



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 02:33 PM UTC

PDB ID : 4KVB / pdb_00004kvb
Title : Thermus thermophilus HB27 30S ribosomal subunit lacking ribosomal protein S17
Authors : Murphy, E.L.; Jogl, G.
Deposited on : 2013-05-22
Resolution : 4.20 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

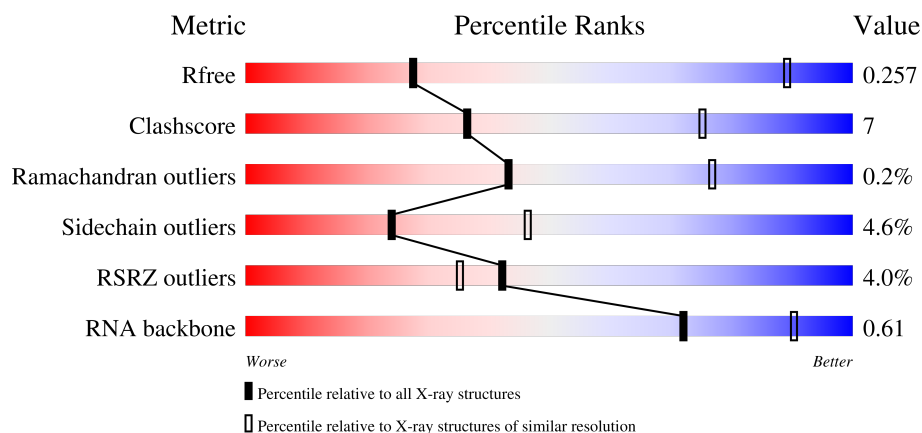
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1004 (4.52-3.88)
Clashscore	190562	1019 (4.50-3.90)
Ramachandran outliers	187476	1020 (4.56-3.84)
Sidechain outliers	187428	1006 (4.56-3.84)
RSRZ outliers	180081	1001 (4.52-3.88)
RNA backbone	3983	1026 (5.04-3.10)

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

Mol	Chain	Length	Quality of chain
1	A	1522	
2	B	256	
3	C	239	
4	D	209	

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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	134	
13	M	126	
14	N	61	
15	O	89	
16	P	88	
17	R	88	
18	S	93	
19	T	106	
20	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
21	MG	A	1607	-	-	-	X
21	MG	A	1608	-	-	-	X
21	MG	A	1615	-	-	-	X
21	MG	A	1616	-	-	-	X
21	MG	A	1619	-	-	-	X
21	MG	A	1621	-	-	-	X
21	MG	A	1623	-	-	-	X
21	MG	A	1624	-	-	-	X
21	MG	A	1625	-	-	-	X
21	MG	A	1626	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	MG	A	1627	-	-	-	X
21	MG	A	1629	-	-	-	X
21	MG	A	1630	-	-	-	X
21	MG	A	1632	-	-	-	X
21	MG	A	1638	-	-	-	X
21	MG	A	1647	-	-	-	X
21	MG	A	1648	-	-	-	X
21	MG	A	1650	-	-	-	X
21	MG	A	1652	-	-	-	X
21	MG	A	1653	-	-	-	X
21	MG	A	1664	-	-	-	X
21	MG	A	1665	-	-	-	X
21	MG	A	1667	-	-	-	X
21	MG	A	1672	-	-	-	X
21	MG	A	1674	-	-	-	X
21	MG	A	1684	-	-	-	X
21	MG	A	1687	-	-	-	X
21	MG	A	1691	-	-	-	X
21	MG	A	1702	-	-	-	X
21	MG	A	1703	-	-	-	X
21	MG	A	1706	-	-	-	X
21	MG	A	1708	-	-	-	X
21	MG	A	1712	-	-	-	X
21	MG	A	1719	-	-	-	X
21	MG	A	1740	-	-	-	X
21	MG	A	1741	-	-	-	X
21	MG	A	1742	-	-	-	X
21	MG	A	1744	-	-	-	X
21	MG	A	1749	-	-	-	X
21	MG	B	301	-	-	-	X
21	MG	E	201	-	-	-	X
22	K	A	1758	-	-	-	X
22	K	A	1771	-	-	-	X
22	K	A	1786	-	-	-	X

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 51128 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1514	Total	C	N	O	P	0	0	0
			32552	14497	6020	10521	1514			

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	235	Total	C	N	O	S	0	0	0
			1905	1217	342	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
			1011	639	198	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
			794	499	156	138	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	119	Total	C	N	O	S	0	0	0
			885	549	168	165	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			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	3	ALA	-	expression tag	UNP P61941
L	4	LEU	-	expression tag	UNP P61941

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	125	Total	C	N	O	S	0	0	0
			997	617	207	171	2			

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

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	88	Total	C	N	O	S	0	0	0
			734	459	147	126	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 S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	R	73	Total	C	N	O	0	0	0
			597	380	118	99			

- Molecule 18 is a protein called 30S ribosomal protein S19.

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

- Molecule 19 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	T	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

- Molecule 20 is a protein called 30S ribosomal protein Thx.

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

- Molecule 21 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	152	Total	Mg	0	0
			152	152		
21	B	1	Total	Mg	0	0
			1	1		
21	D	1	Total	Mg	0	0
			1	1		
21	E	2	Total	Mg	0	0
			2	2		
21	M	1	Total	Mg	0	0
			1	1		
21	U	1	Total	Mg	0	0
			1	1		

- Molecule 22 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	35	Total	K	0	0
			35	35		

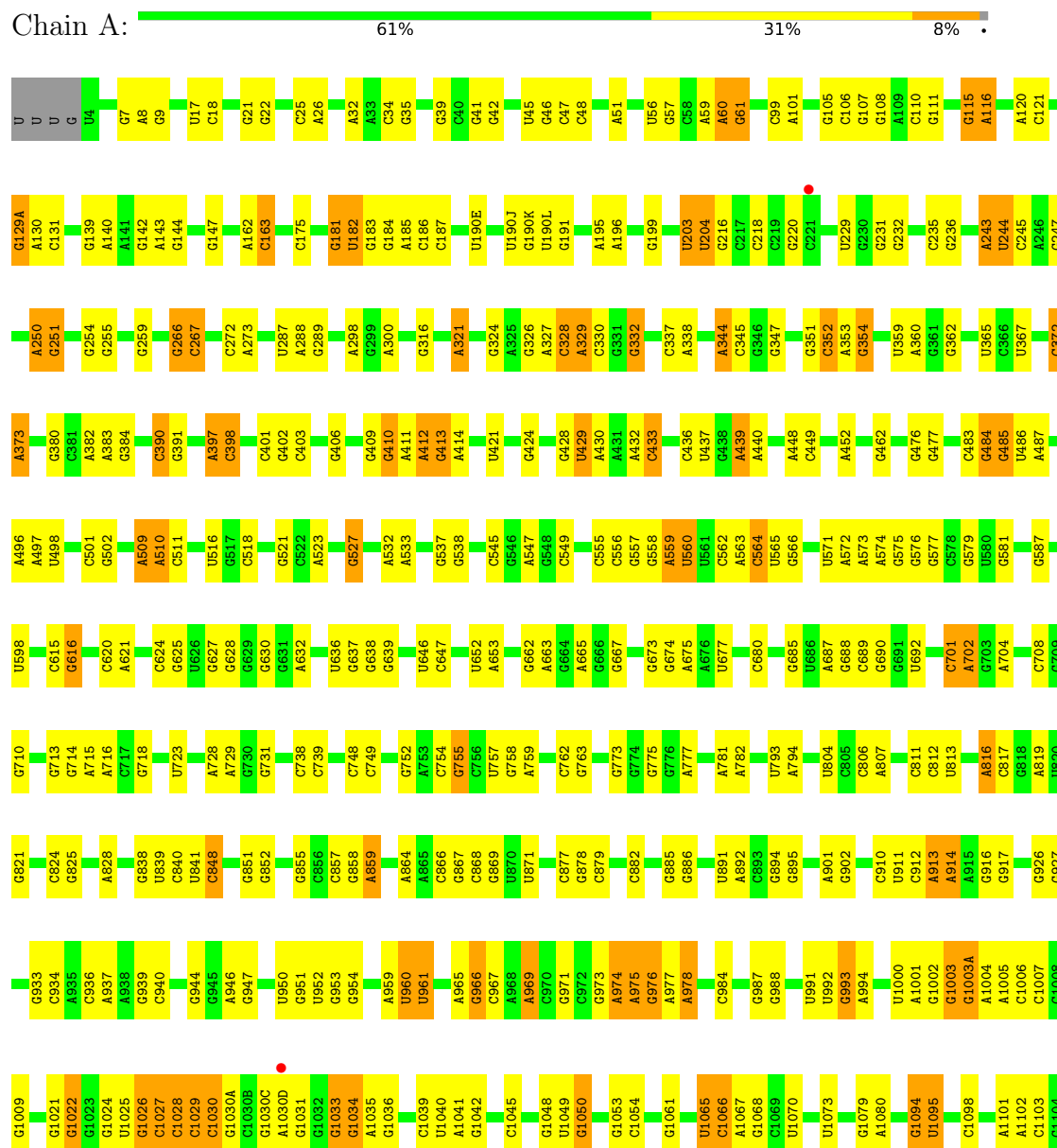
- Molecule 23 is ZINC ION (CCD ID: ZN) (formula: Zn).

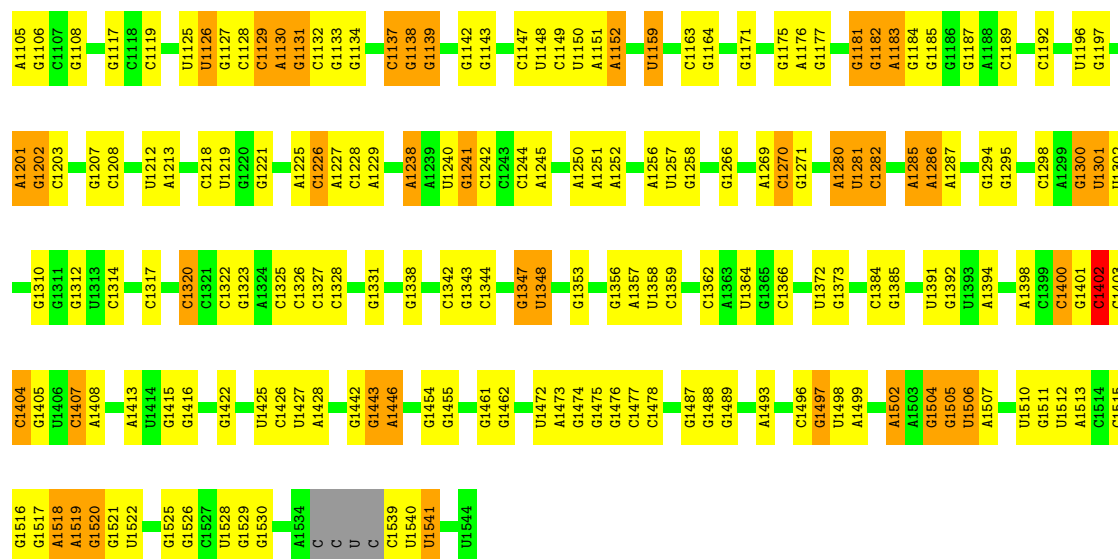
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	D	1	Total	Zn	0	0
			1	1		
23	N	1	Total	Zn	0	0
			1	1		

3 Residue-property plots

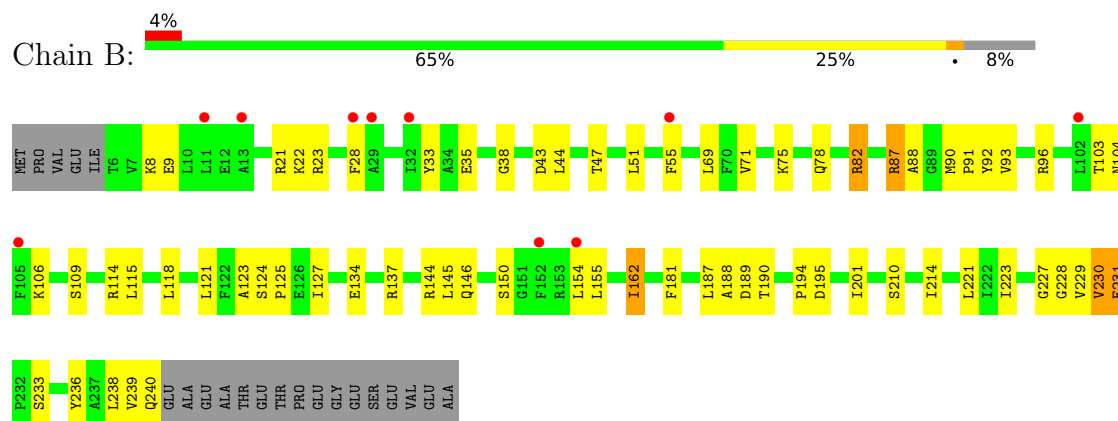
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: 16S rRNA

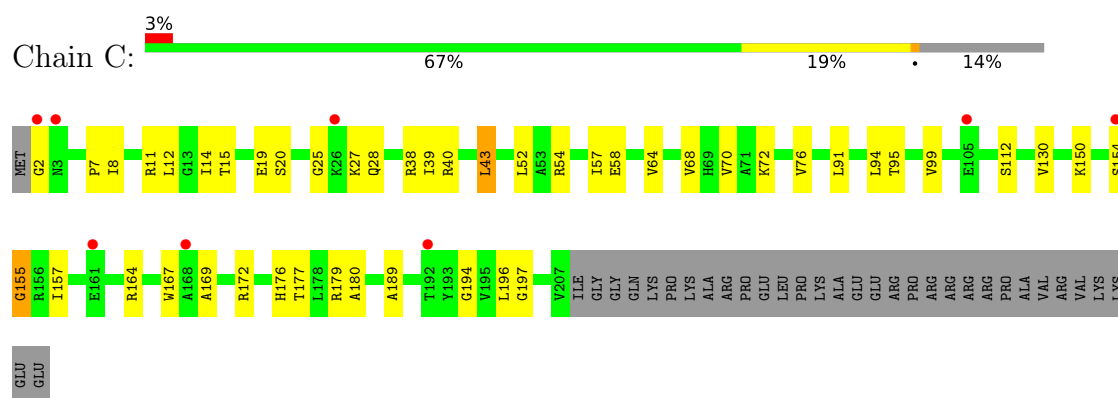




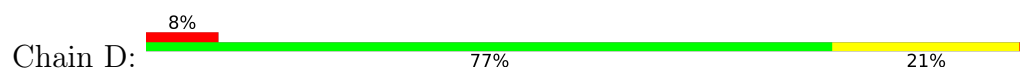
• Molecule 2: 30S ribosomal protein S2

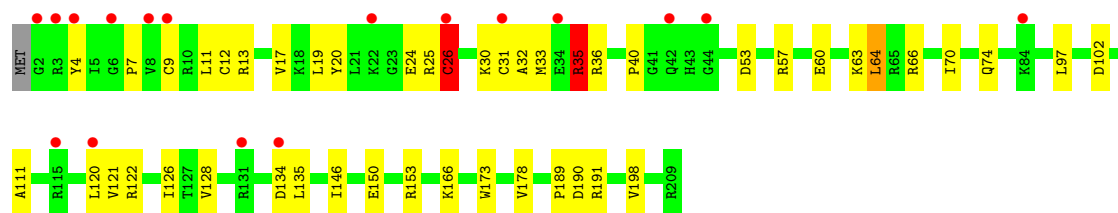


• Molecule 3: 30S ribosomal protein S3

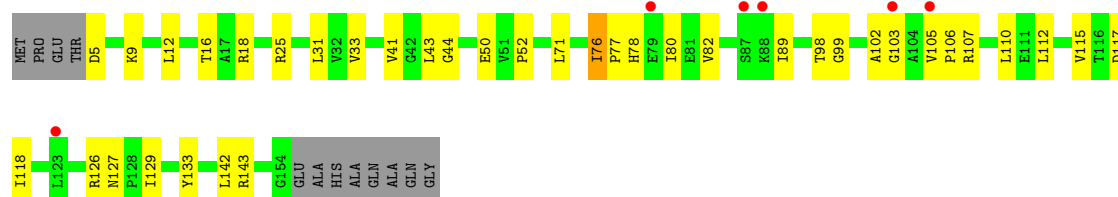


• Molecule 4: 30S ribosomal protein S4

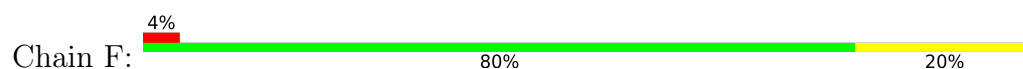




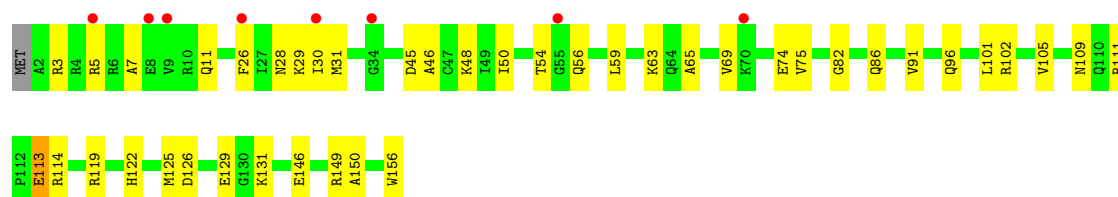
• Molecule 5: 30S ribosomal protein S5



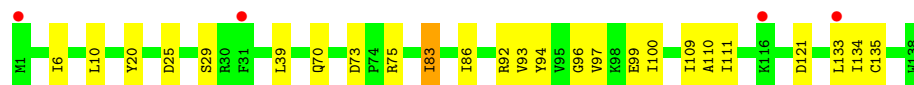
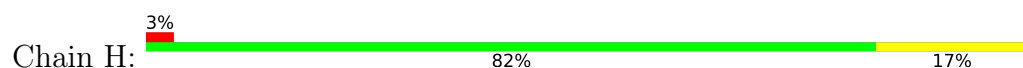
• Molecule 6: 30S ribosomal protein S6



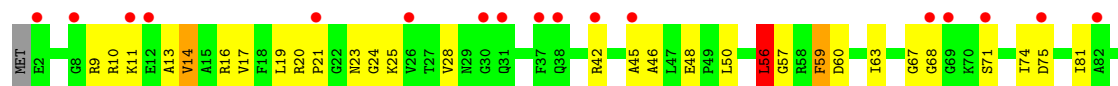
• Molecule 7: 30S ribosomal protein S7

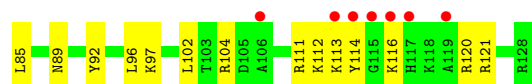


• Molecule 8: 30S ribosomal protein S8

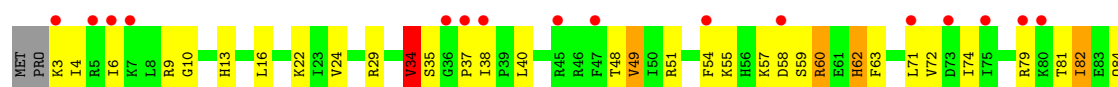


• Molecule 9: 30S ribosomal protein S9





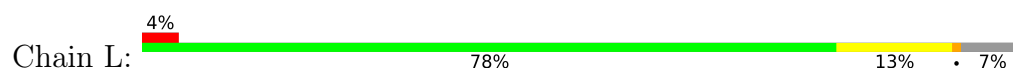
- Molecule 10: 30S ribosomal protein S10



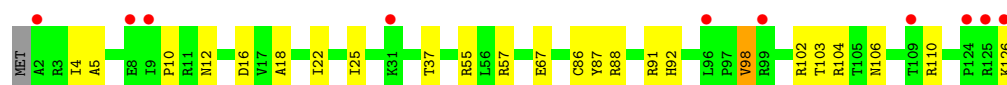
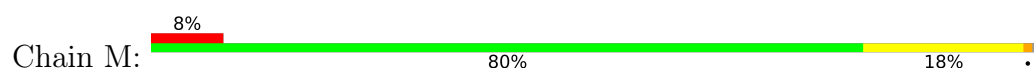
- Molecule 11: 30S ribosomal protein S11



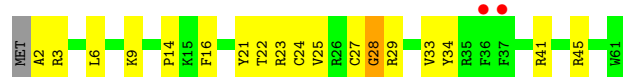
- Molecule 12: 30S ribosomal protein S12



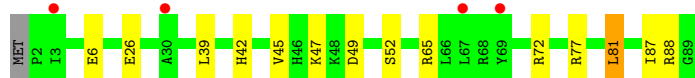
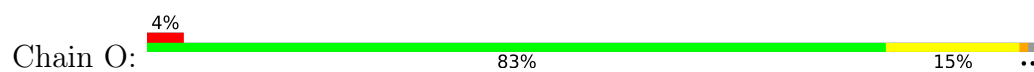
- Molecule 13: 30S ribosomal protein S13



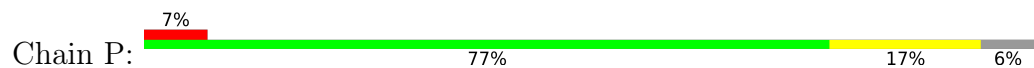
- Molecule 14: 30S ribosomal protein S14 type Z



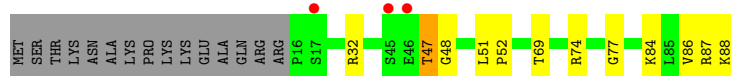
- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16



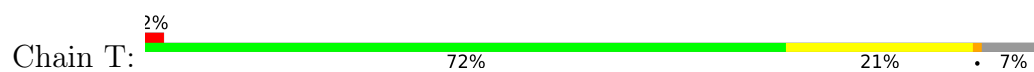
- Molecule 17: 30S ribosomal protein S18



- Molecule 18: 30S ribosomal protein S19



- Molecule 19: 30S ribosomal protein S20



- Molecule 20: 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	397.32Å 397.32Å 215.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.91 – 4.20 29.91 – 4.20	Depositor EDS
% Data completeness (in resolution range)	93.0 (29.91-4.20) 92.7 (29.91-4.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 4.26Å)	Xtriage
Refinement program	PHENIX dev_1370	Depositor
R, R_{free}	0.217 , 0.258 0.219 , 0.257	Depositor DCC
R_{free} test set	5806 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	202.1	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 116.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	51128	wwPDB-VP
Average B, all atoms (Å ²)	200.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.24% 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: 4OC, K, ZN, M2G, 0TD, UR3, 5MC, MG, 7MG, PSU, 2MG, MA6

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	0.09	1/36091 (0.0%)	0.22	0/56323
2	B	0.30	0/1940	0.78	4/2616 (0.2%)
3	C	0.28	0/1636	0.75	1/2205 (0.0%)
4	D	0.26	0/1733	0.75	1/2318 (0.0%)
5	E	0.28	0/1162	0.78	2/1564 (0.1%)
6	F	0.24	0/856	0.74	0/1154
7	G	0.27	0/1276	0.76	0/1709
8	H	0.26	0/1136	0.77	2/1527 (0.1%)
9	I	0.29	0/1029	0.79	0/1378
10	J	0.30	0/807	0.84	1/1085 (0.1%)
11	K	0.27	0/900	0.75	1/1213 (0.1%)
12	L	0.27	0/977	0.83	1/1306 (0.1%)
13	M	0.27	0/1008	0.75	2/1347 (0.1%)
14	N	0.27	0/501	0.75	1/664 (0.2%)
15	O	0.24	0/745	0.65	0/992
16	P	0.26	0/716	0.66	0/963
17	R	0.25	0/603	0.73	1/799 (0.1%)
18	S	0.29	0/661	0.76	1/890 (0.1%)
19	T	0.30	0/764	0.78	0/1006
20	U	0.24	0/212	0.83	0/277
All	All	0.18	1/54753 (0.0%)	0.46	18/81336 (0.0%)

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	1
4	D	0	1
9	I	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1498	UR3	O3'-P	5.83	1.62	1.56

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	R	87	ARG	CB-CA-C	-6.11	109.55	116.63
13	M	67	GLU	CB-CA-C	-6.04	109.60	116.54
13	M	106	ASN	CB-CA-C	-5.86	109.83	116.63
8	H	73	ASP	CA-C-N	5.66	125.36	119.82
8	H	73	ASP	C-N-CA	5.66	125.36	119.82
10	J	60	ARG	CB-CA-C	-5.65	109.54	117.23
12	L	105	TYR	CB-CA-C	-5.54	110.20	116.63
5	E	127	ASN	CA-C-N	5.54	125.63	119.32
5	E	127	ASN	C-N-CA	5.54	125.63	119.32
4	D	26	CYS	N-CA-C	-5.54	106.53	113.28
18	S	6	LYS	CB-CA-C	-5.30	110.48	116.63
2	B	9	GLU	CB-CA-C	-5.25	110.08	117.23
3	C	194	GLY	N-CA-C	5.22	117.06	110.38
2	B	231	GLU	CA-C-N	5.15	125.15	119.89
2	B	231	GLU	C-N-CA	5.15	125.15	119.89
14	N	28	GLY	N-CA-C	-5.08	108.26	115.43
2	B	8	LYS	CB-CA-C	-5.04	110.38	117.23
11	K	116	HIS	N-CA-C	-5.02	107.00	113.02

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	155	GLY	Peptide
4	D	35	ARG	Peptide
9	I	56	LEU	Peptide
9	I	57	GLY	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32552	0	16453	344	0
2	B	1905	0	1958	41	0
3	C	1612	0	1677	28	0
4	D	1703	0	1763	35	0
5	E	1146	0	1207	25	0
6	F	843	0	857	10	0
7	G	1257	0	1296	24	0
8	H	1116	0	1177	14	0
9	I	1011	0	1043	29	0
10	J	794	0	840	33	1
11	K	885	0	904	17	0
12	L	972	0	1058	11	0
13	M	997	0	1072	18	0
14	N	492	0	529	14	0
15	O	734	0	771	9	0
16	P	700	0	720	10	0
17	R	597	0	666	8	0
18	S	647	0	673	14	0
19	T	762	0	859	13	0
20	U	208	0	221	5	0
21	A	152	0	0	0	0
21	B	1	0	0	0	0
21	D	1	0	0	0	0
21	E	2	0	0	0	0
21	M	1	0	0	0	0
21	U	1	0	0	0	0
22	A	35	0	0	0	0
23	D	1	0	0	0	0
23	N	1	0	0	0	0
All	All	51128	0	35744	616	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (616) 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)
9:I:28:VAL:HG22	9:I:63:ILE:HB	1.67	0.76
1:A:1405:G:HO2'	1:A:1518:MA6:HO2'	1.30	0.76
3:C:58:GLU:HB3	10:J:92:THR:HG21	1.69	0.74
6:F:9:VAL:HB	6:F:87:ARG:HB2	1.70	0.74
1:A:1026:G:O6	1:A:1036:G:N2	2.21	0.73
1:A:959:A:HO2'	1:A:984:C:HO2'	1.36	0.71
2:B:75:LYS:HA	2:B:78:GLN:HB2	1.73	0.71
3:C:155:GLY:HA3	3:C:164:ARG:H	1.54	0.71
1:A:993:G:H1	1:A:1045:C:H42	1.39	0.70
10:J:38:ILE:HB	10:J:71:LEU:HB3	1.71	0.70
1:A:110:C:O2'	16:P:25:ARG:O	2.10	0.69
1:A:587:G:N2	1:A:754:C:OP2	2.24	0.69
3:C:64:VAL:HG23	3:C:99:VAL:HG11	1.74	0.69
3:C:7:PRO:HB3	3:C:11:ARG:HH21	1.57	0.69
3:C:70:VAL:HG12	3:C:72:LYS:H	1.58	0.69
1:A:1366:C:O2'	10:J:60:ARG:NH2	2.26	0.69
2:B:43:ASP:O	2:B:47:THR:OG1	2.10	0.68
1:A:501:C:OP1	12:L:117:ARG:NH2	2.28	0.67
1:A:1266:G:N2	1:A:1269:A:OP2	2.24	0.67
1:A:1539:C:H5'	7:G:82:GLY:HA3	1.77	0.67
2:B:134:GLU:HG2	2:B:137:ARG:HH21	1.61	0.66
1:A:816:A:OP2	1:A:1526:G:O2'	2.14	0.66
17:R:48:GLY:O	17:R:74:ARG:NH2	2.28	0.65
4:D:57:ARG:HH22	5:E:107:ARG:HD3	1.60	0.65
1:A:410:G:H5''	4:D:25:ARG:HE	1.62	0.65
1:A:1505:G:O2'	1:A:1506:U:OP2	2.14	0.65
1:A:953:G:N7	13:M:104:ARG:NH2	2.45	0.64
5:E:33:VAL:HG22	5:E:43:LEU:HD23	1.79	0.64
18:S:33:THR:HG22	18:S:35:SER:H	1.62	0.64
1:A:362:G:N2	1:A:365:U:OP2	2.30	0.64
3:C:155:GLY:HA2	3:C:157:ILE:HG13	1.78	0.64
18:S:22:LEU:O	18:S:26:GLY:N	2.31	0.63
1:A:1226:C:OP2	13:M:103:THR:OG1	2.12	0.63
3:C:20:SER:OG	3:C:40:ARG:NH2	2.31	0.63
9:I:50:LEU:HB3	9:I:56:LEU:HA	1.81	0.63
1:A:380:G:N2	1:A:383:A:OP2	2.29	0.63
14:N:9:LYS:HE2	14:N:23:ARG:HB2	1.81	0.63
1:A:448:A:OP2	1:A:485:G:N2	2.26	0.62
1:A:587:G:OP1	8:H:92:ARG:NH2	2.31	0.62
3:C:11:ARG:NH1	3:C:177:THR:O	2.32	0.62
1:A:718:G:O6	17:R:74:ARG:NH1	2.32	0.62
1:A:951:G:OP2	13:M:102:ARG:NH2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1192:C:O2	5:E:25:ARG:NH2	2.33	0.62
1:A:521:G:OP2	12:L:54:LYS:NZ	2.30	0.62
5:E:9:LYS:HB3	5:E:112:LEU:HD11	1.80	0.62
2:B:223:ILE:O	2:B:227:GLY:N	2.32	0.62
19:T:10:LEU:HG	19:T:12:ALA:H	1.64	0.62
1:A:1035:A:H2'	1:A:1036:G:C8	2.35	0.61
1:A:969:A:H61	13:M:126:LYS:HB2	1.64	0.61
1:A:1006:C:N4	1:A:1022:G:O6	2.32	0.61
1:A:196:A:OP1	19:T:68:LYS:NZ	2.32	0.61
1:A:976:G:OP2	1:A:1358:U:O2'	2.19	0.61
5:E:71:LEU:HD21	5:E:115:VAL:HG22	1.83	0.61
1:A:738:C:H5''	6:F:69:GLU:HB2	1.83	0.61
1:A:954:G:O6	1:A:1225:A:N6	2.33	0.61
1:A:1310:G:OP2	13:M:88:ARG:NH2	2.34	0.61
1:A:1392:G:H21	1:A:1502:A:H8	1.49	0.61
1:A:1314:C:N4	18:S:4:SER:OG	2.32	0.61
4:D:13:ARG:HD3	4:D:36:ARG:HG2	1.81	0.61
11:K:15:ALA:HA	11:K:77:MET:HA	1.83	0.61
14:N:23:ARG:NH1	14:N:28:GLY:O	2.33	0.61
1:A:975:A:H4'	1:A:976:G:H5''	1.82	0.61
13:M:88:ARG:HG3	13:M:98:VAL:HG11	1.81	0.61
1:A:1147:C:O2	9:I:16:ARG:NH1	2.34	0.60
18:S:15:LEU:HD23	18:S:33:THR:HG21	1.82	0.60
7:G:122:HIS:HA	7:G:125:MET:HE2	1.83	0.60
15:O:87:ILE:HG13	15:O:88:ARG:HG2	1.83	0.60
2:B:82:ARG:NH2	2:B:92:TYR:OH	2.34	0.60
1:A:401:C:O2'	1:A:621:A:N3	2.34	0.60
13:M:4:ILE:HG12	13:M:5:ALA:H	1.65	0.60
1:A:1106:G:H5''	3:C:172:ARG:HG2	1.84	0.60
6:F:1:MET:HE3	6:F:66:GLU:HG2	1.83	0.60
9:I:13:ALA:HB2	9:I:68:GLY:HA3	1.84	0.59
1:A:708:C:OP1	11:K:85:ARG:NH2	2.36	0.59
1:A:558:G:OP2	1:A:559:A:O2'	2.19	0.59
1:A:1002:G:N2	1:A:1039:C:O2	2.36	0.59
1:A:1029:C:OP1	1:A:1033:G:N2	2.35	0.59
2:B:22:LYS:HG3	2:B:23:ARG:HG3	1.84	0.59
18:S:55:LYS:HG2	18:S:56:GLN:HG3	1.85	0.59
1:A:1003:G:O2'	1:A:1003(A):G:N7	2.36	0.58
4:D:128:VAL:HG22	4:D:146:ILE:HG13	1.85	0.58
1:A:1405:G:H1	1:A:1496:C:H42	1.51	0.58
10:J:24:VAL:HG21	10:J:37:PRO:HD3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:G:H1	1:A:267:C:H42	1.51	0.58
5:E:102:ALA:HB1	5:E:106:PRO:HG2	1.85	0.58
2:B:123:ALA:H	2:B:127:ILE:HD11	1.67	0.58
3:C:14:ILE:HG22	3:C:15:THR:HG23	1.84	0.58
5:E:76:ILE:HG13	5:E:77:PRO:HD2	1.84	0.58
15:O:26:GLU:OE1	15:O:77:ARG:NH1	2.35	0.58
1:A:1203:C:OP1	14:N:2:ALA:N	2.36	0.58
13:M:16:ASP:OD1	13:M:16:ASP:N	2.36	0.58
1:A:1132:C:H2'	1:A:1133:G:H8	1.69	0.58
9:I:25:LYS:N	9:I:60:ASP:OD1	2.37	0.58
1:A:1422:G:H1	1:A:1478:C:H42	1.52	0.58
1:A:115:G:H4'	1:A:116:A:O5'	2.03	0.58
1:A:243:A:H4'	1:A:244:U:O5'	2.02	0.58
1:A:1326:C:OP1	20:U:12:LYS:NZ	2.37	0.58
11:K:123:LYS:HA	11:K:126:ARG:HG3	1.86	0.58
1:A:1413:A:H2	1:A:1487:G:H22	1.51	0.57
18:S:13:ASP:HA	18:S:16:LEU:HB3	1.86	0.57
19:T:54:LYS:HA	19:T:57:ARG:HD2	1.86	0.57
1:A:18:C:H1'	1:A:1079:G:H21	1.69	0.57
1:A:882:C:OP2	12:L:13:LYS:NZ	2.37	0.57
1:A:1128:C:H42	1:A:1143:G:H1	1.50	0.57
9:I:17:VAL:HG11	9:I:81:ILE:HG12	1.87	0.57
1:A:574:A:O2'	1:A:882:C:O2'	2.19	0.57
12:L:46:LYS:HG3	12:L:48:PRO:HD2	1.87	0.57
2:B:69:LEU:HB3	2:B:162:ILE:HG22	1.86	0.57
1:A:1119:C:OP2	9:I:9:ARG:NH2	2.38	0.57
4:D:26:CYS:HA	4:D:31:CYS:HB2	1.87	0.57
1:A:775:G:N2	1:A:804:U:O4	2.37	0.57
6:F:14:LEU:HD11	6:F:84:ASN:HB3	1.86	0.56
10:J:6:ILE:HG12	10:J:98:ILE:HG23	1.86	0.56
10:J:48:THR:O	14:N:34:TYR:OH	2.23	0.56
1:A:574:A:HO2'	1:A:882:C:HO2'	1.54	0.56
1:A:581:G:N2	1:A:759:A:OP2	2.36	0.56
10:J:29:ARG:NH1	10:J:84:GLN:OE1	2.35	0.56
1:A:372:C:H4'	1:A:373:A:O5'	2.05	0.56
3:C:52:LEU:HA	3:C:70:VAL:HG22	1.87	0.56
1:A:652:U:O4	1:A:752:G:O2'	2.20	0.56
2:B:187:LEU:HA	2:B:201:ILE:HB	1.88	0.56
7:G:105:VAL:O	7:G:109:ASN:ND2	2.39	0.56
9:I:45:ALA:O	9:I:48:GLU:HB2	2.06	0.56
1:A:235:C:H2'	1:A:236:G:H8	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:3:LYS:N	10:J:74:ILE:O	2.39	0.55
11:K:110:ASP:OD2	17:R:88:LYS:NZ	2.39	0.55
18:S:31:ILE:HG22	18:S:49:ILE:HA	1.88	0.55
1:A:1515:C:H2'	1:A:1516:G:H8	1.71	0.55
5:E:5:ASP:OD1	5:E:5:ASP:N	2.40	0.55
3:C:91:LEU:HD21	3:C:99:VAL:HG22	1.87	0.55
14:N:3:ARG:HB3	14:N:6:LEU:HD23	1.89	0.55
1:A:484:G:H4'	1:A:485:G:O5'	2.05	0.55
1:A:1150:U:O4	1:A:1151:A:N6	2.40	0.55
1:A:944:G:N1	1:A:1338:G:OP2	2.38	0.55
10:J:79:ARG:HD2	10:J:82:ILE:HD12	1.89	0.55
1:A:1238:A:H62	1:A:1301:U:H3	1.56	0.54
9:I:46:ALA:HB2	9:I:74:ILE:HG23	1.89	0.54
1:A:987:G:H2'	1:A:988:G:H8	1.72	0.54
3:C:130:VAL:HG21	3:C:157:ILE:HG23	1.90	0.54
19:T:10:LEU:HD12	19:T:11:SER:H	1.72	0.54
1:A:523:A:H61	12:L:92:OTD:CG	2.21	0.54
10:J:48:THR:HA	10:J:62:HIS:HB3	1.89	0.54
5:E:102:ALA:O	5:E:107:ARG:NH1	2.40	0.54
1:A:1252:A:H61	1:A:1285:A:H61	1.55	0.54
7:G:29:LYS:HG3	7:G:101:LEU:HB3	1.89	0.54
19:T:67:ALA:O	19:T:73:HIS:ND1	2.41	0.54
19:T:50:GLU:HA	19:T:100:ILE:HG22	1.89	0.53
1:A:231:G:H2'	1:A:232:G:H8	1.73	0.53
1:A:1187:G:O2'	9:I:111:ARG:NH1	2.41	0.53
1:A:1137:C:H4'	1:A:1138:G:C2	2.44	0.53
7:G:150:ALA:HA	11:K:57:THR:HG21	1.91	0.53
1:A:1080:A:H5''	5:E:16:THR:HG21	1.90	0.53
1:A:21:G:H2'	1:A:22:G:C8	2.43	0.53
1:A:1098:C:OP2	2:B:144:ARG:NH2	2.41	0.53
4:D:63:LYS:HD2	4:D:198:VAL:HG22	1.91	0.53
1:A:147:G:H1	1:A:175:C:H42	1.57	0.53
1:A:545:C:O2'	1:A:549:C:OP1	2.26	0.53
2:B:51:LEU:HD21	2:B:201:ILE:HG23	1.91	0.53
1:A:662:G:H2'	1:A:663:A:C8	2.44	0.53
10:J:49:VAL:HG23	14:N:41:ARG:HB2	1.91	0.53
5:E:76:ILE:HG23	5:E:78:HIS:H	1.73	0.53
8:H:10:LEU:HD22	8:H:83:ILE:HD11	1.90	0.52
1:A:139:G:H2'	1:A:140:A:H8	1.73	0.52
1:A:1342:C:H2'	1:A:1343:G:C8	2.44	0.52
1:A:673:G:H2'	1:A:674:G:C8	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:757:U:H2'	1:A:758:G:O4'	2.09	0.52
2:B:121:LEU:O	2:B:124:SER:OG	2.21	0.52
4:D:53:ASP:O	4:D:57:ARG:HG2	2.09	0.52
10:J:16:LEU:HD23	10:J:94:VAL:HG22	1.91	0.52
1:A:410:G:H5'	4:D:30:LYS:HD3	1.92	0.52
1:A:410:G:OP1	4:D:30:LYS:NZ	2.40	0.52
5:E:31:LEU:HD11	5:E:129:ILE:HA	1.91	0.52
1:A:1094:G:O2'	1:A:1108:G:N2	2.43	0.52
1:A:773:G:H1	1:A:806:C:H42	1.57	0.52
13:M:87:TYR:CZ	13:M:91:ARG:HD3	2.44	0.52
1:A:344:A:H5''	1:A:345:C:H5	1.74	0.52
1:A:324:G:N2	1:A:327:A:OP2	2.43	0.51
1:A:563:A:O2'	1:A:566:G:O2'	2.28	0.51
1:A:579:G:H5'	1:A:728:A:H1'	1.92	0.51
1:A:143:A:H2	1:A:220:G:H22	1.58	0.51
1:A:811:C:O2'	1:A:901:A:N1	2.43	0.51
3:C:177:THR:HB	3:C:180:ALA:HB2	1.90	0.51
16:P:21:VAL:HG12	16:P:33:ILE:HD12	1.91	0.51
1:A:1427:U:H2'	1:A:1428:A:H8	1.76	0.51
1:A:715:A:H2'	1:A:716:A:C8	2.46	0.51
9:I:42:ARG:NH2	9:I:71:SER:OG	2.36	0.51
7:G:146:GLU:HA	7:G:149:ARG:HG2	1.93	0.51
1:A:891:U:H2'	1:A:892:A:H8	1.76	0.51
10:J:4:ILE:HG22	10:J:100:THR:HG22	1.93	0.51
1:A:56:U:H2'	1:A:57:G:C8	2.45	0.51
3:C:8:ILE:O	3:C:12:LEU:N	2.44	0.51
1:A:624:C:H2'	1:A:625:G:H8	1.76	0.51
1:A:806:C:H2'	1:A:807:A:H8	1.76	0.51
2:B:188:ALA:N	2:B:201:ILE:O	2.40	0.51
1:A:462:G:N2	16:P:82:GLN:OE1	2.33	0.50
1:A:1454:G:H2'	1:A:1455:G:H8	1.77	0.50
1:A:501:C:H2'	1:A:502:G:C8	2.47	0.50
1:A:855:G:OP2	1:A:871:U:N3	2.45	0.50
1:A:973:G:H3'	1:A:974:A:H5''	1.94	0.50
2:B:28:PHE:HD1	2:B:194:PRO:HG3	1.77	0.50
1:A:559:A:OP2	5:E:126:ARG:NH2	2.44	0.50
1:A:859:A:OP2	1:A:869:G:N2	2.38	0.50
1:A:1516:G:N2	1:A:1519:MA6:OP2	2.33	0.50
8:H:86:ILE:HG22	8:H:93:VAL:HG21	1.93	0.50
11:K:21:ILE:HD11	11:K:98:LEU:HD12	1.94	0.50
2:B:91:PRO:HG2	2:B:155:LEU:HG	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1270:C:H2'	1:A:1271:G:H8	1.76	0.50
1:A:244:U:O4'	1:A:894:G:N2	2.45	0.49
1:A:1218:C:H2'	1:A:1219:U:C6	2.47	0.49
7:G:54:THR:HG22	7:G:56:GLN:H	1.76	0.49
1:A:272:C:H2'	1:A:273:A:H8	1.77	0.49
1:A:987:G:H2'	1:A:988:G:C8	2.47	0.49
4:D:64:LEU:HB2	4:D:198:VAL:HG11	1.93	0.49
15:O:26:GLU:HA	15:O:81:LEU:HD11	1.93	0.49
1:A:523:A:N6	12:L:92:OTD:OD2	2.44	0.49
1:A:913:A:H4'	1:A:914:A:O5'	2.13	0.49
1:A:1159:U:O4'	1:A:1182:G:N2	2.45	0.49
10:J:9:ARG:HG3	10:J:95:GLU:HB3	1.93	0.49
1:A:1373:G:O6	9:I:11:LYS:NZ	2.29	0.49
10:J:40:LEU:HD11	10:J:71:LEU:HB2	1.93	0.49
11:K:58:PRO:HB2	11:K:93:GLN:HG3	1.93	0.49
1:A:1001:A:H2	1:A:1040:U:H3	1.59	0.49
1:A:1152:A:H5''	10:J:13:HIS:HB2	1.94	0.49
1:A:1294:G:H2'	1:A:1295:G:H8	1.76	0.49
15:O:39:LEU:HD11	15:O:52:SER:HB3	1.94	0.49
3:C:64:VAL:H	3:C:99:VAL:HB	1.77	0.49
1:A:974:A:P	14:N:41:ARG:HH12	2.36	0.49
1:A:1108:G:H5''	3:C:176:HIS:CE1	2.47	0.49
2:B:51:LEU:HD22	2:B:55:PHE:HE2	1.78	0.49
1:A:266:G:H4'	1:A:267:C:O5'	2.12	0.49
4:D:11:LEU:HD13	4:D:66:ARG:HD3	1.94	0.49
4:D:102:ASP:OD1	4:D:102:ASP:N	2.45	0.49
1:A:838:G:N2	1:A:848:C:O2	2.44	0.49
1:A:1294:G:H2'	1:A:1295:G:C8	2.48	0.49
4:D:111:ALA:HB2	4:D:120:LEU:HD12	1.95	0.49
1:A:565:U:OP2	1:A:566:G:O2'	2.30	0.48
1:A:946:A:H2'	1:A:947:G:C8	2.47	0.48
4:D:35:ARG:HD2	4:D:35:ARG:O	2.12	0.48
1:A:410:G:H3'	4:D:25:ARG:HH21	1.77	0.48
1:A:636:U:H2'	1:A:637:G:C8	2.48	0.48
1:A:1281:U:H5'	1:A:1282:C:H5	1.78	0.48
1:A:250:A:H4'	1:A:251:G:O5'	2.13	0.48
1:A:974:A:OP2	14:N:29:ARG:NH2	2.45	0.48
4:D:190:ASP:OD1	4:D:191:ARG:N	2.45	0.48
7:G:111:ARG:HB3	7:G:113:GLU:HG2	1.94	0.48
1:A:1427:U:H2'	1:A:1428:A:C8	2.48	0.48
1:A:316:G:OP2	1:A:351:G:O2'	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:C:H2'	1:A:338:A:C8	2.48	0.48
1:A:1028:C:H3'	1:A:1033:G:H22	1.77	0.48
2:B:189:ASP:OD1	2:B:190:THR:N	2.39	0.48
4:D:4:TYR:OH	4:D:7:PRO:O	2.24	0.48
4:D:13:ARG:HB3	4:D:40:PRO:HD3	1.96	0.48
14:N:24:CYS:O	14:N:28:GLY:N	2.42	0.48
7:G:75:VAL:HG21	7:G:86:GLN:HB3	1.96	0.48
11:K:27:ASN:OD1	11:K:28:THR:N	2.46	0.48
13:M:22:ILE:HB	13:M:25:ILE:HB	1.95	0.48
16:P:8:ARG:HE	16:P:15:PRO:HB3	1.78	0.48
1:A:1269:A:HO2'	1:A:1325:C:HO2'	1.61	0.48
5:E:98:THR:N	5:E:117:ASP:OD2	2.47	0.48
7:G:91:VAL:O	7:G:96:GLN:NE2	2.46	0.48
1:A:910:C:OP1	12:L:97:ARG:NH1	2.42	0.48
1:A:1048:G:H5''	14:N:3:ARG:HG3	1.95	0.48
1:A:1250:A:H2'	1:A:1251:A:C8	2.48	0.48
2:B:21:ARG:NE	2:B:38:GLY:HA2	2.28	0.48
1:A:1139:G:N2	1:A:1142:G:O6	2.41	0.47
1:A:1519:MA6:O5'	1:A:1519:MA6:H8	2.14	0.47
1:A:106:C:H2'	1:A:107:G:H8	1.78	0.47
1:A:620:C:C2	4:D:135:LEU:HD13	2.49	0.47
16:P:4:ILE:HG12	16:P:21:VAL:HG22	1.96	0.47
1:A:105:G:OP1	19:T:22:ARG:NH2	2.47	0.47
1:A:328:C:H4'	1:A:329:A:C5'	2.45	0.47
1:A:439:A:C5	1:A:440:A:H1'	2.49	0.47
1:A:950:U:H2'	1:A:951:G:H8	1.78	0.47
1:A:638:G:H2'	1:A:639:G:H8	1.78	0.47
1:A:1095:U:OP1	1:A:1108:G:N2	2.45	0.47
1:A:41:G:H2'	1:A:42:G:H8	1.79	0.47
1:A:757:U:O2'	1:A:879:C:O2	2.32	0.47
5:E:110:LEU:HD13	5:E:118:ILE:HG21	1.94	0.47
7:G:74:GLU:HG2	7:G:91:VAL:HG22	1.96	0.47
1:A:272:C:H2'	1:A:273:A:C8	2.49	0.47
1:A:824:C:H2'	1:A:825:G:C8	2.49	0.47
12:L:117:ARG:HB3	12:L:122:THR:O	2.15	0.47
1:A:571:U:O4	1:A:864:A:N6	2.47	0.47
1:A:627:G:H2'	1:A:628:G:H8	1.80	0.47
1:A:1026:G:H2'	1:A:1027:C:H5''	1.97	0.47
1:A:1175:G:H2'	1:A:1176:A:H8	1.79	0.47
1:A:1347:G:O6	9:I:10:ARG:NH2	2.35	0.47
3:C:25:GLY:H	3:C:28:GLN:HB2	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:63:PHE:HE2	14:N:45:ARG:HA	1.80	0.47
11:K:48:ILE:HG22	11:K:49:GLY:H	1.80	0.47
4:D:24:GLU:HG2	4:D:25:ARG:H	1.79	0.47
9:I:23:ASN:N	9:I:60:ASP:OD2	2.47	0.47
1:A:300:A:O2'	1:A:564:C:N3	2.45	0.47
1:A:885:G:H2'	1:A:886:G:H8	1.79	0.47
2:B:118:LEU:HD23	2:B:121:LEU:HD12	1.96	0.47
1:A:560:U:H5'	1:A:566:G:N2	2.29	0.47
1:A:939:G:O3'	7:G:102:ARG:NH2	2.48	0.47
1:A:1151:A:H5'	10:J:40:LEU:O	2.15	0.47
1:A:41:G:H2'	1:A:42:G:C8	2.50	0.46
1:A:401:C:H2'	1:A:402:G:H8	1.79	0.46
1:A:559:A:H4'	1:A:560:U:O5'	2.15	0.46
18:S:31:ILE:HG12	18:S:32:LYS:H	1.80	0.46
10:J:6:ILE:HG23	10:J:98:ILE:HG12	1.96	0.46
1:A:689:C:H2'	1:A:690:G:O4'	2.15	0.46
7:G:65:ALA:O	7:G:69:VAL:HG23	2.16	0.46
10:J:54:PHE:CD2	10:J:55:LYS:HG2	2.50	0.46
11:K:57:THR:HG22	11:K:60:ALA:H	1.80	0.46
1:A:911:U:H2'	1:A:912:C:C6	2.51	0.46
1:A:1391:U:H2'	1:A:1392:G:C8	2.51	0.46
3:C:19:GLU:HG2	3:C:54:ARG:HH21	1.80	0.46
9:I:21:PRO:HA	9:I:59:PHE:HB3	1.96	0.46
18:S:50:ALA:HB1	18:S:57:HIS:HB3	1.98	0.46
1:A:99:C:H2'	1:A:101:A:C8	2.49	0.46
1:A:1415:G:H2'	1:A:1416:G:C8	2.50	0.46
10:J:82:ILE:HA	10:J:85:LEU:HB2	1.97	0.46
2:B:239:VAL:HG12	2:B:240:GLN:HG2	1.98	0.46
2:B:114:ARG:HH21	2:B:118:LEU:HD21	1.80	0.46
1:A:254:G:H2'	1:A:255:G:H8	1.80	0.46
1:A:674:G:H2'	1:A:675:A:H8	1.80	0.46
1:A:1151:A:HO2'	1:A:1152:A:H8	1.63	0.46
1:A:1443:G:H4'	1:A:1446:A:O5'	2.16	0.46
5:E:142:LEU:O	5:E:143:ARG:NE	2.46	0.46
1:A:191:G:O2'	19:T:102:GLY:O	2.28	0.46
1:A:674:G:H2'	1:A:675:A:C8	2.51	0.46
2:B:87:ARG:NH2	2:B:233:SER:HB2	2.31	0.46
2:B:195:ASP:OD1	2:B:195:ASP:N	2.49	0.46
2:B:103:THR:OG1	2:B:104:ASN:N	2.49	0.46
7:G:46:ALA:O	7:G:50:ILE:HG12	2.15	0.46
1:A:129(A):G:H21	1:A:190(E):U:H3'	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1300:G:O2'	1:A:1301:U:O5'	2.29	0.45
1:A:1344:C:H4'	9:I:120:ARG:HB3	1.98	0.45
1:A:1356:G:H2'	1:A:1357:A:C8	2.51	0.45
1:A:1505:G:O2'	1:A:1541:PSU:OP2	2.31	0.45
1:A:1506:U:N3	1:A:1522:U:OP1	2.41	0.45
2:B:88:ALA:HB1	2:B:90:MET:HG2	1.96	0.45
6:F:11:ASN:HB3	6:F:14:LEU:HG	1.97	0.45
1:A:328:C:H4'	1:A:329:A:O5'	2.16	0.45
1:A:739:C:O2'	15:O:42:HIS:ND1	2.48	0.45
8:H:6:ILE:HD12	8:H:6:ILE:H	1.81	0.45
1:A:476:G:H2'	1:A:477:G:C8	2.52	0.45
1:A:559:A:H1'	1:A:560:U:OP2	2.16	0.45
1:A:701:C:H4'	1:A:702:A:O5'	2.16	0.45
1:A:1281:U:H4'	1:A:1282:C:OP2	2.17	0.45
5:E:50:GLU:HG3	5:E:52:PRO:HD2	1.97	0.45
1:A:352:C:O2'	1:A:354:G:OP1	2.25	0.45
1:A:556:C:H2'	1:A:557:G:O4'	2.16	0.45
1:A:1105:A:H2'	1:A:1106:G:H8	1.81	0.45
1:A:1515:C:H2'	1:A:1516:G:C8	2.50	0.45
2:B:21:ARG:NE	2:B:35:GLU:OE2	2.42	0.45
9:I:96:LEU:HB3	9:I:102:LEU:HD21	1.97	0.45
1:A:692:U:H3	11:K:53:SER:HB3	1.82	0.45
1:A:1510:U:H2'	1:A:1511:G:C8	2.51	0.45
16:P:58:TYR:O	16:P:61:SER:OG	2.32	0.45
1:A:409:G:H1	1:A:433:C:H42	1.65	0.45
8:H:111:ILE:HG22	8:H:134:ILE:HD12	1.99	0.45
12:L:38:THR:N	12:L:57:LYS:O	2.38	0.45
13:M:4:ILE:HA	13:M:57:ARG:HD3	1.98	0.45
1:A:203:U:O2'	1:A:204:U:O5'	2.26	0.45
1:A:403:C:OP2	4:D:74:GLN:NE2	2.47	0.45
1:A:685:G:N1	1:A:704:A:OP2	2.46	0.45
1:A:868:C:H2'	1:A:869:G:O4'	2.15	0.45
1:A:1250:A:O3'	9:I:67:GLY:HA2	2.17	0.45
5:E:43:LEU:HD22	5:E:44:GLY:H	1.82	0.45
1:A:390:C:H2'	1:A:391:G:C8	2.52	0.45
1:A:728:A:H2'	1:A:729:A:H8	1.81	0.45
1:A:1129:C:N4	1:A:1134:G:N7	2.65	0.45
3:C:189:ALA:HB3	3:C:196:LEU:HB2	1.98	0.45
8:H:110:ALA:HB3	8:H:121:ASP:HB3	1.98	0.45
1:A:162:A:C5	1:A:163:C:H1'	2.51	0.45
1:A:190(L):U:O2	19:T:105:SER:OG	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:C:H2'	1:A:338:A:H8	1.81	0.45
1:A:969:A:N6	13:M:126:LYS:HE3	2.32	0.45
1:A:1065:U:H1'	1:A:1066:C:OP2	2.17	0.45
1:A:1461:G:H2'	1:A:1462:G:H8	1.81	0.45
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.99	0.45
1:A:142:G:H2'	1:A:143:A:H8	1.82	0.44
9:I:89:ASN:HB3	9:I:92:TYR:CD2	2.52	0.44
1:A:190(J):U:H2'	1:A:190(K):G:C8	2.52	0.44
19:T:20:LEU:O	19:T:23:ARG:HB3	2.17	0.44
1:A:950:U:H2'	1:A:951:G:C8	2.51	0.44
1:A:1177:G:OP2	9:I:97:LYS:NZ	2.37	0.44
1:A:1488:G:H2'	1:A:1489:G:C8	2.52	0.44
4:D:32:ALA:O	4:D:36:ARG:HB2	2.18	0.44
16:P:1:MET:HE3	16:P:3:LYS:HD2	1.99	0.44
1:A:186:C:H2'	1:A:187:C:C6	2.53	0.44
1:A:509:A:O2'	1:A:510:A:OP1	2.34	0.44
1:A:1320:C:O2	18:S:36:ARG:NH1	2.50	0.44
7:G:111:ARG:NH2	7:G:126:ASP:OD2	2.48	0.44
10:J:57:LYS:O	10:J:58:ASP:HB2	2.18	0.44
1:A:45:U:H2'	1:A:46:G:C8	2.52	0.44
1:A:254:G:H2'	1:A:255:G:C8	2.52	0.44
1:A:1030:C:N4	1:A:1031:G:N7	2.58	0.44
1:A:1298:C:P	7:G:114:ARG:HH22	2.40	0.44
4:D:24:GLU:C	4:D:26:CYS:H	2.25	0.44
18:S:6:LYS:HG2	18:S:7:LYS:HD3	1.98	0.44
1:A:448:A:H2'	1:A:449:C:C6	2.52	0.44
1:A:555:C:H2'	1:A:556:C:C6	2.53	0.44
1:A:713:G:H2'	1:A:714:G:C8	2.53	0.44
2:B:123:ALA:N	2:B:127:ILE:HD11	2.31	0.44
1:A:34:C:H2'	1:A:35:G:C8	2.53	0.44
1:A:1372:U:H2'	1:A:1373:G:O4'	2.17	0.44
6:F:62:TRP:CH2	6:F:64:GLN:HB2	2.52	0.44
1:A:1130:A:H4'	9:I:20:ARG:HH22	1.82	0.44
1:A:1242:C:H42	1:A:1295:G:H1	1.66	0.44
12:L:33:ARG:HD2	12:L:33:ARG:HA	1.76	0.44
1:A:1007:C:H42	1:A:1022:G:H1	1.64	0.44
4:D:57:ARG:HH12	5:E:107:ARG:HE	1.65	0.44
5:E:129:ILE:HD12	5:E:129:ILE:H	1.82	0.44
9:I:24:GLY:H	9:I:60:ASP:CG	2.25	0.44
10:J:10:GLY:N	10:J:16:LEU:HD11	2.33	0.44
1:A:59:A:H1'	1:A:354:G:N2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:A:H61	1:A:332:G:H1	1.66	0.43
1:A:936:C:H2'	1:A:937:A:O4'	2.17	0.43
1:A:1103:C:OP1	2:B:96:ARG:NH1	2.51	0.43
1:A:1131:G:H2'	1:A:1132:C:C6	2.53	0.43
9:I:10:ARG:HG2	9:I:75:ASP:HB2	2.00	0.43
1:A:1240:U:OP1	7:G:119:ARG:NH1	2.41	0.43
1:A:1244:C:H2'	1:A:1245:A:C8	2.53	0.43
2:B:146:GLN:O	2:B:150:SER:HB2	2.17	0.43
8:H:96:GLY:O	8:H:100:ILE:HG13	2.17	0.43
16:P:3:LYS:HD3	16:P:24:ALA:HB2	2.00	0.43
1:A:762:C:H2'	1:A:763:G:C8	2.53	0.43
1:A:851:G:H2'	1:A:852:G:C8	2.53	0.43
1:A:1461:G:H2'	1:A:1462:G:C8	2.53	0.43
1:A:1520:G:H2'	1:A:1521:G:C8	2.53	0.43
10:J:34:VAL:HG12	10:J:35:SER:H	1.83	0.43
11:K:43:SER:HA	11:K:47:VAL:HG21	2.00	0.43
1:A:106:C:H2'	1:A:107:G:C8	2.53	0.43
1:A:486:U:H2'	1:A:487:A:H8	1.83	0.43
1:A:716:A:N3	11:K:118:GLY:HA2	2.33	0.43
1:A:1384:C:H2'	1:A:1385:G:H8	1.83	0.43
4:D:57:ARG:HH12	5:E:107:ARG:NE	2.15	0.43
4:D:60:GLU:HG3	4:D:198:VAL:HG13	2.00	0.43
10:J:79:ARG:HA	10:J:82:ILE:HG13	2.00	0.43
1:A:7:G:H5''	1:A:298:A:O4'	2.18	0.43
1:A:110:C:H2'	1:A:111:G:O4'	2.19	0.43
1:A:667:G:O2'	15:O:49:ASP:OD1	2.31	0.43
1:A:1201:A:H1'	1:A:1202:G:OP2	2.18	0.43
1:A:1472:U:H2'	1:A:1473:A:C8	2.53	0.43
13:M:37:THR:HG22	13:M:55:ARG:HD2	2.00	0.43
1:A:229:U:H5''	16:P:33:ILE:HD13	2.01	0.43
1:A:1035:A:H2'	1:A:1036:G:H8	1.82	0.43
1:A:1270:C:H2'	1:A:1271:G:C8	2.54	0.43
1:A:1425:U:H3	1:A:1475:G:H1	1.67	0.43
9:I:71:SER:O	9:I:74:ILE:HB	2.19	0.43
11:K:117:ASN:N	11:K:117:ASN:OD1	2.52	0.43
1:A:677:U:H3	1:A:713:G:H22	1.65	0.43
1:A:939:G:H2'	1:A:940:C:C6	2.54	0.43
1:A:952:U:H2'	1:A:953:G:C8	2.54	0.43
1:A:1392:G:N2	1:A:1502:A:H8	2.14	0.43
1:A:1454:G:H2'	1:A:1455:G:C8	2.54	0.43
3:C:15:THR:HG21	3:C:179:ARG:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:34:ASP:OD1	11:K:38:ASN:N	2.52	0.43
16:P:28:ARG:NH1	16:P:29:ASP:OD1	2.51	0.43
1:A:1426:C:H2'	1:A:1427:U:C6	2.54	0.43
1:A:537:G:H2'	1:A:538:G:C8	2.54	0.43
1:A:728:A:H2'	1:A:729:A:C8	2.53	0.43
1:A:1244:C:H2'	1:A:1245:A:H8	1.84	0.43
20:U:5:ASP:O	20:U:11:GLY:HA3	2.19	0.43
1:A:1181:G:O2'	1:A:1184:G:H5'	2.19	0.43
2:B:90:MET:HA	2:B:91:PRO:HD3	1.87	0.43
4:D:25:ARG:NH1	4:D:30:LYS:O	2.52	0.43
1:A:25:C:H2'	1:A:26:A:C8	2.54	0.42
1:A:287:U:H2'	1:A:288:A:H8	1.82	0.42
1:A:1132:C:H2'	1:A:1133:G:C8	2.52	0.42
1:A:1504:G:OP1	1:A:1507:A:H4'	2.18	0.42
1:A:1512:U:H2'	1:A:1513:A:C8	2.54	0.42
7:G:59:LEU:HD11	7:G:63:LYS:HE3	2.01	0.42
1:A:108:G:OP2	1:A:326:G:N1	2.47	0.42
1:A:615:C:H2'	1:A:616:G:O4'	2.18	0.42
1:A:680:C:H42	1:A:710:G:H1	1.67	0.42
1:A:978:A:O2'	1:A:1322:C:N3	2.50	0.42
1:A:1050:G:N2	1:A:1208:C:O2	2.52	0.42
1:A:1175:G:H2'	1:A:1176:A:C8	2.54	0.42
1:A:1415:G:H2'	1:A:1416:G:H8	1.84	0.42
2:B:91:PRO:HA	2:B:154:LEU:HD12	2.00	0.42
2:B:124:SER:HB2	2:B:125:PRO:HD2	2.02	0.42
14:N:9:LYS:HD3	14:N:21:TYR:O	2.19	0.42
1:A:824:C:H2'	1:A:825:G:H8	1.83	0.42
1:A:1327:C:H2'	1:A:1328:C:C6	2.54	0.42
1:A:1404:5MC:HN41	1:A:1497:G:H1	1.65	0.42
8:H:86:ILE:HD12	8:H:133:LEU:HG	2.01	0.42
9:I:19:LEU:HD13	9:I:59:PHE:CE1	2.53	0.42
13:M:87:TYR:O	13:M:91:ARG:HG2	2.20	0.42
1:A:181:G:H4'	1:A:182:U:C5'	2.49	0.42
1:A:1126:U:H1'	1:A:1280:A:C5	2.54	0.42
1:A:1228:C:H2'	1:A:1229:A:H8	1.84	0.42
1:A:1516:G:H2'	1:A:1518:MA6:OP2	2.19	0.42
2:B:33:TYR:HB2	2:B:43:ASP:HA	2.00	0.42
3:C:154:SER:OG	3:C:197:GLY:N	2.50	0.42
6:F:2:ARG:HB2	6:F:4:TYR:CE1	2.54	0.42
7:G:5:ARG:HG3	7:G:7:ALA:H	1.84	0.42
10:J:22:LYS:HD3	10:J:89:ASP:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:G:H1	1:A:218:C:H42	1.68	0.42
1:A:412:A:H5'	1:A:413:G:OP1	2.19	0.42
1:A:483:C:OP2	1:A:484:G:O2'	2.35	0.42
1:A:960:U:H4'	1:A:961:U:O5'	2.18	0.42
1:A:1475:G:H2'	1:A:1476:G:C8	2.54	0.42
2:B:51:LEU:HD22	2:B:55:PHE:CE2	2.53	0.42
6:F:82:ARG:HA	6:F:82:ARG:HE	1.84	0.42
9:I:9:ARG:HG2	9:I:14:VAL:HG12	2.02	0.42
11:K:58:PRO:HA	11:K:90:GLY:HA2	2.02	0.42
13:M:86:CYS:SG	18:S:73:GLU:HB3	2.59	0.42
1:A:60:A:H4'	1:A:61:G:O5'	2.19	0.42
1:A:627:G:H2'	1:A:628:G:C8	2.54	0.42
1:A:851:G:H2'	1:A:852:G:H8	1.85	0.42
1:A:1183:A:O2'	1:A:1185:G:OP2	2.38	0.42
3:C:150:LYS:HG3	3:C:169:ALA:HB2	2.00	0.42
4:D:166:LYS:HG2	4:D:178:VAL:HG11	2.01	0.42
5:E:80:ILE:HG22	5:E:82:VAL:HG23	2.01	0.42
8:H:20:TYR:CZ	8:H:75:ARG:HB3	2.55	0.42
17:R:47:THR:HG22	17:R:48:GLY:H	1.85	0.42
19:T:59:ALA:O	19:T:63:ILE:HG13	2.19	0.42
1:A:563:A:O4'	1:A:566:G:N2	2.51	0.42
2:B:91:PRO:HG3	2:B:154:LEU:HB2	2.02	0.42
2:B:106:LYS:O	2:B:109:SER:OG	2.26	0.42
8:H:96:GLY:H	8:H:99:GLU:HB2	1.85	0.42
12:L:70:ILE:HD13	12:L:77:LEU:HD12	2.02	0.42
1:A:250:A:H1'	1:A:251:G:OP2	2.19	0.42
1:A:397:A:H5'	1:A:398:C:OP1	2.20	0.42
1:A:413:G:N2	1:A:429:U:OP2	2.53	0.42
10:J:82:ILE:HA	10:J:85:LEU:CB	2.50	0.42
1:A:952:U:H2'	1:A:953:G:H8	1.85	0.42
1:A:1342:C:H2'	1:A:1343:G:H8	1.85	0.42
4:D:121:VAL:O	4:D:134:ASP:HA	2.20	0.42
4:D:173:TRP:CD2	4:D:189:PRO:HB3	2.55	0.42
18:S:30:LEU:HD23	18:S:48:THR:HB	2.02	0.42
1:A:646:U:H2'	1:A:647:C:C6	2.55	0.42
1:A:1061:G:N7	3:C:2:GLY:HA3	2.34	0.42
1:A:1241:G:H2'	1:A:1242:C:C6	2.54	0.42
1:A:1353:G:OP2	20:U:3:LYS:NZ	2.47	0.42
1:A:1404:5MC:N4	1:A:1497:G:H1	2.18	0.42
2:B:181:PHE:HD2	8:H:70:GLN:HB3	1.84	0.42
2:B:228:GLY:O	2:B:230:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:25:ASP:N	8:H:25:ASP:OD1	2.52	0.42
1:A:598:U:H4'	8:H:94:TYR:CD2	2.55	0.41
1:A:857:C:H2'	1:A:858:G:O4'	2.20	0.41
1:A:877:C:H2'	1:A:878:G:C8	2.54	0.41
1:A:1049:U:O2'	14:N:3:ARG:NH1	2.53	0.41
4:D:9:CYS:O	4:D:12:CYS:HB2	2.19	0.41
4:D:31:CYS:C	4:D:33:MET:H	2.27	0.41
10:J:4:ILE:HD11	10:J:74:ILE:HD12	2.02	0.41
17:R:84:LYS:HE2	17:R:84:LYS:HB3	1.90	0.41
1:A:34:C:H2'	1:A:35:G:H8	1.85	0.41
1:A:184:G:H2'	1:A:185:A:H8	1.83	0.41
4:D:150:GLU:HA	4:D:153:ARG:HG3	2.00	0.41
13:M:92:HIS:HA	13:M:110:ARG:NH2	2.35	0.41
1:A:1041:A:H2'	1:A:1042:G:C8	2.55	0.41
1:A:1285:A:H1'	1:A:1286:A:OP2	2.20	0.41
3:C:27:LYS:HE2	3:C:27:LYS:HB3	1.89	0.41
5:E:99:GLY:H	5:E:117:ASP:CG	2.29	0.41
6:F:42:GLU:OE1	6:F:59:TYR:OH	2.35	0.41
2:B:115:LEU:HD13	2:B:145:LEU:HB3	2.03	0.41
13:M:110:ARG:HD2	13:M:110:ARG:HA	1.82	0.41
14:N:14:PRO:C	14:N:16:PHE:H	2.29	0.41
1:A:21:G:H2'	1:A:22:G:H8	1.84	0.41
1:A:916:G:H2'	1:A:917:G:H8	1.85	0.41
7:G:28:ASN:HA	7:G:31:MET:HE3	2.02	0.41
7:G:126:ASP:HB3	7:G:131:LYS:HG3	2.03	0.41
11:K:120:ARG:HA	11:K:121:PRO:HD3	1.85	0.41
7:G:26:PHE:CE2	7:G:30:ILE:HD11	2.55	0.41
1:A:412:A:H4'	1:A:413:G:O5'	2.21	0.41
1:A:436:C:H2'	1:A:437:U:C6	2.56	0.41
1:A:754:C:P	15:O:72:ARG:HH12	2.44	0.41
1:A:762:C:H2'	1:A:763:G:H8	1.85	0.41
10:J:89:ASP:OD1	10:J:91:PRO:HD2	2.21	0.41
1:A:382:A:H2'	1:A:383:A:C8	2.56	0.41
1:A:638:G:H2'	1:A:639:G:C8	2.56	0.41
1:A:755:G:OP2	15:O:65:ARG:HD2	2.21	0.41
1:A:894:G:H2'	1:A:895:G:C8	2.56	0.41
1:A:933:G:O6	7:G:3:ARG:NH2	2.53	0.41
1:A:1347:G:O2'	1:A:1348:U:P	2.79	0.41
1:A:1402:4OC:H2'	1:A:1403:C:O4'	2.20	0.41
1:A:1525:G:H2'	1:A:1526:G:C8	2.56	0.41
4:D:53:ASP:OD1	4:D:53:ASP:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:50:TYR:CE1	17:R:77:GLY:HA2	2.55	0.41
9:I:9:ARG:HB3	9:I:104:ARG:HH21	1.86	0.41
17:R:51:LEU:HA	17:R:52:PRO:HD3	1.81	0.41
1:A:17:U:H2'	1:A:18:C:C6	2.56	0.41
1:A:984:C:H42	1:A:1221:G:H1	1.69	0.41
1:A:1070:U:OP1	5:E:18:ARG:NH1	2.38	0.41
2:B:210:SER:O	2:B:214:ILE:HG12	2.20	0.41
3:C:38:ARG:HB3	3:C:94:LEU:HD21	2.03	0.41
3:C:39:ILE:O	3:C:43:LEU:HB2	2.20	0.41
3:C:68:VAL:HG12	3:C:70:VAL:HG23	2.02	0.41
8:H:86:ILE:HG13	8:H:135:CYS:HA	2.02	0.41
9:I:114:TYR:HB2	10:J:60:ARG:HG3	2.03	0.41
10:J:81:THR:HG22	10:J:85:LEU:HD23	2.02	0.41
15:O:47:LYS:H	15:O:47:LYS:HG2	1.72	0.41
1:A:1148:U:H2'	1:A:1149:C:O4'	2.21	0.41
1:A:1520:G:H2'	1:A:1521:G:H8	1.86	0.41
20:U:17:THR:O	20:U:22:ARG:NH1	2.54	0.41
1:A:359:U:H2'	1:A:360:A:C8	2.56	0.40
1:A:1033:G:H3'	1:A:1034:G:H5'	2.02	0.40
1:A:1407:5MC:H2'	1:A:1408:A:H8	1.86	0.40
5:E:103:GLY:O	5:E:107:ARG:HB3	2.21	0.40
9:I:116:LYS:HB3	9:I:121:ARG:O	2.20	0.40
1:A:624:C:H2'	1:A:625:G:C8	2.54	0.40
1:A:1163:C:H2'	1:A:1164:G:C8	2.56	0.40
1:A:1201:A:H4'	1:A:1202:G:O5'	2.21	0.40
4:D:97:LEU:HD23	4:D:97:LEU:HA	1.91	0.40
17:R:32:ARG:HA	17:R:69:THR:HG21	2.03	0.40
1:A:1073:U:H3	1:A:1102:A:H61	1.70	0.40
1:A:1269:A:H5'	20:U:19:GLY:HA2	2.03	0.40
1:A:1347:G:H1'	1:A:1348:U:H5	1.87	0.40
1:A:1476:G:H2'	1:A:1477:C:C6	2.57	0.40
19:T:13:LEU:O	19:T:17:ARG:HG3	2.21	0.40
19:T:67:ALA:HB2	19:T:77:ALA:HB2	2.04	0.40
1:A:866:C:C4	1:A:867:G:H1'	2.56	0.40
1:A:1129:C:H4'	1:A:1130:A:H5'	2.04	0.40
1:A:1189:C:OP1	10:J:51:ARG:NH2	2.52	0.40
1:A:1473:A:H2'	1:A:1474:G:C8	2.57	0.40
2:B:71:VAL:HG22	2:B:93:VAL:HB	2.04	0.40
7:G:45:ASP:O	7:G:48:LYS:HG2	2.21	0.40
10:J:38:ILE:N	10:J:71:LEU:O	2.45	0.40
18:S:18:LYS:O	18:S:22:LEU:HG	2.22	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:87:THR:OG1	10:J:87:THR:OG1[8_554]	2.01	0.19

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	233/256 (91%)	204 (88%)	27 (12%)	2 (1%)	14	49
3	C	204/239 (85%)	176 (86%)	28 (14%)	0	100	100
4	D	206/209 (99%)	190 (92%)	16 (8%)	0	100	100
5	E	148/162 (91%)	142 (96%)	6 (4%)	0	100	100
6	F	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
7	G	153/156 (98%)	138 (90%)	15 (10%)	0	100	100
8	H	136/138 (99%)	129 (95%)	7 (5%)	0	100	100
9	I	125/128 (98%)	112 (90%)	13 (10%)	0	100	100
10	J	96/105 (91%)	82 (85%)	13 (14%)	1 (1%)	12	47
11	K	117/129 (91%)	103 (88%)	14 (12%)	0	100	100
12	L	121/134 (90%)	112 (93%)	8 (7%)	1 (1%)	16	52
13	M	123/126 (98%)	112 (91%)	11 (9%)	0	100	100
14	N	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
15	O	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
16	P	81/88 (92%)	78 (96%)	3 (4%)	0	100	100
17	R	71/88 (81%)	66 (93%)	5 (7%)	0	100	100
18	S	78/93 (84%)	71 (91%)	6 (8%)	1 (1%)	9	41
19	T	97/106 (92%)	84 (87%)	13 (13%)	0	100	100
20	U	22/27 (82%)	19 (86%)	3 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2254/2435 (93%)	2045 (91%)	204 (9%)	5 (0%)	43 77

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	229	VAL
10	J	34	VAL
12	L	28	LYS
18	S	31	ILE
2	B	230	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%)	194 (96%)	8 (4%)	28 49
3	C	160/188 (85%)	154 (96%)	6 (4%)	29 51
4	D	180/181 (99%)	171 (95%)	9 (5%)	22 44
5	E	115/123 (94%)	109 (95%)	6 (5%)	21 44
6	F	90/90 (100%)	86 (96%)	4 (4%)	25 48
7	G	126/127 (99%)	122 (97%)	4 (3%)	34 56
8	H	119/119 (100%)	114 (96%)	5 (4%)	26 49
9	I	98/99 (99%)	92 (94%)	6 (6%)	17 40
10	J	88/92 (96%)	78 (89%)	10 (11%)	5 21
11	K	90/99 (91%)	86 (96%)	4 (4%)	25 48
12	L	103/109 (94%)	98 (95%)	5 (5%)	22 45
13	M	100/101 (99%)	98 (98%)	2 (2%)	48 65
14	N	49/50 (98%)	45 (92%)	4 (8%)	10 32
15	O	79/80 (99%)	76 (96%)	3 (4%)	29 51
16	P	72/74 (97%)	71 (99%)	1 (1%)	59 70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	R	64/77 (83%)	62 (97%)	2 (3%)	35	56
18	S	71/80 (89%)	67 (94%)	4 (6%)	19	42
19	T	76/82 (93%)	72 (95%)	4 (5%)	20	43
20	U	19/22 (86%)	18 (95%)	1 (5%)	20	43
All	All	1901/2013 (94%)	1813 (95%)	88 (5%)	24	46

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	44	LEU
2	B	82	ARG
2	B	87	ARG
2	B	162	ILE
2	B	221	LEU
2	B	231	GLU
2	B	236	TYR
2	B	238	LEU
3	C	43	LEU
3	C	57	ILE
3	C	76	VAL
3	C	95	THR
3	C	112	SER
3	C	167	TRP
4	D	17	VAL
4	D	19	LEU
4	D	20	TYR
4	D	26	CYS
4	D	35	ARG
4	D	64	LEU
4	D	70	ILE
4	D	122	ARG
4	D	126	ILE
5	E	12	LEU
5	E	41	VAL
5	E	76	ILE
5	E	89	ILE
5	E	105	VAL
5	E	133	TYR
6	F	45	LEU
6	F	47	ARG
6	F	75	LEU

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Mol	Chain	Res	Type
6	F	100	ASN
7	G	11	GLN
7	G	113	GLU
7	G	129	GLU
7	G	156	TRP
8	H	29	SER
8	H	39	LEU
8	H	83	ILE
8	H	97	VAL
8	H	109	ILE
9	I	14	VAL
9	I	56	LEU
9	I	59	PHE
9	I	85	LEU
9	I	112	LYS
9	I	113	LYS
10	J	34	VAL
10	J	49	VAL
10	J	59	SER
10	J	62	HIS
10	J	72	VAL
10	J	82	ILE
10	J	85	LEU
10	J	87	THR
10	J	90	LEU
10	J	92	THR
11	K	14	VAL
11	K	29	ILE
11	K	117	ASN
11	K	126	ARG
12	L	27	LEU
12	L	28	LYS
12	L	39	VAL
12	L	55	VAL
12	L	110	VAL
13	M	12	ASN
13	M	98	VAL
14	N	22	THR
14	N	25	VAL
14	N	27	CYS
14	N	33	VAL
15	O	6	GLU

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Mol	Chain	Res	Type
15	O	45	VAL
15	O	81	LEU
16	P	2	VAL
17	R	47	THR
17	R	86	VAL
18	S	13	ASP
18	S	25	LYS
18	S	31	ILE
18	S	65	ASN
19	T	55	ILE
19	T	62	LEU
19	T	73	HIS
19	T	74	LYS
20	U	9	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	104	ASN
3	C	69	HIS
3	C	108	ASN
3	C	123	GLN
4	D	42	GLN
4	D	103	ASN
4	D	201	GLN
6	F	100	ASN
7	G	11	GLN
7	G	109	ASN
7	G	148	ASN
9	I	38	GLN
12	L	8	ASN
15	O	51	HIS
16	P	65	GLN
19	T	42	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1512/1522 (99%)	216 (14%)	40 (2%)

All (216) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	8	A
1	A	9	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	51	A
1	A	61	G
1	A	116	A
1	A	120	A
1	A	121	C
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	144	G
1	A	163	C
1	A	182	U
1	A	183	G
1	A	195	A
1	A	204	U
1	A	216	G
1	A	244	U
1	A	245	C
1	A	247	G
1	A	251	G
1	A	267	C
1	A	289	G
1	A	321	A
1	A	328	C
1	A	329	A
1	A	330	C
1	A	332	G
1	A	344	A
1	A	347	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	367	U
1	A	373	A
1	A	384	G
1	A	390	C
1	A	397	A

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Mol	Chain	Res	Type
1	A	398	C
1	A	406	G
1	A	411	A
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	430	A
1	A	432	A
1	A	433	C
1	A	439	A
1	A	452	A
1	A	485	G
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	518	C
1	A	527	7MG
1	A	532	A
1	A	533	A
1	A	547	A
1	A	559	A
1	A	560	U
1	A	562	C
1	A	564	C
1	A	572	A
1	A	573	A
1	A	576	G
1	A	577	G
1	A	616	G
1	A	630	G
1	A	632	A
1	A	653	A
1	A	665	A
1	A	687	A
1	A	688	G
1	A	702	A

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Mol	Chain	Res	Type
1	A	723	U
1	A	731	G
1	A	749	C
1	A	755	G
1	A	777	A
1	A	781	A
1	A	782	A
1	A	793	U
1	A	794	A
1	A	813	U
1	A	816	A
1	A	817	C
1	A	819	A
1	A	821	G
1	A	828	A
1	A	839	U
1	A	840	C
1	A	841	U
1	A	848	C
1	A	859	A
1	A	902	G
1	A	914	A
1	A	926	G
1	A	927	G
1	A	934	C
1	A	960	U
1	A	961	U
1	A	966	M2G
1	A	969	A
1	A	971	G
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	978	A
1	A	991	U
1	A	992	U
1	A	993	G
1	A	994	A
1	A	1000	U
1	A	1003	G
1	A	1003(A)	G

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Mol	Chain	Res	Type
1	A	1004	A
1	A	1005	A
1	A	1009	G
1	A	1021	G
1	A	1022	G
1	A	1024	G
1	A	1025	U
1	A	1026	G
1	A	1027	C
1	A	1028	C
1	A	1029	C
1	A	1030	C
1	A	1030(A)	G
1	A	1030(C)	G
1	A	1030(D)	A
1	A	1033	G
1	A	1034	G
1	A	1050	G
1	A	1053	G
1	A	1054	C
1	A	1065	U
1	A	1066	C
1	A	1068	G
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1117	G
1	A	1125	U
1	A	1126	U
1	A	1127	G
1	A	1129	C
1	A	1130	A
1	A	1131	G
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1152	A
1	A	1159	U
1	A	1171	G
1	A	1181	G
1	A	1183	A
1	A	1196	U

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Mol	Chain	Res	Type
1	A	1197	G
1	A	1201	A
1	A	1202	G
1	A	1212	U
1	A	1213	A
1	A	1226	C
1	A	1227	A
1	A	1238	A
1	A	1241	G
1	A	1256	A
1	A	1257	U
1	A	1258	G
1	A	1270	C
1	A	1280	A
1	A	1281	U
1	A	1282	C
1	A	1286	A
1	A	1287	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1312	G
1	A	1317	C
1	A	1320	C
1	A	1323	G
1	A	1331	G
1	A	1348	U
1	A	1359	C
1	A	1362	C
1	A	1364	U
1	A	1394	A
1	A	1398	A
1	A	1400	5MC
1	A	1401	G
1	A	1402	4OC
1	A	1442	G
1	A	1446	A
1	A	1493	A
1	A	1497	G
1	A	1499	A
1	A	1502	A
1	A	1504	G

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Mol	Chain	Res	Type
1	A	1505	G
1	A	1506	U
1	A	1517	G
1	A	1520	G
1	A	1529	G
1	A	1530	G

All (40) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	60	A
1	A	115	G
1	A	129(A)	G
1	A	181	G
1	A	203	U
1	A	243	A
1	A	250	A
1	A	266	G
1	A	328	C
1	A	372	C
1	A	410	G
1	A	412	A
1	A	428	G
1	A	429	U
1	A	484	G
1	A	509	A
1	A	559	A
1	A	575	G
1	A	687	A
1	A	701	C
1	A	748	C
1	A	812	C
1	A	913	A
1	A	960	U
1	A	965	A
1	A	992	U
1	A	993	G
1	A	1065	U
1	A	1067	A
1	A	1129	C
1	A	1182	G
1	A	1201	A

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Mol	Chain	Res	Type
1	A	1281	U
1	A	1285	A
1	A	1300	G
1	A	1301	U
1	A	1347	G
1	A	1443	G
1	A	1505	G
1	A	1528	U

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

15 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	5MC	A	1404	1	19,22,23	1.11	2 (10%)	26,32,35	0.99	1 (3%)
1	M2G	A	966	1	24,27,28	1.35	4 (16%)	33,40,43	0.89	1 (3%)
1	UR3	A	1498	1	19,22,23	0.71	1 (5%)	26,32,35	0.81	1 (3%)
12	0TD	L	92	12	8,9,10	1.63	1 (12%)	6,11,13	1.64	2 (33%)
1	5MC	A	1407	1	19,22,23	1.08	2 (10%)	26,32,35	0.96	1 (3%)
1	2MG	A	1207	1	23,26,27	1.43	6 (26%)	33,38,41	1.18	5 (15%)
1	PSU	A	516	1,21	18,21,22	1.13	1 (5%)	21,30,33	1.89	4 (19%)
1	PSU	A	1541	1	18,21,22	1.14	1 (5%)	21,30,33	1.92	5 (23%)
1	7MG	A	527	1	23,26,27	3.80	4 (17%)	27,39,42	2.29	9 (33%)
1	5MC	A	1400	1	19,22,23	1.13	3 (15%)	26,32,35	0.97	2 (7%)
1	PSU	A	1540	1	18,21,22	1.14	1 (5%)	21,30,33	1.91	5 (23%)
1	4OC	A	1402	1	20,23,24	1.09	2 (10%)	25,32,35	0.77	0
1	MA6	A	1519	1	23,26,27	1.30	3 (13%)	33,38,41	0.88	0
1	5MC	A	967	1	19,22,23	1.11	3 (15%)	26,32,35	0.95	1 (3%)
1	MA6	A	1518	1	23,26,27	1.27	3 (13%)	33,38,41	0.85	1 (3%)

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	5MC	A	1404	1	-	1/7/25/26	0/2/2/2
1	M2G	A	966	1	-	1/11/29/30	0/3/3/3
1	UR3	A	1498	1	-	0/7/25/26	0/2/2/2
12	0TD	L	92	12	-	5/7/12/14	-
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
1	2MG	A	1207	1	-	0/9/27/28	0/3/3/3
1	PSU	A	516	1,21	-	0/7/25/26	0/2/2/2
1	PSU	A	1541	1	-	0/7/25/26	0/2/2/2
1	7MG	A	527	1	-	0/7/37/38	0/3/3/3
1	5MC	A	1400	1	-	2/7/25/26	0/2/2/2
1	PSU	A	1540	1	-	1/7/25/26	0/2/2/2
1	4OC	A	1402	1	-	2/9/29/30	0/2/2/2
1	MA6	A	1519	1	-	3/11/29/30	0/3/3/3
1	5MC	A	967	1	-	0/7/25/26	0/2/2/2
1	MA6	A	1518	1	-	1/11/29/30	0/3/3/3

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	7MG	C8-N9	-16.77	1.35	1.45
1	A	527	7MG	C2-N2	4.11	1.43	1.34
1	A	527	7MG	C5-N7	4.03	1.40	1.35
1	A	1540	PSU	C6-C5	3.88	1.39	1.35
1	A	1541	PSU	C6-C5	3.80	1.39	1.35
1	A	516	PSU	C6-C5	3.75	1.39	1.35
12	L	92	0TD	CB-CA	-3.60	1.53	1.54
1	A	966	M2G	C2-N2	3.59	1.41	1.35
1	A	1207	2MG	C2-N2	3.38	1.40	1.33
1	A	527	7MG	C4-N3	3.33	1.41	1.34
1	A	1519	MA6	C5-C4	3.10	1.44	1.39
1	A	966	M2G	C4-N3	3.03	1.41	1.34
1	A	1207	2MG	C2-N1	2.92	1.41	1.36
1	A	1518	MA6	C5-C4	2.91	1.44	1.39
1	A	1404	5MC	C2-N1	2.88	1.46	1.40
1	A	1402	4OC	C2-N3	2.78	1.41	1.36
1	A	1400	5MC	C2-N1	2.77	1.45	1.40
1	A	1402	4OC	C2-N1	2.74	1.45	1.40
1	A	967	5MC	C2-N1	2.70	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1407	5MC	C2-N1	2.66	1.45	1.40
1	A	1207	2MG	C4-N3	2.54	1.40	1.34
1	A	1518	MA6	C8-N9	2.46	1.41	1.37
1	A	1519	MA6	C8-N9	2.43	1.41	1.37
1	A	1404	5MC	C2-N3	2.41	1.41	1.36
1	A	967	5MC	C2-N3	2.37	1.41	1.36
1	A	1400	5MC	C2-N3	2.36	1.41	1.36
1	A	1407	5MC	C2-N3	2.36	1.41	1.36
1	A	1519	MA6	C2-N1	2.35	1.38	1.33
1	A	966	M2G	C8-N9	2.31	1.42	1.37
1	A	1207	2MG	C8-N9	2.27	1.42	1.37
1	A	966	M2G	C6-N1	2.26	1.43	1.38
1	A	1207	2MG	C6-N1	2.23	1.43	1.38
1	A	1498	UR3	C2-N1	2.23	1.41	1.38
1	A	1207	2MG	C2-N3	2.22	1.36	1.32
1	A	1518	MA6	C2-N1	2.19	1.37	1.33
1	A	967	5MC	C6-C5	2.03	1.37	1.34
1	A	1400	5MC	C6-C5	2.01	1.37	1.34

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	527	7MG	C5-C6-N1	5.07	119.87	110.94
1	A	527	7MG	N9-C4-N3	5.01	132.79	125.46
1	A	1541	PSU	C4-N3-C2	-4.87	119.66	126.37
1	A	1540	PSU	C4-N3-C2	-4.83	119.72	126.37
1	A	527	7MG	C2-N3-C4	4.76	120.50	112.30
1	A	1541	PSU	N1-C2-N3	4.73	120.16	115.17
1	A	516	PSU	C4-N3-C2	-4.72	119.87	126.37
1	A	1540	PSU	N1-C2-N3	4.72	120.15	115.17
1	A	516	PSU	N1-C2-N3	4.69	120.11	115.17
1	A	527	7MG	C5-C4-N3	-4.38	119.91	128.13
1	A	527	7MG	N9-C8-N7	3.89	108.88	103.37
1	A	527	7MG	O6-C6-C5	-2.90	120.50	127.62
1	A	1207	2MG	C5-C4-N3	-2.89	123.78	128.39
1	A	527	7MG	C2-N1-C6	-2.82	120.00	125.11
1	A	1541	PSU	O2-C2-N1	-2.75	119.95	122.79
1	A	516	PSU	O2-C2-N1	-2.72	119.99	122.79
1	A	1207	2MG	N9-C4-N3	2.72	131.38	125.95
1	A	1540	PSU	O2-C2-N1	-2.68	120.02	122.79
1	A	527	7MG	C6-C5-C4	-2.65	117.73	122.40
12	L	92	0TD	OD1-CG-CB	-2.53	117.15	122.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1407	5MC	N4-C4-N3	-2.44	114.09	118.51
1	A	1400	5MC	N4-C4-N3	-2.43	114.10	118.51
1	A	516	PSU	C6-N1-C2	-2.40	120.46	122.69
1	A	967	5MC	N4-C4-N3	-2.38	114.20	118.51
1	A	1207	2MG	O6-C6-N1	-2.31	115.76	120.11
1	A	1404	5MC	N4-C4-N3	-2.30	114.35	118.51
1	A	966	M2G	C5-C4-N3	-2.24	124.83	128.39
1	A	527	7MG	C6-C5-N7	2.21	135.35	131.93
1	A	1207	2MG	C6-C5-N7	-2.20	126.29	130.29
12	L	92	0TD	O-C-CA	-2.19	119.13	124.77
1	A	1541	PSU	C6-N1-C2	-2.19	120.66	122.69
1	A	1540	PSU	C6-N1-C2	-2.19	120.66	122.69
1	A	1207	2MG	C2-N1-C6	-2.17	121.92	124.55
1	A	1540	PSU	C6-C5-C4	2.12	119.60	118.17
1	A	1541	PSU	C6-C5-C4	2.12	119.60	118.17
1	A	1518	MA6	C2-N1-C6	2.09	116.93	111.83
1	A	1498	UR3	C3U-N3-C4	2.08	120.75	117.87
1	A	1400	5MC	C5-C4-N3	2.04	123.84	121.75

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	966	M2G	C4'-C5'-O5'-P
1	A	1400	5MC	O4'-C4'-C5'-O5'
1	A	1402	4OC	O4'-C4'-C5'-O5'
1	A	1519	MA6	C5-C6-N6-C9
12	L	92	0TD	SB-CB-CG-OD1
1	A	1402	4OC	C3'-C4'-C5'-O5'
1	A	1519	MA6	N1-C6-N6-C9
1	A	1400	5MC	C3'-C4'-C5'-O5'
1	A	1518	MA6	C5-C6-N6-C9
1	A	1519	MA6	C5-C6-N6-C10
12	L	92	0TD	CA-CB-CG-OD1
12	L	92	0TD	CG-CB-SB-CSB
1	A	1540	PSU	O4'-C4'-C5'-O5'
12	L	92	0TD	SB-CB-CG-OD2
12	L	92	0TD	CA-CB-CG-OD2
1	A	1404	5MC	C2'-C1'-N1-C2

There are no ring outliers.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1404	5MC	2	0
12	L	92	0TD	2	0
1	A	1407	5MC	1	0
1	A	1541	PSU	1	0
1	A	1402	4OC	1	0
1	A	1519	MA6	2	0
1	A	1518	MA6	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 195 ligands modelled in this entry, 195 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1500/1522 (98%)	-0.12	2 (0%) 92 87	155, 192, 264, 505	0
2	B	235/256 (91%)	0.40	10 (4%) 40 34	134, 193, 274, 327	0
3	C	206/239 (86%)	0.20	8 (3%) 43 36	134, 182, 248, 311	0
4	D	208/209 (99%)	0.36	17 (8%) 17 21	114, 181, 253, 369	0
5	E	150/162 (92%)	0.25	6 (4%) 42 35	118, 175, 226, 277	0
6	F	101/101 (100%)	0.21	4 (3%) 42 35	143, 207, 273, 471	0
7	G	155/156 (99%)	0.35	8 (5%) 33 30	153, 204, 257, 309	0
8	H	138/138 (100%)	0.17	4 (2%) 53 41	123, 172, 226, 242	0
9	I	127/128 (99%)	1.10	24 (18%) 3 7	179, 238, 348, 501	0
10	J	98/105 (93%)	0.94	21 (21%) 2 5	174, 222, 313, 438	0
11	K	119/129 (92%)	0.23	4 (3%) 48 38	117, 184, 254, 371	0
12	L	123/134 (91%)	0.39	5 (4%) 41 35	139, 181, 231, 259	0
13	M	125/126 (99%)	0.52	10 (8%) 18 21	176, 215, 311, 427	0
14	N	60/61 (98%)	0.34	2 (3%) 49 38	140, 200, 285, 315	0
15	O	88/89 (98%)	0.35	4 (4%) 38 33	155, 197, 253, 326	0
16	P	83/88 (94%)	0.38	6 (7%) 21 23	148, 183, 219, 272	0
17	R	73/88 (82%)	0.61	3 (4%) 41 35	122, 209, 331, 418	0
18	S	80/93 (86%)	0.40	6 (7%) 20 22	189, 220, 289, 312	0
19	T	99/106 (93%)	0.19	2 (2%) 65 50	131, 185, 242, 335	0
20	U	24/27 (88%)	1.14	4 (16%) 4 8	193, 228, 255, 277	0
All	All	3792/3957 (95%)	0.20	150 (3%) 42 35	114, 193, 274, 505	0

All (150) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	U	25	LYS	6.6
9	I	115	GLY	6.0
1	A	1030(D)	A	6.0
13	M	124	PRO	6.0
7	G	8	GLU	5.6
20	U	9	ARG	5.2
2	B	28	PHE	5.0
9	I	30	GLY	5.0
15	O	69	TYR	4.5
14	N	37	PHE	4.4
11	K	100	ALA	4.1
2	B	13	ALA	4.0
13	M	9	ILE	3.9
17	R	17	SER	3.9
13	M	8	GLU	3.9
10	J	54	PHE	3.9
4	D	31	CYS	3.8
17	R	46	GLU	3.8
9	I	106	ALA	3.6
3	C	154	SER	3.5
9	I	37	PHE	3.5
9	I	69	GLY	3.5
10	J	5	ARG	3.5
20	U	6	ARG	3.5
9	I	117	HIS	3.4
9	I	12	GLU	3.4
10	J	47	PHE	3.4
9	I	42	ARG	3.4
13	M	126	LYS	3.3
4	D	2	GLY	3.3
9	I	21	PRO	3.3
2	B	55	PHE	3.2
4	D	26	CYS	3.2
13	M	2	ALA	3.2
3	C	168	ALA	3.2
7	G	5	ARG	3.1
12	L	5	PRO	3.1
13	M	31	LYS	3.1
2	B	154	LEU	3.0
5	E	87	SER	3.0
10	J	71	LEU	3.0
14	N	36	PHE	3.0
11	K	111	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
10	J	6	ILE	2.9
18	S	5	LEU	2.9
19	T	106	ALA	2.9
9	I	2	GLU	2.9
7	G	34	GLY	2.8
4	D	22	LYS	2.8
5	E	123	LEU	2.8
18	S	3	ARG	2.7
16	P	12	LYS	2.7
15	O	67	LEU	2.7
10	J	45	ARG	2.7
10	J	58	ASP	2.7
3	C	105	GLU	2.7
18	S	13	ASP	2.7
2	B	11	LEU	2.7
8	H	1	MET	2.7
12	L	15	ARG	2.7
2	B	102	LEU	2.7
15	O	3	ILE	2.7
9	I	8	GLY	2.6
10	J	90	LEU	2.6
4	D	134	ASP	2.6
3	C	2	GLY	2.6
4	D	4	TYR	2.6
4	D	6	GLY	2.6
15	O	30	ALA	2.6
13	M	109	THR	2.6
7	G	55	GLY	2.5
10	J	88	LEU	2.5
5	E	79	GLU	2.5
7	G	30	ILE	2.5
4	D	42	GLN	2.5
12	L	44	THR	2.5
6	F	89	MET	2.5
4	D	34	GLU	2.5
5	E	88	LYS	2.5
18	S	2	PRO	2.5
7	G	70	LYS	2.5
8	H	116	LYS	2.5
9	I	119	ALA	2.5
9	I	113	LYS	2.5
9	I	114	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
4	D	3	ARG	2.4
10	J	3	LYS	2.4
9	I	31	GLN	2.4
9	I	71	SER	2.4
4	D	120	LEU	2.4
4	D	9	CYS	2.4
4	D	84	LYS	2.4
20	U	18	TYR	2.4
3	C	161	GLU	2.4
9	I	38	GLN	2.4
9	I	11	LYS	2.4
12	L	28	LYS	2.4
9	I	68	GLY	2.4
16	P	11	SER	2.4
2	B	105	PHE	2.4
10	J	100	THR	2.4
2	B	29	ALA	2.3
7	G	26	PHE	2.3
9	I	26	VAL	2.3
3	C	26	LYS	2.3
18	S	81	ARG	2.3
16	P	39	TYR	2.3
16	P	83	GLU	2.3
4	D	44	GLY	2.3
19	T	81	LYS	2.3
9	I	75	ASP	2.3
9	I	45	ALA	2.3
7	G	9	VAL	2.3
13	M	96	LEU	2.3
8	H	31	PHE	2.3
5	E	103	GLY	2.3
9	I	82	ALA	2.2
18	S	8	GLY	2.2
11	K	128	ALA	2.2
6	F	60	PHE	2.2
6	F	58	GLY	2.2
2	B	152	PHE	2.2
10	J	80	LYS	2.2
13	M	125	ARG	2.2
16	P	73	LEU	2.2
12	L	29	GLY	2.1
3	C	3	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
16	P	46	PRO	2.1
10	J	98	ILE	2.1
10	J	79	ARG	2.1
4	D	131	ARG	2.1
3	C	192	THR	2.1
10	J	75	ILE	2.1
5	E	105	VAL	2.1
6	F	9	VAL	2.1
10	J	73	ASP	2.1
10	J	36	GLY	2.1
10	J	38	ILE	2.1
17	R	45	SER	2.1
1	A	221	C	2.1
8	H	133	LEU	2.1
4	D	115	ARG	2.0
9	I	116	LYS	2.0
10	J	7	LYS	2.0
2	B	32	ILE	2.0
10	J	99	LYS	2.0
11	K	25	TYR	2.0
4	D	8	VAL	2.0
10	J	37	PRO	2.0
13	M	99	ARG	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	PSU	A	516	20/21	0.88	0.09	175,181,212,258	0
1	M2G	A	966	25/26	0.91	0.10	158,179,213,255	0
1	2MG	A	1207	24/25	0.93	0.10	182,186,190,197	0
1	MA6	A	1518	24/25	0.93	0.09	185,186,226,235	0
1	PSU	A	1540	20/21	0.93	0.24	194,249,259,261	0
1	5MC	A	967	21/22	0.94	0.12	158,162,188,203	0
1	5MC	A	1400	21/22	0.94	0.10	175,178,193,234	0
1	MA6	A	1519	24/25	0.95	0.10	180,183,202,229	0
1	7MG	A	527	24/25	0.95	0.09	161,162,170,198	0
1	PSU	A	1541	20/21	0.95	0.16	177,179,242,254	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	5MC	A	1404	21/22	0.96	0.14	178,180,182,204	0
1	UR3	A	1498	21/22	0.96	0.14	178,181,221,230	0
12	0TD	L	92	10/11	0.97	0.19	167,204,309,368	0
1	4OC	A	1402	22/23	0.98	0.11	175,177,227,231	0
1	5MC	A	1407	21/22	0.99	0.06	189,192,212,231	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
21	MG	A	1674	1/1	0.01	1.14	192,192,192,192	0
21	MG	A	1647	1/1	0.02	0.59	199,199,199,199	0
21	MG	A	1706	1/1	0.11	0.83	137,137,137,137	0
21	MG	A	1621	1/1	0.25	0.40	134,134,134,134	0
21	MG	A	1606	1/1	0.31	0.30	247,247,247,247	0
21	MG	A	1681	1/1	0.38	0.36	165,165,165,165	0
21	MG	B	301	1/1	0.42	0.41	143,143,143,143	0
21	MG	A	1602	1/1	0.44	0.26	149,149,149,149	0
21	MG	A	1742	1/1	0.45	0.51	143,143,143,143	0
21	MG	A	1691	1/1	0.45	1.05	111,111,111,111	0
22	K	A	1771	1/1	0.47	0.45	197,197,197,197	0
21	MG	A	1687	1/1	0.49	0.84	143,143,143,143	0
21	MG	A	1702	1/1	0.49	0.70	197,197,197,197	0
21	MG	A	1719	1/1	0.49	0.47	196,196,196,196	0
21	MG	A	1615	1/1	0.51	0.47	138,138,138,138	0
21	MG	A	1607	1/1	0.51	1.47	122,122,122,122	0
21	MG	A	1740	1/1	0.51	0.59	114,114,114,114	0
21	MG	A	1627	1/1	0.52	0.87	177,177,177,177	0
21	MG	A	1697	1/1	0.53	0.23	165,165,165,165	0
21	MG	A	1630	1/1	0.54	0.62	90,90,90,90	0
21	MG	A	1653	1/1	0.55	1.01	111,111,111,111	0
21	MG	A	1616	1/1	0.55	1.38	158,158,158,158	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
21	MG	A	1694	1/1	0.56	0.33	133,133,133,133	0
21	MG	A	1628	1/1	0.58	0.27	159,159,159,159	0
21	MG	A	1632	1/1	0.59	0.88	103,103,103,103	0
21	MG	A	1638	1/1	0.61	0.41	116,116,116,116	0
21	MG	A	1667	1/1	0.62	1.46	236,236,236,236	0
22	K	A	1786	1/1	0.62	0.63	215,215,215,215	0
21	MG	A	1624	1/1	0.63	0.79	174,174,174,174	0
21	MG	A	1741	1/1	0.63	0.53	193,193,193,193	0
21	MG	E	201	1/1	0.64	0.92	151,151,151,151	0
21	MG	A	1619	1/1	0.64	0.53	126,126,126,126	0
21	MG	A	1672	1/1	0.64	0.55	171,171,171,171	0
21	MG	A	1633	1/1	0.65	0.34	59,59,59,59	0
21	MG	A	1650	1/1	0.65	1.52	127,127,127,127	0
21	MG	A	1639	1/1	0.67	0.25	157,157,157,157	0
21	MG	A	1652	1/1	0.68	0.52	172,172,172,172	0
21	MG	A	1787	1/1	0.68	0.28	92,92,92,92	0
21	MG	A	1625	1/1	0.69	2.33	140,140,140,140	0
21	MG	A	1648	1/1	0.69	0.41	112,112,112,112	0
21	MG	A	1608	1/1	0.69	1.19	117,117,117,117	0
22	K	A	1776	1/1	0.70	0.30	198,198,198,198	0
21	MG	A	1716	1/1	0.70	0.19	179,179,179,179	0
21	MG	A	1623	1/1	0.71	0.89	154,154,154,154	0
22	K	A	1775	1/1	0.71	0.21	273,273,273,273	0
21	MG	A	1663	1/1	0.72	0.29	147,147,147,147	0
21	MG	A	1626	1/1	0.72	1.22	130,130,130,130	0
21	MG	A	1714	1/1	0.72	0.31	136,136,136,136	0
21	MG	A	1637	1/1	0.73	0.38	68,68,68,68	0
22	K	A	1753	1/1	0.73	0.27	176,176,176,176	0
21	MG	A	1682	1/1	0.74	0.11	128,128,128,128	0
22	K	A	1755	1/1	0.74	0.26	187,187,187,187	0
21	MG	A	1684	1/1	0.74	0.93	150,150,150,150	0
21	MG	A	1744	1/1	0.75	0.69	143,143,143,143	0
22	K	A	1758	1/1	0.75	0.45	199,199,199,199	0
21	MG	A	1732	1/1	0.76	0.26	163,163,163,163	0
21	MG	A	1613	1/1	0.76	0.24	161,161,161,161	0
21	MG	A	1703	1/1	0.76	0.40	115,115,115,115	0
21	MG	A	1668	1/1	0.77	0.18	159,159,159,159	0
21	MG	A	1642	1/1	0.77	0.30	105,105,105,105	0
21	MG	A	1603	1/1	0.78	0.37	98,98,98,98	0
21	MG	A	1712	1/1	0.78	0.44	85,85,85,85	0
21	MG	A	1664	1/1	0.78	0.77	166,166,166,166	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
21	MG	A	1629	1/1	0.78	0.41	171,171,171,171	0
21	MG	A	1708	1/1	0.78	0.83	146,146,146,146	0
21	MG	A	1695	1/1	0.79	0.27	71,71,71,71	0
21	MG	A	1749	1/1	0.79	0.97	130,130,130,130	0
21	MG	A	1675	1/1	0.79	0.26	94,94,94,94	0
21	MG	A	1665	1/1	0.80	0.90	205,205,205,205	0
21	MG	A	1725	1/1	0.81	0.84	208,208,208,208	0
21	MG	A	1612	1/1	0.82	0.23	163,163,163,163	0
22	K	A	1765	1/1	0.82	0.38	168,168,168,168	0
21	MG	A	1736	1/1	0.82	0.16	164,164,164,164	0
21	MG	A	1641	1/1	0.82	0.19	74,74,74,74	0
21	MG	A	1692	1/1	0.82	0.68	101,101,101,101	0
22	K	A	1757	1/1	0.82	0.94	204,204,204,204	0
21	MG	A	1669	1/1	0.83	0.29	85,85,85,85	0
21	MG	A	1693	1/1	0.83	0.34	104,104,104,104	0
21	MG	A	1689	1/1	0.83	0.29	182,182,182,182	0
21	MG	A	1654	1/1	0.83	0.29	114,114,114,114	0
21	MG	A	1727	1/1	0.84	0.40	177,177,177,177	0
22	K	A	1770	1/1	0.84	0.09	202,202,202,202	0
21	MG	A	1658	1/1	0.84	0.24	111,111,111,111	0
22	K	A	1773	1/1	0.84	0.20	116,116,116,116	0
21	MG	A	1696	1/1	0.84	0.78	156,156,156,156	0
21	MG	A	1635	1/1	0.84	0.17	61,61,61,61	0
21	MG	A	1680	1/1	0.84	0.22	88,88,88,88	0
21	MG	A	1700	1/1	0.85	0.79	102,102,102,102	0
22	K	A	1762	1/1	0.85	0.23	181,181,181,181	0
21	MG	A	1655	1/1	0.85	0.18	65,65,65,65	0
22	K	A	1766	1/1	0.85	0.22	168,168,168,168	0
22	K	A	1782	1/1	0.85	0.24	162,162,162,162	0
22	K	A	1785	1/1	0.85	0.27	158,158,158,158	0
21	MG	A	1678	1/1	0.85	0.36	88,88,88,88	0
22	K	A	1752	1/1	0.86	0.29	176,176,176,176	0
21	MG	A	1609	1/1	0.86	0.23	51,51,51,51	0
22	K	A	1784	1/1	0.86	0.25	141,141,141,141	0
21	MG	A	1688	1/1	0.86	0.69	181,181,181,181	0
21	MG	A	1645	1/1	0.86	0.31	55,55,55,55	0
21	MG	A	1747	1/1	0.87	0.39	173,173,173,173	0
21	MG	A	1666	1/1	0.87	0.29	138,138,138,138	0
21	MG	A	1730	1/1	0.88	0.20	188,188,188,188	0
21	MG	A	1610	1/1	0.88	1.29	130,130,130,130	0
21	MG	A	1651	1/1	0.88	0.22	70,70,70,70	0
22	K	A	1768	1/1	0.88	0.28	229,229,229,229	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
21	MG	A	1661	1/1	0.88	0.24	75,75,75,75	0
21	MG	A	1698	1/1	0.88	0.48	104,104,104,104	0
21	MG	A	1617	1/1	0.88	1.43	173,173,173,173	0
22	K	A	1754	1/1	0.88	0.13	168,168,168,168	0
21	MG	A	1611	1/1	0.88	0.09	85,85,85,85	0
22	K	A	1780	1/1	0.88	0.24	149,149,149,149	0
22	K	A	1756	1/1	0.88	0.41	178,178,178,178	0
21	MG	A	1746	1/1	0.88	0.13	114,114,114,114	0
21	MG	A	1710	1/1	0.88	1.02	119,119,119,119	0
22	K	A	1759	1/1	0.88	0.24	186,186,186,186	0
21	MG	A	1721	1/1	0.89	0.35	121,121,121,121	0
21	MG	A	1673	1/1	0.89	0.18	122,122,122,122	0
21	MG	A	1715	1/1	0.89	0.57	105,105,105,105	0
21	MG	A	1686	1/1	0.89	0.63	97,97,97,97	0
22	K	A	1760	1/1	0.89	0.31	207,207,207,207	0
22	K	A	1772	1/1	0.89	0.37	178,178,178,178	0
21	MG	A	1640	1/1	0.89	0.19	90,90,90,90	0
21	MG	A	1699	1/1	0.90	0.27	122,122,122,122	0
21	MG	A	1657	1/1	0.90	0.53	75,75,75,75	0
21	MG	A	1671	1/1	0.90	0.24	48,48,48,48	0
21	MG	A	1728	1/1	0.90	0.64	151,151,151,151	0
21	MG	D	302	1/1	0.90	0.08	100,100,100,100	0
21	MG	A	1620	1/1	0.91	0.28	126,126,126,126	0
21	MG	A	1634	1/1	0.91	0.18	118,118,118,118	0
21	MG	A	1670	1/1	0.91	0.15	74,74,74,74	0
21	MG	A	1748	1/1	0.91	0.09	267,267,267,267	0
22	K	A	1778	1/1	0.91	0.57	208,208,208,208	0
21	MG	A	1659	1/1	0.92	0.20	81,81,81,81	0
21	MG	A	1743	1/1	0.92	0.22	135,135,135,135	0
21	MG	A	1735	1/1	0.92	0.52	167,167,167,167	0
21	MG	A	1745	1/1	0.92	0.96	214,214,214,214	0
21	MG	E	202	1/1	0.92	0.33	99,99,99,99	0
21	MG	M	201	1/1	0.92	0.08	186,186,186,186	0
21	MG	A	1605	1/1	0.92	0.16	92,92,92,92	0
21	MG	A	1738	1/1	0.92	0.96	116,116,116,116	0
22	K	A	1783	1/1	0.92	0.25	187,187,187,187	0
21	MG	A	1713	1/1	0.92	0.47	113,113,113,113	0
22	K	A	1769	1/1	0.92	0.10	193,193,193,193	0
21	MG	A	1646	1/1	0.92	0.18	81,81,81,81	0
21	MG	A	1631	1/1	0.93	0.55	141,141,141,141	0
21	MG	A	1683	1/1	0.93	0.12	133,133,133,133	0
21	MG	A	1622	1/1	0.93	0.32	142,142,142,142	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
21	MG	A	1720	1/1	0.93	0.13	76,76,76,76	0
21	MG	A	1709	1/1	0.94	0.12	89,89,89,89	0
21	MG	A	1705	1/1	0.94	0.39	189,189,189,189	0
21	MG	A	1679	1/1	0.94	0.27	116,116,116,116	0
22	K	A	1763	1/1	0.94	0.20	149,149,149,149	0
21	MG	A	1644	1/1	0.94	0.08	123,123,123,123	0
21	MG	A	1618	1/1	0.94	0.53	193,193,193,193	0
22	K	A	1767	1/1	0.94	0.19	149,149,149,149	0
21	MG	A	1643	1/1	0.94	0.27	170,170,170,170	0
21	MG	A	1701	1/1	0.94	0.23	68,68,68,68	0
21	MG	A	1729	1/1	0.94	0.17	68,68,68,68	0
21	MG	A	1704	1/1	0.94	0.21	112,112,112,112	0
21	MG	A	1718	1/1	0.95	0.06	86,86,86,86	0
21	MG	A	1723	1/1	0.95	0.18	102,102,102,102	0
21	MG	A	1750	1/1	0.95	0.13	134,134,134,134	0
21	MG	A	1737	1/1	0.95	0.05	132,132,132,132	0
22	K	A	1761	1/1	0.95	0.16	181,181,181,181	0
21	MG	A	1656	1/1	0.95	0.34	65,65,65,65	0
21	MG	A	1717	1/1	0.95	0.11	79,79,79,79	0
21	MG	A	1734	1/1	0.95	0.17	366,366,366,366	0
22	K	A	1774	1/1	0.95	0.29	168,168,168,168	0
22	K	A	1777	1/1	0.96	0.15	228,228,228,228	0
21	MG	A	1739	1/1	0.96	0.09	126,126,126,126	0
21	MG	A	1733	1/1	0.96	0.12	170,170,170,170	0
21	MG	A	1660	1/1	0.96	0.15	121,121,121,121	0
21	MG	A	1724	1/1	0.96	0.11	99,99,99,99	0
21	MG	A	1690	1/1	0.96	0.27	74,74,74,74	0
21	MG	A	1731	1/1	0.96	0.05	116,116,116,116	0
21	MG	A	1614	1/1	0.96	0.22	94,94,94,94	0
21	MG	A	1604	1/1	0.97	0.19	311,311,311,311	0
21	MG	A	1662	1/1	0.97	0.14	89,89,89,89	0
21	MG	U	101	1/1	0.97	0.26	523,523,523,523	0
21	MG	A	1711	1/1	0.97	0.17	177,177,177,177	0
21	MG	A	1707	1/1	0.97	0.09	73,73,73,73	0
21	MG	A	1722	1/1	0.97	0.09	55,55,55,55	0
21	MG	A	1677	1/1	0.97	0.05	120,120,120,120	0
22	K	A	1764	1/1	0.98	0.44	206,206,206,206	0
22	K	A	1779	1/1	0.98	0.14	217,217,217,217	0
21	MG	A	1685	1/1	0.98	0.07	82,82,82,82	0
22	K	A	1781	1/1	0.98	0.11	149,149,149,149	0
21	MG	A	1636	1/1	0.98	0.09	59,59,59,59	0
21	MG	A	1676	1/1	0.98	0.14	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
21	MG	A	1649	1/1	0.98	0.15	71,71,71,71	0
21	MG	A	1751	1/1	0.98	0.05	113,113,113,113	0
21	MG	A	1726	1/1	0.98	0.10	129,129,129,129	0
21	MG	A	1601	1/1	0.99	0.29	187,187,187,187	0
23	ZN	D	301	1/1	0.99	0.28	157,157,157,157	0
23	ZN	N	101	1/1	0.99	0.04	124,124,124,124	0

6.5 Other polymers [i](#)

There are no such residues in this entry.