



wwPDB EM Validation Summary Report ⓘ

Mar 15, 2026 – 11:37 AM UTC

PDB ID : 8UU9 / pdb_00008uu9
EMDB ID : EMD-42576
Title : Cryo-EM structure of the ratcheted *Listeria innocua* 70S ribosome (head-swiveled) in complex with HflXr and pe/E-tRNA (structure II-D)
Authors : Seely, S.M.; Basu, R.S.; Gagnon, M.G.
Deposited on : 2023-10-31
Resolution : 3.10 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:

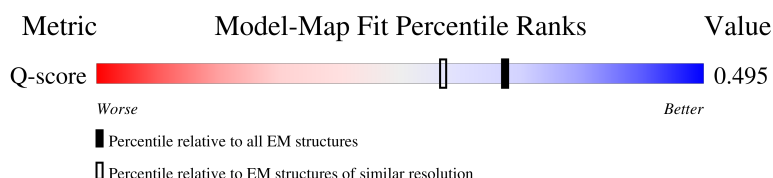
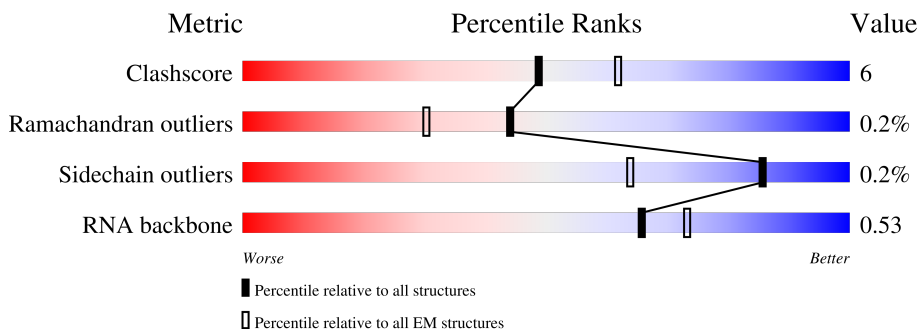
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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.



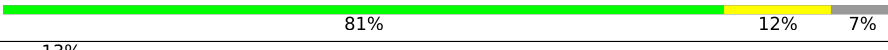
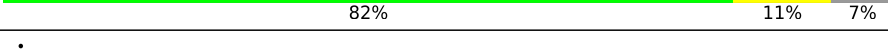
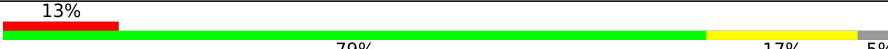
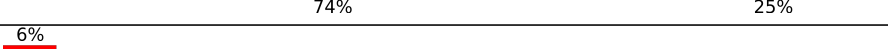
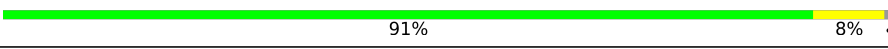
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	

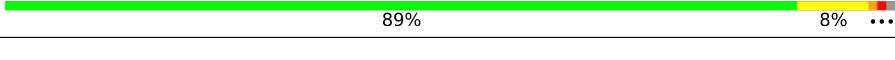
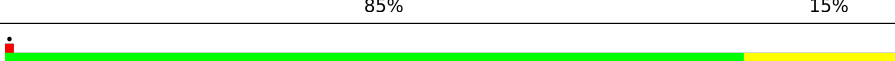
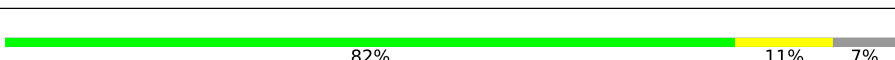
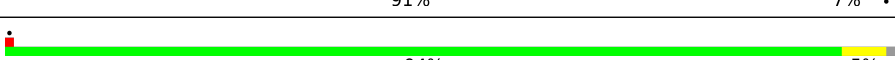
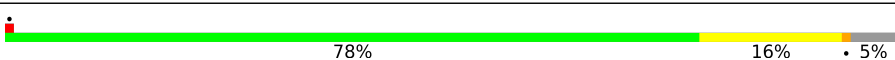
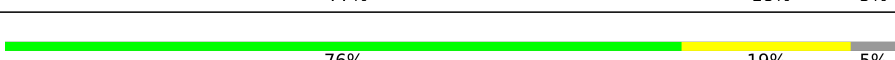
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Mol	Chain	Length	Quality of chain
4	d	200	
5	e	167	
6	f	97	
7	g	156	
8	h	132	
9	i	130	
10	j	102	
11	k	129	
12	l	137	
13	m	121	
14	n	61	
15	o	89	
16	p	90	
17	q	87	
18	r	79	
19	s	92	
20	t	84	
21	x	76	
22	w	21	
23	v	418	
24	A	2932	
25	B	116	
26	C	277	
27	D	209	
28	E	207	

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Mol	Chain	Length	Quality of chain
29	F	179	
30	G	178	
31	L	145	
32	M	122	
33	N	146	
34	O	144	
35	P	135	
36	Q	119	
37	R	114	
38	S	119	
39	T	102	
40	U	118	
41	V	94	
42	W	103	
43	Y	96	
44	Z	62	
45	1	63	
46	2	59	
47	3	81	
48	4	57	
49	5	49	
50	6	44	
51	7	66	
52	8	37	

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 142177 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
1	a	1515	Total	C	N	O	P	0	0
			32493	14494	5955	10529	1515		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	224	Total	C	N	O	S	0	0
			1588	1011	279	292	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	204	Total	C	N	O	S	0	0
			1150	705	223	221	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	199	Total	C	N	O	S	0	0
			1537	961	286	288	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	155	Total	C	N	O	S	0	0
			1116	701	203	210	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	93	Total	C	N	O	S	0	0
			655	423	119	111	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	147	Total	C	N	O	S	0	0
			866	533	173	158	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	131	Total	C	N	O	S	0	0
			1022	651	180	189	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	123	Total	C	N	O	S	0	0
			833	520	163	149	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	96	Total	C	N	O	S	0	0
			608	376	116	115	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	114	Total	C	N	O	S	0	0
			824	508	158	155	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	l	135	Total	C	N	O	S	0	0
			1002	621	198	181	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	114	Total	C	N	O	S	0	0
			616	367	134	114	1		

- 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
			445	283	84	73	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	o	87	Total	C	N	O	S	0	0
			696	433	136	125	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	p	88	Total	C	N	O	S	0	0
			711	450	132	126	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	81	Total	C	N	O	S	0	0
			629	396	120	112	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	r	65	Total	C	N	O	S	0	0
			527	339	96	90	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
19	s	74	Total	C	N	O	0	0
			459	279	96	84		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	t	80	Total	C	N	O	S	0	0
			607	366	124	116	1		

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

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
22	w	8	Total	C	N	O	P		0	0
			168	76	29	55	8			

- Molecule 23 is a protein called GTPase HflX.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	v	416	Total	C	N	O	S		0	0
			3200	2015	558	619	8			

- Molecule 24 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	A	2899	Total	C	N	O	P		0	0
			62278	27794	11524	20061	2899			

- Molecule 25 is a RNA chain called 5S Ribosomal RNA.

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

- Molecule 26 is a protein called Large ribosomal subunit protein uL2.

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

- Molecule 27 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	D	206	Total	C	N	O	S		0	0
			1545	974	287	280	4			

- Molecule 28 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	E	204	Total	C	N	O	0	0
			1564	989	288	287		

- Molecule 29 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	F	175	Total	C	N	O	S	0
			1232	785	211	231	5	0

- Molecule 30 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	G	176	Total	C	N	O	S	0
			1318	830	244	243	1	0

- Molecule 31 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	L	143	Total	C	N	O	S	0
			1128	715	205	205	3	0

- Molecule 32 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	M	122	Total	C	N	O	S	0
			925	573	175	172	5	0

- Molecule 33 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	N	146	Total	C	N	O	S	0
			1112	687	216	208	1	0

- Molecule 34 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	O	134	Total	C	N	O	S	0
			1057	677	203	171	6	0

- Molecule 35 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	P	123	Total	C	N	O	S	0	0
			986	618	194	173	1		

- Molecule 36 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Q	119	Total	C	N	O	S	0	0
			867	530	172	164	1		

- Molecule 37 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	R	113	Total	C	N	O	S	0	0
			879	557	168	153	1		

- Molecule 38 is a protein called Large ribosomal subunit protein bL20.

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

- Molecule 39 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	T	101	Total	C	N	O	S	0	0
			785	506	134	144	1		

- Molecule 40 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	U	112	Total	C	N	O	S	0	0
			864	544	162	158			

- Molecule 41 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	V	93	Total	C	N	O	S	0	0
			760	482	132	143	3		

- Molecule 42 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	W	100	Total	C	N	O	S	0	0
			734	465	137	129	3		

- Molecule 43 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Y	76	Total	C	N	O	S	0	0
			585	357	114	113	1		

- Molecule 44 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Z	59	Total	C	N	O	S	0	0
			462	286	97	77	2		

- Molecule 45 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	1	60	Total	C	N	O	S	0	0
			495	304	95	95	1		

- Molecule 46 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	2	56	Total	C	N	O	S	0	0
			433	272	82	78	1		

- Molecule 47 is a protein called Large ribosomal subunit protein bL31B.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	3	70	Total	C	N	O	0	0
			424	263	78	83		

- Molecule 48 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	4	53	Total	C	N	O	S	0	0
			425	259	87	74	5		

- Molecule 49 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	5	48	Total	C	N	O	S	0	0
			394	241	79	70	4		

- Molecule 50 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	6	43	Total	C	N	O	S	0	0
			365	222	88	53	2		

- Molecule 51 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	7	65	Total	C	N	O	S	0	0
			529	328	116	80	5		

- Molecule 52 is a protein called Large ribosomal subunit protein bL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	8	36	Total	C	N	O	S	0	0
			292	183	59	44	6		

- Molecule 53 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
53	a	202	Total	Mg	0
			202	202	
53	c	1	Total	Mg	0
			1	1	
53	e	1	Total	Mg	0
			1	1	
53	i	1	Total	Mg	0
			1	1	
53	l	1	Total	Mg	0
			1	1	
53	m	1	Total	Mg	0
			1	1	
53	q	1	Total	Mg	0
			1	1	
53	v	3	Total	Mg	0
			3	3	
53	A	256	Total	Mg	0
			256	256	

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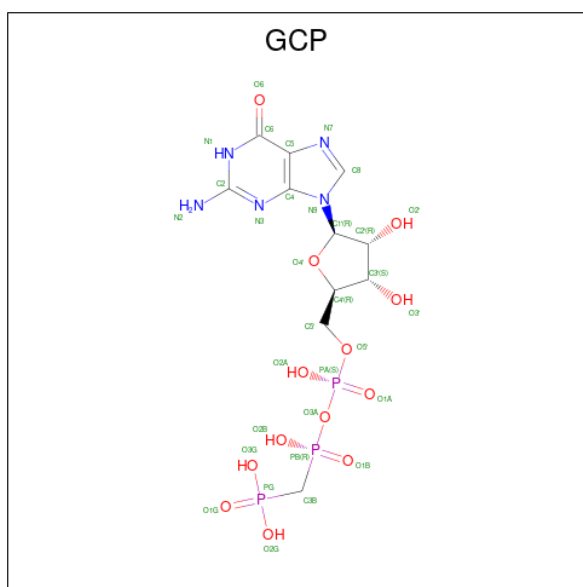
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Mol	Chain	Residues	Atoms		AltConf
53	B	4	Total	Mg	0
			4	4	
53	C	2	Total	Mg	0
			2	2	
53	V	1	Total	Mg	0
			1	1	
53	Y	1	Total	Mg	0
			1	1	

- Molecule 54 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
54	n	1	Total	Zn	0
			1	1	
54	4	1	Total	Zn	0
			1	1	
54	5	1	Total	Zn	0
			1	1	
54	8	1	Total	Zn	0
			1	1	

- Molecule 55 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: C₁₁H₁₈N₅O₁₃P₃).



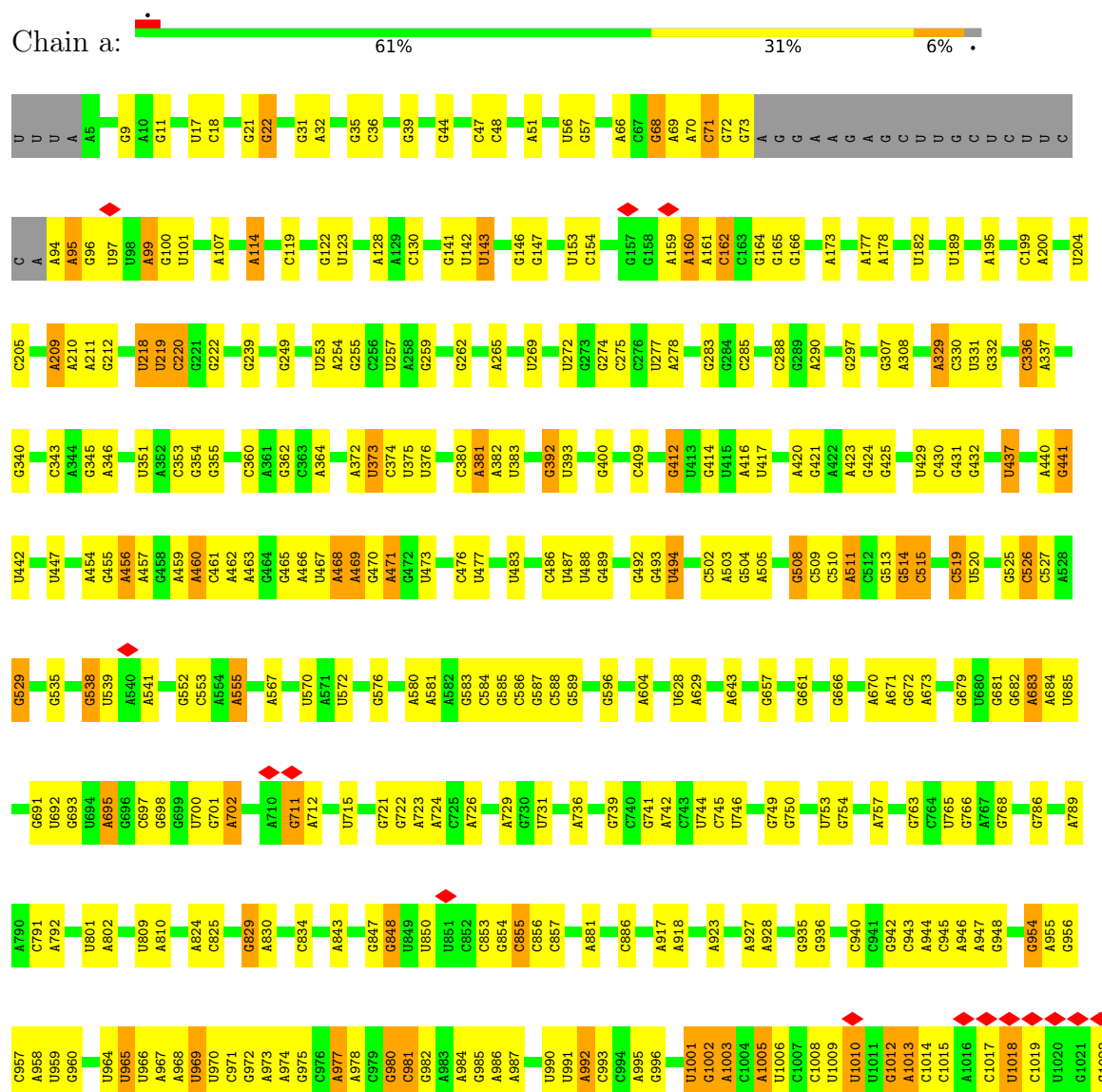
- Molecule 56 is water.

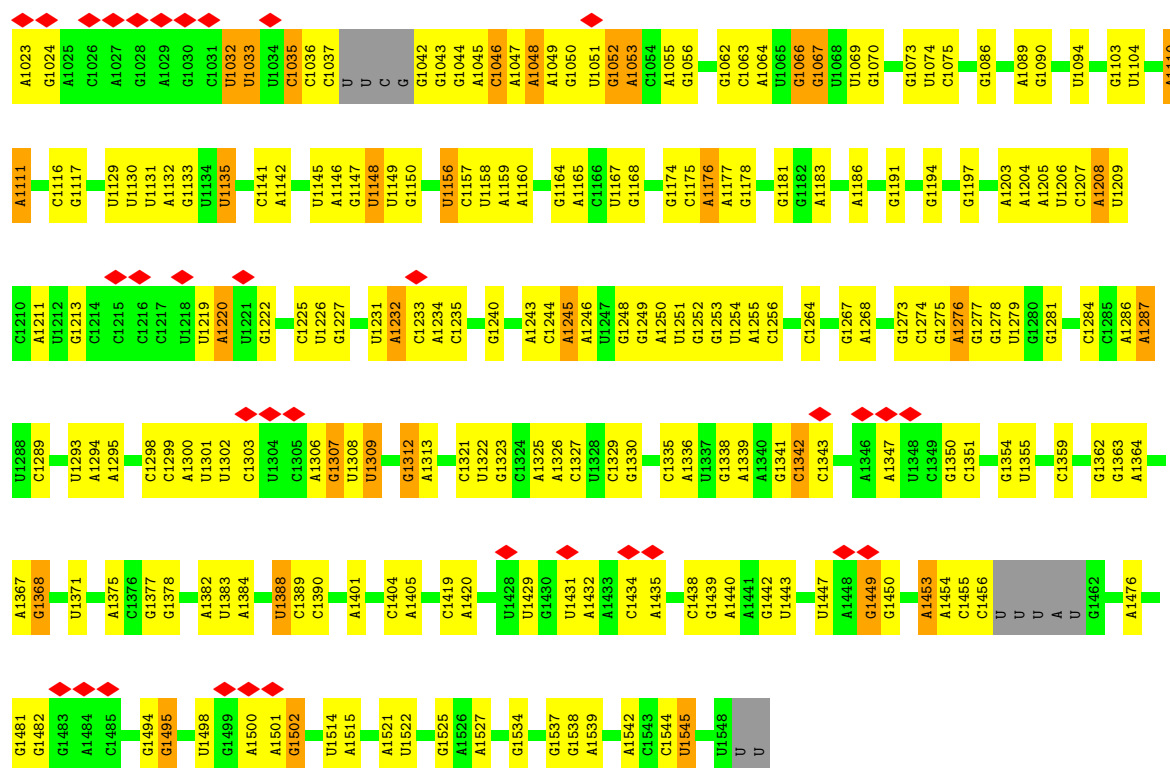
Mol	Chain	Residues	Atoms		AltConf
56	a	105	Total 105	O 105	0
56	c	1	Total 1	O 1	0
56	d	2	Total 2	O 2	0
56	e	1	Total 1	O 1	0
56	m	2	Total 2	O 2	0
56	n	2	Total 2	O 2	0
56	p	1	Total 1	O 1	0
56	v	2	Total 2	O 2	0
56	A	255	Total 255	O 255	0
56	B	5	Total 5	O 5	0
56	C	1	Total 1	O 1	0
56	N	4	Total 4	O 4	0
56	O	2	Total 2	O 2	0
56	P	1	Total 1	O 1	0
56	S	3	Total 3	O 3	0
56	T	1	Total 1	O 1	0
56	U	1	Total 1	O 1	0
56	V	3	Total 3	O 3	0
56	Y	1	Total 1	O 1	0
56	Z	2	Total 2	O 2	0
56	2	1	Total 1	O 1	0

3 Residue-property plots

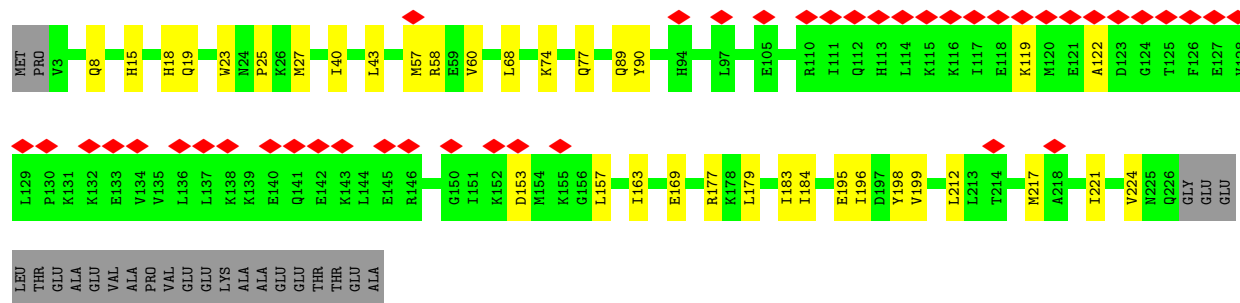
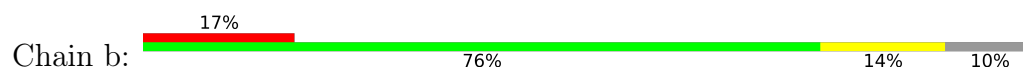
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

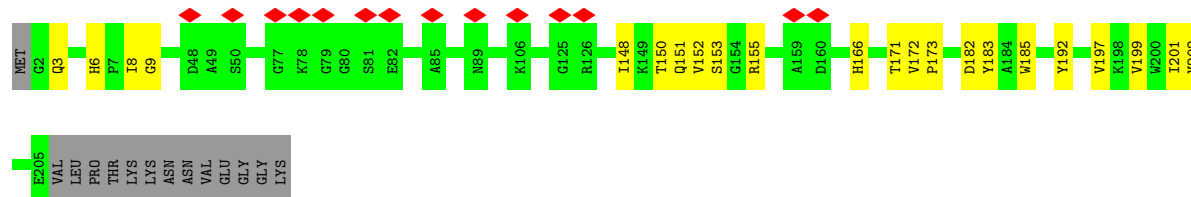
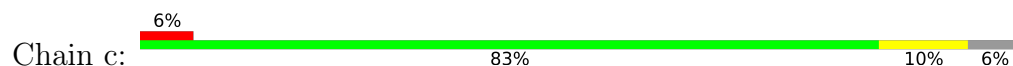




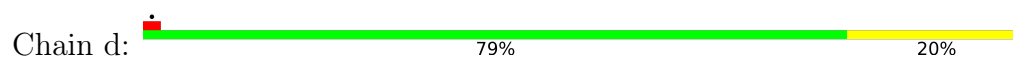
• Molecule 2: Small ribosomal subunit protein uS2



• Molecule 3: Small ribosomal subunit protein uS3



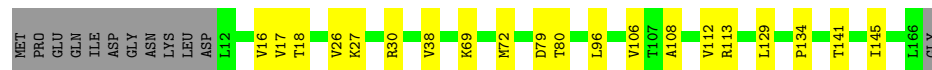
• Molecule 4: Small ribosomal subunit protein uS4





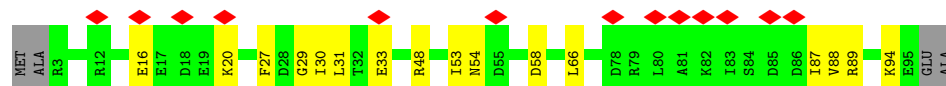
- Molecule 5: Small ribosomal subunit protein uS5

Chain e: 81% 12% 7%



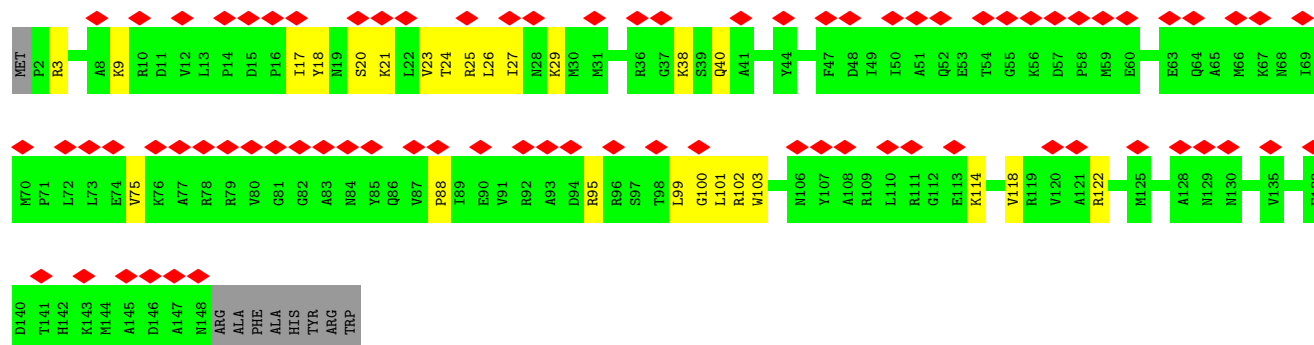
- Molecule 6: Small ribosomal subunit protein bS6

Chain f: 13% 79% 16%



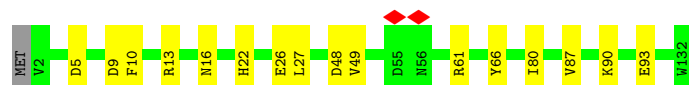
- Molecule 7: Small ribosomal subunit protein uS7

Chain g: 50% 78% 16% 6%



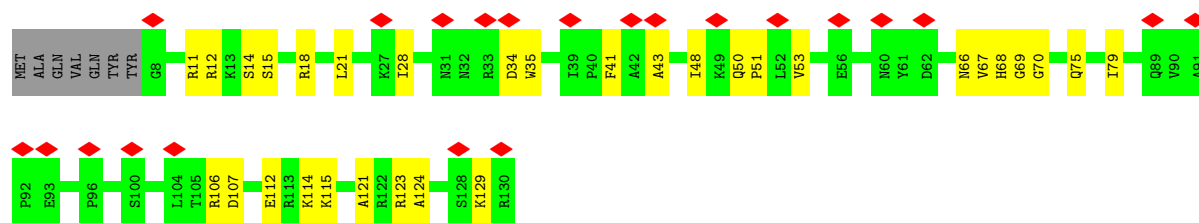
- Molecule 8: Small ribosomal subunit protein uS8

Chain h: 87% 12%

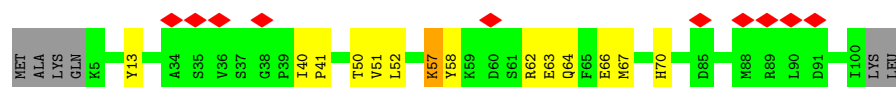
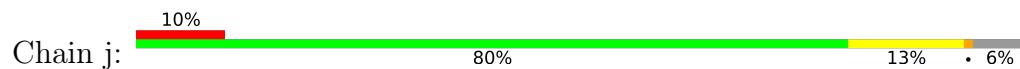


- Molecule 9: Small ribosomal subunit protein uS9

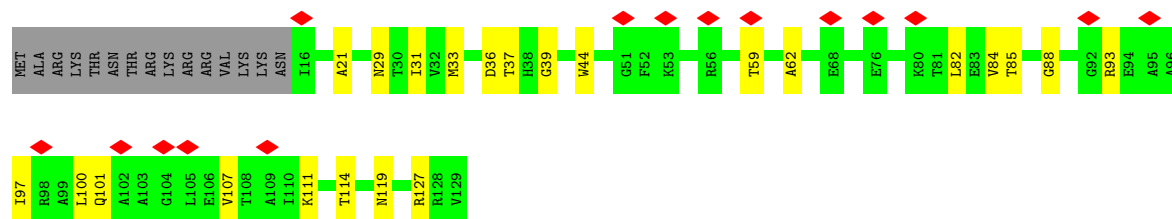
Chain i: 17% 71% 24% 5%



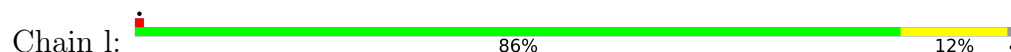
- Molecule 10: Small ribosomal subunit protein uS10



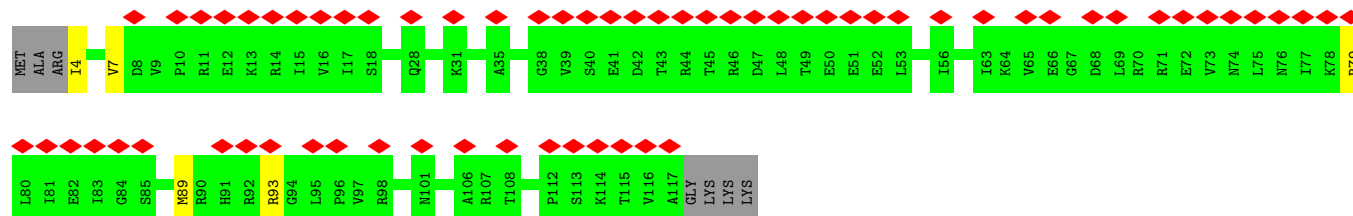
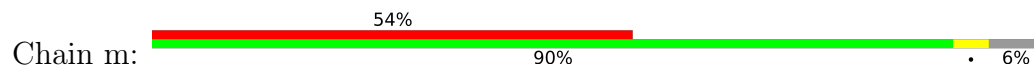
- Molecule 11: Small ribosomal subunit protein uS11



- Molecule 12: Small ribosomal subunit protein uS12

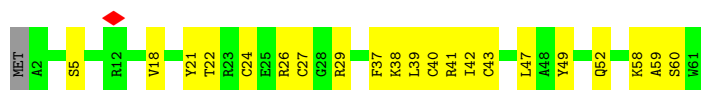


- Molecule 13: Small ribosomal subunit protein uS13

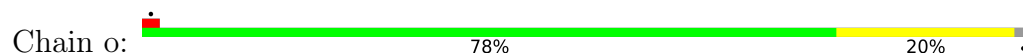


- Molecule 14: Small ribosomal subunit protein uS14

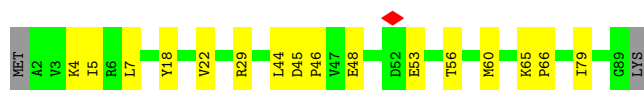
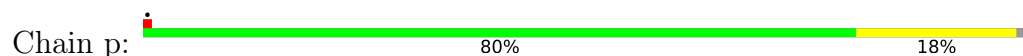




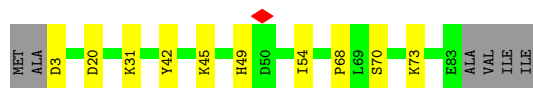
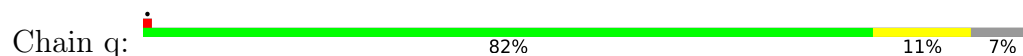
- Molecule 15: Small ribosomal subunit protein uS15



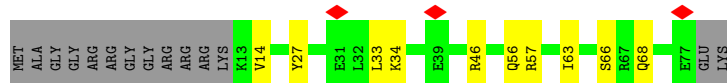
- Molecule 16: Small ribosomal subunit protein bS16



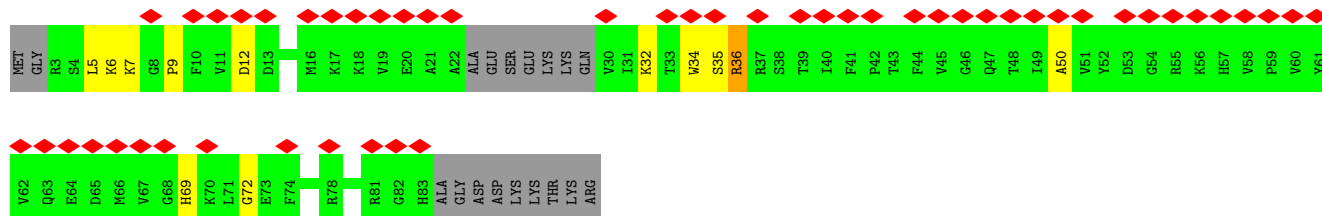
- Molecule 17: Small ribosomal subunit protein uS17



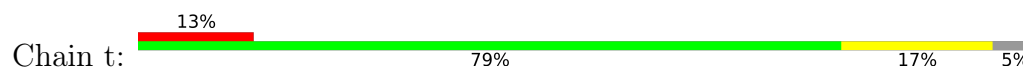
- Molecule 18: Small ribosomal subunit protein bS18

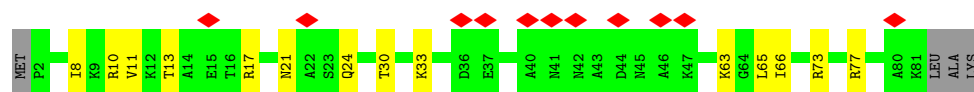


- Molecule 19: Small ribosomal subunit protein uS19

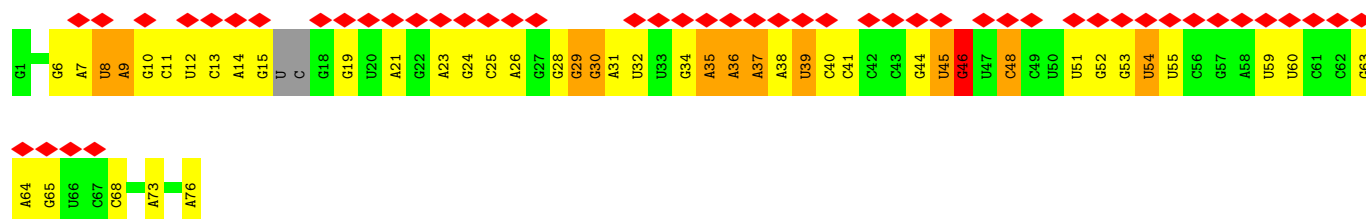


- Molecule 20: Small ribosomal subunit protein bS20

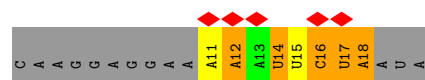




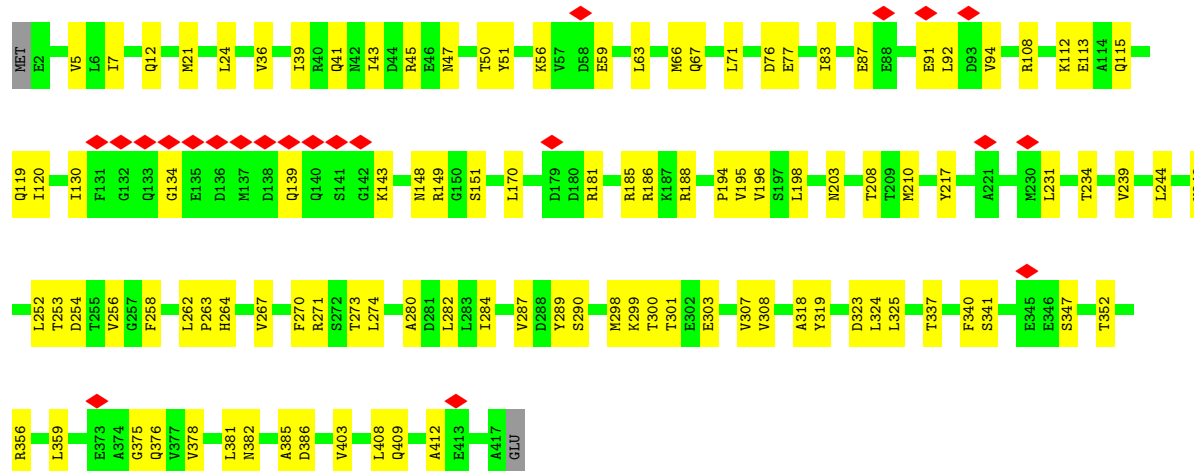
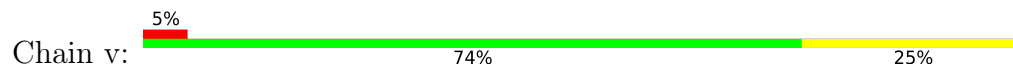
• Molecule 21: pe/E Hybrid State Phenylalanine tRNA



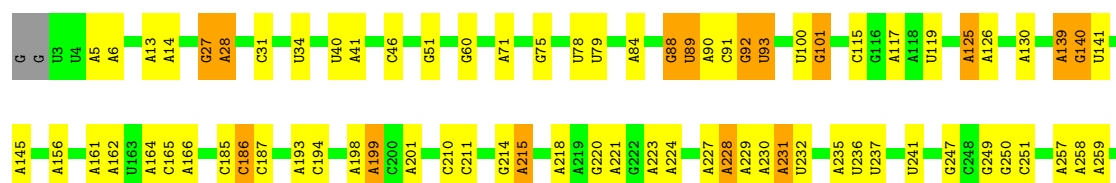
• Molecule 22: F-Stop mRNA



• Molecule 23: GTPase HflX



• Molecule 24: 23S Ribosomal RNA

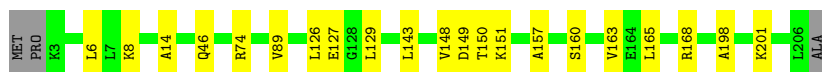






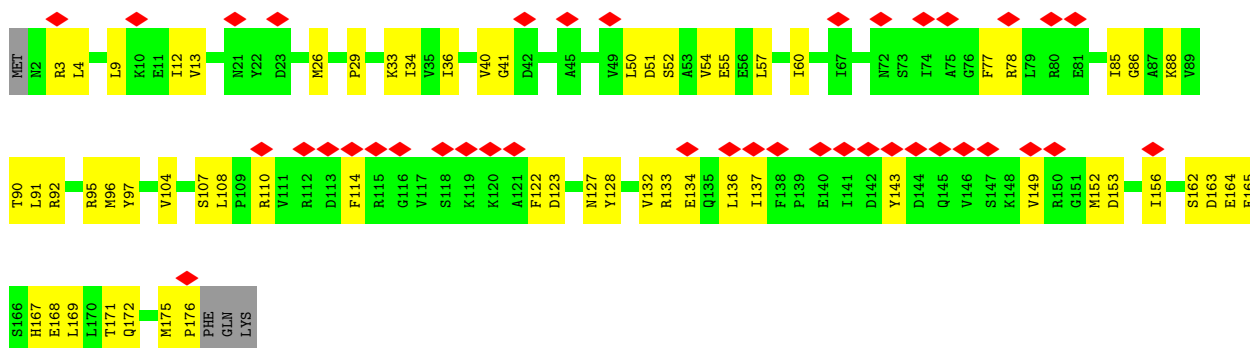
- Molecule 28: Large ribosomal subunit protein uL4

Chain E: 88% 10%



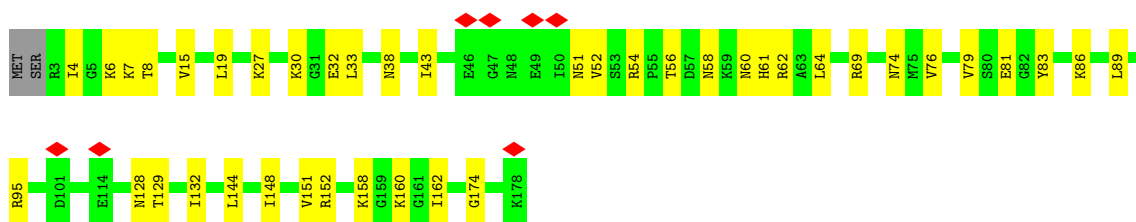
- Molecule 29: Large ribosomal subunit protein uL5

Chain F: 22% 64% 34%



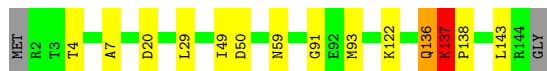
- Molecule 30: Large ribosomal subunit protein uL6

Chain G: 76% 23%



- Molecule 31: Large ribosomal subunit protein uL13

Chain L: 89% 8%

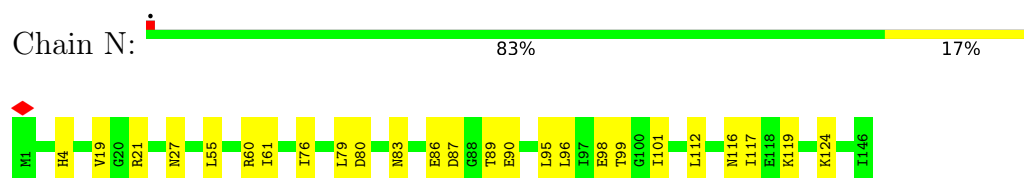


- Molecule 32: Large ribosomal subunit protein uL14

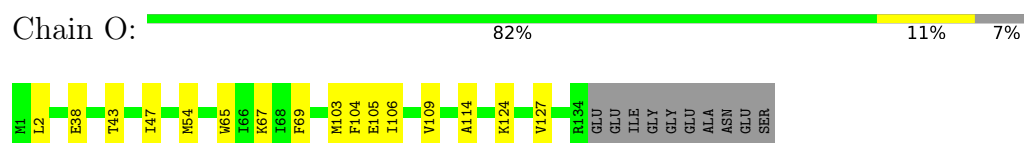
Chain M: 85% 15%



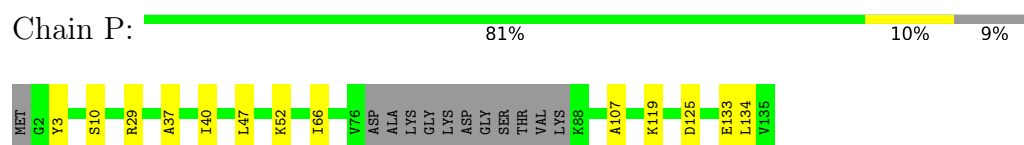
- Molecule 33: Large ribosomal subunit protein uL15



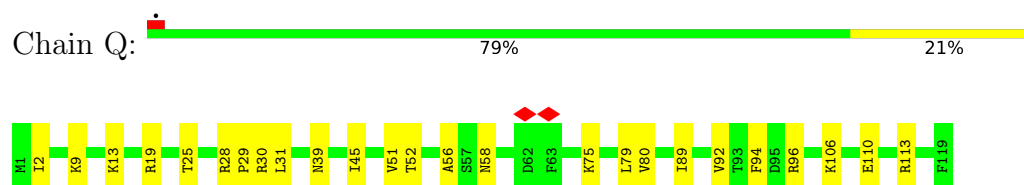
- Molecule 34: Large ribosomal subunit protein uL16



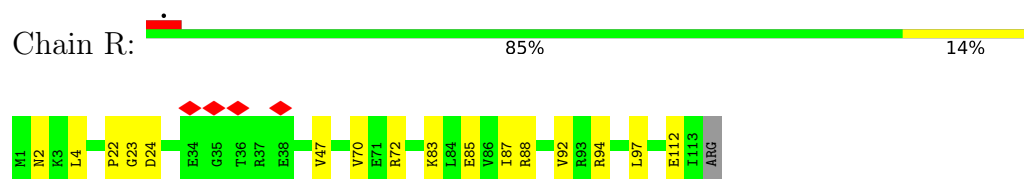
- Molecule 35: Large ribosomal subunit protein bL17



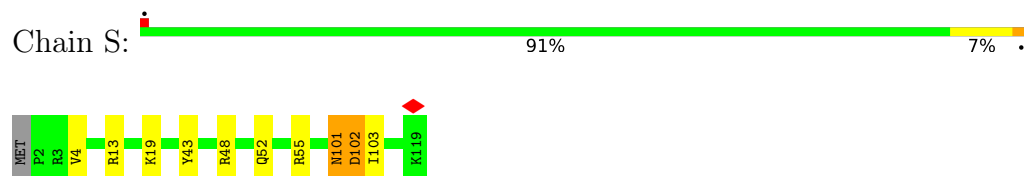
- Molecule 36: Large ribosomal subunit protein uL18



- Molecule 37: Large ribosomal subunit protein bL19

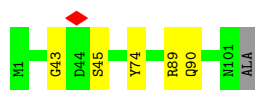


- Molecule 38: Large ribosomal subunit protein bL20

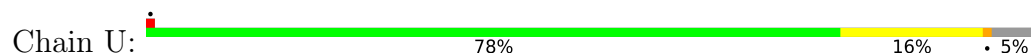


- Molecule 39: Large ribosomal subunit protein bL21

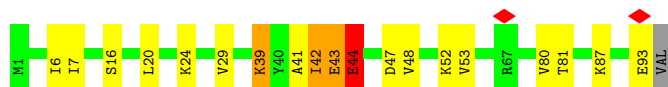
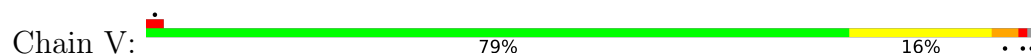




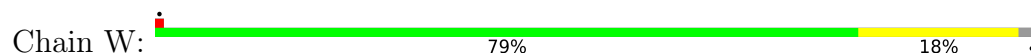
- Molecule 40: Large ribosomal subunit protein uL22



- Molecule 41: Large ribosomal subunit protein uL23



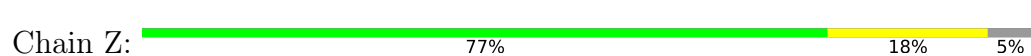
- Molecule 42: Large ribosomal subunit protein uL24



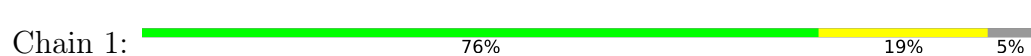
- Molecule 43: Large ribosomal subunit protein bL27



- Molecule 44: Large ribosomal subunit protein bL28



- Molecule 45: Large ribosomal subunit protein uL29



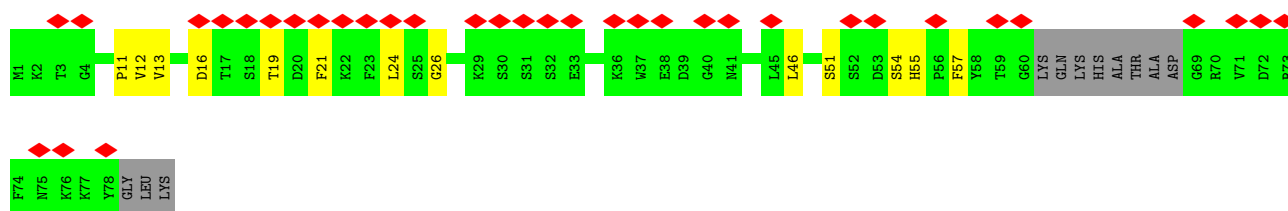
- Molecule 46: Large ribosomal subunit protein uL30

Chain 2:  80% 15% 5%



- Molecule 47: Large ribosomal subunit protein bL31B

Chain 3:  43% 70% 16% 14%



- Molecule 48: Large ribosomal subunit protein bL32

Chain 4:  75% 18% 7%



- Molecule 49: Large ribosomal subunit protein bL33

Chain 5:  82% 16% .



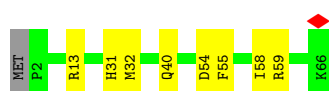
- Molecule 50: Large ribosomal subunit protein bL34

Chain 6:  91% 7% .



- Molecule 51: Large ribosomal subunit protein bL35

Chain 7:  86% 12% .



- Molecule 52: Large ribosomal subunit protein bL36

Chain 8:  65% 32% .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	80381	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	31.784	Depositor
Minimum map value	-18.322	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	1.115	Depositor
Recommended contour level	3.4	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MIA, 7MG, MG, ZN, 5MU, PSU, 4SU, GCP

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	0.28	0/36378	0.34	0/56739
2	b	0.22	0/1612	0.40	0/2195
3	c	0.23	0/1160	0.41	0/1601
4	d	0.24	0/1564	0.34	0/2109
5	e	0.24	0/1129	0.39	0/1530
6	f	0.17	0/666	0.37	0/909
7	g	0.21	0/871	0.44	0/1190
8	h	0.31	0/1035	0.41	0/1392
9	i	0.25	0/845	0.42	0/1146
10	j	0.27	0/617	0.51	2/845 (0.2%)
11	k	0.17	0/838	0.33	0/1132
12	l	0.29	0/1017	0.44	0/1375
13	m	0.15	0/617	0.27	0/843
14	n	0.31	0/453	0.49	0/608
15	o	0.20	0/706	0.36	0/952
16	p	0.28	0/724	0.39	0/970
17	q	0.21	0/638	0.32	0/860
18	r	0.23	0/535	0.37	0/716
19	s	0.22	0/466	0.54	0/636
20	t	0.23	0/610	0.34	0/813
21	x	0.19	0/1605	0.30	0/2497
22	w	0.18	0/187	0.42	0/288
23	v	0.26	0/3240	0.40	0/4380
24	A	0.24	0/69775	0.30	0/108849
25	B	0.14	0/2711	0.21	0/4224
26	C	0.24	0/2144	0.31	0/2875
27	D	0.25	0/1567	0.38	0/2111
28	E	0.21	0/1584	0.34	0/2134
29	F	0.18	0/1249	0.42	0/1704
30	G	0.15	0/1339	0.32	0/1811
31	L	0.23	0/1151	0.39	2/1546 (0.1%)
32	M	0.21	0/932	0.34	0/1248

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	N	0.22	0/1123	0.34	0/1492
34	O	0.22	0/1079	0.28	0/1442
35	P	0.23	0/997	0.34	0/1333
36	Q	0.14	0/874	0.28	0/1175
37	R	0.21	0/891	0.28	0/1199
38	S	0.32	0/966	0.40	0/1284
39	T	0.22	0/798	0.29	0/1071
40	U	0.24	0/874	0.34	0/1182
41	V	0.31	0/769	0.50	1/1029 (0.1%)
42	W	0.18	0/744	0.32	0/998
43	Y	0.24	0/592	0.41	0/788
44	Z	0.23	0/467	0.34	0/619
45	1	0.19	0/496	0.35	0/662
46	2	0.22	0/436	0.36	0/585
47	3	0.09	0/431	0.31	0/591
48	4	0.24	0/433	0.39	0/577
49	5	0.18	0/398	0.27	0/534
50	6	0.24	0/368	0.31	0/479
51	7	0.25	0/536	0.44	0/696
52	8	0.22	0/295	0.36	0/387
All	All	0.24	0/153532	0.33	5/230351 (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
19	s	0	1
31	L	0	1
All	All	0	2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	V	44	GLU	N-CA-C	-6.08	105.99	113.41
10	j	58	TYR	CA-C-N	5.71	131.61	120.99
10	j	58	TYR	C-N-CA	5.71	131.61	120.99
31	L	136	GLN	CA-C-N	5.27	134.67	121.80
31	L	136	GLN	C-N-CA	5.27	134.67	121.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
31	L	137	LYS	Peptide
19	s	36	ARG	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	32493	0	16360	318	0
2	b	1588	0	1450	21	0
3	c	1150	0	774	17	0
4	d	1537	0	1494	32	0
5	e	1116	0	1150	11	0
6	f	655	0	577	12	0
7	g	866	0	645	21	0
8	h	1022	0	1078	9	0
9	i	833	0	754	23	0
10	j	608	0	441	14	0
11	k	824	0	829	17	0
12	l	1002	0	1023	12	0
13	m	616	0	375	3	0
14	n	445	0	430	22	0
15	o	696	0	689	12	0
16	p	711	0	740	11	0
17	q	629	0	629	8	0
18	r	527	0	566	6	0
19	s	459	0	305	8	0
20	t	607	0	632	8	0
21	x	1591	0	819	37	0
22	w	168	0	86	7	0
23	v	3200	0	3158	79	0
24	A	62278	0	31312	437	0
25	B	2428	0	1229	11	0
26	C	2108	0	2184	31	0
27	D	1545	0	1587	12	0
28	E	1564	0	1660	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	F	1232	0	1158	41	0
30	G	1318	0	1346	23	0
31	L	1128	0	1158	8	0
32	M	925	0	982	13	0
33	N	1112	0	1162	16	0
34	O	1057	0	1126	9	0
35	P	986	0	1046	9	0
36	Q	867	0	854	15	0
37	R	879	0	922	13	0
38	S	953	0	1029	7	0
39	T	785	0	823	4	0
40	U	864	0	920	14	0
41	V	760	0	792	12	0
42	W	734	0	782	13	0
43	Y	585	0	586	6	0
44	Z	462	0	507	8	0
45	1	495	0	515	8	0
46	2	433	0	479	7	0
47	3	424	0	297	7	0
48	4	425	0	423	8	0
49	5	394	0	403	5	0
50	6	365	0	417	2	0
51	7	529	0	584	5	0
52	8	292	0	334	9	0
53	A	256	0	0	0	0
53	B	4	0	0	0	0
53	C	2	0	0	0	0
53	V	1	0	0	0	0
53	Y	1	0	0	0	0
53	a	202	0	0	0	0
53	c	1	0	0	0	0
53	e	1	0	0	0	0
53	i	1	0	0	0	0
53	l	1	0	0	0	0
53	m	1	0	0	0	0
53	q	1	0	0	0	0
53	v	3	0	0	0	0
54	4	1	0	0	0	0
54	5	1	0	0	0	0
54	8	1	0	0	0	0
54	n	1	0	0	0	0
55	v	32	0	14	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	2	1	0	0	1	0
56	A	255	0	0	1	0
56	B	5	0	0	0	0
56	C	1	0	0	0	0
56	N	4	0	0	1	0
56	O	2	0	0	0	0
56	P	1	0	0	0	0
56	S	3	0	0	0	0
56	T	1	0	0	0	0
56	U	1	0	0	0	0
56	V	3	0	0	0	0
56	Y	1	0	0	0	0
56	Z	2	0	0	0	0
56	a	105	0	0	6	0
56	c	1	0	0	0	0
56	d	2	0	0	0	0
56	e	1	0	0	0	0
56	m	2	0	0	0	0
56	n	2	0	0	0	0
56	p	1	0	0	0	0
56	v	2	0	0	1	0
All	All	142177	0	91635	1341	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 1341 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1164:G:H21	1:a:1186:A:N6	1.40	1.17
1:a:68:G:H1	1:a:99:A:N6	1.41	1.16
1:a:1164:G:N2	1:a:1186:A:H61	1.47	1.12
24:A:2148:G:H21	24:A:2204:A:N6	1.46	1.11
24:A:2148:G:N2	24:A:2204:A:H61	1.58	0.99

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	b	222/249 (89%)	207 (93%)	15 (7%)	0	100	100
3	c	202/218 (93%)	171 (85%)	31 (15%)	0	100	100
4	d	197/200 (98%)	180 (91%)	17 (9%)	0	100	100
5	e	153/167 (92%)	142 (93%)	11 (7%)	0	100	100
6	f	91/97 (94%)	84 (92%)	7 (8%)	0	100	100
7	g	145/156 (93%)	122 (84%)	23 (16%)	0	100	100
8	h	129/132 (98%)	124 (96%)	5 (4%)	0	100	100
9	i	121/130 (93%)	111 (92%)	10 (8%)	0	100	100
10	j	94/102 (92%)	83 (88%)	10 (11%)	1 (1%)	11	39
11	k	112/129 (87%)	102 (91%)	10 (9%)	0	100	100
12	l	133/137 (97%)	126 (95%)	7 (5%)	0	100	100
13	m	112/121 (93%)	100 (89%)	12 (11%)	0	100	100
14	n	58/61 (95%)	52 (90%)	6 (10%)	0	100	100
15	o	85/89 (96%)	83 (98%)	2 (2%)	0	100	100
16	p	86/90 (96%)	82 (95%)	4 (5%)	0	100	100
17	q	79/87 (91%)	74 (94%)	5 (6%)	0	100	100
18	r	63/79 (80%)	59 (94%)	3 (5%)	1 (2%)	7	30
19	s	70/92 (76%)	54 (77%)	14 (20%)	2 (3%)	3	19
20	t	78/84 (93%)	76 (97%)	2 (3%)	0	100	100
23	v	414/418 (99%)	384 (93%)	30 (7%)	0	100	100
26	C	271/277 (98%)	258 (95%)	13 (5%)	0	100	100
27	D	204/209 (98%)	193 (95%)	11 (5%)	0	100	100
28	E	202/207 (98%)	189 (94%)	13 (6%)	0	100	100
29	F	173/179 (97%)	161 (93%)	12 (7%)	0	100	100
30	G	174/178 (98%)	163 (94%)	11 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	L	141/145 (97%)	137 (97%)	3 (2%)	1 (1%)	18	49
32	M	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
33	N	144/146 (99%)	137 (95%)	7 (5%)	0	100	100
34	O	132/144 (92%)	128 (97%)	4 (3%)	0	100	100
35	P	119/135 (88%)	113 (95%)	5 (4%)	1 (1%)	16	47
36	Q	117/119 (98%)	111 (95%)	6 (5%)	0	100	100
37	R	111/114 (97%)	106 (96%)	5 (4%)	0	100	100
38	S	116/119 (98%)	111 (96%)	4 (3%)	1 (1%)	14	44
39	T	99/102 (97%)	92 (93%)	7 (7%)	0	100	100
40	U	110/118 (93%)	105 (96%)	4 (4%)	1 (1%)	14	44
41	V	91/94 (97%)	84 (92%)	7 (8%)	0	100	100
42	W	98/103 (95%)	95 (97%)	2 (2%)	1 (1%)	12	41
43	Y	74/96 (77%)	67 (90%)	7 (10%)	0	100	100
44	Z	57/62 (92%)	52 (91%)	5 (9%)	0	100	100
45	1	58/63 (92%)	55 (95%)	3 (5%)	0	100	100
46	2	54/59 (92%)	51 (94%)	3 (6%)	0	100	100
47	3	66/81 (82%)	53 (80%)	13 (20%)	0	100	100
48	4	51/57 (90%)	48 (94%)	3 (6%)	0	100	100
49	5	46/49 (94%)	46 (100%)	0	0	100	100
50	6	41/44 (93%)	41 (100%)	0	0	100	100
51	7	63/66 (96%)	58 (92%)	5 (8%)	0	100	100
52	8	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
All	All	5610/5963 (94%)	5217 (93%)	384 (7%)	9 (0%)	44	73

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	s	9	PRO
31	L	137	LYS
10	j	57	LYS
18	r	14	VAL
38	S	102	ASP

5.3.2 Protein sidechains ⓘ

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	138/214 (64%)	137 (99%)	1 (1%)	76	82
3	c	41/177 (23%)	41 (100%)	0	100	100
4	d	154/170 (91%)	154 (100%)	0	100	100
5	e	116/131 (88%)	116 (100%)	0	100	100
6	f	50/85 (59%)	50 (100%)	0	100	100
7	g	38/130 (29%)	38 (100%)	0	100	100
8	h	109/110 (99%)	109 (100%)	0	100	100
9	i	63/102 (62%)	63 (100%)	0	100	100
10	j	35/93 (38%)	35 (100%)	0	100	100
11	k	83/100 (83%)	83 (100%)	0	100	100
12	l	105/118 (89%)	105 (100%)	0	100	100
13	m	13/102 (13%)	13 (100%)	0	100	100
14	n	41/52 (79%)	41 (100%)	0	100	100
15	o	72/81 (89%)	72 (100%)	0	100	100
16	p	78/80 (98%)	78 (100%)	0	100	100
17	q	65/78 (83%)	65 (100%)	0	100	100
18	r	58/67 (87%)	58 (100%)	0	100	100
19	s	21/78 (27%)	21 (100%)	0	100	100
20	t	62/66 (94%)	62 (100%)	0	100	100
23	v	329/365 (90%)	328 (100%)	1 (0%)	86	87
26	C	221/225 (98%)	221 (100%)	0	100	100
27	D	159/171 (93%)	159 (100%)	0	100	100
28	E	170/174 (98%)	170 (100%)	0	100	100
29	F	114/155 (74%)	114 (100%)	0	100	100
30	G	136/147 (92%)	136 (100%)	0	100	100
31	L	120/121 (99%)	120 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	M	101/101 (100%)	101 (100%)	0	100	100
33	N	115/115 (100%)	115 (100%)	0	100	100
34	O	105/113 (93%)	105 (100%)	0	100	100
35	P	102/111 (92%)	102 (100%)	0	100	100
36	Q	83/97 (86%)	83 (100%)	0	100	100
37	R	92/99 (93%)	92 (100%)	0	100	100
38	S	96/97 (99%)	94 (98%)	2 (2%)	47	71
39	T	82/82 (100%)	82 (100%)	0	100	100
40	U	93/97 (96%)	93 (100%)	0	100	100
41	V	83/84 (99%)	79 (95%)	4 (5%)	23	54
42	W	78/88 (89%)	78 (100%)	0	100	100
43	Y	61/76 (80%)	61 (100%)	0	100	100
44	Z	50/53 (94%)	50 (100%)	0	100	100
45	1	53/55 (96%)	53 (100%)	0	100	100
46	2	50/52 (96%)	50 (100%)	0	100	100
47	3	27/73 (37%)	27 (100%)	0	100	100
48	4	47/50 (94%)	47 (100%)	0	100	100
49	5	44/48 (92%)	44 (100%)	0	100	100
50	6	39/39 (100%)	39 (100%)	0	100	100
51	7	55/56 (98%)	55 (100%)	0	100	100
52	8	35/35 (100%)	35 (100%)	0	100	100
All	All	4082/5013 (81%)	4074 (100%)	8 (0%)	85	89

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
41	V	44	GLU
41	V	43	GLU
41	V	39	LYS
38	S	102	ASP
41	V	42	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 74 such sidechains are listed below:

Mol	Chain	Res	Type
35	P	12	GLN
49	5	26	ASN
35	P	96	GLN
43	Y	20	ASN
17	q	49	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1511/1550 (97%)	281 (18%)	0
21	x	72/76 (94%)	17 (23%)	0
22	w	7/21 (33%)	5 (71%)	0
24	A	2895/2932 (98%)	473 (16%)	28 (0%)
25	B	113/116 (97%)	11 (9%)	0
All	All	4598/4695 (97%)	787 (17%)	28 (0%)

5 of 787 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	9	G
1	a	22	G
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
24	A	1497	G
24	A	2908	A
24	A	1533	A
24	A	2615	G
24	A	1532	G

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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	7MG	x	46	21	23,26,27	1.30	3 (13%)	27,39,42	2.70	7 (25%)
21	PSU	x	32	21	18,21,22	1.35	2 (11%)	21,30,33	2.05	3 (14%)
21	4SU	x	8	21	18,21,22	1.87	5 (27%)	25,30,33	2.41	5 (20%)
21	PSU	x	39	21	18,21,22	1.29	2 (11%)	21,30,33	2.25	4 (19%)
21	PSU	x	55	21	18,21,22	1.35	2 (11%)	21,30,33	2.06	4 (19%)
21	MIA	x	37	21	28,31,32	2.33	6 (21%)	38,44,47	2.81	13 (34%)
21	5MU	x	54	21	19,22,23	1.39	6 (31%)	27,32,35	2.05	6 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	7MG	x	46	21	-	5/7/37/38	0/3/3/3
21	PSU	x	32	21	-	0/7/25/26	0/2/2/2
21	4SU	x	8	21	-	0/7/25/26	0/2/2/2
21	PSU	x	39	21	-	0/7/25/26	0/2/2/2
21	PSU	x	55	21	-	0/7/25/26	0/2/2/2
21	MIA	x	37	21	-	2/15/33/34	0/3/3/3
21	5MU	x	54	21	-	0/7/25/26	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	x	37	MIA	C2-S10	-7.04	1.69	1.75
21	x	37	MIA	C13-C14	6.81	1.52	1.32
21	x	8	4SU	C4-S4	-5.05	1.59	1.68
21	x	37	MIA	C5-C4	4.74	1.47	1.39
21	x	8	4SU	C4-N3	-3.41	1.34	1.37

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	x	46	7MG	N9-C4-N3	9.33	139.14	125.46
21	x	37	MIA	C12-C13-C14	-8.63	111.52	127.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	x	37	MIA	C5-C4-N3	-8.31	118.43	127.18
21	x	8	4SU	C4-N3-C2	-7.20	120.41	127.31
21	x	39	PSU	N1-C2-N3	6.75	122.29	115.17

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	46	7MG	O4'-C4'-C5'-O5'
21	x	46	7MG	C3'-C4'-C5'-O5'
21	x	46	7MG	O4'-C1'-N9-C4
21	x	46	7MG	O4'-C1'-N9-C8

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	x	46	7MG	3	0
21	x	39	PSU	3	0
21	x	37	MIA	1	0
21	x	54	5MU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 480 ligands modelled in this entry, 479 are monoatomic - leaving 1 for Mogul analysis.

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
55	GCP	v	502	53	32,34,34	1.42	7 (21%)	49,54,54	1.72	7 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	GCP	v	502	53	-	5/19/38/38	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	v	502	GCP	PG-O3G	2.92	1.61	1.55
55	v	502	GCP	C5-C4	2.88	1.46	1.38
55	v	502	GCP	PG-O2G	2.71	1.61	1.55
55	v	502	GCP	C6-N1	-2.47	1.34	1.38
55	v	502	GCP	PB-O3A	2.31	1.61	1.58

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	v	502	GCP	C5-C4-N3	-5.52	119.60	128.39
55	v	502	GCP	C2-N3-C4	4.69	120.37	112.30
55	v	502	GCP	N9-C4-N3	4.16	134.28	125.95
55	v	502	GCP	C6-C5-N7	3.46	136.59	130.29
55	v	502	GCP	PB-O3A-PA	-3.27	121.69	132.37

There are no chirality outliers.

All (5) torsion outliers are listed below:

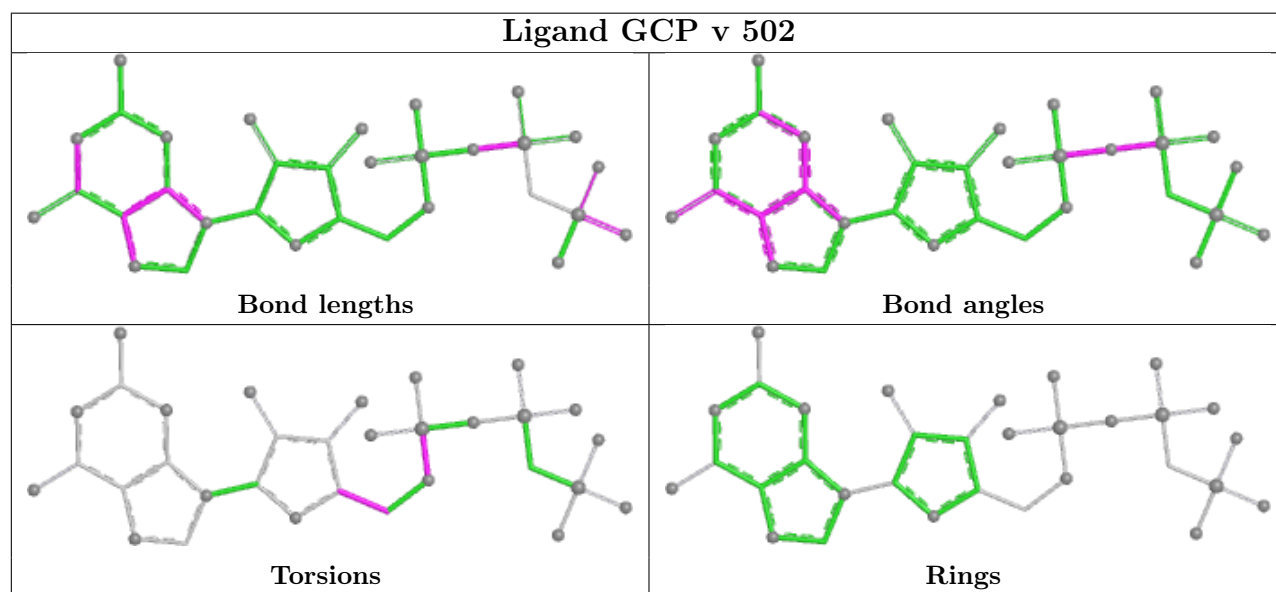
Mol	Chain	Res	Type	Atoms
55	v	502	GCP	C5'-O5'-PA-O1A
55	v	502	GCP	C3'-C4'-C5'-O5'
55	v	502	GCP	O4'-C4'-C5'-O5'
55	v	502	GCP	C5'-O5'-PA-O3A
55	v	502	GCP	C5'-O5'-PA-O2A

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	v	502	GCP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

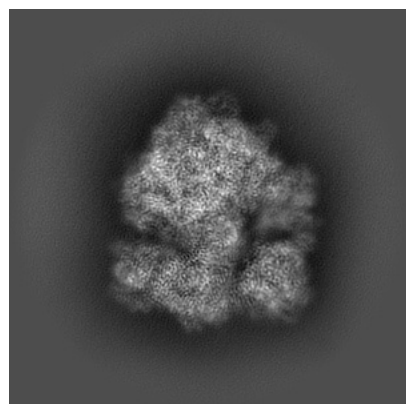
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42576. These allow visual inspection of the internal detail of the map and identification of artifacts.

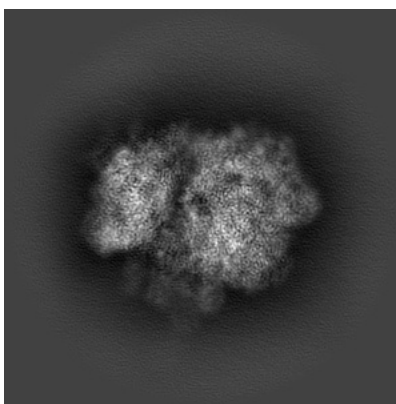
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

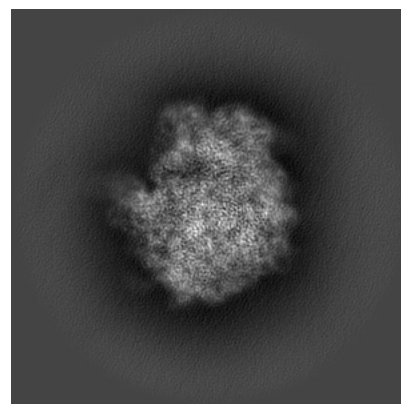
6.1.1 Primary map



X

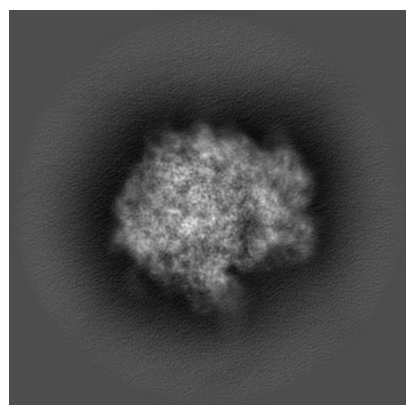


Y

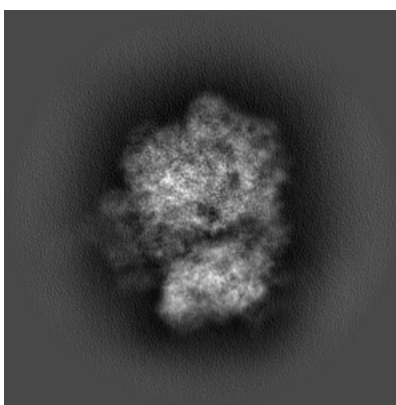


Z

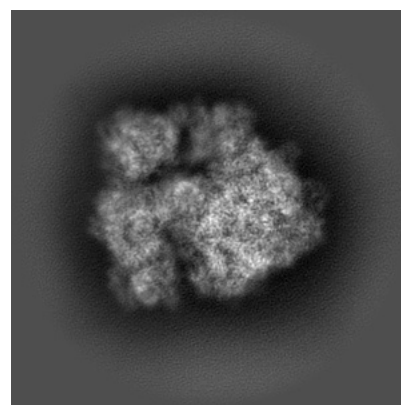
6.1.2 Raw map



X



Y

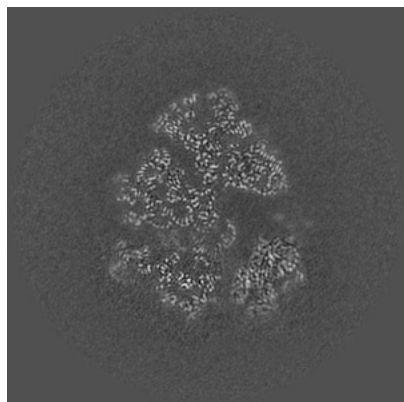


Z

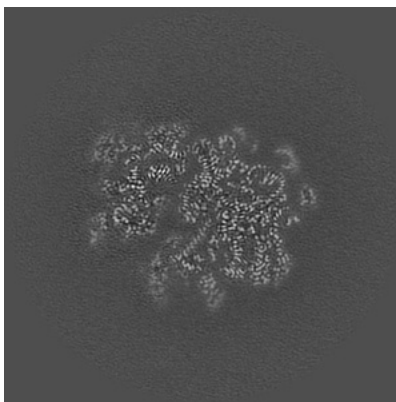
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

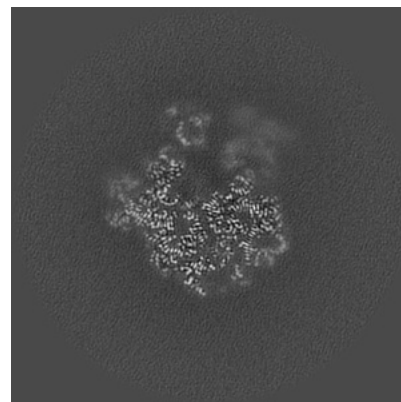
6.2.1 Primary map



X Index: 256

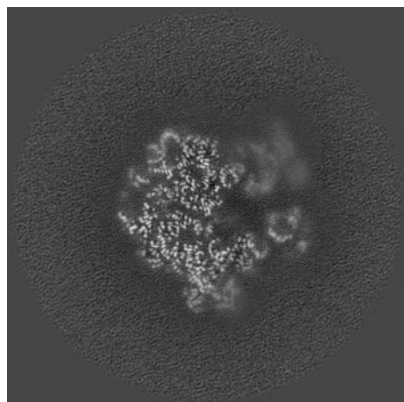


Y Index: 256

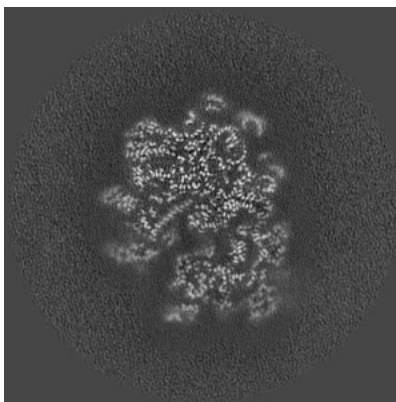


Z Index: 256

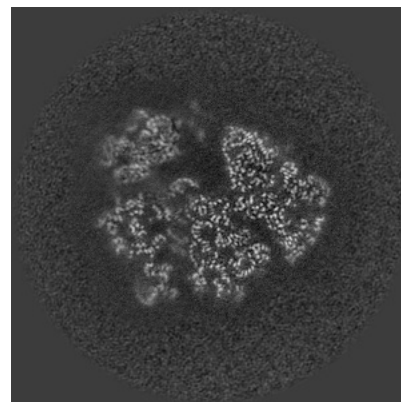
6.2.2 Raw map



X Index: 256



Y Index: 256

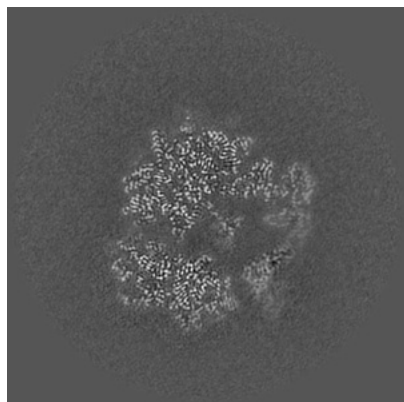


Z Index: 256

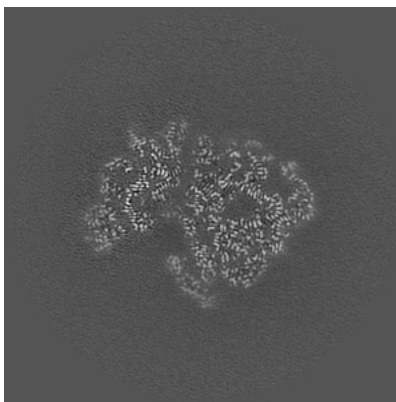
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

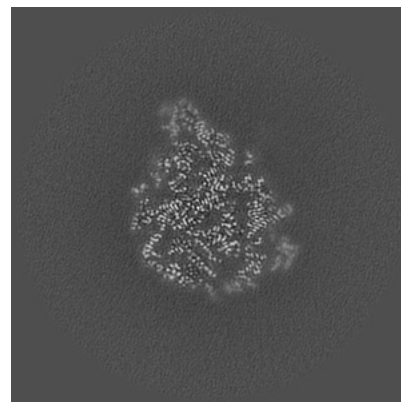
6.3.1 Primary map



X Index: 230

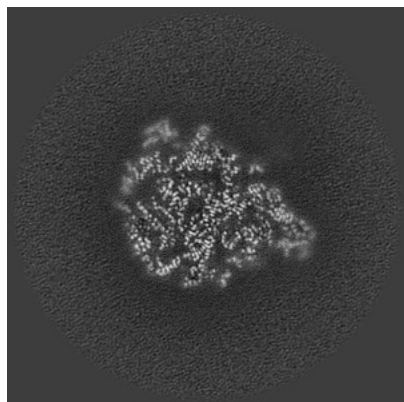


Y Index: 235

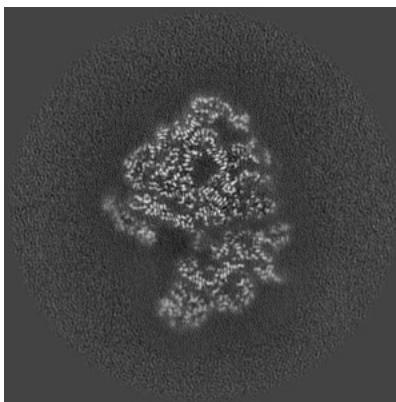


Z Index: 296

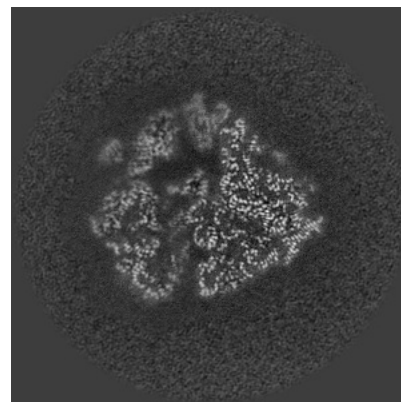
6.3.2 Raw map



X Index: 296



Y Index: 234

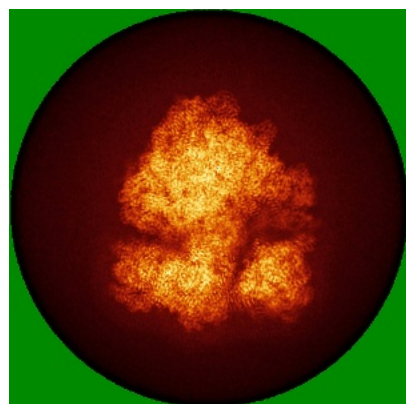


Z Index: 244

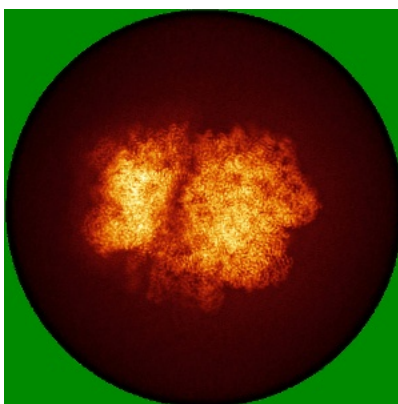
The images above show the largest variance slices of the map in three orthogonal directions.

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

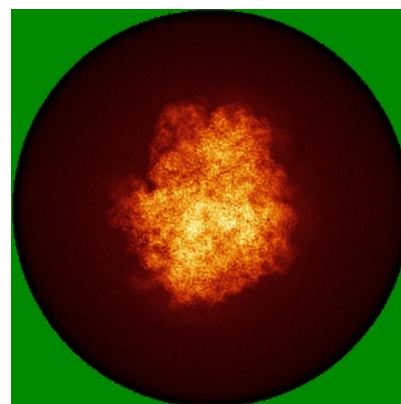
6.4.1 Primary map



X

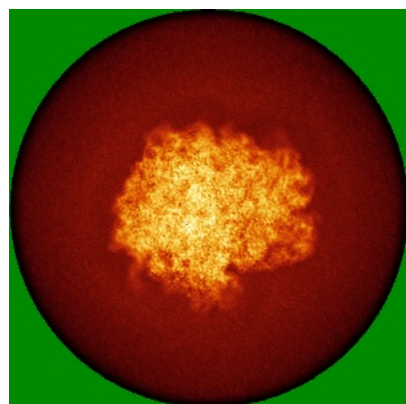


Y

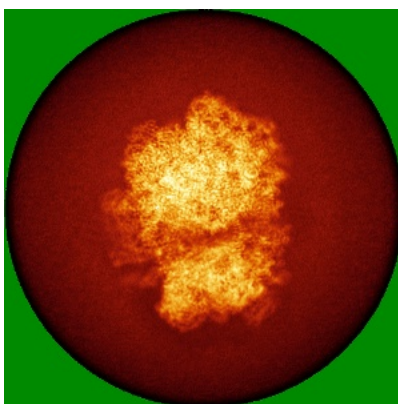


Z

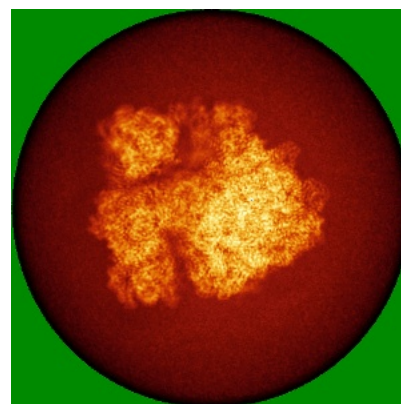
6.4.2 Raw map



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](#)

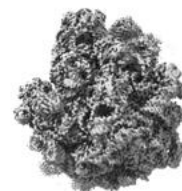
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.4. 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.

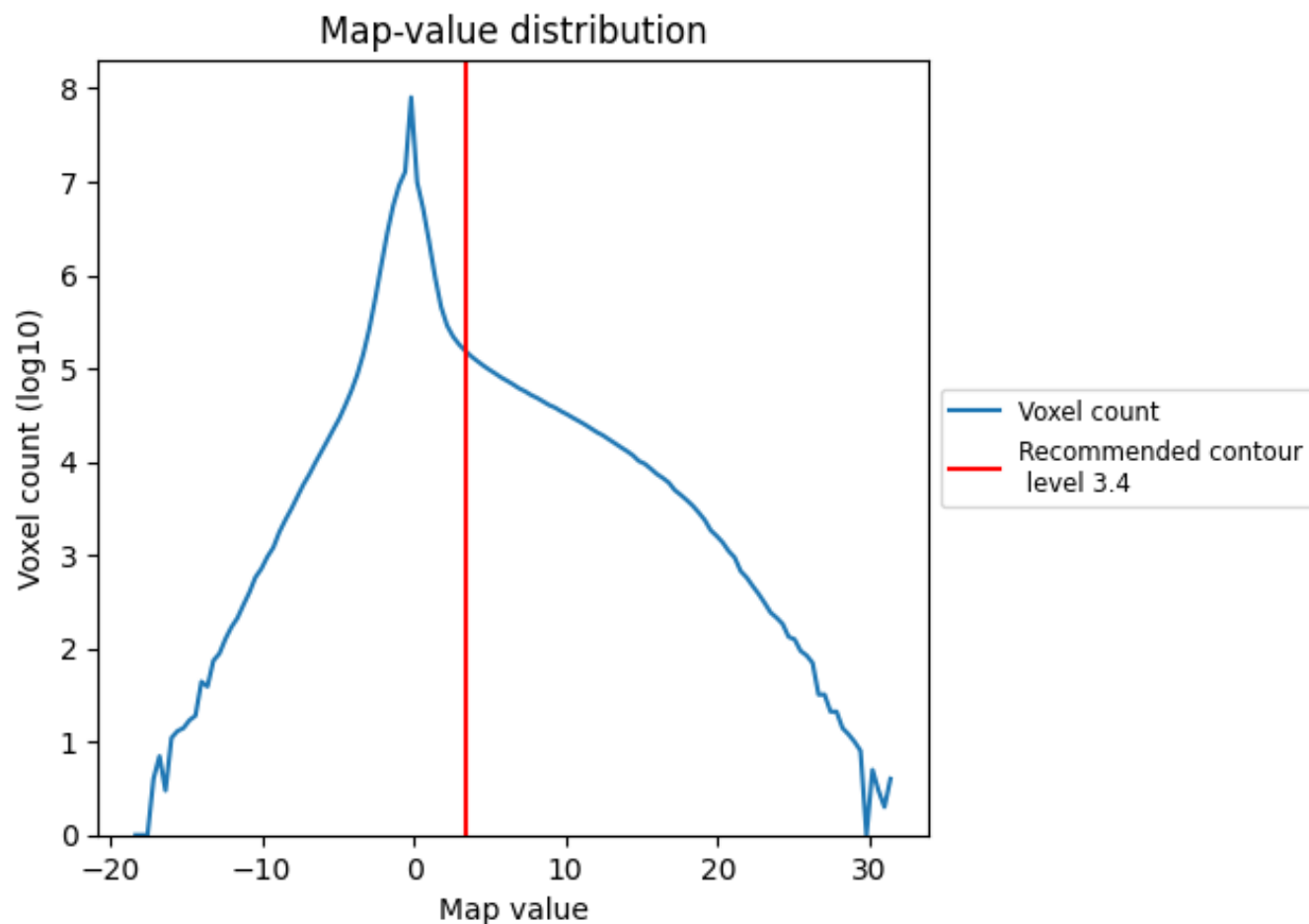
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

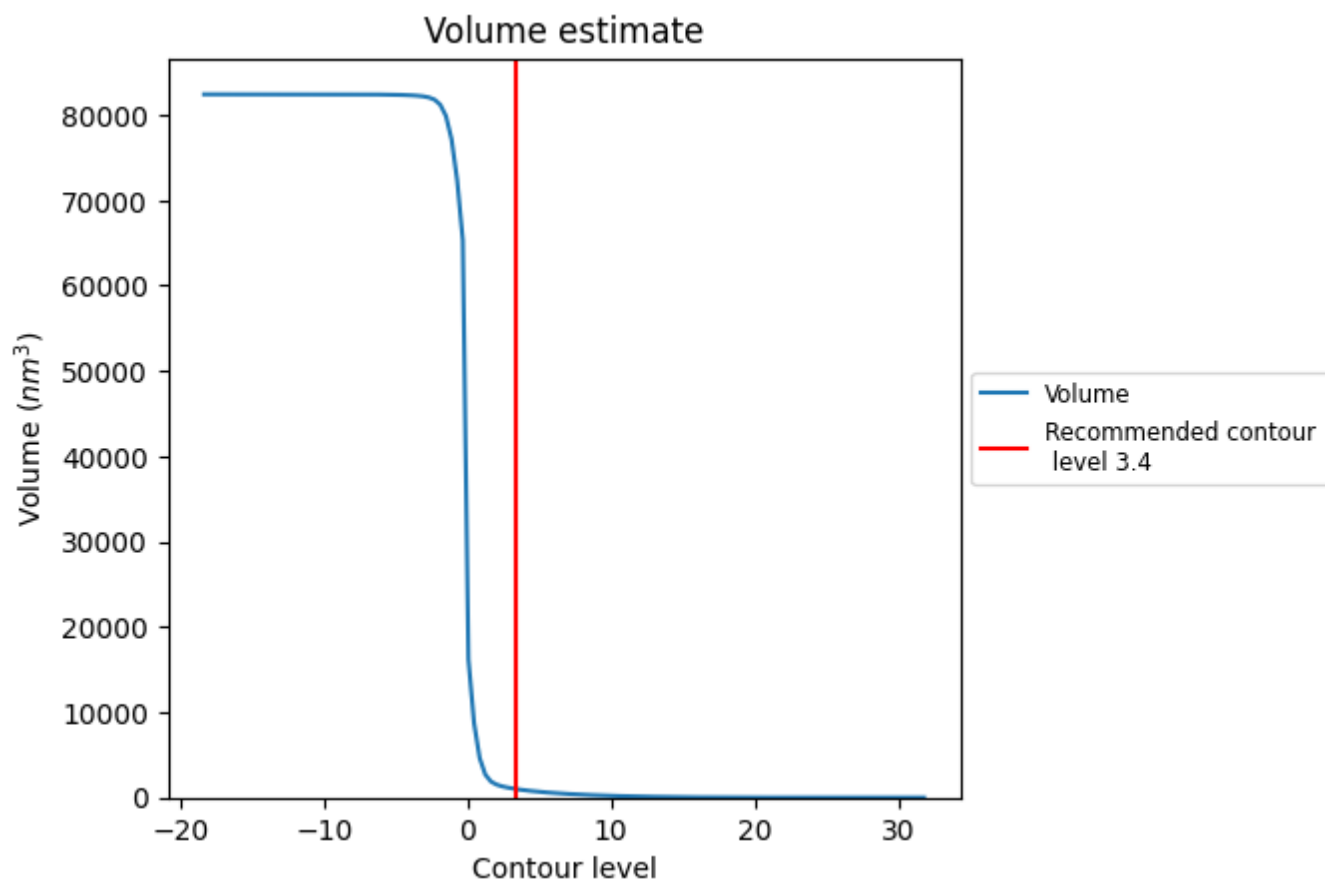
This section contains the results of statistical analysis of the map.

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.

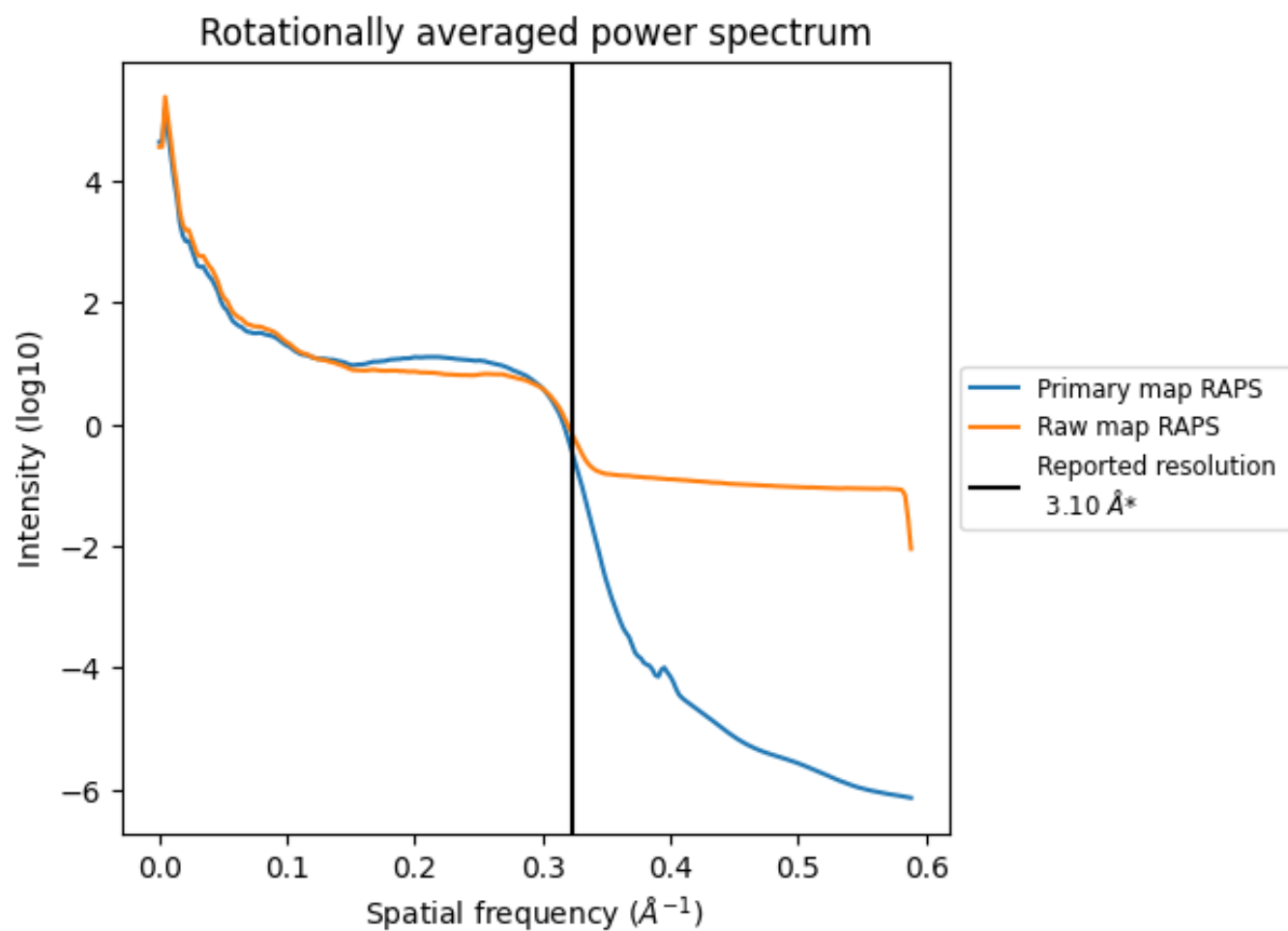
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 997 nm³; this corresponds to an approximate mass of 901 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 ⓘ

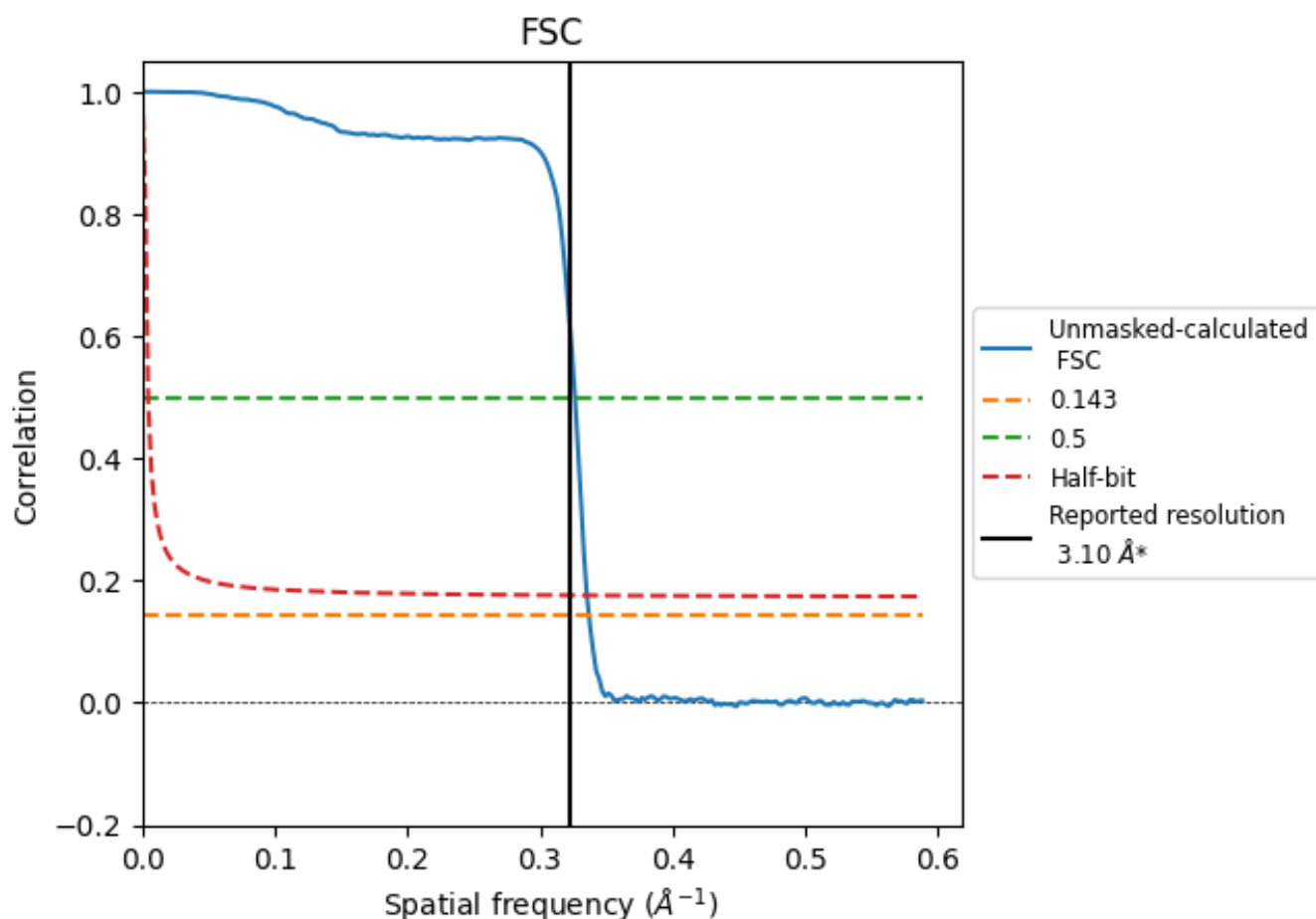


*Reported resolution corresponds to spatial frequency of $0.323 \text{ \AA}^{-1}$

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 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

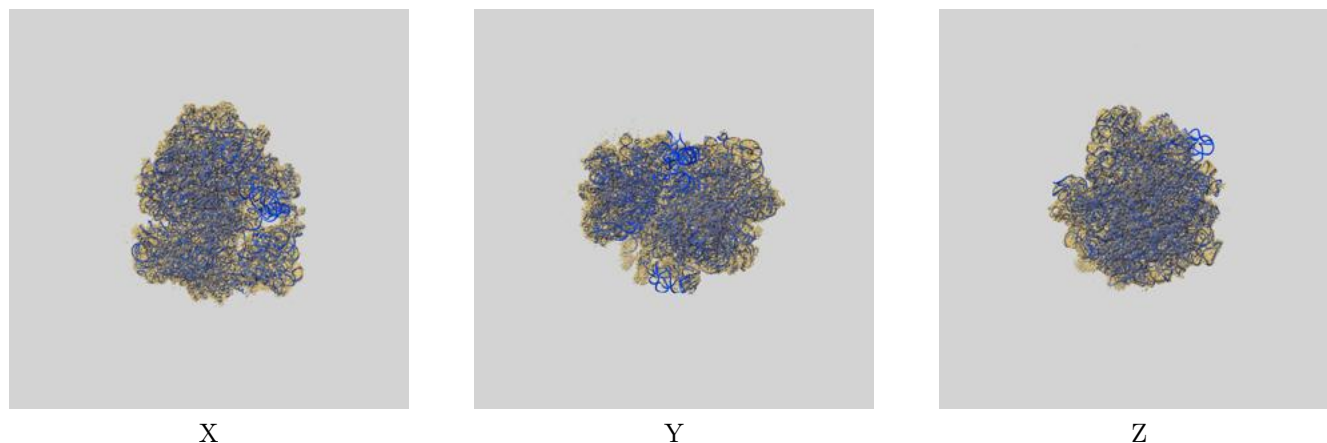
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.97	3.06	2.98

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

9 Map-model fit [i](#)

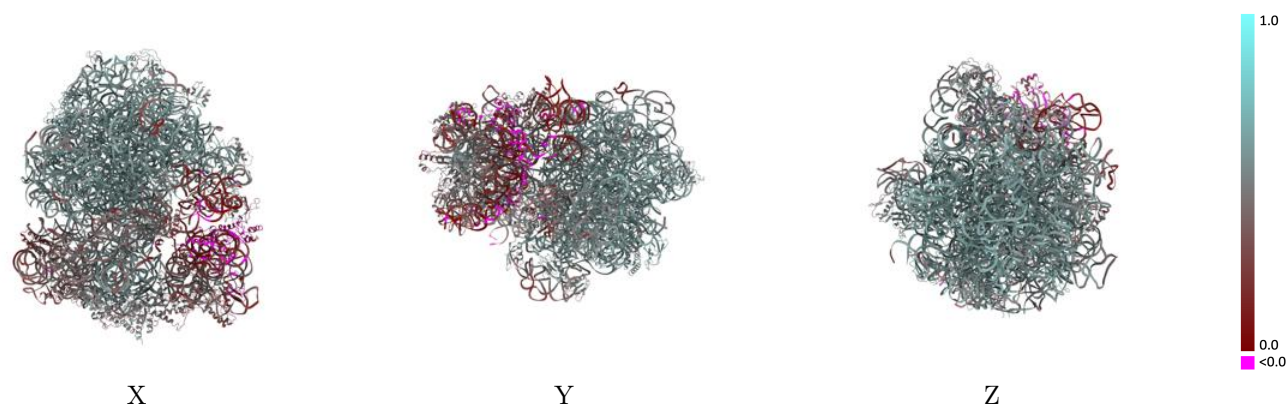
This section contains information regarding the fit between EMDB map EMD-42576 and PDB model 8UU9. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)



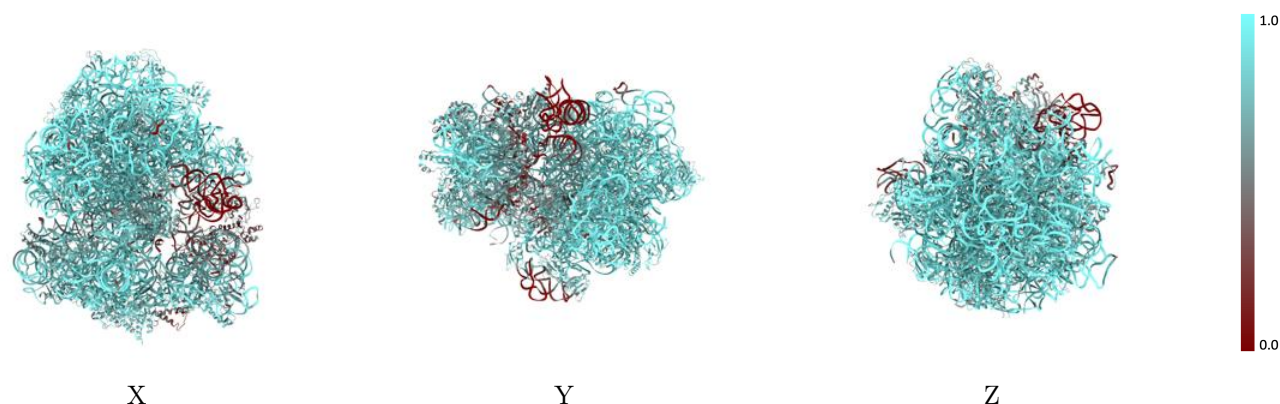
The images above show the 3D surface view of the map at the recommended contour level 3.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



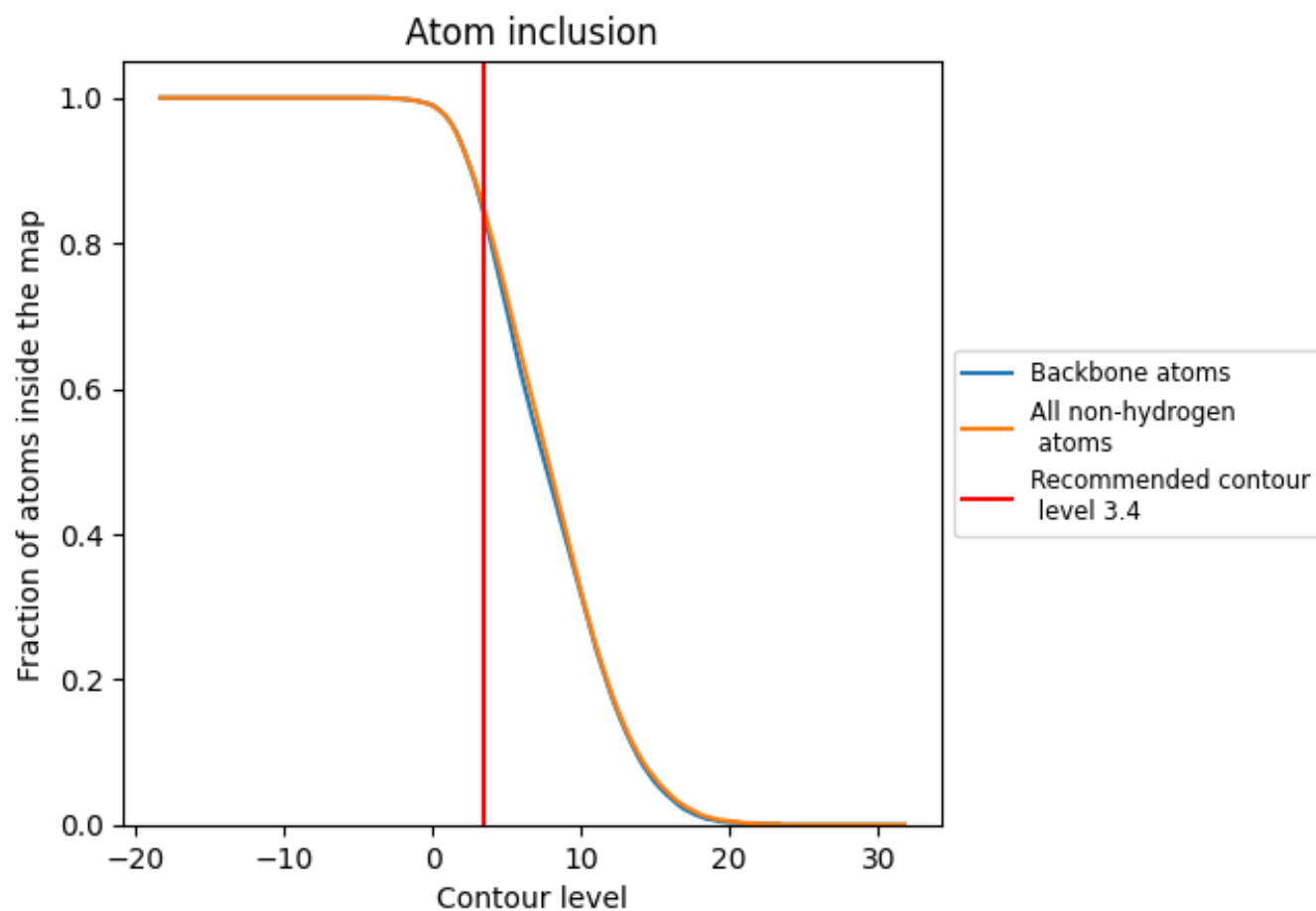
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.4).

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 (3.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8510	 0.4950
1	 0.8620	 0.5420
2	 0.8940	 0.5740
3	 0.4420	 0.3260
4	 0.8860	 0.5630
5	 0.8970	 0.5780
6	 0.9390	 0.6050
7	 0.9220	 0.6050
8	 0.8990	 0.5820
A	 0.9170	 0.5600
B	 0.9350	 0.5130
C	 0.8930	 0.5940
D	 0.9220	 0.5880
E	 0.8850	 0.5720
F	 0.5740	 0.4020
G	 0.7650	 0.5040
L	 0.9140	 0.5930
M	 0.8220	 0.5750
N	 0.8610	 0.5650
O	 0.8940	 0.5850
P	 0.8920	 0.5810
Q	 0.8180	 0.5200
R	 0.8480	 0.5760
S	 0.9230	 0.5910
T	 0.9110	 0.5880
U	 0.8910	 0.5860
V	 0.8520	 0.5620
W	 0.8420	 0.5490
Y	 0.9110	 0.5750
Z	 0.8640	 0.5700
a	 0.8150	 0.3880
b	 0.6720	 0.4670
c	 0.8160	 0.4320
d	 0.7840	 0.4280
e	 0.8550	 0.5450



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Chain	Atom inclusion	Q-score
f	 0.7170	 0.3850
g	 0.4440	 0.1330
h	 0.8600	 0.5120
i	 0.6920	 0.2370
j	 0.8110	 0.4170
k	 0.6440	 0.3450
l	 0.8610	 0.5340
m	 0.4220	 0.0750
n	 0.8370	 0.4080
o	 0.7150	 0.4320
p	 0.7400	 0.3670
q	 0.8090	 0.4140
r	 0.7680	 0.4390
s	 0.3210	 0.0980
t	 0.6540	 0.2830
v	 0.7920	 0.5180
w	 0.2740	 0.1830
x	 0.3410	 0.2300