



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:21 AM UTC

PDB ID : 4DV0 / pdb_00004dv0
Title : Crystal structure of the *Thermus thermophilus* 30S ribosomal subunit with a 16S rRNA mutation, U20G
Authors : Demirci, H.; Murphy IV, F.; Murphy, E.; Gregory, S.T.; Dahlberg, A.E.; Jogl, G.
Deposited on : 2012-02-22
Resolution : 3.85 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

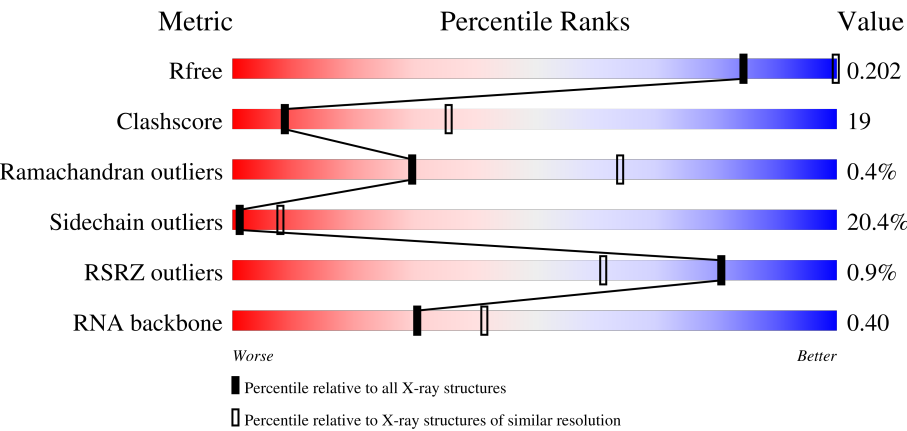
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.85 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.



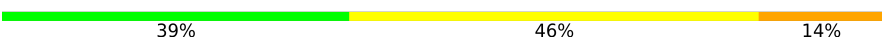
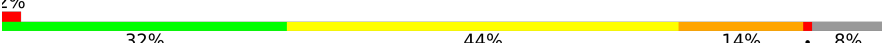
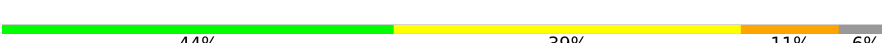
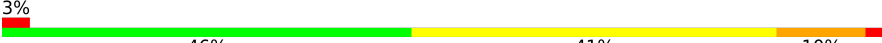
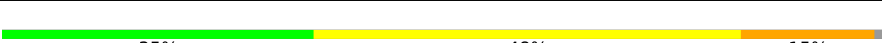
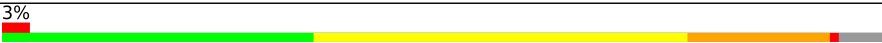
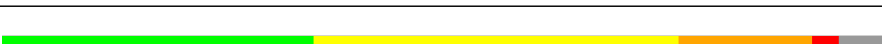
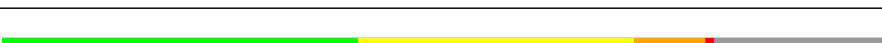
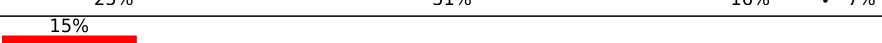
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1165 (4.02-3.70)
Clashscore	190562	1207 (4.02-3.70)
Ramachandran outliers	187476	1149 (4.02-3.70)
Sidechain outliers	187428	1142 (4.02-3.70)
RSRZ outliers	180081	1164 (4.02-3.70)
RNA backbone	3983	1012 (4.62-3.10)

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

Mol	Chain	Length	Quality of chain
1	A	1522	% 40% 45% 14% .
2	B	256	45% 38% 7% . 9%
3	C	239	% 38% 36% 11% . 14%
4	D	209	3% 45% 37% 15% .

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Mol	Chain	Length	Quality of chain
5	E	162	
6	F	101	
7	G	156	
8	H	138	
9	I	128	
10	J	105	
11	K	129	
12	L	135	
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	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	MG	A	1706	-	-	-	X
22	MG	A	1713	-	-	-	X
22	MG	A	1722	-	-	-	X
22	MG	A	1856	-	-	-	X

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 52453 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1512	Total	C	N	O	P	0	6	0
			32647	14541	6042	10546	1518			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	G	U	engineered mutation	GB M26923.1
A	1534	C	A	conflict	GB M26923.1
A	1535	A	C	conflict	GB M26923.1

- Molecule 2 is a protein called ribosomal protein S2.

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

- Molecule 3 is a protein called ribosomal protein S3.

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

- Molecule 4 is a protein called ribosomal protein S4.

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

- Molecule 5 is a protein called ribosomal protein S5.

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

- Molecule 6 is a protein called ribosomal protein S6.

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

- Molecule 7 is a protein called ribosomal protein S7.

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

- Molecule 8 is a protein called ribosomal protein S8.

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

- Molecule 9 is a protein called ribosomal protein S9.

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

- Molecule 10 is a protein called ribosomal protein S10.

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

- Molecule 11 is a protein called ribosomal protein S11.

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

- Molecule 12 is a protein called ribosomal protein S12.

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

- Molecule 13 is a protein called ribosomal protein S13.

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

- Molecule 14 is a protein called ribosomal protein S14.

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

- Molecule 15 is a protein called ribosomal protein S15.

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

- Molecule 16 is a protein called ribosomal protein S16.

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

- Molecule 17 is a protein called ribosomal protein S17.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 18 is a protein called ribosomal protein S18.

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

- Molecule 19 is a protein called ribosomal protein S19.

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

- Molecule 20 is a protein called ribosomal protein S20.

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

- Molecule 21 is a protein called ribosomal protein THX.

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

- Molecule 22 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	262	Total	Mg	0	0
			262	262		
22	B	3	Total	Mg	0	0
			3	3		
22	C	1	Total	Mg	0	0
			1	1		
22	D	2	Total	Mg	0	0
			2	2		
22	E	1	Total	Mg	0	0
			1	1		
22	F	1	Total	Mg	0	0
			1	1		
22	J	2	Total	Mg	0	0
			2	2		
22	M	1	Total	Mg	0	0
			1	1		
22	P	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	Q	1	Total 1	Mg 1	0	0
22	S	1	Total 1	Mg 1	0	0

- Molecule 23 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

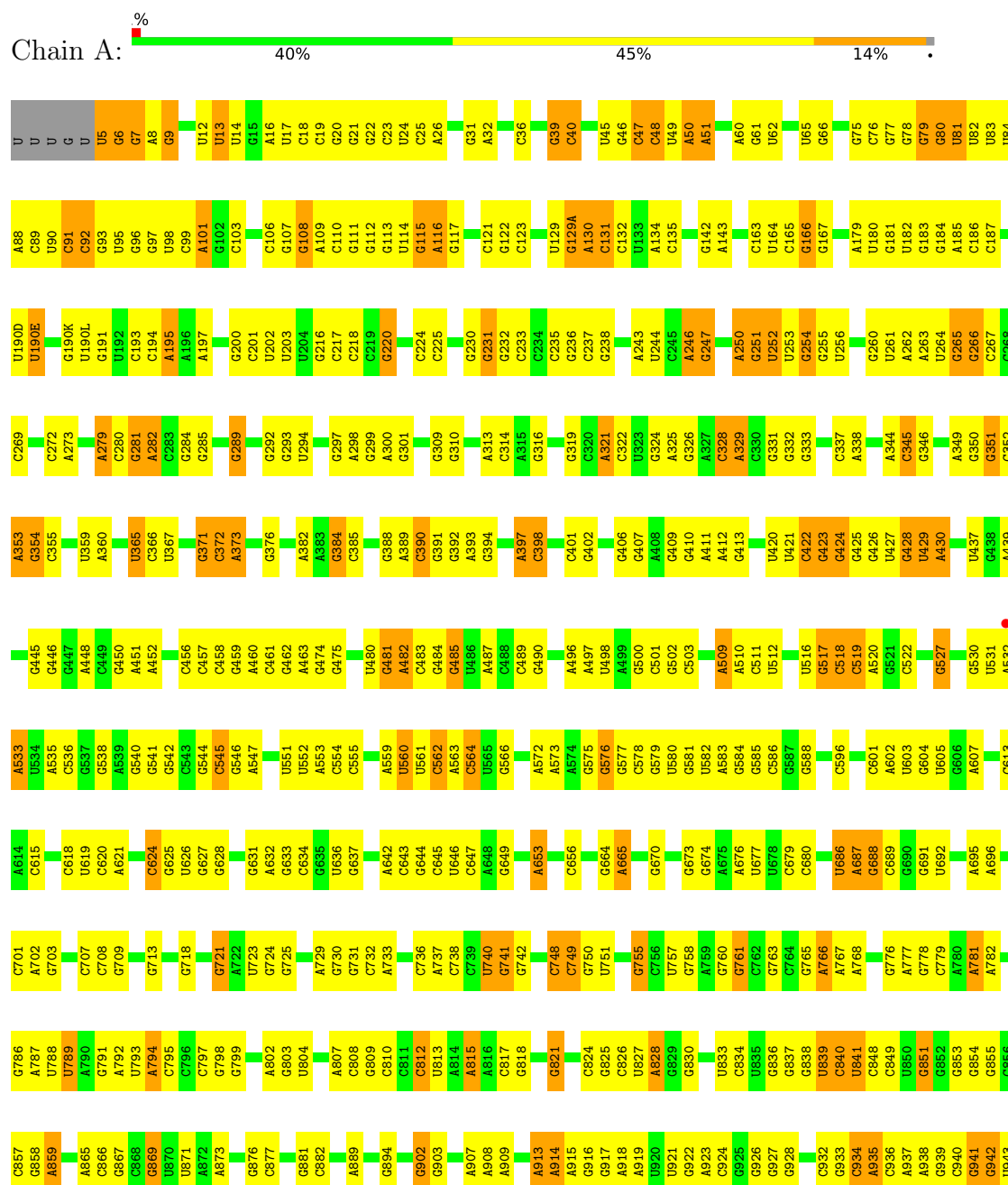
- Molecule 24 is water.

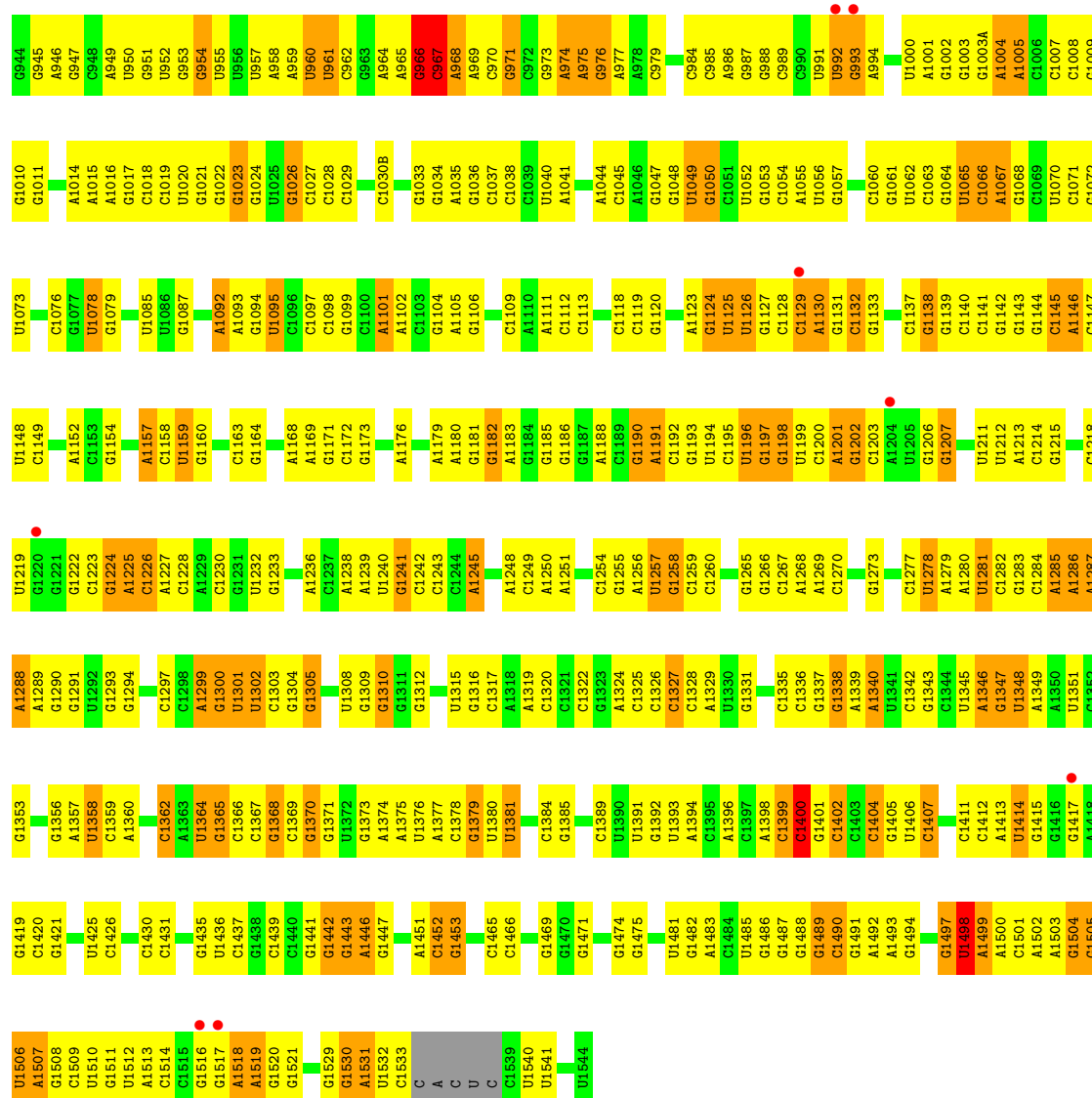
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	A	397	Total 397	O 397	0	0
24	D	1	Total 1	O 1	0	0
24	E	4	Total 4	O 4	0	0
24	G	4	Total 4	O 4	0	0
24	I	1	Total 1	O 1	0	0
24	J	3	Total 3	O 3	0	0
24	L	1	Total 1	O 1	0	0
24	M	8	Total 8	O 8	0	0
24	N	1	Total 1	O 1	0	0
24	P	10	Total 10	O 10	0	0
24	Q	2	Total 2	O 2	0	0
24	S	2	Total 2	O 2	0	0
24	T	5	Total 5	O 5	0	0

3 Residue-property plots

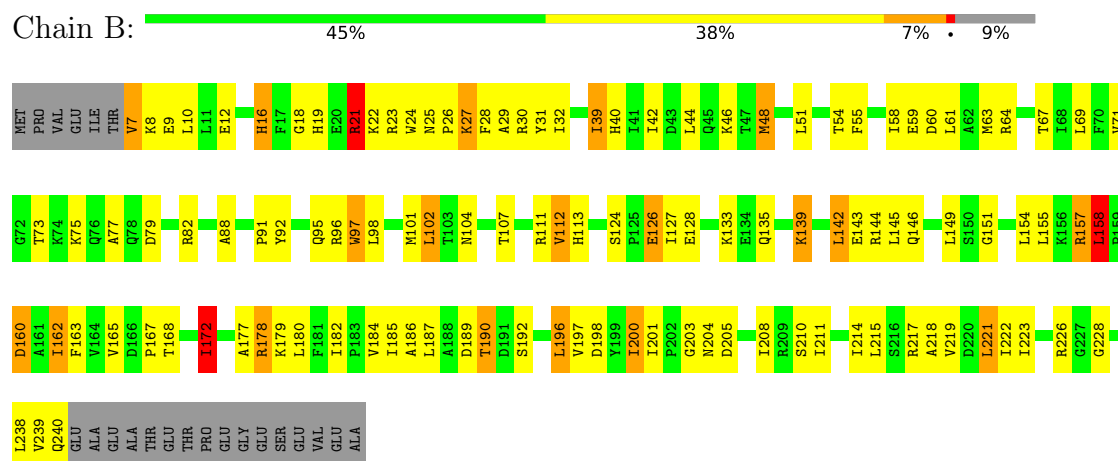
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

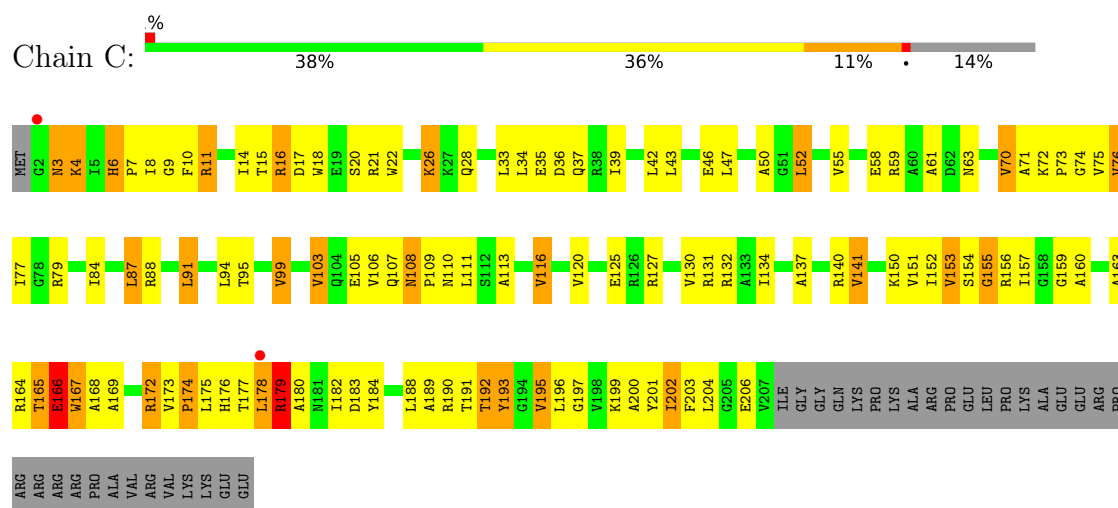
• Molecule 1: 16S rRNA



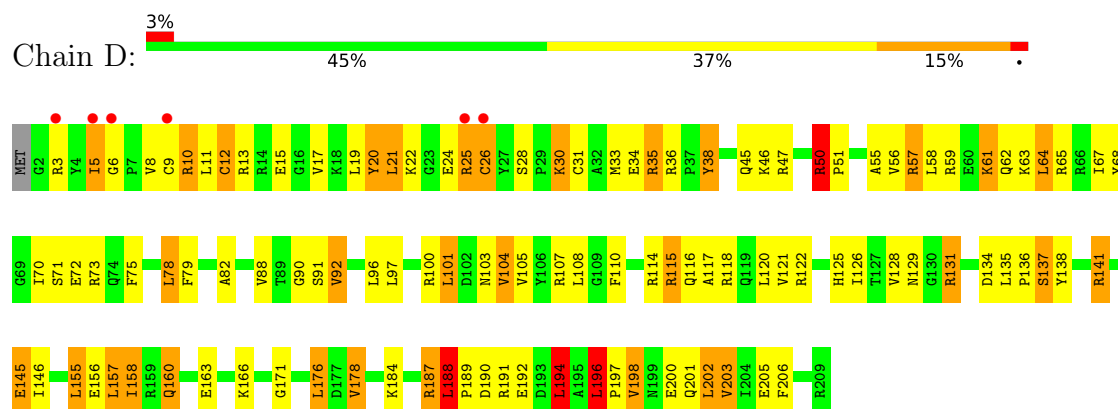


• Molecule 2: ribosomal protein S2

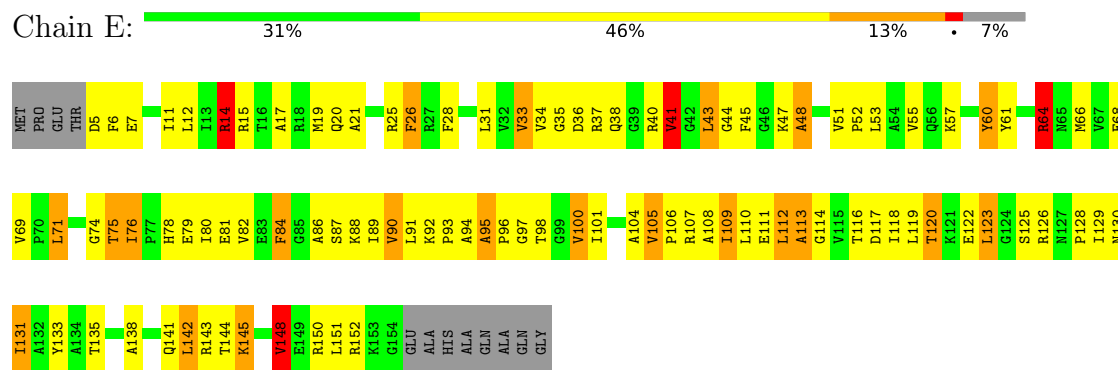




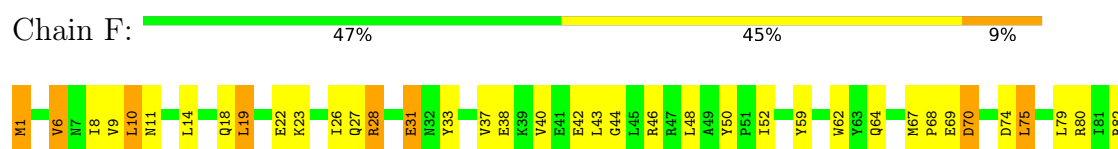
• Molecule 4: ribosomal protein S4

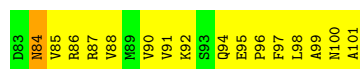


• Molecule 5: ribosomal protein S5

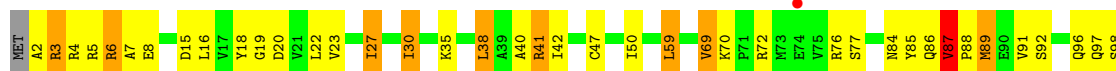


• Molecule 6: ribosomal protein S6

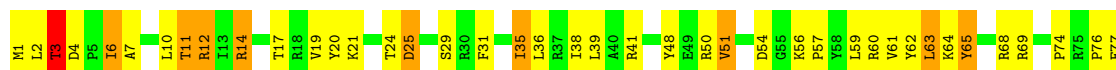




- Molecule 7: ribosomal protein S7



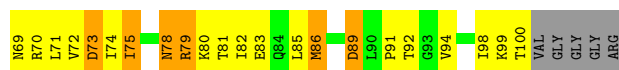
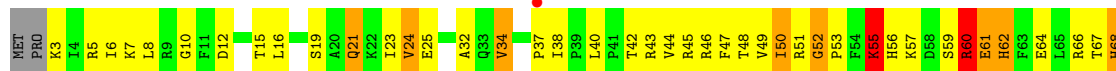
- Molecule 8: ribosomal protein S8



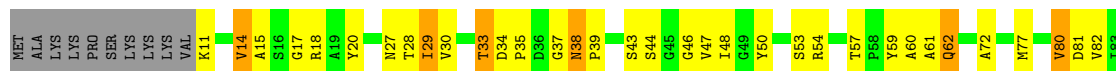
- Molecule 9: ribosomal protein S9



- Molecule 10: ribosomal protein S10



- Molecule 11: ribosomal protein S11





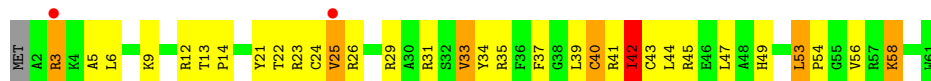
• Molecule 12: ribosomal protein S12



• Molecule 13: ribosomal protein S13



• Molecule 14: ribosomal protein S14

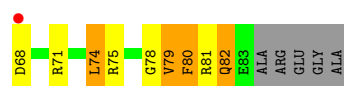


• Molecule 15: ribosomal protein S15



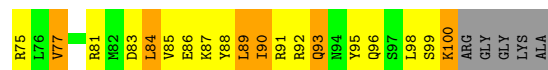
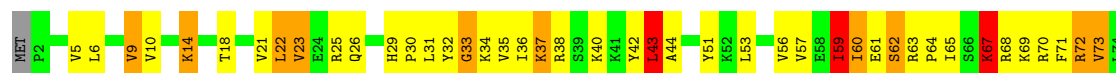
• Molecule 16: ribosomal protein S16





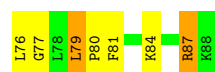
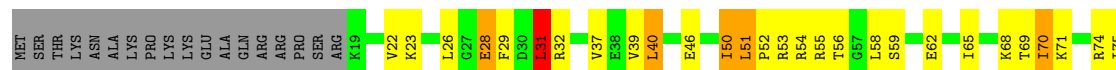
• Molecule 17: ribosomal protein S17

Chain Q: 35% 41% 15% • 6%



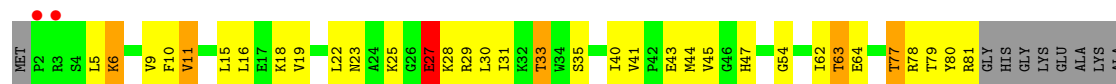
• Molecule 18: ribosomal protein S18

Chain R: 40% 31% 8% • 20%



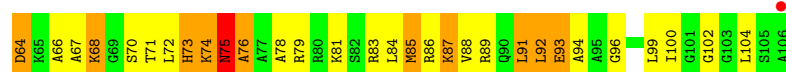
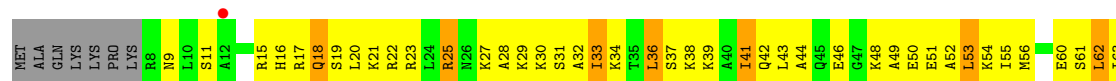
• Molecule 19: ribosomal protein S19

Chain S: 2% 49% 30% 5% • 14%



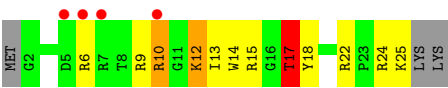
• Molecule 20: ribosomal protein S20

Chain T: 2% 25% 51% 16% • 7%



• Molecule 21: ribosomal protein THX

Chain U: 15% 44% 33% 7% • 11%



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	402.11Å 402.11Å 174.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.82 – 3.85 34.82 – 3.85	Depositor EDS
% Data completeness (in resolution range)	97.7 (34.82-3.85) 97.3 (34.82-3.85)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 3.87Å)	Xtriage
Refinement program	PHENIX dev_978	Depositor
R, R_{free}	0.147 , 0.206 0.147 , 0.202	Depositor DCC
R_{free} test set	6511 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	164.0	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 154.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	52453	wwPDB-VP
Average B, all atoms (Å ²)	196.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.54	1/36143 (0.0%)	0.57	1/56403 (0.0%)
2	B	0.74	0/1935	1.12	7/2609 (0.3%)
3	C	0.71	0/1636	1.16	13/2205 (0.6%)
4	D	0.81	1/1733 (0.1%)	1.34	26/2318 (1.1%)
5	E	1.12	2/1162 (0.2%)	1.45	23/1564 (1.5%)
6	F	0.74	0/856	1.13	3/1154 (0.3%)
7	G	0.76	0/1276	1.20	13/1709 (0.8%)
8	H	1.14	2/1136 (0.2%)	1.54	9/1527 (0.6%)
9	I	0.67	0/1029	1.12	5/1379 (0.4%)
10	J	0.78	0/805	1.25	11/1082 (1.0%)
11	K	0.91	2/879 (0.2%)	1.37	12/1187 (1.0%)
12	L	0.93	1/977 (0.1%)	1.43	14/1306 (1.1%)
13	M	0.72	0/947	1.10	2/1270 (0.2%)
14	N	0.73	0/501	1.12	2/664 (0.3%)
15	O	0.89	1/740 (0.1%)	1.24	4/987 (0.4%)
16	P	1.02	1/716 (0.1%)	1.38	13/963 (1.3%)
17	Q	1.12	2/836 (0.2%)	1.45	12/1117 (1.1%)
18	R	0.88	1/579 (0.2%)	1.39	7/768 (0.9%)
19	S	0.71	0/661	1.13	4/890 (0.4%)
20	T	0.94	0/765	1.40	6/1007 (0.6%)
21	U	0.75	0/212	1.02	1/277 (0.4%)
All	All	0.67	14/55524 (0.0%)	0.86	188/82386 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	2
8	H	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
10	J	0	1
12	L	0	1
20	T	0	1
All	All	0	6

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Q	35	VAL	CA-CB	-6.91	1.46	1.54
5	E	148	VAL	CA-CB	-6.65	1.45	1.54
12	L	85	ILE	CA-CB	-6.62	1.45	1.54
16	P	19	ILE	CA-CB	-6.13	1.46	1.54
15	O	60	VAL	CA-CB	-6.04	1.46	1.54
11	K	120	ARG	CA-C	-5.92	1.46	1.52
8	H	134	ILE	CA-CB	-5.90	1.47	1.54
11	K	61	ALA	CA-CB	-5.27	1.45	1.53
8	H	3	THR	CA-CB	5.26	1.59	1.53
18	R	50	ILE	CA-CB	-5.24	1.48	1.54
4	D	203	VAL	CA-CB	-5.21	1.48	1.54
5	E	90	VAL	CA-CB	-5.18	1.47	1.54
17	Q	99	SER	CA-C	5.16	1.59	1.52
1	A	1346	A	C3'-O3'	5.04	1.50	1.43

All (188) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	100	ILE	CA-C-N	12.42	133.25	119.83
8	H	100	ILE	C-N-CA	12.42	133.25	119.83
4	D	26	CYS	N-CA-C	-11.30	99.15	113.16
11	K	91	ARG	N-CA-C	-11.07	98.29	112.23
12	L	26	ALA	N-CA-C	-10.26	100.78	113.20
4	D	171	GLY	CA-C-N	10.21	132.61	119.84
4	D	171	GLY	C-N-CA	10.21	132.61	119.84
18	R	51	LEU	CA-C-N	9.84	129.77	120.03
18	R	51	LEU	C-N-CA	9.84	129.77	120.03
5	E	69	VAL	CB-CA-C	-9.81	101.82	110.94
11	K	14	VAL	N-CA-C	9.40	122.14	112.83
20	T	94	ALA	N-CA-C	-9.37	93.37	108.55
7	G	111	ARG	CA-C-N	8.95	128.28	118.97
7	G	111	ARG	C-N-CA	8.95	128.28	118.97
6	F	11	ASN	CA-C-N	8.69	128.91	119.87
6	F	11	ASN	C-N-CA	8.69	128.91	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	48	ALA	CA-C-N	8.59	128.17	119.24
5	E	48	ALA	C-N-CA	8.59	128.17	119.24
12	L	105	TYR	CB-CA-C	-8.49	106.78	116.63
8	H	81	HIS	N-CA-C	-8.38	102.49	112.89
3	C	6	HIS	CA-C-N	8.35	127.95	118.85
3	C	6	HIS	C-N-CA	8.35	127.95	118.85
2	B	16	HIS	N-CA-C	8.18	123.44	113.38
7	G	155	ARG	N-CA-C	8.09	122.86	112.34
7	G	84	ASN	N-CA-C	8.09	120.22	110.19
3	C	108	ASN	CA-C-N	8.09	127.74	119.82
3	C	108	ASN	C-N-CA	8.09	127.74	119.82
11	K	117	ASN	N-CA-C	7.69	122.56	111.56
4	D	21	LEU	N-CA-C	-7.48	104.18	113.38
18	R	79	LEU	CA-C-N	7.40	127.98	120.14
18	R	79	LEU	C-N-CA	7.40	127.98	120.14
12	L	85	ILE	CB-CA-C	-7.36	100.32	110.77
4	D	12	CYS	N-CA-C	-7.34	102.30	111.11
5	E	105	VAL	CA-C-N	-7.26	111.49	119.19
5	E	105	VAL	C-N-CA	-7.26	111.49	119.19
17	Q	67	LYS	N-CA-C	-7.23	99.18	109.96
5	E	86	ALA	N-CA-C	-7.21	104.37	113.02
11	K	80	VAL	N-CA-C	7.19	118.17	108.11
12	L	18	VAL	N-CA-C	7.09	119.15	107.24
4	D	38	TYR	CA-C-N	7.07	127.66	120.38
4	D	38	TYR	C-N-CA	7.07	127.66	120.38
20	T	76	ALA	N-CA-C	-7.03	102.83	111.33
16	P	65	GLN	CA-C-N	7.00	127.55	119.99
16	P	65	GLN	C-N-CA	7.00	127.55	119.99
12	L	119	LYS	N-CA-C	-6.99	100.64	110.50
10	J	55	LYS	N-CA-C	6.98	118.33	108.00
7	G	118	VAL	CB-CA-C	-6.94	102.77	112.14
8	H	6	ILE	N-CA-C	6.89	117.68	110.72
20	T	42	GLN	N-CA-C	-6.87	103.73	111.14
4	D	33	MET	N-CA-C	-6.86	104.78	113.01
8	H	3	THR	CA-C-N	-6.80	111.22	121.83
8	H	3	THR	C-N-CA	-6.80	111.22	121.83
9	I	53	VAL	N-CA-C	6.77	118.65	112.29
4	D	6	GLY	CA-C-N	6.75	126.79	119.90
4	D	6	GLY	C-N-CA	6.75	126.79	119.90
20	T	73	HIS	CB-CA-C	-6.69	107.83	115.79
4	D	30	LYS	N-CA-C	6.69	122.26	113.30
4	D	188	LEU	CA-C-N	-6.68	111.49	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	188	LEU	C-N-CA	-6.68	111.49	119.84
5	E	41	VAL	CB-CA-C	-6.68	100.57	110.33
2	B	239	VAL	N-CA-C	6.68	116.83	110.42
20	T	75	ASN	N-CA-C	-6.66	104.78	113.17
5	E	145	LYS	N-CA-C	-6.54	104.07	111.07
5	E	148	VAL	CB-CA-C	-6.53	101.52	112.16
19	S	6	LYS	N-CA-C	6.43	124.50	110.80
12	L	85	ILE	N-CA-C	6.41	117.11	107.75
10	J	62	HIS	N-CA-C	6.41	119.97	109.85
4	D	56	VAL	CB-CA-C	-6.39	103.68	112.24
16	P	62	VAL	N-CA-C	6.38	118.29	112.29
12	L	14	GLY	N-CA-C	-6.37	104.66	112.68
3	C	155	GLY	N-CA-C	6.36	119.32	112.33
10	J	52	GLY	CA-C-N	6.31	126.22	119.85
10	J	52	GLY	C-N-CA	6.31	126.22	119.85
16	P	51	VAL	N-CA-C	6.30	122.45	109.34
7	G	91	VAL	N-CA-C	6.26	122.35	109.34
14	N	42	ILE	N-CA-C	-6.25	104.42	110.42
11	K	38	ASN	CA-C-N	6.22	126.57	119.92
11	K	38	ASN	C-N-CA	6.22	126.57	119.92
7	G	114	ARG	N-CA-C	6.22	118.06	111.28
5	E	109	ILE	N-CA-C	6.12	116.60	110.23
5	E	71	LEU	N-CA-C	6.09	118.11	108.67
16	P	9	PHE	N-CA-C	6.09	121.46	113.30
12	L	24	VAL	CA-C-N	-6.07	107.22	120.89
12	L	24	VAL	C-N-CA	-6.07	107.22	120.89
16	P	31	LYS	N-CA-C	6.07	119.01	109.96
17	Q	43	LEU	N-CA-C	6.05	118.55	108.20
9	I	54	ASP	N-CA-C	6.05	119.45	111.28
3	C	46	GLU	N-CA-C	6.04	119.12	111.69
5	E	142	LEU	N-CA-C	6.02	119.19	110.28
10	J	40	LEU	CA-C-N	5.99	126.01	119.90
10	J	40	LEU	C-N-CA	5.99	126.01	119.90
12	L	66	VAL	N-CA-C	5.99	116.99	108.42
17	Q	99	SER	N-CA-C	5.99	123.56	110.80
16	P	33	ILE	N-CA-C	5.95	118.49	111.05
3	C	74	GLY	N-CA-C	5.93	119.81	112.64
15	O	23	GLY	N-CA-C	5.92	125.74	115.62
17	Q	44	ALA	N-CA-C	5.92	119.04	109.40
5	E	130	ASN	N-CA-C	5.91	117.72	111.28
16	P	19	ILE	CB-CA-C	-5.91	102.95	111.34
7	G	59	LEU	N-CA-C	5.87	118.15	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	25	VAL	N-CA-C	5.84	117.27	110.62
5	E	69	VAL	N-CA-C	5.83	113.65	108.63
17	Q	59	ILE	CA-C-N	-5.83	115.02	123.06
17	Q	59	ILE	C-N-CA	-5.83	115.02	123.06
4	D	141	ARG	CA-C-N	-5.79	113.74	119.99
4	D	141	ARG	C-N-CA	-5.79	113.74	119.99
16	P	79	VAL	CB-CA-C	-5.77	104.32	111.70
10	J	60	ARG	N-CA-C	5.72	118.30	110.24
2	B	71	VAL	N-CA-C	5.69	116.07	108.27
11	K	48	ILE	N-CA-C	-5.68	103.79	110.21
4	D	50	ARG	CA-C-N	5.67	125.85	119.90
4	D	50	ARG	C-N-CA	5.67	125.85	119.90
4	D	178	VAL	N-CA-C	5.67	117.18	111.00
10	J	38	ILE	CA-C-N	5.66	125.85	119.90
10	J	38	ILE	C-N-CA	5.66	125.85	119.90
5	E	14	ARG	N-CA-C	5.64	117.55	109.14
8	H	69	ARG	N-CA-C	5.62	118.42	109.81
5	E	113	ALA	N-CA-C	-5.60	106.22	113.16
2	B	172	ILE	CB-CA-C	-5.59	104.82	111.81
3	C	174	PRO	N-CA-C	5.54	119.96	112.48
11	K	50	TYR	N-CA-C	5.53	118.25	110.23
11	K	116	HIS	CA-C-N	5.52	130.48	122.36
11	K	116	HIS	C-N-CA	5.52	130.48	122.36
17	Q	35	VAL	CB-CA-C	-5.52	103.11	111.33
18	R	87	ARG	CB-CA-C	-5.51	109.73	117.23
4	D	194	LEU	N-CA-C	5.51	118.45	109.59
5	E	64	ARG	N-CA-C	-5.50	103.27	110.53
2	B	21	ARG	N-CA-C	5.45	122.42	110.80
19	S	27	GLU	N-CA-C	5.45	118.22	110.10
16	P	5	ARG	N-CA-C	5.43	115.45	108.34
17	Q	33	GLY	N-CA-C	5.42	122.75	115.59
5	E	41	VAL	N-CA-C	5.42	115.92	108.12
21	U	17	THR	N-CA-C	5.40	118.24	109.86
2	B	158	LEU	CA-C-N	5.39	125.36	120.03
2	B	158	LEU	C-N-CA	5.39	125.36	120.03
10	J	89	ASP	N-CA-C	5.38	118.03	109.96
9	I	22	GLY	N-CA-C	5.37	118.10	110.74
16	P	58	TYR	CB-CA-C	-5.37	102.22	110.81
9	I	58	HIS	N-CA-C	-5.33	106.78	113.28
12	L	57	LYS	N-CA-C	-5.32	101.98	109.96
7	G	89	MET	N-CA-C	5.31	117.83	108.75
8	H	80	ILE	CB-CA-C	-5.31	104.53	111.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	198	VAL	CB-CA-C	-5.28	103.27	110.77
7	G	8	GLU	N-CA-C	5.26	117.94	110.10
3	C	179	ARG	N-CA-C	-5.26	99.59	110.80
5	E	104	ALA	N-CA-C	-5.26	105.62	111.36
9	I	109	VAL	N-CA-C	5.26	115.67	107.99
17	Q	72	ARG	N-CA-C	5.26	117.38	109.23
4	D	12	CYS	CA-CB-SG	5.26	126.49	114.40
19	S	30	LEU	CB-CA-C	-5.24	109.55	115.79
6	F	37	VAL	N-CA-C	5.24	115.39	107.80
4	D	196	LEU	CA-C-N	5.20	128.93	121.91
4	D	196	LEU	C-N-CA	5.20	128.93	121.91
18	R	31	LEU	N-CA-C	-5.17	106.98	113.28
19	S	10	PHE	N-CA-C	5.15	117.14	108.96
12	L	47	LYS	N-CA-C	5.15	120.56	113.77
13	M	118	ALA	N-CA-C	5.14	117.47	109.60
7	G	87	VAL	CA-C-N	5.14	125.59	120.14
7	G	87	VAL	C-N-CA	5.14	125.59	120.14
3	C	87	LEU	N-CA-C	5.13	118.00	111.69
5	E	40	ARG	N-CA-C	5.12	116.76	108.41
17	Q	14	LYS	N-CA-C	5.10	118.97	112.34
1	A	13	U	C2-N1-C1'	5.10	132.99	117.70
17	Q	77	VAL	N-CA-C	-5.10	106.69	111.48
12	L	101	VAL	CB-CA-C	-5.09	105.12	111.08
5	E	120	THR	N-CA-C	5.09	117.71	109.06
15	O	87	ILE	N-CA-C	5.09	117.82	109.78
3	C	166	GLU	N-CA-C	5.07	116.99	109.69
5	E	95	ALA	CA-C-N	5.07	125.07	119.90
5	E	95	ALA	C-N-CA	5.07	125.07	119.90
8	H	80	ILE	N-CA-CB	-5.07	105.52	111.60
11	K	103	LEU	N-CA-C	-5.06	102.99	110.48
3	C	141	VAL	N-CA-C	5.06	116.51	111.00
16	P	7	ALA	CA-C-N	-5.05	115.71	122.42
16	P	7	ALA	C-N-CA	-5.05	115.71	122.42
20	T	11	SER	N-CA-C	5.05	119.08	113.02
13	M	106	ASN	N-CA-C	5.04	118.28	111.17
18	R	52	PRO	CA-C-O	-5.04	115.63	122.08
15	O	73	GLU	CA-C-N	-5.04	113.97	121.83
15	O	73	GLU	C-N-CA	-5.04	113.97	121.83
17	Q	22	LEU	CA-CB-CG	-5.04	98.67	116.30
3	C	55	VAL	CB-CA-C	-5.03	104.74	110.73
11	K	15	ALA	CB-CA-C	-5.03	110.39	117.23
12	L	60	LEU	N-CA-C	5.02	116.30	109.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	24	VAL	CB-CA-C	-5.01	105.48	112.04
7	G	145	ALA	N-CA-C	-5.01	103.98	110.19
4	D	138	TYR	CA-C-N	-5.00	116.34	122.84
4	D	138	TYR	C-N-CA	-5.00	116.34	122.84

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	166	GLU	Peptide
3	C	179	ARG	Peptide
8	H	90	GLY	Peptide
10	J	86	MET	Peptide
12	L	87	GLY	Peptide
20	T	93	GLU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32647	0	16508	772	0
2	B	1900	0	1951	83	0
3	C	1612	0	1677	83	0
4	D	1703	0	1763	94	0
5	E	1146	0	1207	67	0
6	F	843	0	857	46	0
7	G	1257	0	1296	56	0
8	H	1116	0	1177	79	0
9	I	1010	0	1037	70	0
10	J	792	0	835	53	0
11	K	864	0	881	38	0
12	L	972	0	1058	67	0
13	M	937	0	995	51	0
14	N	492	0	529	30	0
15	O	729	0	768	43	0
16	P	700	0	720	37	0
17	Q	823	0	893	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	R	574	0	644	28	0
19	S	647	0	673	20	0
20	T	763	0	861	55	0
21	U	208	0	221	11	0
22	A	262	0	0	0	0
22	B	3	0	0	0	0
22	C	1	0	0	0	0
22	D	2	0	0	0	0
22	E	1	0	0	0	0
22	F	1	0	0	0	0
22	J	2	0	0	0	0
22	M	1	0	0	0	0
22	P	2	0	0	0	0
22	Q	1	0	0	0	0
22	S	1	0	0	0	0
23	D	1	0	0	0	0
23	N	1	0	0	0	0
24	A	397	0	0	11	0
24	D	1	0	0	0	0
24	E	4	0	0	0	0
24	G	4	0	0	0	0
24	I	1	0	0	0	0
24	J	3	0	0	1	0
24	L	1	0	0	0	0
24	M	8	0	0	3	0
24	N	1	0	0	1	0
24	P	10	0	0	4	0
24	Q	2	0	0	0	0
24	S	2	0	0	0	0
24	T	5	0	0	1	0
All	All	52453	0	36551	1630	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (1630) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:G:HO2'	1:A:482:A:H8	1.06	0.96
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.48	0.96
1:A:103:C:OP1	20:T:17:ARG:NH1	2.01	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1377:A:HO2'	7:G:2:ALA:N	1.68	0.90
8:H:83:ILE:HG12	8:H:137:VAL:HG22	1.52	0.90
1:A:1144:G:N2	1:A:1145:C:O2	2.05	0.89
1:A:1338:G:H2'	1:A:1339:A:C8	2.07	0.89
8:H:82:HIS:HD1	8:H:138:TRP:CD1	1.90	0.89
20:T:100:ILE:HG22	20:T:102:GLY:H	1.39	0.87
6:F:23:LYS:NZ	6:F:42:GLU:OE2	2.08	0.86
1:A:1368:G:H5''	9:I:112:LYS:HB3	1.57	0.85
7:G:69:VAL:HG23	7:G:135:VAL:HG22	1.56	0.85
21:U:10:ARG:HD3	21:U:13:ILE:HD12	1.58	0.84
1:A:1195:C:H3'	1:A:1196:U:H5''	1.60	0.83
1:A:1417:G:O2'	1:A:1483:A:N6	2.11	0.83
1:A:1152:A:OP1	10:J:68:HIS:ND1	2.11	0.83
13:M:34:LEU:HD12	13:M:41:PRO:HA	1.61	0.83
1:A:1326:C:OP2	21:U:6:ARG:NH2	2.12	0.83
1:A:263:A:OP2	20:T:79:ARG:NH1	2.11	0.82
18:R:58:LEU:HB3	18:R:62:GLU:HB3	1.59	0.82
8:H:64:LYS:HG2	8:H:79:VAL:HG21	1.61	0.82
3:C:6:HIS:CD2	3:C:9:GLY:H	1.98	0.81
15:O:70:LEU:HB3	15:O:78:TYR:HB2	1.63	0.81
12:L:87:GLY:HA2	12:L:98:TYR:HA	1.63	0.81
1:A:1316:G:N2	1:A:1319:A:OP2	2.14	0.80
2:B:91:PRO:HG3	2:B:154:LEU:HB2	1.62	0.80
7:G:5:ARG:HG3	7:G:7:ALA:H	1.47	0.80
12:L:47:LYS:HG3	12:L:48:PRO:HD3	1.63	0.80
6:F:22:GLU:OE1	6:F:82:ARG:NH1	2.15	0.80
1:A:1243:C:H42	1:A:1294:G:H1	1.27	0.79
11:K:82:VAL:HG11	11:K:95:ILE:HD11	1.64	0.79
11:K:57:THR:HG23	11:K:60:ALA:H	1.48	0.78
15:O:8:LYS:HE3	15:O:31:LEU:HD21	1.66	0.78
10:J:47:PHE:HB3	14:N:34:TYR:HE2	1.48	0.78
1:A:1191:A:H5''	3:C:4:LYS:HE3	1.66	0.78
12:L:89:ARG:HG2	12:L:97:ARG:HA	1.66	0.78
5:E:11:ILE:HB	5:E:31:LEU:HB3	1.65	0.77
1:A:738:C:OP2	6:F:92:LYS:NZ	2.18	0.77
1:A:384:G:H2'	1:A:385:C:C6	2.19	0.77
1:A:1057:G:H5''	3:C:154:SER:HB2	1.67	0.77
1:A:1404:5MC:H1'	1:A:1499:A:C2	2.20	0.77
1:A:1406:U:O2'	1:A:1517[B]:G:N2	2.17	0.76
1:A:1004:A:O2'	1:A:1005:A:OP1	2.04	0.76
1:A:1240:U:OP1	7:G:119:ARG:NH2	2.17	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1435:G:H2'	1:A:1436:U:C6	2.19	0.76
4:D:155:LEU:HD23	4:D:157:LEU:H	1.51	0.76
1:A:1426:C:H42	1:A:1474:G:H1	1.30	0.76
11:K:72:ALA:HB1	11:K:77:MET:HG3	1.66	0.76
10:J:61:GLU:OE1	14:N:45:ARG:NH1	2.19	0.76
1:A:279:A:OP2	17:Q:95:TYR:OH	2.04	0.76
1:A:1202:G:C4	14:N:42:ILE:HD12	2.20	0.75
12:L:25:PRO:C	12:L:27:LEU:H	1.95	0.75
5:E:17:ALA:HA	5:E:26:PHE:HB3	1.67	0.75
1:A:298:A:N6	24:A:2036:HOH:O	2.16	0.75
2:B:223:ILE:HG22	2:B:228:GLY:HA3	1.69	0.74
1:A:115:G:O2'	1:A:116:A:OP2	2.06	0.74
1:A:677:U:H3	1:A:713:G:H22	1.35	0.74
1:A:1414:U:H2'	1:A:1415:G:H8	1.51	0.74
1:A:130:A:H5'	17:Q:63:ARG:HE	1.51	0.74
16:P:74:LEU:HD13	16:P:79:VAL:HG21	1.69	0.74
3:C:174:PRO:HB2	3:C:177:THR:HG22	1.70	0.73
8:H:2:LEU:HD23	8:H:3:THR:N	2.02	0.73
1:A:1278:U:H5'	1:A:1279:A:H5'	1.69	0.73
2:B:24:TRP:CZ3	2:B:26:PRO:HA	2.23	0.73
7:G:16:LEU:HD21	9:I:45:ALA:HB2	1.70	0.73
15:O:36:ILE:HD13	15:O:59:MET:HE3	1.69	0.73
1:A:217:C:H2'	1:A:218:C:H6	1.53	0.73
1:A:411:A:H62	1:A:413:G:H21	1.33	0.73
4:D:64:LEU:HD23	4:D:198:VAL:HG21	1.68	0.73
1:A:337:C:H2'	1:A:338:A:H8	1.54	0.72
10:J:19:SER:HB2	10:J:91:PRO:HG2	1.71	0.72
1:A:1376:U:OP1	7:G:98:SER:OG	2.06	0.72
1:A:190(E):U:O2'	17:Q:63:ARG:NH2	2.23	0.72
2:B:157:ARG:HG3	2:B:158:LEU:HD12	1.71	0.72
3:C:150:LYS:HB3	3:C:201:TYR:HB2	1.69	0.72
14:N:47:LEU:HB3	14:N:53:LEU:HD21	1.70	0.72
2:B:73:THR:HG21	2:B:96:ARG:HD3	1.72	0.72
1:A:1128:C:O2'	1:A:1130:A:N7	2.23	0.72
1:A:1366:C:O2'	10:J:60:ARG:NH2	2.21	0.72
4:D:78:LEU:HD21	4:D:96:LEU:HB3	1.72	0.72
1:A:84:U:H2'	1:A:88:A:H8	1.55	0.71
1:A:918:A:H2'	1:A:919:A:C8	2.25	0.71
1:A:1441:G:H5''	1:A:1442:G:H5'	1.72	0.71
15:O:74:ASP:HB2	15:O:77:ARG:HH21	1.53	0.71
10:J:61:GLU:HA	24:J:303:HOH:O	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:27:LEU:O	12:L:29:GLY:N	2.23	0.71
7:G:70:LYS:O	7:G:72:ARG:NH1	2.23	0.71
9:I:24:GLY:HA3	9:I:56:LEU:HD23	1.72	0.71
1:A:1300:G:OP2	1:A:1335:C:N4	2.24	0.71
2:B:98:LEU:HB2	2:B:101:MET:HG3	1.72	0.71
1:A:262:A:H5'	20:T:74:LYS:HD3	1.73	0.71
12:L:9:GLN:HA	12:L:12:ARG:HG3	1.73	0.71
13:M:4:ILE:HG23	13:M:57:ARG:HA	1.74	0.70
17:Q:40:LYS:HD3	17:Q:42:TYR:CZ	2.26	0.70
1:A:390:C:O3'	16:P:28:ARG:NH2	2.25	0.70
1:A:1143:G:H2'	1:A:1144:G:H8	1.55	0.70
1:A:184:G:H2'	1:A:185:A:H8	1.54	0.70
15:O:6:GLU:N	15:O:6:GLU:OE2	2.25	0.70
20:T:83:ARG:NH2	24:T:203:HOH:O	2.25	0.70
1:A:935:A:N6	7:G:3:ARG:HG3	2.07	0.69
12:L:83:VAL:HG23	12:L:107:ALA:HB2	1.75	0.69
14:N:24:CYS:HB2	14:N:39:LEU:HA	1.74	0.69
1:A:839:U:H5'	1:A:840:C:C5	2.27	0.69
1:A:946:A:H2'	1:A:947:G:C8	2.27	0.69
1:A:1225:A:H2'	1:A:1225:A:N3	2.07	0.69
2:B:167:PRO:HG2	2:B:192:SER:HB2	1.74	0.69
1:A:1347:G:O2'	1:A:1348:U:OP2	2.07	0.69
2:B:178:ARG:NH1	2:B:198:ASP:OD2	2.23	0.69
1:A:337:C:H2'	1:A:338:A:C8	2.28	0.69
1:A:584:G:OP2	17:Q:87:LYS:NZ	2.17	0.69
1:A:1347:G:H3'	9:I:108:VAL:O	1.92	0.69
5:E:100:VAL:HG12	5:E:118:ILE:HG22	1.73	0.69
6:F:42:GLU:OE1	6:F:59:TYR:OH	2.11	0.69
1:A:411:A:H62	1:A:413:G:N2	1.91	0.69
3:C:36:ASP:HA	3:C:39:ILE:HD12	1.75	0.69
12:L:57:LYS:HD3	12:L:67:THR:HG23	1.74	0.69
3:C:130:VAL:HG12	3:C:134:ILE:HD11	1.76	0.68
1:A:250:A:H4'	1:A:251:G:O5'	1.92	0.68
11:K:120:ARG:HH11	11:K:120:ARG:HG2	1.57	0.68
1:A:1498:UR3:O4'	1:A:1519[A]:MA6:H2	1.94	0.68
4:D:163:GLU:HG2	4:D:166:LYS:HE3	1.75	0.68
8:H:82:HIS:HD1	8:H:138:TRP:NE1	1.92	0.68
9:I:42:ARG:NH2	9:I:71:SER:OG	2.26	0.68
5:E:75:THR:OG1	5:E:76:ILE:N	2.25	0.68
1:A:962:C:O2'	24:A:2118:HOH:O	2.11	0.68
1:A:113:G:H1'	1:A:354:G:H5'	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:57:ARG:HG3	4:D:202:LEU:HD13	1.74	0.68
8:H:36:LEU:HA	8:H:39:LEU:HD12	1.75	0.68
1:A:1133:G:H1	1:A:1141:C:H42	1.41	0.67
3:C:137:ALA:HA	3:C:140:ARG:HD2	1.76	0.67
1:A:933:G:O6	7:G:3:ARG:NH2	2.27	0.67
1:A:1347:G:N2	1:A:1373:G:H2'	2.10	0.67
2:B:178:ARG:HD3	2:B:196:LEU:HD22	1.76	0.67
1:A:1474:G:H2'	1:A:1475:G:H8	1.60	0.67
1:A:129(A):G:N3	1:A:190(E):U:H5''	2.10	0.67
3:C:58:GLU:HB3	10:J:92:THR:HG21	1.76	0.67
10:J:50:ILE:HD12	10:J:50:ILE:H	1.59	0.67
1:A:551:U:O2'	12:L:86:ARG:HD2	1.95	0.67
1:A:1124:G:N2	1:A:1126:U:O4	2.28	0.67
2:B:60:ASP:O	2:B:64:ARG:NH1	2.28	0.67
1:A:1065:U:H5''	1:A:1190:G:N2	2.10	0.66
1:A:1305:G:N2	1:A:1331:G:H1'	2.10	0.66
1:A:36:C:OP1	12:L:123:LYS:NZ	2.29	0.66
1:A:401:C:O2'	1:A:621:A:N3	2.23	0.66
1:A:1029:C:N3	1:A:1033:G:N2	2.44	0.66
3:C:42:LEU:HD12	3:C:94:LEU:HD13	1.76	0.66
5:E:109:ILE:HG22	5:E:110:LEU:HD23	1.78	0.66
1:A:633:G:H2'	1:A:634:C:C6	2.31	0.66
8:H:6:ILE:HB	8:H:85:ARG:NH2	2.11	0.66
10:J:6:ILE:HB	10:J:72:VAL:HB	1.75	0.66
13:M:117:VAL:HG12	13:M:118:ALA:H	1.61	0.66
1:A:1310:G:OP1	13:M:77:ASN:ND2	2.27	0.66
1:A:1250:A:H2'	1:A:1251:A:C8	2.30	0.66
3:C:152:ILE:HB	3:C:199:LYS:HB2	1.78	0.66
1:A:664:G:H22	1:A:741:G:H1	1.43	0.66
1:A:957:U:O2'	1:A:959:A:N7	2.27	0.66
1:A:1267:C:N3	1:A:1327:C:O2'	2.29	0.66
1:A:1504:G:OP1	1:A:1507:A:H4'	1.96	0.66
4:D:3:ARG:HH22	4:D:100:ARG:NH2	1.94	0.66
11:K:18:ARG:HG3	11:K:33:THR:HG23	1.78	0.66
9:I:89:ASN:O	9:I:92:TYR:HB2	1.96	0.66
13:M:4:ILE:HD13	13:M:56:LEU:HB3	1.77	0.65
15:O:26:GLU:HA	15:O:81:LEU:HD11	1.78	0.65
1:A:1028:C:H42	1:A:1033:G:H22	1.42	0.65
1:A:1241:G:H2'	1:A:1242:C:H6	1.61	0.65
7:G:108:ALA:O	7:G:119:ARG:HB3	1.96	0.65
19:S:11:VAL:HG12	19:S:15:LEU:HD11	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1300:G:O2'	1:A:1301:U:P	2.55	0.65
8:H:51:VAL:HG11	8:H:60:ARG:HG3	1.78	0.65
1:A:99:C:H2'	1:A:101:A:C8	2.31	0.65
2:B:240:GLN:N	2:B:240:GLN:OE1	2.30	0.65
6:F:80:ARG:NH2	6:F:88:VAL:O	2.30	0.65
5:E:122:GLU:O	5:E:126:ARG:NH1	2.29	0.65
16:P:2:VAL:O	16:P:64:ALA:HA	1.97	0.65
1:A:707:C:H4'	11:K:20:TYR:CD1	2.31	0.64
1:A:767:A:H2'	1:A:768:A:O4'	1.97	0.64
14:N:6:LEU:HD12	14:N:23:ARG:HH21	1.63	0.64
14:N:23:ARG:HA	14:N:29:ARG:O	1.96	0.64
1:A:992:U:O2'	1:A:993:G:OP2	2.11	0.64
3:C:167:TRP:HE3	3:C:168:ALA:H	1.46	0.64
11:K:33:THR:HB	11:K:39:PRO:HA	1.78	0.64
8:H:10:LEU:HD22	8:H:83:ILE:HD13	1.79	0.64
12:L:27:LEU:C	12:L:29:GLY:H	2.06	0.64
1:A:1391:U:H2'	1:A:1392:G:C8	2.33	0.64
3:C:150:LYS:HG3	3:C:169:ALA:HB2	1.78	0.64
8:H:120:THR:HG23	8:H:123:GLU:CD	2.23	0.64
9:I:3:GLN:OE1	9:I:20:ARG:NH2	2.30	0.64
10:J:48:THR:HA	10:J:62:HIS:HB3	1.79	0.64
1:A:1347:G:HO2'	1:A:1373:G:H1	1.44	0.64
2:B:24:TRP:HZ3	2:B:29:ALA:HB2	1.63	0.64
1:A:1198:G:H2'	1:A:1199:U:C6	2.33	0.64
1:A:1520[A]:G:H2'	1:A:1521:G:H8	1.63	0.64
4:D:8:VAL:O	4:D:11:LEU:N	2.29	0.64
4:D:13:ARG:HD2	4:D:38:TYR:O	1.98	0.64
7:G:27:ILE:HA	7:G:30:ILE:HD12	1.79	0.64
8:H:17:THR:HB	8:H:78:GLN:HE22	1.63	0.64
1:A:427:U:OP1	4:D:13:ARG:NH2	2.30	0.64
1:A:1301:U:O2'	1:A:1302:U:O5'	2.12	0.64
1:A:1343:G:H1'	9:I:121:ARG:HH12	1.63	0.64
9:I:20:ARG:HH11	9:I:20:ARG:HB2	1.62	0.64
17:Q:29:HIS:CG	17:Q:30:PRO:HD2	2.32	0.64
20:T:70:SER:HA	20:T:73:HIS:CD2	2.32	0.64
1:A:81:U:H6	1:A:83:U:OP2	1.81	0.64
11:K:84:VAL:HG11	11:K:91:ARG:HD3	1.80	0.64
13:M:115:LYS:H	13:M:115:LYS:HD3	1.63	0.64
1:A:748:C:H4'	1:A:749:C:O5'	1.98	0.63
13:M:34:LEU:HD13	13:M:39:ILE:HD13	1.79	0.63
1:A:839:U:H5'	1:A:840:C:H5	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:85:ILE:CG2	12:L:98:TYR:HB3	2.28	0.63
13:M:14:ARG:HE	13:M:42:ALA:HA	1.62	0.63
1:A:329:A:H5''	24:A:2232:HOH:O	1.98	0.63
3:C:88:ARG:HA	3:C:91:LEU:HD22	1.81	0.63
2:B:69:LEU:HD12	2:B:155:LEU:HD11	1.81	0.63
6:F:95:GLU:HG3	6:F:96:PRO:HD2	1.79	0.63
15:O:26:GLU:OE1	15:O:77:ARG:HD2	1.98	0.63
6:F:70:ASP:OD1	6:F:70:ASP:N	2.32	0.63
1:A:673:G:H2'	1:A:674:G:C8	2.33	0.63
1:A:1300:G:H4'	1:A:1301:U:H5'	1.80	0.63
3:C:26:LYS:H	3:C:26:LYS:HD2	1.62	0.63
1:A:217:C:H2'	1:A:218:C:C6	2.33	0.63
1:A:512:U:O2	1:A:540:G:N2	2.31	0.63
7:G:152:ALA:O	7:G:155:ARG:HG2	1.99	0.63
1:A:1379:G:OP2	7:G:6:ARG:NH2	2.31	0.63
2:B:7:VAL:HG21	2:B:221:LEU:HD23	1.81	0.63
2:B:142:LEU:HD13	2:B:146:GLN:NE2	2.14	0.63
3:C:179:ARG:HG3	3:C:179:ARG:HH11	1.64	0.63
1:A:130:A:H1'	1:A:263:A:O2'	1.99	0.62
16:P:21:VAL:O	16:P:33:ILE:HG12	1.99	0.62
3:C:156:ARG:NE	3:C:160:ALA:O	2.28	0.62
1:A:1119:C:H42	1:A:1154:G:H1	1.47	0.62
2:B:97:TRP:CH2	2:B:101:MET:HB2	2.35	0.62
1:A:166:G:H5''	1:A:167:G:OP2	1.98	0.62
4:D:25:ARG:HH21	4:D:30:LYS:HD3	1.64	0.62
20:T:27:LYS:HA	20:T:30:LYS:HE3	1.80	0.62
4:D:68:TYR:CE2	4:D:97:LEU:HB3	2.33	0.62
1:A:951:G:OP2	13:M:102:ARG:NH1	2.33	0.62
1:A:1505:G:C8	1:A:1505:G:H3'	2.34	0.62
4:D:22:LYS:HB2	4:D:26:CYS:SG	2.40	0.62
1:A:1225:A:H5'	1:A:1226:C:OP2	1.99	0.62
1:A:1435:G:H2'	1:A:1436:U:H6	1.62	0.62
2:B:167:PRO:HG2	2:B:192:SER:CB	2.30	0.62
4:D:55:ALA:O	4:D:59:ARG:HG2	1.99	0.62
18:R:40:LEU:HD11	18:R:69:THR:HG22	1.80	0.62
1:A:1158:C:N3	1:A:1181:G:N2	2.43	0.62
3:C:179:ARG:HD3	3:C:206:GLU:HG3	1.82	0.62
6:F:99:ALA:HB2	18:R:31:LEU:HD12	1.82	0.62
1:A:77:G:H2'	1:A:78:G:H8	1.65	0.61
6:F:6:VAL:HG13	6:F:90:VAL:HG22	1.82	0.61
1:A:1347:G:O2'	1:A:1348:U:P	2.58	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:TRP:HH2	2:B:102:LEU:HD22	1.65	0.61
1:A:949:A:OP1	13:M:101:GLN:HB3	2.00	0.61
3:C:131:ARG:HA	3:C:134:ILE:HD12	1.81	0.61
3:C:180:ALA:HB1	3:C:203:PHE:CE1	2.35	0.61
3:C:180:ALA:HB1	3:C:203:PHE:HE1	1.64	0.61
1:A:77:G:H2'	1:A:78:G:C8	2.34	0.61
16:P:19:ILE:HG22	16:P:36:ILE:HG13	1.82	0.61
1:A:902:G:H2'	1:A:903:G:H8	1.66	0.61
3:C:164:ARG:HG2	3:C:165:THR:H	1.64	0.61
1:A:84:U:H2'	1:A:88:A:C8	2.34	0.61
1:A:1049:U:H4'	1:A:1050:G:O5'	2.00	0.61
7:G:38:LEU:O	7:G:42:ILE:HG13	1.99	0.61
11:K:81:ASP:OD1	11:K:106:LYS:HD3	2.00	0.61
1:A:939:G:H5''	7:G:102:ARG:HH12	1.65	0.61
1:A:1414:U:H3	1:A:1486:G:H1	1.47	0.61
2:B:16:HIS:ND1	2:B:210:SER:HB2	2.15	0.61
1:A:1188:A:H5''	24:A:2229:HOH:O	1.99	0.61
10:J:5:ARG:HA	10:J:73:ASP:OD1	2.01	0.61
11:K:80:VAL:HG21	11:K:103:LEU:HD13	1.81	0.61
1:A:518:C:H1'	12:L:50:SER:HB3	1.83	0.61
1:A:973:G:H3'	1:A:974:A:H5''	1.81	0.60
1:A:1392:G:H21	1:A:1502:A:H8	1.47	0.60
8:H:127:LEU:HB3	8:H:129:VAL:HG23	1.83	0.60
1:A:129:U:O3'	1:A:129(A):G:H3'	2.01	0.60
1:A:1511:G:H2'	1:A:1512:U:O4'	2.01	0.60
5:E:105:VAL:HG11	5:E:131:ILE:HG22	1.83	0.60
1:A:5:U:H4'	1:A:6:G:O5'	2.01	0.60
1:A:1087:G:N2	1:A:1099:G:H1'	2.17	0.60
1:A:1213:A:N6	1:A:1215:G:N3	2.49	0.60
1:A:1356:G:H2'	1:A:1357:A:C8	2.37	0.60
8:H:4:ASP:OD2	8:H:85:ARG:NH1	2.34	0.60
19:S:33:THR:HG22	19:S:35:SER:H	1.65	0.60
1:A:970:C:OP1	10:J:57:LYS:NZ	2.34	0.60
6:F:80:ARG:HH12	6:F:88:VAL:H	1.49	0.60
16:P:74:LEU:O	16:P:79:VAL:HG23	2.00	0.60
8:H:114:THR:HG22	8:H:130:GLY:O	2.02	0.60
9:I:26:VAL:HG13	9:I:61:ALA:HB3	1.82	0.60
1:A:954:G:N2	1:A:1228:C:N3	2.50	0.60
9:I:111:ARG:NH1	9:I:112:LYS:O	2.35	0.60
1:A:413:G:H2'	1:A:428:G:N2	2.17	0.60
1:A:1218:C:H2'	1:A:1219:U:C6	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:U:H2'	1:A:83:U:OP2	2.01	0.60
1:A:916:G:H2'	1:A:917:G:H8	1.65	0.60
1:A:1342:C:H2'	1:A:1343:G:C8	2.36	0.60
1:A:1379:G:N7	7:G:2:ALA:HB3	2.17	0.60
4:D:3:ARG:CG	4:D:118:ARG:HH11	2.13	0.60
5:E:74:GLY:HA3	5:E:116:THR:HG22	1.84	0.60
9:I:50:LEU:HB3	9:I:55:ALA:HB3	1.83	0.60
9:I:118:LYS:O	9:I:120:ARG:N	2.32	0.60
1:A:264:U:H2'	1:A:265:G:O4'	2.02	0.60
1:A:1366:C:HO2'	10:J:60:ARG:HH22	1.47	0.60
1:A:1498:UR3:O2'	1:A:1499:A:OP2	2.10	0.60
6:F:50:TYR:HE1	18:R:77:GLY:HA2	1.67	0.60
1:A:1227:A:O3'	13:M:115:LYS:HE2	2.02	0.59
1:A:1301:U:HO2'	1:A:1302:U:P	2.25	0.59
16:P:74:LEU:HB3	16:P:79:VAL:HG21	1.84	0.59
1:A:19:C:H2'	1:A:20:G:H8	1.67	0.59
10:J:7:LYS:HG3	10:J:71:LEU:HD13	1.83	0.59
1:A:707:C:H2'	1:A:708:C:C6	2.37	0.59
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.38	0.59
1:A:1070:U:H2'	1:A:1071:C:H6	1.68	0.59
1:A:946:A:H2'	1:A:947:G:H8	1.67	0.59
12:L:46:LYS:HG2	12:L:47:LYS:HG2	1.84	0.59
1:A:1076:C:OP1	2:B:179:LYS:NZ	2.36	0.59
1:A:1300:G:O2'	1:A:1301:U:OP2	2.18	0.59
1:A:1399:C:H4'	1:A:1400:5MC:H5''	1.83	0.59
2:B:124:SER:HB2	2:B:126:GLU:HB2	1.84	0.59
15:O:4:THR:H	15:O:7:GLU:CD	2.10	0.59
15:O:56:LEU:O	15:O:60:VAL:HG23	2.03	0.59
1:A:665:A:H1'	1:A:733:A:O4'	2.02	0.59
1:A:1414:U:H2'	1:A:1415:G:C8	2.37	0.59
1:A:1520[B]:G:H2'	1:A:1521:G:H8	1.67	0.59
11:K:92:GLU:HB3	11:K:96:ARG:HH21	1.66	0.59
1:A:1125:U:OP2	1:A:1145:C:N4	2.35	0.59
7:G:139:GLU:O	7:G:143:ARG:HB2	2.03	0.59
8:H:97:VAL:HG23	8:H:129:VAL:O	2.03	0.59
1:A:935:A:H61	7:G:3:ARG:HG3	1.68	0.59
1:A:939:G:H5''	7:G:102:ARG:NH1	2.18	0.59
1:A:1349:A:OP1	9:I:120:ARG:HB2	2.03	0.59
1:A:1490:C:H5'	1:A:1491:G:OP2	2.02	0.59
9:I:50:LEU:HD11	9:I:81:ILE:HD13	1.84	0.59
13:M:96:LEU:HB3	13:M:97:PRO:HD2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:59:SER:H	18:R:62:GLU:HB2	1.68	0.59
1:A:1342:C:H2'	1:A:1343:G:H8	1.67	0.58
20:T:20:LEU:O	20:T:23:ARG:HB3	2.03	0.58
1:A:928:G:H1	1:A:1389:C:H42	1.51	0.58
1:A:1510:U:H2'	1:A:1511:G:C8	2.37	0.58
2:B:25:ASN:O	2:B:27:LYS:N	2.35	0.58
12:L:53:ARG:HH11	12:L:93:LEU:HD21	1.69	0.58
1:A:1070:U:H2'	1:A:1071:C:C6	2.38	0.58
1:A:1488:G:H2'	1:A:1489:G:H8	1.69	0.58
2:B:187:LEU:HA	2:B:201:ILE:HG13	1.83	0.58
8:H:25:ASP:N	8:H:25:ASP:OD1	2.35	0.58
1:A:112:G:O2'	1:A:113:G:H5'	2.04	0.58
1:A:1143:G:H2'	1:A:1144:G:C8	2.38	0.58
9:I:86:VAL:HG21	9:I:102:LEU:HD11	1.86	0.58
1:A:836:G:C6	1:A:851:G:C6	2.92	0.58
1:A:1195:C:H3'	1:A:1196:U:C5'	2.32	0.58
4:D:3:ARG:HG2	4:D:118:ARG:HH11	1.68	0.58
1:A:952:U:H2'	1:A:953:G:H8	1.67	0.58
15:O:85:LEU:N	15:O:85:LEU:HD23	2.18	0.58
15:O:87:ILE:HG22	15:O:88:ARG:HD3	1.84	0.58
1:A:281:G:O2'	1:A:282:A:OP2	2.15	0.58
1:A:527:7MG:C8	1:A:527:7MG:H5''	2.38	0.58
1:A:1488:G:H2'	1:A:1489:G:C8	2.39	0.58
14:N:26:ARG:HD3	14:N:47:LEU:HD21	1.86	0.58
5:E:98:THR:N	5:E:117:ASP:OD1	2.36	0.58
1:A:656:C:O2'	15:O:28:GLN:NE2	2.31	0.58
11:K:43:SER:HA	11:K:47:VAL:HG21	1.85	0.58
1:A:411:A:N7	1:A:413:G:N3	2.51	0.57
1:A:1497:G:C2'	1:A:1498:UR3:H5'	2.35	0.57
1:A:1145:C:O2'	1:A:1146:A:O5'	2.22	0.57
1:A:1305:G:H22	1:A:1331:G:H1'	1.69	0.57
15:O:18:PHE:CE2	15:O:21:ASP:HB2	2.39	0.57
1:A:1326:C:OP1	21:U:12:LYS:NZ	2.33	0.57
10:J:3:LYS:N	10:J:75:ILE:HG23	2.19	0.57
10:J:52:GLY:O	14:N:41:ARG:NH2	2.37	0.57
11:K:27:ASN:OD1	11:K:28:THR:N	2.33	0.57
1:A:1452:C:H4'	1:A:1453:G:O5'	2.05	0.57
17:Q:62:SER:OG	17:Q:72:ARG:HG2	2.05	0.57
1:A:1441:G:O2'	1:A:1442:G:N2	2.38	0.57
1:A:1497:G:H2'	1:A:1498:UR3:H5'	1.86	0.57
12:L:24:VAL:HG13	12:L:98:TYR:CE2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:11:VAL:HG21	15:O:34:LEU:HD12	1.87	0.57
1:A:411:A:C8	1:A:413:G:H1'	2.39	0.57
3:C:174:PRO:O	3:C:177:THR:HG22	2.05	0.57
13:M:79:LYS:HA	13:M:82:MET:HE2	1.86	0.57
1:A:448:A:P	1:A:485:G:H22	2.27	0.57
1:A:576:G:N2	24:A:2214:HOH:O	2.38	0.57
1:A:757:U:H2'	1:A:758:G:O4'	2.04	0.57
3:C:47:LEU:HD22	3:C:52:LEU:HD13	1.87	0.57
5:E:93:PRO:HD2	8:H:105:ARG:NH2	2.19	0.57
12:L:19:ARG:HA	12:L:20:LYS:NZ	2.19	0.57
1:A:1192:C:O2	5:E:25:ARG:NH2	2.38	0.57
1:A:80:G:H3'	1:A:81:U:H5''	1.86	0.57
1:A:1299:A:O2'	1:A:1300:G:O5'	2.20	0.57
3:C:141:VAL:HG11	3:C:202:ILE:HD12	1.87	0.57
12:L:36:VAL:O	12:L:58:VAL:HG13	2.05	0.57
1:A:1371:G:O3'	9:I:69:GLY:HA3	2.05	0.56
1:A:1412:C:H2'	1:A:1413:A:C8	2.40	0.56
1:A:1366:C:H2'	1:A:1367:C:H6	1.70	0.56
6:F:27:GLN:O	6:F:31:GLU:HG3	2.04	0.56
16:P:19:ILE:HD12	16:P:38:TYR:N	2.20	0.56
1:A:76:C:H42	1:A:95:U:H3	1.53	0.56
1:A:164:U:H2'	1:A:165:C:C6	2.40	0.56
1:A:1248:A:H2'	1:A:1249:C:H6	1.70	0.56
1:A:1391:U:H2'	1:A:1392:G:H8	1.71	0.56
1:A:1465:C:H2'	1:A:1466:C:O4'	2.05	0.56
9:I:118:LYS:O	9:I:118:LYS:HD3	2.05	0.56
10:J:24:VAL:HG13	10:J:34:VAL:HG11	1.87	0.56
10:J:51:ARG:HG3	10:J:59:SER:O	2.05	0.56
12:L:97:ARG:HB2	12:L:98:TYR:CE1	2.40	0.56
20:T:63:ILE:HG21	20:T:81:LYS:HG3	1.86	0.56
1:A:372:C:H4'	1:A:373:A:O5'	2.05	0.56
1:A:445:G:H2'	1:A:446:G:H8	1.70	0.56
1:A:859:A:OP2	1:A:869:G:N1	2.30	0.56
2:B:88:ALA:HB2	2:B:219:VAL:HG13	1.86	0.56
1:A:129(A):G:C2	1:A:190(E):U:H5''	2.39	0.56
1:A:309:G:H2'	1:A:310:G:H8	1.70	0.56
1:A:1413:A:H2	1:A:1487:G:H22	1.52	0.56
9:I:17:VAL:HG21	9:I:80:GLY:HA3	1.87	0.56
1:A:392:G:H2'	1:A:393:A:C8	2.41	0.56
1:A:908:A:C2	1:A:909:A:C4	2.93	0.56
1:A:949:A:N6	24:A:2221:HOH:O	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1392:G:N2	1:A:1502:A:H8	2.02	0.56
3:C:91:LEU:HD21	3:C:99:VAL:HG22	1.88	0.56
4:D:65:ARG:HG3	4:D:75:PHE:CD1	2.41	0.56
11:K:121:PRO:HG2	11:K:126:ARG:HG3	1.88	0.56
1:A:512:U:OP1	4:D:46:LYS:NZ	2.39	0.56
4:D:79:PHE:O	4:D:82:ALA:N	2.38	0.56
5:E:122:GLU:C	5:E:123:LEU:HD23	2.31	0.56
3:C:116:VAL:O	3:C:120:VAL:HG23	2.06	0.56
15:O:15:PHE:CE2	15:O:85:LEU:HD21	2.41	0.56
17:Q:59:ILE:HG23	17:Q:71:PHE:HB3	1.88	0.56
1:A:1004:A:HO2'	1:A:1005:A:P	2.28	0.56
1:A:1369:C:H2'	1:A:1370:G:C8	2.41	0.56
1:A:1474:G:H2'	1:A:1475:G:C8	2.41	0.56
2:B:21:ARG:HA	2:B:39:ILE:HA	1.88	0.56
5:E:87:SER:HB3	5:E:131:ILE:HD13	1.88	0.56
7:G:16:LEU:HD12	9:I:44:VAL:HB	1.87	0.56
21:U:12:LYS:HB3	21:U:22:ARG:HD3	1.88	0.56
1:A:627:G:H2'	1:A:628:G:H8	1.70	0.55
1:A:1148:U:H2'	1:A:1149:C:O4'	2.06	0.55
15:O:39:LEU:HD13	15:O:56:LEU:HB2	1.87	0.55
6:F:69:GLU:CD	6:F:69:GLU:H	2.13	0.55
1:A:968:A:C8	1:A:1062:U:H4'	2.41	0.55
1:A:975:A:H5'	1:A:975:A:H8	1.70	0.55
5:E:84:PHE:C	5:E:84:PHE:CD2	2.84	0.55
7:G:152:ALA:HA	7:G:155:ARG:HE	1.71	0.55
1:A:519:C:H2'	1:A:520:A:C8	2.41	0.55
5:E:33:VAL:HG11	5:E:109:ILE:HA	1.89	0.55
8:H:38:ILE:HG13	8:H:41:ARG:HH12	1.70	0.55
12:L:24:VAL:HG13	12:L:98:TYR:HE2	1.70	0.55
1:A:824:C:H2'	1:A:825:G:H8	1.72	0.55
1:A:1206:G:O2'	3:C:192:THR:O	2.24	0.55
1:A:130:A:H5'	17:Q:63:ARG:NE	2.20	0.55
1:A:1425:U:H2'	1:A:1426:C:H6	1.70	0.55
1:A:1197:G:H5''	24:A:2044:HOH:O	2.06	0.55
5:E:118:ILE:HG12	5:E:119:LEU:N	2.22	0.55
10:J:78:ASN:N	10:J:78:ASN:OD1	2.38	0.55
16:P:18:ARG:O	16:P:20:VAL:HG23	2.06	0.55
20:T:50:GLU:HA	20:T:100:ILE:HG13	1.88	0.55
1:A:91:C:H2'	1:A:92:C:C6	2.42	0.55
1:A:976:G:OP2	1:A:1358:U:H1'	2.07	0.55
3:C:6:HIS:NE2	3:C:8:ILE:HB	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:20:TYR:CE1	8:H:76:PRO:HG2	2.42	0.55
11:K:124:LYS:HG3	11:K:125:PHE:CD1	2.42	0.55
17:Q:26:GLN:HG2	17:Q:37:LYS:HB2	1.88	0.55
1:A:501:C:H2'	1:A:502:G:H8	1.71	0.55
1:A:627:G:H2'	1:A:628:G:C8	2.41	0.55
2:B:48:MET:HA	2:B:51:LEU:HB2	1.89	0.55
2:B:142:LEU:HD13	2:B:146:GLN:HE22	1.72	0.55
18:R:22:VAL:HG23	18:R:56:THR:HA	1.88	0.55
1:A:1130:A:H4'	9:I:3:GLN:HE22	1.72	0.55
1:A:1137:C:H5''	1:A:1138:G:OP1	2.07	0.55
1:A:1367:C:H5'	10:J:60:ARG:CZ	2.37	0.55
1:A:1411:C:H2'	1:A:1412:C:H6	1.72	0.55
1:A:1425:U:H2'	1:A:1426:C:C6	2.42	0.55
3:C:20:SER:O	14:N:54:PRO:HB3	2.06	0.54
14:N:40:CYS:O	14:N:44:LEU:N	2.30	0.54
17:Q:9:VAL:HB	17:Q:56:VAL:HG22	1.88	0.54
1:A:131:C:H2'	1:A:132:C:C6	2.42	0.54
3:C:130:VAL:HG21	3:C:157:ILE:HG23	1.87	0.54
1:A:230:G:H2'	1:A:231:G:O4'	2.07	0.54
1:A:737:A:H2'	1:A:738:C:C6	2.43	0.54
1:A:1358:U:H5''	14:N:35:ARG:HD3	1.88	0.54
1:A:913:A:H4'	1:A:914:A:O5'	2.06	0.54
1:A:254:G:H2'	1:A:255:G:C8	2.42	0.54
1:A:316:G:OP2	1:A:351:G:O2'	2.25	0.54
1:A:1338:G:H2'	1:A:1339:A:H8	1.63	0.54
3:C:87:LEU:O	3:C:91:LEU:HB3	2.06	0.54
3:C:182:ILE:HG12	3:C:203:PHE:HB2	1.89	0.54
16:P:79:VAL:N	24:P:210:HOH:O	2.39	0.54
19:S:27:GLU:CD	19:S:27:GLU:H	2.16	0.54
12:L:39:VAL:HG12	12:L:41:ARG:HG3	1.90	0.54
1:A:881:G:H2'	1:A:882:C:O4'	2.07	0.54
10:J:49:VAL:O	10:J:61:GLU:N	2.38	0.54
11:K:85:ARG:HG2	11:K:113:PRO:HD3	1.90	0.54
1:A:411:A:C5	1:A:413:G:H1'	2.42	0.54
1:A:686:U:HO2'	1:A:687:A:H8	1.55	0.54
1:A:830:G:N2	1:A:857:C:C2	2.76	0.54
1:A:936:C:H2'	1:A:937:A:O4'	2.08	0.54
2:B:97:TRP:CZ3	2:B:101:MET:HB2	2.43	0.54
9:I:8:GLY:HA2	9:I:79:LEU:HD13	1.90	0.54
15:O:70:LEU:HD13	15:O:78:TYR:HA	1.89	0.54
6:F:10:LEU:HD23	6:F:85:VAL:HG22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:74:ARG:HB3	18:R:81:PHE:CE1	2.43	0.54
9:I:8:GLY:HA3	9:I:79:LEU:HB3	1.90	0.54
13:M:23:TYR:HE2	13:M:70:LEU:HD22	1.72	0.54
1:A:1250:A:H4'	9:I:68:GLY:N	2.23	0.53
2:B:201:ILE:HD12	2:B:214:ILE:HG21	1.90	0.53
4:D:61:LYS:HE3	4:D:206:PHE:CE2	2.43	0.53
6:F:44:GLY:HA2	6:F:59:TYR:CE2	2.43	0.53
9:I:23:ASN:HB3	9:I:25:LYS:HG2	1.90	0.53
13:M:23:TYR:CE2	13:M:70:LEU:HD22	2.43	0.53
14:N:39:LEU:HD22	14:N:43:CYS:HB3	1.90	0.53
16:P:4:ILE:HG12	16:P:21:VAL:HG22	1.90	0.53
1:A:47:C:C6	1:A:365:U:H2'	2.44	0.53
1:A:781:A:C4	1:A:802:A:C2	2.97	0.53
1:A:1441:G:HO2'	1:A:1442:G:N2	2.06	0.53
1:A:1499:A:H1'	1:A:1520[A]:G:H5'	1.91	0.53
10:J:55:LYS:HB2	10:J:55:LYS:NZ	2.23	0.53
10:J:99:LYS:HG2	10:J:100:THR:H	1.73	0.53
1:A:253:U:H2'	1:A:254:G:H8	1.72	0.53
1:A:840:C:H5''	1:A:841:U:OP1	2.09	0.53
1:A:1001:A:H2'	1:A:1002:G:C8	2.42	0.53
1:A:80:G:C2'	1:A:81:U:OP1	2.57	0.53
1:A:372:C:H1'	1:A:373:A:OP2	2.08	0.53
5:E:7:GLU:HB2	5:E:112:LEU:HD11	1.90	0.53
10:J:42:THR:HG23	10:J:67:THR:O	2.09	0.53
12:L:31:PRO:HB2	12:L:32:PHE:CD2	2.44	0.53
1:A:109:A:H2'	1:A:326:G:N2	2.23	0.53
1:A:324:G:OP1	20:T:22:ARG:NH1	2.41	0.53
1:A:459:G:H1'	1:A:463:A:H61	1.74	0.53
1:A:620:C:H2'	1:A:621:A:O4'	2.07	0.53
3:C:35:GLU:O	3:C:39:ILE:HG13	2.07	0.53
5:E:89:ILE:HD11	5:E:120:THR:HG23	1.90	0.53
16:P:53:VAL:O	16:P:56:ALA:N	2.42	0.53
17:Q:29:HIS:ND1	17:Q:30:PRO:HD2	2.24	0.53
1:A:580:U:H2'	1:A:581:G:O4'	2.08	0.53
1:A:934:C:H42	1:A:938:A:H61	1.56	0.53
9:I:126:SER:OG	9:I:127:LYS:N	2.39	0.53
11:K:92:GLU:HB3	11:K:96:ARG:NH2	2.23	0.53
15:O:36:ILE:HD12	15:O:60:VAL:HG22	1.89	0.53
1:A:80:G:H2'	1:A:81:U:OP1	2.08	0.53
1:A:527:7MG:H5''	1:A:527:7MG:H81	1.91	0.53
1:A:582:U:OP1	15:O:64:ARG:NH2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:750:G:H1'	15:O:23:GLY:H	1.74	0.53
1:A:1105:A:H2'	1:A:1106:G:H8	1.73	0.53
1:A:1239:A:H62	1:A:1299:A:H62	1.57	0.53
3:C:43:LEU:HA	3:C:47:LEU:HD13	1.90	0.53
1:A:299:G:H2'	1:A:300:A:C8	2.43	0.53
1:A:1028:C:N4	1:A:1033:G:H22	2.05	0.53
1:A:1120:G:H22	1:A:1154:G:H1'	1.74	0.53
2:B:9:GLU:O	2:B:10:LEU:HD23	2.09	0.53
8:H:87:SER:OG	8:H:93:VAL:N	2.32	0.53
10:J:80:LYS:H	10:J:80:LYS:HD2	1.73	0.53
1:A:392:G:H2'	1:A:393:A:H8	1.72	0.53
1:A:538:G:OP2	12:L:115:LYS:HB2	2.09	0.53
1:A:656:C:H42	1:A:750:G:H1	1.57	0.53
4:D:61:LYS:NZ	4:D:62:GLN:OE1	2.42	0.53
1:A:1269:A:N1	1:A:1312:G:O2'	2.41	0.52
3:C:150:LYS:HB2	3:C:173:VAL:HG21	1.90	0.52
5:E:95:ALA:HB1	5:E:96:PRO:HD2	1.90	0.52
12:L:27:LEU:HG	12:L:28:LYS:H	1.74	0.52
1:A:501:C:H2'	1:A:502:G:C8	2.44	0.52
2:B:139:LYS:O	2:B:143:GLU:HG2	2.10	0.52
3:C:71:ALA:HA	3:C:106:VAL:HB	1.91	0.52
1:A:653:A:OP1	8:H:56:LYS:NZ	2.36	0.52
1:A:665:A:H2'	1:A:732:C:O2	2.08	0.52
1:A:1000:U:H2'	1:A:1001:A:C8	2.45	0.52
6:F:94:GLN:HB3	18:R:32:ARG:HH11	1.75	0.52
10:J:53:PRO:HA	14:N:41:ARG:HH22	1.74	0.52
16:P:57:ARG:NE	16:P:79:VAL:O	2.27	0.52
1:A:633:G:H2'	1:A:634:C:H6	1.75	0.52
1:A:1123:A:H2'	1:A:1124:G:O4'	2.10	0.52
8:H:20:TYR:HA	8:H:65:TYR:CE2	2.45	0.52
19:S:77:THR:HG22	19:S:78:ARG:HD3	1.90	0.52
20:T:100:ILE:HG22	20:T:102:GLY:N	2.18	0.52
1:A:359:U:H2'	1:A:360:A:C8	2.45	0.52
1:A:778:G:H2'	1:A:779:C:O4'	2.10	0.52
4:D:70:ILE:HG22	4:D:71:SER:H	1.75	0.52
1:A:19:C:H2'	1:A:20:G:C8	2.44	0.52
1:A:1188:A:H4'	24:N:201:HOH:O	2.08	0.52
1:A:1393:U:O2'	1:A:1501:C:O2'	2.27	0.52
11:K:59:TYR:O	11:K:62:GLN:HB3	2.08	0.52
1:A:1123:A:H4'	10:J:37:PRO:HD2	1.92	0.52
1:A:1132:C:N4	1:A:1142:G:H1	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1347:G:O6	9:I:10:ARG:NH2	2.43	0.52
1:A:1377:A:O2'	7:G:2:ALA:N	2.38	0.52
1:A:1439:C:OP2	20:T:38:LYS:NZ	2.43	0.52
2:B:162:ILE:HD12	2:B:177:ALA:HB2	1.92	0.52
3:C:6:HIS:HD2	3:C:9:GLY:H	1.52	0.52
5:E:142:LEU:O	5:E:143:ARG:HD3	2.10	0.52
11:K:90:GLY:HA2	11:K:93:GLN:H	1.75	0.52
1:A:284:G:H2'	1:A:285:G:H8	1.74	0.52
1:A:540:G:H2'	1:A:541:G:O4'	2.10	0.52
1:A:858:G:O2'	1:A:859:A:H5''	2.10	0.52
1:A:1124:G:H3'	1:A:1145:C:H41	1.75	0.52
1:A:1255:G:N2	1:A:1259:C:O2	2.43	0.52
1:A:1407:5MC:H5'	1:A:1517[B]:G:H21	1.75	0.52
4:D:156:GLU:O	4:D:160:GLN:HB2	2.10	0.52
9:I:48:GLU:HA	9:I:51:ARG:HD3	1.91	0.52
13:M:13:LYS:O	13:M:45:VAL:HG23	2.09	0.52
1:A:955:U:H1'	1:A:1227:A:H61	1.75	0.52
1:A:1035:A:H2'	1:A:1036:G:C8	2.45	0.52
1:A:1381:U:N1	7:G:156:TRP:HH2	2.08	0.52
5:E:82:VAL:O	5:E:88:LYS:HA	2.10	0.52
5:E:84:PHE:C	5:E:84:PHE:HD2	2.17	0.52
5:E:109:ILE:HG21	5:E:135:THR:CG2	2.39	0.52
13:M:37:THR:HG23	13:M:55:ARG:HG2	1.92	0.52
1:A:665:A:H3'	1:A:725:G:N2	2.25	0.51
1:A:959:A:O2'	1:A:984:C:O2'	2.27	0.51
1:A:1037:C:H2'	1:A:1038:C:C6	2.45	0.51
3:C:190:ARG:HA	3:C:195:VAL:HG22	1.92	0.51
15:O:84:LYS:C	15:O:85:LEU:HD23	2.35	0.51
1:A:21:G:H2'	1:A:22:G:C8	2.45	0.51
1:A:254:G:H2'	1:A:255:G:H8	1.73	0.51
1:A:552:U:H2'	1:A:553:A:C8	2.46	0.51
1:A:1001:A:H2'	1:A:1002:G:H8	1.75	0.51
1:A:1056:U:H5'	3:C:163:ALA:HB2	1.91	0.51
1:A:1196:U:OP1	1:A:1197:G:H5'	2.10	0.51
1:A:1222:G:OP1	19:S:77:THR:HG21	2.10	0.51
1:A:1257:U:H4'	1:A:1258:G:O5'	2.09	0.51
8:H:114:THR:OG1	8:H:117:GLY:O	2.27	0.51
1:A:371:G:O2'	1:A:372:C:H5'	2.10	0.51
1:A:824:C:H2'	1:A:825:G:C8	2.46	0.51
1:A:833:U:H2'	1:A:834:C:H6	1.75	0.51
1:A:1129:C:OP1	9:I:62:TYR:OH	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1505:G:H3'	1:A:1505:G:H8	1.72	0.51
15:O:12:ILE:HG12	15:O:31:LEU:HD11	1.92	0.51
1:A:106:C:C2'	1:A:107:G:H5'	2.39	0.51
1:A:646:U:H2'	1:A:647:C:C6	2.45	0.51
1:A:679:C:H2'	1:A:680:C:C6	2.45	0.51
1:A:922:G:O2'	1:A:1398:A:N1	2.39	0.51
1:A:1022:G:H22	1:A:1024:G:N2	2.09	0.51
1:A:1040:U:H2'	1:A:1041:A:H8	1.76	0.51
4:D:36:ARG:HG2	4:D:38:TYR:CZ	2.45	0.51
6:F:100:ASN:HA	18:R:23:LYS:HE2	1.92	0.51
18:R:22:VAL:HG23	18:R:55:ARG:O	2.10	0.51
18:R:40:LEU:HD12	18:R:79:LEU:HD11	1.92	0.51
18:R:59:SER:N	18:R:62:GLU:OE1	2.44	0.51
1:A:247:G:OP2	17:Q:100:LYS:HB2	2.11	0.51
1:A:1201:A:H4'	1:A:1202:G:O5'	2.10	0.51
10:J:47:PHE:HB3	14:N:34:TYR:CE2	2.37	0.51
1:A:75:G:C2	1:A:96:G:C2	2.99	0.51
1:A:945:G:O6	1:A:1236:A:N1	2.43	0.51
8:H:87:SER:HG	8:H:93:VAL:H	1.54	0.51
8:H:104:ARG:CZ	8:H:138:TRP:CZ2	2.93	0.51
9:I:25:LYS:HG3	9:I:60:ASP:OD1	2.11	0.51
9:I:69:GLY:O	9:I:73:GLN:HG3	2.10	0.51
13:M:20:THR:HG22	24:M:308:HOH:O	2.10	0.51
1:A:322:C:OP2	1:A:328:C:N4	2.44	0.51
1:A:376:G:N3	1:A:389:A:C2	2.79	0.51
1:A:456:C:H2'	1:A:457:C:C6	2.46	0.51
4:D:50:ARG:HD2	4:D:51:PRO:HD2	1.92	0.51
4:D:187:ARG:NE	4:D:188:LEU:O	2.44	0.51
5:E:98:THR:HB	5:E:117:ASP:HB3	1.92	0.51
8:H:24:THR:O	8:H:60:ARG:HA	2.11	0.51
10:J:12:ASP:OD2	10:J:15:THR:HG22	2.10	0.51
1:A:143:A:H2	1:A:220:G:H22	1.57	0.51
1:A:953:G:H2'	1:A:954:G:O4'	2.11	0.51
1:A:1179:A:H2'	1:A:1180:A:O4'	2.11	0.51
1:A:1243:C:N4	1:A:1294:G:H1	2.04	0.51
1:A:17:U:H2'	1:A:18:C:C6	2.45	0.51
1:A:186:C:H5'	20:T:78:ALA:HB1	1.92	0.51
4:D:187:ARG:NH2	4:D:189:PRO:O	2.44	0.51
13:M:12:ASN:H	13:M:45:VAL:HB	1.75	0.51
1:A:653:A:O4'	8:H:56:LYS:HE2	2.11	0.51
1:A:797:C:H2'	1:A:798:G:H8	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:18:TRP:CD1	14:N:54:PRO:HA	2.46	0.51
15:O:7:GLU:O	15:O:11:VAL:HG23	2.10	0.51
16:P:15:PRO:HG2	16:P:41:PRO:HG2	1.93	0.51
1:A:602:A:H2'	1:A:603:U:O4'	2.11	0.50
1:A:1520[A]:G:H2'	1:A:1521:G:C8	2.43	0.50
20:T:53:LEU:HD22	20:T:56:MET:HE2	1.92	0.50
1:A:193:C:H4'	20:T:61:SER:HB2	1.93	0.50
1:A:755:G:H1'	8:H:1:MET:CE	2.41	0.50
1:A:1009:G:N2	1:A:1010:G:N3	2.59	0.50
1:A:1145:C:HO2'	1:A:1146:A:P	2.33	0.50
1:A:1250:A:C6	1:A:1251:A:C6	3.00	0.50
2:B:210:SER:OG	2:B:211:ILE:N	2.45	0.50
12:L:54:LYS:HD2	12:L:54:LYS:N	2.25	0.50
1:A:235:C:H5'	17:Q:70:ARG:HG2	1.94	0.50
1:A:345:C:OP2	1:A:345:C:H6	1.95	0.50
1:A:463:A:OP1	16:P:75:ARG:NH2	2.44	0.50
1:A:538:G:P	12:L:115:LYS:HB2	2.52	0.50
8:H:4:ASP:OD1	8:H:6:ILE:N	2.41	0.50
13:M:40:ASN:HB3	13:M:43:THR:HG23	1.92	0.50
1:A:826:C:H2'	1:A:827:U:H6	1.76	0.50
1:A:1339:A:H5''	1:A:1340:A:OP2	2.12	0.50
8:H:123:GLU:O	8:H:126:LYS:HG2	2.11	0.50
10:J:53:PRO:HA	14:N:41:ARG:NH2	2.26	0.50
19:S:63:THR:HG22	19:S:64:GLU:H	1.76	0.50
2:B:28:PHE:HD2	2:B:32:ILE:HD11	1.77	0.50
2:B:162:ILE:HG22	2:B:184:VAL:HG13	1.93	0.50
1:A:687:A:H4'	1:A:688:G:O5'	2.10	0.50
1:A:689:C:OP1	11:K:44:SER:OG	2.28	0.50
1:A:1343:G:H1'	9:I:121:ARG:NH1	2.26	0.50
3:C:184:TYR:HA	3:C:200:ALA:O	2.12	0.50
7:G:20:ASP:OD1	7:G:22:LEU:HB3	2.11	0.50
12:L:38:THR:HG22	12:L:39:VAL:HG23	1.93	0.50
1:A:1436:U:H2'	1:A:1437:C:H6	1.76	0.50
8:H:65:TYR:CD1	8:H:65:TYR:N	2.80	0.50
13:M:60:VAL:HG22	13:M:64:TRP:CZ3	2.45	0.50
1:A:191:G:O2'	20:T:102:GLY:O	2.16	0.50
1:A:1104:G:O5'	2:B:111:ARG:HD2	2.12	0.50
3:C:6:HIS:CD2	14:N:49:HIS:HB3	2.47	0.50
4:D:12:CYS:SG	4:D:19:LEU:O	2.70	0.50
7:G:145:ALA:C	7:G:147:ALA:H	2.19	0.50
19:S:18:LYS:O	19:S:22:LEU:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:G:H2'	1:A:23:C:C6	2.46	0.50
1:A:279:A:C6	17:Q:98:LEU:HD13	2.46	0.50
1:A:881:G:P	12:L:12:ARG:NH2	2.85	0.50
1:A:923:A:OP1	5:E:21:ALA:HB2	2.12	0.50
2:B:7:VAL:HG11	2:B:221:LEU:HD23	1.93	0.50
4:D:187:ARG:NH1	4:D:188:LEU:HD12	2.27	0.50
19:S:16:LEU:HA	19:S:19:VAL:HG12	1.94	0.50
4:D:88:VAL:HG12	4:D:90:GLY:N	2.27	0.49
6:F:10:LEU:HD12	6:F:59:TYR:HB3	1.94	0.49
1:A:253:U:H2'	1:A:254:G:C8	2.47	0.49
1:A:803:G:C6	1:A:804:U:C4	3.01	0.49
1:A:857:C:H5'	24:A:2174:HOH:O	2.11	0.49
5:E:84:PHE:O	5:E:87:SER:HB2	2.12	0.49
9:I:96:LEU:O	9:I:100:GLY:N	2.36	0.49
10:J:55:LYS:HZ2	10:J:56:HIS:N	2.10	0.49
13:M:48:LEU:HD13	13:M:53:VAL:HG23	1.93	0.49
20:T:39:LYS:HG2	20:T:55:ILE:HD13	1.93	0.49
21:U:6:ARG:HD2	21:U:15:ARG:HH12	1.76	0.49
1:A:1303:C:H2'	1:A:1304:G:H5'	1.94	0.49
1:A:1412:C:H2'	1:A:1413:A:H8	1.75	0.49
7:G:87:VAL:HG12	7:G:88:PRO:HD2	1.95	0.49
9:I:16:ARG:HB2	9:I:64:THR:HG23	1.94	0.49
13:M:62:ASN:OD1	13:M:62:ASN:N	2.44	0.49
17:Q:29:HIS:O	17:Q:33:GLY:HA2	2.11	0.49
18:R:51:LEU:HB2	18:R:56:THR:HG23	1.94	0.49
1:A:14:U:O2	1:A:16:A:C8	2.65	0.49
1:A:940:C:H2'	1:A:941:G:O4'	2.11	0.49
1:A:1064:G:N2	1:A:1190:G:H2'	2.26	0.49
13:M:37:THR:HB	13:M:39:ILE:HD11	1.93	0.49
17:Q:63:ARG:HG2	17:Q:64:PRO:HD2	1.95	0.49
20:T:92:LEU:O	20:T:96:GLY:HA2	2.12	0.49
1:A:195:A:O2'	20:T:68:LYS:NZ	2.45	0.49
1:A:426:G:OP1	4:D:38:TYR:OH	2.27	0.49
1:A:642:A:H2'	1:A:643:C:C6	2.47	0.49
1:A:665:A:H3'	1:A:725:G:H21	1.76	0.49
2:B:102:LEU:HD22	2:B:102:LEU:H	1.77	0.49
3:C:14:ILE:HG22	3:C:15:THR:HG23	1.94	0.49
5:E:97:GLY:N	5:E:117:ASP:OD1	2.45	0.49
9:I:5:TYR:HD2	9:I:18:PHE:CE2	2.30	0.49
9:I:93:ARG:HD3	9:I:97:LYS:NZ	2.27	0.49
11:K:29:ILE:HG23	11:K:44:SER:CB	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:120:ARG:HG2	11:K:120:ARG:NH1	2.21	0.49
1:A:509:A:C8	1:A:509:A:H3'	2.47	0.49
1:A:828:A:H4'	1:A:828:A:OP1	2.13	0.49
1:A:1003:G:C2	1:A:1003(A):G:C5	3.01	0.49
17:Q:95:TYR:HA	17:Q:98:LEU:HD11	1.95	0.49
1:A:807:A:OP1	15:O:48:LYS:NZ	2.46	0.49
1:A:902:G:H2'	1:A:903:G:C8	2.48	0.49
7:G:88:PRO:HG2	7:G:155:ARG:HH21	1.78	0.49
1:A:376:G:C2	1:A:389:A:C2	3.01	0.49
1:A:451:A:N6	1:A:481:G:C4	2.80	0.49
1:A:462:G:H21	16:P:82:GLN:HE21	1.61	0.49
1:A:1120:G:C2	1:A:1154:G:N3	2.81	0.49
1:A:1531:A:O5'	1:A:1531:A:H8	1.96	0.49
8:H:17:THR:O	8:H:78:GLN:NE2	2.46	0.49
1:A:1328:C:H2'	1:A:1329:A:H8	1.78	0.49
4:D:3:ARG:HH22	4:D:100:ARG:HH22	1.61	0.49
19:S:40:ILE:HD13	19:S:62:ILE:HD11	1.95	0.49
1:A:384:G:H2'	1:A:385:C:H6	1.76	0.49
1:A:1048:G:O3'	1:A:1049:U:H3'	2.13	0.49
3:C:110:ASN:ND2	3:C:140:ARG:HB3	2.28	0.49
16:P:9:PHE:N	16:P:16:HIS:O	2.42	0.49
1:A:91:C:H2'	1:A:92:C:H6	1.78	0.48
1:A:110:C:H2'	1:A:111:G:O4'	2.12	0.48
1:A:451:A:H2	1:A:480:U:C5	2.30	0.48
5:E:90:VAL:O	5:E:91:LEU:HD23	2.13	0.48
9:I:63:ILE:HG21	9:I:77:ILE:HG12	1.94	0.48
11:K:54:ARG:O	11:K:57:THR:HG22	2.12	0.48
1:A:299:G:C6	1:A:300:A:C6	3.02	0.48
1:A:533:A:O2'	1:A:535:A:OP2	2.30	0.48
1:A:636:U:H2'	1:A:637:G:C8	2.48	0.48
1:A:833:U:H2'	1:A:834:C:C6	2.48	0.48
1:A:97:G:H2'	1:A:98:U:O4'	2.13	0.48
1:A:422:C:H4'	1:A:423:G:O5'	2.12	0.48
1:A:914:A:H2'	1:A:915:A:C8	2.48	0.48
7:G:155:ARG:HA	7:G:155:ARG:HD3	1.54	0.48
11:K:17:GLY:HA2	11:K:35:PRO:HD3	1.94	0.48
17:Q:67:LYS:HA	17:Q:70:ARG:HH12	1.78	0.48
6:F:33:TYR:CD1	6:F:75:LEU:HA	2.48	0.48
7:G:88:PRO:HG2	7:G:155:ARG:NH2	2.28	0.48
10:J:45:ARG:O	10:J:64:GLU:HA	2.14	0.48
12:L:27:LEU:C	12:L:29:GLY:N	2.67	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:64:ASP:O	20:T:67:ALA:HB3	2.12	0.48
1:A:260:G:H2'	1:A:261:U:C6	2.49	0.48
1:A:411:A:C6	1:A:429:U:C4	3.01	0.48
1:A:437:U:H5''	4:D:155:LEU:HD11	1.95	0.48
1:A:736:C:H2'	1:A:737:A:C8	2.49	0.48
1:A:755:G:H1'	8:H:1:MET:HE3	1.95	0.48
1:A:1063:C:H2'	1:A:1064:G:C8	2.47	0.48
1:A:1101:A:H4'	1:A:1102:A:O5'	2.14	0.48
1:A:1347:G:H22	1:A:1374:A:P	2.37	0.48
3:C:77:ILE:HD11	3:C:103:VAL:HG21	1.96	0.48
6:F:28:ARG:HA	6:F:31:GLU:CD	2.39	0.48
7:G:40:ALA:HB3	9:I:41:VAL:HG21	1.95	0.48
8:H:17:THR:CB	8:H:78:GLN:HE22	2.25	0.48
1:A:50:A:H4'	1:A:51:A:H5'	1.94	0.48
1:A:114:U:O2'	1:A:115:G:H5'	2.14	0.48
1:A:284:G:H2'	1:A:285:G:C8	2.48	0.48
1:A:794:A:C5	1:A:795:C:C4	3.02	0.48
1:A:938:A:N6	24:A:1937:HOH:O	2.47	0.48
1:A:1499:A:H1'	1:A:1520[A]:G:OP1	2.12	0.48
1:A:1502:A:C2	1:A:1504:G:C2	3.01	0.48
2:B:64:ARG:NH1	2:B:64:ARG:HB2	2.28	0.48
1:A:250:A:O4'	1:A:252:U:C6	2.67	0.48
1:A:676:A:H1'	11:K:115:PRO:HB3	1.95	0.48
1:A:1159:U:OP1	2:B:133:LYS:NZ	2.37	0.48
1:A:1309:G:H5'	13:M:78:ILE:HD11	1.95	0.48
9:I:33:PHE:O	9:I:37:PHE:HB2	2.14	0.48
1:A:89:C:H2'	1:A:90:U:C2	2.49	0.48
1:A:279:A:H5''	1:A:281:G:H5'	1.95	0.48
1:A:960:U:H4'	1:A:961:U:C5'	2.44	0.48
1:A:1180:A:OP1	9:I:103:THR:OG1	2.25	0.48
4:D:28:SER:O	4:D:30:LYS:N	2.42	0.48
4:D:35:ARG:HD2	4:D:35:ARG:N	2.28	0.48
4:D:121:VAL:O	4:D:134:ASP:HA	2.13	0.48
5:E:138:ALA:O	5:E:141:GLN:HB2	2.14	0.48
5:E:151:LEU:HD21	8:H:79:VAL:HA	1.96	0.48
8:H:65:TYR:HA	8:H:79:VAL:HG23	1.96	0.48
9:I:9:ARG:HG2	9:I:14:VAL:HG22	1.95	0.48
12:L:28:LYS:HB3	12:L:30:ALA:HB2	1.94	0.48
1:A:77:G:C6	1:A:93:G:N1	2.82	0.48
1:A:1489:G:H2'	1:A:1490:C:C6	2.49	0.48
3:C:26:LYS:H	3:C:26:LYS:CD	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:G:C2	1:A:76:C:C2	3.02	0.48
1:A:428:G:H1'	1:A:429:U:OP2	2.14	0.48
1:A:1289:A:H2'	1:A:1290:G:H5'	1.95	0.48
1:A:1518[B]:MA6:H93	1:A:1519[B]:MA6:C2	2.44	0.48
2:B:219:VAL:O	2:B:223:ILE:HG13	2.14	0.48
3:C:10:PHE:CE2	3:C:178:LEU:HD12	2.49	0.48
5:E:35:GLY:HA3	5:E:112:LEU:HD12	1.96	0.48
5:E:45:PHE:CE2	5:E:47:LYS:HE3	2.49	0.48
8:H:83:ILE:HG12	8:H:137:VAL:CG2	2.37	0.48
15:O:25:THR:HG21	15:O:70:LEU:HG	1.96	0.48
20:T:31:SER:HA	20:T:34:LYS:HG3	1.94	0.48
1:A:77:G:C4	1:A:93:G:N2	2.82	0.47
1:A:674:G:H5'	6:F:50:TYR:CE2	2.48	0.47
1:A:881:G:P	12:L:12:ARG:HH22	2.37	0.47
1:A:1113:C:H4'	3:C:14:ILE:HD12	1.95	0.47
1:A:1411:C:H2'	1:A:1412:C:C6	2.49	0.47
1:A:619:U:N3	4:D:134:ASP:OD2	2.45	0.47
1:A:1027:C:H42	1:A:1035:A:N6	2.12	0.47
1:A:1087:G:H22	1:A:1099:G:H1'	1.78	0.47
2:B:31:TYR:CE1	2:B:200:ILE:HD11	2.48	0.47
2:B:54:THR:O	2:B:58:ILE:HG13	2.13	0.47
10:J:49:VAL:HG13	14:N:41:ARG:HB2	1.95	0.47
11:K:29:ILE:HG23	11:K:44:SER:HB3	1.96	0.47
14:N:3:ARG:NH2	14:N:5:ALA:HB3	2.28	0.47
1:A:238:G:OP1	17:Q:25:ARG:NH2	2.47	0.47
1:A:280:C:C2	17:Q:38:ARG:HG3	2.48	0.47
1:A:642:A:H2'	1:A:643:C:H6	1.79	0.47
1:A:1498:UR3:C4'	1:A:1519[A]:MA6:H2	2.44	0.47
5:E:105:VAL:HB	5:E:106:PRO:HD3	1.95	0.47
13:M:14:ARG:NE	13:M:42:ALA:HA	2.29	0.47
1:A:24:U:H2'	1:A:25:C:C6	2.49	0.47
1:A:190(K):G:H2'	1:A:190(L):U:C6	2.48	0.47
1:A:988:G:H1'	1:A:1015:A:N1	2.29	0.47
1:A:1513:A:H2'	1:A:1514:C:C6	2.49	0.47
2:B:135:GLN:O	2:B:139:LYS:HB2	2.14	0.47
4:D:21:LEU:CD2	4:D:114:ARG:HB2	2.45	0.47
1:A:113:G:H2'	1:A:114:U:H6	1.80	0.47
1:A:164:U:H2'	1:A:165:C:H6	1.78	0.47
1:A:184:G:H2'	1:A:185:A:C8	2.41	0.47
1:A:459:G:H1'	1:A:463:A:N6	2.29	0.47
1:A:708:C:H2'	1:A:709:G:C8	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:765:G:C6	1:A:812:C:C2	3.03	0.47
1:A:766:A:H2'	1:A:767:A:O4'	2.14	0.47
1:A:1239:A:H62	1:A:1299:A:N6	2.11	0.47
4:D:19:LEU:HD23	4:D:19:LEU:HA	1.56	0.47
8:H:87:SER:HA	8:H:93:VAL:HG12	1.97	0.47
15:O:33:THR:HG23	15:O:63:ARG:HH12	1.79	0.47
20:T:16:HIS:CE1	20:T:20:LEU:HD21	2.49	0.47
1:A:1097:C:H2'	1:A:1098:C:C6	2.49	0.47
1:A:1255:G:O2'	1:A:1258:G:H1'	2.15	0.47
1:A:1329:A:P	13:M:28:ALA:HB3	2.54	0.47
1:A:1399:C:O2	1:A:1401:G:C5	2.68	0.47
2:B:186:ALA:HB3	2:B:197:VAL:HG11	1.96	0.47
4:D:116:GLN:O	4:D:120:LEU:HG	2.15	0.47
4:D:131:ARG:HD2	4:D:131:ARG:N	2.29	0.47
4:D:190:ASP:OD1	4:D:191:ARG:N	2.48	0.47
14:N:13:THR:N	14:N:14:PRO:HD3	2.29	0.47
1:A:708:C:H2'	1:A:709:G:H8	1.80	0.47
2:B:97:TRP:CE3	2:B:98:LEU:O	2.68	0.47
4:D:9:CYS:O	4:D:12:CYS:HB2	2.14	0.47
4:D:63:LYS:O	4:D:67:ILE:HG13	2.14	0.47
6:F:19:LEU:O	6:F:23:LYS:HG3	2.14	0.47
6:F:100:ASN:O	6:F:100:ASN:ND2	2.47	0.47
9:I:36:TYR:O	9:I:70:LYS:NZ	2.35	0.47
16:P:34:GLU:OE1	16:P:55:ARG:HD2	2.15	0.47
20:T:89:ARG:O	20:T:92:LEU:HB2	2.15	0.47
1:A:355:C:H5'	1:A:389:A:OP2	2.14	0.47
1:A:451:A:H2	1:A:480:U:C4	2.32	0.47
1:A:740:U:O2'	1:A:741:G:H5'	2.14	0.47
1:A:922:G:H4'	5:E:20:GLN:HA	1.97	0.47
1:A:1093:A:N3	1:A:1109:C:O2'	2.42	0.47
7:G:70:LYS:HD3	7:G:96:GLN:HB3	1.96	0.47
7:G:149:ARG:HB3	7:G:149:ARG:NH1	2.30	0.47
1:A:865:A:O5'	1:A:865:A:H8	1.97	0.47
1:A:1027:C:H2'	1:A:1028:C:C6	2.50	0.47
1:A:1357:A:H2'	1:A:1358:U:C6	2.50	0.47
1:A:1518[B]:MA6:H102	1:A:1519[B]:MA6:H103	1.97	0.47
7:G:15:ASP:HB3	7:G:19:GLY:H	1.79	0.47
12:L:25:PRO:C	12:L:27:LEU:N	2.64	0.47
13:M:39:ILE:HA	13:M:52:GLU:OE2	2.14	0.47
1:A:78:G:H2'	1:A:79:G:H5''	1.96	0.47
1:A:397:A:H5'	1:A:398:C:OP1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:U:H2'	1:A:422:C:H5	1.80	0.47
1:A:620:C:N1	4:D:135:LEU:HD13	2.29	0.47
1:A:1384:C:H2'	1:A:1385:G:C8	2.50	0.47
1:A:1481:U:H2'	1:A:1482:G:O4'	2.15	0.47
8:H:20:TYR:HE1	8:H:76:PRO:HG2	1.80	0.47
10:J:55:LYS:HZ2	10:J:56:HIS:H	1.63	0.47
15:O:39:LEU:CD1	15:O:56:LEU:HB2	2.45	0.47
1:A:255:G:H2'	1:A:256:U:C6	2.50	0.46
1:A:349:A:H2'	1:A:350:G:O4'	2.14	0.46
1:A:707:C:H2'	1:A:708:C:H6	1.78	0.46
1:A:973:G:C3'	1:A:974:A:H5''	2.45	0.46
1:A:1516[A]:G:H2'	1:A:1518[A]:MA6:OP2	2.15	0.46
6:F:67:MET:HB2	6:F:68:PRO:HD2	1.96	0.46
14:N:12:ARG:HA	14:N:12:ARG:HD3	1.78	0.46
14:N:24:CYS:HB3	14:N:33:VAL:HG12	1.96	0.46
20:T:75:ASN:OD1	20:T:75:ASN:N	2.48	0.46
1:A:542:G:OP1	4:D:10:ARG:NH2	2.47	0.46
2:B:92:TYR:CD2	2:B:151:GLY:HA3	2.50	0.46
3:C:134:ILE:HD11	3:C:153:VAL:HG21	1.98	0.46
1:A:77:G:C6	1:A:93:G:C6	3.04	0.46
1:A:130:A:OP2	1:A:190(E):U:H2'	2.16	0.46
1:A:601:C:H2'	1:A:602:A:C8	2.50	0.46
1:A:620:C:C1'	4:D:135:LEU:HD13	2.45	0.46
1:A:1118:C:H2'	1:A:1119:C:C6	2.50	0.46
1:A:1254:C:OP1	10:J:45:ARG:HD3	2.15	0.46
2:B:180:LEU:HA	2:B:180:LEU:HD23	1.55	0.46
3:C:125:GLU:O	3:C:127:ARG:HG3	2.14	0.46
5:E:148:VAL:O	5:E:152:ARG:HG3	2.16	0.46
10:J:50:ILE:HA	10:J:60:ARG:HB3	1.97	0.46
13:M:37:THR:HB	13:M:39:ILE:CD1	2.45	0.46
18:R:71:LYS:O	18:R:75:ILE:HG12	2.16	0.46
1:A:106:C:O2'	1:A:107:G:H5'	2.16	0.46
1:A:262:A:H5'	20:T:74:LYS:CD	2.44	0.46
1:A:691:G:H2'	1:A:692:U:H6	1.80	0.46
1:A:1206:G:C6	1:A:1207:2MG:C5	3.03	0.46
1:A:1505:G:C8	1:A:1505:G:C3'	2.98	0.46
2:B:55:PHE:CD2	2:B:58:ILE:HD12	2.50	0.46
6:F:67:MET:HE2	6:F:68:PRO:O	2.16	0.46
8:H:11:THR:O	8:H:12:ARG:C	2.57	0.46
9:I:10:ARG:NH1	9:I:75:ASP:OD2	2.49	0.46
12:L:10:LEU:HB3	17:Q:32:TYR:CD1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:24:CYS:SG	14:N:40:CYS:HB3	2.55	0.46
15:O:3:ILE:HD11	15:O:35:ARG:HG3	1.95	0.46
1:A:695:A:H2'	1:A:696:A:C8	2.51	0.46
1:A:881:G:OP2	12:L:12:ARG:NH2	2.48	0.46
1:A:975:A:N6	10:J:60:ARG:HH21	2.14	0.46
1:A:1195:C:C4	1:A:1197:G:C8	3.04	0.46
1:A:1370:G:H5''	9:I:109:VAL:HG21	1.96	0.46
2:B:18:GLY:HA3	2:B:42:ILE:H	1.81	0.46
3:C:28:GLN:H	3:C:28:GLN:HG2	1.49	0.46
7:G:47:CYS:HA	7:G:50:ILE:HG22	1.97	0.46
8:H:2:LEU:HD23	8:H:2:LEU:C	2.40	0.46
17:Q:60:ILE:HD12	17:Q:60:ILE:HG23	1.67	0.46
17:Q:65:ILE:HB	17:Q:69:LYS:HB2	1.97	0.46
1:A:445:G:H2'	1:A:446:G:C8	2.51	0.46
2:B:178:ARG:HE	8:H:74:PRO:HG3	1.81	0.46
4:D:20:TYR:HA	4:D:26:CYS:SG	2.55	0.46
4:D:157:LEU:HD22	4:D:157:LEU:HA	1.67	0.46
9:I:53:VAL:HB	9:I:92:TYR:CE2	2.51	0.46
1:A:781:A:C5	1:A:802:A:C2	3.04	0.46
1:A:1112:C:H42	3:C:178:LEU:H	1.63	0.46
1:A:1172:C:H2'	1:A:1173:G:H8	1.81	0.46
2:B:30:ARG:HD2	2:B:31:TYR:CE2	2.51	0.46
3:C:7:PRO:O	3:C:11:ARG:HD2	2.15	0.46
5:E:31:LEU:HA	5:E:31:LEU:HD23	1.53	0.46
13:M:49:THR:HG22	13:M:50:GLU:H	1.80	0.46
17:Q:5:VAL:C	17:Q:6:LEU:HD23	2.40	0.46
20:T:60:GLU:HA	20:T:63:ILE:HD12	1.98	0.46
1:A:231:G:C2	1:A:232:G:C8	3.04	0.46
1:A:325:A:H2'	1:A:326:G:O4'	2.15	0.46
1:A:457:C:H2'	1:A:458:C:C6	2.51	0.46
1:A:601:C:H2'	1:A:602:A:H8	1.81	0.46
1:A:974:A:H4'	1:A:975:A:H3'	1.97	0.46
1:A:1328:C:H2'	1:A:1329:A:C8	2.51	0.46
6:F:8:ILE:HG23	6:F:85:VAL:HG13	1.98	0.46
8:H:104:ARG:HG2	8:H:138:TRP:CE3	2.50	0.46
9:I:53:VAL:HB	9:I:92:TYR:CZ	2.51	0.46
13:M:23:TYR:HB2	13:M:67:GLU:OE2	2.16	0.46
17:Q:61:GLU:HA	17:Q:71:PHE:CD1	2.51	0.46
19:S:80:TYR:CG	19:S:81:ARG:N	2.84	0.46
1:A:113:G:H2'	1:A:114:U:C6	2.51	0.46
1:A:251:G:H4'	1:A:252:U:OP1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:A:N7	1:A:413:G:H1'	2.31	0.46
1:A:1152:A:P	10:J:70:ARG:HH22	2.39	0.46
1:A:1211:U:H1'	1:A:1213:A:C2	2.50	0.46
1:A:1223:C:H3'	1:A:1224:G:C5'	2.45	0.46
1:A:1283:G:H2'	1:A:1284:C:H6	1.80	0.46
2:B:40:HIS:HD1	2:B:190:THR:HG21	1.81	0.46
2:B:222:ILE:HG22	2:B:226:ARG:HH12	1.81	0.46
4:D:146:ILE:N	4:D:146:ILE:HD12	2.30	0.46
8:H:31:PHE:CE2	8:H:35:ILE:HD11	2.51	0.46
9:I:9:ARG:HG3	9:I:14:VAL:HG13	1.97	0.46
15:O:2:PRO:HB2	15:O:3:ILE:H	1.57	0.46
16:P:43:LYS:HA	16:P:48:TRP:HB3	1.98	0.46
1:A:79:G:C2	1:A:80:G:C8	3.04	0.46
1:A:255:G:O6	1:A:266:G:O6	2.34	0.46
1:A:518:C:H4'	1:A:519:C:O5'	2.16	0.46
1:A:607:A:N3	1:A:607:A:H2'	2.31	0.46
1:A:877:C:O2'	8:H:3:THR:HG23	2.15	0.46
1:A:1347:G:O2'	1:A:1373:G:N1	2.49	0.46
1:A:1504:G:C3'	1:A:1505:G:H5'	2.46	0.46
3:C:151:VAL:C	3:C:152:ILE:HG13	2.41	0.46
12:L:60:LEU:HB2	12:L:64:TYR:O	2.16	0.46
1:A:321:A:C2	1:A:333:G:C2	3.04	0.45
1:A:1111:A:N1	3:C:177:THR:OG1	2.37	0.45
9:I:102:LEU:HD23	9:I:102:LEU:HA	1.78	0.45
1:A:293:G:C6	1:A:294:U:C4	3.04	0.45
1:A:1061:G:H1'	10:J:56:HIS:CE1	2.51	0.45
4:D:61:LYS:HA	4:D:203:VAL:HG22	1.98	0.45
9:I:108:VAL:HG12	9:I:109:VAL:H	1.82	0.45
1:A:393:A:C2	1:A:394:G:C8	3.04	0.45
1:A:1130:A:H8	1:A:1130:A:OP2	1.99	0.45
1:A:1181:G:C2	1:A:1182:G:N2	2.84	0.45
4:D:201:GLN:O	4:D:205:GLU:HG3	2.16	0.45
5:E:11:ILE:HB	5:E:31:LEU:CB	2.43	0.45
8:H:127:LEU:HD13	8:H:127:LEU:HA	1.70	0.45
1:A:564:C:C5	17:Q:31:LEU:HD21	2.51	0.45
1:A:575:G:O2'	1:A:821:G:H5'	2.16	0.45
1:A:949:A:C4	1:A:1233:G:N2	2.85	0.45
1:A:1188:A:O2'	14:N:58:LYS:NZ	2.50	0.45
2:B:73:THR:HG23	2:B:95:GLN:O	2.16	0.45
3:C:155:GLY:O	3:C:196:LEU:HG	2.17	0.45
4:D:91:SER:OG	4:D:92:VAL:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:101:LEU:HA	4:D:104:VAL:HB	1.97	0.45
4:D:196:LEU:HA	4:D:197:PRO:HD3	1.85	0.45
8:H:86:ILE:HG21	8:H:133:LEU:HD22	1.97	0.45
8:H:119:LEU:HD22	8:H:123:GLU:HB3	1.99	0.45
1:A:500:G:C6	1:A:546:G:C2	3.05	0.45
1:A:1193:G:O2'	1:A:1194:U:H5'	2.17	0.45
1:A:1281:U:H5'	1:A:1282:C:C5	2.52	0.45
4:D:26:CYS:HA	4:D:31:CYS:HB2	1.99	0.45
5:E:14:ARG:O	5:E:28:PHE:HD2	1.99	0.45
5:E:51:VAL:HB	5:E:52:PRO:HD3	1.99	0.45
5:E:60:TYR:HE1	5:E:64:ARG:HE	1.63	0.45
6:F:48:LEU:HD13	6:F:52:ILE:HG13	1.99	0.45
8:H:48:TYR:HA	8:H:60:ARG:O	2.16	0.45
9:I:32:ASP:OD2	9:I:33:PHE:N	2.49	0.45
15:O:18:PHE:CZ	15:O:21:ASP:HB2	2.51	0.45
15:O:43:LEU:HD11	15:O:53:HIS:HA	1.98	0.45
17:Q:88:TYR:HA	17:Q:91:ARG:NH1	2.31	0.45
1:A:224:C:H2'	1:A:225:C:H6	1.82	0.45
1:A:424:G:H2'	1:A:425:G:C8	2.51	0.45
1:A:585:G:C6	1:A:586:C:C4	3.04	0.45
1:A:1302:U:C5	13:M:17:VAL:HG21	2.51	0.45
1:A:1505:G:O2'	1:A:1506:U:OP2	2.29	0.45
8:H:120:THR:N	8:H:123:GLU:OE1	2.44	0.45
19:S:22:LEU:HD21	19:S:28:LYS:H	1.82	0.45
1:A:328:C:H2'	1:A:328:C:O2	2.16	0.45
1:A:958:A:O2'	1:A:985:C:O2'	2.32	0.45
4:D:145:GLU:HG3	4:D:184:LYS:HD3	1.98	0.45
16:P:66:PRO:HG2	16:P:71:ARG:HG3	1.99	0.45
1:A:187:C:H4'	20:T:86:ARG:HG3	1.99	0.45
1:A:673:G:O3'	6:F:87:ARG:NH2	2.49	0.45
1:A:923:A:H2'	1:A:924:C:O4'	2.16	0.45
1:A:1112:C:O2	3:C:179:ARG:HB2	2.17	0.45
1:A:1349:A:C2	1:A:1374:A:C4	3.05	0.45
1:A:1520[B]:G:H2'	1:A:1521:G:C8	2.50	0.45
5:E:109:ILE:HG21	5:E:135:THR:HG21	1.99	0.45
12:L:42:THR:CG2	12:L:52:LEU:HB3	2.47	0.45
1:A:642:A:N3	8:H:113:SER:OG	2.41	0.45
1:A:866:C:C4	1:A:867:G:H1'	2.52	0.45
1:A:1420:C:H2'	1:A:1421:G:H8	1.81	0.45
1:A:1499:A:C1'	1:A:1520[A]:G:H5'	2.47	0.45
4:D:114:ARG:O	4:D:117:ALA:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:10:GLY:HA3	16:P:14:ASN:O	2.17	0.45
20:T:60:GLU:HG3	20:T:81:LYS:HE3	1.99	0.45
20:T:62:LEU:HD23	20:T:62:LEU:HA	1.76	0.45
1:A:741:G:H2'	1:A:742:G:O4'	2.17	0.45
2:B:102:LEU:HD11	2:B:162:ILE:HD11	1.99	0.45
15:O:84:LYS:HG2	15:O:85:LEU:HD23	1.98	0.45
17:Q:86:GLU:O	17:Q:90:ILE:HG12	2.17	0.45
1:A:83:U:C4	1:A:84:U:C5	3.05	0.44
1:A:115:G:O2'	1:A:289:G:H5''	2.17	0.44
1:A:263:A:P	20:T:79:ARG:HH11	2.39	0.44
1:A:560:U:H5'	1:A:566:G:N2	2.32	0.44
1:A:959:A:H3'	1:A:960:U:H5''	1.99	0.44
1:A:1066:C:H5	1:A:1067:A:C6	2.35	0.44
1:A:1078:U:C5	1:A:1079:G:C5	3.05	0.44
1:A:1381:U:C2	7:G:156:TRP:HH2	2.34	0.44
1:A:1508:G:C5	1:A:1509:C:C5	3.05	0.44
4:D:88:VAL:HG12	4:D:90:GLY:H	1.81	0.44
4:D:125:HIS:C	4:D:126:ILE:HD12	2.42	0.44
9:I:45:ALA:O	9:I:48:GLU:HB2	2.17	0.44
16:P:78:GLY:N	24:P:208:HOH:O	2.46	0.44
1:A:21:G:C2	1:A:22:G:C6	3.05	0.44
1:A:353:A:H5'	1:A:353:A:H8	1.82	0.44
1:A:411:A:OP1	4:D:30:LYS:NZ	2.45	0.44
1:A:532:A:N6	3:C:159:GLY:O	2.50	0.44
4:D:3:ARG:HG3	4:D:118:ARG:HH11	1.82	0.44
6:F:14:LEU:HD13	6:F:18:GLN:HB3	1.99	0.44
9:I:79:LEU:O	9:I:83:ARG:HG2	2.17	0.44
19:S:16:LEU:O	19:S:19:VAL:HG12	2.17	0.44
1:A:501:C:OP1	12:L:117:ARG:NH2	2.46	0.44
7:G:109:ASN:OD1	7:G:119:ARG:NH2	2.50	0.44
8:H:4:ASP:CG	8:H:7:ALA:H	2.26	0.44
8:H:124:ALA:O	8:H:128:GLY:N	2.47	0.44
9:I:118:LYS:C	9:I:120:ARG:H	2.23	0.44
12:L:48:PRO:CD	12:L:92:OTD:H3	2.48	0.44
15:O:55:GLY:HA2	15:O:58:MET:HE2	1.99	0.44
1:A:92:C:H2'	1:A:92:C:O2	2.17	0.44
1:A:604:G:C5	1:A:605:U:C5	3.05	0.44
1:A:765:G:H1	1:A:812:C:HO2'	1.63	0.44
1:A:921:U:O2'	5:E:19:MET:O	2.35	0.44
1:A:1066:C:C5	1:A:1067:A:C6	3.06	0.44
1:A:1148:U:H4'	9:I:14:VAL:HG11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1291:G:OP1	7:G:41:ARG:NH2	2.50	0.44
2:B:177:ALA:HB1	2:B:182:ILE:HB	1.98	0.44
3:C:70:VAL:HG21	3:C:76:VAL:HG21	1.99	0.44
4:D:25:ARG:HH21	4:D:30:LYS:HB3	1.83	0.44
5:E:81:GLU:CD	5:E:88:LYS:HD2	2.42	0.44
14:N:3:ARG:HH21	14:N:5:ALA:HB3	1.81	0.44
16:P:18:ARG:HD3	16:P:35:LYS:HD2	1.99	0.44
20:T:33:ILE:HD11	20:T:63:ILE:HA	1.99	0.44
20:T:74:LYS:HB2	20:T:76:ALA:H	1.81	0.44
2:B:21:ARG:HD3	2:B:22:LYS:H	1.83	0.44
2:B:189:ASP:OD1	2:B:205:ASP:HB3	2.16	0.44
4:D:57:ARG:HG3	4:D:202:LEU:CD1	2.46	0.44
7:G:76:ARG:HD2	7:G:89:MET:SD	2.58	0.44
13:M:2:ALA:N	13:M:9:ILE:HG23	2.33	0.44
1:A:134:A:H2'	1:A:135:C:O4'	2.18	0.44
1:A:243:A:C2	1:A:246:A:C8	3.05	0.44
1:A:538:G:OP1	12:L:115:LYS:N	2.51	0.44
1:A:553:A:O2'	12:L:29:GLY:O	2.34	0.44
1:A:691:G:H2'	1:A:692:U:C6	2.52	0.44
1:A:922:G:C2	1:A:1396:A:C6	3.06	0.44
1:A:942:G:N2	1:A:943:U:C2	2.86	0.44
1:A:1010:G:N2	1:A:1019:C:O2	2.37	0.44
1:A:1105:A:H2'	1:A:1106:G:C8	2.53	0.44
4:D:19:LEU:HD21	4:D:67:ILE:HG12	1.99	0.44
5:E:28:PHE:HB2	5:E:48:ALA:O	2.18	0.44
5:E:90:VAL:C	5:E:91:LEU:HD23	2.43	0.44
7:G:18:TYR:CE2	7:G:59:LEU:HB2	2.53	0.44
8:H:119:LEU:HD13	8:H:124:ALA:HA	1.98	0.44
8:H:123:GLU:HG2	8:H:126:LYS:NZ	2.33	0.44
20:T:49:ALA:HB3	20:T:99:LEU:HD12	1.99	0.44
1:A:391:G:C6	1:A:392:G:C5	3.05	0.44
1:A:413:G:O6	4:D:36:ARG:NH1	2.51	0.44
4:D:72:GLU:O	4:D:75:PHE:HB3	2.17	0.44
6:F:1:MET:HB3	6:F:67:MET:O	2.18	0.44
7:G:86:GLN:HB2	7:G:148:ASN:ND2	2.32	0.44
7:G:145:ALA:C	7:G:147:ALA:N	2.76	0.44
12:L:19:ARG:HA	12:L:20:LYS:HZ2	1.81	0.44
12:L:70:ILE:HA	12:L:71:PRO:HD3	1.84	0.44
13:M:97:PRO:HB2	13:M:101:GLN:OE1	2.17	0.44
16:P:51:VAL:HG12	16:P:53:VAL:N	2.33	0.44
17:Q:22:LEU:HA	17:Q:22:LEU:HD12	1.24	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:C:H2'	1:A:225:C:C6	2.52	0.44
2:B:215:LEU:HD23	2:B:215:LEU:HA	1.81	0.44
3:C:59:ARG:H	10:J:92:THR:HG23	1.83	0.44
3:C:166:GLU:HA	3:C:166:GLU:OE1	2.18	0.44
4:D:114:ARG:HG3	4:D:114:ARG:HH11	1.82	0.44
6:F:80:ARG:NH1	6:F:88:VAL:H	2.16	0.44
8:H:82:HIS:ND1	8:H:138:TRP:NE1	2.65	0.44
8:H:86:ILE:HG22	8:H:133:LEU:O	2.18	0.44
12:L:46:LYS:HE2	12:L:94:PRO:HG2	2.00	0.44
12:L:124:LYS:HD3	12:L:125:PRO:HD2	2.00	0.44
20:T:41:ILE:HD12	20:T:41:ILE:HA	1.69	0.44
21:U:6:ARG:O	21:U:12:LYS:HE2	2.17	0.44
1:A:9:G:C2	1:A:26:A:N1	2.86	0.44
1:A:624:C:H2'	1:A:625:G:C8	2.53	0.44
1:A:937:A:N6	1:A:1345:U:O4	2.49	0.44
1:A:971:G:H1'	1:A:1365:G:O2'	2.17	0.44
1:A:1226:C:OP1	13:M:91:ARG:NH1	2.49	0.44
1:A:1366:C:H2'	1:A:1367:C:C6	2.51	0.44
1:A:1368:G:OP2	9:I:112:LYS:HD3	2.18	0.44
3:C:61:ALA:C	3:C:63:ASN:H	2.26	0.44
17:Q:65:ILE:HG21	17:Q:69:LYS:HZ3	1.83	0.44
1:A:502:G:H2'	1:A:503:C:O4'	2.17	0.43
1:A:1073:U:OP2	5:E:57:LYS:HE2	2.18	0.43
16:P:43:LYS:HG2	16:P:48:TRP:CG	2.53	0.43
17:Q:51:TYR:CD1	17:Q:73:VAL:HG11	2.53	0.43
17:Q:59:ILE:HD13	17:Q:59:ILE:HA	1.67	0.43
20:T:53:LEU:HD22	20:T:53:LEU:HA	1.52	0.43
1:A:721:G:C6	1:A:733:A:C2	3.05	0.43
1:A:1324:A:H2'	1:A:1325:C:O4'	2.17	0.43
4:D:107:ARG:HH21	4:D:194:LEU:HD11	1.83	0.43
7:G:70:LYS:HG2	7:G:100:ALA:HB2	2.00	0.43
17:Q:5:VAL:HG22	17:Q:60:ILE:HD11	2.00	0.43
1:A:624:C:H2'	1:A:625:G:H8	1.82	0.43
1:A:960:U:H1'	1:A:1223:C:H5'	1.99	0.43
1:A:975:A:H62	10:J:60:ARG:NH2	2.17	0.43
1:A:1118:C:H1'	1:A:1179:A:C4	2.53	0.43
1:A:1202:G:C6	14:N:42:ILE:HG21	2.53	0.43
1:A:1232:U:OP1	9:I:126:SER:HB3	2.18	0.43
2:B:61:LEU:HD21	2:B:160:ASP:HB2	1.99	0.43
2:B:82:ARG:HA	2:B:92:TYR:CE1	2.53	0.43
3:C:11:ARG:HB3	3:C:16:ARG:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:125:GLU:HG2	3:C:189:ALA:HB1	1.99	0.43
4:D:10:ARG:O	4:D:13:ARG:HB2	2.18	0.43
6:F:86:ARG:H	6:F:86:ARG:HG2	1.59	0.43
11:K:38:ASN:HA	11:K:39:PRO:HD3	1.69	0.43
12:L:76:ASN:CG	12:L:108:ALA:HB2	2.44	0.43
17:Q:18:THR:HG23	17:Q:69:LYS:HE3	2.00	0.43
20:T:43:LEU:HG	20:T:55:ILE:CD1	2.48	0.43
1:A:31:G:N2	1:A:48:C:OP1	2.46	0.43
1:A:345:C:OP2	1:A:345:C:C6	2.71	0.43
1:A:561:U:O2'	1:A:562:C:OP1	2.32	0.43
1:A:626:U:H5''	16:P:38:TYR:CD2	2.53	0.43
1:A:1064:G:H21	1:A:1190:G:H2'	1.84	0.43
1:A:1190:G:H5''	1:A:1190:G:H8	1.83	0.43
1:A:1202:G:H2'	1:A:1203:C:O4'	2.19	0.43
1:A:1358:U:H5''	14:N:35:ARG:CD	2.48	0.43
2:B:21:ARG:H	2:B:21:ARG:HG3	1.55	0.43
3:C:10:PHE:CZ	3:C:178:LEU:HD12	2.53	0.43
5:E:84:PHE:CE1	5:E:133:TYR:HB3	2.53	0.43
8:H:104:ARG:HD2	8:H:104:ARG:HA	1.67	0.43
9:I:97:LYS:HA	9:I:97:LYS:HD3	1.78	0.43
15:O:3:ILE:HA	15:O:7:GLU:OE1	2.18	0.43
16:P:68:ASP:OD1	16:P:68:ASP:N	2.50	0.43
16:P:82:GLN:H	16:P:82:GLN:HG2	1.65	0.43
17:Q:93:GLN:HG2	17:Q:96:GLN:HE22	1.83	0.43
18:R:54:ARG:HE	18:R:54:ARG:HB2	1.33	0.43
1:A:409:G:OP1	4:D:24:GLU:O	2.36	0.43
1:A:429:U:H1'	1:A:430:A:H5''	2.01	0.43
1:A:445:G:C2	1:A:490:G:C2	3.07	0.43
1:A:1010:G:H2'	1:A:1011:G:H8	1.84	0.43
1:A:1128:C:H42	1:A:1143:G:H1	1.67	0.43
1:A:1436:U:H2'	1:A:1437:C:C6	2.54	0.43
1:A:1516[B]:G:H2'	1:A:1518[B]:MA6:OP2	2.18	0.43
1:A:1517[A]:G:H2'	1:A:1518[A]:MA6:H8	2.00	0.43
8:H:35:ILE:H	8:H:35:ILE:HG12	1.22	0.43
8:H:105:ARG:HD3	8:H:105:ARG:HA	1.72	0.43
13:M:19:LEU:HD22	13:M:22:ILE:HD13	2.01	0.43
13:M:103:THR:HG23	24:M:304:HOH:O	2.18	0.43
20:T:44:ALA:HB1	20:T:91:LEU:HB3	2.01	0.43
20:T:85:MET:HG2	20:T:104:LEU:HD21	2.00	0.43
21:U:14:TRP:HZ3	21:U:15:ARG:HH21	1.65	0.43
1:A:115:G:H5''	24:A:2264:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:C:H2'	1:A:402:G:C8	2.52	0.43
1:A:501:C:O3'	12:L:118:SER:OG	2.35	0.43
1:A:1182:G:H8	1:A:1182:G:H2'	1.74	0.43
1:A:1197:G:H2'	1:A:1197:G:N3	2.33	0.43
3:C:22:TRP:CD1	3:C:59:ARG:HG3	2.53	0.43
4:D:70:ILE:HG22	4:D:71:SER:N	2.33	0.43
5:E:76:ILE:HG23	5:E:142:LEU:HD11	2.00	0.43
5:E:145:LYS:O	5:E:148:VAL:HG23	2.19	0.43
9:I:27:THR:CG2	9:I:62:TYR:HA	2.49	0.43
11:K:54:ARG:HB3	11:K:54:ARG:HH11	1.84	0.43
12:L:76:ASN:OD1	12:L:76:ASN:N	2.48	0.43
17:Q:89:LEU:HD23	17:Q:89:LEU:HA	1.63	0.43
18:R:31:LEU:HD22	18:R:65:ILE:HG22	2.01	0.43
19:S:5:LEU:HD13	19:S:9:VAL:HG13	2.01	0.43
20:T:52:ALA:HA	20:T:55:ILE:HD12	2.01	0.43
20:T:88:VAL:O	20:T:92:LEU:HD23	2.18	0.43
1:A:190(E):U:C4	17:Q:72:ARG:NH2	2.87	0.43
1:A:760:G:H2'	1:A:761:G:O4'	2.18	0.43
1:A:826:C:C2	1:A:827:U:C5	3.07	0.43
1:A:986:A:H1'	19:S:54:GLY:O	2.19	0.43
3:C:36:ASP:HA	3:C:39:ILE:CD1	2.48	0.43
7:G:97:GLN:O	7:G:101:LEU:HD12	2.19	0.43
8:H:97:VAL:HG23	8:H:129:VAL:C	2.44	0.43
9:I:17:VAL:HA	9:I:63:ILE:HG12	2.01	0.43
12:L:41:ARG:HH21	12:L:43:VAL:HG22	1.84	0.43
13:M:34:LEU:HD13	13:M:39:ILE:HB	2.00	0.43
13:M:87:TYR:HA	13:M:90:LEU:HG	2.00	0.43
19:S:29:ARG:HD2	19:S:29:ARG:N	2.33	0.43
1:A:786:G:C2	1:A:797:C:C2	3.06	0.43
1:A:952:U:H2'	1:A:953:G:C8	2.50	0.43
1:A:1007:C:H1'	1:A:1023:G:H22	1.84	0.43
1:A:1065:U:H4'	1:A:1066:C:O5'	2.17	0.43
1:A:1443:G:H4'	1:A:1446:A:O5'	2.19	0.43
2:B:79:ASP:HA	2:B:82:ARG:HB3	2.01	0.43
3:C:155:GLY:HA2	3:C:164:ARG:H	1.84	0.43
5:E:43:LEU:HG	5:E:44:GLY:N	2.34	0.43
7:G:5:ARG:HA	7:G:5:ARG:HD2	1.79	0.43
8:H:110:ALA:HB3	8:H:121:ASP:HB3	2.00	0.43
10:J:6:ILE:HG12	10:J:98:ILE:HG12	2.00	0.43
11:K:86:GLY:H	11:K:112:THR:HG23	1.84	0.43
12:L:6:THR:N	12:L:9:GLN:HG2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:69:TYR:CD1	12:L:90:VAL:HG21	2.53	0.43
1:A:686:U:O2'	1:A:687:A:H8	2.02	0.43
1:A:786:G:H2'	1:A:787:A:O4'	2.18	0.43
1:A:837:G:H1	1:A:849:C:H42	1.65	0.43
1:A:955:U:H1'	1:A:1227:A:N6	2.34	0.43
1:A:1268:A:H2'	1:A:1269:A:C8	2.54	0.43
1:A:1516[B]:G:N2	1:A:1519[B]:MA6:OP2	2.52	0.43
4:D:115:ARG:HH11	4:D:115:ARG:HB3	1.83	0.43
4:D:128:VAL:HG12	4:D:129:ASN:ND2	2.34	0.43
12:L:7:ILE:HA	12:L:7:ILE:HD13	1.47	0.43
16:P:60:LEU:HD23	16:P:60:LEU:HA	1.60	0.43
1:A:474:G:H2'	1:A:475:G:C8	2.54	0.43
1:A:544:G:C5	1:A:545:C:C5	3.07	0.43
1:A:676:A:C1'	11:K:115:PRO:HB3	2.49	0.43
1:A:907:A:C4	1:A:908:A:C8	3.07	0.43
1:A:957:U:H1'	1:A:960:U:N3	2.34	0.43
1:A:1199:U:O5'	1:A:1199:U:H6	2.02	0.43
1:A:1500:A:OP2	1:A:1505:G:OP1	2.37	0.43
4:D:38:TYR:CE1	4:D:45:GLN:HG3	2.54	0.43
4:D:108:LEU:HD22	4:D:176:LEU:HD12	2.01	0.43
7:G:111:ARG:HG2	7:G:112:PRO:HD2	2.01	0.43
20:T:66:ALA:HB3	20:T:72:LEU:HD12	2.01	0.43
1:A:390:C:H2'	1:A:391:G:C8	2.54	0.42
1:A:613:C:H42	1:A:627:G:H1	1.67	0.42
1:A:1072:G:C5	1:A:1073:U:C4	3.06	0.42
1:A:1232:U:H5''	9:I:124:GLN:O	2.19	0.42
1:A:1337:G:H5''	1:A:1338:G:OP1	2.19	0.42
2:B:55:PHE:HE2	2:B:218:ALA:HA	1.84	0.42
5:E:36:ASP:C	5:E:38:GLN:H	2.27	0.42
8:H:10:LEU:HD23	8:H:10:LEU:HA	1.55	0.42
10:J:46:ARG:CZ	10:J:46:ARG:HB2	2.49	0.42
15:O:56:LEU:HA	15:O:59:MET:HE2	2.00	0.42
16:P:3:LYS:HD3	16:P:24:ALA:HB2	2.00	0.42
19:S:22:LEU:HD22	19:S:47:HIS:CE1	2.54	0.42
19:S:41:VAL:HG22	19:S:44:MET:SD	2.59	0.42
1:A:264:U:H4'	17:Q:63:ARG:HD3	2.01	0.42
1:A:1442:G:C5	1:A:1446:A:N6	2.87	0.42
2:B:75:LYS:HD3	2:B:75:LYS:HA	1.96	0.42
2:B:203:GLY:C	2:B:204:ASN:HD22	2.27	0.42
3:C:50:ALA:O	3:C:70:VAL:HG12	2.19	0.42
4:D:3:ARG:HD3	4:D:3:ARG:HA	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:31:LEU:HD23	5:E:44:GLY:O	2.19	0.42
6:F:62:TRP:CH2	6:F:64:GLN:HB2	2.54	0.42
13:M:102:ARG:HA	24:M:304:HOH:O	2.19	0.42
1:A:522:C:H41	12:L:53:ARG:HH22	1.67	0.42
1:A:688:G:H5'	11:K:46:GLY:C	2.44	0.42
1:A:954:G:C5	1:A:955:U:C4	3.07	0.42
5:E:37:ARG:O	5:E:114:GLY:HA3	2.19	0.42
8:H:21:LYS:O	8:H:65:TYR:OH	2.26	0.42
8:H:111:ILE:HG22	8:H:134:ILE:HD12	2.01	0.42
10:J:32:ALA:O	10:J:34:VAL:HG23	2.19	0.42
12:L:28:LYS:HG3	12:L:33:ARG:NH2	2.34	0.42
12:L:42:THR:HG23	12:L:52:LEU:HB3	2.00	0.42
13:M:17:VAL:O	13:M:20:THR:HB	2.19	0.42
17:Q:43:LEU:HD23	17:Q:43:LEU:HA	1.58	0.42
17:Q:53:LEU:C	17:Q:53:LEU:HD23	2.44	0.42
20:T:18:GLN:O	20:T:21:LYS:HB2	2.19	0.42
1:A:61:G:H2'	1:A:62:U:O4'	2.18	0.42
1:A:115:G:O5'	1:A:115:G:H8	2.02	0.42
1:A:272:C:H2'	1:A:273:A:H8	1.84	0.42
1:A:517:G:N1	1:A:533:A:OP2	2.45	0.42
1:A:945:G:N1	1:A:1337:G:C2	2.87	0.42
1:A:954:G:C6	1:A:955:U:N3	2.87	0.42
1:A:1063:C:OP2	1:A:1064:G:O2'	2.37	0.42
1:A:1126:U:H6	1:A:1126:U:O5'	2.01	0.42
1:A:1265:G:C6	1:A:1266:G:C6	3.07	0.42
1:A:1308:U:OP2	13:M:99:ARG:HG2	2.19	0.42
1:A:1530:G:H4'	1:A:1530:G:OP1	2.18	0.42
2:B:77:ALA:HB2	2:B:211:ILE:HD13	2.01	0.42
3:C:95:THR:O	3:C:95:THR:OG1	2.35	0.42
3:C:182:ILE:HG22	3:C:183:ASP:O	2.19	0.42
5:E:101:ILE:O	5:E:120:THR:HB	2.19	0.42
6:F:94:GLN:HB3	18:R:32:ARG:NH1	2.34	0.42
7:G:136:LYS:HB3	7:G:136:LYS:HE3	1.82	0.42
10:J:79:ARG:NH2	10:J:82:ILE:HB	2.34	0.42
12:L:69:TYR:O	12:L:100:ILE:HB	2.19	0.42
16:P:38:TYR:O	16:P:49:LEU:HD12	2.20	0.42
1:A:22:G:H2'	1:A:23:C:H6	1.83	0.42
1:A:75:G:C2	1:A:76:C:N3	2.88	0.42
1:A:79:G:C2	1:A:80:G:N7	2.87	0.42
1:A:359:U:H2'	1:A:360:A:H8	1.84	0.42
1:A:544:G:C6	1:A:545:C:C4	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:939:G:H5''	7:G:102:ARG:NH2	2.34	0.42
1:A:1047:G:O2'	1:A:1048:G:H5'	2.19	0.42
1:A:1119:C:N4	1:A:1154:G:H1	2.15	0.42
1:A:1190:G:O3'	3:C:3:ASN:HB2	2.19	0.42
1:A:1287:A:H2'	1:A:1288:A:C8	2.55	0.42
1:A:1329:A:OP1	13:M:28:ALA:HB3	2.20	0.42
1:A:1419:G:H1	1:A:1481:U:H3	1.68	0.42
1:A:1420:C:H2'	1:A:1421:G:C8	2.55	0.42
4:D:31:CYS:O	4:D:31:CYS:SG	2.78	0.42
4:D:200:GLU:CD	4:D:200:GLU:H	2.27	0.42
7:G:86:GLN:HB2	7:G:148:ASN:HD22	1.84	0.42
1:A:7:G:H5'	1:A:298:A:O4'	2.19	0.42
1:A:179:A:H2'	1:A:180:U:H6	1.84	0.42
1:A:788:U:H2'	1:A:789:U:H6	1.85	0.42
1:A:918:A:H2'	1:A:919:A:H8	1.82	0.42
1:A:1130:A:H5''	9:I:20:ARG:HH21	1.83	0.42
1:A:1374:A:C4	1:A:1375:A:C8	3.08	0.42
1:A:1516[A]:G:N2	1:A:1519[A]:MA6:OP2	2.26	0.42
20:T:88:VAL:HG12	20:T:89:ARG:N	2.34	0.42
1:A:75:G:N1	1:A:96:G:C6	2.87	0.42
1:A:313:A:H2'	1:A:314:C:C6	2.55	0.42
1:A:393:A:O2'	1:A:394:G:H5'	2.20	0.42
1:A:975:A:H4'	1:A:976:G:O5'	2.20	0.42
1:A:1258:G:H1	1:A:1277:C:H42	1.65	0.42
1:A:1285:A:H4'	1:A:1286:A:O5'	2.19	0.42
8:H:11:THR:O	8:H:14:ARG:N	2.53	0.42
8:H:87:SER:HB2	8:H:133:LEU:O	2.19	0.42
13:M:56:LEU:HD23	13:M:56:LEU:HA	1.73	0.42
16:P:53:VAL:O	16:P:54:GLU:C	2.61	0.42
20:T:87:LYS:O	20:T:91:LEU:HB2	2.19	0.42
1:A:122:G:C2	1:A:123:C:C2	3.08	0.42
1:A:853:G:H2'	1:A:854:G:H5'	2.01	0.42
1:A:976:G:N2	1:A:1362:C:OP2	2.46	0.42
3:C:6:HIS:HA	3:C:7:PRO:HD3	1.72	0.42
3:C:108:ASN:HA	3:C:109:PRO:HD2	1.85	0.42
4:D:15:GLU:OE1	4:D:59:ARG:NH2	2.52	0.42
5:E:41:VAL:HG13	5:E:113:ALA:HA	2.01	0.42
5:E:122:GLU:O	5:E:123:LEU:HD23	2.20	0.42
7:G:47:CYS:O	7:G:50:ILE:HG22	2.19	0.42
9:I:50:LEU:HD11	9:I:81:ILE:HG21	2.01	0.42
12:L:60:LEU:HD13	12:L:60:LEU:HA	1.69	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:60:VAL:HG22	13:M:64:TRP:HZ3	1.82	0.42
18:R:76:LEU:HD23	18:R:76:LEU:HA	1.50	0.42
20:T:25:ARG:HE	20:T:25:ARG:HB2	1.28	0.42
21:U:15:ARG:HG2	21:U:17:THR:OG1	2.20	0.42
1:A:413:G:H2'	1:A:428:G:H22	1.84	0.42
1:A:768:A:N3	1:A:1512:U:O2'	2.53	0.42
3:C:172:ARG:C	3:C:174:PRO:HD3	2.44	0.42
8:H:62:TYR:C	8:H:63:LEU:HD13	2.45	0.42
1:A:424:G:H2'	1:A:425:G:H8	1.84	0.42
1:A:512:U:O2	1:A:540:G:C2	2.73	0.42
1:A:673:G:H5''	6:F:87:ARG:CZ	2.50	0.42
2:B:97:TRP:CH2	2:B:102:LEU:HD22	2.51	0.42
4:D:19:LEU:HD11	4:D:67:ILE:HG12	2.02	0.42
4:D:105:VAL:HG13	4:D:110:PHE:HB2	2.01	0.42
4:D:158:ILE:H	4:D:158:ILE:HG13	1.40	0.42
4:D:196:LEU:HD12	4:D:196:LEU:O	2.20	0.42
8:H:127:LEU:HB3	8:H:129:VAL:CG2	2.50	0.42
15:O:44:LYS:HE3	15:O:44:LYS:HB3	1.59	0.42
1:A:39:G:N1	1:A:40:C:C4	2.88	0.41
1:A:78:G:H2'	1:A:79:G:C5'	2.50	0.41
1:A:949:A:H1'	1:A:1364:U:H3	1.85	0.41
1:A:1093:A:N3	1:A:1095:U:H5'	2.34	0.41
1:A:1283:G:H2'	1:A:1284:C:C6	2.55	0.41
1:A:1315:U:OP2	19:S:6:LYS:NZ	2.53	0.41
11:K:54:ARG:HB3	11:K:54:ARG:NH1	2.35	0.41
12:L:20:LYS:CD	12:L:20:LYS:H	2.33	0.41
13:M:107:ALA:HB3	13:M:111:LYS:HE3	2.02	0.41
15:O:76:GLU:O	15:O:79:ARG:N	2.53	0.41
17:Q:40:LYS:HD3	17:Q:42:TYR:OH	2.19	0.41
1:A:66:G:N3	1:A:66:G:H2'	2.35	0.41
1:A:77:G:O2'	1:A:78:G:H5'	2.20	0.41
1:A:112:G:C2	1:A:113:G:C8	3.08	0.41
1:A:244:U:C6	1:A:894:G:N2	2.88	0.41
1:A:1343:G:H4'	9:I:122:ALA:HB3	2.02	0.41
2:B:64:ARG:HB2	2:B:64:ARG:CZ	2.50	0.41
5:E:66:MET:HE3	5:E:66:MET:HB3	1.93	0.41
7:G:18:TYR:CD2	7:G:59:LEU:HB2	2.55	0.41
14:N:37:PHE:HB3	14:N:39:LEU:HB2	2.01	0.41
16:P:34:GLU:HG2	16:P:36:ILE:HG23	2.02	0.41
16:P:81:ARG:N	24:P:207:HOH:O	2.53	0.41
20:T:48:LYS:HE2	20:T:48:LYS:HB3	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:G:H1	1:A:489:C:H42	1.67	0.41
1:A:966:M2G:HM13	1:A:967:5MC:H1'	2.01	0.41
1:A:1062:U:H2'	1:A:1063:C:C6	2.55	0.41
1:A:1092:A:H5''	1:A:1093:A:OP2	2.20	0.41
1:A:1222:G:P	19:S:77:THR:HG21	2.61	0.41
4:D:25:ARG:HE	4:D:30:LYS:HB2	1.86	0.41
5:E:122:GLU:OE2	5:E:131:ILE:HG21	2.20	0.41
5:E:128:PRO:O	5:E:129:ILE:C	2.62	0.41
8:H:116:LYS:NZ	8:H:127:LEU:HD12	2.35	0.41
11:K:108:ILE:HB	18:R:87:ARG:O	2.21	0.41
13:M:23:TYR:HB3	13:M:67:GLU:H	1.85	0.41
20:T:34:LYS:HB3	20:T:38:LYS:HE3	2.02	0.41
1:A:502:G:P	12:L:118:SER:HG	2.43	0.41
1:A:582:U:H2'	1:A:583:A:C8	2.54	0.41
1:A:755:G:OP2	15:O:65:ARG:HG2	2.21	0.41
1:A:815:A:N6	1:A:1509:C:H1'	2.35	0.41
1:A:1073:U:O2	2:B:104:ASN:ND2	2.54	0.41
1:A:1394:A:N6	1:A:1501:C:H5'	2.35	0.41
1:A:1530:G:H2'	1:A:1531:A:C8	2.56	0.41
5:E:142:LEU:HD23	5:E:142:LEU:HA	1.45	0.41
20:T:25:ARG:O	20:T:28:ALA:HB3	2.20	0.41
1:A:297:G:N2	1:A:300:A:OP2	2.52	0.41
1:A:554:C:O2'	1:A:555:C:H5'	2.20	0.41
1:A:789:U:O2	1:A:791:G:C8	2.74	0.41
1:A:1063:C:C2	1:A:1064:G:N7	2.88	0.41
1:A:1430:C:C2	1:A:1471:G:N2	2.88	0.41
3:C:59:ARG:H	10:J:92:THR:CG2	2.33	0.41
3:C:154:SER:OG	3:C:197:GLY:N	2.50	0.41
4:D:100:ARG:NH1	4:D:137:SER:HA	2.35	0.41
6:F:46:ARG:HH22	18:R:37:VAL:HG21	1.84	0.41
12:L:20:LYS:H	12:L:20:LYS:CE	2.33	0.41
18:R:50:ILE:HD11	18:R:70:ILE:HG21	2.02	0.41
18:R:79:LEU:HA	18:R:80:PRO:HD3	1.72	0.41
20:T:33:ILE:HD11	20:T:62:LEU:C	2.46	0.41
1:A:445:G:C2	1:A:490:G:N1	2.88	0.41
1:A:631:G:H2'	1:A:632:A:C8	2.55	0.41
1:A:644:G:C5	1:A:645:C:C5	3.08	0.41
1:A:964:A:N6	24:A:2280:HOH:O	2.53	0.41
1:A:1015:A:H2'	1:A:1016:A:C8	2.55	0.41
1:A:1144:G:N2	1:A:1145:C:C2	2.84	0.41
1:A:1157:A:C2	1:A:1181:G:N3	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:55:PHE:HD2	2:B:58:ILE:HD12	1.85	0.41
2:B:69:LEU:C	2:B:69:LEU:HD23	2.45	0.41
4:D:88:VAL:HG12	4:D:91:SER:H	1.85	0.41
5:E:118:ILE:O	5:E:119:LEU:HD23	2.21	0.41
6:F:14:LEU:HD21	6:F:84:ASN:OD1	2.21	0.41
6:F:38:GLU:HB2	6:F:64:GLN:HG2	2.03	0.41
6:F:44:GLY:HA2	6:F:59:TYR:CD2	2.56	0.41
9:I:19:LEU:HD23	9:I:60:ASP:O	2.19	0.41
18:R:26:LEU:HD23	18:R:29:PHE:CE2	2.55	0.41
18:R:46:GLU:H	18:R:46:GLU:CD	2.28	0.41
21:U:18:TYR:HB2	21:U:24:ARG:HH21	1.85	0.41
1:A:142:G:H2'	1:A:143:A:H8	1.85	0.41
1:A:200:G:H2'	1:A:201:C:O4'	2.20	0.41
1:A:1014:A:C2	1:A:1219:U:H1'	2.56	0.41
1:A:1018:C:H2'	1:A:1019:C:O4'	2.21	0.41
2:B:178:ARG:HH12	2:B:198:ASP:CG	2.22	0.41
4:D:155:LEU:HD23	4:D:156:GLU:N	2.35	0.41
5:E:78:HIS:ND1	8:H:104:ARG:HG3	2.36	0.41
7:G:40:ALA:CB	9:I:41:VAL:HG21	2.51	0.41
7:G:89:MET:HA	7:G:155:ARG:NH1	2.36	0.41
8:H:2:LEU:HD23	8:H:3:THR:H	1.81	0.41
8:H:59:LEU:HA	8:H:59:LEU:HD23	1.65	0.41
10:J:21:GLN:O	10:J:25:GLU:HG3	2.20	0.41
10:J:81:THR:O	10:J:85:LEU:HD13	2.20	0.41
12:L:19:ARG:HA	12:L:20:LYS:HZ3	1.85	0.41
12:L:114:LYS:HB3	12:L:114:LYS:HE2	1.78	0.41
13:M:82:MET:HA	13:M:89:GLY:HA3	2.02	0.41
17:Q:5:VAL:HG22	17:Q:60:ILE:CD1	2.51	0.41
1:A:77:G:C5	1:A:93:G:C2	3.09	0.41
1:A:1005:A:C2	1:A:1026:G:N3	2.89	0.41
3:C:18:TRP:O	3:C:21:ARG:NH1	2.54	0.41
3:C:73:PRO:O	3:C:76:VAL:HB	2.20	0.41
5:E:107:ARG:O	5:E:111:GLU:HB2	2.20	0.41
10:J:42:THR:HG23	10:J:67:THR:C	2.46	0.41
14:N:39:LEU:HA	14:N:39:LEU:HD23	1.71	0.41
16:P:2:VAL:HG22	16:P:64:ALA:HB2	2.03	0.41
17:Q:83:ASP:OD1	17:Q:84:LEU:HD12	2.21	0.41
19:S:23:ASN:ND2	19:S:43:GLU:O	2.48	0.41
1:A:60:A:N1	1:A:107:G:O2'	2.41	0.41
1:A:91:C:H5''	1:A:92:C:OP2	2.21	0.41
1:A:422:C:H5''	1:A:423:G:C4	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:A:C4	1:A:487:A:C2	3.09	0.41
1:A:674:G:H21	11:K:116:HIS:HB2	1.85	0.41
1:A:737:A:OP1	6:F:91:VAL:HG13	2.20	0.41
1:A:789:U:O2	1:A:789:U:H2'	2.21	0.41
1:A:794:A:N6	1:A:795:C:N4	2.68	0.41
1:A:809:G:C6	1:A:810:C:C5	3.09	0.41
1:A:951:G:H1	1:A:1230:C:H42	1.69	0.41
1:A:1168:A:H2'	1:A:1169:A:C8	2.56	0.41
1:A:1310:G:C2	1:A:1328:C:N3	2.89	0.41
1:A:1405:G:O2'	1:A:1518[A]:MA6:O2'	2.34	0.41
1:A:1491:G:N2	1:A:1492:A:C8	2.89	0.41
7:G:35:LYS:HD3	7:G:38:LEU:HD13	2.02	0.41
8:H:6:ILE:HB	8:H:85:ARG:HH21	1.82	0.41
9:I:118:LYS:HD2	9:I:121:ARG:HB3	2.03	0.41
12:L:84:LEU:HB2	12:L:104:VAL:HG11	2.03	0.41
15:O:38:ARG:HA	15:O:38:ARG:HD3	1.84	0.41
18:R:70:ILE:HG22	18:R:71:LYS:N	2.35	0.41
20:T:51:GLU:O	20:T:54:LYS:HB3	2.21	0.41
1:A:193:C:H2'	1:A:194:C:H6	1.85	0.41
1:A:407:G:OP1	4:D:115:ARG:NH1	2.53	0.41
1:A:854:G:H3'	1:A:871:U:O4	2.21	0.41
1:A:986:A:H2'	1:A:987:G:O4'	2.21	0.41
4:D:50:ARG:HA	4:D:51:PRO:HD2	1.94	0.41
4:D:121:VAL:HG11	4:D:136:PRO:HA	2.03	0.41
6:F:31:GLU:HG3	6:F:31:GLU:H	1.75	0.41
6:F:74:ASP:OD2	6:F:74:ASP:N	2.54	0.41
8:H:56:LYS:HA	8:H:57:PRO:HD3	1.71	0.41
8:H:81:HIS:ND1	8:H:81:HIS:N	2.69	0.41
8:H:83:ILE:HD13	8:H:83:ILE:HG21	1.68	0.41
11:K:34:ASP:O	11:K:37:GLY:N	2.37	0.41
12:L:46:LYS:NZ	12:L:47:LYS:HE2	2.35	0.41
15:O:12:ILE:O	15:O:15:PHE:N	2.54	0.41
16:P:42:ARG:HB2	16:P:44:THR:HG23	2.03	0.41
16:P:80:PHE:N	24:P:210:HOH:O	2.30	0.41
20:T:78:ALA:O	20:T:79:ARG:C	2.63	0.41
1:A:16:A:N1	1:A:919:A:H2	2.20	0.40
1:A:45:U:H2'	1:A:46:G:C8	2.57	0.40
1:A:77:G:C4	1:A:93:G:C2	3.09	0.40
1:A:113:G:H1	1:A:314:C:H42	1.69	0.40
1:A:236:G:H2'	1:A:237:C:O4'	2.21	0.40
1:A:582:U:H2'	1:A:583:A:H8	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:112:VAL:HG22	2:B:149:LEU:HD13	2.02	0.40
2:B:162:ILE:CG2	2:B:184:VAL:HG13	2.51	0.40
2:B:172:ILE:H	2:B:172:ILE:HG13	1.64	0.40
3:C:179:ARG:HG3	3:C:179:ARG:NH1	2.33	0.40
4:D:187:ARG:HH12	4:D:188:LEU:HD12	1.86	0.40
7:G:156:TRP:C	7:G:156:TRP:CD1	3.00	0.40
8:H:120:THR:H	8:H:123:GLU:HB2	1.86	0.40
13:M:48:LEU:HD23	13:M:49:THR:N	2.36	0.40
15:O:58:MET:HE3	15:O:58:MET:HB2	1.86	0.40
15:O:76:GLU:N	15:O:79:ARG:HH21	2.19	0.40
17:Q:23:VAL:HG21	17:Q:42:TYR:CD1	2.56	0.40
20:T:36:LEU:O	20:T:39:LYS:HB3	2.20	0.40
21:U:17:THR:HG22	21:U:18:TYR:H	1.86	0.40
1:A:401:C:OP1	4:D:73:ARG:NH1	2.54	0.40
1:A:765:G:N1	1:A:812:C:O2'	2.44	0.40
2:B:31:TYR:HA	2:B:46:LYS:NZ	2.35	0.40
2:B:163:PHE:HA	2:B:185:ILE:O	2.21	0.40
2:B:187:LEU:HD22	2:B:201:ILE:O	2.21	0.40
2:B:196:LEU:HD23	2:B:196:LEU:HA	1.74	0.40
3:C:159:GLY:HA2	3:C:193:TYR:CG	2.55	0.40
5:E:81:GLU:OE1	5:E:88:LYS:HD2	2.22	0.40
5:E:94:ALA:HB2	5:E:119:LEU:HG	2.03	0.40
9:I:34:ASN:OD1	9:I:34:ASN:N	2.54	0.40
10:J:50:ILE:H	10:J:50:ILE:CD1	2.24	0.40
11:K:33:THR:OG1	11:K:34:ASP:N	2.55	0.40
11:K:95:ILE:HD13	11:K:95:ILE:HA	1.49	0.40
1:A:108:G:C6	20:T:15:ARG:HG3	2.57	0.40
1:A:232:G:H2'	1:A:233:C:H6	1.86	0.40
1:A:578:C:H42	1:A:763:G:H1	1.70	0.40
1:A:689:C:OP1	11:K:27:ASN:ND2	2.45	0.40
1:A:729:A:H2'	1:A:730:G:O4'	2.21	0.40
1:A:932:C:H4'	7:G:4:ARG:NH2	2.37	0.40
1:A:939:G:H5''	7:G:102:ARG:HH22	1.86	0.40
1:A:992:U:H3	1:A:1044:A:H62	1.68	0.40
1:A:1144:G:N2	1:A:1146:A:H62	2.19	0.40
1:A:1245:A:N1	1:A:1293:G:C2	2.89	0.40
3:C:113:ALA:O	3:C:116:VAL:HG23	2.21	0.40
5:E:108:ALA:O	5:E:112:LEU:HB2	2.20	0.40
6:F:101:ALA:HB2	18:R:28:GLU:HG3	2.03	0.40
9:I:7:THR:HG22	9:I:8:GLY:N	2.36	0.40
10:J:10:GLY:O	10:J:67:THR:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:50:HIS:O	15:O:53:HIS:HB3	2.21	0.40
1:A:688:G:H2'	1:A:689:C:C6	2.57	0.40
1:A:736:C:OP1	18:R:68:LYS:HD3	2.21	0.40
1:A:1163:C:H2'	1:A:1164:G:C8	2.56	0.40
1:A:1185:G:O2'	1:A:1186:G:H5'	2.21	0.40
1:A:1431:C:H42	1:A:1469:G:H1	1.68	0.40
2:B:28:PHE:CD2	2:B:32:ILE:HD11	2.55	0.40
2:B:144:ARG:HG3	2:B:145:LEU:N	2.37	0.40
6:F:97:PHE:C	6:F:98:LEU:HD23	2.46	0.40
9:I:10:ARG:HG2	9:I:75:ASP:HB2	2.02	0.40
10:J:69:ASN:O	10:J:70:ARG:HD3	2.21	0.40
12:L:35:GLY:HA3	12:L:60:LEU:HD13	2.03	0.40
12:L:120:TYR:N	12:L:120:TYR:CD2	2.90	0.40
21:U:6:ARG:CD	21:U:15:ARG:HH12	2.33	0.40
1:A:807:A:C6	1:A:808:C:C4	3.09	0.40
1:A:1007:C:O2	1:A:1023:G:C2	2.74	0.40
1:A:1022:G:N2	1:A:1024:G:C2	2.89	0.40
4:D:5:ILE:HD12	4:D:5:ILE:H	1.87	0.40
4:D:105:VAL:HG21	4:D:126:ILE:HG12	2.03	0.40
5:E:92:LYS:HA	5:E:93:PRO:HD3	1.88	0.40
6:F:8:ILE:HG22	6:F:10:LEU:HG	2.04	0.40
8:H:102:ARG:NH1	8:H:105:ARG:HD2	2.36	0.40
9:I:117:HIS:NE2	9:I:123:PRO:HB3	2.37	0.40
10:J:6:ILE:HG12	10:J:98:ILE:CD1	2.52	0.40
12:L:28:LYS:C	12:L:30:ALA:H	2.30	0.40
12:L:113:ARG:HH12	12:L:116:SER:H	1.69	0.40
13:M:51:ALA:HA	13:M:54:VAL:HG12	2.04	0.40
20:T:29:LYS:O	20:T:32:ALA:HB3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	232/256 (91%)	209 (90%)	22 (10%)	1 (0%)	30	64
3	C	204/239 (85%)	180 (88%)	23 (11%)	1 (0%)	24	59
4	D	206/209 (99%)	195 (95%)	11 (5%)	0	100	100
5	E	148/162 (91%)	135 (91%)	13 (9%)	0	100	100
6	F	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
7	G	153/156 (98%)	136 (89%)	17 (11%)	0	100	100
8	H	136/138 (99%)	130 (96%)	6 (4%)	0	100	100
9	I	125/128 (98%)	113 (90%)	11 (9%)	1 (1%)	16	50
10	J	96/105 (91%)	80 (83%)	14 (15%)	2 (2%)	5	32
11	K	114/129 (88%)	101 (89%)	13 (11%)	0	100	100
12	L	121/135 (90%)	108 (89%)	12 (10%)	1 (1%)	16	50
13	M	116/126 (92%)	100 (86%)	15 (13%)	1 (1%)	14	47
14	N	58/61 (95%)	48 (83%)	9 (16%)	1 (2%)	7	35
15	O	85/89 (96%)	77 (91%)	8 (9%)	0	100	100
16	P	81/88 (92%)	79 (98%)	2 (2%)	0	100	100
17	Q	97/105 (92%)	86 (89%)	11 (11%)	0	100	100
18	R	68/88 (77%)	59 (87%)	9 (13%)	0	100	100
19	S	78/93 (84%)	70 (90%)	7 (9%)	1 (1%)	9	40
20	T	97/106 (92%)	79 (81%)	18 (19%)	0	100	100
21	U	22/27 (82%)	18 (82%)	4 (18%)	0	100	100
All	All	2336/2541 (92%)	2097 (90%)	230 (10%)	9 (0%)	30	64

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	L	28	LYS
19	S	31	ILE
2	B	21	ARG
9	I	119	ALA
10	J	86	MET
14	N	31	ARG
10	J	34	VAL
13	M	84	ILE
3	C	76	VAL

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	202/220 (92%)	164 (81%)	38 (19%)	1	10
3	C	160/188 (85%)	123 (77%)	37 (23%)	1	5
4	D	180/181 (99%)	144 (80%)	36 (20%)	1	9
5	E	115/123 (94%)	85 (74%)	30 (26%)	0	3
6	F	90/90 (100%)	76 (84%)	14 (16%)	2	15
7	G	126/127 (99%)	108 (86%)	18 (14%)	3	17
8	H	119/119 (100%)	87 (73%)	32 (27%)	0	3
9	I	98/99 (99%)	86 (88%)	12 (12%)	5	21
10	J	87/92 (95%)	67 (77%)	20 (23%)	1	5
11	K	88/99 (89%)	75 (85%)	13 (15%)	3	16
12	L	103/110 (94%)	79 (77%)	24 (23%)	1	5
13	M	94/101 (93%)	76 (81%)	18 (19%)	1	10
14	N	49/50 (98%)	38 (78%)	11 (22%)	1	6
15	O	79/80 (99%)	60 (76%)	19 (24%)	1	4
16	P	72/74 (97%)	58 (81%)	14 (19%)	1	9
17	Q	94/97 (97%)	68 (72%)	26 (28%)	0	3
18	R	61/77 (79%)	54 (88%)	7 (12%)	5	22
19	S	71/80 (89%)	63 (89%)	8 (11%)	5	23
20	T	76/82 (93%)	54 (71%)	22 (29%)	0	2
21	U	19/22 (86%)	14 (74%)	5 (26%)	0	3
All	All	1983/2111 (94%)	1579 (80%)	404 (20%)	1	8

All (404) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	7	VAL
2	B	8	LYS
2	B	12	GLU

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Mol	Chain	Res	Type
2	B	19	HIS
2	B	21	ARG
2	B	23	ARG
2	B	27	LYS
2	B	39	ILE
2	B	44	LEU
2	B	48	MET
2	B	59	GLU
2	B	63	MET
2	B	67	THR
2	B	97	TRP
2	B	102	LEU
2	B	107	THR
2	B	112	VAL
2	B	113	HIS
2	B	126	GLU
2	B	127	ILE
2	B	128	GLU
2	B	139	LYS
2	B	142	LEU
2	B	157	ARG
2	B	158	LEU
2	B	160	ASP
2	B	162	ILE
2	B	165	VAL
2	B	168	THR
2	B	172	ILE
2	B	178	ARG
2	B	190	THR
2	B	196	LEU
2	B	200	ILE
2	B	208	ILE
2	B	217	ARG
2	B	221	LEU
2	B	238	LEU
3	C	3	ASN
3	C	4	LYS
3	C	11	ARG
3	C	16	ARG
3	C	17	ASP
3	C	26	LYS
3	C	33	LEU

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Mol	Chain	Res	Type
3	C	34	LEU
3	C	37	GLN
3	C	52	LEU
3	C	70	VAL
3	C	72	LYS
3	C	75	VAL
3	C	79	ARG
3	C	84	ILE
3	C	91	LEU
3	C	99	VAL
3	C	103	VAL
3	C	105	GLU
3	C	107	GLN
3	C	111	LEU
3	C	116	VAL
3	C	132	ARG
3	C	153	VAL
3	C	165	THR
3	C	167	TRP
3	C	172	ARG
3	C	175	LEU
3	C	176	HIS
3	C	178	LEU
3	C	188	LEU
3	C	191	THR
3	C	192	THR
3	C	193	TYR
3	C	195	VAL
3	C	202	ILE
3	C	204	LEU
4	D	5	ILE
4	D	10	ARG
4	D	17	VAL
4	D	20	TYR
4	D	25	ARG
4	D	34	GLU
4	D	35	ARG
4	D	47	ARG
4	D	50	ARG
4	D	57	ARG
4	D	58	LEU
4	D	61	LYS

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Mol	Chain	Res	Type
4	D	64	LEU
4	D	78	LEU
4	D	92	VAL
4	D	101	LEU
4	D	103	ASN
4	D	104	VAL
4	D	115	ARG
4	D	122	ARG
4	D	131	ARG
4	D	137	SER
4	D	141	ARG
4	D	145	GLU
4	D	155	LEU
4	D	157	LEU
4	D	158	ILE
4	D	160	GLN
4	D	176	LEU
4	D	178	VAL
4	D	187	ARG
4	D	188	LEU
4	D	192	GLU
4	D	194	LEU
4	D	196	LEU
4	D	202	LEU
5	E	5	ASP
5	E	6	PHE
5	E	12	LEU
5	E	14	ARG
5	E	15	ARG
5	E	26	PHE
5	E	33	VAL
5	E	34	VAL
5	E	41	VAL
5	E	43	LEU
5	E	53	LEU
5	E	55	VAL
5	E	60	TYR
5	E	61	TYR
5	E	64	ARG
5	E	68	GLU
5	E	71	LEU
5	E	75	THR

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Mol	Chain	Res	Type
5	E	76	ILE
5	E	79	GLU
5	E	80	ILE
5	E	84	PHE
5	E	100	VAL
5	E	112	LEU
5	E	123	LEU
5	E	125	SER
5	E	131	ILE
5	E	144	THR
5	E	148	VAL
5	E	150	ARG
6	F	1	MET
6	F	6	VAL
6	F	9	VAL
6	F	10	LEU
6	F	19	LEU
6	F	26	ILE
6	F	28	ARG
6	F	31	GLU
6	F	40	VAL
6	F	43	LEU
6	F	70	ASP
6	F	75	LEU
6	F	79	LEU
6	F	84	ASN
7	G	3	ARG
7	G	6	ARG
7	G	23	VAL
7	G	27	ILE
7	G	30	ILE
7	G	38	LEU
7	G	41	ARG
7	G	69	VAL
7	G	77	SER
7	G	85	TYR
7	G	87	VAL
7	G	92	SER
7	G	113	GLU
7	G	115	ARG
7	G	126	ASP
7	G	135	VAL

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Mol	Chain	Res	Type
7	G	146	GLU
7	G	149	ARG
8	H	3	THR
8	H	11	THR
8	H	12	ARG
8	H	14	ARG
8	H	19	VAL
8	H	25	ASP
8	H	29	SER
8	H	35	ILE
8	H	50	ARG
8	H	51	VAL
8	H	54	ASP
8	H	61	VAL
8	H	63	LEU
8	H	65	TYR
8	H	68	ARG
8	H	77	GLU
8	H	83	ILE
8	H	85	ARG
8	H	86	ILE
8	H	87	SER
8	H	88	LYS
8	H	91	ARG
8	H	95	VAL
8	H	97	VAL
8	H	103	VAL
8	H	109	ILE
8	H	122	ARG
8	H	125	ARG
8	H	127	LEU
8	H	129	VAL
8	H	133	LEU
8	H	137	VAL
9	I	20	ARG
9	I	56	LEU
9	I	64	THR
9	I	91	ASP
9	I	92	TYR
9	I	104	ARG
9	I	108	VAL
9	I	109	VAL

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Mol	Chain	Res	Type
9	I	111	ARG
9	I	118	LYS
9	I	121	ARG
9	I	124	GLN
10	J	8	LEU
10	J	16	LEU
10	J	21	GLN
10	J	23	ILE
10	J	43	ARG
10	J	44	VAL
10	J	50	ILE
10	J	55	LYS
10	J	60	ARG
10	J	61	GLU
10	J	66	ARG
10	J	68	HIS
10	J	73	ASP
10	J	74	ILE
10	J	75	ILE
10	J	78	ASN
10	J	79	ARG
10	J	83	GLU
10	J	89	ASP
10	J	94	VAL
11	K	11	LYS
11	K	14	VAL
11	K	29	ILE
11	K	30	VAL
11	K	33	THR
11	K	53	SER
11	K	62	GLN
11	K	92	GLU
11	K	95	ILE
11	K	105	VAL
11	K	108	ILE
11	K	124	LYS
11	K	126	ARG
12	L	7	ILE
12	L	13	LYS
12	L	18	VAL
12	L	19	ARG
12	L	20	LYS

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Mol	Chain	Res	Type
12	L	28	LYS
12	L	33	ARG
12	L	34	ARG
12	L	36	VAL
12	L	52	LEU
12	L	55	VAL
12	L	60	LEU
12	L	61	THR
12	L	62	SER
12	L	65	GLU
12	L	66	VAL
12	L	67	THR
12	L	79	GLU
12	L	96	VAL
12	L	100	ILE
12	L	104	VAL
12	L	116	SER
12	L	122	THR
12	L	124	LYS
13	M	17	VAL
13	M	19	LEU
13	M	27	LYS
13	M	35	GLU
13	M	39	ILE
13	M	44	ARG
13	M	49	THR
13	M	50	GLU
13	M	53	VAL
13	M	54	VAL
13	M	56	LEU
13	M	60	VAL
13	M	64	TRP
13	M	65	LYS
13	M	77	ASN
13	M	88	ARG
13	M	103	THR
13	M	117	VAL
14	N	3	ARG
14	N	9	LYS
14	N	21	TYR
14	N	22	THR
14	N	25	VAL

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Mol	Chain	Res	Type
14	N	33	VAL
14	N	40	CYS
14	N	42	ILE
14	N	53	LEU
14	N	56	VAL
14	N	58	LYS
15	O	8	LYS
15	O	22	THR
15	O	31	LEU
15	O	32	LEU
15	O	34	LEU
15	O	39	LEU
15	O	41	GLU
15	O	44	LYS
15	O	45	VAL
15	O	56	LEU
15	O	57	LEU
15	O	65	ARG
15	O	66	LEU
15	O	67	LEU
15	O	72	ARG
15	O	78	TYR
15	O	81	LEU
15	O	83	GLU
15	O	85	LEU
16	P	2	VAL
16	P	11	SER
16	P	20	VAL
16	P	31	LYS
16	P	33	ILE
16	P	54	GLU
16	P	55	ARG
16	P	61	SER
16	P	62	VAL
16	P	65	GLN
16	P	67	THR
16	P	74	LEU
16	P	80	PHE
16	P	82	GLN
17	Q	9	VAL
17	Q	10	VAL
17	Q	14	LYS

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Mol	Chain	Res	Type
17	Q	21	VAL
17	Q	23	VAL
17	Q	34	LYS
17	Q	36	ILE
17	Q	37	LYS
17	Q	43	LEU
17	Q	57	VAL
17	Q	59	ILE
17	Q	60	ILE
17	Q	62	SER
17	Q	67	LYS
17	Q	68	ARG
17	Q	73	VAL
17	Q	75	ARG
17	Q	77	VAL
17	Q	81	ARG
17	Q	84	LEU
17	Q	85	VAL
17	Q	89	LEU
17	Q	90	ILE
17	Q	92	ARG
17	Q	93	GLN
17	Q	100	LYS
18	R	28	GLU
18	R	31	LEU
18	R	39	VAL
18	R	40	LEU
18	R	53	ARG
18	R	70	ILE
18	R	84	LYS
19	S	11	VAL
19	S	25	LYS
19	S	27	GLU
19	S	33	THR
19	S	45	VAL
19	S	63	THR
19	S	77	THR
19	S	79	THR
20	T	9	ASN
20	T	18	GLN
20	T	19	SER
20	T	25	ARG

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Mol	Chain	Res	Type
20	T	33	ILE
20	T	36	LEU
20	T	37	SER
20	T	41	ILE
20	T	46	GLU
20	T	53	LEU
20	T	62	LEU
20	T	64	ASP
20	T	68	LYS
20	T	71	THR
20	T	74	LYS
20	T	75	ASN
20	T	84	LEU
20	T	85	MET
20	T	87	LYS
20	T	91	LEU
20	T	92	LEU
20	T	93	GLU
21	U	9	ARG
21	U	10	ARG
21	U	12	LYS
21	U	17	THR
21	U	25	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	19	HIS
2	B	135	GLN
2	B	212	GLN
3	C	6	HIS
3	C	98	ASN
3	C	108	ASN
3	C	176	HIS
4	D	45	GLN
4	D	129	ASN
4	D	161	ASN
5	E	56	GLN
5	E	72	GLN
7	G	28	ASN
9	I	3	GLN
9	I	73	GLN

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Mol	Chain	Res	Type
10	J	21	GLN
10	J	56	HIS
10	J	62	HIS
10	J	76	ASN
11	K	26	ASN
11	K	62	GLN
13	M	40	ASN
15	O	28	GLN
15	O	53	HIS
16	P	16	HIS
16	P	76	GLN
16	P	82	GLN
17	Q	96	GLN
19	S	53	ASN
20	T	18	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1505/1522 (98%)	336 (22%)	50 (3%)

All (336) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	7	G
1	A	8	A
1	A	9	G
1	A	13	U
1	A	32	A
1	A	39	G
1	A	40	C
1	A	47	C
1	A	48	C
1	A	49	U
1	A	50	A
1	A	51	A
1	A	79	G
1	A	80	G
1	A	81	U
1	A	82	U

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Mol	Chain	Res	Type
1	A	91	C
1	A	92	C
1	A	101	A
1	A	108	G
1	A	115	G
1	A	116	A
1	A	117	G
1	A	121	C
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	163	C
1	A	166	G
1	A	182	U
1	A	183	G
1	A	190(D)	U
1	A	190(E)	U
1	A	195	A
1	A	197	A
1	A	202	U
1	A	203	U
1	A	216	G
1	A	220	G
1	A	231	G
1	A	246	A
1	A	247	G
1	A	251	G
1	A	252	U
1	A	254	G
1	A	265	G
1	A	266	G
1	A	267	C
1	A	269	C
1	A	279	A
1	A	281	G
1	A	282	A
1	A	289	G
1	A	292	G
1	A	301	G
1	A	319	G
1	A	321	A
1	A	328	C

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Mol	Chain	Res	Type
1	A	329	A
1	A	331	G
1	A	332	G
1	A	344	A
1	A	345	C
1	A	346	G
1	A	351	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	365	U
1	A	366	C
1	A	367	U
1	A	371	G
1	A	372	C
1	A	373	A
1	A	382	A
1	A	384	G
1	A	388	G
1	A	390	C
1	A	397	A
1	A	398	C
1	A	406	G
1	A	410	G
1	A	412	A
1	A	421	U
1	A	422	C
1	A	423	G
1	A	424	G
1	A	429	U
1	A	430	A
1	A	439	A
1	A	450	G
1	A	452	A
1	A	460	A
1	A	461	C
1	A	481	G
1	A	482	A
1	A	483	C
1	A	484	G
1	A	485	G
1	A	497	A

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Mol	Chain	Res	Type
1	A	498	U
1	A	509	A
1	A	510	A
1	A	511	C
1	A	517	G
1	A	518	C
1	A	519	C
1	A	530	G
1	A	531	U
1	A	533	A
1	A	536	C
1	A	545	C
1	A	547	A
1	A	559	A
1	A	560	U
1	A	562	C
1	A	563	A
1	A	564	C
1	A	572	A
1	A	573	A
1	A	576	G
1	A	577	G
1	A	579	G
1	A	588	G
1	A	596	C
1	A	615	C
1	A	618	C
1	A	624	C
1	A	649	G
1	A	653	A
1	A	665	A
1	A	670	G
1	A	686	U
1	A	687	A
1	A	688	G
1	A	701	C
1	A	702	A
1	A	703	G
1	A	718	G
1	A	721	G
1	A	723	U
1	A	724	G

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Mol	Chain	Res	Type
1	A	731	G
1	A	740	U
1	A	741	G
1	A	749	C
1	A	751	U
1	A	755	G
1	A	761	G
1	A	766	A
1	A	777	A
1	A	781	A
1	A	782	A
1	A	789	U
1	A	792	A
1	A	793	U
1	A	794	A
1	A	799	G
1	A	812	C
1	A	813	U
1	A	815	A
1	A	817	C
1	A	818	G
1	A	821	G
1	A	828	A
1	A	838	G
1	A	839	U
1	A	840	C
1	A	841	U
1	A	848	C
1	A	851	G
1	A	855	G
1	A	859	A
1	A	869	G
1	A	873	A
1	A	876	G
1	A	889	A
1	A	902	G
1	A	914	A
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	941	G

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Mol	Chain	Res	Type
1	A	942	G
1	A	950	U
1	A	954	G
1	A	960	U
1	A	961	U
1	A	966	M2G
1	A	967	5MC
1	A	968	A
1	A	969	A
1	A	971	G
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	979	C
1	A	989	C
1	A	991	U
1	A	992	U
1	A	993	G
1	A	994	A
1	A	1004	A
1	A	1005	A
1	A	1008	C
1	A	1017	G
1	A	1020	U
1	A	1021	G
1	A	1023	G
1	A	1026	G
1	A	1030(B)	C
1	A	1034	G
1	A	1045	C
1	A	1050	G
1	A	1052	U
1	A	1053	G
1	A	1054	C
1	A	1055	A
1	A	1060	C
1	A	1065	U
1	A	1066	C
1	A	1068	G
1	A	1078	U
1	A	1085	U

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Mol	Chain	Res	Type
1	A	1092	A
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1124	G
1	A	1125	U
1	A	1126	U
1	A	1127	G
1	A	1129	C
1	A	1130	A
1	A	1131	G
1	A	1132	C
1	A	1138	G
1	A	1139	G
1	A	1140	C
1	A	1146	A
1	A	1147	C
1	A	1157	A
1	A	1159	U
1	A	1160	G
1	A	1171	G
1	A	1176	A
1	A	1183	A
1	A	1191	A
1	A	1196	U
1	A	1197	G
1	A	1198	G
1	A	1200	C
1	A	1201	A
1	A	1202	G
1	A	1212	U
1	A	1214	C
1	A	1224	G
1	A	1225	A
1	A	1226	C
1	A	1238	A
1	A	1241	G
1	A	1245	A
1	A	1256	A
1	A	1257	U
1	A	1258	G
1	A	1260	C

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Mol	Chain	Res	Type
1	A	1270	C
1	A	1273	G
1	A	1278	U
1	A	1280	A
1	A	1281	U
1	A	1286	A
1	A	1287	A
1	A	1288	A
1	A	1297	C
1	A	1299	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1305	G
1	A	1310	G
1	A	1317	C
1	A	1320	C
1	A	1322	C
1	A	1327	C
1	A	1336	C
1	A	1338	G
1	A	1340	A
1	A	1346	A
1	A	1347	G
1	A	1348	U
1	A	1351	U
1	A	1353	G
1	A	1358	U
1	A	1359	C
1	A	1360	A
1	A	1362	C
1	A	1364	U
1	A	1365	G
1	A	1368	G
1	A	1370	G
1	A	1378	C
1	A	1379	G
1	A	1381	U
1	A	1399	C
1	A	1400	5MC
1	A	1402	4OC
1	A	1414	U

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Mol	Chain	Res	Type
1	A	1442	G
1	A	1443	G
1	A	1446	A
1	A	1447	G
1	A	1451	A
1	A	1452	C
1	A	1453	G
1	A	1485	U
1	A	1489	G
1	A	1490	C
1	A	1493	A
1	A	1494	G
1	A	1497	G
1	A	1498	UR3
1	A	1499	A
1	A	1503	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1507	A
1	A	1529	G
1	A	1530	G
1	A	1531	A
1	A	1532	U
1	A	1533	C

All (50) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U
1	A	12	U
1	A	13	U
1	A	65	U
1	A	115	G
1	A	129(A)	G
1	A	181	G
1	A	246	A
1	A	250	A
1	A	251	G
1	A	281	G
1	A	328	C
1	A	372	C

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Mol	Chain	Res	Type
1	A	428	G
1	A	429	U
1	A	484	G
1	A	496	A
1	A	509	A
1	A	518	C
1	A	559	A
1	A	687	A
1	A	701	C
1	A	748	C
1	A	776	G
1	A	792	A
1	A	812	C
1	A	840	C
1	A	913	A
1	A	960	U
1	A	965	A
1	A	975	A
1	A	992	U
1	A	1004	A
1	A	1049	U
1	A	1065	U
1	A	1067	A
1	A	1129	C
1	A	1145	C
1	A	1182	G
1	A	1190	G
1	A	1201	A
1	A	1257	U
1	A	1285	A
1	A	1300	G
1	A	1301	U
1	A	1346	A
1	A	1347	G
1	A	1380	U
1	A	1443	G
1	A	1505	G

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	UR3	A	1498	1	19,22,23	1.22	2 (10%)	26,32,35	1.45	3 (11%)
1	MA6	A	1518[B]	1	23,26,27	1.44	6 (26%)	33,38,41	0.86	1 (3%)
1	MA6	A	1519[A]	1	23,26,27	1.15	3 (13%)	33,38,41	0.96	2 (6%)
1	M2G	A	966	1	24,27,28	1.02	2 (8%)	33,40,43	1.09	3 (9%)
1	5MC	A	1400	1	19,22,23	1.57	4 (21%)	26,32,35	0.82	0
12	0TD	L	92	12	8,9,10	1.64	1 (12%)	6,11,13	3.11	3 (50%)
1	5MC	A	1407	1	19,22,23	1.39	4 (21%)	26,32,35	1.01	1 (3%)
1	2MG	A	1207	1	23,26,27	1.89	6 (26%)	33,38,41	1.06	4 (12%)
1	MA6	A	1519[B]	1	23,26,27	1.36	5 (21%)	33,38,41	1.15	3 (9%)
1	5MC	A	1404	1	19,22,23	1.41	2 (10%)	26,32,35	1.33	4 (15%)
1	PSU	A	1540	1	18,21,22	1.15	1 (5%)	21,30,33	1.55	3 (14%)
1	PSU	A	1541	1	18,21,22	1.28	1 (5%)	21,30,33	1.59	2 (9%)
1	4OC	A	1402	1	20,23,24	1.42	3 (15%)	25,32,35	0.60	0
1	7MG	A	527	1,22	23,26,27	3.57	6 (26%)	27,39,42	2.52	10 (37%)
1	MA6	A	1518[A]	1	23,26,27	1.19	3 (13%)	33,38,41	0.94	2 (6%)
1	PSU	A	516	1	18,21,22	1.34	1 (5%)	21,30,33	1.66	4 (19%)
1	5MC	A	967	1	19,22,23	1.19	3 (15%)	26,32,35	0.79	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UR3	A	1498	1	-	2/7/25/26	0/2/2/2
1	MA6	A	1518[B]	1	-	0/11/29/30	0/3/3/3
1	MA6	A	1519[A]	1	-	4/11/29/30	0/3/3/3
1	M2G	A	966	1	-	3/11/29/30	0/3/3/3
1	5MC	A	1400	1	-	2/7/25/26	0/2/2/2
12	0TD	L	92	12	-	2/7/12/14	-
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	A	1207	1	-	3/9/27/28	0/3/3/3
1	MA6	A	1519[B]	1	-	6/11/29/30	0/3/3/3
1	5MC	A	1404	1	-	0/7/25/26	0/2/2/2
1	PSU	A	1540	1	-	0/7/25/26	0/2/2/2
1	PSU	A	1541	1	-	1/7/25/26	0/2/2/2
1	4OC	A	1402	1	-	3/9/29/30	0/2/2/2
1	7MG	A	527	1,22	-	0/7/37/38	0/3/3/3
1	MA6	A	1518[A]	1	-	0/11/29/30	0/3/3/3
1	PSU	A	516	1	-	0/7/25/26	0/2/2/2
1	5MC	A	967	1	-	3/7/25/26	0/2/2/2

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	7MG	C8-N9	-14.60	1.36	1.45
1	A	527	7MG	C5-N7	6.08	1.43	1.35
1	A	516	PSU	C6-C5	4.71	1.40	1.35
1	A	1541	PSU	C6-C5	4.48	1.40	1.35
1	A	1207	2MG	C2-N2	4.39	1.42	1.33
1	A	1207	2MG	C2-N1	4.36	1.43	1.36
1	A	1404	5MC	C5-C4	4.36	1.47	1.44
1	A	1402	4OC	C2-N3	3.92	1.44	1.36
1	A	1540	PSU	C6-C5	3.92	1.39	1.35
1	A	1207	2MG	C6-N1	3.89	1.46	1.38
1	A	527	7MG	C2-N2	3.89	1.43	1.34
1	A	1407	5MC	C5-C4	3.79	1.47	1.44
1	A	1400	5MC	C2-N3	3.74	1.43	1.36
12	L	92	0TD	CB-CA	3.72	1.56	1.54
1	A	1400	5MC	C6-C5	3.44	1.40	1.34
1	A	1519[B]	MA6	C5-C4	3.14	1.44	1.39
1	A	967	5MC	C2-N3	3.12	1.42	1.36
1	A	1207	2MG	C4-N3	3.08	1.41	1.34
1	A	1518[A]	MA6	C5-C4	3.01	1.44	1.39
1	A	1400	5MC	C2-N1	2.96	1.46	1.40
1	A	1519[B]	MA6	C2-N1	2.96	1.39	1.33
1	A	1402	4OC	C4-N4	2.96	1.42	1.36
1	A	1519[A]	MA6	C5-C4	2.92	1.44	1.39
1	A	1518[B]	MA6	C5-C4	2.88	1.44	1.39
1	A	1518[B]	MA6	C4-N3	2.72	1.39	1.34
1	A	966	M2G	C4-N3	2.72	1.40	1.34
1	A	1498	UR3	C1'-N1	2.67	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1498	UR3	C4-N3	-2.48	1.35	1.40
1	A	1518[B]	MA6	C6-N1	2.47	1.39	1.34
1	A	1518[A]	MA6	C8-N9	2.47	1.41	1.37
1	A	1207	2MG	C8-N9	2.44	1.43	1.37
1	A	1518[B]	MA6	C8-N9	2.43	1.41	1.37
1	A	1519[A]	MA6	C8-N9	2.40	1.41	1.37
1	A	1407	5MC	C4-N4	2.37	1.40	1.34
1	A	527	7MG	C6-N1	-2.33	1.34	1.38
1	A	1407	5MC	C2-N3	2.19	1.40	1.36
1	A	966	M2G	C4-N9	2.17	1.43	1.38
1	A	1518[B]	MA6	C5-N7	2.16	1.43	1.39
1	A	1519[B]	MA6	C2-N3	2.16	1.37	1.33
1	A	1519[A]	MA6	C8-N7	2.16	1.35	1.31
1	A	1519[B]	MA6	C8-N9	2.14	1.41	1.37
1	A	527	7MG	C4-N3	2.14	1.39	1.34
1	A	1207	2MG	C2-N3	2.11	1.36	1.32
1	A	1404	5MC	O2-C2	-2.10	1.19	1.23
1	A	1400	5MC	C4-N4	2.07	1.39	1.34
1	A	1519[B]	MA6	C4-N9	2.04	1.41	1.37
1	A	527	7MG	C2-N1	-2.03	1.32	1.37
1	A	967	5MC	C6-C5	2.03	1.37	1.34
1	A	1518[B]	MA6	C4-N9	2.02	1.41	1.37
1	A	1518[A]	MA6	C4-N3	2.02	1.38	1.34
1	A	1402	4OC	C2-N1	2.02	1.44	1.40
1	A	1407	5MC	C2-N1	2.01	1.44	1.40
1	A	967	5MC	C4-N4	2.00	1.39	1.34

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	92	0TD	CSB-SB-CB	-6.45	90.77	102.36
1	A	527	7MG	C5-C6-N1	6.27	121.97	110.94
1	A	1498	UR3	C6-N1-C2	-4.81	117.86	121.80
1	A	527	7MG	N9-C4-N3	4.79	132.48	125.46
1	A	527	7MG	C2-N3-C4	4.62	120.26	112.30
1	A	527	7MG	C5-C4-N3	-4.50	119.67	128.13
1	A	1540	PSU	C4-N3-C2	-4.31	120.43	126.37
1	A	1541	PSU	C4-N3-C2	-4.26	120.50	126.37
1	A	516	PSU	N1-C2-N3	4.12	119.51	115.17
1	A	516	PSU	C4-N3-C2	-4.05	120.79	126.37
1	A	527	7MG	N9-C8-N7	4.00	109.03	103.37
1	A	527	7MG	C2-N1-C6	-3.77	118.27	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1541	PSU	N1-C2-N3	3.54	118.90	115.17
1	A	527	7MG	C6-C5-C4	-3.39	116.43	122.40
1	A	1540	PSU	N1-C2-N3	3.32	118.67	115.17
1	A	1519[B]	MA6	C4-C5-C6	3.30	119.33	115.91
1	A	527	7MG	C6-C5-N7	3.17	136.84	131.93
1	A	966	M2G	C5-C4-N3	-3.04	123.55	128.39
1	A	1404	5MC	N4-C4-N3	-2.91	113.23	118.51
1	A	1404	5MC	C5-C6-N1	-2.87	120.19	123.31
1	A	966	M2G	O6-C6-N1	-2.87	114.72	120.11
1	A	1404	5MC	C4-N3-C2	-2.79	116.93	120.81
1	A	1404	5MC	C5-C4-N3	2.68	124.50	121.75
1	A	1407	5MC	N4-C4-N3	-2.67	113.67	118.51
1	A	516	PSU	C6-N1-C2	-2.65	120.23	122.69
1	A	1519[B]	MA6	C5-C4-N3	-2.59	123.15	126.72
1	A	1207	2MG	C6-C5-N7	-2.55	125.64	130.29
1	A	1207	2MG	N9-C4-N3	2.53	131.02	125.95
12	L	92	0TD	OD1-CG-CB	-2.37	117.48	122.44
1	A	966	M2G	O6-C6-C5	2.36	132.78	126.53
1	A	527	7MG	O6-C6-C5	-2.34	121.87	127.62
1	A	1519[B]	MA6	C5-C6-N6	-2.32	121.67	125.33
1	A	1207	2MG	C5-C4-N3	-2.29	124.74	128.39
1	A	1518[A]	MA6	C2-N1-C6	2.25	117.33	111.83
12	L	92	0TD	CB-CA-N	-2.25	104.54	109.10
1	A	516	PSU	O4'-C1'-C2'	2.16	108.13	105.15
1	A	1498	UR3	C1'-N1-C6	2.14	125.36	120.78
1	A	1498	UR3	C5-C4-N3	-2.12	112.24	115.04
1	A	1518[B]	MA6	C2-N1-C6	2.12	117.01	111.83
1	A	527	7MG	O6-C6-N1	-2.10	116.16	120.11
1	A	1519[A]	MA6	C2-N1-C6	2.07	116.89	111.83
1	A	1540	PSU	O4'-C1'-C2'	2.03	107.96	105.15
1	A	1518[A]	MA6	N1-C6-N6	-2.03	114.38	116.86
1	A	1519[A]	MA6	N1-C2-N3	2.02	131.64	128.58
1	A	1207	2MG	C6-C5-C4	2.01	121.85	118.83

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	967	5MC	O4'-C4'-C5'-O5'
1	A	967	5MC	C3'-C4'-C5'-O5'
1	A	1207	2MG	N1-C2-N2-CM2
1	A	1207	2MG	N3-C2-N2-CM2

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Mol	Chain	Res	Type	Atoms
1	A	1402	4OC	O4'-C4'-C5'-O5'
1	A	1519[A]	MA6	O4'-C4'-C5'-O5'
1	A	1519[A]	MA6	C5-C6-N6-C9
1	A	1519[B]	MA6	C5-C6-N6-C9
1	A	1519[B]	MA6	C5-C6-N6-C10
1	A	1519[B]	MA6	N1-C6-N6-C9
1	A	1400	5MC	O4'-C4'-C5'-O5'
1	A	1402	4OC	C3'-C4'-C5'-O5'
1	A	1519[B]	MA6	O4'-C4'-C5'-O5'
1	A	1519[B]	MA6	C3'-C4'-C5'-O5'
1	A	1519[B]	MA6	N1-C6-N6-C10
1	A	966	M2G	C3'-C4'-C5'-O5'
1	A	1519[A]	MA6	C3'-C4'-C5'-O5'
1	A	966	M2G	O4'-C4'-C5'-O5'
1	A	1400	5MC	C3'-C4'-C5'-O5'
1	A	1498	UR3	O4'-C4'-C5'-O5'
1	A	1498	UR3	C3'-C4'-C5'-O5'
12	L	92	0TD	CG-CB-SB-CSB
12	L	92	0TD	SB-CB-CG-OD1
1	A	1541	PSU	O4'-C1'-C5-C4
1	A	966	M2G	C4'-C5'-O5'-P
1	A	1207	2MG	C3'-C4'-C5'-O5'
1	A	1519[A]	MA6	N1-C6-N6-C9
1	A	967	5MC	C2'-C1'-N1-C2
1	A	1402	4OC	C2'-C1'-N1-C2

There are no ring outliers.

13 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1498	UR3	5	0
1	A	1518[B]	MA6	3	0
1	A	1519[A]	MA6	3	0
1	A	966	M2G	1	0
1	A	1400	5MC	1	0
12	L	92	0TD	1	0
1	A	1407	5MC	1	0
1	A	1207	2MG	1	0
1	A	1519[B]	MA6	3	0
1	A	1404	5MC	1	0
1	A	527	7MG	2	0
1	A	1518[A]	MA6	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	967	5MC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 279 ligands modelled in this entry, 279 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1498/1522 (98%)	-0.63	9 (0%) 85 68	70, 178, 309, 393	4 (0%)
2	B	234/256 (91%)	-0.73	0 100 100	145, 220, 326, 363	0
3	C	206/239 (86%)	-0.48	2 (0%) 79 59	190, 245, 287, 310	0
4	D	208/209 (99%)	-0.30	6 (2%) 53 37	120, 190, 253, 286	0
5	E	150/162 (92%)	-0.75	0 100 100	101, 152, 195, 248	0
6	F	101/101 (100%)	-0.71	0 100 100	139, 213, 251, 291	0
7	G	155/156 (99%)	-0.48	1 (0%) 85 68	162, 218, 283, 328	0
8	H	138/138 (100%)	-0.69	0 100 100	94, 136, 183, 228	0
9	I	127/128 (99%)	-0.49	0 100 100	205, 246, 296, 310	0
10	J	98/105 (93%)	-0.16	1 (1%) 79 59	194, 256, 344, 406	0
11	K	116/129 (89%)	-0.67	0 100 100	134, 176, 225, 241	0
12	L	123/135 (91%)	-0.37	3 (2%) 59 42	99, 180, 223, 243	0
13	M	118/126 (93%)	-0.57	0 100 100	158, 213, 251, 306	0
14	N	60/61 (98%)	-0.16	2 (3%) 49 34	187, 237, 295, 326	0
15	O	87/89 (97%)	-0.59	0 100 100	110, 167, 217, 231	0
16	P	83/88 (94%)	-0.41	3 (3%) 46 33	130, 172, 227, 272	0
17	Q	99/105 (94%)	-0.57	0 100 100	115, 152, 216, 241	0
18	R	70/88 (79%)	-0.66	0 100 100	128, 177, 240, 273	0
19	S	80/93 (86%)	-0.21	2 (2%) 58 41	223, 271, 315, 328	0
20	T	99/106 (93%)	-0.19	2 (2%) 65 45	129, 172, 233, 280	0
21	U	24/27 (88%)	-0.01	4 (16%) 4 7	198, 224, 253, 260	0
All	All	3874/4063 (95%)	-0.55	35 (0%) 81 61	70, 194, 292, 406	4 (0%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	T	106	ALA	8.2
1	A	993	G	5.2
3	C	178	LEU	4.3
1	A	1129	C	3.9
3	C	2	GLY	3.5
19	S	3	ARG	3.1
1	A	1417	G	3.1
1	A	1517[A]	G	2.9
1	A	1516[A]	G	2.9
21	U	7	ARG	2.8
1	A	532	A	2.7
19	S	2	PRO	2.6
7	G	74	GLU	2.6
4	D	26	CYS	2.6
1	A	992	U	2.5
12	L	47	LYS	2.4
4	D	3	ARG	2.4
4	D	6	GLY	2.4
16	P	23	ASP	2.4
21	U	6	ARG	2.4
1	A	1220	G	2.4
14	N	3	ARG	2.3
14	N	25	VAL	2.3
4	D	9	CYS	2.3
20	T	12	ALA	2.3
1	A	1204	A	2.3
12	L	115	LYS	2.3
4	D	5	ILE	2.2
16	P	68	ASP	2.2
4	D	25	ARG	2.2
21	U	5	ASP	2.2
21	U	10	ARG	2.1
12	L	48	PRO	2.1
10	J	37	PRO	2.0
16	P	1	MET	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	PSU	A	1540	20/21	0.92	0.12	262,265,277,283	0
1	5MC	A	1407	21/22	0.95	0.11	157,205,219,224	0
1	PSU	A	1541	20/21	0.95	0.10	239,247,262,263	0
1	5MC	A	967	21/22	0.96	0.06	183,190,208,211	0
1	M2G	A	966	25/26	0.96	0.08	192,203,210,221	0
1	5MC	A	1400	21/22	0.97	0.06	141,159,171,180	0
1	UR3	A	1498	21/22	0.97	0.09	155,172,189,197	0
1	5MC	A	1404	21/22	0.98	0.06	141,170,203,221	0
1	7MG	A	527	24/25	0.98	0.07	141,171,178,185	0
1	2MG	A	1207	24/25	0.98	0.05	211,231,295,300	0
1	MA6	A	1518[A]	24/25	0.98	0.18	145,163,168,171	24
1	MA6	A	1518[B]	24/25	0.98	0.18	143,163,180,183	24
1	MA6	A	1519[A]	24/25	0.98	0.11	136,142,149,152	24
1	MA6	A	1519[B]	24/25	0.98	0.11	136,148,164,167	24
1	PSU	A	516	20/21	0.98	0.06	161,204,223,224	0
1	4OC	A	1402	22/23	0.98	0.08	148,156,171,187	0
12	0TD	L	92	10/11	0.99	0.07	158,180,208,372	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides 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. 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	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	A	1722	1/1	0.51	0.73	130,130,130,130	0
22	MG	M	201	1/1	0.51	0.17	160,160,160,160	0
22	MG	S	101	1/1	0.60	0.16	234,234,234,234	0
22	MG	A	1836	1/1	0.61	0.08	207,207,207,207	0
22	MG	A	1846	1/1	0.66	0.25	163,163,163,163	0
22	MG	A	1856	1/1	0.72	0.43	132,132,132,132	0
22	MG	A	1623	1/1	0.73	0.27	185,185,185,185	0
22	MG	A	1706	1/1	0.73	1.36	131,131,131,131	0
22	MG	Q	201	1/1	0.74	0.08	158,158,158,158	0
22	MG	A	1712	1/1	0.77	0.34	171,171,171,171	0
22	MG	P	101	1/1	0.77	0.34	102,102,102,102	0
22	MG	A	1742	1/1	0.78	0.19	148,148,148,148	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	A	1772	1/1	0.78	0.14	150,150,150,150	0
22	MG	A	1735	1/1	0.78	0.24	157,157,157,157	0
22	MG	A	1713	1/1	0.79	1.39	155,155,155,155	0
22	MG	A	1660	1/1	0.79	0.18	135,135,135,135	0
22	MG	A	1844	1/1	0.79	0.34	138,138,138,138	0
22	MG	A	1635	1/1	0.80	0.17	177,177,177,177	0
22	MG	A	1702	1/1	0.80	0.09	165,165,165,165	0
22	MG	A	1754	1/1	0.80	0.27	115,115,115,115	0
22	MG	A	1841	1/1	0.81	0.35	196,196,196,196	0
22	MG	B	301	1/1	0.82	0.10	173,173,173,173	0
22	MG	A	1782	1/1	0.82	0.07	517,517,517,517	0
22	MG	A	1736	1/1	0.82	0.38	110,110,110,110	0
22	MG	A	1663	1/1	0.82	0.17	315,315,315,315	0
22	MG	A	1857	1/1	0.82	0.17	189,189,189,189	0
22	MG	A	1667	1/1	0.83	0.15	128,128,128,128	0
22	MG	A	1775	1/1	0.83	0.17	120,120,120,120	0
22	MG	A	1778	1/1	0.83	0.29	164,164,164,164	0
22	MG	A	1829	1/1	0.84	0.07	317,317,317,317	0
22	MG	A	1685	1/1	0.84	0.17	247,247,247,247	0
22	MG	A	1768	1/1	0.84	0.33	164,164,164,164	0
22	MG	A	1765	1/1	0.85	0.20	149,149,149,149	0
22	MG	A	1664	1/1	0.86	0.24	120,120,120,120	0
22	MG	A	1737	1/1	0.86	0.37	139,139,139,139	0
22	MG	A	1862	1/1	0.86	0.80	129,129,129,129	0
22	MG	A	1838	1/1	0.86	0.16	198,198,198,198	0
22	MG	A	1746	1/1	0.87	0.35	157,157,157,157	0
22	MG	A	1849	1/1	0.87	0.43	141,141,141,141	0
22	MG	A	1640	1/1	0.87	0.23	165,165,165,165	0
22	MG	P	102	1/1	0.87	0.05	360,360,360,360	0
22	MG	A	1783	1/1	0.87	0.10	404,404,404,404	0
22	MG	A	1703	1/1	0.87	0.30	237,237,237,237	0
22	MG	A	1603	1/1	0.88	0.17	170,170,170,170	0
22	MG	A	1860	1/1	0.88	0.21	151,151,151,151	0
22	MG	A	1686	1/1	0.88	0.31	135,135,135,135	0
22	MG	A	1699	1/1	0.88	0.27	126,126,126,126	0
22	MG	A	1708	1/1	0.88	0.21	135,135,135,135	0
22	MG	A	1845	1/1	0.88	0.31	137,137,137,137	0
22	MG	A	1813	1/1	0.88	0.12	460,460,460,460	0
22	MG	A	1816	1/1	0.88	0.11	357,357,357,357	0
22	MG	A	1773	1/1	0.88	0.06	121,121,121,121	0
22	MG	A	1745	1/1	0.89	0.20	126,126,126,126	0
22	MG	C	301	1/1	0.89	0.11	166,166,166,166	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	A	1837	1/1	0.89	0.13	179,179,179,179	0
22	MG	A	1668	1/1	0.89	0.47	153,153,153,153	0
22	MG	A	1748	1/1	0.89	0.36	149,149,149,149	0
22	MG	A	1604	1/1	0.89	0.24	120,120,120,120	0
22	MG	A	1655	1/1	0.89	0.12	136,136,136,136	0
22	MG	A	1779	1/1	0.90	0.22	137,137,137,137	0
22	MG	A	1861	1/1	0.90	0.17	155,155,155,155	0
22	MG	A	1720	1/1	0.90	0.19	171,171,171,171	0
22	MG	A	1666	1/1	0.90	0.21	155,155,155,155	0
22	MG	A	1801	1/1	0.90	0.20	465,465,465,465	0
22	MG	A	1726	1/1	0.90	0.23	132,132,132,132	0
22	MG	A	1734	1/1	0.90	0.09	129,129,129,129	0
22	MG	A	1622	1/1	0.90	0.47	71,71,71,71	0
22	MG	A	1834	1/1	0.90	0.29	113,113,113,113	0
22	MG	A	1649	1/1	0.90	0.09	235,235,235,235	0
22	MG	A	1808	1/1	0.91	0.09	359,359,359,359	0
22	MG	A	1852	1/1	0.91	0.29	152,152,152,152	0
22	MG	A	1710	1/1	0.91	0.13	157,157,157,157	0
22	MG	A	1659	1/1	0.91	0.38	154,154,154,154	0
22	MG	A	1669	1/1	0.91	0.05	306,306,306,306	0
22	MG	A	1717	1/1	0.91	0.14	137,137,137,137	0
22	MG	A	1673	1/1	0.91	0.37	175,175,175,175	0
22	MG	A	1619	1/1	0.91	0.15	179,179,179,179	0
22	MG	A	1725	1/1	0.91	0.15	131,131,131,131	0
22	MG	D	303	1/1	0.91	0.15	138,138,138,138	0
22	MG	E	201	1/1	0.91	0.12	171,171,171,171	0
22	MG	A	1626	1/1	0.91	0.22	127,127,127,127	0
22	MG	A	1733	1/1	0.91	0.22	102,102,102,102	0
22	MG	A	1757	1/1	0.91	0.08	162,162,162,162	0
22	MG	A	1807	1/1	0.91	0.07	500,500,500,500	0
22	MG	A	1847	1/1	0.91	0.11	147,147,147,147	0
22	MG	A	1738	1/1	0.92	0.28	167,167,167,167	0
22	MG	A	1770	1/1	0.92	0.15	185,185,185,185	0
22	MG	A	1683	1/1	0.92	0.06	310,310,310,310	0
22	MG	A	1617	1/1	0.92	0.20	140,140,140,140	0
22	MG	A	1830	1/1	0.92	0.22	321,321,321,321	0
22	MG	A	1621	1/1	0.92	0.12	132,132,132,132	0
22	MG	A	1638	1/1	0.92	0.30	155,155,155,155	0
22	MG	A	1751	1/1	0.92	0.40	160,160,160,160	0
22	MG	A	1780	1/1	0.92	0.20	380,380,380,380	0
22	MG	A	1674	1/1	0.92	0.12	153,153,153,153	0
22	MG	A	1842	1/1	0.92	0.17	173,173,173,173	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	J	201	1/1	0.92	0.16	138,138,138,138	0
22	MG	A	1679	1/1	0.92	0.35	146,146,146,146	0
22	MG	A	1793	1/1	0.92	0.12	189,189,189,189	0
22	MG	A	1764	1/1	0.92	0.12	298,298,298,298	0
22	MG	A	1682	1/1	0.92	0.54	123,123,123,123	0
22	MG	A	1848	1/1	0.92	1.10	173,173,173,173	0
22	MG	A	1792	1/1	0.93	0.11	229,229,229,229	0
22	MG	A	1654	1/1	0.93	0.59	111,111,111,111	0
22	MG	A	1800	1/1	0.93	0.06	237,237,237,237	0
22	MG	A	1743	1/1	0.93	0.14	159,159,159,159	0
22	MG	A	1774	1/1	0.93	0.09	154,154,154,154	0
22	MG	A	1758	1/1	0.93	0.14	172,172,172,172	0
22	MG	A	1811	1/1	0.93	0.21	317,317,317,317	0
22	MG	A	1763	1/1	0.93	0.25	358,358,358,358	0
22	MG	A	1707	1/1	0.93	0.12	131,131,131,131	0
22	MG	A	1818	1/1	0.93	0.05	432,432,432,432	0
22	MG	A	1730	1/1	0.93	0.16	149,149,149,149	0
22	MG	A	1731	1/1	0.93	0.15	106,106,106,106	0
22	MG	A	1854	1/1	0.93	0.07	172,172,172,172	0
22	MG	A	1650	1/1	0.93	0.40	161,161,161,161	0
22	MG	A	1608	1/1	0.94	0.12	150,150,150,150	0
22	MG	A	1610	1/1	0.94	0.05	206,206,206,206	0
22	MG	A	1759	1/1	0.94	0.37	167,167,167,167	0
22	MG	A	1760	1/1	0.94	0.29	189,189,189,189	0
22	MG	A	1732	1/1	0.94	0.21	127,127,127,127	0
22	MG	A	1744	1/1	0.94	0.07	158,158,158,158	0
22	MG	A	1784	1/1	0.94	0.16	250,250,250,250	0
22	MG	A	1624	1/1	0.94	0.33	146,146,146,146	0
22	MG	B	302	1/1	0.94	0.08	219,219,219,219	0
22	MG	A	1767	1/1	0.94	0.14	136,136,136,136	0
22	MG	A	1796	1/1	0.94	0.21	271,271,271,271	0
22	MG	A	1798	1/1	0.94	0.20	514,514,514,514	0
22	MG	A	1647	1/1	0.94	0.14	132,132,132,132	0
22	MG	A	1709	1/1	0.94	0.07	157,157,157,157	0
22	MG	A	1802	1/1	0.94	0.29	225,225,225,225	0
22	MG	A	1616	1/1	0.94	0.17	190,190,190,190	0
22	MG	A	1752	1/1	0.94	0.11	149,149,149,149	0
22	MG	A	1711	1/1	0.94	0.13	101,101,101,101	0
22	MG	A	1850	1/1	0.95	0.28	140,140,140,140	0
22	MG	A	1636	1/1	0.95	0.16	114,114,114,114	0
22	MG	A	1627	1/1	0.95	0.08	113,113,113,113	0
22	MG	A	1855	1/1	0.95	0.08	133,133,133,133	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	A	1651	1/1	0.95	0.20	141,141,141,141	0
22	MG	A	1822	1/1	0.95	0.05	202,202,202,202	0
22	MG	A	1639	1/1	0.95	0.07	227,227,227,227	0
22	MG	A	1785	1/1	0.95	0.10	243,243,243,243	0
22	MG	A	1788	1/1	0.95	0.27	288,288,288,288	0
22	MG	A	1791	1/1	0.95	0.27	444,444,444,444	0
22	MG	A	1766	1/1	0.95	0.41	171,171,171,171	0
22	MG	A	1747	1/1	0.95	0.11	134,134,134,134	0
22	MG	A	1631	1/1	0.95	0.12	175,175,175,175	0
22	MG	A	1643	1/1	0.95	0.07	113,113,113,113	0
22	MG	A	1687	1/1	0.95	0.17	325,325,325,325	0
22	MG	A	1670	1/1	0.95	0.07	209,209,209,209	0
22	MG	A	1755	1/1	0.95	0.08	192,192,192,192	0
22	MG	A	1671	1/1	0.95	0.45	171,171,171,171	0
22	MG	A	1672	1/1	0.95	0.18	163,163,163,163	0
22	MG	A	1605	1/1	0.95	0.11	153,153,153,153	0
22	MG	A	1723	1/1	0.96	0.07	163,163,163,163	0
22	MG	A	1769	1/1	0.96	0.21	161,161,161,161	0
22	MG	A	1815	1/1	0.96	0.83	218,218,218,218	0
22	MG	A	1688	1/1	0.96	0.10	145,145,145,145	0
22	MG	A	1817	1/1	0.96	0.11	489,489,489,489	0
22	MG	A	1789	1/1	0.96	0.67	259,259,259,259	0
22	MG	A	1819	1/1	0.96	0.14	407,407,407,407	0
22	MG	A	1821	1/1	0.96	0.05	449,449,449,449	0
22	MG	A	1790	1/1	0.96	0.11	307,307,307,307	0
22	MG	A	1823	1/1	0.96	0.21	256,256,256,256	0
22	MG	A	1681	1/1	0.96	0.11	154,154,154,154	0
22	MG	A	1729	1/1	0.96	0.32	169,169,169,169	0
22	MG	A	1831	1/1	0.96	0.20	322,322,322,322	0
22	MG	A	1832	1/1	0.96	0.25	435,435,435,435	0
22	MG	A	1618	1/1	0.96	0.11	137,137,137,137	0
22	MG	A	1794	1/1	0.96	0.12	173,173,173,173	0
22	MG	A	1615	1/1	0.96	0.14	104,104,104,104	0
22	MG	A	1776	1/1	0.96	0.39	159,159,159,159	0
22	MG	J	202	1/1	0.96	0.06	501,501,501,501	0
22	MG	A	1705	1/1	0.96	0.29	129,129,129,129	0
22	MG	A	1628	1/1	0.96	0.13	189,189,189,189	0
22	MG	A	1676	1/1	0.96	0.06	173,173,173,173	0
22	MG	A	1721	1/1	0.96	0.04	166,166,166,166	0
22	MG	A	1662	1/1	0.96	0.08	182,182,182,182	0
22	MG	A	1840	1/1	0.97	0.21	153,153,153,153	0
22	MG	A	1634	1/1	0.97	0.07	118,118,118,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	A	1728	1/1	0.97	0.12	129,129,129,129	0
22	MG	A	1601	1/1	0.97	0.29	210,210,210,210	0
22	MG	A	1749	1/1	0.97	0.10	113,113,113,113	0
22	MG	A	1750	1/1	0.97	0.15	152,152,152,152	0
22	MG	A	1606	1/1	0.97	0.07	174,174,174,174	0
22	MG	A	1689	1/1	0.97	0.04	223,223,223,223	0
22	MG	A	1809	1/1	0.97	0.22	249,249,249,249	0
22	MG	A	1810	1/1	0.97	0.46	344,344,344,344	0
22	MG	A	1753	1/1	0.97	0.10	128,128,128,128	0
22	MG	A	1777	1/1	0.97	0.18	119,119,119,119	0
22	MG	A	1692	1/1	0.97	0.07	148,148,148,148	0
22	MG	A	1695	1/1	0.97	0.29	386,386,386,386	0
22	MG	A	1756	1/1	0.97	0.28	126,126,126,126	0
22	MG	A	1858	1/1	0.97	0.25	127,127,127,127	0
22	MG	A	1781	1/1	0.97	0.18	247,247,247,247	0
22	MG	A	1696	1/1	0.97	0.13	151,151,151,151	0
22	MG	A	1716	1/1	0.97	0.16	131,131,131,131	0
22	MG	A	1697	1/1	0.97	0.06	119,119,119,119	0
22	MG	A	1719	1/1	0.97	0.11	136,136,136,136	0
22	MG	A	1827	1/1	0.97	0.09	507,507,507,507	0
22	MG	D	302	1/1	0.97	0.04	140,140,140,140	0
22	MG	A	1787	1/1	0.97	0.07	254,254,254,254	0
22	MG	A	1761	1/1	0.97	0.04	205,205,205,205	0
22	MG	F	201	1/1	0.97	0.05	170,170,170,170	0
22	MG	A	1762	1/1	0.97	0.07	365,365,365,365	0
22	MG	A	1629	1/1	0.97	0.08	154,154,154,154	0
22	MG	A	1607	1/1	0.97	0.21	130,130,130,130	0
22	MG	A	1653	1/1	0.97	0.15	129,129,129,129	0
22	MG	A	1684	1/1	0.97	0.10	222,222,222,222	0
22	MG	A	1632	1/1	0.97	0.42	109,109,109,109	0
22	MG	A	1839	1/1	0.97	0.13	170,170,170,170	0
22	MG	A	1843	1/1	0.98	0.42	156,156,156,156	0
22	MG	A	1661	1/1	0.98	0.04	136,136,136,136	0
22	MG	A	1690	1/1	0.98	0.08	154,154,154,154	0
22	MG	A	1609	1/1	0.98	0.11	151,151,151,151	0
22	MG	A	1693	1/1	0.98	0.14	394,394,394,394	0
22	MG	A	1715	1/1	0.98	0.15	155,155,155,155	0
22	MG	A	1675	1/1	0.98	0.12	269,269,269,269	0
22	MG	A	1630	1/1	0.98	0.07	104,104,104,104	0
22	MG	A	1851	1/1	0.98	0.04	182,182,182,182	0
22	MG	A	1718	1/1	0.98	0.15	145,145,145,145	0
22	MG	A	1853	1/1	0.98	0.16	171,171,171,171	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	A	1739	1/1	0.98	0.17	158,158,158,158	0
22	MG	A	1740	1/1	0.98	0.07	138,138,138,138	0
22	MG	A	1741	1/1	0.98	0.44	145,145,145,145	0
22	MG	A	1625	1/1	0.98	0.14	114,114,114,114	0
22	MG	A	1665	1/1	0.98	0.06	180,180,180,180	0
22	MG	A	1652	1/1	0.98	0.10	188,188,188,188	0
22	MG	A	1824	1/1	0.98	0.17	424,424,424,424	0
22	MG	A	1826	1/1	0.98	0.15	178,178,178,178	0
22	MG	A	1602	1/1	0.98	0.25	237,237,237,237	0
22	MG	A	1704	1/1	0.98	0.16	105,105,105,105	0
22	MG	A	1724	1/1	0.98	0.07	127,127,127,127	0
22	MG	A	1642	1/1	0.98	0.08	129,129,129,129	0
22	MG	A	1795	1/1	0.98	0.19	416,416,416,416	0
22	MG	A	1771	1/1	0.98	0.12	139,139,139,139	0
22	MG	A	1835	1/1	0.98	0.11	161,161,161,161	0
22	MG	A	1797	1/1	0.98	0.19	387,387,387,387	0
22	MG	A	1611	1/1	0.98	0.06	234,234,234,234	0
22	MG	A	1799	1/1	0.98	0.08	224,224,224,224	0
22	MG	A	1657	1/1	0.98	0.06	190,190,190,190	0
22	MG	A	1612	1/1	0.98	0.21	172,172,172,172	0
22	MG	A	1648	1/1	0.98	0.05	139,139,139,139	0
22	MG	A	1804	1/1	0.98	0.18	228,228,228,228	0
22	MG	A	1698	1/1	0.99	0.10	180,180,180,180	0
22	MG	A	1633	1/1	0.99	0.08	368,368,368,368	0
22	MG	A	1820	1/1	0.99	0.06	437,437,437,437	0
22	MG	A	1700	1/1	0.99	0.10	143,143,143,143	0
22	MG	A	1701	1/1	0.99	0.06	101,101,101,101	0
22	MG	A	1644	1/1	0.99	0.12	143,143,143,143	0
22	MG	A	1645	1/1	0.99	0.07	87,87,87,87	0
22	MG	A	1825	1/1	0.99	0.09	264,264,264,264	0
22	MG	A	1646	1/1	0.99	0.08	205,205,205,205	0
22	MG	A	1614	1/1	0.99	0.22	194,194,194,194	0
22	MG	A	1828	1/1	0.99	0.24	281,281,281,281	0
22	MG	A	1656	1/1	0.99	0.04	146,146,146,146	0
22	MG	A	1859	1/1	0.99	0.09	161,161,161,161	0
22	MG	A	1677	1/1	0.99	0.10	189,189,189,189	0
22	MG	A	1803	1/1	0.99	0.21	413,413,413,413	0
22	MG	A	1691	1/1	0.99	0.08	197,197,197,197	0
22	MG	A	1833	1/1	0.99	0.12	338,338,338,338	0
22	MG	A	1805	1/1	0.99	0.10	450,450,450,450	0
22	MG	B	303	1/1	0.99	0.24	260,260,260,260	0
22	MG	A	1806	1/1	0.99	0.34	279,279,279,279	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	A	1727	1/1	0.99	0.08	113,113,113,113	0
22	MG	A	1613	1/1	0.99	0.04	144,144,144,144	0
22	MG	A	1786	1/1	0.99	0.09	449,449,449,449	0
22	MG	A	1680	1/1	0.99	0.10	165,165,165,165	0
22	MG	A	1694	1/1	0.99	0.13	346,346,346,346	0
22	MG	A	1812	1/1	0.99	0.20	450,450,450,450	0
22	MG	A	1658	1/1	0.99	0.10	210,210,210,210	0
22	MG	A	1814	1/1	0.99	0.16	336,336,336,336	0
22	MG	A	1641	1/1	0.99	0.23	139,139,139,139	0
22	MG	A	1714	1/1	0.99	0.09	118,118,118,118	0
22	MG	A	1620	1/1	0.99	0.03	107,107,107,107	0
23	ZN	D	301	1/1	0.99	0.15	147,147,147,147	0
23	ZN	N	101	1/1	0.99	0.05	258,258,258,258	0
22	MG	A	1678	1/1	1.00	0.15	180,180,180,180	0
22	MG	A	1637	1/1	1.00	0.12	283,283,283,283	0

6.5 Other polymers ⓘ

There are no such residues in this entry.