



wwPDB EM Validation Summary Report ⓘ

Dec 12, 2022 – 09:12 AM EST

PDB ID : 6VWN
EMDB ID : EMD-21422
Title : 70S ribosome bound to HIV frameshifting stem-loop (FSS) and P-site tRNA (non-rotated conformation, Structure II)
Authors : Loerch, S.; Bao, C.; Ling, C.; Korostelev, A.A.; Grigorieff, N.; Ermolenko, D.M.
Deposited on : 2020-02-20
Resolution : 3.40 Å(reported)

This is a wwPDB EM Validation Summary 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/EMValidationReportHelp>

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:

EMDB validation analysis : **FAILED**
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

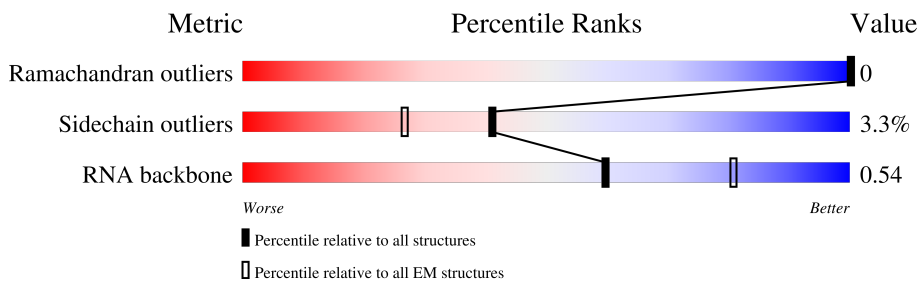
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	3	120	72% 27% .
2	5	76	75% 25%
3	A	273	97% ..
4	B	209	97% .
5	C	201	99% .
6	D	179	94% ..
7	E	177	95% ..
8	F	149	30% . 68%
9	G	142	98% .

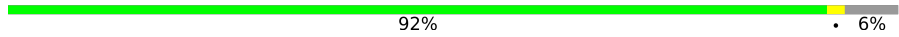


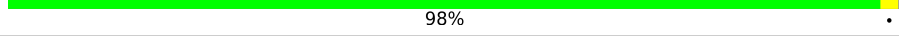




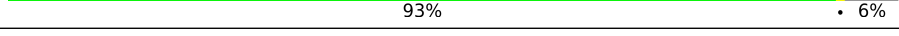
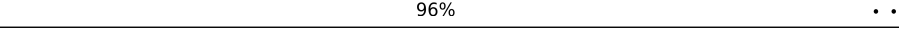
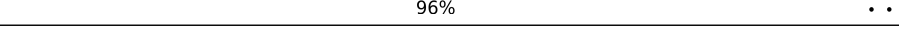
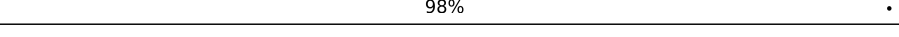

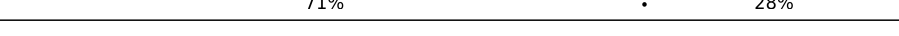

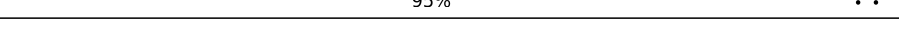
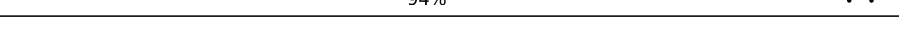

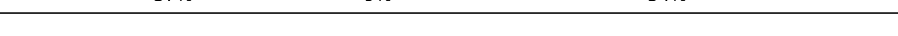
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Mol	Chain	Length	Quality of chain
10	I	123	98%
11	J	144	98%
12	K	136	98%
13	L	127	94%
14	M	117	94%
15	N	115	95%
16	O	118	97%
17	P	103	97%
18	Q	110	95%
19	R	100	87%
20	S	104	91%
21	T	94	95%
22	U	85	86%
23	V	78	96%
24	W	63	95%
25	X	59	98%
26	Y	57	93%
27	Z	55	84%
28	AA	46	100%
29	AB	65	95%
30	AC	38	95%
31	2	2903	78%
32	a	241	90%
33	b	233	82%
34	c	206	73%

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Mol	Chain	Length	Quality of chain
35	d	167	 92% 6%
36	e	135	 73% 25%
37	f	179	 54% 46%
38	g	130	 98%
39	h	130	 89% 7%
40	i	103	 84% 14%
41	j	129	 88% 9%
42	k	124	 83% 6% 10%
43	l	118	 93% 6%
44	m	101	 96%
45	n	89	 96%
46	o	82	 98%
47	p	84	 89% 7%
48	q	75	 71% 28%
49	r	92	 83% 14%
50	s	87	 95%
51	t	71	 94%
52	1	1540	 77% 20%
53	4	93	 37% 9% 54%

2 Entry composition i

There are 54 unique types of molecules in this entry. The entry contains 140036 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 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	3	120	2568	1145	471	833	119	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	120	A	U	conflict	GB 984297099

- Molecule 2 is a RNA chain called tRNAPhe.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	5	76	1619	723	290	531	75	0	0

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	A	271	2082	1288	423	364	7	0	0

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	B	209	1565	979	288	294	4	0	0

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	C	201	1552	974	283	290	5	0	0

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	D	177	1410	899	249	256	6	0	0

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	E	173	1298	817	238	241	2	0	0

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	F	48	368	238	63	66	1	0	0

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	G	142	1129	714	212	199	4	0	0

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	I	123	947	593	181	167	6	0	0

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	J	143	1043	649	206	186	2	0	0

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	K	136	1074	686	205	177	6	0	0

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	L	119	951	588	195	163	5	0	0

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	M	114	875	542	175	158		0	0

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	N	114	917	574	179	163	1	0	0

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	O	117	947	604	192	151		0	0

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	P	103	816	516	153	145	2	0	0

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	Q	110	857	532	166	156	3	0	0

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	R	90	714	449	136	128	1	0	0

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	S	96	Total	C	N	O	0	0
			735	464	138	133		

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	93	Total	C	N	O	S	0	0
			745	474	136	133	2		

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	60	Total	C	N	O	S	0	0
			491	303	96	91	1		

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 26 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Y	55	Total	C	N	O	S	0	0
			434	263	92	78	1		

- Molecule 27 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
27	Z	48	396	255	72	69	0	0

- Molecule 28 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	AA	46	377	228	90	57	2	0	0

- Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	AB	64	504	323	105	74	2	0	0

- Molecule 30 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	AC	38	302	185	65	48	4	0	0

- Molecule 31 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
31	2	2833	60819	27131	11192	19664	2832	0	0

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	208	C	-	insertion	GB 984297099
2	284	U	C	conflict	GB 984297099
2	285	G	A	conflict	GB 984297099
2	356	G	A	conflict	GB 984297099
2	542	C	U	conflict	GB 984297099
2	747	C	U	conflict	GB 984297099
2	1174	U	G	conflict	GB 984297099
2	1211	C	U	conflict	GB 984297099
2	1513	U	C	conflict	GB 984297099
2	1723	G	A	conflict	GB 984297099
2	1730	C	U	conflict	GB 984297099
2	1865	U	C	conflict	GB 984297099
2	2163	A	G	conflict	GB 984297099

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Chain	Residue	Modelled	Actual	Comment	Reference
2	2712	C	U	conflict	GB 984297099
2	2794	C	U	conflict	GB 984297099
2	2796	U	C	conflict	GB 984297099
2	2797	U	C	conflict	GB 984297099
2	2799	A	G	conflict	GB 984297099
2	2802	G	A	conflict	GB 984297099

- Molecule 32 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	a	220	1672	1062	293	310	7	0	0

- Molecule 33 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	b	197	1502	957	276	266	3	0	0

- Molecule 34 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	c	159	1273	796	240	234	3	0	0

- Molecule 35 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	d	157	1146	714	215	211	6	0	0

- Molecule 36 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	e	101	824	520	149	149	6	0	0

- Molecule 37 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	f	97	Total	C	N	O	S	0	0
			742	467	133	139	3		

- Molecule 38 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	g	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 39 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	h	121	Total	C	N	O	S	0	0
			950	591	189	168	2		

- Molecule 40 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	i	89	Total	C	N	O	S	0	0
			726	455	141	129	1		

- Molecule 41 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	j	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 42 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	k	111	Total	C	N	O	S	0	0
			867	535	180	148	4		

- Molecule 43 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	l	111	Total	C	N	O	S	0	0
			859	531	172	153	3		

- Molecule 44 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	m	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 45 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	n	87	Total	C	N	O	S	0	0
			702	433	140	128	1		

- Molecule 46 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	o	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 47 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	p	78	Total	C	N	O	S	0	0
			632	400	118	111	3		

- Molecule 48 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	q	54	Total	C	N	O	0	0
			443	281	81	81		

- Molecule 49 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	r	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 50 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	s	84	Total	C	N	O	S	0	0
			655	406	136	110	3		

- Molecule 51 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	t	68	566	351	120	94	1	0	0

- Molecule 52 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
52	1	1508	32365	14434	5945	10478	1508	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	1517	A	G	conflict	GB 1726036237

- Molecule 53 is a RNA chain called HIV1 frameshift stimulating sequence mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
53	4	43	926	413	174	296	43	0	0

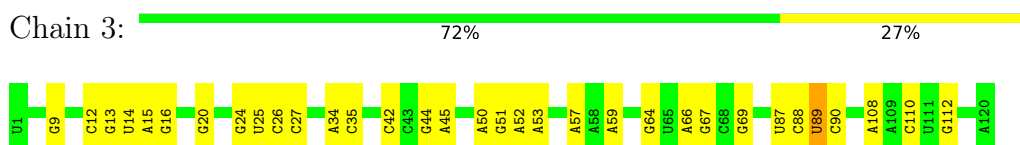
- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
54	A	2	Total	Mg	0
			2	2	
54	Y	1	Total	Mg	0
			1	1	
54	2	45	Total	Mg	0
			45	45	
54	1	7	Total	Mg	0
			7	7	

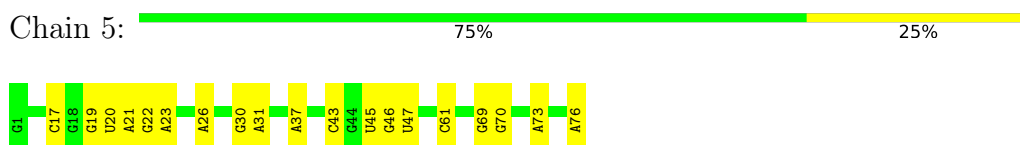
3 Residue-property plots [i](#)

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. 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.

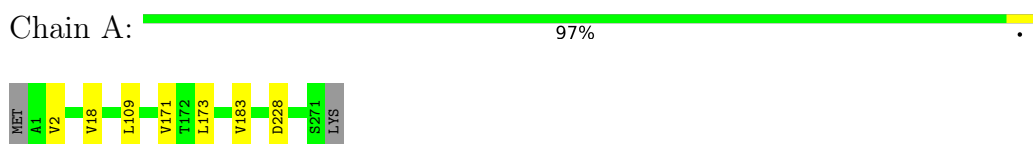
- Molecule 1: 5S ribosomal RNA



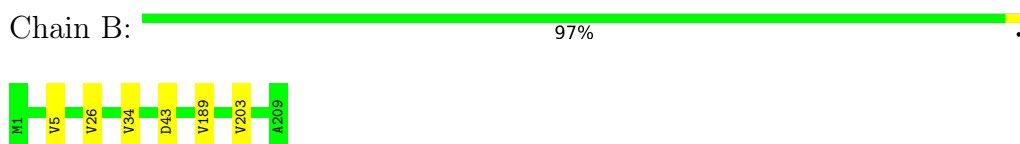
- Molecule 2: tRNAPhe



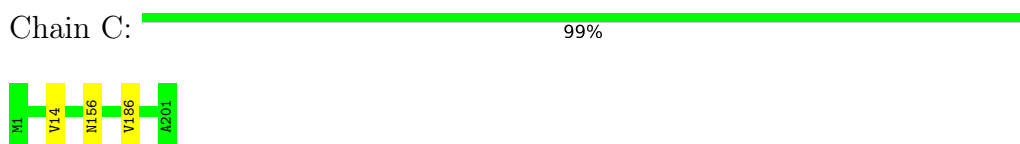
- Molecule 3: 50S ribosomal protein L2



- Molecule 4: 50S ribosomal protein L3



- Molecule 5: 50S ribosomal protein L4



- Molecule 6: 50S ribosomal protein L5





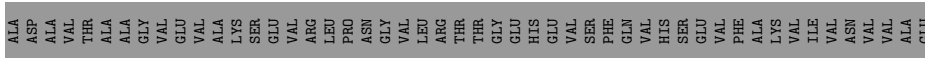
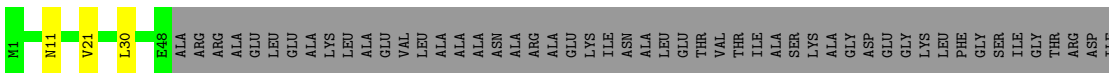
- Molecule 7: 50S ribosomal protein L6

Chain E: 95%



- Molecule 8: 50S ribosomal protein L9

Chain F: 30% 68%



- Molecule 9: 50S ribosomal protein L13

Chain G: 98%



- Molecule 10: 50S ribosomal protein L14

Chain I: 98%



- Molecule 11: 50S ribosomal protein L15

Chain J: 98%



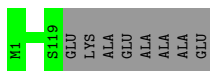
- Molecule 12: 50S ribosomal protein L16

Chain K: 98%



- Molecule 13: 50S ribosomal protein L17

Chain L:  94% 6%



- Molecule 14: 50S ribosomal protein L18

Chain M:  94%



- Molecule 15: 50S ribosomal protein L19

Chain N:  95%



- Molecule 16: 50S ribosomal protein L20

Chain O:  97%



- Molecule 17: 50S ribosomal protein L21

Chain P:  97%




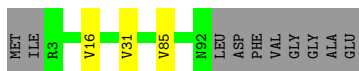
- Molecule 18: 50S ribosomal protein L22

Chain Q:  95% 5%




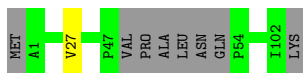
- Molecule 19: 50S ribosomal protein L23

Chain R:  87% 10%



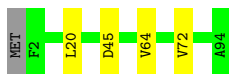
- Molecule 20: 50S ribosomal protein L24

Chain S:  91% • 8%




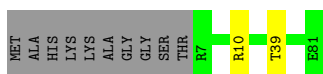
- Molecule 21: 50S ribosomal protein L25

Chain T:  95% ••



- Molecule 22: 50S ribosomal protein L27

Chain U:  86% • 12%



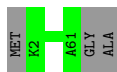
- Molecule 23: 50S ribosomal protein L28

Chain V:  96% ••



- Molecule 24: 50S ribosomal protein L29

Chain W:  95% 5%



- Molecule 25: 50S ribosomal protein L30

Chain X:  98% •

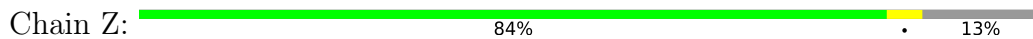


- Molecule 26: 50S ribosomal protein L32

Chain Y:  93% ••



- Molecule 27: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L34



There are no outlier residues recorded for this chain.

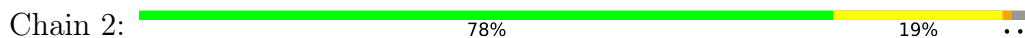
- Molecule 29: 50S ribosomal protein L35

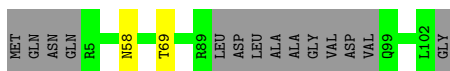


- Molecule 30: 50S ribosomal protein L36

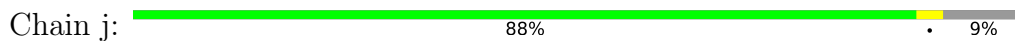


- Molecule 31: 23S ribosomal RNA

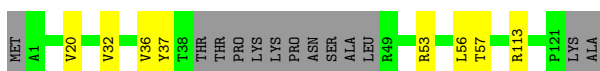
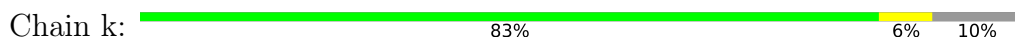




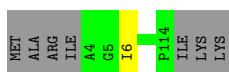
- Molecule 41: 30S ribosomal protein S11



- Molecule 42: 30S ribosomal protein S12



- Molecule 43: 30S ribosomal protein S13



- Molecule 44: 30S ribosomal protein S14



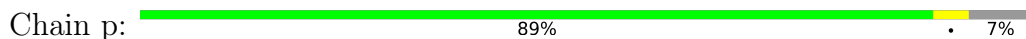
- Molecule 45: 30S ribosomal protein S15



- Molecule 46: 30S ribosomal protein S16

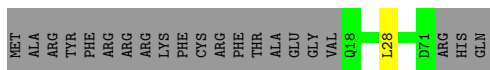


- Molecule 47: 30S ribosomal protein S17

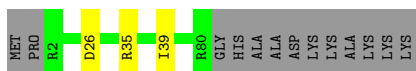
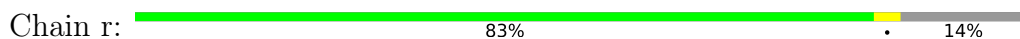




● Molecule 48: 30S ribosomal protein S18



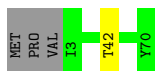
● Molecule 49: 30S ribosomal protein S19



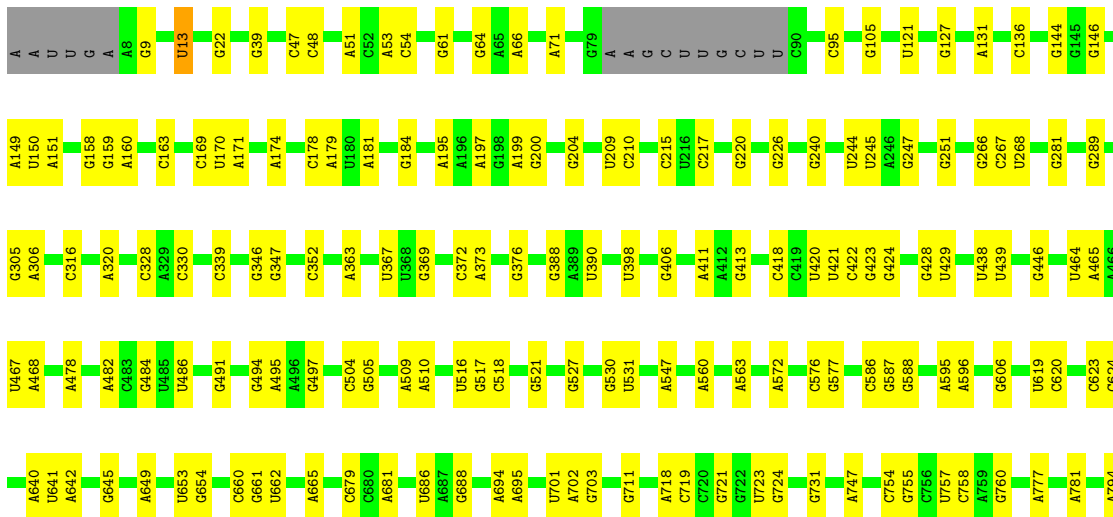
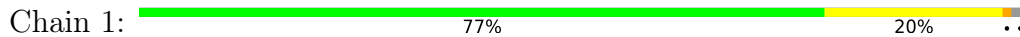
● Molecule 50: 30S ribosomal protein S20



● Molecule 51: 30S ribosomal protein S21



● Molecule 52: 16S ribosomal RNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	640261	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	75	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

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: MG

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	3	0.24	0/2872	0.86	1/4479 (0.0%)
2	5	0.27	0/1809	0.97	0/2819
3	A	0.25	0/2121	0.44	0/2852
4	B	0.25	0/1586	0.46	0/2134
5	C	0.24	0/1571	0.42	0/2113
6	D	0.25	0/1434	0.45	0/1926
7	E	0.25	0/1318	0.45	0/1786
8	F	0.25	0/373	0.48	0/502
9	G	0.24	0/1152	0.43	0/1551
10	I	0.25	0/956	0.46	0/1279
11	J	0.24	0/1052	0.44	0/1401
12	K	0.24	0/1093	0.42	0/1460
13	L	0.25	0/964	0.44	0/1289
14	M	0.25	0/885	0.44	0/1187
15	N	0.25	0/929	0.44	0/1242
16	O	0.25	0/960	0.35	0/1278
17	P	0.26	0/829	0.48	0/1107
18	Q	0.24	0/864	0.43	0/1156
19	R	0.24	0/720	0.43	0/962
20	S	0.25	0/741	0.44	0/984
21	T	0.24	0/758	0.43	0/1015
22	U	0.25	0/582	0.44	0/769
23	V	0.24	0/635	0.45	0/848
24	W	0.23	0/492	0.39	0/655
25	X	0.24	0/453	0.43	0/605
26	Y	0.24	0/440	0.45	0/588
27	Z	0.23	0/403	0.45	0/538
28	AA	0.23	0/380	0.40	0/498
29	AB	0.25	0/513	0.45	0/676
30	AC	0.25	0/303	0.46	0/397
31	2	0.25	0/68117	0.87	58/106268 (0.1%)
32	a	0.25	0/1703	0.43	0/2305

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	b	0.24	0/1528	0.43	0/2069
34	c	0.24	0/1289	0.44	0/1729
35	d	0.25	0/1159	0.47	0/1561
36	e	0.24	0/843	0.48	0/1140
37	f	0.24	0/750	0.46	0/1009
38	g	0.25	0/989	0.46	0/1326
39	h	0.26	0/960	0.53	1/1280 (0.1%)
40	i	0.24	0/735	0.46	0/991
41	j	0.25	0/893	0.47	0/1205
42	k	0.26	0/878	0.51	0/1176
43	l	0.23	0/868	0.44	0/1161
44	m	0.23	0/817	0.42	0/1088
45	n	0.23	0/710	0.41	0/950
46	o	0.25	0/659	0.42	0/884
47	p	0.24	0/641	0.46	0/860
48	q	0.24	0/449	0.43	0/604
49	r	0.28	0/652	0.51	0/877
50	s	0.25	0/661	0.37	0/876
51	t	0.23	0/573	0.36	0/759
52	1	0.25	0/36240	0.89	39/56532 (0.1%)
53	4	0.32	0/1037	0.98	3/1616 (0.2%)
All	All	0.25	0/152339	0.79	102/228362 (0.0%)

There are no bond length outliers.

The worst 5 of 102 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	2	2794	C	N3-C2-O2	-10.15	114.79	121.90
52	1	1141	C	N3-C2-O2	-9.63	115.16	121.90
31	2	2210	U	C2-N1-C1'	9.44	129.03	117.70
31	2	2210	U	N1-C2-O2	9.07	129.15	122.80
31	2	268	C	N3-C2-O2	-8.56	115.91	121.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [\(i\)](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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 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	
3	A	269/273 (98%)	260 (97%)	9 (3%)	0	100	100
4	B	207/209 (99%)	202 (98%)	5 (2%)	0	100	100
5	C	199/201 (99%)	192 (96%)	7 (4%)	0	100	100
6	D	175/179 (98%)	167 (95%)	8 (5%)	0	100	100
7	E	171/177 (97%)	160 (94%)	11 (6%)	0	100	100
8	F	46/149 (31%)	39 (85%)	7 (15%)	0	100	100
9	G	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
10	I	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
11	J	141/144 (98%)	136 (96%)	5 (4%)	0	100	100
12	K	134/136 (98%)	132 (98%)	2 (2%)	0	100	100
13	L	117/127 (92%)	112 (96%)	5 (4%)	0	100	100
14	M	112/117 (96%)	106 (95%)	6 (5%)	0	100	100
15	N	112/115 (97%)	103 (92%)	9 (8%)	0	100	100
16	O	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
17	P	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
18	Q	108/110 (98%)	103 (95%)	5 (5%)	0	100	100
19	R	88/100 (88%)	86 (98%)	2 (2%)	0	100	100
20	S	92/104 (88%)	92 (100%)	0	0	100	100
21	T	91/94 (97%)	87 (96%)	4 (4%)	0	100	100
22	U	73/85 (86%)	73 (100%)	0	0	100	100
23	V	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
24	W	58/63 (92%)	58 (100%)	0	0	100	100
25	X	56/59 (95%)	56 (100%)	0	0	100	100
26	Y	53/57 (93%)	53 (100%)	0	0	100	100
27	Z	46/55 (84%)	45 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	AA	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
29	AB	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
30	AC	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
32	a	218/241 (90%)	208 (95%)	10 (5%)	0	100	100
33	b	193/233 (83%)	188 (97%)	5 (3%)	0	100	100
34	c	157/206 (76%)	148 (94%)	9 (6%)	0	100	100
35	d	155/167 (93%)	152 (98%)	3 (2%)	0	100	100
36	e	99/135 (73%)	90 (91%)	9 (9%)	0	100	100
37	f	93/179 (52%)	86 (92%)	7 (8%)	0	100	100
38	g	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
39	h	119/130 (92%)	104 (87%)	15 (13%)	0	100	100
40	i	85/103 (82%)	80 (94%)	5 (6%)	0	100	100
41	j	115/129 (89%)	105 (91%)	10 (9%)	0	100	100
42	k	107/124 (86%)	93 (87%)	14 (13%)	0	100	100
43	l	109/118 (92%)	101 (93%)	8 (7%)	0	100	100
44	m	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
45	n	85/89 (96%)	84 (99%)	1 (1%)	0	100	100
46	o	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
47	p	76/84 (90%)	67 (88%)	9 (12%)	0	100	100
48	q	52/75 (69%)	50 (96%)	2 (4%)	0	100	100
49	r	77/92 (84%)	69 (90%)	8 (10%)	0	100	100
50	s	82/87 (94%)	80 (98%)	2 (2%)	0	100	100
51	t	66/71 (93%)	65 (98%)	1 (2%)	0	100	100
All	All	5235/5843 (90%)	5008 (96%)	227 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain 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 sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	216/218 (99%)	209 (97%)	7 (3%)	39	67
4	B	164/164 (100%)	158 (96%)	6 (4%)	34	62
5	C	165/165 (100%)	162 (98%)	3 (2%)	59	79
6	D	148/150 (99%)	140 (95%)	8 (5%)	22	52
7	E	134/138 (97%)	130 (97%)	4 (3%)	41	68
8	F	39/114 (34%)	36 (92%)	3 (8%)	13	40
9	G	116/116 (100%)	113 (97%)	3 (3%)	46	72
10	I	104/104 (100%)	102 (98%)	2 (2%)	57	78
11	J	102/103 (99%)	100 (98%)	2 (2%)	55	77
12	K	109/109 (100%)	106 (97%)	3 (3%)	43	70
13	L	99/103 (96%)	99 (100%)	0	100	100
14	M	84/87 (97%)	80 (95%)	4 (5%)	25	56
15	N	99/100 (99%)	94 (95%)	5 (5%)	24	54
16	O	89/90 (99%)	87 (98%)	2 (2%)	52	75
17	P	84/84 (100%)	81 (96%)	3 (4%)	35	63
18	Q	93/93 (100%)	87 (94%)	6 (6%)	17	46
19	R	77/84 (92%)	74 (96%)	3 (4%)	32	61
20	S	78/85 (92%)	77 (99%)	1 (1%)	69	84
21	T	77/78 (99%)	73 (95%)	4 (5%)	23	53
22	U	57/63 (90%)	55 (96%)	2 (4%)	36	65
23	V	67/68 (98%)	65 (97%)	2 (3%)	41	68
24	W	54/55 (98%)	54 (100%)	0	100	100
25	X	48/49 (98%)	48 (100%)	0	100	100
26	Y	46/48 (96%)	44 (96%)	2 (4%)	29	59
27	Z	44/49 (90%)	42 (96%)	2 (4%)	27	58
28	AA	38/38 (100%)	38 (100%)	0	100	100
29	AB	51/52 (98%)	49 (96%)	2 (4%)	32	61
30	AC	34/34 (100%)	32 (94%)	2 (6%)	19	49
32	a	171/199 (86%)	167 (98%)	4 (2%)	50	74
33	b	152/190 (80%)	147 (97%)	5 (3%)	38	66
34	c	133/173 (77%)	125 (94%)	8 (6%)	19	49
35	d	117/126 (93%)	114 (97%)	3 (3%)	46	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	e	88/116 (76%)	85 (97%)	3 (3%)	37	65
37	f	77/147 (52%)	76 (99%)	1 (1%)	69	84
38	g	104/105 (99%)	102 (98%)	2 (2%)	57	78
39	h	97/107 (91%)	93 (96%)	4 (4%)	30	59
40	i	80/90 (89%)	78 (98%)	2 (2%)	47	72
41	j	90/99 (91%)	86 (96%)	4 (4%)	28	58
42	k	93/104 (89%)	85 (91%)	8 (9%)	10	35
43	l	90/96 (94%)	89 (99%)	1 (1%)	73	86
44	m	83/84 (99%)	80 (96%)	3 (4%)	35	63
45	n	75/77 (97%)	73 (97%)	2 (3%)	44	70
46	o	65/65 (100%)	63 (97%)	2 (3%)	40	68
47	p	72/78 (92%)	69 (96%)	3 (4%)	30	59
48	q	47/65 (72%)	46 (98%)	1 (2%)	53	76
49	r	70/79 (89%)	67 (96%)	3 (4%)	29	59
50	s	64/66 (97%)	63 (98%)	1 (2%)	62	81
51	t	56/61 (92%)	55 (98%)	1 (2%)	59	79
All	All	4340/4768 (91%)	4198 (97%)	142 (3%)	41	66

5 of 142 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
41	j	64	VAL
42	k	36	VAL
45	n	69	LEU
15	N	59	THR
15	N	46	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
33	b	99	GLN
44	m	65	GLN
34	c	73	ASN
36	e	17	GLN
45	n	45	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	3	119/120 (99%)	33 (27%)	2 (1%)
2	5	75/76 (98%)	19 (25%)	0
31	2	2831/2903 (97%)	549 (19%)	9 (0%)
52	1	1505/1540 (97%)	303 (20%)	7 (0%)
53	4	42/93 (45%)	9 (21%)	0
All	All	4572/4732 (96%)	913 (19%)	18 (0%)

5 of 913 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	3	9	G
1	3	12	C
1	3	13	G
1	3	14	U
1	3	15	A

5 of 18 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
52	1	595	A
52	1	1300	G
52	1	1201	A
31	2	1340	U
52	1	509	A

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 55 ligands modelled in this entry, 55 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.