



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:17 PM UTC

PDB ID : 4JI7 / pdb_00004ji7
Title : Crystal Structure of 30S ribosomal subunit from *Thermus thermophilus*
Authors : Demirci, H.; Wang, L.; Murphy IV, F.; Murphy, E.; Carr, J.; Blanchard, S.;
Jogl, G.; Dahlberg, A.E.; Gregory, S.T.
Deposited on : 2013-03-05
Resolution : 3.50 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

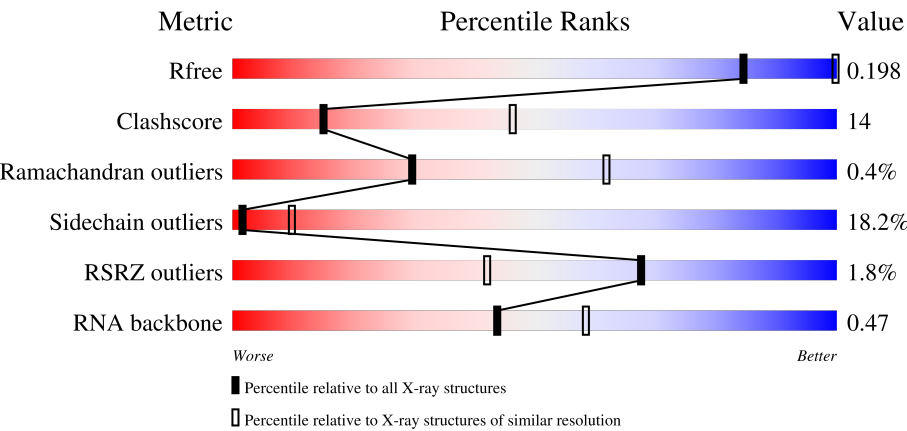
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)
RNA backbone	3983	1010 (3.98-3.02)

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	50%39%10% 3%
2	B	256	51%32%7%9% 3%
3	C	239	44%30%12%14%
4	D	209	54%35%9% 5%

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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	1695	-	-	-	X
22	MG	A	1707	-	-	-	X

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 53810 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	1514	Total	C	N	O	P	0	6	0
			32687	14559	6046	10562	1520			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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
			977	617	196	163	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	94	TRP	PRO	conflict	UNP F6DEQ7

- Molecule 13 is a protein called RIBOSOMAL PROTEIN S13.

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

- Molecule 14 is a protein called RIBOSOMAL PROTEIN S14.

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

- Molecule 15 is a protein called RIBOSOMAL PROTEIN S15.

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

- Molecule 16 is a protein called RIBOSOMAL PROTEIN S16.

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

- Molecule 17 is a protein called RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 18 is a protein called RIBOSOMAL PROTEIN S18.

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

- Molecule 19 is a protein called RIBOSOMAL PROTEIN S19.

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

- Molecule 20 is a protein called RIBOSOMAL PROTEIN S20.

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

- Molecule 21 is a protein called RIBOSOMAL PROTEIN THX.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	418	Total	Mg	0	0
			418	418		
22	B	3	Total	Mg	0	0
			3	3		
22	C	4	Total	Mg	0	0
			4	4		
22	D	6	Total	Mg	0	0
			6	6		
22	E	6	Total	Mg	0	0
			6	6		
22	F	1	Total	Mg	0	0
			1	1		
22	H	1	Total	Mg	0	0
			1	1		
22	K	1	Total	Mg	0	0
			1	1		
22	L	1	Total	Mg	0	0
			1	1		
22	N	1	Total	Mg	0	0
			1	1		
22	O	1	Total	Mg	0	0
			1	1		
22	P	4	Total	Mg	0	0
			4	4		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	Q	3	Total 3	Mg 3	0	0
22	S	1	Total 1	Mg 1	0	0

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

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

- Molecule 24 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	A	1483	Total 1483	O 1483	0	0
24	C	15	Total 15	O 15	0	0
24	D	26	Total 26	O 26	0	0
24	E	21	Total 21	O 21	0	0
24	F	6	Total 6	O 6	0	0
24	H	3	Total 3	O 3	0	0
24	K	1	Total 1	O 1	0	0
24	L	7	Total 7	O 7	0	0
24	M	2	Total 2	O 2	0	0
24	N	1	Total 1	O 1	0	0
24	O	2	Total 2	O 2	0	0
24	P	2	Total 2	O 2	0	0
24	Q	7	Total 7	O 7	0	0

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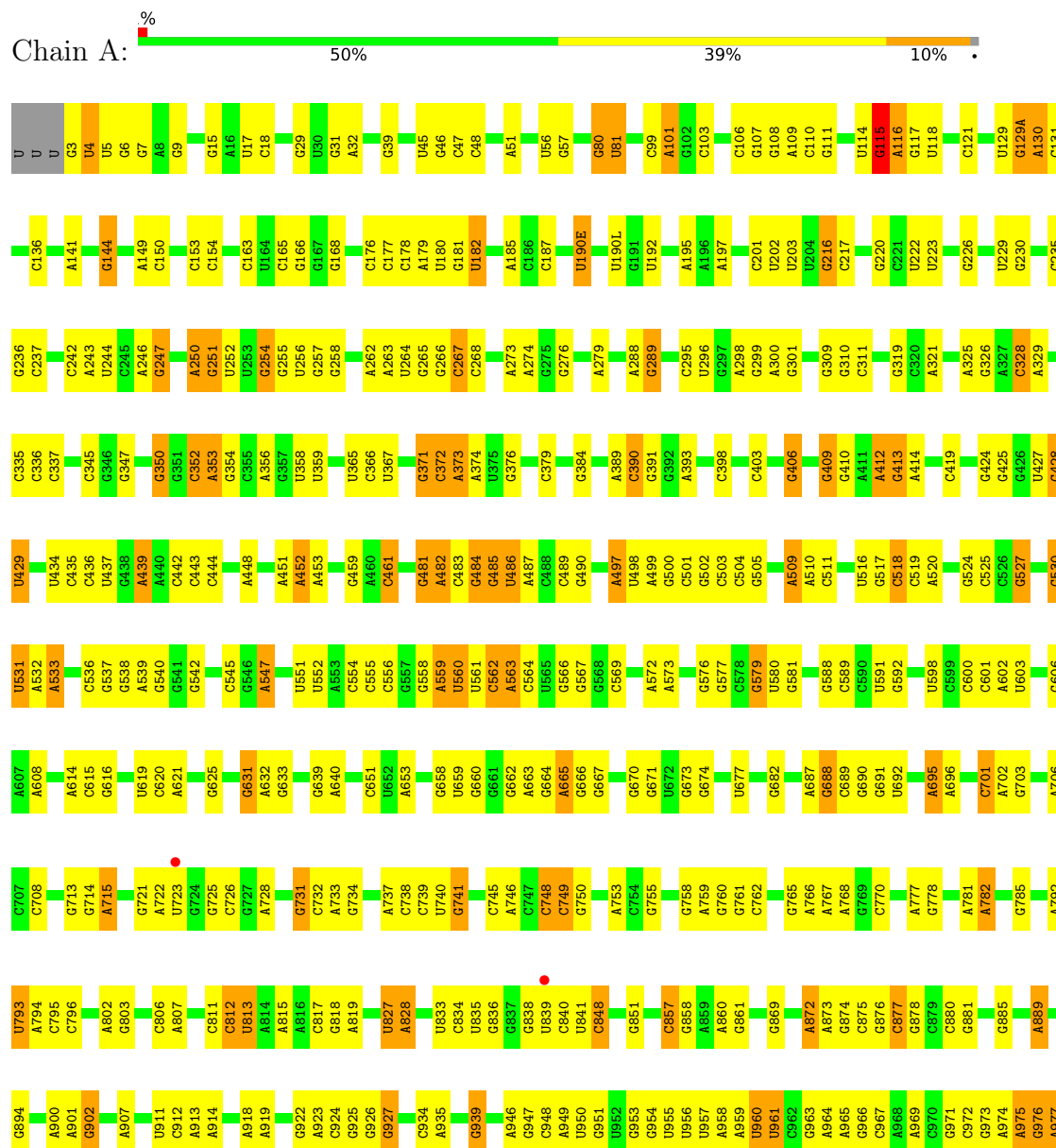
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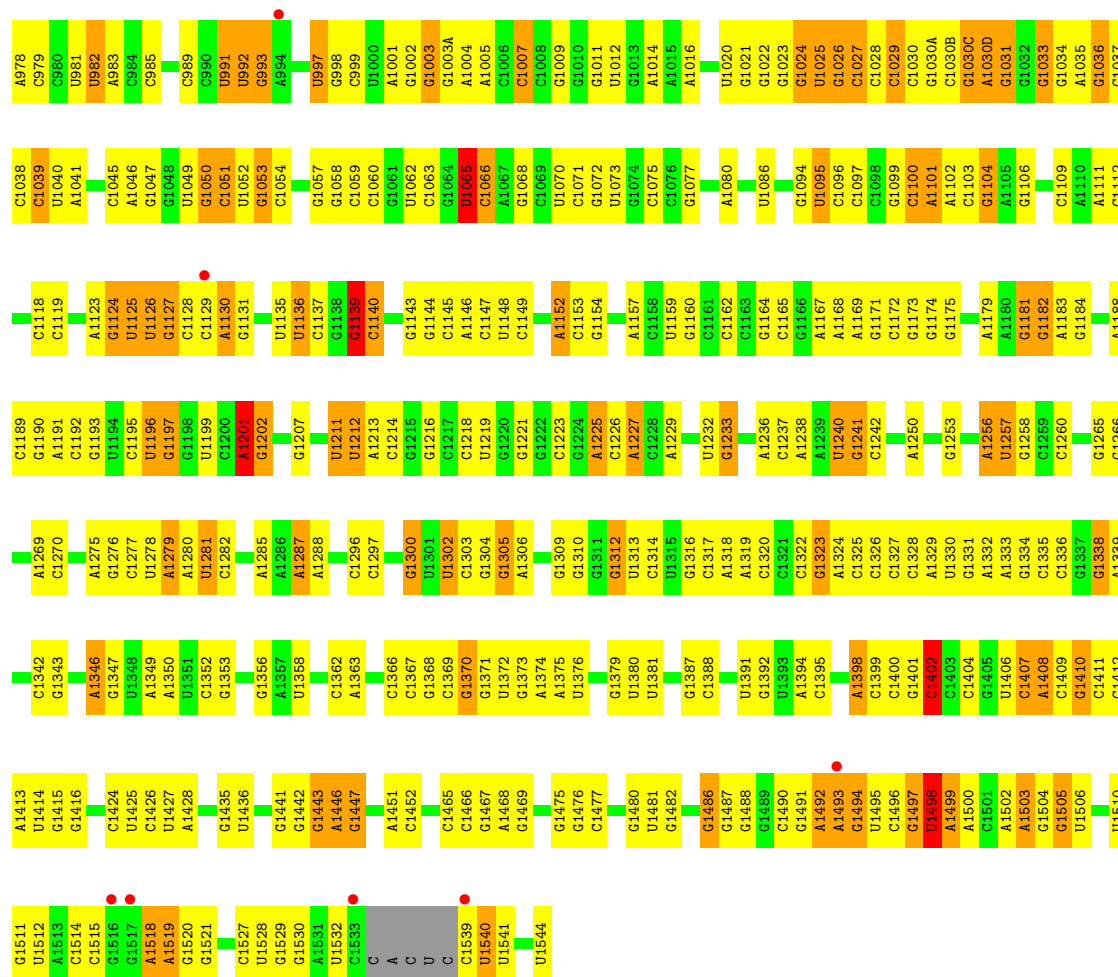
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	T	1	Total	O	0	0
			1	1		

3 Residue-property plots

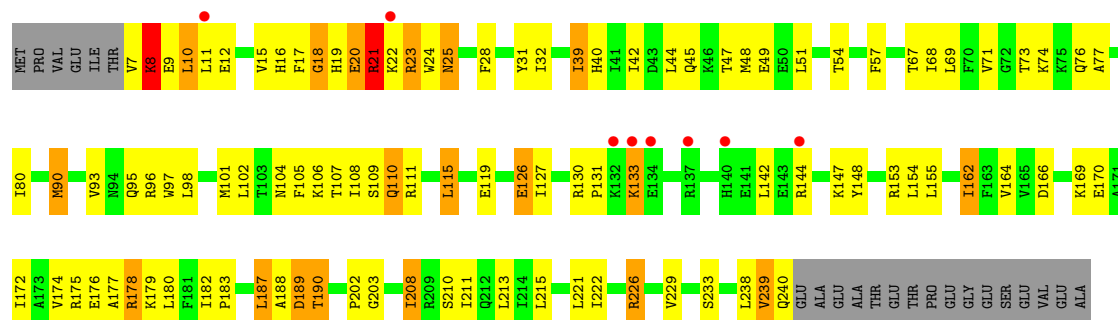
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: 16S rRNA

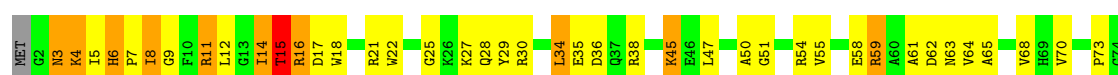


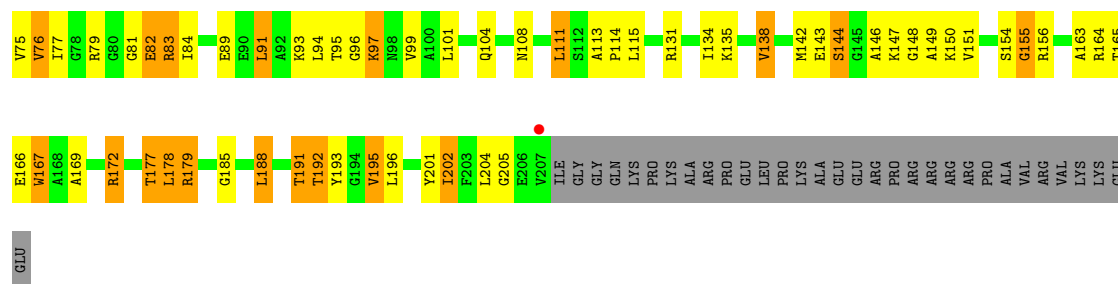


• Molecule 2: RIBOSOMAL PROTEIN S2

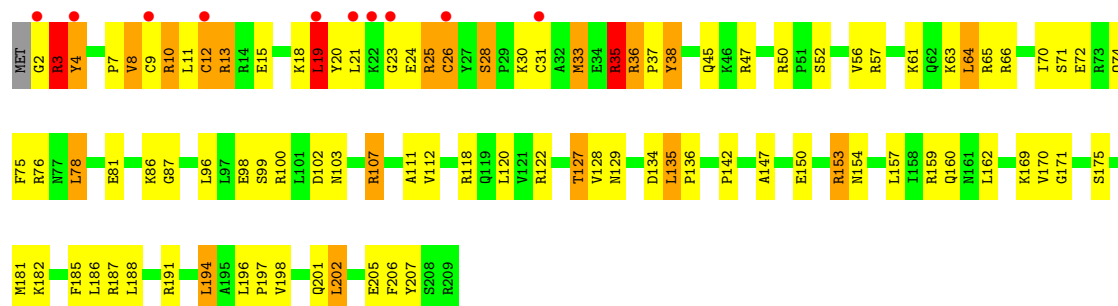


• Molecule 3: RIBOSOMAL PROTEIN S3

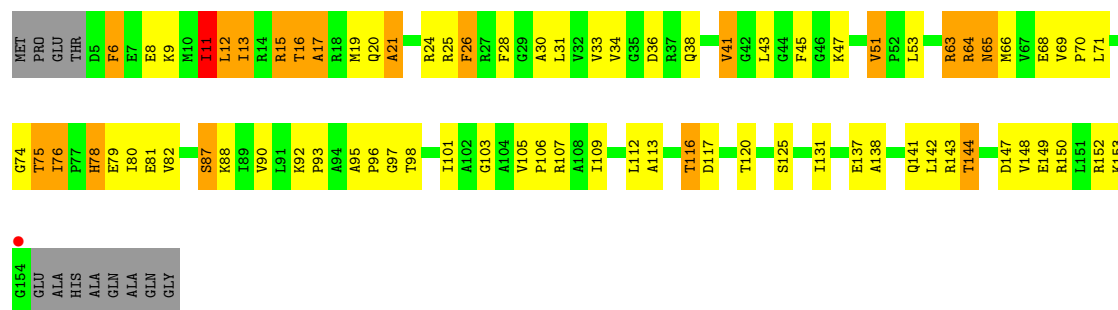
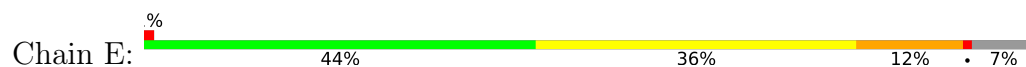




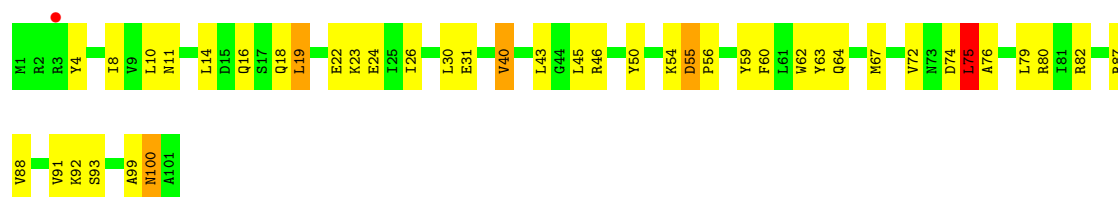
• Molecule 4: RIBOSOMAL PROTEIN S4



• Molecule 5: RIBOSOMAL PROTEIN S5

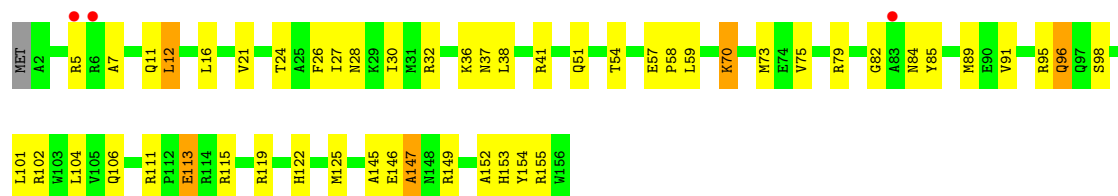


• Molecule 6: RIBOSOMAL PROTEIN S6

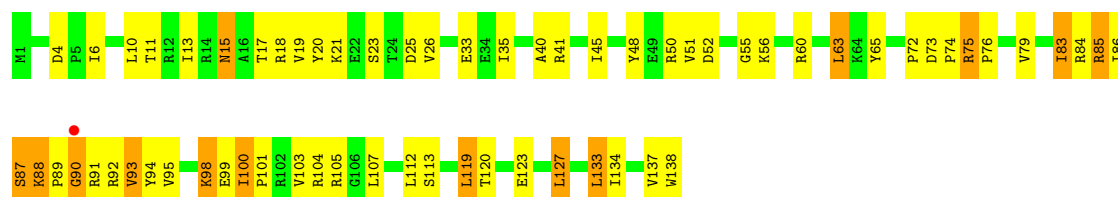


• Molecule 7: RIBOSOMAL PROTEIN S7

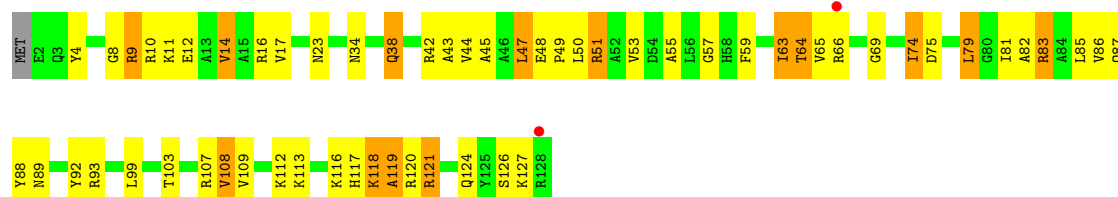




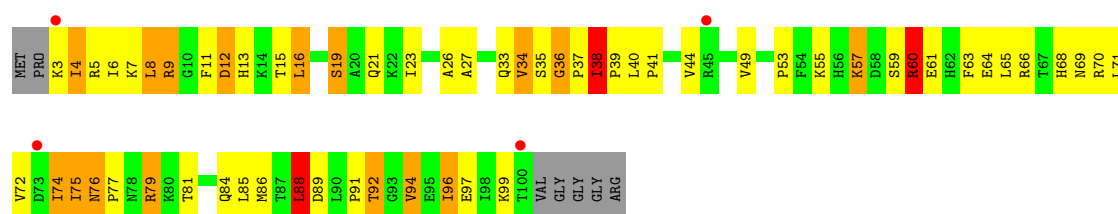
• Molecule 8: RIBOSOMAL PROTEIN S8



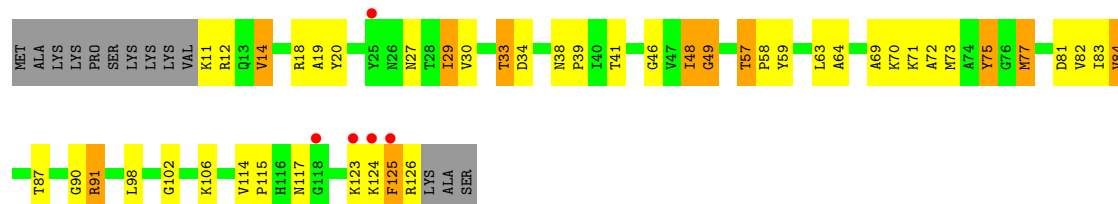
• Molecule 9: RIBOSOMAL PROTEIN S9



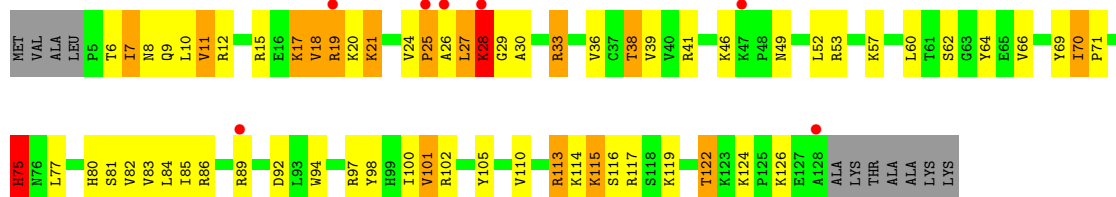
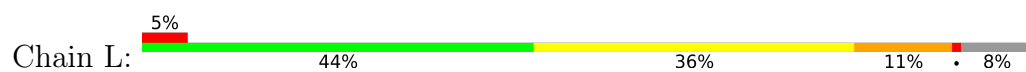
• Molecule 10: RIBOSOMAL PROTEIN S10



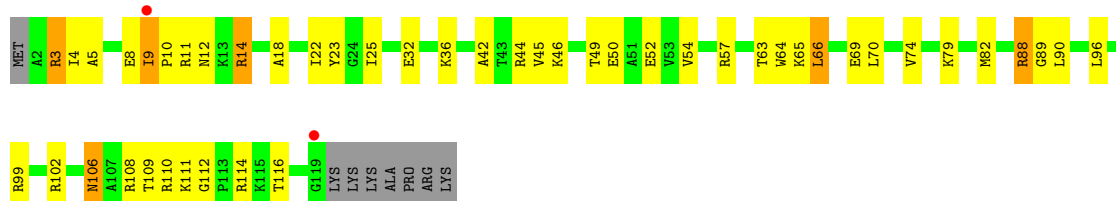
• Molecule 11: RIBOSOMAL PROTEIN S11



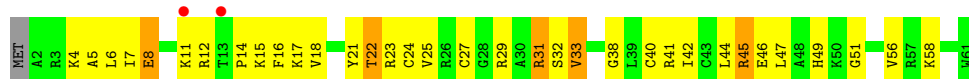
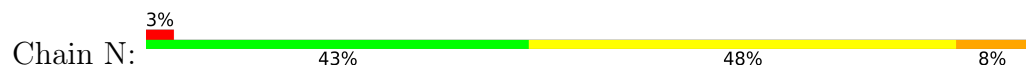
• Molecule 12: RIBOSOMAL PROTEIN S12



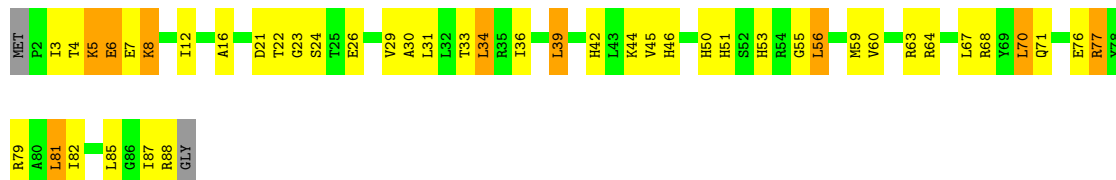
• Molecule 13: RIBOSOMAL PROTEIN S13



• Molecule 14: RIBOSOMAL PROTEIN S14



• Molecule 15: RIBOSOMAL PROTEIN S15

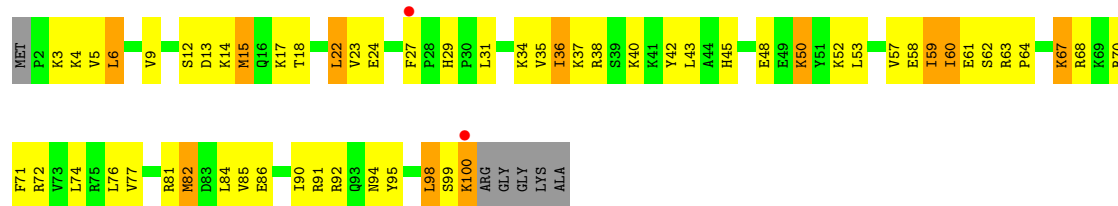


• Molecule 16: RIBOSOMAL PROTEIN S16

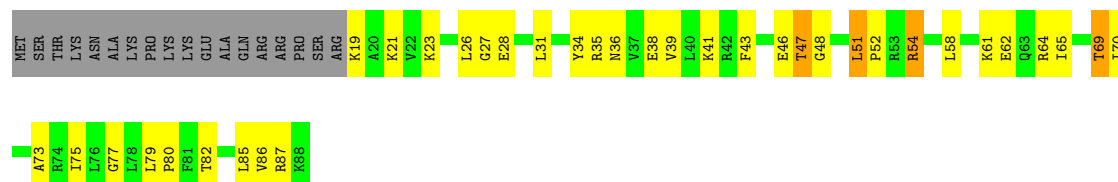


• Molecule 17: RIBOSOMAL PROTEIN S17

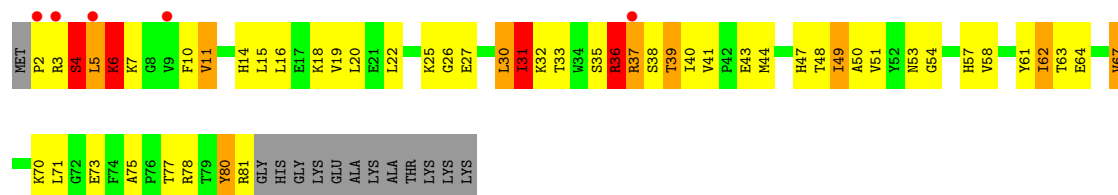




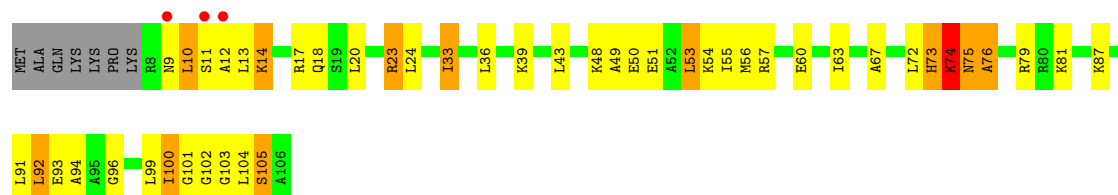
• Molecule 18: RIBOSOMAL PROTEIN S18



• 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	397.81Å 397.81Å 214.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.84 – 3.50 49.84 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.84-3.50) 99.7 (49.84-3.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 3.48Å)	Xtriage
Refinement program	PHENIX dev_1119	Depositor
R, R_{free}	0.158 , 0.201 0.159 , 0.198	Depositor DCC
R_{free} test set	10715 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	123.2	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 116.6	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	53810	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% 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, UR3, PSU, MG, 2MG, 7MG, M2G, 4OC, MA6, 5MC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.42	0/36187	0.63	10/56471 (0.0%)
2	B	0.70	0/1935	1.17	12/2609 (0.5%)
3	C	0.73	0/1636	1.16	7/2205 (0.3%)
4	D	0.69	0/1733	1.16	10/2318 (0.4%)
5	E	0.98	0/1162	1.26	8/1564 (0.5%)
6	F	0.70	0/856	1.15	3/1154 (0.3%)
7	G	0.57	0/1276	1.05	5/1709 (0.3%)
8	H	0.79	0/1136	1.26	12/1527 (0.8%)
9	I	0.56	0/1029	1.02	3/1379 (0.2%)
10	J	0.73	0/805	1.28	9/1082 (0.8%)
11	K	0.68	1/879 (0.1%)	1.16	8/1187 (0.7%)
12	L	0.86	2/994 (0.2%)	1.43	15/1331 (1.1%)
13	M	0.60	0/947	1.04	5/1270 (0.4%)
14	N	0.63	0/501	1.10	2/664 (0.3%)
15	O	0.72	0/740	1.04	1/987 (0.1%)
16	P	0.73	0/716	1.20	6/963 (0.6%)
17	Q	0.77	0/836	1.28	7/1117 (0.6%)
18	R	0.70	0/579	1.07	1/768 (0.1%)
19	S	0.64	0/661	1.34	12/890 (1.3%)
20	T	0.72	0/765	1.22	7/1007 (0.7%)
21	U	0.50	0/212	0.99	2/277 (0.7%)
All	All	0.54	3/55585 (0.0%)	0.84	145/82479 (0.2%)

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

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

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Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	2
8	H	0	1
10	J	0	2
20	T	0	2
All	All	0	11

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	25	PRO	CA-C	6.17	1.60	1.53
11	K	48	ILE	CA-CB	-5.46	1.48	1.54
12	L	36	VAL	CA-CB	-5.01	1.48	1.54

All (145) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	26	CYS	N-CA-C	-10.93	99.95	113.28
16	P	51	VAL	N-CA-C	10.66	120.73	111.56
12	L	26	ALA	N-CA-C	-10.24	100.97	113.15
3	C	179	ARG	N-CA-C	-10.12	89.24	110.80
8	H	75	ARG	CA-C-N	10.11	130.17	119.76
8	H	75	ARG	C-N-CA	10.11	130.17	119.76
20	T	74	LYS	CB-CA-C	-9.26	104.77	115.79
10	J	60	ARG	N-CA-C	9.08	122.05	110.24
12	L	115	LYS	CA-C-N	-9.02	109.42	122.77
12	L	115	LYS	C-N-CA	-9.02	109.42	122.77
2	B	8	LYS	N-CA-C	8.48	119.14	108.45
12	L	119	LYS	N-CA-C	-8.38	98.68	110.50
19	S	80	TYR	N-CA-C	8.37	122.05	110.24
3	C	25	GLY	N-CA-C	-8.20	99.13	111.10
7	G	147	ALA	N-CA-C	-8.16	101.94	112.23
19	S	4	SER	N-CA-C	8.15	121.89	107.80
8	H	73	ASP	CA-C-N	8.06	127.72	119.82
8	H	73	ASP	C-N-CA	8.06	127.72	119.82
19	S	73	GLU	N-CA-C	-7.91	103.52	113.01
5	E	41	VAL	CB-CA-C	-7.87	98.59	110.55
3	C	4	LYS	N-CA-C	7.63	127.05	110.80
9	I	23	ASN	N-CA-C	7.61	122.28	112.92
4	D	12	CYS	N-CA-C	-7.42	102.21	111.11
10	J	59	SER	N-CA-C	7.33	121.93	112.92
4	D	33	MET	N-CA-C	-7.32	104.32	113.18
10	J	55	LYS	N-CA-C	7.32	118.83	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	S	54	GLY	N-CA-C	-7.21	106.11	114.69
5	E	80	ILE	N-CA-C	7.12	120.10	108.99
11	K	14	VAL	N-CA-C	7.08	118.95	112.29
20	T	94	ALA	N-CA-C	-6.93	95.80	107.80
12	L	18	VAL	N-CA-C	6.91	117.85	108.17
6	F	55	ASP	CA-C-N	6.89	126.52	119.56
6	F	55	ASP	C-N-CA	6.89	126.52	119.56
5	E	6	PHE	N-CA-C	6.84	120.05	108.90
17	Q	60	ILE	N-CA-C	6.78	118.49	108.45
5	E	17	ALA	N-CA-C	6.77	119.69	110.55
19	S	31	ILE	N-CA-C	-6.73	95.35	109.34
19	S	30	LEU	CB-CA-C	-6.69	107.83	115.79
4	D	171	GLY	CA-C-N	6.68	126.82	119.87
4	D	171	GLY	C-N-CA	6.68	126.82	119.87
20	T	76	ALA	N-CA-C	-6.66	104.02	111.28
19	S	36	ARG	N-CA-C	-6.65	104.92	113.16
11	K	48	ILE	CB-CA-C	-6.44	102.95	111.13
11	K	102	GLY	N-CA-C	-6.43	107.04	114.69
5	E	21	ALA	N-CA-C	-6.38	100.86	110.24
4	D	35	ARG	N-CA-C	6.33	120.25	111.90
21	U	22	ARG	CA-C-N	6.32	126.29	119.78
21	U	22	ARG	C-N-CA	6.32	126.29	119.78
3	C	155	GLY	N-CA-C	6.28	120.66	112.25
8	H	84	ARG	N-CA-C	6.26	118.93	109.23
9	I	57	GLY	N-CA-C	-6.23	105.92	114.64
4	D	4	TYR	N-CA-C	6.14	119.27	110.24
5	E	78	HIS	CB-CA-C	-6.13	99.48	113.33
1	A	1139	G	C2'-C3'-O3'	6.11	118.67	109.50
2	B	23	ARG	N-CA-C	-6.07	97.87	110.80
12	L	17	LYS	CA-C-N	-6.02	115.72	123.19
12	L	17	LYS	C-N-CA	-6.02	115.72	123.19
17	Q	67	LYS	N-CA-C	-6.01	102.18	110.35
20	T	92	LEU	CA-C-N	-5.99	113.91	122.77
20	T	92	LEU	C-N-CA	-5.99	113.91	122.77
13	M	112	GLY	CA-C-N	5.97	127.30	119.84
13	M	112	GLY	C-N-CA	5.97	127.30	119.84
8	H	50	ARG	N-CA-C	-5.97	100.77	110.20
2	B	90	MET	CA-C-N	5.91	126.11	120.31
2	B	90	MET	C-N-CA	5.91	126.11	120.31
11	K	125	PHE	N-CA-C	5.90	120.18	112.92
12	L	70	ILE	CA-C-N	5.89	125.86	120.03
12	L	70	ILE	C-N-CA	5.89	125.86	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Q	82	MET	N-CA-C	-5.88	105.76	113.17
7	G	70	LYS	CA-C-N	5.88	126.08	119.90
7	G	70	LYS	C-N-CA	5.88	126.08	119.90
11	K	57	THR	CA-C-N	5.88	125.08	118.97
11	K	57	THR	C-N-CA	5.88	125.08	118.97
1	A	328	C	P-O3'-C3'	5.86	129.00	120.20
19	S	6	LYS	CB-CA-C	-5.86	109.26	117.23
10	J	89	ASP	N-CA-C	5.86	117.84	108.41
8	H	100	ILE	CA-C-N	5.85	125.86	119.89
8	H	100	ILE	C-N-CA	5.85	125.86	119.89
4	D	28	SER	CA-C-N	-5.84	112.54	119.84
4	D	28	SER	C-N-CA	-5.84	112.54	119.84
5	E	75	THR	N-CA-C	5.84	118.76	109.65
16	P	64	ALA	N-CA-C	-5.83	102.28	110.50
6	F	75	LEU	N-CA-C	-5.80	104.87	111.07
16	P	9	PHE	N-CA-C	5.80	120.36	112.88
2	B	187	LEU	N-CA-C	-5.78	101.10	109.59
2	B	18	GLY	N-CA-C	5.72	120.70	112.81
1	A	509	A	C2'-C3'-O3'	5.68	122.23	113.70
17	Q	29	HIS	CA-C-N	5.65	125.32	119.56
17	Q	29	HIS	C-N-CA	5.65	125.32	119.56
19	S	6	LYS	N-CA-C	5.64	118.09	108.67
1	A	1498	UR3	P-O3'-C3'	5.63	126.46	119.70
20	T	9	ASN	N-CA-C	5.61	117.47	110.91
2	B	21	ARG	N-CA-C	5.61	122.74	110.80
1	A	1201	A	P-O3'-C3'	5.60	128.60	120.20
7	G	84	ASN	N-CA-C	5.59	118.12	110.24
1	A	1065	U	C2'-C3'-O3'	5.58	117.86	109.50
8	H	103	VAL	N-CA-C	5.57	115.90	108.11
7	G	89	MET	N-CA-C	5.53	117.25	108.79
12	L	49	ASN	N-CA-C	5.51	117.89	109.95
1	A	812	C	C2'-C3'-O3'	5.51	117.77	109.50
12	L	38	THR	N-CA-C	-5.50	104.75	112.12
5	E	11	ILE	N-CA-C	5.48	118.78	111.44
10	J	4	ILE	N-CA-C	5.44	116.22	107.73
11	K	49	GLY	N-CA-C	5.43	120.49	113.27
12	L	80	HIS	N-CA-C	5.40	119.97	113.17
3	C	6	HIS	CA-C-N	5.40	124.91	119.19
3	C	6	HIS	C-N-CA	5.40	124.91	119.19
4	D	19	LEU	N-CA-C	-5.39	100.92	109.76
19	S	5	LEU	N-CA-C	5.38	120.50	113.30
20	T	101	GLY	N-CA-C	-5.34	107.61	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	190	THR	N-CA-C	5.33	118.89	112.38
17	Q	99	SER	N-CA-C	5.32	122.14	110.80
1	A	115	G	C2'-C3'-O3'	5.32	117.47	109.50
12	L	27	LEU	CB-CA-C	-5.32	109.46	115.79
12	L	105	TYR	CB-CA-C	-5.31	110.47	116.63
10	J	36	GLY	CA-C-N	5.30	126.46	119.84
10	J	36	GLY	C-N-CA	5.30	126.46	119.84
10	J	38	ILE	CB-CA-C	-5.27	105.07	110.71
13	M	89	GLY	N-CA-C	-5.26	106.40	112.50
17	Q	12	SER	N-CA-C	5.26	116.96	108.34
2	B	233	SER	CA-C-N	5.22	124.73	119.19
2	B	233	SER	C-N-CA	5.22	124.73	119.19
3	C	28	GLN	N-CA-C	5.22	119.80	113.38
9	I	59	PHE	N-CA-C	5.20	117.64	108.75
18	R	85	LEU	N-CA-C	5.15	116.80	108.41
13	M	5	ALA	N-CA-C	-5.14	103.26	110.35
1	A	1201	A	C4'-C3'-O3'	5.13	117.09	109.40
8	H	88	LYS	CA-C-N	-5.11	114.65	119.76
8	H	88	LYS	C-N-CA	-5.11	114.65	119.76
11	K	91	ARG	N-CA-C	-5.10	104.77	111.96
19	S	27	GLU	N-CA-C	5.10	117.82	110.28
12	L	75	HIS	N-CA-C	5.09	116.99	108.99
13	M	25	ILE	N-CA-C	5.09	115.19	107.75
2	B	25	ASN	N-CA-C	-5.08	98.59	109.81
1	A	1139	G	P-O3'-C3'	5.07	127.81	120.20
10	J	55	LYS	CB-CA-C	-5.07	109.24	116.34
2	B	174	VAL	CB-CA-C	-5.05	105.23	111.70
16	P	5	ARG	N-CA-C	5.04	115.70	108.74
14	N	31	ARG	CA-C-N	-5.03	115.01	122.41
14	N	31	ARG	C-N-CA	-5.03	115.01	122.41
15	O	68	ARG	N-CA-C	-5.03	105.69	111.07
16	P	45	THR	CA-C-N	5.03	124.47	119.24
16	P	45	THR	C-N-CA	5.03	124.47	119.24
19	S	67	VAL	N-CA-C	5.02	115.17	110.30
8	H	35	ILE	CB-CA-C	-5.01	105.46	111.88

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	11	LEU	Peptide
2	B	8	LYS	Peptide

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Mol	Chain	Res	Type	Group
2	B	9	GLU	Peptide
3	C	166	GLU	Peptide
4	D	3	ARG	Peptide
4	D	35	ARG	Peptide
8	H	90	GLY	Peptide
10	J	12	ASP	Peptide
10	J	88	LEU	Peptide
20	T	12	ALA	Peptide
20	T	93	GLU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32687	0	16528	559	0
2	B	1900	0	1951	73	0
3	C	1612	0	1677	66	0
4	D	1703	0	1763	69	0
5	E	1146	0	1207	57	0
6	F	843	0	857	26	0
7	G	1257	0	1296	30	0
8	H	1116	0	1177	46	0
9	I	1010	0	1037	46	0
10	J	792	0	835	46	0
11	K	864	0	881	32	0
12	L	977	0	1060	41	0
13	M	937	0	995	26	0
14	N	492	0	529	29	0
15	O	729	0	768	37	0
16	P	700	0	720	17	0
17	Q	823	0	891	37	0
18	R	574	0	644	29	0
19	S	647	0	673	40	0
20	T	763	0	861	36	0
21	U	208	0	221	11	0
22	A	418	0	0	0	0
22	B	3	0	0	0	0
22	C	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	D	6	0	0	0	0
22	E	6	0	0	0	0
22	F	1	0	0	0	0
22	H	1	0	0	0	0
22	K	1	0	0	0	0
22	L	1	0	0	0	0
22	N	1	0	0	0	0
22	O	1	0	0	0	0
22	P	4	0	0	0	0
22	Q	3	0	0	0	0
22	S	1	0	0	0	0
23	D	1	0	0	0	0
23	N	1	0	0	0	0
24	A	1483	0	0	49	0
24	C	15	0	0	0	0
24	D	26	0	0	0	0
24	E	21	0	0	1	0
24	F	6	0	0	0	0
24	H	3	0	0	1	0
24	K	1	0	0	0	0
24	L	7	0	0	0	0
24	M	2	0	0	1	0
24	N	1	0	0	0	0
24	O	2	0	0	0	0
24	P	2	0	0	0	0
24	Q	7	0	0	2	0
24	T	1	0	0	0	0
All	All	53810	0	36571	1200	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (1200) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:G:HO2'	1:A:482:A:H8	1.13	0.90
3:C:142:MET:HE1	3:C:148:GLY:HA2	1.52	0.90
14:N:21:TYR:HE2	14:N:23:ARG:HE	1.20	0.90
15:O:64:ARG:HG3	15:O:88:ARG:HH22	1.36	0.89
1:A:190(L):U:H3	20:T:105:SER:HG	1.21	0.88
1:A:372:C:O2'	24:A:3555:HOH:O	1.93	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.58	0.86
2:B:178:ARG:HH21	8:H:74:PRO:HG3	1.38	0.85
1:A:745:C:N4	24:A:2511:HOH:O	2.06	0.85
1:A:413:G:H8	1:A:428:G:H21	1.22	0.84
5:E:12:LEU:HD13	5:E:31:LEU:HB2	1.59	0.84
1:A:975:A:H5'	1:A:975:A:H8	1.40	0.84
20:T:57:ARG:HH12	20:T:100:ILE:HD12	1.44	0.83
2:B:16:HIS:HB3	2:B:210:SER:HB2	1.58	0.83
1:A:1128:C:H5'	9:I:16:ARG:HH22	1.42	0.83
4:D:11:LEU:HD13	4:D:66:ARG:HD2	1.57	0.82
3:C:35:GLU:HG3	3:C:95:THR:HG21	1.61	0.82
10:J:57:LYS:HD3	10:J:60:ARG:HH12	1.43	0.82
1:A:1491:G:H3'	1:A:1492:A:H5''	1.61	0.82
10:J:38:ILE:HG13	10:J:71:LEU:HB3	1.61	0.81
1:A:677:U:H3	1:A:713:G:H22	1.27	0.80
8:H:4:ASP:OD2	8:H:85:ARG:NH1	2.14	0.80
12:L:24:VAL:HG13	12:L:98:TYR:HE2	1.43	0.80
3:C:91:LEU:HB3	3:C:99:VAL:HG11	1.62	0.80
1:A:975:A:H4'	1:A:976:G:H5''	1.64	0.79
1:A:376:G:H5''	16:P:5:ARG:HD2	1.64	0.79
3:C:14:ILE:HB	3:C:15:THR:HG23	1.65	0.79
1:A:337:C:N4	24:A:2760:HOH:O	2.17	0.78
7:G:122:HIS:HA	7:G:125:MET:HE2	1.66	0.78
1:A:451:A:O2'	24:A:2851:HOH:O	2.02	0.77
8:H:10:LEU:HD22	8:H:83:ILE:HD11	1.66	0.77
4:D:25:ARG:HA	4:D:28:SER:HB3	1.67	0.77
11:K:57:THR:HG22	11:K:59:TYR:H	1.49	0.77
12:L:27:LEU:O	12:L:29:GLY:N	2.18	0.77
1:A:393:A:N6	24:A:2968:HOH:O	2.18	0.77
18:R:51:LEU:HD23	18:R:52:PRO:HD2	1.65	0.76
19:S:80:TYR:CE1	19:S:81:ARG:HD3	2.20	0.75
1:A:1047:G:H5''	14:N:4:LYS:HD3	1.69	0.75
1:A:279:A:OP2	17:Q:95:TYR:OH	2.00	0.75
20:T:100:ILE:HB	20:T:102:GLY:H	1.52	0.75
1:A:1100:C:N4	24:A:3186:HOH:O	2.19	0.74
8:H:17:THR:HG22	8:H:63:LEU:HG	1.70	0.74
1:A:542:G:OP1	4:D:10:ARG:NH2	2.20	0.73
11:K:18:ARG:HB2	11:K:33:THR:HG23	1.70	0.73
12:L:33:ARG:HD3	12:L:62:SER:HB3	1.68	0.73
19:S:50:ALA:HB1	19:S:57:HIS:HB3	1.69	0.73
9:I:45:ALA:HA	9:I:48:GLU:HG2	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:G:O2'	1:A:482:A:H8	1.71	0.73
1:A:1057:G:H5''	3:C:154:SER:HB2	1.70	0.72
8:H:83:ILE:HG13	8:H:137:VAL:HG22	1.72	0.72
12:L:28:LYS:HB3	12:L:30:ALA:HB2	1.71	0.72
18:R:46:GLU:N	18:R:46:GLU:OE2	2.21	0.72
1:A:530:G:H2'	1:A:530:G:N3	2.05	0.72
3:C:147:LYS:HD3	3:C:205:GLY:H	1.55	0.72
1:A:80:G:H2'	1:A:81:U:H5'	1.72	0.71
1:A:1427:U:H2'	1:A:1428:A:C8	2.26	0.71
1:A:1499:A:H1'	1:A:1520[A]:G:H5'	1.71	0.71
3:C:14:ILE:O	3:C:16:ARG:N	2.24	0.71
3:C:77:ILE:HG22	3:C:81:GLY:HA2	1.73	0.71
2:B:97:TRP:HH2	2:B:176:GLU:CD	1.99	0.71
5:E:81:GLU:OE1	5:E:88:LYS:NZ	2.20	0.71
14:N:8:GLU:HG2	14:N:11:LYS:HE3	1.71	0.71
1:A:673:G:H2'	1:A:674:G:C8	2.26	0.70
8:H:41:ARG:NH2	8:H:123:GLU:OE2	2.24	0.70
21:U:17:THR:O	21:U:22:ARG:NH1	2.24	0.70
1:A:1100:C:OP2	2:B:96:ARG:NH1	2.25	0.70
3:C:18:TRP:O	3:C:21:ARG:NH1	2.23	0.70
1:A:298:A:N6	24:A:2223:HOH:O	2.23	0.70
15:O:45:VAL:HG23	15:O:46:HIS:HD2	1.57	0.70
1:A:518:C:H2'	1:A:530:G:C8	2.26	0.70
1:A:1196:U:OP1	1:A:1197:G:H5''	1.91	0.70
4:D:4:TYR:OH	4:D:7:PRO:O	2.08	0.70
12:L:33:ARG:HB3	12:L:60:LEU:HD12	1.74	0.69
8:H:19:VAL:HG23	8:H:21:LYS:HG3	1.75	0.69
13:M:66:LEU:HA	13:M:70:LEU:HD12	1.73	0.69
1:A:1196:U:O2'	24:A:2229:HOH:O	2.09	0.69
3:C:58:GLU:H	3:C:65:ALA:HB3	1.56	0.69
1:A:975:A:H5'	1:A:975:A:C8	2.26	0.69
2:B:98:LEU:HD12	2:B:101:MET:HE3	1.74	0.68
1:A:1124:G:H4'	10:J:38:ILE:HD13	1.74	0.68
10:J:6:ILE:HB	10:J:72:VAL:HB	1.74	0.68
15:O:70:LEU:HD21	15:O:77:ARG:HB2	1.75	0.68
1:A:1195:C:H3'	1:A:1196:U:H5''	1.75	0.68
3:C:95:THR:HB	3:C:97:LYS:HG2	1.75	0.68
12:L:86:ARG:HB3	12:L:101:VAL:HG22	1.76	0.68
1:A:1443:G:H5''	1:A:1446:A:H5'	1.75	0.68
4:D:175:SER:HB3	4:D:186:LEU:HD21	1.76	0.68
17:Q:67:LYS:HA	17:Q:70:ARG:HH12	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:THR:HA	2:B:202:PRO:HG2	1.74	0.68
7:G:5:ARG:HG3	7:G:7:ALA:H	1.59	0.68
12:L:38:THR:HG22	12:L:39:VAL:HG23	1.74	0.68
5:E:116:THR:HG23	5:E:117:ASP:OD2	1.93	0.68
16:P:22:THR:HA	16:P:33:ILE:HG13	1.75	0.68
1:A:452:A:HO2'	1:A:453:A:H8	1.41	0.67
1:A:1367:C:H5'	10:J:60:ARG:HH21	1.57	0.67
1:A:1052:U:O2'	24:A:3216:HOH:O	2.01	0.67
10:J:53:PRO:HA	14:N:41:ARG:HH21	1.58	0.67
1:A:1502:A:H2	1:A:1505:G:H1	1.43	0.67
4:D:150:GLU:CD	4:D:150:GLU:H	2.01	0.67
9:I:8:GLY:HA2	9:I:79:LEU:HD13	1.77	0.67
1:A:983:A:O2'	1:A:1050:G:OP2	2.13	0.66
1:A:1281:U:H5'	1:A:1282:C:C5	2.30	0.66
3:C:6:HIS:CD2	14:N:49:HIS:HB3	2.30	0.66
14:N:5:ALA:O	14:N:8:GLU:HB3	1.95	0.66
2:B:42:ILE:HG13	2:B:203:GLY:HA2	1.76	0.66
6:F:14:LEU:HD22	6:F:18:GLN:HB3	1.77	0.66
1:A:972:C:H4'	10:J:57:LYS:HG2	1.76	0.66
1:A:1059:C:N4	24:A:2868:HOH:O	2.28	0.66
1:A:1391:U:H2'	1:A:1392:G:C8	2.31	0.66
5:E:64:ARG:O	5:E:65:ASN:ND2	2.28	0.65
1:A:250:A:H4'	1:A:251:G:O5'	1.96	0.65
1:A:1392:G:N2	1:A:1502:A:H8	1.94	0.65
19:S:36:ARG:NH2	19:S:75:ALA:O	2.29	0.65
5:E:20:GLN:HG2	5:E:25:ARG:HE	1.62	0.65
20:T:74:LYS:HB2	20:T:76:ALA:H	1.61	0.65
1:A:1128:C:O2'	1:A:1130:A:OP1	2.13	0.65
2:B:10:LEU:HA	2:B:48:MET:HE1	1.79	0.65
3:C:36:ASP:OD1	3:C:59:ARG:NH2	2.30	0.65
4:D:100:ARG:NH2	4:D:102:ASP:OD2	2.28	0.65
1:A:1001:A:H2'	1:A:1002:G:H8	1.62	0.65
1:A:1104:G:O5'	2:B:111:ARG:NH1	2.29	0.65
8:H:86:ILE:HG21	8:H:133:LEU:HD13	1.78	0.65
1:A:1515[B]:C:N4	1:A:1520[B]:G:O6	2.29	0.64
10:J:85:LEU:HA	10:J:88:LEU:HD11	1.79	0.64
1:A:410:G:OP1	4:D:30:LYS:NZ	2.30	0.64
4:D:111:ALA:HB2	4:D:120:LEU:HD12	1.79	0.64
15:O:56:LEU:HA	15:O:59:MET:HE2	1.79	0.64
8:H:119:LEU:HB3	8:H:123:GLU:HB3	1.79	0.64
1:A:1103:C:H5''	2:B:98:LEU:HD22	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1241:G:H2'	1:A:1242:C:C6	2.33	0.64
1:A:1392:G:H21	1:A:1502:A:H8	1.44	0.64
1:A:538:G:H5''	12:L:114:LYS:HB2	1.80	0.64
1:A:99:C:N4	24:A:2677:HOH:O	2.31	0.64
13:M:79:LYS:HA	13:M:82:MET:HE2	1.78	0.64
3:C:73:PRO:O	3:C:77:ILE:HG12	1.98	0.63
1:A:1415:G:H2'	1:A:1416:G:H8	1.61	0.63
3:C:50:ALA:HB2	3:C:75:VAL:HB	1.81	0.63
12:L:110:VAL:H	12:L:122:THR:HG22	1.63	0.63
2:B:16:HIS:ND1	2:B:17:PHE:O	2.29	0.63
16:P:74:LEU:HD13	16:P:79:VAL:HG21	1.80	0.63
19:S:10:PHE:O	19:S:39:THR:OG1	2.15	0.63
1:A:1327:C:OP2	21:U:12:LYS:NZ	2.31	0.63
2:B:126:GLU:O	2:B:130:ARG:NH2	2.32	0.63
17:Q:40:LYS:HE2	17:Q:42:TYR:CZ	2.33	0.63
1:A:15:G:H1'	5:E:19:MET:HE2	1.80	0.63
1:A:1125:U:H3'	24:A:3301:HOH:O	1.98	0.63
1:A:1226:C:H4'	1:A:1227:A:OP1	1.99	0.63
1:A:1007:C:N4	1:A:1023:G:O6	2.32	0.62
1:A:1030(C):G:N2	1:A:1030(D):A:N1	2.45	0.62
11:K:57:THR:HG22	11:K:59:TYR:N	2.13	0.62
21:U:6:ARG:HE	21:U:15:ARG:CZ	2.11	0.62
12:L:27:LEU:C	12:L:29:GLY:H	2.07	0.62
6:F:62:TRP:CH2	6:F:64:GLN:HB2	2.33	0.62
1:A:951:G:OP2	13:M:102:ARG:NH2	2.33	0.62
12:L:113:ARG:HH11	12:L:116:SER:H	1.46	0.62
5:E:15:ARG:HG3	5:E:15:ARG:HH11	1.63	0.62
1:A:598:U:H4'	8:H:94:TYR:CD1	2.35	0.62
1:A:1373:G:H5''	7:G:36:LYS:HD2	1.81	0.62
1:A:1305:G:OP2	21:U:2:GLY:N	2.33	0.62
2:B:20:GLU:HB3	2:B:190:THR:HB	1.82	0.62
8:H:51:VAL:HG22	8:H:52:ASP:H	1.65	0.62
7:G:70:LYS:HB3	7:G:96:GLN:HG2	1.82	0.61
4:D:66:ARG:HG3	4:D:66:ARG:HH11	1.63	0.61
1:A:1281:U:H5'	1:A:1282:C:H5	1.64	0.61
1:A:149:A:H2'	1:A:150:C:C6	2.36	0.61
7:G:85:TYR:HD1	7:G:154:TYR:HE1	1.49	0.61
8:H:11:THR:HG22	8:H:15:ASN:HD21	1.65	0.61
4:D:61:LYS:HD2	4:D:207:TYR:OH	2.01	0.61
5:E:11:ILE:HG22	5:E:31:LEU:HB3	1.82	0.61
10:J:8:LEU:HD22	10:J:96:ILE:HG22	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:51:GLY:O	3:C:115:LEU:HD21	2.01	0.61
1:A:1139:G:O2'	1:A:1140:C:OP2	2.16	0.61
5:E:78:HIS:HD2	5:E:142:LEU:HA	1.65	0.61
13:M:49:THR:HB	13:M:52:GLU:H	1.66	0.61
3:C:138:VAL:HG23	3:C:151:VAL:HG23	1.82	0.60
5:E:31:LEU:HD22	5:E:43:LEU:HD11	1.83	0.60
9:I:16:ARG:HB2	9:I:64:THR:HG22	1.84	0.60
2:B:172:ILE:HD12	2:B:172:ILE:H	1.65	0.60
5:E:64:ARG:CZ	5:E:65:ASN:HB3	2.31	0.60
4:D:194:LEU:H	4:D:194:LEU:HD22	1.66	0.60
7:G:16:LEU:HD13	9:I:44:VAL:HB	1.82	0.60
11:K:41:THR:HG21	11:K:71:LYS:HB3	1.84	0.60
19:S:40:ILE:HD13	19:S:62:ILE:HD13	1.82	0.60
1:A:1435:G:H2'	1:A:1436:U:C6	2.36	0.60
10:J:15:THR:O	10:J:19:SER:HB2	2.02	0.60
13:M:4:ILE:HG23	13:M:57:ARG:HA	1.84	0.60
16:P:34:GLU:OE1	16:P:55:ARG:NH1	2.30	0.60
3:C:76:VAL:O	3:C:83:ARG:HG2	2.02	0.60
13:M:23:TYR:CD2	13:M:70:LEU:HD13	2.37	0.60
21:U:6:ARG:HG2	21:U:15:ARG:HH11	1.66	0.60
1:A:1346:A:N6	1:A:1375:A:OP2	2.33	0.60
14:N:42:ILE:O	14:N:46:GLU:HG3	2.01	0.60
1:A:1366:C:O3'	10:J:60:ARG:NH2	2.35	0.59
1:A:1054:C:H3'	24:A:3211:HOH:O	2.02	0.59
2:B:32:ILE:HD11	2:B:190:THR:HG23	1.84	0.59
18:R:34:TYR:HB3	18:R:69:THR:HG22	1.83	0.59
1:A:976:G:H22	1:A:1362:C:H5''	1.67	0.59
1:A:1174:G:H2'	1:A:1175:G:H8	1.67	0.59
1:A:1241:G:H2'	1:A:1242:C:H6	1.67	0.59
20:T:67:ALA:O	20:T:73:HIS:ND1	2.35	0.59
20:T:33:ILE:HD13	20:T:63:ILE:HG12	1.84	0.59
1:A:948:C:H42	1:A:1233:G:H1	1.49	0.59
5:E:78:HIS:CD2	5:E:142:LEU:HA	2.37	0.59
6:F:26:ILE:HG21	6:F:63:TYR:HE2	1.68	0.59
1:A:3:G:H1	4:D:87:GLY:H	1.50	0.59
2:B:71:VAL:HG13	2:B:93:VAL:HB	1.83	0.59
1:A:667:G:H4'	15:O:51:HIS:ND1	2.17	0.59
1:A:1232:U:H5''	9:I:124:GLN:O	2.02	0.59
1:A:1497:G:H2'	1:A:1498:UR3:H5'	1.85	0.59
1:A:371:G:C2'	1:A:372:C:H5'	2.32	0.59
1:A:667:G:H4'	15:O:51:HIS:CE1	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:21:LYS:O	8:H:65:TYR:OH	2.20	0.59
19:S:18:LYS:HD3	19:S:31:ILE:HD11	1.85	0.59
1:A:547:A:OP2	4:D:2:GLY:N	2.36	0.58
1:A:1510:U:H2'	1:A:1511:G:C8	2.37	0.58
11:K:20:TYR:CZ	11:K:83:ILE:HD12	2.38	0.58
1:A:682:G:H1	1:A:708:C:H42	1.50	0.58
1:A:1277:C:HO2'	1:A:1279:A:H8	1.51	0.58
2:B:107:THR:O	2:B:110:GLN:HG3	2.03	0.58
7:G:102:ARG:O	7:G:106:GLN:HG3	2.03	0.58
1:A:243:A:C2	1:A:246:A:C8	2.91	0.58
1:A:1126:U:H4'	24:A:3272:HOH:O	2.03	0.58
1:A:1126:U:C5	1:A:1127:G:N2	2.72	0.58
1:A:1441:G:H4'	1:A:1442:G:C5	2.38	0.58
4:D:70:ILE:HG22	4:D:71:SER:O	2.03	0.58
12:L:25:PRO:C	12:L:27:LEU:H	2.07	0.58
12:L:84:LEU:HD23	12:L:101:VAL:HG21	1.84	0.58
1:A:589:C:N4	24:A:2443:HOH:O	2.31	0.58
1:A:1442:G:N7	1:A:1446:A:N6	2.52	0.58
12:L:24:VAL:HG13	12:L:98:TYR:CE2	2.32	0.58
2:B:17:PHE:HA	2:B:44:LEU:HD11	1.84	0.58
1:A:827:U:H5''	1:A:828:A:OP2	2.03	0.58
1:A:1033:G:O6	1:A:1034:G:N2	2.37	0.58
2:B:21:ARG:HA	2:B:39:ILE:HA	1.86	0.58
1:A:524:G:H2'	1:A:525:C:C6	2.39	0.58
1:A:560:U:H4'	1:A:561:U:H5''	1.86	0.58
4:D:8:VAL:O	4:D:11:LEU:N	2.33	0.58
1:A:185:A:N6	24:A:2739:HOH:O	2.36	0.58
1:A:371:G:O2'	1:A:372:C:H5'	2.03	0.58
1:A:1415:G:H2'	1:A:1416:G:C8	2.38	0.58
4:D:13:ARG:HG2	4:D:38:TYR:O	2.04	0.58
5:E:74:GLY:HA3	5:E:116:THR:HG22	1.85	0.58
5:E:17:ALA:HB2	5:E:26:PHE:CD2	2.38	0.57
10:J:63:PHE:HE2	14:N:58:LYS:HG2	1.69	0.57
13:M:3:ARG:HH12	13:M:9:ILE:HD11	1.69	0.57
7:G:26:PHE:HD1	7:G:101:LEU:HD22	1.68	0.57
15:O:26:GLU:HA	15:O:81:LEU:HD11	1.86	0.57
19:S:39:THR:HG23	19:S:70:LYS:HD2	1.86	0.57
3:C:6:HIS:ND1	3:C:7:PRO:HD2	2.18	0.57
4:D:65:ARG:HG3	4:D:75:PHE:CG	2.39	0.57
1:A:530:G:H4'	1:A:531:U:OP2	2.04	0.57
2:B:105:PHE:O	2:B:109:SER:OG	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:123:LYS:HA	11:K:126:ARG:HG2	1.85	0.57
20:T:10:LEU:HD23	20:T:13:LEU:H	1.69	0.57
1:A:869:G:N7	24:A:3468:HOH:O	2.33	0.57
1:A:1279:A:OP1	10:J:99:LYS:NZ	2.27	0.57
1:A:255:G:N2	24:A:3205:HOH:O	2.14	0.57
1:A:860:A:H2'	1:A:861:G:O4'	2.05	0.57
1:A:946:A:H2'	1:A:947:G:C8	2.39	0.57
3:C:22:TRP:NE1	3:C:59:ARG:HH21	2.02	0.57
1:A:141:A:H1'	1:A:182:U:O2	2.05	0.57
9:I:42:ARG:NH2	9:I:75:ASP:OD1	2.36	0.57
5:E:15:ARG:HH11	5:E:15:ARG:CG	2.18	0.57
1:A:235:C:H5'	17:Q:70:ARG:HG2	1.87	0.56
1:A:1179:A:OP2	9:I:93:ARG:NH2	2.38	0.56
3:C:155:GLY:HA3	3:C:163:ALA:HB1	1.87	0.56
10:J:40:LEU:HB2	10:J:69:ASN:HB2	1.86	0.56
8:H:41:ARG:HB3	8:H:41:ARG:NH1	2.20	0.56
1:A:1033:G:H2'	1:A:1034:G:O4'	2.04	0.56
8:H:113:SER:HB2	8:H:134:ILE:HD11	1.86	0.56
4:D:187:ARG:CZ	4:D:188:LEU:H	2.18	0.56
12:L:46:LYS:HE2	12:L:94:TRP:CE3	2.40	0.56
1:A:1112:C:N3	3:C:178:LEU:HD12	2.21	0.56
7:G:37:ASN:O	7:G:41:ARG:HG2	2.06	0.56
18:R:38:GLU:HA	18:R:41:LYS:HE2	1.88	0.56
1:A:296:U:O2'	1:A:556:C:O2	2.18	0.56
1:A:1004:A:N6	1:A:1037:C:H42	2.04	0.56
2:B:69:LEU:HD21	2:B:93:VAL:HG23	1.87	0.56
10:J:61:GLU:OE2	14:N:45:ARG:NH1	2.34	0.56
1:A:373:A:H1'	1:A:481:G:N3	2.20	0.56
1:A:390:C:H2'	1:A:391:G:C8	2.41	0.56
1:A:975:A:H4'	1:A:976:G:C5'	2.35	0.56
1:A:1316:G:N1	1:A:1319:A:OP2	2.38	0.56
2:B:31:TYR:CD2	2:B:202:PRO:HG3	2.41	0.56
2:B:97:TRP:CH2	2:B:176:GLU:CD	2.82	0.56
15:O:55:GLY:O	15:O:59:MET:HG3	2.06	0.56
3:C:11:ARG:NH1	3:C:177:THR:O	2.39	0.56
13:M:106:ASN:ND2	24:M:202:HOH:O	2.38	0.56
5:E:97:GLY:N	5:E:117:ASP:OD1	2.39	0.56
20:T:50:GLU:H	20:T:99:LEU:HD12	1.70	0.56
19:S:39:THR:HA	19:S:70:LYS:HA	1.87	0.55
1:A:108:G:H5'	1:A:109:A:H5''	1.89	0.55
2:B:101:MET:HA	2:B:108:ILE:HG13	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:3:LYS:N	10:J:77:PRO:HG3	2.21	0.55
15:O:4:THR:OG1	15:O:7:GLU:HG3	2.07	0.55
1:A:235:C:N4	24:A:2170:HOH:O	2.38	0.55
1:A:881:G:OP2	12:L:12:ARG:NH2	2.39	0.55
1:A:1040:U:H2'	1:A:1041:A:C8	2.40	0.55
1:A:1149:C:OP1	9:I:9:ARG:NH1	2.39	0.55
1:A:1490:C:H2'	1:A:1491:G:H5'	1.89	0.55
8:H:13:ILE:O	8:H:17:THR:HG23	2.07	0.55
20:T:39:LYS:HB3	20:T:55:ILE:HG21	1.88	0.55
20:T:49:ALA:HB3	20:T:99:LEU:HG	1.89	0.55
1:A:1442:G:N2	1:A:1447:G:N7	2.44	0.55
9:I:53:VAL:HB	9:I:92:TYR:CE2	2.41	0.55
1:A:130:A:OP2	1:A:190(E):U:O2'	2.19	0.55
1:A:114:U:O2'	1:A:115:G:H5'	2.06	0.55
18:R:73:ALA:HB3	18:R:79:LEU:HD12	1.89	0.55
1:A:537:G:H2'	1:A:538:G:C8	2.41	0.55
1:A:912:C:OP1	12:L:46:LYS:NZ	2.29	0.55
1:A:1287:A:H2'	1:A:1288:A:C8	2.41	0.55
4:D:23:GLY:HA3	4:D:112:VAL:HG12	1.89	0.55
5:E:92:LYS:NZ	24:E:316:HOH:O	2.31	0.55
1:A:409:G:N2	24:A:3446:HOH:O	2.39	0.55
1:A:1127:G:H5''	9:I:66:ARG:HH12	1.72	0.55
20:T:92:LEU:O	20:T:96:GLY:HA2	2.06	0.55
1:A:740:U:O2'	1:A:741:G:H5'	2.07	0.55
18:R:38:GLU:N	18:R:38:GLU:OE1	2.39	0.55
1:A:974:A:OP1	14:N:29:ARG:NH2	2.40	0.55
1:A:1256:A:H4'	1:A:1257:U:H5'	1.89	0.55
1:A:1323:G:H2'	1:A:1324:A:C8	2.42	0.55
3:C:156:ARG:H	3:C:163:ALA:HA	1.71	0.55
4:D:25:ARG:O	4:D:25:ARG:HG2	2.07	0.55
9:I:43:ALA:HA	9:I:74:ILE:HG12	1.88	0.55
1:A:939:G:H5'	7:G:102:ARG:HH22	1.72	0.54
1:A:1086:U:H3	1:A:1099:G:H22	1.52	0.54
1:A:1297:C:OP2	13:M:44:ARG:NH2	2.40	0.54
6:F:100:ASN:H	18:R:23:LYS:HD2	1.72	0.54
1:A:452:A:O2'	1:A:453:A:H8	1.90	0.54
1:A:701:C:H5''	1:A:703:G:H5'	1.89	0.54
1:A:881:G:P	12:L:12:ARG:HH22	2.29	0.54
1:A:1527:C:H2'	1:A:1528:U:C6	2.42	0.54
20:T:67:ALA:HA	20:T:73:HIS:H	1.72	0.54
3:C:79:ARG:O	3:C:82:GLU:HG3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:A:H61	4:D:35:ARG:HB3	1.73	0.54
13:M:108:ARG:HD3	13:M:114:ARG:CZ	2.37	0.54
14:N:32:SER:O	14:N:40:CYS:HA	2.08	0.54
17:Q:86:GLU:O	17:Q:90:ILE:HG13	2.08	0.54
15:O:3:ILE:HA	15:O:7:GLU:OE1	2.08	0.54
18:R:47:THR:OG1	18:R:48:GLY:N	2.39	0.54
3:C:6:HIS:CD2	3:C:9:GLY:H	2.26	0.54
1:A:1126:U:H5'	24:A:3271:HOH:O	2.07	0.54
8:H:21:LYS:O	8:H:63:LEU:HD23	2.08	0.54
15:O:6:GLU:CD	15:O:6:GLU:H	2.16	0.54
1:A:390:C:O3'	16:P:28:ARG:NH2	2.41	0.53
1:A:1406:U:H5'	1:A:1518[B]:MA6:H1'	1.90	0.53
10:J:27:ALA:HB1	10:J:34:VAL:HG21	1.90	0.53
1:A:551:U:H2'	1:A:552:U:C6	2.43	0.53
1:A:581:G:N7	24:A:3575:HOH:O	2.40	0.53
2:B:18:GLY:HA2	2:B:42:ILE:HG12	1.90	0.53
1:A:372:C:H4'	1:A:373:A:O5'	2.08	0.53
1:A:714:G:H2'	1:A:715:A:C8	2.43	0.53
1:A:957:U:O2	1:A:959:A:H8	1.90	0.53
1:A:581:G:N2	1:A:760:G:N7	2.55	0.53
1:A:1057:G:H5''	3:C:154:SER:CB	2.39	0.53
4:D:76:ARG:HD3	4:D:207:TYR:CE2	2.44	0.53
10:J:4:ILE:HB	10:J:74:ILE:HG13	1.90	0.53
16:P:8:ARG:NH2	16:P:15:PRO:HB3	2.23	0.53
1:A:350:G:H8	1:A:350:G:H5''	1.74	0.53
1:A:352:C:H5'	24:A:3246:HOH:O	2.08	0.53
1:A:539:A:H2'	1:A:540:G:C8	2.43	0.53
1:A:1499:A:H1'	1:A:1520[B]:G:H5'	1.90	0.53
6:F:30:LEU:HD23	6:F:75:LEU:HD11	1.91	0.53
11:K:126:ARG:HG3	11:K:126:ARG:HH11	1.73	0.53
1:A:1201:A:H5''	24:A:3229:HOH:O	2.08	0.53
8:H:120:THR:OG1	8:H:123:GLU:HB2	2.09	0.53
10:J:88:LEU:N	10:J:88:LEU:HD22	2.23	0.53
18:R:43:PHE:C	18:R:51:LEU:HD12	2.34	0.53
1:A:748:C:H6	1:A:748:C:O5'	1.92	0.53
1:A:1126:U:H2'	1:A:1127:G:H5'	1.90	0.53
4:D:64:LEU:HG	4:D:198:VAL:HG11	1.91	0.53
4:D:142:PRO:HA	4:D:185:PHE:HD2	1.73	0.53
1:A:1147:C:O2'	9:I:16:ARG:HD3	2.09	0.53
8:H:11:THR:O	8:H:15:ASN:ND2	2.42	0.53
1:A:658:G:H2'	1:A:659:U:C6	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:836:G:C6	1:A:851:G:C6	2.97	0.53
1:A:1112:C:O2	3:C:179:ARG:HG3	2.09	0.53
1:A:1497:G:C2'	1:A:1498:UR3:H5'	2.38	0.53
1:A:923:A:OP1	5:E:21:ALA:HB2	2.08	0.52
1:A:1218:C:H2'	1:A:1219:U:C6	2.44	0.52
1:A:1532:U:H6	1:A:1532:U:O5'	1.92	0.52
6:F:45:LEU:HG	6:F:59:TYR:HD1	1.73	0.52
1:A:1313:U:O4	19:S:4:SER:OG	2.24	0.52
11:K:12:ARG:HB2	11:K:75:TYR:HE2	1.73	0.52
1:A:731:G:OP1	1:A:766:A:H1'	2.09	0.52
1:A:748:C:H4'	1:A:749:C:O5'	2.08	0.52
6:F:80:ARG:HD3	6:F:88:VAL:HB	1.92	0.52
16:P:19:ILE:HG22	16:P:36:ILE:HG13	1.91	0.52
1:A:110:C:H2'	1:A:111:G:O4'	2.09	0.52
1:A:658:G:H2'	1:A:659:U:H6	1.72	0.52
1:A:792:A:H4'	1:A:793:U:H5''	1.91	0.52
1:A:1375:A:P	7:G:28:ASN:HD22	2.32	0.52
13:M:11:ARG:HA	13:M:45:VAL:HG11	1.91	0.52
1:A:806:C:H2'	1:A:807:A:C8	2.45	0.52
1:A:1196:U:O2'	1:A:1197:G:OP1	2.25	0.52
1:A:1425:U:H2'	1:A:1426:C:C6	2.44	0.52
1:A:1519[B]:MA6:C5	1:A:1520[B]:G:H1'	2.39	0.52
10:J:16:LEU:HD12	10:J:70:ARG:HD2	1.90	0.52
10:J:76:ASN:N	10:J:76:ASN:OD1	2.42	0.52
1:A:560:U:H5'	1:A:566:G:N2	2.25	0.52
12:L:25:PRO:HB2	12:L:64:TYR:HE2	1.73	0.52
13:M:108:ARG:O	13:M:111:LYS:N	2.43	0.52
19:S:49:ILE:HD12	19:S:71:LEU:HD11	1.90	0.52
1:A:981:U:H5'	14:N:21:TYR:CE1	2.45	0.52
1:A:551:U:H2'	1:A:552:U:H6	1.75	0.52
1:A:963:G:H5'	24:A:2803:HOH:O	2.09	0.52
1:A:1023:G:N2	1:A:1024:G:O2'	2.43	0.52
1:A:1060:C:OP1	14:N:45:ARG:NH2	2.43	0.52
21:U:6:ARG:HG2	21:U:15:ARG:NH1	2.25	0.52
1:A:168:G:N2	24:A:3296:HOH:O	2.26	0.51
1:A:1111:A:N1	3:C:177:THR:OG1	2.39	0.51
1:A:1191:A:H2'	1:A:1192:C:C6	2.45	0.51
1:A:1221:G:H4'	19:S:77:THR:HG21	1.92	0.51
2:B:131:PRO:HB2	2:B:133:LYS:HD2	1.91	0.51
3:C:35:GLU:OE1	3:C:59:ARG:NH1	2.40	0.51
9:I:4:TYR:CD2	9:I:88:TYR:HA	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:124:LYS:HD2	11:K:125:PHE:CE1	2.46	0.51
20:T:43:LEU:HD22	20:T:51:GLU:HB3	1.92	0.51
1:A:1511:G:H2'	1:A:1512:U:O4'	2.10	0.51
3:C:81:GLY:O	3:C:84:ILE:HG22	2.10	0.51
4:D:31:CYS:C	4:D:33:MET:H	2.18	0.51
1:A:185:A:N3	20:T:81:LYS:NZ	2.56	0.51
1:A:434:U:H2'	1:A:435:C:C6	2.45	0.51
3:C:191:THR:HG21	3:C:193:TYR:CE2	2.45	0.51
1:A:187:C:N3	20:T:105:SER:HB2	2.25	0.51
1:A:485:G:O2'	1:A:486:U:P	2.68	0.51
2:B:74:LYS:HD2	2:B:166:ASP:HB2	1.93	0.51
16:P:74:LEU:O	16:P:79:VAL:HG23	2.10	0.51
1:A:45:U:H2'	1:A:46:G:C8	2.45	0.51
1:A:939:G:H5'	7:G:102:ARG:NH2	2.26	0.51
10:J:65:LEU:HD12	14:N:56:VAL:HG22	1.92	0.51
19:S:38:SER:O	19:S:71:LEU:N	2.43	0.51
1:A:1192:C:H2'	1:A:1193:G:O4'	2.10	0.51
5:E:78:HIS:O	5:E:93:PRO:HD3	2.11	0.51
10:J:75:ILE:HG22	10:J:76:ASN:H	1.76	0.51
1:A:256:U:H1'	24:A:3207:HOH:O	2.10	0.51
1:A:335:C:H2'	1:A:336:C:C6	2.45	0.51
1:A:390:C:H4'	16:P:28:ARG:HH21	1.75	0.51
1:A:750:G:N3	15:O:23:GLY:HA3	2.25	0.51
1:A:806:C:H2'	1:A:807:A:H8	1.75	0.51
1:A:811:C:H4'	1:A:900:A:N6	2.26	0.51
1:A:1029:C:N4	1:A:1031:G:N7	2.58	0.51
2:B:97:TRP:HZ2	2:B:102:LEU:HD13	1.76	0.51
3:C:17:ASP:O	3:C:54:ARG:NH2	2.43	0.51
5:E:64:ARG:NH2	5:E:65:ASN:HB3	2.26	0.51
6:F:40:VAL:HB	6:F:63:TYR:HD1	1.76	0.51
1:A:222:U:H2'	1:A:223:U:C6	2.45	0.51
2:B:101:MET:HG2	2:B:108:ILE:HG21	1.92	0.51
3:C:12:LEU:HD11	14:N:51:GLY:HA2	1.92	0.51
1:A:4:U:H4'	1:A:5:U:OP2	2.10	0.51
1:A:17:U:H2'	1:A:18:C:C6	2.46	0.51
1:A:949:A:H2'	1:A:950:U:O4'	2.11	0.51
1:A:1106:G:H5''	3:C:172:ARG:HG2	1.92	0.51
3:C:134:ILE:HG23	3:C:151:VAL:HB	1.93	0.51
4:D:35:ARG:O	4:D:36:ARG:HG2	2.10	0.51
17:Q:22:LEU:HD12	17:Q:23:VAL:N	2.26	0.51
19:S:40:ILE:HG23	19:S:44:MET:SD	2.50	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:G:O6	4:D:86:LYS:HA	2.11	0.51
1:A:1269:A:H2	1:A:1312:G:N3	2.09	0.51
3:C:134:ILE:HG21	3:C:167:TRP:O	2.10	0.51
17:Q:27:PHE:CE1	17:Q:36:ILE:HD11	2.46	0.51
1:A:1277:C:O2'	1:A:1279:A:H8	1.94	0.50
1:A:1350:A:OP1	9:I:121:ARG:NH1	2.44	0.50
2:B:97:TRP:HH2	2:B:176:GLU:OE1	1.94	0.50
5:E:98:THR:HB	5:E:117:ASP:HB3	1.93	0.50
9:I:17:VAL:HG22	9:I:63:ILE:HD13	1.93	0.50
13:M:12:ASN:H	13:M:45:VAL:HB	1.76	0.50
1:A:129:U:O3'	1:A:129(A):G:H3'	2.10	0.50
1:A:1191:A:OP1	3:C:4:LYS:NZ	2.37	0.50
1:A:1305:G:N2	1:A:1331:G:H1'	2.26	0.50
5:E:8:GLU:HG2	5:E:34:VAL:HG22	1.93	0.50
6:F:16:GLN:OE1	6:F:16:GLN:HA	2.11	0.50
12:L:75:HIS:ND1	12:L:75:HIS:C	2.69	0.50
1:A:216:G:H2'	1:A:217:C:C6	2.46	0.50
1:A:436:C:H2'	1:A:437:U:H6	1.76	0.50
1:A:689:C:OP1	11:K:27:ASN:ND2	2.43	0.50
1:A:665:A:N3	1:A:732:C:H2'	2.26	0.50
1:A:673:G:H5''	6:F:87:ARG:NH1	2.27	0.50
1:A:778:G:O5'	1:A:778:G:H8	1.95	0.50
1:A:1077:G:N2	1:A:1080:A:OP2	2.40	0.50
5:E:6:PHE:CZ	5:E:66:MET:HE1	2.46	0.50
6:F:99:ALA:HB2	18:R:31:LEU:HG	1.93	0.50
1:A:767:A:H2'	1:A:768:A:O4'	2.12	0.50
1:A:982:U:OP2	14:N:23:ARG:NH2	2.44	0.50
5:E:64:ARG:NH1	5:E:65:ASN:HB3	2.27	0.50
16:P:1:MET:HE3	16:P:1:MET:H3	1.76	0.50
1:A:413:G:OP1	1:A:413:G:H4'	2.12	0.50
1:A:1174:G:H2'	1:A:1175:G:C8	2.46	0.50
1:A:1216:G:H5''	14:N:5:ALA:HB2	1.93	0.50
1:A:1190:G:OP1	3:C:5:ILE:HG22	2.12	0.50
1:A:1223:C:OP1	19:S:78:ARG:NH2	2.41	0.50
10:J:92:THR:C	10:J:94:VAL:H	2.20	0.50
1:A:276:G:O2'	17:Q:68:ARG:NH1	2.44	0.50
1:A:579:G:H5'	1:A:728:A:H1'	1.94	0.50
1:A:955:U:H2'	1:A:956:U:H6	1.77	0.50
1:A:985:C:N4	24:A:2902:HOH:O	2.45	0.50
1:A:1168:A:H2'	1:A:1169:A:C8	2.47	0.50
17:Q:48:GLU:HB2	17:Q:50:LYS:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:62:SER:OG	17:Q:72:ARG:HG2	2.11	0.50
18:R:87:ARG:HH11	18:R:87:ARG:HA	1.76	0.50
1:A:520:A:OP1	12:L:52:LEU:HD12	2.11	0.50
1:A:1240:U:C2	7:G:32:ARG:HD2	2.47	0.50
1:A:1328:C:OP1	21:U:21:TYR:OH	2.25	0.50
1:A:1466:C:H2'	1:A:1467:G:O4'	2.12	0.50
2:B:17:PHE:HD1	2:B:18:GLY:H	1.58	0.50
4:D:201:GLN:O	4:D:205:GLU:HG3	2.11	0.50
10:J:9:ARG:HA	10:J:68:HIS:O	2.12	0.50
1:A:758:G:N7	24:A:3576:HOH:O	2.43	0.49
1:A:1125:U:H5''	24:A:3301:HOH:O	2.12	0.49
1:A:1126:U:C4	1:A:1127:G:N3	2.79	0.49
1:A:1189:C:OP1	14:N:58:LYS:NZ	2.44	0.49
8:H:33:GLU:HG2	8:H:48:TYR:OH	2.12	0.49
9:I:112:LYS:HA	9:I:119:ALA:HB2	1.92	0.49
1:A:1314:C:H41	19:S:4:SER:HB2	1.76	0.49
4:D:57:ARG:HB3	4:D:206:PHE:HB2	1.94	0.49
1:A:1057:G:H2'	1:A:1058:G:O4'	2.11	0.49
3:C:6:HIS:NE2	3:C:8:ILE:HB	2.27	0.49
20:T:14:LYS:O	20:T:17:ARG:HB3	2.12	0.49
1:A:560:U:H5'	1:A:566:G:C2	2.47	0.49
1:A:1014:A:H4'	19:S:14:HIS:CD2	2.48	0.49
1:A:1148:U:H2'	1:A:1149:C:O4'	2.12	0.49
2:B:240:GLN:N	2:B:240:GLN:OE1	2.46	0.49
3:C:111:LEU:HD11	3:C:146:ALA:HB2	1.94	0.49
5:E:90:VAL:O	5:E:120:THR:HA	2.12	0.49
15:O:5:LYS:H	15:O:5:LYS:HZ3	1.59	0.49
1:A:1118:C:H1'	1:A:1179:A:C4	2.47	0.49
1:A:1502:A:H2	1:A:1505:G:N1	2.08	0.49
4:D:3:ARG:HD3	4:D:71:SER:HB3	1.95	0.49
4:D:52:SER:O	4:D:56:VAL:HG23	2.12	0.49
4:D:63:LYS:HD2	4:D:197:PRO:O	2.13	0.49
12:L:27:LEU:C	12:L:29:GLY:N	2.69	0.49
14:N:14:PRO:HB2	14:N:16:PHE:O	2.12	0.49
1:A:620:C:H2'	1:A:621:A:O4'	2.13	0.49
4:D:36:ARG:N	4:D:37:PRO:HD3	2.27	0.49
1:A:298:A:H2'	1:A:299:G:O4'	2.13	0.49
1:A:414:A:OP2	1:A:428:G:N2	2.35	0.49
1:A:1167:A:H2'	1:A:1168:A:C8	2.48	0.49
1:A:1181:G:H1'	1:A:1182:G:C5	2.47	0.49
1:A:1424:C:H42	1:A:1476:G:H1	1.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:58:LEU:HD22	18:R:62:GLU:HB3	1.95	0.49
1:A:1035:A:H2'	1:A:1036:G:C8	2.48	0.49
1:A:1277:C:H3'	1:A:1277:C:C6	2.48	0.49
1:A:1288:A:N3	1:A:1352:C:O2'	2.45	0.49
14:N:11:LYS:HG3	14:N:12:ARG:O	2.13	0.49
17:Q:3:LYS:HD3	17:Q:61:GLU:O	2.13	0.49
1:A:977:A:H2'	1:A:978:A:H5''	1.95	0.49
1:A:1036:G:N2	1:A:1037:C:H1'	2.28	0.49
1:A:1101:A:H4'	1:A:1102:A:O5'	2.13	0.49
17:Q:13:ASP:HA	24:Q:307:HOH:O	2.12	0.49
4:D:61:LYS:HD3	4:D:206:PHE:CE2	2.48	0.49
4:D:187:ARG:HH22	4:D:188:LEU:HD12	1.77	0.49
7:G:16:LEU:HD11	9:I:45:ALA:HB2	1.93	0.49
11:K:69:ALA:O	11:K:73:MET:HG2	2.13	0.49
1:A:7:G:N7	5:E:92:LYS:HD3	2.28	0.48
1:A:956:U:C2	1:A:1225:A:C2	3.01	0.48
1:A:1330:U:H2'	1:A:1331:G:H5'	1.94	0.48
1:A:1399:C:C2	1:A:1502:A:N6	2.81	0.48
3:C:148:GLY:HA3	3:C:172:ARG:O	2.13	0.48
5:E:76:ILE:O	5:E:93:PRO:HB3	2.12	0.48
10:J:86:MET:HE2	10:J:86:MET:HB2	1.69	0.48
12:L:7:ILE:O	12:L:11:VAL:HG23	2.13	0.48
13:M:22:ILE:HG21	13:M:66:LEU:HD13	1.94	0.48
17:Q:37:LYS:O	17:Q:38:ARG:HD3	2.13	0.48
1:A:706:A:H1'	11:K:29:ILE:HD11	1.94	0.48
1:A:1338:G:H2'	1:A:1339:A:C8	2.49	0.48
1:A:1366:C:H2'	1:A:1367:C:C6	2.49	0.48
1:A:444:C:N4	24:A:2334:HOH:O	2.47	0.48
1:A:1237:C:H4'	1:A:1300:G:H22	1.78	0.48
1:A:1401:G:C2	1:A:1402:4OC:H1'	2.48	0.48
4:D:100:ARG:HH22	4:D:118:ARG:HH22	1.60	0.48
6:F:76:ALA:HB1	6:F:80:ARG:NH1	2.28	0.48
15:O:3:ILE:HD11	15:O:34:LEU:HB3	1.95	0.48
1:A:179:A:H2'	1:A:180:U:C6	2.47	0.48
1:A:1173:G:H2'	1:A:1174:G:C8	2.48	0.48
1:A:1499:A:C1'	1:A:1520[A]:G:H5'	2.41	0.48
20:T:14:LYS:O	20:T:18:GLN:HG2	2.12	0.48
1:A:182:U:OP2	1:A:182:U:H6	1.95	0.48
1:A:365:U:H5''	1:A:366:C:OP1	2.14	0.48
1:A:739:C:O2'	15:O:42:HIS:ND1	2.40	0.48
1:A:1103:C:H2'	1:A:1104:G:O4'	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1296:C:H4'	1:A:1302:U:C5	2.48	0.48
4:D:28:SER:OG	4:D:30:LYS:N	2.41	0.48
7:G:12:LEU:HD12	7:G:12:LEU:H	1.77	0.48
9:I:79:LEU:HD22	9:I:83:ARG:HG2	1.95	0.48
10:J:4:ILE:HD12	10:J:74:ILE:HD12	1.96	0.48
16:P:1:MET:HE1	16:P:3:LYS:HE3	1.94	0.48
4:D:153:ARG:HD3	4:D:181:MET:HG3	1.96	0.48
11:K:19:ALA:HB3	11:K:82:VAL:HG22	1.96	0.48
1:A:165:C:H2'	1:A:166:G:C8	2.47	0.48
1:A:403:C:OP1	4:D:136:PRO:HD2	2.14	0.48
1:A:1265:G:O5'	1:A:1265:G:H8	1.97	0.48
12:L:46:LYS:N	12:L:92:ASP:O	2.42	0.48
1:A:187:C:C2	20:T:105:SER:HB2	2.49	0.48
1:A:1062:U:H2'	1:A:1063:C:C6	2.49	0.48
16:P:4:ILE:HG23	16:P:36:ILE:HD11	1.95	0.48
1:A:31:G:N2	24:A:3285:HOH:O	2.46	0.48
2:B:162:ILE:HD13	2:B:162:ILE:HA	1.61	0.48
5:E:63:ARG:HE	5:E:63:ARG:HB2	1.46	0.48
8:H:41:ARG:HB3	8:H:41:ARG:HH11	1.79	0.48
9:I:89:ASN:HB3	9:I:92:TYR:HD1	1.78	0.48
1:A:262:A:C6	1:A:263:A:C6	3.02	0.48
1:A:276:G:O3'	17:Q:68:ARG:NH1	2.43	0.48
1:A:922:G:H1	1:A:1395:C:H42	1.61	0.48
1:A:1236:A:H4'	1:A:1304:G:H4'	1.96	0.48
12:L:70:ILE:HD13	12:L:77:LEU:HD12	1.96	0.48
15:O:56:LEU:HD22	15:O:60:VAL:HG23	1.96	0.48
1:A:353:A:H5'	1:A:353:A:C8	2.48	0.47
1:A:927:G:O2'	1:A:1503:A:N7	2.46	0.47
19:S:30:LEU:HD22	19:S:50:ALA:HB2	1.96	0.47
19:S:64:GLU:O	19:S:67:VAL:HG23	2.14	0.47
20:T:72:LEU:HD23	20:T:72:LEU:HA	1.72	0.47
1:A:295:C:H2'	1:A:296:U:O4'	2.14	0.47
13:M:88:ARG:HD3	19:S:3:ARG:HH21	1.79	0.47
1:A:1317:C:OP2	14:N:17:LYS:HE3	2.14	0.47
15:O:87:ILE:HG22	15:O:88:ARG:N	2.29	0.47
16:P:28:ARG:HG2	16:P:29:ASP:OD2	2.15	0.47
1:A:750:G:H1'	15:O:23:GLY:H	1.79	0.47
1:A:922:G:O2'	1:A:1398:A:N1	2.29	0.47
1:A:1053:G:H4'	1:A:1054:C:H5'	1.96	0.47
11:K:48:ILE:HG22	11:K:49:GLY:N	2.30	0.47
1:A:765:G:H5''	1:A:766:A:OP1	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:885:G:O2'	1:A:914:A:N1	2.45	0.47
1:A:991:U:O4	1:A:1212:U:O2'	2.24	0.47
4:D:18:LYS:HD3	4:D:20:TYR:HE2	1.78	0.47
6:F:74:ASP:OD1	6:F:74:ASP:N	2.47	0.47
9:I:50:LEU:HA	9:I:53:VAL:HG22	1.96	0.47
11:K:29:ILE:HD12	11:K:30:VAL:N	2.30	0.47
1:A:620:C:N1	4:D:135:LEU:HD13	2.29	0.47
1:A:878:G:H5'	8:H:89:PRO:HG2	1.96	0.47
3:C:113:ALA:HB2	3:C:202:ILE:HG13	1.96	0.47
3:C:195:VAL:C	3:C:196:LEU:HD12	2.40	0.47
15:O:76:GLU:N	15:O:79:ARG:HH21	2.12	0.47
17:Q:63:ARG:HG2	17:Q:64:PRO:HD2	1.96	0.47
1:A:165:C:H2'	1:A:166:G:H8	1.79	0.47
1:A:499:A:H4'	1:A:500:G:OP1	2.15	0.47
1:A:802:A:O2'	24:A:2610:HOH:O	2.20	0.47
1:A:1305:G:O2'	1:A:1331:G:N2	2.47	0.47
1:A:1425:U:H3	1:A:1475:G:H1	1.63	0.47
2:B:69:LEU:HB3	2:B:162:ILE:CD1	2.45	0.47
2:B:111:ARG:HG3	2:B:111:ARG:HH11	1.80	0.47
7:G:113:GLU:HG2	7:G:119:ARG:HG2	1.95	0.47
10:J:26:ALA:HB1	10:J:84:GLN:HB3	1.96	0.47
15:O:36:ILE:HG12	15:O:59:MET:HE3	1.96	0.47
2:B:177:ALA:HB1	2:B:182:ILE:HB	1.95	0.47
5:E:82:VAL:HG21	5:E:138:ALA:HA	1.97	0.47
15:O:87:ILE:HG22	15:O:88:ARG:HD3	1.97	0.47
20:T:54:LYS:HA	20:T:57:ARG:NH2	2.30	0.47
1:A:263:A:OP1	20:T:79:ARG:NH1	2.48	0.47
1:A:267:C:H2'	1:A:268:C:H6	1.80	0.47
3:C:114:PRO:HA	3:C:185:GLY:HA3	1.96	0.47
5:E:148:VAL:HG21	8:H:107:LEU:HD13	1.97	0.47
8:H:85:ARG:NE	8:H:87:SER:O	2.48	0.47
9:I:17:VAL:HG11	9:I:81:ILE:HA	1.97	0.47
12:L:60:LEU:HD21	12:L:66:VAL:HG22	1.97	0.47
15:O:26:GLU:HG3	15:O:81:LEU:HG	1.96	0.47
15:O:87:ILE:HG22	15:O:88:ARG:H	1.80	0.47
17:Q:43:LEU:HD23	17:Q:43:LEU:HA	1.53	0.47
1:A:662:G:O2'	1:A:836:G:OP1	2.33	0.47
1:A:1486:G:H2'	1:A:1487:G:C8	2.50	0.47
4:D:66:ARG:HG3	4:D:66:ARG:NH1	2.29	0.47
17:Q:6:LEU:HD12	17:Q:23:VAL:HG21	1.97	0.47
4:D:57:ARG:HG3	4:D:202:LEU:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:31:LEU:HA	5:E:31:LEU:HD23	1.68	0.46
8:H:40:ALA:HB2	8:H:45:ILE:HD11	1.97	0.46
1:A:1277:C:H3'	1:A:1277:C:H6	1.80	0.46
2:B:115:LEU:HD21	2:B:153:ARG:CZ	2.45	0.46
3:C:96:GLY:N	3:C:97:LYS:HZ2	2.13	0.46
8:H:119:LEU:CB	8:H:123:GLU:HB3	2.45	0.46
1:A:5:U:H4'	1:A:6:G:O5'	2.15	0.46
1:A:176:C:H2'	1:A:177:C:H6	1.80	0.46
1:A:616:G:H1'	1:A:625:G:N2	2.30	0.46
1:A:957:U:O2	1:A:959:A:C8	2.69	0.46
1:A:976:G:H5'	1:A:1358:U:O2'	2.15	0.46
1:A:1051:C:N4	24:A:3238:HOH:O	2.48	0.46
1:A:1143:G:H2'	1:A:1144:G:C8	2.50	0.46
2:B:21:ARG:H	2:B:21:ARG:HG2	1.42	0.46
3:C:150:LYS:HB3	3:C:201:TYR:HB2	1.98	0.46
1:A:4:U:H5''	1:A:4:U:H6	1.81	0.46
1:A:109:A:C6	1:A:326:G:C6	3.03	0.46
18:R:61:LYS:O	18:R:65:ILE:HG12	2.16	0.46
19:S:16:LEU:O	19:S:20:LEU:HG	2.15	0.46
20:T:36:LEU:HD23	20:T:36:LEU:HA	1.71	0.46
1:A:1182:G:H4'	1:A:1183:A:H5''	1.97	0.46
2:B:80:ILE:HD11	2:B:208:ILE:HG12	1.96	0.46
10:J:9:ARG:NH2	10:J:97:GLU:OE2	2.47	0.46
20:T:50:GLU:O	20:T:100:ILE:HD11	2.16	0.46
1:A:242:C:H2'	1:A:243:A:H5''	1.97	0.46
5:E:9:LYS:HB2	5:E:112:LEU:HD11	1.98	0.46
8:H:87:SER:HA	8:H:93:VAL:HG13	1.98	0.46
11:K:84:VAL:HG11	11:K:91:ARG:HH11	1.81	0.46
1:A:299:G:H2'	1:A:300:A:C8	2.50	0.46
1:A:606:G:H1'	1:A:632:A:N6	2.30	0.46
1:A:689:C:H2'	1:A:690:G:O4'	2.16	0.46
1:A:1152:A:H2'	1:A:1153:C:O4'	2.16	0.46
2:B:23:ARG:HG3	2:B:24:TRP:H	1.79	0.46
17:Q:15:MET:HE1	17:Q:43:LEU:HD13	1.96	0.46
20:T:14:LYS:HB2	20:T:17:ARG:CZ	2.45	0.46
1:A:279:A:H5'	1:A:279:A:H8	1.81	0.46
1:A:353:A:H5'	1:A:353:A:H8	1.80	0.46
1:A:448:A:C4	1:A:487:A:C2	3.04	0.46
1:A:554:C:O2'	24:A:3278:HOH:O	2.21	0.46
1:A:833:U:H2'	1:A:834:C:C6	2.51	0.46
1:A:913:A:H4'	1:A:914:A:H4'	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:90:GLY:O	17:Q:34:LYS:HE2	2.15	0.46
1:A:965:A:H3'	24:A:3435:HOH:O	2.15	0.46
6:F:14:LEU:HB2	6:F:19:LEU:HD12	1.97	0.46
6:F:19:LEU:HD21	6:F:59:TYR:CZ	2.51	0.46
7:G:51:GLN:HB2	7:G:58:PRO:HG3	1.98	0.46
19:S:19:VAL:HG23	19:S:47:HIS:CD2	2.50	0.46
1:A:29:G:N2	24:A:3277:HOH:O	2.48	0.46
1:A:136:C:O4'	16:P:1:MET:HG2	2.16	0.46
1:A:154:C:H1'	24:A:3297:HOH:O	2.16	0.46
1:A:439:A:C4	1:A:497:A:C2	3.04	0.46
1:A:688:G:H5'	11:K:46:GLY:C	2.40	0.46
1:A:918:A:H2'	1:A:919:A:C8	2.50	0.46
1:A:1493:A:H1'	1:A:1494:G:P	2.56	0.46
6:F:8:ILE:HD12	6:F:26:ILE:HD13	1.98	0.46
19:S:53:ASN:O	19:S:77:THR:HG22	2.16	0.46
20:T:53:LEU:HD13	20:T:103:GLY:H	1.81	0.46
1:A:1371:G:OP1	9:I:12:GLU:HB2	2.16	0.45
5:E:95:ALA:HB1	5:E:96:PRO:HD2	1.98	0.45
9:I:112:LYS:HG3	9:I:118:LYS:HA	1.98	0.45
21:U:9:ARG:O	21:U:13:ILE:HG12	2.16	0.45
1:A:489:C:H2'	1:A:490:G:H8	1.81	0.45
1:A:974:A:OP2	14:N:41:ARG:NH1	2.48	0.45
1:A:1004:A:H5''	1:A:1025:U:C4	2.51	0.45
4:D:38:TYR:H	4:D:38:TYR:HD2	1.64	0.45
5:E:141:GLN:HA	5:E:143:ARG:HH12	1.79	0.45
8:H:51:VAL:HG21	8:H:60:ARG:NH1	2.31	0.45
10:J:79:ARG:NH1	10:J:79:ARG:HA	2.31	0.45
15:O:5:LYS:H	15:O:5:LYS:CE	2.29	0.45
19:S:61:TYR:HD2	19:S:62:ILE:N	2.14	0.45
1:A:691:G:H2'	1:A:692:U:C6	2.50	0.45
18:R:36:ASN:OD1	18:R:39:VAL:HG12	2.17	0.45
1:A:1096:C:H2'	1:A:1097:C:H6	1.82	0.45
1:A:1392:G:N2	1:A:1502:A:C8	2.80	0.45
1:A:1486:G:H2'	1:A:1487:G:H8	1.82	0.45
2:B:68:ILE:O	2:B:90:MET:HB3	2.16	0.45
2:B:73:THR:HG23	2:B:95:GLN:O	2.17	0.45
5:E:11:ILE:HD13	5:E:11:ILE:HA	1.51	0.45
11:K:124:LYS:HD2	11:K:125:PHE:CZ	2.51	0.45
19:S:25:LYS:HD3	19:S:26:GLY:O	2.17	0.45
20:T:104:LEU:HA	20:T:104:LEU:HD23	1.66	0.45
1:A:1493:A:O2'	1:A:1494:G:OP1	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:226:ARG:H	2:B:226:ARG:HG2	1.57	0.45
3:C:191:THR:HG22	3:C:192:THR:HG23	1.99	0.45
4:D:202:LEU:HA	4:D:202:LEU:HD13	1.70	0.45
8:H:20:TYR:HA	8:H:65:TYR:CZ	2.52	0.45
11:K:48:ILE:HD13	11:K:63:LEU:HB2	1.99	0.45
11:K:70:LYS:HE2	11:K:70:LYS:HB3	1.80	0.45
11:K:115:PRO:C	11:K:117:ASN:H	2.23	0.45
1:A:660:G:H1	1:A:745:C:H42	1.65	0.45
1:A:1070:U:H2'	1:A:1071:C:H6	1.81	0.45
1:A:1376:U:OP1	7:G:98:SER:OG	2.31	0.45
1:A:1480:G:C6	1:A:1481:U:C4	3.05	0.45
1:A:1514:C:H2'	1:A:1515[A]:C:O4'	2.17	0.45
2:B:98:LEU:HB2	2:B:101:MET:HG3	1.98	0.45
4:D:102:ASP:OD1	4:D:103:ASN:N	2.48	0.45
5:E:28:PHE:CG	5:E:51:VAL:HG23	2.52	0.45
17:Q:45:HIS:HB3	17:Q:72:ARG:HB3	1.99	0.45
17:Q:81:ARG:HH21	17:Q:84:LEU:HD11	1.81	0.45
1:A:761:G:H2'	1:A:762:C:O4'	2.16	0.45
1:A:828:A:H4'	1:A:828:A:OP1	2.16	0.45
20:T:23:ARG:HB3	20:T:23:ARG:HH11	1.82	0.45
1:A:659:U:OP2	15:O:8:LYS:NZ	2.36	0.45
1:A:872:A:C8	1:A:874:G:C8	3.04	0.45
1:A:964:A:N6	24:A:2817:HOH:O	2.39	0.45
1:A:1001:A:H2'	1:A:1002:G:C8	2.47	0.45
1:A:1026:G:H3'	1:A:1027:C:H5''	1.99	0.45
1:A:1152:A:O3'	10:J:13:HIS:NE2	2.50	0.45
7:G:91:VAL:HG13	7:G:95:ARG:HG2	1.99	0.45
14:N:23:ARG:HA	14:N:29:ARG:O	2.16	0.45
1:A:389:A:C6	1:A:390:C:H1'	2.52	0.45
1:A:442:C:H2'	1:A:443:C:C6	2.52	0.45
1:A:1004:A:H5''	1:A:1025:U:N3	2.31	0.45
4:D:65:ARG:HD2	4:D:72:GLU:HA	1.99	0.45
6:F:67:MET:HB2	6:F:67:MET:HE3	1.59	0.45
1:A:192:U:O2'	20:T:57:ARG:HG2	2.17	0.45
1:A:600:C:H2'	1:A:601:C:C6	2.51	0.45
1:A:602:A:H2'	1:A:603:U:O4'	2.16	0.45
1:A:614:A:H2'	1:A:615:C:C6	2.52	0.45
1:A:806:C:O2'	1:A:807:A:H5'	2.17	0.45
1:A:922:G:H2'	1:A:923:A:C8	2.52	0.45
1:A:1075:C:H5''	2:B:179:LYS:NZ	2.31	0.45
1:A:1233:G:OP2	9:I:124:GLN:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:30:ALA:O	5:E:45:PHE:HA	2.16	0.45
5:E:65:ASN:O	5:E:65:ASN:CG	2.60	0.45
6:F:10:LEU:HD12	6:F:59:TYR:HB3	1.99	0.45
8:H:127:LEU:HD22	8:H:127:LEU:HA	1.67	0.45
20:T:87:LYS:O	20:T:91:LEU:HB2	2.17	0.45
1:A:176:C:N4	24:A:3047:HOH:O	2.48	0.44
1:A:975:A:N6	1:A:1366:C:O2'	2.42	0.44
1:A:1068:G:N2	1:A:1191:A:N3	2.53	0.44
1:A:1070:U:H2'	1:A:1071:C:C6	2.53	0.44
1:A:1347:G:C8	9:I:107:ARG:HB3	2.52	0.44
7:G:26:PHE:CE2	7:G:30:ILE:HD11	2.52	0.44
7:G:111:ARG:NH1	7:G:113:GLU:OE2	2.48	0.44
10:J:39:PRO:HA	10:J:70:ARG:HG3	1.98	0.44
19:S:49:ILE:HG22	19:S:51:VAL:HG22	2.00	0.44
1:A:558:G:C4	1:A:559:A:C2	3.05	0.44
1:A:663:A:H5''	18:R:61:LYS:HE3	1.99	0.44
1:A:725:G:O2'	1:A:726:C:H5'	2.16	0.44
1:A:973:G:O5'	1:A:973:G:H8	2.00	0.44
1:A:1065:U:O2'	1:A:1066:C:OP2	2.26	0.44
1:A:1148:U:O3'	9:I:14:VAL:HG11	2.17	0.44
1:A:1406:U:C5'	1:A:1518[B]:MA6:H1'	2.47	0.44
1:A:1413:A:N1	1:A:1488:G:C2	2.86	0.44
1:A:1442:G:H5''	24:A:3034:HOH:O	2.18	0.44
1:A:1502:A:C2	1:A:1504:G:C2	3.05	0.44
4:D:71:SER:HG	4:D:74:GLN:H	1.63	0.44
14:N:25:VAL:HG12	14:N:38:GLY:O	2.18	0.44
17:Q:57:VAL:HG12	17:Q:76:LEU:HA	2.00	0.44
1:A:103:C:P	20:T:17:ARG:HH11	2.40	0.44
1:A:273:A:N6	1:A:274:A:N6	2.65	0.44
1:A:1369:C:H2'	1:A:1370:G:C8	2.53	0.44
4:D:9:CYS:O	4:D:12:CYS:HB2	2.17	0.44
8:H:104:ARG:HG3	8:H:138:TRP:CD2	2.52	0.44
1:A:99:C:H2'	1:A:101:A:C8	2.53	0.44
1:A:501:C:H2'	1:A:502:G:H8	1.82	0.44
1:A:959:A:H3'	1:A:960:U:H5''	1.99	0.44
1:A:1332:A:H2'	1:A:1333:A:C8	2.51	0.44
1:A:1465:C:H2'	1:A:1466:C:O4'	2.18	0.44
1:A:1491:G:H3'	1:A:1492:A:C5'	2.41	0.44
24:A:2434:HOH:O	17:Q:98:LEU:HA	2.18	0.44
4:D:127:THR:HG23	4:D:147:ALA:HB3	1.99	0.44
15:O:8:LYS:O	15:O:12:ILE:HG13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:21:ASP:OD2	15:O:24:SER:HB3	2.17	0.44
19:S:30:LEU:HB3	19:S:31:ILE:H	1.42	0.44
9:I:51:ARG:H	9:I:51:ARG:HG2	1.56	0.44
9:I:113:LYS:HG2	9:I:119:ALA:HA	2.00	0.44
11:K:58:PRO:HA	11:K:90:GLY:HA3	2.00	0.44
1:A:256:U:OP1	17:Q:17:LYS:NZ	2.33	0.44
1:A:1029:C:H2'	1:A:1030:C:C6	2.53	0.44
1:A:1410:G:O6	1:A:1490:C:N4	2.50	0.44
7:G:85:TYR:CD1	7:G:154:TYR:HE1	2.31	0.44
17:Q:15:MET:HE2	17:Q:18:THR:HG21	1.99	0.44
21:U:6:ARG:HE	21:U:15:ARG:NH1	2.15	0.44
1:A:56:U:H2'	1:A:57:G:C8	2.53	0.44
1:A:310:G:C5	1:A:311:C:C5	3.06	0.44
1:A:489:C:H2'	1:A:490:G:C8	2.53	0.44
1:A:1182:G:H5'	1:A:1184:G:H5''	1.99	0.44
4:D:3:ARG:H	4:D:3:ARG:HG2	1.50	0.44
4:D:150:GLU:CD	4:D:150:GLU:N	2.74	0.44
4:D:196:LEU:HA	4:D:197:PRO:HD3	1.83	0.44
8:H:104:ARG:HG3	8:H:138:TRP:CG	2.53	0.44
12:L:38:THR:HB	12:L:57:LYS:HB3	2.00	0.44
1:A:289:G:P	24:A:2104:HOH:O	2.76	0.44
1:A:325:A:H2'	1:A:326:G:O4'	2.17	0.44
1:A:1072:G:C5	1:A:1073:U:C4	3.06	0.44
2:B:222:ILE:O	2:B:226:ARG:HG2	2.18	0.44
9:I:4:TYR:HB3	9:I:87:GLN:HG2	1.99	0.44
9:I:10:ARG:HG2	9:I:75:ASP:HB2	2.00	0.44
1:A:802:A:H2'	1:A:803:G:O4'	2.17	0.44
1:A:1300:G:C6	1:A:1334:G:C5	3.06	0.44
3:C:155:GLY:O	3:C:196:LEU:HG	2.18	0.44
13:M:50:GLU:O	13:M:54:VAL:HG23	2.18	0.44
1:A:485:G:O2'	1:A:486:U:O5'	2.36	0.43
1:A:659:U:H2'	1:A:660:G:C8	2.53	0.43
1:A:1338:G:C6	1:A:1339:A:C6	3.06	0.43
1:A:1505:G:H8	1:A:1505:G:H3'	1.84	0.43
3:C:34:LEU:O	3:C:38:ARG:HG3	2.17	0.43
3:C:108:ASN:HD21	3:C:144:SER:CB	2.31	0.43
12:L:83:VAL:HG21	12:L:100:ILE:HD13	1.99	0.43
19:S:30:LEU:HD23	19:S:48:THR:HG22	1.99	0.43
1:A:503:C:O2'	1:A:504:C:H5'	2.18	0.43
1:A:1371:G:O3'	9:I:69:GLY:HA3	2.18	0.43
1:A:1505:G:H3'	1:A:1505:G:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:77:ALA:HB2	2:B:211:ILE:HD13	2.01	0.43
3:C:11:ARG:O	3:C:14:ILE:O	2.36	0.43
3:C:58:GLU:HB3	10:J:92:THR:HG21	2.00	0.43
5:E:15:ARG:HH11	5:E:15:ARG:HB2	1.83	0.43
6:F:4:TYR:CZ	6:F:72:VAL:HG21	2.53	0.43
11:K:98:LEU:HD23	11:K:98:LEU:HA	1.81	0.43
18:R:87:ARG:HA	18:R:87:ARG:NH1	2.33	0.43
1:A:256:U:H2'	1:A:257:G:C8	2.53	0.43
1:A:770:C:N4	24:A:2622:HOH:O	2.34	0.43
1:A:857:C:H5''	1:A:857:C:H6	1.83	0.43
1:A:1191:A:H5''	3:C:4:LYS:NZ	2.34	0.43
2:B:119:GLU:OE2	2:B:153:ARG:NH2	2.50	0.43
5:E:103:GLY:O	5:E:106:PRO:HD2	2.18	0.43
6:F:55:ASP:HA	6:F:56:PRO:HD3	1.79	0.43
15:O:33:THR:HG21	15:O:85:LEU:HD22	2.00	0.43
16:P:51:VAL:O	16:P:52:ASP:HB3	2.18	0.43
1:A:216:G:H2'	1:A:217:C:H6	1.83	0.43
1:A:911:U:H2'	1:A:912:C:C6	2.53	0.43
1:A:953:G:H2'	1:A:954:G:O4'	2.17	0.43
1:A:1075:C:H5''	2:B:179:LYS:HZ3	1.84	0.43
1:A:1128:C:H5'	9:I:16:ARG:NH2	2.20	0.43
1:A:1427:U:H2'	1:A:1428:A:H8	1.79	0.43
4:D:98:GLU:CD	4:D:103:ASN:HD21	2.26	0.43
6:F:46:ARG:HB2	6:F:60:PHE:CE1	2.53	0.43
8:H:55:GLY:C	8:H:56:LYS:HD2	2.44	0.43
19:S:36:ARG:H	19:S:36:ARG:HG2	1.42	0.43
1:A:412:A:N6	4:D:35:ARG:HB3	2.33	0.43
1:A:1356:G:O5'	1:A:1356:G:H8	2.01	0.43
1:A:1411:C:O2'	1:A:1412:C:H5'	2.18	0.43
3:C:111:LEU:HA	3:C:111:LEU:HD13	1.65	0.43
4:D:8:VAL:HG12	4:D:21:LEU:HD13	1.99	0.43
5:E:13:ILE:HD13	5:E:13:ILE:HG21	1.76	0.43
7:G:26:PHE:CD1	7:G:101:LEU:HD22	2.50	0.43
9:I:82:ALA:O	9:I:86:VAL:HG23	2.19	0.43
14:N:27:CYS:SG	14:N:29:ARG:HB2	2.59	0.43
20:T:20:LEU:HA	20:T:20:LEU:HD23	1.86	0.43
1:A:144:G:H1	1:A:178:C:H42	1.66	0.43
1:A:254:G:OP1	17:Q:67:LYS:O	2.35	0.43
1:A:309:G:H1'	1:A:608:A:C2	2.54	0.43
1:A:734:G:H21	18:R:75:ILE:HD11	1.83	0.43
1:A:1310:G:N2	1:A:1327:C:O2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:15:VAL:HG21	2:B:213:LEU:HD12	2.00	0.43
8:H:98:LYS:H	8:H:98:LYS:HG2	1.57	0.43
19:S:44:MET:O	19:S:47:HIS:HB2	2.18	0.43
1:A:815:A:N3	1:A:1527:C:O2'	2.50	0.43
1:A:1232:U:OP1	9:I:126:SER:HB2	2.18	0.43
1:A:1342:C:H2'	1:A:1343:G:C8	2.54	0.43
1:A:1426:C:H2'	1:A:1427:U:C6	2.53	0.43
2:B:45:GLN:O	2:B:49:GLU:HG3	2.19	0.43
3:C:178:LEU:HD12	3:C:178:LEU:H	1.83	0.43
17:Q:31:LEU:HD12	17:Q:31:LEU:HA	1.79	0.43
1:A:501:C:H2'	1:A:502:G:C8	2.53	0.43
1:A:1073:U:O2	2:B:104:ASN:ND2	2.51	0.43
1:A:1309:G:N7	13:M:99:ARG:NH2	2.67	0.43
1:A:1495:U:H2'	1:A:1496:C:C6	2.54	0.43
4:D:76:ARG:HD2	4:D:76:ARG:HA	1.79	0.43
10:J:36:GLY:HA2	10:J:37:PRO:HD3	1.81	0.43
13:M:99:ARG:HH12	19:S:2:PRO:HG2	1.83	0.43
15:O:50:HIS:O	15:O:53:HIS:HB3	2.19	0.43
1:A:115:G:H1'	1:A:116:A:N7	2.34	0.43
1:A:924:C:O2'	1:A:1502:A:N6	2.49	0.43
1:A:1053:G:O2'	1:A:1199:U:H5	2.01	0.43
1:A:1387:G:C6	1:A:1388:C:C4	3.07	0.43
2:B:166:ASP:HB3	2:B:169:LYS:HB3	2.01	0.43
3:C:29:TYR:HE1	10:J:11:PHE:CE1	2.37	0.43
3:C:45:LYS:HE3	3:C:45:LYS:HB2	1.82	0.43
8:H:100:ILE:HA	8:H:101:PRO:HD2	1.78	0.43
13:M:3:ARG:HH11	13:M:3:ARG:HB2	1.84	0.43
17:Q:3:LYS:HB3	17:Q:61:GLU:HB3	2.01	0.43
1:A:130:A:H1'	1:A:263:A:O2'	2.19	0.43
1:A:591:U:H2'	1:A:592:G:C8	2.53	0.43
1:A:958:A:C6	1:A:959:A:N1	2.87	0.43
1:A:1095:U:H5''	1:A:1109:C:O2	2.19	0.43
1:A:1314:C:C5	19:S:6:LYS:HE2	2.54	0.43
1:A:1367:C:H5'	10:J:60:ARG:NH2	2.28	0.43
5:E:69:VAL:HA	5:E:70:PRO:HD3	1.78	0.43
5:E:131:ILE:HD13	5:E:131:ILE:HA	1.82	0.43
7:G:79:ARG:NH2	7:G:82:GLY:HA2	2.33	0.43
18:R:26:LEU:HD12	18:R:27:GLY:H	1.84	0.43
19:S:40:ILE:HG21	19:S:62:ILE:HD11	2.01	0.43
1:A:235:C:N4	24:A:2169:HOH:O	2.52	0.42
1:A:795:C:H5''	1:A:796:C:OP2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:974:A:P	14:N:41:ARG:HH12	2.42	0.42
1:A:1196:U:HO2'	1:A:1197:G:P	2.39	0.42
11:K:81:ASP:OD2	11:K:106:LYS:HE3	2.19	0.42
12:L:102:ARG:HE	12:L:102:ARG:HB3	1.67	0.42
18:R:46:GLU:H	18:R:46:GLU:CD	2.18	0.42
19:S:31:ILE:HG22	19:S:49:ILE:HA	2.01	0.42
1:A:406:G:N2	1:A:437:U:C2	2.87	0.42
1:A:689:C:P	11:K:46:GLY:HA3	2.59	0.42
1:A:1468:A:H2'	1:A:1469:G:O4'	2.19	0.42
5:E:16:THR:O	5:E:16:THR:OG1	2.30	0.42
7:G:111:ARG:HB3	7:G:113:GLU:OE2	2.19	0.42
7:G:145:ALA:C	7:G:147:ALA:H	2.26	0.42
17:Q:53:LEU:HD23	17:Q:82:MET:SD	2.59	0.42
1:A:1011:G:H2'	1:A:1012:U:O4'	2.19	0.42
1:A:1103:C:C5'	2:B:98:LEU:HD22	2.46	0.42
1:A:1143:G:H2'	1:A:1144:G:H8	1.83	0.42
1:A:1229:A:OP1	13:M:116:THR:OG1	2.32	0.42
5:E:36:ASP:O	5:E:38:GLN:HG2	2.18	0.42
8:H:83:ILE:O	8:H:83:ILE:HG23	2.20	0.42
1:A:665:A:H1'	1:A:733:A:O4'	2.20	0.42
1:A:765:G:N2	1:A:813:U:OP2	2.48	0.42
1:A:880:C:OP1	12:L:8:ASN:ND2	2.52	0.42
1:A:1171:G:O2'	1:A:1172:C:H5'	2.20	0.42
3:C:188:LEU:HD11	3:C:195:VAL:HG22	2.02	0.42
4:D:24:GLU:O	4:D:25:ARG:HB3	2.20	0.42
4:D:31:CYS:O	4:D:31:CYS:SG	2.77	0.42
5:E:15:ARG:HG2	5:E:16:THR:N	2.25	0.42
9:I:8:GLY:N	9:I:83:ARG:HD2	2.34	0.42
9:I:118:LYS:O	9:I:120:ARG:N	2.48	0.42
10:J:57:LYS:O	10:J:60:ARG:NH1	2.53	0.42
14:N:22:THR:HB	14:N:33:VAL:HG21	2.02	0.42
18:R:51:LEU:CD2	18:R:52:PRO:HD2	2.42	0.42
19:S:19:VAL:HG21	19:S:44:MET:HA	2.01	0.42
1:A:149:A:H2'	1:A:150:C:H6	1.83	0.42
1:A:436:C:H2'	1:A:437:U:C6	2.53	0.42
1:A:875:C:H1'	8:H:15:ASN:OD1	2.19	0.42
1:A:1481:U:H2'	1:A:1482:G:O4'	2.20	0.42
1:A:1518[A]:MA6:H93	1:A:1519[A]:MA6:H92	2.01	0.42
4:D:57:ARG:CG	4:D:202:LEU:HD12	2.49	0.42
4:D:103:ASN:O	4:D:107:ARG:HB2	2.19	0.42
5:E:71:LEU:HD11	5:E:113:ALA:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:148:VAL:O	5:E:152:ARG:HG2	2.20	0.42
8:H:51:VAL:HG21	8:H:60:ARG:HH12	1.85	0.42
10:J:41:PRO:O	10:J:69:ASN:ND2	2.53	0.42
13:M:14:ARG:CZ	13:M:42:ALA:HA	2.49	0.42
14:N:14:PRO:O	14:N:15:LYS:HB3	2.19	0.42
17:Q:45:HIS:H	17:Q:72:ARG:HA	1.84	0.42
1:A:257:G:H2'	1:A:258:G:O4'	2.20	0.42
1:A:517:G:N1	1:A:533:A:OP2	2.50	0.42
1:A:619:U:N3	4:D:134:ASP:OD2	2.44	0.42
1:A:737:A:OP1	6:F:92:LYS:HG2	2.19	0.42
1:A:1325:C:H2'	1:A:1326:C:H6	1.85	0.42
1:A:1325:C:H2'	1:A:1326:C:C6	2.54	0.42
24:A:3306:HOH:O	10:J:38:ILE:HB	2.19	0.42
9:I:47:LEU:C	9:I:49:PRO:HD2	2.44	0.42
12:L:117:ARG:NH2	12:L:124:LYS:HB2	2.35	0.42
1:A:997:U:H5'	1:A:998:G:OP2	2.19	0.42
1:A:1038:C:O2'	1:A:1039:C:H5'	2.19	0.42
1:A:1123:A:C2'	1:A:1124:G:H5'	2.50	0.42
2:B:154:LEU:HD23	2:B:154:LEU:HA	1.91	0.42
8:H:95:VAL:HB	8:H:99:GLU:HB2	2.00	0.42
11:K:38:ASN:HA	11:K:39:PRO:HD3	1.81	0.42
12:L:7:ILE:O	12:L:10:LEU:N	2.48	0.42
19:S:80:TYR:HE1	19:S:81:ARG:HH11	1.68	0.42
1:A:229:U:H2'	1:A:230:G:C8	2.55	0.42
1:A:236:G:H2'	1:A:237:C:O4'	2.20	0.42
1:A:247:G:OP2	17:Q:100:LYS:HB3	2.19	0.42
1:A:632:A:H2'	1:A:633:G:O4'	2.20	0.42
1:A:659:U:C2	1:A:660:G:C8	3.08	0.42
1:A:835:U:OP1	18:R:64:ARG:NH2	2.41	0.42
1:A:977:A:O2'	1:A:979:C:OP2	2.36	0.42
1:A:1127:G:H4'	1:A:1148:U:O2	2.19	0.42
1:A:1191:A:OP2	3:C:3:ASN:ND2	2.53	0.42
1:A:1211:U:H2'	24:A:2779:HOH:O	2.20	0.42
1:A:1329:A:H2'	1:A:1330:U:O4'	2.20	0.42
1:A:1476:G:H2'	1:A:1477:C:C6	2.54	0.42
5:E:101:ILE:O	5:E:120:THR:HB	2.19	0.42
6:F:19:LEU:HD21	6:F:59:TYR:CE2	2.55	0.42
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.55	0.42
10:J:36:GLY:O	10:J:38:ILE:HG12	2.20	0.42
20:T:92:LEU:HD23	20:T:92:LEU:HA	1.83	0.42
1:A:153:C:O5'	1:A:153:C:H6	2.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:C:O2	20:T:105:SER:HB2	2.20	0.42
1:A:262:A:H4'	20:T:75:ASN:OD1	2.20	0.42
1:A:1004:A:H3'	1:A:1025:U:H3	1.85	0.42
3:C:11:ARG:HG3	3:C:178:LEU:HB3	2.00	0.42
5:E:6:PHE:CE2	5:E:36:ASP:HB3	2.55	0.42
5:E:87:SER:HB3	5:E:131:ILE:HD13	2.02	0.42
13:M:96:LEU:HD23	13:M:96:LEU:HA	1.85	0.42
18:R:79:LEU:HA	18:R:80:PRO:HD3	1.88	0.42
1:A:517:G:N2	1:A:533:A:OP2	2.46	0.42
1:A:1349:A:H1'	1:A:1374:A:N6	2.34	0.42
2:B:10:LEU:O	2:B:12:GLU:HG2	2.20	0.42
8:H:105:ARG:NH2	24:H:302:HOH:O	2.17	0.42
15:O:85:LEU:HA	15:O:85:LEU:HD23	1.73	0.42
1:A:7:G:H5'	1:A:298:A:H5'	2.02	0.41
1:A:459:G:C6	1:A:461:C:H5'	2.55	0.41
1:A:606:G:H1'	1:A:632:A:H61	1.86	0.41
1:A:1054:C:H6	1:A:1054:C:H2'	1.69	0.41
1:A:1275:A:H2'	1:A:1276:G:O4'	2.20	0.41
1:A:1539:C:H2'	1:A:1540:PSU:H5''	2.01	0.41
2:B:10:LEU:HD23	2:B:48:MET:HE1	2.02	0.41
2:B:215:LEU:HD23	2:B:215:LEU:HA	1.85	0.41
10:J:91:PRO:HB2	10:J:94:VAL:HG11	2.02	0.41
17:Q:74:LEU:HD12	17:Q:74:LEU:HA	1.66	0.41
18:R:26:LEU:HD12	18:R:26:LEU:HA	1.82	0.41
19:S:33:THR:HG22	19:S:50:ALA:O	2.20	0.41
1:A:229:U:O2'	1:A:230:G:H5'	2.20	0.41
1:A:782:A:OP1	1:A:1521:G:N2	2.51	0.41
2:B:24:TRP:CG	2:B:25:ASN:N	2.88	0.41
3:C:59:ARG:HG3	3:C:63:ASN:O	2.21	0.41
4:D:12:CYS:HA	4:D:19:LEU:HD12	2.01	0.41
9:I:34:ASN:O	9:I:38:GLN:HB2	2.20	0.41
9:I:38:GLN:HE21	9:I:38:GLN:HB3	1.69	0.41
12:L:19:ARG:H	12:L:19:ARG:HD2	1.84	0.41
13:M:46:LYS:H	13:M:46:LYS:HG3	1.62	0.41
13:M:106:ASN:C	13:M:108:ARG:H	2.28	0.41
15:O:5:LYS:H	15:O:5:LYS:NZ	2.18	0.41
1:A:1136:U:H6	1:A:1136:U:H2'	1.64	0.41
1:A:1372:U:H2'	1:A:1373:G:O4'	2.20	0.41
3:C:61:ALA:C	3:C:63:ASN:H	2.28	0.41
3:C:111:LEU:O	3:C:202:ILE:HD12	2.20	0.41
7:G:101:LEU:HA	7:G:101:LEU:HD23	1.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:25:ASP:N	8:H:25:ASP:OD1	2.51	0.41
11:K:126:ARG:HG3	11:K:126:ARG:NH1	2.36	0.41
15:O:16:ALA:HB1	15:O:21:ASP:HB3	2.03	0.41
1:A:639:G:O2'	1:A:640:A:H5'	2.20	0.41
2:B:182:ILE:HA	2:B:183:PRO:HD3	1.95	0.41
4:D:78:LEU:HA	4:D:78:LEU:HD23	1.49	0.41
5:E:144:THR:HB	5:E:147:ASP:H	1.85	0.41
8:H:4:ASP:CG	8:H:85:ARG:HH11	2.22	0.41
9:I:50:LEU:HB3	9:I:55:ALA:HB3	2.03	0.41
18:R:70:ILE:HG23	18:R:79:LEU:HD13	2.02	0.41
20:T:13:LEU:HD12	20:T:13:LEU:C	2.45	0.41
1:A:106:C:O2	1:A:379:C:H4'	2.21	0.41
1:A:427:U:OP1	4:D:13:ARG:NH2	2.52	0.41
1:A:1201:A:H4'	1:A:1202:G:O5'	2.21	0.41
2:B:102:LEU:HB3	2:B:180:LEU:CD1	2.50	0.41
5:E:76:ILE:HG22	5:E:78:HIS:O	2.21	0.41
7:G:104:LEU:HD23	7:G:104:LEU:HA	1.88	0.41
1:A:118:U:H3'	1:A:288:A:H61	1.84	0.41
1:A:950:U:H2'	1:A:951:G:C8	2.55	0.41
1:A:991:U:O2'	1:A:992:U:O5'	2.37	0.41
1:A:1023:G:H2'	1:A:1023:G:N3	2.35	0.41
1:A:1306:A:P	21:U:6:ARG:HH12	2.43	0.41
2:B:19:HIS:HB3	2:B:189:ASP:OD2	2.21	0.41
2:B:28:PHE:CD2	2:B:190:THR:HA	2.55	0.41
3:C:149:ALA:O	3:C:169:ALA:HB1	2.21	0.41
12:L:21:LYS:H	12:L:21:LYS:HG2	1.62	0.41
12:L:53:ARG:NH1	12:L:92:ASP:OD1	2.53	0.41
18:R:26:LEU:HD21	18:R:39:VAL:HG23	2.01	0.41
19:S:49:ILE:HG21	19:S:71:LEU:HD11	2.03	0.41
1:A:264:U:H2'	1:A:265:G:O4'	2.21	0.41
1:A:1152:A:H4'	10:J:13:HIS:NE2	2.35	0.41
2:B:19:HIS:CG	2:B:20:GLU:H	2.38	0.41
5:E:75:THR:C	5:E:76:ILE:HD13	2.46	0.41
7:G:152:ALA:O	7:G:155:ARG:HG3	2.21	0.41
15:O:33:THR:OG1	15:O:63:ARG:NH1	2.48	0.41
15:O:67:LEU:HD23	15:O:67:LEU:HA	1.77	0.41
16:P:52:ASP:OD2	16:P:55:ARG:HB2	2.20	0.41
17:Q:52:LYS:HD3	24:Q:305:HOH:O	2.20	0.41
18:R:34:TYR:CE1	18:R:35:ARG:HG3	2.55	0.41
1:A:518:C:H2'	1:A:530:G:N7	2.36	0.41
1:A:538:G:P	12:L:115:LYS:HB2	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:562:C:H1'	12:L:15:ARG:HB3	2.02	0.41
1:A:695:A:H2'	1:A:696:A:C8	2.55	0.41
1:A:1451:A:H5''	1:A:1452:C:H5	1.85	0.41
2:B:179:LYS:HA	8:H:72:PRO:HD3	2.02	0.41
5:E:33:VAL:HG11	5:E:109:ILE:HA	2.01	0.41
6:F:11:ASN:HB3	6:F:14:LEU:HG	2.02	0.41
8:H:75:ARG:HA	8:H:76:PRO:HD3	1.70	0.41
9:I:8:GLY:CA	9:I:79:LEU:HB3	2.50	0.41
12:L:24:VAL:O	12:L:24:VAL:HG12	2.20	0.41
1:A:484:G:H5'	1:A:486:U:O4'	2.21	0.41
1:A:554:C:H2'	1:A:555:C:C6	2.56	0.41
1:A:563:A:H2'	1:A:567:G:C8	2.56	0.41
1:A:659:U:H2'	1:A:660:G:H8	1.85	0.41
1:A:1164:G:C6	1:A:1165:C:C4	3.09	0.41
1:A:1179:A:O3'	9:I:103:THR:HG23	2.21	0.41
1:A:1296:C:H4'	1:A:1302:U:H5	1.86	0.41
1:A:1402:4OC:O2	1:A:1500:A:N1	2.53	0.41
2:B:17:PHE:CD1	2:B:18:GLY:N	2.88	0.41
2:B:22:LYS:HG3	2:B:40:HIS:NE2	2.35	0.41
2:B:48:MET:HA	2:B:51:LEU:HB2	2.03	0.41
3:C:59:ARG:HE	3:C:59:ARG:HB2	1.20	0.41
9:I:108:VAL:HG12	9:I:109:VAL:H	1.86	0.41
9:I:117:HIS:HB2	9:I:121:ARG:HG3	2.01	0.41
9:I:127:LYS:HA	9:I:127:LYS:HD3	1.72	0.41
10:J:88:LEU:HD22	10:J:88:LEU:H	1.86	0.41
16:P:40:ASP:HA	16:P:41:PRO:HD3	1.91	0.41
17:Q:84:LEU:HA	17:Q:84:LEU:HD23	1.67	0.41
19:S:35:SER:O	19:S:35:SER:OG	2.39	0.41
1:A:106:C:C2'	1:A:107:G:H5'	2.51	0.41
1:A:428:G:H4'	1:A:429:U:O5'	2.20	0.41
1:A:566:G:N2	24:A:3565:HOH:O	2.36	0.41
1:A:580:U:H2'	1:A:581:G:O4'	2.20	0.41
1:A:631:G:H8	1:A:631:G:OP2	2.03	0.41
1:A:1002:G:H2'	1:A:1003:G:O4'	2.21	0.41
11:K:84:VAL:HG11	11:K:91:ARG:HD2	2.03	0.41
14:N:31:ARG:O	14:N:33:VAL:HG22	2.21	0.41
20:T:60:GLU:HG3	20:T:81:LYS:HD2	2.02	0.41
21:U:8:THR:OG1	21:U:10:ARG:N	2.54	0.41
1:A:838:G:H1	1:A:848:C:H42	1.69	0.40
1:A:869:G:C8	24:A:3466:HOH:O	2.71	0.40
1:A:961:U:OP1	1:A:1223:C:O2'	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1196:U:H3'	1:A:1197:G:H5''	2.03	0.40
2:B:24:TRP:HB2	2:B:190:THR:HG22	2.03	0.40
2:B:188:ALA:O	2:B:202:PRO:HA	2.21	0.40
5:E:81:GLU:HB3	5:E:88:LYS:HZ2	1.86	0.40
6:F:75:LEU:O	6:F:79:LEU:HG	2.20	0.40
10:J:79:ARG:HA	10:J:79:ARG:HH11	1.87	0.40
11:K:48:ILE:HD11	11:K:64:ALA:HA	2.02	0.40
15:O:21:ASP:OD1	15:O:24:SER:HB3	2.21	0.40
18:R:19:LYS:HE2	18:R:19:LYS:HB2	1.87	0.40
18:R:21:LYS:HD2	18:R:54:ARG:O	2.21	0.40
1:A:1265:G:H2'	1:A:1266:G:O4'	2.21	0.40
1:A:1408:A:H2'	1:A:1409:C:C6	2.57	0.40
2:B:147:LYS:HE2	2:B:148:TYR:CE1	2.56	0.40
4:D:10:ARG:HG2	4:D:11:LEU:N	2.33	0.40
4:D:15:GLU:OE2	4:D:15:GLU:HA	2.21	0.40
11:K:72:ALA:HB1	11:K:77:MET:HE2	2.02	0.40
12:L:6:THR:HG23	12:L:9:GLN:HG3	2.03	0.40
13:M:3:ARG:HA	13:M:8:GLU:O	2.21	0.40
17:Q:59:ILE:HG23	17:Q:71:PHE:HD1	1.87	0.40
17:Q:91:ARG:O	17:Q:94:ASN:HB2	2.20	0.40
1:A:244:U:C6	1:A:894:G:N2	2.89	0.40
1:A:419:C:C2	1:A:425:G:C2	3.09	0.40
1:A:664:G:H22	1:A:741:G:H1	1.69	0.40
1:A:738:C:H2'	1:A:739:C:H6	1.86	0.40
1:A:992:U:H4'	1:A:993:G:O5'	2.22	0.40
1:A:1046:A:H3'	1:A:1047:G:H8	1.86	0.40
1:A:1367:C:H5'	10:J:60:ARG:HE	1.86	0.40
2:B:54:THR:O	2:B:57:PHE:HB3	2.21	0.40
4:D:128:VAL:HG12	4:D:129:ASN:HD22	1.86	0.40
1:A:358:U:H2'	1:A:359:U:C6	2.55	0.40
1:A:1318:A:O2'	19:S:37:ARG:HG3	2.22	0.40
2:B:208:ILE:HG21	2:B:239:VAL:HA	2.04	0.40
7:G:149:ARG:HD3	11:K:59:TYR:CE1	2.57	0.40
10:J:64:GLU:OE2	10:J:66:ARG:NE	2.55	0.40
12:L:6:THR:HG23	12:L:9:GLN:OE1	2.22	0.40
12:L:69:TYR:HE2	12:L:71:PRO:HA	1.87	0.40
15:O:30:ALA:HB2	15:O:85:LEU:HD11	2.04	0.40
17:Q:40:LYS:HE2	17:Q:42:TYR:OH	2.21	0.40
19:S:11:VAL:HG22	19:S:38:SER:HB3	2.03	0.40
1:A:877:C:OP1	8:H:88:LYS:NZ	2.40	0.40
1:A:889:A:N1	1:A:907:A:H5''	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:901:A:C5	1:A:902:G:H1'	2.56	0.40
1:A:924:C:H2'	1:A:925:G:C8	2.56	0.40
5:E:15:ARG:HG3	5:E:15:ARG:NH1	2.33	0.40
11:K:34:ASP:OD1	11:K:38:ASN:N	2.48	0.40
15:O:39:LEU:HD12	15:O:59:MET:HE2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	232/256 (91%)	209 (90%)	21 (9%)	2 (1%)	14	47
3	C	204/239 (85%)	179 (88%)	24 (12%)	1 (0%)	24	57
4	D	206/209 (99%)	199 (97%)	7 (3%)	0	100	100
5	E	148/162 (91%)	138 (93%)	10 (7%)	0	100	100
6	F	99/101 (98%)	97 (98%)	2 (2%)	0	100	100
7	G	153/156 (98%)	143 (94%)	10 (6%)	0	100	100
8	H	136/138 (99%)	132 (97%)	4 (3%)	0	100	100
9	I	125/128 (98%)	113 (90%)	11 (9%)	1 (1%)	16	49
10	J	96/105 (91%)	78 (81%)	16 (17%)	2 (2%)	5	31
11	K	114/129 (88%)	103 (90%)	11 (10%)	0	100	100
12	L	122/135 (90%)	111 (91%)	10 (8%)	1 (1%)	16	49
13	M	116/126 (92%)	104 (90%)	12 (10%)	0	100	100
14	N	58/61 (95%)	51 (88%)	7 (12%)	0	100	100
15	O	85/89 (96%)	82 (96%)	3 (4%)	0	100	100
16	P	81/88 (92%)	79 (98%)	2 (2%)	0	100	100
17	Q	97/105 (92%)	90 (93%)	7 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	R	68/88 (77%)	63 (93%)	4 (6%)	1 (2%)	8	37
19	S	78/93 (84%)	73 (94%)	4 (5%)	1 (1%)	9	39
20	T	97/106 (92%)	85 (88%)	12 (12%)	0	100	100
21	U	22/27 (82%)	21 (96%)	1 (4%)	0	100	100
All	All	2337/2541 (92%)	2150 (92%)	178 (8%)	9 (0%)	30	62

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	21	ARG
12	L	28	LYS
19	S	31	ILE
3	C	15	THR
10	J	35	SER
9	I	119	ALA
10	J	34	VAL
18	R	86	VAL
2	B	229	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%)	173 (86%)	29 (14%)	3	18
3	C	160/188 (85%)	115 (72%)	45 (28%)	0	3
4	D	180/181 (99%)	147 (82%)	33 (18%)	2	10
5	E	115/123 (94%)	88 (76%)	27 (24%)	1	4
6	F	90/90 (100%)	77 (86%)	13 (14%)	3	18
7	G	126/127 (99%)	110 (87%)	16 (13%)	4	21
8	H	119/119 (100%)	101 (85%)	18 (15%)	3	16
9	I	98/99 (99%)	80 (82%)	18 (18%)	1	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	J	87/92 (95%)	63 (72%)	24 (28%)	0	3
11	K	88/99 (89%)	79 (90%)	9 (10%)	7	28
12	L	104/111 (94%)	84 (81%)	20 (19%)	1	8
13	M	94/101 (93%)	78 (83%)	16 (17%)	2	12
14	N	49/50 (98%)	39 (80%)	10 (20%)	1	7
15	O	79/80 (99%)	64 (81%)	15 (19%)	1	8
16	P	72/74 (97%)	62 (86%)	10 (14%)	3	19
17	Q	94/97 (97%)	75 (80%)	19 (20%)	1	7
18	R	61/77 (79%)	55 (90%)	6 (10%)	7	30
19	S	71/80 (89%)	53 (75%)	18 (25%)	0	3
20	T	76/82 (93%)	62 (82%)	14 (18%)	1	9
21	U	19/22 (86%)	17 (90%)	2 (10%)	6	27
All	All	1984/2112 (94%)	1622 (82%)	362 (18%)	2	10

All (362) 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	20	GLU
2	B	21	ARG
2	B	39	ILE
2	B	67	THR
2	B	76	GLN
2	B	106	LYS
2	B	110	GLN
2	B	115	LEU
2	B	126	GLU
2	B	127	ILE
2	B	133	LYS
2	B	142	LEU
2	B	144	ARG
2	B	155	LEU
2	B	162	ILE
2	B	164	VAL
2	B	170	GLU
2	B	175	ARG

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Mol	Chain	Res	Type
2	B	178	ARG
2	B	187	LEU
2	B	189	ASP
2	B	208	ILE
2	B	221	LEU
2	B	226	ARG
2	B	238	LEU
2	B	239	VAL
3	C	3	ASN
3	C	8	ILE
3	C	11	ARG
3	C	14	ILE
3	C	15	THR
3	C	16	ARG
3	C	27	LYS
3	C	30	ARG
3	C	34	LEU
3	C	45	LYS
3	C	47	LEU
3	C	55	VAL
3	C	59	ARG
3	C	62	ASP
3	C	64	VAL
3	C	68	VAL
3	C	70	VAL
3	C	76	VAL
3	C	82	GLU
3	C	83	ARG
3	C	89	GLU
3	C	91	LEU
3	C	93	LYS
3	C	94	LEU
3	C	97	LYS
3	C	101	LEU
3	C	104	GLN
3	C	111	LEU
3	C	131	ARG
3	C	135	LYS
3	C	138	VAL
3	C	143	GLU
3	C	144	SER
3	C	164	ARG

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Mol	Chain	Res	Type
3	C	165	THR
3	C	167	TRP
3	C	172	ARG
3	C	177	THR
3	C	178	LEU
3	C	188	LEU
3	C	191	THR
3	C	192	THR
3	C	195	VAL
3	C	202	ILE
3	C	204	LEU
4	D	3	ARG
4	D	8	VAL
4	D	10	ARG
4	D	13	ARG
4	D	19	LEU
4	D	25	ARG
4	D	26	CYS
4	D	36	ARG
4	D	38	TYR
4	D	45	GLN
4	D	47	ARG
4	D	50	ARG
4	D	64	LEU
4	D	78	LEU
4	D	81	GLU
4	D	96	LEU
4	D	99	SER
4	D	107	ARG
4	D	122	ARG
4	D	127	THR
4	D	135	LEU
4	D	153	ARG
4	D	154	ASN
4	D	157	LEU
4	D	159	ARG
4	D	160	GLN
4	D	162	LEU
4	D	169	LYS
4	D	170	VAL
4	D	182	LYS
4	D	191	ARG

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Mol	Chain	Res	Type
4	D	194	LEU
4	D	202	LEU
5	E	11	ILE
5	E	12	LEU
5	E	13	ILE
5	E	15	ARG
5	E	16	THR
5	E	24	ARG
5	E	26	PHE
5	E	41	VAL
5	E	47	LYS
5	E	51	VAL
5	E	53	LEU
5	E	63	ARG
5	E	64	ARG
5	E	65	ASN
5	E	68	GLU
5	E	76	ILE
5	E	79	GLU
5	E	87	SER
5	E	105	VAL
5	E	107	ARG
5	E	116	THR
5	E	125	SER
5	E	137	GLU
5	E	144	THR
5	E	149	GLU
5	E	150	ARG
5	E	153	LYS
6	F	19	LEU
6	F	22	GLU
6	F	23	LYS
6	F	24	GLU
6	F	31	GLU
6	F	40	VAL
6	F	43	LEU
6	F	54	LYS
6	F	75	LEU
6	F	82	ARG
6	F	91	VAL
6	F	93	SER
6	F	100	ASN

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Mol	Chain	Res	Type
7	G	11	GLN
7	G	12	LEU
7	G	21	VAL
7	G	24	THR
7	G	27	ILE
7	G	38	LEU
7	G	54	THR
7	G	57	GLU
7	G	59	LEU
7	G	73	MET
7	G	75	VAL
7	G	96	GLN
7	G	113	GLU
7	G	115	ARG
7	G	146	GLU
7	G	153	HIS
8	H	6	ILE
8	H	15	ASN
8	H	18	ARG
8	H	23	SER
8	H	26	VAL
8	H	63	LEU
8	H	79	VAL
8	H	83	ILE
8	H	85	ARG
8	H	87	SER
8	H	91	ARG
8	H	92	ARG
8	H	93	VAL
8	H	98	LYS
8	H	112	LEU
8	H	119	LEU
8	H	127	LEU
8	H	133	LEU
9	I	9	ARG
9	I	11	LYS
9	I	14	VAL
9	I	38	GLN
9	I	47	LEU
9	I	51	ARG
9	I	63	ILE
9	I	64	THR

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Mol	Chain	Res	Type
9	I	65	VAL
9	I	74	ILE
9	I	79	LEU
9	I	83	ARG
9	I	85	LEU
9	I	99	LEU
9	I	108	VAL
9	I	116	LYS
9	I	118	LYS
9	I	121	ARG
10	J	5	ARG
10	J	7	LYS
10	J	8	LEU
10	J	9	ARG
10	J	12	ASP
10	J	16	LEU
10	J	19	SER
10	J	21	GLN
10	J	23	ILE
10	J	33	GLN
10	J	38	ILE
10	J	44	VAL
10	J	49	VAL
10	J	57	LYS
10	J	60	ARG
10	J	74	ILE
10	J	75	ILE
10	J	76	ASN
10	J	79	ARG
10	J	81	THR
10	J	88	LEU
10	J	92	THR
10	J	94	VAL
10	J	96	ILE
11	K	11	LYS
11	K	14	VAL
11	K	29	ILE
11	K	33	THR
11	K	75	TYR
11	K	77	MET
11	K	84	VAL
11	K	87	THR

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Mol	Chain	Res	Type
11	K	114	VAL
12	L	7	ILE
12	L	11	VAL
12	L	17	LYS
12	L	18	VAL
12	L	19	ARG
12	L	20	LYS
12	L	21	LYS
12	L	28	LYS
12	L	33	ARG
12	L	41	ARG
12	L	75	HIS
12	L	81	SER
12	L	82	VAL
12	L	85	ILE
12	L	89	ARG
12	L	97	ARG
12	L	101	VAL
12	L	113	ARG
12	L	122	THR
12	L	126	LYS
13	M	3	ARG
13	M	9	ILE
13	M	14	ARG
13	M	32	GLU
13	M	36	LYS
13	M	63	THR
13	M	64	TRP
13	M	65	LYS
13	M	66	LEU
13	M	69	GLU
13	M	74	VAL
13	M	88	ARG
13	M	90	LEU
13	M	106	ASN
13	M	109	THR
13	M	110	ARG
14	N	6	LEU
14	N	7	ILE
14	N	8	GLU
14	N	18	VAL
14	N	22	THR

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Mol	Chain	Res	Type
14	N	24	CYS
14	N	33	VAL
14	N	44	LEU
14	N	45	ARG
14	N	47	LEU
15	O	5	LYS
15	O	6	GLU
15	O	8	LYS
15	O	22	THR
15	O	29	VAL
15	O	31	LEU
15	O	34	LEU
15	O	39	LEU
15	O	44	LYS
15	O	56	LEU
15	O	70	LEU
15	O	71	GLN
15	O	77	ARG
15	O	81	LEU
15	O	82	ILE
16	P	1	MET
16	P	2	VAL
16	P	20	VAL
16	P	33	ILE
16	P	43	LYS
16	P	46	PRO
16	P	53	VAL
16	P	65	GLN
16	P	69	THR
16	P	74	LEU
17	Q	4	LYS
17	Q	5	VAL
17	Q	6	LEU
17	Q	9	VAL
17	Q	14	LYS
17	Q	15	MET
17	Q	22	LEU
17	Q	24	GLU
17	Q	35	VAL
17	Q	36	ILE
17	Q	50	LYS
17	Q	58	GLU

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Mol	Chain	Res	Type
17	Q	59	ILE
17	Q	60	ILE
17	Q	77	VAL
17	Q	85	VAL
17	Q	92	ARG
17	Q	98	LEU
17	Q	100	LYS
18	R	28	GLU
18	R	47	THR
18	R	51	LEU
18	R	54	ARG
18	R	69	THR
18	R	82	THR
19	S	4	SER
19	S	5	LEU
19	S	6	LYS
19	S	7	LYS
19	S	11	VAL
19	S	15	LEU
19	S	22	LEU
19	S	31	ILE
19	S	32	LYS
19	S	36	ARG
19	S	37	ARG
19	S	39	THR
19	S	41	VAL
19	S	43	GLU
19	S	49	ILE
19	S	58	VAL
19	S	62	ILE
19	S	63	THR
20	T	10	LEU
20	T	11	SER
20	T	14	LYS
20	T	23	ARG
20	T	24	LEU
20	T	33	ILE
20	T	48	LYS
20	T	53	LEU
20	T	56	MET
20	T	73	HIS
20	T	74	LYS

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Mol	Chain	Res	Type
20	T	75	ASN
20	T	100	ILE
20	T	105	SER
21	U	8	THR
21	U	22	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	37	ASN
2	B	110	GLN
3	C	6	HIS
3	C	108	ASN
3	C	123	GLN
4	D	129	ASN
4	D	161	ASN
5	E	38	GLN
5	E	56	GLN
5	E	78	HIS
6	F	73	ASN
6	F	100	ASN
8	H	15	ASN
9	I	124	GLN
10	J	56	HIS
12	L	8	ASN
15	O	62	GLN
16	P	76	GLN
20	T	18	GLN
20	T	90	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1506/1522 (98%)	290 (19%)	34 (2%)

All (290) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	4	U
1	A	9	G

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Mol	Chain	Res	Type
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	51	A
1	A	80	G
1	A	81	U
1	A	101	A
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	144	G
1	A	163	C
1	A	182	U
1	A	190(E)	U
1	A	195	A
1	A	197	A
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	247	G
1	A	251	G
1	A	252	U
1	A	254	G
1	A	266	G
1	A	267	C
1	A	289	G
1	A	301	G
1	A	319	G
1	A	321	A
1	A	328	C
1	A	329	A
1	A	345	C
1	A	347	G
1	A	350	G

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Mol	Chain	Res	Type
1	A	352	C
1	A	353	A
1	A	354	G
1	A	356	A
1	A	367	U
1	A	371	G
1	A	372	C
1	A	373	A
1	A	374	A
1	A	384	G
1	A	390	C
1	A	398	C
1	A	406	G
1	A	409	G
1	A	412	A
1	A	413	G
1	A	424	G
1	A	429	U
1	A	439	A
1	A	452	A
1	A	461	C
1	A	481	G
1	A	482	A
1	A	483	C
1	A	484	G
1	A	485	G
1	A	486	U
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	527	7MG
1	A	530	G
1	A	531	U
1	A	532	A
1	A	533	A
1	A	536	C
1	A	545	C

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Mol	Chain	Res	Type
1	A	547	A
1	A	559	A
1	A	560	U
1	A	562	C
1	A	563	A
1	A	564	C
1	A	569	C
1	A	572	A
1	A	573	A
1	A	576	G
1	A	577	G
1	A	579	G
1	A	588	G
1	A	631	G
1	A	651	C
1	A	653	A
1	A	665	A
1	A	666	G
1	A	670	G
1	A	671	G
1	A	687	A
1	A	688	G
1	A	695	A
1	A	701	C
1	A	702	A
1	A	715	A
1	A	721	G
1	A	722	A
1	A	723	U
1	A	731	G
1	A	741	G
1	A	746	A
1	A	749	C
1	A	753	A
1	A	755	G
1	A	759	A
1	A	777	A
1	A	781	A
1	A	782	A
1	A	785	G
1	A	793	U
1	A	794	A

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Mol	Chain	Res	Type
1	A	813	U
1	A	817	C
1	A	818	G
1	A	819	A
1	A	827	U
1	A	828	A
1	A	839	U
1	A	840	C
1	A	841	U
1	A	848	C
1	A	857	C
1	A	858	G
1	A	872	A
1	A	873	A
1	A	876	G
1	A	877	C
1	A	889	A
1	A	902	G
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	939	G
1	A	961	U
1	A	966	M2G
1	A	969	A
1	A	971	G
1	A	975	A
1	A	976	G
1	A	977	A
1	A	982	U
1	A	989	C
1	A	991	U
1	A	992	U
1	A	993	G
1	A	997	U
1	A	999	C
1	A	1003	G
1	A	1003(A)	G
1	A	1005	A
1	A	1007	C
1	A	1009	G

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Mol	Chain	Res	Type
1	A	1016	A
1	A	1020	U
1	A	1021	G
1	A	1022	G
1	A	1024	G
1	A	1025	U
1	A	1026	G
1	A	1027	C
1	A	1028	C
1	A	1029	C
1	A	1030(A)	G
1	A	1030(B)	C
1	A	1030(C)	G
1	A	1030(D)	A
1	A	1031	G
1	A	1033	G
1	A	1036	G
1	A	1039	C
1	A	1045	C
1	A	1049	U
1	A	1050	G
1	A	1051	C
1	A	1053	G
1	A	1065	U
1	A	1066	C
1	A	1094	G
1	A	1095	U
1	A	1100	C
1	A	1101	A
1	A	1104	G
1	A	1119	C
1	A	1124	G
1	A	1125	U
1	A	1126	U
1	A	1127	G
1	A	1129	C
1	A	1130	A
1	A	1131	G
1	A	1135	U
1	A	1136	U
1	A	1137	C
1	A	1139	G

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Mol	Chain	Res	Type
1	A	1140	C
1	A	1146	A
1	A	1152	A
1	A	1154	G
1	A	1157	A
1	A	1159	U
1	A	1160	G
1	A	1162	C
1	A	1182	G
1	A	1188	A
1	A	1196	U
1	A	1197	G
1	A	1201	A
1	A	1202	G
1	A	1211	U
1	A	1212	U
1	A	1213	A
1	A	1214	C
1	A	1225	A
1	A	1227	A
1	A	1233	G
1	A	1238	A
1	A	1240	U
1	A	1241	G
1	A	1250	A
1	A	1253	G
1	A	1256	A
1	A	1257	U
1	A	1258	G
1	A	1260	C
1	A	1270	C
1	A	1278	U
1	A	1279	A
1	A	1280	A
1	A	1281	U
1	A	1285	A
1	A	1287	A
1	A	1300	G
1	A	1302	U
1	A	1303	C
1	A	1305	G
1	A	1312	G

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Mol	Chain	Res	Type
1	A	1320	C
1	A	1322	C
1	A	1323	G
1	A	1335	C
1	A	1336	C
1	A	1338	G
1	A	1346	A
1	A	1353	G
1	A	1363	A
1	A	1368	G
1	A	1370	G
1	A	1379	G
1	A	1380	U
1	A	1381	U
1	A	1394	A
1	A	1398	A
1	A	1402	4OC
1	A	1407	5MC
1	A	1408	A
1	A	1410	G
1	A	1414	U
1	A	1443	G
1	A	1446	A
1	A	1447	G
1	A	1486	G
1	A	1492	A
1	A	1493	A
1	A	1494	G
1	A	1497	G
1	A	1498	UR3
1	A	1499	A
1	A	1503	A
1	A	1506	U
1	A	1529	G
1	A	1530	G
1	A	1544	U

All (34) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	115	G
1	A	129(A)	G

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Mol	Chain	Res	Type
1	A	181	G
1	A	250	A
1	A	251	G
1	A	328	C
1	A	353	A
1	A	372	C
1	A	428	G
1	A	484	G
1	A	485	G
1	A	509	A
1	A	518	C
1	A	530	G
1	A	532	A
1	A	559	A
1	A	687	A
1	A	701	C
1	A	748	C
1	A	793	U
1	A	812	C
1	A	960	U
1	A	991	U
1	A	992	U
1	A	1049	U
1	A	1065	U
1	A	1129	C
1	A	1139	G
1	A	1145	C
1	A	1181	G
1	A	1201	A
1	A	1380	U
1	A	1493	A
1	A	1505	G

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

16 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	MA6	A	1519[A]	1	23,26,27	1.12	2 (8%)	33,38,41	1.04	1 (3%)
1	M2G	A	966	1	24,27,28	0.87	0	33,40,43	0.82	0
1	MA6	A	1518[A]	1	23,26,27	0.88	2 (8%)	33,38,41	0.90	1 (3%)
1	MA6	A	1518[B]	1	23,26,27	1.35	5 (21%)	33,38,41	0.94	1 (3%)
1	PSU	A	516	1,22	18,21,22	1.05	2 (11%)	21,30,33	2.75	6 (28%)
1	MA6	A	1519[B]	1	23,26,27	1.47	5 (21%)	33,38,41	0.91	3 (9%)
1	4OC	A	1402	1	20,23,24	0.88	1 (5%)	25,32,35	0.82	1 (4%)
1	2MG	A	1207	1	23,26,27	1.24	3 (13%)	33,38,41	1.30	5 (15%)
1	7MG	A	527	1	23,26,27	4.26	6 (26%)	27,39,42	2.14	9 (33%)
1	5MC	A	1404	1	19,22,23	0.92	1 (5%)	26,32,35	1.17	4 (15%)
1	PSU	A	1540	1	18,21,22	1.04	1 (5%)	21,30,33	1.71	5 (23%)
1	5MC	A	1407	1	19,22,23	1.01	1 (5%)	26,32,35	1.14	3 (11%)
1	PSU	A	1541	1	18,21,22	1.06	1 (5%)	21,30,33	1.94	4 (19%)
1	5MC	A	967	1	19,22,23	1.11	2 (10%)	26,32,35	1.12	4 (15%)
1	UR3	A	1498	1	19,22,23	1.00	2 (10%)	26,32,35	1.08	1 (3%)
1	5MC	A	1400	1	19,22,23	1.10	2 (10%)	26,32,35	1.01	2 (7%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	A	1541	1	-	1/7/25/26	0/2/2/2
1	5MC	A	967	1	-	0/7/25/26	0/2/2/2
1	UR3	A	1498	1	-	0/7/25/26	0/2/2/2
1	5MC	A	1400	1	-	1/7/25/26	0/2/2/2

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	7MG	C8-N9	-18.54	1.33	1.45
1	A	527	7MG	C5-N7	5.48	1.42	1.35
1	A	1540	PSU	C6-C5	3.65	1.39	1.35
1	A	1207	2MG	C2-N2	3.62	1.41	1.33
1	A	527	7MG	C4-N9	-3.58	1.33	1.37
1	A	1519[B]	MA6	C5-C4	3.39	1.45	1.39
1	A	527	7MG	C2-N2	3.26	1.41	1.34
1	A	1541	PSU	C6-C5	3.12	1.38	1.35
1	A	1519[A]	MA6	C5-C4	3.10	1.44	1.39
1	A	1518[B]	MA6	C5-C4	3.05	1.44	1.39
1	A	967	5MC	C2-N1	2.93	1.46	1.40
1	A	1400	5MC	C6-C5	2.88	1.39	1.34
1	A	1519[A]	MA6	C8-N9	2.82	1.42	1.37
1	A	516	PSU	C6-C5	2.73	1.38	1.35
1	A	1519[B]	MA6	C2-N1	2.61	1.38	1.33
1	A	1519[B]	MA6	C8-N9	2.57	1.41	1.37
1	A	967	5MC	C2-N3	2.56	1.41	1.36
1	A	1518[B]	MA6	C8-N9	2.55	1.41	1.37
1	A	1407	5MC	C2-N1	2.53	1.45	1.40
1	A	1400	5MC	C2-N3	2.35	1.41	1.36
1	A	1404	5MC	C2-N3	2.25	1.40	1.36
1	A	1518[A]	MA6	C5-C4	2.22	1.43	1.39
1	A	527	7MG	C4-N3	2.18	1.39	1.34
1	A	1518[A]	MA6	C8-N9	2.17	1.41	1.37
1	A	1519[B]	MA6	C6-N1	2.17	1.38	1.34
1	A	1207	2MG	C2-N1	2.09	1.40	1.36
1	A	1498	UR3	C2-N1	2.08	1.41	1.38
1	A	1519[B]	MA6	C6-N6	2.08	1.42	1.36
1	A	1498	UR3	C4-N3	-2.08	1.36	1.40
1	A	1207	2MG	C5-C6	-2.07	1.36	1.44
1	A	1518[B]	MA6	C2-N1	2.06	1.37	1.33
1	A	1518[B]	MA6	C4-N9	2.05	1.42	1.37
1	A	1402	4OC	C2-N3	2.04	1.40	1.36
1	A	516	PSU	O4'-C1'	-2.02	1.41	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1518[B]	MA6	C8-N7	2.02	1.35	1.31
1	A	527	7MG	C8-N7	-2.01	1.32	1.42

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	516	PSU	N1-C2-N3	6.66	122.19	115.17
1	A	516	PSU	O2-C2-N1	-6.21	116.39	122.79
1	A	516	PSU	C4-N3-C2	-5.50	118.80	126.37
1	A	1541	PSU	C4-N3-C2	-5.15	119.28	126.37
1	A	527	7MG	C5-C6-N1	4.88	119.52	110.94
1	A	1541	PSU	N1-C2-N3	4.57	119.98	115.17
1	A	516	PSU	C6-C5-C4	4.34	121.10	118.17
1	A	1540	PSU	N1-C2-N3	4.31	119.71	115.17
1	A	1540	PSU	C4-N3-C2	-4.27	120.49	126.37
1	A	527	7MG	C2-N3-C4	4.23	119.58	112.30
1	A	527	7MG	C6-C5-N7	4.19	138.43	131.93
1	A	527	7MG	C6-C5-C4	-3.89	115.57	122.40
1	A	516	PSU	C6-N1-C2	-3.79	119.17	122.69
1	A	1207	2MG	C6-C5-N7	-3.30	124.28	130.29
1	A	527	7MG	N9-C4-N3	3.14	130.06	125.46
1	A	1207	2MG	N9-C4-N3	3.07	132.10	125.95
1	A	1407	5MC	N4-C4-N3	-3.04	113.00	118.51
1	A	527	7MG	C5-C4-N3	-2.84	122.79	128.13
1	A	1207	2MG	C5-C4-N3	-2.77	123.98	128.39
1	A	1541	PSU	O2-C2-N1	-2.71	119.99	122.79
1	A	1207	2MG	C6-C5-C4	2.68	122.86	118.83
1	A	1540	PSU	O2-C2-N1	-2.68	120.03	122.79
1	A	527	7MG	C2-N1-C6	-2.68	120.25	125.11
1	A	527	7MG	O6-C6-C5	-2.66	121.10	127.62
1	A	1404	5MC	C5-C4-N3	2.55	124.37	121.75
1	A	1498	UR3	O3'-C3'-C2'	2.45	119.68	111.82
1	A	1400	5MC	N4-C4-N3	-2.42	114.13	118.51
1	A	1404	5MC	N4-C4-N3	-2.39	114.19	118.51
1	A	516	PSU	O4'-C1'-C2'	2.38	108.45	105.15
1	A	527	7MG	N9-C8-N7	2.38	106.74	103.37
1	A	967	5MC	C1'-N1-C6	-2.36	117.27	121.15
1	A	1540	PSU	C6-N1-C2	-2.32	120.53	122.69
1	A	967	5MC	C5-C4-N3	2.30	124.12	121.75
1	A	1404	5MC	C4-N3-C2	-2.30	117.61	120.81
1	A	1518[B]	MA6	C5-C4-N3	-2.30	123.54	126.72
1	A	1404	5MC	C1'-N1-C6	-2.28	117.40	121.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1407	5MC	C5-C4-N3	2.24	124.05	121.75
1	A	1519[B]	MA6	C4-C5-C6	2.19	118.18	115.91
1	A	1518[A]	MA6	C2-N1-C6	2.17	117.14	111.83
1	A	1402	4OC	C2'-C1'-N1	-2.15	110.16	114.24
1	A	1541	PSU	O4'-C1'-C2'	2.13	108.10	105.15
1	A	1207	2MG	C2-N1-C6	-2.10	122.01	124.55
1	A	1400	5MC	C5-C6-N1	-2.09	121.05	123.31
1	A	1519[B]	MA6	C5-C4-N3	-2.08	123.85	126.72
1	A	1407	5MC	O2-C2-N3	-2.07	119.07	122.33
1	A	1540	PSU	O4'-C1'-C2'	2.06	108.01	105.15
1	A	967	5MC	N4-C4-N3	-2.06	114.77	118.51
1	A	1519[B]	MA6	C2-N1-C6	2.04	116.81	111.83
1	A	1519[A]	MA6	C5-C4-N3	-2.03	123.92	126.72
1	A	967	5MC	C4-N3-C2	-2.02	118.00	120.81

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	527	7MG	O4'-C4'-C5'-O5'
1	A	966	M2G	O4'-C4'-C5'-O5'
1	A	1207	2MG	N1-C2-N2-CM2
1	A	1207	2MG	N3-C2-N2-CM2
1	A	1402	4OC	O4'-C4'-C5'-O5'
1	A	1407	5MC	O4'-C4'-C5'-O5'
1	A	1518[B]	MA6	O4'-C4'-C5'-O5'
1	A	1518[B]	MA6	C5-C6-N6-C9
1	A	1519[A]	MA6	O4'-C4'-C5'-O5'
1	A	1519[A]	MA6	C3'-C4'-C5'-O5'
1	A	1519[B]	MA6	C5-C6-N6-C9
1	A	527	7MG	C3'-C4'-C5'-O5'
1	A	1407	5MC	C3'-C4'-C5'-O5'
1	A	1518[A]	MA6	O4'-C4'-C5'-O5'
1	A	1518[B]	MA6	C3'-C4'-C5'-O5'
1	A	1519[B]	MA6	C3'-C4'-C5'-O5'
1	A	1519[B]	MA6	O4'-C4'-C5'-O5'
1	A	1518[B]	MA6	N1-C6-N6-C9
1	A	1519[B]	MA6	N1-C6-N6-C9
1	A	1402	4OC	C3'-C4'-C5'-O5'
1	A	966	M2G	C3'-C4'-C5'-O5'
1	A	1518[A]	MA6	C3'-C4'-C5'-O5'
1	A	1519[A]	MA6	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
1	A	1519[B]	MA6	C5-C6-N6-C10
1	A	1541	PSU	O4'-C1'-C5-C4
1	A	1518[B]	MA6	C5-C6-N6-C10
1	A	1400	5MC	O4'-C4'-C5'-O5'

There are no ring outliers.

7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1519[A]	MA6	1	0
1	A	1518[A]	MA6	1	0
1	A	1518[B]	MA6	2	0
1	A	1519[B]	MA6	1	0
1	A	1402	4OC	2	0
1	A	1540	PSU	1	0
1	A	1498	UR3	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 453 ligands modelled in this entry, 453 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [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	1500/1522 (98%)	-0.56	9 (0%) 85 65	39, 103, 182, 296	4 (0%)
2	B	234/256 (91%)	-0.22	8 (3%) 48 27	83, 115, 192, 217	0
3	C	206/239 (86%)	-0.36	1 (0%) 87 68	87, 114, 150, 183	0
4	D	208/209 (99%)	-0.00	10 (4%) 35 19	71, 103, 143, 192	0
5	E	150/162 (92%)	-0.42	1 (0%) 84 63	64, 90, 123, 150	0
6	F	101/101 (100%)	-0.26	1 (0%) 79 56	92, 120, 150, 213	0
7	G	155/156 (99%)	-0.25	3 (1%) 66 41	109, 133, 184, 220	0
8	H	138/138 (100%)	-0.45	1 (0%) 84 63	66, 92, 122, 155	0
9	I	127/128 (99%)	0.02	2 (1%) 70 45	100, 139, 175, 200	0
10	J	98/105 (93%)	0.38	4 (4%) 41 22	91, 140, 161, 196	0
11	K	116/129 (89%)	-0.16	5 (4%) 40 21	92, 119, 157, 183	0
12	L	124/135 (91%)	-0.16	7 (5%) 30 17	70, 89, 121, 192	0
13	M	118/126 (93%)	-0.08	2 (1%) 69 43	110, 144, 180, 242	0
14	N	60/61 (98%)	0.32	2 (3%) 49 28	98, 119, 153, 198	0
15	O	87/89 (97%)	-0.44	0 100 100	92, 115, 137, 157	0
16	P	83/88 (94%)	-0.17	0 100 100	79, 97, 125, 165	0
17	Q	99/105 (94%)	-0.03	2 (2%) 65 39	75, 97, 125, 145	0
18	R	70/88 (79%)	-0.44	0 100 100	81, 114, 195, 226	0
19	S	80/93 (86%)	0.21	5 (6%) 26 15	117, 155, 191, 206	0
20	T	99/106 (93%)	-0.14	3 (3%) 52 30	79, 105, 146, 169	0
21	U	24/27 (88%)	0.79	3 (12%) 8 6	129, 142, 156, 169	0
All	All	3877/4063 (95%)	-0.31	69 (1%) 67 42	39, 111, 173, 296	4 (0%)

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
21	U	25	LYS	8.9
1	A	1516[A]	G	7.6
19	S	3	ARG	7.6
10	J	100	THR	7.1
19	S	2	PRO	6.6
1	A	1129	C	5.6
4	D	31	CYS	5.1
7	G	5	ARG	4.8
2	B	132	LYS	4.6
1	A	1517[A]	G	4.5
20	T	12	ALA	4.4
4	D	9	CYS	4.2
2	B	133	LYS	4.2
4	D	26	CYS	4.2
7	G	83	ALA	4.0
4	D	4	TYR	3.8
4	D	22	LYS	3.8
12	L	28	LYS	3.7
4	D	2	GLY	3.6
17	Q	100	LYS	3.6
3	C	207	VAL	3.3
10	J	3	LYS	3.2
4	D	19	LEU	3.2
4	D	21	LEU	3.1
10	J	45	ARG	3.1
12	L	47	LYS	3.0
21	U	24	ARG	3.0
4	D	12	CYS	3.0
11	K	125	PHE	3.0
1	A	994	A	3.0
1	A	723	U	2.9
19	S	5	LEU	2.9
11	K	25	TYR	2.9
2	B	22	LYS	2.9
17	Q	27	PHE	2.8
14	N	11	LYS	2.8
1	A	1533	C	2.7
5	E	154	GLY	2.7
2	B	134	GLU	2.7
20	T	9	ASN	2.7
4	D	23	GLY	2.6
21	U	7	ARG	2.6
9	I	66	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
13	M	119	GLY	2.6
6	F	3	ARG	2.5
9	I	128	ARG	2.5
11	K	124	LYS	2.5
2	B	11	LEU	2.5
11	K	118	GLY	2.3
13	M	9	ILE	2.3
12	L	89	ARG	2.3
14	N	13	THR	2.3
10	J	73	ASP	2.3
19	S	9	VAL	2.3
19	S	37	ARG	2.3
12	L	26	ALA	2.3
12	L	128	ALA	2.2
7	G	6	ARG	2.2
8	H	90	GLY	2.2
2	B	144	ARG	2.2
1	A	1539	C	2.1
2	B	137	ARG	2.1
12	L	19	ARG	2.1
2	B	140	HIS	2.1
1	A	1493	A	2.1
12	L	25	PRO	2.1
11	K	123	LYS	2.1
20	T	11	SER	2.0
1	A	839	U	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	1540	20/21	0.85	0.19	210,230,255,256	0
1	PSU	A	1541	20/21	0.90	0.16	209,230,242,244	0
1	MA6	A	1518[A]	24/25	0.92	0.15	73,79,83,87	24
1	MA6	A	1518[B]	24/25	0.92	0.15	80,83,91,94	24
1	5MC	A	1407	21/22	0.95	0.07	93,104,118,120	0
1	MA6	A	1519[A]	24/25	0.96	0.09	68,73,77,81	24
1	MA6	A	1519[B]	24/25	0.96	0.09	69,74,75,77	24

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	5MC	A	1404	21/22	0.96	0.14	70,87,96,102	0
1	2MG	A	1207	24/25	0.96	0.06	111,117,122,131	0
1	4OC	A	1402	22/23	0.97	0.10	80,92,108,108	0
1	PSU	A	516	20/21	0.98	0.04	88,102,114,116	0
1	5MC	A	1400	21/22	0.98	0.09	65,79,104,105	0
1	7MG	A	527	24/25	0.98	0.06	81,89,105,113	0
1	M2G	A	966	25/26	0.98	0.07	85,98,120,126	0
1	5MC	A	967	21/22	0.98	0.08	94,105,113,116	0
1	UR3	A	1498	21/22	0.98	0.07	76,85,96,100	0

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	A	1817	1/1	0.26	0.25	499,499,499,499	0
22	MG	A	1778	1/1	0.36	0.35	111,111,111,111	0
22	MG	A	1941	1/1	0.36	0.13	457,457,457,457	0
22	MG	A	1970	1/1	0.38	0.18	394,394,394,394	0
22	MG	A	1870	1/1	0.39	0.13	449,449,449,449	0
22	MG	A	1948	1/1	0.41	0.14	503,503,503,503	0
22	MG	A	1806	1/1	0.44	0.10	444,444,444,444	0
22	MG	A	1786	1/1	0.44	0.22	115,115,115,115	0
22	MG	A	1949	1/1	0.44	0.10	481,481,481,481	0
22	MG	A	1802	1/1	0.44	0.12	464,464,464,464	0
22	MG	A	1937	1/1	0.45	0.09	443,443,443,443	0
22	MG	A	1944	1/1	0.46	0.10	461,461,461,461	0
22	MG	A	1764	1/1	0.46	0.20	148,148,148,148	0
22	MG	A	1920	1/1	0.47	0.15	444,444,444,444	0
22	MG	A	1878	1/1	0.50	0.11	455,455,455,455	0
22	MG	A	1889	1/1	0.51	0.15	392,392,392,392	0
22	MG	D	305	1/1	0.52	0.13	418,418,418,418	0
22	MG	A	2015	1/1	0.53	0.17	414,414,414,414	0
22	MG	A	1845	1/1	0.55	0.21	521,521,521,521	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	A	1871	1/1	0.56	0.11	417,417,417,417	0
22	MG	A	1803	1/1	0.56	0.15	447,447,447,447	0
22	MG	A	1911	1/1	0.57	0.16	425,425,425,425	0
22	MG	A	1801	1/1	0.57	0.12	392,392,392,392	0
22	MG	A	1798	1/1	0.60	0.15	374,374,374,374	0
22	MG	A	1959	1/1	0.61	0.32	382,382,382,382	0
22	MG	A	1919	1/1	0.61	0.20	440,440,440,440	0
22	MG	A	2011	1/1	0.62	0.37	96,96,96,96	0
22	MG	E	205	1/1	0.62	0.15	550,550,550,550	0
22	MG	A	1912	1/1	0.63	0.14	429,429,429,429	0
22	MG	A	1695	1/1	0.63	0.59	127,127,127,127	0
22	MG	A	1916	1/1	0.64	0.13	445,445,445,445	0
22	MG	A	1666	1/1	0.66	0.27	100,100,100,100	0
22	MG	A	1992	1/1	0.66	0.12	495,495,495,495	0
22	MG	A	1866	1/1	0.67	0.10	354,354,354,354	0
22	MG	A	1904	1/1	0.67	0.18	469,469,469,469	0
22	MG	A	1872	1/1	0.67	0.11	378,378,378,378	0
22	MG	A	1926	1/1	0.67	0.13	439,439,439,439	0
22	MG	A	1851	1/1	0.67	0.23	365,365,365,365	0
22	MG	A	1961	1/1	0.67	0.27	379,379,379,379	0
22	MG	A	1672	1/1	0.68	0.27	121,121,121,121	0
22	MG	A	1835	1/1	0.68	0.18	516,516,516,516	0
22	MG	A	1702	1/1	0.69	0.40	105,105,105,105	0
22	MG	A	1760	1/1	0.69	0.27	115,115,115,115	0
22	MG	A	1694	1/1	0.69	0.15	94,94,94,94	0
22	MG	A	1658	1/1	0.69	0.34	99,99,99,99	0
22	MG	A	1890	1/1	0.69	0.12	469,469,469,469	0
22	MG	A	1669	1/1	0.70	0.27	99,99,99,99	0
22	MG	A	1707	1/1	0.70	0.40	99,99,99,99	0
22	MG	A	1820	1/1	0.70	0.14	382,382,382,382	0
22	MG	O	1001	1/1	0.70	0.08	183,183,183,183	0
22	MG	L	201	1/1	0.71	0.24	342,342,342,342	0
22	MG	A	1930	1/1	0.71	0.07	510,510,510,510	0
22	MG	A	1833	1/1	0.73	0.11	497,497,497,497	0
22	MG	A	1797	1/1	0.73	0.14	427,427,427,427	0
22	MG	A	1780	1/1	0.74	0.23	119,119,119,119	0
22	MG	A	1950	1/1	0.74	0.12	424,424,424,424	0
22	MG	A	1768	1/1	0.74	0.29	119,119,119,119	0
22	MG	A	1939	1/1	0.74	0.17	392,392,392,392	0
22	MG	Q	203	1/1	0.74	0.12	406,406,406,406	0
22	MG	A	1651	1/1	0.75	0.27	112,112,112,112	0
22	MG	C	304	1/1	0.75	0.33	475,475,475,475	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
22	MG	A	1795	1/1	0.75	0.26	534,534,534,534	0
22	MG	A	1927	1/1	0.75	0.14	440,440,440,440	0
22	MG	A	1862	1/1	0.75	0.11	474,474,474,474	0
22	MG	A	1931	1/1	0.75	0.10	397,397,397,397	0
22	MG	A	1936	1/1	0.75	0.08	388,388,388,388	0
22	MG	A	1882	1/1	0.76	0.10	443,443,443,443	0
22	MG	A	2004	1/1	0.76	0.14	402,402,402,402	0
22	MG	A	1819	1/1	0.76	0.22	508,508,508,508	0
22	MG	A	1774	1/1	0.76	0.16	263,263,263,263	0
22	MG	A	1616	1/1	0.76	0.21	91,91,91,91	0
22	MG	A	1864	1/1	0.77	0.13	450,450,450,450	0
22	MG	A	1727	1/1	0.77	0.25	97,97,97,97	0
22	MG	A	1701	1/1	0.78	0.29	106,106,106,106	0
22	MG	A	1844	1/1	0.78	0.17	415,415,415,415	0
22	MG	A	1830	1/1	0.78	0.08	331,331,331,331	0
22	MG	A	1808	1/1	0.78	0.07	335,335,335,335	0
22	MG	A	1925	1/1	0.78	0.22	447,447,447,447	0
22	MG	A	1958	1/1	0.79	0.08	431,431,431,431	0
22	MG	A	1839	1/1	0.79	0.20	533,533,533,533	0
22	MG	A	1913	1/1	0.79	0.23	432,432,432,432	0
22	MG	A	1825	1/1	0.79	0.13	409,409,409,409	0
22	MG	A	1974	1/1	0.79	0.34	503,503,503,503	0
22	MG	A	1837	1/1	0.80	0.20	500,500,500,500	0
22	MG	A	1877	1/1	0.80	0.20	407,407,407,407	0
22	MG	A	1815	1/1	0.80	0.14	516,516,516,516	0
22	MG	A	1879	1/1	0.80	0.11	396,396,396,396	0
22	MG	A	1787	1/1	0.80	0.14	98,98,98,98	0
22	MG	A	1917	1/1	0.80	0.27	430,430,430,430	0
22	MG	A	1748	1/1	0.80	0.20	98,98,98,98	0
22	MG	A	1678	1/1	0.80	0.28	105,105,105,105	0
22	MG	A	1902	1/1	0.80	0.12	395,395,395,395	0
22	MG	A	1984	1/1	0.81	0.14	360,360,360,360	0
22	MG	A	1867	1/1	0.81	0.14	364,364,364,364	0
22	MG	A	1706	1/1	0.81	0.11	114,114,114,114	0
22	MG	A	1951	1/1	0.81	0.23	476,476,476,476	0
22	MG	A	1804	1/1	0.81	0.12	506,506,506,506	0
22	MG	A	2016	1/1	0.81	0.23	104,104,104,104	0
22	MG	A	1752	1/1	0.82	0.17	115,115,115,115	0
22	MG	A	1601	1/1	0.82	0.17	101,101,101,101	0
22	MG	A	1670	1/1	0.82	0.20	92,92,92,92	0
22	MG	A	1602	1/1	0.82	0.13	155,155,155,155	0
22	MG	A	1990	1/1	0.83	0.12	259,259,259,259	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	A	1886	1/1	0.83	0.09	361,361,361,361	0
22	MG	A	1929	1/1	0.83	0.13	346,346,346,346	0
22	MG	A	1647	1/1	0.83	0.20	70,70,70,70	0
22	MG	A	1821	1/1	0.83	0.18	377,377,377,377	0
22	MG	A	1893	1/1	0.83	0.22	453,453,453,453	0
22	MG	A	1901	1/1	0.83	0.21	536,536,536,536	0
22	MG	A	1686	1/1	0.83	0.28	99,99,99,99	0
22	MG	A	1969	1/1	0.83	0.29	550,550,550,550	0
22	MG	A	1857	1/1	0.83	0.26	436,436,436,436	0
22	MG	A	1942	1/1	0.83	0.36	487,487,487,487	0
22	MG	A	1749	1/1	0.83	0.26	123,123,123,123	0
22	MG	A	1703	1/1	0.84	0.14	187,187,187,187	0
22	MG	A	1868	1/1	0.84	0.17	452,452,452,452	0
22	MG	A	1826	1/1	0.84	0.22	441,441,441,441	0
22	MG	A	1848	1/1	0.84	0.10	330,330,330,330	0
22	MG	A	1895	1/1	0.84	0.32	472,472,472,472	0
22	MG	A	1784	1/1	0.84	0.22	109,109,109,109	0
22	MG	A	1732	1/1	0.84	0.31	98,98,98,98	0
22	MG	A	1770	1/1	0.84	0.06	122,122,122,122	0
22	MG	A	1754	1/1	0.84	1.02	108,108,108,108	0
22	MG	A	1714	1/1	0.84	0.64	104,104,104,104	0
22	MG	A	1842	1/1	0.85	0.17	424,424,424,424	0
22	MG	A	1975	1/1	0.85	0.23	459,459,459,459	0
22	MG	A	1627	1/1	0.85	0.16	333,333,333,333	0
22	MG	A	1923	1/1	0.85	0.13	427,427,427,427	0
22	MG	A	1785	1/1	0.85	0.28	103,103,103,103	0
22	MG	A	1903	1/1	0.85	0.24	475,475,475,475	0
22	MG	A	1709	1/1	0.85	0.59	105,105,105,105	0
22	MG	A	1614	1/1	0.85	0.36	100,100,100,100	0
22	MG	A	1887	1/1	0.85	0.11	321,321,321,321	0
22	MG	A	1856	1/1	0.85	0.27	461,461,461,461	0
22	MG	A	1661	1/1	0.85	0.52	115,115,115,115	0
22	MG	D	307	1/1	0.85	0.23	376,376,376,376	0
22	MG	A	1964	1/1	0.85	0.08	382,382,382,382	0
22	MG	A	1860	1/1	0.85	0.13	411,411,411,411	0
22	MG	A	1918	1/1	0.85	0.15	441,441,441,441	0
22	MG	A	1971	1/1	0.85	0.16	410,410,410,410	0
22	MG	D	302	1/1	0.86	0.13	87,87,87,87	0
22	MG	A	1996	1/1	0.86	0.17	445,445,445,445	0
22	MG	A	1977	1/1	0.86	0.37	419,419,419,419	0
22	MG	A	1899	1/1	0.86	0.15	345,345,345,345	0
22	MG	A	1838	1/1	0.86	0.22	350,350,350,350	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	A	1991	1/1	0.86	0.14	473,473,473,473	0
22	MG	A	1824	1/1	0.86	0.16	354,354,354,354	0
22	MG	A	1759	1/1	0.87	0.11	111,111,111,111	0
22	MG	A	1715	1/1	0.87	0.27	109,109,109,109	0
22	MG	A	1790	1/1	0.87	0.15	115,115,115,115	0
22	MG	A	1794	1/1	0.87	0.28	103,103,103,103	0
22	MG	A	1876	1/1	0.87	0.21	460,460,460,460	0
22	MG	A	1957	1/1	0.87	0.52	482,482,482,482	0
22	MG	A	1657	1/1	0.87	0.23	110,110,110,110	0
22	MG	E	202	1/1	0.87	0.48	105,105,105,105	0
22	MG	A	1841	1/1	0.87	0.12	315,315,315,315	0
22	MG	A	1648	1/1	0.87	0.55	109,109,109,109	0
22	MG	A	1812	1/1	0.87	0.26	484,484,484,484	0
22	MG	A	1733	1/1	0.87	0.13	85,85,85,85	0
22	MG	A	1943	1/1	0.88	0.37	341,341,341,341	0
22	MG	A	1988	1/1	0.88	0.38	402,402,402,402	0
22	MG	A	1892	1/1	0.88	0.14	329,329,329,329	0
22	MG	A	1852	1/1	0.88	0.30	473,473,473,473	0
22	MG	A	1854	1/1	0.88	0.20	364,364,364,364	0
22	MG	A	1789	1/1	0.88	0.07	118,118,118,118	0
22	MG	A	2000	1/1	0.88	0.21	441,441,441,441	0
22	MG	A	1900	1/1	0.88	0.27	410,410,410,410	0
22	MG	A	1955	1/1	0.88	0.16	374,374,374,374	0
22	MG	A	1606	1/1	0.88	0.26	69,69,69,69	0
22	MG	A	1791	1/1	0.88	0.39	114,114,114,114	0
22	MG	B	302	1/1	0.88	0.20	88,88,88,88	0
22	MG	C	303	1/1	0.88	0.09	429,429,429,429	0
22	MG	A	1805	1/1	0.88	0.14	503,503,503,503	0
22	MG	A	1880	1/1	0.88	0.37	498,498,498,498	0
22	MG	A	1782	1/1	0.88	0.31	89,89,89,89	0
22	MG	A	1932	1/1	0.88	0.17	402,402,402,402	0
22	MG	A	1705	1/1	0.88	0.78	99,99,99,99	0
22	MG	A	1758	1/1	0.88	0.16	96,96,96,96	0
22	MG	A	1914	1/1	0.88	0.22	376,376,376,376	0
22	MG	A	1634	1/1	0.88	0.11	88,88,88,88	0
22	MG	A	1750	1/1	0.88	0.21	109,109,109,109	0
22	MG	A	1813	1/1	0.89	0.18	438,438,438,438	0
22	MG	A	1793	1/1	0.89	0.65	124,124,124,124	0
22	MG	A	1777	1/1	0.89	0.22	112,112,112,112	0
22	MG	A	1952	1/1	0.89	0.28	397,397,397,397	0
22	MG	A	2001	1/1	0.89	0.13	346,346,346,346	0
22	MG	A	1662	1/1	0.89	0.43	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	A	2008	1/1	0.89	0.18	373,373,373,373	0
22	MG	A	1652	1/1	0.89	0.21	76,76,76,76	0
22	MG	A	1873	1/1	0.89	0.25	473,473,473,473	0
22	MG	A	1874	1/1	0.89	0.20	384,384,384,384	0
22	MG	A	2017	1/1	0.89	0.06	80,80,80,80	0
22	MG	A	1736	1/1	0.89	0.13	142,142,142,142	0
22	MG	A	1737	1/1	0.89	0.28	68,68,68,68	0
22	MG	A	1740	1/1	0.89	0.15	81,81,81,81	0
22	MG	A	1667	1/1	0.89	0.23	103,103,103,103	0
22	MG	A	1827	1/1	0.89	0.39	515,515,515,515	0
22	MG	A	1766	1/1	0.89	0.58	93,93,93,93	0
22	MG	A	1720	1/1	0.89	0.19	100,100,100,100	0
22	MG	A	1620	1/1	0.89	0.15	83,83,83,83	0
22	MG	A	1751	1/1	0.89	0.24	69,69,69,69	0
22	MG	A	1946	1/1	0.89	0.40	503,503,503,503	0
22	MG	A	1792	1/1	0.89	0.29	93,93,93,93	0
22	MG	A	1623	1/1	0.90	0.15	112,112,112,112	0
22	MG	A	1883	1/1	0.90	0.12	304,304,304,304	0
22	MG	A	1696	1/1	0.90	0.14	94,94,94,94	0
22	MG	A	1816	1/1	0.90	0.17	458,458,458,458	0
22	MG	A	1947	1/1	0.90	0.17	440,440,440,440	0
22	MG	A	1888	1/1	0.90	0.28	481,481,481,481	0
22	MG	A	2018	1/1	0.90	0.22	82,82,82,82	0
22	MG	A	1828	1/1	0.90	0.19	417,417,417,417	0
22	MG	A	1875	1/1	0.90	0.14	451,451,451,451	0
22	MG	A	1983	1/1	0.90	0.12	393,393,393,393	0
22	MG	A	1725	1/1	0.90	0.27	98,98,98,98	0
22	MG	A	1915	1/1	0.90	0.11	185,185,185,185	0
22	MG	A	1953	1/1	0.90	0.09	295,295,295,295	0
22	MG	A	1796	1/1	0.90	0.23	383,383,383,383	0
22	MG	A	1697	1/1	0.90	0.21	106,106,106,106	0
22	MG	F	201	1/1	0.90	0.12	351,351,351,351	0
22	MG	A	1731	1/1	0.90	0.20	68,68,68,68	0
22	MG	A	1700	1/1	0.90	0.29	97,97,97,97	0
22	MG	A	1960	1/1	0.90	0.21	293,293,293,293	0
22	MG	A	1968	1/1	0.91	0.56	503,503,503,503	0
22	MG	A	2009	1/1	0.91	0.20	79,79,79,79	0
22	MG	A	1681	1/1	0.91	0.34	115,115,115,115	0
22	MG	A	2012	1/1	0.91	0.11	196,196,196,196	0
22	MG	A	1834	1/1	0.91	0.06	265,265,265,265	0
22	MG	A	1818	1/1	0.91	0.12	391,391,391,391	0
22	MG	A	1753	1/1	0.91	0.18	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	A	1861	1/1	0.91	0.15	444,444,444,444	0
22	MG	A	1633	1/1	0.91	0.29	124,124,124,124	0
22	MG	A	1723	1/1	0.91	0.15	81,81,81,81	0
22	MG	A	1905	1/1	0.91	0.24	506,506,506,506	0
22	MG	A	1608	1/1	0.91	0.11	165,165,165,165	0
22	MG	A	1746	1/1	0.91	0.22	86,86,86,86	0
22	MG	A	1622	1/1	0.91	0.38	81,81,81,81	0
22	MG	A	1729	1/1	0.91	0.24	106,106,106,106	0
22	MG	A	1710	1/1	0.91	0.15	124,124,124,124	0
22	MG	A	1999	1/1	0.91	0.36	438,438,438,438	0
22	MG	A	1829	1/1	0.91	0.09	436,436,436,436	0
22	MG	A	1631	1/1	0.91	0.15	173,173,173,173	0
22	MG	A	1853	1/1	0.91	0.36	543,543,543,543	0
22	MG	S	101	1/1	0.91	0.15	101,101,101,101	0
22	MG	A	1630	1/1	0.92	0.29	100,100,100,100	0
22	MG	A	1743	1/1	0.92	0.44	88,88,88,88	0
22	MG	A	1933	1/1	0.92	0.27	374,374,374,374	0
22	MG	A	1763	1/1	0.92	0.31	94,94,94,94	0
22	MG	A	1855	1/1	0.92	0.40	525,525,525,525	0
22	MG	A	1781	1/1	0.92	0.20	95,95,95,95	0
22	MG	A	1744	1/1	0.92	0.23	94,94,94,94	0
22	MG	D	304	1/1	0.92	0.33	526,526,526,526	0
22	MG	A	1896	1/1	0.92	0.22	172,172,172,172	0
22	MG	A	1807	1/1	0.92	0.15	511,511,511,511	0
22	MG	A	1682	1/1	0.92	0.08	187,187,187,187	0
22	MG	A	1809	1/1	0.92	0.33	517,517,517,517	0
22	MG	A	1677	1/1	0.92	0.17	125,125,125,125	0
22	MG	A	1769	1/1	0.92	0.07	134,134,134,134	0
22	MG	N	102	1/1	0.92	0.17	79,79,79,79	0
22	MG	A	1756	1/1	0.92	0.34	132,132,132,132	0
22	MG	P	101	1/1	0.92	0.12	78,78,78,78	0
22	MG	Q	202	1/1	0.92	0.36	538,538,538,538	0
22	MG	A	1849	1/1	0.92	0.10	412,412,412,412	0
22	MG	A	1668	1/1	0.92	0.08	165,165,165,165	0
22	MG	A	1742	1/1	0.93	0.50	81,81,81,81	0
22	MG	A	1921	1/1	0.93	0.29	412,412,412,412	0
22	MG	A	1972	1/1	0.93	0.10	420,420,420,420	0
22	MG	A	1846	1/1	0.93	0.47	490,490,490,490	0
22	MG	A	1674	1/1	0.93	0.17	146,146,146,146	0
22	MG	A	1881	1/1	0.93	0.11	357,357,357,357	0
22	MG	A	1626	1/1	0.93	0.15	70,70,70,70	0
22	MG	A	1928	1/1	0.93	0.19	490,490,490,490	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	A	1604	1/1	0.93	0.05	89,89,89,89	0
22	MG	A	1869	1/1	0.93	0.30	339,339,339,339	0
22	MG	A	1635	1/1	0.93	0.20	66,66,66,66	0
22	MG	A	1643	1/1	0.93	0.26	132,132,132,132	0
22	MG	A	1615	1/1	0.93	0.14	93,93,93,93	0
22	MG	A	1997	1/1	0.93	0.51	172,172,172,172	0
22	MG	A	1765	1/1	0.93	0.20	84,84,84,84	0
22	MG	A	1840	1/1	0.93	0.20	525,525,525,525	0
22	MG	A	1624	1/1	0.93	0.16	100,100,100,100	0
22	MG	A	1738	1/1	0.93	0.47	88,88,88,88	0
22	MG	A	2006	1/1	0.93	0.07	302,302,302,302	0
22	MG	P	102	1/1	0.93	0.15	89,89,89,89	0
22	MG	Q	201	1/1	0.93	0.12	64,64,64,64	0
22	MG	A	1965	1/1	0.93	0.17	296,296,296,296	0
22	MG	A	1673	1/1	0.93	0.12	121,121,121,121	0
22	MG	A	1898	1/1	0.93	0.22	406,406,406,406	0
22	MG	A	1689	1/1	0.94	0.16	138,138,138,138	0
22	MG	A	1607	1/1	0.94	0.18	65,65,65,65	0
22	MG	A	1985	1/1	0.94	0.08	278,278,278,278	0
22	MG	A	1986	1/1	0.94	0.07	225,225,225,225	0
22	MG	A	1922	1/1	0.94	0.16	433,433,433,433	0
22	MG	A	1989	1/1	0.94	0.36	475,475,475,475	0
22	MG	A	1773	1/1	0.94	0.14	69,69,69,69	0
22	MG	A	1863	1/1	0.94	0.15	413,413,413,413	0
22	MG	A	1741	1/1	0.94	0.13	87,87,87,87	0
22	MG	A	1962	1/1	0.94	0.26	273,273,273,273	0
22	MG	A	1945	1/1	0.94	0.36	436,436,436,436	0
22	MG	A	1865	1/1	0.94	0.36	484,484,484,484	0
22	MG	E	206	1/1	0.94	0.26	412,412,412,412	0
22	MG	A	1638	1/1	0.94	0.12	180,180,180,180	0
22	MG	K	201	1/1	0.94	0.19	74,74,74,74	0
22	MG	A	1724	1/1	0.94	0.26	74,74,74,74	0
22	MG	A	1779	1/1	0.94	0.20	101,101,101,101	0
22	MG	A	1665	1/1	0.94	0.47	81,81,81,81	0
22	MG	A	1745	1/1	0.94	0.14	88,88,88,88	0
22	MG	A	1973	1/1	0.94	0.27	446,446,446,446	0
22	MG	A	1619	1/1	0.94	0.24	95,95,95,95	0
22	MG	A	1884	1/1	0.94	0.55	546,546,546,546	0
22	MG	A	2013	1/1	0.94	0.08	227,227,227,227	0
22	MG	A	1954	1/1	0.94	0.17	459,459,459,459	0
22	MG	A	1908	1/1	0.95	0.40	354,354,354,354	0
22	MG	A	1909	1/1	0.95	0.22	312,312,312,312	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	A	1683	1/1	0.95	0.09	110,110,110,110	0
22	MG	A	1772	1/1	0.95	0.06	72,72,72,72	0
22	MG	A	1717	1/1	0.95	0.14	87,87,87,87	0
22	MG	A	1814	1/1	0.95	0.31	481,481,481,481	0
22	MG	A	1610	1/1	0.95	0.06	94,94,94,94	0
22	MG	A	1688	1/1	0.95	0.13	178,178,178,178	0
22	MG	B	301	1/1	0.95	0.08	76,76,76,76	0
22	MG	A	1704	1/1	0.95	0.24	66,66,66,66	0
22	MG	A	1980	1/1	0.95	0.21	340,340,340,340	0
22	MG	A	1639	1/1	0.95	0.11	92,92,92,92	0
22	MG	A	1843	1/1	0.95	0.18	393,393,393,393	0
22	MG	D	303	1/1	0.95	0.12	81,81,81,81	0
22	MG	A	1891	1/1	0.95	0.25	308,308,308,308	0
22	MG	A	1676	1/1	0.95	0.13	63,63,63,63	0
22	MG	A	1987	1/1	0.95	0.13	238,238,238,238	0
22	MG	A	1617	1/1	0.95	0.15	85,85,85,85	0
22	MG	A	1799	1/1	0.95	0.24	446,446,446,446	0
22	MG	A	1644	1/1	0.95	0.12	96,96,96,96	0
22	MG	A	1783	1/1	0.95	0.07	69,69,69,69	0
22	MG	H	201	1/1	0.95	0.12	281,281,281,281	0
22	MG	A	1664	1/1	0.95	0.06	95,95,95,95	0
22	MG	A	1994	1/1	0.95	0.09	158,158,158,158	0
22	MG	A	1712	1/1	0.95	0.20	96,96,96,96	0
22	MG	A	1767	1/1	0.95	0.09	61,61,61,61	0
22	MG	A	1735	1/1	0.95	0.10	73,73,73,73	0
22	MG	A	1788	1/1	0.95	0.14	81,81,81,81	0
22	MG	P	104	1/1	0.95	0.04	89,89,89,89	0
22	MG	A	1831	1/1	0.95	0.08	233,233,233,233	0
22	MG	A	1963	1/1	0.95	0.20	335,335,335,335	0
22	MG	A	1656	1/1	0.95	0.15	100,100,100,100	0
22	MG	A	1906	1/1	0.95	0.11	180,180,180,180	0
22	MG	A	1775	1/1	0.96	0.10	168,168,168,168	0
22	MG	A	1650	1/1	0.96	0.20	112,112,112,112	0
22	MG	A	1711	1/1	0.96	0.07	68,68,68,68	0
22	MG	A	1659	1/1	0.96	0.15	72,72,72,72	0
22	MG	A	1858	1/1	0.96	0.39	473,473,473,473	0
22	MG	A	1859	1/1	0.96	0.07	151,151,151,151	0
22	MG	A	2010	1/1	0.96	0.27	87,87,87,87	0
22	MG	A	1660	1/1	0.96	0.07	160,160,160,160	0
22	MG	A	1924	1/1	0.96	0.11	336,336,336,336	0
22	MG	A	1637	1/1	0.96	0.18	94,94,94,94	0
22	MG	A	1625	1/1	0.96	0.16	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	A	1832	1/1	0.96	0.32	453,453,453,453	0
22	MG	A	1894	1/1	0.96	0.16	227,227,227,227	0
22	MG	A	1739	1/1	0.96	0.07	74,74,74,74	0
22	MG	A	1761	1/1	0.96	0.24	57,57,57,57	0
22	MG	A	1762	1/1	0.96	0.12	69,69,69,69	0
22	MG	C	301	1/1	0.96	0.04	77,77,77,77	0
22	MG	C	302	1/1	0.96	0.05	95,95,95,95	0
22	MG	A	1836	1/1	0.96	0.24	424,424,424,424	0
22	MG	A	1719	1/1	0.96	0.17	102,102,102,102	0
22	MG	A	1934	1/1	0.96	0.22	349,349,349,349	0
22	MG	A	1935	1/1	0.96	0.32	363,363,363,363	0
22	MG	A	1810	1/1	0.96	0.25	460,460,460,460	0
22	MG	A	1685	1/1	0.96	0.13	87,87,87,87	0
22	MG	A	1938	1/1	0.96	0.20	496,496,496,496	0
22	MG	A	1722	1/1	0.96	0.05	89,89,89,89	0
22	MG	A	1940	1/1	0.96	0.24	425,425,425,425	0
22	MG	A	1653	1/1	0.96	0.07	114,114,114,114	0
22	MG	A	1613	1/1	0.96	0.15	58,58,58,58	0
22	MG	A	1675	1/1	0.96	0.16	150,150,150,150	0
22	MG	A	1907	1/1	0.96	0.14	310,310,310,310	0
22	MG	A	1726	1/1	0.96	0.10	77,77,77,77	0
22	MG	A	1690	1/1	0.96	0.14	137,137,137,137	0
22	MG	A	1771	1/1	0.96	0.08	101,101,101,101	0
22	MG	A	1693	1/1	0.96	0.08	209,209,209,209	0
22	MG	A	1730	1/1	0.96	0.27	85,85,85,85	0
22	MG	A	1995	1/1	0.96	0.44	355,355,355,355	0
22	MG	A	1822	1/1	0.96	0.07	229,229,229,229	0
22	MG	A	1823	1/1	0.96	0.17	337,337,337,337	0
22	MG	A	1998	1/1	0.96	0.46	464,464,464,464	0
22	MG	A	1642	1/1	0.96	0.08	81,81,81,81	0
23	ZN	D	301	1/1	0.96	0.26	97,97,97,97	0
22	MG	A	1713	1/1	0.97	0.28	85,85,85,85	0
22	MG	A	1628	1/1	0.97	0.13	130,130,130,130	0
22	MG	A	1612	1/1	0.97	0.18	145,145,145,145	0
22	MG	A	1716	1/1	0.97	0.08	53,53,53,53	0
22	MG	D	306	1/1	0.97	0.29	350,350,350,350	0
22	MG	A	1641	1/1	0.97	0.09	122,122,122,122	0
22	MG	A	1718	1/1	0.97	0.07	65,65,65,65	0
22	MG	E	204	1/1	0.97	0.13	74,74,74,74	0
22	MG	A	1978	1/1	0.97	0.10	184,184,184,184	0
22	MG	A	1847	1/1	0.97	0.14	414,414,414,414	0
22	MG	A	1663	1/1	0.97	0.10	125,125,125,125	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	A	1755	1/1	0.97	0.18	83,83,83,83	0
22	MG	A	1811	1/1	0.97	0.09	181,181,181,181	0
22	MG	A	1691	1/1	0.97	0.19	160,160,160,160	0
22	MG	A	1721	1/1	0.97	0.10	77,77,77,77	0
22	MG	A	1776	1/1	0.97	0.23	460,460,460,460	0
22	MG	A	1679	1/1	0.97	0.14	102,102,102,102	0
22	MG	A	1897	1/1	0.97	0.29	424,424,424,424	0
22	MG	P	103	1/1	0.97	0.20	60,60,60,60	0
22	MG	A	1680	1/1	0.97	0.07	81,81,81,81	0
22	MG	A	1708	1/1	0.97	0.10	117,117,117,117	0
22	MG	A	1671	1/1	0.97	0.28	153,153,153,153	0
22	MG	A	1649	1/1	0.97	0.10	79,79,79,79	0
22	MG	A	1605	1/1	0.97	0.04	112,112,112,112	0
22	MG	A	1632	1/1	0.97	0.07	73,73,73,73	0
22	MG	A	2002	1/1	0.98	0.06	176,176,176,176	0
22	MG	A	1981	1/1	0.98	0.24	451,451,451,451	0
22	MG	A	2005	1/1	0.98	0.32	327,327,327,327	0
22	MG	A	1982	1/1	0.98	0.13	340,340,340,340	0
22	MG	E	201	1/1	0.98	0.08	115,115,115,115	0
22	MG	A	2007	1/1	0.98	0.13	159,159,159,159	0
22	MG	E	203	1/1	0.98	0.04	72,72,72,72	0
22	MG	A	1692	1/1	0.98	0.14	231,231,231,231	0
22	MG	A	1684	1/1	0.98	0.06	86,86,86,86	0
22	MG	A	1621	1/1	0.98	0.21	130,130,130,130	0
22	MG	A	1728	1/1	0.98	0.17	91,91,91,91	0
22	MG	A	1885	1/1	0.98	0.04	132,132,132,132	0
22	MG	A	1967	1/1	0.98	0.30	459,459,459,459	0
22	MG	A	1655	1/1	0.98	0.09	72,72,72,72	0
22	MG	A	1687	1/1	0.98	0.10	81,81,81,81	0
22	MG	A	1609	1/1	0.98	0.05	125,125,125,125	0
22	MG	A	1698	1/1	0.98	0.18	138,138,138,138	0
22	MG	A	1699	1/1	0.98	0.11	89,89,89,89	0
22	MG	A	1747	1/1	0.98	0.04	70,70,70,70	0
22	MG	A	1734	1/1	0.98	0.09	84,84,84,84	0
22	MG	A	1640	1/1	0.98	0.06	49,49,49,49	0
22	MG	A	1976	1/1	0.98	0.06	127,127,127,127	0
22	MG	A	1645	1/1	0.98	0.13	137,137,137,137	0
22	MG	A	1910	1/1	0.98	0.12	222,222,222,222	0
22	MG	A	1603	1/1	0.98	0.09	90,90,90,90	0
22	MG	A	1646	1/1	0.99	0.10	80,80,80,80	0
22	MG	A	1618	1/1	0.99	0.05	71,71,71,71	0
22	MG	A	1629	1/1	0.99	0.11	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	A	1654	1/1	0.99	0.06	127,127,127,127	0
22	MG	A	1757	1/1	0.99	0.17	163,163,163,163	0
22	MG	A	1966	1/1	0.99	0.15	349,349,349,349	0
22	MG	A	2003	1/1	0.99	0.11	400,400,400,400	0
22	MG	A	1956	1/1	0.99	0.14	322,322,322,322	0
22	MG	A	1979	1/1	0.99	0.08	113,113,113,113	0
22	MG	A	1800	1/1	0.99	0.04	124,124,124,124	0
22	MG	B	303	1/1	0.99	0.16	88,88,88,88	0
22	MG	A	1636	1/1	0.99	0.02	63,63,63,63	0
22	MG	A	1850	1/1	0.99	0.05	96,96,96,96	0
22	MG	A	1611	1/1	0.99	0.05	104,104,104,104	0
22	MG	A	1993	1/1	1.00	0.08	36,36,36,36	0
22	MG	A	2014	1/1	1.00	0.05	75,75,75,75	0
23	ZN	N	101	1/1	1.00	0.03	100,100,100,100	0

6.5 Other polymers [i](#)

There are no such residues in this entry.