2'	1:A:937:A:O4'	2.17	0.45
4:D:146:ILE:HD12	4:D:146:ILE:N	2.32	0.45
1:A:1487:G:O5'	1:A:1487:G:H8	2.00	0.45
1:A:923:A:H2'	1:A:924:C:C6	2.52	0.45
1:A:1354:C:N3	1:A:1368:G:O6	2.49	0.45
5:E:98:THR:HG22	5:E:99:GLY:N	2.32	0.45
1:A:730:G:C5	1:A:731:G:H1'	2.52	0.45
15:O:24:SER:O	15:O:27:VAL:N	2.50	0.45
19:S:62:ILE:HD12	19:S:62:ILE:H	1.82	0.45
1:A:987:G:H1	1:A:1218:C:H42	1.65	0.45
1:A:1305:G:N1	1:A:1331:G:O2'	2.46	0.45
2:B:18:GLY:HA2	2:B:42:ILE:HG13	1.99	0.45
1:A:429:U:H1'	1:A:430:A:H5''	1.99	0.45
8:H:127:LEU:HD13	8:H:127:LEU:HA	1.69	0.45
10:J:69:ASN:O	10:J:70:ARG:HG2	2.18	0.44
3:C:18:TRP:N	3:C:18:TRP:CE3	2.82	0.44
1:A:1348:U:H4'	9:I:120:ARG:HG3	1.99	0.44
1:A:819:A:H4'	1:A:820:U:OP2	2.17	0.44
1:A:675:A:H2'	1:A:676:A:H8	1.81	0.44
1:A:678:U:H2'	1:A:679:C:H6	1.82	0.44
1:A:1435:G:H2'	1:A:1436:U:C6	2.52	0.44
1:A:923:A:OP1	5:E:21:ALA:HB2	2.17	0.44
10:J:51:ARG:HG3	10:J:60:ARG:HA	1.99	0.44
1:A:129(A):G:N1	1:A:189(D):C:O2	2.50	0.44
1:A:243:A:C2	1:A:246:A:C8	3.05	0.44
1:A:1328:C:OP2	21:U:7:ARG:NH1	2.50	0.44
1:A:590:C:H2'	1:A:591:U:C6	2.52	0.44
1:A:436:C:O2'	1:A:437:U:P	2.76	0.44
5:E:151:LEU:CD1	8:H:77:GLU:HG2	2.47	0.44
1:A:1382:C:H2'	1:A:1383:C:C6	2.52	0.44
1:A:991:U:C5	1:A:1212:U:H1'	2.52	0.44
11:K:67:ASP:O	11:K:71:LYS:HG3	2.17	0.44
5:E:84:PHE:HB2	5:E:134:ALA:HB2	1.98	0.44
1:A:1370:G:O6	26:A:1954:HOH:O	2.21	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:36:ARG:HG2	4:D:38:TYR:CZ	2.52	0.44
2:B:132:LYS:O	2:B:135:GLN:HG2	2.17	0.44
1:A:174:C:H2'	1:A:175:C:H6	1.81	0.44
1:A:1008:C:O2	1:A:1009:G:H1'	2.17	0.44
1:A:880:C:H2'	1:A:881:G:H8	1.82	0.44
13:M:15:VAL:HG22	13:M:42:ALA:O	2.18	0.44
19:S:52:TYR:HB2	19:S:57:HIS:CE1	2.52	0.44
4:D:173:TRP:HB2	4:D:187:ARG:O	2.18	0.44
13:M:66:LEU:HA	13:M:66:LEU:HD22	1.74	0.44
16:P:68:ASP:C	16:P:70:ALA:H	2.20	0.44
3:C:92:ALA:HB2	3:C:99:VAL:CB	2.48	0.44
1:A:814:A:N7	1:A:816:A:C4	2.85	0.44
17:Q:81:ARG:NH2	17:Q:84:LEU:HD11	2.32	0.44
1:A:1043:C:H2'	1:A:1044:A:O4'	2.18	0.44
1:A:376:G:H2'	1:A:377:G:C8	2.52	0.44
1:A:425:G:N2	1:A:426:G:H1'	2.33	0.44
1:A:727:G:N2	1:A:730:G:OP2	2.48	0.44
1:A:1309:G:H5'	13:M:78:ILE:HD11	1.99	0.44
5:E:88:LYS:HB3	5:E:123:LEU:HB2	2.00	0.44
1:A:1516:G:H2'	1:A:1518:A:OP2	2.18	0.44
17:Q:67:LYS:O	17:Q:68:ARG:HB3	2.17	0.44
1:A:838:G:H2'	1:A:839:U:H5''	2.00	0.44
1:A:119:A:H5'	1:A:120:A:C4	2.52	0.44
9:I:69:GLY:O	9:I:73:GLN:N	2.37	0.44
1:A:384:G:C6	1:A:385:C:N4	2.85	0.44
6:F:26:ILE:O	6:F:30:LEU:HD12	2.17	0.44
1:A:1347:G:N1	1:A:1374:A:OP2	2.42	0.44
1:A:39:G:C6	1:A:40:C:C5	3.06	0.44
4:D:73:ARG:O	4:D:77:ASN:HB2	2.18	0.44
20:T:38:LYS:HA	20:T:41:ILE:HD11	1.99	0.44
5:E:88:LYS:HG2	5:E:123:LEU:HB2	2.00	0.44
3:C:114:PRO:O	3:C:118:GLN:HG2	2.17	0.44
1:A:663:A:H2'	1:A:664:G:O4'	2.18	0.44
3:C:4:LYS:HE3	3:C:4:LYS:HB2	1.82	0.44
14:N:45:ARG:O	14:N:49:HIS:HD2	1.99	0.44
1:A:587:G:N1	1:A:754:C:OP2	2.51	0.44
22:V:40:C:O2'	22:V:41:C:H5'	2.17	0.44
2:B:194:PRO:HB2	2:B:195:ASP:OD1	2.18	0.44
3:C:52:LEU:HA	3:C:70:VAL:HA	1.99	0.44
1:A:1107:C:C4	1:A:1108:G:N7	2.86	0.44
13:M:106:ASN:N	13:M:106:ASN:OD1	2.49	0.44
13:M:33:ALA:HA	13:M:59:TYR:HE1	1.79	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1305:G:N2	1:A:1331:G:O2'	2.49	0.44
7:G:10:ARG:HG2	7:G:10:ARG:NH1	2.33	0.44
1:A:790:A:N6	1:A:1498:U:OP1	2.51	0.44
4:D:103:ASN:OD1	4:D:114:ARG:NE	2.45	0.44
1:A:1508:G:H2'	1:A:1509:C:O4'	2.17	0.44
5:E:39:GLY:O	5:E:69:VAL:HG13	2.17	0.44
8:H:29:SER:O	8:H:32:LYS:HB2	2.17	0.44
12:L:84:LEU:HD23	12:L:105:TYR:HE1	1.82	0.44
3:C:37:GLN:NE2	14:N:52:GLN:OE1	2.39	0.44
10:J:40:LEU:HA	10:J:40:LEU:HD23	1.70	0.44
1:A:1298:C:H2'	7:G:114:ARG:NH1	2.33	0.44
1:A:503:C:H2'	1:A:504:C:C6	2.53	0.44
3:C:134:ILE:HG23	3:C:151:VAL:HB	1.98	0.44
1:A:1073:U:O4	1:A:1102:A:N1	2.51	0.44
2:B:78:GLN:NE2	2:B:94:ASN:O	2.51	0.44
1:A:1300:G:O2'	1:A:1301:U:P	2.76	0.44
12:L:66:VAL:HG11	12:L:98:TYR:CE1	2.52	0.44
1:A:673:G:H5''	6:F:87:ARG:NH1	2.33	0.44
14:N:26:ARG:HB3	14:N:43:CYS:SG	2.58	0.44
1:A:939:G:H1	1:A:1344:C:N4	2.16	0.44
1:A:634:C:H2'	1:A:635:G:H8	1.83	0.44
1:A:1266:G:N2	1:A:1269:A:OP2	2.48	0.44
1:A:1134:G:H2'	1:A:1134:G:N3	2.33	0.44
4:D:64:LEU:HB2	4:D:198:VAL:HG21	1.99	0.44
1:A:850:U:H2'	1:A:851:G:H5''	2.00	0.44
1:A:779:C:H5''	11:K:122:LYS:HG2	2.00	0.44
22:V:43:A:C2	22:V:44:A:C4	3.06	0.44
22:V:69:C:C2'	22:V:70:G:H5'	2.47	0.43
1:A:176:C:H2'	1:A:177:C:C6	2.53	0.43
1:A:1452:C:O2'	1:A:1456:G:OP1	2.31	0.43
7:G:99:LEU:HD22	7:G:103:TRP:CZ2	2.53	0.43
1:A:558:G:H8	1:A:558:G:O5'	2.01	0.43
1:A:35:G:O2'	12:L:118:SER:O	2.35	0.43
1:A:1471:G:H2'	1:A:1472:U:H6	1.83	0.43
1:A:717:C:H6	1:A:717:C:H5''	1.82	0.43
10:J:50:ILE:HA	10:J:60:ARG:HG2	2.00	0.43
2:B:206:ASP:O	2:B:211:ILE:HD11	2.18	0.43
1:A:1319:A:H61	1:A:1361:G:H21	1.67	0.43
1:A:1310:G:OP1	13:M:77:ASN:ND2	2.48	0.43
1:A:589:C:H2'	1:A:590:C:C6	2.53	0.43
22:V:25:C:H2'	22:V:26:G:O4'	2.17	0.43
1:A:928:G:H1	1:A:1389:C:N4	2.16	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:J:8:LEU:HD13	10:J:19:SER:OG	2.18	0.43
1:A:665:A:H2'	1:A:725:G:N2	2.33	0.43
8:H:5:PRO:O	8:H:8:ASP:HB3	2.18	0.43
1:A:1181:G:H2'	1:A:1182:G:C5	2.53	0.43
1:A:874:G:H2'	1:A:875:C:H6	1.83	0.43
22:V:3:C:N4	22:V:70:G:H1	2.10	0.43
2:B:211:ILE:O	2:B:215:LEU:HB2	2.18	0.43
2:B:72:GLY:O	2:B:94:ASN:HA	2.18	0.43
1:A:1329:A:H2'	1:A:1330:U:O4'	2.19	0.43
4:D:65:ARG:HG2	4:D:75:PHE:CD1	2.53	0.43
1:A:33:A:H2'	1:A:34:C:C6	2.53	0.43
1:A:257:G:H2'	1:A:258:G:H8	1.84	0.43
2:B:24:TRP:HZ3	2:B:29:ALA:HB2	1.82	0.43
7:G:75:VAL:HG13	7:G:145:ALA:HB2	2.01	0.43
1:A:1323:G:H4'	1:A:1363:C:N3	2.34	0.43
1:A:1123:A:H2	10:J:39:PRO:HD2	1.83	0.43
1:A:502:G:H4'	1:A:550:G:H4'	2.00	0.43
15:O:88:ARG:HG3	15:O:88:ARG:HH11	1.84	0.43
1:A:1049:U:H4'	1:A:1050:G:O5'	2.19	0.43
1:A:1134:G:C2	1:A:1135:U:O4'	2.72	0.43
2:B:24:TRP:CZ3	2:B:26:PRO:HA	2.53	0.43
1:A:1434:A:H2'	1:A:1435:G:O4'	2.18	0.43
9:I:97:LYS:O	9:I:100:GLY:N	2.46	0.43
1:A:37:U:O2'	1:A:547:A:N1	2.40	0.43
5:E:68:GLU:HG2	5:E:70:PRO:HD3	2.00	0.43
1:A:631:G:H2'	1:A:631:G:N3	2.32	0.43
17:Q:74:LEU:HD22	17:Q:74:LEU:HA	1.72	0.43
5:E:51:VAL:O	5:E:54:ALA:HB3	2.17	0.43
16:P:72:ARG:CG	16:P:72:ARG:HH11	2.22	0.43
1:A:1128:C:O2'	1:A:1130:A:C8	2.71	0.43
7:G:113:GLU:CD	7:G:119:ARG:HG2	2.39	0.43
1:A:1238:A:C8	1:A:1303:C:H1'	2.54	0.43
1:A:675:A:H2'	1:A:676:A:C8	2.53	0.43
17:Q:29:HIS:HB3	17:Q:33:GLY:N	2.33	0.43
1:A:1053:G:N7	1:A:1200:C:C5'	2.81	0.43
8:H:58:TYR:O	8:H:59:LEU:HD23	2.19	0.43
1:A:1339:A:H2'	1:A:1340:A:O4'	2.19	0.43
1:A:1273:G:C5	1:A:1274:G:C8	3.07	0.43
15:O:79:ARG:HA	15:O:82:ILE:HD11	2.01	0.43
15:O:81:LEU:HG	15:O:85:LEU:HD12	1.99	0.43
1:A:1415:G:H1	1:A:1485:U:H3	1.66	0.43
1:A:93:G:H1'	1:A:96:U:H5'	2.00	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:25:C:H5'	1:A:524:G:H1'	2.00	0.43
1:A:683:G:C2	1:A:684:A:C4	3.06	0.43
1:A:1068:G:N3	1:A:1191:A:C2	2.86	0.43
17:Q:89:LEU:HD23	17:Q:89:LEU:HA	1.85	0.43
2:B:102:LEU:O	2:B:105:PHE:HB2	2.19	0.43
2:B:105:PHE:HD2	2:B:158:LEU:HD22	1.83	0.43
1:A:401:C:H6	1:A:401:C:O5'	2.01	0.43
22:V:19:G:H5'	22:V:20:U:C5	2.54	0.43
1:A:5:U:H5'	1:A:6:G:C5	2.54	0.43
22:V:64:G:C6	22:V:65:C:C4	3.06	0.43
1:A:392:G:H2'	1:A:393:A:C8	2.53	0.43
6:F:53:ALA:HB3	6:F:86:ARG:NH1	2.33	0.43
11:K:55:LYS:H	11:K:55:LYS:HG2	1.60	0.43
9:I:4:TYR:CE1	9:I:88:TYR:HA	2.54	0.43
11:K:98:LEU:HA	11:K:98:LEU:HD22	1.84	0.43
1:A:569:C:H42	1:A:881:G:H1	1.66	0.43
1:A:1061:G:H5''	10:J:59:SER:CB	2.49	0.43
1:A:832:C:HO2'	1:A:833:U:P	2.41	0.43
1:A:854:G:N1	1:A:855:G:C5	2.87	0.43
11:K:79:SER:HA	11:K:104:GLN:HB2	2.00	0.43
5:E:19:MET:SD	5:E:24:ARG:HB3	2.58	0.43
1:A:93:G:HO2'	1:A:96:U:H6	1.66	0.43
1:A:683:G:C6	1:A:684:A:C6	3.07	0.43
17:Q:32:TYR:O	17:Q:34:LYS:N	2.51	0.43
16:P:2:VAL:O	16:P:64:ALA:HA	2.18	0.43
15:O:43:LEU:HA	15:O:43:LEU:HD23	1.59	0.43
1:A:1332:A:O5'	1:A:1332:A:H8	2.02	0.43
2:B:216:SER:O	2:B:219:VAL:N	2.52	0.43
1:A:1291:G:C6	1:A:1292:U:C4	3.06	0.43
1:A:1084:G:H5'	1:A:1102:A:OP2	2.18	0.43
1:A:1057:G:C5	1:A:1204:A:C2	3.07	0.43
2:B:111:ARG:O	2:B:115:LEU:N	2.52	0.43
1:A:452:A:C2	1:A:453:A:C4	3.07	0.43
5:E:57:LYS:HD3	5:E:61:TYR:HE2	1.83	0.43
14:N:53:LEU:HD23	14:N:53:LEU:HA	1.70	0.43
3:C:68:VAL:HG12	3:C:70:VAL:HG22	2.00	0.43
13:M:23:TYR:CD1	13:M:71:ARG:NH1	2.87	0.43
1:A:942:G:C2	1:A:1342:C:C2	3.06	0.43
1:A:1058:G:H1	1:A:1199:U:H3	1.67	0.43
9:I:49:PRO:O	9:I:52:ALA:N	2.44	0.43
1:A:447:G:H2'	1:A:485:G:N2	2.34	0.43
11:K:120:ARG:HA	11:K:121:PRO:HD3	1.82	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:41:G:H2'	1:A:42:G:C8	2.54	0.43
1:A:1046:A:H3'	1:A:1047:G:H8	1.84	0.43
20:T:43:LEU:O	20:T:47:GLY:N	2.52	0.42
1:A:171:A:C2	1:A:172:A:C4	3.07	0.42
1:A:1207:G:H2'	1:A:1208:C:H6	1.83	0.42
1:A:1061:G:HO2'	1:A:1062:U:P	2.40	0.42
12:L:85:ILE:HA	12:L:85:ILE:HD13	1.85	0.42
16:P:55:ARG:O	16:P:58:TYR:HB3	2.19	0.42
9:I:99:LEU:HB3	9:I:101:PHE:HE1	1.82	0.42
1:A:1300:G:O2'	1:A:1303:C:N4	2.52	0.42
1:A:499:A:H4'	1:A:500:G:H5'	2.00	0.42
1:A:841:U:H6	1:A:841:U:OP1	2.02	0.42
12:L:7:ILE:O	12:L:11:VAL:HG23	2.18	0.42
4:D:50:ARG:HA	4:D:51:PRO:HD3	1.88	0.42
1:A:153:C:H2'	1:A:154:C:C6	2.54	0.42
17:Q:10:VAL:HG13	17:Q:19:VAL:HG23	2.00	0.42
6:F:3:ARG:HB2	6:F:93:SER:HB2	2.00	0.42
7:G:52:GLU:H	7:G:52:GLU:HG2	1.57	0.42
15:O:37:ASN:HA	15:O:40:SER:HB2	2.01	0.42
1:A:673:G:H5''	6:F:87:ARG:CZ	2.49	0.42
1:A:1346:A:N1	1:A:1374:A:H5''	2.33	0.42
2:B:158:LEU:HA	2:B:159:PRO:HD3	1.94	0.42
2:B:97:TRP:CH2	2:B:176:GLU:CD	2.92	0.42
1:A:1375:A:H2'	1:A:1376:U:C6	2.54	0.42
7:G:26:PHE:CE2	7:G:30:ILE:HD11	2.55	0.42
1:A:689:C:OP2	11:K:55:LYS:NZ	2.41	0.42
2:B:14:GLY:O	2:B:15:VAL:HG22	2.19	0.42
1:A:1480:G:H2'	1:A:1481:U:O4'	2.19	0.42
10:J:42:THR:HG21	10:J:66:ARG:HB3	2.02	0.42
1:A:131:C:H2'	1:A:132:C:H6	1.84	0.42
6:F:2:ARG:NE	6:F:69:GLU:HG2	2.34	0.42
6:F:10:LEU:HD21	6:F:61:LEU:HD22	2.02	0.42
3:C:153:VAL:O	3:C:165:THR:HG23	2.19	0.42
2:B:86:GLU:C	2:B:89:GLY:H	2.23	0.42
1:A:1310:G:H1	1:A:1327:C:N4	2.18	0.42
13:M:69:GLU:HG3	13:M:70:LEU:H	1.84	0.42
22:V:63:G:N1	22:V:64:G:C5	2.87	0.42
20:T:51:GLU:O	20:T:54:LYS:HB3	2.19	0.42
1:A:189(F):U:C5	17:Q:72:ARG:NH2	2.87	0.42
3:C:12:LEU:HD23	3:C:12:LEU:HA	1.87	0.42
1:A:866:C:C4	1:A:867:G:H1'	2.55	0.42
1:A:1468:A:H2'	1:A:1469:G:O4'	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:170:GLU:O	2:B:173:ALA:N	2.50	0.42
1:A:881:G:P	12:L:12:ARG:NH2	2.92	0.42
1:A:625:G:H4'	16:P:16:HIS:CD2	2.55	0.42
7:G:65:ALA:O	7:G:69:VAL:HG23	2.18	0.42
8:H:48:TYR:HA	8:H:60:ARG:O	2.20	0.42
15:O:30:ALA:HA	15:O:85:LEU:HD21	2.01	0.42
15:O:4:THR:N	15:O:7:GLU:OE2	2.46	0.42
17:Q:18:THR:HG22	17:Q:19:VAL:N	2.34	0.42
6:F:49:ALA:HB2	18:R:78:LEU:O	2.19	0.42
8:H:46:LYS:HB3	8:H:46:LYS:HE2	1.75	0.42
1:A:66:G:N3	1:A:66:G:H2'	2.34	0.42
1:A:404:U:H5''	4:D:122:ARG:HD3	2.01	0.42
9:I:11:LYS:HE3	9:I:11:LYS:HB2	1.72	0.42
1:A:1080:A:H5''	1:A:1081:G:OP2	2.19	0.42
4:D:200:GLU:O	4:D:204:ILE:HG12	2.20	0.42
1:A:353:A:H5'	1:A:353:A:C8	2.47	0.42
1:A:303:A:O2'	1:A:555:C:H4'	2.20	0.42
8:H:112:LEU:HB3	8:H:133:LEU:HA	2.00	0.42
11:K:38:ASN:HA	11:K:39:PRO:HD3	1.92	0.42
22:V:22:G:O5'	22:V:22:G:H8	2.02	0.42
17:Q:45:HIS:CD2	17:Q:47:PRO:HG3	2.54	0.42
1:A:119:A:H4'	1:A:120:A:O5'	2.19	0.42
2:B:77:ALA:O	2:B:81:VAL:HG23	2.18	0.42
8:H:121:ASP:O	8:H:125:ARG:HG3	2.19	0.42
1:A:346:G:H2'	1:A:347:G:O4'	2.20	0.42
1:A:601:C:C2	1:A:638:G:N2	2.87	0.42
1:A:451:A:N7	1:A:481:G:C6	2.87	0.42
1:A:112:G:H21	1:A:354:G:C4'	2.33	0.42
14:N:4:LYS:HA	14:N:4:LYS:HZ2	1.85	0.42
1:A:149:A:O2'	1:A:150:C:O4'	2.38	0.42
2:B:215:LEU:HD23	2:B:215:LEU:HA	1.65	0.42
2:B:95:GLN:HG3	2:B:147:LYS:O	2.19	0.42
4:D:67:ILE:HG22	4:D:68:TYR:CD1	2.55	0.42
1:A:433:C:O2'	1:A:434:U:H5'	2.20	0.42
1:A:948:C:OP2	13:M:108:ARG:HB2	2.19	0.42
8:H:49:GLU:HG2	8:H:62:TYR:HE2	1.85	0.42
1:A:406:G:N3	4:D:119:GLN:NE2	2.68	0.42
1:A:1269:A:H2	1:A:1312:G:H21	1.67	0.42
1:A:105:G:H2'	1:A:106:C:C6	2.55	0.42
20:T:13:LEU:HG	20:T:13:LEU:H	1.53	0.42
1:A:563:A:C8	1:A:567:G:H1'	2.55	0.42
13:M:64:TRP:N	13:M:64:TRP:CE3	2.86	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1151:A:N3	10:J:39:PRO:HG3	2.34	0.42
1:A:1179:A:O3'	9:I:103:THR:HB	2.20	0.42
1:A:540:G:H2'	1:A:541:G:O4'	2.20	0.42
1:A:981:U:H2'	1:A:982:U:C5	2.55	0.42
17:Q:5:VAL:O	17:Q:6:LEU:HD13	2.20	0.42
22:V:73:A:H5''	22:V:74:C:O5'	2.20	0.42
1:A:160:A:O5'	1:A:160:A:H8	2.03	0.42
1:A:617:G:H4'	16:P:44:THR:O	2.18	0.42
9:I:14:VAL:O	9:I:65:VAL:HG23	2.19	0.42
13:M:90:LEU:C	13:M:92:HIS:H	2.23	0.42
2:B:100:GLY:C	2:B:108:ILE:HG13	2.40	0.42
1:A:1101:A:C4	2:B:99:GLY:HA3	2.55	0.42
1:A:590:C:H2'	1:A:591:U:H6	1.84	0.42
9:I:99:LEU:HB3	9:I:101:PHE:CD1	2.55	0.42
1:A:494:U:H6	1:A:494:U:O5'	2.02	0.42
2:B:42:ILE:HG22	2:B:43:ASP:N	2.34	0.42
1:A:1154:G:C4	1:A:1155:G:C8	3.07	0.42
6:F:55:ASP:OD1	6:F:56:PRO:HD2	2.20	0.42
19:S:41:VAL:HA	19:S:42:PRO:HD3	1.92	0.42
5:E:60:TYR:C	5:E:60:TYR:CD1	2.92	0.42
14:N:9:LYS:HE3	14:N:9:LYS:HB3	1.90	0.42
1:A:1370:G:N7	9:I:109:VAL:HG11	2.34	0.42
1:A:1013:G:N2	1:A:1016:A:OP2	2.48	0.42
1:A:473:G:H2'	1:A:474:G:C8	2.48	0.42
2:B:127:ILE:C	2:B:129:GLU:H	2.21	0.42
7:G:58:PRO:HA	7:G:61:VAL:CG1	2.50	0.42
22:V:49:G:O6	22:V:65:C:N4	2.53	0.42
1:A:1381:U:H2'	1:A:1382:C:H5'	2.02	0.42
1:A:391:G:C6	1:A:392:G:C5	3.08	0.42
1:A:1427:U:H2'	1:A:1428:A:H8	1.83	0.42
1:A:617:G:C2	1:A:618:C:C5	3.08	0.42
1:A:612:C:H2'	1:A:613:C:C6	2.55	0.42
1:A:1465:C:H2'	1:A:1466:C:O4'	2.19	0.42
3:C:22:TRP:HB3	3:C:59:ARG:HB2	2.01	0.42
5:E:142:LEU:O	5:E:143:ARG:NE	2.42	0.42
1:A:1401:G:C2	1:A:1402:C:H1'	2.55	0.42
7:G:115:ARG:O	7:G:118:VAL:HG23	2.20	0.42
2:B:105:PHE:HA	2:B:108:ILE:HB	2.02	0.42
1:A:1327:C:H2'	1:A:1328:C:C6	2.55	0.42
1:A:1170:A:N6	1:A:1171:G:C2	2.87	0.42
1:A:1219:U:O2'	19:S:34:TRP:HB3	2.20	0.42
1:A:1241:G:H2'	1:A:1242:C:C6	2.54	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:I:45:ALA:HB1	9:I:48:GLU:N	2.35	0.42
1:A:1502:A:H5'	1:A:1504:G:N7	2.35	0.41
9:I:17:VAL:HG21	9:I:80:GLY:O	2.20	0.41
1:A:401:C:OP2	4:D:73:ARG:NH1	2.53	0.41
1:A:473:G:C5	1:A:474:G:N7	2.88	0.41
1:A:32:A:N3	1:A:32:A:H2'	2.34	0.41
16:P:52:ASP:OD2	16:P:55:ARG:N	2.26	0.41
4:D:170:VAL:HG13	4:D:174:LEU:O	2.20	0.41
1:A:1192:C:N4	1:A:1193:G:C4	2.88	0.41
1:A:1288:A:H2'	1:A:1289:A:C8	2.55	0.41
1:A:930:C:C4	1:A:931:C:C5	3.08	0.41
10:J:35:SER:CB	10:J:73:ASP:HB2	2.41	0.41
7:G:18:TYR:CD2	7:G:59:LEU:HD22	2.51	0.41
15:O:87:ILE:CG2	15:O:88:ARG:N	2.83	0.41
22:V:18:G:C4	22:V:58:A:C2	3.08	0.41
13:M:69:GLU:OE1	13:M:73:GLU:N	2.53	0.41
1:A:722:A:H2'	1:A:724:G:C8	2.56	0.41
5:E:69:VAL:HG22	5:E:69:VAL:O	2.20	0.41
1:A:255:G:H1'	17:Q:16:GLN:OE1	2.20	0.41
1:A:616:G:H5''	26:A:1926:HOH:O	2.19	0.41
21:U:5:ASP:O	21:U:11:GLY:HA3	2.20	0.41
1:A:922:G:H2'	1:A:923:A:H8	1.84	0.41
1:A:1092:A:C5	1:A:1183:A:N7	2.88	0.41
1:A:1077:G:C2	1:A:1081:G:C6	3.08	0.41
7:G:48:LYS:O	7:G:52:GLU:HG2	2.21	0.41
3:C:149:ALA:HA	3:C:201:TYR:O	2.19	0.41
16:P:9:PHE:CD2	16:P:18:ARG:HG3	2.55	0.41
7:G:101:LEU:HA	7:G:101:LEU:HD13	1.87	0.41
2:B:102:LEU:HB2	2:B:176:GLU:HB3	2.03	0.41
1:A:1015:A:O5'	1:A:1015:A:H8	2.03	0.41
16:P:51:VAL:HG12	16:P:53:VAL:H	1.84	0.41
1:A:533:A:O2'	1:A:535:A:OP2	2.26	0.41
1:A:1107:C:N4	1:A:1108:G:N7	2.67	0.41
1:A:475:G:H2'	1:A:476:G:C8	2.55	0.41
1:A:929:G:C6	1:A:930:C:C4	3.08	0.41
10:J:5:ARG:N	10:J:74:ILE:H	2.19	0.41
1:A:1076:C:C2	1:A:1082:G:N2	2.89	0.41
6:F:41:GLU:HG2	6:F:43:LEU:CD1	2.51	0.41
16:P:12:LYS:C	16:P:14:ASN:H	2.24	0.41
5:E:139:LEU:HA	5:E:139:LEU:HD23	1.81	0.41
3:C:178:LEU:HD13	3:C:178:LEU:HA	1.78	0.41
9:I:107:ARG:HH11	9:I:107:ARG:CG	2.26	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:338:A:H2'	1:A:339:C:C6	2.56	0.41
1:A:1292:U:C2	1:A:1293:G:C8	3.08	0.41
1:A:1309:G:C6	1:A:1329:A:C2	3.08	0.41
4:D:74:GLN:O	4:D:78:LEU:HD13	2.20	0.41
20:T:36:LEU:HA	20:T:36:LEU:HD13	1.83	0.41
20:T:51:GLU:HG2	20:T:54:LYS:HD3	2.03	0.41
1:A:557:G:C6	1:A:558:G:N1	2.88	0.41
7:G:56:GLN:HB2	7:G:57:GLU:H	1.64	0.41
12:L:93:LEU:HD23	12:L:93:LEU:HA	1.75	0.41
1:A:1323:G:H4'	1:A:1363:C:C2	2.56	0.41
8:H:63:LEU:HD23	8:H:65:TYR:OH	2.21	0.41
2:B:88:ALA:HB1	2:B:222:ILE:HG21	2.02	0.41
1:A:620:C:H2'	1:A:621:A:O4'	2.20	0.41
1:A:509:A:C6	1:A:510:A:N1	2.87	0.41
8:H:7:ALA:HB2	8:H:85:ARG:HD2	2.03	0.41
1:A:1330:U:H4'	13:M:23:TYR:CE2	2.55	0.41
1:A:604:G:C6	1:A:635:G:C6	3.09	0.41
11:K:80:VAL:HG23	11:K:105:VAL:H	1.85	0.41
1:A:723:U:O2'	1:A:724:G:P	2.79	0.41
4:D:110:PHE:HD1	4:D:110:PHE:N	2.18	0.41
1:A:936:C:C4	1:A:937:A:C5	3.08	0.41
1:A:375:U:OP1	16:P:69:THR:HG21	2.20	0.41
7:G:72:ARG:HG2	7:G:142:GLU:OE2	2.21	0.41
2:B:69:LEU:HD12	2:B:70:PHE:H	1.86	0.41
1:A:403:C:O2'	1:A:404:U:H5'	2.20	0.41
2:B:100:GLY:HA3	2:B:104:ASN:HB3	2.03	0.41
1:A:1144:G:H22	1:A:1146:A:H62	1.68	0.41
5:E:99:GLY:O	5:E:117:ASP:HA	2.21	0.41
1:A:511:C:HO2'	1:A:512:U:H6	1.65	0.41
5:E:126:ARG:CG	5:E:126:ARG:NH1	2.81	0.41
4:D:74:GLN:NE2	4:D:137:SER:HB3	2.36	0.41
4:D:10:ARG:CB	4:D:40:PRO:HG3	2.49	0.41
1:A:792:A:N3	1:A:794:A:C5	2.89	0.41
7:G:145:ALA:C	7:G:147:ALA:H	2.24	0.41
1:A:25:C:O2'	1:A:26:A:H5'	2.21	0.41
1:A:451:A:C5	1:A:481:G:C6	3.09	0.41
8:H:96:GLY:H	8:H:99:GLU:CD	2.24	0.41
1:A:719:C:N4	18:R:71:LYS:HE2	2.35	0.41
1:A:579:G:C5	1:A:580:U:C4	3.08	0.41
5:E:144:THR:HG22	5:E:146:ALA:H	1.85	0.41
3:C:180:ALA:HB1	3:C:203:PHE:HE1	1.86	0.41
8:H:42:GLU:HG3	8:H:109:ILE:HD13	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1368:G:H2'	1:A:1369:C:C6	2.56	0.41
6:F:22:GLU:O	6:F:26:ILE:HG13	2.21	0.41
1:A:1367:C:H5''	9:I:114:TYR:HA	2.02	0.41
3:C:111:LEU:HD12	3:C:111:LEU:N	2.35	0.41
1:A:129(A):G:C2	1:A:189(H):G:C8	3.09	0.41
1:A:65:U:C5	1:A:381:C:N4	2.89	0.41
1:A:175:C:H2'	1:A:176:C:H6	1.86	0.41
1:A:202:U:O2'	1:A:203:U:O5'	2.27	0.41
10:J:55:LYS:HG2	10:J:56:HIS:N	2.36	0.41
1:A:1203:C:H2'	1:A:1204:A:O4'	2.21	0.41
1:A:791:G:H2'	1:A:792:A:H5'	2.02	0.41
17:Q:10:VAL:HG22	17:Q:19:VAL:HG21	2.02	0.41
5:E:78:HIS:NE2	5:E:142:LEU:HD23	2.35	0.41
11:K:61:ALA:CB	11:K:90:GLY:HA3	2.51	0.41
1:A:1194:U:H2'	1:A:1195:C:C6	2.55	0.41
1:A:1322:C:OP1	1:A:1322:C:H6	2.04	0.41
1:A:736:C:N4	1:A:737:A:H62	2.18	0.41
3:C:36:ASP:OD1	3:C:57:ILE:HD12	2.21	0.41
6:F:10:LEU:HD23	6:F:61:LEU:HD13	2.03	0.41
1:A:324:G:OP1	20:T:22:ARG:NE	2.54	0.41
1:A:1342:C:H1'	9:I:124:GLN:NE2	2.36	0.41
12:L:33:ARG:O	12:L:85:ILE:HB	2.21	0.41
16:P:55:ARG:HD2	16:P:55:ARG:HA	1.69	0.41
1:A:1067:A:O5'	1:A:1067:A:C8	2.72	0.41
2:B:54:THR:O	2:B:58:ILE:HG13	2.21	0.41
1:A:1300:G:O2'	1:A:1301:U:OP2	2.24	0.41
22:V:47:U:H2'	22:V:50:U:OP1	2.20	0.41
1:A:1057:G:C2'	1:A:1058:G:H5'	2.50	0.41
1:A:1318:A:O2'	19:S:37:ARG:HB3	2.20	0.41
1:A:286:G:C6	1:A:287:U:C4	3.09	0.41
5:E:137:GLU:O	5:E:141:GLN:HB2	2.20	0.41
20:T:91:LEU:HD22	20:T:91:LEU:HA	1.78	0.41
17:Q:27:PHE:CZ	17:Q:36:ILE:HD11	2.56	0.41
19:S:20:LEU:HA	19:S:23:ASN:HB3	2.01	0.41
16:P:41:PRO:O	16:P:43:LYS:HD2	2.21	0.41
15:O:24:SER:O	15:O:25:THR:C	2.60	0.41
17:Q:94:ASN:O	17:Q:98:LEU:HD13	2.21	0.41
13:M:4:ILE:HG12	13:M:9:ILE:HG13	2.03	0.41
13:M:25:ILE:HD11	13:M:66:LEU:HD11	2.02	0.41
6:F:80:ARG:HG3	6:F:80:ARG:NH2	2.36	0.41
1:A:1285:A:H1'	1:A:1286:A:OP2	2.21	0.41
3:C:5:ILE:HA	3:C:5:ILE:HD12	1.90	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:G:118:VAL:O	7:G:121:ALA:HB3	2.21	0.41
1:A:719:C:O2'	18:R:49:LYS:HB3	2.21	0.41
16:P:8:ARG:HA	16:P:17:TYR:CD2	2.56	0.41
1:A:367:U:C2	1:A:369:C:C5	3.09	0.41
20:T:20:LEU:O	20:T:24:LEU:HD23	2.21	0.41
1:A:1357:A:H5''	1:A:1358:U:OP2	2.20	0.40
1:A:1321:C:C3'	1:A:1322:C:H5''	2.51	0.40
7:G:23:VAL:HG13	7:G:43:PHE:CE2	2.34	0.40
8:H:33:GLU:HG2	8:H:59:LEU:CD1	2.52	0.40
3:C:18:TRP:HE3	3:C:18:TRP:N	2.12	0.40
3:C:66:VAL:O	3:C:68:VAL:HG23	2.21	0.40
20:T:22:ARG:O	20:T:25:ARG:N	2.53	0.40
17:Q:68:ARG:H	17:Q:70:ARG:HH11	1.68	0.40
16:P:68:ASP:O	16:P:70:ALA:N	2.54	0.40
16:P:18:ARG:NH1	16:P:32:TYR:OH	2.55	0.40
1:A:1324:A:O4'	1:A:1362:C:H4'	2.21	0.40
14:N:60:SER:O	14:N:61:TRP:HB3	2.20	0.40
2:B:20:GLU:HB2	2:B:190:THR:OG1	2.20	0.40
4:D:9:CYS:O	4:D:13:ARG:HG3	2.20	0.40
1:A:1298:C:H2'	7:G:114:ARG:HH12	1.86	0.40
16:P:53:VAL:O	16:P:56:ALA:N	2.55	0.40
1:A:1319:A:N6	1:A:1361:G:H21	2.17	0.40
1:A:1492:A:C4'	1:A:1493:A:OP1	2.67	0.40
8:H:132:GLU:O	8:H:134:ILE:HG12	2.21	0.40
22:V:18:G:C2	22:V:58:A:C4	3.10	0.40
1:A:908:A:H8	1:A:908:A:O5'	2.05	0.40
1:A:983:A:H1'	1:A:1049:U:O2	2.21	0.40
1:A:1237:C:H5''	1:A:1238:A:O4'	2.22	0.40
1:A:254:G:OP1	17:Q:67:LYS:O	2.39	0.40
1:A:283:C:H2'	1:A:284:G:O4'	2.22	0.40
1:A:683:G:H2'	1:A:684:A:O4'	2.21	0.40
1:A:579:G:H2'	1:A:580:U:C6	2.56	0.40
1:A:309:G:H1'	1:A:608:A:C2	2.56	0.40
13:M:82:MET:HA	13:M:89:GLY:HA3	2.03	0.40
1:A:15:G:C5	1:A:1396:A:C2	3.10	0.40
4:D:13:ARG:HD2	4:D:38:TYR:O	2.21	0.40
1:A:736:C:C2	1:A:737:A:N7	2.90	0.40
13:M:70:LEU:O	13:M:70:LEU:HD22	2.21	0.40
1:A:1342:C:H2'	1:A:1343:G:C8	2.56	0.40
19:S:57:HIS:O	19:S:59:PRO:HD3	2.21	0.40
4:D:119:GLN:OE1	4:D:123:HIS:CE1	2.74	0.40
1:A:1178:G:N2	1:A:1180:A:H3'	2.36	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:I:18:PHE:O	9:I:62:TYR:N	2.37	0.40
3:C:34:LEU:CD1	3:C:38:ARG:HD2	2.51	0.40
2:B:118:LEU:HB3	2:B:142:LEU:HG	2.03	0.40
8:H:49:GLU:O	8:H:51:VAL:HG13	2.21	0.40
1:A:393:A:C4	1:A:394:G:C8	3.10	0.40
1:A:307:C:C5	1:A:308:C:C5	3.10	0.40
1:A:57:G:C5	1:A:58:C:C4	3.10	0.40
1:A:409:G:C6	1:A:410:G:C4	3.10	0.40
7:G:71:PRO:HG3	7:G:103:TRP:CZ3	2.56	0.40
1:A:1332:A:O5'	1:A:1332:A:C8	2.74	0.40
1:A:431:A:H5''	1:A:432:A:OP2	2.21	0.40
1:A:196:A:H5''	26:A:1907:HOH:O	2.20	0.40
5:E:152:ARG:HB3	8:H:43:GLY:HA3	2.03	0.40
1:A:960:U:H2'	1:A:960:U:O2	2.22	0.40
5:E:121:LYS:HD3	5:E:121:LYS:HA	1.97	0.40
1:A:450:G:H5'	16:P:41:PRO:O	2.22	0.40
2:B:21:ARG:HB2	2:B:38:GLY:O	2.22	0.40
13:M:92:HIS:CD2	13:M:98:VAL:HG11	2.56	0.40
1:A:425:G:C2'	1:A:426:G:H5'	2.51	0.40
1:A:1118:C:OP1	9:I:104:ARG:HG3	2.21	0.40
1:A:738:C:OP1	6:F:2:ARG:NH1	2.53	0.40
1:A:51:A:C6	1:A:353:A:C2	3.10	0.40
1:A:624:C:H2'	1:A:625:G:C8	2.57	0.40
1:A:435:C:H2'	1:A:436:C:H5'	2.03	0.40
1:A:373:A:N3	1:A:374:A:C8	2.89	0.40
17:Q:37:LYS:O	17:Q:38:ARG:NH2	2.55	0.40
1:A:1426:C:O2	1:A:1475:G:C2	2.74	0.40
17:Q:8:GLY:HA3	17:Q:22:LEU:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	233/256 (91%)	182 (78%)	45 (19%)	6 (3%)	8 47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	204/239 (85%)	168 (82%)	36 (18%)	0	100	100
4	D	206/209 (99%)	178 (86%)	23 (11%)	5 (2%)	9	51
5	E	147/162 (91%)	129 (88%)	13 (9%)	5 (3%)	6	38
6	F	98/101 (97%)	89 (91%)	9 (9%)	0	100	100
7	G	152/156 (97%)	131 (86%)	20 (13%)	1 (1%)	30	80
8	H	136/138 (99%)	126 (93%)	10 (7%)	0	100	100
9	I	123/128 (96%)	106 (86%)	13 (11%)	4 (3%)	6	38
10	J	94/105 (90%)	74 (79%)	17 (18%)	3 (3%)	6	39
11	K	112/129 (87%)	98 (88%)	14 (12%)	0	100	100
12	L	120/132 (91%)	111 (92%)	7 (6%)	2 (2%)	14	62
13	M	110/126 (87%)	82 (74%)	21 (19%)	7 (6%)	2	17
14	N	57/61 (93%)	48 (84%)	8 (14%)	1 (2%)	13	60
15	O	86/89 (97%)	75 (87%)	11 (13%)	0	100	100
16	P	80/88 (91%)	66 (82%)	10 (12%)	4 (5%)	3	26
17	Q	97/105 (92%)	83 (86%)	13 (13%)	1 (1%)	22	74
18	R	66/88 (75%)	58 (88%)	8 (12%)	0	100	100
19	S	73/93 (78%)	60 (82%)	13 (18%)	0	100	100
20	T	102/106 (96%)	73 (72%)	26 (26%)	3 (3%)	7	43
21	U	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
All	All	2317/2538 (91%)	1956 (84%)	319 (14%)	42 (2%)	13	60

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	15	VAL
5	E	73	ASN
9	I	54	ASP
13	M	7	VAL
13	M	45	VAL
16	P	44	THR
17	Q	14	LYS
20	T	46	GLU
2	B	23	ARG
5	E	8	GLU
9	I	119	ALA

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Mol	Chain	Res	Type
13	M	10	PRO
16	P	16	HIS
20	T	96	GLY
2	B	22	LYS
4	D	7	PRO
4	D	177	ASP
5	E	9	LYS
9	I	21	PRO
12	L	26	ALA
16	P	15	PRO
16	P	53	VAL
20	T	95	ALA
4	D	176	LEU
5	E	98	THR
5	E	146	ALA
9	I	88	TYR
13	M	66	LEU
10	J	89	ASP
10	J	90	LEU
13	M	51	ALA
2	B	177	ALA
4	D	5	ILE
7	G	55	GLY
13	M	63	THR
14	N	14	PRO
10	J	34	VAL
2	B	239	VAL
2	B	131	PRO
12	L	25	PRO
13	M	40	ASN
4	D	197	PRO

5.3.2 Protein sidechains ⓘ

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	181/220 (82%)	132 (73%)	49 (27%)	1 2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	114/188 (61%)	96 (84%)	18 (16%)	4	16
4	D	142/181 (78%)	112 (79%)	30 (21%)	1	8
5	E	109/123 (89%)	84 (77%)	25 (23%)	1	5
6	F	76/90 (84%)	61 (80%)	15 (20%)	2	10
7	G	102/127 (80%)	78 (76%)	24 (24%)	1	5
8	H	104/119 (87%)	89 (86%)	15 (14%)	5	22
9	I	62/99 (63%)	52 (84%)	10 (16%)	3	16
10	J	52/92 (56%)	36 (69%)	16 (31%)	0	1
11	K	81/99 (82%)	61 (75%)	20 (25%)	1	3
12	L	91/109 (84%)	71 (78%)	20 (22%)	1	7
13	M	62/101 (61%)	39 (63%)	23 (37%)	0	0
14	N	45/50 (90%)	30 (67%)	15 (33%)	0	0
15	O	77/80 (96%)	64 (83%)	13 (17%)	3	14
16	P	65/74 (88%)	49 (75%)	16 (25%)	1	3
17	Q	93/97 (96%)	77 (83%)	16 (17%)	3	14
18	R	49/77 (64%)	36 (74%)	13 (26%)	1	2
19	S	42/80 (52%)	28 (67%)	14 (33%)	0	0
20	T	72/82 (88%)	56 (78%)	16 (22%)	1	6
21	U	14/22 (64%)	13 (93%)	1 (7%)	21	63
All	All	1633/2110 (77%)	1264 (77%)	369 (23%)	1	6

All (369) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	17	PHE
2	B	21	ARG
2	B	24	TRP
2	B	30	ARG
2	B	45	GLN
2	B	48	MET
2	B	50	GLU
2	B	58	ILE
2	B	60	ASP
2	B	63	MET
2	B	67	THR

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Mol	Chain	Res	Type
2	B	71	VAL
2	B	73	THR
2	B	80	ILE
2	B	87	ARG
2	B	90	MET
2	B	93	VAL
2	B	101	MET
2	B	105	PHE
2	B	107	THR
2	B	108	ILE
2	B	111	ARG
2	B	116	GLU
2	B	119	GLU
2	B	121	LEU
2	B	122	PHE
2	B	126	GLU
2	B	127	ILE
2	B	138	LEU
2	B	140	HIS
2	B	142	LEU
2	B	153	ARG
2	B	154	LEU
2	B	158	LEU
2	B	164	VAL
2	B	174	VAL
2	B	175	ARG
2	B	185	ILE
2	B	187	LEU
2	B	191	ASP
2	B	193	ASP
2	B	198	ASP
2	B	200	ILE
2	B	205	ASP
2	B	221	LEU
2	B	222	ILE
2	B	229	VAL
2	B	230	VAL
2	B	231	GLU
3	C	5	ILE
3	C	18	TRP
3	C	30	ARG
3	C	31	HIS

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Mol	Chain	Res	Type
3	C	46	GLU
3	C	47	LEU
3	C	52	LEU
3	C	57	ILE
3	C	67	THR
3	C	131	ARG
3	C	132	ARG
3	C	140	ARG
3	C	153	VAL
3	C	167	TRP
3	C	178	LEU
3	C	179	ARG
3	C	193	TYR
3	C	207	VAL
4	D	5	ILE
4	D	8	VAL
4	D	10	ARG
4	D	12	CYS
4	D	15	GLU
4	D	19	LEU
4	D	26	CYS
4	D	28	SER
4	D	36	ARG
4	D	58	LEU
4	D	59	ARG
4	D	65	ARG
4	D	77	ASN
4	D	97	LEU
4	D	101	LEU
4	D	106	TYR
4	D	107	ARG
4	D	119	GLN
4	D	126	ILE
4	D	127	THR
4	D	135	LEU
4	D	137	SER
4	D	152	SER
4	D	153	ARG
4	D	156	GLU
4	D	158	ILE
4	D	162	LEU
4	D	177	ASP

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Mol	Chain	Res	Type
4	D	188	LEU
4	D	201	GLN
5	E	11	ILE
5	E	13	ILE
5	E	31	LEU
5	E	37	ARG
5	E	38	GLN
5	E	41	VAL
5	E	47	LYS
5	E	51	VAL
5	E	55	VAL
5	E	71	LEU
5	E	78	HIS
5	E	81	GLU
5	E	89	ILE
5	E	90	VAL
5	E	91	LEU
5	E	101	ILE
5	E	107	ARG
5	E	112	LEU
5	E	116	THR
5	E	120	THR
5	E	121	LYS
5	E	126	ARG
5	E	136	MET
5	E	141	GLN
5	E	153	LYS
6	F	15	ASP
6	F	19	LEU
6	F	22	GLU
6	F	25	ILE
6	F	30	LEU
6	F	36	ARG
6	F	41	GLU
6	F	42	GLU
6	F	61	LEU
6	F	63	TYR
6	F	64	GLN
6	F	70	ASP
6	F	75	LEU
6	F	80	ARG
6	F	82	ARG

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Mol	Chain	Res	Type
7	G	12	LEU
7	G	21	VAL
7	G	27	ILE
7	G	38	LEU
7	G	51	GLN
7	G	52	GLU
7	G	56	GLN
7	G	57	GLU
7	G	72	ARG
7	G	75	VAL
7	G	80	VAL
7	G	85	TYR
7	G	96	GLN
7	G	98	SER
7	G	101	LEU
7	G	104	LEU
7	G	106	GLN
7	G	111	ARG
7	G	113	GLU
7	G	118	VAL
7	G	124	LEU
7	G	142	GLU
7	G	146	GLU
7	G	155	ARG
8	H	3	THR
8	H	12	ARG
8	H	13	ILE
8	H	37	ARG
8	H	83	ILE
8	H	84	ARG
8	H	85	ARG
8	H	99	GLU
8	H	112	LEU
8	H	119	LEU
8	H	123	GLU
8	H	129	VAL
8	H	134	ILE
8	H	137	VAL
8	H	138	TRP
9	I	11	LYS
9	I	31	GLN
9	I	36	TYR

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Mol	Chain	Res	Type
9	I	74	ILE
9	I	75	ASP
9	I	86	VAL
9	I	99	LEU
9	I	107	ARG
9	I	114	TYR
9	I	124	GLN
10	J	8	LEU
10	J	13	HIS
10	J	16	LEU
10	J	19	SER
10	J	33	GLN
10	J	47	PHE
10	J	48	THR
10	J	49	VAL
10	J	55	LYS
10	J	59	SER
10	J	61	GLU
10	J	62	HIS
10	J	68	HIS
10	J	95	GLU
10	J	96	ILE
10	J	100	THR
11	K	18	ARG
11	K	24	SER
11	K	30	VAL
11	K	31	THR
11	K	33	THR
11	K	38	ASN
11	K	48	ILE
11	K	55	LYS
11	K	57	THR
11	K	63	LEU
11	K	67	ASP
11	K	70	LYS
11	K	83	ILE
11	K	95	ILE
11	K	96	ARG
11	K	98	LEU
11	K	109	VAL
11	K	111	ASP
11	K	114	VAL

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Mol	Chain	Res	Type
11	K	119	CYS
12	L	6	THR
12	L	24	VAL
12	L	33	ARG
12	L	39	VAL
12	L	40	VAL
12	L	43	VAL
12	L	44	THR
12	L	46	LYS
12	L	52	LEU
12	L	60	LEU
12	L	66	VAL
12	L	67	THR
12	L	70	ILE
12	L	79	GLU
12	L	84	LEU
12	L	92	ASP
12	L	97	ARG
12	L	99	HIS
12	L	104	VAL
12	L	112	ASP
13	M	4	ILE
13	M	17	VAL
13	M	23	TYR
13	M	27	LYS
13	M	37	THR
13	M	40	ASN
13	M	43	THR
13	M	47	ASP
13	M	52	GLU
13	M	60	VAL
13	M	64	TRP
13	M	65	LYS
13	M	66	LEU
13	M	70	LEU
13	M	77	ASN
13	M	88	ARG
13	M	91	ARG
13	M	102	ARG
13	M	105	THR
13	M	106	ASN
13	M	108	ARG

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Mol	Chain	Res	Type
13	M	109	THR
13	M	110	ARG
14	N	3	ARG
14	N	4	LYS
14	N	7	ILE
14	N	13	THR
14	N	17	LYS
14	N	22	THR
14	N	29	ARG
14	N	31	ARG
14	N	33	VAL
14	N	40	CYS
14	N	41	ARG
14	N	42	ILE
14	N	44	LEU
14	N	56	VAL
14	N	60	SER
15	O	3	ILE
15	O	13	GLN
15	O	17	ARG
15	O	26	GLU
15	O	38	ARG
15	O	39	LEU
15	O	40	SER
15	O	41	GLU
15	O	65	ARG
15	O	71	GLN
15	O	72	ARG
15	O	87	ILE
15	O	88	ARG
16	P	1	MET
16	P	2	VAL
16	P	6	LEU
16	P	20	VAL
16	P	21	VAL
16	P	28	ARG
16	P	29	ASP
16	P	42	ARG
16	P	51	VAL
16	P	54	GLU
16	P	60	LEU
16	P	62	VAL

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Mol	Chain	Res	Type
16	P	67	THR
16	P	69	THR
16	P	72	ARG
16	P	76	GLN
17	Q	7	THR
17	Q	9	VAL
17	Q	13	ASP
17	Q	14	LYS
17	Q	19	VAL
17	Q	39	SER
17	Q	49	GLU
17	Q	50	LYS
17	Q	63	ARG
17	Q	68	ARG
17	Q	72	ARG
17	Q	74	LEU
17	Q	77	VAL
17	Q	79	SER
17	Q	90	ILE
17	Q	97	SER
18	R	21	LYS
18	R	31	LEU
18	R	32	ARG
18	R	35	ARG
18	R	36	ASN
18	R	37	VAL
18	R	47	THR
18	R	69	THR
18	R	75	ILE
18	R	76	LEU
18	R	82	THR
18	R	85	LEU
18	R	86	VAL
19	S	11	VAL
19	S	12	ASP
19	S	14	HIS
19	S	22	LEU
19	S	23	ASN
19	S	32	LYS
19	S	33	THR
19	S	36	ARG
19	S	53	ASN

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Mol	Chain	Res	Type
19	S	57	HIS
19	S	66	MET
19	S	77	THR
19	S	78	ARG
19	S	79	THR
20	T	4	LYS
20	T	13	LEU
20	T	14	LYS
20	T	19	SER
20	T	21	LYS
20	T	50	GLU
20	T	51	GLU
20	T	56	MET
20	T	71	THR
20	T	72	LEU
20	T	73	HIS
20	T	75	ASN
20	T	84	LEU
20	T	90	GLN
20	T	91	LEU
20	T	93	GLU
21	U	10	ARG

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

Mol	Chain	Res	Type
2	B	16	HIS
4	D	123	HIS
6	F	73	ASN
7	G	28	ASN
9	I	3	GLN
11	K	99	GLN
13	M	40	ASN
14	N	49	HIS
15	O	28	GLN
18	R	63	GLN
19	S	14	HIS
19	S	23	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1457/1522 (95%)	367 (25%)	33 (2%)
22	V	76/77 (98%)	21 (27%)	0
23	X	5/16 (31%)	0	0
All	All	1538/1615 (95%)	388 (25%)	33 (2%)

All (388) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	7	G
1	A	9	G
1	A	10	A
1	A	13	U
1	A	22	G
1	A	26	A
1	A	32	A
1	A	39	G
1	A	40	C
1	A	47	C
1	A	48	C
1	A	50	A
1	A	51	A
1	A	58	C
1	A	60	A
1	A	61	G
1	A	65	U
1	A	66	G
1	A	73	G
1	A	76	C
1	A	96	U
1	A	97	G
1	A	101	A
1	A	105	G
1	A	112	G
1	A	115	G
1	A	116	A
1	A	117	G
1	A	120	A
1	A	121	C
1	A	129(A)	G
1	A	131	C
1	A	144	G
1	A	146	G

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Mol	Chain	Res	Type
1	A	150	C
1	A	154	C
1	A	163	C
1	A	173	U
1	A	182	U
1	A	189(B)	C
1	A	189(F)	U
1	A	189(H)	G
1	A	195	A
1	A	197	A
1	A	199	G
1	A	200	G
1	A	201	C
1	A	202	U
1	A	203	U
1	A	204	U
1	A	216	G
1	A	227	G
1	A	245	C
1	A	247	G
1	A	250	A
1	A	251	G
1	A	253	U
1	A	266	G
1	A	267	C
1	A	275	G
1	A	281	G
1	A	289	G
1	A	300	A
1	A	305	G
1	A	314	C
1	A	319	G
1	A	321	A
1	A	328	C
1	A	329	A
1	A	331	G
1	A	332	G
1	A	344	A
1	A	349	A
1	A	352	C
1	A	353	A
1	A	354	G

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Mol	Chain	Res	Type
1	A	355	C
1	A	363	A
1	A	365	U
1	A	366	C
1	A	367	U
1	A	372	C
1	A	373	A
1	A	381	C
1	A	382	A
1	A	389	A
1	A	397	A
1	A	398	C
1	A	404	U
1	A	406	G
1	A	412	A
1	A	413	G
1	A	414	A
1	A	419	C
1	A	421	U
1	A	422	C
1	A	424	G
1	A	427	U
1	A	429	U
1	A	430	A
1	A	431	A
1	A	436	C
1	A	437	U
1	A	439	A
1	A	441	A
1	A	442	C
1	A	445	G
1	A	452	A
1	A	461	A
1	A	475	G
1	A	484	G
1	A	485	G
1	A	491	G
1	A	496	A
1	A	498	U
1	A	499	A
1	A	505	G
1	A	509	A

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Mol	Chain	Res	Type
1	A	510	A
1	A	511	C
1	A	513	C
1	A	518	C
1	A	527	G
1	A	532	A
1	A	533	A
1	A	541	G
1	A	547	A
1	A	549	C
1	A	550	G
1	A	558	G
1	A	559	A
1	A	561	U
1	A	562	C
1	A	564	C
1	A	573	A
1	A	575	G
1	A	576	G
1	A	577	G
1	A	587	G
1	A	588	G
1	A	595	G
1	A	596	C
1	A	597	G
1	A	602	A
1	A	617	G
1	A	623	C
1	A	630	G
1	A	632	A
1	A	633	G
1	A	650	G
1	A	653	A
1	A	657	G
1	A	665	A
1	A	666	G
1	A	687	A
1	A	688	G
1	A	711	G
1	A	721	G
1	A	723	U
1	A	724	G

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Mol	Chain	Res	Type
1	A	729	A
1	A	731	G
1	A	749	C
1	A	754	C
1	A	755	G
1	A	760	G
1	A	763	G
1	A	765	G
1	A	776	G
1	A	777	A
1	A	782	A
1	A	788	U
1	A	792	A
1	A	793	U
1	A	794	A
1	A	796	C
1	A	799	G
1	A	810	C
1	A	812	C
1	A	817	C
1	A	819	A
1	A	820	U
1	A	821	G
1	A	828	A
1	A	829	G
1	A	833	U
1	A	839	U
1	A	840	C
1	A	841	U
1	A	848	C
1	A	851	G
1	A	858	G
1	A	859	A
1	A	870	U
1	A	872	A
1	A	873	A
1	A	876	G
1	A	877	C
1	A	878	G
1	A	884	U
1	A	885	G
1	A	902	G

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Mol	Chain	Res	Type
1	A	906	G
1	A	914	A
1	A	919	A
1	A	926	G
1	A	927	G
1	A	934	C
1	A	954	G
1	A	960	U
1	A	961	U
1	A	966	G
1	A	969	A
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	980	C
1	A	984	C
1	A	992	U
1	A	993	G
1	A	995	C
1	A	1009	G
1	A	1011	G
1	A	1017	G
1	A	1045	C
1	A	1050	G
1	A	1053	G
1	A	1054	C
1	A	1055	A
1	A	1057	G
1	A	1058	G
1	A	1062	U
1	A	1065	U
1	A	1066	C
1	A	1068	G
1	A	1069	C
1	A	1079	G
1	A	1081	G
1	A	1086	U
1	A	1093	A
1	A	1095	U

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Mol	Chain	Res	Type
1	A	1101	A
1	A	1104	G
1	A	1113	C
1	A	1117	G
1	A	1124	G
1	A	1125	U
1	A	1126	U
1	A	1127	G
1	A	1134	G
1	A	1136	U
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1140	C
1	A	1147	C
1	A	1148	U
1	A	1152	A
1	A	1154	G
1	A	1159	U
1	A	1160	G
1	A	1170	A
1	A	1171	G
1	A	1178	G
1	A	1179	A
1	A	1182	G
1	A	1185	G
1	A	1188	A
1	A	1190	G
1	A	1193	G
1	A	1196	U
1	A	1197	G
1	A	1201	A
1	A	1202	G
1	A	1203	C
1	A	1211	U
1	A	1212	U
1	A	1213	A
1	A	1215	G
1	A	1218	C
1	A	1224	G
1	A	1225	A
1	A	1226	C

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Mol	Chain	Res	Type
1	A	1227	A
1	A	1228	C
1	A	1236	A
1	A	1238	A
1	A	1239	A
1	A	1240	U
1	A	1241	G
1	A	1248	A
1	A	1256	A
1	A	1257	U
1	A	1258	G
1	A	1260	C
1	A	1263	C
1	A	1269	A
1	A	1270	C
1	A	1273	G
1	A	1277	C
1	A	1279	A
1	A	1280	A
1	A	1282	C
1	A	1283	G
1	A	1286	A
1	A	1287	A
1	A	1299	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1305	G
1	A	1311	G
1	A	1312	G
1	A	1317	C
1	A	1320	C
1	A	1321	C
1	A	1322	C
1	A	1323	G
1	A	1331	G
1	A	1335	C
1	A	1336	C
1	A	1346	A
1	A	1347	G
1	A	1353	G
1	A	1358	U

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Mol	Chain	Res	Type
1	A	1359	C
1	A	1363	C
1	A	1365	G
1	A	1369	C
1	A	1370	G
1	A	1378	C
1	A	1382	C
1	A	1388	C
1	A	1389	C
1	A	1397	C
1	A	1398	A
1	A	1406	U
1	A	1411	C
1	A	1419	G
1	A	1425	U
1	A	1442	G
1	A	1442(A)	G
1	A	1447	A
1	A	1452	C
1	A	1456	G
1	A	1457	G
1	A	1487	G
1	A	1492	A
1	A	1493	A
1	A	1494	G
1	A	1499	A
1	A	1502	A
1	A	1503	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1507	A
1	A	1517	G
1	A	1519	A
1	A	1520	G
1	A	1529	G
1	A	1530	G
1	A	1531	A
22	V	7	G
22	V	8	U
22	V	9	G
22	V	10	G

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Mol	Chain	Res	Type
22	V	13	C
22	V	17	C
22	V	18	G
22	V	19	G
22	V	20	U
22	V	21	A
22	V	22	G
22	V	47	U
22	V	48	C
22	V	49	G
22	V	50	U
22	V	52	G
22	V	56	C
22	V	65	C
22	V	70	G
22	V	74	C
22	V	76	A

All (33) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	60	A
1	A	65	U
1	A	115	G
1	A	119	A
1	A	149	A
1	A	266	G
1	A	366	C
1	A	428	G
1	A	429	U
1	A	509	A
1	A	560	U
1	A	562	C
1	A	687	A
1	A	748	C
1	A	793	U
1	A	828	A
1	A	840	C
1	A	913	A
1	A	991	U
1	A	992	U
1	A	1049	U

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Mol	Chain	Res	Type
1	A	1061	G
1	A	1064	G
1	A	1065	U
1	A	1067	A
1	A	1201	A
1	A	1256	A
1	A	1279	A
1	A	1285	A
1	A	1300	G
1	A	1492	A
1	A	1504	G
1	A	1530	G

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 249 ligands modelled in this entry, 249 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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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	1461/1522 (95%)	0.07	21 (1%) 72 22	55, 104, 145, 167	0
2	B	235/256 (91%)	-0.03	1 (0%) 90 51	100, 125, 139, 147	0
3	C	206/239 (86%)	-0.07	2 (0%) 79 29	110, 125, 136, 142	0
4	D	208/209 (99%)	-0.04	4 (1%) 64 18	85, 98, 114, 120	0
5	E	149/162 (91%)	-0.14	2 (1%) 74 24	83, 99, 110, 131	0
6	F	100/101 (99%)	-0.25	0 100 100	78, 96, 110, 117	0
7	G	154/156 (98%)	0.10	10 (6%) 18 4	107, 119, 133, 144	0
8	H	138/138 (100%)	-0.07	3 (2%) 59 14	82, 100, 111, 116	0
9	I	125/128 (97%)	0.19	5 (4%) 36 7	101, 130, 138, 142	0
10	J	96/105 (91%)	0.19	2 (2%) 60 15	111, 133, 141, 143	0
11	K	114/129 (88%)	0.01	0 100 100	78, 103, 118, 127	0
12	L	122/132 (92%)	0.04	2 (1%) 68 20	72, 90, 105, 114	0
13	M	112/126 (88%)	0.11	2 (1%) 65 18	102, 127, 135, 139	0
14	N	59/61 (96%)	0.50	2 (3%) 43 9	116, 125, 133, 135	0
15	O	88/89 (98%)	-0.08	0 100 100	74, 96, 114, 118	0
16	P	82/88 (93%)	-0.05	1 (1%) 75 26	84, 94, 112, 122	0
17	Q	99/105 (94%)	-0.09	0 100 100	77, 95, 110, 113	0
18	R	68/88 (77%)	-0.07	1 (1%) 70 21	82, 92, 111, 115	0
19	S	75/93 (80%)	0.10	0 100 100	107, 131, 142, 146	0
20	T	104/106 (98%)	0.01	2 (1%) 64 18	81, 101, 123, 139	0
21	U	23/27 (85%)	1.18	5 (21%) 1 1	115, 126, 132, 134	0
22	V	77/77 (100%)	-0.18	1 (1%) 74 24	73, 109, 133, 156	0
23	X	6/16 (37%)	0.99	1 (16%) 2 1	89, 96, 142, 147	0
All	All	3901/4153 (93%)	0.03	67 (1%) 64 19	55, 108, 139, 167	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1149	C	4.8
1	A	422	C	4.2
23	X	1	A	3.8
21	U	14	TRP	3.8
5	E	124	GLY	3.7
3	C	170	GLN	3.7
1	A	977	A	3.6
1	A	1260	C	3.4
22	V	63	G	3.3
13	M	115	LYS	3.2
21	U	24	ARG	3.1
21	U	15	ARG	3.1
1	A	1148	U	3.1
7	G	2	ALA	3.0
8	H	56	LYS	2.9
18	R	46	GLU	2.9
14	N	58	LYS	2.9
7	G	12	LEU	2.9
1	A	1150	U	2.8
9	I	30	GLY	2.8
1	A	1394	A	2.7
1	A	1224	G	2.7
7	G	133	GLY	2.6
2	B	241	GLU	2.6
9	I	103	THR	2.5
8	H	33	GLU	2.5
1	A	1363	C	2.5
7	G	132	GLY	2.5
1	A	1108	G	2.5
13	M	86	CYS	2.4
10	J	62	HIS	2.4
1	A	1125	U	2.4
1	A	1235	U	2.4
14	N	59	ALA	2.4
3	C	19	GLU	2.4
9	I	101	PHE	2.4
1	A	1018	C	2.3
1	A	575	G	2.3
1	A	149	A	2.3
9	I	126	SER	2.3
4	D	3	ARG	2.3
8	H	54	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
16	P	10	GLY	2.3
21	U	16	GLY	2.3
1	A	963	G	2.2
10	J	64	GLU	2.2
12	L	89	ARG	2.2
5	E	81	GLU	2.2
20	T	78	ALA	2.2
20	T	77	ALA	2.2
1	A	1257	U	2.2
7	G	82	GLY	2.1
7	G	83	ALA	2.1
7	G	29	LYS	2.1
7	G	79	ARG	2.1
9	I	102	LEU	2.1
12	L	111	LYS	2.1
1	A	1258	G	2.1
1	A	980	C	2.1
4	D	68	TYR	2.1
21	U	3	LYS	2.1
1	A	1066	C	2.1
7	G	39	ALA	2.0
7	G	32	ARG	2.0
4	D	70	ILE	2.0
4	D	69	GLY	2.0
1	A	962	C	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 95th percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
24	MG	A	1794	1/1	0.43	-	118,118,118,118	0
24	MG	A	1694	1/1	0.46	-	84,84,84,84	0
24	MG	A	1688	1/1	0.20	-	70,70,70,70	0
24	MG	A	1732	1/1	0.20	-	70,70,70,70	0
24	MG	A	1672	1/1	0.38	-	78,78,78,78	0
24	MG	A	1635	1/1	0.42	-	81,81,81,81	0
24	MG	A	1713	1/1	1.01	-	91,91,91,91	0
24	MG	A	1612	1/1	0.37	-	84,84,84,84	0
24	MG	A	1636	1/1	0.36	-	63,63,63,63	0
24	MG	A	1601	1/1	0.50	-	79,79,79,79	0
24	MG	A	1763	1/1	0.28	-	94,94,94,94	0
24	MG	A	1761	1/1	0.25	-	93,93,93,93	0
24	MG	D	302	1/1	0.15	-	53,53,53,53	0
24	MG	A	1696	1/1	0.31	-	53,53,53,53	0
24	MG	A	1714	1/1	0.85	-	82,82,82,82	0
24	MG	A	1819	1/1	0.15	-	92,92,92,92	0
24	MG	A	1766	1/1	0.46	-	103,103,103,103	0
24	MG	A	1817	1/1	0.27	-	102,102,102,102	0
24	MG	A	1652	1/1	0.27	-	61,61,61,61	0
24	MG	A	1606	1/1	0.21	-	77,77,77,77	0
24	MG	A	1641	1/1	0.29	-	96,96,96,96	0
24	MG	V	109	1/1	0.28	-	79,79,79,79	0
24	MG	A	1750	1/1	0.26	-	80,80,80,80	0
24	MG	A	1631	1/1	1.02	-	74,74,74,74	0
24	MG	A	1778	1/1	0.15	-	77,77,77,77	0
24	MG	A	1632	1/1	0.32	-	70,70,70,70	0
24	MG	A	1824	1/1	0.17	-	119,119,119,119	0
24	MG	V	101	1/1	0.29	-	59,59,59,59	0
24	MG	A	1827	1/1	0.44	-	87,87,87,87	0
24	MG	A	1657	1/1	0.52	-	66,66,66,66	0
24	MG	A	1825	1/1	0.13	-	110,110,110,110	0
24	MG	A	1756	1/1	0.24	-	56,56,56,56	0
24	MG	A	1602	1/1	0.50	-	72,72,72,72	0
24	MG	A	1802	1/1	0.28	-	102,102,102,102	0
24	MG	A	1700	1/1	0.22	-	94,94,94,94	0
24	MG	A	1818	1/1	0.23	-	101,101,101,101	0
24	MG	A	1755	1/1	0.40	-	92,92,92,92	0
24	MG	A	1643	1/1	0.23	-	80,80,80,80	0
24	MG	A	1796	1/1	0.37	-	64,64,64,64	0
24	MG	A	1651	1/1	0.26	-	78,78,78,78	0
24	MG	A	1624	1/1	0.83	-	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	MG	A	1753	1/1	0.22	-	96,96,96,96	0
24	MG	A	1620	1/1	0.39	-	71,71,71,71	0
24	MG	A	1667	1/1	1.16	-	76,76,76,76	0
24	MG	O	101	1/1	0.29	-	90,90,90,90	0
24	MG	V	104	1/1	0.25	-	92,92,92,92	0
24	MG	A	1810	1/1	0.21	-	83,83,83,83	0
24	MG	A	1691	1/1	0.33	-	72,72,72,72	0
24	MG	A	1608	1/1	0.27	-	80,80,80,80	0
24	MG	A	1682	1/1	0.22	-	65,65,65,65	0
24	MG	A	1730	1/1	0.15	-	88,88,88,88	0
24	MG	A	1604	1/1	0.83	-	114,114,114,114	0
24	MG	A	1647	1/1	0.81	-	74,74,74,74	0
24	MG	A	1617	1/1	0.28	-	54,54,54,54	0
24	MG	A	1758	1/1	0.18	-	58,58,58,58	0
24	MG	A	1733	1/1	0.44	-	74,74,74,74	0
24	MG	A	1807	1/1	0.10	-	94,94,94,94	0
24	MG	A	1662	1/1	0.45	-	85,85,85,85	0
24	MG	A	1745	1/1	0.20	-	79,79,79,79	0
24	MG	A	1718	1/1	0.52	-	71,71,71,71	0
24	MG	A	1698	1/1	0.37	-	83,83,83,83	0
24	MG	A	1716	1/1	0.26	-	70,70,70,70	0
24	MG	A	1775	1/1	0.36	-	93,93,93,93	0
24	MG	A	1665	1/1	0.20	-	92,92,92,92	0
24	MG	A	1735	1/1	0.13	-	80,80,80,80	0
24	MG	A	1768	1/1	0.13	-	76,76,76,76	0
24	MG	A	1715	1/1	0.09	-	95,95,95,95	0
24	MG	A	1769	1/1	0.14	-	62,62,62,62	0
24	MG	A	1792	1/1	0.57	-	80,80,80,80	0
24	MG	A	1747	1/1	0.07	-	92,92,92,92	0
24	MG	A	1813	1/1	0.58	-	103,103,103,103	0
24	MG	A	1772	1/1	0.17	-	106,106,106,106	0
24	MG	A	1723	1/1	1.15	-	88,88,88,88	0
24	MG	A	1740	1/1	0.14	-	80,80,80,80	0
24	MG	A	1633	1/1	0.71	-	66,66,66,66	0
24	MG	A	1674	1/1	0.62	-	82,82,82,82	0
24	MG	A	1704	1/1	0.85	-	97,97,97,97	0
24	MG	A	1668	1/1	0.49	-	64,64,64,64	0
24	MG	A	1712	1/1	0.98	-	72,72,72,72	0
24	MG	V	110	1/1	0.18	-	102,102,102,102	0
24	MG	A	1695	1/1	0.36	-	74,74,74,74	0
24	MG	A	1613	1/1	0.19	-	58,58,58,58	0
24	MG	A	1780	1/1	0.48	-	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	MG	A	1655	1/1	0.40	-	78,78,78,78	0
24	MG	A	1711	1/1	0.48	-	75,75,75,75	0
24	MG	A	1685	1/1	0.31	-	73,73,73,73	0
24	MG	A	1720	1/1	0.54	-	66,66,66,66	0
24	MG	A	1603	1/1	0.76	-	72,72,72,72	0
24	MG	A	1671	1/1	0.64	-	59,59,59,59	0
24	MG	V	112	1/1	0.18	-	66,66,66,66	0
24	MG	A	1806	1/1	0.16	-	121,121,121,121	0
24	MG	A	1628	1/1	0.32	-	50,50,50,50	0
24	MG	A	1661	1/1	0.56	-	91,91,91,91	0
24	MG	A	1626	1/1	0.41	-	71,71,71,71	0
24	MG	A	1609	1/1	0.25	-	70,70,70,70	0
24	MG	A	1722	1/1	0.28	-	77,77,77,77	0
24	MG	A	1649	1/1	0.55	-	71,71,71,71	0
24	MG	A	1706	1/1	0.22	-	109,109,109,109	0
24	MG	A	1677	1/1	0.58	-	79,79,79,79	0
24	MG	A	1786	1/1	0.32	-	90,90,90,90	0
24	MG	A	1679	1/1	0.21	-	83,83,83,83	0
24	MG	A	1681	1/1	0.25	-	84,84,84,84	0
24	MG	A	1642	1/1	0.65	-	72,72,72,72	0
24	MG	A	1646	1/1	0.72	-	69,69,69,69	0
24	MG	A	1689	1/1	0.78	-	75,75,75,75	0
24	MG	A	1731	1/1	0.19	-	79,79,79,79	0
24	MG	A	1634	1/1	1.25	-	77,77,77,77	0
24	MG	A	1812	1/1	0.31	-	102,102,102,102	0
24	MG	A	1788	1/1	0.56	-	96,96,96,96	0
25	ZN	N	101	1/1	0.14	-	165,165,165,165	0
24	MG	A	1622	1/1	0.19	-	100,100,100,100	0
24	MG	A	1784	1/1	0.41	-	81,81,81,81	0
24	MG	V	106	1/1	0.20	-	78,78,78,78	0
24	MG	A	1660	1/1	0.24	-	64,64,64,64	0
24	MG	A	1702	1/1	0.32	-	117,117,117,117	0
24	MG	A	1639	1/1	0.40	-	80,80,80,80	0
24	MG	A	1610	1/1	0.14	-	63,63,63,63	0
24	MG	V	102	1/1	0.45	-	85,85,85,85	0
24	MG	A	1719	1/1	0.27	-	74,74,74,74	0
24	MG	A	1697	1/1	0.38	-	84,84,84,84	0
24	MG	A	1767	1/1	0.22	-	68,68,68,68	0
24	MG	A	1658	1/1	0.18	-	80,80,80,80	0
24	MG	A	1738	1/1	0.21	-	81,81,81,81	0
25	ZN	D	301	1/1	0.08	-	90,90,90,90	0
24	MG	V	107	1/1	0.34	-	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	MG	A	1770	1/1	0.12	-	75,75,75,75	0
24	MG	A	1814	1/1	0.21	-	88,88,88,88	0
24	MG	A	1760	1/1	0.18	-	70,70,70,70	0
24	MG	A	1773	1/1	0.31	-	62,62,62,62	0
24	MG	A	1726	1/1	0.81	-	84,84,84,84	0
24	MG	V	105	1/1	0.23	-	106,106,106,106	0
24	MG	A	1684	1/1	0.25	-	70,70,70,70	0
24	MG	A	1619	1/1	0.28	-	78,78,78,78	0
24	MG	A	1710	1/1	0.57	-	112,112,112,112	0
24	MG	A	1669	1/1	0.16	-	73,73,73,73	0
24	MG	A	1757	1/1	0.06	-	86,86,86,86	0
24	MG	A	1721	1/1	0.21	-	66,66,66,66	0
24	MG	A	1803	1/1	0.25	-	56,56,56,56	0
24	MG	A	1751	1/1	0.11	-	99,99,99,99	0
24	MG	A	1809	1/1	0.26	-	105,105,105,105	0
24	MG	A	1686	1/1	0.48	-	43,43,43,43	0
24	MG	A	1774	1/1	0.14	-	94,94,94,94	0
24	MG	A	1830	1/1	0.15	-	95,95,95,95	0
24	MG	A	1734	1/1	0.27	-	83,83,83,83	0
24	MG	A	1673	1/1	0.20	-	69,69,69,69	0
24	MG	A	1777	1/1	0.32	-	78,78,78,78	0
24	MG	A	1727	1/1	0.40	-	75,75,75,75	0
24	MG	A	1748	1/1	0.35	-	89,89,89,89	0
24	MG	A	1759	1/1	0.18	-	61,61,61,61	0
24	MG	A	1823	1/1	0.18	-	114,114,114,114	0
24	MG	A	1828	1/1	0.14	-	96,96,96,96	0
24	MG	A	1629	1/1	0.36	-	69,69,69,69	0
24	MG	X	101	1/1	0.44	-	99,99,99,99	0
24	MG	A	1752	1/1	0.08	-	65,65,65,65	0
24	MG	A	1762	1/1	0.33	-	84,84,84,84	0
24	MG	A	1653	1/1	0.22	-	54,54,54,54	0
24	MG	A	1725	1/1	0.22	-	85,85,85,85	0
24	MG	A	1764	1/1	0.40	-	56,56,56,56	0
24	MG	A	1640	1/1	0.28	-	99,99,99,99	0
24	MG	A	1623	1/1	0.71	-	80,80,80,80	0
24	MG	A	1650	1/1	0.82	-	73,73,73,73	0
24	MG	A	1821	1/1	0.45	-	114,114,114,114	0
24	MG	A	1801	1/1	0.11	-	100,100,100,100	0
24	MG	A	1616	1/1	0.25	-	74,74,74,74	0
24	MG	A	1754	1/1	0.25	-	75,75,75,75	0
24	MG	A	1693	1/1	0.24	-	68,68,68,68	0
24	MG	A	1707	1/1	0.85	-	114,114,114,114	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	MG	A	1785	1/1	0.15	-	95,95,95,95	0
24	MG	A	1656	1/1	0.99	-	74,74,74,74	0
24	MG	A	1703	1/1	0.54	-	114,114,114,114	0
24	MG	T	201	1/1	0.77	-	67,67,67,67	0
24	MG	A	1744	1/1	0.66	-	98,98,98,98	0
24	MG	A	1611	1/1	0.17	-	74,74,74,74	0
24	MG	A	1717	1/1	0.23	-	83,83,83,83	0
24	MG	A	1808	1/1	0.22	-	94,94,94,94	0
24	MG	A	1644	1/1	0.20	-	84,84,84,84	0
24	MG	A	1648	1/1	0.18	-	73,73,73,73	0
24	MG	A	1793	1/1	1.82	-	98,98,98,98	0
24	MG	A	1765	1/1	0.08	-	76,76,76,76	0
24	MG	A	1805	1/1	0.43	-	82,82,82,82	0
24	MG	A	1678	1/1	0.45	-	77,77,77,77	0
24	MG	A	1737	1/1	0.25	-	84,84,84,84	0
24	MG	A	1741	1/1	0.14	-	78,78,78,78	0
24	MG	A	1739	1/1	0.16	-	90,90,90,90	0
24	MG	A	1666	1/1	0.38	-	63,63,63,63	0
24	MG	A	1615	1/1	0.29	-	81,81,81,81	0
24	MG	A	1654	1/1	0.97	-	75,75,75,75	0
24	MG	A	1787	1/1	0.30	-	103,103,103,103	0
24	MG	A	1630	1/1	0.16	-	51,51,51,51	0
24	MG	A	1746	1/1	0.13	-	73,73,73,73	0
24	MG	A	1789	1/1	0.12	-	78,78,78,78	0
24	MG	A	1779	1/1	0.16	-	124,124,124,124	0
24	MG	A	1618	1/1	0.38	-	61,61,61,61	0
24	MG	A	1729	1/1	0.30	-	96,96,96,96	0
24	MG	A	1708	1/1	0.25	-	100,100,100,100	0
24	MG	V	113	1/1	0.13	-	76,76,76,76	0
24	MG	A	1664	1/1	0.12	-	101,101,101,101	0
24	MG	A	1795	1/1	0.54	-	66,66,66,66	0
24	MG	A	1749	1/1	0.13	-	86,86,86,86	0
24	MG	A	1637	1/1	0.52	-	72,72,72,72	0
24	MG	A	1791	1/1	0.11	-	87,87,87,87	0
24	MG	A	1663	1/1	0.21	-	92,92,92,92	0
24	MG	A	1776	1/1	0.19	-	93,93,93,93	0
24	MG	A	1687	1/1	0.15	-	71,71,71,71	0
24	MG	A	1822	1/1	0.23	-	113,113,113,113	0
24	MG	A	1627	1/1	0.50	-	50,50,50,50	0
24	MG	A	1790	1/1	0.14	-	96,96,96,96	0
24	MG	A	1815	1/1	0.26	-	102,102,102,102	0
24	MG	A	1797	1/1	0.18	-	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	MG	A	1659	1/1	0.59	-	77,77,77,77	0
24	MG	A	1811	1/1	0.16	-	115,115,115,115	0
24	MG	A	1699	1/1	0.76	-	80,80,80,80	0
24	MG	A	1816	1/1	0.23	-	100,100,100,100	0
24	MG	A	1709	1/1	0.75	-	93,93,93,93	0
24	MG	V	103	1/1	0.34	-	88,88,88,88	0
24	MG	A	1607	1/1	0.14	-	73,73,73,73	0
24	MG	A	1724	1/1	0.33	-	73,73,73,73	0
24	MG	A	1680	1/1	0.19	-	88,88,88,88	0
24	MG	A	1798	1/1	0.39	-	82,82,82,82	0
24	MG	A	1683	1/1	0.22	-	70,70,70,70	0
24	MG	A	1675	1/1	0.66	-	76,76,76,76	0
24	MG	A	1826	1/1	0.27	-	111,111,111,111	0
24	MG	A	1742	1/1	0.25	-	97,97,97,97	0
24	MG	A	1705	1/1	1.04	-	90,90,90,90	0
24	MG	A	1645	1/1	0.14	-	53,53,53,53	0
24	MG	A	1676	1/1	0.21	-	54,54,54,54	0
24	MG	A	1605	1/1	0.25	-	59,59,59,59	0
24	MG	A	1625	1/1	0.14	-	64,64,64,64	0
24	MG	A	1638	1/1	0.28	-	50,50,50,50	0
24	MG	A	1799	1/1	0.15	-	73,73,73,73	0
24	MG	A	1781	1/1	0.16	-	99,99,99,99	0
24	MG	A	1728	1/1	0.71	-	76,76,76,76	0
24	MG	A	1800	1/1	0.14	-	59,59,59,59	0
24	MG	A	1782	1/1	0.23	-	90,90,90,90	0
24	MG	A	1670	1/1	0.20	-	66,66,66,66	0
24	MG	A	1804	1/1	0.29	-	84,84,84,84	0
24	MG	A	1690	1/1	0.23	-	64,64,64,64	0
24	MG	A	1736	1/1	0.19	-	69,69,69,69	0
24	MG	A	1829	1/1	0.30	-	108,108,108,108	0
24	MG	A	1771	1/1	0.21	-	61,61,61,61	0
24	MG	A	1783	1/1	0.45	-	82,82,82,82	0
24	MG	A	1701	1/1	0.19	-	99,99,99,99	0
24	MG	A	1820	1/1	0.10	-	102,102,102,102	0
24	MG	A	1743	1/1	0.31	-	90,90,90,90	0
24	MG	A	1621	1/1	0.26	-	70,70,70,70	0
24	MG	A	1692	1/1	0.24	-	81,81,81,81	0
24	MG	A	1614	1/1	0.43	-	75,75,75,75	0
24	MG	V	108	1/1	0.41	-	78,78,78,78	0
24	MG	V	111	1/1	0.07	-	100,100,100,100	0

6.5 Other polymers ⓘ

There are no such residues in this entry.