



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:00 AM UTC

PDB ID : 4DR1 / pdb_00004dr1
Title : Crystal structure of the apo 30S ribosomal subunit from *Thermus thermophilus* (HB8)
Authors : Demirci, H.; Murphy IV, F.; Murphy, E.; Gregory, S.T.; Dahlberg, A.E.; Jogl, G.
Deposited on : 2012-02-16
Resolution : 3.60 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

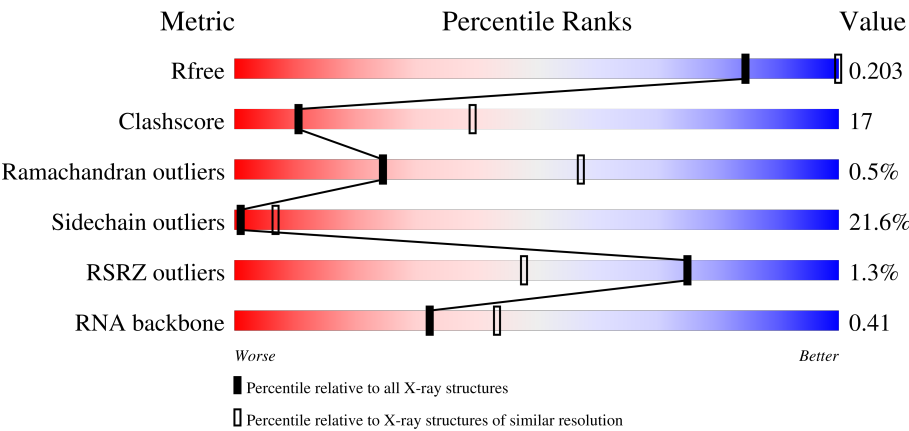
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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.



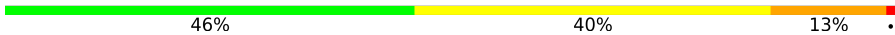
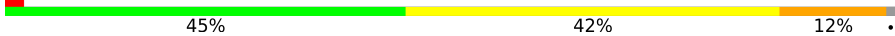
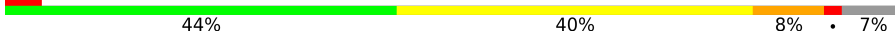
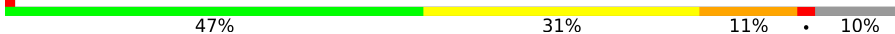
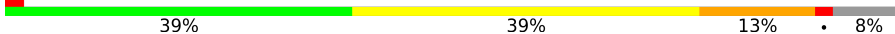
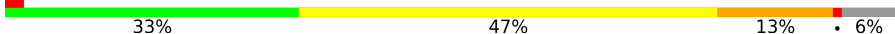
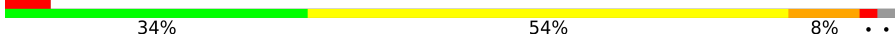
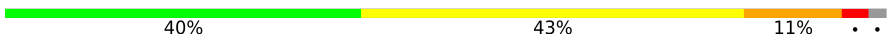
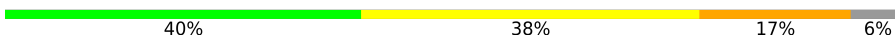
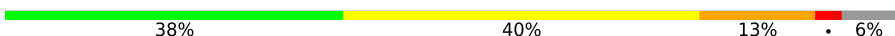
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)
RNA backbone	3983	1014 (4.14-3.06)

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

Mol	Chain	Length	Quality of chain
1	A	1522	44% 41% 14% .
2	B	256	43% 34% 13% . 9%
3	C	239	40% 35% 10% . 14%
4	D	209	4% 51% 36% 11% .

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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	1605	-	-	-	X
22	MG	A	1634	-	-	-	X
22	MG	A	1687	-	-	-	X
22	MG	A	1725	-	-	-	X
22	MG	A	1736	-	-	-	X
22	MG	A	1737	-	-	-	X
22	MG	A	1742	-	-	-	X
22	MG	A	1745	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	MG	A	1758	-	-	-	X
22	MG	A	1794	-	-	-	X
22	MG	A	1810	-	-	-	X
22	MG	A	1828	-	-	-	X

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 52227 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1512	Total	C	N	O	P	0	6	0
			32644	14540	6039	10547	1518			

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 30S 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 30S 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 30S 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 30S 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 30S 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 30S 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 30S 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 30S 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 30S 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 30S 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 30S ribosomal protein S12.

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

- Molecule 13 is a protein called 30S 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 30S 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 30S 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 30S 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 30S ribosomal protein S17.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 18 is a protein called 30S 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 30S 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 30S 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 30S 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	239	Total	Mg	0	0
			239	239		
22	B	2	Total	Mg	0	0
			2	2		
22	C	3	Total	Mg	0	0
			3	3		
22	D	4	Total	Mg	0	0
			4	4		
22	E	1	Total	Mg	0	0
			1	1		
22	F	1	Total	Mg	0	0
			1	1		
22	L	1	Total	Mg	0	0
			1	1		
22	P	2	Total	Mg	0	0
			2	2		
22	Q	1	Total	Mg	0	0
			1	1		

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

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

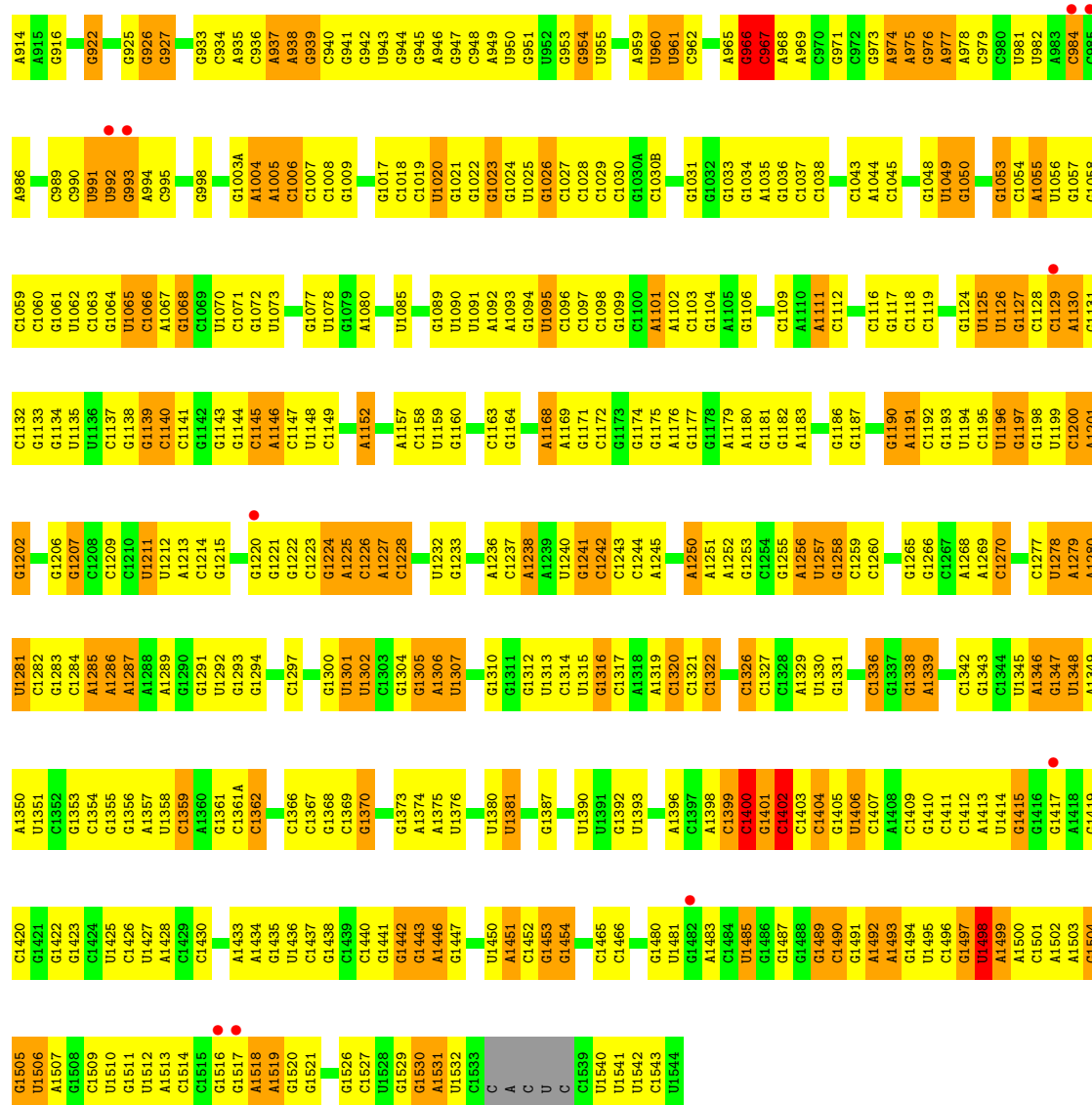
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	N	1	Total	Zn	0	0
			1	1		

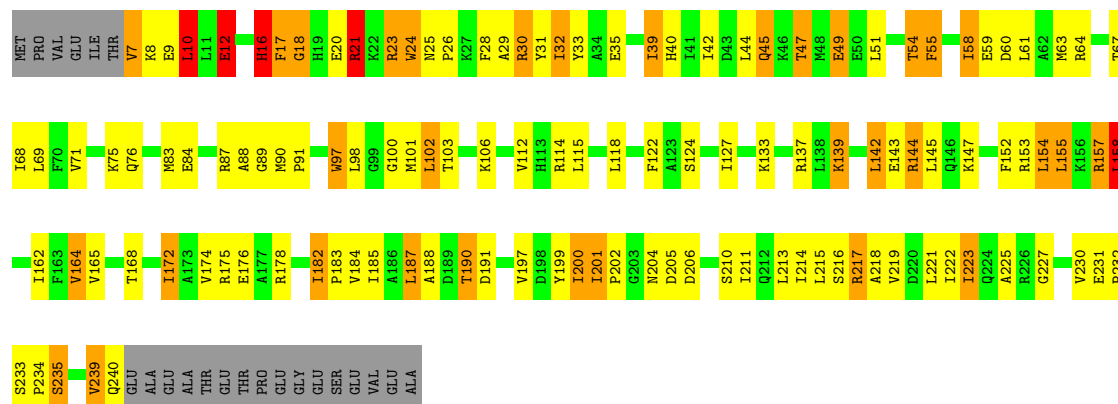
- Molecule 24 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	A	232	Total	O	0	0
			232	232		
24	E	3	Total	O	0	0
			3	3		
24	L	1	Total	O	0	0
			1	1		
24	Q	1	Total	O	0	0
			1	1		
24	T	2	Total	O	0	0
			2	2		

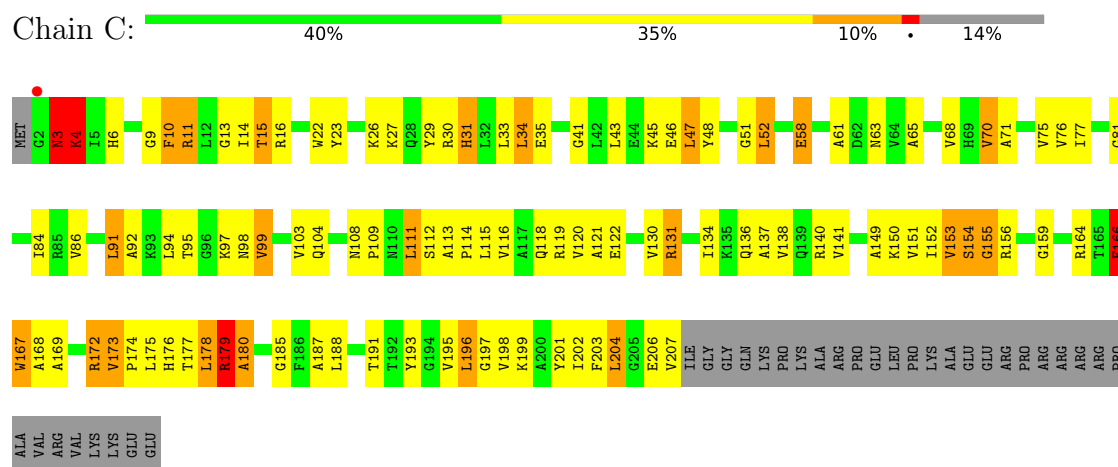


• Molecule 2: 30S ribosomal protein S2

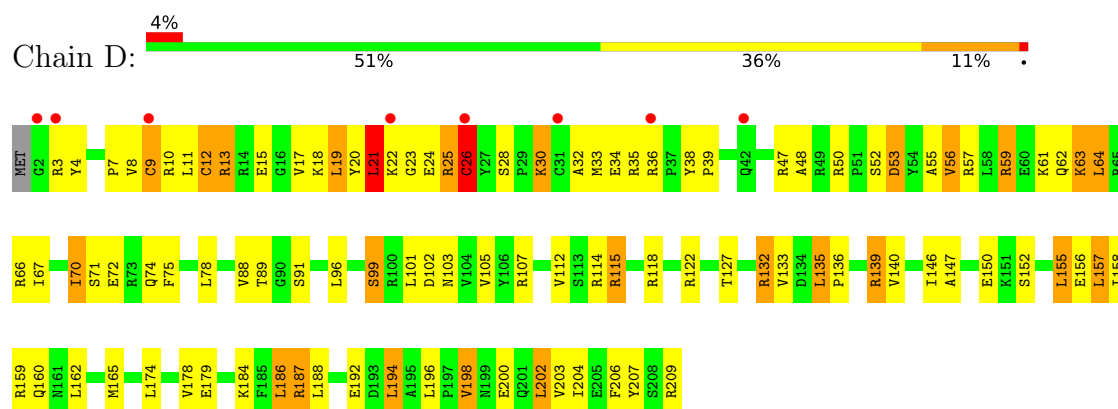
Chain B: 43% 34% 13% 9%



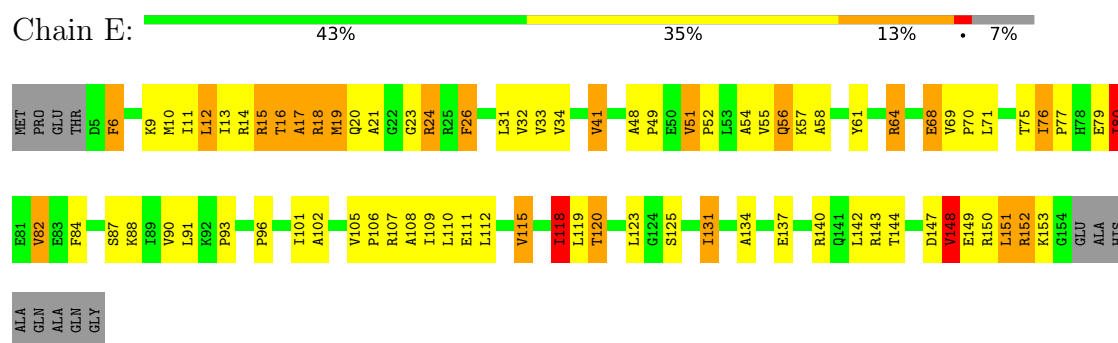
- Molecule 3: 30S ribosomal protein S3



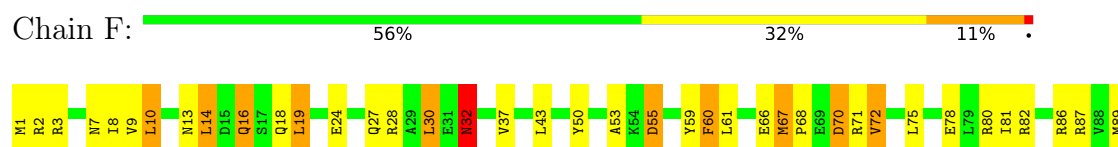
- Molecule 4: 30S ribosomal protein S4

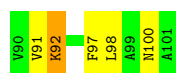


- Molecule 5: 30S ribosomal protein S5



- Molecule 6: 30S ribosomal protein S6





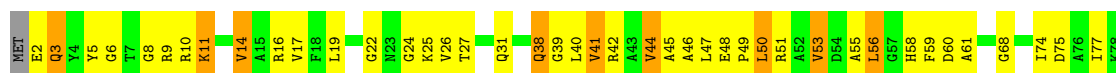
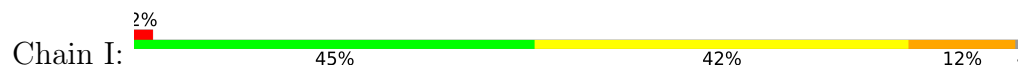
• Molecule 7: 30S ribosomal protein S7



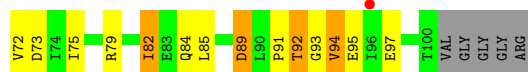
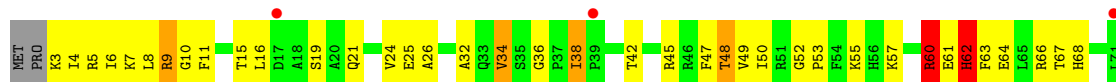
• Molecule 8: 30S ribosomal protein S8



• Molecule 9: 30S ribosomal protein S9

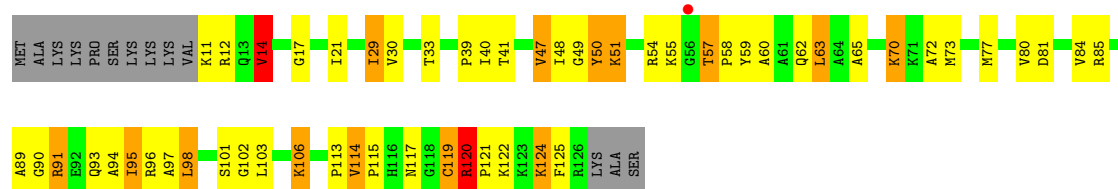


• Molecule 10: 30S ribosomal protein S10

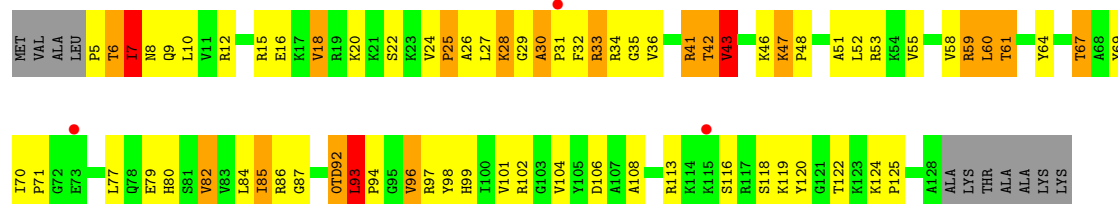


• Molecule 11: 30S ribosomal protein S11

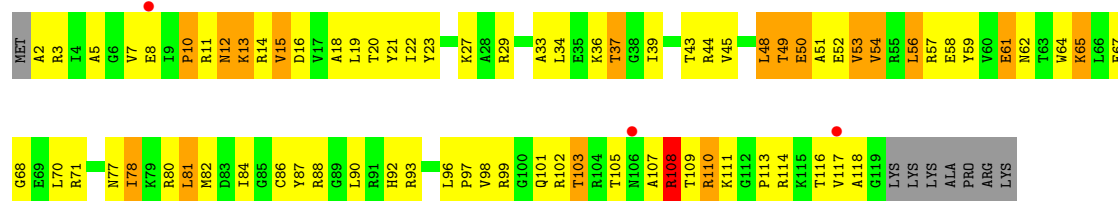




• Molecule 12: 30S ribosomal protein S12



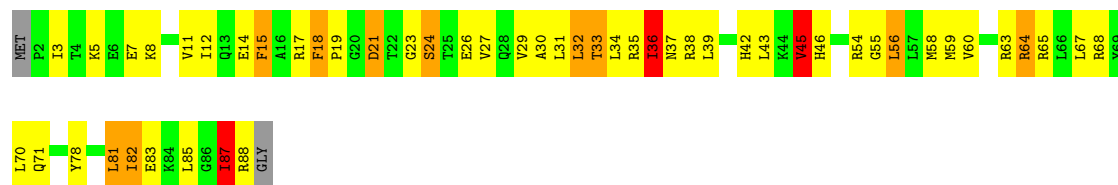
• Molecule 13: 30S ribosomal protein S13



• Molecule 14: 30S ribosomal protein S14

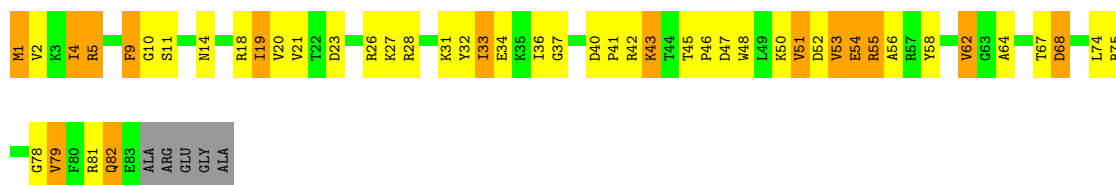


• Molecule 15: 30S ribosomal protein S15

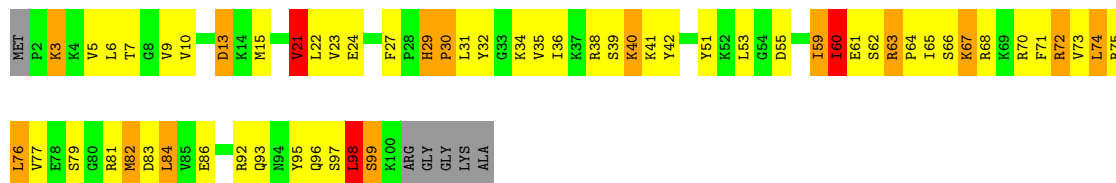


• Molecule 16: 30S ribosomal protein S16

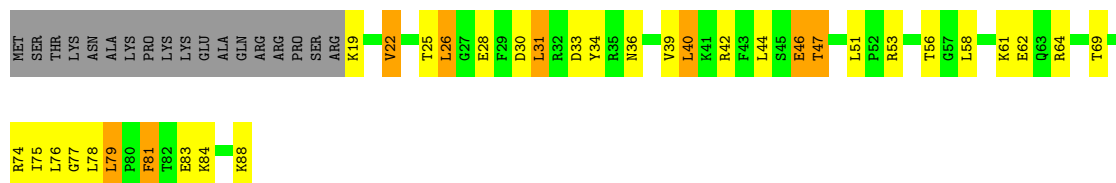




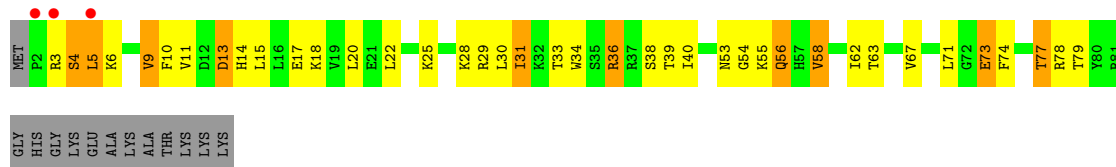
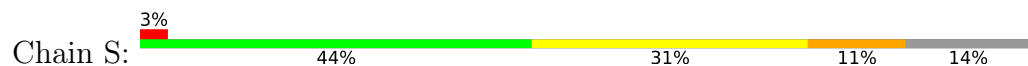
• Molecule 17: 30S ribosomal protein S17



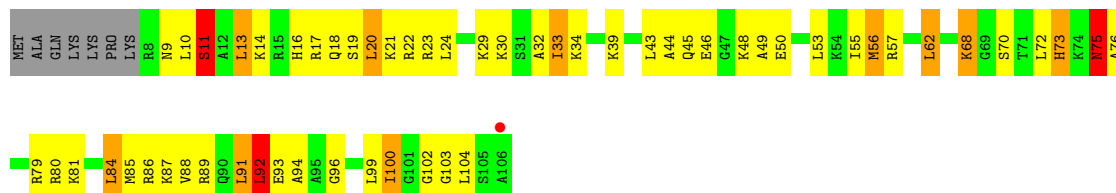
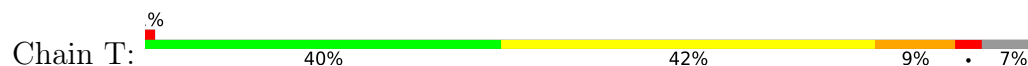
• Molecule 18: 30S ribosomal protein S18



• Molecule 19: 30S ribosomal protein S19

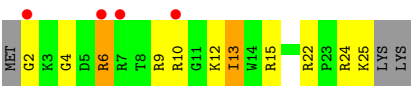


• Molecule 20: 30S ribosomal protein S20



• Molecule 21: 30S ribosomal protein THX





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	403.04Å 403.04Å 174.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.64 – 3.60 34.64 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.2 (34.64-3.60) 98.8 (34.64-3.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 3.56Å)	Xtriage
Refinement program	PHENIX dev_978	Depositor
R, R_{free}	0.157 , 0.207 0.155 , 0.203	Depositor DCC
R_{free} test set	8156 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	138.5	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 141.7	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	0.97	EDS
Total number of atoms	52227	wwPDB-VP
Average B, all atoms (Å ²)	167.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.59	1/36139 (0.0%)	0.60	0/56396
2	B	0.91	0/1935	1.29	20/2609 (0.8%)
3	C	0.74	0/1636	1.16	10/2205 (0.5%)
4	D	0.83	1/1733 (0.1%)	1.26	14/2318 (0.6%)
5	E	1.26	6/1162 (0.5%)	1.53	13/1564 (0.8%)
6	F	0.74	0/856	1.11	6/1154 (0.5%)
7	G	0.78	0/1276	1.17	8/1709 (0.5%)
8	H	1.25	2/1136 (0.2%)	1.59	15/1527 (1.0%)
9	I	0.76	0/1029	1.13	1/1379 (0.1%)
10	J	0.86	1/805 (0.1%)	1.29	12/1082 (1.1%)
11	K	0.95	1/879 (0.1%)	1.32	9/1187 (0.8%)
12	L	0.99	2/977 (0.2%)	1.50	14/1306 (1.1%)
13	M	0.80	0/947	1.24	5/1270 (0.4%)
14	N	0.75	0/501	1.19	2/664 (0.3%)
15	O	0.99	2/740 (0.3%)	1.22	8/987 (0.8%)
16	P	0.98	1/716 (0.1%)	1.35	7/963 (0.7%)
17	Q	1.17	3/836 (0.4%)	1.52	8/1117 (0.7%)
18	R	0.92	0/579	1.28	5/768 (0.7%)
19	S	0.72	0/661	1.24	11/890 (1.2%)
20	T	0.92	0/765	1.38	7/1007 (0.7%)
21	U	0.74	0/212	1.11	1/277 (0.4%)
All	All	0.73	20/55520 (0.0%)	0.89	176/82379 (0.2%)

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

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

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Mol	Chain	#Chirality outliers	#Planarity outliers
17	Q	0	1
20	T	0	2
All	All	0	7

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	76	ILE	CA-CB	-7.77	1.44	1.54
8	H	111	ILE	CA-CB	-7.07	1.45	1.54
16	P	19	ILE	CA-CB	-6.96	1.46	1.54
12	L	25	PRO	CA-C	6.63	1.60	1.53
8	H	134	ILE	CA-CB	-6.46	1.46	1.54
5	E	51	VAL	CA-CB	6.18	1.57	1.54
11	K	120	ARG	CA-C	-5.92	1.46	1.53
17	Q	21	VAL	CA-CB	-5.71	1.47	1.54
12	L	85	ILE	CA-CB	-5.66	1.47	1.54
5	E	115	VAL	CA-CB	-5.63	1.47	1.54
10	J	4	ILE	CA-CB	5.61	1.60	1.53
17	Q	99	SER	CA-C	5.56	1.60	1.52
17	Q	60	ILE	CA-CB	-5.54	1.47	1.54
5	E	148	VAL	CA-CB	-5.31	1.47	1.54
15	O	45	VAL	CA-CB	-5.14	1.47	1.54
4	D	30	LYS	CA-C	5.12	1.59	1.52
5	E	108	ALA	CA-CB	-5.11	1.45	1.53
15	O	60	VAL	CA-CB	-5.08	1.48	1.54
1	A	1498	UR3	O3'-P	5.02	1.61	1.56
5	E	118	ILE	CA-CB	-5.01	1.50	1.55

All (176) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	100	ILE	CA-C-N	13.59	133.78	119.78
8	H	100	ILE	C-N-CA	13.59	133.78	119.78
12	L	26	ALA	N-CA-C	-11.02	100.08	113.19
3	C	167	TRP	N-CA-C	9.59	121.47	108.23
4	D	26	CYS	N-CA-C	-9.50	101.38	113.16
5	E	64	ARG	N-CA-C	-9.26	98.58	110.53
7	G	111	ARG	CA-C-N	9.05	128.71	118.85
7	G	111	ARG	C-N-CA	9.05	128.71	118.85
11	K	91	ARG	N-CA-C	-8.98	101.57	111.36
8	H	134	ILE	N-CA-C	8.92	119.47	110.82
4	D	70	ILE	N-CA-C	8.49	119.81	110.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	180	ALA	N-CA-C	8.19	122.84	113.02
20	T	94	ALA	N-CA-C	-8.05	94.89	108.26
4	D	12	CYS	N-CA-C	-8.02	101.62	111.33
10	J	52	GLY	CA-C-N	7.86	127.87	119.78
10	J	52	GLY	C-N-CA	7.86	127.87	119.78
8	H	73	ASP	CA-C-N	7.79	127.97	119.87
8	H	73	ASP	C-N-CA	7.79	127.97	119.87
5	E	41	VAL	CB-CA-C	-7.77	98.01	110.28
4	D	56	VAL	CB-CA-C	-7.73	101.99	111.88
20	T	76	ALA	N-CA-C	-7.65	102.89	111.07
8	H	81	HIS	N-CA-C	-7.29	103.36	111.82
19	S	4	SER	N-CA-C	7.24	120.92	108.02
5	E	15	ARG	N-CA-C	7.18	121.28	112.23
11	K	50	TYR	N-CA-C	7.17	119.82	110.43
4	D	33	MET	N-CA-C	-7.02	103.98	112.54
2	B	211	ILE	CB-CA-C	-6.96	102.97	111.88
2	B	172	ILE	CB-CA-C	-6.95	102.92	112.24
13	M	108	ARG	N-CA-C	6.92	119.41	111.11
20	T	75	ASN	N-CA-C	-6.90	104.89	113.38
17	Q	67	LYS	N-CA-C	-6.87	100.27	110.23
11	K	49	GLY	N-CA-C	6.85	120.93	112.64
10	J	60	ARG	N-CA-C	6.81	119.84	110.24
17	Q	98	LEU	N-CA-C	6.80	120.94	112.24
8	H	134	ILE	CB-CA-C	-6.79	103.14	112.04
17	Q	99	SER	N-CA-C	6.77	125.22	110.80
10	J	89	ASP	N-CA-C	6.77	121.33	109.96
12	L	119	LYS	N-CA-C	-6.66	101.29	110.35
19	S	67	VAL	N-CA-C	6.66	117.35	110.36
12	L	18	VAL	N-CA-C	6.66	117.86	107.28
18	R	79	LEU	CA-C-N	6.62	126.85	119.90
18	R	79	LEU	C-N-CA	6.62	126.85	119.90
3	C	179	ARG	N-CA-C	-6.61	96.72	110.80
10	J	38	ILE	CA-C-N	6.61	127.59	120.13
10	J	38	ILE	C-N-CA	6.61	127.59	120.13
16	P	5	ARG	N-CA-C	6.59	116.75	108.45
11	K	125	PHE	N-CA-C	6.58	121.01	112.92
2	B	12	GLU	N-CA-C	6.56	120.74	112.87
7	G	19	GLY	N-CA-C	-6.55	106.08	115.64
12	L	85	ILE	N-CA-C	6.54	117.53	107.99
15	O	11	VAL	N-CA-C	6.49	116.65	110.42
6	F	55	ASP	CA-C-N	6.44	126.57	119.87
6	F	55	ASP	C-N-CA	6.44	126.57	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Q	63	ARG	N-CA-C	-6.44	101.94	109.93
19	S	58	VAL	N-CA-C	6.38	114.84	107.89
15	O	18	PHE	N-CA-C	-6.33	102.44	108.13
18	R	51	LEU	CA-C-N	6.31	126.68	119.92
18	R	51	LEU	C-N-CA	6.31	126.68	119.92
21	U	13	ILE	N-CA-C	6.31	116.47	110.42
3	C	173	VAL	CA-C-N	6.28	127.69	119.84
3	C	173	VAL	C-N-CA	6.28	127.69	119.84
12	L	30	ALA	CA-C-N	6.27	125.89	119.56
12	L	30	ALA	C-N-CA	6.27	125.89	119.56
5	E	76	ILE	N-CA-CB	-6.26	102.44	111.21
19	S	30	LEU	CB-CA-C	-6.25	108.35	115.79
7	G	87	VAL	CA-C-N	6.25	126.61	119.92
7	G	87	VAL	C-N-CA	6.25	126.61	119.92
8	H	35	ILE	CB-CA-C	-6.23	103.90	111.88
9	I	58	HIS	N-CA-C	-6.22	104.39	112.23
10	J	62	HIS	N-CA-C	6.20	119.30	109.50
8	H	89	PRO	CA-C-N	-6.20	113.41	122.46
8	H	89	PRO	C-N-CA	-6.20	113.41	122.46
10	J	55	LYS	N-CA-C	6.20	117.17	108.00
14	N	32	SER	N-CA-C	6.15	118.72	108.20
19	S	73	GLU	N-CA-C	-6.15	105.27	112.89
13	M	15	VAL	N-CA-C	6.14	116.31	110.53
4	D	158	ILE	N-CA-C	6.14	116.25	110.30
3	C	46	GLU	N-CA-C	6.10	118.84	111.40
6	F	60	PHE	N-CA-C	6.09	118.87	109.07
12	L	85	ILE	CB-CA-C	-6.08	102.66	110.98
12	L	6	THR	CA-C-N	-6.07	112.79	120.56
12	L	6	THR	C-N-CA	-6.07	112.79	120.56
7	G	84	ASN	N-CA-C	6.05	118.52	110.53
13	M	10	PRO	CA-C-O	-6.05	114.34	122.08
4	D	12	CYS	CA-CB-SG	6.03	128.28	114.40
8	H	69	ARG	N-CA-C	6.03	118.37	109.69
10	J	10	GLY	N-CA-C	6.03	119.59	110.18
20	T	92	LEU	CA-C-N	-5.99	113.83	123.23
20	T	92	LEU	C-N-CA	-5.99	113.83	123.23
19	S	6	LYS	N-CA-C	5.97	123.53	110.80
8	H	3	THR	N-CA-C	5.96	120.71	112.90
5	E	17	ALA	N-CA-C	5.95	119.29	110.48
5	E	80	ILE	N-CA-C	5.95	116.92	108.42
5	E	48	ALA	CA-C-N	5.94	126.36	119.47
5	E	48	ALA	C-N-CA	5.94	126.36	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	50	ARG	CA-C-N	5.92	126.11	119.90
4	D	50	ARG	C-N-CA	5.92	126.11	119.90
6	F	16	GLN	N-CA-C	5.91	117.52	111.14
16	P	79	VAL	N-CA-C	-5.88	103.75	111.09
16	P	51	VAL	N-CA-C	5.85	121.51	109.34
16	P	19	ILE	CB-CA-C	-5.85	102.62	111.33
8	H	3	THR	CA-C-N	-5.82	115.26	122.42
8	H	3	THR	C-N-CA	-5.82	115.26	122.42
4	D	30	LYS	N-CA-C	5.82	121.09	113.30
11	K	102	GLY	N-CA-C	-5.82	107.15	115.64
2	B	165	VAL	N-CA-C	5.80	117.32	111.00
17	Q	29	HIS	N-CA-C	-5.80	102.27	109.64
5	E	6	PHE	N-CA-C	5.78	118.38	109.07
15	O	36	ILE	CB-CA-C	-5.78	104.49	111.88
2	B	58	ILE	CB-CA-C	-5.77	104.49	111.88
10	J	75	ILE	N-CA-C	5.75	115.87	107.37
8	H	101	PRO	CB-CA-C	-5.72	103.91	111.23
20	T	103	GLY	N-CA-C	5.70	119.57	112.73
5	E	115	VAL	CB-CA-C	-5.70	102.84	111.33
2	B	16	HIS	N-CA-C	5.69	122.92	110.80
11	K	17	GLY	N-CA-C	5.65	119.93	110.56
17	Q	98	LEU	CA-CB-CG	5.64	136.06	116.30
19	S	10	PHE	N-CA-C	5.64	117.93	108.96
7	G	62	PHE	N-CA-C	-5.62	104.85	110.97
15	O	23	GLY	N-CA-C	5.59	126.44	113.18
4	D	21	LEU	N-CA-C	-5.58	106.14	113.17
3	C	3	ASN	N-CA-C	-5.54	101.08	108.34
15	O	15	PHE	N-CA-C	5.54	120.15	113.17
5	E	148	VAL	CB-CA-C	-5.53	104.67	112.14
4	D	198	VAL	CB-CA-C	-5.52	101.56	110.28
2	B	190	THR	N-CA-C	5.52	118.01	111.33
2	B	158	LEU	CA-C-N	5.51	125.82	119.92
2	B	158	LEU	C-N-CA	5.51	125.82	119.92
2	B	90	MET	N-CA-C	5.50	117.48	109.84
16	P	82	GLN	N-CA-C	5.46	120.05	113.17
6	F	13	ASN	N-CA-C	5.46	119.42	112.87
10	J	36	GLY	CA-C-N	5.44	126.64	119.84
10	J	36	GLY	C-N-CA	5.44	126.64	119.84
19	S	36	ARG	N-CA-C	-5.43	106.33	113.17
5	E	23	GLY	N-CA-C	5.41	117.92	110.56
12	L	7	ILE	N-CA-C	-5.41	105.44	110.53
12	L	93	LEU	CA-C-N	-5.40	114.20	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	93	LEU	C-N-CA	-5.40	114.20	119.76
19	S	38	SER	N-CA-C	5.40	118.62	109.76
12	L	43	VAL	N-CA-C	5.40	116.25	108.48
19	S	58	VAL	CA-C-N	5.39	125.56	119.90
19	S	58	VAL	C-N-CA	5.39	125.56	119.90
3	C	166	GLU	N-CA-C	5.37	118.38	109.94
3	C	4	LYS	N-CA-C	5.36	122.21	110.80
15	O	11	VAL	CB-CA-C	-5.36	105.11	111.97
4	D	204	ILE	CB-CA-C	-5.33	105.14	111.97
2	B	89	GLY	N-CA-C	-5.32	108.06	114.66
13	M	20	THR	CA-C-N	5.32	129.11	120.60
13	M	20	THR	C-N-CA	5.32	129.11	120.60
15	O	87	ILE	N-CA-C	5.26	116.49	108.80
2	B	239	VAL	N-CA-C	5.26	115.48	110.53
5	E	14	ARG	N-CA-C	5.26	117.19	109.24
11	K	14	VAL	N-CA-C	5.26	118.85	112.80
2	B	10	LEU	CA-C-N	5.24	131.55	121.54
2	B	10	LEU	C-N-CA	5.24	131.55	121.54
20	T	11	SER	N-CA-C	5.23	119.29	113.02
2	B	174	VAL	CB-CA-C	-5.21	105.30	111.97
17	Q	84	LEU	CA-CB-CG	-5.18	98.15	116.30
15	O	24	SER	CB-CA-C	-5.16	100.50	109.64
4	D	13	ARG	N-CA-C	5.15	118.03	111.69
14	N	42	ILE	N-CA-C	-5.12	105.72	110.53
2	B	122	PHE	N-CA-C	-5.11	106.73	113.17
2	B	103	THR	CB-CA-C	-5.10	102.33	110.79
2	B	18	GLY	N-CA-C	5.08	119.82	112.81
16	P	9	PHE	N-CA-C	5.08	119.43	112.88
3	C	155	GLY	N-CA-C	5.08	119.82	112.82
16	P	32	TYR	N-CA-C	5.07	117.56	109.65
11	K	57	THR	CA-C-N	5.07	124.86	119.28
11	K	57	THR	C-N-CA	5.07	124.86	119.28
12	L	22	SER	N-CA-C	5.04	117.00	109.59
6	F	32	ASN	N-CA-C	5.04	117.50	111.71
18	R	31	LEU	N-CA-C	-5.03	107.09	113.18
7	G	88	PRO	CA-C-O	-5.03	115.67	121.95
17	Q	3	LYS	N-CA-C	-5.02	102.42	109.96
2	B	182	ILE	CA-C-N	5.01	124.99	120.03
2	B	182	ILE	C-N-CA	5.01	124.99	120.03

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	166	GLU	Peptide
3	C	179	ARG	Peptide
8	H	27	PRO	Peptide
8	H	90	GLY	Peptide
17	Q	13	ASP	Peptide
20	T	11	SER	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	32644	0	16505	665	0
2	B	1900	0	1951	82	0
3	C	1612	0	1677	83	0
4	D	1703	0	1763	73	0
5	E	1146	0	1207	51	0
6	F	843	0	857	27	0
7	G	1257	0	1296	55	0
8	H	1116	0	1177	56	0
9	I	1010	0	1037	75	0
10	J	792	0	835	45	0
11	K	864	0	881	39	0
12	L	972	0	1058	59	0
13	M	937	0	995	51	0
14	N	492	0	529	35	0
15	O	729	0	768	42	0
16	P	700	0	720	28	0
17	Q	823	0	893	45	0
18	R	574	0	644	28	0
19	S	647	0	673	24	0
20	T	763	0	861	39	0
21	U	208	0	221	14	0
22	A	239	0	0	0	0
22	B	2	0	0	0	0
22	C	3	0	0	0	0
22	D	4	0	0	0	0
22	E	1	0	0	0	0
22	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	L	1	0	0	0	0
22	P	2	0	0	0	0
22	Q	1	0	0	0	0
23	D	1	0	0	0	0
23	N	1	0	0	0	0
24	A	232	0	0	12	0
24	E	3	0	0	0	0
24	L	1	0	0	0	0
24	Q	1	0	0	0	0
24	T	2	0	0	0	0
All	All	52227	0	36548	1464	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 17.

All (1464) 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:1195:C:H3'	1:A:1196:U:H5''	1.46	0.95
20:T:100:ILE:HG22	20:T:102:GLY:H	1.32	0.90
12:L:41:ARG:HH21	12:L:43:VAL:HG13	1.36	0.90
1:A:103:C:OP1	20:T:17:ARG:NH1	2.03	0.90
1:A:279:A:OP2	17:Q:95:TYR:OH	1.90	0.88
1:A:1060:C:OP1	14:N:45:ARG:NH2	2.07	0.87
3:C:137:ALA:HA	3:C:140:ARG:HD2	1.55	0.87
2:B:114:ARG:HH11	2:B:118:LEU:HD21	1.41	0.85
1:A:992:U:H3	1:A:1044:A:H62	1.25	0.85
1:A:664:G:H22	1:A:741:G:H1	1.23	0.84
12:L:27:LEU:O	12:L:29:GLY:N	2.10	0.83
1:A:144:G:H1	1:A:178:C:H42	1.25	0.83
1:A:481:G:HO2'	1:A:482:A:H8	1.27	0.82
8:H:83:ILE:HG12	8:H:137:VAL:HG22	1.61	0.82
1:A:1417:G:O2'	1:A:1483:A:N6	2.13	0.82
17:Q:81:ARG:HE	17:Q:84:LEU:HD12	1.45	0.81
1:A:1497:G:H2'	1:A:1498:UR3:H5'	1.61	0.81
3:C:6:HIS:HD2	3:C:9:GLY:H	1.27	0.80
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.64	0.80
8:H:4:ASP:OD2	8:H:85:ARG:NH1	2.15	0.79
1:A:1347:G:H1'	1:A:1348:U:H5	1.48	0.79
1:A:1368:G:H5''	9:I:112:LYS:HB3	1.64	0.79
17:Q:66:SER:O	17:Q:70:ARG:NH1	2.16	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1316:G:N2	1:A:1319:A:OP2	2.16	0.78
1:A:1406:U:O2'	1:A:1517[B]:G:N2	2.16	0.78
1:A:1111:A:H61	3:C:177:THR:HB	1.49	0.77
10:J:47:PHE:HB3	14:N:34:TYR:HE2	1.49	0.77
1:A:1356:G:H2'	1:A:1357:A:C8	2.20	0.77
5:E:11:ILE:HB	5:E:31:LEU:HB3	1.65	0.77
15:O:55:GLY:HA2	15:O:58:MET:HE2	1.64	0.77
15:O:33:THR:OG1	15:O:63:ARG:NH1	2.18	0.77
1:A:1240:U:OP1	7:G:119:ARG:NH2	2.17	0.77
3:C:156:ARG:NH1	3:C:193:TYR:O	2.17	0.77
12:L:25:PRO:C	12:L:27:LEU:H	1.88	0.77
4:D:11:LEU:HD13	4:D:66:ARG:HD2	1.67	0.76
20:T:56:MET:HG3	20:T:88:VAL:HG21	1.66	0.76
6:F:70:ASP:OD1	6:F:70:ASP:N	2.15	0.76
1:A:1126:U:O4	1:A:1127:G:N2	2.19	0.75
9:I:25:LYS:NZ	9:I:60:ASP:OD2	2.15	0.75
1:A:1125:U:OP2	1:A:1145:C:N4	2.19	0.75
6:F:97:PHE:HE1	18:R:61:LYS:HE2	1.51	0.75
10:J:49:VAL:HG13	14:N:41:ARG:HB2	1.69	0.75
1:A:869:G:N7	24:A:2109:HOH:O	2.19	0.75
10:J:50:ILE:HA	10:J:60:ARG:HB3	1.68	0.75
1:A:1195:C:H3'	1:A:1196:U:C5'	2.16	0.74
1:A:1504:G:OP1	1:A:1507:A:H4'	1.87	0.74
12:L:24:VAL:HG13	12:L:98:TYR:HE2	1.51	0.74
15:O:17:ARG:HG3	15:O:17:ARG:HH11	1.52	0.74
1:A:979:C:O2	1:A:1317:C:N4	2.19	0.74
6:F:10:LEU:HD12	6:F:59:TYR:HB3	1.69	0.74
18:R:46:GLU:CD	18:R:46:GLU:H	1.95	0.74
12:L:27:LEU:HB3	12:L:28:LYS:HG2	1.69	0.74
1:A:1145:C:O2'	1:A:1146:A:O5'	2.06	0.74
3:C:150:LYS:HB3	3:C:201:TYR:HB2	1.68	0.74
3:C:180:ALA:HB1	3:C:203:PHE:HE1	1.51	0.74
3:C:13:GLY:HA3	14:N:57:ARG:HH21	1.53	0.73
10:J:64:GLU:OE2	10:J:66:ARG:NH2	2.20	0.73
17:Q:29:HIS:CG	17:Q:30:PRO:HD2	2.24	0.73
1:A:269:C:H2'	1:A:270:A:C8	2.24	0.73
1:A:281:G:O2'	1:A:282:A:OP2	2.07	0.73
10:J:82:ILE:HA	10:J:85:LEU:HB2	1.68	0.72
1:A:1147:C:H4'	9:I:5:TYR:HE1	1.54	0.72
2:B:55:PHE:HD2	2:B:58:ILE:HD12	1.54	0.72
17:Q:62:SER:OG	17:Q:72:ARG:HG3	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1152:A:OP1	10:J:68:HIS:ND1	2.22	0.72
9:I:126:SER:OG	9:I:127:LYS:N	2.21	0.72
3:C:112:SER:HB3	3:C:115:LEU:HD12	1.71	0.72
1:A:1125:U:H3	10:J:5:ARG:HH21	1.37	0.72
4:D:61:LYS:NZ	4:D:62:GLN:OE1	2.18	0.72
2:B:91:PRO:HG2	2:B:155:LEU:HD23	1.73	0.71
1:A:951:G:OP2	13:M:102:ARG:NH2	2.23	0.71
1:A:975:A:H5'	1:A:975:A:H8	1.55	0.71
7:G:17:VAL:HG12	7:G:18:TYR:HD1	1.55	0.71
20:T:50:GLU:HA	20:T:100:ILE:HG13	1.72	0.71
1:A:1256:A:O2'	1:A:1257:U:OP2	2.08	0.71
10:J:61:GLU:OE1	14:N:45:ARG:NH1	2.24	0.71
1:A:1049:U:O2'	14:N:3:ARG:NH1	2.24	0.71
3:C:52:LEU:HD12	3:C:68:VAL:HG13	1.72	0.71
1:A:250:A:H4'	1:A:251:G:O5'	1.91	0.71
1:A:95:U:H2'	1:A:96:G:H8	1.55	0.70
1:A:1510:U:H2'	1:A:1511:G:C8	2.26	0.70
3:C:179:ARG:HD3	3:C:206:GLU:HG3	1.73	0.70
9:I:50:LEU:HD11	9:I:81:ILE:HD13	1.72	0.70
1:A:1435:G:H2'	1:A:1436:U:C6	2.26	0.70
1:A:1257:U:O2'	1:A:1258:G:OP2	2.08	0.70
9:I:46:ALA:HB2	9:I:74:ILE:HG23	1.73	0.70
4:D:22:LYS:HB2	4:D:26:CYS:SG	2.31	0.69
5:E:144:THR:O	5:E:148:VAL:HG23	1.91	0.69
10:J:21:GLN:NE2	10:J:25:GLU:OE2	2.25	0.69
12:L:53:ARG:NH1	12:L:92:OTD:OD2	2.24	0.69
3:C:26:LYS:O	3:C:30:ARG:NH1	2.25	0.69
3:C:150:LYS:HG3	3:C:169:ALA:HB2	1.73	0.69
1:A:1222:G:OP2	1:A:1322:C:N4	2.26	0.69
7:G:16:LEU:HD12	9:I:44:VAL:HG12	1.74	0.69
1:A:1497:G:C2'	1:A:1498:UR3:H5'	2.22	0.69
1:A:542:G:OP1	4:D:10:ARG:NH2	2.26	0.68
16:P:68:ASP:OD1	16:P:68:ASP:N	2.26	0.68
13:M:16:ASP:OD1	13:M:16:ASP:N	2.26	0.68
1:A:1414:U:H2'	1:A:1415:G:C8	2.28	0.68
3:C:131:ARG:HA	3:C:134:ILE:HD12	1.76	0.68
16:P:9:PHE:HD1	16:P:18:ARG:HG3	1.59	0.68
1:A:1305:G:N2	1:A:1331:G:H1'	2.09	0.67
12:L:27:LEU:C	12:L:29:GLY:H	1.95	0.67
13:M:11:ARG:HG3	13:M:12:ASN:HB2	1.75	0.67
1:A:1399:C:H4'	1:A:1400:5MC:H5''	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:10:LEU:HD22	8:H:83:ILE:HD13	1.77	0.67
1:A:263:A:OP2	20:T:79:ARG:NH1	2.27	0.67
1:A:1443:G:H5''	1:A:1446:A:H5'	1.76	0.67
3:C:23:TYR:OH	10:J:9:ARG:NH1	2.26	0.67
9:I:55:ALA:HB1	9:I:59:PHE:HB2	1.76	0.67
15:O:12:ILE:HG12	15:O:31:LEU:HD11	1.76	0.67
1:A:1255:G:C6	1:A:1279:A:N7	2.63	0.67
6:F:14:LEU:HD13	6:F:18:GLN:HB3	1.77	0.67
1:A:1338:G:H2'	1:A:1339:A:C8	2.30	0.67
1:A:113:G:H1'	1:A:354:G:H5'	1.78	0.66
1:A:1498:UR3:O4'	1:A:1519[A]:MA6:H2	1.96	0.66
1:A:103:C:P	20:T:17:ARG:HH12	2.18	0.66
1:A:1190:G:OP1	3:C:4:LYS:HA	1.95	0.66
1:A:1144:G:N2	1:A:1145:C:O2	2.28	0.66
1:A:1128:C:O2'	1:A:1130:A:N7	2.28	0.66
8:H:20:TYR:CE1	8:H:76:PRO:HD2	2.31	0.66
10:J:61:GLU:OE2	14:N:58:LYS:NZ	2.28	0.66
1:A:310:G:OP2	16:P:27:LYS:NZ	2.25	0.66
1:A:1148:U:H2'	1:A:1149:C:O4'	1.96	0.66
1:A:966:M2G:HM22	1:A:967:5MC:C2	2.30	0.66
1:A:269:C:H2'	1:A:270:A:H8	1.61	0.65
20:T:100:ILE:HG22	20:T:102:GLY:N	2.09	0.65
1:A:77:G:H2'	1:A:78:G:C8	2.30	0.65
1:A:560:U:H5'	1:A:566:G:N2	2.12	0.65
1:A:443:C:H42	1:A:491:G:H1	1.45	0.65
1:A:1222:G:OP1	19:S:77:THR:HG21	1.95	0.65
15:O:33:THR:HG21	15:O:85:LEU:HD13	1.77	0.65
5:E:80:ILE:HG22	8:H:104:ARG:HH21	1.60	0.65
1:A:407:G:OP1	4:D:115:ARG:NH1	2.29	0.65
1:A:1255:G:O2'	1:A:1258:G:H1'	1.97	0.65
1:A:1349:A:P	9:I:118:LYS:HZ1	2.20	0.65
11:K:40:ILE:HG22	11:K:41:THR:HG23	1.79	0.65
17:Q:95:TYR:HA	17:Q:98:LEU:HD11	1.79	0.65
20:T:39:LYS:HG2	20:T:55:ILE:HD13	1.77	0.65
14:N:18:VAL:HG23	14:N:19:ARG:HG3	1.79	0.65
21:U:6:ARG:HD2	21:U:15:ARG:NH2	2.11	0.65
1:A:858:G:N7	24:A:2109:HOH:O	2.29	0.64
1:A:76:C:H2'	1:A:77:G:H8	1.61	0.64
1:A:1049:U:H4'	1:A:1050:G:O5'	1.97	0.64
3:C:41:GLY:O	3:C:45:LYS:HG2	1.97	0.64
1:A:452:A:O2'	1:A:453:A:O4'	2.08	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:21:ARG:HA	2:B:39:ILE:HA	1.80	0.64
3:C:108:ASN:HB3	3:C:111:LEU:HB2	1.80	0.64
8:H:85:ARG:NE	8:H:87:SER:O	2.31	0.64
1:A:89:C:H2'	1:A:90:U:H6	1.62	0.64
1:A:427:U:OP1	4:D:13:ARG:NH2	2.31	0.64
1:A:517:G:N1	1:A:533:A:OP2	2.29	0.64
1:A:1387:G:O2'	24:A:2061:HOH:O	2.14	0.64
7:G:40:ALA:HB3	9:I:41:VAL:HG21	1.80	0.63
13:M:15:VAL:HG21	13:M:48:LEU:HD21	1.80	0.63
8:H:104:ARG:HH11	8:H:104:ARG:HG2	1.62	0.63
11:K:57:THR:HG23	11:K:60:ALA:H	1.62	0.63
1:A:328:C:H2'	1:A:328:C:O2	1.96	0.63
1:A:707:C:H2'	1:A:708:C:C6	2.32	0.63
7:G:84:ASN:OD1	7:G:84:ASN:N	2.30	0.63
11:K:29:ILE:HG12	11:K:30:VAL:N	2.13	0.63
16:P:21:VAL:HG12	16:P:33:ILE:HD12	1.81	0.63
20:T:46:GLU:OE1	20:T:48:LYS:NZ	2.32	0.63
1:A:686:U:HO2'	1:A:687:A:H8	1.45	0.63
10:J:50:ILE:HD12	10:J:50:ILE:H	1.62	0.63
1:A:553:A:O2'	12:L:29:GLY:O	2.16	0.63
3:C:154:SER:OG	3:C:155:GLY:N	2.29	0.63
12:L:28:LYS:C	12:L:30:ALA:H	2.04	0.63
1:A:1128:C:H5'	9:I:16:ARG:HH12	1.63	0.62
11:K:48:ILE:HD12	11:K:63:LEU:HB2	1.81	0.62
1:A:864:A:H2'	1:A:865:A:C8	2.35	0.62
7:G:91:VAL:HG11	7:G:96:GLN:HG3	1.81	0.62
13:M:117:VAL:HG12	13:M:118:ALA:H	1.64	0.62
15:O:45:VAL:HB	15:O:46:HIS:ND1	2.13	0.62
1:A:537:G:OP1	12:L:113:ARG:NH2	2.33	0.62
1:A:1064:G:N2	1:A:1190:G:O2'	2.33	0.62
1:A:1143:G:H2'	1:A:1144:G:C8	2.35	0.62
3:C:33:LEU:HD21	14:N:53:LEU:HD22	1.82	0.62
3:C:137:ALA:O	3:C:141:VAL:HG23	1.99	0.62
4:D:64:LEU:HD23	4:D:198:VAL:HG21	1.81	0.62
1:A:77:G:C6	1:A:93:G:N1	2.68	0.62
1:A:1148:U:H1'	9:I:16:ARG:HH21	1.64	0.62
1:A:1373:G:H5''	7:G:36:LYS:HE3	1.82	0.62
2:B:240:GLN:N	2:B:240:GLN:OE1	2.31	0.62
12:L:5:PRO:HG2	12:L:15:ARG:NH2	2.14	0.62
15:O:56:LEU:HA	15:O:59:MET:HE2	1.82	0.62
1:A:1164:G:H1	1:A:1172:C:H42	1.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:23:GLY:HA3	4:D:112:VAL:HG12	1.81	0.62
1:A:501:C:H2'	1:A:502:G:C8	2.35	0.61
1:A:673:G:H2'	1:A:674:G:C8	2.34	0.61
1:A:967:5MC:O2'	9:I:128:ARG:NH1	2.33	0.61
1:A:1090:U:H2'	1:A:1091:U:H6	1.65	0.61
4:D:107:ARG:HH12	4:D:114:ARG:HH21	1.47	0.61
1:A:707:C:H2'	1:A:708:C:H6	1.65	0.61
1:A:1349:A:OP1	9:I:118:LYS:NZ	2.32	0.61
19:S:11:VAL:HG22	19:S:39:THR:HB	1.82	0.61
1:A:1513:A:H2'	1:A:1514:C:C6	2.36	0.61
9:I:24:GLY:HA3	9:I:56:LEU:HD23	1.83	0.61
5:E:88:LYS:HB3	5:E:123:LEU:HB2	1.82	0.61
16:P:74:LEU:O	16:P:79:VAL:HG23	2.01	0.61
1:A:1224:G:N2	1:A:1362:C:O2	2.33	0.61
1:A:1499:A:H1'	1:A:1520[A]:G:H5'	1.81	0.61
15:O:87:ILE:HG22	15:O:88:ARG:H	1.64	0.61
1:A:1143:G:H2'	1:A:1144:G:H8	1.64	0.61
14:N:39:LEU:HD22	14:N:43:CYS:HB3	1.81	0.61
1:A:827:U:H5''	1:A:828:A:OP2	2.00	0.61
1:A:1291:G:H2'	1:A:1292:U:C6	2.35	0.61
1:A:858:G:O6	24:A:2107:HOH:O	2.16	0.61
1:A:1101:A:H4'	1:A:1102:A:O5'	1.99	0.61
12:L:25:PRO:HB2	12:L:64:TYR:HE2	1.66	0.61
17:Q:74:LEU:HD23	17:Q:75:ARG:HG2	1.83	0.61
1:A:130:A:H5'	17:Q:63:ARG:HE	1.66	0.61
1:A:1020:U:H2'	1:A:1021:G:H8	1.66	0.61
1:A:1368:G:OP2	9:I:112:LYS:HD3	2.01	0.61
2:B:223:ILE:HD13	2:B:230:VAL:HG21	1.82	0.61
1:A:1314:C:H2'	1:A:1315:U:C6	2.35	0.60
1:A:581:G:N7	24:A:1973:HOH:O	2.31	0.60
1:A:1006:C:H42	1:A:1022:G:H22	1.47	0.60
1:A:1305:G:OP1	21:U:2:GLY:N	2.34	0.60
3:C:22:TRP:HA	10:J:93:GLY:HA2	1.83	0.60
4:D:78:LEU:HD21	4:D:96:LEU:HB3	1.83	0.60
20:T:56:MET:HE1	20:T:104:LEU:HD21	1.83	0.60
4:D:187:ARG:NH2	4:D:188:LEU:HB2	2.17	0.60
9:I:26:VAL:HG13	9:I:61:ALA:HB3	1.83	0.60
16:P:43:LYS:HG2	16:P:48:TRP:CD2	2.36	0.60
1:A:76:C:H42	1:A:95:U:H3	1.49	0.60
5:E:33:VAL:HG11	5:E:109:ILE:HA	1.82	0.60
9:I:45:ALA:HA	9:I:48:GLU:HB2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:4:ILE:HG12	16:P:21:VAL:HG22	1.82	0.60
1:A:1347:G:H3'	9:I:108:VAL:O	2.02	0.60
2:B:16:HIS:CD2	2:B:204:ASN:H	2.19	0.60
7:G:17:VAL:HG12	7:G:18:TYR:CD1	2.34	0.60
1:A:89:C:H2'	1:A:90:U:O4'	2.00	0.60
1:A:992:U:H3	1:A:1044:A:N6	1.97	0.60
1:A:1392:G:H21	1:A:1502:A:H8	1.47	0.60
7:G:38:LEU:O	7:G:42:ILE:HG13	2.02	0.60
15:O:29:VAL:HG11	15:O:67:LEU:HD21	1.83	0.60
1:A:1349:A:C2	1:A:1374:A:C4	2.90	0.60
8:H:116:LYS:NZ	8:H:127:LEU:HD12	2.17	0.60
11:K:62:GLN:HG3	11:K:97:ALA:HB2	1.83	0.60
13:M:96:LEU:O	13:M:110:ARG:NH1	2.35	0.60
20:T:81:LYS:O	20:T:85:MET:HG3	2.01	0.60
2:B:63:MET:HB3	2:B:225:ALA:HB1	1.83	0.60
3:C:31:HIS:HA	3:C:34:LEU:HB2	1.84	0.60
1:A:204:U:H4'	1:A:216:G:OP1	2.02	0.59
6:F:55:ASP:HB3	6:F:86:ARG:HH12	1.66	0.59
1:A:89:C:H2'	1:A:90:U:C6	2.38	0.59
1:A:1376:U:OP1	7:G:98:SER:OG	2.16	0.59
20:T:33:ILE:HD13	20:T:62:LEU:HB3	1.84	0.59
1:A:757:U:H2'	1:A:758:G:O4'	2.01	0.59
1:A:1366:C:H2'	1:A:1367:C:H6	1.67	0.59
5:E:32:VAL:HB	5:E:58:ALA:HB1	1.83	0.59
1:A:973:G:H3'	1:A:974:A:H5''	1.84	0.59
8:H:41:ARG:NH1	8:H:123:GLU:OE2	2.35	0.59
12:L:25:PRO:C	12:L:27:LEU:N	2.56	0.59
14:N:6:LEU:HB3	14:N:23:ARG:NH2	2.17	0.59
6:F:78:GLU:HA	6:F:81:ILE:HD12	1.83	0.59
8:H:118:VAL:C	8:H:119:LEU:HD23	2.27	0.59
1:A:235:C:N4	24:A:1988:HOH:O	2.36	0.59
1:A:345:C:OP2	1:A:345:C:H6	1.85	0.59
1:A:1443:G:C5'	1:A:1446:A:H5'	2.33	0.59
20:T:92:LEU:O	20:T:96:GLY:HA2	2.03	0.59
1:A:1301:U:O2'	1:A:1302:U:O5'	2.20	0.59
1:A:390:C:O3'	16:P:28:ARG:NH2	2.36	0.59
2:B:7:VAL:HG11	2:B:221:LEU:HD23	1.83	0.59
5:E:77:PRO:HD2	5:E:142:LEU:HD13	1.85	0.59
10:J:79:ARG:NH1	10:J:79:ARG:HA	2.18	0.59
11:K:94:ALA:O	11:K:98:LEU:HB2	2.03	0.59
1:A:737:A:H2'	1:A:738:C:C6	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1009:G:H1	1:A:1020:U:H3	1.51	0.58
19:S:5:LEU:HB2	19:S:9:VAL:HG22	1.84	0.58
1:A:5:U:H4'	1:A:6:G:O5'	2.02	0.58
1:A:35:G:O2'	12:L:118:SER:O	2.21	0.58
1:A:1313:U:O4	19:S:4:SER:OG	2.12	0.58
8:H:2:LEU:C	8:H:2:LEU:HD23	2.28	0.58
18:R:22:VAL:HG23	18:R:56:THR:HA	1.84	0.58
3:C:134:ILE:HG23	3:C:151:VAL:HB	1.85	0.58
1:A:1048:G:H1	1:A:1209:C:H42	1.50	0.58
1:A:1409:C:H2'	1:A:1410:G:C8	2.37	0.58
2:B:91:PRO:HG2	2:B:155:LEU:CD2	2.33	0.58
1:A:216:G:H2'	1:A:217:C:C6	2.37	0.58
14:N:27:CYS:HB2	14:N:43:CYS:SG	2.33	0.58
18:R:47:THR:HA	18:R:83:GLU:HB2	1.85	0.58
1:A:344:A:H5'	1:A:345:C:C5	2.38	0.58
1:A:1126:U:O2'	1:A:1127:G:OP1	2.19	0.58
1:A:1225:A:H2'	1:A:1225:A:N3	2.19	0.58
2:B:97:TRP:HZ2	2:B:102:LEU:HD22	1.69	0.58
17:Q:24:GLU:HG2	17:Q:39:SER:HB3	1.86	0.58
1:A:1347:G:O2'	1:A:1348:U:P	2.62	0.58
3:C:179:ARG:HG3	3:C:179:ARG:HH11	1.68	0.58
4:D:107:ARG:HH21	4:D:194:LEU:HD12	1.67	0.58
9:I:8:GLY:HA3	9:I:79:LEU:HB3	1.84	0.58
12:L:87:GLY:HA2	12:L:98:TYR:HA	1.85	0.58
1:A:836:G:C6	1:A:851:G:C6	2.92	0.58
4:D:15:GLU:O	4:D:17:VAL:HG23	2.04	0.58
4:D:187:ARG:CZ	4:D:188:LEU:HB2	2.34	0.58
11:K:80:VAL:HG21	11:K:103:LEU:HD13	1.86	0.58
15:O:39:LEU:HD13	15:O:56:LEU:HB2	1.86	0.58
16:P:19:ILE:HD12	16:P:37:GLY:HA3	1.86	0.58
1:A:324:G:OP1	20:T:22:ARG:NH1	2.37	0.58
1:A:457:C:H2'	1:A:458:C:H6	1.68	0.58
1:A:1347:G:O6	9:I:10:ARG:NH2	2.29	0.58
3:C:155:GLY:HA2	3:C:164:ARG:H	1.69	0.58
9:I:19:LEU:HD23	9:I:61:ALA:HB2	1.84	0.58
9:I:117:HIS:NE2	9:I:123:PRO:HB3	2.18	0.58
1:A:372:C:H4'	1:A:373:A:O5'	2.03	0.58
1:A:858:G:O6	1:A:869:G:C8	2.57	0.58
3:C:138:VAL:HG13	3:C:149:ALA:HB3	1.85	0.58
1:A:90:U:O2'	1:A:91:C:H5'	2.04	0.57
1:A:937:A:N6	1:A:1345:U:O4	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:967:5MC:H4'	9:I:128:ARG:HG3	1.85	0.57
1:A:1243:C:H42	1:A:1294:G:H1	1.52	0.57
8:H:25:ASP:N	8:H:25:ASP:OD1	2.36	0.57
1:A:580:U:H2'	1:A:581:G:O4'	2.05	0.57
9:I:10:ARG:HG2	9:I:75:ASP:HB2	1.85	0.57
1:A:299:G:H2'	1:A:300:A:C8	2.40	0.57
1:A:442:C:H42	1:A:492:G:H1	1.52	0.57
1:A:579:G:H4'	15:O:54:ARG:HH21	1.69	0.57
1:A:1106:G:H5''	3:C:172:ARG:HB3	1.85	0.57
8:H:31:PHE:O	8:H:35:ILE:HG12	2.04	0.57
16:P:2:VAL:O	16:P:64:ALA:HA	2.04	0.57
1:A:235:C:H5'	17:Q:70:ARG:HG2	1.87	0.57
1:A:1118:C:H5'	9:I:104:ARG:HG3	1.87	0.57
2:B:88:ALA:HB2	2:B:219:VAL:HG13	1.87	0.57
1:A:633:G:H2'	1:A:634:C:C6	2.40	0.57
20:T:49:ALA:HB3	20:T:99:LEU:HD12	1.87	0.57
20:T:75:ASN:OD1	20:T:75:ASN:N	2.36	0.57
1:A:298:A:N6	24:A:2058:HOH:O	2.08	0.57
8:H:82:HIS:HD1	8:H:138:TRP:CD1	2.23	0.57
9:I:117:HIS:HB2	9:I:121:ARG:HG2	1.86	0.57
1:A:129:U:O3'	1:A:129(A):G:H3'	2.05	0.57
1:A:384:G:H2'	1:A:385:C:C6	2.40	0.57
1:A:509:A:C8	1:A:509:A:H3'	2.39	0.57
14:N:24:CYS:HA	14:N:38:GLY:O	2.05	0.57
17:Q:63:ARG:HG2	17:Q:64:PRO:HD2	1.87	0.57
1:A:1139:G:H4'	1:A:1140:C:C5'	2.35	0.57
1:A:1511:G:H2'	1:A:1512:U:O4'	2.05	0.57
11:K:65:ALA:HB1	11:K:98:LEU:HD23	1.87	0.57
12:L:124:LYS:HD2	12:L:125:PRO:HD2	1.87	0.57
1:A:569:C:H42	1:A:881:G:H1	1.53	0.56
1:A:975:A:H5'	1:A:975:A:C8	2.38	0.56
1:A:1139:G:H4'	1:A:1140:C:O5'	2.05	0.56
3:C:153:VAL:HG12	3:C:196:LEU:HD22	1.87	0.56
1:A:1129:C:H4'	1:A:1130:A:OP2	2.05	0.56
1:A:1225:A:H5'	1:A:1226:C:OP2	2.05	0.56
3:C:14:ILE:HG22	3:C:15:THR:HG23	1.87	0.56
4:D:55:ALA:O	4:D:59:ARG:HG2	2.06	0.56
9:I:38:GLN:OE1	9:I:39:GLY:N	2.37	0.56
1:A:1112:C:H1'	3:C:179:ARG:NH2	2.20	0.56
2:B:55:PHE:CD2	2:B:58:ILE:HD12	2.38	0.56
10:J:50:ILE:HG13	10:J:60:ARG:HD3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:102:ARG:NH2	12:L:108:ALA:O	2.24	0.56
19:S:53:ASN:ND2	19:S:56:GLN:HB2	2.20	0.56
1:A:758:G:C8	24:A:1974:HOH:O	2.59	0.56
3:C:29:TYR:HE1	10:J:11:PHE:HE1	1.54	0.56
3:C:43:LEU:HA	3:C:47:LEU:HD13	1.87	0.56
3:C:180:ALA:CB	3:C:203:PHE:HE1	2.18	0.56
5:E:93:PRO:HD2	8:H:105:ARG:HH21	1.69	0.56
6:F:100:ASN:O	18:R:28:GLU:HG3	2.06	0.56
1:A:532:A:H2'	1:A:533:A:H5''	1.87	0.56
1:A:792:A:H4'	1:A:793:U:O5'	2.06	0.56
1:A:1437:C:H2'	1:A:1438:G:H8	1.71	0.56
12:L:24:VAL:HG13	12:L:98:TYR:CE2	2.36	0.56
12:L:25:PRO:HA	12:L:27:LEU:H	1.71	0.56
1:A:481:G:O2'	1:A:482:A:H8	1.86	0.56
13:M:99:ARG:HB2	13:M:101:GLN:NE2	2.21	0.56
1:A:451:A:N6	1:A:481:G:C4	2.73	0.56
5:E:17:ALA:HB2	5:E:26:PHE:HD2	1.71	0.56
1:A:45:U:H2'	1:A:46:G:C8	2.41	0.56
1:A:254:G:OP1	17:Q:67:LYS:O	2.23	0.56
4:D:162:LEU:HA	4:D:165:MET:HB2	1.88	0.56
2:B:47:THR:OG1	2:B:202:PRO:O	2.23	0.56
7:G:115:ARG:HB2	7:G:118:VAL:HG23	1.88	0.56
10:J:63:PHE:HB3	14:N:57:ARG:O	2.05	0.56
12:L:113:ARG:NH1	12:L:116:SER:H	2.03	0.56
1:A:411:A:N7	1:A:413:G:N3	2.55	0.55
1:A:1516[B]:G:N2	1:A:1519[B]:MA6:OP2	2.34	0.55
2:B:28:PHE:HD2	2:B:32:ILE:HD11	1.71	0.55
3:C:58:GLU:HB3	10:J:92:THR:HG21	1.88	0.55
5:E:101:ILE:O	5:E:120:THR:HB	2.06	0.55
13:M:90:LEU:HD23	13:M:93:ARG:HD2	1.88	0.55
1:A:1392:G:N2	1:A:1502:A:H8	2.04	0.55
8:H:87:SER:HA	8:H:93:VAL:HG13	1.87	0.55
10:J:48:THR:HA	10:J:62:HIS:HB3	1.88	0.55
21:U:9:ARG:HE	21:U:22:ARG:HG3	1.70	0.55
1:A:500:G:C6	1:A:546:G:C2	2.95	0.55
1:A:869:G:H5''	1:A:870:U:OP1	2.06	0.55
6:F:97:PHE:CE1	18:R:61:LYS:HE2	2.39	0.55
8:H:104:ARG:HG3	8:H:138:TRP:CD2	2.41	0.55
17:Q:60:ILE:HD13	17:Q:61:GLU:N	2.22	0.55
1:A:544:G:OP1	4:D:62:GLN:NE2	2.37	0.55
1:A:1347:G:O2'	1:A:1348:U:OP2	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1509:C:H42	1:A:1526:G:H1	1.53	0.55
4:D:9:CYS:O	4:D:12:CYS:HB2	2.06	0.55
7:G:18:TYR:HE2	7:G:59:LEU:HA	1.72	0.55
1:A:401:C:O2'	1:A:621:A:N3	2.31	0.55
1:A:1006:C:H2'	1:A:1007:C:H6	1.71	0.55
1:A:1028:C:H42	1:A:1033:G:H1	1.55	0.55
1:A:1128:C:H5'	9:I:16:ARG:NH1	2.21	0.55
3:C:150:LYS:HB2	3:C:173:VAL:HG21	1.88	0.55
7:G:111:ARG:HG2	7:G:112:PRO:HD2	1.87	0.55
9:I:50:LEU:HB3	9:I:55:ALA:HB3	1.89	0.55
9:I:112:LYS:HA	9:I:119:ALA:HB2	1.89	0.55
20:T:68:LYS:HE3	20:T:68:LYS:HA	1.88	0.55
1:A:353:A:H5'	1:A:353:A:H8	1.72	0.55
1:A:1130:A:O2'	9:I:3:GLN:NE2	2.24	0.55
1:A:1256:A:H4'	1:A:1257:U:O5'	2.05	0.55
17:Q:29:HIS:CD2	17:Q:30:PRO:HD2	2.42	0.55
1:A:948:C:OP2	13:M:108:ARG:HB2	2.07	0.55
1:A:1403:C:H1'	1:A:1500:A:N1	2.22	0.55
3:C:172:ARG:NH2	3:C:174:PRO:HG3	2.21	0.55
8:H:121:ASP:OD2	8:H:122:ARG:N	2.38	0.55
9:I:48:GLU:N	9:I:49:PRO:HD2	2.22	0.55
13:M:62:ASN:OD1	13:M:62:ASN:N	2.39	0.55
14:N:50:LYS:HG2	14:N:52:GLN:HE21	1.72	0.55
3:C:154:SER:HB3	3:C:197:GLY:H	1.72	0.55
10:J:79:ARG:NH1	10:J:82:ILE:HB	2.21	0.55
1:A:1531:A:O5'	1:A:1531:A:H8	1.90	0.55
10:J:6:ILE:HD13	10:J:72:VAL:HB	1.88	0.55
20:T:45:GLN:HA	20:T:91:LEU:HD12	1.87	0.55
4:D:35:ARG:O	4:D:36:ARG:HG3	2.07	0.54
4:D:174:LEU:O	4:D:186:LEU:HD11	2.07	0.54
12:L:5:PRO:HG2	12:L:15:ARG:HH22	1.71	0.54
1:A:1286:A:H2'	1:A:1287:A:H4'	1.88	0.54
15:O:30:ALA:HA	15:O:85:LEU:HD11	1.89	0.54
18:R:74:ARG:HB3	18:R:81:PHE:CE1	2.42	0.54
20:T:16:HIS:NE2	20:T:20:LEU:HD21	2.22	0.54
1:A:451:A:H8	1:A:451:A:OP1	1.90	0.54
1:A:706:A:O2'	11:K:29:ILE:HD11	2.07	0.54
1:A:707:C:OP1	11:K:85:ARG:NH1	2.41	0.54
1:A:974:A:OP2	14:N:29:ARG:NH2	2.40	0.54
3:C:58:GLU:H	3:C:65:ALA:HB3	1.73	0.54
15:O:21:ASP:OD1	15:O:24:SER:OG	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:A:C2	1:A:246:A:C8	2.96	0.54
1:A:1193:G:H2'	1:A:1194:U:H6	1.73	0.54
13:M:86:CYS:SG	13:M:87:TYR:N	2.81	0.54
15:O:34:LEU:HD23	15:O:34:LEU:C	2.32	0.54
1:A:581:G:C8	24:A:1973:HOH:O	2.60	0.54
1:A:1048:G:H5''	14:N:3:ARG:HD2	1.89	0.54
1:A:1359:C:H1'	1:A:1361(A):C:H41	1.72	0.54
4:D:18:LYS:HE2	4:D:20:TYR:HE2	1.72	0.54
12:L:93:LEU:HD12	12:L:96:VAL:HG21	1.88	0.54
15:O:18:PHE:HD1	15:O:19:PRO:O	1.91	0.54
1:A:594:G:H1	1:A:645:C:H42	1.56	0.54
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.42	0.54
1:A:998:G:N2	1:A:1043:C:O2	2.41	0.54
1:A:1065:U:H5''	1:A:1190:G:N2	2.23	0.54
3:C:91:LEU:HD21	3:C:99:VAL:HG22	1.89	0.54
3:C:112:SER:O	3:C:116:VAL:HG23	2.08	0.54
5:E:71:LEU:HD21	5:E:115:VAL:HG22	1.90	0.54
1:A:1008:C:H42	1:A:1021:G:H1	1.55	0.54
1:A:1191:A:H2'	1:A:1192:C:C6	2.42	0.54
5:E:84:PHE:HB2	5:E:134:ALA:HB2	1.90	0.54
7:G:69:VAL:HG21	7:G:104:LEU:HD21	1.90	0.54
13:M:5:ALA:HB3	13:M:8:GLU:HG3	1.90	0.54
16:P:52:ASP:OD2	16:P:55:ARG:HB2	2.08	0.54
1:A:103:C:OP2	20:T:14:LYS:HD2	2.08	0.53
1:A:130:A:C8	17:Q:63:ARG:HG3	2.43	0.53
1:A:500:G:C5	1:A:546:G:N2	2.77	0.53
1:A:1198:G:H2'	1:A:1199:U:C6	2.43	0.53
1:A:1281:U:H5'	1:A:1282:C:H5	1.72	0.53
3:C:6:HIS:CD2	3:C:9:GLY:H	2.16	0.53
1:A:77:G:C4	1:A:93:G:N2	2.77	0.53
1:A:353:A:H5'	1:A:353:A:C8	2.43	0.53
1:A:946:A:H2'	1:A:947:G:C8	2.43	0.53
1:A:1304:G:OP2	24:A:2087:HOH:O	2.19	0.53
7:G:26:PHE:O	7:G:30:ILE:HG13	2.08	0.53
1:A:279:A:H5'	1:A:279:A:H8	1.73	0.53
2:B:158:LEU:HD12	2:B:158:LEU:H	1.73	0.53
8:H:9:MET:HG3	8:H:26:VAL:HG21	1.89	0.53
13:M:13:LYS:O	13:M:45:VAL:HG23	2.07	0.53
1:A:660:G:H1	1:A:745:C:H42	1.56	0.53
1:A:1393:U:HO2'	1:A:1501:C:HO2'	1.54	0.53
18:R:53:ARG:NH1	18:R:58:LEU:O	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1343:G:H1'	9:I:121:ARG:NH1	2.23	0.53
13:M:82:MET:HE3	13:M:92:HIS:HB3	1.90	0.53
1:A:192:U:H5'	20:T:102:GLY:O	2.09	0.53
1:A:596:C:C2'	1:A:597:G:H5'	2.38	0.53
1:A:1139:G:H4'	1:A:1140:C:H5'	1.91	0.53
1:A:1145:C:HO2'	1:A:1146:A:P	2.30	0.53
15:O:36:ILE:HA	15:O:59:MET:HE1	1.91	0.53
1:A:503:C:H2'	1:A:504:C:C6	2.44	0.53
6:F:8:ILE:HB	6:F:61:LEU:HB2	1.90	0.53
9:I:22:GLY:HA3	9:I:60:ASP:HB2	1.90	0.53
12:L:69:TYR:HE2	12:L:71:PRO:HA	1.73	0.53
15:O:78:TYR:CZ	15:O:82:ILE:HD12	2.44	0.53
17:Q:31:LEU:HD23	17:Q:32:TYR:CE2	2.44	0.53
1:A:141:A:H1'	1:A:182:U:O2	2.09	0.53
1:A:1305:G:O2'	1:A:1306:A:H8	1.91	0.53
4:D:36:ARG:HG2	4:D:38:TYR:CZ	2.44	0.53
1:A:1004:A:H5''	1:A:1025:U:C4	2.44	0.53
9:I:88:TYR:HD2	9:I:89:ASN:HB2	1.74	0.53
1:A:1116:C:O2'	9:I:108:VAL:HG21	2.09	0.52
15:O:24:SER:HB2	15:O:27:VAL:HG23	1.91	0.52
19:S:77:THR:HG22	19:S:78:ARG:HD2	1.91	0.52
1:A:383:A:C6	1:A:384:G:H1'	2.44	0.52
1:A:1442:G:C2	1:A:1446:A:N7	2.77	0.52
1:A:1499:A:H1'	1:A:1520[A]:G:OP1	2.09	0.52
1:A:76:C:H2'	1:A:77:G:C8	2.43	0.52
3:C:11:ARG:HA	3:C:178:LEU:HD11	1.90	0.52
4:D:127:THR:HB	4:D:147:ALA:HB3	1.91	0.52
1:A:95:U:H2'	1:A:96:G:C8	2.41	0.52
1:A:866:C:H2'	1:A:867:G:O4'	2.08	0.52
12:L:82:VAL:HG13	12:L:106:ASP:OD1	2.09	0.52
1:A:80:G:H2'	1:A:81:U:H5'	1.91	0.52
4:D:72:GLU:OE1	4:D:207:TYR:OH	2.27	0.52
11:K:70:LYS:HA	11:K:73:MET:HG2	1.92	0.52
12:L:35:GLY:HA3	12:L:60:LEU:HD13	1.91	0.52
13:M:2:ALA:O	13:M:10:PRO:HD2	2.10	0.52
1:A:943:U:H1'	9:I:124:GLN:HE22	1.74	0.52
1:A:968:A:C8	1:A:1062:U:H4'	2.44	0.52
3:C:116:VAL:HG21	3:C:202:ILE:HD11	1.92	0.52
11:K:48:ILE:CD1	11:K:63:LEU:HB2	2.39	0.52
14:N:37:PHE:C	14:N:39:LEU:H	2.15	0.52
15:O:26:GLU:HA	15:O:81:LEU:HD11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:146:ILE:N	4:D:146:ILE:HD12	2.24	0.52
13:M:54:VAL:HG22	13:M:58:GLU:OE1	2.10	0.52
1:A:1061:G:H1	1:A:1195:C:H42	1.58	0.52
1:A:1349:A:OP1	9:I:120:ARG:HB2	2.09	0.52
2:B:200:ILE:HG12	2:B:202:PRO:HD3	1.92	0.52
3:C:174:PRO:HB2	3:C:177:THR:CG2	2.40	0.52
4:D:3:ARG:HH22	4:D:74:GLN:NE2	2.07	0.52
4:D:36:ARG:HG2	4:D:38:TYR:OH	2.09	0.52
9:I:19:LEU:HD22	9:I:59:PHE:HD2	1.75	0.52
13:M:57:ARG:O	13:M:61:GLU:HB2	2.10	0.52
1:A:1073:U:OP2	5:E:57:LYS:NZ	2.35	0.52
1:A:1250:A:C6	1:A:1251:A:C6	2.97	0.52
1:A:1403:C:H1'	1:A:1500:A:C2	2.45	0.52
11:K:72:ALA:HB1	11:K:77:MET:HG3	1.92	0.52
14:N:48:ALA:HB1	14:N:56:VAL:HG11	1.92	0.52
14:N:50:LYS:HB3	14:N:52:GLN:HG3	1.92	0.52
1:A:501:C:H2'	1:A:502:G:H8	1.74	0.52
1:A:943:U:H2'	1:A:944:G:H5'	1.92	0.52
1:A:960:U:H4'	1:A:961:U:C5'	2.40	0.52
13:M:3:ARG:HA	13:M:8:GLU:O	2.10	0.52
17:Q:93:GLN:HG2	17:Q:96:GLN:HE21	1.75	0.52
1:A:677:U:H3	1:A:713:G:H22	1.58	0.51
4:D:152:SER:O	4:D:155:LEU:HB2	2.09	0.51
8:H:114:THR:HG21	8:H:129:VAL:HG23	1.91	0.51
18:R:58:LEU:HD22	18:R:62:GLU:HB3	1.92	0.51
1:A:143:A:O3'	1:A:144:G:H8	1.93	0.51
1:A:838:G:H2'	1:A:839:U:H5''	1.91	0.51
1:A:1055:A:N7	1:A:1200:C:N4	2.54	0.51
1:A:1117:G:H5''	9:I:104:ARG:NH2	2.25	0.51
1:A:1201:A:H4'	1:A:1202:G:O5'	2.10	0.51
5:E:142:LEU:O	5:E:143:ARG:HD3	2.10	0.51
10:J:32:ALA:O	10:J:34:VAL:HG23	2.09	0.51
11:K:14:VAL:HG11	11:K:40:ILE:HD11	1.90	0.51
14:N:29:ARG:HB3	14:N:33:VAL:HG22	1.91	0.51
1:A:476:G:H2'	1:A:477:G:C8	2.45	0.51
1:A:695:A:H61	1:A:797:C:H1'	1.75	0.51
1:A:1068:G:H8	1:A:1068:G:OP2	1.92	0.51
1:A:1374:A:C4	1:A:1375:A:C8	2.99	0.51
1:A:1518[B]:MA6:H102	1:A:1519[B]:MA6:H103	1.91	0.51
10:J:79:ARG:HA	10:J:79:ARG:CZ	2.40	0.51
12:L:28:LYS:C	12:L:30:ALA:N	2.69	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:G:H2'	1:A:541:G:C8	2.45	0.51
1:A:721:G:OP2	18:R:53:ARG:HG3	2.11	0.51
1:A:1004:A:H5''	1:A:1025:U:C5	2.46	0.51
1:A:1327:C:OP2	21:U:12:LYS:NZ	2.42	0.51
6:F:91:VAL:HG12	6:F:92:LYS:O	2.11	0.51
7:G:108:ALA:O	7:G:119:ARG:HB3	2.10	0.51
1:A:1003(A):G:C5	1:A:1004:A:H1'	2.45	0.51
1:A:1006:C:H2'	1:A:1007:C:C6	2.46	0.51
1:A:1026:G:O6	1:A:1035:A:N6	2.36	0.51
4:D:78:LEU:HD21	4:D:96:LEU:CB	2.40	0.51
4:D:102:ASP:OD1	4:D:103:ASN:N	2.44	0.51
7:G:78:ARG:HG3	7:G:156:TRP:CE3	2.45	0.51
12:L:87:GLY:H	12:L:99:HIS:H	1.59	0.51
2:B:23:ARG:O	2:B:24:TRP:HD1	1.94	0.51
3:C:51:GLY:O	3:C:71:ALA:N	2.26	0.51
15:O:14:GLU:HG3	15:O:15:PHE:CD1	2.45	0.51
15:O:29:VAL:O	15:O:33:THR:HB	2.10	0.51
17:Q:65:ILE:HD12	17:Q:65:ILE:N	2.26	0.51
1:A:278:G:C6	17:Q:95:TYR:HD2	2.28	0.51
1:A:337:C:H2'	1:A:338:A:C8	2.45	0.51
1:A:503:C:H2'	1:A:504:C:H6	1.76	0.51
3:C:130:VAL:HG22	3:C:134:ILE:HD11	1.93	0.51
4:D:101:LEU:O	4:D:105:VAL:HG23	2.11	0.51
10:J:19:SER:HB2	10:J:91:PRO:HG3	1.93	0.51
10:J:89:ASP:HB2	10:J:91:PRO:HD2	1.92	0.51
12:L:48:PRO:HD2	12:L:92:OTD:H3	1.92	0.51
1:A:216:G:H2'	1:A:217:C:H6	1.75	0.51
1:A:1008:C:N4	1:A:1021:G:H1	2.09	0.51
1:A:1175:G:H2'	1:A:1176:A:C8	2.45	0.51
1:A:976:G:OP1	14:N:32:SER:HB2	2.10	0.51
1:A:1057:G:H4'	3:C:154:SER:HG	1.76	0.51
1:A:1359:C:O2'	1:A:1361:G:N7	2.43	0.51
4:D:107:ARG:HH12	4:D:114:ARG:NH2	2.08	0.51
11:K:47:VAL:HG12	11:K:48:ILE:HG23	1.92	0.51
17:Q:63:ARG:HG2	17:Q:64:PRO:CD	2.40	0.51
20:T:23:ARG:HG2	20:T:24:LEU:HD12	1.93	0.51
20:T:89:ARG:NH2	20:T:104:LEU:HB3	2.26	0.51
1:A:1034:G:H2'	1:A:1035:A:H8	1.76	0.51
2:B:213:LEU:HD23	2:B:214:ILE:HD13	1.92	0.51
3:C:114:PRO:O	3:C:118:GLN:HG3	2.11	0.51
4:D:107:ARG:NH1	4:D:114:ARG:HH21	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:104:ARG:HG2	8:H:104:ARG:NH1	2.26	0.51
18:R:28:GLU:N	18:R:28:GLU:OE1	2.44	0.51
1:A:106:C:C2'	1:A:107:G:H5'	2.41	0.50
1:A:1305:G:O2'	1:A:1306:A:P	2.69	0.50
1:A:1369:C:H2'	1:A:1370:G:C8	2.46	0.50
1:A:1518[B]:MA6:H93	1:A:1519[B]:MA6:N1	2.26	0.50
9:I:112:LYS:HE2	9:I:113:LYS:O	2.11	0.50
16:P:53:VAL:O	16:P:56:ALA:N	2.44	0.50
1:A:514:C:H2'	1:A:515:G:C8	2.46	0.50
1:A:633:G:H2'	1:A:634:C:H6	1.76	0.50
1:A:943:U:C2'	1:A:944:G:H5'	2.42	0.50
1:A:1133:G:H1	1:A:1141:C:H42	1.59	0.50
8:H:114:THR:HG22	8:H:130:GLY:O	2.10	0.50
1:A:92:C:O2'	1:A:93:G:H5'	2.12	0.50
11:K:50:TYR:CE2	11:K:54:ARG:HD2	2.46	0.50
1:A:41:G:H2'	1:A:42:G:C8	2.46	0.50
1:A:491:G:C2	1:A:492:G:C8	2.99	0.50
1:A:691:G:H2'	1:A:692:U:C6	2.46	0.50
1:A:858:G:O2'	1:A:859:A:H5'	2.11	0.50
1:A:1305:G:H22	1:A:1331:G:H1'	1.76	0.50
1:A:1530:G:H4'	1:A:1530:G:OP1	2.11	0.50
14:N:24:CYS:HB2	14:N:39:LEU:C	2.36	0.50
18:R:74:ARG:HD3	18:R:81:PHE:HA	1.92	0.50
1:A:1131:G:H2'	1:A:1132:C:C6	2.47	0.50
5:E:118:ILE:HG12	5:E:119:LEU:N	2.26	0.50
10:J:79:ARG:HH12	10:J:82:ILE:HB	1.76	0.50
12:L:42:THR:HG22	12:L:52:LEU:HB3	1.93	0.50
17:Q:40:LYS:HE2	17:Q:42:TYR:CZ	2.47	0.50
1:A:374:A:N3	1:A:374:A:H2'	2.26	0.50
1:A:457:C:H2'	1:A:458:C:C6	2.46	0.50
1:A:981:U:H5'	14:N:21:TYR:CZ	2.47	0.50
2:B:60:ASP:CG	2:B:64:ARG:HH12	2.16	0.50
2:B:84:GLU:HB3	2:B:219:VAL:HG21	1.93	0.50
3:C:70:VAL:HG21	3:C:76:VAL:HG21	1.93	0.50
4:D:19:LEU:HB3	4:D:67:ILE:HG12	1.94	0.50
1:A:1260:C:O5'	1:A:1284:C:H4'	2.12	0.50
3:C:114:PRO:HA	3:C:185:GLY:HA3	1.94	0.50
7:G:47:CYS:HA	7:G:50:ILE:HG22	1.94	0.50
13:M:48:LEU:HB3	13:M:53:VAL:HG23	1.94	0.50
12:L:7:ILE:O	12:L:10:LEU:N	2.41	0.50
1:A:819:A:H4'	1:A:820:U:OP2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1221:G:OP1	19:S:36:ARG:HD3	2.11	0.50
1:A:1399:C:O2	1:A:1401:G:C5	2.65	0.50
1:A:1406:U:H4'	1:A:1518[B]:MA6:H1'	1.94	0.50
1:A:56:U:H2'	1:A:57:G:H8	1.76	0.49
1:A:421:U:H5'	1:A:422:C:H5	1.77	0.49
1:A:661:G:H8	1:A:661:G:H5''	1.77	0.49
1:A:1409:C:H2'	1:A:1410:G:H8	1.77	0.49
2:B:153:ARG:HB3	2:B:154:LEU:HD23	1.94	0.49
1:A:321:A:H2'	1:A:322:C:H6	1.77	0.49
1:A:1305:G:O2'	1:A:1306:A:O5'	2.30	0.49
2:B:188:ALA:O	2:B:202:PRO:HA	2.12	0.49
7:G:22:LEU:HD13	7:G:97:GLN:NE2	2.27	0.49
1:A:17:U:H2'	1:A:18:C:C6	2.48	0.49
1:A:514:C:H2'	1:A:515:G:H8	1.76	0.49
1:A:736:C:H2'	1:A:737:A:C8	2.47	0.49
5:E:76:ILE:HG23	5:E:142:LEU:CD1	2.41	0.49
1:A:92:C:O2	1:A:93:G:C8	2.65	0.49
1:A:701:C:H5''	1:A:703:G:H5'	1.94	0.49
1:A:1366:C:H2'	1:A:1367:C:C6	2.45	0.49
4:D:21:LEU:HD11	4:D:67:ILE:HA	1.95	0.49
4:D:25:ARG:O	4:D:25:ARG:HG2	2.11	0.49
12:L:113:ARG:HH11	12:L:116:SER:H	1.60	0.49
18:R:25:THR:HG22	18:R:42:ARG:HH22	1.77	0.49
1:A:77:G:H2'	1:A:78:G:H8	1.77	0.49
1:A:266:G:H5''	1:A:266:G:H8	1.77	0.49
1:A:371:G:O2'	1:A:372:C:H5'	2.11	0.49
1:A:742:G:H2'	1:A:743:U:O4'	2.12	0.49
1:A:1077:G:N2	1:A:1080:A:OP2	2.43	0.49
1:A:1405:G:O2'	1:A:1518[A]:MA6:O2'	2.28	0.49
2:B:16:HIS:NE2	2:B:204:ASN:N	2.60	0.49
3:C:202:ILE:HG22	3:C:204:LEU:HD23	1.95	0.49
5:E:82:VAL:HG12	5:E:134:ALA:HB1	1.94	0.49
12:L:84:LEU:HD23	12:L:101:VAL:HG21	1.93	0.49
1:A:858:G:O6	1:A:869:G:N7	2.45	0.49
3:C:77:ILE:HD13	3:C:84:ILE:HD12	1.94	0.49
3:C:130:VAL:HG21	3:C:153:VAL:HG21	1.94	0.49
6:F:89:MET:HE2	18:R:76:LEU:HG	1.94	0.49
1:A:688:G:O2'	1:A:704:A:N1	2.43	0.49
1:A:692:U:OP1	11:K:124:LYS:HE3	2.12	0.49
3:C:167:TRP:HE3	3:C:168:ALA:H	1.58	0.49
12:L:27:LEU:HD23	12:L:28:LYS:HE2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:G:N2	1:A:79:G:H1'	2.28	0.49
1:A:349:A:H2'	1:A:350:G:H5''	1.95	0.49
1:A:731:G:O2'	1:A:732:C:H5'	2.12	0.49
1:A:1168:A:H2'	1:A:1169:A:C8	2.47	0.49
1:A:1305:G:O2'	1:A:1306:A:C8	2.65	0.49
1:A:1465:C:H2'	1:A:1466:C:O4'	2.13	0.49
2:B:10:LEU:C	2:B:12:GLU:H	2.20	0.49
7:G:78:ARG:HG3	7:G:156:TRP:HE3	1.78	0.49
9:I:48:GLU:OE1	9:I:51:ARG:NH1	2.45	0.49
1:A:463:A:H2'	1:A:474:G:O4'	2.12	0.49
1:A:571:U:H5''	1:A:572:A:OP2	2.13	0.49
1:A:1480:G:C6	1:A:1481:U:C4	3.00	0.49
2:B:157:ARG:HG2	2:B:158:LEU:N	2.28	0.49
4:D:157:LEU:O	4:D:160:GLN:HB2	2.12	0.49
15:O:18:PHE:CZ	15:O:21:ASP:HB2	2.47	0.49
18:R:39:VAL:HG13	18:R:40:LEU:HD23	1.95	0.49
1:A:723:U:H2'	1:A:723:U:O2	2.13	0.49
1:A:758:G:N7	24:A:1974:HOH:O	2.33	0.49
1:A:887:G:H1	1:A:910:C:H42	1.61	0.49
1:A:1201:A:H4'	1:A:1202:G:C5'	2.42	0.49
2:B:17:PHE:HD1	2:B:18:GLY:N	2.11	0.49
5:E:69:VAL:HG12	5:E:71:LEU:HG	1.94	0.49
1:A:60:A:P	1:A:331:G:H22	2.36	0.48
1:A:77:G:N2	1:A:78:G:C4	2.81	0.48
1:A:79:G:C2	1:A:80:G:N7	2.81	0.48
1:A:279:A:H5'	1:A:279:A:C8	2.48	0.48
1:A:646:U:H2'	1:A:647:C:C6	2.48	0.48
1:A:686:U:O2'	1:A:687:A:H8	1.94	0.48
1:A:986:A:H1'	19:S:55:LYS:HA	1.95	0.48
1:A:1063:C:OP2	1:A:1064:G:O2'	2.30	0.48
1:A:1269:A:N1	1:A:1312:G:O2'	2.41	0.48
1:A:1346:A:O2'	1:A:1347:G:OP2	2.24	0.48
1:A:1516[A]:G:N1	1:A:1519[A]:MA6:OP2	2.46	0.48
6:F:53:ALA:HB3	6:F:86:ARG:CZ	2.43	0.48
10:J:42:THR:HG23	10:J:67:THR:O	2.13	0.48
15:O:55:GLY:O	15:O:59:MET:HG3	2.13	0.48
19:S:18:LYS:HD3	19:S:31:ILE:HD11	1.94	0.48
1:A:66:G:N3	1:A:66:G:H2'	2.28	0.48
1:A:1111:A:N6	3:C:177:THR:HB	2.24	0.48
1:A:1158:C:N3	1:A:1181:G:N2	2.53	0.48
1:A:1191:A:H2'	1:A:1192:C:H6	1.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:48:PRO:HG2	12:L:92:0TD:H3	1.96	0.48
1:A:500:G:H2'	1:A:501:C:C6	2.48	0.48
1:A:737:A:H2'	1:A:738:C:H6	1.77	0.48
8:H:100:ILE:HG23	8:H:112:LEU:HD11	1.95	0.48
9:I:19:LEU:HD22	9:I:59:PHE:CD2	2.48	0.48
15:O:17:ARG:HG3	15:O:17:ARG:NH1	2.23	0.48
16:P:10:GLY:HA3	16:P:14:ASN:O	2.12	0.48
1:A:7:G:H5'	1:A:298:A:H5'	1.95	0.48
1:A:77:G:O2'	1:A:78:G:H5'	2.13	0.48
1:A:828:A:H4'	1:A:828:A:OP1	2.14	0.48
1:A:937:A:H5''	1:A:938:A:OP2	2.13	0.48
1:A:1425:U:H2'	1:A:1426:C:H6	1.77	0.48
1:A:1425:U:H2'	1:A:1426:C:C6	2.48	0.48
1:A:1520[A]:G:H2'	1:A:1521:G:H8	1.78	0.48
3:C:27:LYS:HA	3:C:30:ARG:HH12	1.78	0.48
3:C:29:TYR:HE1	10:J:11:PHE:CE1	2.31	0.48
7:G:26:PHE:CE2	7:G:30:ILE:HD11	2.49	0.48
9:I:8:GLY:HA2	9:I:79:LEU:HD13	1.95	0.48
1:A:130:A:H5'	17:Q:63:ARG:NE	2.29	0.48
1:A:219:C:O2'	1:A:381:C:H5'	2.13	0.48
1:A:381:C:H2'	1:A:382:A:O4'	2.14	0.48
1:A:933:G:O6	7:G:3:ARG:NH2	2.46	0.48
1:A:1526:G:H2'	1:A:1527:C:H6	1.79	0.48
3:C:121:ALA:HB2	3:C:187:ALA:HB1	1.95	0.48
7:G:91:VAL:CG1	7:G:96:GLN:HG3	2.43	0.48
9:I:10:ARG:O	9:I:11:LYS:C	2.57	0.48
15:O:87:ILE:HG22	15:O:88:ARG:N	2.28	0.48
1:A:142:G:N3	1:A:196:A:H2	2.12	0.48
1:A:320:C:O2'	1:A:1435:G:H1'	2.14	0.48
4:D:4:TYR:OH	4:D:7:PRO:O	2.24	0.48
4:D:57:ARG:HG3	4:D:202:LEU:HD13	1.96	0.48
6:F:80:ARG:HH11	6:F:80:ARG:HG2	1.78	0.48
9:I:111:ARG:O	9:I:113:LYS:HD2	2.13	0.48
12:L:25:PRO:CA	12:L:27:LEU:H	2.26	0.48
15:O:64:ARG:HG3	15:O:88:ARG:NH1	2.29	0.48
1:A:253:U:H2'	1:A:254:G:H8	1.79	0.48
1:A:551:U:O2'	12:L:86:ARG:HD2	2.14	0.48
1:A:1326:C:OP2	21:U:6:ARG:NH2	2.47	0.48
3:C:91:LEU:HD23	3:C:92:ALA:N	2.29	0.48
17:Q:59:ILE:HG23	17:Q:71:PHE:HB3	1.96	0.48
19:S:25:LYS:HD2	19:S:25:LYS:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:G:OP1	12:L:61:THR:HG22	2.14	0.48
1:A:448:A:P	1:A:485:G:H22	2.37	0.48
1:A:522:C:OP2	12:L:69:TYR:OH	2.28	0.48
1:A:960:U:H1'	1:A:1223:C:H5'	1.96	0.48
1:A:1493:A:H2'	1:A:1494:G:H8	1.79	0.48
2:B:59:GLU:HB2	2:B:221:LEU:HD11	1.96	0.48
2:B:217:ARG:HD3	2:B:217:ARG:HA	1.58	0.48
4:D:18:LYS:HE2	4:D:20:TYR:CE2	2.49	0.48
7:G:31:MET:HE1	7:G:36:LYS:HD3	1.95	0.48
1:A:41:G:H2'	1:A:42:G:H8	1.79	0.48
1:A:321:A:H2'	1:A:322:C:C6	2.48	0.48
1:A:1053:G:HO2'	1:A:1199:U:H5	1.60	0.48
1:A:1057:G:C4	1:A:1058:G:C8	3.02	0.48
2:B:115:LEU:HD13	2:B:145:LEU:HB3	1.95	0.48
5:E:137:GLU:HG2	5:E:140:ARG:HH11	1.79	0.48
21:U:6:ARG:NH1	21:U:15:ARG:HH12	2.11	0.48
5:E:18:ARG:HG2	5:E:19:MET:N	2.25	0.48
7:G:144:MET:O	7:G:147:ALA:HB3	2.12	0.48
9:I:126:SER:HB2	9:I:127:LYS:HD2	1.96	0.48
1:A:18:C:H2'	1:A:19:C:O4'	2.14	0.47
1:A:1305:G:H3'	21:U:4:GLY:O	2.14	0.47
1:A:1498:UR3:O2'	1:A:1499:A:OP2	2.21	0.47
3:C:15:THR:HG21	3:C:179:ARG:O	2.14	0.47
12:L:28:LYS:HG3	12:L:33:ARG:CZ	2.44	0.47
13:M:33:ALA:O	13:M:37:THR:OG1	2.16	0.47
1:A:75:G:C2	1:A:96:G:C2	3.01	0.47
1:A:79:G:H5'	1:A:80:G:OP2	2.13	0.47
1:A:346:G:H2'	1:A:347:G:O4'	2.14	0.47
1:A:664:G:OP1	18:R:64:ARG:HD2	2.14	0.47
1:A:835:U:H3	1:A:851:G:H1	1.62	0.47
1:A:1097:C:H2'	1:A:1098:C:C6	2.49	0.47
1:A:1098:C:H2'	1:A:1099:G:O4'	2.14	0.47
1:A:1126:U:H6	1:A:1126:U:O5'	1.97	0.47
1:A:1258:G:H2'	1:A:1259:C:C6	2.49	0.47
1:A:1505:G:O2'	1:A:1506:U:OP2	2.25	0.47
2:B:71:VAL:HB	2:B:164:VAL:HG12	1.97	0.47
14:N:37:PHE:C	14:N:39:LEU:N	2.72	0.47
18:R:76:LEU:HD23	18:R:76:LEU:HA	1.56	0.47
1:A:21:G:H2'	1:A:22:G:C8	2.49	0.47
1:A:337:C:H2'	1:A:338:A:H8	1.78	0.47
1:A:476:G:H2'	1:A:477:G:H8	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:675:A:O2'	11:K:114:VAL:O	2.31	0.47
1:A:1354:C:H2'	1:A:1355:G:H8	1.80	0.47
1:A:1451:A:H5''	1:A:1452:C:H5	1.79	0.47
1:A:1498:UR3:C4'	1:A:1519[A]:MA6:H2	2.43	0.47
2:B:76:GLN:HG3	2:B:206:ASP:CG	2.39	0.47
4:D:187:ARG:HD2	4:D:187:ARG:HA	1.43	0.47
12:L:46:LYS:NZ	12:L:47:LYS:HE2	2.29	0.47
16:P:58:TYR:CE1	16:P:62:VAL:HG21	2.48	0.47
1:A:1211:U:H1'	1:A:1213:A:N3	2.30	0.47
14:N:40:CYS:H	14:N:43:CYS:HB2	1.78	0.47
18:R:39:VAL:CG1	18:R:40:LEU:HD23	2.44	0.47
1:A:78:G:N1	1:A:92:C:N4	2.62	0.47
1:A:833:U:H2'	1:A:834:C:C6	2.49	0.47
1:A:1118:C:H1'	1:A:1179:A:C4	2.49	0.47
2:B:98:LEU:HB2	2:B:101:MET:CG	2.45	0.47
2:B:223:ILE:H	2:B:223:ILE:HG13	1.59	0.47
3:C:11:ARG:HB3	3:C:16:ARG:HB2	1.95	0.47
8:H:11:THR:O	8:H:12:ARG:C	2.58	0.47
12:L:85:ILE:HG23	12:L:98:TYR:HB3	1.95	0.47
13:M:19:LEU:O	13:M:22:ILE:HG13	2.14	0.47
1:A:255:G:C2	1:A:272:C:C2	3.03	0.47
1:A:1126:U:HO2'	1:A:1127:G:P	2.37	0.47
1:A:1250:A:H4'	9:I:68:GLY:N	2.30	0.47
1:A:1405:G:HO2'	1:A:1518[A]:MA6:HO2'	1.58	0.47
5:E:87:SER:HB3	5:E:131:ILE:HD13	1.96	0.47
9:I:5:TYR:CD2	9:I:6:GLY:N	2.82	0.47
11:K:93:GLN:HA	11:K:96:ARG:HG3	1.96	0.47
17:Q:5:VAL:C	17:Q:6:LEU:HD23	2.39	0.47
20:T:10:LEU:O	20:T:13:LEU:HD12	2.14	0.47
1:A:778:G:H2'	1:A:779:C:O4'	2.13	0.47
1:A:1516[A]:G:H2'	1:A:1518[A]:MA6:OP2	2.15	0.47
11:K:114:VAL:HG23	11:K:115:PRO:HD2	1.97	0.47
13:M:36:LYS:HB2	13:M:59:TYR:CE2	2.50	0.47
1:A:1093:A:N3	1:A:1109:C:O2'	2.44	0.47
1:A:1435:G:H2'	1:A:1436:U:H6	1.79	0.47
4:D:184:LYS:HE3	4:D:184:LYS:HB2	1.74	0.47
8:H:86:ILE:HG21	8:H:133:LEU:HD22	1.96	0.47
11:K:70:LYS:NZ	11:K:70:LYS:HB3	2.30	0.47
15:O:14:GLU:HG3	15:O:15:PHE:CE1	2.50	0.47
17:Q:22:LEU:HA	17:Q:22:LEU:HD12	1.58	0.47
17:Q:83:ASP:OD1	17:Q:83:ASP:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1313:U:H5	19:S:4:SER:HB2	1.79	0.47
2:B:215:LEU:HD23	2:B:215:LEU:HA	1.72	0.47
2:B:218:ALA:O	2:B:222:ILE:HG13	2.14	0.47
2:B:219:VAL:HA	2:B:222:ILE:HD12	1.97	0.47
1:A:186:C:H2'	1:A:187:C:C6	2.49	0.46
1:A:502:G:H2'	1:A:503:C:O4'	2.15	0.46
1:A:542:G:H2'	1:A:543:C:H6	1.80	0.46
1:A:925:G:C2	1:A:927:G:C8	3.03	0.46
1:A:1402:4OC:O2	1:A:1500:A:N1	2.48	0.46
2:B:24:TRP:HZ3	2:B:29:ALA:HB2	1.80	0.46
4:D:132:ARG:HG3	4:D:133:VAL:N	2.29	0.46
7:G:69:VAL:HG12	7:G:100:ALA:HA	1.97	0.46
10:J:64:GLU:HG2	14:N:59:ALA:HA	1.96	0.46
11:K:60:ALA:HA	11:K:63:LEU:HD12	1.97	0.46
13:M:8:GLU:CD	13:M:22:ILE:HA	2.40	0.46
15:O:12:ILE:HG23	15:O:27:VAL:HG11	1.95	0.46
1:A:1063:C:H2'	1:A:1064:G:C8	2.49	0.46
6:F:2:ARG:O	6:F:66:GLU:HA	2.15	0.46
7:G:41:ARG:HH11	7:G:41:ARG:HB3	1.80	0.46
15:O:42:HIS:CD2	15:O:43:LEU:HD23	2.50	0.46
17:Q:27:PHE:CE1	17:Q:36:ILE:HD11	2.50	0.46
17:Q:97:SER:O	17:Q:98:LEU:HD12	2.14	0.46
18:R:40:LEU:HB3	18:R:79:LEU:HD11	1.97	0.46
1:A:451:A:OP1	1:A:451:A:C8	2.67	0.46
1:A:1070:U:H2'	1:A:1071:C:H6	1.80	0.46
2:B:30:ARG:HD2	2:B:31:TYR:CZ	2.49	0.46
7:G:16:LEU:HD21	9:I:42:ARG:HG2	1.97	0.46
8:H:4:ASP:CG	8:H:85:ARG:NH1	2.72	0.46
13:M:97:PRO:HB2	13:M:101:GLN:OE1	2.15	0.46
1:A:78:G:H1	1:A:92:C:N4	2.14	0.46
1:A:283:C:C2	1:A:284:G:C8	3.02	0.46
1:A:299:G:C6	1:A:300:A:C6	3.03	0.46
1:A:992:U:O2'	1:A:993:G:OP2	2.29	0.46
2:B:98:LEU:O	2:B:101:MET:HG3	2.16	0.46
4:D:64:LEU:HD12	4:D:75:PHE:CZ	2.50	0.46
4:D:70:ILE:HG22	4:D:71:SER:O	2.16	0.46
6:F:67:MET:HE3	6:F:67:MET:HB2	1.72	0.46
11:K:58:PRO:HD3	11:K:89:ALA:HB1	1.96	0.46
13:M:88:ARG:NH1	19:S:3:ARG:HH21	2.14	0.46
19:S:28:LYS:HG2	19:S:29:ARG:H	1.81	0.46
20:T:84:LEU:HD23	20:T:84:LEU:HA	1.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:C:O2	1:A:262:A:H2	1.99	0.46
1:A:532:A:O2'	1:A:533:A:OP1	2.20	0.46
1:A:1242:C:OP1	21:U:10:ARG:NH1	2.45	0.46
2:B:35:GLU:HG2	2:B:40:HIS:HD2	1.79	0.46
3:C:174:PRO:HB2	3:C:177:THR:HG22	1.96	0.46
4:D:61:LYS:HZ2	4:D:62:GLN:N	2.13	0.46
5:E:51:VAL:HB	5:E:52:PRO:HD3	1.97	0.46
7:G:51:GLN:HB2	7:G:58:PRO:HD3	1.97	0.46
8:H:111:ILE:HG22	8:H:134:ILE:HD12	1.96	0.46
9:I:2:GLU:HG3	9:I:3:GLN:N	2.31	0.46
21:U:6:ARG:CZ	21:U:15:ARG:HH12	2.29	0.46
1:A:397:A:H5'	1:A:398:C:OP1	2.15	0.46
1:A:687:A:H4'	1:A:688:G:O5'	2.16	0.46
1:A:1005:A:H1'	1:A:1026:G:H22	1.81	0.46
1:A:1037:C:H2'	1:A:1038:C:C6	2.51	0.46
1:A:1063:C:C6	1:A:1064:G:C8	3.04	0.46
1:A:1305:G:C8	1:A:1305:G:OP2	2.68	0.46
2:B:51:LEU:O	2:B:55:PHE:HB2	2.15	0.46
4:D:70:ILE:HG22	4:D:71:SER:N	2.30	0.46
9:I:88:TYR:CD2	9:I:89:ASN:HB2	2.49	0.46
10:J:57:LYS:O	10:J:60:ARG:NH1	2.48	0.46
1:A:824:C:H2'	1:A:825:G:C8	2.50	0.46
1:A:1186:G:H2'	1:A:1187:G:O4'	2.15	0.46
1:A:1443:G:H5''	1:A:1446:A:OP1	2.16	0.46
1:A:1499:A:C1'	1:A:1520[A]:G:H5'	2.46	0.46
3:C:71:ALA:HB1	3:C:109:PRO:HG3	1.97	0.46
5:E:12:LEU:HD13	5:E:31:LEU:HB2	1.96	0.46
9:I:39:GLY:O	9:I:40:LEU:HD23	2.16	0.46
1:A:1035:A:H2'	1:A:1036:G:C8	2.50	0.46
1:A:1257:U:H4'	1:A:1258:G:O5'	2.15	0.46
1:A:1301:U:HO2'	1:A:1302:U:P	2.38	0.46
6:F:28:ARG:O	6:F:32:ASN:HB2	2.16	0.46
12:L:58:VAL:HG12	12:L:59:ARG:O	2.15	0.46
13:M:48:LEU:HD12	13:M:53:VAL:HG23	1.98	0.46
1:A:222:U:H2'	1:A:223:U:C6	2.50	0.46
1:A:949:A:C2	1:A:1233:G:N3	2.84	0.46
2:B:223:ILE:O	2:B:227:GLY:N	2.48	0.46
7:G:18:TYR:OH	7:G:58:PRO:HG2	2.16	0.46
10:J:48:THR:OG1	10:J:62:HIS:CD2	2.69	0.46
17:Q:82:MET:HE3	17:Q:82:MET:HB3	1.82	0.46
1:A:75:G:N1	1:A:96:G:C6	2.83	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1504:G:H4'	1:A:1505:G:H5'	1.98	0.46
2:B:84:GLU:OE1	2:B:216:SER:HA	2.16	0.46
12:L:27:LEU:HG	12:L:28:LYS:H	1.81	0.46
14:N:46:GLU:O	14:N:49:HIS:HB2	2.15	0.46
21:U:13:ILE:HG22	21:U:22:ARG:CZ	2.46	0.46
1:A:200:G:H2'	1:A:201:C:C6	2.50	0.45
1:A:679:C:H2'	1:A:680:C:C6	2.51	0.45
1:A:880:C:OP1	12:L:8:ASN:ND2	2.46	0.45
1:A:922:G:C2	1:A:1396:A:C6	3.04	0.45
1:A:1197:G:H5''	24:A:2066:HOH:O	2.16	0.45
5:E:17:ALA:CB	5:E:26:PHE:HD2	2.29	0.45
19:S:39:THR:HG22	19:S:40:ILE:O	2.16	0.45
1:A:436:C:H5'	4:D:156:GLU:OE1	2.16	0.45
1:A:1065:U:H4'	1:A:1066:C:O5'	2.16	0.45
1:A:1228:C:O3'	13:M:116:THR:HG23	2.16	0.45
1:A:1330:U:H2'	1:A:1331:G:H5'	1.99	0.45
2:B:33:TYR:C	2:B:33:TYR:CD2	2.93	0.45
3:C:81:GLY:O	3:C:84:ILE:HG22	2.17	0.45
8:H:86:ILE:HG22	8:H:87:SER:N	2.31	0.45
13:M:39:ILE:HG23	13:M:52:GLU:OE2	2.15	0.45
1:A:455:C:H6	1:A:455:C:O5'	1.99	0.45
1:A:892:A:H2'	1:A:893:C:C6	2.51	0.45
1:A:1196:U:OP1	1:A:1197:G:H5'	2.17	0.45
1:A:1355:G:H2'	1:A:1356:G:C8	2.51	0.45
1:A:1485:U:O2	1:A:1485:U:H2'	2.16	0.45
2:B:133:LYS:O	2:B:137:ARG:HG3	2.16	0.45
3:C:112:SER:O	3:C:115:LEU:HB2	2.15	0.45
5:E:105:VAL:HB	5:E:106:PRO:HD3	1.99	0.45
7:G:22:LEU:O	7:G:25:ALA:HB3	2.16	0.45
8:H:105:ARG:HA	8:H:105:ARG:HD3	1.77	0.45
11:K:85:ARG:HD3	11:K:113:PRO:HD3	1.98	0.45
14:N:32:SER:O	14:N:40:CYS:HB2	2.16	0.45
19:S:74:PHE:CD1	19:S:74:PHE:N	2.84	0.45
1:A:35:G:H2'	1:A:36:C:C6	2.51	0.45
1:A:959:A:H3'	1:A:960:U:H5''	1.98	0.45
2:B:20:GLU:HB2	2:B:190:THR:HB	1.98	0.45
8:H:46:LYS:HG3	8:H:64:LYS:HB3	1.98	0.45
13:M:88:ARG:HG3	13:M:98:VAL:HG13	1.97	0.45
17:Q:5:VAL:O	17:Q:6:LEU:HD23	2.15	0.45
1:A:109:A:H2'	1:A:326:G:N2	2.31	0.45
1:A:544:G:C6	1:A:545:C:C4	3.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:731:G:OP1	1:A:766:A:H1'	2.17	0.45
7:G:94:ARG:O	7:G:97:GLN:HB3	2.16	0.45
10:J:24:VAL:HG13	10:J:34:VAL:HG11	1.98	0.45
15:O:45:VAL:HG12	15:O:46:HIS:H	1.80	0.45
1:A:79:G:C5	1:A:91:C:N3	2.84	0.45
1:A:1306:A:C2	1:A:1307:U:H1'	2.52	0.45
1:A:1412:C:H2'	1:A:1413:A:C8	2.52	0.45
13:M:27:LYS:HA	13:M:27:LYS:HD2	1.53	0.45
13:M:50:GLU:HG3	13:M:51:ALA:N	2.32	0.45
15:O:29:VAL:HG13	15:O:63:ARG:HG3	1.99	0.45
16:P:53:VAL:O	16:P:55:ARG:N	2.49	0.45
20:T:70:SER:HA	20:T:73:HIS:CD2	2.51	0.45
1:A:328:C:O2'	1:A:329:A:OP2	2.27	0.45
1:A:909:A:H2'	1:A:910:C:O4'	2.17	0.45
1:A:1509:C:N4	1:A:1526:G:H1	2.15	0.45
3:C:116:VAL:O	3:C:120:VAL:HG23	2.16	0.45
4:D:200:GLU:H	4:D:200:GLU:CD	2.24	0.45
5:E:93:PRO:HD2	8:H:105:ARG:NH2	2.31	0.45
10:J:7:LYS:HB3	10:J:97:GLU:HB2	1.99	0.45
10:J:50:ILE:H	10:J:50:ILE:CD1	2.28	0.45
12:L:46:LYS:HD2	12:L:94:PRO:CG	2.47	0.45
1:A:1381:U:N1	7:G:156:TRP:HH2	2.15	0.45
7:G:135:VAL:HG12	7:G:139:GLU:OE2	2.17	0.45
8:H:1:MET:HG2	8:H:2:LEU:N	2.32	0.45
12:L:60:LEU:HD13	12:L:60:LEU:HA	1.68	0.45
16:P:4:ILE:HG21	16:P:74:LEU:HD11	1.98	0.45
17:Q:21:VAL:O	17:Q:41:LYS:HA	2.16	0.45
1:A:140:A:H2'	1:A:141:A:O4'	2.17	0.45
1:A:273:A:N6	1:A:274:A:C6	2.85	0.45
2:B:114:ARG:HD2	2:B:118:LEU:HG	1.99	0.45
4:D:203:VAL:O	4:D:206:PHE:HB3	2.17	0.45
6:F:86:ARG:O	6:F:87:ARG:HG2	2.16	0.45
7:G:44:TYR:O	7:G:48:LYS:HG3	2.17	0.45
9:I:17:VAL:HG11	9:I:81:ILE:HA	1.99	0.45
9:I:118:LYS:HZ2	9:I:118:LYS:HG3	1.54	0.45
18:R:58:LEU:HD23	18:R:58:LEU:HA	1.60	0.45
20:T:56:MET:HE2	20:T:85:MET:HA	1.99	0.45
1:A:1190:G:O3'	3:C:3:ASN:HB2	2.17	0.45
3:C:10:PHE:CE2	3:C:178:LEU:HB2	2.51	0.45
4:D:155:LEU:HD23	4:D:156:GLU:H	1.82	0.45
20:T:56:MET:HG2	20:T:84:LEU:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:92:LEU:HD22	20:T:92:LEU:HA	1.60	0.45
1:A:475:G:C4	1:A:476:G:C8	3.05	0.44
5:E:19:MET:HE1	5:E:24:ARG:NH1	2.32	0.44
7:G:27:ILE:HD11	7:G:43:PHE:HB3	1.98	0.44
16:P:75:ARG:C	16:P:78:GLY:H	2.24	0.44
17:Q:10:VAL:HG23	17:Q:55:ASP:O	2.17	0.44
19:S:18:LYS:O	19:S:22:LEU:HG	2.16	0.44
1:A:112:G:O2'	1:A:113:G:H5'	2.18	0.44
1:A:253:U:H2'	1:A:254:G:C8	2.53	0.44
1:A:1305:G:H5''	21:U:4:GLY:HA3	1.99	0.44
5:E:76:ILE:HG23	5:E:142:LEU:HD11	1.99	0.44
6:F:98:LEU:HD23	6:F:98:LEU:HA	1.68	0.44
7:G:32:ARG:C	7:G:34:GLY:H	2.25	0.44
7:G:113:GLU:H	7:G:113:GLU:HG2	1.31	0.44
11:K:119:CYS:O	11:K:121:PRO:HD3	2.18	0.44
15:O:21:ASP:CG	15:O:24:SER:OG	2.59	0.44
17:Q:40:LYS:HG2	17:Q:42:TYR:CE1	2.52	0.44
1:A:976:G:C8	1:A:1358:U:O2	2.70	0.44
1:A:1241:G:H2'	1:A:1242:C:H6	1.82	0.44
1:A:1278:U:H5'	1:A:1279:A:O4'	2.16	0.44
2:B:51:LEU:HG	2:B:201:ILE:HG23	1.99	0.44
2:B:100:GLY:N	2:B:176:GLU:OE2	2.39	0.44
3:C:187:ALA:HB3	3:C:198:VAL:HB	1.99	0.44
1:A:106:C:O2'	1:A:107:G:H5'	2.18	0.44
1:A:130:A:H1'	1:A:263:A:O2'	2.18	0.44
1:A:376:G:OP2	16:P:67:THR:HG21	2.17	0.44
1:A:518:C:H4'	1:A:519:C:O5'	2.16	0.44
1:A:629:G:H2'	1:A:630:G:O4'	2.18	0.44
1:A:1211:U:H1'	1:A:1213:A:C2	2.52	0.44
3:C:172:ARG:CZ	3:C:172:ARG:HB2	2.47	0.44
5:E:110:LEU:HA	5:E:110:LEU:HD23	1.59	0.44
7:G:74:GLU:O	7:G:88:PRO:HA	2.16	0.44
1:A:858:G:C6	1:A:869:G:C8	3.05	0.44
1:A:877:C:O2'	1:A:878:G:H5'	2.17	0.44
1:A:955:U:H1'	1:A:1227:A:H61	1.83	0.44
2:B:24:TRP:CZ3	2:B:26:PRO:HA	2.51	0.44
2:B:87:ARG:HH21	2:B:219:VAL:HB	1.82	0.44
2:B:97:TRP:CZ2	2:B:101:MET:HB2	2.52	0.44
1:A:824:C:H2'	1:A:825:G:H8	1.83	0.44
1:A:1157:A:H4'	1:A:1158:C:O5'	2.17	0.44
1:A:1191:A:C4	1:A:1192:C:C5	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:167:TRP:HE3	3:C:168:ALA:N	2.16	0.44
4:D:61:LYS:HD3	4:D:206:PHE:CE2	2.53	0.44
7:G:47:CYS:O	7:G:50:ILE:HG22	2.18	0.44
11:K:91:ARG:HH12	18:R:88:LYS:NZ	2.15	0.44
13:M:88:ARG:HH11	19:S:3:ARG:HH21	1.66	0.44
17:Q:31:LEU:HD12	17:Q:31:LEU:HA	1.83	0.44
17:Q:76:LEU:HD11	17:Q:79:SER:HB2	1.98	0.44
1:A:407:G:N2	1:A:436:C:C2	2.85	0.44
1:A:447:G:H2'	1:A:485:G:N2	2.32	0.44
1:A:540:G:H2'	1:A:541:G:H8	1.80	0.44
1:A:1244:C:H42	1:A:1293:G:H1	1.66	0.44
1:A:1250:A:O2'	9:I:68:GLY:HA2	2.18	0.44
1:A:1505:G:C8	1:A:1505:G:H3'	2.52	0.44
1:A:92:C:H2'	1:A:93:G:C8	2.53	0.44
1:A:393:A:C2	1:A:394:G:C8	3.06	0.44
1:A:1237:C:N4	1:A:1336:C:O2	2.51	0.44
1:A:1241:G:H2'	1:A:1242:C:C6	2.53	0.44
1:A:1450:U:O2'	1:A:1451:A:H8	2.01	0.44
2:B:139:LYS:NZ	2:B:143:GLU:HG3	2.33	0.44
4:D:8:VAL:O	4:D:11:LEU:N	2.37	0.44
4:D:99:SER:HB3	4:D:139:ARG:HG3	1.99	0.44
4:D:187:ARG:HH22	4:D:188:LEU:HD12	1.82	0.44
8:H:119:LEU:HD12	8:H:124:ALA:HA	1.99	0.44
20:T:20:LEU:O	20:T:23:ARG:HB3	2.18	0.44
1:A:234:C:H2'	1:A:235:C:C6	2.53	0.44
1:A:243:A:H4'	1:A:244:U:H5''	2.00	0.44
1:A:440:A:H5'	1:A:442:C:OP2	2.18	0.44
1:A:560:U:H5'	1:A:566:G:C2	2.52	0.44
1:A:820:U:H4'	1:A:821:G:OP2	2.18	0.44
1:A:959:A:O2'	1:A:984:C:O2'	2.34	0.44
1:A:1059:C:OP2	3:C:199:LYS:NZ	2.47	0.44
5:E:90:VAL:C	5:E:91:LEU:HD23	2.43	0.44
8:H:20:TYR:HA	8:H:65:TYR:CZ	2.52	0.44
8:H:116:LYS:HZ3	8:H:127:LEU:HD12	1.82	0.44
12:L:82:VAL:O	12:L:106:ASP:HB2	2.18	0.44
13:M:107:ALA:HB3	13:M:111:LYS:HE3	2.00	0.44
15:O:81:LEU:HA	15:O:81:LEU:HD23	1.79	0.44
19:S:73:GLU:HB2	19:S:74:PHE:CE1	2.53	0.44
1:A:229:U:O2'	16:P:23:ASP:HB2	2.18	0.43
1:A:1285:A:H4'	1:A:1286:A:O5'	2.18	0.43
3:C:134:ILE:HG21	3:C:167:TRP:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:24:GLU:HG2	4:D:25:ARG:H	1.83	0.43
4:D:47:ARG:HG2	4:D:48:ALA:N	2.33	0.43
9:I:27:THR:OG1	9:I:31:GLN:O	2.30	0.43
11:K:115:PRO:C	11:K:117:ASN:H	2.25	0.43
12:L:41:ARG:HG2	12:L:42:THR:N	2.33	0.43
1:A:88:A:H2'	1:A:89:C:O4'	2.18	0.43
1:A:945:G:O6	1:A:1236:A:N1	2.50	0.43
1:A:1265:G:C6	1:A:1266:G:C6	3.06	0.43
6:F:7:ASN:HD21	18:R:34:TYR:HE1	1.66	0.43
9:I:79:LEU:HD23	9:I:79:LEU:HA	1.88	0.43
13:M:8:GLU:HG3	13:M:22:ILE:HG23	1.99	0.43
17:Q:81:ARG:HE	17:Q:84:LEU:CD1	2.24	0.43
20:T:29:LYS:O	20:T:32:ALA:HB3	2.17	0.43
1:A:376:G:H5''	16:P:5:ARG:HD2	1.99	0.43
1:A:452:A:O2'	1:A:453:A:O5'	2.35	0.43
1:A:1071:C:O2'	1:A:1072:G:H5'	2.17	0.43
1:A:1417:G:HO2'	1:A:1483:A:N6	2.15	0.43
2:B:144:ARG:O	2:B:147:LYS:HB3	2.18	0.43
2:B:185:ILE:HA	2:B:199:TYR:O	2.19	0.43
2:B:187:LEU:HD22	2:B:187:LEU:HA	1.73	0.43
6:F:14:LEU:HB2	6:F:19:LEU:HD12	2.00	0.43
7:G:129:GLU:OE1	7:G:131:LYS:HE2	2.18	0.43
8:H:104:ARG:HG3	8:H:138:TRP:CE3	2.53	0.43
12:L:6:THR:H	12:L:9:GLN:HB2	1.82	0.43
12:L:124:LYS:HA	12:L:125:PRO:HD3	1.84	0.43
13:M:12:ASN:N	13:M:45:VAL:HB	2.33	0.43
15:O:85:LEU:HA	15:O:85:LEU:HD23	1.65	0.43
1:A:79:G:C4	1:A:91:C:O2	2.71	0.43
1:A:93:G:O2'	1:A:95:U:H5'	2.17	0.43
1:A:539:A:H2'	1:A:540:G:C8	2.54	0.43
1:A:1029:C:H2'	1:A:1030:C:H6	1.83	0.43
1:A:1119:C:OP1	9:I:9:ARG:NH2	2.51	0.43
1:A:1226:C:H2'	13:M:103:THR:OG1	2.19	0.43
1:A:1493:A:H2'	1:A:1494:G:C8	2.54	0.43
1:A:1497:G:O2'	1:A:1518[A]:MA6:H92	2.18	0.43
2:B:114:ARG:NH1	2:B:118:LEU:HD21	2.21	0.43
4:D:35:ARG:HD2	4:D:35:ARG:N	2.33	0.43
8:H:13:ILE:HG21	8:H:13:ILE:HD13	1.72	0.43
8:H:50:ARG:HA	8:H:59:LEU:HD23	2.00	0.43
8:H:124:ALA:O	8:H:128:GLY:N	2.49	0.43
10:J:53:PRO:HA	14:N:41:ARG:NH2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:36:ILE:HD13	15:O:59:MET:HE3	2.00	0.43
1:A:115:G:O2'	1:A:116:A:OP2	2.24	0.43
1:A:981:U:H5'	14:N:21:TYR:CE1	2.54	0.43
1:A:1018:C:H2'	1:A:1019:C:O4'	2.18	0.43
1:A:1148:U:O2'	9:I:14:VAL:HG21	2.19	0.43
2:B:233:SER:HA	2:B:234:PRO:HD3	1.91	0.43
3:C:159:GLY:HA2	3:C:193:TYR:CG	2.54	0.43
4:D:38:TYR:HB2	4:D:39:PRO:HD2	2.00	0.43
11:K:59:TYR:CE1	11:K:63:LEU:HD21	2.54	0.43
11:K:95:ILE:H	11:K:95:ILE:HG13	1.51	0.43
12:L:31:PRO:HB2	12:L:32:PHE:CD2	2.54	0.43
12:L:120:TYR:N	12:L:120:TYR:CD2	2.86	0.43
13:M:36:LYS:HB2	13:M:59:TYR:HE2	1.83	0.43
20:T:22:ARG:O	20:T:23:ARG:C	2.59	0.43
1:A:60:A:H4'	1:A:61:G:O5'	2.18	0.43
1:A:355:C:C4	1:A:356:A:N7	2.86	0.43
1:A:524:G:H2'	1:A:525:C:C6	2.53	0.43
1:A:858:G:C6	1:A:869:G:N7	2.87	0.43
1:A:1091:U:O2	1:A:1093:A:C8	2.71	0.43
1:A:1145:C:HO2'	1:A:1146:A:C5'	2.28	0.43
1:A:1329:A:H2'	1:A:1330:U:O4'	2.18	0.43
1:A:1355:G:H2'	1:A:1356:G:H8	1.83	0.43
3:C:27:LYS:O	3:C:30:ARG:NH2	2.52	0.43
5:E:76:ILE:H	5:E:76:ILE:HG13	1.38	0.43
13:M:78:ILE:O	13:M:81:LEU:HD12	2.18	0.43
17:Q:38:ARG:HA	17:Q:38:ARG:HD3	1.57	0.43
1:A:953:G:H2'	1:A:954:G:O4'	2.19	0.43
1:A:1437:C:H2'	1:A:1438:G:C8	2.53	0.43
2:B:191:ASP:OD1	2:B:191:ASP:N	2.50	0.43
4:D:15:GLU:HB3	4:D:63:LYS:HD3	2.00	0.43
5:E:56:GLN:NE2	5:E:56:GLN:HA	2.34	0.43
7:G:88:PRO:O	7:G:89:MET:HB3	2.19	0.43
11:K:106:LYS:HD2	11:K:106:LYS:HA	1.85	0.43
1:A:344:A:H5'	1:A:345:C:H5	1.81	0.43
2:B:54:THR:O	2:B:58:ILE:HG13	2.19	0.43
2:B:142:LEU:HD23	2:B:142:LEU:HA	1.83	0.43
3:C:23:TYR:HE1	10:J:67:THR:HG23	1.83	0.43
8:H:45:ILE:HD12	8:H:61:VAL:HG13	2.01	0.43
1:A:509:A:C8	1:A:509:A:C3'	3.02	0.43
1:A:986:A:H1'	19:S:54:GLY:O	2.18	0.43
1:A:991:U:O2	1:A:993:G:H8	2.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1007:C:O2	1:A:1023:G:N1	2.51	0.43
1:A:1149:C:O2'	1:A:1280:A:N1	2.51	0.43
1:A:1255:G:N2	1:A:1283:G:H1'	2.34	0.43
4:D:53:ASP:OD1	4:D:53:ASP:N	2.51	0.43
9:I:8:GLY:CA	9:I:79:LEU:HB3	2.49	0.43
13:M:23:TYR:HB2	13:M:67:GLU:OE2	2.18	0.43
15:O:67:LEU:O	15:O:68:ARG:C	2.61	0.43
17:Q:29:HIS:ND1	17:Q:30:PRO:HD2	2.33	0.43
18:R:26:LEU:HA	18:R:26:LEU:HD12	1.62	0.43
18:R:31:LEU:HA	18:R:31:LEU:HD23	1.63	0.43
1:A:436:C:H2'	1:A:437:U:H6	1.83	0.43
1:A:620:C:H2'	1:A:621:A:O4'	2.18	0.43
1:A:990:C:H5'	1:A:1017:G:O2'	2.19	0.43
1:A:1089:G:C6	1:A:1090:U:C4	3.07	0.43
2:B:83:MET:SD	2:B:234:PRO:HB2	2.59	0.43
2:B:187:LEU:HD22	2:B:201:ILE:O	2.19	0.43
4:D:52:SER:O	4:D:56:VAL:HG23	2.19	0.43
7:G:6:ARG:O	7:G:6:ARG:HG3	2.17	0.43
7:G:15:ASP:OD1	7:G:44:TYR:OH	2.37	0.43
8:H:104:ARG:CZ	8:H:138:TRP:CZ2	3.02	0.43
8:H:134:ILE:H	8:H:134:ILE:HG13	1.61	0.43
9:I:19:LEU:HD12	9:I:84:ALA:HB3	2.01	0.43
12:L:70:ILE:HA	12:L:71:PRO:HD3	1.70	0.43
14:N:14:PRO:O	14:N:15:LYS:HB3	2.18	0.43
1:A:1063:C:H2'	1:A:1064:G:H8	1.83	0.42
1:A:1238:A:OP1	1:A:1336:C:N4	2.52	0.42
1:A:1251:A:H2'	1:A:1252:A:C8	2.54	0.42
2:B:55:PHE:HD2	2:B:55:PHE:HA	1.66	0.42
3:C:151:VAL:C	3:C:152:ILE:HD12	2.44	0.42
4:D:23:GLY:CA	4:D:112:VAL:HG12	2.47	0.42
15:O:37:ASN:O	15:O:38:ARG:C	2.62	0.42
16:P:1:MET:HE2	16:P:1:MET:HB3	1.79	0.42
21:U:10:ARG:O	21:U:13:ILE:HG12	2.19	0.42
1:A:56:U:H2'	1:A:57:G:C8	2.53	0.42
1:A:451:A:N7	1:A:481:G:C2	2.86	0.42
1:A:474:G:N1	1:A:475:G:C5	2.87	0.42
1:A:1202:G:C4	14:N:42:ILE:HD12	2.54	0.42
5:E:69:VAL:HA	5:E:70:PRO:HD3	1.76	0.42
7:G:28:ASN:HA	7:G:31:MET:HE2	2.02	0.42
7:G:152:ALA:O	7:G:155:ARG:HG2	2.20	0.42
13:M:68:GLY:HA2	13:M:71:ARG:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:18:ARG:O	16:P:20:VAL:HG23	2.19	0.42
21:U:6:ARG:HD2	21:U:15:ARG:HH22	1.83	0.42
1:A:79:G:C4	1:A:91:C:C2	3.07	0.42
1:A:481:G:O2'	1:A:482:A:C8	2.65	0.42
1:A:1190:G:O2'	1:A:1191:A:OP2	2.37	0.42
1:A:1350:A:OP2	9:I:118:LYS:HE3	2.19	0.42
1:A:1491:G:N2	1:A:1492:A:H62	2.16	0.42
5:E:51:VAL:O	5:E:54:ALA:HB3	2.19	0.42
8:H:53:VAL:O	8:H:53:VAL:HG12	2.19	0.42
9:I:89:ASN:HB3	9:I:92:TYR:CD1	2.54	0.42
9:I:113:LYS:H	9:I:119:ALA:HA	1.84	0.42
12:L:47:LYS:H	12:L:47:LYS:HG3	1.51	0.42
14:N:24:CYS:HB3	14:N:40:CYS:HB3	1.99	0.42
19:S:17:GLU:HA	19:S:20:LEU:HG	2.00	0.42
1:A:79:G:H2'	1:A:79:G:N3	2.34	0.42
1:A:190(K):G:H2'	1:A:190(L):U:C6	2.55	0.42
1:A:197:A:H1'	1:A:198:G:O4'	2.20	0.42
1:A:1526:G:C4	1:A:1527:C:C5	3.08	0.42
5:E:31:LEU:HA	5:E:31:LEU:HD23	1.54	0.42
13:M:65:LYS:H	13:M:65:LYS:HG2	1.36	0.42
20:T:44:ALA:HB1	20:T:92:LEU:HD23	2.02	0.42
20:T:87:LYS:O	20:T:91:LEU:HB2	2.19	0.42
1:A:443:C:N4	1:A:491:G:H1	2.13	0.42
1:A:784:C:H2'	1:A:785:G:O4'	2.19	0.42
1:A:1232:U:H5''	9:I:124:GLN:O	2.19	0.42
1:A:1321:C:C5	1:A:1322:C:C2	3.08	0.42
1:A:1427:U:H2'	1:A:1428:A:C8	2.54	0.42
1:A:1440:C:H2'	1:A:1441:G:O4'	2.19	0.42
6:F:67:MET:HB2	6:F:68:PRO:HD2	2.02	0.42
7:G:28:ASN:O	7:G:31:MET:HB3	2.19	0.42
12:L:41:ARG:HE	12:L:43:VAL:HG22	1.84	0.42
1:A:284:G:H2'	1:A:285:G:C8	2.54	0.42
1:A:391:G:C6	1:A:392:G:C5	3.07	0.42
3:C:61:ALA:C	3:C:63:ASN:H	2.27	0.42
3:C:113:ALA:N	3:C:114:PRO:HD2	2.34	0.42
8:H:10:LEU:HD23	8:H:10:LEU:HA	1.70	0.42
8:H:127:LEU:HD13	8:H:127:LEU:HA	1.73	0.42
11:K:120:ARG:HH11	11:K:120:ARG:HG2	1.85	0.42
13:M:77:ASN:O	13:M:80:ARG:HB3	2.19	0.42
2:B:18:GLY:HA3	2:B:42:ILE:H	1.85	0.42
2:B:184:VAL:HG12	2:B:197:VAL:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:151:LEU:HA	5:E:151:LEU:HD23	1.65	0.42
7:G:104:LEU:HD22	7:G:104:LEU:HA	1.81	0.42
8:H:100:ILE:HD12	8:H:125:ARG:HG3	2.01	0.42
10:J:19:SER:CB	10:J:91:PRO:HG3	2.50	0.42
11:K:73:MET:HE1	11:K:103:LEU:HG	2.02	0.42
16:P:43:LYS:HG2	16:P:48:TRP:CG	2.55	0.42
18:R:33:ASP:OD2	18:R:36:ASN:N	2.52	0.42
1:A:16:A:HO2'	1:A:1080:A:HO2'	1.65	0.42
1:A:31:G:N2	1:A:48:C:OP1	2.45	0.42
1:A:36:C:C4	1:A:37:U:C5	3.08	0.42
1:A:77:G:C2	1:A:78:G:C4	3.08	0.42
1:A:690:G:H2'	1:A:691:G:O4'	2.19	0.42
1:A:1095:U:H2'	1:A:1096:C:C6	2.54	0.42
1:A:1220:G:H5'	19:S:34:TRP:O	2.20	0.42
2:B:45:GLN:O	2:B:49:GLU:HG3	2.20	0.42
4:D:30:LYS:O	4:D:32:ALA:N	2.53	0.42
13:M:34:LEU:HD13	13:M:39:ILE:HB	2.02	0.42
13:M:49:THR:HB	13:M:52:GLU:H	1.85	0.42
1:A:79:G:N1	1:A:80:G:N7	2.68	0.42
1:A:540:G:C4	1:A:541:G:C8	3.08	0.42
1:A:940:C:H2'	1:A:941:G:O4'	2.20	0.42
1:A:1255:G:C6	1:A:1283:G:C2	3.08	0.42
1:A:1329:A:C5'	13:M:29:ARG:HD2	2.49	0.42
4:D:28:SER:O	4:D:30:LYS:N	2.51	0.42
5:E:102:ALA:HB3	5:E:107:ARG:HB2	2.02	0.42
10:J:48:THR:OG1	10:J:62:HIS:HB3	2.20	0.42
12:L:67:THR:O	12:L:96:VAL:HG12	2.20	0.42
1:A:461:C:H4'	1:A:462:G:OP2	2.20	0.42
1:A:1103:C:H2'	1:A:1104:G:O4'	2.20	0.42
1:A:1148:U:H4'	9:I:14:VAL:HG11	2.02	0.42
1:A:1368:G:H5'	9:I:112:LYS:O	2.19	0.42
1:A:1433:A:N6	1:A:1434:A:C6	2.88	0.42
1:A:1453:G:H2'	1:A:1454:G:O4'	2.20	0.42
2:B:33:TYR:C	2:B:33:TYR:HD2	2.28	0.42
7:G:103:TRP:CZ2	7:G:141:VAL:HG21	2.54	0.42
13:M:21:TYR:N	13:M:21:TYR:CD2	2.87	0.42
15:O:34:LEU:HD23	15:O:35:ARG:N	2.35	0.42
16:P:50:LYS:HG2	16:P:51:VAL:H	1.85	0.42
16:P:53:VAL:O	16:P:54:GLU:C	2.63	0.42
20:T:11:SER:C	20:T:13:LEU:N	2.78	0.42
1:A:794:A:N6	1:A:795:C:N4	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:830:G:C6	1:A:831:U:C4	3.08	0.41
1:A:938:A:C6	1:A:939:G:C5	3.08	0.41
5:E:10:MET:SD	5:E:13:ILE:HG23	2.60	0.41
5:E:11:ILE:HG22	5:E:12:LEU:N	2.34	0.41
5:E:112:LEU:HA	5:E:112:LEU:HD23	1.51	0.41
5:E:119:LEU:HA	5:E:119:LEU:HD23	1.50	0.41
7:G:89:MET:HB3	7:G:89:MET:HE2	1.78	0.41
7:G:136:LYS:HB3	7:G:136:LYS:NZ	2.35	0.41
8:H:107:LEU:N	8:H:107:LEU:HD23	2.35	0.41
11:K:98:LEU:HA	11:K:98:LEU:HD22	1.68	0.41
1:A:191:G:O2'	20:T:102:GLY:O	2.17	0.41
1:A:804:U:H5''	1:A:805:C:OP2	2.20	0.41
1:A:1342:C:H2'	1:A:1343:G:C8	2.55	0.41
5:E:148:VAL:O	5:E:152:ARG:HG3	2.20	0.41
7:G:22:LEU:HD12	7:G:22:LEU:HA	1.74	0.41
8:H:59:LEU:HD23	8:H:59:LEU:HA	1.81	0.41
11:K:33:THR:HB	11:K:39:PRO:HA	2.02	0.41
15:O:38:ARG:HA	15:O:38:ARG:HD3	1.62	0.41
17:Q:51:TYR:CE1	17:Q:73:VAL:HB	2.55	0.41
1:A:79:G:N2	1:A:80:G:C8	2.88	0.41
1:A:1419:G:H2'	1:A:1420:C:C6	2.55	0.41
1:A:1543:C:O5'	1:A:1543:C:H6	2.03	0.41
2:B:71:VAL:O	2:B:164:VAL:HA	2.19	0.41
3:C:119:ARG:O	3:C:122:GLU:HB2	2.20	0.41
3:C:164:ARG:NH1	3:C:166:GLU:OE1	2.51	0.41
5:E:15:ARG:O	5:E:16:THR:C	2.63	0.41
7:G:40:ALA:CB	9:I:41:VAL:HG21	2.48	0.41
9:I:46:ALA:HB1	9:I:77:ILE:HG21	2.02	0.41
17:Q:3:LYS:HD3	17:Q:61:GLU:O	2.19	0.41
20:T:18:GLN:O	20:T:21:LYS:HB2	2.20	0.41
1:A:107:G:C2	1:A:108:G:H1'	2.56	0.41
1:A:266:G:H5''	1:A:266:G:C8	2.56	0.41
1:A:1270:C:OP2	21:U:24:ARG:NH2	2.53	0.41
2:B:16:HIS:CE1	2:B:210:SER:HB2	2.56	0.41
3:C:153:VAL:HG12	3:C:154:SER:H	1.84	0.41
8:H:121:ASP:HB2	8:H:125:ARG:NH2	2.35	0.41
11:K:47:VAL:HG12	11:K:48:ILE:N	2.34	0.41
11:K:51:LYS:O	11:K:55:LYS:HE2	2.20	0.41
13:M:56:LEU:HD23	13:M:56:LEU:HA	1.62	0.41
15:O:32:LEU:HD12	15:O:63:ARG:HB2	2.01	0.41
1:A:123:C:OP1	1:A:312:C:H5'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:966:M2G:HM22	1:A:967:5MC:O2	2.20	0.41
5:E:20:GLN:O	5:E:21:ALA:C	2.63	0.41
10:J:26:ALA:HB1	10:J:84:GLN:HB3	2.03	0.41
13:M:12:ASN:H	13:M:45:VAL:HB	1.85	0.41
16:P:40:ASP:HA	16:P:41:PRO:HD3	1.82	0.41
20:T:33:ILE:O	20:T:34:LYS:C	2.63	0.41
20:T:100:ILE:C	20:T:102:GLY:H	2.27	0.41
1:A:369:C:O2'	1:A:370:C:H5'	2.21	0.41
1:A:622:A:C8	1:A:623:C:C6	3.08	0.41
1:A:881:G:OP2	12:L:12:ARG:NH2	2.53	0.41
1:A:1053:G:O2'	1:A:1199:U:H5	2.04	0.41
2:B:84:GLU:OE2	2:B:235:SER:OG	2.35	0.41
4:D:194:LEU:HB3	4:D:196:LEU:HG	2.02	0.41
9:I:53:VAL:HB	9:I:92:TYR:CZ	2.56	0.41
10:J:6:ILE:HG22	10:J:8:LEU:HD21	2.03	0.41
13:M:71:ARG:NH1	13:M:71:ARG:HG2	2.36	0.41
19:S:13:ASP:OD2	19:S:13:ASP:N	2.51	0.41
1:A:661:G:H5''	1:A:661:G:C8	2.55	0.41
1:A:883:C:C2	1:A:884:U:C5	3.09	0.41
1:A:927:G:H1	1:A:1390:U:H3	1.67	0.41
1:A:1152:A:OP1	10:J:68:HIS:CE1	2.74	0.41
1:A:1201:A:H4'	1:A:1202:G:H5''	2.03	0.41
1:A:1213:A:N6	1:A:1215:G:N3	2.69	0.41
1:A:1354:C:H2'	1:A:1355:G:C8	2.54	0.41
1:A:1415:G:H1	1:A:1485:U:H3	1.69	0.41
1:A:1422:G:C2	1:A:1423:G:N7	2.88	0.41
4:D:88:VAL:O	4:D:89:THR:C	2.62	0.41
5:E:9:LYS:NZ	5:E:111:GLU:OE1	2.53	0.41
5:E:106:PRO:O	5:E:107:ARG:C	2.64	0.41
6:F:1:MET:HB3	6:F:66:GLU:HG2	2.02	0.41
6:F:67:MET:SD	6:F:72:VAL:HG23	2.61	0.41
7:G:115:ARG:HB2	7:G:118:VAL:CG2	2.50	0.41
10:J:91:PRO:HB2	10:J:94:VAL:HB	2.03	0.41
1:A:95:U:O2'	1:A:96:G:H5'	2.21	0.41
1:A:125:U:O3'	1:A:633:G:N2	2.54	0.41
1:A:179:A:H2'	1:A:180:U:C6	2.55	0.41
1:A:257:G:C6	1:A:258:G:N7	2.89	0.41
1:A:1027:C:N4	1:A:1034:G:H1	2.19	0.41
5:E:68:GLU:O	5:E:68:GLU:HG3	2.21	0.41
18:R:19:LYS:HB2	18:R:19:LYS:HE3	1.76	0.41
1:A:292:G:H1	1:A:308:C:H42	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:U:OP2	4:D:36:ARG:NH2	2.54	0.41
1:A:564:C:C5	17:Q:31:LEU:HD21	2.56	0.41
1:A:620:C:N1	4:D:135:LEU:HD13	2.35	0.41
1:A:659:U:H2'	1:A:660:G:C8	2.56	0.41
1:A:1026:G:N7	1:A:1027:C:C4	2.89	0.41
1:A:1402:4OC:H2'	1:A:1403:C:H6	1.84	0.41
1:A:1495:U:H2'	1:A:1496:C:C6	2.56	0.41
4:D:24:GLU:O	4:D:25:ARG:HB3	2.20	0.41
6:F:27:GLN:HA	6:F:30:LEU:HD12	2.03	0.41
7:G:111:ARG:NH1	7:G:113:GLU:OE2	2.54	0.41
9:I:8:GLY:HA2	9:I:79:LEU:CD1	2.51	0.41
9:I:50:LEU:HA	9:I:53:VAL:HG22	2.03	0.41
10:J:50:ILE:CA	10:J:60:ARG:HB3	2.45	0.41
11:K:90:GLY:HA2	11:K:93:GLN:HB2	2.01	0.41
12:L:67:THR:C	12:L:96:VAL:HG12	2.46	0.41
13:M:84:ILE:HG13	13:M:86:CYS:H	1.86	0.41
14:N:16:PHE:HB2	14:N:19:ARG:HD2	2.03	0.41
15:O:32:LEU:HA	15:O:32:LEU:HD22	1.72	0.41
17:Q:7:THR:O	17:Q:23:VAL:HG13	2.20	0.41
1:A:147:G:N2	1:A:148:G:C4	2.89	0.41
1:A:276:G:O3'	17:Q:68:ARG:NH1	2.51	0.41
1:A:811:C:O2'	1:A:901:A:N1	2.51	0.41
1:A:1003(A):G:H2'	1:A:1004:A:H4'	2.03	0.41
1:A:1320:C:N4	19:S:36:ARG:HG3	2.36	0.41
1:A:1401:G:O6	1:A:1504:G:N2	2.54	0.41
2:B:68:ILE:HG21	2:B:68:ILE:HD13	1.74	0.41
4:D:135:LEU:HA	4:D:136:PRO:HD3	1.92	0.41
4:D:155:LEU:HD23	4:D:156:GLU:N	2.36	0.41
5:E:61:TYR:HD1	5:E:61:TYR:HA	1.72	0.41
12:L:85:ILE:CG2	12:L:98:TYR:HB3	2.50	0.41
17:Q:63:ARG:HA	17:Q:64:PRO:HD3	1.85	0.41
1:A:256:U:H2'	1:A:257:G:C8	2.57	0.40
1:A:398:C:O2'	1:A:399:G:H5'	2.21	0.40
1:A:794:A:C6	1:A:795:C:C4	3.09	0.40
1:A:875:C:O2'	8:H:14:ARG:NH1	2.54	0.40
1:A:926:G:N2	1:A:1542:U:OP1	2.44	0.40
1:A:977:A:H2'	1:A:978:A:H5''	2.04	0.40
1:A:1134:G:H1	1:A:1140:C:H42	1.67	0.40
1:A:1163:C:N3	1:A:1174:G:C2	2.89	0.40
1:A:1532:U:H6	1:A:1532:U:O5'	2.04	0.40
2:B:158:LEU:H	2:B:158:LEU:CD1	2.32	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:182:ILE:HA	2:B:183:PRO:HD3	1.86	0.40
2:B:187:LEU:HD12	2:B:205:ASP:HA	2.03	0.40
5:E:90:VAL:O	5:E:91:LEU:HD23	2.21	0.40
8:H:100:ILE:H	8:H:100:ILE:HG13	1.68	0.40
8:H:100:ILE:CG2	8:H:112:LEU:HD11	2.51	0.40
9:I:53:VAL:HG21	9:I:85:LEU:HD21	2.03	0.40
10:J:42:THR:HG23	10:J:67:THR:C	2.46	0.40
1:A:523:A:O5'	1:A:523:A:H8	2.04	0.40
1:A:1163:C:H2'	1:A:1164:G:O4'	2.22	0.40
1:A:1221:G:H4'	19:S:53:ASN:O	2.21	0.40
1:A:1277:C:O2'	1:A:1279:A:H1'	2.21	0.40
2:B:23:ARG:O	2:B:24:TRP:CD1	2.73	0.40
2:B:97:TRP:HZ3	2:B:176:GLU:OE2	2.04	0.40
2:B:231:GLU:HB3	2:B:232:PRO:HD2	2.02	0.40
3:C:136:GLN:O	3:C:140:ARG:HG3	2.21	0.40
6:F:68:PRO:HG2	6:F:71:ARG:HG3	2.03	0.40
8:H:9:MET:HE2	8:H:9:MET:HB3	1.87	0.40
11:K:50:TYR:CD2	11:K:54:ARG:HD2	2.57	0.40
15:O:39:LEU:HD23	15:O:43:LEU:HG	2.03	0.40
16:P:45:THR:HB	16:P:46:PRO:HD2	2.04	0.40
1:A:127:G:N2	1:A:234:C:O2	2.52	0.40
1:A:344:A:H4'	1:A:345:C:OP2	2.22	0.40
1:A:881:G:H2'	1:A:882:C:O4'	2.21	0.40
1:A:979:C:OP1	1:A:1222:G:O6	2.40	0.40
1:A:1056:U:H2'	1:A:1057:G:H8	1.87	0.40
1:A:1338:G:C6	1:A:1339:A:C6	3.10	0.40
1:A:1489:G:H2'	1:A:1490:C:C6	2.56	0.40
2:B:33:TYR:HD2	2:B:33:TYR:O	2.03	0.40
10:J:89:ASP:CB	10:J:91:PRO:HD2	2.52	0.40
17:Q:15:MET:HE3	17:Q:15:MET:HB2	1.81	0.40
1:A:397:A:H3'	1:A:397:A:N3	2.35	0.40
1:A:825:G:H21	8:H:11:THR:HG21	1.86	0.40
2:B:25:ASN:O	2:B:26:PRO:C	2.63	0.40
6:F:60:PHE:CZ	18:R:78:LEU:HD21	2.56	0.40
11:K:11:LYS:HB3	11:K:11:LYS:HE2	1.87	0.40
1:A:35:G:C6	1:A:36:C:N4	2.89	0.40
1:A:74:C:C4	1:A:75:G:N7	2.90	0.40
1:A:376:G:P	16:P:67:THR:HG21	2.61	0.40
1:A:663:A:H2'	1:A:664:G:O4'	2.22	0.40
1:A:1179:A:H2'	1:A:1180:A:O4'	2.20	0.40
1:A:1255:G:H22	1:A:1283:G:H1'	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1404:5MC:H1'	1:A:1499:A:C2	2.57	0.40
2:B:101:MET:HE2	2:B:152:PHE:CD1	2.57	0.40
4:D:114:ARG:HH11	4:D:114:ARG:HG3	1.86	0.40
5:E:80:ILE:CG2	8:H:104:ARG:HH21	2.32	0.40
5:E:102:ALA:O	5:E:107:ARG:NH1	2.54	0.40
8:H:116:LYS:HD2	8:H:129:VAL:HG11	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%)	208 (90%)	22 (10%)	2 (1%)	14	46
3	C	204/239 (85%)	180 (88%)	23 (11%)	1 (0%)	24	57
4	D	206/209 (99%)	196 (95%)	10 (5%)	0	100	100
5	E	148/162 (91%)	140 (95%)	8 (5%)	0	100	100
6	F	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
7	G	153/156 (98%)	136 (89%)	17 (11%)	0	100	100
8	H	136/138 (99%)	132 (97%)	4 (3%)	0	100	100
9	I	125/128 (98%)	114 (91%)	10 (8%)	1 (1%)	16	49
10	J	96/105 (91%)	79 (82%)	16 (17%)	1 (1%)	12	45
11	K	114/129 (88%)	100 (88%)	14 (12%)	0	100	100
12	L	121/135 (90%)	109 (90%)	10 (8%)	2 (2%)	7	35
13	M	116/126 (92%)	103 (89%)	12 (10%)	1 (1%)	14	46
14	N	58/61 (95%)	51 (88%)	7 (12%)	0	100	100
15	O	85/89 (96%)	77 (91%)	7 (8%)	1 (1%)	10	41
16	P	81/88 (92%)	77 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	Q	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
18	R	68/88 (77%)	63 (93%)	5 (7%)	0	100	100
19	S	78/93 (84%)	72 (92%)	5 (6%)	1 (1%)	9	39
20	T	97/106 (92%)	85 (88%)	11 (11%)	1 (1%)	12	45
21	U	22/27 (82%)	21 (96%)	1 (4%)	0	100	100
All	All	2336/2541 (92%)	2128 (91%)	197 (8%)	11 (0%)	24	57

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	21	ARG
19	S	31	ILE
12	L	28	LYS
2	B	24	TRP
20	T	73	HIS
9	I	119	ALA
12	L	51	ALA
3	C	86	VAL
10	J	34	VAL
13	M	7	VAL
15	O	45	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	202/220 (92%)	154 (76%)	48 (24%)	1	5
3	C	160/188 (85%)	123 (77%)	37 (23%)	1	6
4	D	180/181 (99%)	149 (83%)	31 (17%)	2	12
5	E	115/123 (94%)	85 (74%)	30 (26%)	0	4
6	F	90/90 (100%)	73 (81%)	17 (19%)	1	9
7	G	126/127 (99%)	107 (85%)	19 (15%)	3	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	119/119 (100%)	90 (76%)	29 (24%)	1	4
9	I	98/99 (99%)	76 (78%)	22 (22%)	1	6
10	J	87/92 (95%)	73 (84%)	14 (16%)	2	15
11	K	88/99 (89%)	69 (78%)	19 (22%)	1	7
12	L	103/110 (94%)	78 (76%)	25 (24%)	1	5
13	M	94/101 (93%)	69 (73%)	25 (27%)	0	3
14	N	49/50 (98%)	38 (78%)	11 (22%)	1	6
15	O	79/80 (99%)	61 (77%)	18 (23%)	1	6
16	P	72/74 (97%)	54 (75%)	18 (25%)	0	4
17	Q	94/97 (97%)	75 (80%)	19 (20%)	1	8
18	R	61/77 (79%)	50 (82%)	11 (18%)	2	11
19	S	71/80 (89%)	58 (82%)	13 (18%)	2	11
20	T	76/82 (93%)	56 (74%)	20 (26%)	0	3
21	U	19/22 (86%)	17 (90%)	2 (10%)	6	29
All	All	1983/2111 (94%)	1555 (78%)	428 (22%)	1	7

All (428) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	7	VAL
2	B	8	LYS
2	B	9	GLU
2	B	10	LEU
2	B	12	GLU
2	B	16	HIS
2	B	17	PHE
2	B	21	ARG
2	B	23	ARG
2	B	30	ARG
2	B	32	ILE
2	B	39	ILE
2	B	44	LEU
2	B	45	GLN
2	B	47	THR
2	B	49	GLU
2	B	54	THR
2	B	55	PHE

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Mol	Chain	Res	Type
2	B	61	LEU
2	B	67	THR
2	B	69	LEU
2	B	75	LYS
2	B	97	TRP
2	B	102	LEU
2	B	106	LYS
2	B	112	VAL
2	B	124	SER
2	B	127	ILE
2	B	139	LYS
2	B	142	LEU
2	B	144	ARG
2	B	154	LEU
2	B	155	LEU
2	B	157	ARG
2	B	158	LEU
2	B	162	ILE
2	B	164	VAL
2	B	168	THR
2	B	172	ILE
2	B	175	ARG
2	B	178	ARG
2	B	187	LEU
2	B	200	ILE
2	B	201	ILE
2	B	217	ARG
2	B	223	ILE
2	B	235	SER
2	B	239	VAL
3	C	3	ASN
3	C	4	LYS
3	C	10	PHE
3	C	11	ARG
3	C	15	THR
3	C	31	HIS
3	C	34	LEU
3	C	35	GLU
3	C	47	LEU
3	C	48	TYR
3	C	52	LEU
3	C	58	GLU

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Mol	Chain	Res	Type
3	C	70	VAL
3	C	75	VAL
3	C	91	LEU
3	C	94	LEU
3	C	95	THR
3	C	97	LYS
3	C	98	ASN
3	C	99	VAL
3	C	103	VAL
3	C	104	GLN
3	C	111	LEU
3	C	131	ARG
3	C	153	VAL
3	C	154	SER
3	C	166	GLU
3	C	172	ARG
3	C	175	LEU
3	C	176	HIS
3	C	178	LEU
3	C	188	LEU
3	C	191	THR
3	C	195	VAL
3	C	196	LEU
3	C	204	LEU
3	C	207	VAL
4	D	9	CYS
4	D	19	LEU
4	D	21	LEU
4	D	25	ARG
4	D	26	CYS
4	D	34	GLU
4	D	53	ASP
4	D	59	ARG
4	D	63	LYS
4	D	64	LEU
4	D	91	SER
4	D	99	SER
4	D	115	ARG
4	D	118	ARG
4	D	122	ARG
4	D	132	ARG
4	D	135	LEU

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Mol	Chain	Res	Type
4	D	139	ARG
4	D	140	VAL
4	D	150	GLU
4	D	155	LEU
4	D	157	LEU
4	D	159	ARG
4	D	178	VAL
4	D	179	GLU
4	D	186	LEU
4	D	187	ARG
4	D	192	GLU
4	D	194	LEU
4	D	202	LEU
4	D	209	ARG
5	E	6	PHE
5	E	12	LEU
5	E	16	THR
5	E	18	ARG
5	E	19	MET
5	E	24	ARG
5	E	26	PHE
5	E	34	VAL
5	E	41	VAL
5	E	49	PRO
5	E	55	VAL
5	E	56	GLN
5	E	64	ARG
5	E	68	GLU
5	E	75	THR
5	E	79	GLU
5	E	80	ILE
5	E	82	VAL
5	E	96	PRO
5	E	118	ILE
5	E	120	THR
5	E	125	SER
5	E	131	ILE
5	E	147	ASP
5	E	148	VAL
5	E	149	GLU
5	E	150	ARG
5	E	151	LEU

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Mol	Chain	Res	Type
5	E	152	ARG
5	E	153	LYS
6	F	3	ARG
6	F	9	VAL
6	F	10	LEU
6	F	14	LEU
6	F	16	GLN
6	F	19	LEU
6	F	24	GLU
6	F	30	LEU
6	F	32	ASN
6	F	37	VAL
6	F	43	LEU
6	F	67	MET
6	F	70	ASP
6	F	72	VAL
6	F	75	LEU
6	F	82	ARG
6	F	92	LYS
7	G	3	ARG
7	G	8	GLU
7	G	9	VAL
7	G	23	VAL
7	G	27	ILE
7	G	31	MET
7	G	32	ARG
7	G	47	CYS
7	G	61	VAL
7	G	67	GLU
7	G	75	VAL
7	G	79	ARG
7	G	84	ASN
7	G	104	LEU
7	G	113	GLU
7	G	125	MET
7	G	135	VAL
7	G	136	LYS
7	G	141	VAL
8	H	6	ILE
8	H	11	THR
8	H	19	VAL
8	H	24	THR

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Mol	Chain	Res	Type
8	H	25	ASP
8	H	26	VAL
8	H	37	ARG
8	H	45	ILE
8	H	51	VAL
8	H	52	ASP
8	H	53	VAL
8	H	63	LEU
8	H	83	ILE
8	H	85	ARG
8	H	86	ILE
8	H	88	LYS
8	H	91	ARG
8	H	93	VAL
8	H	95	VAL
8	H	97	VAL
8	H	98	LYS
8	H	104	ARG
8	H	105	ARG
8	H	115	SER
8	H	119	LEU
8	H	125	ARG
8	H	127	LEU
8	H	129	VAL
8	H	134	ILE
9	I	3	GLN
9	I	11	LYS
9	I	14	VAL
9	I	38	GLN
9	I	41	VAL
9	I	44	VAL
9	I	47	LEU
9	I	50	LEU
9	I	53	VAL
9	I	56	LEU
9	I	79	LEU
9	I	83	ARG
9	I	85	LEU
9	I	91	ASP
9	I	96	LEU
9	I	99	LEU
9	I	107	ARG

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Mol	Chain	Res	Type
9	I	109	VAL
9	I	113	LYS
9	I	118	LYS
9	I	121	ARG
9	I	127	LYS
10	J	3	LYS
10	J	9	ARG
10	J	15	THR
10	J	16	LEU
10	J	38	ILE
10	J	45	ARG
10	J	48	THR
10	J	60	ARG
10	J	62	HIS
10	J	73	ASP
10	J	82	ILE
10	J	92	THR
10	J	94	VAL
10	J	95	GLU
11	K	12	ARG
11	K	14	VAL
11	K	21	ILE
11	K	29	ILE
11	K	47	VAL
11	K	51	LYS
11	K	63	LEU
11	K	70	LYS
11	K	81	ASP
11	K	84	VAL
11	K	95	ILE
11	K	98	LEU
11	K	101	SER
11	K	106	LYS
11	K	114	VAL
11	K	119	CYS
11	K	120	ARG
11	K	122	LYS
11	K	124	LYS
12	L	7	ILE
12	L	16	GLU
12	L	18	VAL
12	L	20	LYS

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Mol	Chain	Res	Type
12	L	33	ARG
12	L	34	ARG
12	L	36	VAL
12	L	41	ARG
12	L	42	THR
12	L	43	VAL
12	L	47	LYS
12	L	55	VAL
12	L	59	ARG
12	L	60	LEU
12	L	61	THR
12	L	67	THR
12	L	77	LEU
12	L	79	GLU
12	L	80	HIS
12	L	82	VAL
12	L	93	LEU
12	L	96	VAL
12	L	97	ARG
12	L	104	VAL
12	L	122	THR
13	M	12	ASN
13	M	13	LYS
13	M	14	ARG
13	M	37	THR
13	M	43	THR
13	M	44	ARG
13	M	48	LEU
13	M	49	THR
13	M	50	GLU
13	M	53	VAL
13	M	54	VAL
13	M	56	LEU
13	M	61	GLU
13	M	64	TRP
13	M	65	LYS
13	M	70	LEU
13	M	78	ILE
13	M	81	LEU
13	M	103	THR
13	M	105	THR
13	M	108	ARG

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Mol	Chain	Res	Type
13	M	109	THR
13	M	110	ARG
13	M	113	PRO
13	M	114	ARG
14	N	9	LYS
14	N	13	THR
14	N	22	THR
14	N	24	CYS
14	N	25	VAL
14	N	27	CYS
14	N	31	ARG
14	N	42	ILE
14	N	47	LEU
14	N	50	LYS
14	N	53	LEU
15	O	3	ILE
15	O	5	LYS
15	O	7	GLU
15	O	8	LYS
15	O	21	ASP
15	O	32	LEU
15	O	33	THR
15	O	36	ILE
15	O	45	VAL
15	O	56	LEU
15	O	64	ARG
15	O	65	ARG
15	O	70	LEU
15	O	71	GLN
15	O	81	LEU
15	O	82	ILE
15	O	83	GLU
15	O	87	ILE
16	P	1	MET
16	P	4	ILE
16	P	11	SER
16	P	26	ARG
16	P	31	LYS
16	P	33	ILE
16	P	34	GLU
16	P	36	ILE
16	P	42	ARG

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Mol	Chain	Res	Type
16	P	43	LYS
16	P	47	ASP
16	P	53	VAL
16	P	54	GLU
16	P	55	ARG
16	P	62	VAL
16	P	68	ASP
16	P	81	ARG
16	P	82	GLN
17	Q	9	VAL
17	Q	13	ASP
17	Q	21	VAL
17	Q	30	PRO
17	Q	34	LYS
17	Q	35	VAL
17	Q	40	LYS
17	Q	53	LEU
17	Q	59	ILE
17	Q	60	ILE
17	Q	72	ARG
17	Q	74	LEU
17	Q	76	LEU
17	Q	77	VAL
17	Q	82	MET
17	Q	86	GLU
17	Q	92	ARG
17	Q	98	LEU
17	Q	99	SER
18	R	22	VAL
18	R	26	LEU
18	R	30	ASP
18	R	40	LEU
18	R	44	LEU
18	R	46	GLU
18	R	47	THR
18	R	69	THR
18	R	75	ILE
18	R	81	PHE
18	R	84	LYS
19	S	5	LEU
19	S	9	VAL
19	S	13	ASP

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Mol	Chain	Res	Type
19	S	14	HIS
19	S	15	LEU
19	S	33	THR
19	S	56	GLN
19	S	58	VAL
19	S	62	ILE
19	S	63	THR
19	S	71	LEU
19	S	77	THR
19	S	79	THR
20	T	9	ASN
20	T	13	LEU
20	T	19	SER
20	T	20	LEU
20	T	30	LYS
20	T	33	ILE
20	T	43	LEU
20	T	53	LEU
20	T	56	MET
20	T	57	ARG
20	T	62	LEU
20	T	68	LYS
20	T	72	LEU
20	T	75	ASN
20	T	80	ARG
20	T	84	LEU
20	T	86	ARG
20	T	91	LEU
20	T	92	LEU
20	T	100	ILE
21	U	6	ARG
21	U	25	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	40	HIS
2	B	113	HIS
2	B	204	ASN
3	C	6	HIS
5	E	38	GLN
5	E	72	GLN

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Mol	Chain	Res	Type
7	G	86	GLN
7	G	97	GLN
9	I	3	GLN
9	I	73	GLN
9	I	124	GLN
11	K	26	ASN
12	L	80	HIS
14	N	52	GLN
17	Q	96	GLN
19	S	53	ASN
19	S	56	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1505/1522 (98%)	341 (22%)	51 (3%)

All (341) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	8	A
1	A	9	G
1	A	31	G
1	A	32	A
1	A	33	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	50	A
1	A	51	A
1	A	54	C
1	A	80	G
1	A	81	U
1	A	92	C
1	A	93	G
1	A	101	A
1	A	108	G
1	A	115	G
1	A	116	A
1	A	117	G

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Mol	Chain	Res	Type
1	A	121	C
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	163	C
1	A	180	U
1	A	181	G
1	A	182	U
1	A	183	G
1	A	188	C
1	A	195	A
1	A	201	C
1	A	202	U
1	A	203	U
1	A	204	U
1	A	216	G
1	A	226	G
1	A	231	G
1	A	247	G
1	A	250	A
1	A	251	G
1	A	252	U
1	A	258	G
1	A	266	G
1	A	267	C
1	A	281	G
1	A	282	A
1	A	289	G
1	A	299	G
1	A	319	G
1	A	321	A
1	A	328	C
1	A	329	A
1	A	331	G
1	A	332	G
1	A	344	A
1	A	345	C
1	A	346	G
1	A	350	G
1	A	351	G
1	A	352	C
1	A	353	A

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Mol	Chain	Res	Type
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	382	A
1	A	384	G
1	A	390	C
1	A	397	A
1	A	398	C
1	A	406	G
1	A	409	G
1	A	412	A
1	A	413	G
1	A	414	A
1	A	421	U
1	A	424	G
1	A	429	U
1	A	439	A
1	A	442	C
1	A	451	A
1	A	460	A
1	A	461	C
1	A	481	G
1	A	482	A
1	A	485	G
1	A	486	U
1	A	496	A
1	A	497	A
1	A	498	U
1	A	509	A
1	A	510	A
1	A	511	C
1	A	517	G
1	A	518	C
1	A	519	C
1	A	524	G
1	A	527	7MG
1	A	531	U
1	A	532	A

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Mol	Chain	Res	Type
1	A	533	A
1	A	538	G
1	A	545	C
1	A	547	A
1	A	559	A
1	A	560	U
1	A	562	C
1	A	564	C
1	A	568	G
1	A	571	U
1	A	572	A
1	A	573	A
1	A	576	G
1	A	577	G
1	A	579	G
1	A	588	G
1	A	596	C
1	A	597	G
1	A	598	U
1	A	616	G
1	A	621	A
1	A	624	C
1	A	653	A
1	A	658	G
1	A	665	A
1	A	671	G
1	A	687	A
1	A	688	G
1	A	695	A
1	A	697	U
1	A	701	C
1	A	702	A
1	A	703	G
1	A	722	A
1	A	723	U
1	A	724	G
1	A	731	G
1	A	733	A
1	A	740	U
1	A	741	G
1	A	749	C
1	A	751	U

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Mol	Chain	Res	Type
1	A	755	G
1	A	760	G
1	A	777	A
1	A	781	A
1	A	782	A
1	A	785	G
1	A	792	A
1	A	793	U
1	A	794	A
1	A	812	C
1	A	813	U
1	A	815	A
1	A	817	C
1	A	818	G
1	A	827	U
1	A	828	A
1	A	837	G
1	A	838	G
1	A	839	U
1	A	840	C
1	A	841	U
1	A	848	C
1	A	849	C
1	A	853	G
1	A	869	G
1	A	873	A
1	A	889	A
1	A	902	G
1	A	910	C
1	A	914	A
1	A	916	G
1	A	922	G
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	936	C
1	A	937	A
1	A	938	A
1	A	939	G
1	A	942	G
1	A	950	U

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Mol	Chain	Res	Type
1	A	954	G
1	A	961	U
1	A	962	C
1	A	966	M2G
1	A	967	5MC
1	A	969	A
1	A	971	G
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	982	U
1	A	984	C
1	A	989	C
1	A	991	U
1	A	992	U
1	A	993	G
1	A	994	A
1	A	995	C
1	A	1004	A
1	A	1005	A
1	A	1006	C
1	A	1020	U
1	A	1023	G
1	A	1024	G
1	A	1026	G
1	A	1030(B)	C
1	A	1031	G
1	A	1045	C
1	A	1050	G
1	A	1053	G
1	A	1054	C
1	A	1055	A
1	A	1065	U
1	A	1066	C
1	A	1068	G
1	A	1078	U
1	A	1085	U
1	A	1092	A
1	A	1094	G
1	A	1095	U
1	A	1101	A

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Mol	Chain	Res	Type
1	A	1111	A
1	A	1124	G
1	A	1125	U
1	A	1126	U
1	A	1127	G
1	A	1129	C
1	A	1130	A
1	A	1135	U
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1140	C
1	A	1146	A
1	A	1152	A
1	A	1159	U
1	A	1160	G
1	A	1168	A
1	A	1171	G
1	A	1177	G
1	A	1183	A
1	A	1191	A
1	A	1196	U
1	A	1197	G
1	A	1200	C
1	A	1201	A
1	A	1202	G
1	A	1206	G
1	A	1207	2MG
1	A	1211	U
1	A	1212	U
1	A	1214	C
1	A	1224	G
1	A	1225	A
1	A	1226	C
1	A	1227	A
1	A	1228	C
1	A	1238	A
1	A	1241	G
1	A	1242	C
1	A	1245	A
1	A	1250	A
1	A	1253	G

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Mol	Chain	Res	Type
1	A	1256	A
1	A	1257	U
1	A	1258	G
1	A	1268	A
1	A	1270	C
1	A	1278	U
1	A	1279	A
1	A	1280	A
1	A	1281	U
1	A	1286	A
1	A	1287	A
1	A	1289	A
1	A	1297	C
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1305	G
1	A	1306	A
1	A	1307	U
1	A	1310	G
1	A	1316	G
1	A	1320	C
1	A	1322	C
1	A	1326	C
1	A	1336	C
1	A	1338	G
1	A	1339	A
1	A	1346	A
1	A	1347	G
1	A	1348	U
1	A	1351	U
1	A	1353	G
1	A	1359	C
1	A	1362	C
1	A	1370	G
1	A	1381	U
1	A	1398	A
1	A	1399	C
1	A	1400	5MC
1	A	1401	G
1	A	1402	4OC
1	A	1406	U

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Mol	Chain	Res	Type
1	A	1411	C
1	A	1415	G
1	A	1430	C
1	A	1442	G
1	A	1443	G
1	A	1446	A
1	A	1447	G
1	A	1451	A
1	A	1453	G
1	A	1454	G
1	A	1485	U
1	A	1487	G
1	A	1489	G
1	A	1490	C
1	A	1492	A
1	A	1493	A
1	A	1497	G
1	A	1498	UR3
1	A	1499	A
1	A	1503	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1529	G
1	A	1530	G
1	A	1531	A

All (51) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U
1	A	92	C
1	A	115	G
1	A	129(A)	G
1	A	181	G
1	A	204	U
1	A	250	A
1	A	251	G
1	A	281	G
1	A	328	C
1	A	350	G
1	A	353	A

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Mol	Chain	Res	Type
1	A	372	C
1	A	428	G
1	A	484	G
1	A	485	G
1	A	496	A
1	A	509	A
1	A	518	C
1	A	532	A
1	A	559	A
1	A	575	G
1	A	687	A
1	A	701	C
1	A	748	C
1	A	792	A
1	A	812	C
1	A	913	A
1	A	960	U
1	A	965	A
1	A	992	U
1	A	1049	U
1	A	1065	U
1	A	1067	A
1	A	1126	U
1	A	1129	C
1	A	1139	G
1	A	1145	C
1	A	1182	G
1	A	1190	G
1	A	1201	A
1	A	1256	A
1	A	1257	U
1	A	1285	A
1	A	1300	G
1	A	1301	U
1	A	1305	G
1	A	1346	A
1	A	1347	G
1	A	1380	U
1	A	1505	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MA6	A	1518[B]	1	23,26,27	1.57	6 (26%)	33,38,41	1.05	2 (6%)
1	PSU	A	1540	1	18,21,22	1.17	1 (5%)	21,30,33	1.46	3 (14%)
1	M2G	A	966	1	24,27,28	0.94	2 (8%)	33,40,43	0.85	2 (6%)
1	UR3	A	1498	1	19,22,23	1.23	2 (10%)	26,32,35	1.26	2 (7%)
1	PSU	A	1541	1	18,21,22	1.16	1 (5%)	21,30,33	1.65	3 (14%)
1	2MG	A	1207	1	23,26,27	1.78	6 (26%)	33,38,41	1.14	3 (9%)
1	MA6	A	1519[A]	1	23,26,27	1.16	3 (13%)	33,38,41	0.96	2 (6%)
1	5MC	A	1404	1	19,22,23	1.59	2 (10%)	26,32,35	1.34	4 (15%)
1	PSU	A	516	1,22	18,21,22	1.05	1 (5%)	21,30,33	1.67	5 (23%)
1	4OC	A	1402	1	20,23,24	1.03	1 (5%)	25,32,35	0.74	0
1	MA6	A	1519[B]	1	23,26,27	1.43	3 (13%)	33,38,41	0.99	1 (3%)
12	0TD	L	92	12	8,9,10	1.07	0	6,11,13	3.28	4 (66%)
1	7MG	A	527	1,22	23,26,27	3.64	5 (21%)	27,39,42	2.49	9 (33%)
1	5MC	A	967	1	19,22,23	0.89	1 (5%)	26,32,35	0.91	2 (7%)
1	5MC	A	1400	1	19,22,23	1.46	3 (15%)	26,32,35	1.03	1 (3%)
1	MA6	A	1518[A]	1	23,26,27	1.22	4 (17%)	33,38,41	0.87	1 (3%)
1	5MC	A	1407	1	19,22,23	1.82	3 (15%)	26,32,35	1.48	4 (15%)

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	1518[B]	1	-	0/11/29/30	0/3/3/3
1	PSU	A	1540	1	-	0/7/25/26	0/2/2/2
1	M2G	A	966	1	-	5/11/29/30	0/3/3/3

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

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	7MG	C8-N9	-14.77	1.36	1.45
1	A	527	7MG	C5-N7	6.36	1.43	1.35
1	A	1407	5MC	C5-C4	5.74	1.48	1.44
1	A	1404	5MC	C5-C4	5.65	1.48	1.44
1	A	1540	PSU	C6-C5	4.10	1.39	1.35
1	A	527	7MG	C2-N2	4.02	1.43	1.34
1	A	1541	PSU	C6-C5	3.97	1.39	1.35
1	A	1407	5MC	C2-N1	3.95	1.48	1.40
1	A	516	PSU	C6-C5	3.62	1.39	1.35
1	A	1207	2MG	C2-N1	3.62	1.42	1.36
1	A	1518[B]	MA6	C8-N9	3.53	1.43	1.37
1	A	1400	5MC	C2-N1	3.52	1.47	1.40
1	A	1207	2MG	C4-N3	3.50	1.42	1.34
1	A	1207	2MG	C6-N1	3.45	1.45	1.38
1	A	1207	2MG	C2-N2	3.37	1.40	1.33
1	A	1498	UR3	C6-N1	-3.21	1.30	1.38
1	A	1518[B]	MA6	C5-C4	3.20	1.44	1.39
1	A	1518[A]	MA6	C5-C4	3.12	1.44	1.39
1	A	1519[A]	MA6	C5-C4	3.07	1.44	1.39
1	A	1519[B]	MA6	C5-C4	3.07	1.44	1.39
1	A	527	7MG	O6-C6	-3.05	1.17	1.23
1	A	527	7MG	C4-N3	2.97	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1498	UR3	C4-N3	-2.91	1.34	1.40
1	A	1404	5MC	C2-N3	2.75	1.41	1.36
1	A	1519[B]	MA6	C4-N3	2.73	1.39	1.34
1	A	1519[B]	MA6	C2-N1	2.69	1.38	1.33
1	A	1407	5MC	C2-N3	2.63	1.41	1.36
1	A	1400	5MC	C6-C5	2.62	1.38	1.34
1	A	1518[A]	MA6	C8-N9	2.59	1.42	1.37
1	A	1207	2MG	C8-N9	2.56	1.43	1.37
1	A	1207	2MG	C2-N3	2.56	1.36	1.32
1	A	1518[B]	MA6	C5-N7	2.49	1.43	1.39
1	A	1400	5MC	C2-N3	2.48	1.41	1.36
1	A	1519[A]	MA6	C2-N1	2.47	1.38	1.33
1	A	1402	4OC	C2-N1	2.46	1.45	1.40
1	A	966	M2G	C8-N9	2.41	1.42	1.37
1	A	1518[B]	MA6	C8-N7	2.35	1.36	1.31
1	A	967	5MC	C2-N3	2.26	1.40	1.36
1	A	1518[A]	MA6	C4-N3	2.18	1.38	1.34
1	A	1518[B]	MA6	C4-N3	2.13	1.38	1.34
1	A	1518[A]	MA6	C2-N1	2.13	1.37	1.33
1	A	1519[A]	MA6	C8-N7	2.09	1.35	1.31
1	A	966	M2G	C4-N3	2.09	1.39	1.34
1	A	1518[B]	MA6	C4-N9	2.08	1.42	1.37

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	527	7MG	C5-C6-N1	6.41	122.22	110.94
12	L	92	0TD	CSB-SB-CB	-6.36	90.94	102.36
1	A	527	7MG	C2-N3-C4	4.48	120.01	112.30
1	A	516	PSU	N1-C2-N3	4.22	119.62	115.17
1	A	1541	PSU	C4-N3-C2	-4.16	120.64	126.37
1	A	516	PSU	C4-N3-C2	-4.13	120.68	126.37
1	A	527	7MG	C6-C5-C4	-4.09	115.20	122.40
1	A	527	7MG	C6-C5-N7	4.00	138.14	131.93
1	A	527	7MG	N9-C4-N3	3.82	131.05	125.46
1	A	1540	PSU	C4-N3-C2	-3.77	121.17	126.37
1	A	1404	5MC	N4-C4-N3	-3.60	111.99	118.51
1	A	527	7MG	C5-C4-N3	-3.59	121.38	128.13
1	A	1541	PSU	N1-C2-N3	3.58	118.94	115.17
1	A	1540	PSU	N1-C2-N3	3.43	118.79	115.17
1	A	527	7MG	C2-N1-C6	-3.40	118.95	125.11
1	A	1407	5MC	C1'-N1-C6	-3.36	115.61	121.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1407	5MC	N4-C4-N3	-3.34	112.45	118.51
1	A	527	7MG	N9-C8-N7	3.32	108.08	103.37
1	A	527	7MG	O6-C6-C5	-3.21	119.73	127.62
12	L	92	0TD	CB-CA-N	-3.16	102.69	109.10
1	A	1498	UR3	C6-N1-C2	-3.08	119.28	121.80
1	A	1404	5MC	C5-C6-N1	-3.00	120.06	123.31
1	A	1404	5MC	C5-C4-N3	2.80	124.63	121.75
1	A	1541	PSU	O2-C2-N1	-2.80	119.91	122.79
1	A	1207	2MG	C5-C4-N3	-2.79	123.95	128.39
1	A	1407	5MC	C5-C4-N3	2.77	124.59	121.75
1	A	1518[A]	MA6	C2-N1-C6	2.74	118.53	111.83
1	A	967	5MC	N4-C4-N3	-2.74	113.55	118.51
1	A	1207	2MG	N9-C4-N3	2.71	131.38	125.95
1	A	1404	5MC	C4-N3-C2	-2.67	117.10	120.81
1	A	1400	5MC	C5-C4-N3	2.48	124.30	121.75
12	L	92	0TD	OD1-CG-CB	-2.47	117.27	122.44
1	A	516	PSU	C6-N1-C2	-2.46	120.41	122.69
1	A	966	M2G	O6-C6-N1	-2.29	115.81	120.11
1	A	1518[B]	MA6	N1-C6-N6	-2.24	114.12	116.86
1	A	967	5MC	C5-C4-N3	2.21	124.02	121.75
1	A	516	PSU	O4'-C1'-C2'	2.21	108.20	105.15
1	A	966	M2G	C5-C4-N3	-2.21	124.88	128.39
1	A	1207	2MG	O6-C6-N1	-2.17	116.04	120.11
1	A	1519[B]	MA6	C4-C5-N7	-2.12	108.16	110.58
1	A	516	PSU	O2-C2-N1	-2.10	120.62	122.79
12	L	92	0TD	O-C-CA	-2.09	119.39	124.77
1	A	1519[A]	MA6	N1-C2-N3	2.09	131.75	128.58
1	A	1498	UR3	O2-C2-N3	-2.08	118.45	121.33
1	A	1519[A]	MA6	C4-C5-C6	2.06	118.04	115.91
1	A	1407	5MC	O2-C2-N1	2.05	122.92	118.90
1	A	1518[B]	MA6	C4-C5-N7	-2.01	108.28	110.58
1	A	1540	PSU	O2-C2-N1	-2.01	120.72	122.79

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	967	5MC	O4'-C4'-C5'-O5'
1	A	1207	2MG	O4'-C4'-C5'-O5'
1	A	1400	5MC	O4'-C4'-C5'-O5'
1	A	1402	4OC	O4'-C4'-C5'-O5'
1	A	1402	4OC	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	A	527	7MG	C3'-C4'-C5'-O5'
1	A	1207	2MG	C3'-C4'-C5'-O5'
1	A	1519[B]	MA6	O4'-C4'-C5'-O5'
1	A	527	7MG	O4'-C4'-C5'-O5'
1	A	966	M2G	C3'-C4'-C5'-O5'
1	A	1400	5MC	C3'-C4'-C5'-O5'
1	A	966	M2G	O4'-C4'-C5'-O5'
1	A	967	5MC	C3'-C4'-C5'-O5'
1	A	1498	UR3	O4'-C4'-C5'-O5'
1	A	1519[A]	MA6	C5-C6-N6-C9
1	A	1498	UR3	C3'-C4'-C5'-O5'
1	A	1519[B]	MA6	C3'-C4'-C5'-O5'
1	A	966	M2G	N1-C2-N2-CM1
12	L	92	0TD	CG-CB-SB-CSB
12	L	92	0TD	SB-CB-CG-OD1
1	A	966	M2G	C4'-C5'-O5'-P
1	A	1541	PSU	O4'-C1'-C5-C4
1	A	966	M2G	N3-C2-N2-CM1
1	A	1519[A]	MA6	O4'-C4'-C5'-O5'

There are no ring outliers.

11 monomers are involved in 25 short contacts:

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 256 ligands modelled in this entry, 256 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1498/1522 (98%)	-0.43	16 (1%) 78 52	56, 149, 294, 392	4 (0%)
2	B	234/256 (91%)	-0.48	0 100 100	107, 163, 248, 282	0
3	C	206/239 (86%)	-0.17	1 (0%) 87 66	167, 228, 284, 310	0
4	D	208/209 (99%)	-0.20	8 (3%) 44 25	105, 155, 204, 238	0
5	E	150/162 (92%)	-0.70	0 100 100	80, 121, 160, 178	0
6	F	101/101 (100%)	-0.69	0 100 100	122, 176, 205, 223	0
7	G	155/156 (99%)	-0.27	2 (1%) 75 48	135, 193, 257, 275	0
8	H	138/138 (100%)	-0.67	0 100 100	74, 109, 147, 192	0
9	I	127/128 (99%)	-0.11	2 (1%) 70 43	151, 217, 251, 272	0
10	J	98/105 (93%)	0.17	4 (4%) 41 23	190, 234, 309, 344	0
11	K	116/129 (89%)	-0.51	1 (0%) 81 56	118, 148, 198, 218	0
12	L	123/135 (91%)	-0.39	3 (2%) 59 34	86, 150, 190, 221	0
13	M	118/126 (93%)	-0.27	3 (2%) 58 34	138, 184, 221, 319	0
14	N	60/61 (98%)	0.03	3 (5%) 34 19	167, 208, 268, 285	0
15	O	87/89 (97%)	-0.58	0 100 100	93, 134, 179, 189	0
16	P	83/88 (94%)	-0.40	0 100 100	102, 145, 176, 226	0
17	Q	99/105 (94%)	-0.56	0 100 100	95, 123, 167, 189	0
18	R	70/88 (79%)	-0.49	0 100 100	110, 146, 206, 216	0
19	S	80/93 (86%)	-0.02	3 (3%) 44 25	198, 244, 285, 305	0
20	T	99/106 (93%)	-0.17	1 (1%) 79 54	113, 150, 202, 238	0
21	U	24/27 (88%)	0.30	4 (16%) 4 5	167, 192, 215, 235	0
All	All	3874/4063 (95%)	-0.38	51 (1%) 75 48	56, 160, 266, 392	4 (0%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1129	C	7.4
20	T	106	ALA	6.8
1	A	985	C	5.0
1	A	984	C	4.8
19	S	3	ARG	4.6
4	D	9	CYS	4.4
10	J	39	PRO	4.0
21	U	6	ARG	4.0
1	A	80	G	4.0
19	S	2	PRO	3.9
4	D	31	CYS	3.8
14	N	4	LYS	3.7
10	J	17	ASP	3.6
4	D	2	GLY	3.4
9	I	127	LYS	3.3
13	M	106	ASN	3.3
1	A	993	G	3.2
12	L	73	GLU	3.2
4	D	3	ARG	3.2
1	A	1417	G	3.1
13	M	117	VAL	3.1
1	A	1220	G	3.0
4	D	36	ARG	2.9
19	S	5	LEU	2.7
10	J	96	ILE	2.7
9	I	110	GLU	2.7
1	A	1517[A]	G	2.6
1	A	202	U	2.6
13	M	8	GLU	2.6
14	N	2	ALA	2.6
14	N	3	ARG	2.5
21	U	2	GLY	2.5
4	D	22	LYS	2.5
1	A	77	G	2.5
1	A	1482	G	2.5
3	C	2	GLY	2.5
4	D	26	CYS	2.4
1	A	992	U	2.4
1	A	532	A	2.4
7	G	141	VAL	2.3
11	K	56	GLY	2.3
21	U	7	ARG	2.3
21	U	10	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
4	D	42	GLN	2.2
1	A	353	A	2.2
12	L	115	LYS	2.1
1	A	1516[A]	G	2.1
1	A	64	G	2.1
12	L	31	PRO	2.0
10	J	71	LEU	2.0
7	G	147	ALA	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	PSU	A	1541	20/21	0.90	0.11	211,234,251,253	0
1	M2G	A	966	25/26	0.95	0.08	153,180,185,193	0
1	2MG	A	1207	24/25	0.95	0.08	207,227,293,300	0
1	PSU	A	1540	20/21	0.95	0.12	239,244,264,268	0
1	7MG	A	527	24/25	0.95	0.08	128,140,159,170	0
1	5MC	A	967	21/22	0.96	0.07	152,157,177,181	0
1	PSU	A	516	20/21	0.96	0.07	138,167,192,192	0
1	5MC	A	1400	21/22	0.97	0.07	114,137,145,148	0
1	5MC	A	1407	21/22	0.97	0.09	134,175,190,192	0
1	UR3	A	1498	21/22	0.98	0.12	118,145,161,171	0
1	MA6	A	1518[A]	24/25	0.98	0.12	115,120,128,130	24
1	MA6	A	1518[B]	24/25	0.98	0.12	116,127,138,148	24
1	5MC	A	1404	21/22	0.98	0.08	118,133,162,167	0
1	4OC	A	1402	22/23	0.98	0.09	122,134,156,160	0
12	0TD	L	92	10/11	0.98	0.09	150,171,185,382	0
1	MA6	A	1519[B]	24/25	0.99	0.11	107,127,131,133	24
1	MA6	A	1519[A]	24/25	0.99	0.11	109,121,132,133	24

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
22	MG	A	1758	1/1	0.35	0.65	139,139,139,139	0
22	MG	A	1733	1/1	0.46	0.21	261,261,261,261	0
22	MG	A	1693	1/1	0.48	0.27	176,176,176,176	0
22	MG	A	1835	1/1	0.58	0.39	149,149,149,149	0
22	MG	A	1827	1/1	0.62	0.25	140,140,140,140	0
22	MG	A	1810	1/1	0.62	0.59	150,150,150,150	0
22	MG	A	1716	1/1	0.64	0.32	211,211,211,211	0
22	MG	A	1675	1/1	0.65	0.17	143,143,143,143	0
22	MG	A	1750	1/1	0.66	0.21	149,149,149,149	0
22	MG	A	1681	1/1	0.67	0.37	121,121,121,121	0
22	MG	A	1794	1/1	0.68	1.20	150,150,150,150	0
22	MG	A	1680	1/1	0.68	0.17	275,275,275,275	0
22	MG	A	1838	1/1	0.69	0.30	144,144,144,144	0
22	MG	A	1787	1/1	0.71	0.23	126,126,126,126	0
22	MG	A	1819	1/1	0.72	0.28	132,132,132,132	0
22	MG	A	1799	1/1	0.72	0.09	157,157,157,157	0
22	MG	A	1772	1/1	0.73	0.39	108,108,108,108	0
22	MG	A	1736	1/1	0.74	0.98	121,121,121,121	0
22	MG	A	1775	1/1	0.74	0.27	132,132,132,132	0
22	MG	A	1784	1/1	0.76	0.13	149,149,149,149	0
22	MG	A	1643	1/1	0.76	0.32	111,111,111,111	0
22	MG	A	1745	1/1	0.76	0.84	132,132,132,132	0
22	MG	A	1839	1/1	0.76	0.21	138,138,138,138	0
22	MG	A	1828	1/1	0.78	0.68	154,154,154,154	0
22	MG	A	1687	1/1	0.78	0.63	130,130,130,130	0
22	MG	A	1634	1/1	0.78	0.45	124,124,124,124	0
22	MG	A	1801	1/1	0.78	0.21	142,142,142,142	0
22	MG	L	201	1/1	0.78	0.10	140,140,140,140	0
22	MG	A	1669	1/1	0.79	0.18	136,136,136,136	0
22	MG	A	1737	1/1	0.79	0.40	145,145,145,145	0
22	MG	A	1834	1/1	0.79	0.09	146,146,146,146	0
22	MG	A	1742	1/1	0.79	0.42	108,108,108,108	0
22	MG	A	1725	1/1	0.79	0.44	115,115,115,115	0
22	MG	A	1817	1/1	0.79	0.38	127,127,127,127	0
22	MG	A	1605	1/1	0.79	0.42	109,109,109,109	0
22	MG	A	1781	1/1	0.80	0.32	123,123,123,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	A	1764	1/1	0.80	0.24	126,126,126,126	0
22	MG	A	1685	1/1	0.80	0.28	111,111,111,111	0
22	MG	D	305	1/1	0.80	0.38	123,123,123,123	0
22	MG	A	1677	1/1	0.80	0.21	130,130,130,130	0
22	MG	A	1806	1/1	0.81	0.12	157,157,157,157	0
22	MG	A	1679	1/1	0.81	0.23	138,138,138,138	0
22	MG	A	1629	1/1	0.81	0.50	208,208,208,208	0
22	MG	P	102	1/1	0.81	0.07	119,119,119,119	0
22	MG	A	1601	1/1	0.82	0.20	132,132,132,132	0
22	MG	A	1832	1/1	0.82	0.12	118,118,118,118	0
22	MG	A	1804	1/1	0.82	0.31	121,121,121,121	0
22	MG	A	1765	1/1	0.82	0.24	113,113,113,113	0
22	MG	A	1769	1/1	0.82	0.34	145,145,145,145	0
22	MG	A	1816	1/1	0.82	0.17	149,149,149,149	0
22	MG	A	1790	1/1	0.82	0.21	130,130,130,130	0
22	MG	A	1754	1/1	0.82	0.24	130,130,130,130	0
22	MG	A	1691	1/1	0.82	0.52	128,128,128,128	0
22	MG	A	1774	1/1	0.83	0.17	167,167,167,167	0
22	MG	A	1624	1/1	0.84	0.12	124,124,124,124	0
22	MG	A	1604	1/1	0.84	0.17	137,137,137,137	0
22	MG	C	301	1/1	0.84	0.18	139,139,139,139	0
22	MG	A	1704	1/1	0.84	0.07	178,178,178,178	0
22	MG	A	1756	1/1	0.84	0.07	122,122,122,122	0
22	MG	A	1824	1/1	0.84	0.39	127,127,127,127	0
22	MG	A	1785	1/1	0.85	0.26	82,82,82,82	0
22	MG	A	1833	1/1	0.85	0.21	112,112,112,112	0
22	MG	A	1803	1/1	0.86	0.16	160,160,160,160	0
22	MG	A	1709	1/1	0.86	0.59	132,132,132,132	0
22	MG	A	1738	1/1	0.86	0.30	122,122,122,122	0
22	MG	A	1786	1/1	0.86	0.11	174,174,174,174	0
22	MG	A	1731	1/1	0.86	0.13	140,140,140,140	0
22	MG	A	1649	1/1	0.87	0.12	165,165,165,165	0
22	MG	A	1797	1/1	0.87	0.26	163,163,163,163	0
22	MG	A	1743	1/1	0.87	0.18	104,104,104,104	0
22	MG	A	1732	1/1	0.87	0.42	138,138,138,138	0
22	MG	A	1703	1/1	0.87	0.44	120,120,120,120	0
22	MG	A	1753	1/1	0.87	0.20	138,138,138,138	0
22	MG	A	1700	1/1	0.88	0.27	129,129,129,129	0
22	MG	A	1830	1/1	0.88	0.12	114,114,114,114	0
22	MG	A	1721	1/1	0.88	0.12	154,154,154,154	0
22	MG	A	1782	1/1	0.88	0.65	148,148,148,148	0
22	MG	A	1694	1/1	0.89	0.14	133,133,133,133	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	A	1818	1/1	0.89	0.47	129,129,129,129	0
22	MG	A	1663	1/1	0.89	0.24	102,102,102,102	0
22	MG	A	1667	1/1	0.89	0.41	102,102,102,102	0
22	MG	A	1807	1/1	0.89	0.57	106,106,106,106	0
22	MG	B	302	1/1	0.89	0.07	185,185,185,185	0
22	MG	A	1808	1/1	0.89	0.10	141,141,141,141	0
22	MG	A	1829	1/1	0.89	0.30	97,97,97,97	0
22	MG	A	1648	1/1	0.89	0.14	226,226,226,226	0
22	MG	A	1706	1/1	0.89	0.35	148,148,148,148	0
22	MG	A	1789	1/1	0.90	0.28	134,134,134,134	0
22	MG	A	1707	1/1	0.90	0.17	143,143,143,143	0
22	MG	A	1791	1/1	0.90	0.17	147,147,147,147	0
22	MG	A	1805	1/1	0.90	0.20	138,138,138,138	0
22	MG	A	1761	1/1	0.90	0.34	129,129,129,129	0
22	MG	A	1771	1/1	0.90	0.29	105,105,105,105	0
22	MG	A	1688	1/1	0.90	0.08	169,169,169,169	0
22	MG	A	1684	1/1	0.91	0.14	145,145,145,145	0
22	MG	A	1726	1/1	0.91	0.33	341,341,341,341	0
22	MG	A	1831	1/1	0.91	0.10	121,121,121,121	0
22	MG	A	1739	1/1	0.91	0.20	116,116,116,116	0
22	MG	A	1757	1/1	0.91	0.28	102,102,102,102	0
22	MG	A	1628	1/1	0.91	0.25	89,89,89,89	0
22	MG	A	1619	1/1	0.91	0.33	121,121,121,121	0
22	MG	A	1744	1/1	0.91	0.27	133,133,133,133	0
22	MG	A	1802	1/1	0.91	0.12	122,122,122,122	0
22	MG	B	301	1/1	0.91	0.15	120,120,120,120	0
22	MG	A	1823	1/1	0.91	0.23	123,123,123,123	0
22	MG	A	1656	1/1	0.91	0.14	124,124,124,124	0
22	MG	A	1825	1/1	0.91	0.70	132,132,132,132	0
22	MG	A	1767	1/1	0.91	0.23	104,104,104,104	0
22	MG	A	1662	1/1	0.91	0.28	151,151,151,151	0
22	MG	A	1722	1/1	0.92	0.10	88,88,88,88	0
22	MG	A	1783	1/1	0.92	0.17	142,142,142,142	0
22	MG	A	1603	1/1	0.92	0.18	121,121,121,121	0
22	MG	A	1630	1/1	0.92	0.26	123,123,123,123	0
22	MG	A	1800	1/1	0.92	0.22	126,126,126,126	0
22	MG	A	1773	1/1	0.92	0.10	128,128,128,128	0
22	MG	A	1674	1/1	0.92	0.40	155,155,155,155	0
22	MG	A	1622	1/1	0.92	0.18	146,146,146,146	0
22	MG	A	1682	1/1	0.92	0.48	156,156,156,156	0
22	MG	A	1822	1/1	0.92	0.23	136,136,136,136	0
22	MG	A	1668	1/1	0.93	0.13	129,129,129,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	A	1639	1/1	0.93	0.37	105,105,105,105	0
22	MG	A	1755	1/1	0.93	0.16	139,139,139,139	0
22	MG	A	1717	1/1	0.93	0.16	131,131,131,131	0
22	MG	A	1719	1/1	0.93	0.17	267,267,267,267	0
22	MG	A	1720	1/1	0.93	0.11	150,150,150,150	0
22	MG	A	1686	1/1	0.93	0.27	112,112,112,112	0
22	MG	A	1672	1/1	0.93	0.11	164,164,164,164	0
22	MG	A	1664	1/1	0.93	0.12	115,115,115,115	0
22	MG	A	1632	1/1	0.93	0.36	113,113,113,113	0
22	MG	A	1809	1/1	0.93	0.12	133,133,133,133	0
22	MG	A	1837	1/1	0.93	0.38	156,156,156,156	0
22	MG	A	1768	1/1	0.93	0.13	92,92,92,92	0
22	MG	A	1730	1/1	0.93	0.37	124,124,124,124	0
22	MG	A	1770	1/1	0.93	0.31	100,100,100,100	0
22	MG	A	1792	1/1	0.93	0.06	127,127,127,127	0
22	MG	A	1793	1/1	0.93	0.05	176,176,176,176	0
22	MG	C	302	1/1	0.93	0.09	172,172,172,172	0
22	MG	D	303	1/1	0.93	0.17	122,122,122,122	0
22	MG	D	304	1/1	0.93	0.12	112,112,112,112	0
22	MG	A	1821	1/1	0.93	0.15	144,144,144,144	0
22	MG	E	201	1/1	0.93	0.06	146,146,146,146	0
22	MG	A	1692	1/1	0.93	0.16	131,131,131,131	0
22	MG	A	1751	1/1	0.93	0.31	125,125,125,125	0
22	MG	Q	201	1/1	0.93	0.11	116,116,116,116	0
22	MG	A	1652	1/1	0.94	0.09	93,93,93,93	0
22	MG	A	1621	1/1	0.94	0.11	143,143,143,143	0
22	MG	A	1759	1/1	0.94	0.12	132,132,132,132	0
22	MG	A	1760	1/1	0.94	0.08	143,143,143,143	0
22	MG	A	1658	1/1	0.94	0.15	92,92,92,92	0
22	MG	A	1776	1/1	0.94	0.33	98,98,98,98	0
22	MG	A	1698	1/1	0.94	0.24	99,99,99,99	0
22	MG	A	1796	1/1	0.94	0.07	98,98,98,98	0
22	MG	A	1661	1/1	0.94	0.07	154,154,154,154	0
22	MG	A	1644	1/1	0.94	0.22	105,105,105,105	0
22	MG	A	1617	1/1	0.94	0.14	84,84,84,84	0
22	MG	A	1613	1/1	0.94	0.09	153,153,153,153	0
22	MG	A	1651	1/1	0.94	0.12	132,132,132,132	0
22	MG	A	1836	1/1	0.94	0.30	109,109,109,109	0
22	MG	A	1711	1/1	0.95	0.09	101,101,101,101	0
22	MG	A	1608	1/1	0.95	0.10	146,146,146,146	0
22	MG	A	1788	1/1	0.95	0.25	115,115,115,115	0
22	MG	A	1620	1/1	0.95	0.13	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	A	1626	1/1	0.95	0.33	172,172,172,172	0
22	MG	A	1645	1/1	0.95	0.08	90,90,90,90	0
22	MG	A	1814	1/1	0.95	0.19	250,250,250,250	0
22	MG	A	1647	1/1	0.95	0.31	132,132,132,132	0
22	MG	A	1741	1/1	0.95	0.13	127,127,127,127	0
22	MG	A	1676	1/1	0.95	0.23	153,153,153,153	0
22	MG	A	1795	1/1	0.95	0.22	96,96,96,96	0
22	MG	A	1705	1/1	0.95	0.08	157,157,157,157	0
22	MG	A	1777	1/1	0.95	0.36	94,94,94,94	0
22	MG	A	1798	1/1	0.95	0.09	108,108,108,108	0
22	MG	A	1778	1/1	0.95	0.20	136,136,136,136	0
22	MG	A	1612	1/1	0.95	0.05	194,194,194,194	0
22	MG	A	1635	1/1	0.95	0.11	221,221,221,221	0
22	MG	A	1748	1/1	0.95	0.30	116,116,116,116	0
22	MG	A	1766	1/1	0.95	0.26	134,134,134,134	0
22	MG	A	1636	1/1	0.95	0.21	203,203,203,203	0
23	ZN	N	101	1/1	0.95	0.06	319,319,319,319	0
22	MG	A	1826	1/1	0.96	0.24	104,104,104,104	0
22	MG	A	1752	1/1	0.96	0.07	122,122,122,122	0
22	MG	A	1729	1/1	0.96	0.09	112,112,112,112	0
22	MG	A	1670	1/1	0.96	0.19	108,108,108,108	0
22	MG	A	1708	1/1	0.96	0.10	152,152,152,152	0
22	MG	A	1640	1/1	0.96	0.09	202,202,202,202	0
22	MG	A	1780	1/1	0.96	0.40	136,136,136,136	0
22	MG	A	1710	1/1	0.96	0.10	208,208,208,208	0
22	MG	A	1734	1/1	0.96	0.13	101,101,101,101	0
22	MG	A	1609	1/1	0.96	0.16	106,106,106,106	0
22	MG	A	1713	1/1	0.96	0.11	122,122,122,122	0
22	MG	A	1695	1/1	0.96	0.07	167,167,167,167	0
22	MG	A	1762	1/1	0.96	0.20	118,118,118,118	0
22	MG	A	1763	1/1	0.96	0.09	90,90,90,90	0
22	MG	A	1812	1/1	0.96	0.07	228,228,228,228	0
22	MG	A	1638	1/1	0.96	0.17	76,76,76,76	0
22	MG	A	1815	1/1	0.96	0.08	202,202,202,202	0
22	MG	A	1699	1/1	0.96	0.12	113,113,113,113	0
22	MG	A	1666	1/1	0.96	0.25	120,120,120,120	0
22	MG	A	1659	1/1	0.96	0.12	112,112,112,112	0
22	MG	A	1660	1/1	0.96	0.07	122,122,122,122	0
22	MG	A	1723	1/1	0.96	0.24	114,114,114,114	0
22	MG	F	201	1/1	0.96	0.08	134,134,134,134	0
22	MG	A	1690	1/1	0.96	0.29	179,179,179,179	0
22	MG	A	1749	1/1	0.96	0.15	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	1627	1/1	0.96	0.58	98,98,98,98	0
22	MG	A	1727	1/1	0.96	0.21	118,118,118,118	0
22	MG	A	1618	1/1	0.97	0.10	123,123,123,123	0
22	MG	A	1820	1/1	0.97	0.28	148,148,148,148	0
22	MG	A	1610	1/1	0.97	0.07	111,111,111,111	0
22	MG	A	1740	1/1	0.97	0.23	86,86,86,86	0
22	MG	A	1712	1/1	0.97	0.09	182,182,182,182	0
22	MG	A	1728	1/1	0.97	0.47	150,150,150,150	0
22	MG	A	1702	1/1	0.97	0.10	143,143,143,143	0
22	MG	A	1653	1/1	0.97	0.13	114,114,114,114	0
22	MG	A	1625	1/1	0.97	0.32	61,61,61,61	0
22	MG	A	1746	1/1	0.97	0.10	91,91,91,91	0
22	MG	A	1614	1/1	0.97	0.28	160,160,160,160	0
22	MG	A	1779	1/1	0.97	0.13	115,115,115,115	0
22	MG	A	1602	1/1	0.97	0.22	152,152,152,152	0
22	MG	A	1642	1/1	0.97	0.10	119,119,119,119	0
22	MG	P	101	1/1	0.97	0.10	86,86,86,86	0
22	MG	A	1735	1/1	0.97	0.25	112,112,112,112	0
22	MG	A	1696	1/1	0.97	0.16	174,174,174,174	0
22	MG	A	1678	1/1	0.97	0.06	98,98,98,98	0
22	MG	A	1607	1/1	0.98	0.17	107,107,107,107	0
22	MG	A	1650	1/1	0.98	0.29	121,121,121,121	0
22	MG	A	1637	1/1	0.98	0.13	85,85,85,85	0
22	MG	A	1671	1/1	0.98	0.05	119,119,119,119	0
22	MG	A	1606	1/1	0.98	0.08	101,101,101,101	0
22	MG	A	1811	1/1	0.98	0.15	165,165,165,165	0
22	MG	C	303	1/1	0.98	0.08	175,175,175,175	0
22	MG	A	1611	1/1	0.98	0.10	90,90,90,90	0
22	MG	A	1813	1/1	0.98	0.14	264,264,264,264	0
22	MG	A	1697	1/1	0.98	0.12	183,183,183,183	0
22	MG	A	1655	1/1	0.98	0.07	74,74,74,74	0
22	MG	A	1665	1/1	0.98	0.07	127,127,127,127	0
22	MG	A	1616	1/1	0.98	0.08	92,92,92,92	0
22	MG	A	1715	1/1	0.98	0.09	114,114,114,114	0
22	MG	A	1701	1/1	0.98	0.23	134,134,134,134	0
22	MG	A	1689	1/1	0.98	0.15	270,270,270,270	0
22	MG	A	1641	1/1	0.98	0.05	80,80,80,80	0
22	MG	A	1673	1/1	0.99	0.07	141,141,141,141	0
22	MG	D	302	1/1	0.99	0.07	109,109,109,109	0
22	MG	A	1646	1/1	0.99	0.03	84,84,84,84	0
22	MG	A	1747	1/1	0.99	0.17	138,138,138,138	0
22	MG	A	1615	1/1	0.99	0.04	123,123,123,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	A	1718	1/1	0.99	0.13	301,301,301,301	0
22	MG	A	1631	1/1	0.99	0.09	123,123,123,123	0
22	MG	A	1683	1/1	0.99	0.09	186,186,186,186	0
22	MG	A	1623	1/1	0.99	0.06	91,91,91,91	0
22	MG	A	1633	1/1	0.99	0.05	112,112,112,112	0
22	MG	A	1714	1/1	0.99	0.04	146,146,146,146	0
23	ZN	D	301	1/1	0.99	0.20	130,130,130,130	0
22	MG	A	1724	1/1	0.99	0.05	132,132,132,132	0
22	MG	A	1657	1/1	1.00	0.10	170,170,170,170	0
22	MG	A	1654	1/1	1.00	0.01	126,126,126,126	0

6.5 Other polymers

There are no such residues in this entry.