



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 28, 2020 – 08:24 pm BST

PDB ID : 1FFK  
Title : CRYSTAL STRUCTURE OF THE LARGE RIBOSOMAL SUBUNIT FROM  
HALOARCULA MARISMORTUI AT 2.4 ANGSTROM RESOLUTION  
Authors : Ban, N.; Nissen, P.; Hansen, J.; Moore, P.B.; Steitz, T.A.  
Deposited on : 2000-07-25  
Resolution : 2.40 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

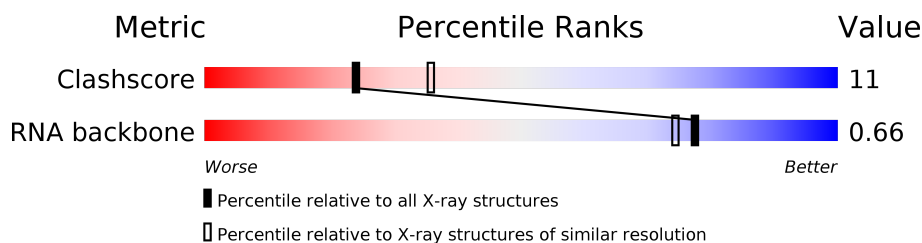
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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.







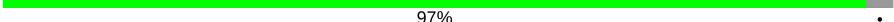

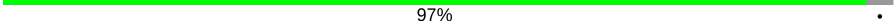

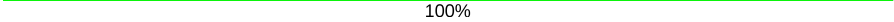


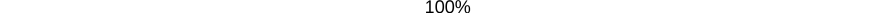

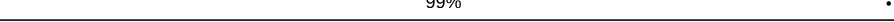
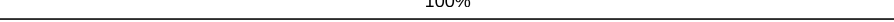
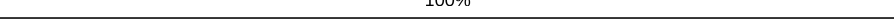

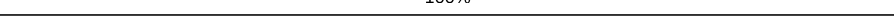
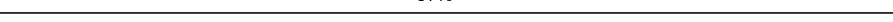
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	4398 (2.40-2.40)
RNA backbone	3102	1174 (2.80-2.00)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	0	2922	49% 34% 8% 7%
2	9	122	43% 43% 11%
3	A	239	98% ..
4	B	337	99% .
5	C	246	100%
6	D	176	80% 20%
7	E	119	97% ..
8	F	157	100%
9	G	145	98% .
10	H	132	99% .

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Mol	Chain	Length	Quality of chain
11	I	194	 100%
12	J	164	 87% 13%
13	K	186	 100%
14	L	115	 100%
15	M	148	 97% .
16	N	95	 100%
17	O	154	 97% .
18	P	84	 93% 7%
19	Q	119	 100%
20	R	66	 80% 20%
21	S	70	 93% 7%
22	T	154	 100%
23	U	91	 92% . 7%
24	V	143	 99% .
25	W	73	 100%
26	X	56	 100%
27	Y	49	 63% 37%
28	Z	92	 100%
29	1	177	 97% .

## 2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 64281 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 23S RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	2706	Total	C	N	O	P	0	0	0
			58012	25885	10685	18737	2705			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	560	C	U	CONFLICT	GB 3377779

- Molecule 2 is a RNA chain called 5S RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	9	122	Total	C	N	O	P	0	0	0
			2600	1160	472	847	121			

- Molecule 3 is a protein called RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
3	A	237	Total	C	0	0	237
			237	237			

- Molecule 4 is a protein called RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
4	B	337	Total	C	0	0	337
			337	337			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLU	DELETION	UNP P20279
B	311	PHE	-	INSERTION	UNP P20279

- Molecule 5 is a protein called RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	C	246	Total C 246 246	0	0	246

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	73	LEU	GLN	CONFLICT	UNP P12735

- Molecule 6 is a protein called RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	D	140	Total C 140 140	0	0	140

- Molecule 7 is a protein called RIBOSOMAL PROTEIN L7AE.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	E	118	Total C 118 118	0	0	118

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	108	LEU	-	INSERTION	UNP P12743
E	109	GLU	-	INSERTION	UNP P12743
E	110	GLU	-	INSERTION	UNP P12743

- Molecule 8 is a protein called RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
8	F	157	Total C 157 157	0	0	157

- Molecule 9 is a protein called RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
9	G	142	Total C 142 142	0	0	142

- Molecule 10 is a protein called RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	H	132	Total C 132 132	0	0	132

- Molecule 11 is a protein called RIBOSOMAL PROTEIN L15E.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
11	I	194	Total C 194 194	0	0	194

- Molecule 12 is a protein called RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
12	J	143	Total C 143 143	0	0	143

- Molecule 13 is a protein called RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
13	K	186	Total C 186 186	0	0	186

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	186	LEU	-	INSERTION	UNP P14123

- Molecule 14 is a protein called RIBOSOMAL PROTEIN L18E.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
14	L	115	Total C 115 115	0	0	115

- Molecule 15 is a protein called RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
15	M	143	Total C 143 143	0	0	143

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	71	LYS	TYR	CONFLICT	UNP P14119

- Molecule 16 is a protein called RIBOSOMAL PROTEIN L21E.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
16	N	95	Total C 95 95	0	0	95

- Molecule 17 is a protein called RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
17	O	150	Total C 150 150	0	0	150

- Molecule 18 is a protein called RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
18	P	78	Total C 78 78	0	0	78

- Molecule 19 is a protein called RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
19	Q	119	Total C 119 119	0	0	119

- Molecule 20 is a protein called RIBOSOMAL PROTEIN L24E.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
20	R	53	Total C 53 53	0	0	53

- Molecule 21 is a protein called RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
21	S	65	Total C 65 65	0	0	65

- Molecule 22 is a protein called RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
22	T	154	Total C 154 154	0	0	154

- Molecule 23 is a protein called RIBOSOMAL PROTEIN L31E.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
23	U	85	Total C 85 85	0	0	85

- Molecule 24 is a protein called RIBOSOMAL PROTEIN L32E.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
24	V	143	Total C 143 143	0	0	143

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	109	ASN	ALA	CONFLICT	UNP P12736

- Molecule 25 is a protein called RIBOSOMAL PROTEIN L37AE.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
25	W	73	Total C 73 73	0	0	73

- Molecule 26 is a protein called RIBOSOMAL PROTEIN L37E.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
26	X	56	Total C 56 56	0	0	56

- Molecule 27 is a protein called RIBOSOMAL PROTEIN L39E.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
27	Y	31	Total C 31 31	0	0	31

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	11	LYS	LEU	CONFLICT	UNP P22452
Y	24	TYR	TRP	CONFLICT	UNP P22452
Y	42	TRP	TYR	CONFLICT	UNP P22452

- Molecule 28 is a protein called RIBOSOMAL PROTEIN L44E.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
28	Z	92	Total C 92 92	0	0	92

- Molecule 29 is a protein called RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
29	1	172	Total C 172 172	0	0	172

- Molecule 30 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	0	1	Total K 1 1	0	0

- Molecule 31 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	0	2	Total Mg 2 2	0	0

- Molecule 32 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	X	1	Total Cd 1 1	0	0
32	W	1	Total Cd 1 1	0	0
32	R	1	Total Cd 1 1	0	0
32	Z	1	Total Cd 1 1	0	0

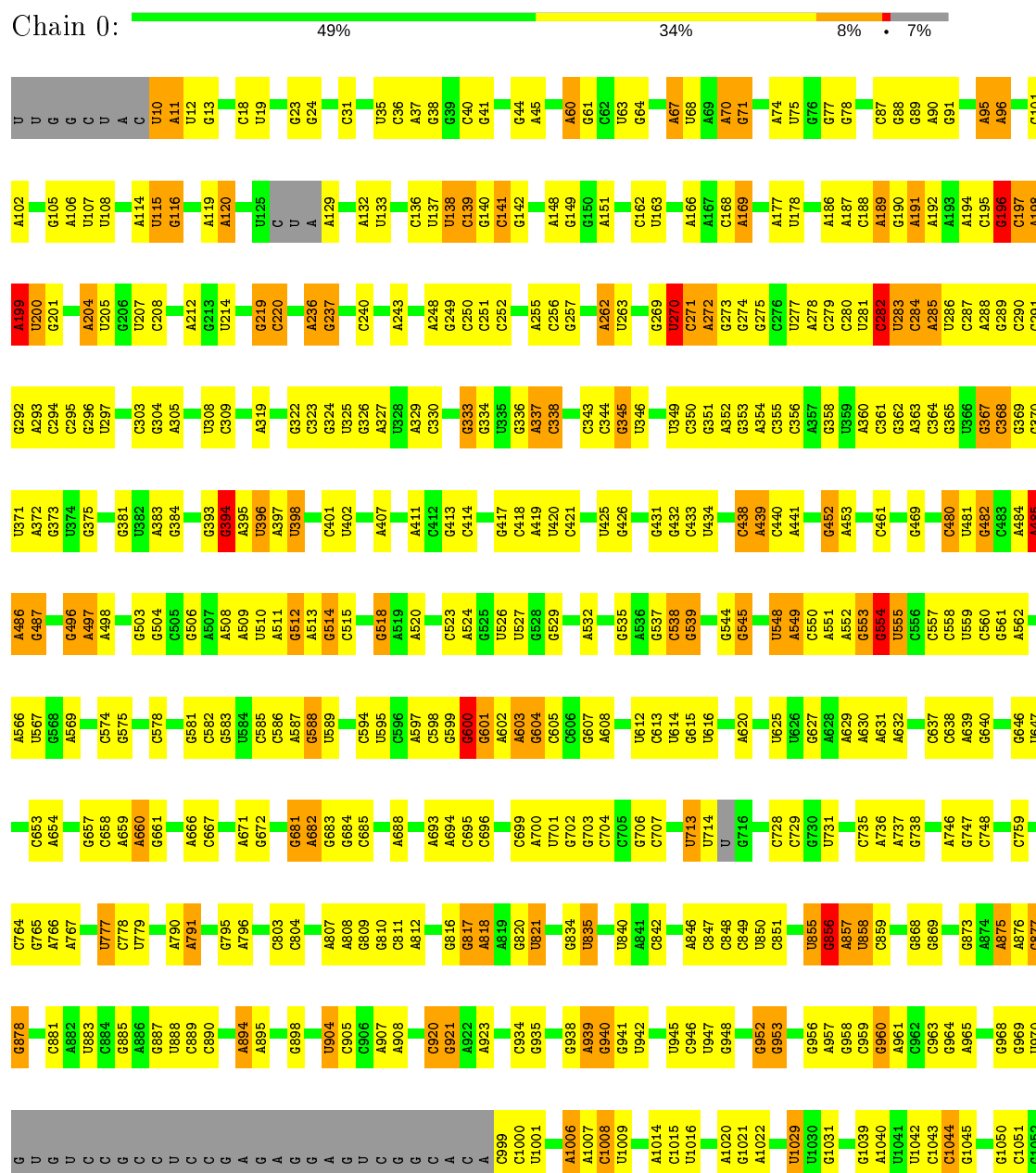
- Molecule 33 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	0	6	Total O 6 6	0	0

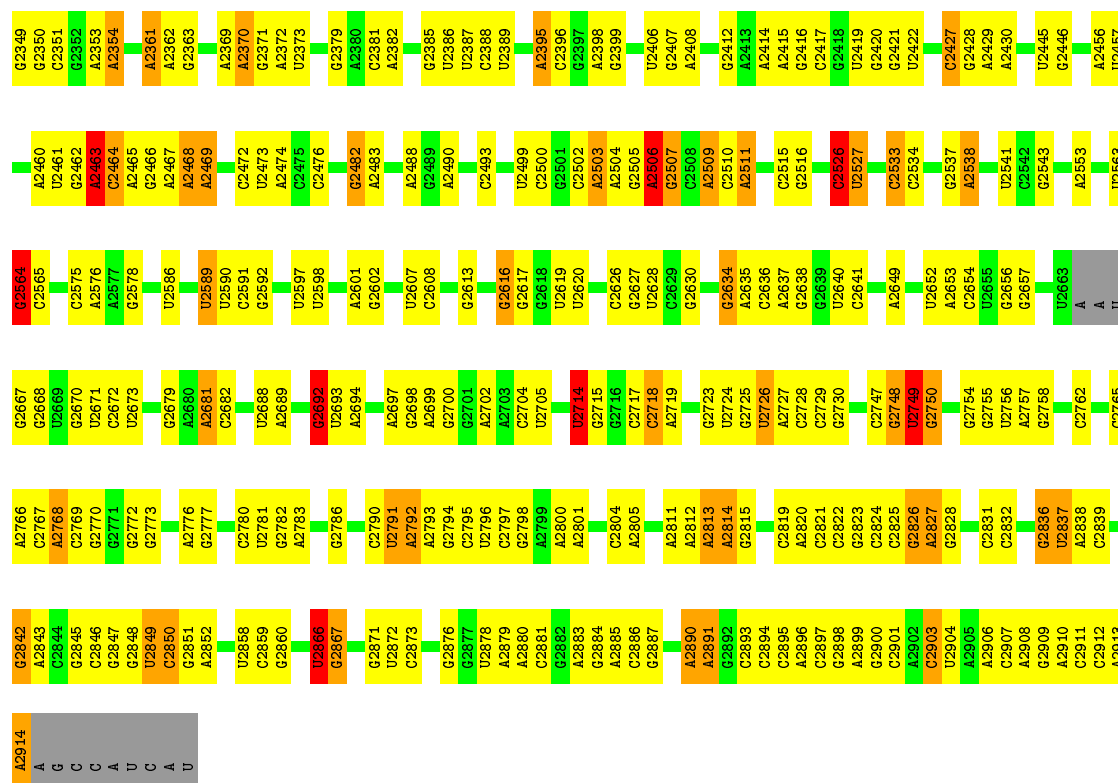
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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: 23S rRNA

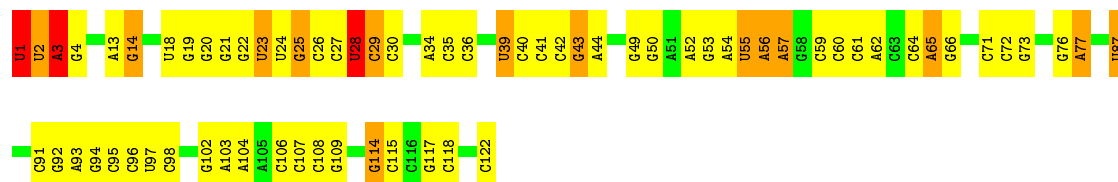






• Molecule 2: 5S RRNA

Chain 9: 43% 43% 11%



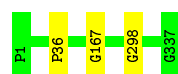
• Molecule 3: RIBOSOMAL PROTEIN L2

Chain A: 98%



• Molecule 4: RIBOSOMAL PROTEIN L3

Chain B: 99%



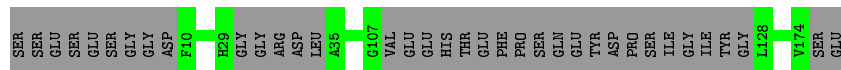
• Molecule 5: RIBOSOMAL PROTEIN L4

Chain C: 100%

There are no outlier residues recorded for this chain.

- Molecule 6: RIBOSOMAL PROTEIN L5

Chain D:  80% 20%



- Molecule 7: RIBOSOMAL PROTEIN L7AE

Chain E:  97% ..



- Molecule 8: RIBOSOMAL PROTEIN L10E

Chain F:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: RIBOSOMAL PROTEIN L13

Chain G:  98% .



- Molecule 10: RIBOSOMAL PROTEIN L14

Chain H:  99% .




- Molecule 11: RIBOSOMAL PROTEIN L15E

Chain I:  100%

There are no outlier residues recorded for this chain.

- Molecule 12: RIBOSOMAL PROTEIN L15

Chain J:  87% 13%



- Molecule 13: RIBOSOMAL PROTEIN L18

Chain K:  100%

There are no outlier residues recorded for this chain.

- Molecule 14: RIBOSOMAL PROTEIN L18E

Chain L:  100%

There are no outlier residues recorded for this chain.

- Molecule 15: RIBOSOMAL PROTEIN L19

Chain M:  97%



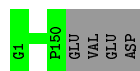
- Molecule 16: RIBOSOMAL PROTEIN L21E

Chain N:  100%

There are no outlier residues recorded for this chain.

- Molecule 17: RIBOSOMAL PROTEIN L22

Chain O:  97%



- Molecule 18: RIBOSOMAL PROTEIN L23

Chain P:  93% 7%



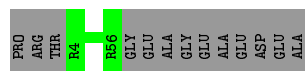
- Molecule 19: RIBOSOMAL PROTEIN L24

Chain Q:  100%

There are no outlier residues recorded for this chain.

- Molecule 20: RIBOSOMAL PROTEIN L24E

Chain R:  80% 20%



- Molecule 21: RIBOSOMAL PROTEIN L29

Chain S:  93% 7%



- Molecule 22: RIBOSOMAL PROTEIN L30

Chain T: 100%

There are no outlier residues recorded for this chain.

- Molecule 23: RIBOSOMAL PROTEIN L31E

Chain U: 92% • 7%



- Molecule 24: RIBOSOMAL PROTEIN L32E

Chain V: 99% •



- Molecule 25: RIBOSOMAL PROTEIN L37AE

Chain W: 100%

There are no outlier residues recorded for this chain.

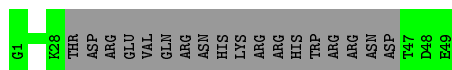
- Molecule 26: RIBOSOMAL PROTEIN L37E

Chain X: 100%

There are no outlier residues recorded for this chain.

- Molecule 27: RIBOSOMAL PROTEIN L39E

Chain Y: 63% 37%



- Molecule 28: RIBOSOMAL PROTEIN L44E

Chain Z: 100%

There are no outlier residues recorded for this chain.

- Molecule 29: RIBOSOMAL PROTEIN L6

Chain 1: 97% •





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	211.66Å 299.67Å 573.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	90.00 – 2.40 89.24 – 2.40	Depositor EDS
% Data completeness (in resolution range)	82.3 (90.00-2.40) 95.5 (89.24-2.40)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.28 (at 2.40Å)	Xtriage
Refinement program	CNS, TNT & CNS	Depositor
R, $R_{free}$	0.252 , 0.261 0.345 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.3	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.04 , -7.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.82	EDS
Total number of atoms	64281	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: K, MG, CD

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	0	0.47	0/64945	0.72	73/101281 (0.1%)
2	9	0.35	0/2905	0.75	4/4528 (0.1%)
All	All	0.46	0/67850	0.72	77/105809 (0.1%)

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
1	0	18	45
2	9	2	0
All	All	20	45

There are no bond length outliers.

The worst 5 of 77 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	0	2749	U	C2'-C3'-O3'	11.07	133.85	109.50
1	0	904	U	C2'-C3'-O3'	10.39	132.35	109.50
1	0	1981	A	C2'-C3'-O3'	10.23	132.00	109.50
1	0	2692	G	N9-C1'-C2'	10.09	127.12	114.00
2	9	3	A	C2'-C3'-O3'	9.58	130.57	109.50

5 of 20 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	191	A	C3'
1	0	282	C	C3'
1	0	600	G	C3'

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Mol	Chain	Res	Type	Atom
1	0	894	A	C3'
1	0	904	U	C3'

5 of 45 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	138	U	Sidechain
1	0	189	A	Sidechain
1	0	262	A	Sidechain
1	0	270	U	Sidechain
1	0	333	G	Sidechain

## 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	0	58012	0	29282	976	0
2	9	2600	0	1326	62	0
3	A	237	0	0	1	0
4	B	337	0	0	2	0
5	C	246	0	0	0	0
6	D	140	0	0	0	0
7	E	118	0	0	1	0
8	F	157	0	0	0	0
9	G	142	0	0	0	0
10	H	132	0	0	1	0
11	I	194	0	0	0	0
12	J	143	0	0	0	0
13	K	186	0	0	0	0
14	L	115	0	0	0	0
15	M	143	0	0	0	0
16	N	95	0	0	0	0
17	O	150	0	0	0	0
18	P	78	0	0	0	0
19	Q	119	0	0	0	0
20	R	53	0	0	0	0
21	S	65	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	T	154	0	0	0	0
23	U	85	0	0	1	0
24	V	143	0	0	2	0
25	W	73	0	0	0	0
26	X	56	0	0	0	0
27	Y	31	0	0	0	0
28	Z	92	0	0	0	0
29	1	172	0	0	0	0
30	0	1	0	0	0	0
31	0	2	0	0	0	0
32	R	1	0	0	0	0
32	W	1	0	0	0	0
32	X	1	0	0	0	0
32	Z	1	0	0	0	0
33	0	6	0	0	0	0
All	All	64281	0	30608	1040	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 11.

The worst 5 of 1040 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)
2:9:76:G:H3'	2:9:77:A:H5''	1.29	1.10
1:0:1682:A:H2	1:0:1696:U:H3	1.05	1.01
1:0:795:G:H2'	1:0:817:G:H22	1.25	1.00
1:0:326:G:H1	1:0:330:C:H5	1.03	1.00
1:0:1355:A:O2'	1:0:1356:A:H3'	1.60	1.00

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2697/2922 (92%)	334 (12%)	107 (3%)
2	9	122/122 (100%)	17 (13%)	5 (4%)
All	All	2819/3044 (92%)	351 (12%)	112 (3%)

5 of 351 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	11	A
1	0	31	C
1	0	60	A
1	0	67	A
1	0	70	A

5 of 112 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1379	A
1	0	1690	C
1	0	2836	G
1	0	1408	U
1	0	1534	C

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 7 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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.