



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:44 PM UTC

PDB ID : 4DV2 / pdb_00004dv2
Title : Crystal structure of the *Thermus thermophilus* 30S ribosomal subunit with a 16S rRNA mutation, C912A
Authors : Demirci, H.; Murphy IV, F.; Murphy, E.; Gregory, S.T.; Dahlberg, A.E.; Jogl, G.
Deposited on : 2012-02-22
Resolution : 3.65 Å(reported)

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

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

A user guide is available at

<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

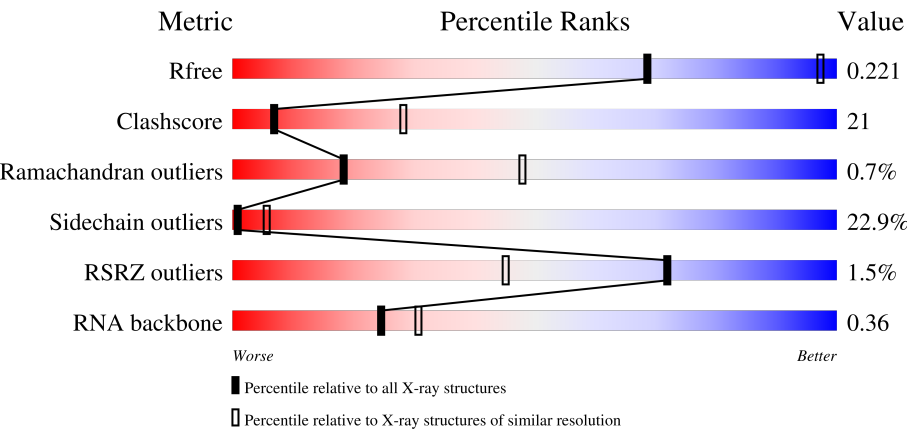
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.65 Å.

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



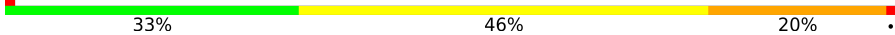
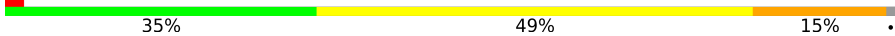
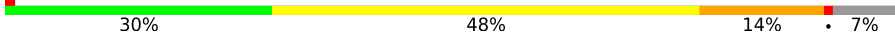
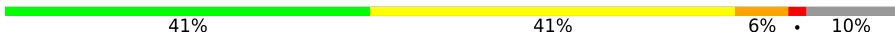
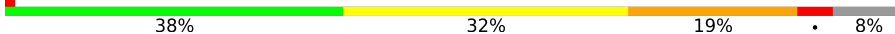
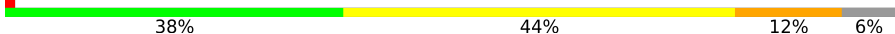
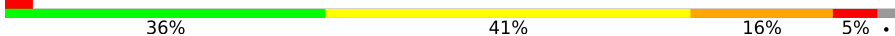
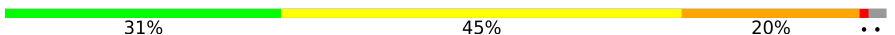
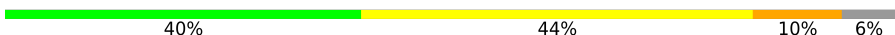
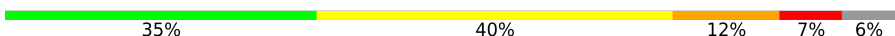
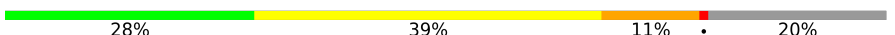
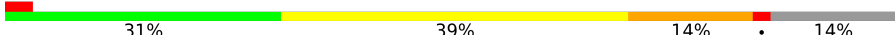
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1132 (3.76-3.52)
Clashscore	190562	1014 (3.74-3.54)
Ramachandran outliers	187476	1123 (3.76-3.52)
Sidechain outliers	187428	1121 (3.76-3.52)
RSRZ outliers	180081	1130 (3.76-3.52)
RNA backbone	3983	1026 (4.22-3.06)

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	2% 37% 45% 17% .
2	B	256	% 37% 41% 12% . 9%
3	C	239	% 29% 43% 12% . 14%
4	D	209	4% 49% 38% 12%

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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	1672	-	-	-	X
22	MG	A	1713	-	-	-	X
22	MG	A	1751	-	-	-	X

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 52441 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
			32646	14541	6041	10546	1518			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	912	A	C	engineered mutation	GB M26923.1
A	1534	C	A	conflict	GB M26923.1
A	1535	A	C	conflict	GB M26923.1

- Molecule 2 is a protein called ribosomal protein S2.

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

- Molecule 3 is a protein called ribosomal protein S3.

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

- Molecule 4 is a protein called ribosomal protein S4.

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

- Molecule 5 is a protein called ribosomal protein S5.

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

- Molecule 6 is a protein called ribosomal protein S6.

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

- Molecule 7 is a protein called ribosomal protein S7.

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

- Molecule 8 is a protein called ribosomal protein S8.

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

- Molecule 9 is a protein called ribosomal protein S9.

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

- Molecule 10 is a protein called ribosomal protein S10.

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

- Molecule 11 is a protein called ribosomal protein S11.

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

- Molecule 12 is a protein called ribosomal protein S12.

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

- Molecule 13 is a protein called ribosomal protein S13.

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

- Molecule 14 is a protein called ribosomal protein S14.

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

- Molecule 15 is a protein called ribosomal protein S15.

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

- Molecule 16 is a protein called ribosomal protein S16.

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

- Molecule 17 is a protein called ribosomal protein S17.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 18 is a protein called ribosomal protein S18.

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

- Molecule 19 is a protein called ribosomal protein S19.

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

- Molecule 20 is a protein called ribosomal protein S20.

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

- Molecule 21 is a protein called ribosomal protein THX.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	268	Total	Mg	0	0
			268	268		
22	B	2	Total	Mg	0	0
			2	2		
22	C	2	Total	Mg	0	0
			2	2		
22	D	4	Total	Mg	0	0
			4	4		
22	E	1	Total	Mg	0	0
			1	1		
22	F	1	Total	Mg	0	0
			1	1		
22	I	1	Total	Mg	0	0
			1	1		
22	J	1	Total	Mg	0	0
			1	1		
22	L	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	M	2	Total 2	Mg 2	0	0
22	P	2	Total 2	Mg 2	0	0
22	Q	2	Total 2	Mg 2	0	0
22	T	2	Total 2	Mg 2	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

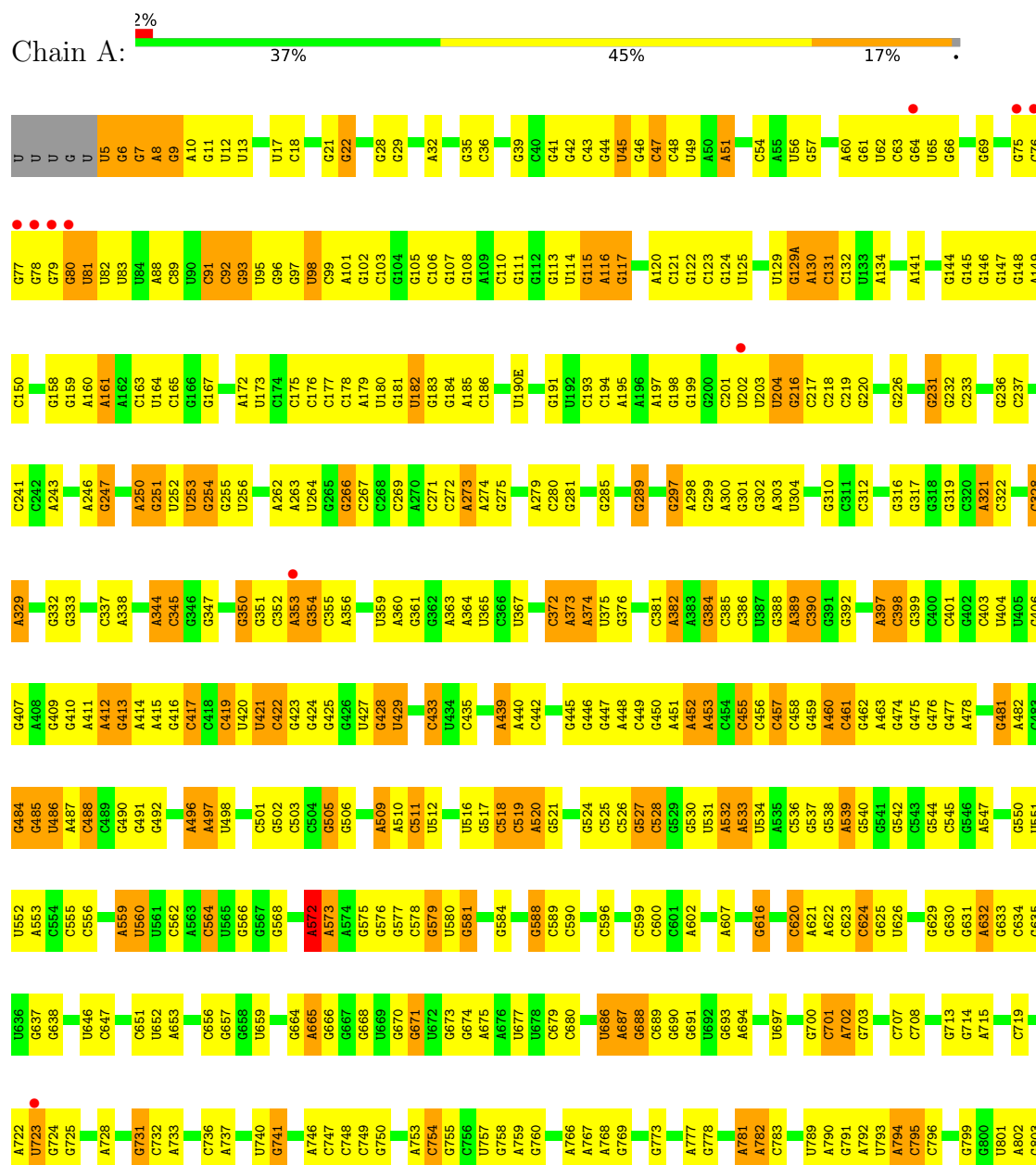
- Molecule 24 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	A	391	Total 391	O 391	0	0
24	B	1	Total 1	O 1	0	0
24	D	3	Total 3	O 3	0	0
24	E	4	Total 4	O 4	0	0
24	G	2	Total 2	O 2	0	0
24	J	2	Total 2	O 2	0	0
24	K	1	Total 1	O 1	0	0
24	M	3	Total 3	O 3	0	0
24	N	4	Total 4	O 4	0	0
24	P	4	Total 4	O 4	0	0
24	T	1	Total 1	O 1	0	0

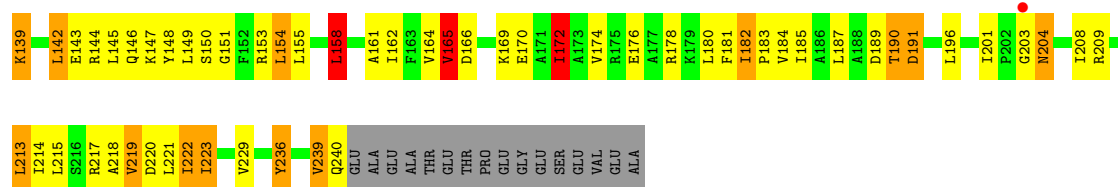
3 Residue-property plots

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.

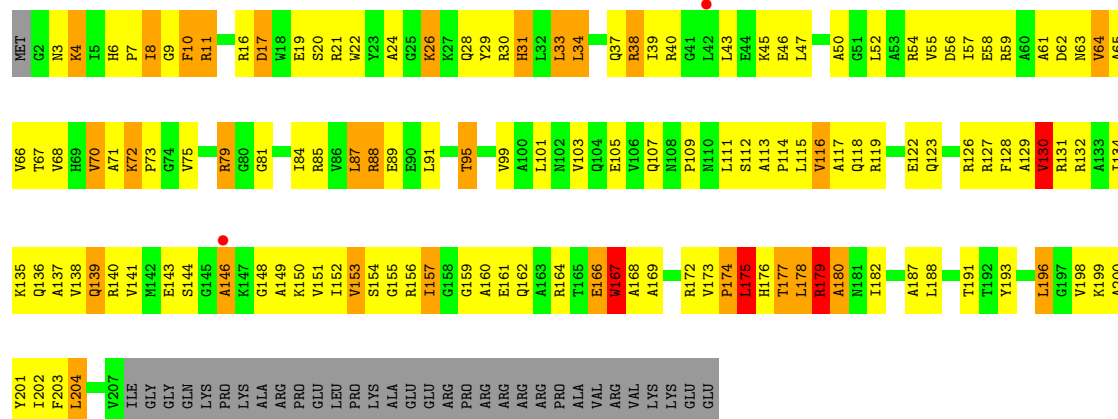
• Molecule 1: 16S rRNA



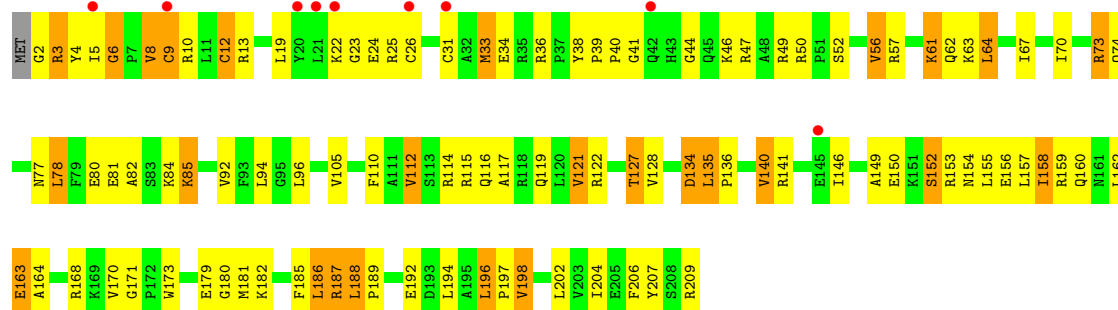




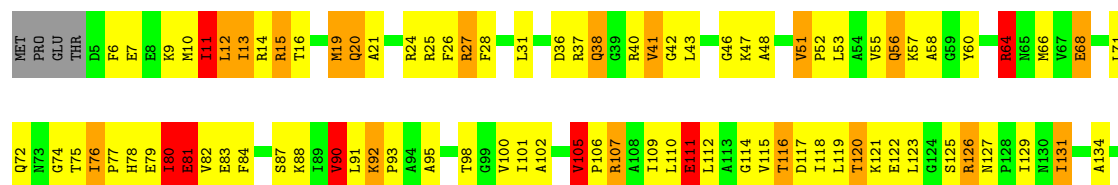
- Molecule 3: ribosomal protein S3



- Molecule 4: ribosomal protein S4



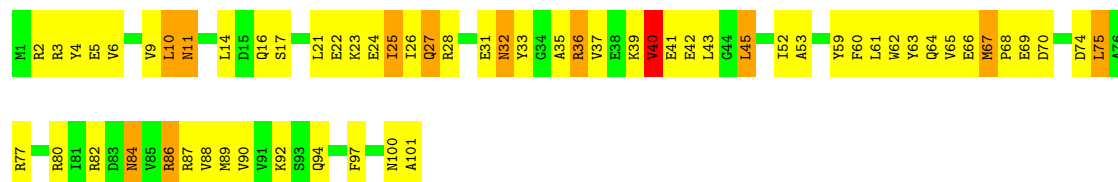
- Molecule 5: ribosomal protein S5





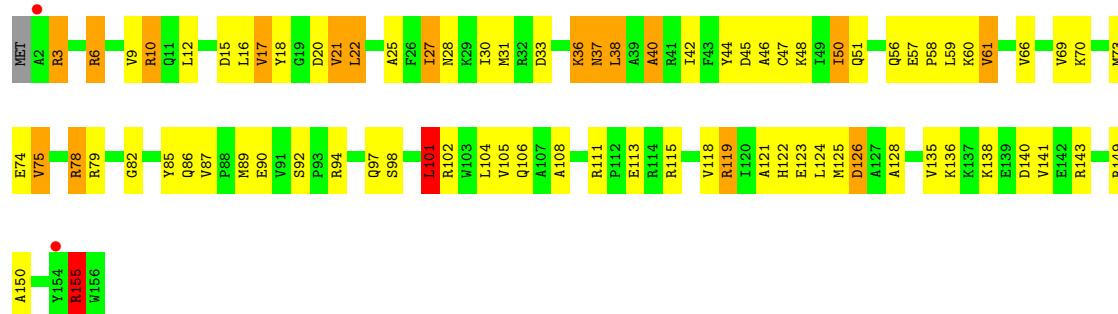
• Molecule 6: ribosomal protein S6

Chain F: 40% 49% 11% .



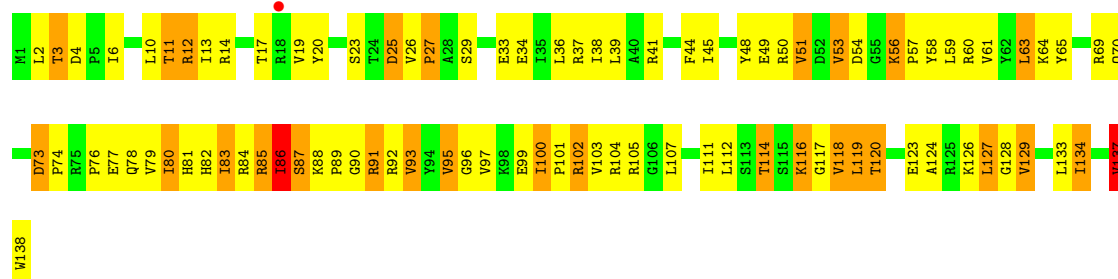
• Molecule 7: ribosomal protein S7

Chain G: 47% 40% 11% ..



• Molecule 8: ribosomal protein S8

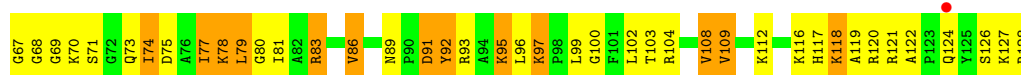
Chain H: 33% 46% 20% .



• Molecule 9: ribosomal protein S9

Chain I: 35% 49% 15% .





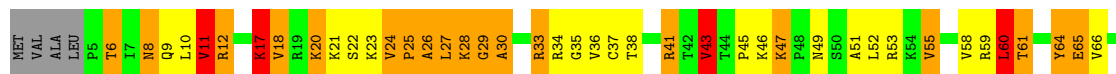
• Molecule 10: ribosomal protein S10



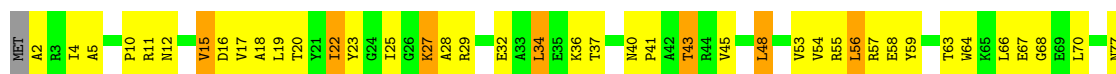
• Molecule 11: ribosomal protein S11



• Molecule 12: ribosomal protein S12



• Molecule 13: ribosomal protein S13

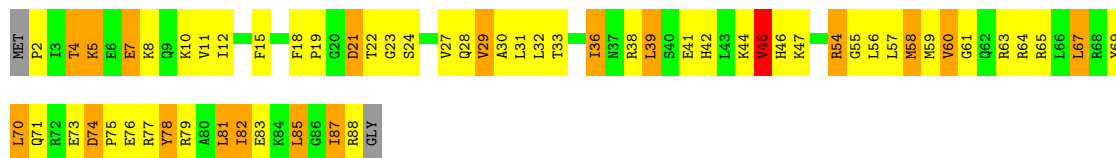


• Molecule 14: ribosomal protein S14

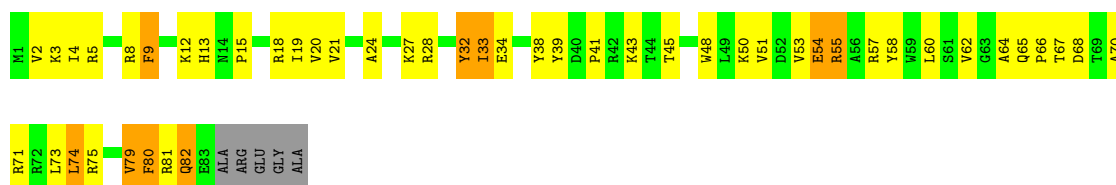




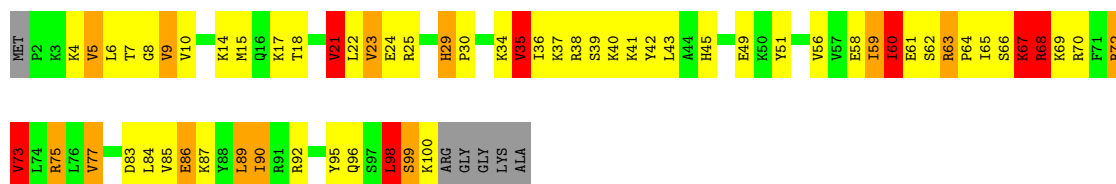
• Molecule 15: ribosomal protein S15



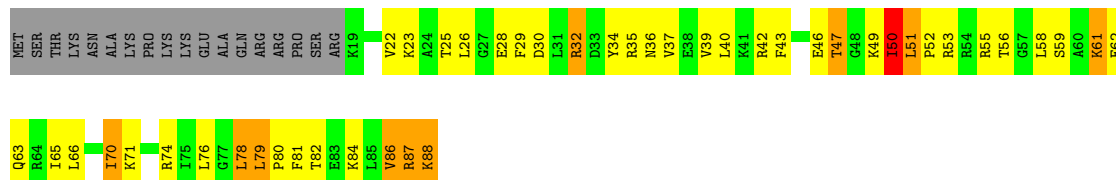
• Molecule 16: ribosomal protein S16



• Molecule 17: ribosomal protein S17

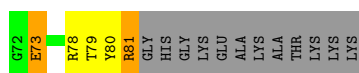


• Molecule 18: ribosomal protein S18

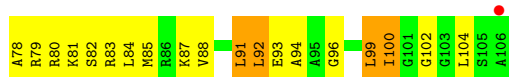


• Molecule 19: ribosomal protein S19

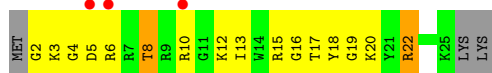




- Molecule 20: ribosomal protein S20



- Molecule 21: ribosomal protein THX



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	403.74Å 403.74Å 173.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.77 – 3.65 29.77 – 3.65	Depositor EDS
% Data completeness (in resolution range)	97.0 (29.77-3.65) 96.6 (29.77-3.65)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 3.65Å)	Xtriage
Refinement program	PHENIX dev_978	Depositor
R, R_{free}	0.165 , 0.223 0.164 , 0.221	Depositor DCC
R_{free} test set	7644 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	137.5	Xtriage
Anisotropy	0.320	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 129.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	52441	wwPDB-VP
Average B, all atoms (Å ²)	173.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.78% 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: ZN, MA6, 7MG, 5MC, 2MG, 4OC, PSU, UR3, 0TD, M2G, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.64	2/36142 (0.0%)	0.63	1/56401 (0.0%)
2	B	1.02	4/1935 (0.2%)	1.34	18/2609 (0.7%)
3	C	0.81	0/1636	1.21	12/2205 (0.5%)
4	D	0.91	0/1733	1.37	15/2318 (0.6%)
5	E	1.26	4/1162 (0.3%)	1.55	20/1564 (1.3%)
6	F	0.84	2/856 (0.2%)	1.17	9/1154 (0.8%)
7	G	0.84	0/1276	1.21	8/1709 (0.5%)
8	H	1.33	3/1136 (0.3%)	1.67	30/1527 (2.0%)
9	I	0.90	0/1029	1.23	6/1379 (0.4%)
10	J	0.82	1/805 (0.1%)	1.35	9/1082 (0.8%)
11	K	1.05	1/879 (0.1%)	1.46	10/1187 (0.8%)
12	L	1.06	1/977 (0.1%)	1.61	28/1306 (2.1%)
13	M	0.89	0/947	1.27	6/1270 (0.5%)
14	N	0.78	1/501 (0.2%)	1.18	3/664 (0.5%)
15	O	1.04	2/740 (0.3%)	1.35	7/987 (0.7%)
16	P	1.12	2/716 (0.3%)	1.41	4/963 (0.4%)
17	Q	1.28	6/836 (0.7%)	1.58	16/1117 (1.4%)
18	R	0.96	1/579 (0.2%)	1.37	7/768 (0.9%)
19	S	0.71	0/661	1.17	5/890 (0.6%)
20	T	1.03	1/765 (0.1%)	1.43	8/1007 (0.8%)
21	U	0.86	0/212	1.24	1/277 (0.4%)
All	All	0.79	31/55523 (0.1%)	0.93	223/82384 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
3	C	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
5	E	0	1
8	H	0	2
10	J	0	2
12	L	0	1
13	M	0	1
20	T	0	1
All	All	0	11

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	48	ILE	CA-CB	-9.48	1.43	1.54
8	H	134	ILE	CA-CB	-8.77	1.44	1.54
2	B	201	ILE	CA-CB	-8.47	1.46	1.54
5	E	138	ALA	CA-C	-7.31	1.45	1.53
12	L	85	ILE	CA-CB	-7.03	1.46	1.54
5	E	115	VAL	CA-CB	-6.95	1.45	1.54
15	O	45	VAL	CA-CB	-6.59	1.45	1.54
17	Q	60	ILE	CA-CB	-6.54	1.46	1.54
16	P	19	ILE	CA-CB	-6.27	1.46	1.54
6	F	9	VAL	CA-CB	-6.07	1.46	1.54
14	N	13	THR	CA-CB	6.00	1.56	1.52
5	E	109	ILE	CA-CB	-5.96	1.47	1.54
10	J	4	ILE	CA-CB	5.88	1.60	1.53
2	B	184	VAL	CA-CB	-5.83	1.47	1.54
5	E	90	VAL	CA-CB	-5.78	1.47	1.54
20	T	63	ILE	CA-CB	-5.71	1.48	1.54
8	H	61	VAL	CA-CB	-5.62	1.47	1.54
17	Q	9	VAL	CA-CB	-5.53	1.47	1.54
17	Q	7	THR	CA-CB	-5.52	1.44	1.53
6	F	37	VAL	CA-CB	-5.51	1.47	1.53
17	Q	90	ILE	CA-CB	-5.46	1.47	1.54
2	B	174	VAL	CA-CB	-5.42	1.48	1.54
1	A	572	A	P-OP1	5.38	1.59	1.49
8	H	119	LEU	CA-C	-5.36	1.46	1.52
18	R	50	ILE	CA-CB	-5.35	1.49	1.54
15	O	69	TYR	CA-C	-5.33	1.46	1.52
2	B	172	ILE	CA-CB	-5.20	1.47	1.54
17	Q	10	VAL	CA-CB	-5.20	1.48	1.54
1	A	1498	UR3	O3'-P	5.07	1.61	1.56
17	Q	23	VAL	CA-CB	-5.07	1.47	1.53
16	P	51	VAL	CA-CB	-5.03	1.47	1.54

All (223) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	91	ARG	N-CA-C	-13.16	95.50	111.69
8	H	100	ILE	CA-C-N	12.21	133.18	119.99
8	H	100	ILE	C-N-CA	12.21	133.18	119.99
4	D	171	GLY	CA-C-N	11.23	133.87	119.84
4	D	171	GLY	C-N-CA	11.23	133.87	119.84
3	C	167	TRP	N-CA-C	11.02	121.16	108.49
4	D	26	CYS	N-CA-C	-10.78	100.08	113.02
10	J	38	ILE	CA-C-N	9.92	130.32	119.90
10	J	38	ILE	C-N-CA	9.92	130.32	119.90
13	M	118	ALA	N-CA-C	9.11	124.01	109.79
11	K	14	VAL	N-CA-C	9.05	121.79	112.83
12	L	70	ILE	CA-C-N	8.98	128.74	119.76
12	L	70	ILE	C-N-CA	8.98	128.74	119.76
10	J	10	GLY	N-CA-C	8.45	124.59	110.56
20	T	11	SER	N-CA-C	8.22	122.93	113.15
8	H	134	ILE	CB-CA-C	-8.11	101.41	111.87
10	J	89	ASP	N-CA-C	8.05	122.03	109.96
12	L	30	ALA	CA-C-N	8.04	127.67	119.56
12	L	30	ALA	C-N-CA	8.04	127.67	119.56
3	C	130	VAL	N-CA-C	-8.00	102.74	110.42
20	T	75	ASN	N-CA-C	-8.00	103.09	113.17
12	L	85	ILE	CB-CA-C	-7.84	100.23	110.98
11	K	88	GLY	N-CA-C	-7.84	101.64	110.96
8	H	81	HIS	N-CA-C	-7.76	102.15	111.69
13	M	15	VAL	N-CA-C	7.64	117.75	110.42
16	P	80	PHE	N-CA-C	7.61	122.28	112.92
2	B	90	MET	N-CA-C	7.59	120.56	110.08
15	O	11	VAL	CB-CA-C	-7.57	102.19	111.88
11	K	125	PHE	N-CA-C	7.55	122.20	112.92
5	E	15	ARG	N-CA-C	7.54	122.46	112.13
17	Q	5	VAL	CB-CA-C	-7.42	101.34	110.99
16	P	51	VAL	N-CA-C	7.38	124.70	109.34
17	Q	29	HIS	CA-C-N	7.35	127.51	119.87
17	Q	29	HIS	C-N-CA	7.35	127.51	119.87
17	Q	98	LEU	N-CA-C	7.20	121.36	112.58
20	T	94	ALA	N-CA-C	-7.18	95.38	107.80
10	J	72	VAL	N-CA-C	7.15	117.76	110.82
4	D	33	MET	N-CA-C	-7.11	103.53	111.71
12	L	89	ARG	N-CA-C	-7.11	100.54	110.35
12	L	26	ALA	N-CA-C	-7.05	104.40	112.87
17	Q	67	LYS	N-CA-C	-7.02	100.05	110.23
3	C	180	ALA	N-CA-C	6.99	121.40	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	O	69	TYR	CB-CA-C	-6.98	100.13	110.95
8	H	107	LEU	N-CA-C	-6.98	104.77	113.28
5	E	80	ILE	N-CA-C	6.94	120.41	108.90
6	F	11	ASN	CA-C-N	6.93	127.22	119.32
6	F	11	ASN	C-N-CA	6.93	127.22	119.32
4	D	50	ARG	CA-C-N	6.93	127.17	119.90
4	D	50	ARG	C-N-CA	6.93	127.17	119.90
7	G	40	ALA	N-CA-C	-6.88	103.47	110.97
10	J	96	ILE	N-CA-C	6.87	117.78	108.17
8	H	3	THR	CA-C-N	-6.86	113.42	123.30
8	H	3	THR	C-N-CA	-6.86	113.42	123.30
11	K	117	ASN	N-CA-C	6.85	125.38	110.80
7	G	111	ARG	CA-C-N	6.84	126.30	118.85
7	G	111	ARG	C-N-CA	6.84	126.30	118.85
2	B	239	VAL	N-CA-C	6.83	116.95	110.53
13	M	108	ARG	N-CA-C	6.83	120.49	111.75
18	R	51	LEU	CA-C-N	6.81	127.21	119.92
18	R	51	LEU	C-N-CA	6.81	127.21	119.92
16	P	9	PHE	N-CA-C	6.72	121.64	113.17
5	E	105	VAL	CA-C-N	-6.69	112.10	119.19
5	E	105	VAL	C-N-CA	-6.69	112.10	119.19
14	N	42	ILE	N-CA-C	-6.66	103.84	110.30
8	H	56	LYS	CA-C-N	6.65	126.88	119.90
8	H	56	LYS	C-N-CA	6.65	126.88	119.90
2	B	204	ASN	N-CA-C	6.64	119.36	109.59
20	T	76	ALA	N-CA-C	-6.63	103.75	110.97
10	J	55	LYS	N-CA-C	6.60	117.77	108.00
3	C	174	PRO	CA-C-O	-6.59	116.30	121.38
9	I	70	LYS	N-CA-C	6.54	119.73	111.69
4	D	6	GLY	CA-C-N	6.52	126.54	119.89
4	D	6	GLY	C-N-CA	6.52	126.54	119.89
4	D	204	ILE	CB-CA-C	-6.52	103.54	111.88
3	C	130	VAL	CB-CA-C	-6.50	103.65	111.97
18	R	55	ARG	N-CA-C	6.48	121.46	112.45
12	L	24	VAL	CA-C-N	-6.46	106.35	120.89
12	L	24	VAL	C-N-CA	-6.46	106.35	120.89
8	H	13	ILE	CB-CA-C	-6.45	103.63	111.88
12	L	43	VAL	N-CA-C	6.43	118.04	108.46
4	D	12	CYS	N-CA-C	-6.42	103.40	111.11
12	L	114	LYS	N-CA-C	6.42	121.90	113.30
5	E	11	ILE	N-CA-C	6.41	116.57	110.74
15	O	74	ASP	CA-C-N	-6.39	113.10	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	O	74	ASP	C-N-CA	-6.39	113.10	119.56
15	O	36	ILE	CB-CA-C	-6.37	103.85	111.81
8	H	73	ASP	CA-C-N	6.35	126.47	119.87
8	H	73	ASP	C-N-CA	6.35	126.47	119.87
12	L	8	ASN	N-CA-C	-6.31	103.70	111.40
2	B	165	VAL	N-CA-C	6.26	121.17	112.35
3	C	146	ALA	N-CA-C	6.25	118.84	111.02
2	B	33	TYR	N-CA-C	6.22	118.99	111.40
5	E	109	ILE	N-CA-C	6.21	116.88	110.36
18	R	79	LEU	CA-C-N	6.20	126.71	120.14
18	R	79	LEU	C-N-CA	6.20	126.71	120.14
17	Q	60	ILE	N-CA-C	6.17	117.18	108.17
12	L	119	LYS	N-CA-C	-6.15	102.41	110.53
18	R	50	ILE	CB-CA-C	-6.15	101.37	111.51
5	E	64	ARG	N-CA-C	-6.11	102.31	110.55
10	J	90	LEU	N-CA-C	6.04	123.16	109.81
9	I	23	ASN	N-CA-C	6.02	118.80	111.82
5	E	81	GLU	N-CA-C	6.02	118.25	108.26
12	L	105	TYR	CB-CA-C	-5.98	109.66	116.54
2	B	172	ILE	CB-CA-C	-5.96	102.60	112.26
8	H	101	PRO	CA-C-O	-5.95	114.34	121.48
5	E	38	GLN	N-CA-C	5.92	120.21	112.92
16	P	19	ILE	CB-CA-C	-5.92	104.16	111.08
19	S	4	SER	N-CA-C	5.90	119.25	107.62
4	D	56	VAL	CB-CA-C	-5.88	103.05	112.16
9	I	77	ILE	CB-CA-C	-5.84	104.40	111.88
19	S	58	VAL	CB-CA-C	-5.84	104.46	110.71
4	D	12	CYS	CA-CB-SG	5.83	127.81	114.40
10	J	62	HIS	N-CA-C	5.82	118.96	109.59
9	I	67	GLY	N-CA-C	5.82	119.97	112.18
2	B	166	ASP	CA-C-N	5.81	125.52	119.82
2	B	166	ASP	C-N-CA	5.81	125.52	119.82
8	H	103	VAL	N-CA-C	5.81	116.22	107.80
17	Q	73	VAL	N-CA-C	5.80	116.15	107.51
4	D	70	ILE	N-CA-C	5.80	118.94	109.78
5	E	41	VAL	CB-CA-C	-5.79	100.69	110.71
7	G	155	ARG	N-CA-C	5.78	123.11	110.80
2	B	150	SER	N-CA-C	5.78	118.04	111.11
8	H	87	SER	N-CA-C	-5.78	99.77	108.96
20	T	63	ILE	CB-CA-C	-5.76	104.50	111.88
20	T	99	LEU	N-CA-C	5.76	118.67	111.24
6	F	9	VAL	CB-CA-C	-5.76	102.64	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	58	HIS	N-CA-C	-5.75	104.61	111.69
12	L	85	ILE	N-CA-C	5.75	116.39	107.99
12	L	18	VAL	N-CA-C	5.74	116.40	107.28
12	L	17	LYS	CA-C-N	-5.70	115.50	123.13
12	L	17	LYS	C-N-CA	-5.70	115.50	123.13
8	H	102	ARG	CA-C-N	-5.69	115.72	123.12
8	H	102	ARG	C-N-CA	-5.69	115.72	123.12
14	N	25	VAL	N-CA-C	5.69	115.88	110.53
17	Q	90	ILE	CB-CA-C	-5.68	104.59	112.04
5	E	102	ALA	N-CA-C	5.68	117.11	108.07
15	O	57	LEU	CB-CA-C	-5.68	101.02	110.68
6	F	67	MET	CA-C-N	5.67	125.61	119.78
6	F	67	MET	C-N-CA	5.67	125.61	119.78
3	C	179	ARG	N-CA-C	-5.66	98.74	110.80
5	E	82	VAL	N-CA-C	5.65	116.02	108.11
7	G	101	LEU	N-CA-C	5.64	117.11	111.07
12	L	29	GLY	N-CA-C	-5.64	108.25	115.42
8	H	80	ILE	CB-CA-C	-5.64	104.08	111.81
18	R	65	ILE	CB-CA-C	-5.63	104.45	112.22
4	D	121	VAL	N-CA-C	-5.62	104.85	110.30
7	G	37	ASN	N-CA-C	-5.61	104.56	111.40
12	L	11	VAL	N-CA-C	5.61	115.74	110.30
8	H	53	VAL	CB-CA-C	-5.60	103.30	110.98
13	M	112	GLY	CA-C-N	5.60	125.61	119.90
13	M	112	GLY	C-N-CA	5.60	125.61	119.90
8	H	49	GLU	N-CA-C	-5.58	100.92	109.41
5	E	127	ASN	CA-C-N	5.58	125.42	119.28
5	E	127	ASN	C-N-CA	5.58	125.42	119.28
8	H	57	PRO	CB-CA-C	-5.56	104.74	111.46
15	O	5	LYS	N-CA-C	-5.53	105.17	111.14
12	L	66	VAL	CB-CA-C	-5.52	102.86	110.91
2	B	98	LEU	CA-C-N	-5.51	116.02	120.98
2	B	98	LEU	C-N-CA	-5.51	116.02	120.98
12	L	60	LEU	N-CA-C	5.51	118.54	109.72
5	E	48	ALA	CA-C-N	5.51	125.16	119.05
5	E	48	ALA	C-N-CA	5.51	125.16	119.05
20	T	30	LYS	N-CA-C	-5.51	105.18	111.07
12	L	81	SER	N-CA-C	5.50	117.80	110.53
17	Q	68	ARG	CA-C-N	-5.49	115.70	122.84
17	Q	68	ARG	C-N-CA	-5.49	115.70	122.84
8	H	3	THR	CB-CA-C	5.49	121.34	110.42
3	C	87	LEU	N-CA-C	5.47	118.41	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	32	ILE	N-CA-C	5.45	115.81	108.17
19	S	54	GLY	N-CA-C	-5.45	107.50	114.37
2	B	145	LEU	N-CA-C	-5.43	105.47	111.71
12	L	118	SER	N-CA-C	-5.42	105.07	110.97
13	M	97	PRO	N-CA-C	5.40	119.35	111.03
14	N	39	LEU	N-CA-C	5.39	118.02	109.50
17	Q	99	SER	N-CA-C	5.39	122.28	110.80
5	E	148	VAL	CB-CA-C	-5.38	105.03	112.24
2	B	158	LEU	N-CA-C	5.38	115.78	109.60
17	Q	63	ARG	N-CA-C	-5.35	103.03	109.83
19	S	33	THR	N-CA-C	5.33	118.13	108.69
3	C	6	HIS	CA-C-N	5.31	124.63	118.85
3	C	6	HIS	C-N-CA	5.31	124.63	118.85
2	B	222	ILE	CB-CA-C	-5.30	105.18	111.97
17	Q	35	VAL	CA-C-N	-5.30	114.30	122.68
17	Q	35	VAL	C-N-CA	-5.30	114.30	122.68
5	E	111	GLU	N-CA-C	-5.29	105.52	111.28
11	K	48	ILE	CB-CA-C	-5.28	105.54	111.45
8	H	86	ILE	CA-C-N	-5.27	115.18	122.30
8	H	86	ILE	C-N-CA	-5.27	115.18	122.30
2	B	81	VAL	CB-CA-C	-5.26	105.24	111.97
8	H	12	ARG	NE-CZ-NH2	5.26	123.93	119.20
2	B	148	TYR	N-CA-C	5.25	117.08	111.36
19	S	10	PHE	N-CA-C	5.22	117.26	108.96
12	L	55	VAL	N-CA-C	5.21	116.51	108.44
8	H	137	VAL	CB-CA-C	-5.20	102.37	110.69
17	Q	5	VAL	N-CA-C	5.20	115.55	107.28
5	E	90	VAL	CB-CA-C	-5.19	103.38	110.96
3	C	175	LEU	N-CA-C	5.18	118.38	111.75
12	L	38	THR	N-CA-C	-5.16	104.69	111.96
4	D	185	PHE	N-CA-C	-5.12	98.22	107.75
12	L	124	LYS	CA-C-N	5.12	125.39	119.92
12	L	124	LYS	C-N-CA	5.12	125.39	119.92
17	Q	21	VAL	CB-CA-C	-5.12	104.20	111.21
6	F	89	MET	CA-C-N	-5.11	115.83	122.94
6	F	89	MET	C-N-CA	-5.11	115.83	122.94
7	G	70	LYS	CA-C-N	5.10	125.50	119.99
7	G	70	LYS	C-N-CA	5.10	125.50	119.99
8	H	96	GLY	CA-C-N	-5.08	112.30	120.64
8	H	96	GLY	C-N-CA	-5.08	112.30	120.64
2	B	68	ILE	CB-CA-C	-5.08	104.61	110.91
6	F	40	VAL	N-CA-C	5.08	116.03	108.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	T	55	ILE	CB-CA-C	-5.08	105.20	111.70
5	E	115	VAL	CB-CA-C	-5.08	103.31	111.59
11	K	118	GLY	CA-C-N	-5.07	115.33	122.94
11	K	118	GLY	C-N-CA	-5.07	115.33	122.94
3	C	46	GLU	N-CA-C	5.04	117.89	111.69
11	K	15	ALA	CB-CA-C	-5.04	110.37	117.23
21	U	17	THR	N-CA-C	5.04	117.65	109.79
6	F	37	VAL	N-CA-C	5.02	114.81	107.37
1	A	1498	UR3	P-O3'-C3'	5.02	125.73	119.70
8	H	26	VAL	CA-C-N	-5.02	115.06	120.03
8	H	26	VAL	C-N-CA	-5.02	115.06	120.03
11	K	37	GLY	N-CA-C	5.02	120.69	114.37
9	I	122	ALA	N-CA-C	-5.01	102.58	110.14

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	77	ALA	Peptide
3	C	166	GLU	Peptide
3	C	179	ARG	Peptide
5	E	20	GLN	Peptide
8	H	27	PRO	Peptide
8	H	90	GLY	Peptide
10	J	35	SER	Peptide
10	J	87	THR	Peptide
12	L	25	PRO	Peptide
13	M	117	VAL	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	32646	0	16503	873	1
2	B	1900	0	1951	108	0
3	C	1612	0	1677	113	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1703	0	1763	71	0
5	E	1146	0	1207	75	0
6	F	843	0	857	48	0
7	G	1257	0	1296	60	0
8	H	1116	0	1177	73	0
9	I	1010	0	1037	78	0
10	J	792	0	835	59	0
11	K	864	0	881	40	0
12	L	972	0	1058	62	0
13	M	937	0	995	55	0
14	N	492	0	529	47	0
15	O	729	0	768	41	0
16	P	700	0	720	45	0
17	Q	823	0	893	58	0
18	R	574	0	644	38	0
19	S	647	0	673	36	0
20	T	763	0	861	42	0
21	U	208	0	221	14	0
22	A	268	0	0	0	0
22	B	2	0	0	0	0
22	C	2	0	0	0	0
22	D	4	0	0	0	0
22	E	1	0	0	0	0
22	F	1	0	0	0	0
22	I	1	0	0	0	0
22	J	1	0	0	0	0
22	L	1	0	0	0	0
22	M	2	0	0	0	0
22	P	2	0	0	0	0
22	Q	2	0	0	0	0
22	T	2	0	0	0	0
23	D	1	0	0	0	0
23	N	1	0	0	0	0
24	A	391	0	0	6	0
24	B	1	0	0	2	0
24	D	3	0	0	0	0
24	E	4	0	0	0	0
24	G	2	0	0	1	0
24	J	2	0	0	2	0
24	K	1	0	0	0	0
24	M	3	0	0	1	0
24	N	4	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	P	4	0	0	3	0
24	T	1	0	0	1	0
All	All	52441	0	36546	1843	1

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

All (1843) 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:967:5MC:H4'	9:I:128:ARG:HG3	1.33	1.06
1:A:75:G:N2	1:A:76:C:N3	2.07	1.02
1:A:949:A:N6	24:A:2225:HOH:O	1.90	1.02
1:A:1152:A:H5''	10:J:13:HIS:HB2	1.44	1.00
20:T:50:GLU:HA	20:T:100:ILE:HG13	1.47	0.95
1:A:1532:U:H2'	1:A:1533:C:H3'	1.50	0.92
1:A:1073:U:OP2	5:E:57:LYS:NZ	2.01	0.92
1:A:184:G:H2'	1:A:185:A:H8	1.35	0.91
1:A:1347:G:H3'	9:I:108:VAL:O	1.70	0.91
3:C:182:ILE:HG12	3:C:203:PHE:HB2	1.51	0.91
13:M:23:TYR:HE2	13:M:70:LEU:HD22	1.36	0.90
1:A:1125:U:OP2	1:A:1145:C:N4	2.04	0.89
1:A:130:A:OP2	1:A:190(E):U:O2'	1.89	0.89
8:H:4:ASP:OD2	8:H:85:ARG:NH1	2.06	0.89
3:C:138:VAL:HG13	3:C:149:ALA:HB3	1.54	0.88
10:J:55:LYS:HB2	10:J:57:LYS:HE3	1.56	0.88
16:P:21:VAL:HG12	16:P:33:ILE:HD12	1.56	0.87
1:A:1415:G:H2'	1:A:1416:G:H8	1.38	0.87
1:A:1417:G:O2'	1:A:1483:A:N6	2.06	0.87
1:A:1426:C:H42	1:A:1474:G:H1	1.23	0.86
20:T:100:ILE:HG22	20:T:102:GLY:H	1.39	0.86
1:A:1368:G:H5''	9:I:112:LYS:HB3	1.56	0.86
3:C:137:ALA:HA	3:C:140:ARG:HD2	1.55	0.86
1:A:1415:G:H2'	1:A:1416:G:C8	2.09	0.85
1:A:446:G:H1	1:A:488:C:H42	1.21	0.84
11:K:121:PRO:HG2	11:K:126:ARG:HG2	1.60	0.84
10:J:12:ASP:HB3	10:J:15:THR:HB	1.60	0.84
1:A:517:G:N1	1:A:533:A:OP2	2.09	0.84
8:H:41:ARG:NH1	8:H:123:GLU:OE2	2.11	0.84
12:L:24:VAL:HG13	12:L:98:TYR:HE2	1.42	0.83
1:A:91:C:O2'	1:A:92:C:OP1	1.95	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1515[B]:C:H42	1:A:1520[B]:G:H1	1.27	0.82
3:C:150:LYS:HB2	3:C:173:VAL:HG21	1.60	0.81
1:A:664:G:H22	1:A:741:G:H1	1.27	0.81
1:A:101:A:H2'	1:A:102:G:H8	1.46	0.81
1:A:501:C:H2'	1:A:502:G:C8	2.15	0.81
19:S:41:VAL:HG22	19:S:44:MET:HG3	1.61	0.81
1:A:1195:C:H3'	1:A:1196:U:H5''	1.60	0.81
1:A:1436:U:H2'	1:A:1437:C:H6	1.46	0.80
1:A:1149:C:O2'	1:A:1280:A:N1	2.15	0.80
1:A:279:A:H5'	1:A:279:A:H8	1.47	0.80
1:A:279:A:OP2	17:Q:95:TYR:OH	1.98	0.80
7:G:56:GLN:HG2	7:G:60:LYS:HD3	1.64	0.80
1:A:1518[B]:MA6:H102	1:A:1519[B]:MA6:H103	1.65	0.79
8:H:6:ILE:HB	8:H:85:ARG:HH12	1.45	0.79
15:O:39:LEU:HD13	15:O:56:LEU:HB2	1.64	0.79
1:A:103:C:OP1	20:T:17:ARG:NH1	2.15	0.79
1:A:951:G:OP2	13:M:102:ARG:NH2	2.16	0.79
1:A:1009:G:H1	1:A:1020:U:H3	1.30	0.79
4:D:57:ARG:HG2	4:D:202:LEU:HD12	1.65	0.79
1:A:184:G:H2'	1:A:185:A:C8	2.17	0.79
7:G:140:ASP:HA	7:G:143:ARG:HB2	1.65	0.79
1:A:384:G:H2'	1:A:385:C:C6	2.18	0.78
3:C:85:ARG:HD2	3:C:88:ARG:HH11	1.48	0.78
1:A:1426:C:N3	1:A:1474:G:N2	2.29	0.78
20:T:45:GLN:HG3	20:T:91:LEU:HD11	1.65	0.77
1:A:1198:G:H2'	1:A:1199:U:C6	2.20	0.77
1:A:1314:C:H5	19:S:6:LYS:HD3	1.49	0.77
4:D:64:LEU:HD23	4:D:198:VAL:HG21	1.65	0.77
1:A:505:G:O6	1:A:526:C:N4	2.17	0.77
1:A:1266:G:N2	1:A:1269:A:OP2	2.15	0.77
13:M:23:TYR:CE2	13:M:70:LEU:HD22	2.20	0.77
1:A:1250:A:O2'	1:A:1370:G:O2'	2.02	0.77
10:J:53:PRO:HA	14:N:41:ARG:HH22	1.51	0.76
1:A:79:G:N1	1:A:80:G:N7	2.34	0.76
3:C:130:VAL:HG11	3:C:153:VAL:HG21	1.65	0.76
12:L:34:ARG:O	12:L:61:THR:OG1	2.04	0.76
16:P:3:LYS:HG3	16:P:24:ALA:HB2	1.67	0.76
3:C:43:LEU:HA	3:C:47:LEU:HD13	1.68	0.75
8:H:85:ARG:NE	8:H:87:SER:O	2.17	0.75
1:A:1404:5MC:H1'	1:A:1499:A:C2	2.21	0.75
1:A:1415:G:N2	1:A:1486:G:N3	2.34	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:180:ALA:HB1	3:C:203:PHE:HE1	1.51	0.75
1:A:9:G:OP2	5:E:121:LYS:NZ	2.16	0.75
16:P:80:PHE:N	24:P:204:HOH:O	2.10	0.75
1:A:36:C:H5''	12:L:123:LYS:HD3	1.69	0.75
10:J:47:PHE:HB3	14:N:34:TYR:HE2	1.49	0.75
1:A:115:G:O2'	1:A:116:A:OP2	2.05	0.75
1:A:953:G:H5'	1:A:965:A:H61	1.52	0.75
12:L:24:VAL:HG13	12:L:98:TYR:CE2	2.21	0.75
14:N:24:CYS:HB2	14:N:39:LEU:HA	1.67	0.74
1:A:1373:G:H5''	7:G:36:LYS:HE2	1.70	0.74
1:A:1497:G:H2'	1:A:1498:UR3:H5'	1.70	0.74
1:A:1249:C:O2'	9:I:73:GLN:NE2	2.19	0.74
1:A:584:G:OP2	17:Q:87:LYS:NZ	2.21	0.73
1:A:455:C:H2'	1:A:456:C:H6	1.53	0.73
14:N:40:CYS:O	14:N:44:LEU:N	2.17	0.73
1:A:1435:G:H2'	1:A:1436:U:C6	2.24	0.73
1:A:1310:G:OP1	13:M:77:ASN:ND2	2.22	0.73
8:H:6:ILE:HB	8:H:85:ARG:NH1	2.04	0.73
13:M:22:ILE:HG22	13:M:23:TYR:H	1.52	0.73
13:M:96:LEU:O	13:M:110:ARG:NH1	2.22	0.73
1:A:1241:G:H2'	1:A:1242:C:H6	1.54	0.72
4:D:13:ARG:NH1	4:D:38:TYR:O	2.22	0.72
8:H:114:THR:HB	8:H:116:LYS:H	1.54	0.72
1:A:81:U:H2'	1:A:83:U:OP2	1.89	0.72
1:A:1003:G:N2	1:A:1039:C:N3	2.35	0.72
1:A:1242:C:H42	1:A:1295:G:H1	1.37	0.72
1:A:1145:C:O2'	1:A:1146:A:O5'	2.07	0.72
1:A:1188:A:O3'	14:N:58:LYS:NZ	2.22	0.72
1:A:1316:G:N2	1:A:1319:A:OP2	2.22	0.72
1:A:992:U:H3	1:A:1044:A:N6	1.87	0.72
1:A:1399:C:H4'	1:A:1400:5MC:H5''	1.71	0.72
1:A:1192:C:O2	5:E:25:ARG:NH2	2.22	0.72
1:A:113:G:H1'	1:A:354:G:H5'	1.70	0.72
1:A:1113:C:H42	1:A:1187:G:H1	1.37	0.72
1:A:836:G:OP1	18:R:61:LYS:NZ	2.23	0.71
9:I:5:TYR:HD1	9:I:6:GLY:N	1.88	0.71
20:T:44:ALA:HB1	20:T:91:LEU:HB3	1.72	0.71
13:M:91:ARG:HB3	13:M:98:VAL:HG22	1.72	0.71
19:S:12:ASP:OD1	19:S:35:SER:OG	2.08	0.71
2:B:16:HIS:CD2	2:B:204:ASN:H	2.08	0.71
10:J:61:GLU:HA	24:J:302:HOH:O	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:27:LEU:HG	12:L:28:LYS:H	1.56	0.71
1:A:686:U:HO2'	1:A:687:A:H8	1.38	0.71
1:A:1498:UR3:O2'	1:A:1499:A:OP2	2.06	0.71
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.73	0.71
1:A:1201:A:H4'	1:A:1202:G:C5'	2.21	0.71
2:B:97:TRP:HH2	2:B:176:GLU:CD	1.99	0.71
11:K:57:THR:HG23	11:K:60:ALA:H	1.53	0.71
1:A:1300:G:O2'	1:A:1301:U:OP2	2.09	0.70
10:J:39:PRO:HA	10:J:70:ARG:HG3	1.72	0.70
17:Q:75:ARG:HH22	17:Q:77:VAL:HG13	1.57	0.70
1:A:216:G:H2'	1:A:217:C:C6	2.27	0.70
13:M:108:ARG:NH2	13:M:112:GLY:O	2.23	0.70
16:P:57:ARG:NE	16:P:79:VAL:O	2.19	0.70
10:J:79:ARG:HH12	10:J:82:ILE:HB	1.56	0.70
7:G:10:ARG:HH11	7:G:10:ARG:HB2	1.57	0.70
3:C:129:ALA:HB3	3:C:132:ARG:HG3	1.73	0.70
1:A:1078:U:H5''	1:A:1079:G:OP2	1.92	0.69
7:G:113:GLU:O	7:G:119:ARG:HD3	1.92	0.69
3:C:134:ILE:HG23	3:C:151:VAL:HB	1.75	0.69
1:A:103:C:P	20:T:17:ARG:HH12	2.16	0.69
21:U:5:ASP:HB3	21:U:8:THR:OG1	1.92	0.69
1:A:298:A:N6	24:A:2047:HOH:O	2.09	0.69
1:A:411:A:OP2	4:D:25:ARG:NH2	2.25	0.69
5:E:137:GLU:O	5:E:141:GLN:HG3	1.93	0.69
20:T:33:ILE:HG12	20:T:62:LEU:HD13	1.75	0.69
21:U:6:ARG:HD3	21:U:15:ARG:HH12	1.57	0.69
1:A:255:G:H1	1:A:271:C:H42	1.38	0.69
1:A:975:A:H5'	1:A:975:A:H8	1.57	0.69
7:G:69:VAL:HG21	7:G:104:LEU:HD21	1.75	0.69
17:Q:4:LYS:HG2	17:Q:6:LEU:HD21	1.75	0.69
17:Q:66:SER:O	17:Q:70:ARG:NH1	2.26	0.69
21:U:10:ARG:HA	21:U:13:ILE:HD12	1.74	0.69
1:A:537:G:H5''	12:L:113:ARG:HH21	1.57	0.68
1:A:1144:G:H22	1:A:1146:A:H62	1.40	0.68
7:G:47:CYS:HB3	7:G:58:PRO:HG2	1.76	0.68
8:H:10:LEU:HD22	8:H:83:ILE:HD12	1.74	0.68
8:H:20:TYR:CE1	8:H:76:PRO:HG2	2.29	0.68
20:T:60:GLU:HA	20:T:63:ILE:HD12	1.74	0.68
1:A:359:U:H2'	1:A:360:A:C8	2.29	0.68
8:H:87:SER:HA	8:H:93:VAL:HG13	1.76	0.68
13:M:20:THR:HG22	24:M:303:HOH:O	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:18:GLY:HA3	2:B:41:ILE:HA	1.74	0.68
1:A:198:G:H1	1:A:219:C:H42	1.42	0.68
8:H:25:ASP:OD1	8:H:25:ASP:N	2.26	0.68
1:A:972:C:H4'	10:J:57:LYS:HG2	1.76	0.68
13:M:54:VAL:HG22	13:M:57:ARG:HH12	1.59	0.68
1:A:501:C:H2'	1:A:502:G:H8	1.59	0.67
1:A:1053:G:N2	1:A:1058:G:O6	2.26	0.67
1:A:130:A:O2'	1:A:131:C:H5''	1.94	0.67
5:E:142:LEU:O	5:E:143:ARG:HD3	1.95	0.67
1:A:559:A:OP1	5:E:126:ARG:NH2	2.26	0.67
2:B:139:LYS:NZ	2:B:139:LYS:O	2.27	0.67
4:D:187:ARG:HD2	4:D:188:LEU:H	1.56	0.67
1:A:1510:U:H2'	1:A:1511:G:C8	2.30	0.67
4:D:80:GLU:O	4:D:84:LYS:HG2	1.95	0.67
8:H:20:TYR:HE1	8:H:76:PRO:HG2	1.58	0.67
1:A:1250:A:HO2'	1:A:1370:G:HO2'	1.38	0.67
14:N:24:CYS:HB2	14:N:39:LEU:HD23	1.77	0.67
1:A:781:A:H2'	1:A:782:A:H5'	1.76	0.67
5:E:84:PHE:HB2	5:E:134:ALA:HB2	1.76	0.67
4:D:13:ARG:NH2	4:D:40:PRO:HA	2.10	0.67
1:A:966:M2G:HM22	1:A:967:5MC:H1'	1.77	0.66
6:F:2:ARG:O	6:F:66:GLU:HA	1.95	0.66
9:I:50:LEU:HB3	9:I:55:ALA:HB3	1.76	0.66
12:L:25:PRO:C	12:L:27:LEU:H	2.03	0.66
1:A:1338:G:H2'	1:A:1339:A:C8	2.30	0.66
1:A:1418:A:H61	1:A:1482:G:H1'	1.60	0.66
1:A:1195:C:H3'	1:A:1196:U:C5'	2.24	0.66
5:E:126:ARG:HG3	5:E:126:ARG:HH11	1.59	0.66
4:D:19:LEU:HD21	4:D:67:ILE:HG12	1.78	0.66
20:T:92:LEU:O	20:T:96:GLY:HA2	1.95	0.66
12:L:27:LEU:C	12:L:29:GLY:H	2.03	0.66
19:S:53:ASN:HB2	19:S:55:LYS:H	1.60	0.66
1:A:838:G:H1	1:A:848:C:H42	1.44	0.66
7:G:20:ASP:OD2	7:G:22:LEU:N	2.27	0.66
1:A:216:G:H2'	1:A:217:C:H6	1.61	0.65
1:A:1118:C:H1'	1:A:1179:A:C4	2.31	0.65
1:A:1497:G:C2'	1:A:1498:UR3:H5'	2.26	0.65
1:A:1139:G:O2'	1:A:1140:C:OP2	2.13	0.65
14:N:23:ARG:NH1	14:N:28:GLY:O	2.29	0.65
1:A:279:A:H5'	1:A:279:A:C8	2.31	0.65
1:A:1007:C:H1'	1:A:1023:G:H1	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:158:LEU:H	2:B:158:LEU:HD12	1.60	0.65
7:G:15:ASP:OD2	7:G:44:TYR:OH	2.13	0.65
9:I:19:LEU:HD21	9:I:59:PHE:HB3	1.79	0.65
1:A:1515[B]:C:N4	1:A:1520[B]:G:H1	1.94	0.65
1:A:457:C:H2'	1:A:458:C:C6	2.32	0.65
3:C:123:GLN:HA	3:C:126:ARG:HD2	1.78	0.65
17:Q:86:GLU:HG3	17:Q:90:ILE:HD11	1.79	0.65
1:A:1143:G:H2'	1:A:1144:G:C8	2.32	0.65
14:N:2:ALA:N	14:N:27:CYS:O	2.29	0.65
1:A:77:G:H2'	1:A:78:G:C8	2.32	0.65
17:Q:24:GLU:HA	17:Q:39:SER:HB3	1.79	0.65
1:A:17:U:H2'	1:A:18:C:C6	2.33	0.65
1:A:485:G:O2'	1:A:486:U:OP2	2.15	0.64
8:H:17:THR:O	8:H:78:GLN:NE2	2.30	0.64
12:L:87:GLY:HA2	12:L:98:TYR:HA	1.78	0.64
17:Q:40:LYS:HD3	17:Q:42:TYR:CZ	2.32	0.64
1:A:77:G:H2'	1:A:78:G:H8	1.62	0.64
7:G:18:TYR:HE2	7:G:59:LEU:HB2	1.62	0.64
20:T:87:LYS:O	20:T:91:LEU:HB2	1.96	0.64
1:A:1305:G:O2'	1:A:1306:A:H8	1.80	0.64
1:A:1347:G:N2	1:A:1374:A:OP2	2.26	0.64
3:C:11:ARG:HA	3:C:178:LEU:HD11	1.77	0.64
10:J:62:HIS:ND1	24:J:301:HOH:O	2.27	0.64
17:Q:51:TYR:HE1	17:Q:73:VAL:HB	1.62	0.64
1:A:572:A:H5'	1:A:573:A:OP2	1.98	0.64
12:L:84:LEU:HD23	12:L:101:VAL:HG21	1.79	0.64
1:A:973:G:H3'	1:A:974:A:H5''	1.79	0.64
1:A:1006:C:N4	1:A:1024:G:H21	1.95	0.64
1:A:279:A:H5''	1:A:281:G:O4'	1.97	0.64
9:I:21:PRO:HA	9:I:59:PHE:HA	1.79	0.64
1:A:967:5MC:O2'	9:I:128:ARG:NH1	2.31	0.64
1:A:1098:C:OP2	2:B:144:ARG:NH2	2.31	0.64
1:A:1241:G:H2'	1:A:1242:C:C6	2.33	0.64
17:Q:5:VAL:HG22	17:Q:60:ILE:HD12	1.80	0.64
1:A:250:A:H4'	1:A:251:G:O5'	1.98	0.63
1:A:1314:C:C5	19:S:6:LYS:HD3	2.33	0.63
5:E:42:GLY:N	5:E:66:MET:SD	2.71	0.63
1:A:447:G:H1	1:A:485:G:HO2'	1.44	0.63
1:A:1240:U:OP1	7:G:119:ARG:NH2	2.30	0.63
1:A:217:C:H2'	1:A:218:C:H6	1.63	0.63
6:F:94:GLN:HB2	18:R:32:ARG:HD3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:108:VAL:HG12	9:I:109:VAL:H	1.63	0.63
12:L:53:ARG:HD3	12:L:93:LEU:HD21	1.80	0.63
1:A:551:U:O2'	12:L:86:ARG:HD2	1.97	0.63
1:A:980:C:H3'	1:A:981:U:H6	1.63	0.63
1:A:1305:G:O2'	1:A:1306:A:O5'	2.16	0.63
6:F:41:GLU:OE1	18:R:35:ARG:NH1	2.31	0.63
11:K:101:SER:HG	11:K:103:LEU:H	1.45	0.63
1:A:588:G:H1	1:A:651:C:H42	1.44	0.63
2:B:61:LEU:HD13	2:B:66:GLY:HA3	1.80	0.63
7:G:115:ARG:HB2	7:G:118:VAL:HG23	1.80	0.63
12:L:27:LEU:O	12:L:29:GLY:N	2.32	0.63
1:A:129:U:O3'	1:A:129(A):G:H3'	1.98	0.63
1:A:1318:A:H4'	19:S:10:PHE:CE2	2.34	0.63
1:A:1244:C:H42	1:A:1293:G:H1	1.44	0.63
1:A:1255:G:C6	1:A:1279:A:N7	2.67	0.63
2:B:131:PRO:HG2	2:B:134:GLU:HG2	1.80	0.63
13:M:4:ILE:HG12	13:M:56:LEU:HD12	1.81	0.63
15:O:2:PRO:O	15:O:38:ARG:NH1	2.32	0.63
1:A:78:G:C2	1:A:92:C:N4	2.66	0.63
3:C:29:TYR:HD2	3:C:33:LEU:HD22	1.64	0.63
1:A:512:U:OP1	4:D:46:LYS:NZ	2.31	0.62
5:E:126:ARG:HH11	5:E:126:ARG:CG	2.12	0.62
10:J:24:VAL:HG21	10:J:37:PRO:HG3	1.80	0.62
12:L:55:VAL:HG12	12:L:69:TYR:HA	1.80	0.62
1:A:1168:A:H2'	1:A:1169:A:C8	2.34	0.62
12:L:93:LEU:O	12:L:96:VAL:HG23	1.99	0.62
1:A:407:G:H5''	4:D:115:ARG:HB3	1.82	0.62
1:A:1111:A:N1	3:C:177:THR:HB	2.13	0.62
1:A:1465:C:H2'	1:A:1466:C:O4'	2.00	0.62
1:A:1096:C:H2'	1:A:1097:C:H6	1.65	0.62
1:A:1045:C:H2'	1:A:1046:A:H8	1.64	0.62
1:A:1436:U:H2'	1:A:1437:C:C6	2.32	0.62
1:A:299:G:H2'	1:A:300:A:C8	2.35	0.62
1:A:457:C:H2'	1:A:458:C:H6	1.64	0.62
1:A:1001:A:H2'	1:A:1002:G:H8	1.65	0.62
19:S:19:VAL:HG13	19:S:22:LEU:HD12	1.81	0.62
7:G:40:ALA:HB1	9:I:41:VAL:HG21	1.82	0.61
2:B:116:GLU:HG2	2:B:153:ARG:HH12	1.65	0.61
1:A:992:U:H3	1:A:1044:A:H61	1.47	0.61
2:B:240:GLN:OE1	2:B:240:GLN:N	2.33	0.61
9:I:26:VAL:HG23	9:I:33:PHE:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:38:GLN:OE1	9:I:39:GLY:N	2.34	0.61
14:N:39:LEU:HD13	14:N:43:CYS:HB3	1.83	0.61
15:O:36:ILE:HD13	15:O:59:MET:HE3	1.82	0.61
17:Q:95:TYR:HA	17:Q:98:LEU:HD11	1.81	0.61
4:D:156:GLU:O	4:D:160:GLN:HG2	1.99	0.61
1:A:75:G:N2	1:A:96:G:H1	1.98	0.61
1:A:1305:G:HO2'	1:A:1306:A:H8	1.49	0.61
1:A:1328:C:H2'	1:A:1329:A:H8	1.64	0.61
3:C:58:GLU:H	3:C:65:ALA:HB3	1.65	0.61
10:J:45:ARG:HB3	10:J:45:ARG:HH11	1.65	0.61
1:A:578:C:O2'	1:A:728:A:N3	2.28	0.61
2:B:98:LEU:HB2	2:B:101:MET:SD	2.40	0.61
7:G:17:VAL:HG12	7:G:18:TYR:HD1	1.66	0.61
3:C:132:ARG:HA	3:C:135:LYS:HE2	1.82	0.61
14:N:12:ARG:HG3	14:N:14:PRO:HD3	1.82	0.61
1:A:427:U:OP1	4:D:13:ARG:NH2	2.34	0.60
1:A:1243:C:H2'	1:A:1244:C:H6	1.65	0.60
1:A:1473:A:H2'	1:A:1474:G:C8	2.36	0.60
17:Q:60:ILE:O	17:Q:62:SER:OG	2.20	0.60
1:A:247:G:OP2	17:Q:100:LYS:HG3	2.00	0.60
1:A:989:C:H42	1:A:1216:G:H1	1.49	0.60
1:A:1113:C:N4	1:A:1187:G:H1	1.99	0.60
9:I:96:LEU:HD23	9:I:102:LEU:HD21	1.82	0.60
9:I:28:VAL:HG12	9:I:29:ASN:OD1	2.01	0.60
8:H:127:LEU:O	8:H:127:LEU:HD12	2.01	0.60
17:Q:18:THR:HG23	17:Q:69:LYS:HE3	1.84	0.60
18:R:86:VAL:HG12	18:R:87:ARG:H	1.67	0.60
21:U:6:ARG:HD3	21:U:15:ARG:NH1	2.17	0.60
1:A:92:C:H2'	1:A:92:C:O2	2.00	0.60
1:A:275:G:H5'	17:Q:14:LYS:HD3	1.84	0.60
1:A:1347:G:O2'	1:A:1348:U:O5'	2.19	0.60
3:C:56:ASP:HB2	3:C:67:THR:HB	1.83	0.60
8:H:111:ILE:HG22	8:H:134:ILE:HD12	1.83	0.60
9:I:45:ALA:HA	9:I:48:GLU:HB2	1.83	0.60
11:K:84:VAL:HG11	11:K:91:ARG:HD3	1.84	0.60
11:K:108:ILE:HB	18:R:87:ARG:O	2.02	0.60
2:B:181:PHE:CE2	8:H:70:GLN:HB3	2.37	0.60
6:F:11:ASN:HB2	6:F:86:ARG:NH2	2.17	0.60
17:Q:63:ARG:O	17:Q:65:ILE:HD12	2.02	0.60
1:A:1347:G:HO2'	1:A:1348:U:H6	1.49	0.60
1:A:1504:G:OP1	1:A:1507:A:H4'	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:98:LEU:HA	24:B:401:HOH:O	2.02	0.60
4:D:39:PRO:HG2	4:D:44:GLY:HA2	1.82	0.60
4:D:187:ARG:HD2	4:D:188:LEU:N	2.16	0.60
1:A:1152:A:H2'	1:A:1153:C:C6	2.37	0.59
7:G:75:VAL:HG11	7:G:86:GLN:HB3	1.83	0.59
1:A:5:U:H4'	1:A:6:G:O5'	2.02	0.59
1:A:1347:G:O2'	1:A:1348:U:H6	1.85	0.59
1:A:1368:G:OP2	9:I:112:LYS:HD3	2.01	0.59
11:K:21:ILE:HD12	11:K:95:ILE:HG23	1.84	0.59
1:A:36:C:OP1	12:L:123:LYS:NZ	2.28	0.59
1:A:668:G:H1'	15:O:46:HIS:HD2	1.67	0.59
1:A:1326:C:OP2	21:U:6:ARG:NH1	2.35	0.59
1:A:1499:A:H1'	1:A:1520[A]:G:OP1	2.02	0.59
7:G:46:ALA:O	7:G:50:ILE:HB	2.02	0.59
1:A:877:C:O2'	8:H:3:THR:HG23	2.03	0.59
1:A:1402:4OC:H2'	1:A:1403:C:C6	2.38	0.59
1:A:345:C:OP2	1:A:345:C:H6	1.86	0.59
1:A:376:G:OP2	16:P:67:THR:HG21	2.03	0.59
17:Q:29:HIS:CG	17:Q:30:PRO:HD2	2.37	0.59
1:A:79:G:C4	1:A:91:C:N3	2.70	0.59
1:A:101:A:H2'	1:A:102:G:C8	2.34	0.59
1:A:802:A:H2'	1:A:803:G:O4'	2.03	0.59
1:A:1257:U:O2'	1:A:1258:G:H8	1.84	0.59
1:A:1442:G:N7	1:A:1446:A:N6	2.50	0.59
2:B:23:ARG:O	2:B:24:TRP:HD1	1.86	0.59
4:D:36:ARG:HG2	4:D:38:TYR:OH	2.02	0.59
8:H:82:HIS:ND1	8:H:138:TRP:NE1	2.50	0.59
8:H:83:ILE:HG12	8:H:137:VAL:HG13	1.84	0.59
9:I:3:GLN:O	9:I:3:GLN:NE2	2.35	0.59
1:A:1238:A:OP1	1:A:1336:C:N4	2.32	0.59
1:A:1349:A:OP1	9:I:118:LYS:NZ	2.35	0.59
2:B:15:VAL:HG21	2:B:209:ARG:HG2	1.83	0.59
1:A:836:G:C6	1:A:851:G:C6	2.90	0.59
1:A:1187:G:H1'	14:N:61:TRP:OXT	2.02	0.59
13:M:59:TYR:CE1	13:M:63:THR:HG21	2.37	0.59
1:A:719:C:H42	18:R:74:ARG:HH12	1.50	0.59
1:A:1127:G:H1	1:A:1145:C:H42	1.50	0.59
1:A:1221:G:H5'	19:S:36:ARG:HH11	1.66	0.59
1:A:1356:G:H2'	1:A:1357:A:C8	2.38	0.59
12:L:84:LEU:O	12:L:101:VAL:HG23	2.02	0.59
15:O:18:PHE:HB2	15:O:19:PRO:HD2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:43:LYS:HG2	16:P:48:TRP:CG	2.37	0.59
1:A:344:A:H5'	1:A:345:C:C5	2.38	0.59
3:C:39:ILE:HG21	3:C:57:ILE:HD11	1.84	0.59
9:I:28:VAL:N	9:I:31:GLN:O	2.30	0.59
1:A:1033:G:H2'	1:A:1034:G:C8	2.38	0.58
3:C:155:GLY:HA2	3:C:164:ARG:O	2.03	0.58
9:I:71:SER:HA	9:I:74:ILE:HG13	1.84	0.58
13:M:107:ALA:HB3	13:M:111:LYS:HE3	1.85	0.58
19:S:56:GLN:HG2	19:S:57:HIS:H	1.68	0.58
1:A:1025:U:O2'	1:A:1026:G:O4'	2.21	0.58
1:A:1152:A:H2'	1:A:1153:C:H6	1.68	0.58
2:B:189:ASP:HB3	2:B:203:GLY:O	2.03	0.58
12:L:82:VAL:HG13	12:L:106:ASP:OD1	2.03	0.58
13:M:22:ILE:HG22	13:M:23:TYR:N	2.18	0.58
18:R:87:ARG:H	18:R:87:ARG:NH1	2.00	0.58
1:A:92:C:O2	1:A:93:G:C8	2.57	0.58
1:A:967:5MC:C4'	9:I:128:ARG:HG3	2.22	0.58
1:A:1474:G:H2'	1:A:1475:G:C8	2.38	0.58
3:C:148:GLY:HA3	3:C:172:ARG:O	2.03	0.58
4:D:112:VAL:HG23	4:D:116:GLN:OE1	2.02	0.58
17:Q:8:GLY:O	17:Q:56:VAL:HA	2.03	0.58
19:S:3:ARG:NH2	19:S:73:GLU:OE2	2.35	0.58
19:S:7:LYS:NZ	19:S:7:LYS:HB3	2.17	0.58
19:S:31:ILE:HG21	19:S:49:ILE:HD13	1.85	0.58
1:A:948:C:H42	1:A:1233:G:H1	1.49	0.58
2:B:55:PHE:CD2	2:B:58:ILE:HD12	2.38	0.58
3:C:30:ARG:HE	3:C:31:HIS:CE1	2.20	0.58
1:A:528:C:H41	12:L:49:ASN:HD21	1.52	0.58
1:A:933:G:OP2	7:G:3:ARG:HB3	2.03	0.58
1:A:1160:G:O4'	2:B:132:LYS:NZ	2.36	0.58
1:A:1328:C:H2'	1:A:1329:A:C8	2.39	0.58
1:A:753:A:H4'	1:A:754:C:O5'	2.03	0.58
11:K:59:TYR:O	11:K:62:GLN:HB3	2.04	0.58
2:B:82:ARG:HA	2:B:92:TYR:CE1	2.39	0.58
15:O:36:ILE:HA	15:O:59:MET:HE1	1.85	0.58
1:A:328:C:O2	1:A:328:C:H2'	2.02	0.58
1:A:1366:C:O3'	10:J:60:ARG:NH2	2.36	0.58
16:P:74:LEU:HB3	16:P:79:VAL:HG21	1.86	0.58
7:G:22:LEU:O	7:G:25:ALA:HB3	2.04	0.58
1:A:1358:U:H5''	14:N:35:ARG:HG3	1.85	0.57
1:A:1443:G:H5''	1:A:1446:A:H5''	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:124:ALA:O	8:H:128:GLY:N	2.34	0.57
16:P:39:TYR:HE2	16:P:41:PRO:HB3	1.69	0.57
1:A:237:C:OP2	17:Q:40:LYS:NZ	2.36	0.57
1:A:263:A:OP2	20:T:79:ARG:NH1	2.37	0.57
5:E:92:LYS:O	5:E:118:ILE:HG13	2.04	0.57
19:S:18:LYS:O	19:S:22:LEU:HG	2.05	0.57
1:A:463:A:H2'	1:A:474:G:H8	1.70	0.57
1:A:1057:G:H5''	3:C:154:SER:HB2	1.86	0.57
9:I:96:LEU:HB3	9:I:102:LEU:HG	1.85	0.57
1:A:76:C:H41	1:A:93:G:H1	1.49	0.57
1:A:719:C:H42	18:R:74:ARG:NH1	2.02	0.57
1:A:1006:C:H42	1:A:1024:G:H21	1.51	0.57
1:A:1370:G:H5''	9:I:109:VAL:HG11	1.86	0.57
19:S:51:VAL:HG12	19:S:52:TYR:H	1.68	0.57
1:A:372:C:H4'	1:A:373:A:O5'	2.05	0.57
1:A:946:A:H2'	1:A:947:G:C8	2.39	0.57
1:A:1347:G:H2'	1:A:1373:G:H1	1.68	0.57
1:A:1370:G:C5'	9:I:109:VAL:HG11	2.34	0.57
20:T:63:ILE:HG21	20:T:81:LYS:HG3	1.85	0.57
1:A:1305:G:N2	1:A:1331:G:H1'	2.19	0.57
1:A:403:C:H4'	4:D:122:ARG:NH1	2.19	0.57
1:A:945:G:O6	1:A:1236:A:N1	2.38	0.57
1:A:1216:G:OP1	14:N:3:ARG:NH2	2.38	0.57
20:T:79:ARG:O	20:T:83:ARG:HG3	2.04	0.57
1:A:77:G:C2	1:A:93:G:C2	2.93	0.57
13:M:99:ARG:HH12	19:S:2:PRO:HD2	1.70	0.57
1:A:60:A:H4'	1:A:61:G:O5'	2.05	0.57
1:A:355:C:H5'	1:A:389:A:OP2	2.05	0.57
1:A:1267:C:H1'	21:U:20:LYS:HE3	1.86	0.57
1:A:1357:A:H2'	1:A:1358:U:C6	2.40	0.57
3:C:38:ARG:HH11	3:C:38:ARG:HB2	1.69	0.57
4:D:9:CYS:O	4:D:12:CYS:HB2	2.04	0.57
1:A:1255:G:O2'	1:A:1258:G:H1'	2.04	0.57
13:M:79:LYS:HA	13:M:82:MET:HE2	1.86	0.57
1:A:926:G:H3'	1:A:1505:G:H21	1.70	0.56
15:O:56:LEU:HA	15:O:59:MET:HE2	1.87	0.56
18:R:43:PHE:C	18:R:51:LEU:HD12	2.29	0.56
1:A:407:G:OP1	4:D:115:ARG:HD3	2.05	0.56
1:A:1127:G:H1	1:A:1145:C:N4	2.03	0.56
1:A:1261:A:H1'	1:A:1283:G:H5''	1.87	0.56
4:D:78:LEU:O	4:D:81:GLU:HB3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:C:H2'	1:A:92:C:C5	2.40	0.56
1:A:95:U:H2'	1:A:96:G:C8	2.40	0.56
2:B:23:ARG:NH1	2:B:23:ARG:HB2	2.20	0.56
5:E:27:ARG:HG2	5:E:27:ARG:HH11	1.70	0.56
9:I:50:LEU:HD11	9:I:81:ILE:HD12	1.87	0.56
8:H:83:ILE:HD11	8:H:137:VAL:HG22	1.88	0.56
9:I:17:VAL:HG21	9:I:80:GLY:HA3	1.88	0.56
12:L:27:LEU:C	12:L:29:GLY:N	2.63	0.56
1:A:44:G:OP2	16:P:12:LYS:HB2	2.06	0.56
1:A:620:C:H2'	1:A:621:A:O4'	2.06	0.56
1:A:1031:G:H2'	1:A:1032:G:C8	2.41	0.56
1:A:1352:C:H2'	1:A:1353:G:C8	2.41	0.56
3:C:159:GLY:HA2	3:C:193:TYR:CZ	2.40	0.56
10:J:49:VAL:HG13	14:N:41:ARG:HB2	1.87	0.56
16:P:66:PRO:HG2	16:P:71:ARG:NH1	2.20	0.56
1:A:131:C:O2	1:A:231:G:N2	2.39	0.56
1:A:552:U:H2'	1:A:553:A:C8	2.41	0.56
1:A:1337:G:H5''	1:A:1338:G:OP1	2.06	0.56
9:I:48:GLU:N	9:I:49:PRO:HD2	2.21	0.56
17:Q:75:ARG:HH12	17:Q:77:VAL:HA	1.71	0.56
1:A:106:C:C2'	1:A:107:G:H5'	2.35	0.56
1:A:686:U:O2'	1:A:687:A:H8	1.88	0.56
1:A:1133:G:N2	1:A:1141:C:O2	2.38	0.56
1:A:1172:C:H2'	1:A:1173:G:H8	1.71	0.56
21:U:13:ILE:O	21:U:16:GLY:N	2.34	0.56
1:A:976:G:C8	1:A:1358:U:O2	2.59	0.56
1:A:1043:C:H2'	1:A:1044:A:C8	2.41	0.56
1:A:1484:C:H2'	1:A:1485:U:O4'	2.06	0.56
3:C:139:GLN:O	3:C:143:GLU:N	2.33	0.56
1:A:130:A:H5'	17:Q:63:ARG:HE	1.71	0.56
1:A:986:A:O2'	19:S:52:TYR:OH	2.14	0.56
14:N:22:THR:HB	14:N:33:VAL:HB	1.87	0.56
1:A:509:A:C8	1:A:509:A:H3'	2.41	0.56
1:A:975:A:H5'	1:A:975:A:C8	2.38	0.56
1:A:1351:U:H4'	7:G:33:ASP:CG	2.31	0.56
1:A:1242:C:N4	1:A:1295:G:H1	2.03	0.55
1:A:1255:G:N2	1:A:1259:C:O2	2.37	0.55
2:B:23:ARG:HH11	2:B:23:ARG:N	2.04	0.55
4:D:155:LEU:HB2	4:D:158:ILE:HG12	1.88	0.55
7:G:38:LEU:O	7:G:42:ILE:HG13	2.06	0.55
12:L:89:ARG:HH21	12:L:97:ARG:HB3	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:73:HIS:O	20:T:76:ALA:HB3	2.06	0.55
1:A:344:A:H4'	1:A:345:C:OP2	2.06	0.55
3:C:8:ILE:HD11	3:C:16:ARG:NH2	2.22	0.55
12:L:55:VAL:HA	12:L:70:ILE:HG13	1.87	0.55
13:M:15:VAL:HG21	13:M:48:LEU:HD21	1.89	0.55
1:A:976:G:OP2	1:A:1358:U:O2'	2.22	0.55
15:O:70:LEU:HD13	15:O:78:TYR:HB2	1.89	0.55
10:J:57:LYS:H	10:J:57:LYS:HD2	1.70	0.55
15:O:55:GLY:O	15:O:59:MET:HG3	2.06	0.55
17:Q:6:LEU:HD23	17:Q:6:LEU:N	2.22	0.55
1:A:147:G:H1	1:A:175:C:H42	1.53	0.55
1:A:373:A:H1'	1:A:481:G:H1'	1.88	0.55
1:A:401:C:H1'	1:A:622:A:H1'	1.89	0.55
1:A:673:G:H2'	1:A:674:G:C8	2.42	0.55
1:A:1254:C:OP1	10:J:45:ARG:HD2	2.06	0.55
1:A:1329:A:P	13:M:28:ALA:HB3	2.47	0.55
1:A:1367:C:H5'	10:J:60:ARG:HE	1.71	0.55
2:B:115:LEU:O	2:B:119:GLU:HB2	2.06	0.55
1:A:64:G:H4'	1:A:65:U:H5''	1.88	0.55
7:G:123:GLU:O	7:G:126:ASP:N	2.40	0.55
13:M:2:ALA:O	13:M:10:PRO:HD2	2.06	0.55
14:N:19:ARG:HB3	14:N:19:ARG:HH11	1.70	0.55
1:A:191:G:H21	20:T:104:LEU:HA	1.72	0.55
1:A:359:U:H2'	1:A:360:A:H8	1.70	0.55
3:C:131:ARG:HA	3:C:134:ILE:HD12	1.89	0.55
5:E:101:ILE:O	5:E:120:THR:HB	2.07	0.55
17:Q:86:GLU:O	17:Q:89:LEU:N	2.40	0.55
19:S:5:LEU:HD13	19:S:9:VAL:HG13	1.87	0.55
1:A:77:G:C6	1:A:93:G:N1	2.74	0.55
1:A:1505:G:C8	1:A:1505:G:H3'	2.42	0.55
1:A:1435:G:H2'	1:A:1436:U:H6	1.72	0.55
5:E:68:GLU:O	5:E:68:GLU:HG3	2.07	0.55
5:E:78:HIS:HD1	8:H:104:ARG:HG3	1.71	0.55
6:F:36:ARG:HB3	6:F:36:ARG:HH11	1.71	0.55
10:J:87:THR:HG23	10:J:89:ASP:H	1.72	0.55
11:K:41:THR:HG21	11:K:71:LYS:HB3	1.88	0.55
1:A:411:A:N7	1:A:413:G:N3	2.54	0.55
1:A:1143:G:H2'	1:A:1144:G:H8	1.71	0.55
1:A:1437:C:H5''	1:A:1438:G:OP2	2.06	0.55
3:C:116:VAL:O	3:C:119:ARG:HB3	2.07	0.55
7:G:20:ASP:OD2	7:G:21:VAL:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:A:H2'	1:A:474:G:C8	2.42	0.54
1:A:1147:C:O2'	9:I:5:TYR:OH	2.14	0.54
1:A:1188:A:H4'	24:N:202:HOH:O	2.06	0.54
8:H:119:LEU:HD12	8:H:124:ALA:HB2	1.89	0.54
15:O:15:PHE:CD2	15:O:30:ALA:HB2	2.41	0.54
1:A:579:G:O3'	15:O:54:ARG:NH2	2.38	0.54
1:A:1257:U:O2'	1:A:1258:G:O5'	2.26	0.54
1:A:1498:UR3:O4'	1:A:1519[A]:MA6:H2	2.06	0.54
2:B:22:LYS:O	2:B:23:ARG:HD3	2.07	0.54
5:E:88:LYS:HB3	5:E:123:LEU:HB2	1.89	0.54
11:K:94:ALA:O	11:K:98:LEU:HB2	2.07	0.54
1:A:103:C:O2'	1:A:172:A:N1	2.39	0.54
1:A:384:G:H2'	1:A:385:C:C5	2.41	0.54
1:A:633:G:H2'	1:A:634:C:C6	2.43	0.54
1:A:746:A:O2'	1:A:747:C:H5'	2.06	0.54
1:A:1181:G:O2'	1:A:1182:G:O5'	2.22	0.54
1:A:1416:G:C2'	1:A:1417:G:H5'	2.38	0.54
11:K:71:LYS:O	11:K:74:ALA:HB3	2.07	0.54
1:A:838:G:H1	1:A:848:C:N4	2.05	0.54
1:A:1200:C:H1'	1:A:1204:A:N6	2.23	0.54
1:A:1378:C:H2'	1:A:1379:G:O4'	2.08	0.54
1:A:1499:A:C1'	1:A:1520[A]:G:H5'	2.37	0.54
4:D:117:ALA:O	4:D:121:VAL:HG23	2.07	0.54
12:L:46:LYS:NZ	12:L:47:LYS:HE3	2.23	0.54
1:A:1355:G:H2'	1:A:1356:G:H8	1.71	0.54
3:C:131:ARG:O	3:C:134:ILE:HB	2.08	0.54
4:D:52:SER:O	4:D:56:VAL:HG23	2.07	0.54
1:A:1237:C:N4	1:A:1336:C:O2	2.41	0.54
1:A:1342:C:O2'	9:I:124:GLN:HG2	2.07	0.54
1:A:1369:C:H2'	1:A:1370:G:C8	2.42	0.54
2:B:17:PHE:HA	2:B:44:LEU:HD11	1.90	0.54
3:C:43:LEU:O	3:C:47:LEU:HB2	2.07	0.54
7:G:79:ARG:NE	7:G:82:GLY:O	2.37	0.54
1:A:853:G:C2'	1:A:854:G:H5'	2.37	0.54
1:A:1048:G:H5''	14:N:3:ARG:HH21	1.73	0.54
1:A:1085:U:C6	1:A:1094:G:N1	2.76	0.54
1:A:1406:U:H4'	1:A:1518[B]:MA6:H1'	1.90	0.54
4:D:127:THR:OG1	4:D:149:ALA:HB2	2.08	0.54
5:E:72:GLN:O	5:E:75:THR:HG22	2.07	0.54
1:A:560:U:H5'	1:A:566:G:C2	2.42	0.54
3:C:26:LYS:H	3:C:26:LYS:HD3	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:152:ILE:HB	3:C:199:LYS:HB2	1.90	0.54
10:J:82:ILE:H	10:J:82:ILE:HD12	1.72	0.54
13:M:25:ILE:HD11	13:M:66:LEU:HD11	1.90	0.54
18:R:87:ARG:HH11	18:R:87:ARG:HA	1.73	0.54
1:A:75:G:N2	1:A:96:G:N1	2.56	0.54
1:A:390:C:O3'	16:P:28:ARG:NH2	2.41	0.54
1:A:707:C:H2'	1:A:708:C:C6	2.43	0.54
1:A:1332:A:H2'	1:A:1333:A:C8	2.43	0.54
6:F:35:ALA:HA	6:F:67:MET:HB3	1.87	0.54
1:A:707:C:H2'	1:A:708:C:H6	1.72	0.54
2:B:172:ILE:H	2:B:172:ILE:HD12	1.71	0.54
2:B:191:ASP:OD1	2:B:191:ASP:N	2.37	0.54
18:R:86:VAL:HG12	18:R:87:ARG:NH1	2.23	0.54
1:A:1197:G:H5''	24:A:2054:HOH:O	2.08	0.53
1:A:1422:G:H2'	1:A:1423:G:H8	1.73	0.53
5:E:105:VAL:HG11	5:E:131:ILE:HG22	1.90	0.53
10:J:4:ILE:HG22	10:J:6:ILE:HD11	1.90	0.53
1:A:1181:G:C2	1:A:1182:G:N2	2.76	0.53
1:A:1329:A:C2	1:A:1330:U:C2	2.96	0.53
5:E:27:ARG:HG2	5:E:27:ARG:NH1	2.24	0.53
1:A:1014:A:H4'	19:S:14:HIS:CE1	2.43	0.53
2:B:91:PRO:HB3	2:B:154:LEU:HB3	1.91	0.53
4:D:114:ARG:HH11	4:D:114:ARG:HG3	1.74	0.53
16:P:79:VAL:N	24:P:204:HOH:O	2.40	0.53
1:A:62:U:OP1	1:A:385:C:O2'	2.25	0.53
1:A:381:C:H2'	1:A:382:A:O4'	2.09	0.53
1:A:1128:C:OP1	9:I:66:ARG:NH2	2.41	0.53
1:A:1244:C:H5''	1:A:1245:A:OP2	2.08	0.53
2:B:126:GLU:HG3	2:B:129:GLU:HB2	1.90	0.53
9:I:22:GLY:HA3	9:I:60:ASP:HB2	1.89	0.53
13:M:11:ARG:HA	13:M:45:VAL:HG11	1.90	0.53
1:A:241:C:H42	1:A:285:G:H1	1.57	0.53
1:A:677:U:H3	1:A:713:G:H22	1.55	0.53
1:A:1526:G:H2'	1:A:1527:C:H6	1.74	0.53
12:L:28:LYS:C	12:L:30:ALA:H	2.16	0.53
14:N:24:CYS:H	14:N:33:VAL:HG21	1.73	0.53
1:A:665:A:N3	1:A:732:C:H2'	2.23	0.53
2:B:139:LYS:NZ	2:B:143:GLU:HG3	2.23	0.53
4:D:121:VAL:HG11	4:D:136:PRO:HA	1.88	0.53
15:O:29:VAL:HG11	15:O:81:LEU:HD11	1.91	0.53
17:Q:21:VAL:HG21	17:Q:59:ILE:HG13	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:66:SER:HB3	17:Q:69:LYS:HG3	1.90	0.53
1:A:1305:G:O2'	1:A:1306:A:P	2.67	0.53
3:C:70:VAL:HG12	3:C:72:LYS:H	1.73	0.53
5:E:84:PHE:CB	5:E:134:ALA:HB2	2.38	0.53
10:J:52:GLY:O	14:N:41:ARG:NH2	2.41	0.53
1:A:404:U:O4	4:D:2:GLY:N	2.42	0.53
1:A:778:G:H8	1:A:778:G:O5'	1.92	0.53
1:A:1305:G:H5''	21:U:4:GLY:HA3	1.90	0.53
1:A:1320:C:N4	19:S:36:ARG:HG3	2.24	0.53
1:A:1329:A:OP1	13:M:28:ALA:HB3	2.08	0.53
3:C:114:PRO:O	3:C:118:GLN:NE2	2.42	0.53
4:D:150:GLU:HA	4:D:153:ARG:HG3	1.91	0.53
9:I:28:VAL:O	9:I:31:GLN:N	2.39	0.53
9:I:118:LYS:NZ	9:I:118:LYS:O	2.41	0.53
18:R:46:GLU:OE1	18:R:46:GLU:N	2.37	0.53
20:T:81:LYS:O	20:T:85:MET:HG3	2.09	0.53
1:A:47:C:H6	1:A:365:U:H2'	1.74	0.53
1:A:939:G:H5''	7:G:102:ARG:NH1	2.24	0.53
1:A:1190:G:OP1	3:C:4:LYS:HA	2.07	0.53
1:A:1250:A:H4'	9:I:68:GLY:O	2.09	0.53
1:A:1399:C:O2	1:A:1401:G:C5	2.62	0.53
2:B:19:HIS:ND1	2:B:20:GLU:HG2	2.24	0.53
6:F:4:TYR:HD1	6:F:92:LYS:HA	1.74	0.53
12:L:58:VAL:O	12:L:65:GLU:HA	2.08	0.53
15:O:4:THR:N	15:O:7:GLU:OE1	2.28	0.53
1:A:56:U:H2'	1:A:57:G:H8	1.74	0.53
1:A:1032:G:H2'	1:A:1033:G:O4'	2.08	0.53
1:A:1064:G:H1'	1:A:1190:G:H21	1.74	0.53
4:D:209:ARG:HG2	4:D:209:ARG:O	2.08	0.53
5:E:19:MET:HE1	5:E:24:ARG:NH1	2.24	0.53
8:H:83:ILE:CD1	8:H:137:VAL:HG22	2.39	0.53
15:O:29:VAL:HG21	15:O:67:LEU:HD23	1.91	0.53
1:A:273:A:N6	1:A:274:A:C6	2.77	0.52
1:A:416:G:H2'	1:A:417:C:C6	2.44	0.52
1:A:1311:G:H1	1:A:1326:C:H42	1.57	0.52
1:A:1397:C:O2'	1:A:1398:A:OP1	2.26	0.52
3:C:202:ILE:HG22	3:C:204:LEU:HD23	1.91	0.52
1:A:409:G:OP2	4:D:22:LYS:HD3	2.10	0.52
1:A:731:G:OP1	1:A:766:A:H1'	2.08	0.52
1:A:1093:A:N3	1:A:1109:C:O2'	2.41	0.52
2:B:51:LEU:O	2:B:55:PHE:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:180:LEU:O	2:B:181:PHE:HB2	2.09	0.52
4:D:152:SER:HA	4:D:155:LEU:HG	1.91	0.52
13:M:84:ILE:HG13	13:M:86:CYS:H	1.74	0.52
13:M:96:LEU:HB3	13:M:97:PRO:HD2	1.91	0.52
18:R:22:VAL:HG23	18:R:56:THR:HA	1.89	0.52
1:A:579:G:H5'	1:A:728:A:H1'	1.90	0.52
1:A:864:A:H2'	1:A:865:A:C8	2.44	0.52
1:A:885:G:H1	1:A:912:A:H2	1.57	0.52
1:A:1285:A:H4'	1:A:1286:A:O5'	2.09	0.52
5:E:19:MET:HE1	5:E:24:ARG:HH11	1.74	0.52
11:K:72:ALA:HB1	11:K:77:MET:HG3	1.91	0.52
13:M:16:ASP:OD1	13:M:16:ASP:N	2.41	0.52
16:P:53:VAL:O	16:P:54:GLU:C	2.51	0.52
1:A:421:U:H5'	1:A:422:C:H5	1.74	0.52
1:A:502:G:P	12:L:118:SER:HG	2.32	0.52
1:A:659:U:OP2	15:O:8:LYS:NZ	2.42	0.52
1:A:790:A:H2'	1:A:791:G:C8	2.44	0.52
1:A:1391:U:H2'	1:A:1392:G:C8	2.44	0.52
2:B:36:ARG:O	2:B:39:ILE:HD12	2.09	0.52
3:C:156:ARG:NH1	3:C:160:ALA:O	2.40	0.52
3:C:187:ALA:HB3	3:C:198:VAL:HB	1.91	0.52
12:L:45:PRO:HD3	12:L:51:ALA:O	2.09	0.52
1:A:589:C:O2'	1:A:590:C:H5'	2.09	0.52
1:A:902:G:H2'	1:A:903:G:H8	1.75	0.52
1:A:943:U:C2'	1:A:944:G:H5'	2.39	0.52
1:A:949:A:C2	1:A:1233:G:N3	2.78	0.52
12:L:53:ARG:NH1	12:L:92:0TD:OD2	2.43	0.52
21:U:12:LYS:O	21:U:22:ARG:NH1	2.41	0.52
1:A:459:G:H1'	1:A:463:A:H61	1.75	0.52
1:A:551:U:H2'	1:A:552:U:C6	2.44	0.52
1:A:1499:A:H1'	1:A:1520[A]:G:H5'	1.90	0.52
20:T:39:LYS:HG2	20:T:55:ILE:HD13	1.91	0.52
1:A:581:G:O3'	15:O:64:ARG:NH2	2.42	0.52
1:A:1172:C:H2'	1:A:1173:G:C8	2.45	0.52
5:E:91:LEU:HB3	5:E:118:ILE:HD11	1.91	0.52
6:F:97:PHE:HE1	18:R:61:LYS:HE2	1.74	0.52
8:H:77:GLU:HG2	8:H:78:GLN:H	1.73	0.52
12:L:8:ASN:O	12:L:12:ARG:HG2	2.09	0.52
1:A:350:G:H5''	1:A:350:G:H8	1.74	0.52
1:A:766:A:H2'	1:A:767:A:O4'	2.10	0.52
3:C:11:ARG:NH2	3:C:175:LEU:O	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:113:ARG:HB3	12:L:122:THR:HG21	1.92	0.52
1:A:423:G:H3'	1:A:423:G:N3	2.24	0.52
1:A:673:G:H5''	6:F:87:ARG:NH1	2.25	0.52
2:B:23:ARG:HB2	2:B:23:ARG:CZ	2.39	0.52
20:T:56:MET:HE1	20:T:104:LEU:HD21	1.92	0.52
1:A:1045:C:H2'	1:A:1046:A:C8	2.44	0.52
2:B:134:GLU:HA	2:B:137:ARG:HG3	1.92	0.52
3:C:136:GLN:HA	3:C:139:GLN:HG3	1.90	0.52
9:I:5:TYR:CD1	9:I:6:GLY:N	2.75	0.52
11:K:54:ARG:O	11:K:57:THR:HG22	2.08	0.52
19:S:22:LEU:HD22	19:S:28:LYS:HB2	1.92	0.52
1:A:337:C:H2'	1:A:338:A:H8	1.74	0.51
1:A:981:U:H5''	1:A:982:U:H5''	1.92	0.51
1:A:1118:C:O2'	1:A:1119:C:H5'	2.10	0.51
4:D:46:LYS:HG2	4:D:47:ARG:H	1.75	0.51
5:E:107:ARG:O	5:E:111:GLU:HB2	2.10	0.51
1:A:47:C:C6	1:A:365:U:H2'	2.46	0.51
1:A:528:C:N4	12:L:49:ASN:HD21	2.08	0.51
1:A:1305:G:O2'	1:A:1306:A:C8	2.58	0.51
3:C:130:VAL:O	3:C:134:ILE:HG13	2.10	0.51
1:A:254:G:OP1	17:Q:67:LYS:O	2.28	0.51
1:A:1338:G:C6	1:A:1339:A:C6	2.98	0.51
1:A:1502:A:C2	1:A:1504:G:C4	2.97	0.51
1:A:412:A:H5''	1:A:413:G:OP1	2.09	0.51
1:A:1000:U:H2'	1:A:1001:A:C8	2.46	0.51
1:A:1188:A:H5''	24:A:2233:HOH:O	2.10	0.51
1:A:1376:U:OP1	7:G:98:SER:OG	2.20	0.51
6:F:100:ASN:HB2	18:R:23:LYS:HG3	1.92	0.51
10:J:79:ARG:NH1	10:J:79:ARG:O	2.43	0.51
13:M:82:MET:HA	13:M:89:GLY:HA3	1.91	0.51
1:A:236:G:H2'	1:A:237:C:O4'	2.10	0.51
1:A:1163:C:H2'	1:A:1164:G:O4'	2.11	0.51
2:B:23:ARG:O	2:B:24:TRP:CD1	2.63	0.51
11:K:32:ILE:HD12	11:K:72:ALA:HB2	1.93	0.51
12:L:89:ARG:NH2	12:L:97:ARG:HB3	2.25	0.51
13:M:27:LYS:HE2	13:M:27:LYS:HA	1.93	0.51
1:A:1221:G:OP1	19:S:36:ARG:HD3	2.10	0.51
1:A:1358:U:O2'	1:A:1359:C:OP1	2.28	0.51
7:G:22:LEU:HD21	7:G:66:VAL:HG21	1.93	0.51
15:O:75:PRO:O	15:O:79:ARG:HG3	2.11	0.51
21:U:10:ARG:O	21:U:13:ILE:HB	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:90:GLY:HA2	11:K:93:GLN:HB2	1.92	0.51
15:O:74:ASP:CG	15:O:77:ARG:HG3	2.36	0.51
20:T:71:THR:O	20:T:72:LEU:HD23	2.10	0.51
5:E:36:ASP:OD1	5:E:38:GLN:N	2.38	0.51
5:E:60:TYR:HE1	5:E:64:ARG:HE	1.58	0.51
1:A:79:G:C2	1:A:80:G:C8	2.99	0.51
1:A:204:U:H4'	1:A:216:G:O4'	2.09	0.51
1:A:1355:G:H2'	1:A:1356:G:C8	2.46	0.51
1:A:1412:C:C5	1:A:1413:A:C6	2.99	0.51
1:A:1483:A:H2'	1:A:1484:C:O4'	2.11	0.51
2:B:24:TRP:HZ3	2:B:29:ALA:HB2	1.75	0.51
7:G:115:ARG:H	7:G:115:ARG:HD2	1.76	0.51
7:G:118:VAL:O	7:G:122:HIS:HB2	2.10	0.51
9:I:103:THR:HG22	9:I:104:ARG:O	2.11	0.51
14:N:3:ARG:NH1	14:N:3:ARG:HB3	2.26	0.51
6:F:23:LYS:NZ	6:F:42:GLU:OE1	2.40	0.51
9:I:79:LEU:O	9:I:83:ARG:HG2	2.11	0.51
10:J:27:ALA:HB2	10:J:85:LEU:HD21	1.93	0.51
14:N:9:LYS:HD2	14:N:23:ARG:HB2	1.91	0.51
16:P:8:ARG:NH2	16:P:15:PRO:HB3	2.26	0.51
1:A:1125:U:H5	10:J:73:ASP:OD2	1.94	0.50
1:A:1225:A:H2'	1:A:1225:A:N3	2.26	0.50
2:B:161:ALA:HB1	2:B:185:ILE:HD11	1.92	0.50
4:D:23:GLY:HA3	4:D:112:VAL:HG12	1.93	0.50
7:G:10:ARG:HB2	7:G:10:ARG:NH1	2.25	0.50
8:H:95:VAL:HG12	8:H:99:GLU:HB2	1.92	0.50
13:M:12:ASN:H	13:M:45:VAL:HB	1.76	0.50
18:R:70:ILE:HG22	18:R:71:LYS:N	2.26	0.50
7:G:22:LEU:HD12	7:G:97:GLN:HE22	1.77	0.50
7:G:28:ASN:O	7:G:31:MET:HB3	2.11	0.50
12:L:25:PRO:C	12:L:27:LEU:N	2.64	0.50
18:R:59:SER:H	18:R:62:GLU:HB2	1.76	0.50
1:A:144:G:H1	1:A:178:C:H42	1.57	0.50
1:A:985:C:N3	1:A:1221:G:N2	2.59	0.50
1:A:1003(A):G:N1	1:A:1038:C:N3	2.59	0.50
1:A:1222:G:OP2	1:A:1322:C:N4	2.41	0.50
7:G:40:ALA:CB	9:I:41:VAL:HG21	2.40	0.50
9:I:91:ASP:N	9:I:91:ASP:OD1	2.44	0.50
12:L:11:VAL:HG12	12:L:12:ARG:N	2.26	0.50
1:A:616:G:H1'	1:A:625:G:N2	2.26	0.50
1:A:736:C:H2'	1:A:737:A:C8	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:757:U:H2'	1:A:758:G:O4'	2.12	0.50
1:A:795:C:H5''	1:A:796:C:OP2	2.12	0.50
1:A:1092:A:N3	1:A:1183:A:N6	2.60	0.50
2:B:21:ARG:HA	2:B:39:ILE:HG23	1.94	0.50
3:C:58:GLU:HB3	10:J:92:THR:HG21	1.91	0.50
5:E:81:GLU:OE2	5:E:88:LYS:HE2	2.11	0.50
11:K:32:ILE:O	11:K:40:ILE:N	2.44	0.50
19:S:50:ALA:HA	19:S:58:VAL:O	2.12	0.50
1:A:620:C:C2	4:D:135:LEU:HD13	2.46	0.50
1:A:835:U:H3	1:A:851:G:H1	1.59	0.50
1:A:1128:C:O2'	1:A:1130:A:N7	2.40	0.50
1:A:1214:C:O2'	1:A:1215:G:H5'	2.11	0.50
2:B:136:VAL:HA	2:B:139:LYS:HB3	1.93	0.50
2:B:142:LEU:HD22	2:B:146:GLN:NE2	2.27	0.50
6:F:60:PHE:CZ	18:R:78:LEU:HD21	2.46	0.50
7:G:17:VAL:HG12	7:G:18:TYR:CD1	2.45	0.50
1:A:518:C:H4'	1:A:519:C:O5'	2.11	0.50
1:A:946:A:H2'	1:A:947:G:H8	1.76	0.50
1:A:1104:G:H4'	2:B:111:ARG:NH2	2.27	0.50
1:A:1257:U:HO2'	1:A:1258:G:P	2.34	0.50
1:A:1314:C:H2'	1:A:1315:U:C6	2.46	0.50
3:C:95:THR:O	3:C:95:THR:OG1	2.30	0.50
3:C:116:VAL:HG21	3:C:202:ILE:HD11	1.92	0.50
6:F:36:ARG:HB3	6:F:36:ARG:NH1	2.27	0.50
15:O:55:GLY:HA2	15:O:58:MET:HG3	1.92	0.50
1:A:1148:U:H4'	9:I:14:VAL:HG11	1.94	0.50
1:A:1443:G:H4'	1:A:1446:A:H5''	1.93	0.50
3:C:180:ALA:HB1	3:C:203:PHE:CE1	2.40	0.50
6:F:33:TYR:CD1	6:F:75:LEU:HA	2.46	0.50
13:M:4:ILE:HG12	13:M:56:LEU:CD1	2.40	0.50
1:A:123:C:OP1	1:A:312:C:H5'	2.12	0.50
3:C:29:TYR:CD2	3:C:33:LEU:HD22	2.46	0.50
10:J:6:ILE:HD13	10:J:72:VAL:HB	1.93	0.50
17:Q:63:ARG:HG2	17:Q:64:PRO:CD	2.42	0.50
1:A:114:U:O2'	1:A:115:G:H5'	2.12	0.50
1:A:552:U:H2'	1:A:553:A:H8	1.76	0.50
1:A:580:U:H2'	1:A:581:G:O4'	2.12	0.50
1:A:600:C:H42	1:A:638:G:H1	1.60	0.50
1:A:789:U:O2	1:A:791:G:C8	2.65	0.50
1:A:953:G:H2'	1:A:954:G:O4'	2.12	0.50
1:A:1058:G:H2'	1:A:1059:C:O4'	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1101:A:H4'	1:A:1102:A:O5'	2.12	0.50
1:A:1201:A:H4'	1:A:1202:G:O5'	2.11	0.50
2:B:142:LEU:HD13	2:B:146:GLN:HE22	1.76	0.50
3:C:156:ARG:HA	3:C:160:ALA:HB3	1.94	0.50
3:C:167:TRP:HE3	3:C:168:ALA:H	1.58	0.50
18:R:50:ILE:HD13	18:R:70:ILE:HD13	1.94	0.50
1:A:10:A:OP2	5:E:126:ARG:HD3	2.12	0.49
1:A:385:C:H2'	1:A:386:C:H6	1.77	0.49
1:A:918:A:H2'	1:A:919:A:O4'	2.12	0.49
1:A:980:C:H3'	1:A:981:U:C6	2.46	0.49
1:A:1505:G:H3'	1:A:1505:G:H8	1.77	0.49
1:A:44:G:N2	1:A:399:G:C4	2.80	0.49
1:A:45:U:H2'	1:A:46:G:C8	2.47	0.49
1:A:96:G:O2'	1:A:97:G:H5'	2.12	0.49
1:A:442:C:H42	1:A:492:G:H1	1.59	0.49
1:A:451:A:N6	1:A:481:G:C4	2.80	0.49
1:A:485:G:O2'	1:A:486:U:P	2.71	0.49
1:A:814:A:H2'	1:A:816:A:H5''	1.94	0.49
1:A:1065:U:H4'	1:A:1066:C:O5'	2.12	0.49
1:A:1481:U:C2	1:A:1482:G:C8	3.00	0.49
3:C:19:GLU:HB3	3:C:40:ARG:NH2	2.27	0.49
3:C:37:GLN:HE22	14:N:52:GLN:CD	2.21	0.49
4:D:36:ARG:HA	4:D:38:TYR:CE2	2.46	0.49
13:M:108:ARG:CZ	13:M:114:ARG:HG2	2.41	0.49
17:Q:67:LYS:O	17:Q:68:ARG:HB2	2.11	0.49
1:A:409:G:H1	1:A:433:C:H42	1.60	0.49
1:A:1521:G:H2'	1:A:1522:U:O4'	2.11	0.49
7:G:16:LEU:HD11	9:I:45:ALA:HB2	1.95	0.49
5:E:116:THR:HG23	5:E:117:ASP:OD1	2.12	0.49
6:F:3:ARG:HA	6:F:65:VAL:O	2.13	0.49
12:L:46:LYS:HZ2	12:L:47:LYS:HE3	1.78	0.49
14:N:53:LEU:HD12	14:N:56:VAL:HG21	1.94	0.49
18:R:34:TYR:CE1	18:R:35:ARG:HG3	2.47	0.49
1:A:117:G:O5'	1:A:117:G:H8	1.95	0.49
1:A:1339:A:H2'	1:A:1340:A:O4'	2.12	0.49
1:A:1398:A:H5'	1:A:1401:G:H4'	1.94	0.49
9:I:26:VAL:HG12	9:I:61:ALA:HB3	1.93	0.49
18:R:86:VAL:HG12	18:R:87:ARG:HH12	1.76	0.49
1:A:1518[A]:MA6:H93	1:A:1519[A]:MA6:H92	1.93	0.49
1:A:56:U:H2'	1:A:57:G:C8	2.47	0.49
1:A:496:A:H4'	1:A:497:A:OP1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1163:C:H2'	1:A:1164:G:C8	2.48	0.49
5:E:144:THR:O	5:E:147:ASP:HB2	2.13	0.49
10:J:48:THR:OG1	10:J:62:HIS:HB3	2.13	0.49
15:O:39:LEU:CD1	15:O:56:LEU:HB2	2.37	0.49
16:P:20:VAL:CG1	16:P:32:TYR:HB2	2.43	0.49
1:A:255:G:H2'	1:A:256:U:C6	2.47	0.49
1:A:477:G:H2'	1:A:478:A:C8	2.48	0.49
1:A:629:G:H2'	1:A:630:G:O4'	2.13	0.49
1:A:1287:A:H2'	1:A:1288:A:C8	2.48	0.49
5:E:46:GLY:H	5:E:58:ALA:HB2	1.78	0.49
11:K:48:ILE:HG22	11:K:49:GLY:H	1.78	0.49
11:K:91:ARG:HB3	11:K:91:ARG:HH11	1.77	0.49
1:A:193:C:H2'	1:A:194:C:H6	1.78	0.49
1:A:1269:A:N1	1:A:1312:G:O2'	2.42	0.49
3:C:8:ILE:HD11	3:C:16:ARG:HH21	1.78	0.49
1:A:299:G:C6	1:A:300:A:C6	3.01	0.49
5:E:118:ILE:O	5:E:119:LEU:HD23	2.11	0.49
9:I:53:VAL:HG21	9:I:59:PHE:HE1	1.77	0.49
1:A:21:G:H2'	1:A:22:G:C8	2.48	0.48
1:A:182:U:H3'	1:A:182:U:P	2.53	0.48
1:A:456:C:C2	1:A:457:C:C5	3.01	0.48
9:I:69:GLY:O	9:I:73:GLN:HG3	2.13	0.48
9:I:126:SER:HB2	9:I:127:LYS:HD2	1.95	0.48
13:M:36:LYS:HD3	13:M:59:TYR:CE2	2.48	0.48
1:A:91:C:HO2'	1:A:92:C:P	2.32	0.48
1:A:231:G:O2'	1:A:232:G:H5'	2.13	0.48
1:A:865:A:C2	1:A:918:A:H4'	2.48	0.48
2:B:139:LYS:HZ2	2:B:143:GLU:HG3	1.78	0.48
3:C:52:LEU:HD13	3:C:68:VAL:HG13	1.95	0.48
3:C:150:LYS:HB3	3:C:201:TYR:HB2	1.94	0.48
4:D:63:LYS:NZ	4:D:197:PRO:O	2.46	0.48
10:J:10:GLY:O	10:J:67:THR:HA	2.12	0.48
15:O:39:LEU:HB3	15:O:56:LEU:HD12	1.95	0.48
17:Q:63:ARG:HG2	17:Q:64:PRO:HD2	1.94	0.48
19:S:11:VAL:HG22	19:S:39:THR:HB	1.93	0.48
1:A:491:G:N2	1:A:492:G:H1'	2.28	0.48
1:A:679:C:H2'	1:A:680:C:H6	1.79	0.48
1:A:1347:G:H2'	1:A:1373:G:N1	2.27	0.48
1:A:1366:C:H2'	1:A:1367:C:H6	1.77	0.48
1:A:1418:A:N6	1:A:1482:G:H1'	2.27	0.48
5:E:78:HIS:ND1	8:H:104:ARG:HG3	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:11:THR:OG1	8:H:14:ARG:NH1	2.34	0.48
1:A:459:G:H1'	1:A:463:A:N6	2.28	0.48
1:A:912:A:H8	1:A:912:A:O5'	1.96	0.48
1:A:1022:G:N2	1:A:1023:G:O6	2.46	0.48
1:A:1300:G:HO2'	1:A:1301:U:P	2.34	0.48
1:A:1499:A:O5'	1:A:1499:A:H8	1.96	0.48
2:B:144:ARG:O	2:B:147:LYS:N	2.46	0.48
5:E:7:GLU:OE1	5:E:37:ARG:NE	2.46	0.48
6:F:39:LYS:HB2	6:F:39:LYS:HE3	1.44	0.48
8:H:34:GLU:HB3	8:H:118:VAL:HG21	1.95	0.48
9:I:97:LYS:HB2	9:I:102:LEU:HD12	1.94	0.48
18:R:74:ARG:HB3	18:R:81:PHE:CE1	2.48	0.48
19:S:40:ILE:HA	19:S:44:MET:SD	2.53	0.48
1:A:1065:U:H5''	1:A:1190:G:N2	2.28	0.48
1:A:1152:A:H5'	10:J:70:ARG:NH2	2.28	0.48
1:A:1191:A:H2'	1:A:1192:C:H6	1.78	0.48
1:A:1244:C:N4	1:A:1293:G:H1	2.11	0.48
1:A:1402:4OC:H2'	1:A:1403:C:O4'	2.13	0.48
1:A:1416:G:H2'	1:A:1417:G:H5'	1.95	0.48
4:D:173:TRP:HB2	4:D:187:ARG:O	2.14	0.48
16:P:82:GLN:H	16:P:82:GLN:HG2	1.50	0.48
1:A:78:G:N2	1:A:92:C:C4	2.82	0.48
1:A:1029:C:H42	1:A:1033:G:N2	2.11	0.48
1:A:1265:G:C6	1:A:1266:G:C6	3.00	0.48
1:A:1417:G:C8	1:A:1417:G:OP2	2.67	0.48
2:B:17:PHE:CD1	2:B:18:GLY:N	2.81	0.48
2:B:101:MET:HB2	2:B:102:LEU:HD12	1.94	0.48
3:C:112:SER:O	3:C:115:LEU:HB2	2.13	0.48
4:D:78:LEU:HD21	4:D:96:LEU:HB3	1.95	0.48
7:G:97:GLN:O	7:G:101:LEU:HD12	2.13	0.48
10:J:27:ALA:HB2	10:J:85:LEU:HD11	1.95	0.48
1:A:264:U:H4'	17:Q:63:ARG:HD3	1.96	0.48
1:A:550:G:C5	1:A:551:U:C5	3.02	0.48
1:A:992:U:O2'	1:A:993:G:OP2	2.25	0.48
1:A:1249:C:H2'	1:A:1250:A:H5'	1.95	0.48
1:A:1313:U:O4	19:S:4:SER:OG	2.25	0.48
1:A:1350:A:C5	1:A:1351:U:C5	3.02	0.48
8:H:104:ARG:CZ	8:H:138:TRP:CZ2	2.96	0.48
9:I:33:PHE:CE2	9:I:47:LEU:HD11	2.49	0.48
11:K:18:ARG:O	11:K:33:THR:HG23	2.14	0.48
12:L:6:THR:HB	12:L:8:ASN:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:72:LEU:HD21	20:T:80:ARG:HH12	1.79	0.48
1:A:303:A:H2'	1:A:304:U:O4'	2.13	0.48
1:A:646:U:H2'	1:A:647:C:C6	2.49	0.48
1:A:679:C:H2'	1:A:680:C:C6	2.49	0.48
1:A:1516[A]:G:H2'	1:A:1518[A]:MA6:OP2	2.14	0.48
3:C:157:ILE:HD13	3:C:166:GLU:HG2	1.96	0.48
4:D:164:ALA:O	4:D:168:ARG:HD3	2.13	0.48
11:K:110:ASP:HB2	18:R:88:LYS:HD2	1.94	0.48
15:O:12:ILE:HG23	15:O:27:VAL:CG1	2.43	0.48
1:A:77:G:N1	1:A:93:G:C2	2.82	0.48
1:A:217:C:H2'	1:A:218:C:C6	2.47	0.48
1:A:481:G:O2'	1:A:482:A:H8	1.97	0.48
1:A:502:G:H2'	1:A:503:C:O4'	2.14	0.48
1:A:625:G:H2'	1:A:626:U:C6	2.49	0.48
4:D:19:LEU:HA	4:D:19:LEU:HD23	1.45	0.48
13:M:67:GLU:HG3	13:M:68:GLY:H	1.78	0.48
15:O:12:ILE:HG12	15:O:31:LEU:HD11	1.94	0.48
17:Q:5:VAL:C	17:Q:6:LEU:HD23	2.39	0.48
1:A:76:C:C6	1:A:77:G:C8	3.02	0.48
1:A:106:C:H2'	1:A:107:G:H5'	1.95	0.48
1:A:176:C:H2'	1:A:177:C:C6	2.49	0.48
1:A:1437:C:O2	1:A:1437:C:H2'	2.13	0.48
7:G:73:MET:SD	7:G:90:GLU:HA	2.54	0.48
9:I:79:LEU:HD21	9:I:102:LEU:O	2.14	0.48
1:A:35:G:C6	1:A:36:C:N4	2.82	0.47
1:A:484:G:O2'	1:A:485:G:OP2	2.26	0.47
1:A:501:C:O3'	12:L:118:SER:OG	2.31	0.47
1:A:1049:U:H5'	1:A:1201:A:OP2	2.14	0.47
1:A:1058:G:C2	1:A:1059:C:C2	3.02	0.47
1:A:1413:A:H2'	1:A:1414:U:C6	2.49	0.47
4:D:31:CYS:C	4:D:33:MET:H	2.21	0.47
12:L:35:GLY:HA3	12:L:60:LEU:HD13	1.96	0.47
1:A:1116:C:O2'	9:I:108:VAL:HG21	2.14	0.47
1:A:1144:G:N2	1:A:1146:A:H62	2.11	0.47
1:A:1157:A:C8	1:A:1158:C:C4	3.02	0.47
1:A:1203:C:O5'	1:A:1203:C:H6	1.97	0.47
1:A:1347:G:O2'	1:A:1348:U:P	2.72	0.47
2:B:219:VAL:HG13	2:B:223:ILE:HD11	1.96	0.47
10:J:87:THR:HG23	10:J:89:ASP:N	2.29	0.47
1:A:723:U:O2	1:A:723:U:H2'	2.14	0.47
1:A:757:U:O2'	1:A:879:C:O2	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:833:U:H2'	1:A:834:C:C6	2.48	0.47
2:B:21:ARG:HG3	2:B:22:LYS:H	1.80	0.47
2:B:62:ALA:HB1	2:B:222:ILE:HG23	1.95	0.47
5:E:10:MET:SD	5:E:13:ILE:HG23	2.55	0.47
6:F:53:ALA:HB3	6:F:86:ARG:NH1	2.29	0.47
12:L:46:LYS:HG2	12:L:47:LYS:HG3	1.96	0.47
1:A:115:G:H5''	24:A:2260:HOH:O	2.14	0.47
1:A:902:G:H2'	1:A:903:G:C8	2.49	0.47
1:A:1496:C:H2'	1:A:1497:G:O4'	2.14	0.47
13:M:106:ASN:HA	13:M:108:ARG:HG2	1.97	0.47
16:P:18:ARG:O	16:P:20:VAL:HG23	2.14	0.47
16:P:53:VAL:O	16:P:55:ARG:N	2.47	0.47
20:T:39:LYS:O	20:T:43:LEU:HD23	2.14	0.47
1:A:164:U:H2'	1:A:165:C:C6	2.49	0.47
1:A:945:G:N1	1:A:1337:G:C2	2.82	0.47
1:A:986:A:H2'	1:A:987:G:C8	2.49	0.47
1:A:1007:C:H2'	1:A:1008:C:C6	2.50	0.47
1:A:1064:G:N2	1:A:1190:G:O2'	2.48	0.47
1:A:1160:G:O6	1:A:1181:G:C6	2.67	0.47
3:C:22:TRP:CD1	3:C:59:ARG:HG3	2.49	0.47
6:F:27:GLN:O	6:F:31:GLU:HG3	2.14	0.47
9:I:97:LYS:HB2	9:I:97:LYS:HE2	1.68	0.47
10:J:15:THR:HG23	10:J:94:VAL:HG13	1.95	0.47
11:K:63:LEU:HD23	11:K:63:LEU:HA	1.52	0.47
16:P:9:PHE:HD1	16:P:18:ARG:HG3	1.79	0.47
17:Q:86:GLU:CG	17:Q:90:ILE:HD11	2.44	0.47
20:T:30:LYS:O	20:T:34:LYS:HG2	2.14	0.47
1:A:310:G:OP2	16:P:27:LYS:NZ	2.35	0.47
5:E:83:GLU:HG2	5:E:88:LYS:HG3	1.96	0.47
11:K:29:ILE:HD12	11:K:30:VAL:N	2.30	0.47
16:P:3:LYS:HD2	16:P:65:GLN:O	2.15	0.47
1:A:79:G:N1	1:A:80:G:C5	2.83	0.47
1:A:124:G:H2'	1:A:125:U:C6	2.49	0.47
1:A:316:G:H1	1:A:337:C:H42	1.61	0.47
1:A:923:A:OP1	5:E:21:ALA:HB2	2.15	0.47
1:A:1157:A:C4	1:A:1181:G:N2	2.82	0.47
1:A:1526:G:C4	1:A:1527:C:C5	3.03	0.47
2:B:10:LEU:C	2:B:12:GLU:H	2.21	0.47
4:D:152:SER:O	4:D:155:LEU:HG	2.14	0.47
5:E:6:PHE:HD2	5:E:36:ASP:HB3	1.80	0.47
14:N:36:PHE:C	14:N:36:PHE:CD1	2.93	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:30:ALA:HA	15:O:85:LEU:HD11	1.96	0.47
16:P:20:VAL:HG13	16:P:32:TYR:HB2	1.96	0.47
17:Q:40:LYS:HD3	17:Q:42:TYR:OH	2.15	0.47
18:R:39:VAL:HG13	18:R:40:LEU:HD23	1.96	0.47
20:T:36:LEU:HA	20:T:36:LEU:HD23	1.61	0.47
20:T:36:LEU:O	20:T:39:LYS:HB3	2.14	0.47
1:A:8:A:C2	4:D:209:ARG:HD2	2.50	0.47
1:A:88:A:H2'	1:A:89:C:O4'	2.14	0.47
1:A:113:G:C1'	1:A:354:G:H5'	2.41	0.47
1:A:236:G:OP1	17:Q:40:LYS:NZ	2.38	0.47
1:A:1029:C:H42	1:A:1033:G:H21	1.61	0.47
1:A:1068:G:OP2	1:A:1068:G:H8	1.98	0.47
1:A:1336:C:H6	1:A:1336:C:H5''	1.80	0.47
4:D:206:PHE:CD2	4:D:207:TYR:CE2	3.03	0.47
8:H:33:GLU:OE2	8:H:50:ARG:NH2	2.48	0.47
8:H:36:LEU:HA	8:H:39:LEU:HD12	1.96	0.47
9:I:74:ILE:HA	9:I:77:ILE:HD12	1.96	0.47
10:J:6:ILE:O	10:J:71:LEU:HD12	2.15	0.47
10:J:49:VAL:CG1	14:N:41:ARG:HB2	2.44	0.47
15:O:87:ILE:HG22	15:O:88:ARG:N	2.30	0.47
16:P:38:TYR:HE2	16:P:50:LYS:HE2	1.80	0.47
1:A:1096:C:H2'	1:A:1097:C:C6	2.49	0.47
1:A:1366:C:H2'	1:A:1367:C:C6	2.49	0.47
2:B:54:THR:O	2:B:58:ILE:HG13	2.15	0.47
2:B:217:ARG:HA	2:B:217:ARG:HD3	1.71	0.47
3:C:64:VAL:HG12	3:C:65:ALA:H	1.80	0.47
3:C:123:GLN:O	3:C:128:PHE:HB2	2.15	0.47
7:G:124:LEU:HD23	7:G:124:LEU:HA	1.63	0.47
8:H:11:THR:O	8:H:12:ARG:C	2.58	0.47
9:I:126:SER:OG	9:I:127:LYS:N	2.48	0.47
10:J:6:ILE:C	10:J:71:LEU:HD12	2.39	0.47
16:P:4:ILE:HG22	16:P:70:ALA:HB1	1.96	0.47
1:A:110:C:H2'	1:A:111:G:O4'	2.15	0.47
1:A:376:G:H5''	16:P:5:ARG:HB2	1.97	0.47
1:A:1053:G:H4'	1:A:1054:C:H5'	1.97	0.47
1:A:1103:C:H2'	1:A:1104:G:O4'	2.15	0.47
1:A:1174:G:H2'	1:A:1175:G:H8	1.80	0.47
1:A:1349:A:OP1	9:I:120:ARG:HB2	2.15	0.47
3:C:24:ALA:HB1	3:C:28:GLN:HB2	1.97	0.47
5:E:37:ARG:O	5:E:114:GLY:HA3	2.14	0.47
10:J:15:THR:HG23	10:J:94:VAL:CG1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:61:GLU:OE1	14:N:45:ARG:NH1	2.42	0.47
13:M:34:LEU:HG	13:M:41:PRO:HA	1.97	0.47
1:A:1150:U:O4	1:A:1151:A:N6	2.48	0.46
1:A:1218:C:H2'	1:A:1219:U:C6	2.49	0.46
3:C:117:ALA:HB1	3:C:187:ALA:HB2	1.97	0.46
14:N:9:LYS:HE2	14:N:12:ARG:HH12	1.80	0.46
15:O:18:PHE:CE2	15:O:21:ASP:HB2	2.50	0.46
1:A:1003(A):G:N2	1:A:1038:C:O2	2.49	0.46
2:B:97:TRP:HH2	2:B:176:GLU:OE2	1.96	0.46
3:C:199:LYS:HB3	3:C:201:TYR:HE1	1.81	0.46
7:G:150:ALA:HA	11:K:59:TYR:CD2	2.51	0.46
10:J:21:GLN:O	10:J:25:GLU:HG3	2.15	0.46
18:R:79:LEU:CD2	18:R:80:PRO:HD2	2.45	0.46
1:A:397:A:H3'	1:A:397:A:N3	2.30	0.46
1:A:978:A:N7	1:A:1361:G:N2	2.64	0.46
1:A:997:U:H2'	1:A:998:G:C8	2.51	0.46
1:A:1202:G:N3	14:N:42:ILE:HD12	2.31	0.46
1:A:1376:U:O4	7:G:10:ARG:NH1	2.49	0.46
1:A:1414:U:O2	1:A:1414:U:H2'	2.15	0.46
1:A:1434:A:N7	1:A:1435:G:C5	2.83	0.46
1:A:1498:UR3:H4'	1:A:1519[A]:MA6:N1	2.31	0.46
4:D:73:ARG:O	4:D:77:ASN:HB2	2.15	0.46
5:E:31:LEU:HA	5:E:31:LEU:HD23	1.60	0.46
5:E:152:ARG:O	8:H:64:LYS:NZ	2.48	0.46
6:F:26:ILE:HG21	6:F:63:TYR:HE2	1.81	0.46
8:H:84:ARG:HG3	8:H:85:ARG:N	2.28	0.46
8:H:112:LEU:N	8:H:112:LEU:HD23	2.29	0.46
10:J:42:THR:HG23	10:J:67:THR:C	2.41	0.46
1:A:78:G:N2	1:A:79:G:H1'	2.30	0.46
1:A:892:A:C2	1:A:907:A:C4	3.04	0.46
1:A:966:M2G:HM22	1:A:967:5MC:C2	2.50	0.46
1:A:988:G:N1	1:A:989:C:O2	2.48	0.46
1:A:1435:G:C2	1:A:1436:U:C4	3.04	0.46
2:B:118:LEU:O	2:B:122:PHE:N	2.49	0.46
8:H:114:THR:OG1	8:H:117:GLY:O	2.22	0.46
10:J:32:ALA:O	10:J:34:VAL:HG23	2.15	0.46
18:R:36:ASN:OD1	18:R:39:VAL:HG12	2.16	0.46
1:A:1145:C:HO2'	1:A:1146:A:P	2.37	0.46
1:A:1214:C:H3'	1:A:1215:G:C8	2.50	0.46
2:B:98:LEU:HD13	24:B:401:HOH:O	2.16	0.46
3:C:21:ARG:HG3	3:C:58:GLU:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:101:SER:OG	11:K:102:GLY:N	2.49	0.46
14:N:36:PHE:C	14:N:36:PHE:HD1	2.22	0.46
1:A:78:G:N2	1:A:92:C:C5	2.84	0.46
1:A:564:C:O2'	8:H:91:ARG:NH2	2.44	0.46
1:A:1202:G:O2'	14:N:27:CYS:SG	2.64	0.46
1:A:1425:U:O2'	1:A:1426:C:H5'	2.16	0.46
2:B:31:TYR:N	2:B:31:TYR:CD1	2.84	0.46
6:F:10:LEU:HB3	6:F:84:ASN:O	2.16	0.46
8:H:51:VAL:HG21	8:H:60:ARG:NH2	2.31	0.46
10:J:34:VAL:HG13	10:J:74:ILE:HA	1.97	0.46
1:A:297:G:H5''	1:A:298:A:OP2	2.15	0.46
1:A:881:G:H2'	1:A:882:C:O4'	2.15	0.46
1:A:989:C:N3	1:A:1216:G:N2	2.64	0.46
1:A:1371:G:O3'	9:I:69:GLY:HA3	2.15	0.46
1:A:1422:G:H2'	1:A:1423:G:C8	2.51	0.46
9:I:126:SER:CB	9:I:127:LYS:HD2	2.46	0.46
12:L:25:PRO:HA	12:L:27:LEU:H	1.81	0.46
16:P:75:ARG:HH11	16:P:75:ARG:HG3	1.81	0.46
20:T:83:ARG:NH2	24:T:301:HOH:O	2.49	0.46
1:A:991:U:O2'	1:A:992:U:P	2.74	0.46
1:A:1015:A:N6	1:A:1016:A:C6	2.84	0.46
1:A:1196:U:H3'	1:A:1197:G:H5'	1.98	0.46
4:D:140:VAL:HG11	4:D:146:ILE:HD11	1.98	0.46
6:F:33:TYR:CE1	6:F:75:LEU:HA	2.51	0.46
12:L:60:LEU:HD13	12:L:60:LEU:HA	1.52	0.46
13:M:29:ARG:HB3	13:M:64:TRP:CH2	2.51	0.46
16:P:43:LYS:HG2	16:P:48:TRP:CD2	2.50	0.46
1:A:129(A):G:H1'	1:A:190(E):U:H2'	1.97	0.46
1:A:316:G:H2'	1:A:317:G:H8	1.81	0.46
1:A:446:G:N2	1:A:488:C:N3	2.50	0.46
1:A:981:U:H4'	14:N:21:TYR:CE2	2.51	0.46
1:A:1030:C:H42	1:A:1031:G:H22	1.64	0.46
1:A:1174:G:C2	1:A:1175:G:C5	3.04	0.46
1:A:1278:U:H5'	1:A:1279:A:H5'	1.96	0.46
1:A:1369:C:H2'	1:A:1370:G:H8	1.80	0.46
1:A:1518[B]:MA6:H93	1:A:1519[B]:MA6:C2	2.46	0.46
2:B:134:GLU:HB2	2:B:137:ARG:HE	1.80	0.46
3:C:151:VAL:O	3:C:152:ILE:HD13	2.15	0.46
11:K:27:ASN:OD1	11:K:28:THR:N	2.49	0.46
15:O:76:GLU:O	15:O:77:ARG:C	2.59	0.46
17:Q:4:LYS:CG	17:Q:6:LEU:HD21	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:51:LEU:HD23	18:R:52:PRO:HD2	1.98	0.46
19:S:15:LEU:HD21	19:S:71:LEU:HD11	1.97	0.46
1:A:106:C:O2'	1:A:107:G:H5'	2.16	0.46
1:A:130:A:H1'	1:A:263:A:O2'	2.16	0.46
1:A:935:A:O2'	1:A:1383:C:N3	2.48	0.46
1:A:1067:A:N1	1:A:1108:G:O2'	2.44	0.46
3:C:61:ALA:C	3:C:63:ASN:H	2.24	0.46
5:E:80:ILE:HD11	5:E:138:ALA:HA	1.98	0.46
10:J:91:PRO:HB2	10:J:94:VAL:CG2	2.46	0.46
12:L:20:LYS:H	12:L:20:LYS:HG3	1.57	0.46
12:L:58:VAL:HG12	12:L:59:ARG:O	2.14	0.46
13:M:40:ASN:HD22	13:M:43:THR:HG23	1.81	0.46
17:Q:83:ASP:OD1	17:Q:83:ASP:N	2.45	0.46
1:A:280:C:H4'	1:A:281:G:OP2	2.15	0.45
1:A:877:C:O2	8:H:3:THR:HG21	2.15	0.45
1:A:1090:U:H2'	1:A:1091:U:H6	1.81	0.45
1:A:1243:C:H2'	1:A:1244:C:C6	2.48	0.45
1:A:1300:G:OP2	1:A:1335:C:N4	2.50	0.45
1:A:1417:G:H21	1:A:1484:C:H42	1.63	0.45
5:E:95:ALA:O	5:E:98:THR:OG1	2.28	0.45
11:K:59:TYR:CE1	11:K:63:LEU:HD11	2.51	0.45
1:A:130:A:H5'	17:Q:63:ARG:NE	2.30	0.45
1:A:344:A:H5'	1:A:345:C:H5	1.79	0.45
1:A:1332:A:H2'	1:A:1333:A:H8	1.81	0.45
2:B:24:TRP:HA	2:B:190:THR:O	2.16	0.45
8:H:10:LEU:HD23	8:H:10:LEU:HA	1.48	0.45
8:H:65:TYR:HA	8:H:79:VAL:HG23	1.98	0.45
11:K:90:GLY:HA2	11:K:93:GLN:H	1.80	0.45
17:Q:38:ARG:N	17:Q:38:ARG:HD2	2.32	0.45
20:T:75:ASN:HA	20:T:78:ALA:HB3	1.98	0.45
1:A:452:A:H2'	1:A:453:A:C8	2.52	0.45
1:A:939:G:H2'	1:A:940:C:C6	2.51	0.45
1:A:1117:G:H5''	9:I:104:ARG:NH2	2.30	0.45
2:B:122:PHE:CZ	2:B:139:LYS:HE2	2.51	0.45
11:K:44:SER:O	11:K:47:VAL:HB	2.16	0.45
16:P:38:TYR:CE2	16:P:50:LYS:HE2	2.51	0.45
16:P:39:TYR:CD1	16:P:73:LEU:HD13	2.51	0.45
1:A:51:A:C6	1:A:353:A:C2	3.05	0.45
1:A:120:A:H2'	1:A:122:G:C8	2.52	0.45
1:A:419:C:H42	1:A:424:G:H1	1.63	0.45
1:A:926:G:H3'	1:A:1505:G:N2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1417:G:H21	1:A:1484:C:N4	2.15	0.45
2:B:97:TRP:CZ3	2:B:98:LEU:O	2.70	0.45
10:J:8:LEU:HD11	10:J:72:VAL:HG22	1.98	0.45
17:Q:37:LYS:C	17:Q:38:ARG:HD2	2.41	0.45
1:A:542:G:H5'	4:D:41:GLY:HA3	1.99	0.45
1:A:544:G:C6	1:A:545:C:C4	3.04	0.45
1:A:1035:A:H2'	1:A:1036:G:C8	2.51	0.45
2:B:55:PHE:HD2	2:B:58:ILE:HD12	1.80	0.45
5:E:51:VAL:HB	5:E:52:PRO:HD3	1.98	0.45
6:F:14:LEU:HD21	6:F:84:ASN:OD1	2.15	0.45
8:H:97:VAL:HG23	8:H:129:VAL:O	2.17	0.45
10:J:89:ASP:OD2	10:J:91:PRO:HD2	2.15	0.45
13:M:80:ARG:NH1	13:M:81:LEU:HB3	2.32	0.45
1:A:588:G:H1	1:A:651:C:N4	2.12	0.45
1:A:838:G:N2	1:A:849:C:C2	2.85	0.45
1:A:1361(A):C:O2'	1:A:1362:C:H6	2.00	0.45
5:E:87:SER:HB3	5:E:131:ILE:HD13	1.98	0.45
6:F:4:TYR:HB2	6:F:65:VAL:HG22	1.98	0.45
6:F:10:LEU:HD11	6:F:61:LEU:HD11	1.98	0.45
7:G:102:ARG:O	7:G:106:GLN:HG3	2.16	0.45
8:H:102:ARG:HG3	8:H:102:ARG:O	2.17	0.45
9:I:83:ARG:O	9:I:86:VAL:HG12	2.17	0.45
11:K:47:VAL:HG12	11:K:48:ILE:N	2.31	0.45
1:A:1174:G:H2'	1:A:1175:G:C8	2.51	0.45
1:A:1406:U:O2'	1:A:1517[B]:G:N2	2.50	0.45
2:B:87:ARG:HB3	2:B:87:ARG:HH11	1.82	0.45
3:C:64:VAL:HB	3:C:99:VAL:HG23	1.99	0.45
3:C:117:ALA:HB2	3:C:200:ALA:CB	2.46	0.45
5:E:36:ASP:OD2	5:E:40:ARG:HB2	2.16	0.45
8:H:87:SER:CA	8:H:93:VAL:HG13	2.44	0.45
11:K:70:LYS:HE2	11:K:70:LYS:HB3	1.76	0.45
12:L:46:LYS:HD2	12:L:94:PRO:HG3	1.99	0.45
16:P:34:GLU:OE2	16:P:55:ARG:HD2	2.17	0.45
17:Q:43:LEU:HD12	17:Q:68:ARG:HB3	1.99	0.45
17:Q:60:ILE:HG13	17:Q:61:GLU:N	2.31	0.45
18:R:26:LEU:HD23	18:R:29:PHE:CE2	2.52	0.45
20:T:82:SER:O	20:T:83:ARG:C	2.60	0.45
1:A:445:G:C2	1:A:490:G:C2	3.05	0.45
1:A:1112:C:H1'	3:C:179:ARG:NH2	2.31	0.45
1:A:1288:A:H2'	1:A:1289:A:H8	1.82	0.45
1:A:1481:U:C4	1:A:1482:G:N7	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:24:TRP:CZ3	2:B:26:PRO:HA	2.52	0.45
2:B:108:ILE:HD12	2:B:108:ILE:HA	1.74	0.45
2:B:162:ILE:HG22	2:B:164:VAL:HG23	1.98	0.45
8:H:86:ILE:HG22	8:H:87:SER:N	2.30	0.45
13:M:54:VAL:O	13:M:58:GLU:HG2	2.16	0.45
18:R:76:LEU:HD23	18:R:76:LEU:HA	1.58	0.45
1:A:452:A:O2'	1:A:453:A:O5'	2.34	0.45
1:A:832:C:H2'	1:A:833:U:O4'	2.17	0.45
1:A:955:U:H1'	1:A:1227:A:N6	2.31	0.45
1:A:1346:A:H62	1:A:1375:A:H62	1.65	0.45
1:A:1397:C:HO2'	1:A:1398:A:P	2.40	0.45
2:B:21:ARG:HA	2:B:39:ILE:HA	1.98	0.45
4:D:73:ARG:HD3	4:D:77:ASN:OD1	2.16	0.45
7:G:108:ALA:O	7:G:119:ARG:HG2	2.17	0.45
9:I:9:ARG:CG	9:I:14:VAL:HG13	2.47	0.45
9:I:75:ASP:O	9:I:78:LYS:HB3	2.17	0.45
10:J:7:LYS:HB3	10:J:97:GLU:HB2	1.98	0.45
11:K:80:VAL:HG21	11:K:103:LEU:HD13	1.99	0.45
12:L:17:LYS:HB2	12:L:17:LYS:HE3	1.74	0.45
21:U:18:TYR:HE2	21:U:22:ARG:HE	1.65	0.45
1:A:7:G:H5'	1:A:298:A:H5'	1.98	0.45
1:A:410:G:C2	1:A:429:U:C2	3.05	0.45
1:A:1417:G:N2	1:A:1484:C:H42	2.15	0.45
1:A:1513:A:H2'	1:A:1514:C:C6	2.52	0.45
2:B:101:MET:O	2:B:105:PHE:HD1	2.00	0.45
3:C:66:VAL:HG21	3:C:91:LEU:HD21	1.99	0.45
4:D:121:VAL:HG12	4:D:134:ASP:C	2.42	0.45
6:F:22:GLU:OE1	6:F:82:ARG:NH2	2.50	0.45
8:H:36:LEU:HA	8:H:36:LEU:HD23	1.70	0.45
13:M:79:LYS:O	13:M:83:ASP:HB2	2.17	0.45
1:A:75:G:N2	1:A:96:G:H22	2.15	0.44
1:A:980:C:H5''	1:A:981:U:C5	2.52	0.44
1:A:1124:G:H2'	1:A:1145:C:H41	1.81	0.44
2:B:107:THR:HG23	2:B:110:GLN:OE1	2.17	0.44
5:E:90:VAL:HG23	5:E:121:LYS:O	2.16	0.44
7:G:37:ASN:HB3	24:G:201:HOH:O	2.17	0.44
8:H:27:PRO:HA	8:H:58:TYR:CD2	2.51	0.44
9:I:117:HIS:HB2	9:I:121:ARG:HG2	1.98	0.44
17:Q:15:MET:HE3	17:Q:18:THR:HB	1.99	0.44
1:A:11:G:C5	1:A:12:U:C5	3.05	0.44
1:A:191:G:O2'	20:T:102:GLY:O	2.24	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:A:P	1:A:485:G:H22	2.40	0.44
1:A:853:G:H2'	1:A:854:G:H5'	1.99	0.44
1:A:970:C:OP1	10:J:57:LYS:NZ	2.26	0.44
1:A:1215:G:H2'	1:A:1215:G:N3	2.32	0.44
3:C:85:ARG:HA	3:C:88:ARG:HD2	1.99	0.44
5:E:98:THR:HB	5:E:117:ASP:HB3	1.99	0.44
7:G:89:MET:HA	7:G:155:ARG:NH1	2.32	0.44
7:G:136:LYS:HE3	7:G:136:LYS:HB3	1.77	0.44
8:H:120:THR:H	8:H:123:GLU:HB2	1.83	0.44
10:J:91:PRO:HB2	10:J:94:VAL:HG21	1.99	0.44
11:K:114:VAL:HG23	11:K:115:PRO:HD2	2.00	0.44
15:O:60:VAL:HG12	15:O:61:GLY:N	2.33	0.44
20:T:33:ILE:CD1	20:T:63:ILE:HA	2.47	0.44
1:A:28:G:C6	1:A:29:G:C5	3.06	0.44
1:A:981:U:H5'	14:N:21:TYR:OH	2.17	0.44
1:A:1124:G:C8	1:A:1145:C:C5	3.06	0.44
3:C:84:ILE:HG23	3:C:88:ARG:NH1	2.32	0.44
3:C:112:SER:HB3	3:C:115:LEU:HD12	1.97	0.44
10:J:51:ARG:NH1	10:J:61:GLU:OE1	2.50	0.44
12:L:33:ARG:NH1	12:L:61:THR:HB	2.32	0.44
20:T:56:MET:HE1	20:T:104:LEU:CD2	2.48	0.44
1:A:333:G:H4'	20:T:16:HIS:CE1	2.52	0.44
1:A:460:A:O2'	1:A:461:C:H5''	2.18	0.44
1:A:519:C:H2'	1:A:520:A:C8	2.51	0.44
1:A:803:G:H2'	1:A:804:U:O4'	2.17	0.44
1:A:923:A:H8	1:A:923:A:O5'	2.00	0.44
3:C:4:LYS:HB2	3:C:4:LYS:NZ	2.32	0.44
3:C:10:PHE:HD2	3:C:10:PHE:O	2.00	0.44
6:F:69:GLU:OE1	6:F:69:GLU:N	2.48	0.44
7:G:108:ALA:HB2	7:G:123:GLU:HG2	1.99	0.44
8:H:85:ARG:HH11	8:H:85:ARG:HG3	1.82	0.44
13:M:40:ASN:ND2	13:M:43:THR:HG23	2.33	0.44
18:R:79:LEU:HD23	18:R:79:LEU:HA	1.66	0.44
1:A:93:G:C2	1:A:95:U:N3	2.86	0.44
1:A:415:A:H2'	1:A:416:G:O4'	2.17	0.44
1:A:719:C:N4	18:R:74:ARG:HH12	2.14	0.44
1:A:828:A:H4'	1:A:828:A:OP1	2.16	0.44
2:B:25:ASN:O	2:B:26:PRO:C	2.61	0.44
2:B:215:LEU:HD23	2:B:215:LEU:HA	1.43	0.44
3:C:9:GLY:HA3	14:N:49:HIS:HD1	1.81	0.44
3:C:91:LEU:HG	3:C:99:VAL:HG11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:3:ARG:NH1	4:D:74:GLN:OE1	2.51	0.44
5:E:112:LEU:HA	5:E:112:LEU:HD23	1.70	0.44
7:G:85:TYR:O	7:G:87:VAL:HG13	2.17	0.44
8:H:20:TYR:HA	8:H:65:TYR:CE2	2.53	0.44
10:J:11:PHE:HB3	14:N:55:GLY:HA2	2.00	0.44
16:P:58:TYR:CD1	16:P:58:TYR:C	2.96	0.44
1:A:505:G:H2'	1:A:506:G:C8	2.52	0.44
1:A:579:G:H2'	1:A:580:U:C6	2.53	0.44
1:A:1417:G:OP2	1:A:1417:G:H8	2.01	0.44
3:C:119:ARG:O	3:C:122:GLU:HB2	2.18	0.44
3:C:200:ALA:C	3:C:201:TYR:HD1	2.26	0.44
4:D:159:ARG:O	4:D:163:GLU:HB2	2.18	0.44
5:E:116:THR:HG23	5:E:117:ASP:CG	2.41	0.44
5:E:144:THR:O	5:E:148:VAL:HG23	2.17	0.44
9:I:9:ARG:HG3	9:I:14:VAL:HG13	1.99	0.44
9:I:89:ASN:O	9:I:92:TYR:HB2	2.17	0.44
15:O:70:LEU:HA	15:O:70:LEU:HD23	1.51	0.44
1:A:524:G:H2'	1:A:525:C:C6	2.53	0.44
1:A:1054:C:OP1	1:A:1197:G:OP1	2.36	0.44
1:A:1219:U:C4	1:A:1220:G:N7	2.86	0.44
1:A:1223:C:P	19:S:78:ARG:HH22	2.41	0.44
3:C:79:ARG:H	3:C:79:ARG:HG3	1.73	0.44
5:E:121:LYS:HG2	5:E:123:LEU:HD21	1.99	0.44
10:J:63:PHE:HE1	14:N:45:ARG:HA	1.83	0.44
14:N:6:LEU:O	14:N:23:ARG:NE	2.39	0.44
15:O:36:ILE:HD12	15:O:60:VAL:HG23	1.99	0.44
20:T:27:LYS:O	20:T:28:ALA:C	2.61	0.44
1:A:651:C:O2'	1:A:652:U:H5'	2.18	0.44
1:A:1069:C:O2'	1:A:1192:C:H1'	2.18	0.44
1:A:1185:G:O2'	1:A:1186:G:H5'	2.18	0.44
2:B:10:LEU:C	2:B:12:GLU:N	2.75	0.44
2:B:17:PHE:HD1	2:B:18:GLY:N	2.15	0.44
2:B:25:ASN:O	2:B:27:LYS:N	2.51	0.44
2:B:55:PHE:HE2	2:B:218:ALA:HA	1.83	0.44
5:E:28:PHE:O	5:E:47:LYS:HA	2.18	0.44
5:E:51:VAL:HG12	5:E:52:PRO:N	2.32	0.44
5:E:92:LYS:HB3	5:E:119:LEU:HB2	1.99	0.44
6:F:10:LEU:HD12	6:F:59:TYR:HB3	1.99	0.44
9:I:118:LYS:O	9:I:120:ARG:N	2.44	0.44
11:K:58:PRO:O	11:K:61:ALA:HB3	2.18	0.44
1:A:80:G:H2'	1:A:81:U:H5'	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:A:N6	1:A:329:A:OP2	2.50	0.44
1:A:673:G:H5''	6:F:87:ARG:CZ	2.47	0.44
1:A:825:G:H21	8:H:11:THR:HG21	1.83	0.44
1:A:990:C:N3	1:A:1216:G:N2	2.66	0.44
1:A:1257:U:O2'	1:A:1258:G:C8	2.70	0.44
1:A:1290:G:H2'	1:A:1291:G:H8	1.83	0.44
4:D:186:LEU:H	4:D:186:LEU:HG	1.47	0.44
11:K:87:THR:HG22	11:K:88:GLY:N	2.32	0.44
12:L:120:TYR:N	12:L:120:TYR:CD2	2.86	0.44
16:P:12:LYS:O	16:P:13:HIS:HB2	2.17	0.44
1:A:176:C:H2'	1:A:177:C:C5	2.53	0.43
1:A:701:C:H4'	1:A:702:A:O5'	2.18	0.43
1:A:1136:U:H4'	1:A:1137:C:OP2	2.17	0.43
1:A:1196:U:OP1	1:A:1197:G:H5'	2.18	0.43
1:A:1329:A:H2'	1:A:1330:U:O4'	2.18	0.43
1:A:1354:C:H2'	1:A:1355:G:H8	1.83	0.43
1:A:1375:A:C2	1:A:1376:U:C2	3.06	0.43
1:A:1473:A:C6	1:A:1474:G:C6	3.06	0.43
4:D:121:VAL:HG12	4:D:134:ASP:O	2.17	0.43
5:E:12:LEU:O	5:E:12:LEU:HD22	2.18	0.43
8:H:114:THR:HG21	8:H:129:VAL:HB	2.00	0.43
12:L:11:VAL:HG22	17:Q:29:HIS:CD2	2.53	0.43
13:M:23:TYR:HB2	13:M:67:GLU:OE2	2.18	0.43
16:P:65:GLN:HA	16:P:66:PRO:HD2	1.76	0.43
18:R:63:GLN:O	18:R:66:LEU:HB3	2.18	0.43
19:S:31:ILE:HG23	19:S:32:LYS:N	2.33	0.43
20:T:100:ILE:HG22	20:T:102:GLY:N	2.20	0.43
1:A:98:U:H6	1:A:98:U:OP2	2.00	0.43
1:A:602:A:C2	1:A:637:G:C2	3.06	0.43
1:A:815:A:N3	1:A:1527:C:O2'	2.43	0.43
1:A:988:G:C6	1:A:989:C:C2	3.07	0.43
1:A:1221:G:H5'	19:S:36:ARG:NH1	2.32	0.43
5:E:60:TYR:O	5:E:64:ARG:HG2	2.18	0.43
6:F:80:ARG:HG3	6:F:88:VAL:HB	2.00	0.43
13:M:37:THR:HG23	13:M:55:ARG:HB3	2.00	0.43
13:M:80:ARG:HB3	13:M:80:ARG:HH11	1.83	0.43
1:A:773:G:N2	1:A:806:C:O2	2.50	0.43
1:A:1254:C:H4'	1:A:1357:A:OP1	2.18	0.43
1:A:1311:G:H1	1:A:1326:C:N4	2.16	0.43
1:A:1349:A:C2	1:A:1374:A:C4	3.06	0.43
4:D:173:TRP:CD1	4:D:189:PRO:HD3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:63:LEU:HD23	8:H:65:TYR:OH	2.18	0.43
8:H:78:GLN:OE1	8:H:78:GLN:HA	2.18	0.43
11:K:98:LEU:HD23	11:K:98:LEU:HA	1.70	0.43
14:N:23:ARG:HD3	14:N:28:GLY:O	2.19	0.43
1:A:147:G:C2	1:A:148:G:C8	3.06	0.43
1:A:403:C:H4'	4:D:122:ARG:HH11	1.82	0.43
1:A:448:A:C4	1:A:487:A:C2	3.06	0.43
1:A:539:A:H2'	1:A:540:G:C8	2.53	0.43
1:A:622:A:H2'	1:A:623:C:H5'	2.00	0.43
1:A:671:G:H5'	6:F:77:ARG:NH2	2.33	0.43
1:A:1341:U:O5'	1:A:1341:U:H6	2.00	0.43
1:A:1374:A:C4	1:A:1375:A:C8	3.07	0.43
1:A:1399:C:C2	1:A:1502:A:N6	2.86	0.43
2:B:180:LEU:HD23	2:B:180:LEU:HA	1.59	0.43
5:E:71:LEU:HD23	5:E:71:LEU:HA	1.66	0.43
6:F:4:TYR:CD1	6:F:92:LYS:HA	2.53	0.43
8:H:89:PRO:HA	8:H:92:ARG:NH1	2.33	0.43
11:K:92:GLU:HB3	11:K:96:ARG:NH2	2.33	0.43
15:O:39:LEU:HB3	15:O:56:LEU:CD1	2.47	0.43
15:O:78:TYR:CZ	15:O:82:ILE:HD12	2.54	0.43
16:P:68:ASP:OD1	16:P:68:ASP:N	2.50	0.43
17:Q:67:LYS:HA	17:Q:70:ARG:HH12	1.84	0.43
1:A:253:U:H2'	1:A:254:G:H8	1.84	0.43
1:A:1320:C:C4	19:S:36:ARG:HG3	2.53	0.43
1:A:1371:G:C5	1:A:1372:U:C5	3.07	0.43
1:A:1408:A:C6	1:A:1494:G:C6	3.07	0.43
3:C:113:ALA:O	3:C:116:VAL:HG23	2.18	0.43
5:E:11:ILE:HD13	5:E:11:ILE:HA	1.61	0.43
5:E:122:GLU:HG2	5:E:131:ILE:HG13	1.99	0.43
12:L:60:LEU:HB2	12:L:64:TYR:O	2.19	0.43
12:L:84:LEU:HB3	12:L:104:VAL:HG11	2.00	0.43
13:M:80:ARG:HH12	13:M:81:LEU:HB3	1.83	0.43
14:N:17:LYS:HE2	14:N:17:LYS:HB2	1.79	0.43
17:Q:22:LEU:HD12	17:Q:23:VAL:N	2.34	0.43
20:T:74:LYS:HB2	20:T:76:ALA:H	1.82	0.43
1:A:455:C:H2'	1:A:456:C:C6	2.43	0.43
1:A:657:G:H4'	15:O:28:GLN:HG2	2.01	0.43
1:A:1001:A:H2'	1:A:1002:G:C8	2.48	0.43
1:A:1007:C:O2	1:A:1023:G:N1	2.51	0.43
1:A:1370:G:C2	1:A:1371:G:N7	2.87	0.43
1:A:1419:G:H2'	1:A:1420:C:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:22:LYS:C	2:B:23:ARG:HH11	2.27	0.43
2:B:55:PHE:HA	2:B:58:ILE:HD12	2.00	0.43
3:C:17:ASP:O	3:C:54:ARG:NH1	2.48	0.43
3:C:40:ARG:HE	3:C:55:VAL:HB	1.81	0.43
3:C:81:GLY:O	3:C:84:ILE:HG22	2.17	0.43
3:C:87:LEU:HD13	3:C:87:LEU:HA	1.82	0.43
4:D:207:TYR:HD2	4:D:207:TYR:HA	1.66	0.43
7:G:47:CYS:HB3	7:G:58:PRO:CG	2.47	0.43
12:L:77:LEU:HA	12:L:77:LEU:HD23	1.63	0.43
1:A:9:G:H5'	5:E:122:GLU:OE2	2.19	0.43
1:A:49:U:C2	1:A:361:G:N2	2.86	0.43
1:A:289:G:H5'	1:A:289:G:H8	1.83	0.43
1:A:1067:A:N6	1:A:1109:C:H5'	2.34	0.43
2:B:149:LEU:O	2:B:153:ARG:HB2	2.18	0.43
5:E:76:ILE:HG22	5:E:93:PRO:HG3	2.00	0.43
6:F:45:LEU:HA	6:F:45:LEU:HD23	1.80	0.43
16:P:32:TYR:HD2	16:P:32:TYR:C	2.27	0.43
1:A:8:A:N1	4:D:209:ARG:HD2	2.34	0.43
1:A:78:G:C6	1:A:79:G:C8	3.07	0.43
1:A:145:G:C2	1:A:146:G:C5	3.07	0.43
1:A:475:G:H2'	1:A:476:G:C8	2.54	0.43
1:A:631:G:H5''	1:A:632:A:OP1	2.19	0.43
1:A:673:G:O3'	6:F:87:ARG:NH2	2.52	0.43
1:A:687:A:H4'	1:A:688:G:O5'	2.19	0.43
1:A:902:G:O2'	1:A:903:G:H5'	2.19	0.43
1:A:1167:A:C6	1:A:1168:A:C6	3.07	0.43
1:A:1220:G:H2'	1:A:1221:G:O4'	2.19	0.43
7:G:45:ASP:HA	7:G:48:LYS:HG3	1.99	0.43
8:H:112:LEU:HD22	8:H:133:LEU:HA	2.01	0.43
9:I:37:PHE:CZ	9:I:74:ILE:HG12	2.53	0.43
16:P:32:TYR:C	16:P:32:TYR:CD2	2.97	0.43
17:Q:75:ARG:NH2	17:Q:77:VAL:HG13	2.30	0.43
19:S:33:THR:HG22	19:S:35:SER:H	1.84	0.43
1:A:675:A:H1'	11:K:116:HIS:CG	2.53	0.43
1:A:980:C:H5''	1:A:981:U:H5	1.84	0.43
1:A:992:U:N3	1:A:1044:A:N6	2.60	0.43
1:A:1346:A:OP1	9:I:120:ARG:NH1	2.45	0.43
1:A:1421:G:H2'	1:A:1422:G:O4'	2.19	0.43
1:A:1491:G:N2	1:A:1492:A:H62	2.16	0.43
2:B:204:ASN:N	2:B:204:ASN:OD1	2.51	0.43
5:E:77:PRO:HD2	5:E:142:LEU:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:18:TYR:OH	7:G:58:PRO:HB2	2.19	0.43
7:G:118:VAL:HG12	7:G:122:HIS:HD1	1.83	0.43
17:Q:83:ASP:OD1	17:Q:84:LEU:N	2.49	0.43
1:A:120:A:H2'	1:A:122:G:N7	2.34	0.43
1:A:1268:A:O3'	21:U:19:GLY:HA2	2.19	0.43
1:A:1305:G:H22	1:A:1331:G:H1'	1.81	0.43
2:B:114:ARG:O	2:B:114:ARG:HD3	2.19	0.43
4:D:82:ALA:HA	4:D:85:LYS:HG3	2.00	0.43
12:L:53:ARG:HH12	12:L:92:OTD:CG	2.31	0.43
15:O:15:PHE:CZ	15:O:85:LEU:HD21	2.53	0.43
15:O:70:LEU:O	15:O:73:GLU:N	2.50	0.43
20:T:20:LEU:O	20:T:23:ARG:HB3	2.18	0.43
1:A:321:A:H2'	1:A:322:C:C6	2.54	0.42
1:A:337:C:H2'	1:A:338:A:C8	2.54	0.42
1:A:376:G:H5''	16:P:5:ARG:HD2	2.00	0.42
1:A:631:G:O3'	1:A:632:A:H8	2.01	0.42
1:A:1526:G:H2'	1:A:1527:C:C6	2.53	0.42
2:B:10:LEU:HD12	2:B:10:LEU:H	1.84	0.42
2:B:92:TYR:O	2:B:151:GLY:HA3	2.19	0.42
3:C:10:PHE:CE2	3:C:178:LEU:HB2	2.54	0.42
6:F:11:ASN:HB2	6:F:86:ARG:CZ	2.49	0.42
6:F:62:TRP:CH2	6:F:64:GLN:HB2	2.54	0.42
7:G:115:ARG:HB2	7:G:118:VAL:CG2	2.47	0.42
8:H:83:ILE:HD12	8:H:83:ILE:HG23	1.73	0.42
1:A:376:G:H4'	16:P:5:ARG:HD2	2.01	0.42
1:A:688:G:C5	1:A:700:G:C2	3.07	0.42
1:A:1123:A:H2'	1:A:1124:G:C8	2.54	0.42
1:A:1148:U:H2'	1:A:1149:C:O4'	2.19	0.42
1:A:1491:G:C5	1:A:1493:A:C2	3.07	0.42
1:A:1514:C:H2'	1:A:1515[A]:C:O4'	2.19	0.42
2:B:88:ALA:O	2:B:90:MET:N	2.52	0.42
2:B:172:ILE:H	2:B:172:ILE:CD1	2.26	0.42
3:C:19:GLU:O	3:C:56:ASP:HA	2.19	0.42
3:C:24:ALA:HB3	3:C:29:TYR:CD1	2.54	0.42
5:E:6:PHE:CD2	5:E:36:ASP:HB3	2.54	0.42
5:E:80:ILE:HD11	5:E:138:ALA:HB1	2.01	0.42
13:M:82:MET:HA	13:M:89:GLY:CA	2.49	0.42
16:P:32:TYR:HD2	16:P:32:TYR:O	2.02	0.42
17:Q:17:LYS:N	17:Q:49:GLU:OE2	2.36	0.42
17:Q:43:LEU:HD23	17:Q:43:LEU:HA	1.77	0.42
17:Q:59:ILE:HA	17:Q:59:ILE:HD13	1.64	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:U:H2'	1:A:63:C:C6	2.55	0.42
1:A:75:G:N2	1:A:96:G:N2	2.68	0.42
1:A:160:A:N6	1:A:161:A:C2	2.88	0.42
1:A:665:A:H3'	1:A:725:G:N2	2.34	0.42
2:B:222:ILE:HD13	2:B:222:ILE:HG21	1.77	0.42
4:D:180:GLY:C	4:D:182:LYS:H	2.27	0.42
5:E:106:PRO:O	5:E:110:LEU:HG	2.18	0.42
8:H:53:VAL:HB	8:H:58:TYR:CE1	2.54	0.42
10:J:36:GLY:HA3	10:J:37:PRO:HD3	1.70	0.42
11:K:48:ILE:HD13	11:K:63:LEU:HB3	2.01	0.42
15:O:7:GLU:H	15:O:7:GLU:HG3	1.63	0.42
19:S:80:TYR:CG	19:S:81:ARG:N	2.87	0.42
1:A:439:A:C4	1:A:497:A:C2	3.07	0.42
1:A:599:C:O2'	8:H:129:VAL:HG12	2.20	0.42
1:A:740:U:O2'	1:A:741:G:H5'	2.19	0.42
1:A:768:A:C5	1:A:769:G:C8	3.08	0.42
1:A:865:A:H2	1:A:918:A:H4'	1.84	0.42
1:A:905:U:H2'	1:A:906:G:H5'	2.01	0.42
1:A:1370:G:C2	1:A:1371:G:C8	3.08	0.42
2:B:9:GLU:C	2:B:10:LEU:HG	2.43	0.42
2:B:102:LEU:HB3	2:B:180:LEU:HD12	2.01	0.42
2:B:217:ARG:O	2:B:220:ASP:HB2	2.20	0.42
3:C:7:PRO:O	3:C:11:ARG:NE	2.52	0.42
5:E:11:ILE:HB	5:E:31:LEU:HB3	2.00	0.42
5:E:74:GLY:HA3	5:E:116:THR:HG22	2.00	0.42
6:F:67:MET:HB2	6:F:68:PRO:HD2	2.02	0.42
9:I:54:ASP:O	9:I:58:HIS:ND1	2.52	0.42
9:I:97:LYS:O	9:I:100:GLY:N	2.51	0.42
1:A:76:C:N4	1:A:93:G:H1	2.16	0.42
1:A:266:G:H5''	1:A:266:G:H8	1.83	0.42
1:A:403:C:O3'	4:D:122:ARG:HD3	2.19	0.42
1:A:424:G:H2'	1:A:425:G:C8	2.55	0.42
1:A:511:C:O2'	1:A:534:U:H1'	2.20	0.42
1:A:690:G:C6	1:A:691:G:C6	3.07	0.42
1:A:994:A:C8	1:A:1216:G:H4'	2.54	0.42
1:A:1149:C:H6	1:A:1149:C:O5'	2.03	0.42
1:A:1304:G:OP1	21:U:2:GLY:N	2.53	0.42
3:C:34:LEU:HD21	14:N:25:VAL:HG21	2.01	0.42
3:C:115:LEU:HA	3:C:115:LEU:HD23	1.77	0.42
12:L:22:SER:C	12:L:24:VAL:H	2.26	0.42
13:M:34:LEU:HA	13:M:34:LEU:HD13	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:87:TYR:O	13:M:90:LEU:N	2.52	0.42
15:O:4:THR:HG23	15:O:7:GLU:OE1	2.20	0.42
16:P:4:ILE:HG13	16:P:64:ALA:HB1	2.01	0.42
1:A:77:G:C4	1:A:93:G:N2	2.87	0.42
1:A:1324:A:H2'	1:A:1325:C:O4'	2.18	0.42
1:A:1474:G:H8	1:A:1474:G:O5'	2.02	0.42
1:A:1520[A]:G:H2'	1:A:1521:G:C8	2.54	0.42
2:B:7:VAL:O	2:B:8:LYS:HB3	2.19	0.42
3:C:87:LEU:O	3:C:91:LEU:HB2	2.18	0.42
3:C:155:GLY:O	3:C:196:LEU:HG	2.20	0.42
7:G:6:ARG:HG3	7:G:6:ARG:O	2.20	0.42
9:I:102:LEU:HA	9:I:102:LEU:HD23	1.70	0.42
10:J:47:PHE:HB3	14:N:34:TYR:CE2	2.40	0.42
12:L:127:GLU:H	12:L:127:GLU:HG2	1.68	0.42
13:M:4:ILE:HG22	13:M:5:ALA:N	2.35	0.42
1:A:97:G:C2'	1:A:98:U:H5'	2.49	0.42
1:A:105:G:H2'	1:A:106:C:C6	2.54	0.42
1:A:429:U:OP1	4:D:36:ARG:NH1	2.52	0.42
1:A:912:A:H5''	12:L:46:LYS:HZ1	1.84	0.42
1:A:1169:A:H2'	1:A:1171:G:O4'	2.19	0.42
1:A:1208:C:C4	1:A:1209:C:C5	3.08	0.42
3:C:11:ARG:HB3	3:C:16:ARG:HB2	2.02	0.42
4:D:162:LEU:HA	4:D:162:LEU:HD23	1.64	0.42
6:F:5:GLU:HG2	6:F:62:TRP:CZ2	2.55	0.42
9:I:52:ALA:HB1	9:I:95:LYS:HD2	2.01	0.42
14:N:39:LEU:HA	14:N:39:LEU:HD23	1.77	0.42
20:T:33:ILE:O	20:T:34:LYS:C	2.62	0.42
1:A:79:G:C2	1:A:80:G:N7	2.87	0.42
1:A:149:A:H2'	1:A:150:C:C6	2.55	0.42
1:A:363:A:N6	1:A:364:A:N1	2.67	0.42
1:A:461:C:H4'	1:A:462:G:OP2	2.20	0.42
1:A:943:U:H2'	1:A:944:G:H5'	2.00	0.42
1:A:1037:C:N3	1:A:1038:C:N4	2.68	0.42
1:A:1191:A:H2'	1:A:1192:C:C6	2.55	0.42
1:A:1374:A:H2'	1:A:1375:A:C8	2.54	0.42
8:H:4:ASP:CG	8:H:85:ARG:NH1	2.75	0.42
8:H:51:VAL:HG11	8:H:60:ARG:HB2	2.01	0.42
9:I:14:VAL:O	9:I:65:VAL:HG23	2.20	0.42
20:T:43:LEU:HG	20:T:55:ILE:CD1	2.50	0.42
20:T:60:GLU:O	20:T:63:ILE:HB	2.19	0.42
1:A:77:G:C2	1:A:93:G:N3	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:G:H2'	1:A:146:G:H8	1.85	0.42
1:A:539:A:H2'	1:A:540:G:H8	1.83	0.42
1:A:782:A:C6	1:A:801:U:C2	3.08	0.42
1:A:956:U:H2'	1:A:957:U:O4'	2.20	0.42
1:A:1109:C:H2'	1:A:1110:A:O4'	2.19	0.42
1:A:1402:4OC:HM23	1:A:1402:4OC:H1'	1.48	0.42
2:B:46:LYS:HE3	2:B:46:LYS:HB2	1.95	0.42
2:B:51:LEU:HD23	2:B:51:LEU:HA	1.88	0.42
2:B:236:TYR:CD2	2:B:239:VAL:HG21	2.55	0.42
5:E:11:ILE:HG23	5:E:11:ILE:HD12	1.59	0.42
7:G:79:ARG:HH21	7:G:82:GLY:HA2	1.84	0.42
8:H:54:ASP:C	8:H:56:LYS:H	2.28	0.42
13:M:23:TYR:C	13:M:25:ILE:H	2.28	0.42
1:A:374:A:C6	1:A:375:U:C4	3.08	0.42
1:A:1056:U:O2'	1:A:1057:G:H5'	2.20	0.42
1:A:1098:C:H2'	1:A:1099:G:O4'	2.20	0.42
1:A:1178:G:OP2	9:I:97:LYS:NZ	2.48	0.42
2:B:24:TRP:CZ3	2:B:29:ALA:HB2	2.54	0.42
2:B:95:GLN:NE2	2:B:147:LYS:HE2	2.35	0.42
3:C:200:ALA:C	3:C:201:TYR:CD1	2.98	0.42
5:E:55:VAL:HG12	5:E:56:GLN:N	2.34	0.42
5:E:131:ILE:HD13	5:E:131:ILE:HA	1.54	0.42
9:I:28:VAL:HA	9:I:63:ILE:O	2.19	0.42
12:L:24:VAL:HG12	12:L:26:ALA:H	1.85	0.42
14:N:6:LEU:HB3	14:N:23:ARG:HH21	1.85	0.42
1:A:596:C:O5'	1:A:596:C:H6	2.02	0.41
1:A:1250:A:H2'	1:A:1251:A:C8	2.55	0.41
1:A:1311:G:C2	1:A:1327:C:N3	2.88	0.41
1:A:1406:U:C6	1:A:1407:5MC:HM52	2.55	0.41
3:C:73:PRO:HG3	3:C:105:GLU:OE1	2.20	0.41
3:C:161:GLU:O	3:C:161:GLU:HG2	2.20	0.41
10:J:19:SER:CB	10:J:94:VAL:HG11	2.50	0.41
11:K:106:LYS:HD3	11:K:106:LYS:HA	1.95	0.41
1:A:141:A:H1'	1:A:182:U:O2	2.19	0.41
1:A:532:A:H2'	1:A:533:A:H5''	2.01	0.41
1:A:623:C:H2'	1:A:624:C:O4'	2.19	0.41
1:A:689:C:H2'	1:A:690:G:O4'	2.19	0.41
1:A:1004:A:H4'	1:A:1005:A:OP1	2.20	0.41
1:A:1114:C:H42	1:A:1186:G:H1	1.68	0.41
1:A:1196:U:H3'	1:A:1197:G:C5'	2.50	0.41
2:B:88:ALA:HB3	2:B:219:VAL:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:10:PHE:HD2	3:C:10:PHE:C	2.28	0.41
3:C:150:LYS:O	3:C:201:TYR:HB2	2.20	0.41
6:F:97:PHE:C	6:F:97:PHE:CD2	2.97	0.41
12:L:46:LYS:HE3	12:L:47:LYS:NZ	2.35	0.41
14:N:48:ALA:HA	14:N:53:LEU:HB2	2.02	0.41
20:T:40:ALA:HB2	20:T:55:ILE:CG2	2.50	0.41
1:A:428:G:H1'	1:A:429:U:OP2	2.20	0.41
1:A:794:A:C5	1:A:795:C:C4	3.09	0.41
1:A:1084:G:O2'	1:A:1085:U:OP1	2.26	0.41
1:A:1201:A:H4'	1:A:1202:G:H5''	2.00	0.41
1:A:1221:G:C4	1:A:1222:G:C8	3.08	0.41
2:B:95:GLN:OE1	2:B:95:GLN:HA	2.19	0.41
4:D:4:TYR:HE2	4:D:6:GLY:O	2.03	0.41
4:D:105:VAL:HG13	4:D:110:PHE:HB2	2.02	0.41
4:D:196:LEU:O	4:D:198:VAL:N	2.51	0.41
8:H:48:TYR:CD1	8:H:59:LEU:HD22	2.55	0.41
17:Q:60:ILE:HG22	17:Q:72:ARG:O	2.20	0.41
1:A:901:A:C5	1:A:902:G:H1'	2.56	0.41
1:A:1257:U:O2'	1:A:1258:G:P	2.78	0.41
1:A:1279:A:H5''	10:J:7:LYS:HE2	2.02	0.41
1:A:1354:C:H2'	1:A:1355:G:C8	2.55	0.41
1:A:1417:G:O3'	1:A:1418:A:H8	2.03	0.41
1:A:1434:A:H2'	1:A:1435:G:O4'	2.20	0.41
2:B:74:LYS:O	2:B:78:GLN:HG3	2.20	0.41
4:D:8:VAL:O	4:D:10:ARG:N	2.54	0.41
6:F:70:ASP:OD1	6:F:70:ASP:N	2.49	0.41
7:G:78:ARG:HG3	7:G:87:VAL:HG21	2.01	0.41
16:P:54:GLU:C	16:P:54:GLU:CD	2.88	0.41
17:Q:35:VAL:O	17:Q:35:VAL:HG12	2.21	0.41
17:Q:45:HIS:CD2	17:Q:45:HIS:C	2.98	0.41
1:A:255:G:O6	1:A:266:G:O6	2.38	0.41
1:A:446:G:H1	1:A:488:C:N4	2.03	0.41
1:A:750:G:N3	15:O:23:GLY:HA3	2.34	0.41
1:A:973:G:C3'	1:A:974:A:H5''	2.49	0.41
1:A:980:C:H5'	1:A:981:U:OP2	2.20	0.41
1:A:1103:C:H5'	2:B:98:LEU:HD12	2.03	0.41
1:A:1376:U:H2'	1:A:1377:A:C8	2.56	0.41
1:A:1408:A:N6	1:A:1494:G:C6	2.89	0.41
1:A:1416:G:N2	1:A:1484:C:O2	2.53	0.41
1:A:1443:G:C4'	1:A:1446:A:H5''	2.50	0.41
2:B:102:LEU:HB2	2:B:176:GLU:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:134:GLU:O	2:B:138:LEU:HD12	2.21	0.41
3:C:154:SER:OG	3:C:155:GLY:N	2.48	0.41
3:C:175:LEU:HD21	3:C:201:TYR:CE2	2.56	0.41
6:F:21:LEU:O	6:F:25:ILE:HG12	2.20	0.41
8:H:80:ILE:HG21	8:H:80:ILE:HD13	1.72	0.41
9:I:93:ARG:HG3	9:I:102:LEU:HD11	2.03	0.41
1:A:289:G:P	24:A:1909:HOH:O	2.79	0.41
1:A:302:G:N3	1:A:556:C:H4'	2.36	0.41
1:A:397:A:H5'	1:A:398:C:P	2.61	0.41
1:A:460:A:C6	1:A:462:G:C5	3.09	0.41
1:A:506:G:H1	1:A:525:C:H42	1.68	0.41
1:A:854:G:H3'	1:A:871:U:O4	2.21	0.41
1:A:938:A:H2'	1:A:939:G:O4'	2.20	0.41
1:A:981:U:H5''	1:A:982:U:C5'	2.50	0.41
1:A:1048:G:N2	1:A:1050:G:C4	2.88	0.41
1:A:1228:C:O3'	13:M:116:THR:HG23	2.20	0.41
1:A:1443:G:C5'	1:A:1446:A:H5''	2.50	0.41
1:A:1486:G:N2	1:A:1487:G:N3	2.68	0.41
3:C:113:ALA:HA	3:C:116:VAL:CG2	2.51	0.41
4:D:187:ARG:NH2	4:D:188:LEU:HD12	2.36	0.41
6:F:4:TYR:HD1	6:F:92:LYS:CA	2.34	0.41
6:F:74:ASP:OD2	6:F:74:ASP:N	2.48	0.41
7:G:27:ILE:HA	7:G:30:ILE:HD12	2.03	0.41
8:H:27:PRO:HB3	8:H:58:TYR:CE2	2.56	0.41
8:H:73:ASP:HA	8:H:74:PRO:HD2	1.75	0.41
10:J:72:VAL:O	10:J:73:ASP:HB2	2.20	0.41
11:K:48:ILE:H	11:K:48:ILE:HG13	1.36	0.41
13:M:19:LEU:O	13:M:22:ILE:HG13	2.20	0.41
1:A:7:G:H5'	1:A:298:A:O4'	2.20	0.41
1:A:92:C:O2	1:A:92:C:C2'	2.66	0.41
1:A:262:A:C6	1:A:263:A:C6	3.08	0.41
1:A:413:G:C8	1:A:413:G:H3'	2.55	0.41
1:A:555:C:H2'	1:A:556:C:C6	2.55	0.41
1:A:620:C:N1	4:D:135:LEU:HD13	2.35	0.41
1:A:634:C:H2'	1:A:635:G:H8	1.85	0.41
1:A:1030(C):G:C6	1:A:1030(D):A:N1	2.89	0.41
1:A:1228:C:OP1	13:M:115:LYS:NZ	2.39	0.41
1:A:1372:U:N3	1:A:1373:G:C4	2.89	0.41
3:C:149:ALA:O	3:C:169:ALA:HB1	2.20	0.41
4:D:110:PHE:CZ	4:D:181:MET:O	2.73	0.41
5:E:12:LEU:HD13	5:E:31:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:4:TYR:CE1	6:F:92:LYS:HB3	2.56	0.41
7:G:61:VAL:HG22	7:G:128:ALA:HB1	2.03	0.41
8:H:2:LEU:HD23	8:H:2:LEU:HA	1.88	0.41
10:J:34:VAL:HG22	10:J:75:ILE:H	1.86	0.41
17:Q:58:GLU:O	17:Q:59:ILE:HD13	2.20	0.41
1:A:474:G:H8	1:A:474:G:O5'	2.04	0.41
1:A:517:G:N2	1:A:530:G:OP1	2.50	0.41
1:A:841:U:H3	2:B:37:ASN:HA	1.84	0.41
1:A:938:A:N3	1:A:1376:U:O2'	2.40	0.41
1:A:1133:G:C2	1:A:1142:G:C2	3.08	0.41
1:A:1251:A:H4'	9:I:12:GLU:OE2	2.21	0.41
1:A:1320:C:H2'	1:A:1321:C:O4'	2.20	0.41
1:A:1433:A:C8	1:A:1467:G:N2	2.89	0.41
2:B:80:ILE:HD12	2:B:80:ILE:N	2.36	0.41
2:B:213:LEU:HD23	2:B:214:ILE:HG12	2.02	0.41
3:C:72:LYS:HB2	3:C:75:VAL:HG23	2.02	0.41
3:C:141:VAL:O	3:C:146:ALA:HB3	2.21	0.41
5:E:152:ARG:NE	8:H:44:PHE:CE1	2.89	0.41
6:F:6:VAL:HG22	6:F:90:VAL:HG22	2.03	0.41
7:G:135:VAL:HA	7:G:138:LYS:HB3	2.03	0.41
8:H:77:GLU:HG2	8:H:78:GLN:N	2.35	0.41
12:L:6:THR:OG1	12:L:9:GLN:HG3	2.21	0.41
19:S:80:TYR:CE1	19:S:81:ARG:HB3	2.56	0.41
1:A:179:A:H2'	1:A:180:U:C6	2.56	0.41
1:A:255:G:C2	1:A:272:C:C2	3.08	0.41
1:A:985:C:C4	1:A:1221:G:N2	2.89	0.41
1:A:999:C:O2'	1:A:1000:U:H5'	2.21	0.41
1:A:1003:G:N2	1:A:1039:C:C2	2.89	0.41
2:B:71:VAL:O	2:B:165:VAL:HG23	2.20	0.41
2:B:132:LYS:HA	2:B:135:GLN:HB3	2.03	0.41
3:C:8:ILE:HA	3:C:11:ARG:HB2	2.03	0.41
3:C:10:PHE:C	3:C:10:PHE:CD2	2.98	0.41
3:C:68:VAL:HG12	3:C:70:VAL:HG22	2.03	0.41
3:C:71:ALA:CB	3:C:109:PRO:HB3	2.51	0.41
3:C:174:PRO:O	3:C:177:THR:HG23	2.21	0.41
3:C:178:LEU:HA	3:C:178:LEU:HD23	1.69	0.41
6:F:10:LEU:HD12	6:F:10:LEU:H	1.86	0.41
9:I:43:ALA:HA	9:I:74:ILE:HD13	2.02	0.41
9:I:116:LYS:HB3	9:I:121:ARG:O	2.20	0.41
11:K:34:ASP:OD1	11:K:38:ASN:N	2.54	0.41
12:L:41:ARG:HD3	12:L:43:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:98:TYR:CD1	12:L:98:TYR:N	2.88	0.41
15:O:44:LYS:HE2	15:O:44:LYS:HB3	1.82	0.41
17:Q:29:HIS:ND1	17:Q:30:PRO:HD2	2.35	0.41
18:R:47:THR:O	18:R:49:LYS:N	2.54	0.41
19:S:63:THR:HG22	19:S:64:GLU:H	1.86	0.41
20:T:33:ILE:HD11	20:T:63:ILE:HA	2.03	0.41
1:A:35:G:C6	1:A:36:C:C4	3.09	0.41
1:A:184:G:C4	1:A:185:A:N7	2.89	0.41
1:A:409:G:OP1	4:D:24:GLU:O	2.38	0.41
1:A:462:G:C6	1:A:463:A:C5	3.09	0.41
1:A:463:A:O2'	16:P:82:GLN:HG2	2.20	0.41
1:A:1236:A:OP1	21:U:3:LYS:HG3	2.21	0.41
1:A:1380:U:H1'	1:A:1381:U:OP2	2.21	0.41
1:A:1495:U:H2'	1:A:1496:C:C6	2.56	0.41
6:F:101:ALA:HA	18:R:28:GLU:HG3	2.03	0.41
7:G:44:TYR:O	7:G:48:LYS:HG3	2.21	0.41
8:H:63:LEU:N	8:H:63:LEU:HD13	2.36	0.41
10:J:79:ARG:NH2	10:J:82:ILE:HD13	2.36	0.41
13:M:54:VAL:HG22	13:M:57:ARG:NH1	2.32	0.41
18:R:58:LEU:HD23	18:R:58:LEU:HA	1.70	0.41
1:A:42:G:H2'	1:A:43:C:O4'	2.20	0.40
1:A:232:G:H2'	1:A:233:C:C6	2.56	0.40
1:A:934:C:H42	1:A:938:A:H61	1.69	0.40
1:A:948:C:N4	1:A:1233:G:H1	2.18	0.40
1:A:1135:U:O2'	1:A:1136:U:H2'	2.21	0.40
1:A:1251:A:H2'	1:A:1252:A:C8	2.56	0.40
1:A:1261:A:H5''	1:A:1262:C:OP2	2.21	0.40
1:A:1338:G:C6	1:A:1339:A:N6	2.89	0.40
1:A:1402:4OC:H2'	1:A:1403:C:H6	1.83	0.40
6:F:28:ARG:O	6:F:32:ASN:HB2	2.21	0.40
14:N:7:ILE:HG22	14:N:7:ILE:O	2.21	0.40
15:O:42:HIS:O	15:O:46:HIS:HB2	2.20	0.40
17:Q:84:LEU:N	17:Q:84:LEU:HD23	2.36	0.40
19:S:41:VAL:HG23	19:S:43:GLU:HG2	2.01	0.40
1:A:35:G:C5	1:A:36:C:C5	3.09	0.40
1:A:782:A:H2'	1:A:783:C:O4'	2.21	0.40
1:A:1014:A:H2'	1:A:1015:A:C8	2.57	0.40
1:A:1474:G:H2'	1:A:1475:G:H8	1.80	0.40
3:C:123:GLN:O	3:C:126:ARG:HB2	2.21	0.40
4:D:61:LYS:HD3	4:D:62:GLN:HG2	2.03	0.40
7:G:22:LEU:CD2	7:G:66:VAL:HG21	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:126:SER:OG	9:I:127:LYS:HD2	2.21	0.40
10:J:53:PRO:HA	14:N:41:ARG:NH2	2.28	0.40
12:L:33:ARG:C	12:L:84:LEU:HD12	2.46	0.40
16:P:81:ARG:N	24:P:201:HOH:O	2.53	0.40
17:Q:65:ILE:HD12	17:Q:65:ILE:N	2.36	0.40
18:R:47:THR:C	18:R:49:LYS:H	2.29	0.40
1:A:1200:C:H1'	1:A:1204:A:H62	1.86	0.40
1:A:1202:G:C4	14:N:42:ILE:HD12	2.56	0.40
1:A:1231:G:H2'	1:A:1232:U:O4'	2.22	0.40
1:A:1263:C:C2	1:A:1273:G:N2	2.89	0.40
5:E:25:ARG:C	5:E:26:PHE:CD2	3.00	0.40
8:H:137:VAL:HG12	8:H:138:TRP:N	2.36	0.40
16:P:60:LEU:HD23	16:P:60:LEU:HA	1.68	0.40
17:Q:59:ILE:CD1	17:Q:73:VAL:HG13	2.51	0.40
1:A:102:G:H2'	1:A:103:C:H6	1.86	0.40
1:A:241:C:N4	1:A:285:G:H1	2.20	0.40
1:A:416:G:C5	1:A:417:C:C4	3.10	0.40
1:A:449:C:C5	1:A:450:G:C5	3.09	0.40
1:A:581:G:O6	1:A:758:G:C8	2.75	0.40
1:A:714:G:H2'	1:A:715:A:C8	2.56	0.40
1:A:934:C:N4	1:A:938:A:H61	2.19	0.40
1:A:1157:A:H8	1:A:1158:C:C4	2.39	0.40
2:B:182:ILE:HA	2:B:183:PRO:HD3	1.98	0.40
3:C:50:ALA:HA	3:C:72:LYS:HD3	2.04	0.40
3:C:157:ILE:HB	3:C:164:ARG:HH12	1.86	0.40
3:C:172:ARG:NH1	3:C:174:PRO:HG3	2.37	0.40
5:E:80:ILE:HA	8:H:104:ARG:NH2	2.36	0.40
14:N:41:ARG:HA	14:N:44:LEU:HB3	2.03	0.40
15:O:33:THR:OG1	15:O:63:ARG:HD2	2.21	0.40
16:P:43:LYS:HA	16:P:48:TRP:HB3	2.03	0.40
20:T:10:LEU:HD22	20:T:11:SER:H	1.87	0.40
1:A:449:C:H3'	1:A:450:G:H8	1.87	0.40
1:A:778:G:O5'	1:A:778:G:C8	2.73	0.40
1:A:794:A:C6	1:A:795:C:C4	3.10	0.40
1:A:865:A:O5'	1:A:865:A:H8	2.05	0.40
1:A:1288:A:H2'	1:A:1289:A:C8	2.56	0.40
1:A:1296:C:H4'	1:A:1302:U:C5	2.56	0.40
1:A:1367:C:P	10:J:60:ARG:HH21	2.45	0.40
1:A:1399:C:C2	1:A:1401:G:C5	3.09	0.40
2:B:9:GLU:HG2	2:B:10:LEU:H	1.86	0.40
6:F:40:VAL:HB	6:F:63:TYR:CD1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:46:ALA:HB1	7:G:121:ALA:HB2	2.04	0.40
8:H:82:HIS:ND1	8:H:138:TRP:CD1	2.89	0.40
12:L:22:SER:C	12:L:24:VAL:N	2.80	0.40
13:M:70:LEU:C	13:M:70:LEU:HD23	2.47	0.40
18:R:30:ASP:OD2	18:R:32:ARG:HB3	2.22	0.40
18:R:79:LEU:HD22	18:R:80:PRO:HD2	2.02	0.40
19:S:41:VAL:CG2	19:S:44:MET:HG3	2.41	0.40
20:T:11:SER:C	20:T:13:LEU:N	2.79	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:C:O2'	1:A:1338:G:O2'[3_545]	2.18	0.02

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	232/256 (91%)	195 (84%)	33 (14%)	4 (2%)	7	31
3	C	204/239 (85%)	172 (84%)	32 (16%)	0	100	100
4	D	206/209 (99%)	197 (96%)	9 (4%)	0	100	100
5	E	148/162 (91%)	137 (93%)	10 (7%)	1 (1%)	18	48
6	F	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
7	G	153/156 (98%)	139 (91%)	13 (8%)	1 (1%)	18	48
8	H	136/138 (99%)	125 (92%)	11 (8%)	0	100	100
9	I	125/128 (98%)	109 (87%)	15 (12%)	1 (1%)	16	45
10	J	96/105 (91%)	82 (85%)	12 (12%)	2 (2%)	5	27
11	K	114/129 (88%)	104 (91%)	10 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	L	121/135 (90%)	111 (92%)	8 (7%)	2 (2%)	7	31
13	M	116/126 (92%)	99 (85%)	17 (15%)	0	100	100
14	N	58/61 (95%)	51 (88%)	7 (12%)	0	100	100
15	O	85/89 (96%)	80 (94%)	4 (5%)	1 (1%)	10	38
16	P	81/88 (92%)	77 (95%)	4 (5%)	0	100	100
17	Q	97/105 (92%)	88 (91%)	9 (9%)	0	100	100
18	R	68/88 (77%)	59 (87%)	9 (13%)	0	100	100
19	S	78/93 (84%)	69 (88%)	7 (9%)	2 (3%)	4	23
20	T	97/106 (92%)	81 (84%)	14 (14%)	2 (2%)	5	27
21	U	22/27 (82%)	19 (86%)	3 (14%)	0	100	100
All	All	2336/2541 (92%)	2087 (89%)	233 (10%)	16 (1%)	18	48

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	21	ARG
7	G	155	ARG
19	S	31	ILE
9	I	119	ALA
10	J	86	MET
12	L	28	LYS
2	B	87	ARG
20	T	73	HIS
2	B	16	HIS
12	L	27	LEU
19	S	14	HIS
10	J	34	VAL
5	E	129	ILE
20	T	88	VAL
2	B	229	VAL
15	O	45	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%)	157 (78%)	45 (22%)	1	6
3	C	160/188 (85%)	118 (74%)	42 (26%)	0	3
4	D	180/181 (99%)	145 (81%)	35 (19%)	1	8
5	E	115/123 (94%)	80 (70%)	35 (30%)	0	2
6	F	90/90 (100%)	75 (83%)	15 (17%)	2	12
7	G	126/127 (99%)	98 (78%)	28 (22%)	1	6
8	H	119/119 (100%)	91 (76%)	28 (24%)	1	5
9	I	98/99 (99%)	76 (78%)	22 (22%)	1	6
10	J	87/92 (95%)	66 (76%)	21 (24%)	1	5
11	K	88/99 (89%)	74 (84%)	14 (16%)	2	13
12	L	103/110 (94%)	77 (75%)	26 (25%)	0	4
13	M	94/101 (93%)	78 (83%)	16 (17%)	2	12
14	N	49/50 (98%)	34 (69%)	15 (31%)	0	2
15	O	79/80 (99%)	53 (67%)	26 (33%)	0	1
16	P	72/74 (97%)	62 (86%)	10 (14%)	3	17
17	Q	94/97 (97%)	72 (77%)	22 (23%)	1	5
18	R	61/77 (79%)	46 (75%)	15 (25%)	1	4
19	S	71/80 (89%)	52 (73%)	19 (27%)	0	3
20	T	76/82 (93%)	58 (76%)	18 (24%)	1	5
21	U	19/22 (86%)	17 (90%)	2 (10%)	6	26
All	All	1983/2111 (94%)	1529 (77%)	454 (23%)	1	6

All (454) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	7	VAL
2	B	8	LYS
2	B	10	LEU
2	B	11	LEU
2	B	12	GLU
2	B	16	HIS
2	B	17	PHE
2	B	23	ARG
2	B	39	ILE

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Mol	Chain	Res	Type
2	B	46	LYS
2	B	53	ARG
2	B	55	PHE
2	B	60	ASP
2	B	61	LEU
2	B	67	THR
2	B	69	LEU
2	B	73	THR
2	B	83	MET
2	B	108	ILE
2	B	109	SER
2	B	110	GLN
2	B	112	VAL
2	B	119	GLU
2	B	127	ILE
2	B	139	LYS
2	B	142	LEU
2	B	154	LEU
2	B	155	LEU
2	B	158	LEU
2	B	165	VAL
2	B	169	LYS
2	B	170	GLU
2	B	172	ILE
2	B	178	ARG
2	B	182	ILE
2	B	187	LEU
2	B	190	THR
2	B	191	ASP
2	B	196	LEU
2	B	208	ILE
2	B	213	LEU
2	B	219	VAL
2	B	221	LEU
2	B	223	ILE
2	B	236	TYR
3	C	3	ASN
3	C	4	LYS
3	C	8	ILE
3	C	10	PHE
3	C	11	ARG
3	C	17	ASP

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Mol	Chain	Res	Type
3	C	20	SER
3	C	26	LYS
3	C	31	HIS
3	C	33	LEU
3	C	34	LEU
3	C	38	ARG
3	C	45	LYS
3	C	62	ASP
3	C	64	VAL
3	C	70	VAL
3	C	72	LYS
3	C	79	ARG
3	C	88	ARG
3	C	89	GLU
3	C	95	THR
3	C	101	LEU
3	C	103	VAL
3	C	107	GLN
3	C	111	LEU
3	C	116	VAL
3	C	127	ARG
3	C	130	VAL
3	C	139	GLN
3	C	144	SER
3	C	153	VAL
3	C	157	ILE
3	C	162	GLN
3	C	167	TRP
3	C	175	LEU
3	C	176	HIS
3	C	177	THR
3	C	178	LEU
3	C	188	LEU
3	C	191	THR
3	C	196	LEU
3	C	204	LEU
4	D	3	ARG
4	D	5	ILE
4	D	8	VAL
4	D	9	CYS
4	D	34	GLU
4	D	49	ARG

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Mol	Chain	Res	Type
4	D	61	LYS
4	D	64	LEU
4	D	73	ARG
4	D	78	LEU
4	D	85	LYS
4	D	92	VAL
4	D	94	LEU
4	D	112	VAL
4	D	119	GLN
4	D	127	THR
4	D	128	VAL
4	D	134	ASP
4	D	135	LEU
4	D	140	VAL
4	D	141	ARG
4	D	152	SER
4	D	154	ASN
4	D	157	LEU
4	D	158	ILE
4	D	163	GLU
4	D	170	VAL
4	D	179	GLU
4	D	186	LEU
4	D	187	ARG
4	D	188	LEU
4	D	192	GLU
4	D	194	LEU
4	D	196	LEU
4	D	198	VAL
5	E	9	LYS
5	E	11	ILE
5	E	12	LEU
5	E	13	ILE
5	E	14	ARG
5	E	15	ARG
5	E	16	THR
5	E	19	MET
5	E	20	GLN
5	E	27	ARG
5	E	41	VAL
5	E	43	LEU
5	E	51	VAL

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Mol	Chain	Res	Type
5	E	53	LEU
5	E	56	GLN
5	E	64	ARG
5	E	68	GLU
5	E	76	ILE
5	E	79	GLU
5	E	80	ILE
5	E	81	GLU
5	E	90	VAL
5	E	92	LYS
5	E	100	VAL
5	E	105	VAL
5	E	107	ARG
5	E	111	GLU
5	E	116	THR
5	E	120	THR
5	E	125	SER
5	E	126	ARG
5	E	131	ILE
5	E	148	VAL
5	E	150	ARG
5	E	151	LEU
6	F	10	LEU
6	F	16	GLN
6	F	17	SER
6	F	24	GLU
6	F	25	ILE
6	F	27	GLN
6	F	32	ASN
6	F	36	ARG
6	F	40	VAL
6	F	43	LEU
6	F	45	LEU
6	F	52	ILE
6	F	75	LEU
6	F	84	ASN
6	F	86	ARG
7	G	3	ARG
7	G	6	ARG
7	G	9	VAL
7	G	10	ARG
7	G	12	LEU

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Mol	Chain	Res	Type
7	G	17	VAL
7	G	21	VAL
7	G	22	LEU
7	G	27	ILE
7	G	36	LYS
7	G	38	LEU
7	G	50	ILE
7	G	51	GLN
7	G	57	GLU
7	G	61	VAL
7	G	74	GLU
7	G	75	VAL
7	G	78	ARG
7	G	92	SER
7	G	94	ARG
7	G	101	LEU
7	G	105	VAL
7	G	119	ARG
7	G	125	MET
7	G	126	ASP
7	G	141	VAL
7	G	149	ARG
7	G	155	ARG
8	H	11	THR
8	H	19	VAL
8	H	23	SER
8	H	25	ASP
8	H	29	SER
8	H	37	ARG
8	H	38	ILE
8	H	45	ILE
8	H	51	VAL
8	H	63	LEU
8	H	69	ARG
8	H	83	ILE
8	H	85	ARG
8	H	86	ILE
8	H	88	LYS
8	H	91	ARG
8	H	93	VAL
8	H	95	VAL
8	H	100	ILE

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Mol	Chain	Res	Type
8	H	105	ARG
8	H	114	THR
8	H	116	LYS
8	H	118	VAL
8	H	120	THR
8	H	126	LYS
8	H	127	LEU
8	H	129	VAL
8	H	137	VAL
9	I	12	GLU
9	I	14	VAL
9	I	19	LEU
9	I	20	ARG
9	I	26	VAL
9	I	40	LEU
9	I	53	VAL
9	I	56	LEU
9	I	64	THR
9	I	74	ILE
9	I	78	LYS
9	I	79	LEU
9	I	83	ARG
9	I	86	VAL
9	I	91	ASP
9	I	92	TYR
9	I	95	LYS
9	I	97	LYS
9	I	99	LEU
9	I	108	VAL
9	I	109	VAL
9	I	118	LYS
10	J	8	LEU
10	J	9	ARG
10	J	15	THR
10	J	16	LEU
10	J	23	ILE
10	J	24	VAL
10	J	38	ILE
10	J	40	LEU
10	J	45	ARG
10	J	46	ARG
10	J	48	THR

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Mol	Chain	Res	Type
10	J	50	ILE
10	J	62	HIS
10	J	66	ARG
10	J	68	HIS
10	J	78	ASN
10	J	79	ARG
10	J	80	LYS
10	J	82	ILE
10	J	83	GLU
10	J	88	LEU
11	K	11	LYS
11	K	12	ARG
11	K	29	ILE
11	K	33	THR
11	K	47	VAL
11	K	48	ILE
11	K	53	SER
11	K	79	SER
11	K	84	VAL
11	K	91	ARG
11	K	95	ILE
11	K	98	LEU
11	K	119	CYS
11	K	126	ARG
12	L	6	THR
12	L	10	LEU
12	L	11	VAL
12	L	12	ARG
12	L	17	LYS
12	L	18	VAL
12	L	20	LYS
12	L	21	LYS
12	L	23	LYS
12	L	33	ARG
12	L	36	VAL
12	L	37	CYS
12	L	41	ARG
12	L	43	VAL
12	L	47	LYS
12	L	52	LEU
12	L	60	LEU
12	L	61	THR

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Mol	Chain	Res	Type
12	L	64	TYR
12	L	65	GLU
12	L	79	GLU
12	L	80	HIS
12	L	82	VAL
12	L	89	ARG
12	L	113	ARG
12	L	122	THR
13	M	17	VAL
13	M	22	ILE
13	M	27	LYS
13	M	32	GLU
13	M	34	LEU
13	M	43	THR
13	M	48	LEU
13	M	53	VAL
13	M	56	LEU
13	M	80	ARG
13	M	81	LEU
13	M	90	LEU
13	M	91	ARG
13	M	103	THR
13	M	109	THR
13	M	117	VAL
14	N	3	ARG
14	N	6	LEU
14	N	7	ILE
14	N	17	LYS
14	N	19	ARG
14	N	21	TYR
14	N	22	THR
14	N	25	VAL
14	N	36	PHE
14	N	39	LEU
14	N	42	ILE
14	N	47	LEU
14	N	53	LEU
14	N	57	ARG
14	N	58	LYS
15	O	4	THR
15	O	5	LYS
15	O	7	GLU

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Mol	Chain	Res	Type
15	O	10	LYS
15	O	21	ASP
15	O	22	THR
15	O	24	SER
15	O	29	VAL
15	O	32	LEU
15	O	39	LEU
15	O	41	GLU
15	O	45	VAL
15	O	47	LYS
15	O	54	ARG
15	O	58	MET
15	O	60	VAL
15	O	65	ARG
15	O	67	LEU
15	O	70	LEU
15	O	71	GLN
15	O	78	TYR
15	O	81	LEU
15	O	82	ILE
15	O	83	GLU
15	O	85	LEU
15	O	87	ILE
16	P	2	VAL
16	P	32	TYR
16	P	33	ILE
16	P	45	THR
16	P	54	GLU
16	P	55	ARG
16	P	62	VAL
16	P	74	LEU
16	P	79	VAL
16	P	82	GLN
17	Q	9	VAL
17	Q	21	VAL
17	Q	25	ARG
17	Q	34	LYS
17	Q	35	VAL
17	Q	36	ILE
17	Q	41	LYS
17	Q	59	ILE
17	Q	60	ILE

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Mol	Chain	Res	Type
17	Q	67	LYS
17	Q	68	ARG
17	Q	72	ARG
17	Q	73	VAL
17	Q	75	ARG
17	Q	77	VAL
17	Q	85	VAL
17	Q	86	GLU
17	Q	89	LEU
17	Q	92	ARG
17	Q	96	GLN
17	Q	98	LEU
17	Q	99	SER
18	R	25	THR
18	R	32	ARG
18	R	37	VAL
18	R	42	ARG
18	R	47	THR
18	R	50	ILE
18	R	53	ARG
18	R	61	LYS
18	R	70	ILE
18	R	78	LEU
18	R	82	THR
18	R	84	LYS
18	R	86	VAL
18	R	87	ARG
18	R	88	LYS
19	S	6	LYS
19	S	7	LYS
19	S	15	LEU
19	S	16	LEU
19	S	19	VAL
19	S	20	LEU
19	S	23	ASN
19	S	25	LYS
19	S	27	GLU
19	S	30	LEU
19	S	31	ILE
19	S	33	THR
19	S	49	ILE
19	S	51	VAL

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Mol	Chain	Res	Type
19	S	62	ILE
19	S	63	THR
19	S	73	GLU
19	S	79	THR
19	S	81	ARG
20	T	10	LEU
20	T	13	LEU
20	T	19	SER
20	T	24	LEU
20	T	36	LEU
20	T	45	GLN
20	T	51	GLU
20	T	54	LYS
20	T	56	MET
20	T	62	LEU
20	T	70	SER
20	T	72	LEU
20	T	75	ASN
20	T	84	LEU
20	T	91	LEU
20	T	92	LEU
20	T	99	LEU
20	T	100	ILE
21	U	8	THR
21	U	22	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	16	HIS
2	B	78	GLN
2	B	146	GLN
2	B	224	GLN
3	C	28	GLN
3	C	37	GLN
3	C	63	ASN
3	C	176	HIS
4	D	42	GLN
7	G	51	GLN
7	G	56	GLN
9	I	73	GLN
10	J	56	HIS

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Mol	Chain	Res	Type
10	J	62	HIS
10	J	68	HIS
11	K	26	ASN
15	O	37	ASN
15	O	46	HIS
19	S	14	HIS
19	S	23	ASN
19	S	65	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1505/1522 (98%)	403 (26%)	50 (3%)

All (403) 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	22	G
1	A	32	A
1	A	39	G
1	A	41	G
1	A	45	U
1	A	47	C
1	A	48	C
1	A	51	A
1	A	54	C
1	A	66	G
1	A	69	G
1	A	80	G
1	A	81	U
1	A	82	U
1	A	91	C
1	A	92	C
1	A	93	G
1	A	98	U
1	A	99	C

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Mol	Chain	Res	Type
1	A	108	G
1	A	115	G
1	A	116	A
1	A	117	G
1	A	121	C
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	132	C
1	A	134	A
1	A	158	G
1	A	159	G
1	A	161	A
1	A	163	C
1	A	167	G
1	A	173	U
1	A	182	U
1	A	183	G
1	A	186	C
1	A	195	A
1	A	197	A
1	A	199	G
1	A	201	C
1	A	202	U
1	A	203	U
1	A	216	G
1	A	220	G
1	A	226	G
1	A	231	G
1	A	246	A
1	A	247	G
1	A	250	A
1	A	251	G
1	A	252	U
1	A	253	U
1	A	254	G
1	A	266	G
1	A	267	C
1	A	269	C
1	A	273	A
1	A	289	G
1	A	297	G

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Mol	Chain	Res	Type
1	A	301	G
1	A	319	G
1	A	321	A
1	A	328	C
1	A	329	A
1	A	332	G
1	A	344	A
1	A	345	C
1	A	347	G
1	A	350	G
1	A	351	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	356	A
1	A	367	U
1	A	372	C
1	A	373	A
1	A	374	A
1	A	382	A
1	A	384	G
1	A	388	G
1	A	389	A
1	A	390	C
1	A	392	G
1	A	397	A
1	A	398	C
1	A	406	G
1	A	412	A
1	A	413	G
1	A	414	A
1	A	417	C
1	A	419	C
1	A	420	U
1	A	421	U
1	A	422	C
1	A	428	G
1	A	429	U
1	A	433	C
1	A	435	C
1	A	439	A
1	A	440	A

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Mol	Chain	Res	Type
1	A	452	A
1	A	453	A
1	A	455	C
1	A	457	C
1	A	460	A
1	A	461	C
1	A	481	G
1	A	485	G
1	A	486	U
1	A	488	C
1	A	497	A
1	A	498	U
1	A	505	G
1	A	509	A
1	A	510	A
1	A	511	C
1	A	518	C
1	A	519	C
1	A	520	A
1	A	521	G
1	A	527	7MG
1	A	528	C
1	A	531	U
1	A	532	A
1	A	533	A
1	A	536	C
1	A	538	G
1	A	539	A
1	A	547	A
1	A	559	A
1	A	560	U
1	A	562	C
1	A	564	C
1	A	568	G
1	A	572	A
1	A	573	A
1	A	576	G
1	A	577	G
1	A	579	G
1	A	581	G
1	A	588	G
1	A	607	A

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Mol	Chain	Res	Type
1	A	616	G
1	A	620	C
1	A	624	C
1	A	632	A
1	A	653	A
1	A	656	C
1	A	665	A
1	A	666	G
1	A	670	G
1	A	671	G
1	A	686	U
1	A	687	A
1	A	688	G
1	A	693	G
1	A	694	A
1	A	697	U
1	A	701	C
1	A	702	A
1	A	703	G
1	A	722	A
1	A	723	U
1	A	724	G
1	A	731	G
1	A	733	A
1	A	741	G
1	A	748	C
1	A	749	C
1	A	754	C
1	A	755	G
1	A	759	A
1	A	760	G
1	A	777	A
1	A	781	A
1	A	782	A
1	A	792	A
1	A	793	U
1	A	794	A
1	A	795	C
1	A	799	G
1	A	812	C
1	A	813	U
1	A	815	A

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Mol	Chain	Res	Type
1	A	817	C
1	A	818	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	852	G
1	A	857	C
1	A	858	G
1	A	859	A
1	A	873	A
1	A	874	G
1	A	876	G
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	938	A
1	A	940	C
1	A	942	G
1	A	944	G
1	A	954	G
1	A	960	U
1	A	961	U
1	A	964	A
1	A	966	M2G
1	A	969	A
1	A	971	G
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	978	A
1	A	981	U
1	A	982	U
1	A	983	A
1	A	984	C
1	A	988	G

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Mol	Chain	Res	Type
1	A	990	C
1	A	992	U
1	A	993	G
1	A	994	A
1	A	1004	A
1	A	1005	A
1	A	1006	C
1	A	1007	C
1	A	1016	A
1	A	1019	C
1	A	1023	G
1	A	1025	U
1	A	1026	G
1	A	1028	C
1	A	1030(B)	C
1	A	1031	G
1	A	1038	C
1	A	1045	C
1	A	1051	C
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	1072	G
1	A	1078	U
1	A	1085	U
1	A	1092	A
1	A	1094	G
1	A	1095	U
1	A	1096	C
1	A	1101	A
1	A	1120	G
1	A	1124	G
1	A	1125	U
1	A	1126	U
1	A	1127	G
1	A	1128	C
1	A	1129	C
1	A	1130	A

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Mol	Chain	Res	Type
1	A	1132	C
1	A	1135	U
1	A	1137	C
1	A	1139	G
1	A	1140	C
1	A	1141	C
1	A	1145	C
1	A	1146	A
1	A	1152	A
1	A	1153	C
1	A	1157	A
1	A	1159	U
1	A	1160	G
1	A	1162	C
1	A	1164	G
1	A	1171	G
1	A	1176	A
1	A	1182	G
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	1207	2MG
1	A	1211	U
1	A	1212	U
1	A	1214	C
1	A	1224	G
1	A	1225	A
1	A	1226	C
1	A	1227	A
1	A	1228	C
1	A	1229	A
1	A	1238	A
1	A	1241	G
1	A	1242	C
1	A	1243	C
1	A	1244	C
1	A	1249	C

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Mol	Chain	Res	Type
1	A	1256	A
1	A	1258	G
1	A	1261	A
1	A	1268	A
1	A	1270	C
1	A	1278	U
1	A	1280	A
1	A	1285	A
1	A	1286	A
1	A	1287	A
1	A	1289	A
1	A	1297	C
1	A	1298	C
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1303	C
1	A	1305	G
1	A	1306	A
1	A	1315	U
1	A	1316	G
1	A	1320	C
1	A	1336	C
1	A	1338	G
1	A	1346	A
1	A	1347	G
1	A	1348	U
1	A	1349	A
1	A	1353	G
1	A	1359	C
1	A	1362	C
1	A	1364	U
1	A	1365	G
1	A	1370	G
1	A	1378	C
1	A	1381	U
1	A	1394	A
1	A	1396	A
1	A	1397	C
1	A	1398	A
1	A	1399	C
1	A	1400	5MC

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Mol	Chain	Res	Type
1	A	1402	4OC
1	A	1406	U
1	A	1408	A
1	A	1411	C
1	A	1412	C
1	A	1414	U
1	A	1415	G
1	A	1416	G
1	A	1417	G
1	A	1418	A
1	A	1419	G
1	A	1430	C
1	A	1437	C
1	A	1442	G
1	A	1443	G
1	A	1446	A
1	A	1447	G
1	A	1451	A
1	A	1452	C
1	A	1453	G
1	A	1454	G
1	A	1459	C
1	A	1475	G
1	A	1479	C
1	A	1487	G
1	A	1489	G
1	A	1490	C
1	A	1491	G
1	A	1492	A
1	A	1493	A
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

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Mol	Chain	Res	Type
1	A	1533	C

All (50) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U
1	A	91	C
1	A	115	G
1	A	129(A)	G
1	A	181	G
1	A	204	U
1	A	243	A
1	A	246	A
1	A	250	A
1	A	251	G
1	A	328	C
1	A	350	G
1	A	372	C
1	A	428	G
1	A	484	G
1	A	485	G
1	A	496	A
1	A	509	A
1	A	518	C
1	A	559	A
1	A	575	G
1	A	686	U
1	A	687	A
1	A	701	C
1	A	748	C
1	A	792	A
1	A	812	C
1	A	872	A
1	A	913	A
1	A	960	U
1	A	975	A
1	A	991	U
1	A	992	U
1	A	1004	A
1	A	1065	U
1	A	1067	A
1	A	1139	G

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Mol	Chain	Res	Type
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	1305	G
1	A	1346	A
1	A	1347	G
1	A	1358	U
1	A	1380	U
1	A	1505	G

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

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	7MG	A	527	1	23,26,27	3.47	4 (17%)	27,39,42	2.26	9 (33%)
1	M2G	A	966	1	24,27,28	1.60	5 (20%)	33,40,43	1.17	3 (9%)
1	5MC	A	1400	1	19,22,23	1.87	4 (21%)	26,32,35	1.27	4 (15%)
1	MA6	A	1518[B]	1	23,26,27	1.46	6 (26%)	33,38,41	0.90	1 (3%)
1	4OC	A	1402	1	20,23,24	1.54	4 (20%)	25,32,35	0.87	0
1	PSU	A	1541	1	18,21,22	1.17	1 (5%)	21,30,33	1.69	3 (14%)
1	UR3	A	1498	1,22	19,22,23	1.41	3 (15%)	26,32,35	1.31	1 (3%)
1	MA6	A	1519[A]	1	23,26,27	1.36	4 (17%)	33,38,41	1.08	3 (9%)
1	PSU	A	1540	1	18,21,22	1.10	1 (5%)	21,30,33	1.72	4 (19%)
1	MA6	A	1518[A]	1	23,26,27	1.08	2 (8%)	33,38,41	1.00	1 (3%)
1	5MC	A	1404	1	19,22,23	1.33	2 (10%)	26,32,35	1.11	3 (11%)
1	2MG	A	1207	1	23,26,27	1.41	5 (21%)	33,38,41	1.14	4 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	A	967	1	19,22,23	0.91	1 (5%)	26,32,35	1.07	2 (7%)
1	PSU	A	516	1,22	18,21,22	1.24	2 (11%)	21,30,33	2.09	6 (28%)
1	5MC	A	1407	1	19,22,23	1.47	4 (21%)	26,32,35	0.98	1 (3%)
12	0TD	L	92	12	8,9,10	1.36	0	6,11,13	2.64	3 (50%)
1	MA6	A	1519[B]	1	23,26,27	1.42	2 (8%)	33,38,41	1.00	3 (9%)

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	7MG	A	527	1	-	2/7/37/38	0/3/3/3
1	M2G	A	966	1	-	4/11/29/30	0/3/3/3
1	5MC	A	1400	1	-	2/7/25/26	0/2/2/2
1	MA6	A	1518[B]	1	-	0/11/29/30	0/3/3/3
1	4OC	A	1402	1	-	3/9/29/30	0/2/2/2
1	PSU	A	1541	1	-	0/7/25/26	0/2/2/2
1	UR3	A	1498	1,22	-	2/7/25/26	0/2/2/2
1	MA6	A	1519[A]	1	-	2/11/29/30	0/3/3/3
1	PSU	A	1540	1	-	1/7/25/26	0/2/2/2
1	MA6	A	1518[A]	1	-	1/11/29/30	0/3/3/3
1	5MC	A	1404	1	-	0/7/25/26	0/2/2/2
1	2MG	A	1207	1	-	2/9/27/28	0/3/3/3
1	5MC	A	967	1	-	0/7/25/26	0/2/2/2
1	PSU	A	516	1,22	-	0/7/25/26	0/2/2/2
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
12	0TD	L	92	12	-	2/7/12/14	-
1	MA6	A	1519[B]	1	-	5/11/29/30	0/3/3/3

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	7MG	C8-N9	-14.06	1.36	1.45
1	A	527	7MG	C5-N7	7.21	1.44	1.35
1	A	1400	5MC	C2-N1	5.01	1.50	1.40
1	A	1541	PSU	C6-C5	4.16	1.39	1.35
1	A	1498	UR3	C4-N3	-4.10	1.32	1.40
1	A	516	PSU	C6-C5	4.07	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1400	5MC	C2-N3	4.01	1.44	1.36
1	A	1540	PSU	C6-C5	3.99	1.39	1.35
1	A	966	M2G	C4-N3	3.67	1.42	1.34
1	A	1519[B]	MA6	C5-C4	3.63	1.45	1.39
1	A	1407	5MC	C5-C4	3.52	1.46	1.44
1	A	1519[A]	MA6	C5-C4	3.48	1.45	1.39
1	A	966	M2G	C4-N9	3.45	1.46	1.38
1	A	527	7MG	C2-N2	3.41	1.42	1.34
1	A	1404	5MC	C2-N3	3.26	1.42	1.36
1	A	1519[B]	MA6	C2-N1	3.22	1.39	1.33
1	A	1207	2MG	C2-N2	3.09	1.39	1.33
1	A	1518[B]	MA6	C5-C4	3.06	1.44	1.39
1	A	1207	2MG	C2-N1	3.05	1.41	1.36
1	A	1407	5MC	C2-N3	3.00	1.42	1.36
1	A	1400	5MC	C6-C5	2.98	1.39	1.34
1	A	1518[A]	MA6	C8-N9	2.97	1.42	1.37
1	A	1407	5MC	C4-N4	2.90	1.41	1.34
1	A	1519[A]	MA6	C2-N1	2.89	1.39	1.33
1	A	966	M2G	C2-N2	2.84	1.40	1.35
1	A	966	M2G	C8-N9	2.80	1.43	1.37
1	A	1402	4OC	C2-N1	2.80	1.45	1.40
1	A	1207	2MG	C8-N9	2.76	1.43	1.37
1	A	1404	5MC	C2-N1	2.71	1.45	1.40
1	A	1518[B]	MA6	C4-N3	2.56	1.39	1.34
1	A	1498	UR3	C6-N1	-2.54	1.32	1.38
1	A	1402	4OC	O2-C2	-2.49	1.19	1.23
1	A	1402	4OC	C2-N3	2.48	1.41	1.36
1	A	1402	4OC	CM4-N4	2.47	1.50	1.45
1	A	1498	UR3	C3U-N3	-2.47	1.42	1.47
1	A	1400	5MC	C4-N3	2.46	1.38	1.34
1	A	1207	2MG	C6-N1	2.46	1.43	1.38
1	A	1407	5MC	C2-N1	2.45	1.45	1.40
1	A	1519[A]	MA6	C8-N9	2.41	1.41	1.37
1	A	1518[B]	MA6	C8-N9	2.39	1.41	1.37
1	A	1518[B]	MA6	C2-N1	2.36	1.38	1.33
1	A	1519[A]	MA6	C8-N7	2.32	1.36	1.31
1	A	1518[B]	MA6	C6-N1	2.26	1.38	1.34
1	A	1518[A]	MA6	C5-C4	2.20	1.43	1.39
1	A	967	5MC	O2-C2	-2.15	1.19	1.23
1	A	966	M2G	O6-C6	-2.13	1.19	1.23
1	A	1207	2MG	C4-N3	2.04	1.38	1.34
1	A	1518[B]	MA6	C5-N7	2.02	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	7MG	C5-C6	2.01	1.48	1.43
1	A	516	PSU	C4-C5	-2.00	1.38	1.44

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	516	PSU	N1-C2-N3	5.36	120.82	115.17
12	L	92	0TD	CSB-SB-CB	-5.06	93.27	102.36
1	A	516	PSU	C4-N3-C2	-4.89	119.64	126.37
1	A	527	7MG	C5-C6-N1	4.74	119.29	110.94
1	A	1541	PSU	C4-N3-C2	-4.51	120.16	126.37
1	A	1540	PSU	N1-C2-N3	4.43	119.84	115.17
1	A	527	7MG	C6-C5-N7	4.41	138.77	131.93
1	A	527	7MG	C2-N3-C4	4.34	119.78	112.30
1	A	1540	PSU	C4-N3-C2	-4.34	120.39	126.37
1	A	1541	PSU	N1-C2-N3	4.23	119.63	115.17
1	A	966	M2G	C5-C4-N3	-3.65	122.58	128.39
1	A	527	7MG	C5-C4-N3	-3.47	121.62	128.13
1	A	527	7MG	C6-C5-C4	-3.45	116.32	122.40
1	A	527	7MG	C2-N1-C6	-3.44	118.87	125.11
1	A	516	PSU	C6-N1-C2	-3.38	119.56	122.69
1	A	966	M2G	O6-C6-N1	-3.36	113.80	120.11
1	A	1498	UR3	C6-N1-C2	-3.33	119.08	121.80
1	A	1400	5MC	C1'-N1-C6	-3.12	116.02	121.15
1	A	527	7MG	N9-C8-N7	3.07	107.71	103.37
1	A	527	7MG	N9-C4-N3	2.79	129.55	125.46
1	A	1519[B]	MA6	C4-C5-C6	2.78	118.79	115.91
1	A	1400	5MC	C5-C4-N3	2.76	124.58	121.75
1	A	1207	2MG	C5-C4-N3	-2.65	124.17	128.39
1	A	1407	5MC	N4-C4-N3	-2.61	113.79	118.51
1	A	967	5MC	N4-C4-N3	-2.58	113.84	118.51
1	A	1519[A]	MA6	C2-N1-C6	2.57	118.11	111.83
1	A	967	5MC	C1'-N1-C6	-2.54	116.97	121.15
1	A	516	PSU	C6-C5-C4	2.53	119.88	118.17
1	A	1518[A]	MA6	C2-N1-C6	2.47	117.86	111.83
1	A	1404	5MC	N4-C4-N3	-2.46	114.05	118.51
1	A	1404	5MC	C5-C4-N3	2.44	124.26	121.75
1	A	527	7MG	N2-C2-N3	-2.40	114.99	119.67
1	A	1207	2MG	C2-N1-C6	-2.33	121.73	124.55
1	A	1540	PSU	C6-N1-C2	-2.31	120.55	122.69
1	A	1207	2MG	N9-C4-N3	2.28	130.52	125.95
1	A	1207	2MG	C6-C5-N7	-2.26	126.17	130.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1540	PSU	O2-C2-N1	-2.26	120.46	122.79
1	A	1400	5MC	C1'-N1-C2	2.24	123.38	118.44
1	A	516	PSU	O2-C2-N1	-2.23	120.49	122.79
1	A	516	PSU	O4'-C1'-C2'	2.20	108.19	105.15
1	A	1519[B]	MA6	C5-C4-N3	-2.19	123.70	126.72
12	L	92	0TD	CB-CA-N	-2.18	104.68	109.10
1	A	1400	5MC	O2-C2-N1	2.17	123.15	118.90
1	A	1541	PSU	C6-N1-C2	-2.16	120.68	122.69
1	A	1519[A]	MA6	C4-C5-N7	-2.14	108.14	110.58
1	A	966	M2G	N9-C4-N3	2.12	130.20	125.95
1	A	1518[B]	MA6	C2-N1-C6	2.12	117.01	111.83
12	L	92	0TD	OD1-CG-CB	-2.11	118.02	122.44
1	A	1519[B]	MA6	C2-N1-C6	2.09	116.93	111.83
1	A	1404	5MC	C4-N3-C2	-2.03	118.00	120.81
1	A	1519[A]	MA6	C5-C4-N9	2.00	107.99	105.81

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	527	7MG	O4'-C4'-C5'-O5'
1	A	966	M2G	N1-C2-N2-CM1
1	A	966	M2G	N1-C2-N2-CM2
1	A	966	M2G	N3-C2-N2-CM1
1	A	966	M2G	N3-C2-N2-CM2
1	A	1400	5MC	O4'-C4'-C5'-O5'
1	A	1402	4OC	O4'-C4'-C5'-O5'
1	A	1402	4OC	C1'-C2'-O2'-CM2
1	A	1519[A]	MA6	O4'-C4'-C5'-O5'
1	A	1519[B]	MA6	C5-C6-N6-C9
1	A	1519[B]	MA6	N1-C6-N6-C9
1	A	527	7MG	C3'-C4'-C5'-O5'
1	A	1207	2MG	O4'-C4'-C5'-O5'
1	A	1207	2MG	C3'-C4'-C5'-O5'
1	A	1400	5MC	C3'-C4'-C5'-O5'
1	A	1519[A]	MA6	C3'-C4'-C5'-O5'
1	A	1402	4OC	C3'-C4'-C5'-O5'
1	A	1519[B]	MA6	C3'-C4'-C5'-O5'
1	A	1498	UR3	O4'-C4'-C5'-O5'
1	A	1518[A]	MA6	C5-C6-N6-C9
1	A	1498	UR3	C3'-C4'-C5'-O5'
1	A	1519[B]	MA6	C5-C6-N6-C10

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Mol	Chain	Res	Type	Atoms
1	A	1519[B]	MA6	O4'-C4'-C5'-O5'
12	L	92	0TD	CG-CB-SB-CSB
12	L	92	0TD	SB-CB-CG-OD1
1	A	1540	PSU	O4'-C4'-C5'-O5'

There are no ring outliers.

12 monomers are involved in 24 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 291 ligands modelled in this entry, 291 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.37	30 (2%) 65 39	56, 156, 308, 384	4 (0%)
2	B	234/256 (91%)	-0.49	2 (0%) 81 57	105, 165, 249, 269	0
3	C	206/239 (86%)	-0.18	2 (0%) 79 54	164, 235, 290, 329	0
4	D	208/209 (99%)	-0.32	9 (4%) 40 23	99, 159, 211, 239	0
5	E	150/162 (92%)	-0.69	0 100 100	79, 122, 163, 194	0
6	F	101/101 (100%)	-0.52	0 100 100	130, 175, 208, 240	0
7	G	155/156 (99%)	-0.36	2 (1%) 75 49	150, 203, 268, 323	0
8	H	138/138 (100%)	-0.65	1 (0%) 84 62	74, 108, 152, 181	0
9	I	127/128 (99%)	-0.10	2 (1%) 70 44	173, 226, 272, 298	0
10	J	98/105 (93%)	-0.09	1 (1%) 79 54	194, 237, 302, 326	0
11	K	116/129 (89%)	-0.55	0 100 100	111, 146, 197, 222	0
12	L	123/135 (91%)	-0.38	1 (0%) 82 60	79, 155, 195, 227	0
13	M	118/126 (93%)	-0.28	1 (0%) 82 60	139, 190, 229, 290	0
14	N	60/61 (98%)	0.05	2 (3%) 49 29	185, 222, 274, 306	0
15	O	87/89 (97%)	-0.61	0 100 100	92, 132, 179, 209	0
16	P	83/88 (94%)	-0.38	0 100 100	110, 146, 187, 230	0
17	Q	99/105 (94%)	-0.56	0 100 100	95, 125, 176, 185	0
18	R	70/88 (79%)	-0.53	0 100 100	107, 145, 200, 231	0
19	S	80/93 (86%)	0.03	3 (3%) 44 26	197, 254, 313, 320	0
20	T	99/106 (93%)	-0.27	1 (1%) 79 54	112, 149, 204, 232	0
21	U	24/27 (88%)	0.54	3 (12%) 8 8	169, 204, 229, 238	0
All	All	3874/4063 (95%)	-0.37	60 (1%) 72 45	56, 166, 278, 384	4 (0%)

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	985	C	6.9
20	T	106	ALA	5.7
1	A	1204	A	4.4
4	D	31	CYS	4.2
4	D	9	CYS	4.2
9	I	9	ARG	4.1
1	A	1520[A]	G	4.0
1	A	1516[A]	G	3.9
1	A	1220	G	3.8
1	A	1129	C	3.7
1	A	64	G	3.4
1	A	1417	G	3.3
1	A	1517[A]	G	3.3
12	L	73	GLU	3.2
21	U	6	ARG	3.1
4	D	5	ILE	3.1
1	A	79	G	3.1
1	A	984	C	3.1
4	D	21	LEU	3.1
14	N	35	ARG	3.0
13	M	117	VAL	3.0
4	D	26	CYS	2.9
1	A	353	A	2.9
19	S	51	VAL	2.9
1	A	80	G	2.9
1	A	1532	U	2.8
7	G	2	ALA	2.8
1	A	1006	C	2.7
1	A	1222	G	2.7
21	U	5	ASP	2.7
1	A	1416	G	2.5
19	S	2	PRO	2.5
1	A	1221	G	2.5
1	A	1362	C	2.5
4	D	22	LYS	2.5
1	A	1017	G	2.5
9	I	124	GLN	2.5
2	B	16	HIS	2.4
3	C	42	LEU	2.4
1	A	76	C	2.4
1	A	1255	G	2.4
1	A	75	G	2.4
19	S	35	SER	2.3

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Mol	Chain	Res	Type	RSRZ
3	C	146	ALA	2.3
1	A	78	G	2.3
7	G	154	TYR	2.3
21	U	10	ARG	2.3
1	A	202	U	2.3
10	J	56	HIS	2.2
1	A	1314	C	2.2
4	D	145	GLU	2.2
1	A	1019	C	2.2
2	B	203	GLY	2.2
1	A	77	G	2.1
8	H	18	ARG	2.1
14	N	4	LYS	2.1
1	A	993	G	2.1
1	A	723	U	2.0
4	D	42	GLN	2.0
4	D	20	TYR	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(Å ²)	Q<0.9
1	PSU	A	1541	20/21	0.89	0.10	223,263,279,284	0
1	PSU	A	1540	20/21	0.91	0.09	271,280,285,287	0
1	5MC	A	967	21/22	0.95	0.06	162,170,190,199	0
1	PSU	A	516	20/21	0.95	0.06	162,181,197,197	0
1	M2G	A	966	25/26	0.95	0.07	165,177,184,186	0
1	5MC	A	1400	21/22	0.96	0.07	114,142,154,174	0
1	4OC	A	1402	22/23	0.96	0.13	124,137,170,187	0
1	7MG	A	527	24/25	0.96	0.08	116,135,155,161	0
1	2MG	A	1207	24/25	0.96	0.12	263,291,297,309	0
1	MA6	A	1518[A]	24/25	0.97	0.14	118,131,141,143	24
1	MA6	A	1518[B]	24/25	0.97	0.14	126,135,138,138	24
1	5MC	A	1407	21/22	0.97	0.07	149,172,180,188	0
1	UR3	A	1498	21/22	0.97	0.10	117,143,151,155	0
12	0TD	L	92	10/11	0.97	0.08	157,170,178,331	0
1	5MC	A	1404	21/22	0.98	0.09	112,135,164,183	0
1	MA6	A	1519[B]	24/25	0.99	0.10	106,118,129,130	24

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	MA6	A	1519[A]	24/25	0.99	0.10	109,115,125,137	24

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B	301	1/1	0.40	0.24	154,154,154,154	0
22	MG	A	1672	1/1	0.53	0.52	130,130,130,130	0
22	MG	A	1779	1/1	0.54	0.09	159,159,159,159	0
22	MG	M	202	1/1	0.59	0.11	122,122,122,122	0
22	MG	A	1626	1/1	0.61	0.31	150,150,150,150	0
22	MG	A	1776	1/1	0.71	0.14	129,129,129,129	0
22	MG	A	1679	1/1	0.71	0.24	177,177,177,177	0
22	MG	A	1751	1/1	0.72	0.50	136,136,136,136	0
22	MG	A	1769	1/1	0.73	0.25	142,142,142,142	0
22	MG	A	1840	1/1	0.75	0.16	149,149,149,149	0
22	MG	A	1713	1/1	0.77	0.65	106,106,106,106	0
22	MG	A	1780	1/1	0.78	0.33	162,162,162,162	0
22	MG	A	1783	1/1	0.79	0.39	133,133,133,133	0
22	MG	A	1768	1/1	0.79	0.37	118,118,118,118	0
22	MG	A	1744	1/1	0.81	0.18	151,151,151,151	0
22	MG	A	1799	1/1	0.81	0.38	287,287,287,287	0
22	MG	A	1823	1/1	0.81	0.19	168,168,168,168	0
22	MG	A	1773	1/1	0.82	0.14	164,164,164,164	0
22	MG	A	1601	1/1	0.82	0.24	137,137,137,137	0
22	MG	A	1656	1/1	0.82	0.20	133,133,133,133	0
22	MG	A	1863	1/1	0.82	0.15	103,103,103,103	0
22	MG	A	1864	1/1	0.82	0.25	123,123,123,123	0
22	MG	A	1689	1/1	0.82	0.07	238,238,238,238	0
22	MG	A	1668	1/1	0.82	0.24	111,111,111,111	0
22	MG	T	201	1/1	0.82	0.09	155,155,155,155	0
22	MG	A	1825	1/1	0.83	0.13	404,404,404,404	0
22	MG	A	1685	1/1	0.83	0.35	116,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	A	1847	1/1	0.83	0.17	145,145,145,145	0
22	MG	A	1680	1/1	0.83	0.15	139,139,139,139	0
22	MG	A	1748	1/1	0.84	0.27	144,144,144,144	0
22	MG	A	1664	1/1	0.85	0.12	126,126,126,126	0
22	MG	A	1618	1/1	0.85	0.35	125,125,125,125	0
22	MG	A	1671	1/1	0.85	0.21	162,162,162,162	0
22	MG	A	1729	1/1	0.85	0.25	120,120,120,120	0
22	MG	A	1742	1/1	0.85	0.21	132,132,132,132	0
22	MG	A	1758	1/1	0.86	0.18	107,107,107,107	0
22	MG	A	1782	1/1	0.86	0.37	144,144,144,144	0
22	MG	A	1749	1/1	0.86	0.19	121,121,121,121	0
22	MG	C	301	1/1	0.86	0.19	150,150,150,150	0
22	MG	A	1724	1/1	0.86	0.43	146,146,146,146	0
22	MG	A	1859	1/1	0.86	0.24	132,132,132,132	0
22	MG	A	1798	1/1	0.87	0.17	208,208,208,208	0
22	MG	A	1760	1/1	0.87	0.15	137,137,137,137	0
22	MG	A	1816	1/1	0.87	0.14	170,170,170,170	0
22	MG	A	1763	1/1	0.87	0.10	240,240,240,240	0
22	MG	A	1716	1/1	0.87	0.12	95,95,95,95	0
22	MG	A	1745	1/1	0.87	0.11	127,127,127,127	0
22	MG	A	1695	1/1	0.87	0.11	125,125,125,125	0
22	MG	A	1608	1/1	0.88	0.35	127,127,127,127	0
22	MG	A	1720	1/1	0.88	0.20	109,109,109,109	0
22	MG	A	1765	1/1	0.88	0.51	390,390,390,390	0
22	MG	A	1867	1/1	0.88	0.18	139,139,139,139	0
22	MG	A	1692	1/1	0.88	0.11	167,167,167,167	0
22	MG	A	1756	1/1	0.88	0.22	140,140,140,140	0
22	MG	D	304	1/1	0.88	0.15	106,106,106,106	0
22	MG	A	1726	1/1	0.88	0.53	106,106,106,106	0
22	MG	A	1856	1/1	0.88	0.25	108,108,108,108	0
22	MG	A	1607	1/1	0.89	0.08	165,165,165,165	0
22	MG	A	1693	1/1	0.89	0.43	146,146,146,146	0
22	MG	A	1820	1/1	0.89	0.06	495,495,495,495	0
22	MG	A	1623	1/1	0.89	0.07	125,125,125,125	0
22	MG	A	1674	1/1	0.89	0.09	168,168,168,168	0
22	MG	A	1677	1/1	0.89	0.36	125,125,125,125	0
22	MG	A	1788	1/1	0.89	0.10	330,330,330,330	0
22	MG	A	1853	1/1	0.89	0.05	91,91,91,91	0
22	MG	Q	201	1/1	0.89	0.18	140,140,140,140	0
22	MG	A	1717	1/1	0.89	1.18	146,146,146,146	0
22	MG	A	1795	1/1	0.90	0.15	253,253,253,253	0
22	MG	A	1709	1/1	0.90	0.08	165,165,165,165	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	A	1846	1/1	0.90	0.08	131,131,131,131	0
22	MG	A	1631	1/1	0.90	0.40	118,118,118,118	0
22	MG	A	1813	1/1	0.90	0.12	210,210,210,210	0
22	MG	L	201	1/1	0.90	0.06	122,122,122,122	0
22	MG	A	1640	1/1	0.90	0.23	111,111,111,111	0
22	MG	A	1704	1/1	0.90	0.08	118,118,118,118	0
22	MG	A	1735	1/1	0.90	0.49	114,114,114,114	0
22	MG	A	1644	1/1	0.91	0.09	253,253,253,253	0
22	MG	A	1655	1/1	0.91	0.16	141,141,141,141	0
22	MG	A	1737	1/1	0.91	0.23	142,142,142,142	0
22	MG	A	1603	1/1	0.91	0.13	111,111,111,111	0
22	MG	A	1762	1/1	0.91	0.22	219,219,219,219	0
22	MG	A	1635	1/1	0.91	0.26	151,151,151,151	0
22	MG	A	1838	1/1	0.91	0.31	386,386,386,386	0
22	MG	A	1667	1/1	0.91	0.16	274,274,274,274	0
22	MG	A	1845	1/1	0.91	0.33	106,106,106,106	0
22	MG	A	1790	1/1	0.91	0.22	159,159,159,159	0
22	MG	A	1703	1/1	0.91	0.10	138,138,138,138	0
22	MG	A	1620	1/1	0.91	0.21	136,136,136,136	0
22	MG	A	1678	1/1	0.92	0.18	143,143,143,143	0
22	MG	A	1865	1/1	0.92	0.16	120,120,120,120	0
22	MG	A	1801	1/1	0.92	0.21	152,152,152,152	0
22	MG	A	1722	1/1	0.92	0.29	129,129,129,129	0
22	MG	A	1710	1/1	0.92	0.15	162,162,162,162	0
22	MG	D	302	1/1	0.92	0.13	142,142,142,142	0
22	MG	A	1851	1/1	0.92	0.13	126,126,126,126	0
22	MG	A	1771	1/1	0.92	0.21	158,158,158,158	0
22	MG	A	1639	1/1	0.92	0.16	173,173,173,173	0
22	MG	A	1691	1/1	0.92	0.18	136,136,136,136	0
22	MG	A	1609	1/1	0.92	0.14	113,113,113,113	0
22	MG	A	1774	1/1	0.93	0.53	134,134,134,134	0
22	MG	A	1673	1/1	0.93	0.24	130,130,130,130	0
22	MG	A	1805	1/1	0.93	0.46	153,153,153,153	0
22	MG	A	1778	1/1	0.93	0.10	137,137,137,137	0
22	MG	A	1860	1/1	0.93	0.13	115,115,115,115	0
22	MG	A	1687	1/1	0.93	0.07	151,151,151,151	0
22	MG	A	1659	1/1	0.93	0.27	95,95,95,95	0
22	MG	A	1721	1/1	0.93	0.12	128,128,128,128	0
22	MG	A	1736	1/1	0.93	0.07	99,99,99,99	0
22	MG	A	1827	1/1	0.93	0.08	148,148,148,148	0
22	MG	A	1621	1/1	0.93	0.08	118,118,118,118	0
22	MG	A	1752	1/1	0.93	0.14	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	D	303	1/1	0.93	0.14	141,141,141,141	0
22	MG	A	1843	1/1	0.93	0.43	163,163,163,163	0
22	MG	E	201	1/1	0.93	0.11	152,152,152,152	0
22	MG	J	201	1/1	0.93	0.08	497,497,497,497	0
22	MG	A	1792	1/1	0.93	0.12	398,398,398,398	0
22	MG	A	1753	1/1	0.93	0.21	169,169,169,169	0
22	MG	A	1739	1/1	0.93	0.07	126,126,126,126	0
22	MG	Q	202	1/1	0.93	0.08	105,105,105,105	0
22	MG	A	1849	1/1	0.93	0.45	123,123,123,123	0
22	MG	A	1732	1/1	0.94	0.23	134,134,134,134	0
22	MG	A	1733	1/1	0.94	0.12	91,91,91,91	0
22	MG	A	1850	1/1	0.94	0.05	134,134,134,134	0
22	MG	A	1791	1/1	0.94	0.10	160,160,160,160	0
22	MG	A	1636	1/1	0.94	0.43	112,112,112,112	0
22	MG	A	1854	1/1	0.94	0.06	94,94,94,94	0
22	MG	A	1665	1/1	0.94	0.13	117,117,117,117	0
22	MG	A	1857	1/1	0.94	0.09	115,115,115,115	0
22	MG	A	1858	1/1	0.94	0.17	90,90,90,90	0
22	MG	A	1714	1/1	0.94	0.21	116,116,116,116	0
22	MG	A	1766	1/1	0.94	0.17	282,282,282,282	0
22	MG	A	1800	1/1	0.94	0.10	389,389,389,389	0
22	MG	A	1682	1/1	0.94	0.14	137,137,137,137	0
22	MG	A	1646	1/1	0.94	0.38	143,143,143,143	0
22	MG	A	1696	1/1	0.94	0.07	193,193,193,193	0
22	MG	A	1697	1/1	0.94	0.11	139,139,139,139	0
22	MG	B	302	1/1	0.94	0.08	166,166,166,166	0
22	MG	A	1653	1/1	0.94	0.05	118,118,118,118	0
22	MG	A	1688	1/1	0.94	0.28	113,113,113,113	0
22	MG	A	1777	1/1	0.94	0.06	93,93,93,93	0
22	MG	A	1707	1/1	0.94	0.39	120,120,120,120	0
22	MG	A	1828	1/1	0.94	0.24	156,156,156,156	0
22	MG	I	201	1/1	0.94	0.33	143,143,143,143	0
22	MG	A	1829	1/1	0.94	0.34	286,286,286,286	0
22	MG	A	1727	1/1	0.94	0.19	178,178,178,178	0
22	MG	A	1661	1/1	0.94	0.15	148,148,148,148	0
22	MG	A	1755	1/1	0.94	0.17	131,131,131,131	0
22	MG	A	1731	1/1	0.94	0.17	103,103,103,103	0
22	MG	A	1787	1/1	0.94	0.19	140,140,140,140	0
22	MG	A	1797	1/1	0.95	0.51	367,367,367,367	0
22	MG	A	1754	1/1	0.95	0.10	107,107,107,107	0
22	MG	A	1861	1/1	0.95	0.12	135,135,135,135	0
22	MG	A	1830	1/1	0.95	0.09	199,199,199,199	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	A	1836	1/1	0.95	0.21	231,231,231,231	0
22	MG	A	1708	1/1	0.95	0.11	113,113,113,113	0
22	MG	A	1701	1/1	0.95	0.20	216,216,216,216	0
22	MG	A	1841	1/1	0.95	0.14	175,175,175,175	0
22	MG	A	1757	1/1	0.95	0.12	123,123,123,123	0
22	MG	A	1803	1/1	0.95	0.14	147,147,147,147	0
22	MG	A	1804	1/1	0.95	0.30	305,305,305,305	0
22	MG	A	1784	1/1	0.95	0.21	318,318,318,318	0
22	MG	A	1811	1/1	0.95	0.24	242,242,242,242	0
22	MG	D	305	1/1	0.95	0.22	122,122,122,122	0
22	MG	A	1750	1/1	0.95	0.07	128,128,128,128	0
22	MG	F	201	1/1	0.95	0.09	149,149,149,149	0
22	MG	A	1743	1/1	0.95	0.41	135,135,135,135	0
22	MG	A	1819	1/1	0.95	0.42	141,141,141,141	0
22	MG	A	1761	1/1	0.95	0.30	156,156,156,156	0
22	MG	A	1855	1/1	0.95	0.17	139,139,139,139	0
22	MG	P	101	1/1	0.95	0.15	90,90,90,90	0
22	MG	P	102	1/1	0.95	0.08	128,128,128,128	0
22	MG	A	1705	1/1	0.95	0.11	118,118,118,118	0
22	MG	A	1698	1/1	0.95	0.18	192,192,192,192	0
22	MG	A	1764	1/1	0.95	0.12	290,290,290,290	0
22	MG	T	202	1/1	0.95	0.45	96,96,96,96	0
22	MG	A	1616	1/1	0.96	0.11	79,79,79,79	0
22	MG	A	1741	1/1	0.96	0.20	111,111,111,111	0
22	MG	A	1818	1/1	0.96	0.33	247,247,247,247	0
22	MG	A	1759	1/1	0.96	0.27	98,98,98,98	0
22	MG	A	1602	1/1	0.96	0.19	168,168,168,168	0
22	MG	A	1862	1/1	0.96	0.11	99,99,99,99	0
22	MG	A	1604	1/1	0.96	0.17	141,141,141,141	0
22	MG	A	1785	1/1	0.96	0.21	394,394,394,394	0
22	MG	A	1786	1/1	0.96	0.12	234,234,234,234	0
22	MG	A	1725	1/1	0.96	0.06	142,142,142,142	0
22	MG	A	1663	1/1	0.96	0.18	148,148,148,148	0
22	MG	A	1746	1/1	0.96	0.45	126,126,126,126	0
22	MG	A	1833	1/1	0.96	0.06	450,450,450,450	0
22	MG	A	1747	1/1	0.96	0.10	137,137,137,137	0
22	MG	A	1648	1/1	0.96	0.13	82,82,82,82	0
22	MG	A	1794	1/1	0.96	0.25	422,422,422,422	0
22	MG	A	1767	1/1	0.96	0.09	184,184,184,184	0
22	MG	A	1796	1/1	0.96	0.20	383,383,383,383	0
22	MG	A	1652	1/1	0.96	0.13	126,126,126,126	0
22	MG	A	1711	1/1	0.96	0.15	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	A	1770	1/1	0.96	0.56	166,166,166,166	0
22	MG	A	1666	1/1	0.96	0.17	147,147,147,147	0
22	MG	M	201	1/1	0.96	0.19	388,388,388,388	0
22	MG	A	1605	1/1	0.96	0.13	102,102,102,102	0
22	MG	A	1734	1/1	0.96	0.35	99,99,99,99	0
22	MG	A	1852	1/1	0.96	0.42	121,121,121,121	0
22	MG	A	1654	1/1	0.96	0.05	117,117,117,117	0
22	MG	A	1686	1/1	0.96	0.13	124,124,124,124	0
22	MG	A	1807	1/1	0.96	0.11	141,141,141,141	0
22	MG	A	1612	1/1	0.96	0.04	136,136,136,136	0
23	ZN	N	101	1/1	0.96	0.06	395,395,395,395	0
22	MG	A	1793	1/1	0.97	0.06	182,182,182,182	0
22	MG	A	1772	1/1	0.97	0.18	126,126,126,126	0
22	MG	A	1641	1/1	0.97	0.07	78,78,78,78	0
22	MG	A	1832	1/1	0.97	0.21	364,364,364,364	0
22	MG	A	1719	1/1	0.97	0.18	143,143,143,143	0
22	MG	A	1835	1/1	0.97	0.21	317,317,317,317	0
22	MG	A	1868	1/1	0.97	0.18	139,139,139,139	0
22	MG	A	1775	1/1	0.97	0.10	101,101,101,101	0
22	MG	A	1700	1/1	0.97	0.30	438,438,438,438	0
22	MG	A	1669	1/1	0.97	0.14	145,145,145,145	0
22	MG	A	1670	1/1	0.97	0.07	129,129,129,129	0
22	MG	A	1629	1/1	0.97	0.19	106,106,106,106	0
22	MG	A	1613	1/1	0.97	0.13	117,117,117,117	0
22	MG	A	1781	1/1	0.97	0.39	116,116,116,116	0
22	MG	A	1647	1/1	0.97	0.09	110,110,110,110	0
22	MG	A	1848	1/1	0.97	0.10	166,166,166,166	0
22	MG	A	1619	1/1	0.97	0.08	95,95,95,95	0
22	MG	A	1728	1/1	0.97	0.08	129,129,129,129	0
22	MG	A	1650	1/1	0.97	0.14	118,118,118,118	0
22	MG	A	1814	1/1	0.97	0.22	224,224,224,224	0
22	MG	A	1730	1/1	0.97	0.10	107,107,107,107	0
22	MG	A	1817	1/1	0.97	0.19	297,297,297,297	0
22	MG	A	1617	1/1	0.97	0.03	97,97,97,97	0
22	MG	A	1694	1/1	0.97	0.10	376,376,376,376	0
22	MG	A	1789	1/1	0.97	0.26	174,174,174,174	0
22	MG	A	1627	1/1	0.97	0.06	96,96,96,96	0
22	MG	A	1628	1/1	0.97	0.10	69,69,69,69	0
22	MG	A	1681	1/1	0.97	0.06	162,162,162,162	0
22	MG	A	1633	1/1	0.98	0.03	105,105,105,105	0
22	MG	A	1702	1/1	0.98	0.15	322,322,322,322	0
22	MG	A	1821	1/1	0.98	0.20	399,399,399,399	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	A	1643	1/1	0.98	0.13	102,102,102,102	0
22	MG	A	1634	1/1	0.98	0.10	73,73,73,73	0
22	MG	A	1826	1/1	0.98	0.21	447,447,447,447	0
22	MG	A	1645	1/1	0.98	0.13	132,132,132,132	0
22	MG	A	1706	1/1	0.98	0.10	151,151,151,151	0
22	MG	A	1610	1/1	0.98	0.11	110,110,110,110	0
22	MG	A	1690	1/1	0.98	0.07	160,160,160,160	0
22	MG	A	1866	1/1	0.98	0.18	149,149,149,149	0
22	MG	A	1831	1/1	0.98	0.08	191,191,191,191	0
22	MG	A	1662	1/1	0.98	0.08	144,144,144,144	0
22	MG	A	1675	1/1	0.98	0.15	275,275,275,275	0
22	MG	A	1834	1/1	0.98	0.18	232,232,232,232	0
22	MG	A	1611	1/1	0.98	0.04	182,182,182,182	0
22	MG	C	302	1/1	0.98	0.07	163,163,163,163	0
22	MG	A	1712	1/1	0.98	0.23	103,103,103,103	0
22	MG	A	1802	1/1	0.98	0.10	137,137,137,137	0
22	MG	A	1839	1/1	0.98	0.34	318,318,318,318	0
22	MG	A	1637	1/1	0.98	0.06	329,329,329,329	0
22	MG	A	1649	1/1	0.98	0.11	145,145,145,145	0
22	MG	A	1715	1/1	0.98	0.07	148,148,148,148	0
22	MG	A	1844	1/1	0.98	0.15	276,276,276,276	0
22	MG	A	1806	1/1	0.98	0.21	408,408,408,408	0
22	MG	A	1738	1/1	0.98	0.34	102,102,102,102	0
22	MG	A	1808	1/1	0.98	0.08	278,278,278,278	0
22	MG	A	1809	1/1	0.98	0.08	330,330,330,330	0
22	MG	A	1638	1/1	0.98	0.08	124,124,124,124	0
22	MG	A	1624	1/1	0.98	0.24	68,68,68,68	0
22	MG	A	1718	1/1	0.98	0.08	96,96,96,96	0
22	MG	A	1815	1/1	0.98	0.06	197,197,197,197	0
22	MG	A	1606	1/1	0.98	0.07	114,114,114,114	0
22	MG	A	1699	1/1	0.98	0.07	117,117,117,117	0
22	MG	A	1683	1/1	0.98	0.12	237,237,237,237	0
22	MG	A	1632	1/1	0.99	0.08	231,231,231,231	0
22	MG	A	1822	1/1	0.99	0.33	333,333,333,333	0
22	MG	A	1723	1/1	0.99	0.03	122,122,122,122	0
22	MG	A	1614	1/1	0.99	0.06	152,152,152,152	0
22	MG	A	1676	1/1	0.99	0.12	136,136,136,136	0
22	MG	A	1615	1/1	0.99	0.05	86,86,86,86	0
22	MG	A	1740	1/1	0.99	0.11	107,107,107,107	0
22	MG	A	1812	1/1	0.99	0.12	365,365,365,365	0
22	MG	A	1625	1/1	0.99	0.31	214,214,214,214	0
22	MG	A	1658	1/1	0.99	0.08	123,123,123,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	A	1642	1/1	0.99	0.12	176,176,176,176	0
22	MG	A	1660	1/1	0.99	0.04	129,129,129,129	0
22	MG	A	1630	1/1	0.99	0.09	129,129,129,129	0
22	MG	A	1651	1/1	0.99	0.08	173,173,173,173	0
22	MG	A	1684	1/1	0.99	0.17	128,128,128,128	0
22	MG	A	1837	1/1	0.99	0.17	226,226,226,226	0
23	ZN	D	301	1/1	0.99	0.20	127,127,127,127	0
22	MG	A	1622	1/1	0.99	0.05	75,75,75,75	0
22	MG	A	1810	1/1	1.00	0.02	122,122,122,122	0
22	MG	A	1657	1/1	1.00	0.06	124,124,124,124	0
22	MG	A	1842	1/1	1.00	0.23	244,244,244,244	0
22	MG	A	1824	1/1	1.00	0.29	435,435,435,435	0

6.5 Other polymers [i](#)

There are no such residues in this entry.