



wwPDB EM Validation Summary Report ⓘ

Mar 4, 2024 – 12:33 PM EST

PDB ID : 8UU5
EMDB ID : EMD-42557
Title : Cryo-EM structure of the *Listeria innocua* 70S ribosome (head-swiveled) in complex with pe/E-tRNA (structure I-B)
Authors : Seely, S.M.; Basu, R.S.; Gagnon, M.G.
Deposited on : 2023-10-31
Resolution : 3.00 Å (reported)
Based on initial model : 7NHN

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:

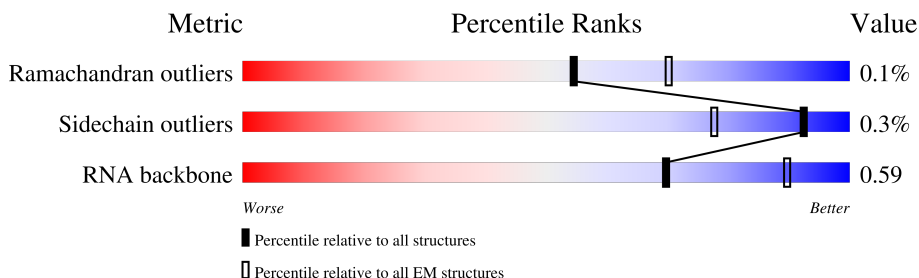
EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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 3.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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 $\leq 5\%$. 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	1550	
2	b	249	
3	c	218	
4	d	200	
5	e	167	
6	f	97	
7	g	156	
8	h	132	


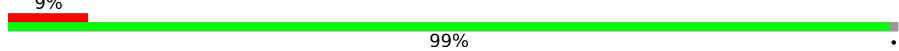
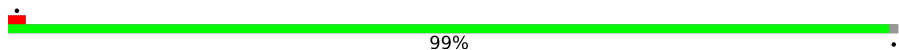
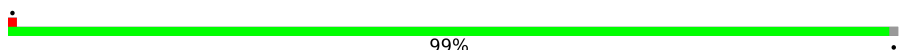

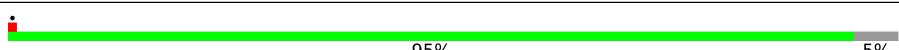
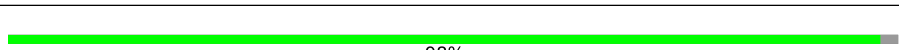
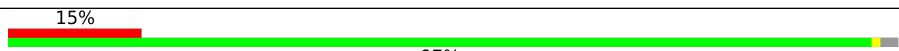
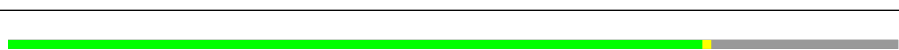

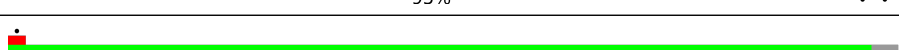
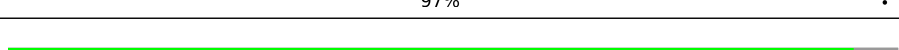
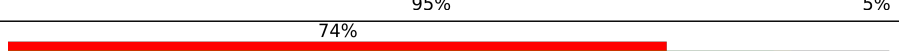
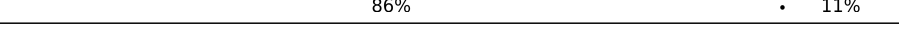
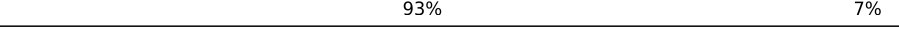
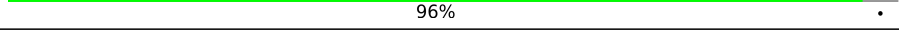
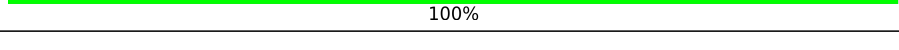
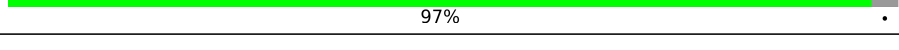
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Mol	Chain	Length	Quality of chain
9	i	130	96%
10	j	102	95% 5%
11	k	129	21% 88% 11%
12	l	137	21% 98%
13	m	121	94% 6%
14	n	61	98%
15	o	89	9% 96%
16	p	90	24% 96%
17	q	87	32% 92% 8%
18	r	79	9% 80% 19%
19	s	92	9% 87% 12%
20	t	84	19% 95%
21	x	76	28% 68% 25%
22	w	21	57% 10% 33%
23	A	2932	6% 83% 16%
24	B	116	86% 12%
25	C	277	99%
26	D	209	99%
27	E	207	99%
28	F	179	59% 96%
29	G	178	17% 96%
30	L	145	99%
31	M	122	100%
32	N	146	99%
33	O	144	93% 7%

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Mol	Chain	Length	Quality of chain
34	P	135	 91% 9%
35	Q	119	 9% 99%
36	R	114	 99%
37	S	119	 99%
38	T	102	 99%
39	U	118	 95% 5%
40	V	94	 98%
41	W	103	 15% 97%
42	Y	96	 78% 21%
43	Z	62	 95%
44	1	63	 97%
45	2	59	 95% 5%
46	3	81	 74% 86% 11%
47	4	57	 93% 7%
48	5	49	 96%
49	6	44	 100%
50	7	66	 97%
51	8	37	 97%

2 Entry composition i

There are 54 unique types of molecules in this entry. The entry contains 140861 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 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	a	1523	32665	14571	5988	10583	1523	0	0

- Molecule 2 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	b	221	1765	1128	308	322	7	0	0

- Molecule 3 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	c	204	1547	967	296	282	2	0	0

- Molecule 4 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	d	199	1562	978	289	293	2	0	0

- Molecule 5 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	e	156	1146	719	210	215	2	0	0

- Molecule 6 is a protein called Small ribosomal subunit protein bS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	f	93	771	488	132	149	2	0	0

- Molecule 7 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	g	149	1143	709	216	209	9	0	0

- Molecule 8 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	h	130	1002	641	178	181	2	0	0

- Molecule 9 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	i	127	998	629	195	173	1	0	0

- Molecule 10 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	j	97	738	463	139	135	1	0	0

- Molecule 11 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	k	115	845	520	163	159	3	0	0

- Molecule 12 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	l	134	1003	623	199	179	2	0	0

- Molecule 13 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	m	114	900	554	177	168	1	0	0

- Molecule 14 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	60	Total	C	N	O	S	0	0
			490	313	97	75	5		

- Molecule 15 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	o	86	Total	C	N	O	S	0	0
			716	445	142	127	2		

- Molecule 16 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	p	87	Total	C	N	O	S	0	0
			691	439	130	119	3		

- Molecule 17 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	80	Total	C	N	O	S	0	0
			612	391	112	108	1		

- Molecule 18 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	r	64	Total	C	N	O	S	0	0
			509	328	92	87	2		

- Molecule 19 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	s	81	Total	C	N	O	S	0	0
			632	405	115	110	2		

- Molecule 20 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	t	81	Total	C	N	O	S	0	0
			610	369	123	117	1		

- Molecule 21 is a RNA chain called pe/E Hybrid State Phenylalanine tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	N	O	P			S
21	x	74	1591	713	285	517	74	2	0	0

- Molecule 22 is a RNA chain called F-Stop mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
22	w	14	304	136	59	95	14	0	0

- Molecule 23 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
23	A	2902	62340	27821	11532	20085	2902	0	0

- Molecule 24 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
24	B	114	2428	1082	428	804	114	0	0

- Molecule 25 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	C	273	2108	1307	415	379	7	0	0

- Molecule 26 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	D	206	1583	995	291	293	4	0	0

- Molecule 27 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
27	E	204	1537	974	285	278	0	0

- Molecule 28 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	F	174	1189	745	210	229	5	0	0

- Molecule 29 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	G	172	1283	802	239	241	1	0	0

- Molecule 30 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	L	143	1124	713	205	203	3	0	0

- Molecule 31 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	M	122	915	569	174	167	5	0	0

- Molecule 32 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
32	N	145	1040	644	209	187	0	0

- Molecule 33 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	O	134	1045	669	201	169	6	0	0

- Molecule 34 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	P	123	967	607	188	171	1	0	0

- Molecule 35 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
35	Q	118	846	522	169	155	0	0

- Molecule 36 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	R	113	893	564	177	151	1	0	0

- Molecule 37 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	S	118	953	605	188	156	4	0	0

- Molecule 38 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	T	101	774	502	134	137	1	0	0

- Molecule 39 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
39	U	112	858	541	159	158	0	0

- Molecule 40 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	V	92	720	461	123	134	2	0	0

- Molecule 41 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	W	101	755	479	140	133	3	0	0

- Molecule 42 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Y	76	Total	C	N	O	S	0	0
			572	350	110	111	1		

- Molecule 43 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Z	60	Total	C	N	O	S	0	0
			451	277	95	77	2		

- Molecule 44 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	1	61	Total	C	N	O	S	0	0
			504	310	97	96	1		

- Molecule 45 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	2	56	Total	C	N	O	S	0	0
			421	265	81	74	1		

- Molecule 46 is a protein called Large ribosomal subunit protein bL31B.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	3	72	Total	C	N	O	S	0	0
			555	352	95	107	1		

- Molecule 47 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	4	53	Total	C	N	O	S	0	0
			410	251	85	69	5		

- Molecule 48 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	5	47	Total	C	N	O	S	0	0
			377	231	73	70	3		

- Molecule 49 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	6	44	370	225	89	54	2	0	0

- Molecule 50 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	7	64	520	322	114	79	5	0	0

- Molecule 51 is a protein called Large ribosomal subunit protein bL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	8	36	266	166	52	42	6	0	0

- Molecule 52 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
52	a	219	Total 219	Mg 219	0
52	c	2	Total 2	Mg 2	0
52	g	2	Total 2	Mg 2	0
52	i	7	Total 7	Mg 7	0
52	j	1	Total 1	Mg 1	0
52	m	1	Total 1	Mg 1	0
52	s	1	Total 1	Mg 1	0
52	t	1	Total 1	Mg 1	0
52	w	1	Total 1	Mg 1	0
52	A	248	Total 248	Mg 248	0
52	B	3	Total 3	Mg 3	0
52	C	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
52	N	1	Total 1	Mg 1	0
52	S	1	Total 1	Mg 1	0
52	6	1	Total 1	Mg 1	0

- Molecule 53 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
53	n	1	Total 1	Zn 1	0
53	4	1	Total 1	Zn 1	0
53	5	1	Total 1	Zn 1	0
53	8	1	Total 1	Zn 1	0

- Molecule 54 is water.

Mol	Chain	Residues	Atoms		AltConf
54	a	122	Total 122	O 122	0
54	c	1	Total 1	O 1	0
54	d	1	Total 1	O 1	0
54	g	2	Total 2	O 2	0
54	i	2	Total 2	O 2	0
54	m	3	Total 3	O 3	0
54	n	2	Total 2	O 2	0
54	t	1	Total 1	O 1	0
54	A	175	Total 175	O 175	0
54	B	1	Total 1	O 1	0

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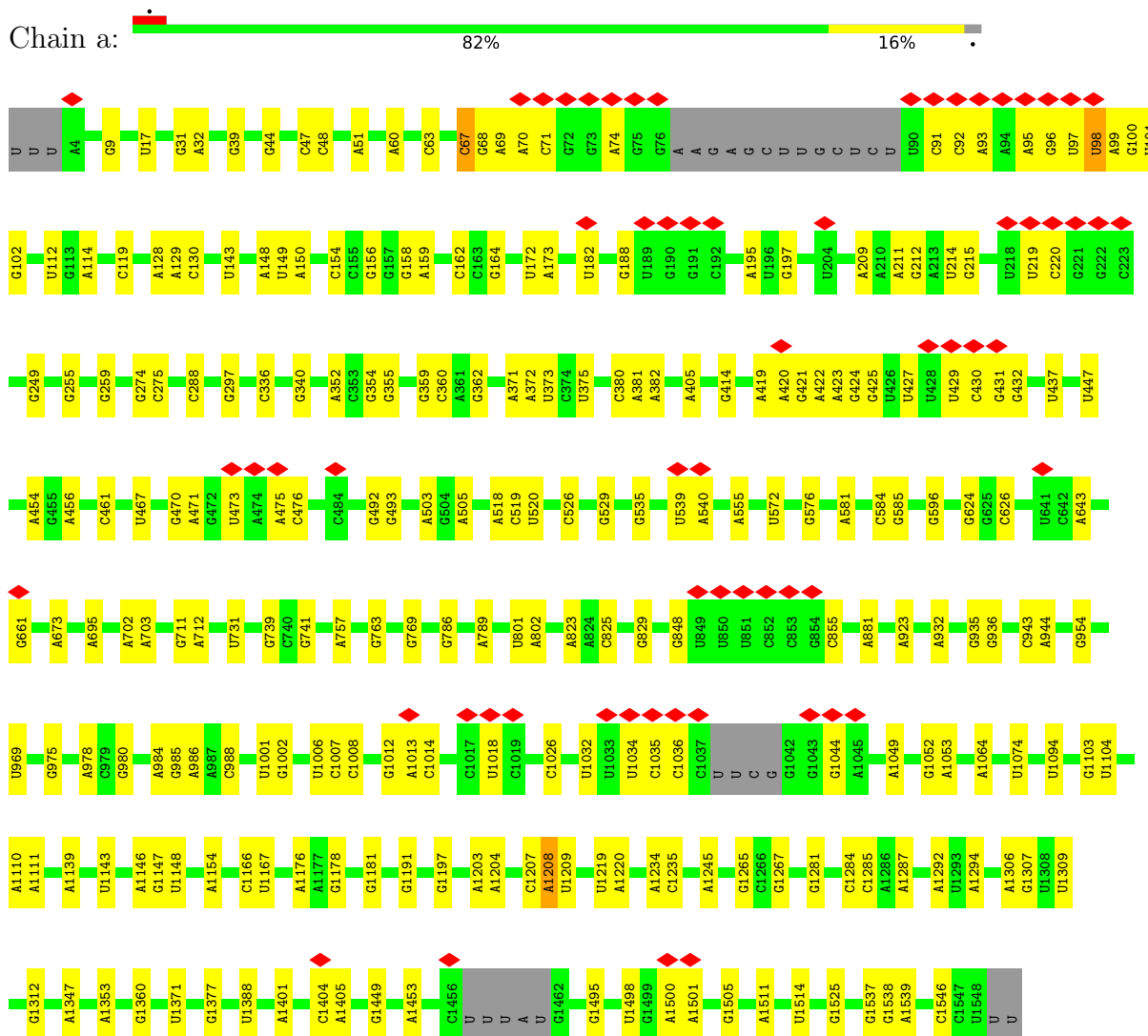
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Mol	Chain	Residues	Atoms		AltConf
54	C	4	Total 4	O 4	0
54	D	1	Total 1	O 1	0
54	N	2	Total 2	O 2	0
54	O	1	Total 1	O 1	0
54	P	1	Total 1	O 1	0
54	S	1	Total 1	O 1	0
54	T	1	Total 1	O 1	0
54	U	2	Total 2	O 2	0

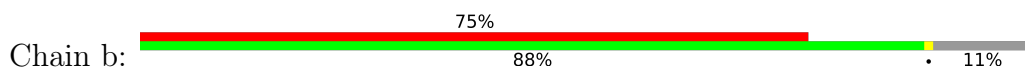
3 Residue-property plots

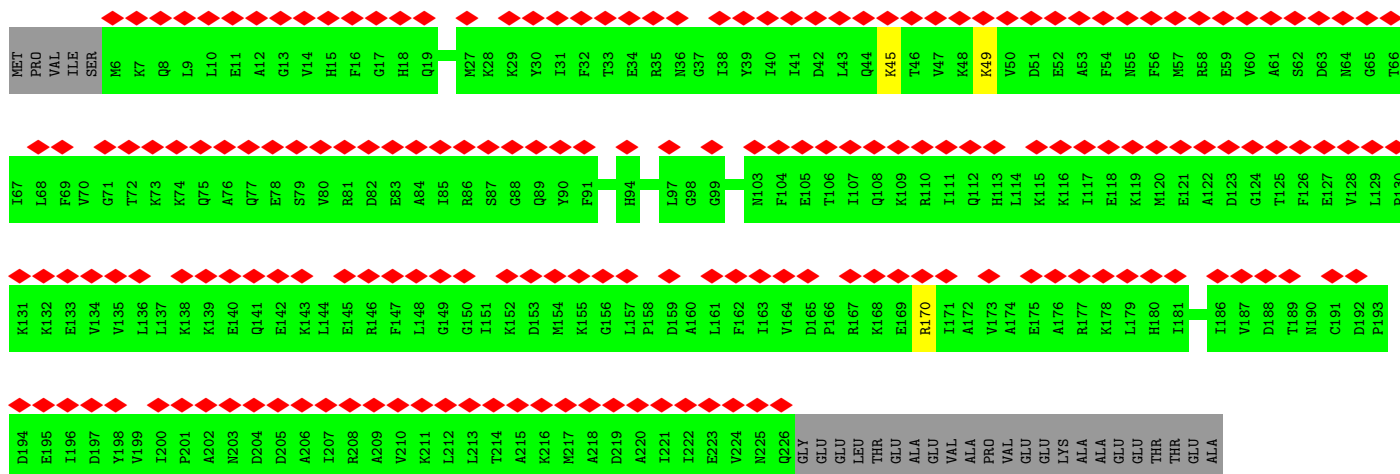
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 16S Ribosomal RNA

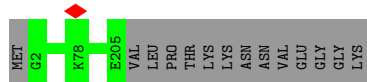


- Molecule 2: Small ribosomal subunit protein uS2

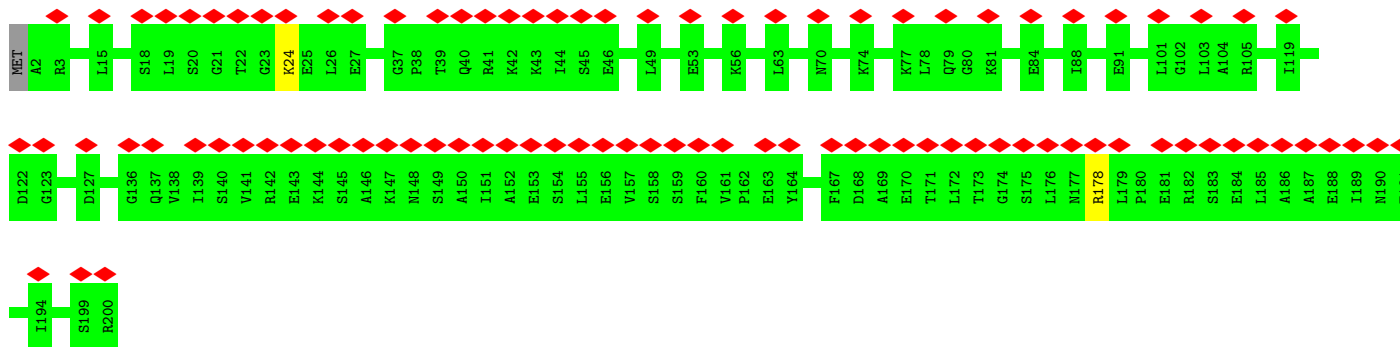




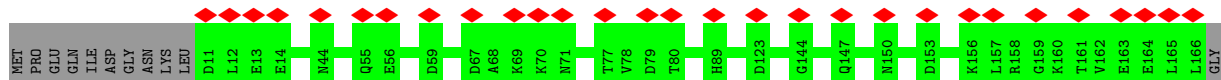
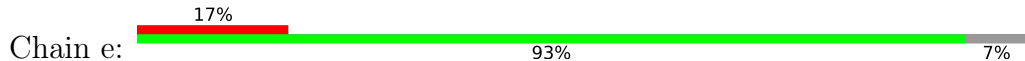
• Molecule 3: Small ribosomal subunit protein uS3



• Molecule 4: Small ribosomal subunit protein uS4

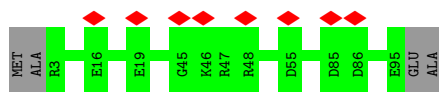


• Molecule 5: Small ribosomal subunit protein uS5



• Molecule 6: Small ribosomal subunit protein bS6

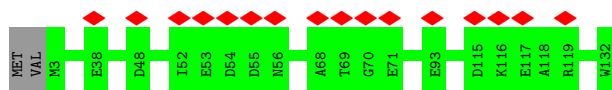




- Molecule 7: Small ribosomal subunit protein uS7



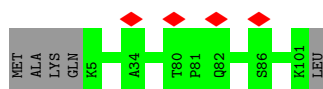
- Molecule 8: Small ribosomal subunit protein uS8



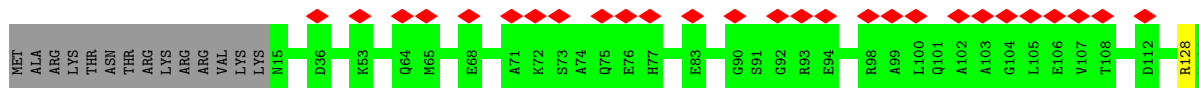
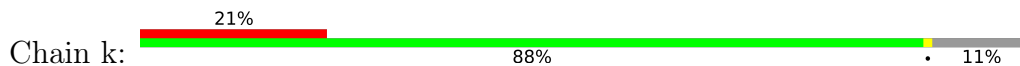
- Molecule 9: Small ribosomal subunit protein uS9



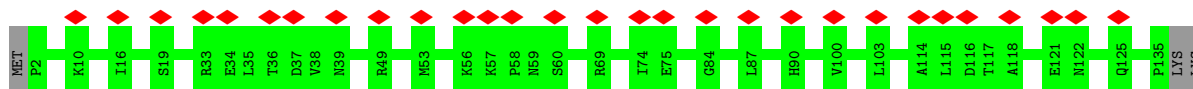
- Molecule 10: Small ribosomal subunit protein uS10



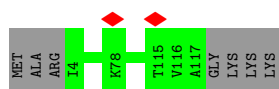
- Molecule 11: Small ribosomal subunit protein uS11



- Molecule 12: Small ribosomal subunit protein uS12



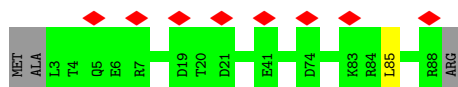
- Molecule 13: Small ribosomal subunit protein uS13



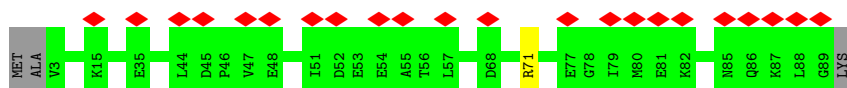
- Molecule 14: Small ribosomal subunit protein uS14



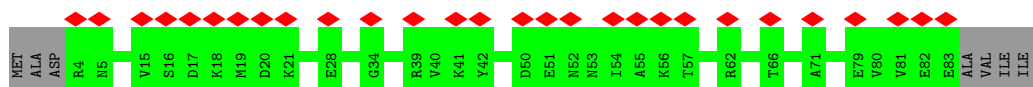
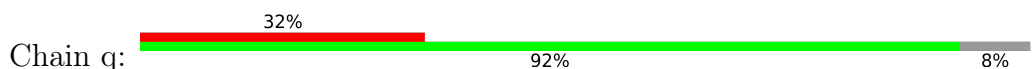
- Molecule 15: Small ribosomal subunit protein uS15



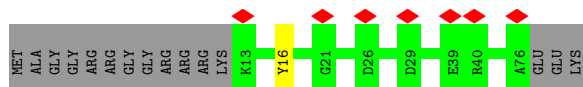
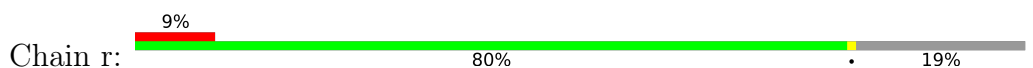
- Molecule 16: Small ribosomal subunit protein bS16



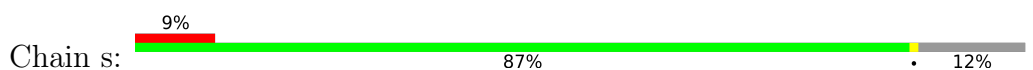
- Molecule 17: Small ribosomal subunit protein uS17



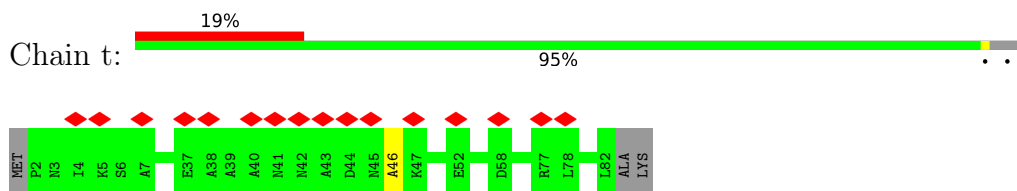
- Molecule 18: Small ribosomal subunit protein bS18



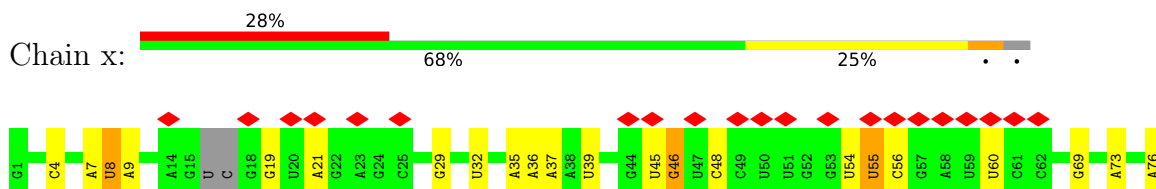
- Molecule 19: Small ribosomal subunit protein uS19



- Molecule 20: Small ribosomal subunit protein bS20



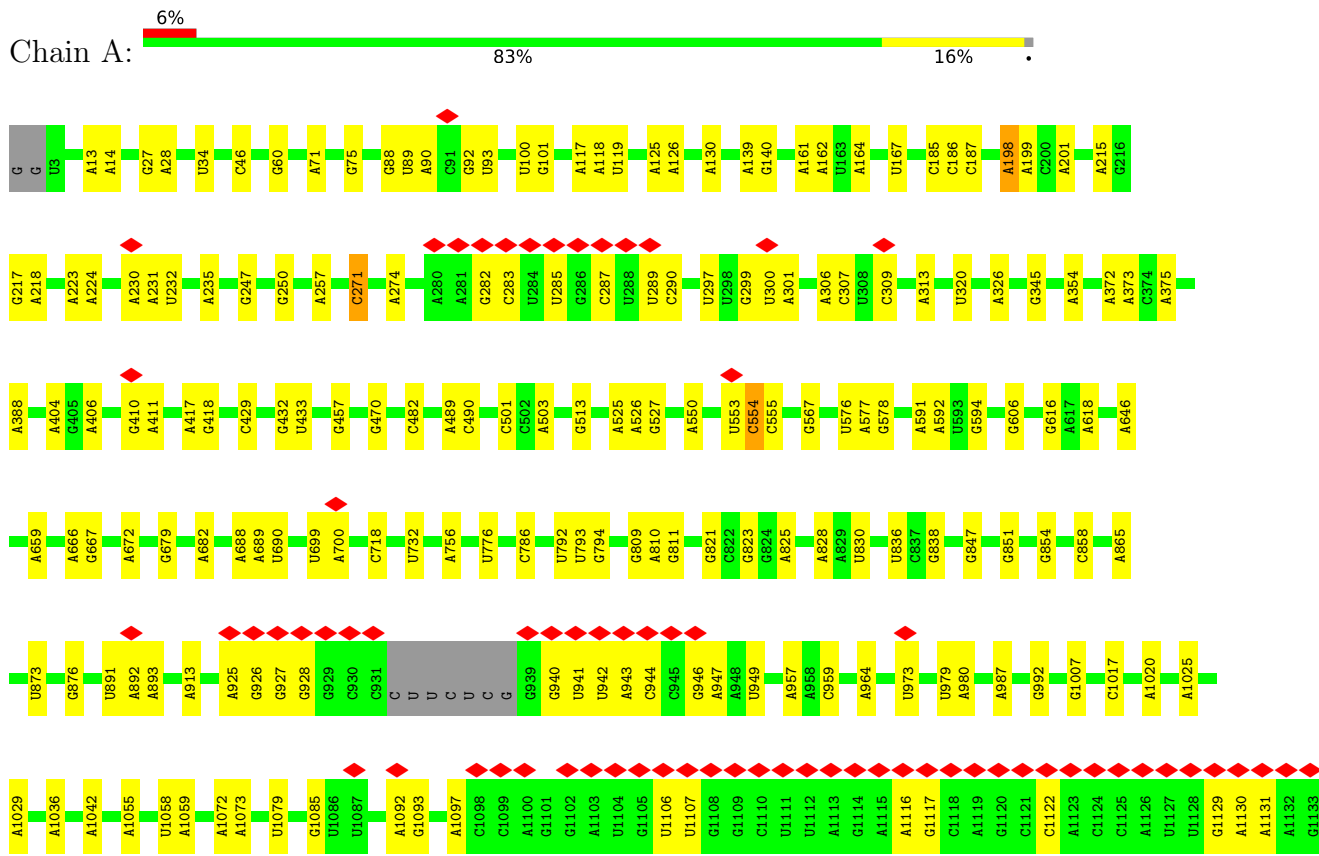
- Molecule 21: pe/E Hybrid State Phenylalanine tRNA

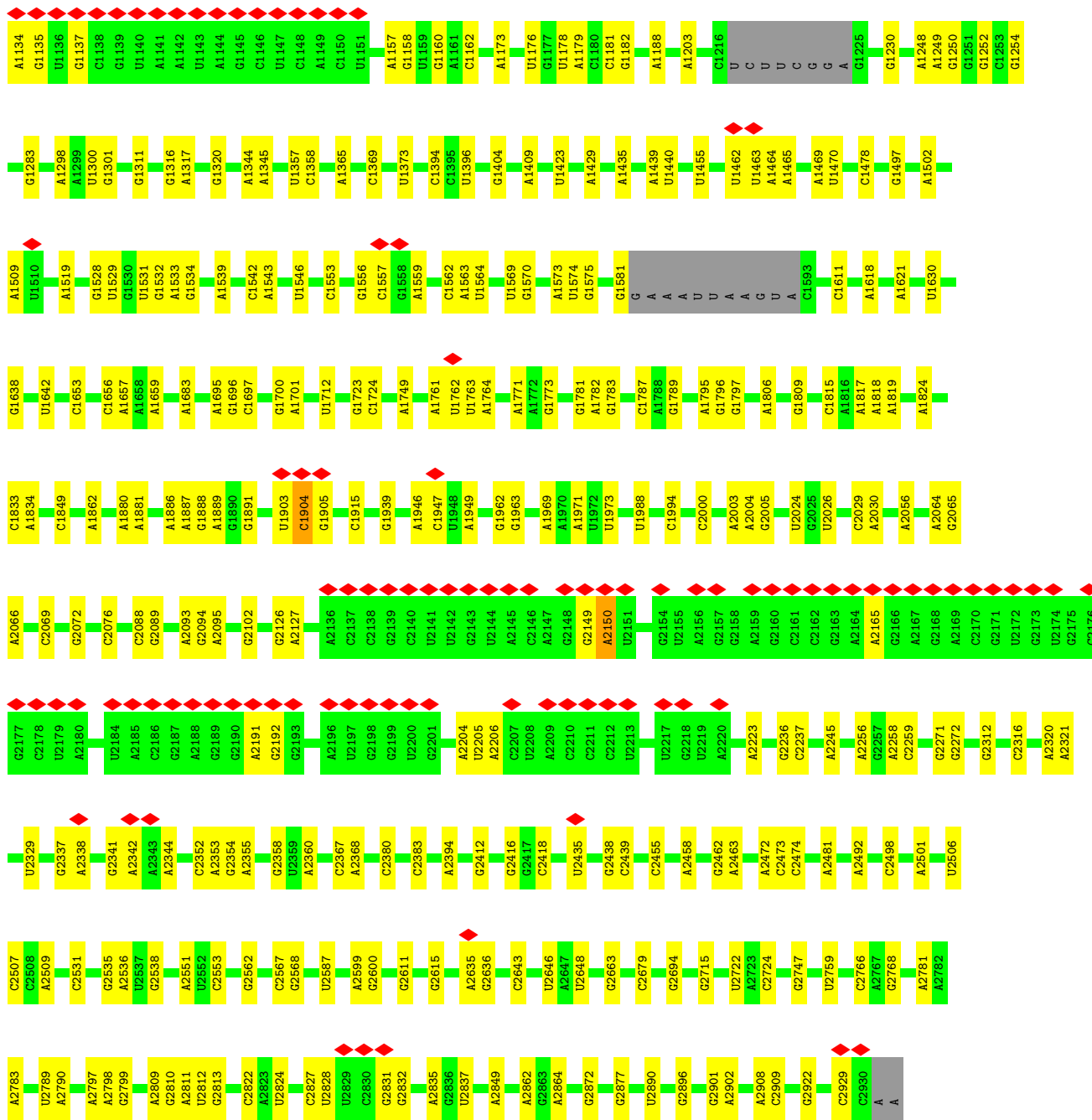


- Molecule 22: F-Stop mRNA

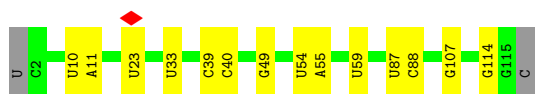
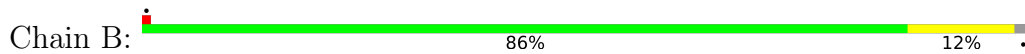


- Molecule 23: 23S Ribosomal RNA



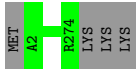


- Molecule 24: 5S Ribosomal RNA

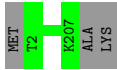


- Molecule 25: Large ribosomal subunit protein uL2

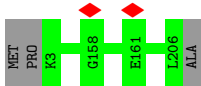




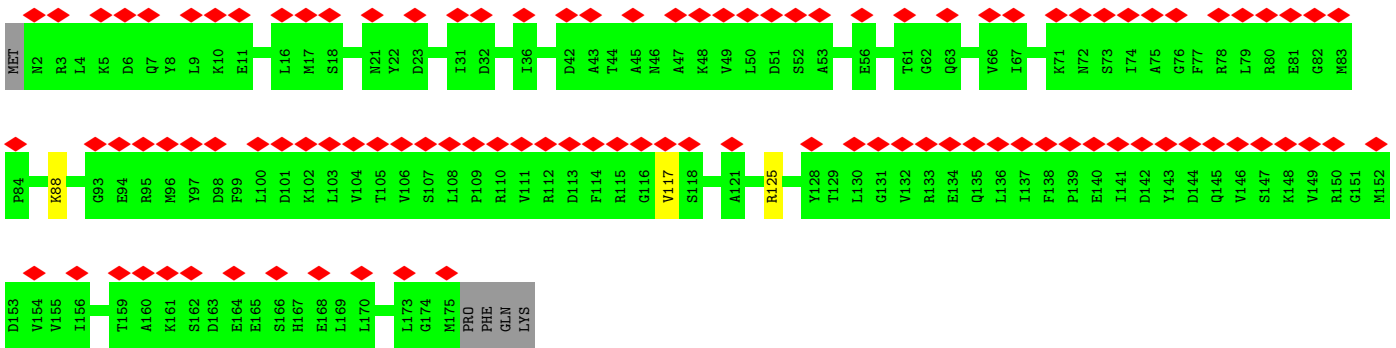
- Molecule 26: Large ribosomal subunit protein uL3



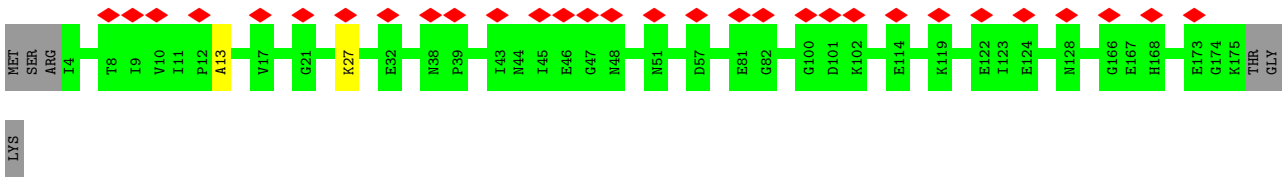
- Molecule 27: Large ribosomal subunit protein uL4



- Molecule 28: Large ribosomal subunit protein uL5



- Molecule 29: Large ribosomal subunit protein uL6



- Molecule 30: Large ribosomal subunit protein uL13



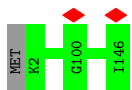
- Molecule 31: Large ribosomal subunit protein uL14

Chain M:  100%

There are no outlier residues recorded for this chain.

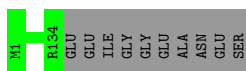
- Molecule 32: Large ribosomal subunit protein uL15

Chain N:  99%



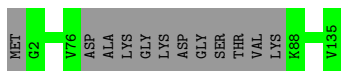
- Molecule 33: Large ribosomal subunit protein uL16

Chain O:  93% 7%



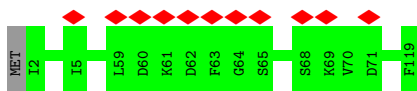
- Molecule 34: Large ribosomal subunit protein bL17

Chain P:  91% 9%



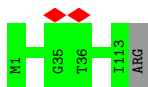
- Molecule 35: Large ribosomal subunit protein uL18

Chain Q:  99% 9%



- Molecule 36: Large ribosomal subunit protein bL19

Chain R:  99%



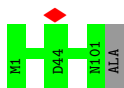
- Molecule 37: Large ribosomal subunit protein bL20

Chain S:  99%



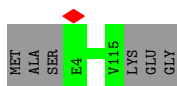
- Molecule 38: Large ribosomal subunit protein bL21

Chain T:  99%



- Molecule 39: Large ribosomal subunit protein uL22

Chain U:  95%



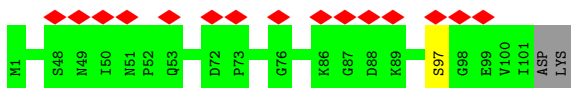
- Molecule 40: Large ribosomal subunit protein uL23

Chain V:  98%




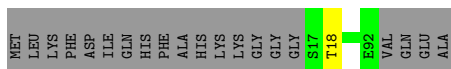
- Molecule 41: Large ribosomal subunit protein uL24

Chain W:  15% 97%



- Molecule 42: Large ribosomal subunit protein bL27

Chain Y:  78% 21%



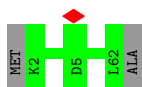
- Molecule 43: Large ribosomal subunit protein bL28

Chain Z:  95%



- Molecule 44: Large ribosomal subunit protein uL29

Chain 1:  97%




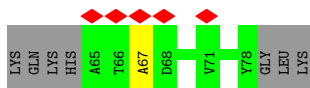
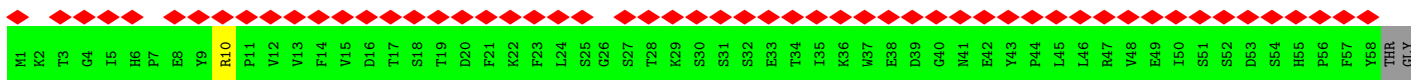
- Molecule 45: Large ribosomal subunit protein uL30

Chain 2:  95% 5%



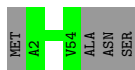
- Molecule 46: Large ribosomal subunit protein bL31B

Chain 3:  74% 86% 11%



- Molecule 47: Large ribosomal subunit protein bL32

Chain 4:  93% 7%



- Molecule 48: Large ribosomal subunit protein bL33

Chain 5:  96%



- Molecule 49: Large ribosomal subunit protein bL34

Chain 6:  100%

There are no outlier residues recorded for this chain.

- Molecule 50: Large ribosomal subunit protein bL35

Chain 7:  97%



- Molecule 51: Large ribosomal subunit protein bL36

Chain 8:  97%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	196886	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.0	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	47.649	Depositor
Minimum map value	-27.659	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.089	Depositor
Recommended contour level	3.28	Depositor
Map size (Å)	435.2, 435.2, 435.2	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	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, PSU, G7M, 5MU, 4SU, MIA, ZN

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	0.21	0/36571	0.79	8/57040 (0.0%)
2	b	0.30	0/1794	0.58	1/2414 (0.0%)
3	c	0.24	0/1572	0.54	0/2129
4	d	0.24	0/1590	0.53	0/2142
5	e	0.24	0/1159	0.51	0/1565
6	f	0.26	0/783	0.55	0/1051
7	g	0.24	0/1156	0.52	0/1552
8	h	0.25	0/1015	0.51	0/1365
9	i	0.26	0/1017	0.60	0/1369
10	j	0.23	0/747	0.54	0/1006
11	k	0.24	0/859	0.55	0/1159
12	l	0.25	0/1019	0.56	0/1376
13	m	0.26	0/906	0.63	0/1213
14	n	0.25	0/500	0.58	0/664
15	o	0.25	0/726	0.58	1/973 (0.1%)
16	p	0.24	0/704	0.56	0/945
17	q	0.23	0/621	0.51	0/836
18	r	0.25	0/516	0.53	0/692
19	s	0.26	0/648	0.57	1/876 (0.1%)
20	t	0.26	0/612	0.53	0/816
21	x	0.20	0/1605	0.83	0/2497
22	w	0.16	0/341	0.71	0/530
23	A	0.22	0/69843	0.78	15/108955 (0.0%)
24	B	0.18	0/2711	0.75	0/4224
25	C	0.25	0/2144	0.56	0/2875
26	D	0.25	0/1605	0.52	0/2156
27	E	0.24	0/1557	0.52	0/2103
28	F	0.26	0/1202	0.51	0/1634
29	G	0.25	0/1304	0.52	0/1762
30	L	0.23	0/1147	0.48	0/1541
31	M	0.25	0/922	0.56	0/1235
32	N	0.24	0/1050	0.53	0/1401

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	O	0.24	0/1067	0.54	0/1429
34	P	0.23	0/978	0.57	0/1310
35	Q	0.24	0/854	0.52	0/1149
36	R	0.26	0/905	0.60	0/1215
37	S	0.23	0/966	0.49	0/1284
38	T	0.25	0/787	0.47	0/1057
39	U	0.24	0/868	0.53	0/1175
40	V	0.23	0/729	0.47	0/981
41	W	0.25	0/764	0.49	0/1021
42	Y	0.25	0/579	0.58	0/773
43	Z	0.23	0/456	0.62	0/607
44	1	0.22	0/505	0.52	0/673
45	2	0.23	0/424	0.54	0/571
46	3	0.24	0/566	0.50	0/763
47	4	0.23	0/418	0.56	0/559
48	5	0.22	0/381	0.56	0/514
49	6	0.23	0/373	0.64	0/486
50	7	0.24	0/527	0.58	0/685
51	8	0.23	0/269	0.50	0/359
All	All	0.22	0/152362	0.73	26/228707 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
7	g	0	2

There are no bond length outliers.

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	98	U	O4'-C1'-N1	-7.64	102.09	108.20
1	a	1036	C	N3-C2-O2	-7.13	116.91	121.90
1	a	67	C	C6-N1-C2	-6.55	117.68	120.30
23	A	1357	U	C2-N1-C1'	6.34	125.31	117.70
23	A	1824	A	N1-C2-N3	6.28	132.44	129.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	g	1	MET	Peptide
7	g	2	PRO	Peptide

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	
2	b	219/249 (88%)	192 (88%)	27 (12%)	0	100	100
3	c	202/218 (93%)	185 (92%)	17 (8%)	0	100	100
4	d	197/200 (98%)	184 (93%)	13 (7%)	0	100	100
5	e	154/167 (92%)	152 (99%)	2 (1%)	0	100	100
6	f	91/97 (94%)	84 (92%)	7 (8%)	0	100	100
7	g	147/156 (94%)	144 (98%)	3 (2%)	0	100	100
8	h	128/132 (97%)	123 (96%)	5 (4%)	0	100	100
9	i	125/130 (96%)	123 (98%)	2 (2%)	0	100	100
10	j	95/102 (93%)	91 (96%)	4 (4%)	0	100	100
11	k	113/129 (88%)	106 (94%)	7 (6%)	0	100	100
12	l	132/137 (96%)	129 (98%)	3 (2%)	0	100	100
13	m	112/121 (93%)	105 (94%)	7 (6%)	0	100	100
14	n	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
15	o	84/89 (94%)	84 (100%)	0	0	100	100
16	p	85/90 (94%)	82 (96%)	3 (4%)	0	100	100
17	q	78/87 (90%)	73 (94%)	5 (6%)	0	100	100
18	r	62/79 (78%)	60 (97%)	1 (2%)	1 (2%)	9	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	s	79/92 (86%)	76 (96%)	3 (4%)	0	100	100
20	t	79/84 (94%)	75 (95%)	3 (4%)	1 (1%)	12	45
25	C	271/277 (98%)	260 (96%)	11 (4%)	0	100	100
26	D	204/209 (98%)	195 (96%)	9 (4%)	0	100	100
27	E	202/207 (98%)	194 (96%)	8 (4%)	0	100	100
28	F	172/179 (96%)	154 (90%)	17 (10%)	1 (1%)	25	64
29	G	170/178 (96%)	150 (88%)	19 (11%)	1 (1%)	25	64
30	L	141/145 (97%)	141 (100%)	0	0	100	100
31	M	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
32	N	143/146 (98%)	136 (95%)	7 (5%)	0	100	100
33	O	132/144 (92%)	132 (100%)	0	0	100	100
34	P	119/135 (88%)	115 (97%)	4 (3%)	0	100	100
35	Q	116/119 (98%)	112 (97%)	4 (3%)	0	100	100
36	R	111/114 (97%)	104 (94%)	7 (6%)	0	100	100
37	S	116/119 (98%)	113 (97%)	3 (3%)	0	100	100
38	T	99/102 (97%)	96 (97%)	3 (3%)	0	100	100
39	U	110/118 (93%)	108 (98%)	2 (2%)	0	100	100
40	V	90/94 (96%)	88 (98%)	2 (2%)	0	100	100
41	W	99/103 (96%)	95 (96%)	3 (3%)	1 (1%)	15	53
42	Y	74/96 (77%)	68 (92%)	5 (7%)	1 (1%)	11	43
43	Z	58/62 (94%)	49 (84%)	9 (16%)	0	100	100
44	1	59/63 (94%)	57 (97%)	2 (3%)	0	100	100
45	2	54/59 (92%)	52 (96%)	2 (4%)	0	100	100
46	3	68/81 (84%)	63 (93%)	4 (6%)	1 (2%)	10	42
47	4	51/57 (90%)	48 (94%)	3 (6%)	0	100	100
48	5	45/49 (92%)	45 (100%)	0	0	100	100
49	6	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
50	7	62/66 (94%)	55 (89%)	7 (11%)	0	100	100
51	8	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
All	All	5202/5545 (94%)	4941 (95%)	254 (5%)	7 (0%)	54	85

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	r	16	TYR
20	t	46	ALA
42	Y	18	THR
41	W	97	SER
29	G	13	ALA

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	
2	b	188/214 (88%)	186 (99%)	2 (1%)	73	90
3	c	145/177 (82%)	145 (100%)	0	100	100
4	d	162/170 (95%)	160 (99%)	2 (1%)	71	90
5	e	122/131 (93%)	122 (100%)	0	100	100
6	f	81/85 (95%)	81 (100%)	0	100	100
7	g	116/130 (89%)	116 (100%)	0	100	100
8	h	104/110 (94%)	104 (100%)	0	100	100
9	i	100/102 (98%)	98 (98%)	2 (2%)	55	83
10	j	73/93 (78%)	73 (100%)	0	100	100
11	k	87/100 (87%)	86 (99%)	1 (1%)	73	90
12	l	105/118 (89%)	105 (100%)	0	100	100
13	m	96/102 (94%)	96 (100%)	0	100	100
14	n	51/52 (98%)	51 (100%)	0	100	100
15	o	78/81 (96%)	78 (100%)	0	100	100
16	p	74/80 (92%)	73 (99%)	1 (1%)	67	88
17	q	63/78 (81%)	63 (100%)	0	100	100
18	r	55/67 (82%)	55 (100%)	0	100	100
19	s	64/78 (82%)	64 (100%)	0	100	100
20	t	62/66 (94%)	62 (100%)	0	100	100
25	C	221/225 (98%)	221 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	D	169/171 (99%)	169 (100%)	0	100	100
27	E	162/174 (93%)	162 (100%)	0	100	100
28	F	101/155 (65%)	99 (98%)	2 (2%)	55	83
29	G	127/147 (86%)	126 (99%)	1 (1%)	81	93
30	L	119/121 (98%)	119 (100%)	0	100	100
31	M	98/101 (97%)	98 (100%)	0	100	100
32	N	97/115 (84%)	97 (100%)	0	100	100
33	O	102/113 (90%)	102 (100%)	0	100	100
34	P	97/111 (87%)	97 (100%)	0	100	100
35	Q	77/97 (79%)	77 (100%)	0	100	100
36	R	94/99 (95%)	94 (100%)	0	100	100
37	S	96/97 (99%)	96 (100%)	0	100	100
38	T	78/82 (95%)	78 (100%)	0	100	100
39	U	92/97 (95%)	92 (100%)	0	100	100
40	V	74/84 (88%)	74 (100%)	0	100	100
41	W	82/88 (93%)	82 (100%)	0	100	100
42	Y	58/76 (76%)	58 (100%)	0	100	100
43	Z	45/53 (85%)	44 (98%)	1 (2%)	52	81
44	1	54/55 (98%)	54 (100%)	0	100	100
45	2	47/52 (90%)	47 (100%)	0	100	100
46	3	57/73 (78%)	56 (98%)	1 (2%)	59	85
47	4	43/50 (86%)	43 (100%)	0	100	100
48	5	41/48 (85%)	41 (100%)	0	100	100
49	6	39/39 (100%)	39 (100%)	0	100	100
50	7	54/56 (96%)	54 (100%)	0	100	100
51	8	29/35 (83%)	29 (100%)	0	100	100
All	All	4179/4648 (90%)	4166 (100%)	13 (0%)	92	97

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	p	71	ARG
28	F	88	LYS

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Mol	Chain	Res	Type
46	3	10	ARG
29	G	27	LYS
43	Z	61	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
27	E	9	GLN
35	Q	43	GLN
50	7	35	ASN
27	E	46	GLN
32	N	17	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1519/1550 (98%)	242 (15%)	0
21	x	71/76 (93%)	18 (25%)	0
22	w	13/21 (61%)	2 (15%)	0
23	A	2898/2932 (98%)	453 (15%)	28 (0%)
24	B	113/116 (97%)	14 (12%)	0
All	All	4614/4695 (98%)	729 (15%)	28 (0%)

5 of 729 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	9	G
1	a	17	U
1	a	31	G
1	a	32	A
1	a	39	G

5 of 28 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	A	1248	A
23	A	2908	A
23	A	1528	G
23	A	2438	G
23	A	1497	G

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

7 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	PSU	x	32	21	18,21,22	1.37	2 (11%)	22,30,33	1.86	3 (13%)
21	4SU	x	8	21	18,21,22	1.75	5 (27%)	26,30,33	2.15	5 (19%)
21	5MU	x	54	21	19,22,23	1.41	5 (26%)	28,32,35	2.02	7 (25%)
21	MIA	x	37	21	24,31,32	2.22	3 (12%)	26,44,47	2.48	9 (34%)
21	PSU	x	39	21	18,21,22	1.21	1 (5%)	22,30,33	2.36	4 (18%)
21	PSU	x	55	21	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
21	G7M	x	46	21	20,26,27	2.66	4 (20%)	17,39,42	0.90	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. ^{1,2} means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	PSU	x	32	21	-	0/7/25/26	0/2/2/2
21	4SU	x	8	21	-	2/7/25/26	0/2/2/2
21	5MU	x	54	21	-	0/7/25/26	0/2/2/2
21	MIA	x	37	21	-	1/11/33/34	0/3/3/3
21	PSU	x	39	21	-	0/7/25/26	0/2/2/2
21	PSU	x	55	21	-	3/7/25/26	0/2/2/2
21	G7M	x	46	21	-	1/3/25/26	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	x	46	G7M	C8-N9	7.56	1.47	1.33
21	x	46	G7M	C8-N7	7.26	1.46	1.33
21	x	37	MIA	C13-C14	7.18	1.53	1.32
21	x	37	MIA	C2-S10	-6.73	1.70	1.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	x	8	4SU	C4-S4	-4.47	1.59	1.68

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	x	37	MIA	C12-C13-C14	-7.96	111.66	127.14
21	x	39	PSU	N1-C2-N3	6.96	123.02	115.13
21	x	8	4SU	C4-N3-C2	-6.42	121.10	127.34
21	x	32	PSU	N1-C2-N3	6.02	121.95	115.13
21	x	55	PSU	N1-C2-N3	6.00	121.93	115.13

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	x	37	MIA	C12-C13-C14-C16
21	x	55	PSU	C3'-C4'-C5'-O5'
21	x	55	PSU	O4'-C4'-C5'-O5'
21	x	55	PSU	C4'-C5'-O5'-P
21	x	8	4SU	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 494 ligands modelled in this entry, 494 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.

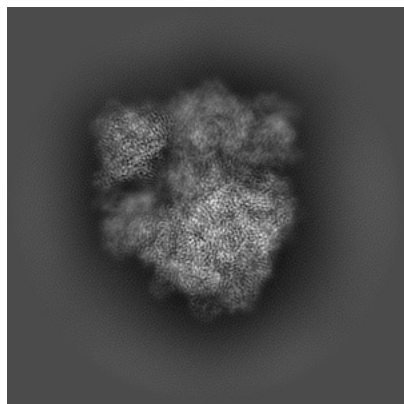
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42557. These allow visual inspection of the internal detail of the map and identification of artifacts.

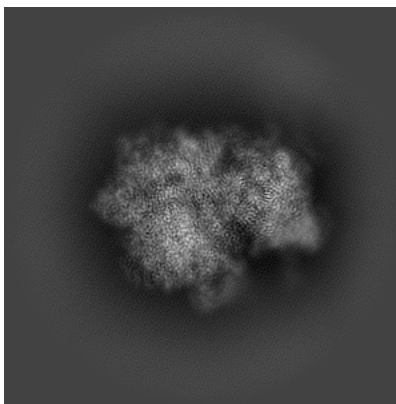
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

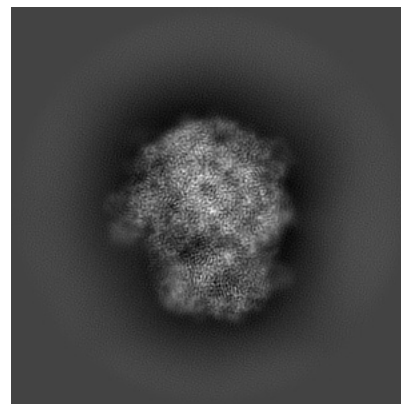
6.1.1 Primary map



X

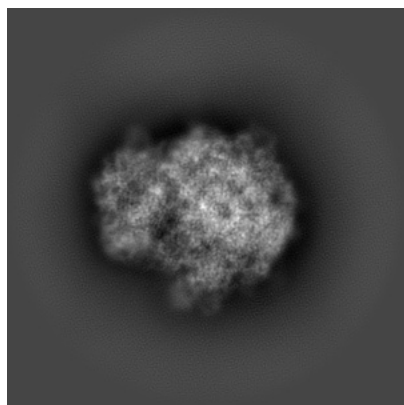


Y

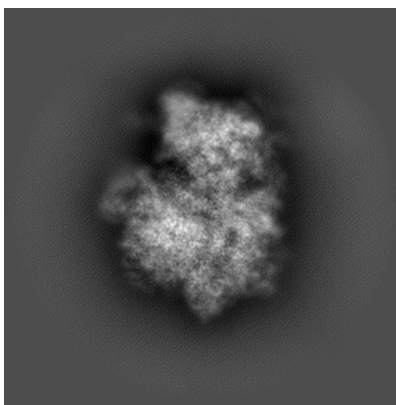


Z

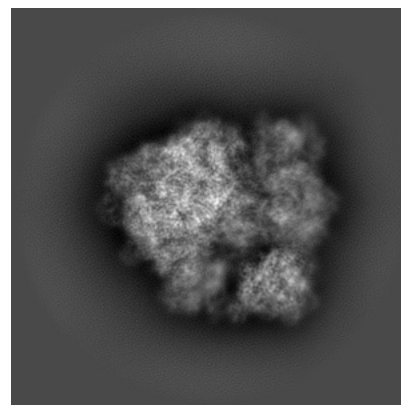
6.1.2 Raw map



X



Y

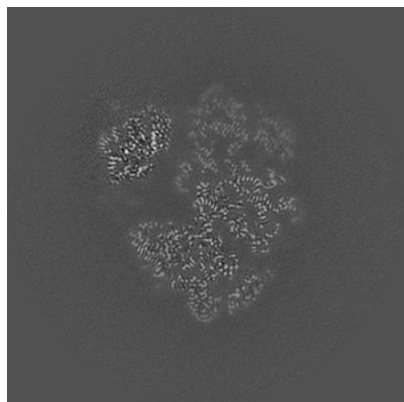


Z

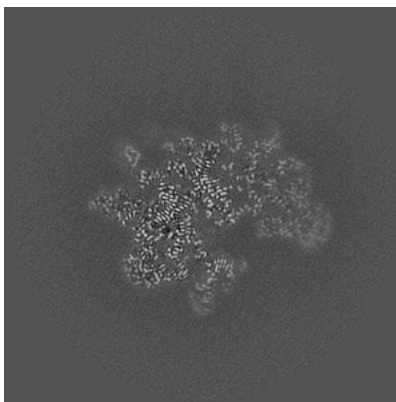
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

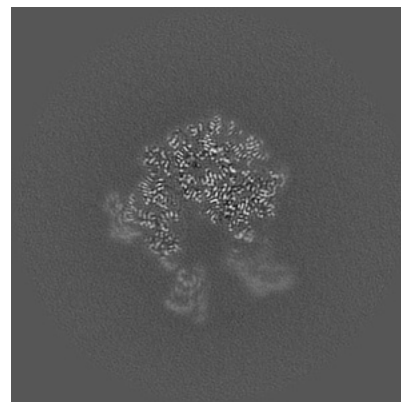
6.2.1 Primary map



X Index: 256

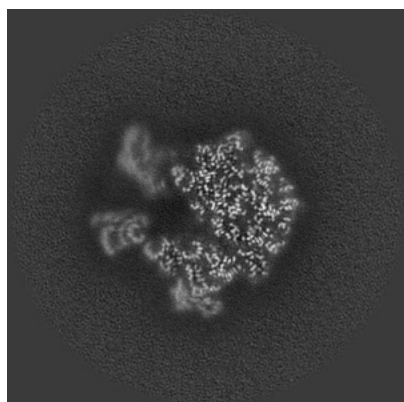


Y Index: 256

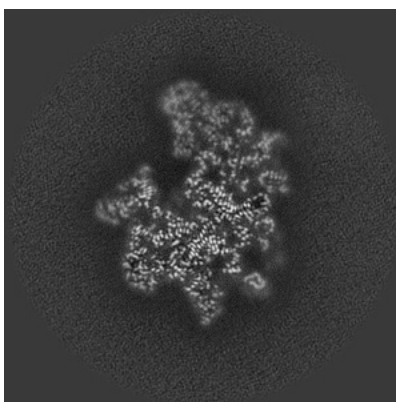


Z Index: 256

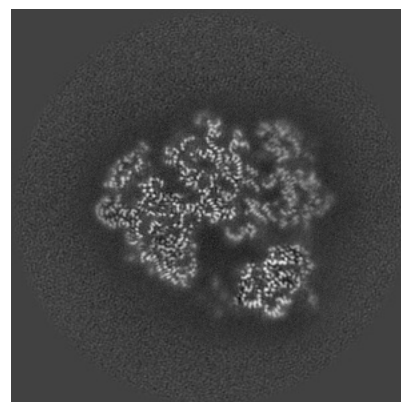
6.2.2 Raw map



X Index: 256



Y Index: 256

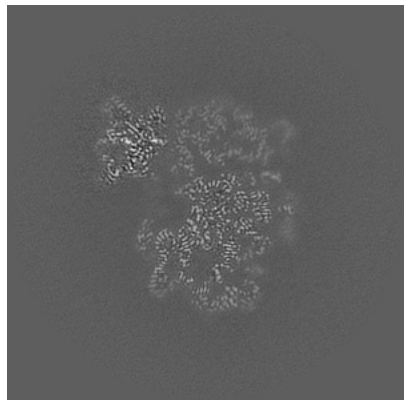


Z Index: 256

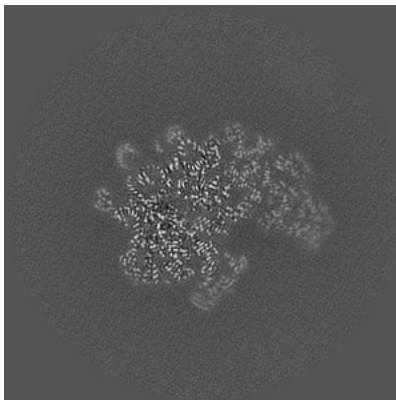
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

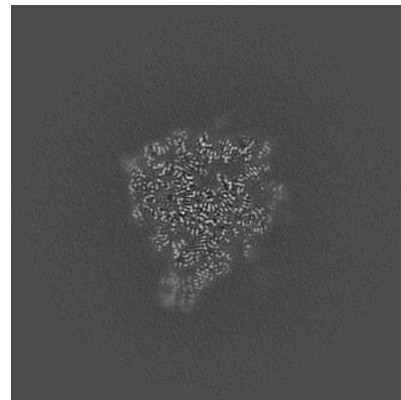
6.3.1 Primary map



X Index: 269

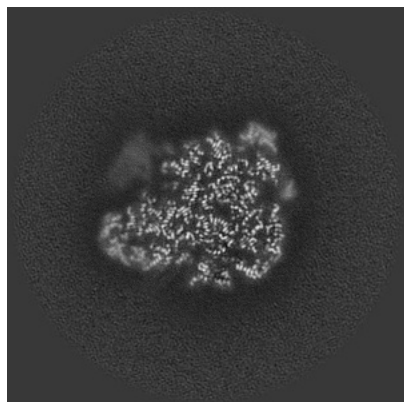


Y Index: 265

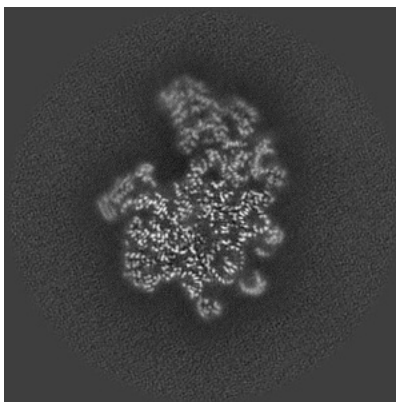


Z Index: 209

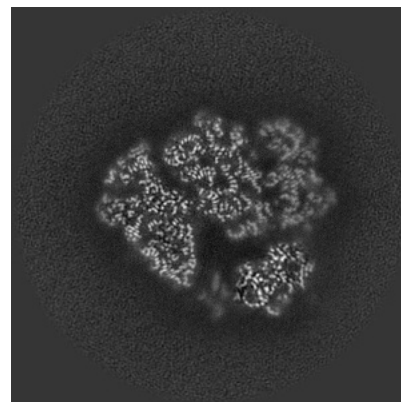
6.3.2 Raw map



X Index: 228



Y Index: 265

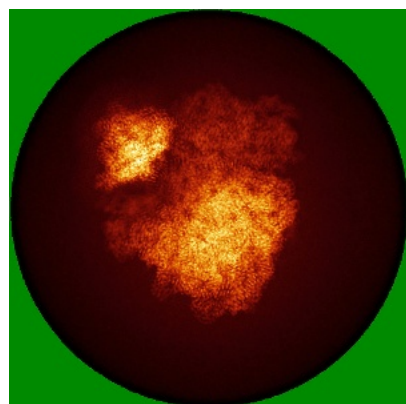


Z Index: 252

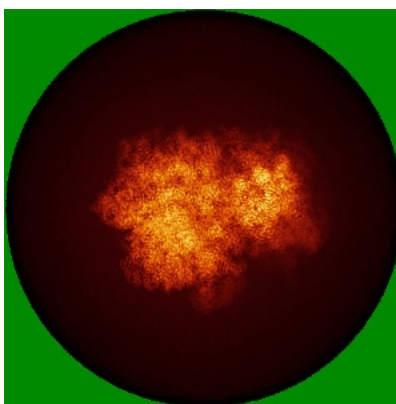
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

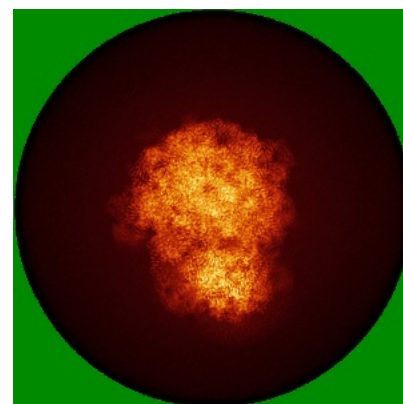
6.4.1 Primary map



X

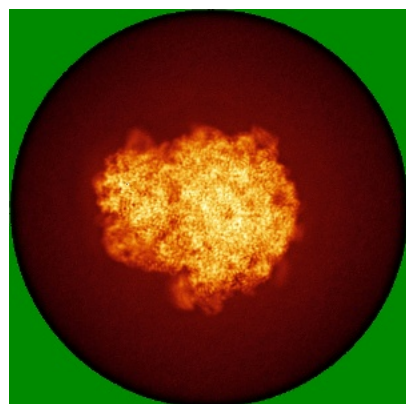


Y

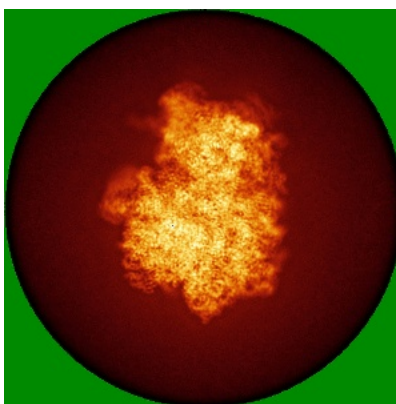


Z

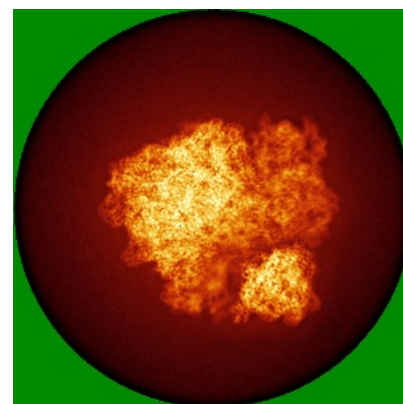
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



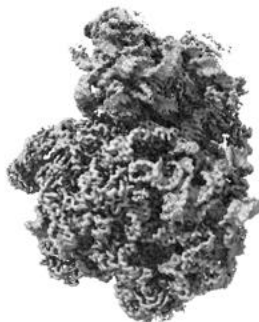
Z

The images above show the 3D surface view of the map at the recommended contour level 3.28. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

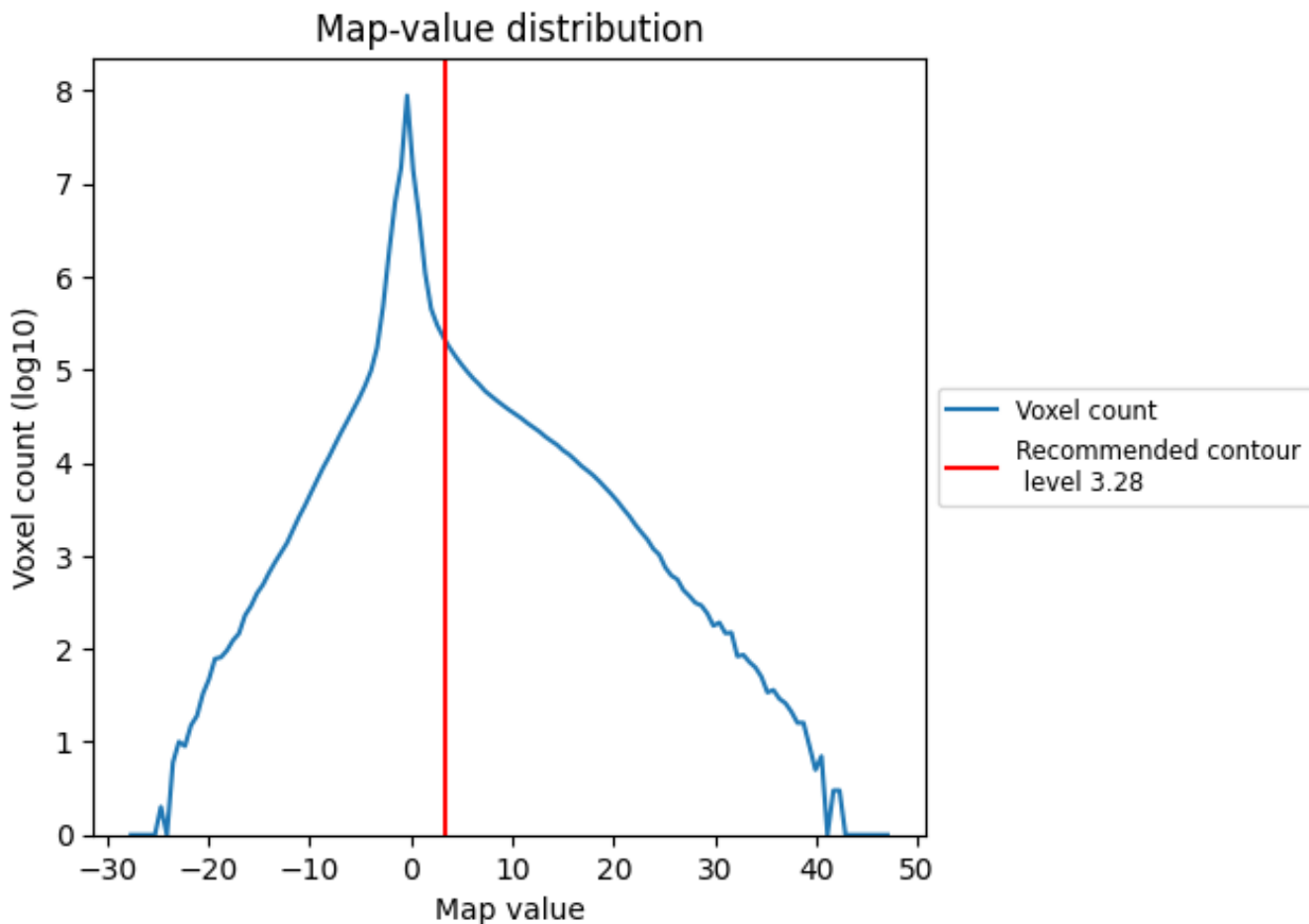
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

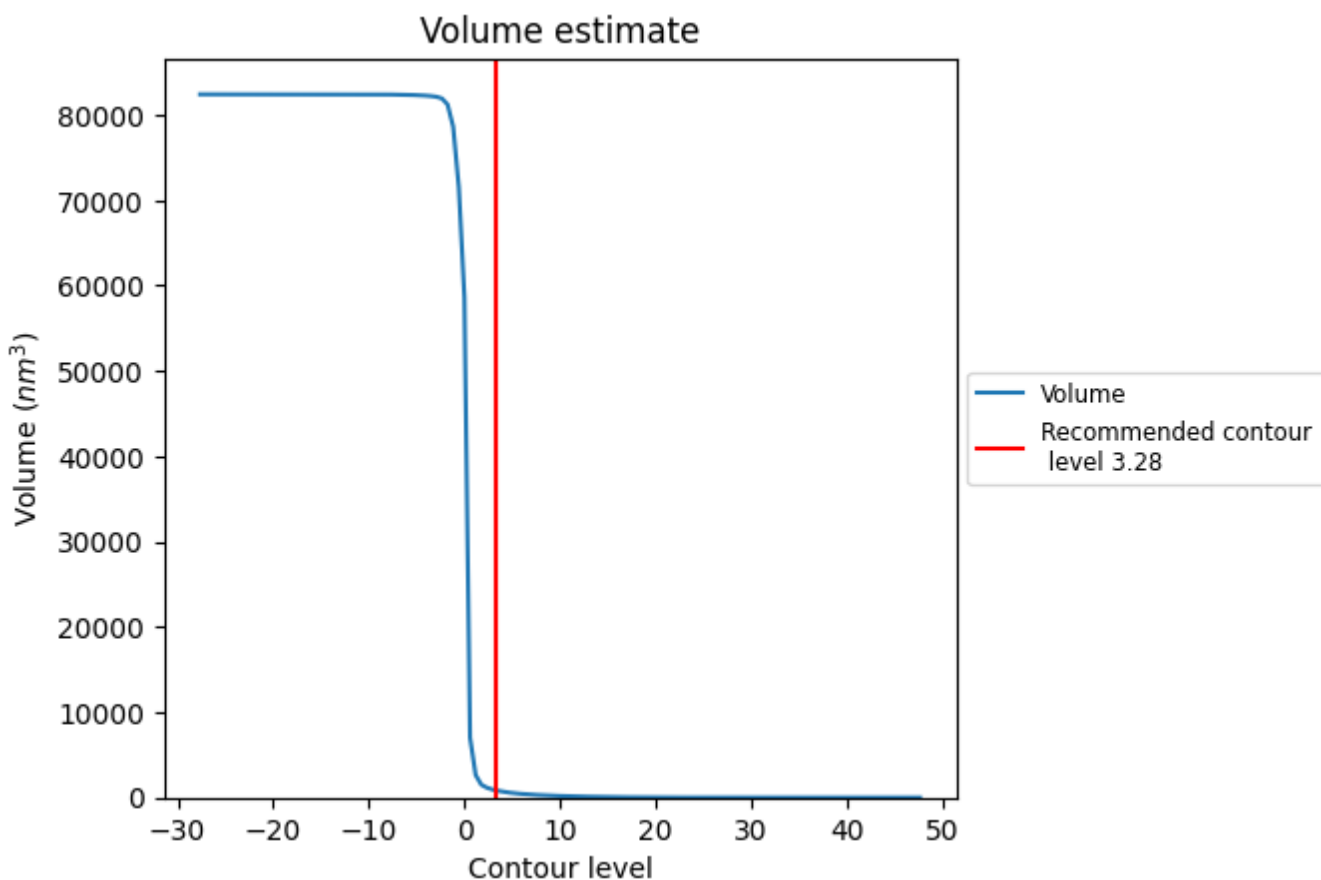
This section contains the results of statistical analysis of the map.

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.

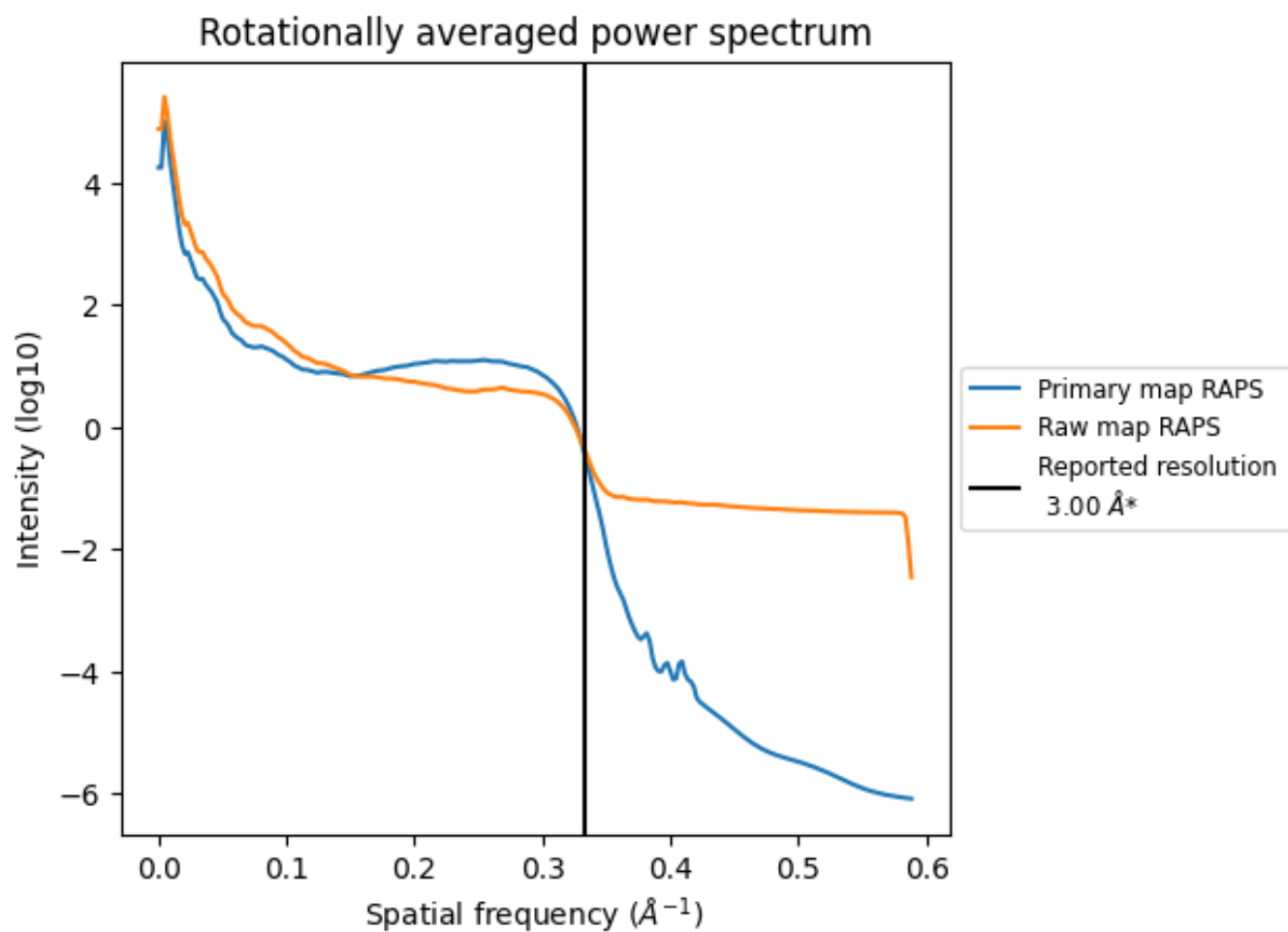
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 853 nm³; this corresponds to an approximate mass of 770 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](#)

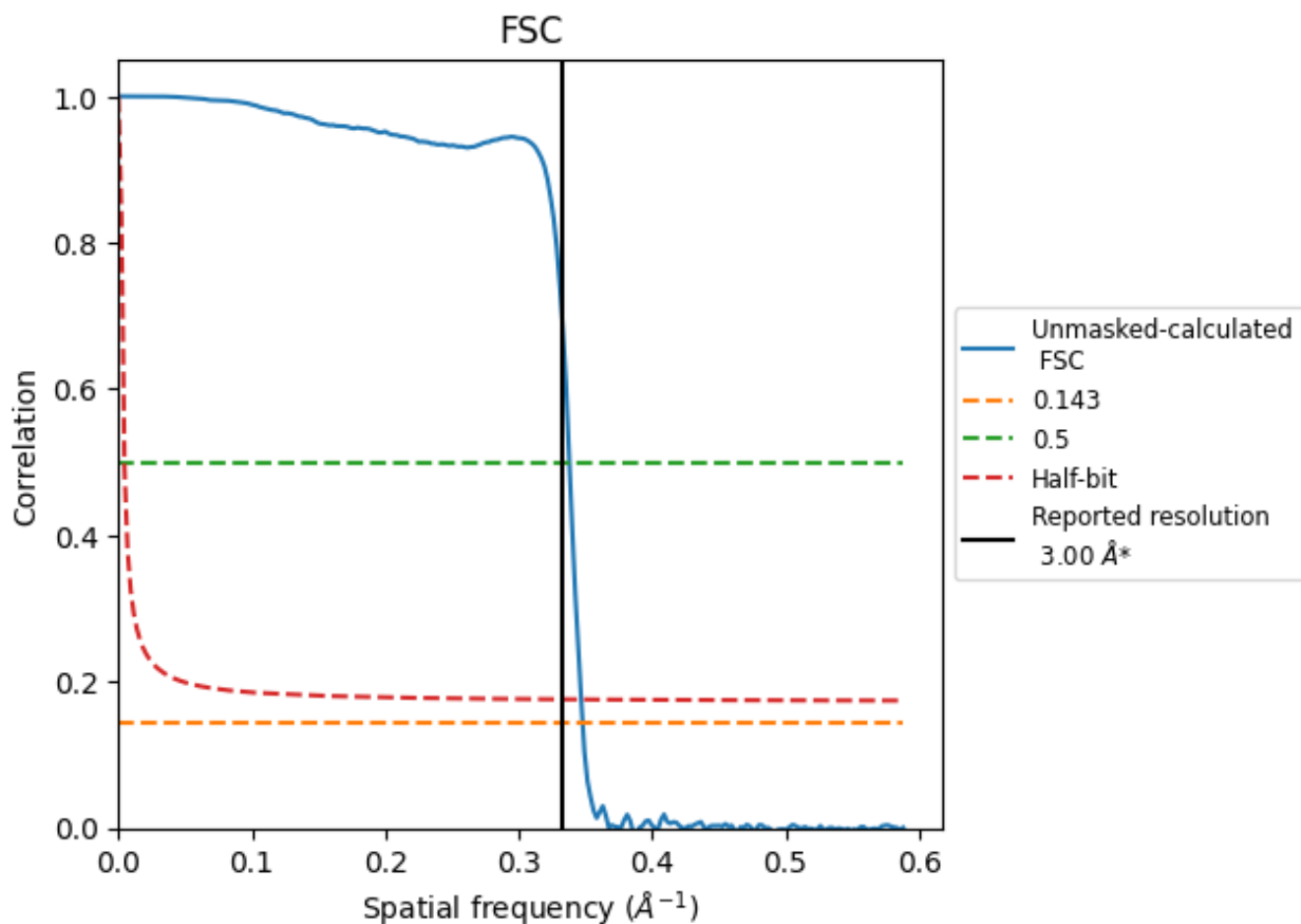


*Reported resolution corresponds to spatial frequency of 0.333 \AA^{-1}

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 0.333\AA^{-1}

8.2 Resolution estimates [i](#)

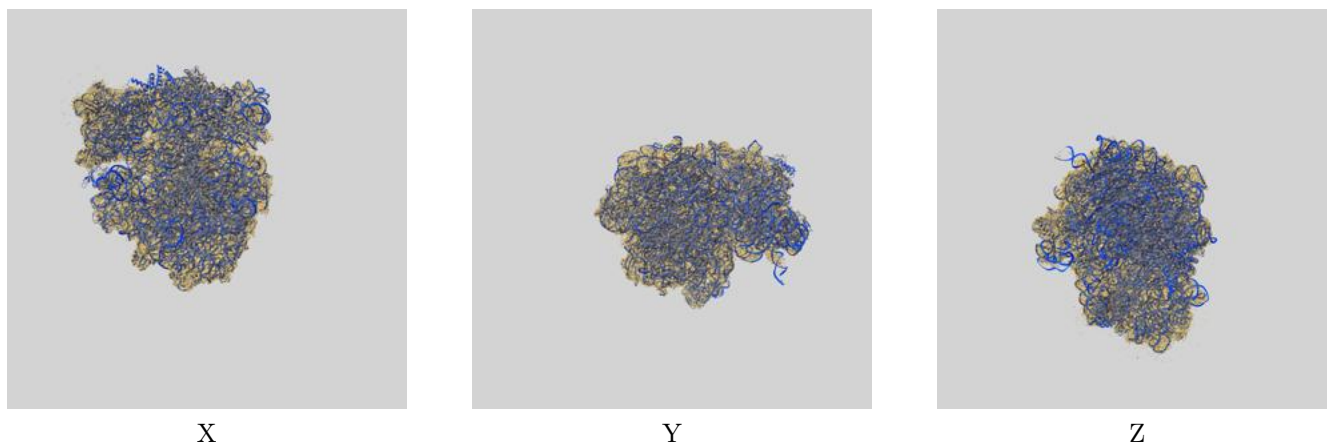
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.87	2.96	2.88

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

9 Map-model fit [i](#)

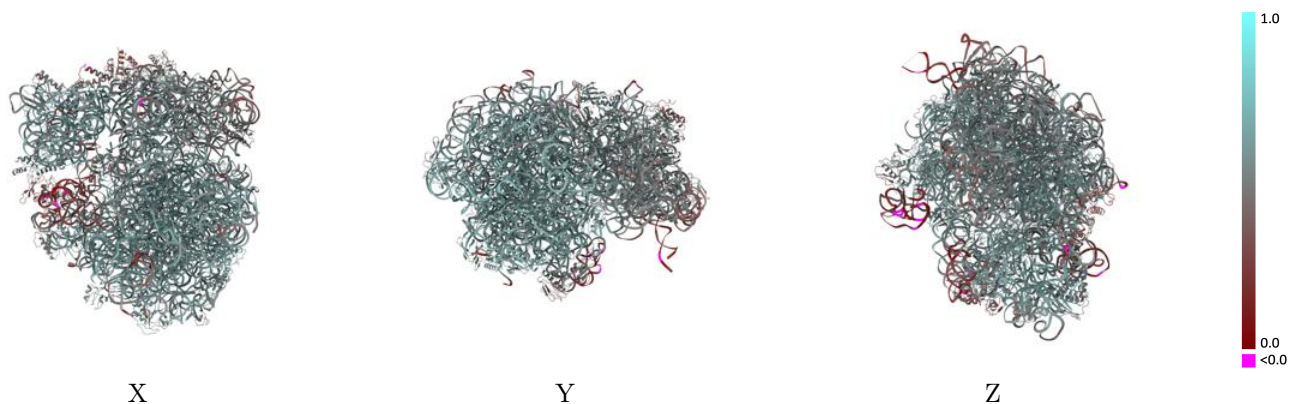
This section contains information regarding the fit between EMDB map EMD-42557 and PDB model 8UU5. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



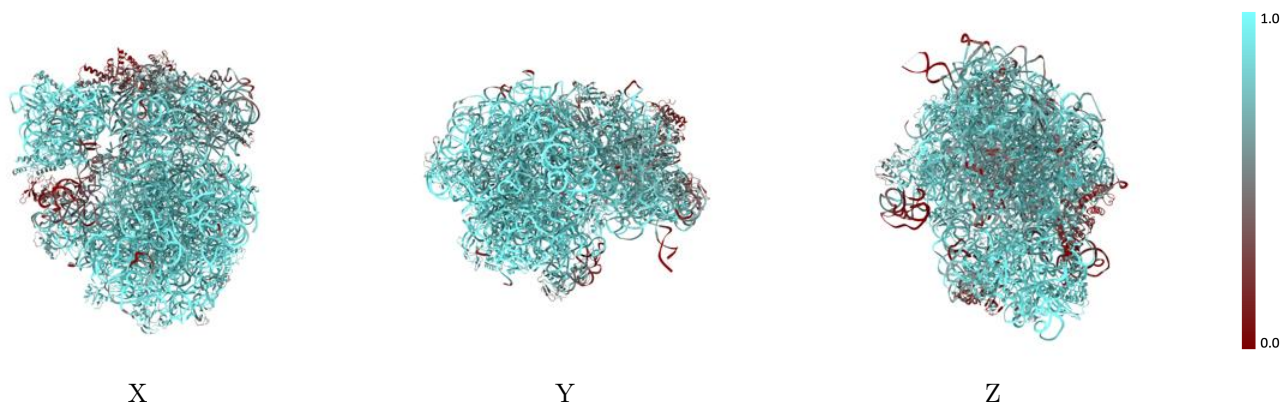
The images above show the 3D surface view of the map at the recommended contour level 3.28 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



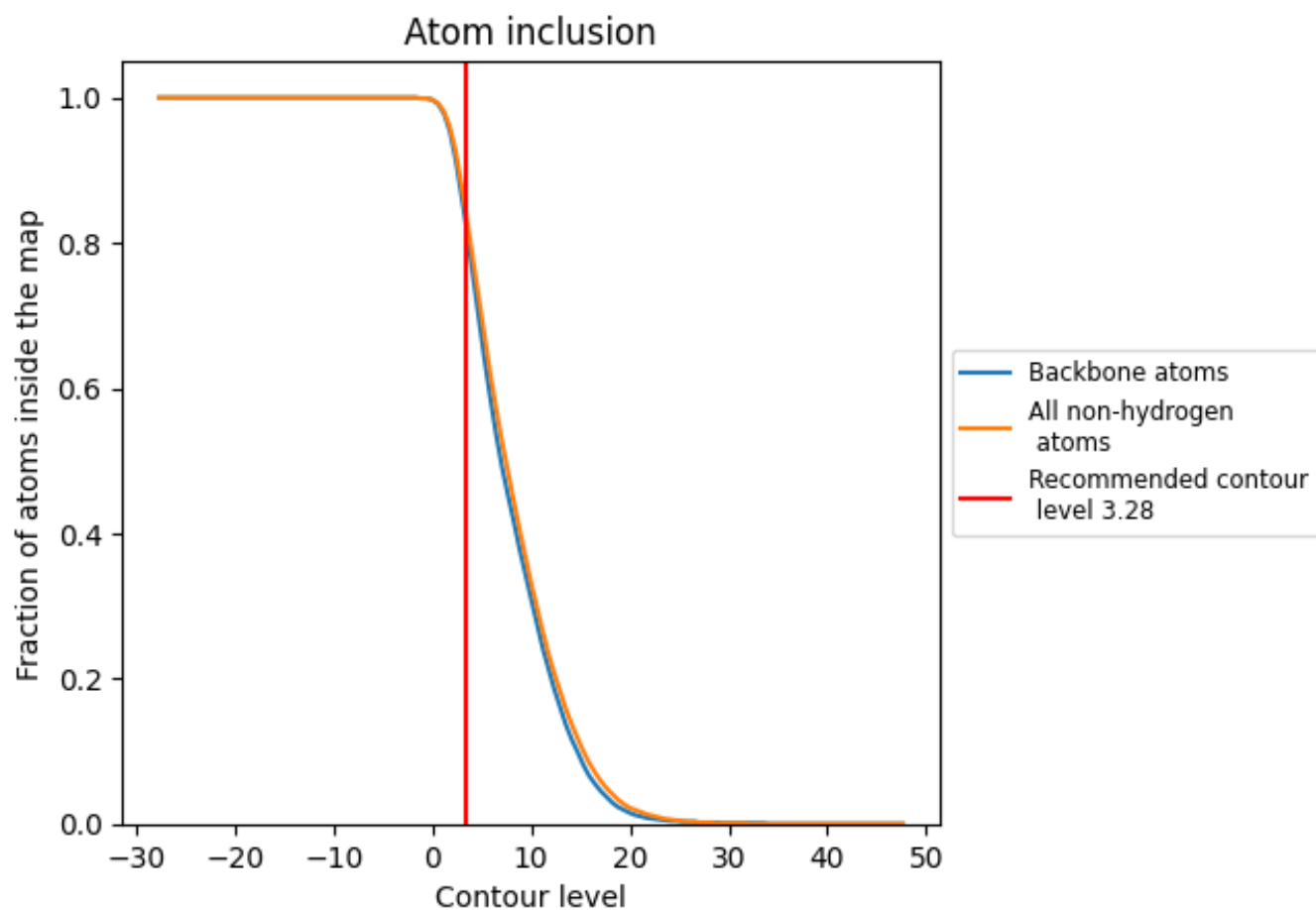
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.28).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 85% 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 (3.28) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8520	 0.5520
1	 0.8320	 0.5580
2	 0.9180	 0.6050
3	 0.2040	 0.3190
4	 0.9520	 0.6120
5	 0.8960	 0.5820
6	 0.9660	 0.6290
7	 0.9540	 0.6170
8	 0.9430	 0.6080
A	 0.9140	 0.5690
B	 0.8790	 0.5050
C	 0.9320	 0.6110
D	 0.9230	 0.6070
E	 0.8890	 0.5920
F	 0.3700	 0.4020
G	 0.6550	 0.4780
L	 0.9390	 0.6130
M	 0.9040	 0.6030
N	 0.8850	 0.5890
O	 0.9110	 0.5940
P	 0.9180	 0.6010
Q	 0.7360	 0.5110
R	 0.9120	 0.6020
S	 0.9390	 0.6110
T	 0.9110	 0.6070
U	 0.9240	 0.6060
V	 0.9080	 0.6020
W	 0.7460	 0.5400
Y	 0.9220	 0.6060
Z	 0.9130	 0.5870
a	 0.8610	 0.5340
b	 0.2210	 0.4040
c	 0.9030	 0.5760
d	 0.4380	 0.4600
e	 0.6020	 0.5280



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Chain	Atom inclusion	Q-score
f	 0.6990	 0.5330
g	 0.7930	 0.5240
h	 0.6400	 0.5250
i	 0.9250	 0.5700
j	 0.8650	 0.5480
k	 0.5810	 0.4960
l	 0.6010	 0.5150
m	 0.8410	 0.5460
n	 0.9510	 0.5990
o	 0.7170	 0.5190
p	 0.5510	 0.4960
q	 0.5020	 0.4830
r	 0.6920	 0.5430
s	 0.8080	 0.5590
t	 0.5710	 0.4800
w	 0.6980	 0.5240
x	 0.6070	 0.4390