



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:36 PM BST

PDB ID : 5FL8
EMDB ID: : 3199
Title : CRYO-EM STRUCTURE OF THE RIX1-REA1 PRE-60S PARTICLE
Authors : BARRIO-GARCIA, C.; THOMS, M.; FLEMMING, D.; KATER, L.; BERN-
INGHAUSEN, O.; BASSLER, J.; BECKMANN, R.; HURT, E.
Deposited on : 2015-10-22
Resolution : 9.50 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

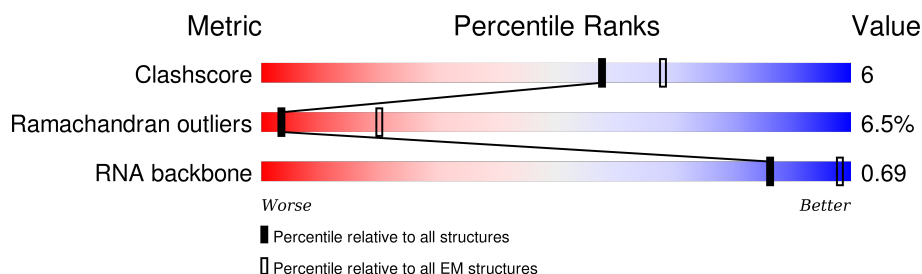
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 9.50 Å.

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



















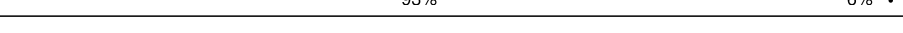


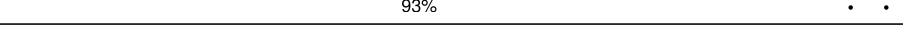
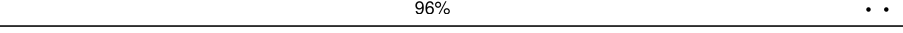


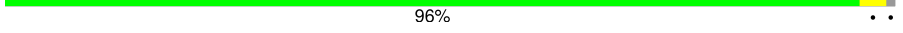

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
RNA backbone	3027	244

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	254	85% 13% ..
2	B	387	92% 7% .
3	C	362	90% 9% .
4	D	297	95% .
5	E	176	84% 5% 11%
6	F	244	85% 6% 9%
7	G	256	87% . 9%
8	H	191	95% 5% .
9	I	217	94% 6%

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Mol	Chain	Length	Quality of chain
10	J	174	
11	K	165	
12	L	199	
13	M	138	
14	N	204	
15	O	199	
16	P	184	
17	Q	186	
18	R	189	
19	S	172	
20	T	160	
21	U	121	
22	V	137	
23	X	142	
24	Y	127	
25	Z	136	
26	a	149	
27	c	105	
28	d	113	
29	e	130	
30	f	107	
31	g	121	
32	h	120	
33	i	100	
34	j	88	

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Mol	Chain	Length	Quality of chain
35	k	78	
36	l	51	
37	m	245	
38	n	236	
39	o	647	
40	p	92	
41	q	515	
42	r	767	
43	s	4914	
44	t	199	
45	u	380	
46	x	2779	
47	y	158	
48	z	121	

2 Entry composition [i](#)

There are 48 unique types of molecules in this entry. The entry contains 105808 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 protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	252	Total	C	N	O	0	0
			1007	504	252	251		

- Molecule 2 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	386	Total	C	N	O	0	0
			1543	772	386	385		

- Molecule 3 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	361	Total	C	N	O	0	0
			1443	722	361	360		

- Molecule 4 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	296	Total	C	N	O	0	0
			1183	592	296	295		

- Molecule 5 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	156	Total	C	N	O	0	0
			622	312	156	154		

- Molecule 6 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	222	Total	C	N	O	0	0
			887	444	222	221		

- Molecule 7 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	233	Total	C	N	O	0	0
			931	466	233	232		

- Molecule 8 is a protein called Rpl9ap.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	H	191	Total	C	N	O	0	0
			763	382	191	190		

- Molecule 9 is a protein called 60S ribosomal protein L1-B.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	217	Total	C	N	O	0	0
			867	434	217	216		

- Molecule 10 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	169	Total	C	N	O	0	0
			675	338	169	168		

- Molecule 11 is a protein called 60S ribosomal protein L12-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	K	127	Total	C	N	O	0	0
			507	254	127	126		

- Molecule 12 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	L	193	Total	C	N	O	0	0
			771	386	193	192		

- Molecule 13 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	136	Total	C	N	O	0	0
			543	272	136	135		

- Molecule 14 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	N	203	Total	C	N	O	0	0
			811	406	203	202		

- Molecule 15 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	O	197	Total	C	N	O	0	0
			787	394	197	196		

- Molecule 16 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	P	183	Total	C	N	O	0	0
			731	366	183	182		

- Molecule 17 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Q	185	Total	C	N	O	0	0
			739	370	185	184		

- Molecule 18 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	R	188	Total	C	N	O	0	0
			751	376	188	187		

- Molecule 19 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	S	172	Total	C	N	O	0	0
			687	344	172	171		

- Molecule 20 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	T	159	Total	C	N	O	0	0
			635	318	159	158		

- Molecule 21 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	U	100	Total	C	N	O	0	0
			399	200	100	99		

- Molecule 22 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	V	136	Total	C	N	O	0	0
			543	272	136	135		

- Molecule 23 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	X	121	Total	C	N	O	0	0
			483	242	121	120		

- Molecule 24 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	Y	126	Total	C	N	O	0	0
			503	252	126	125		

- Molecule 25 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	Z	135	Total	C	N	O	0	0
			539	270	135	134		

- Molecule 26 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	a	148	Total	C	N	O	0	0
			591	296	148	147		

- Molecule 27 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	c	97	Total	C	N	O	0	0
			387	194	97	96		

- Molecule 28 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	d	109	Total	C	N	O	0	0
			435	218	109	108		

- Molecule 29 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	e	127	Total	C	N	O	0	0
			507	254	127	126		

- Molecule 30 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	f	106	Total	C	N	O	0	0
			423	212	106	105		

- Molecule 31 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	g	112	Total	C	N	O	0	0
			447	224	112	111		

- Molecule 32 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	h	119	Total	C	N	O	0	0
			475	238	119	118		

- Molecule 33 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	i	99	Total	C	N	O	0	0
			395	198	99	98		

- Molecule 34 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	j	87	Total	C	N	O	0	0
			347	174	87	86		

- Molecule 35 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	k	77	Total	C	N	O	0	0
			307	154	77	76		

- Molecule 36 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	l	50	Total	C	N	O	0	0
			199	100	50	49		

- Molecule 37 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	m	224	Total	C	N	O	0	0
			895	448	224	223		

- Molecule 38 is a protein called Ribosome assembly factor MRT4.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	n	212	Total	C	N	O	0	0
			847	424	212	211		

- Molecule 39 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	o	347	Total	C	N	O	0	0
			1387	694	347	346		

- Molecule 40 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	p	91	Total	C	N	O	0	0
			363	182	91	90		

- Molecule 41 is a protein called Ribosome assembly protein 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	q	488	Total	C	N	O	0	0
			1951	976	488	487		

- Molecule 42 is a protein called Protein SDA1.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	r	333	Total	C	N	O	0	0
			1304	666	333	305		

- Molecule 43 is a protein called Midasin.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	s	2008	Total	C	N	O	0	0
			8027	4016	2008	2003		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
s	804	ASN	-	insertion	UNP Q12019
s	805	SER	-	insertion	UNP Q12019
s	999	LYS	-	insertion	UNP Q12019
s	1643	ALA	-	insertion	UNP Q12019

- Molecule 44 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	t	63	Total	C	N	O	0	0
			251	126	63	62		

- Molecule 45 is a protein called ARX1.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	u	380	Total	C	N	O	0	0
			1519	760	380	379		

- Molecule 46 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	x	2779	Total	C	N	O	P	0	0
			59475	26560	10747	19390	2778		

- Molecule 47 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	y	158	Total	C	N	O	P	0	0
			3350	1500	586	1107	157		

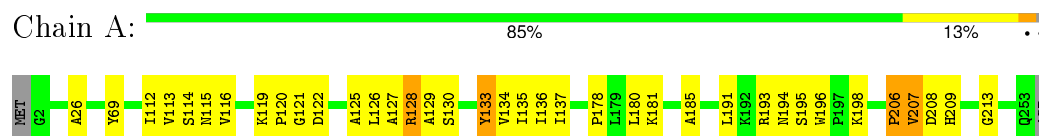
- Molecule 48 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	z	121	Total	C	N	O	P	0	0
			2576	1152	461	843	120		

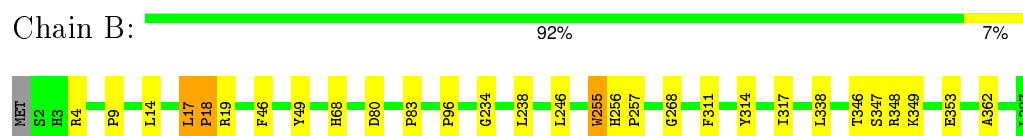
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

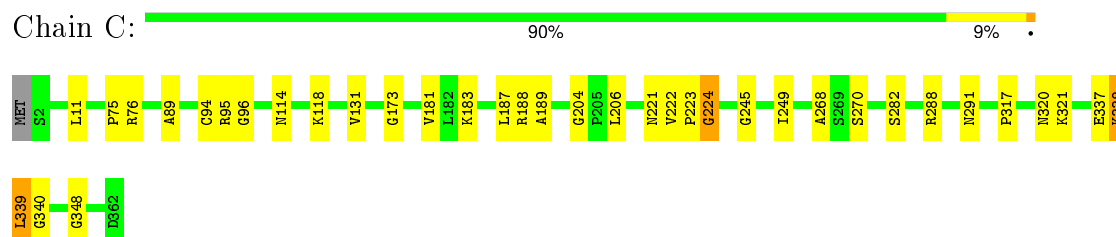
- Molecule 1: 60S ribosomal protein L2-A



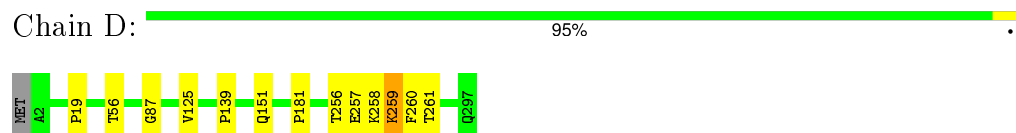
- Molecule 2: 60S ribosomal protein L3



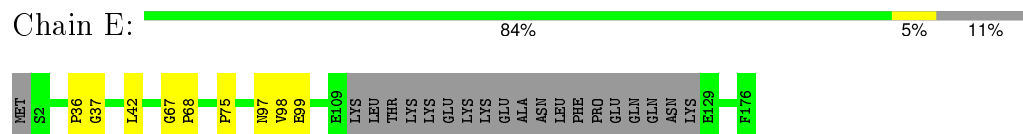
- Molecule 3: 60S ribosomal protein L4-A




- Molecule 4: 60S ribosomal protein L5

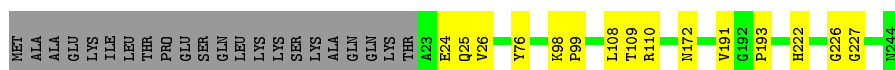


- Molecule 5: 60S ribosomal protein L6-A



- Molecule 6: 60S ribosomal protein L7-A

Chain F: 



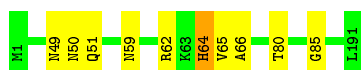
- Molecule 7: 60S ribosomal protein L8-A

Chain G: 



- Molecule 8: Rpl9ap

Chain H: 



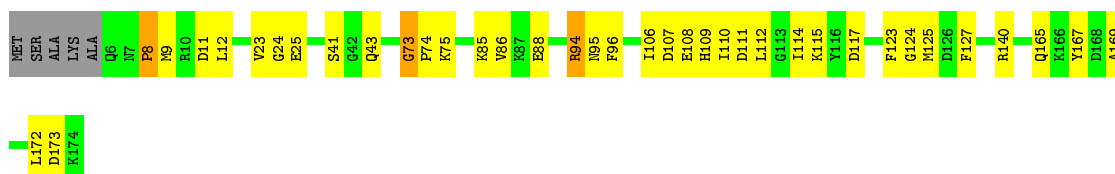
- Molecule 9: 60S ribosomal protein L1-B

Chain I: 



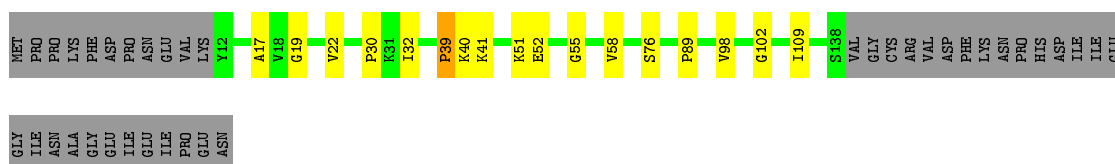
- Molecule 10: 60S ribosomal protein L11-A

Chain J: 




- Molecule 11: 60S ribosomal protein L12-A

Chain K: 



- Molecule 12: 60S ribosomal protein L13-A

Chain L: 



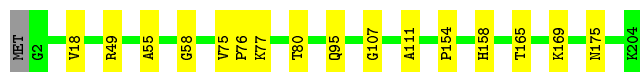
- Molecule 13: 60S ribosomal protein L14-A

Chain M: 93% 6% .



- Molecule 14: 60S ribosomal protein L15-A

Chain N: 92% 8%



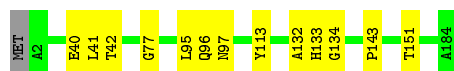
- Molecule 15: 60S ribosomal protein L16-A

Chain O: 87% 11% . .



- Molecule 16: 60S ribosomal protein L17-A

Chain P: 92% 7% .



- Molecule 17: 60S ribosomal protein L18-A

Chain Q: 93% 6% .



- Molecule 18: 60S ribosomal protein L19-A

Chain R: 88% 12% .

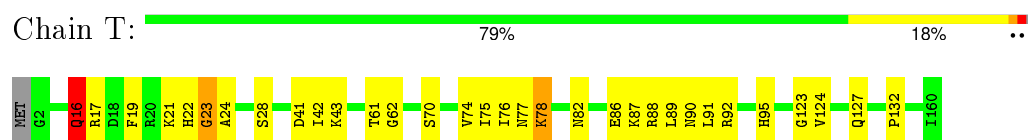


- Molecule 19: 60S ribosomal protein L20-A

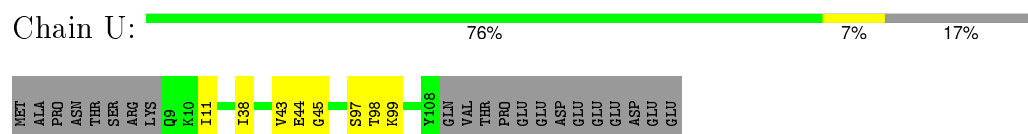
Chain S: 95% 5% .



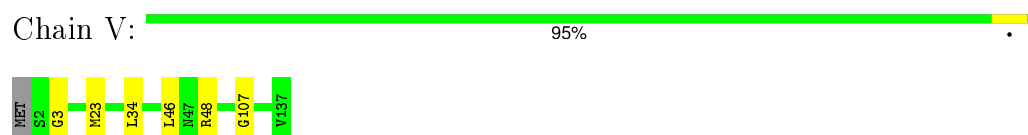
- Molecule 20: 60S ribosomal protein L21-A



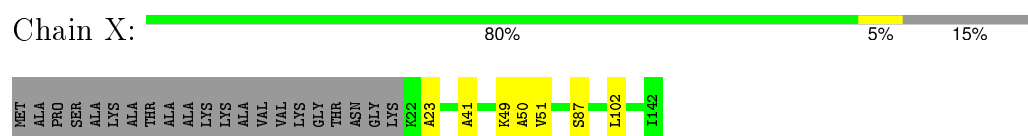
- Molecule 21: 60S ribosomal protein L22-A



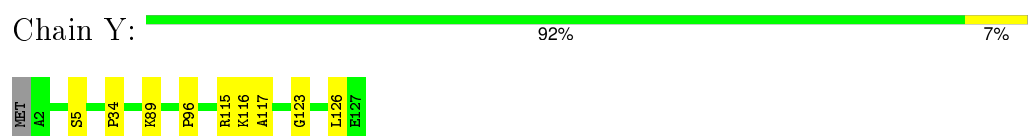
- Molecule 22: 60S ribosomal protein L23-A



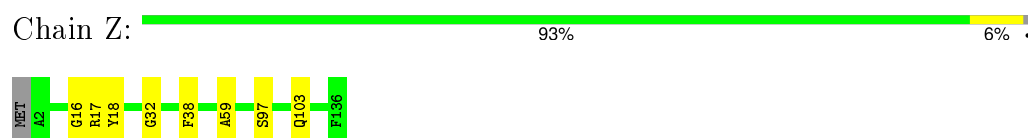
- Molecule 23: 60S ribosomal protein L25



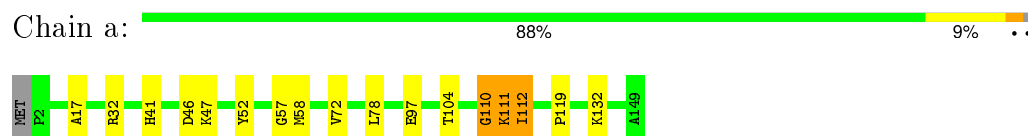
- Molecule 24: 60S ribosomal protein L26-A




- Molecule 25: 60S ribosomal protein L27-A

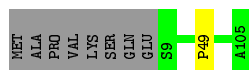


- Molecule 26: 60S ribosomal protein L28



- Molecule 27: 60S ribosomal protein L30

Chain c:  91% • 8%



- Molecule 28: 60S ribosomal protein L31-A

Chain d:  93% • •




- Molecule 29: 60S ribosomal protein L32

Chain e:  96% • •




- Molecule 30: 60S ribosomal protein L33-A

Chain f:  92% 6% • •



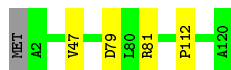
- Molecule 31: 60S ribosomal protein L34-A

Chain g:  88% • 7%



- Molecule 32: 60S ribosomal protein L35-A

Chain h:  96% • •



- Molecule 33: 60S ribosomal protein L36-A

Chain i:  93% 6% •



- Molecule 34: 60S ribosomal protein L37-A

Chain j:  91% 7% • •

-
- A diagram of a protein structure represented as a horizontal bar. The bar is divided into segments of different colors: grey, green, yellow, yellow, and green. The segments are labeled with residue numbers: MET (grey), A2 (green), K7 (yellow), R23 and R24 (yellow), and A92 (green). The labels are placed below the corresponding segments.

- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|
| Met | Ser | Thr | Leu | Ile | Pro | Pro | Pro | Ser | Lys | Lys | Gln | Lys | Lys | Glu | Gln | Leu | Pro | Arg | Glu | Val | Ala | Ile | Ile | Pro | Lys | D28 | S89 | K93 | V126 | F127 | K128 | V129 | P249 | H515 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|

- [illegible]

Chain s: 37% 0 59%

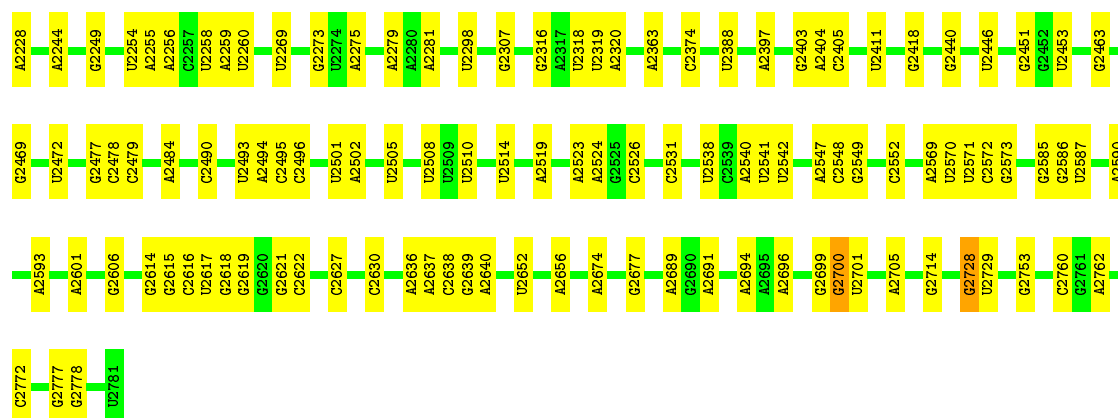












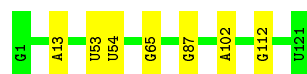
- Molecule 47: 5.8S ribosomal RNA

Chain y: 87% 13%



- Molecule 48: 5S ribosomal RNA

Chain z: 94% 6%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	SUBVOLUMES, Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	4200	Depositor
Magnification	75000	Depositor
Image detector	TVIPS	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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
1	A	0.35	1/1006 (0.1%)	0.47	0/1256
10	J	0.53	0/674	0.78	0/841
11	K	0.18	0/506	0.35	0/631
12	L	0.17	0/770	0.35	0/961
13	M	0.17	0/542	0.30	0/676
14	N	0.19	0/810	0.38	0/1011
15	O	0.20	0/786	0.47	1/981 (0.1%)
16	P	0.17	0/730	0.33	0/911
17	Q	0.17	0/738	0.30	0/921
18	R	0.20	0/750	0.41	0/936
19	S	0.16	0/686	0.32	0/856
2	B	0.32	1/1542 (0.1%)	0.44	2/1926 (0.1%)
20	T	0.44	1/634 (0.2%)	0.64	2/791 (0.3%)
21	U	0.17	0/398	0.31	0/496
22	V	0.22	0/542	0.34	0/676
23	X	0.17	0/482	0.29	0/601
24	Y	0.17	0/502	0.30	0/626
25	Z	0.17	0/538	0.31	0/671
26	a	0.80	3/590 (0.5%)	0.71	3/736 (0.4%)
27	c	0.17	0/386	0.27	0/481
28	d	0.17	0/434	0.31	0/541
29	e	0.17	0/506	0.32	0/631
3	C	0.19	0/1442	0.37	1/1801 (0.1%)
30	f	0.49	1/422 (0.2%)	0.71	1/526 (0.2%)
31	g	0.17	0/446	0.32	0/556
32	h	0.17	0/474	0.29	0/591
33	i	0.17	0/394	0.31	0/491
34	j	0.57	1/346 (0.3%)	0.57	1/431 (0.2%)
35	k	0.17	0/306	0.29	0/381
36	l	0.17	0/198	0.36	0/246
37	m	0.17	0/894	0.30	0/1116
38	n	0.17	0/846	0.31	0/1056
39	o	0.60	3/1386 (0.2%)	0.86	9/1731 (0.5%)
4	D	0.17	0/1182	0.32	0/1476

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
40	p	0.17	0/362	0.30	0/451
41	q	0.94	0/1950	0.91	1/2436 (0.0%)
42	r	0.56	1/1276 (0.1%)	0.92	4/1553 (0.3%)
43	s	0.43	4/8022 (0.0%)	0.50	9/10020 (0.1%)
44	t	0.34	0/250	0.52	0/311
45	u	0.92	0/1518	0.86	1/1896 (0.1%)
46	x	0.26	5/66581 (0.0%)	0.76	154/103823 (0.1%)
47	y	0.11	0/3743	0.64	0/5828
48	z	0.12	0/2880	0.64	0/4487
5	E	0.55	1/620 (0.2%)	0.70	4/772 (0.5%)
6	F	0.17	0/886	0.32	0/1106
7	G	0.17	0/930	0.32	0/1161
8	H	0.17	0/762	0.30	0/951
9	I	0.17	0/866	0.31	0/1081
All	All	0.32	22/113534 (0.0%)	0.69	193/164435 (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	A	0	1
10	J	0	1
2	B	0	3
20	T	0	3
26	a	0	1
30	f	0	2
39	o	0	1
42	r	0	3
43	s	0	12
44	t	0	1
5	E	0	1
All	All	0	29

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	x	2699	G	O3'-P	41.80	2.11	1.61
43	s	825	TRP	C-N	-18.64	0.91	1.34
43	s	826	LEU	N-CA	17.84	1.82	1.46
26	a	111	LYS	N-CA	14.18	1.74	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a	110	GLY	C-N	9.94	1.56	1.34

The worst 5 of 193 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	x	2699	G	P-O3'-C3'	-26.90	87.42	119.70
46	x	2700	G	O5'-P-OP2	26.12	142.05	110.70
46	x	2700	G	O5'-P-OP1	-25.82	79.71	110.70
43	s	858	GLU	O-C-N	-21.29	88.64	122.70
46	x	440	A	O5'-P-OP1	-19.66	87.11	110.70

There are no chirality outliers.

5 of 29 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	198	LYS	Peptide
2	B	18	PRO	Peptide
2	B	255	TRP	Peptide
2	B	256	HIS	Peptide
5	E	42	LEU	Mainchain

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	1007	0	310	18	0
2	B	1543	0	433	4	0
3	C	1443	0	399	7	0
4	D	1183	0	325	1	0
5	E	622	0	160	1	0
6	F	887	0	241	3	0
7	G	931	0	242	1	0
8	H	763	0	215	3	0
9	I	867	0	230	2	0
10	J	675	0	191	11	0
11	K	507	0	140	1	0
12	L	771	0	199	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	M	543	0	145	2	0
14	N	811	0	221	3	0
15	O	787	0	214	7	0
16	P	731	0	197	4	0
17	Q	739	0	205	1	0
18	R	751	0	203	14	0
19	S	687	0	175	3	0
20	T	635	0	174	14	0
21	U	399	0	109	2	0
22	V	543	0	162	2	0
23	X	483	0	121	1	0
24	Y	503	0	134	1	0
25	Z	539	0	144	1	0
26	a	591	0	176	0	0
27	c	387	0	113	0	0
28	d	435	0	114	0	0
29	e	507	0	135	0	0
30	f	423	0	117	0	0
31	g	447	0	121	0	0
32	h	475	0	118	0	0
33	i	395	0	109	0	0
34	j	347	0	104	0	0
35	k	307	0	79	0	0
36	l	199	0	47	0	0
37	m	895	0	257	0	0
38	n	847	0	224	0	0
39	o	1387	0	358	0	0
40	p	363	0	108	0	0
41	q	1951	0	539	0	0
42	r	1304	0	336	0	0
43	s	8027	0	2141	0	0
44	t	251	0	68	0	0
45	u	1519	0	416	0	0
46	x	59475	0	29874	0	0
47	y	3350	0	1696	0	0
48	z	2576	0	1304	0	0
All	All	105808	0	43843	111	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 6.

The worst 5 of 111 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)
15:O:75:ALA:O	15:O:77:SER:N	1.85	1.10
20:T:62:GLY:N	20:T:75:ILE:H	1.51	1.08
20:T:43:LYS:O	20:T:95:HIS:CA	2.03	1.06
18:R:158:GLU:O	18:R:162:ARG:N	1.90	1.03
20:T:62:GLY:CA	20:T:75:ILE:H	1.72	1.03

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	
1	A	250/254 (98%)	156 (62%)	70 (28%)	24 (10%)	1	15
2	B	384/387 (99%)	294 (77%)	71 (18%)	19 (5%)	3	31
3	C	359/362 (99%)	254 (71%)	80 (22%)	25 (7%)	1	22
4	D	294/297 (99%)	229 (78%)	53 (18%)	12 (4%)	3	35
5	E	152/176 (86%)	113 (74%)	35 (23%)	4 (3%)	7	45
6	F	220/244 (90%)	181 (82%)	30 (14%)	9 (4%)	3	35
7	G	231/256 (90%)	179 (78%)	43 (19%)	9 (4%)	4	36
8	H	189/191 (99%)	147 (78%)	37 (20%)	5 (3%)	7	45
9	I	215/217 (99%)	159 (74%)	48 (22%)	8 (4%)	4	38
10	J	167/174 (96%)	116 (70%)	29 (17%)	22 (13%)	0	7
11	K	125/165 (76%)	80 (64%)	29 (23%)	16 (13%)	0	8
12	L	191/199 (96%)	141 (74%)	39 (20%)	11 (6%)	2	27
13	M	134/138 (97%)	106 (79%)	22 (16%)	6 (4%)	3	33
14	N	201/204 (98%)	147 (73%)	44 (22%)	10 (5%)	3	31
15	O	195/199 (98%)	142 (73%)	38 (20%)	15 (8%)	1	20
16	P	181/184 (98%)	141 (78%)	35 (19%)	5 (3%)	6	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	Q	183/186 (98%)	143 (78%)	30 (16%)	10 (6%)	2	29
18	R	186/189 (98%)	136 (73%)	44 (24%)	6 (3%)	5	41
19	S	170/172 (99%)	133 (78%)	31 (18%)	6 (4%)	4	39
20	T	157/160 (98%)	90 (57%)	46 (29%)	21 (13%)	0	7
21	U	98/121 (81%)	77 (79%)	17 (17%)	4 (4%)	3	35
22	V	134/137 (98%)	95 (71%)	37 (28%)	2 (2%)	13	57
23	X	119/142 (84%)	91 (76%)	23 (19%)	5 (4%)	3	34
24	Y	124/127 (98%)	91 (73%)	26 (21%)	7 (6%)	2	28
25	Z	133/136 (98%)	97 (73%)	30 (23%)	6 (4%)	3	33
26	a	146/149 (98%)	91 (62%)	39 (27%)	16 (11%)	0	11
27	c	95/105 (90%)	84 (88%)	10 (10%)	1 (1%)	17	63
28	d	107/113 (95%)	88 (82%)	15 (14%)	4 (4%)	4	38
29	e	125/130 (96%)	99 (79%)	24 (19%)	2 (2%)	12	56
30	f	104/107 (97%)	78 (75%)	19 (18%)	7 (7%)	1	24
31	g	110/121 (91%)	78 (71%)	27 (24%)	5 (4%)	3	33
32	h	117/120 (98%)	92 (79%)	21 (18%)	4 (3%)	5	40
33	i	97/100 (97%)	78 (80%)	13 (13%)	6 (6%)	2	26
34	j	85/88 (97%)	53 (62%)	26 (31%)	6 (7%)	1	22
35	k	75/78 (96%)	66 (88%)	8 (11%)	1 (1%)	15	60
36	l	48/51 (94%)	33 (69%)	11 (23%)	4 (8%)	1	18
37	m	222/245 (91%)	170 (77%)	44 (20%)	8 (4%)	4	38
38	n	210/236 (89%)	156 (74%)	48 (23%)	6 (3%)	6	43
39	o	345/647 (53%)	218 (63%)	76 (22%)	51 (15%)	0	5
40	p	89/92 (97%)	72 (81%)	14 (16%)	3 (3%)	5	40
41	q	486/515 (94%)	459 (94%)	21 (4%)	6 (1%)	16	61
42	r	277/767 (36%)	152 (55%)	58 (21%)	67 (24%)	0	2
43	s	1998/4914 (41%)	1595 (80%)	228 (11%)	175 (9%)	1	17
44	t	61/199 (31%)	53 (87%)	6 (10%)	2 (3%)	5	40
45	u	378/380 (100%)	359 (95%)	9 (2%)	10 (3%)	7	45
All	All	9967/14174 (70%)	7612 (76%)	1704 (17%)	651 (6%)	3	25

5 of 651 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	ASP
1	A	128	ARG
1	A	133	TYR
1	A	135	ILE
1	A	137	ILE

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
46	x	2778/2779 (99%)	291 (10%)	0
47	y	157/158 (99%)	20 (12%)	0
48	z	120/121 (99%)	7 (5%)	0
All	All	3055/3058 (99%)	318 (10%)	0

5 of 318 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
46	x	22	G
46	x	49	A
46	x	60	A
46	x	66	A
46	x	92	G

There are no RNA pucker outliers to report.

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

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

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
42	r	14
46	x	1
43	s	1

The worst 5 of 16 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	r	576:GLY	C	629:GLU	N	23.87
1	r	472:VAL	C	476:GLU	N	19.67
1	r	121:MET	C	126:LEU	N	18.70
1	r	228:GLY	C	240:ASN	N	15.12
1	r	436:VAL	C	440:ALA	N	14.62