



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 11:08 am GMT

PDB ID : 1ML5
EMDB ID: : EMD-1005
Title : Structure of the E. coli ribosomal termination complex with release factor 2
Authors : Klaholz, B.P.; Pape, T.; Zavialov, A.V.; Myasnikov, A.G.; Orlova, E.V.; Vestergaard, B.; Ehrenberg, M.; van Heel, M.
Deposited on : 2002-08-30
Resolution : 14.00 Å(reported)
Based on PDB ID : 1GQE, 1GIX, 1GIY

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : recalc29047

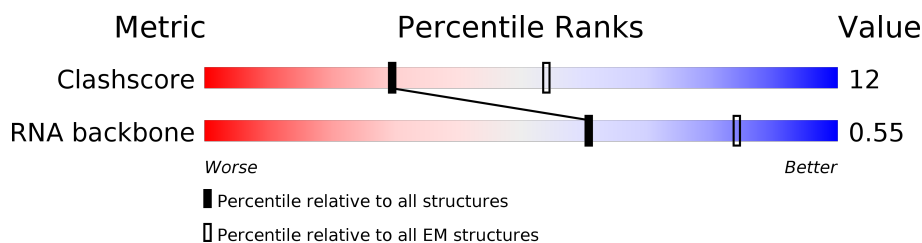
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 14.00 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.



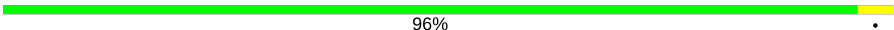

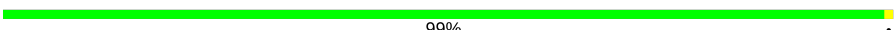
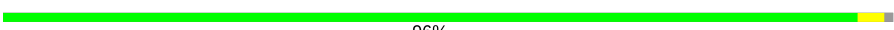













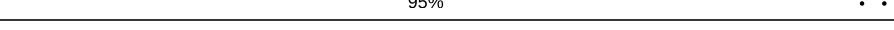
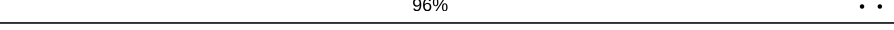






Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
RNA backbone	3398	335

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	A	1522	97% .
2	B	76	32% 47% 16% 5%
3	C	6	17% 67% 17%
4	a	2916	97% ..
5	b	123	98% .
6	Z	365	96% . .
7	E	256	90% . 9%
8	F	239	84% . 14%
9	G	209	96% .
10	H	162	91% . 7%


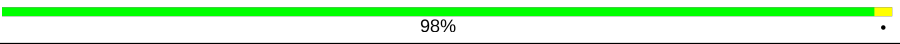


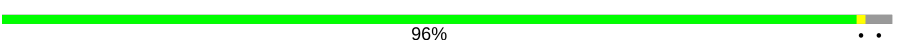





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Mol	Chain	Length	Quality of chain
11	I	101	 96% .
12	J	156	 97% ..
13	K	138	 99% .
14	L	128	 96% ..
15	M	105	 88% 6% 7%
16	N	129	 89% . 8%
17	O	135	 89% . 8%
18	P	126	 96% ..
19	Q	61	 87% 11% .
20	R	89	 94% ..
21	S	91	 90% . 9%
22	T	105	 95% ..
23	U	88	 80% . 17%
24	V	93	 86% 14%
25	W	106	 92% . 7%
26	X	26	 92% 8%
27	c	228	 95% ..
28	d	178	 96% ..
29	e	338	 55% . 43%
30	f	246	 75% . 23%
31	g	176	 67% . 31%
32	h	177	 92% . 7%
33	l	141	 94% . 6%
34	m	145	 79% . 19%
35	n	122	 97% .

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Mol	Chain	Length	Quality of chain
36	o	164	
37	p	138	
38	q	186	
39	r	66	
40	s	113	
41	t	84	
42	u	119	
43	v	94	
44	w	70	
45	x	60	

2 Entry composition

There are 45 unique types of molecules in this entry. The entry contains 11392 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 30S 16S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms		AltConf	Trace
1	A	1519	Total	P	0	1519
			1519	1519		

- Molecule 2 is a RNA chain called T-RNA(PHE).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	76	Total	C	N	O	P	0	0
			1652	746	294	536	76		

- Molecule 3 is a RNA chain called A- AND P-SITE MESSENGER RNA CODONS.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	6	Total	C	N	O	P	0	0
			120	54	12	48	6		

- Molecule 4 is a RNA chain called 50S 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms		AltConf	Trace
4	a	2889	Total	P	0	2889
			2889	2889		

- Molecule 5 is a RNA chain called 50S 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms		AltConf	Trace
5	b	123	Total	P	0	123
			123	123		

- Molecule 6 is a protein called Peptide chain release factor 2.

Mol	Chain	Residues	Atoms		AltConf	Trace
6	Z	362	Total	C	0	362
			362	362		

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms		AltConf	Trace
7	E	234	Total	C	0	234
			234	234		

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms		AltConf	Trace
8	F	206	Total	C	0	206
			206	206		

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S4.

Mol	Chain	Residues	Atoms		AltConf	Trace
9	G	208	Total	C	0	208
			208	208		

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms		AltConf	Trace
10	H	150	Total	C	0	150
			150	150		

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms		AltConf	Trace
11	I	101	Total	C	0	101
			101	101		

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms		AltConf	Trace
12	J	155	Total	C	0	155
			155	155		

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms		AltConf	Trace
13	K	138	Total	C	0	138
			138	138		

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms		AltConf	Trace
14	L	127	Total	C	0	127
			127	127		

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms		AltConf	Trace
15	M	98	Total	C	0	98
			98	98		

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms		AltConf	Trace
16	N	119	Total	C	0	119
			119	119		

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms		AltConf	Trace
17	O	124	Total	C	0	124
			124	124		

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms		AltConf	Trace
18	P	125	Total	C	0	125
			125	125		

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S14.

Mol	Chain	Residues	Atoms		AltConf	Trace
19	Q	60	Total	C	0	60
			60	60		

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms		AltConf	Trace
20	R	88	Total	C	0	88
			88	88		

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms		AltConf	Trace
21	S	83	Total	C	0	83
			83	83		

- Molecule 22 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms		AltConf	Trace
22	T	104	Total	C	0	104
			104	104		

- Molecule 23 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms		AltConf	Trace
23	U	73	Total	C	0	73
			73	73		

- Molecule 24 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms		AltConf	Trace
24	V	80	Total	C	0	80
			80	80		

- Molecule 25 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms		AltConf	Trace
25	W	99	Total	C	0	99
			99	99		

- Molecule 26 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms		AltConf	Trace
26	X	24	Total	C	0	24
			24	24		

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L1.

Mol	Chain	Residues	Atoms		AltConf	Trace
27	c	224	Total	C	0	224
			224	224		

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms		AltConf	Trace
28	d	173	Total	C	0	173
			173	173		

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms		AltConf	Trace
29	e	191	Total	C	0	191
			191	191		

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms		AltConf	Trace
30	f	189	Total	C	0	189
			189	189		

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms		AltConf	Trace
31	g	122	Total	C	0	122
			122	122		

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms		AltConf	Trace
32	h	164	Total	C	0	164
			164	164		

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L11.

Mol	Chain	Residues	Atoms		AltConf	Trace
33	l	133	Total	C	0	133
			133	133		

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms		AltConf	Trace
34	m	117	Total	C	0	117
			117	117		

- Molecule 35 is a protein called 50S RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms		AltConf	Trace
35	n	122	Total	C	0	122
			122	122		

- Molecule 36 is a protein called 50S RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms		AltConf	Trace
36	o	84	Total	C	0	84
			84	84		

- Molecule 37 is a protein called 50S RIBOSOMAL PROTEIN L16.

Mol	Chain	Residues	Atoms		AltConf	Trace
37	p	138	Total	C	0	138
			138	138		

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms		AltConf	Trace
38	q	113	Total	C	0	113
			113	113		

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms		AltConf	Trace
39	r	52	Total	C	0	52
			52	52		

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms		AltConf	Trace
40	s	110	Total	C	0	110
			110	110		

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms		AltConf	Trace
41	t	76	Total	C	0	76
			76	76		

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms		AltConf	Trace
42	u	110	Total	C	0	110
			110	110		

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms		AltConf	Trace
43	v	89	Total	C	0	89
			89	89		

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms		AltConf	Trace
44	w	64	Total	C	0	64
			64	64		

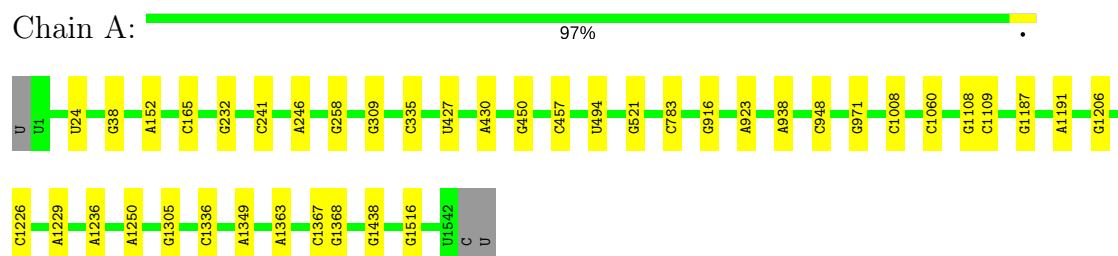
- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms		AltConf	Trace
45	x	60	Total	C	0	60
			60	60		

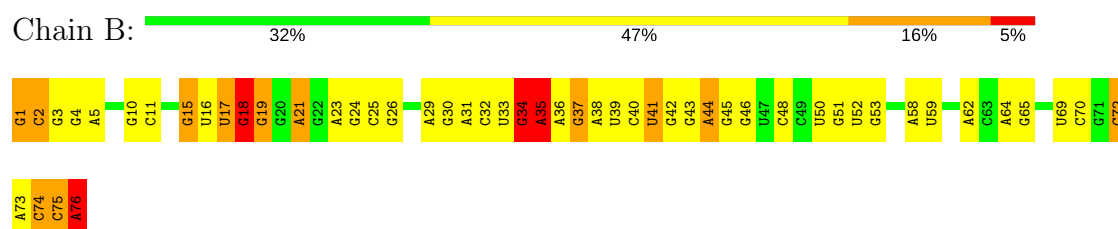
3 Residue-property plots

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.

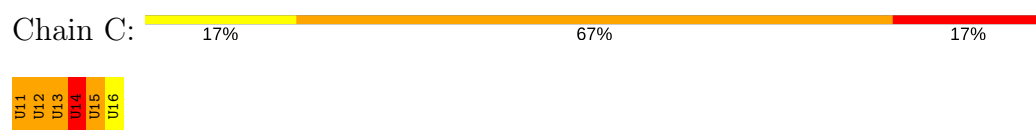
• Molecule 1: 30S 16S RIBOSOMAL RNA



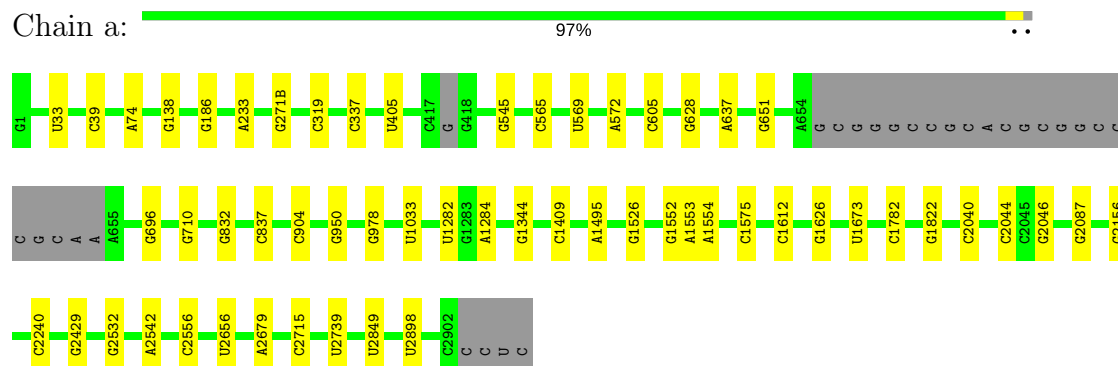
• Molecule 2: T-RNA(PHE)



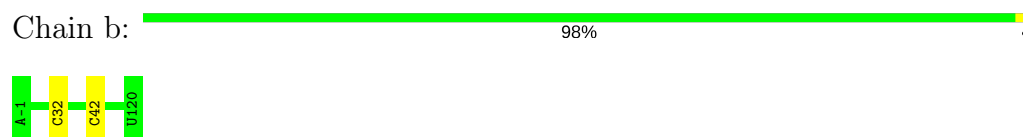
• Molecule 3: A- AND P-SITE MESSENGER RNA CODONS



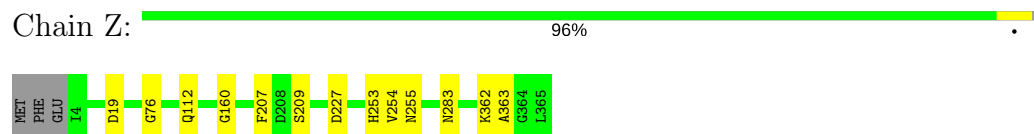
• Molecule 4: 50S 23S RIBOSOMAL RNA



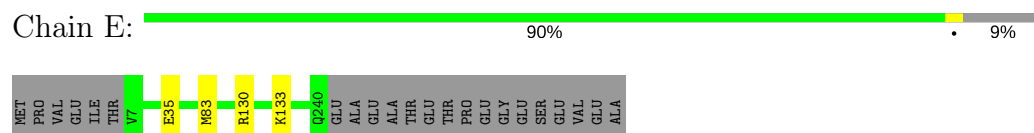
- Molecule 5: 50S 5S RIBOSOMAL RNA



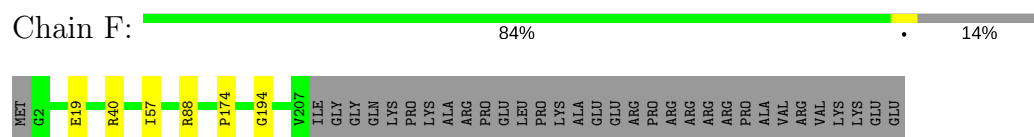
- Molecule 6: Peptide chain release factor 2



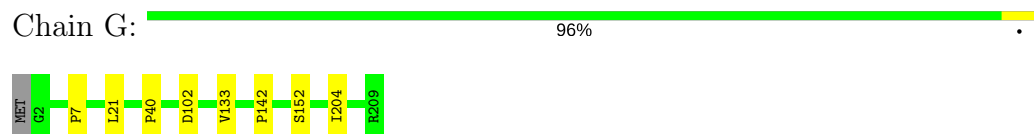
- Molecule 7: 30S RIBOSOMAL PROTEIN S2



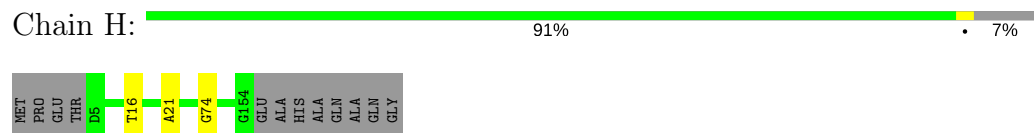
- Molecule 8: 30S RIBOSOMAL PROTEIN S3



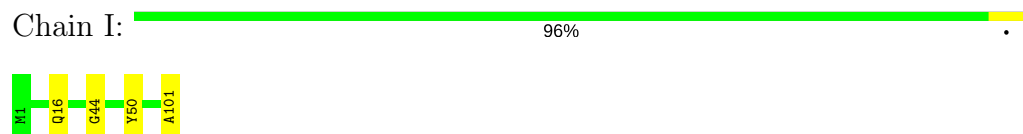
- Molecule 9: 30S RIBOSOMAL PROTEIN S4



- Molecule 10: 30S RIBOSOMAL PROTEIN S5



- Molecule 11: 30S RIBOSOMAL PROTEIN S6



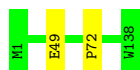
- Molecule 12: 30S RIBOSOMAL PROTEIN S7





- Molecule 13: 30S RIBOSOMAL PROTEIN S8

Chain K: 99%



- Molecule 14: 30S RIBOSOMAL PROTEIN S9

Chain L: 96%



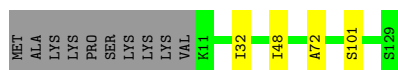
- Molecule 15: 30S RIBOSOMAL PROTEIN S10

Chain M: 88% 6% 7%



- Molecule 16: 30S RIBOSOMAL PROTEIN S11

Chain N: 89% 8%



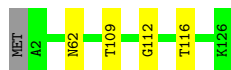
- Molecule 17: 30S RIBOSOMAL PROTEIN S12

Chain O: 89% 8%



- Molecule 18: 30S RIBOSOMAL PROTEIN S13

Chain P: 96%



- Molecule 19: 30S RIBOSOMAL PROTEIN S14

Chain Q: 87% 11%



- Molecule 20: 30S RIBOSOMAL PROTEIN S15

Chain R:  94%



- Molecule 21: 30S RIBOSOMAL PROTEIN S16

Chain S:  90%



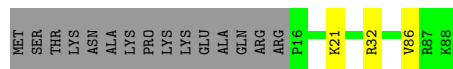
- Molecule 22: 30S RIBOSOMAL PROTEIN S17

Chain T:  95%




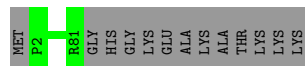
- Molecule 23: 30S RIBOSOMAL PROTEIN S18

Chain U:  80%



- Molecule 24: 30S RIBOSOMAL PROTEIN S19

Chain V:  86%



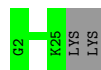
- Molecule 25: 30S RIBOSOMAL PROTEIN S20

Chain W:  92%



- Molecule 26: 30S RIBOSOMAL PROTEIN THX

Chain X:  92%



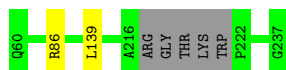
- Molecule 27: 50S RIBOSOMAL PROTEIN L1

Chain c:  95%



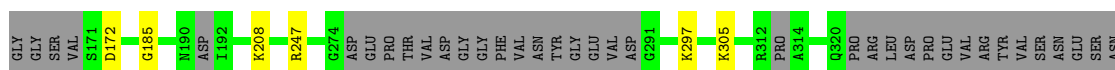
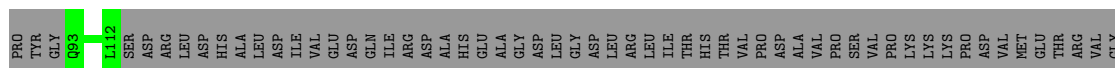
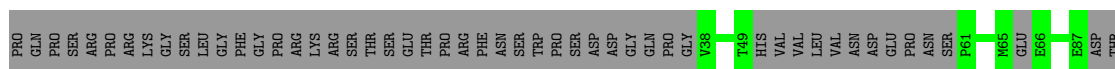
• Molecule 28: 50S RIBOSOMAL PROTEIN L2

Chain d: 96%



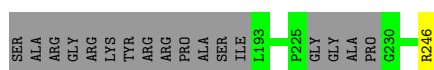
• Molecule 29: 50S RIBOSOMAL PROTEIN L3

Chain e: 55% 43%



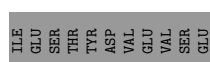
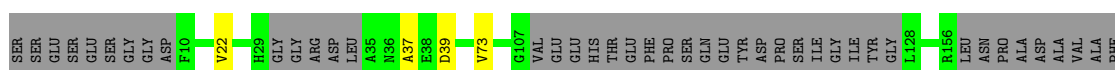
• Molecule 30: 50S RIBOSOMAL PROTEIN L4

Chain f: 75% 23%



• Molecule 31: 50S RIBOSOMAL PROTEIN L5

Chain g: 67% 31%

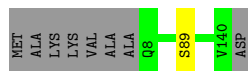


• Molecule 32: 50S RIBOSOMAL PROTEIN L6


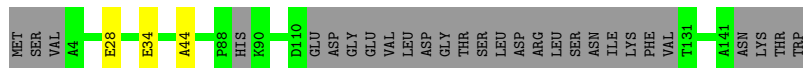
Chain h: 92% 7%



• Molecule 33: 50S RIBOSOMAL PROTEIN L11

Chain l:  94% • 6%

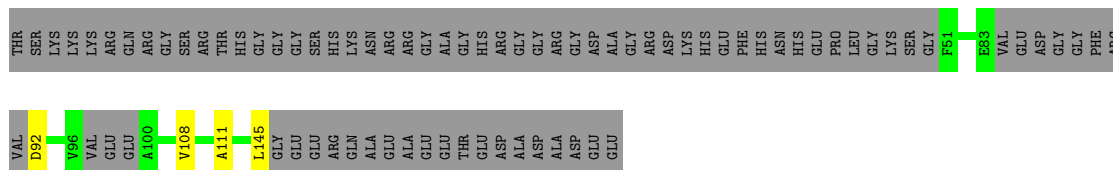
• Molecule 34: 50S RIBOSOMAL PROTEIN L13

Chain m:  79% • 19%

• Molecule 35: 50S RIBOSOMAL PROTEIN L14

Chain n:  97% •

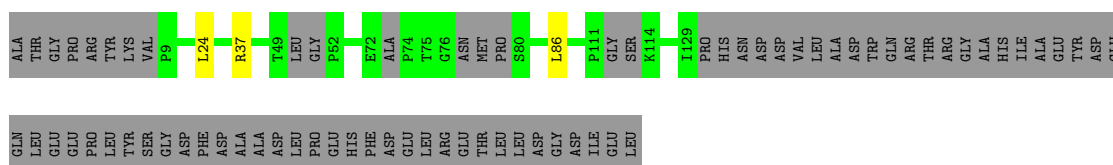
• Molecule 36: 50S RIBOSOMAL PROTEIN L15

Chain o:  49% • 49%


• Molecule 37: 50S RIBOSOMAL PROTEIN L16

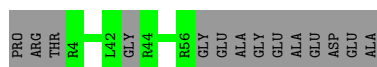
Chain p:  98% •

• Molecule 38: 50S RIBOSOMAL PROTEIN L18

Chain q:  59% • 39%

• Molecule 39: 50S RIBOSOMAL PROTEIN L19

Chain r:  79% • 21%



- Molecule 40: 50S RIBOSOMAL PROTEIN L22

Chain s: 96%



- Molecule 41: 50S RIBOSOMAL PROTEIN L23

Chain t: 90%



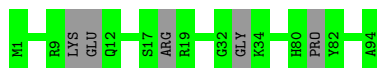
- Molecule 42: 50S RIBOSOMAL PROTEIN L24

Chain u: 88%



- Molecule 43: 50S RIBOSOMAL PROTEIN L25

Chain v: 95%



- Molecule 44: 50S RIBOSOMAL PROTEIN L29

Chain w: 87%



- Molecule 45: 50S RIBOSOMAL PROTEIN L30

Chain x: 97%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	phase flipping CTF correction of each particle as function of position in the micrograph	Depositor
Microscope	FEI/PHILIPS CM200FEG/ST	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1000	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2900	Depositor
Magnification	48000	Depositor
Image detector	KODAK SO163 FILM	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, 5MU, OMG, H2U, YG, 2MG, 5MC, 1MA, M2G, 7MG, PSU

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	$\# Z > 2$	RMSZ	$\# Z > 2$
2	B	1.44	7/1487 (0.5%)	1.47	22/2315 (1.0%)
3	C	2.34	5/131 (3.8%)	2.47	3/200 (1.5%)
All	All	1.53	12/1618 (0.7%)	1.57	25/2515 (1.0%)

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
2	B	0	3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	74	C	O3'-P	-26.96	1.28	1.61
2	B	75	C	O3'-P	-25.74	1.30	1.61
2	B	44	A	O3'-P	-16.95	1.40	1.61
2	B	72	C	O3'-P	-15.83	1.42	1.61
3	C	14	U	O3'-P	-12.23	1.46	1.61

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	13	U	P-O3'-C3'	27.70	152.94	119.70
2	B	35	A	P-O3'-C3'	27.03	152.14	119.70
2	B	74	C	O3'-P-O5'	24.45	150.46	104.00
2	B	35	A	OP1-P-O3'	14.59	137.30	105.20
2	B	72	C	O3'-P-O5'	13.95	130.50	104.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	18	G	Sidechain
2	B	19	G	Sidechain
2	B	62	A	Sidechain

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	1519	0	0	15	24
2	B	1652	0	862	67	29
3	C	120	0	61	11	1
4	a	2889	0	0	0	52
5	b	123	0	0	0	2
6	Z	362	0	0	23	7
7	E	234	0	0	0	4
8	F	206	0	0	2	4
9	G	208	0	0	2	8
10	H	150	0	0	1	2
11	I	101	0	0	0	4
12	J	155	0	0	0	4
13	K	138	0	0	0	2
14	L	127	0	0	3	1
15	M	98	0	0	5	3
16	N	119	0	0	0	4
17	O	124	0	0	1	3
18	P	125	0	0	2	2
19	Q	60	0	0	5	3
20	R	88	0	0	0	4
21	S	83	0	0	0	1
22	T	104	0	0	0	4
23	U	73	0	0	0	3
24	V	80	0	0	0	0
25	W	99	0	0	0	2
26	X	24	0	0	0	0
27	c	224	0	0	0	7

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	d	173	0	0	0	2
29	e	191	0	0	0	6
30	f	189	0	0	0	5
31	g	122	0	0	0	4
32	h	164	0	0	0	2
33	l	133	0	0	0	1
34	m	117	0	0	0	3
35	n	122	0	0	0	4
36	o	84	0	0	0	4
37	p	138	0	0	0	3
38	q	113	0	0	0	3
39	r	52	0	0	0	0
40	s	110	0	0	0	1
41	t	76	0	0	0	0
42	u	110	0	0	0	6
43	v	89	0	0	0	0
44	w	64	0	0	0	3
45	x	60	0	0	0	2
All	All	11392	0	923	98	117

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 12.

The worst 5 of 98 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:B:73:A:H3'	6:Z:255:ASN:CA	1.33	1.51
1:A:430:A:P	9:G:7:PRO:CA	2.16	1.34
2:B:73:A:C3'	6:Z:255:ASN:CA	2.05	1.33
2:B:1:G:N2	2:B:2:C:H41	1.22	1.32
2:B:1:G:N2	2:B:2:C:N4	1.77	1.30

The worst 5 of 117 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)
4:a:904:C:P	4:a:2715:C:P[1_657]	0.14	2.06
1:A:241:C:P	29:e:172:ASP:CA[1_435]	0.38	1.82
4:a:1552:G:P	7:E:35:GLU:CA[1_574]	0.41	1.79
2:B:40:5MC:C2	4:a:1673:U:P[1_546]	0.47	1.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:A:P	15:M:53:PRO:CA[1_563]	0.57	1.63

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 [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	0/1522	-	-
2	B	75/76 (98%)	13 (17%)	0
3	C	5/6 (83%)	1 (20%)	0
4	a	0/2916	-	-
5	b	0/123	-	-
All	All	80/4643 (1%)	14 (17%)	0

5 of 14 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	2	C
2	B	3	G
2	B	17	H2U
2	B	18	G
2	B	19	G

There are no RNA pucker outliers to report.

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

14 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
2	2MG	B	10	2	19,26,27	1.05	1 (5%)	20,38,41	2.52	4 (20%)
2	H2U	B	16	2	17,21,22	0.78	1 (5%)	21,30,33	1.16	3 (14%)
2	H2U	B	17	2	17,21,22	0.78	1 (5%)	21,30,33	1.07	2 (9%)
2	M2G	B	26	2	20,27,28	1.23	3 (15%)	21,40,43	2.67	4 (19%)
2	OMC	B	32	2	15,22,23	0.87	0	19,31,34	0.62	0
2	OMG	B	34	3,2	18,26,27	1.32	2 (11%)	22,38,41	2.57	4 (18%)
2	YG	B	37	2	29,42,43	1.04	2 (6%)	29,62,65	2.23	8 (27%)
2	PSU	B	39	2	16,21,22	1.26	2 (12%)	20,30,33	6.11	4 (20%)
2	5MC	B	40	2	15,22,23	0.99	1 (6%)	17,32,35	1.02	2 (11%)
2	7MG	B	46	2	20,26,27	1.19	2 (10%)	22,39,42	2.10	2 (9%)
2	5MC	B	49	2	15,22,23	0.93	0	17,32,35	1.16	2 (11%)
2	5MU	B	54	2	14,22,23	1.25	2 (14%)	16,32,35	4.33	2 (12%)
2	PSU	B	55	2	16,21,22	1.45	3 (18%)	20,30,33	5.96	6 (30%)
2	1MA	B	58	2	16,25,26	2.76	4 (25%)	13,37,40	1.20	1 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2MG	B	10	2	-	0/5/27/28	0/3/3/3
2	H2U	B	16	2	-	0/7/38/39	0/2/2/2
2	H2U	B	17	2	-	0/7/38/39	0/2/2/2
2	M2G	B	26	2	-	0/7/29/30	0/3/3/3
2	OMC	B	32	2	-	0/5/27/28	0/2/2/2
2	OMG	B	34	3,2	-	0/5/27/28	0/3/3/3
2	YG	B	37	2	-	0/20/42/43	0/4/4/4
2	PSU	B	39	2	-	0/7/25/26	0/2/2/2
2	5MC	B	40	2	-	0/3/25/26	0/2/2/2
2	7MG	B	46	2	-	0/7/37/38	0/3/3/3
2	5MC	B	49	2	-	0/3/25/26	0/2/2/2
2	5MU	B	54	2	-	0/3/25/26	0/2/2/2
2	PSU	B	55	2	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	1MA	B	58	2	-	0/3/25/26	0/3/3/3

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	39	PSU	C6-C5	-3.37	1.33	1.38
2	B	55	PSU	C6-C5	-3.07	1.34	1.38
2	B	58	1MA	O5'-C5'	-2.65	1.41	1.44
2	B	54	5MU	O5'-C5'	-2.63	1.41	1.44
2	B	26	M2G	C8-N7	-2.20	1.30	1.34

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	39	PSU	N1-C2-N3	-19.62	114.29	128.40
2	B	55	PSU	N1-C2-N3	-19.54	114.35	128.40
2	B	39	PSU	C5-C4-N3	-12.94	114.81	125.43
2	B	55	PSU	C5-C4-N3	-12.21	115.41	125.43
2	B	54	5MU	C5-C4-N3	-10.04	114.17	125.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	10	2MG	3	0
2	B	16	H2U	3	0
2	B	17	H2U	3	1
2	B	26	M2G	6	0
2	B	32	OMC	1	0
2	B	34	OMG	4	0
2	B	37	YG	7	2
2	B	39	PSU	1	1
2	B	40	5MC	3	2
2	B	46	7MG	0	1
2	B	58	1MA	0	1

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.