



## wwPDB EM Validation Summary Report ⓘ

Oct 28, 2024 – 08:08 pm GMT

PDB ID : 5GAE  
EMDB ID : EMD-8001  
Title : RNC in complex with a translocating SecYEG  
Authors : Jomaa, A.; Boehringer, D.; Leibundgut, M.; Ban, N.  
Deposited on : 2015-11-25  
Resolution : 3.33 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev113  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

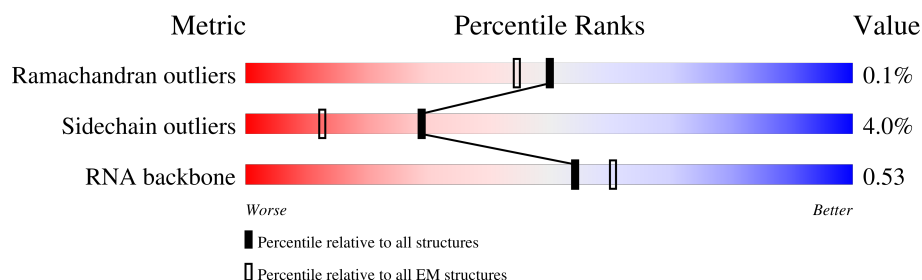
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.33 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	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2903	
2	B	120	
3	C	273	
4	D	209	
5	E	201	
6	F	179	
7	G	177	
8	H	149	


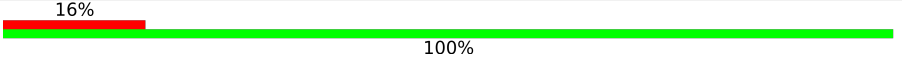

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Mol	Chain	Length	Quality of chain
9	I	165	
10	J	142	
11	K	142	
12	L	123	
13	M	144	
14	N	136	
15	O	127	
16	P	117	
17	Q	115	
18	R	118	
19	S	103	
20	T	110	
21	U	100	
22	V	104	
23	W	94	
24	X	85	
25	Y	78	
26	Z	63	
27	a	59	
28	b	57	
29	c	55	
30	d	46	
31	e	65	
32	f	38	
33	g	443	

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Mol	Chain	Length	Quality of chain
34	h	127	
35	i	25	
36	x	3	

## 2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 95192 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 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2884	Total	C	N	O	P	0	0
			61923	27622	11400	20017	2884		

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	149	Total	C	N	O	S	0	0
			1110	699	197	213	1		

- Molecule 9 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	125	Total	C	N	O	S	0	0
			946	599	169	175	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	85	VAL	SER	conflict	UNP P0A7J3
I	86	THR	MET	conflict	UNP P0A7J3

- Molecule 10 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	70	Total	C	N	O	S	0	0
			502	309	92	98	3		

- Molecule 11 is a protein called 50S ribosomal protein L13.

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

- Molecule 12 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 13 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 14 is a protein called 50S ribosomal protein L16.

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

- Molecule 15 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	125	Total	C	N	O	S	0	0
			993	613	202	173	5		

- Molecule 16 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	117	Total	C	N	O	S	0	0
			900	557	179	163	1		

- Molecule 17 is a protein called 50S ribosomal protein L19.

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

- Molecule 18 is a protein called 50S ribosomal protein L20.

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

- Molecule 19 is a protein called 50S ribosomal protein L21.

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

- Molecule 20 is a protein called 50S ribosomal protein L22.

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

- Molecule 21 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	95	Total	C	N	O	S	0	0
			756	479	141	135	1		

- Molecule 22 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	102	Total	C	N	O	S	0	0
			779	492	146	141			

- Molecule 23 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	76	Total	C	N	O	S	0	0
			580	359	117	103	1		

- Molecule 25 is a protein called 50S ribosomal protein L28.

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

- Molecule 26 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 27 is a protein called 50S ribosomal protein L30.



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

- Molecule 28 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 29 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	51	Total	C	N	O	S	0	0
			414	266	76	72			

- Molecule 30 is a protein called 50S ribosomal protein L34.

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

- Molecule 31 is a protein called 50S ribosomal protein L35.

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

- Molecule 32 is a protein called 50S ribosomal protein L36.

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

- Molecule 33 is a protein called Protein translocase subunit SecY.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	399	Total	C	N	O	S	0	0
			3099	2056	508	520	15		

- Molecule 34 is a protein called Protein translocase subunit SecE.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	h	59	Total	C	N	O	S	0	0
			459	298	82	78	1		

- Molecule 35 is a protein called SecG.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	i	25	Total	C	N	O	0	0
			150	100	25	25		

- Molecule 36 is a RNA chain called tRNA CCA end (5'-R(P\*CP\*CP\*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
36	x	3	Total	C	N	O	P	0	0
			62	28	11	20	3		

- Molecule 37 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
37	A	313	Total	Mg	0
			313	313	
37	B	8	Total	Mg	0
			8	8	
37	R	1	Total	Mg	0
			1	1	
37	b	1	Total	Mg	0
			1	1	

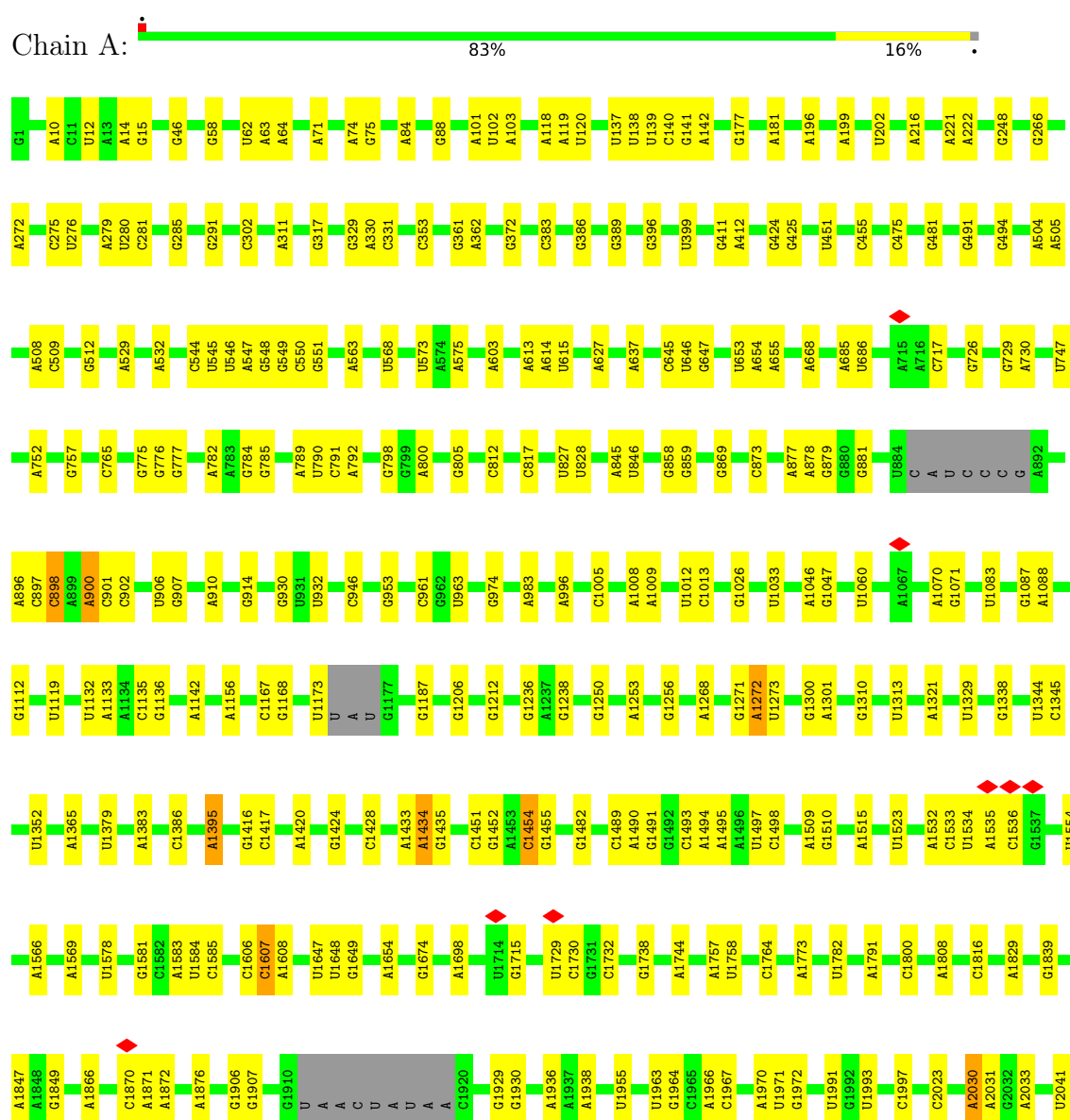
- Molecule 38 is ZINC ION (three-letter code: ZN) (formula: Zn).

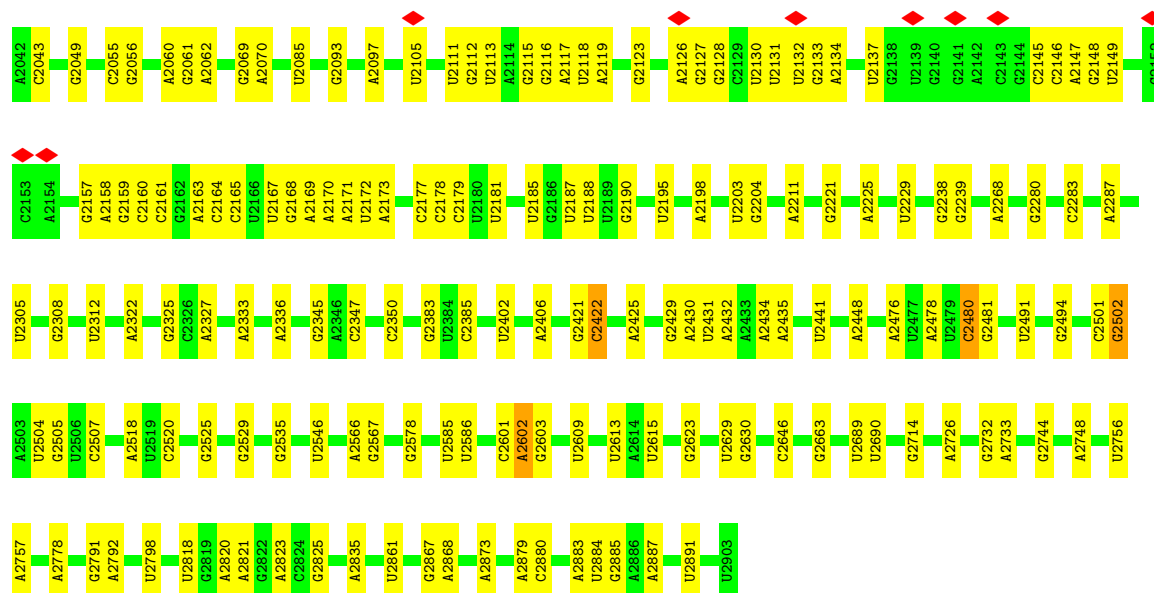
Mol	Chain	Residues	Atoms		AltConf
38	f	1	Total	Zn	0
			1	1	

### 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.

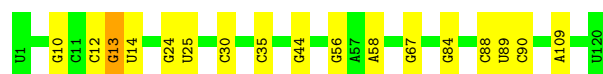
#### • Molecule 1: 23S rRNA





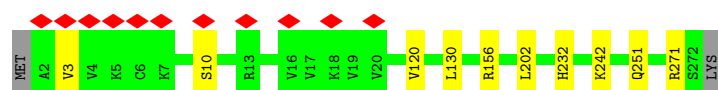
• Molecule 2: 5S rRNA

Chain B: 86% 13%



• Molecule 3: 50S ribosomal protein L2

Chain C: 96%



• Molecule 4: 50S ribosomal protein L3

Chain D: 98%



• Molecule 5: 50S ribosomal protein L4

Chain E: 99%



• Molecule 6: 50S ribosomal protein L5

Chain F: 92% 7%





- Molecule 13: 50S ribosomal protein L15

Chain M: 99%



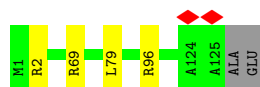
- Molecule 14: 50S ribosomal protein L16

Chain N: 98%



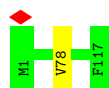
- Molecule 15: 50S ribosomal protein L17

Chain O: 95%



- Molecule 16: 50S ribosomal protein L18

Chain P: 99%



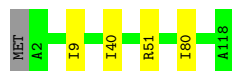
- Molecule 17: 50S ribosomal protein L19

Chain Q: 95%



- Molecule 18: 50S ribosomal protein L20

Chain R: 96%



- Molecule 19: 50S ribosomal protein L21

Chain S: 93%



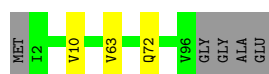
- Molecule 20: 50S ribosomal protein L22

Chain T: 99%



- Molecule 21: 50S ribosomal protein L23

Chain U: 92% 5%



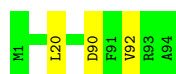
- Molecule 22: 50S ribosomal protein L24

Chain V: 94%



- Molecule 23: 50S ribosomal protein L25

Chain W: 97%



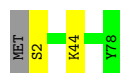
- Molecule 24: 50S ribosomal protein L27

Chain X: 86% 11%



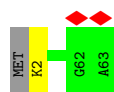
- Molecule 25: 50S ribosomal protein L28

Chain Y: 96%

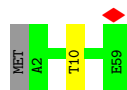


- Molecule 26: 50S ribosomal protein L29

Chain Z: 97%



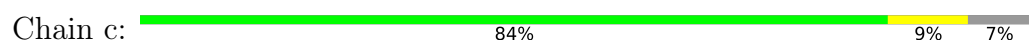
- Molecule 27: 50S ribosomal protein L30



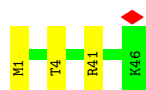
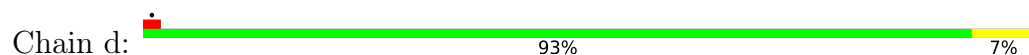
- Molecule 28: 50S ribosomal protein L32



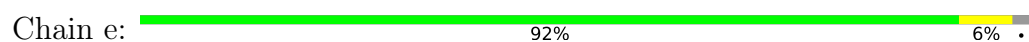
- Molecule 29: 50S ribosomal protein L33



- Molecule 30: 50S ribosomal protein L34



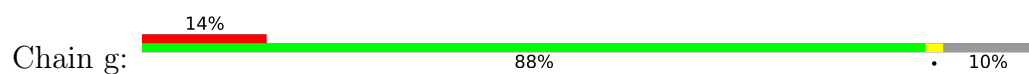
- Molecule 31: 50S ribosomal protein L35



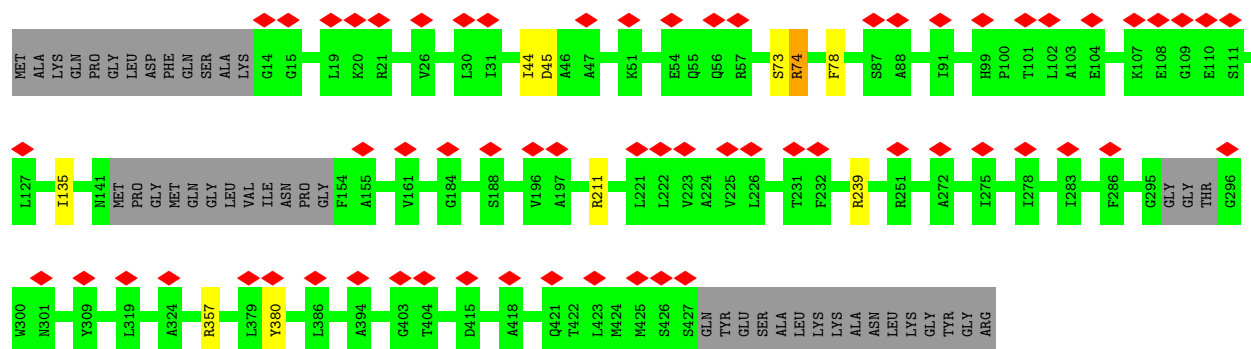
- Molecule 32: 50S ribosomal protein L36



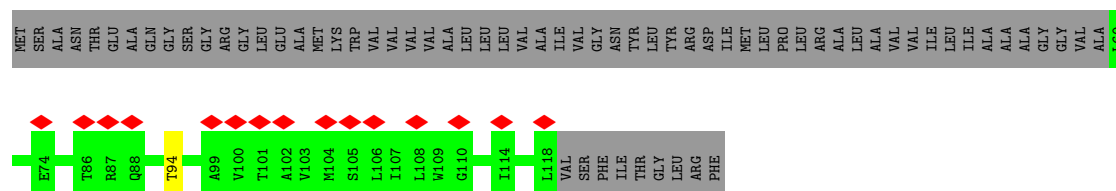
- Molecule 33: Protein translocase subunit SecY



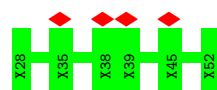




• Molecule 34: Protein translocase subunit SecE



• Molecule 35: SecG



• Molecule 36: tRNA CCA end (5'-R(P\*CP\*CP\*A)-3')



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	216907	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	20	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	101083	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.380	Depositor
Minimum map value	-0.139	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	443.2, 443.2, 443.2	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.385, 1.385, 1.385	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0.56	0/69352	0.96	54/108188 (0.0%)
2	B	0.44	0/2872	0.89	2/4478 (0.0%)
3	C	0.36	0/2121	0.54	0/2852
4	D	0.38	0/1586	0.55	0/2134
5	E	0.37	0/1571	0.50	0/2113
6	F	0.36	0/1434	0.50	0/1926
7	G	0.30	0/1343	0.48	0/1816
8	H	0.34	0/1121	0.48	0/1515
9	I	0.45	0/958	0.52	0/1292
10	J	0.45	0/504	0.54	0/673
11	K	0.37	0/1152	0.50	0/1551
12	L	0.38	0/955	0.55	0/1279
13	M	0.36	0/1062	0.55	0/1413
14	N	0.39	0/1093	0.52	0/1460
15	O	0.39	0/1006	0.56	0/1345
16	P	0.31	0/910	0.47	0/1219
17	Q	0.39	0/929	0.54	0/1242
18	R	0.48	0/960	0.55	0/1278
19	S	0.38	0/829	0.53	0/1107
20	T	0.38	0/864	0.58	0/1156
21	U	0.35	0/763	0.51	0/1021
22	V	0.32	0/787	0.47	0/1051
23	W	0.31	0/766	0.50	0/1025
24	X	0.42	0/587	0.53	0/776
25	Y	0.38	0/635	0.52	0/848
26	Z	0.30	0/502	0.41	0/667
27	a	0.34	0/453	0.51	0/605
28	b	0.37	0/450	0.54	0/599
29	c	0.32	0/421	0.48	0/561
30	d	0.41	0/380	0.57	0/498
31	e	0.37	0/513	0.55	0/676
32	f	0.31	0/303	0.48	0/397

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	g	0.45	0/3169	0.53	0/4299
34	h	0.48	0/465	0.47	0/633
36	x	0.32	0/68	0.99	0/103
All	All	0.51	0/102884	0.86	56/153796 (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
3	C	0	1
33	g	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1607	C	N1-C2-O2	8.21	123.82	118.90
1	A	550	C	C2-N1-C1'	7.67	127.24	118.80
1	A	1607	C	N3-C2-O2	-7.58	116.59	121.90
1	A	280	U	C6-N1-C2	-7.38	116.57	121.00
1	A	1584	U	C2-N1-C1'	7.33	126.50	117.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	232	HIS	Peptide
33	g	74	ARG	Peptide

## 5.2 Too-close contacts

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

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	269/273 (98%)	264 (98%)	5 (2%)	0	100	100
4	D	207/209 (99%)	203 (98%)	4 (2%)	0	100	100
5	E	199/201 (99%)	194 (98%)	5 (2%)	0	100	100
6	F	175/179 (98%)	170 (97%)	5 (3%)	0	100	100
7	G	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
8	H	147/149 (99%)	137 (93%)	10 (7%)	0	100	100
9	I	123/165 (74%)	114 (93%)	8 (6%)	1 (1%)	16	47
10	J	68/142 (48%)	64 (94%)	4 (6%)	0	100	100
11	K	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
12	L	121/123 (98%)	118 (98%)	3 (2%)	0	100	100
13	M	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
14	N	134/136 (98%)	131 (98%)	3 (2%)	0	100	100
15	O	123/127 (97%)	120 (98%)	3 (2%)	0	100	100
16	P	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
17	Q	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
18	R	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
19	S	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
20	T	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
21	U	93/100 (93%)	89 (96%)	4 (4%)	0	100	100
22	V	100/104 (96%)	98 (98%)	2 (2%)	0	100	100
23	W	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
24	X	74/85 (87%)	72 (97%)	2 (3%)	0	100	100
25	Y	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
26	Z	60/63 (95%)	59 (98%)	1 (2%)	0	100	100
27	a	56/59 (95%)	55 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	b	54/57 (95%)	54 (100%)	0	0	100	100
29	c	49/55 (89%)	48 (98%)	1 (2%)	0	100	100
30	d	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
31	e	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
32	f	36/38 (95%)	36 (100%)	0	0	100	100
33	g	393/443 (89%)	370 (94%)	22 (6%)	1 (0%)	37	66
34	h	57/127 (45%)	55 (96%)	2 (4%)	0	100	100
All	All	3818/4144 (92%)	3700 (97%)	116 (3%)	2 (0%)	50	76

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
33	g	135	ILE
9	I	108	VAL

### 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	
3	C	216/218 (99%)	207 (96%)	9 (4%)	25	54
4	D	164/164 (100%)	160 (98%)	4 (2%)	44	68
5	E	165/165 (100%)	162 (98%)	3 (2%)	54	74
6	F	148/150 (99%)	135 (91%)	13 (9%)	8	30
7	G	137/138 (99%)	133 (97%)	4 (3%)	37	63
8	H	114/114 (100%)	108 (95%)	6 (5%)	19	47
9	I	95/123 (77%)	88 (93%)	7 (7%)	11	36
10	J	52/110 (47%)	50 (96%)	2 (4%)	28	56
11	K	116/116 (100%)	115 (99%)	1 (1%)	75	85
12	L	104/104 (100%)	98 (94%)	6 (6%)	17	45
13	M	103/103 (100%)	101 (98%)	2 (2%)	52	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	109/109 (100%)	106 (97%)	3 (3%)	38	64
15	O	102/103 (99%)	98 (96%)	4 (4%)	27	55
16	P	87/87 (100%)	86 (99%)	1 (1%)	70	82
17	Q	99/100 (99%)	94 (95%)	5 (5%)	20	49
18	R	89/90 (99%)	85 (96%)	4 (4%)	23	52
19	S	84/84 (100%)	77 (92%)	7 (8%)	9	32
20	T	93/93 (100%)	92 (99%)	1 (1%)	70	82
21	U	82/84 (98%)	79 (96%)	3 (4%)	29	57
22	V	83/85 (98%)	79 (95%)	4 (5%)	21	51
23	W	78/78 (100%)	75 (96%)	3 (4%)	28	56
24	X	57/63 (90%)	54 (95%)	3 (5%)	19	47
25	Y	67/68 (98%)	65 (97%)	2 (3%)	36	62
26	Z	54/55 (98%)	53 (98%)	1 (2%)	52	72
27	a	48/49 (98%)	47 (98%)	1 (2%)	48	70
28	b	47/48 (98%)	46 (98%)	1 (2%)	48	70
29	c	45/49 (92%)	40 (89%)	5 (11%)	5	20
30	d	38/38 (100%)	35 (92%)	3 (8%)	10	34
31	e	51/52 (98%)	47 (92%)	4 (8%)	10	34
32	f	34/34 (100%)	32 (94%)	2 (6%)	16	44
33	g	327/359 (91%)	318 (97%)	9 (3%)	38	64
34	h	49/99 (50%)	48 (98%)	1 (2%)	50	72
All	All	3137/3332 (94%)	3013 (96%)	124 (4%)	29	54

5 of 124 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	N	12	MET
31	e	31	HIS
18	R	40	ILE
31	e	8	ARG
33	g	78	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
14	N	3	GLN
17	Q	41	GLN
26	Z	27	ASN
15	O	18	GLN
17	Q	66	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2879/2903 (99%)	438 (15%)	14 (0%)
2	B	119/120 (99%)	17 (14%)	1 (0%)
36	x	2/3 (66%)	1 (50%)	0
All	All	3000/3026 (99%)	456 (15%)	15 (0%)

5 of 456 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	A
1	A	12	U
1	A	14	A
1	A	15	G
1	A	46	G

5 of 15 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1454	C
1	A	2756	U
1	A	1494	A
2	B	13	G
1	A	2158	A

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.



## 5.6 Ligand geometry [i](#)

Of 324 ligands modelled in this entry, 324 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
33	g	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	g	398:PRO	C	399:PHE	N	5.57
1	A	2789:C	O3'	2790:U	P	3.00

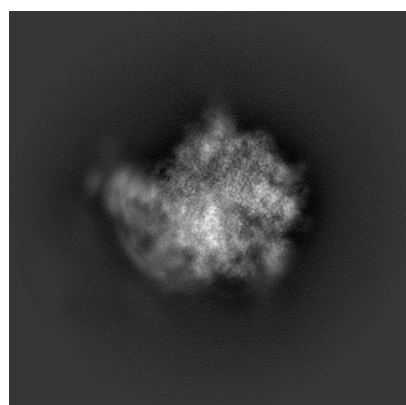
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8001. These allow visual inspection of the internal detail of the map and identification of artifacts.

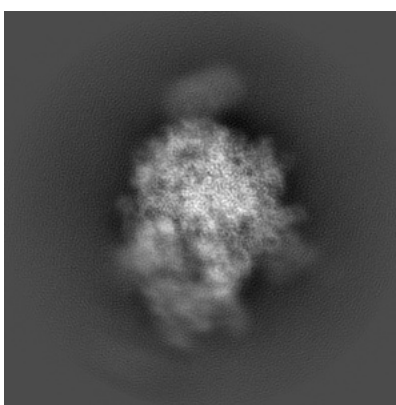
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

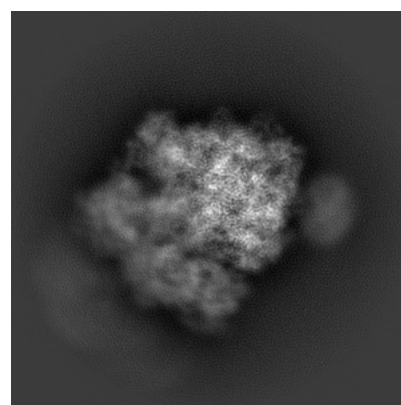
#### 6.1.1 Primary map



X



Y

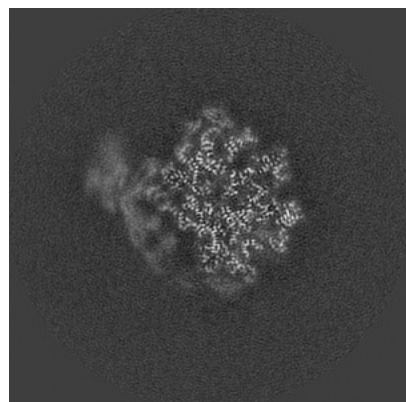


Z

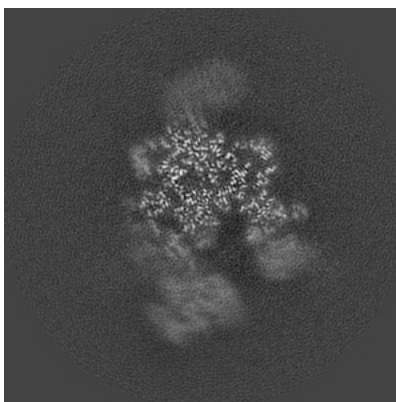
The images above show the map projected in three orthogonal directions.

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

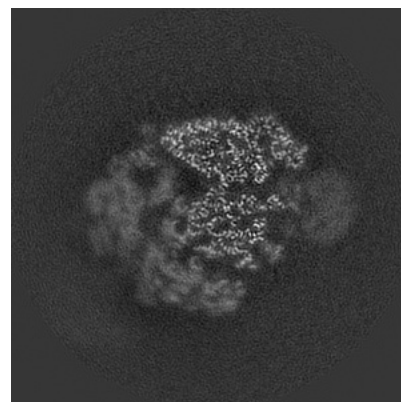
#### 6.2.1 Primary map



X Index: 160



Y Index: 160

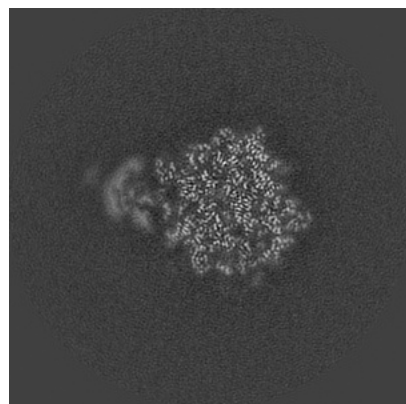


Z Index: 160

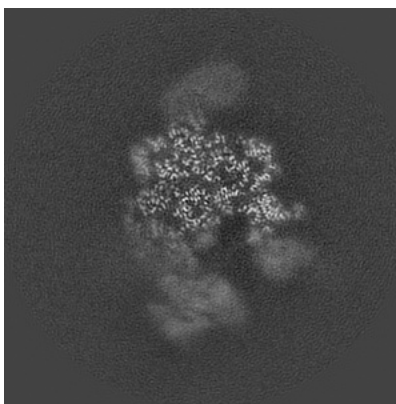
The images above show central slices of the map in three orthogonal directions.

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

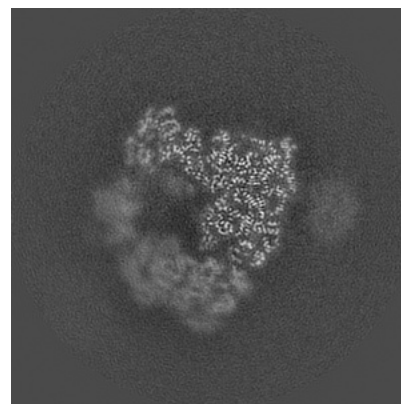
### 6.3.1 Primary map



X Index: 173



Y Index: 158

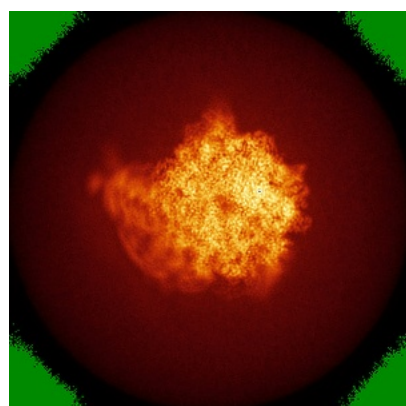


Z Index: 175

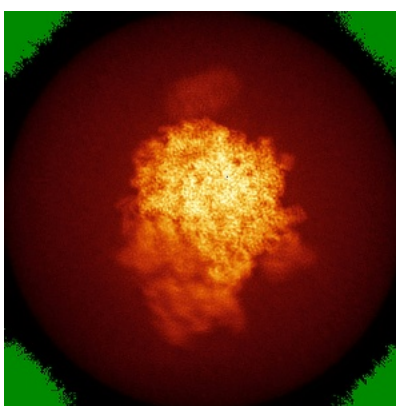
The images above show the largest variance slices of the map in three orthogonal directions.

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

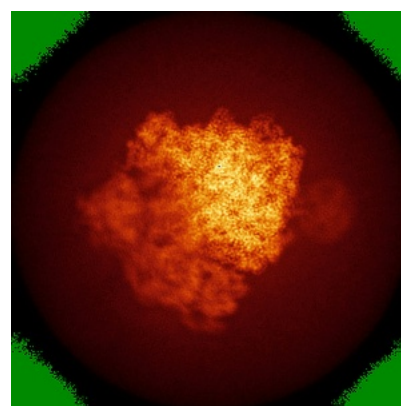
### 6.4.1 Primary map



X



Y

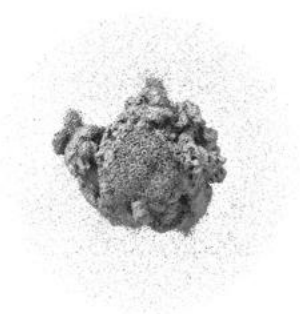


Z

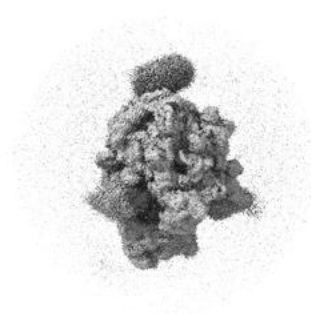
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

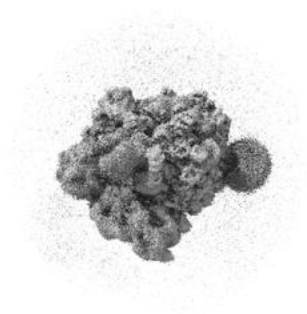
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

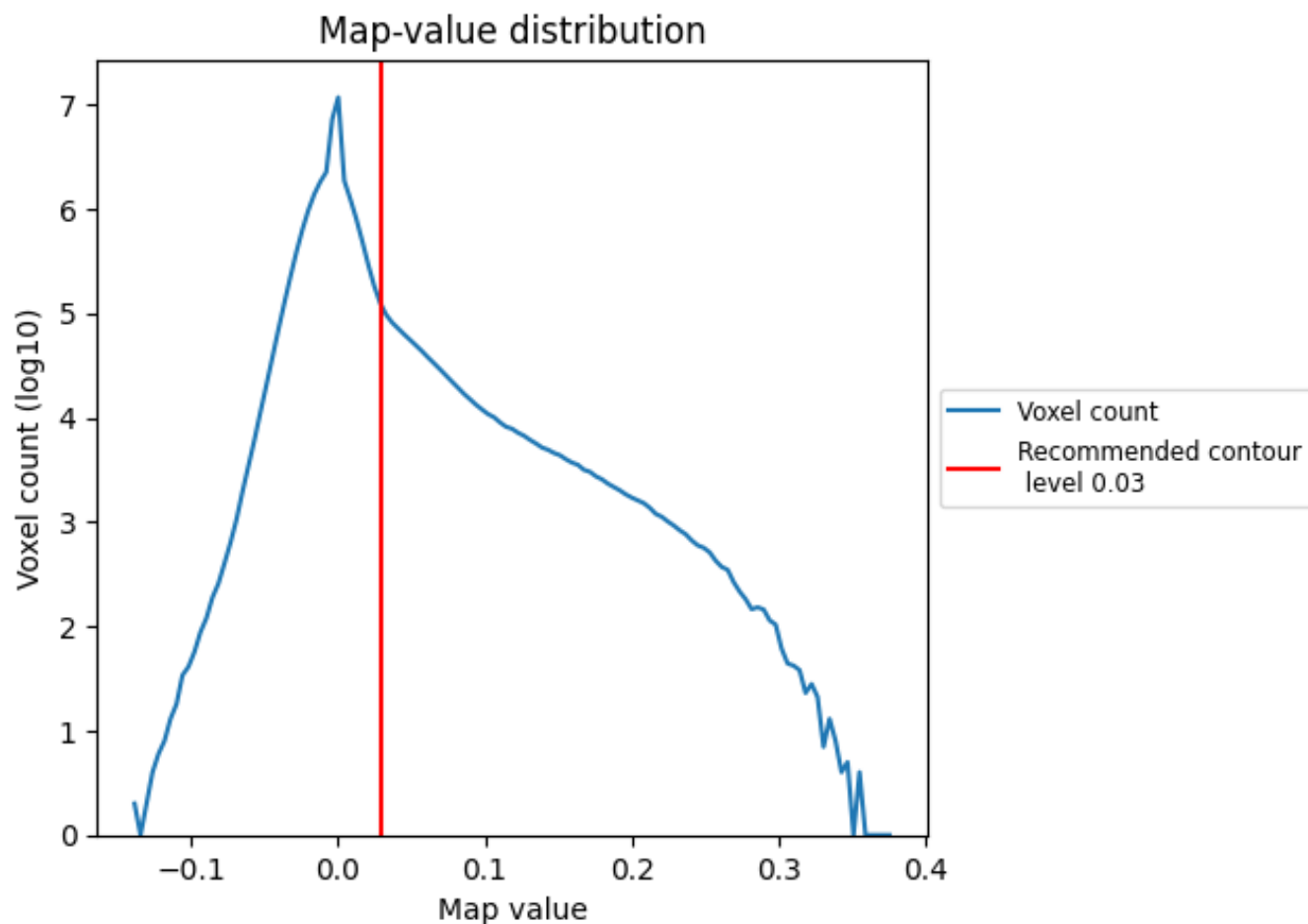
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

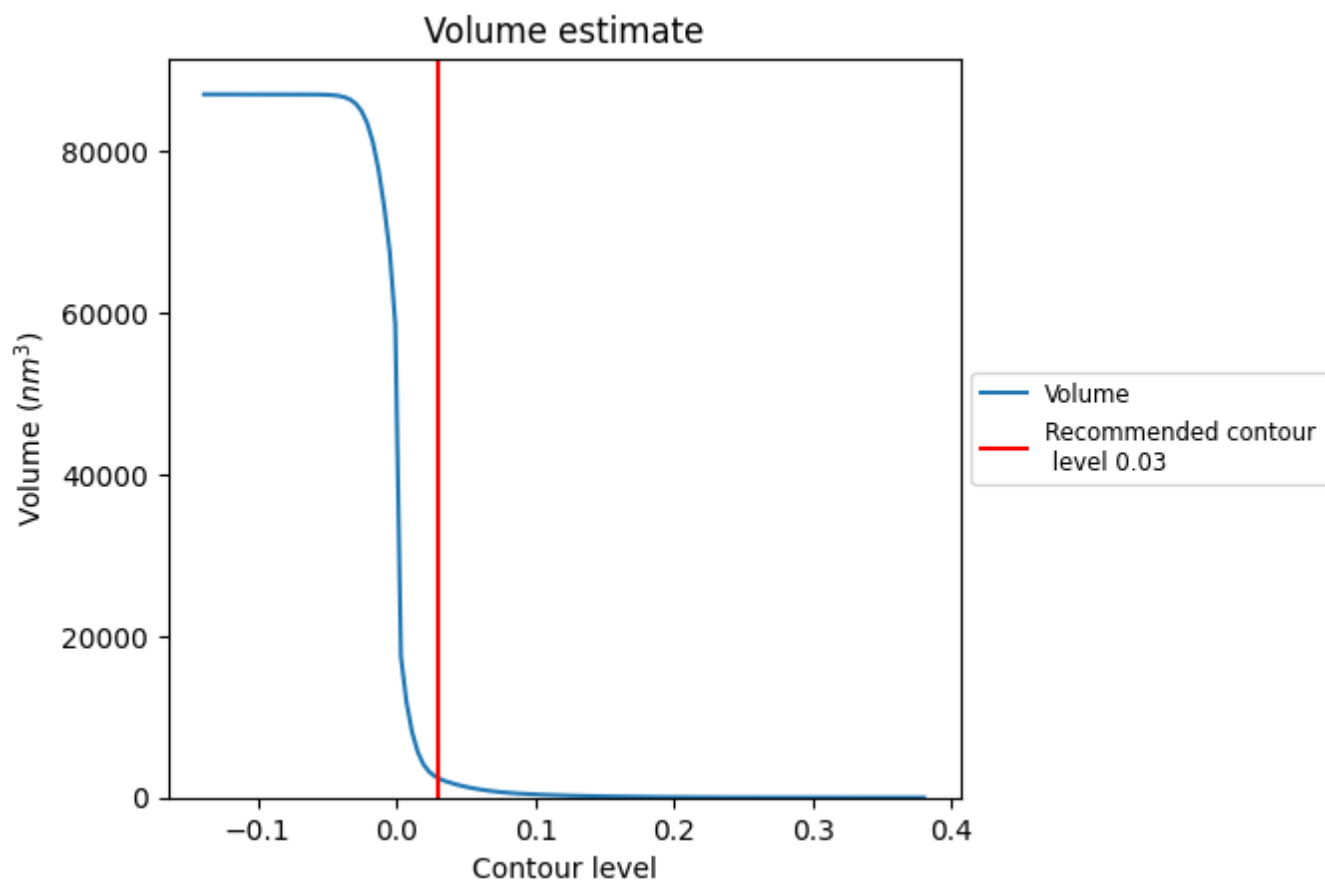
This section contains the results of statistical analysis of the map.

### 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.

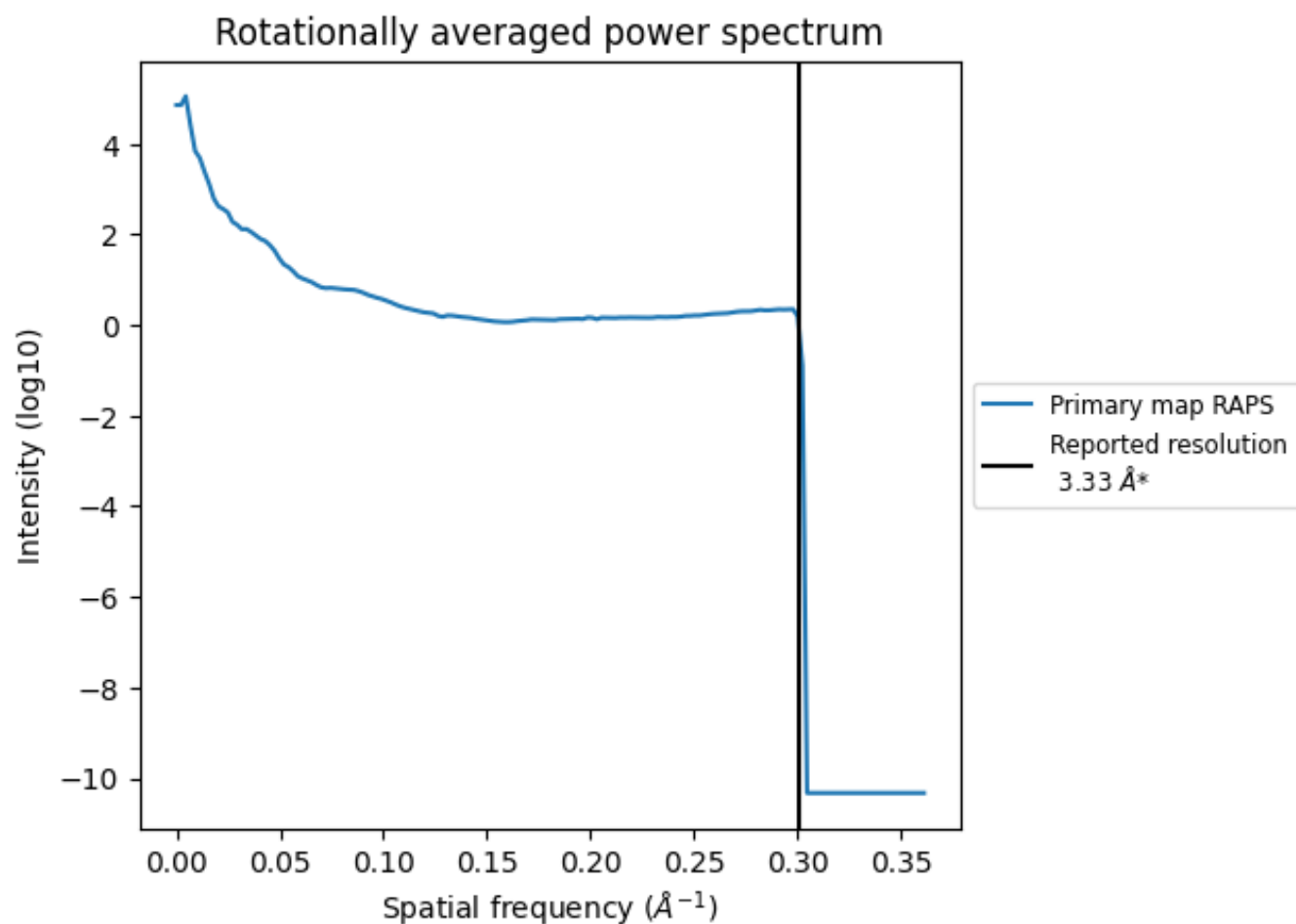
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2415  $\text{nm}^3$ ; this corresponds to an approximate mass of 2182 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 0.300 Å<sup>-1</sup>

## 8 Fourier-Shell correlation

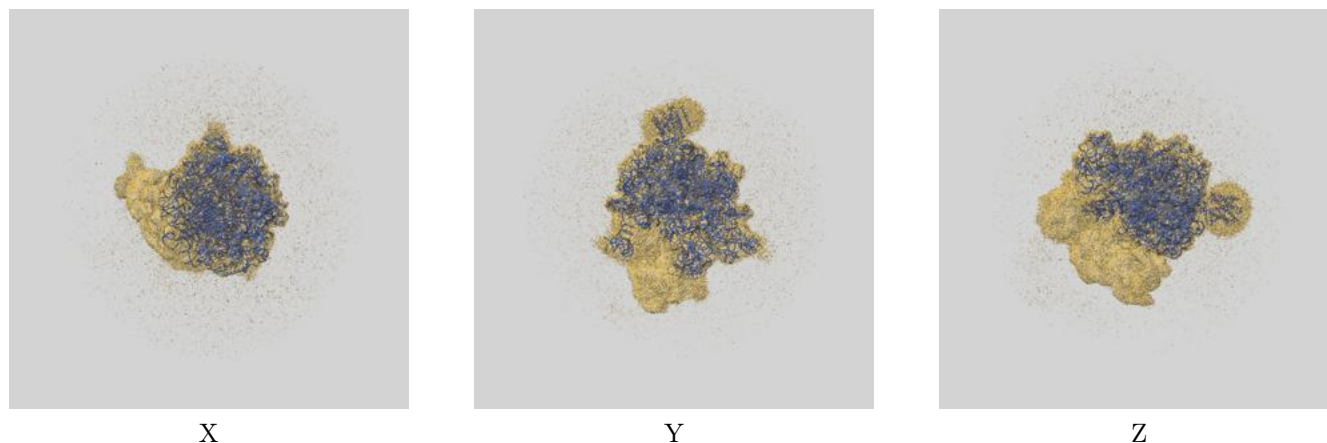
This section was not generated. No FSC curve or half-maps provided.



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

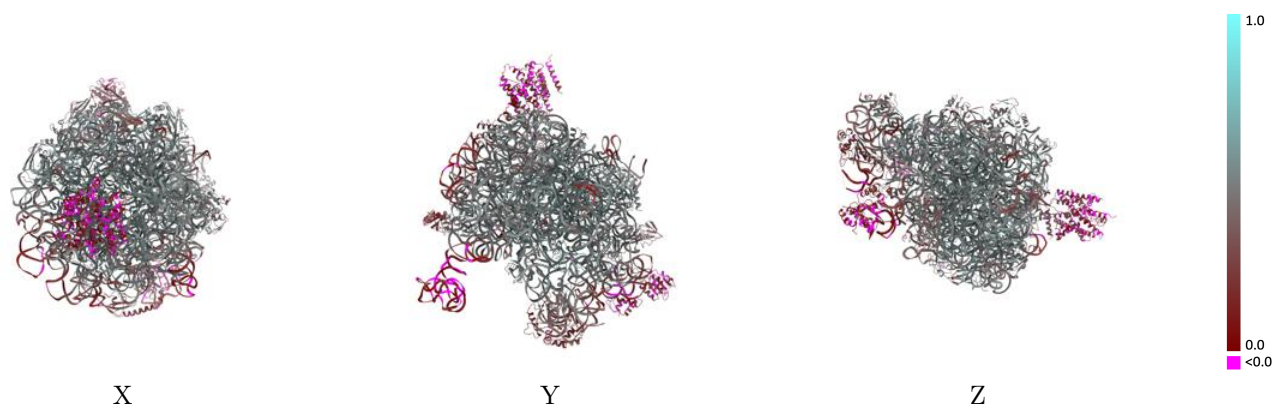
This section contains information regarding the fit between EMDB map EMD-8001 and PDB model 5GAE. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

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



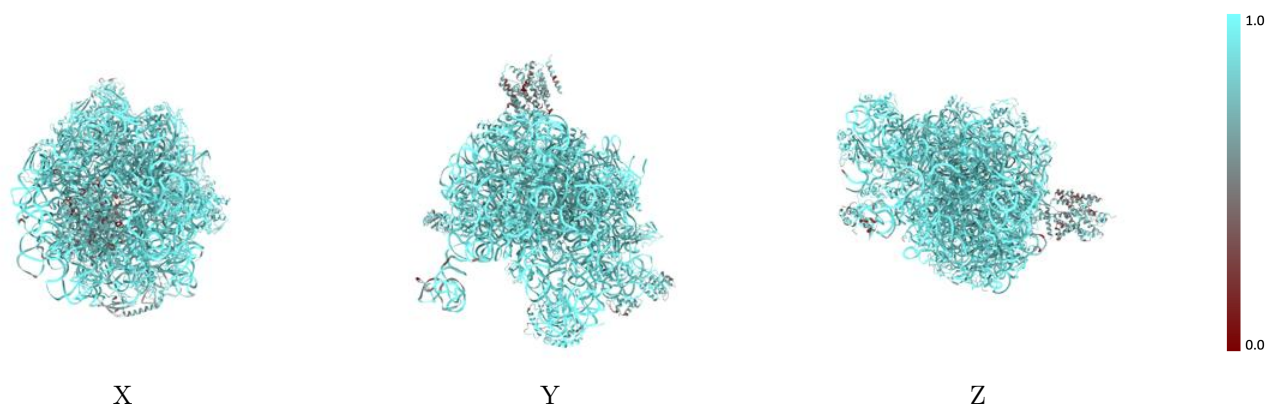
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



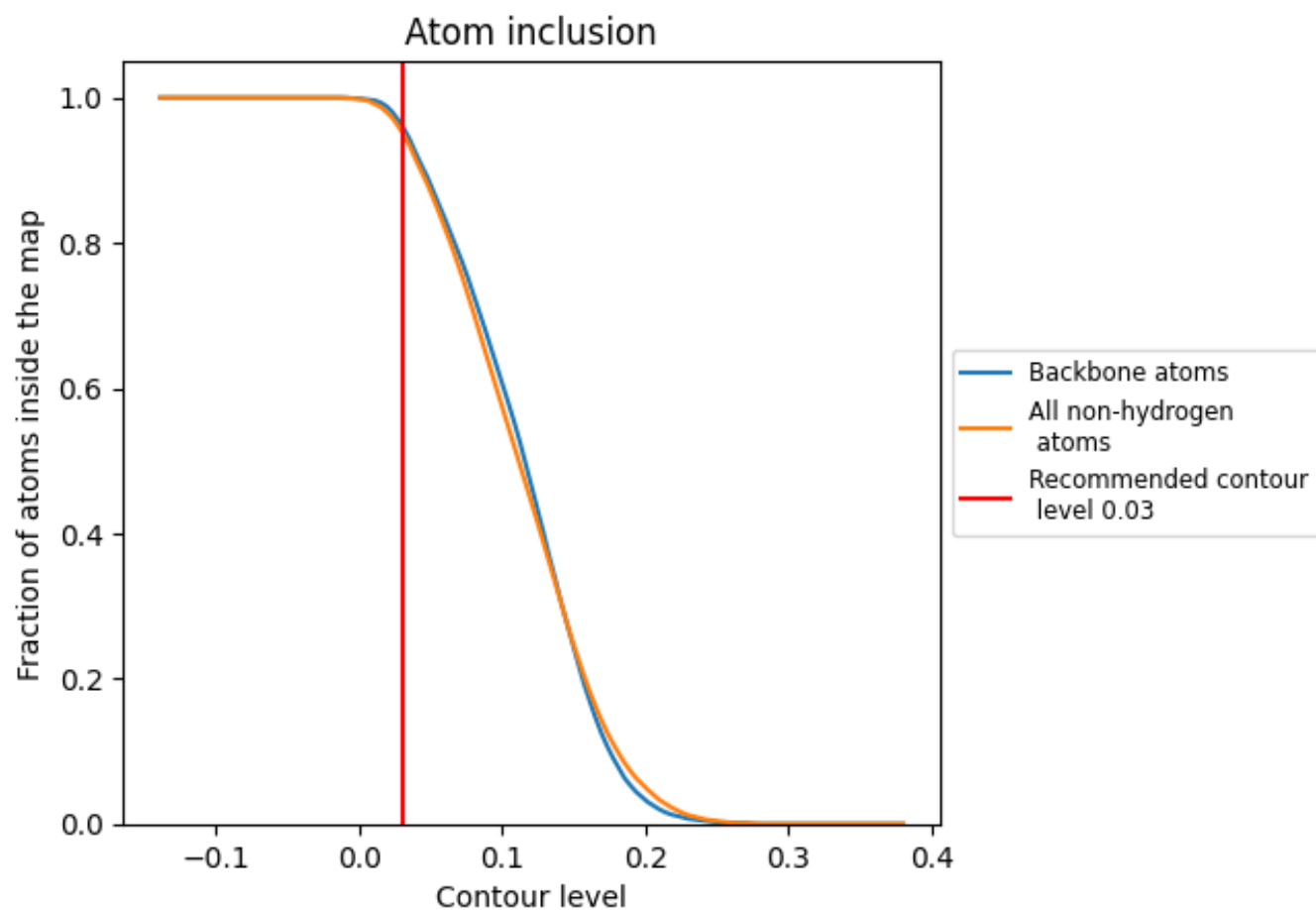
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 95% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9530	 0.4410
A	 0.9810	 0.4600
B	 0.9940	 0.4040
C	 0.9090	 0.4990
D	 0.9580	 0.5180
E	 0.9520	 0.4890
F	 0.8910	 0.2540
G	 0.9240	 0.3740
H	 0.7260	 0.2930
I	 0.7720	 0.1130
J	 0.7000	 0.0730
K	 0.9690	 0.5150
L	 0.9210	 0.5120
M	 0.9540	 0.4920
N	 0.9620	 0.5080
O	 0.9560	 0.5100
P	 0.9530	 0.4340
Q	 0.9210	 0.4870
R	 0.9820	 0.5330
S	 0.9400	 0.4950
T	 0.9450	 0.5050
U	 0.9180	 0.4730
V	 0.9350	 0.4520
W	 0.9490	 0.4780
X	 0.9420	 0.5130
Y	 0.9580	 0.4760
Z	 0.9160	 0.4240
a	 0.9470	 0.5010
b	 0.9460	 0.5030
c	 0.9090	 0.4690
d	 0.9660	 0.5390
e	 0.9720	 0.5340
f	 0.9760	 0.4850
g	 0.6790	 0.1190
h	 0.5550	 0.0700



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Chain	Atom inclusion	Q-score
i	 0.6000	 0.0380
x	 0.9680	 0.4800