



## wwPDB EM Validation Summary Report ⓘ

Nov 13, 2022 – 08:10 PM EST

PDB ID : 6VWL  
EMDB ID : EMD-21420  
Title : 70S ribosome bound to HIV frameshifting stem-loop (FSS) and P/E tRNA  
(rotated conformation)  
Authors : Loerch, S.; Bao, C.; Ling, C.; Korostelev, A.A.; Grigorieff, N.; Ermolenko,  
D.M.  
Deposited on : 2020-02-20  
Resolution : 3.10 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](mailto: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:

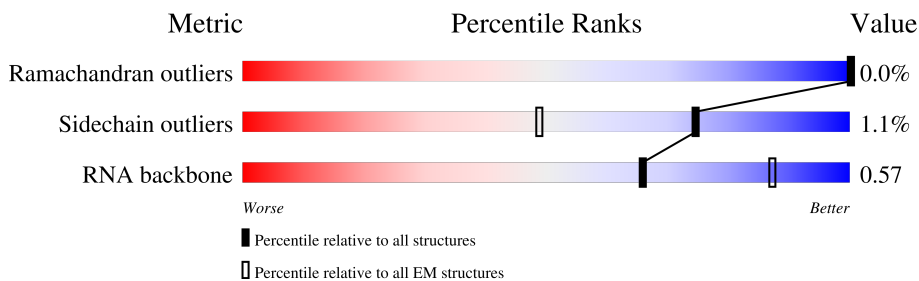
EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.10 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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	273	99%
2	B	209	98%
3	C	201	9% 100%
4	D	179	64% 96%
5	E	177	19% 97%
6	F	149	26% 38% 62%
7	G	142	100%
8	I	123	98%

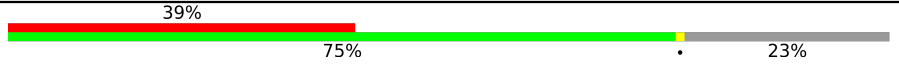
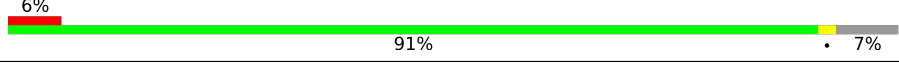


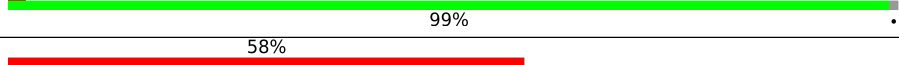
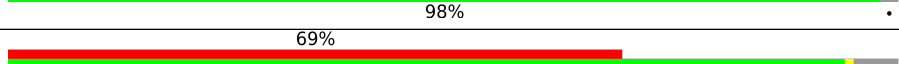
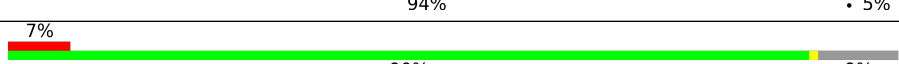
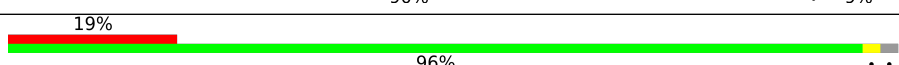
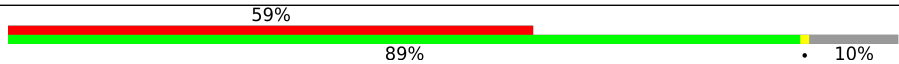
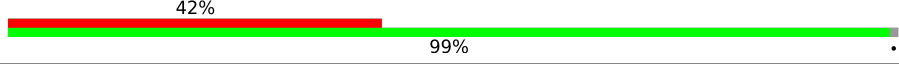
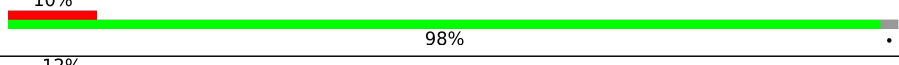
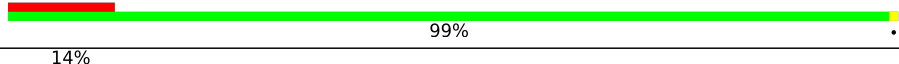
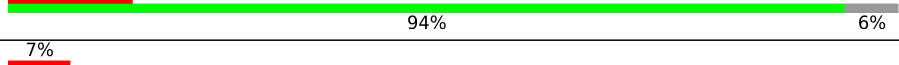

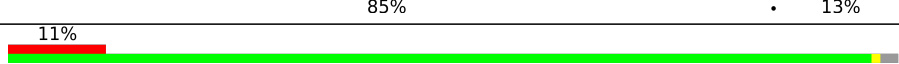
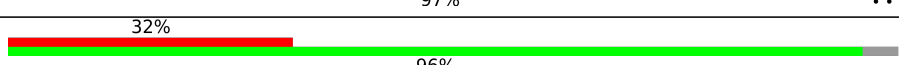




Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	J	144	99%
10	K	136	99%
11	L	127	93% 6%
12	M	117	15% 96%
13	N	115	99%
14	O	118	99%
15	P	103	6% 100%
16	Q	110	99%
17	R	100	89% 10%
18	S	104	91% 8%
19	T	94	7% 98%
20	U	85	87% 12%
21	V	78	97%
22	W	63	95% 5%
23	X	59	5% 98%
24	Y	57	95%
25	Z	55	15% 87% 13%
26	AA	46	98%
27	AB	65	98%
28	3	120	10% 84% 16%
29	5	76	18% 61% 39%
30	AC	38	100%
31	2	2903	8% 81% 16%
32	a	241	64% 91% 8%
33	b	233	37% 84% 15%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	c	206	
35	d	167	
36	e	135	
37	f	179	
38	g	130	
39	h	130	
40	i	103	
41	j	129	
42	k	124	
43	l	118	
44	m	101	
45	n	89	
46	o	82	
47	p	84	
48	q	75	
49	r	92	
50	s	87	
51	t	71	
52	1	1540	
53	4	93	

## 2 Entry composition [i](#)

There are 54 unique types of molecules in this entry. The entry contains 140603 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 50S ribosomal protein L2.

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

- Molecule 2 is a protein called 50S ribosomal protein L3.

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

- Molecule 3 is a protein called 50S ribosomal protein L4.

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

- Molecule 4 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	175	1396	890	246	254	6	0	0

- Molecule 5 is a protein called 50S ribosomal protein L6.

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

- Molecule 6 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	57	440	281	79	79	1	0	0

- Molecule 7 is a protein called 50S ribosomal protein L13.

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

- Molecule 8 is a protein called 50S ribosomal protein L14.

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

- Molecule 9 is a protein called 50S ribosomal protein L15.

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

- Molecule 10 is a protein called 50S ribosomal protein L16.

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

- Molecule 11 is a protein called 50S ribosomal protein L17.

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

- Molecule 12 is a protein called 50S ribosomal protein L18.

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

- Molecule 13 is a protein called 50S ribosomal protein L19.

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

- Molecule 14 is a protein called 50S ribosomal protein L20.

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

- Molecule 15 is a protein called 50S ribosomal protein L21.

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

- Molecule 16 is a protein called 50S ribosomal protein L22.

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

- Molecule 17 is a protein called 50S ribosomal protein L23.

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

- Molecule 18 is a protein called 50S ribosomal protein L24.

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

- Molecule 19 is a protein called 50S ribosomal protein L25.

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

- Molecule 20 is a protein called 50S ribosomal protein L27.

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

- Molecule 21 is a protein called 50S ribosomal protein L28.

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

- Molecule 22 is a protein called 50S ribosomal protein L29.

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

- Molecule 23 is a protein called 50S ribosomal protein L30.

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

- Molecule 24 is a protein called 50S ribosomal protein L32.

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

- Molecule 25 is a protein called 50S ribosomal protein L33.

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

- Molecule 26 is a protein called 50S ribosomal protein L34.

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

- Molecule 27 is a protein called 50S ribosomal protein L35.

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

- Molecule 28 is a RNA chain called 5S ribosomal RNA.



Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
28	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 29 is a RNA chain called tRNAPhe.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
29	5	76	1625	724	292	533	76	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	47	G	U	conflict	GB 984297099
5	48	U	C	conflict	GB 984297099

- 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

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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
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	222	1689	1071	296	315	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	158	1262	790	236	233	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	156	1137	709	214	208	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	e	102	Total	C	N	O	S	0	0
			832	525	150	150	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	f	108	Total	C	N	O	S	0	0
			837	525	158	151	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	127	Total	C	N	O	S	0	0
			1006	626	200	178	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	i	98	Total	C	N	O	S	0	0
			786	493	150	142	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	121	Total	C	N	O	S	0	0
			940	581	193	162	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	l	106	Total	C	N	O	S	0	0
			806	500	156	147	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	79	Total	C	N	O	S	0	0
			641	406	120	112	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	80	Total	C	N	O	S	0	0
			644	413	121	108	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	s	85	660	409	137	111	3	0	0

- 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	1521	32632	14554	5986	10571	1521	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 HIV 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

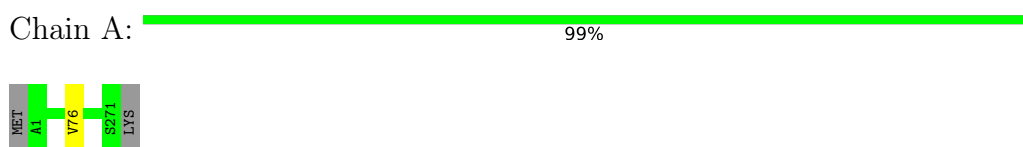
- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
54	A	1	Total	Mg	0
			1	1	
54	B	1	Total	Mg	0
			1	1	
54	3	5	Total	Mg	0
			5	5	
54	2	26	Total	Mg	0
			26	26	
54	1	1	Total	Mg	0
			1	1	

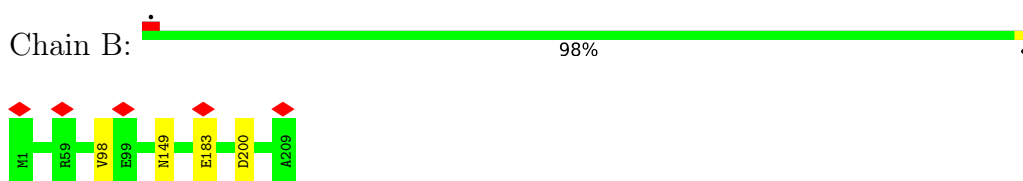
### 3 Residue-property plots [i](#)

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 and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

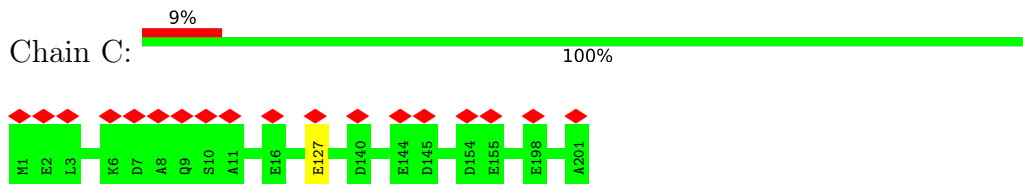
- Molecule 1: 50S ribosomal protein L2



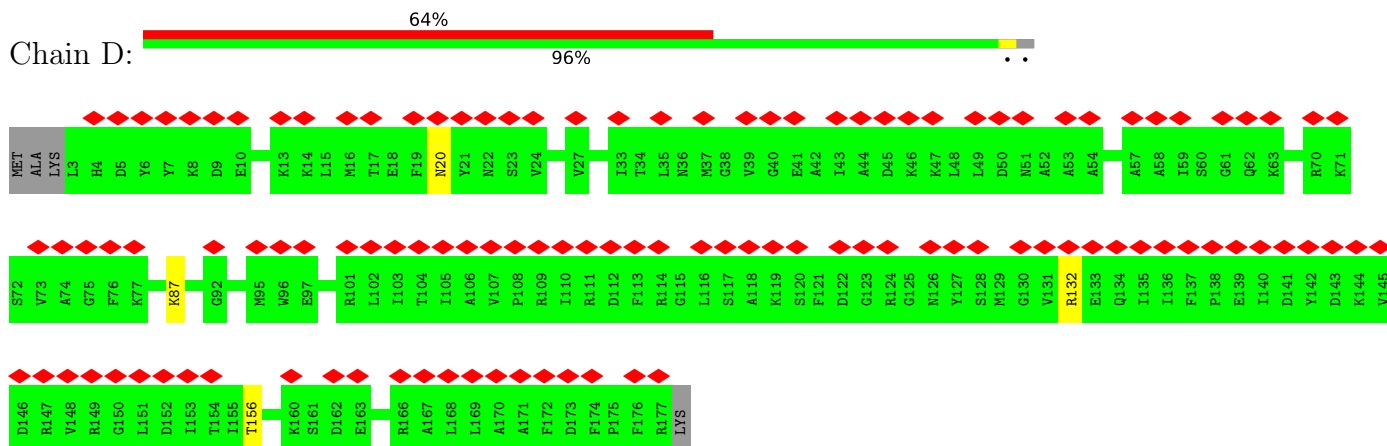
- Molecule 2: 50S ribosomal protein L3



- Molecule 3: 50S ribosomal protein L4

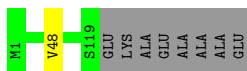


- Molecule 4: 50S ribosomal protein L5



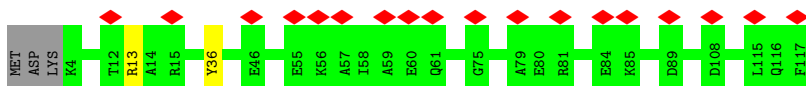


Chain L:  93% • 6%



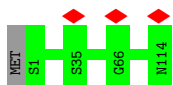
- Molecule 12: 50S ribosomal protein L18

Chain M:  15% 96%



- Molecule 13: 50S ribosomal protein L19

Chain N:  99%



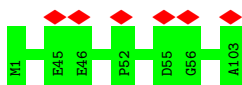
- Molecule 14: 50S ribosomal protein L20

Chain O:  99%



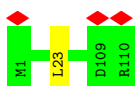
- Molecule 15: 50S ribosomal protein L21

Chain P:  6% 100%




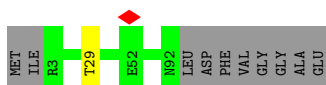
- Molecule 16: 50S ribosomal protein L22

Chain Q:  99%




- Molecule 17: 50S ribosomal protein L23

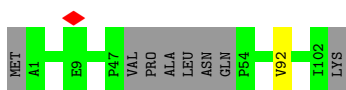
Chain R:  89% • 10%





- Molecule 18: 50S ribosomal protein L24

Chain S:  91% 8%



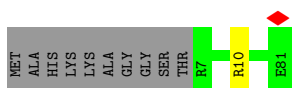
- Molecule 19: 50S ribosomal protein L25

Chain T:  98% 7%



- Molecule 20: 50S ribosomal protein L27

Chain U:  87% 12%



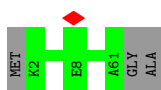
- Molecule 21: 50S ribosomal protein L28

Chain V:  97%



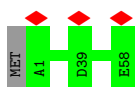
- Molecule 22: 50S ribosomal protein L29

Chain W:  95% 5%



- Molecule 23: 50S ribosomal protein L30

Chain X:  98% 5%

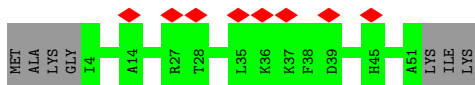
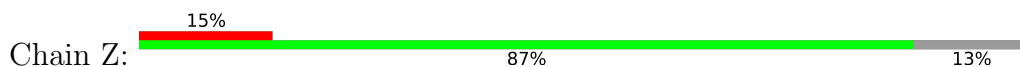


- Molecule 24: 50S ribosomal protein L32

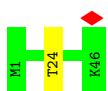
Chain Y:  95%



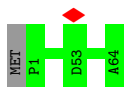
- Molecule 25: 50S ribosomal protein L33



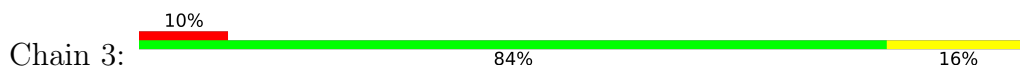
- Molecule 26: 50S ribosomal protein L34



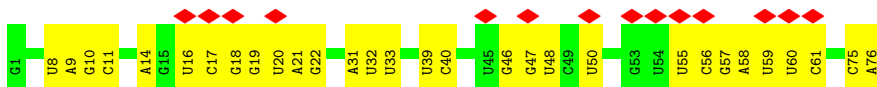
- Molecule 27: 50S ribosomal protein L35



- Molecule 28: 5S ribosomal RNA



- Molecule 29: tRNAPhe

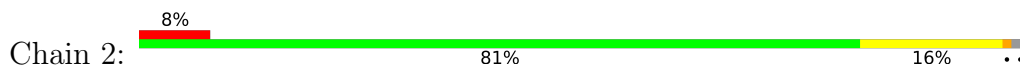


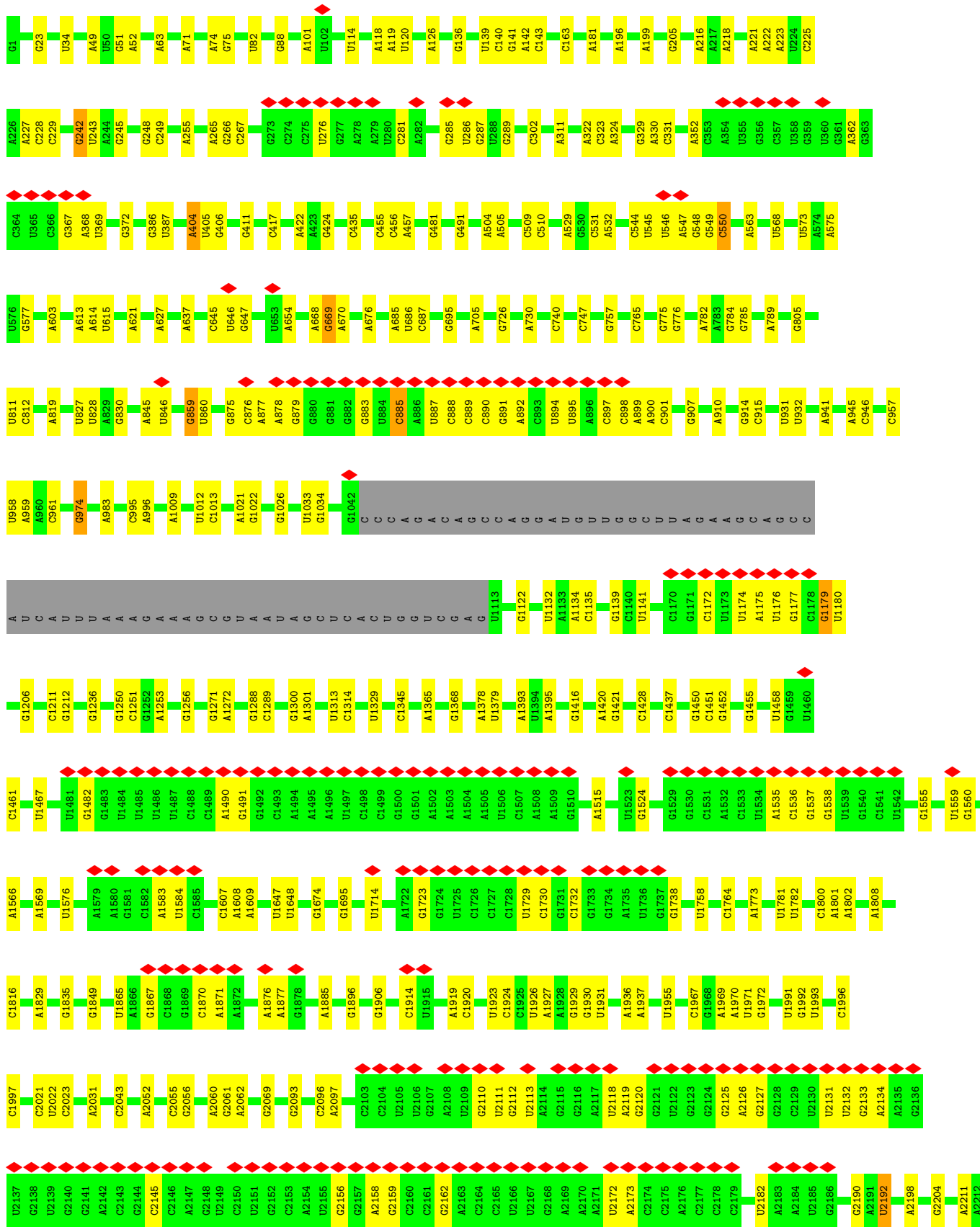
- Molecule 30: 50S ribosomal protein L36

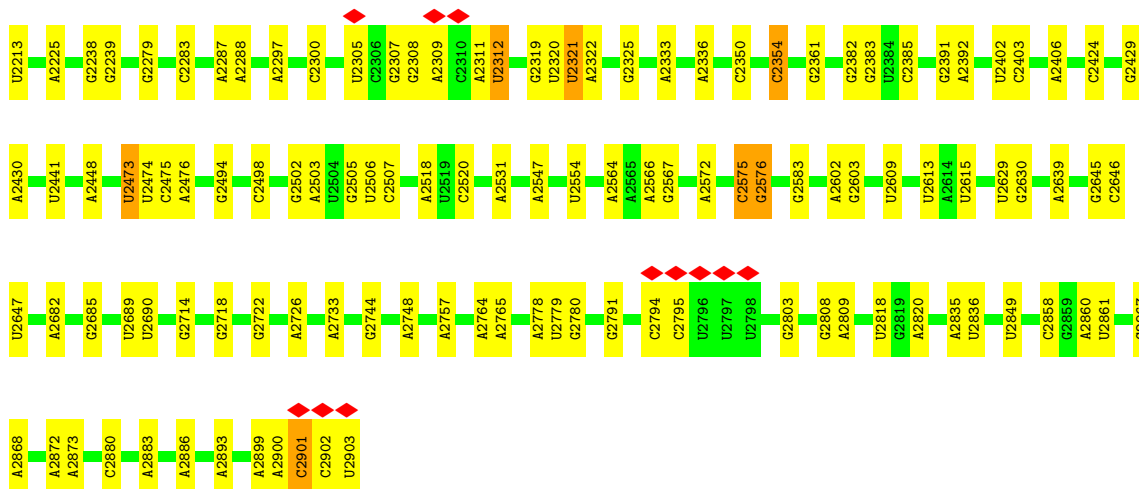


There are no outlier residues recorded for this chain.

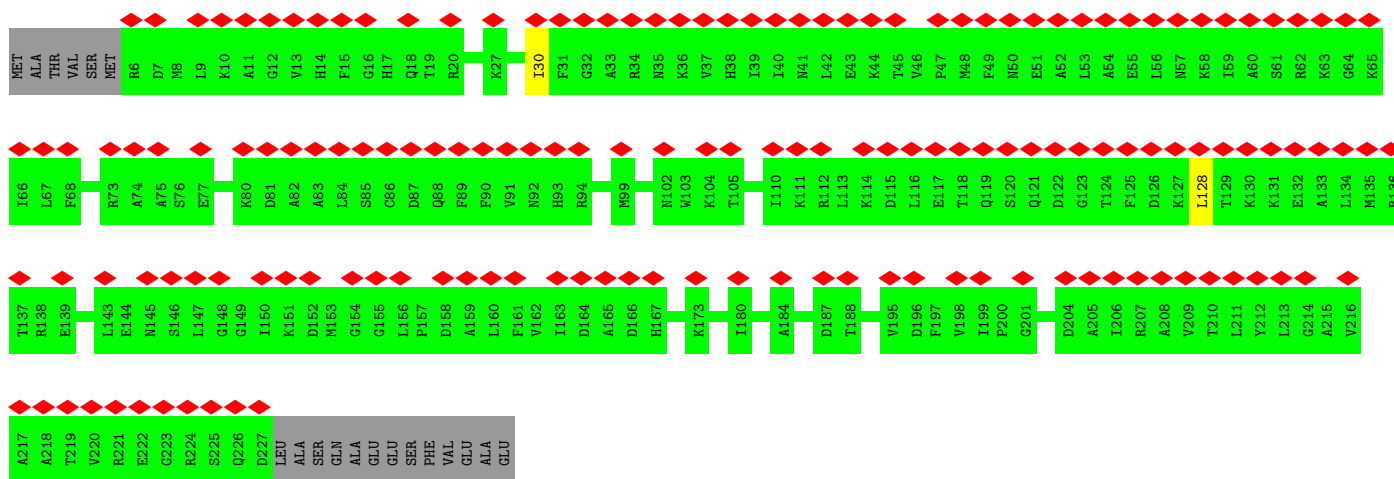
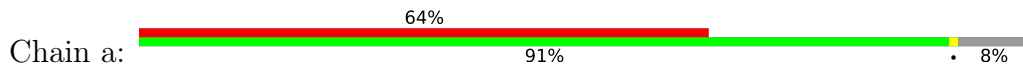
- Molecule 31: 23S ribosomal RNA



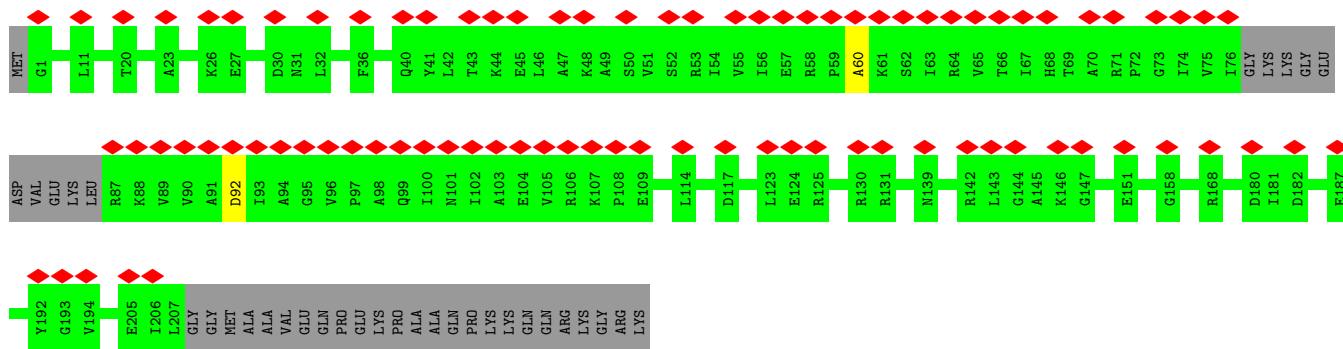
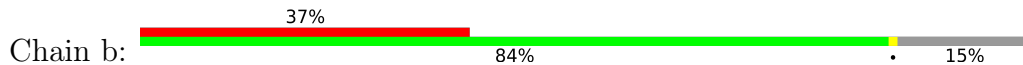




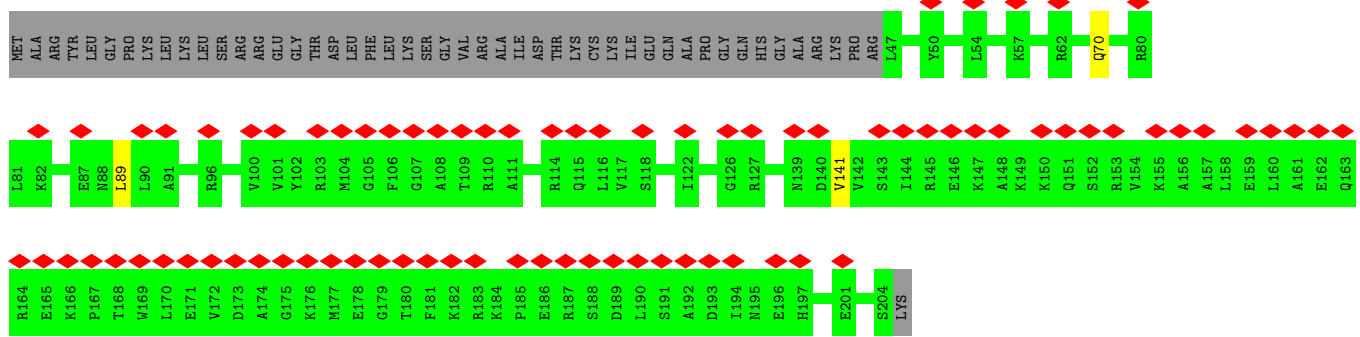
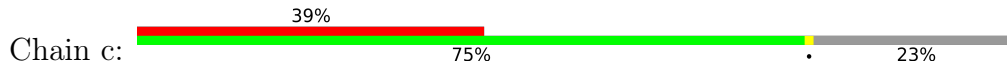
• Molecule 32: 30S ribosomal protein S2



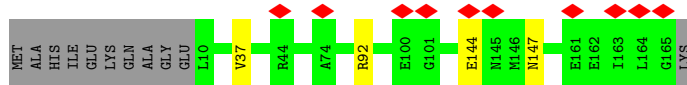
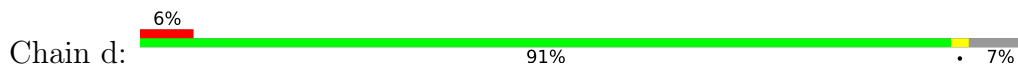
• Molecule 33: 30S ribosomal protein S3



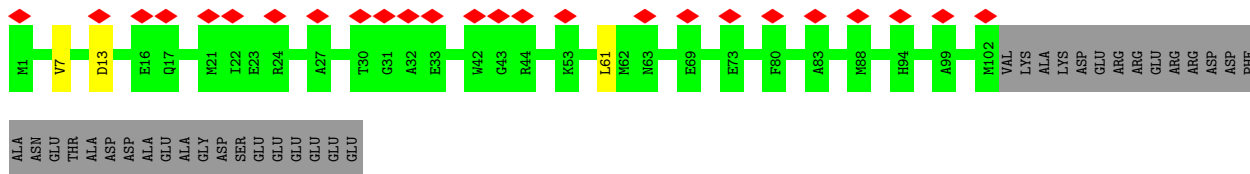
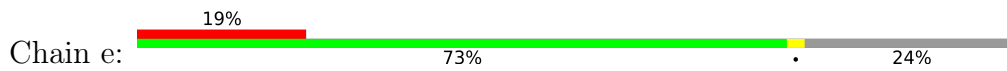
• Molecule 34: 30S ribosomal protein S4



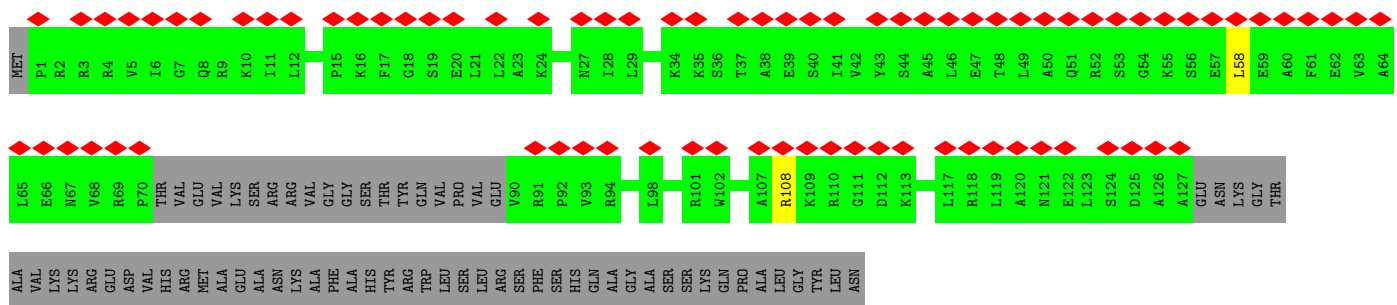
- Molecule 35: 30S ribosomal protein S5



- Molecule 36: 30S ribosomal protein S6

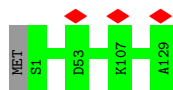


- Molecule 37: 30S ribosomal protein S7

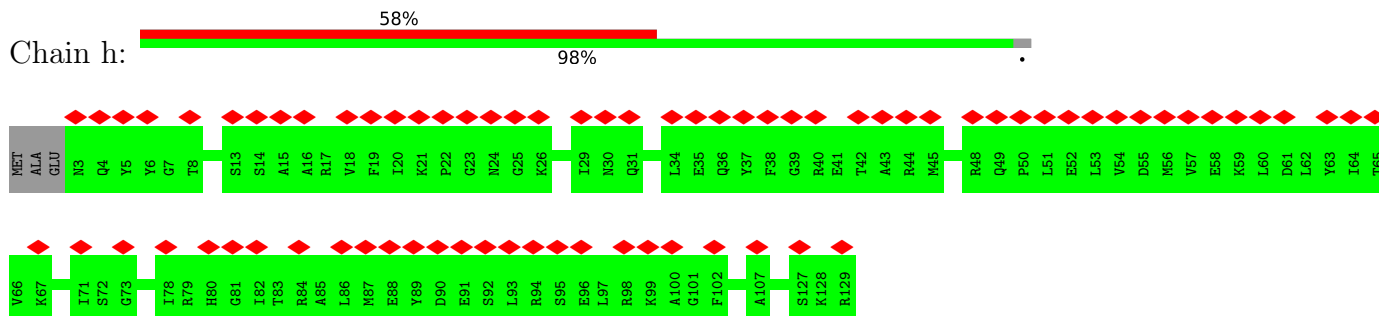


- Molecule 38: 30S ribosomal protein S8

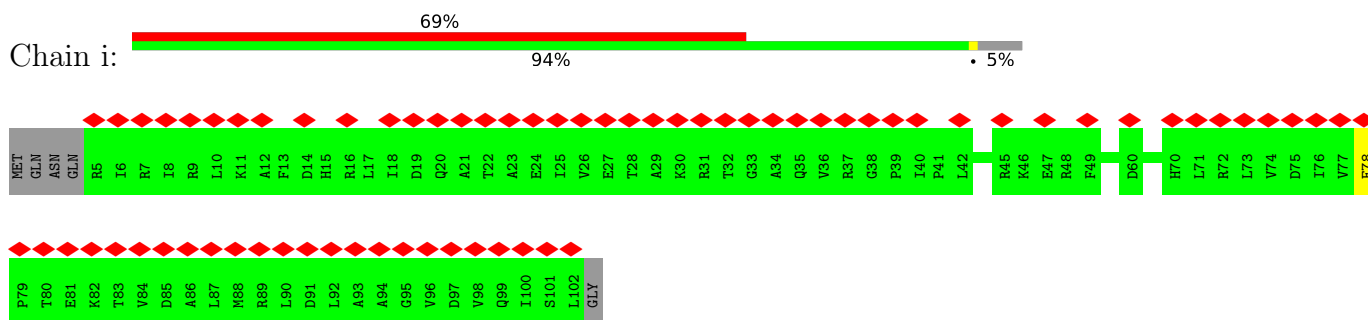




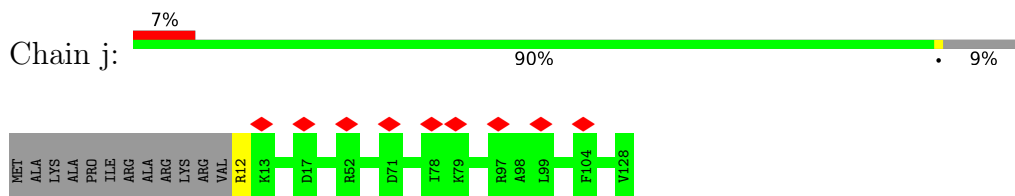
- Molecule 39: 30S ribosomal protein S9



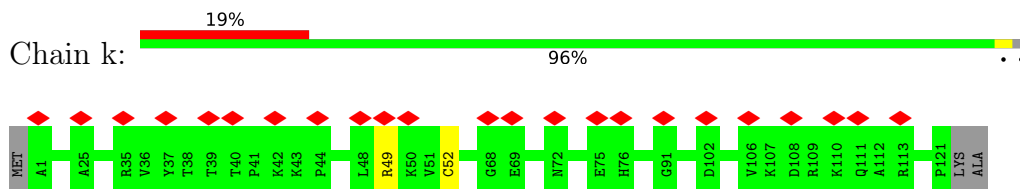
- Molecule 40: 30S ribosomal protein S10



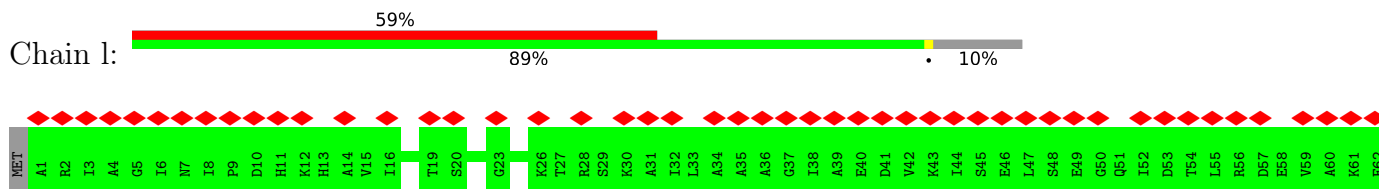
- Molecule 41: 30S ribosomal protein S11

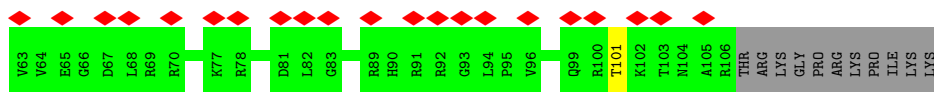


- Molecule 42: 30S ribosomal protein S12

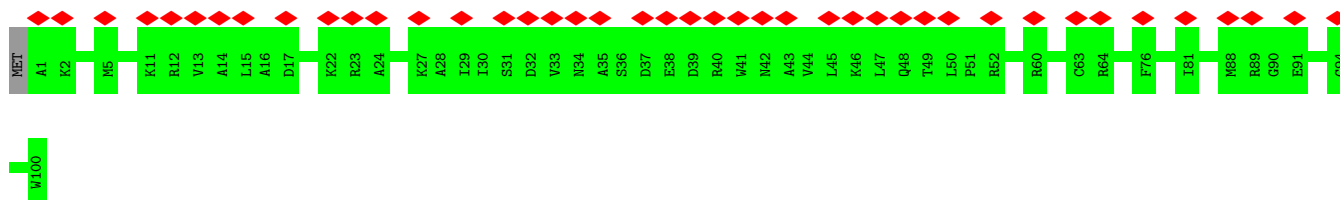
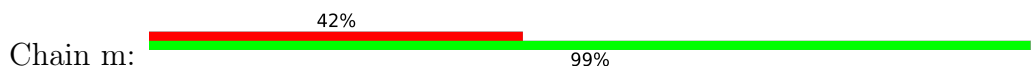


- Molecule 43: 30S ribosomal protein S13

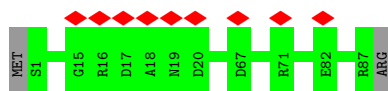




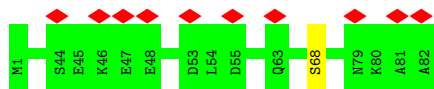
- Molecule 44: 30S ribosomal protein S14



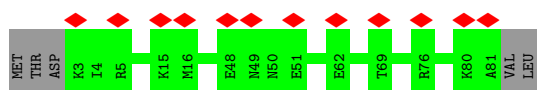
- Molecule 45: 30S ribosomal protein S15



- Molecule 46: 30S ribosomal protein S16



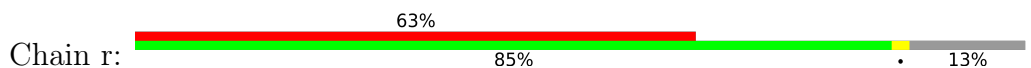
- Molecule 47: 30S ribosomal protein S17

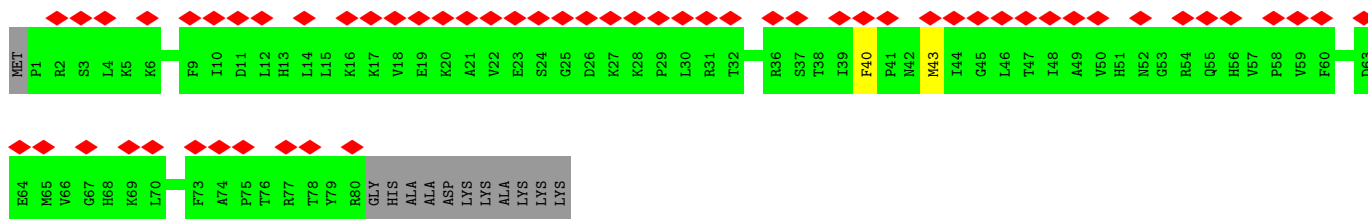


- Molecule 48: 30S ribosomal protein S18

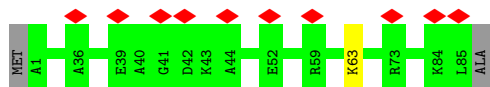


- Molecule 49: 30S ribosomal protein S19

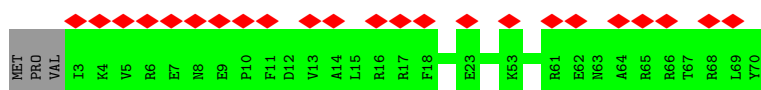




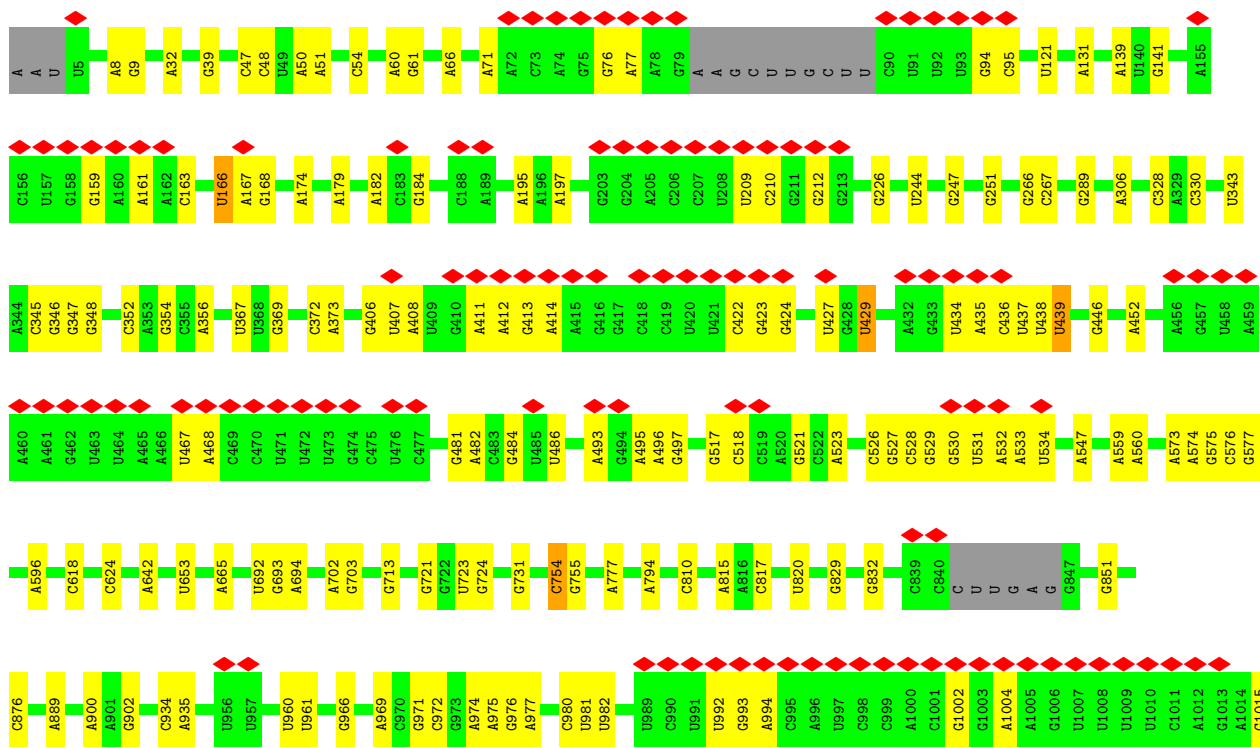
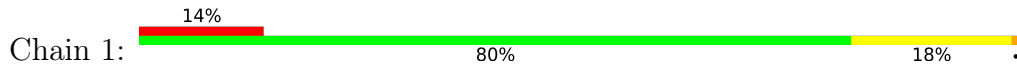
• Molecule 50: 30S ribosomal protein S20



• 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
Maximum map value	32.492	Depositor
Minimum map value	-11.578	Depositor
Average map value	0.189	Depositor
Map value standard deviation	1.179	Depositor
Recommended contour level	7.0	Depositor
Map size (Å)	654.48, 654.48, 654.48	wwPDB
Map dimensions	648, 648, 648	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.01, 1.01, 1.01	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	A	0.37	0/2121	0.49	0/2852
2	B	0.37	0/1586	0.50	0/2134
3	C	0.34	0/1571	0.44	0/2113
4	D	0.28	0/1420	0.44	0/1908
5	E	0.30	0/1318	0.46	0/1786
6	F	0.29	0/445	0.49	0/597
7	G	0.36	0/1152	0.45	0/1551
8	I	0.35	0/956	0.48	0/1279
9	J	0.35	0/1052	0.48	0/1401
10	K	0.33	0/1093	0.46	0/1460
11	L	0.33	0/964	0.47	0/1289
12	M	0.28	0/885	0.44	0/1187
13	N	0.34	0/929	0.47	0/1242
14	O	0.38	0/960	0.40	0/1278
15	P	0.36	0/829	0.48	0/1107
16	Q	0.34	0/864	0.48	0/1156
17	R	0.31	0/720	0.44	0/962
18	S	0.32	0/741	0.46	0/984
19	T	0.31	0/758	0.45	0/1015
20	U	0.35	0/582	0.44	0/769
21	V	0.32	0/635	0.45	0/848
22	W	0.27	0/492	0.39	0/655
23	X	0.33	0/453	0.46	0/605
24	Y	0.36	0/440	0.49	0/588
25	Z	0.29	0/403	0.45	0/538
26	AA	0.34	0/380	0.43	0/498
27	AB	0.31	0/513	0.47	0/676
28	3	0.43	0/2872	0.85	0/4479
29	5	0.33	0/1816	0.89	0/2830
30	AC	0.30	0/303	0.50	0/397
31	2	0.62	1/68117 (0.0%)	0.88	48/106268 (0.0%)
32	a	0.27	0/1720	0.42	0/2328

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	b	0.28	0/1528	0.45	0/2069
34	c	0.26	0/1278	0.44	0/1715
35	d	0.29	0/1150	0.47	0/1549
36	e	0.29	0/851	0.49	0/1150
37	f	0.26	0/846	0.46	0/1135
38	g	0.31	0/989	0.45	0/1326
39	h	0.26	0/1018	0.47	0/1358
40	i	0.27	0/796	0.48	0/1077
41	j	0.28	0/893	0.45	0/1205
42	k	0.30	0/954	0.51	0/1282
43	l	0.27	0/813	0.48	0/1090
44	m	0.25	0/817	0.42	0/1088
45	n	0.29	0/710	0.41	0/950
46	o	0.29	0/659	0.44	0/884
47	p	0.30	0/650	0.46	0/871
48	q	0.30	0/449	0.43	0/604
49	r	0.29	0/660	0.53	0/888
50	s	0.26	0/666	0.40	0/883
51	t	0.26	0/573	0.38	0/759
52	1	0.44	0/36536	0.87	53/56991 (0.1%)
53	4	0.30	0/1037	0.89	0/1616
All	All	0.50	1/152963 (0.0%)	0.79	101/229270 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	2	887	U	C1'-N1	5.45	1.56	1.48

The worst 5 of 101 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	2	2473	U	C2-N1-C1'	10.35	130.12	117.70
52	1	429	U	C2-N1-C1'	9.12	128.64	117.70
52	1	166	U	C2-N1-C1'	8.62	128.04	117.70
52	1	1516	G	C2-N3-C4	8.41	116.10	111.90
31	2	2473	U	N1-C2-O2	8.32	128.62	122.80

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 [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	269/273 (98%)	263 (98%)	6 (2%)	0	100	100
2	B	207/209 (99%)	201 (97%)	6 (3%)	0	100	100
3	C	199/201 (99%)	192 (96%)	7 (4%)	0	100	100
4	D	173/179 (97%)	164 (95%)	9 (5%)	0	100	100
5	E	171/177 (97%)	166 (97%)	5 (3%)	0	100	100
6	F	55/149 (37%)	54 (98%)	1 (2%)	0	100	100
7	G	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
8	I	121/123 (98%)	118 (98%)	3 (2%)	0	100	100
9	J	141/144 (98%)	134 (95%)	7 (5%)	0	100	100
10	K	134/136 (98%)	129 (96%)	5 (4%)	0	100	100
11	L	117/127 (92%)	110 (94%)	7 (6%)	0	100	100
12	M	112/117 (96%)	106 (95%)	6 (5%)	0	100	100
13	N	112/115 (97%)	105 (94%)	7 (6%)	0	100	100
14	O	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
15	P	101/103 (98%)	93 (92%)	8 (8%)	0	100	100
16	Q	108/110 (98%)	104 (96%)	4 (4%)	0	100	100
17	R	88/100 (88%)	86 (98%)	2 (2%)	0	100	100
18	S	92/104 (88%)	91 (99%)	1 (1%)	0	100	100
19	T	91/94 (97%)	89 (98%)	2 (2%)	0	100	100
20	U	73/85 (86%)	70 (96%)	3 (4%)	0	100	100
21	V	75/78 (96%)	74 (99%)	1 (1%)	0	100	100

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	W	58/63 (92%)	58 (100%)	0	0	100	100
23	X	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
24	Y	53/57 (93%)	53 (100%)	0	0	100	100
25	Z	46/55 (84%)	46 (100%)	0	0	100	100
26	AA	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
27	AB	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
30	AC	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
32	a	220/241 (91%)	206 (94%)	14 (6%)	0	100	100
33	b	193/233 (83%)	187 (97%)	5 (3%)	1 (0%)	29	64
34	c	156/206 (76%)	147 (94%)	9 (6%)	0	100	100
35	d	154/167 (92%)	149 (97%)	5 (3%)	0	100	100
36	e	100/135 (74%)	96 (96%)	4 (4%)	0	100	100
37	f	104/179 (58%)	101 (97%)	3 (3%)	0	100	100
38	g	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
39	h	125/130 (96%)	114 (91%)	11 (9%)	0	100	100
40	i	96/103 (93%)	88 (92%)	8 (8%)	0	100	100
41	j	115/129 (89%)	111 (96%)	4 (4%)	0	100	100
42	k	119/124 (96%)	109 (92%)	10 (8%)	0	100	100
43	l	104/118 (88%)	95 (91%)	9 (9%)	0	100	100
44	m	98/101 (97%)	91 (93%)	7 (7%)	0	100	100
45	n	85/89 (96%)	83 (98%)	2 (2%)	0	100	100
46	o	80/82 (98%)	77 (96%)	3 (4%)	0	100	100
47	p	77/84 (92%)	72 (94%)	5 (6%)	0	100	100
48	q	52/75 (69%)	51 (98%)	1 (2%)	0	100	100
49	r	78/92 (85%)	67 (86%)	10 (13%)	1 (1%)	12	42
50	s	83/87 (95%)	80 (96%)	3 (4%)	0	100	100
51	t	66/71 (93%)	61 (92%)	5 (8%)	0	100	100
All	All	5281/5843 (90%)	5056 (96%)	223 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
33	b	60	ALA

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
49	r	40	PHE

### 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
1	A	216/218 (99%)	215 (100%)	1 (0%)	88 94
2	B	164/164 (100%)	160 (98%)	4 (2%)	49 76
3	C	165/165 (100%)	164 (99%)	1 (1%)	86 94
4	D	147/150 (98%)	143 (97%)	4 (3%)	44 74
5	E	134/138 (97%)	133 (99%)	1 (1%)	84 93
6	F	45/114 (40%)	45 (100%)	0	100 100
7	G	116/116 (100%)	116 (100%)	0	100 100
8	I	104/104 (100%)	101 (97%)	3 (3%)	42 72
9	J	102/103 (99%)	101 (99%)	1 (1%)	76 90
10	K	109/109 (100%)	108 (99%)	1 (1%)	78 91
11	L	99/103 (96%)	98 (99%)	1 (1%)	76 90
12	M	84/87 (97%)	82 (98%)	2 (2%)	49 76
13	N	99/100 (99%)	99 (100%)	0	100 100
14	O	89/90 (99%)	89 (100%)	0	100 100
15	P	84/84 (100%)	84 (100%)	0	100 100
16	Q	93/93 (100%)	92 (99%)	1 (1%)	73 89
17	R	77/84 (92%)	76 (99%)	1 (1%)	69 87
18	S	78/85 (92%)	77 (99%)	1 (1%)	69 87
19	T	77/78 (99%)	76 (99%)	1 (1%)	69 87
20	U	57/63 (90%)	56 (98%)	1 (2%)	59 82
21	V	67/68 (98%)	66 (98%)	1 (2%)	65 85
22	W	54/55 (98%)	54 (100%)	0	100 100
23	X	48/49 (98%)	48 (100%)	0	100 100

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	Y	46/48 (96%)	45 (98%)	1 (2%)	52	78
25	Z	44/49 (90%)	44 (100%)	0	100	100
26	AA	38/38 (100%)	37 (97%)	1 (3%)	46	74
27	AB	51/52 (98%)	51 (100%)	0	100	100
30	AC	34/34 (100%)	34 (100%)	0	100	100
32	a	173/199 (87%)	171 (99%)	2 (1%)	71	88
33	b	152/190 (80%)	151 (99%)	1 (1%)	84	93
34	c	132/173 (76%)	129 (98%)	3 (2%)	50	77
35	d	116/126 (92%)	112 (97%)	4 (3%)	37	69
36	e	89/116 (77%)	86 (97%)	3 (3%)	37	69
37	f	87/147 (59%)	85 (98%)	2 (2%)	50	77
38	g	104/105 (99%)	104 (100%)	0	100	100
39	h	102/107 (95%)	102 (100%)	0	100	100
40	i	86/90 (96%)	85 (99%)	1 (1%)	71	88
41	j	90/99 (91%)	89 (99%)	1 (1%)	73	89
42	k	102/104 (98%)	100 (98%)	2 (2%)	55	80
43	l	83/96 (86%)	82 (99%)	1 (1%)	71	88
44	m	83/84 (99%)	83 (100%)	0	100	100
45	n	75/77 (97%)	75 (100%)	0	100	100
46	o	65/65 (100%)	64 (98%)	1 (2%)	65	85
47	p	73/78 (94%)	73 (100%)	0	100	100
48	q	47/65 (72%)	47 (100%)	0	100	100
49	r	71/79 (90%)	70 (99%)	1 (1%)	67	86
50	s	64/66 (97%)	63 (98%)	1 (2%)	62	84
51	t	56/61 (92%)	56 (100%)	0	100	100
All	All	4371/4768 (92%)	4321 (99%)	50 (1%)	74	89

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
32	a	128	LEU
35	d	144	GLU
50	s	63	LYS

Continued on next page...



*Continued from previous page...*

Mol	Chain	Res	Type
33	b	92	ASP
34	c	141	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
20	U	42	HIS
34	c	70	GLN
49	r	42	ASN
21	V	5	GLN
24	Y	5	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
28	3	119/120 (99%)	19 (15%)	0
29	5	75/76 (98%)	28 (37%)	5 (6%)
31	2	2831/2903 (97%)	454 (16%)	9 (0%)
52	1	1518/1540 (98%)	268 (17%)	6 (0%)
53	4	42/93 (45%)	10 (23%)	0
All	All	4585/4732 (96%)	779 (16%)	20 (0%)

5 of 779 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
28	3	4	C
28	3	12	C
28	3	13	G
28	3	14	U
28	3	15	A

5 of 20 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
52	1	407	U
52	1	1167	A
52	1	1474	U
52	1	1347	G
31	2	242	G

## 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 34 ligands modelled in this entry, 34 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

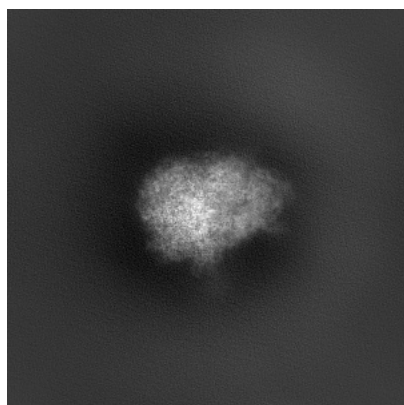
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21420. These allow visual inspection of the internal detail of the map and identification of artifacts.

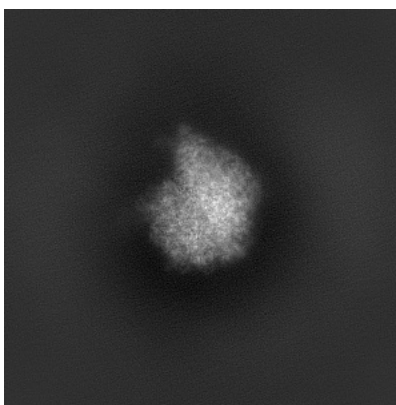
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

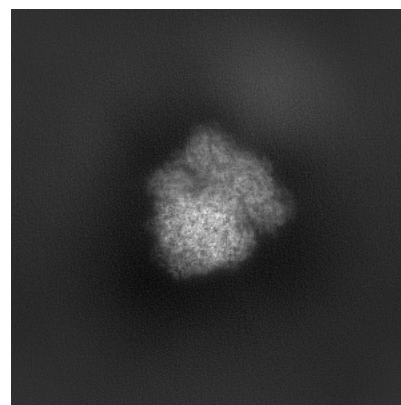
#### 6.1.1 Primary map



X



Y

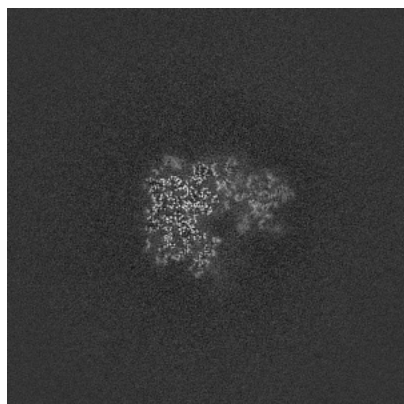


Z

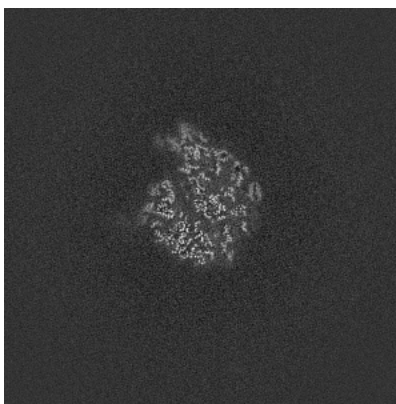
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

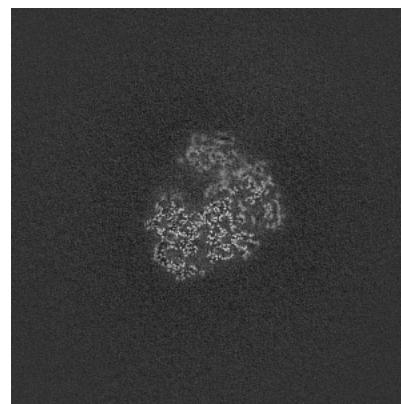
#### 6.2.1 Primary map



X Index: 324



Y Index: 324

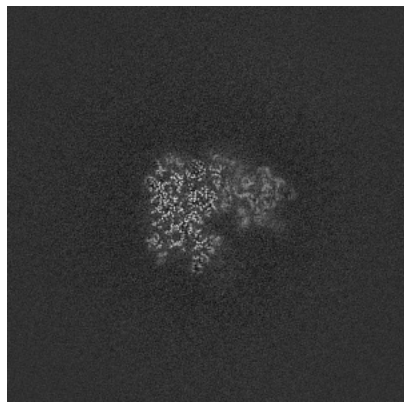


Z Index: 324

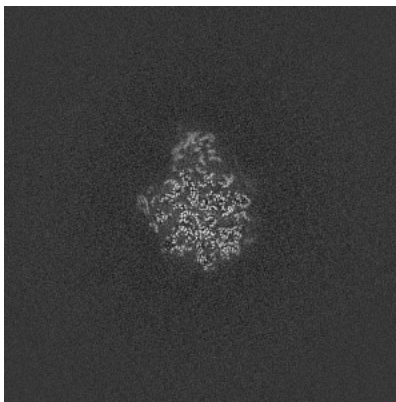
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

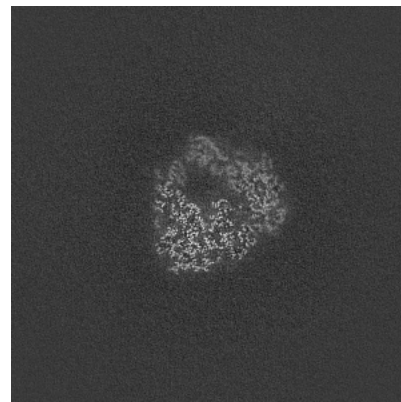
### 6.3.1 Primary map



X Index: 330



Y Index: 302



Z Index: 310

The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

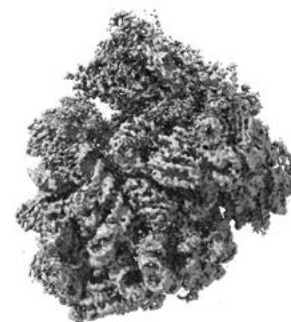
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 7.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

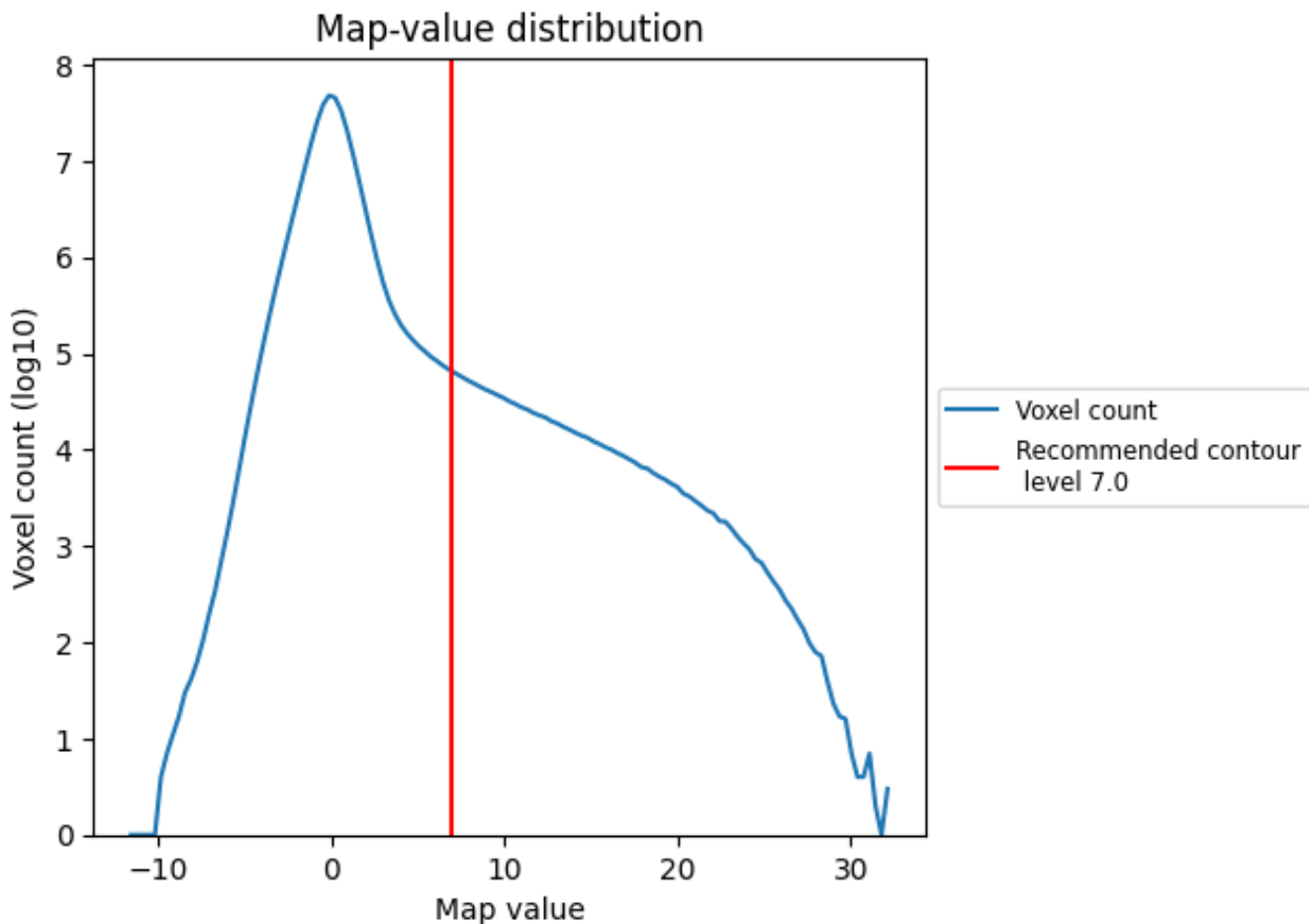
## 6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

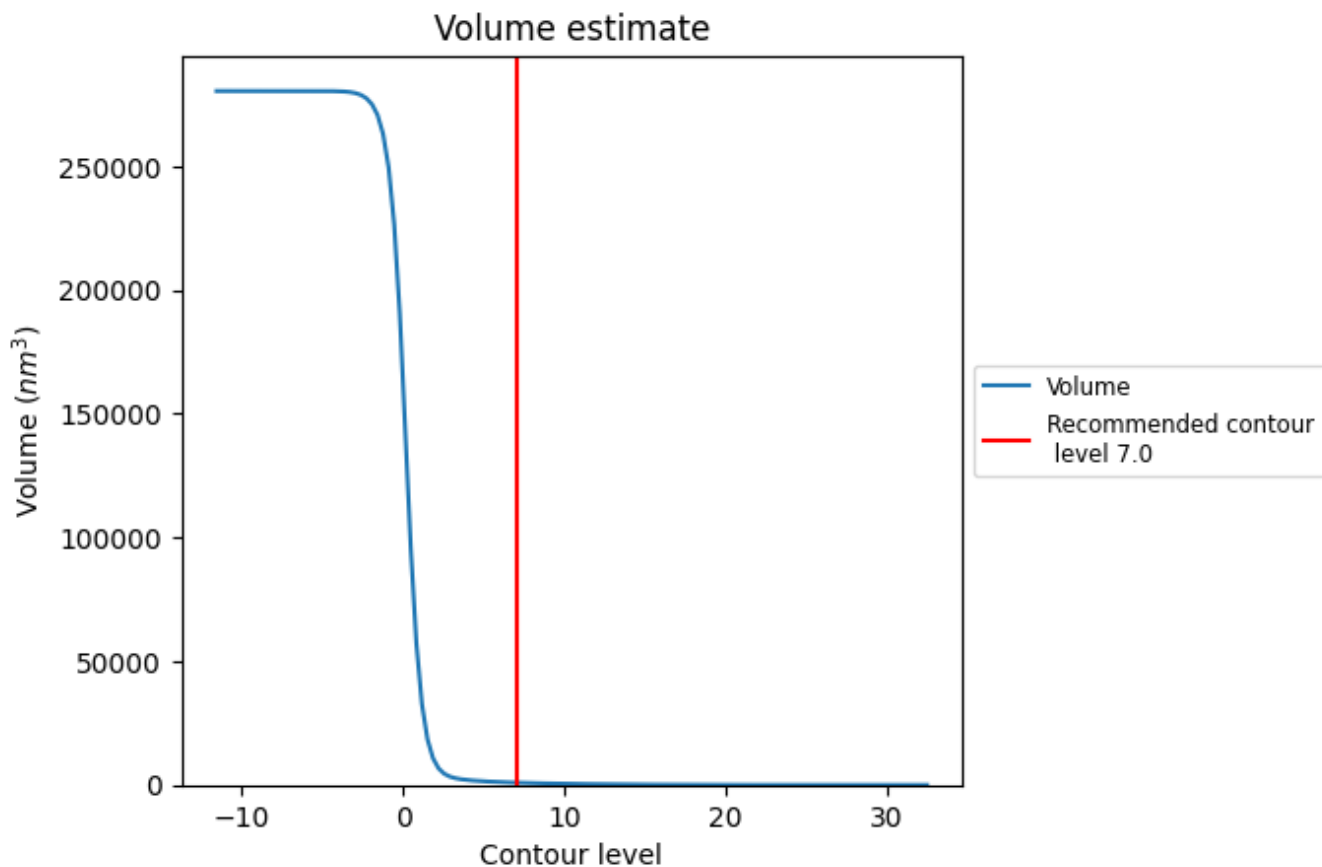
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

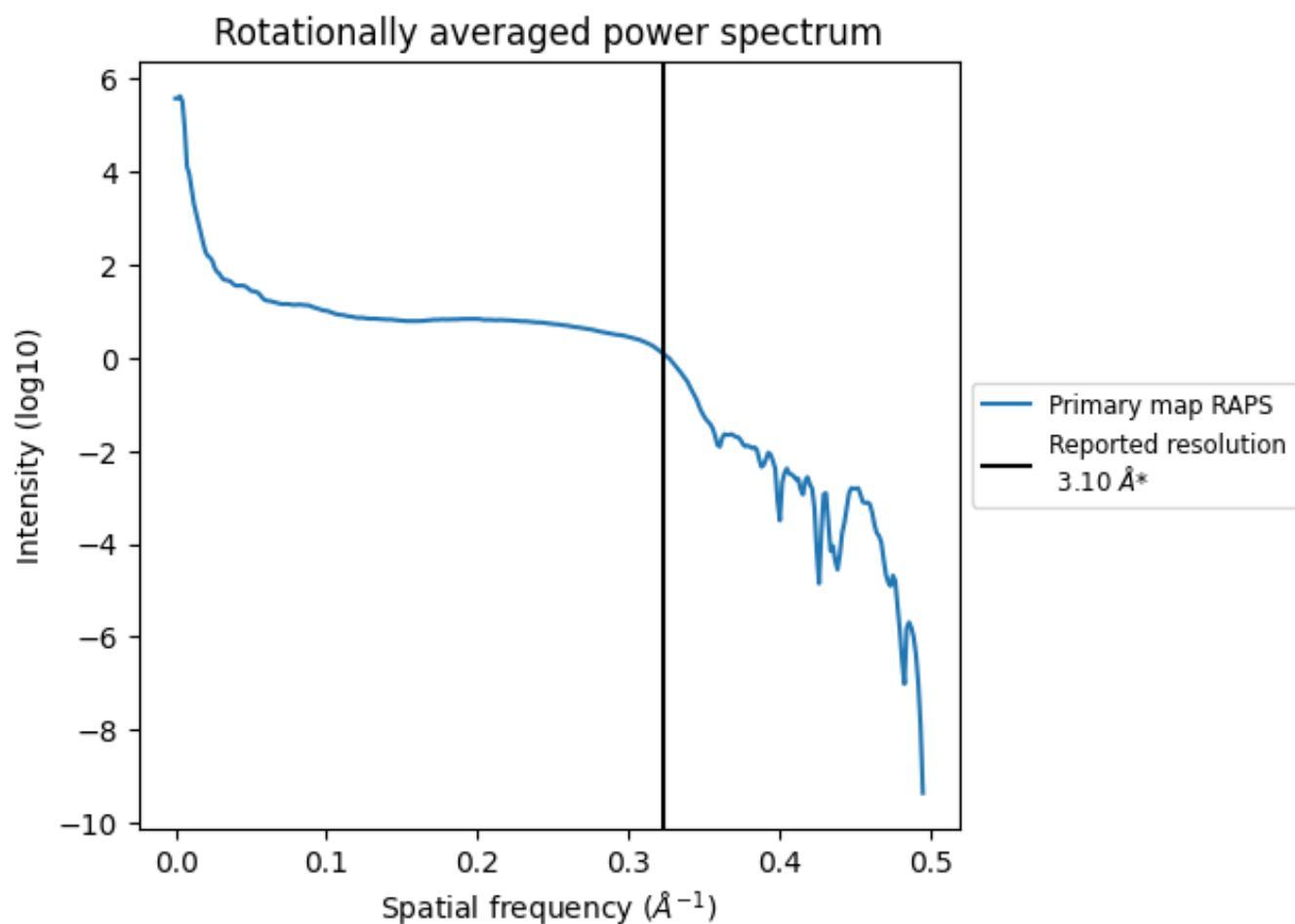
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 922 nm<sup>3</sup>; this corresponds to an approximate mass of 833 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum i



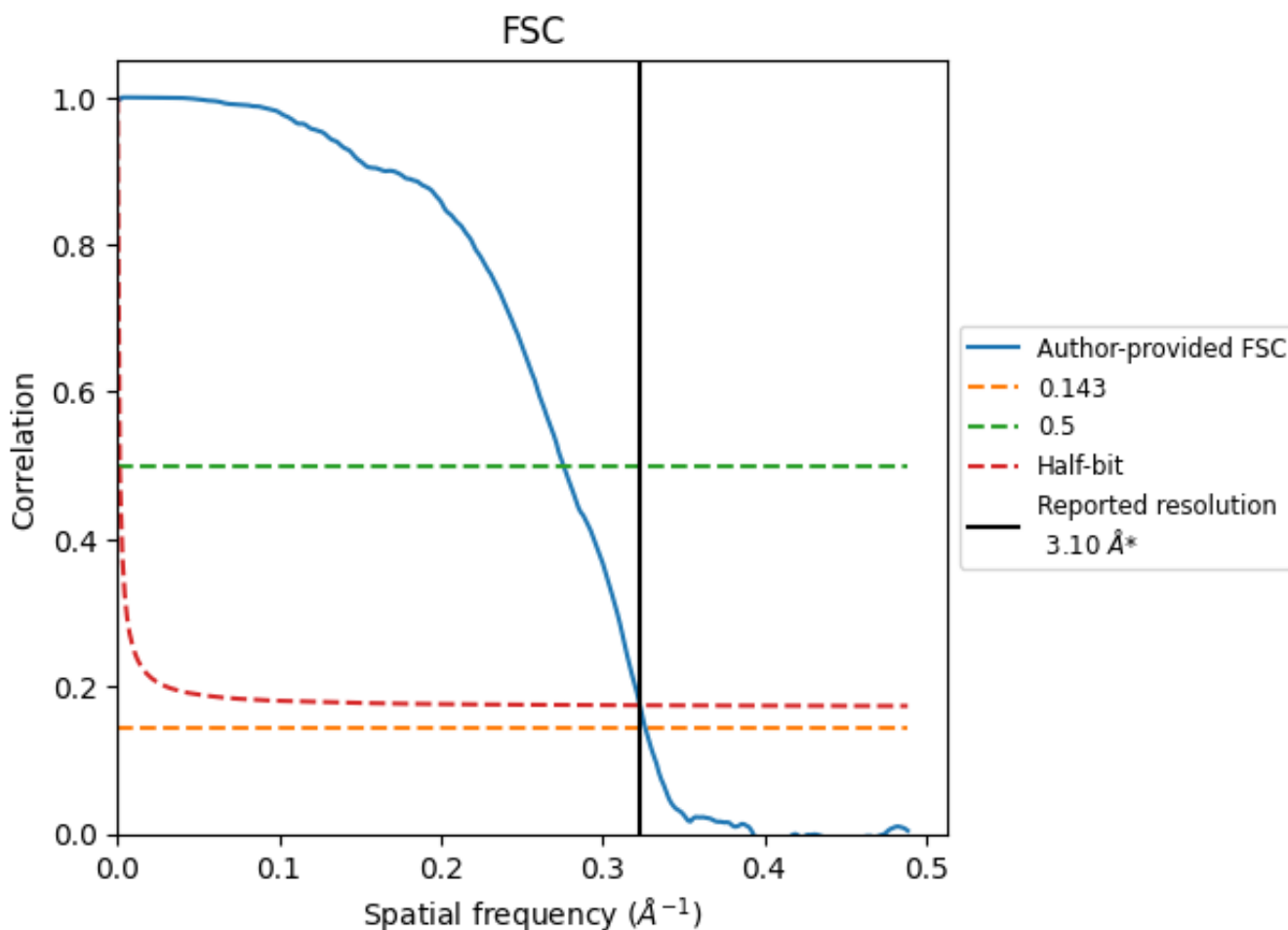
\*Reported resolution corresponds to spatial frequency of 0.323 Å<sup>-1</sup>



## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.323 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

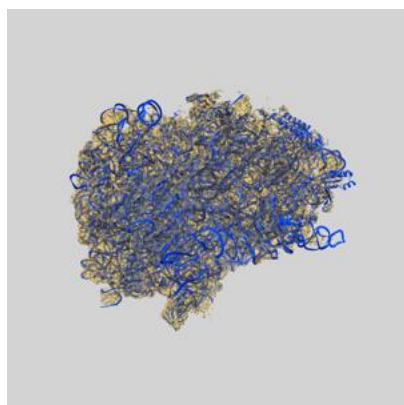
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.06	3.63	3.10
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

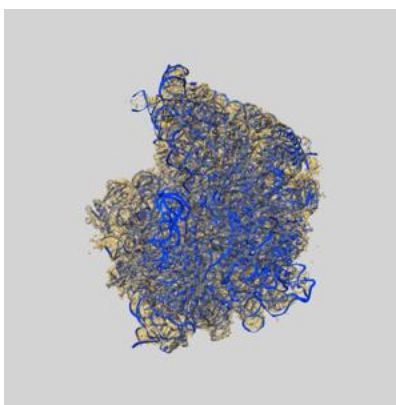
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21420 and PDB model 6VWL. Per-residue inclusion information can be found in section [3](#) on page [14](#).

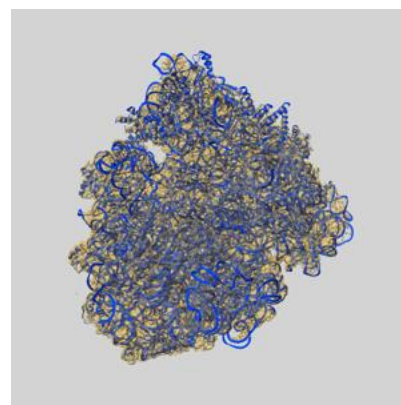
### 9.1 Map-model overlay [i](#)



X



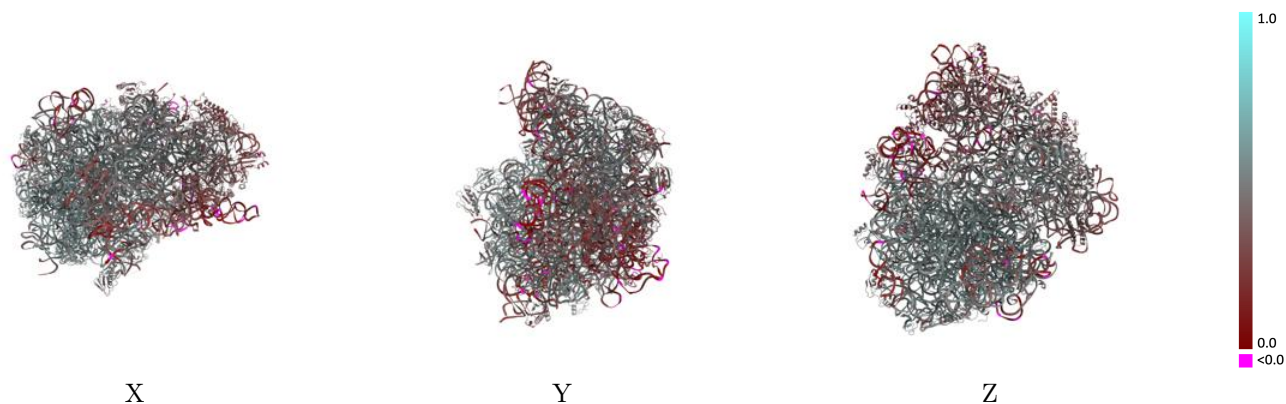
Y



Z

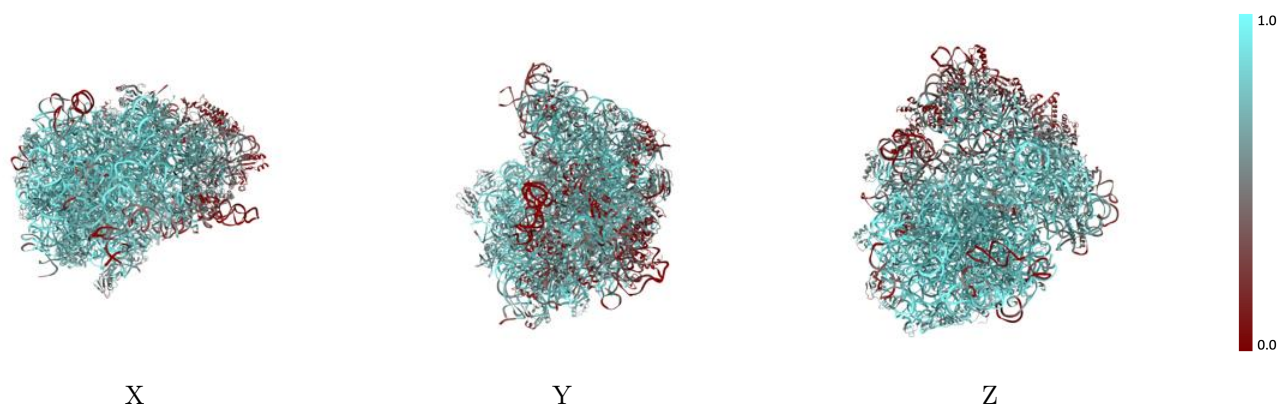
The images above show the 3D surface view of the map at the recommended contour level 7.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



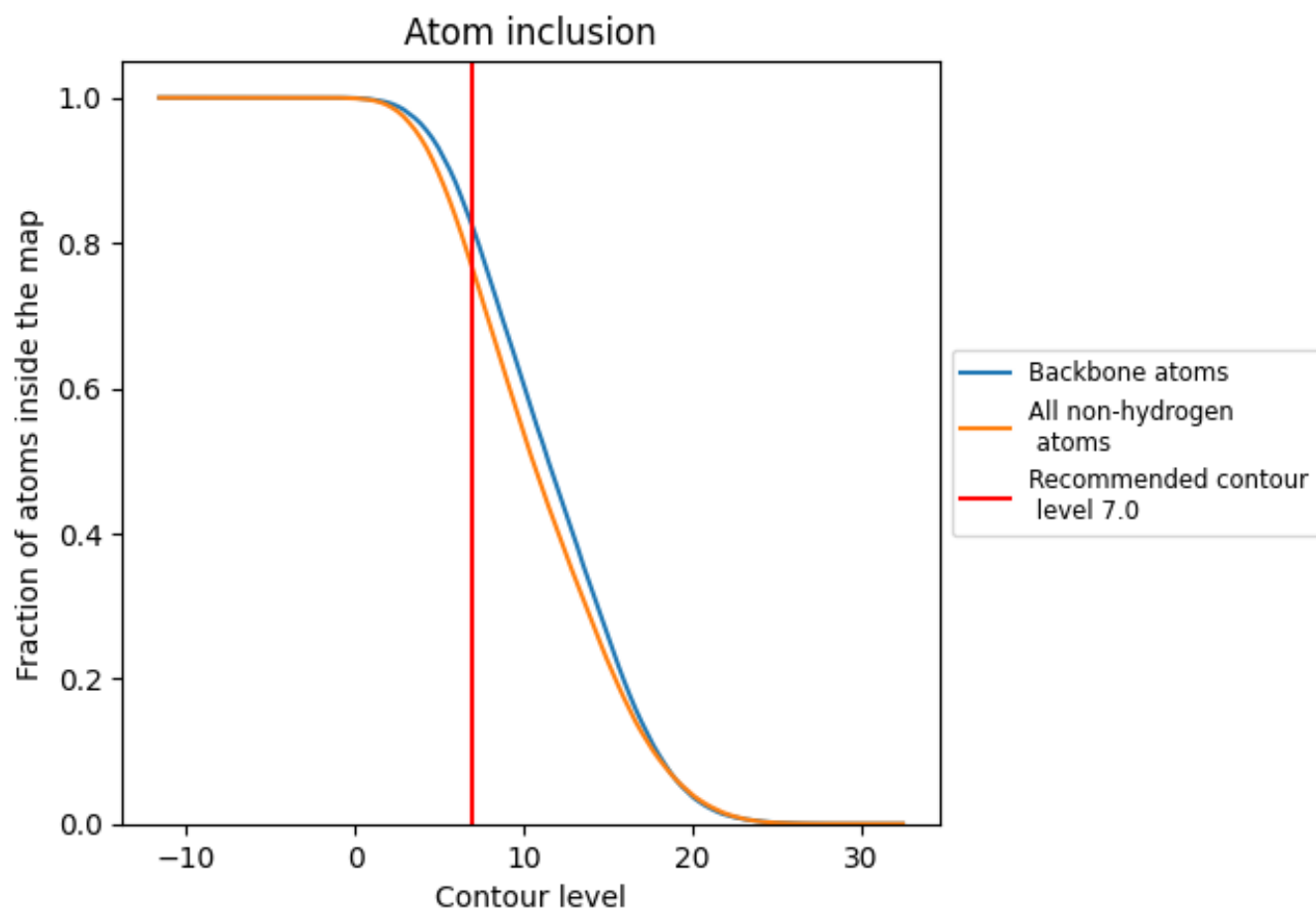
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (7.0).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary







































The table lists the average atom inclusion at the recommended contour level (7.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7638	 0.4490
1	 0.7572	 0.3940
2	 0.8645	 0.4870
3	 0.7353	 0.3720
4	 0.3726	 0.1650
5	 0.6135	 0.2950
A	 0.8622	 0.5500
AA	 0.9155	 0.5670
AB	 0.9043	 0.5410
AC	 0.7945	 0.5170
B	 0.8122	 0.5450
C	 0.7382	 0.5150
D	 0.3149	 0.2980
E	 0.5810	 0.4500
F	 0.3048	 0.3900
G	 0.8291	 0.5390
I	 0.8406	 0.5410
J	 0.8107	 0.5330
K	 0.8234	 0.5240
L	 0.8675	 0.5420
M	 0.5839	 0.4020
N	 0.7804	 0.5170
O	 0.8458	 0.5440
P	 0.7378	 0.5240
Q	 0.8134	 0.5340
R	 0.7808	 0.5260
S	 0.7220	 0.5230
T	 0.6849	 0.4830
U	 0.8247	 0.5440
V	 0.8336	 0.5180
W	 0.6994	 0.4730
X	 0.7872	 0.5370
Y	 0.8254	 0.5350
Z	 0.5490	 0.4900
a	 0.3127	 0.3800



*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
b	 0.4407	 0.3600
c	 0.3922	 0.3170
d	 0.6920	 0.4700
e	 0.5228	 0.4020
f	 0.2552	 0.2790
g	 0.6969	 0.4970
h	 0.3340	 0.3140
i	 0.2536	 0.3010
j	 0.6729	 0.4580
k	 0.6026	 0.4140
l	 0.3133	 0.2810
m	 0.4703	 0.3420
n	 0.6794	 0.4450
o	 0.6619	 0.4500
p	 0.6592	 0.4640
q	 0.6479	 0.4530
r	 0.2866	 0.2730
s	 0.6186	 0.3750
t	 0.5335	 0.3880