



wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 12:56 pm GMT

PDB ID : 5MMJ
EMDB ID : EMD-3532
Title : Structure of the small subunit of the chloroplast ribosome
Authors : Bieri, P.; Leibundgut, M.; Saurer, M.; Boehringer, D.; Ban, N.
Deposited on : 2016-12-10
Resolution : 3.65 Å (reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

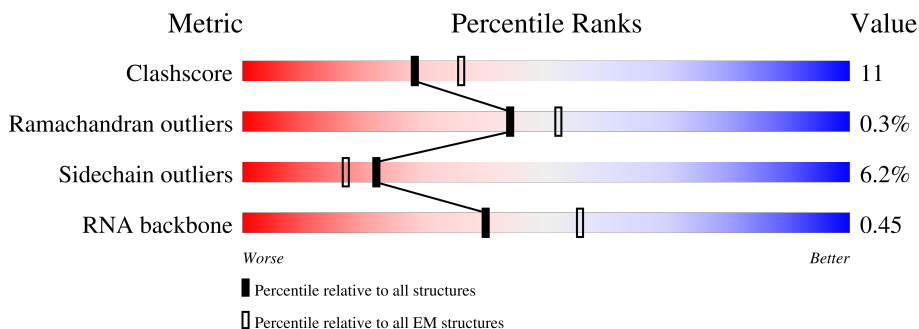
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 3.65 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.



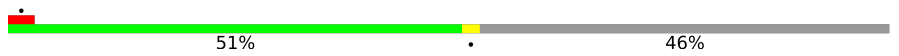
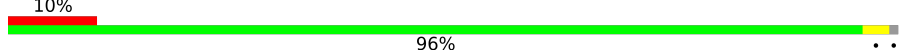
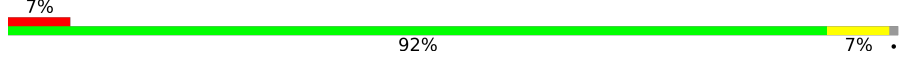



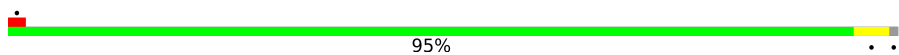





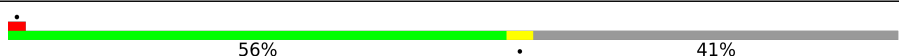

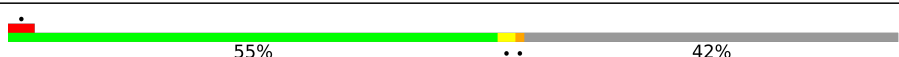
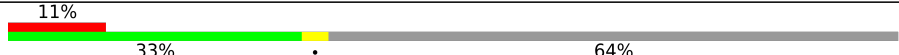




Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	0	130	
2	8	174	
3	a	1491	
4	b	236	
5	c	218	
6	d	201	
7	e	308	

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Mol	Chain	Length	Quality of chain
8	f	211	
9	g	155	
10	h	134	
11	i	208	
12	j	195	
13	k	138	
14	l	123	
15	m	172	
16	n	100	
17	o	90	
18	p	88	
19	q	165	
20	r	101	
21	s	92	
22	t	183	
23	u	180	
24	v	260	
25	w	179	
26	x	101	
27	y	302	

2 Entry composition [i](#)

There are 28 unique types of molecules in this entry. The entry contains 55315 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	0	11	98	63	18	17	0	0

- Molecule 2 is a protein called plastid ribosomal protein bS1c.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	8	174	870	522	174	174	0	0

- Molecule 3 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	a	1484	31868	14208	5881	10295	1484	0	0

- Molecule 4 is a protein called 30S ribosomal protein S2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	b	233	1844	1163	339	329	13	0	0

- Molecule 5 is a protein called 30S ribosomal protein S3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	c	216	1736	1108	313	309	6	0	0

- Molecule 6 is a protein called 30S ribosomal protein S4, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	d	199	1633	1032	319	278	4	0	0

- Molecule 7 is a protein called 30S ribosomal protein S5, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	e	187	Total	C	N	O	S	0	0
			1331	826	259	240	6		

- Molecule 8 is a protein called plastid ribosomal protein bS6c.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	f	113	Total	C	N	O	S	0	0
			911	583	152	172	4		

- Molecule 9 is a protein called 30S ribosomal protein S7, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	g	154	Total	C	N	O	S	0	0
			1210	753	244	210	3		

- Molecule 10 is a protein called 30S ribosomal protein S8, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	h	133	Total	C	N	O	S	0	0
			1079	679	210	185	5		

- Molecule 11 is a protein called plastid ribosomal protein uS9c.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	i	144	Total	C	N	O	S	0	0
			1119	712	211	195	1		

- Molecule 12 is a protein called plastid ribosomal protein uS10c.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	j	99	Total	C	N	O	S	0	0
			805	517	144	139	5		

- Molecule 13 is a protein called 30S ribosomal protein S11, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	k	117	Total	C	N	O	S	0	0
			882	546	181	150	5		

- Molecule 14 is a protein called 30S ribosomal protein S12, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	l	122	Total	C	N	O	S	0	0
			959	599	197	161	2		

- Molecule 15 is a protein called plastid ribosomal protein uS13c.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	m	110	Total	C	N	O	S	0	0
			904	556	182	161	5		

- Molecule 16 is a protein called 30S ribosomal protein S14, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	n	99	Total	C	N	O	S	0	0
			820	507	174	136	3		

- Molecule 17 is a protein called 30S ribosomal protein S15, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	o	75	Total	C	N	O	S	0	0
			635	404	123	107	1		

- Molecule 18 is a protein called 30S ribosomal protein S16, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	p	80	Total	C	N	O	S	0	0
			664	425	123	114	2		

- Molecule 19 is a protein called plastid ribosomal protein uS17c.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	q	86	Total	C	N	O	S	0	0
			693	434	136	119	4		

- Molecule 20 is a protein called 30S ribosomal protein S18, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	r	60	Total	C	N	O	S	0	0
			490	308	96	85	1		

- Molecule 21 is a protein called 30S ribosomal protein S19 alpha, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	s	78	Total	C	N	O	S	0	0
			631	406	119	104	2		

- Molecule 22 is a protein called plastid ribosomal protein bS20c.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	t	107	Total	C	N	O	S	0	0
			853	528	173	151	1		

- Molecule 23 is a protein called plastid ribosomal protein bS21c.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	u	65	Total	C	N	O	S	0	0
			568	339	127	100	2		

- Molecule 24 is a protein called 30S ribosomal protein 2, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	v	80	Total	C	N	O	0	0
			613	388	104	121		

- Molecule 25 is a protein called 30S ribosomal protein 3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	w	82	Total	C	N	O	S	0	0
			686	454	113	116	3		

- Molecule 26 is a protein called 30S ribosomal protein S31, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	x	40	Total	C	N	O	0	0
			309	192	69	48		

- Molecule 27 is a protein called Ribosome-binding factor PSRP1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	y	116	Total	C	N	O	S	0	0
			919	567	181	169	2		

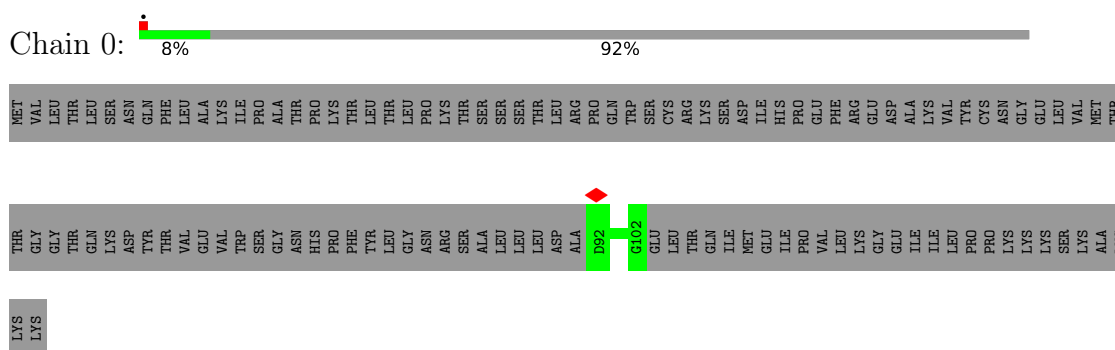
- Molecule 28 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
28	a	182	Total 182	Mg 182	0
28	k	1	Total 1	Mg 1	0
28	l	1	Total 1	Mg 1	0
28	x	1	Total 1	Mg 1	0

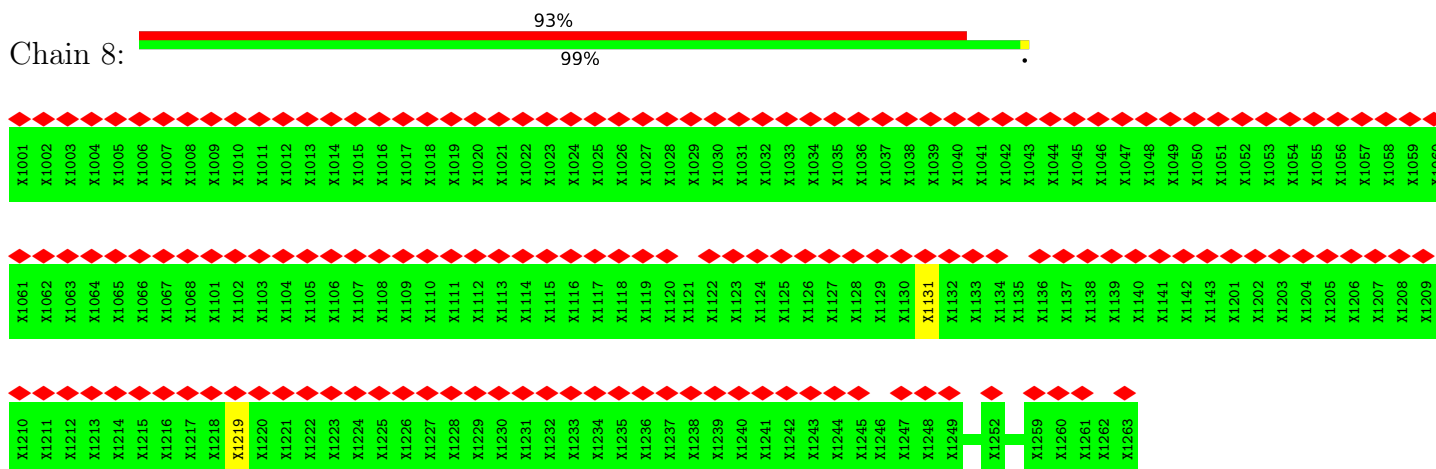
3 Residue-property plots

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.

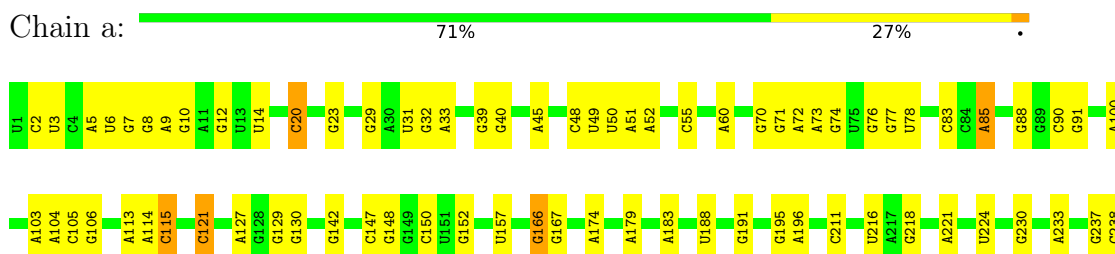
- Molecule 1: 50S ribosomal protein L31

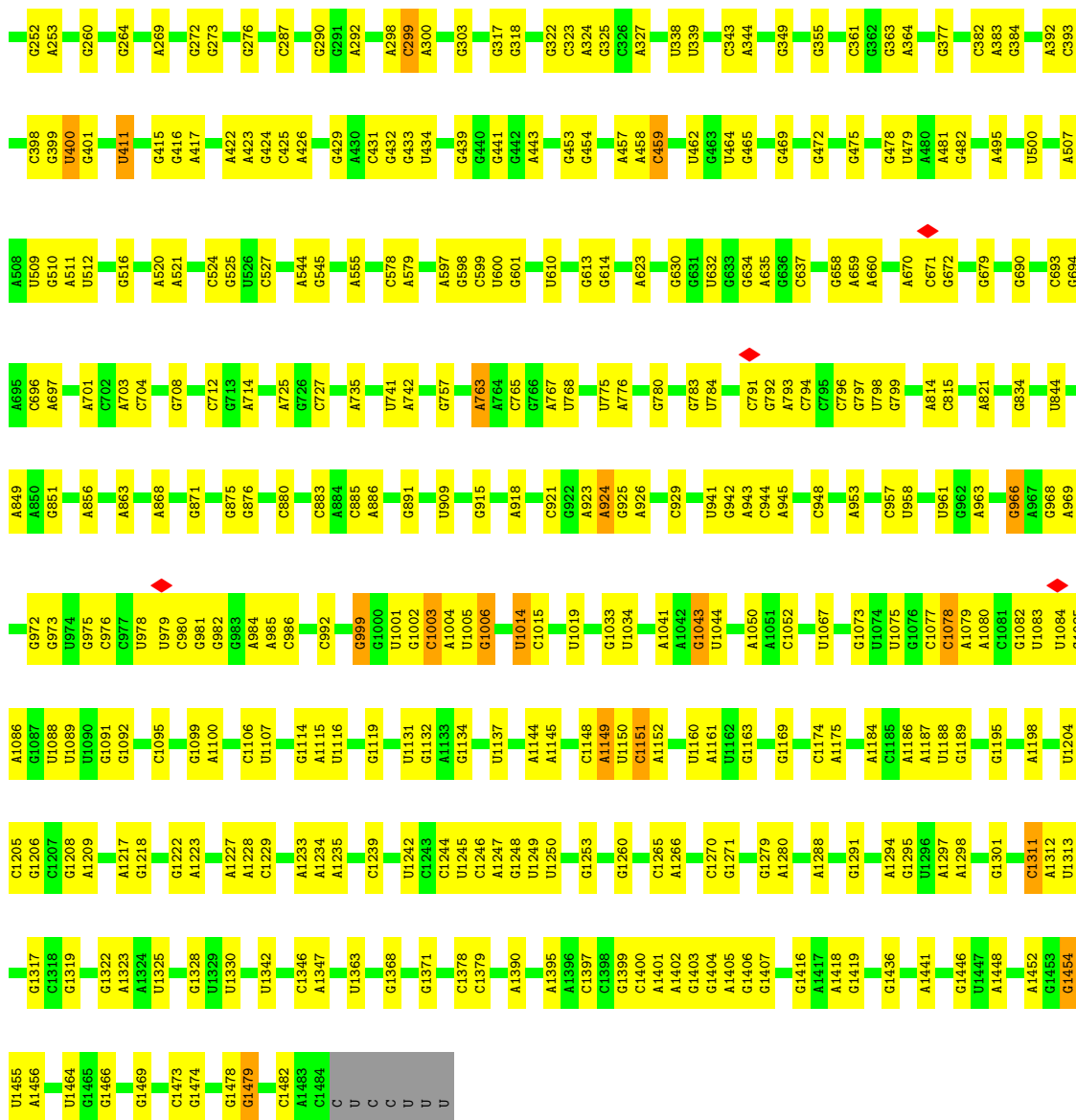


- Molecule 2: plastid ribosomal protein bS1c

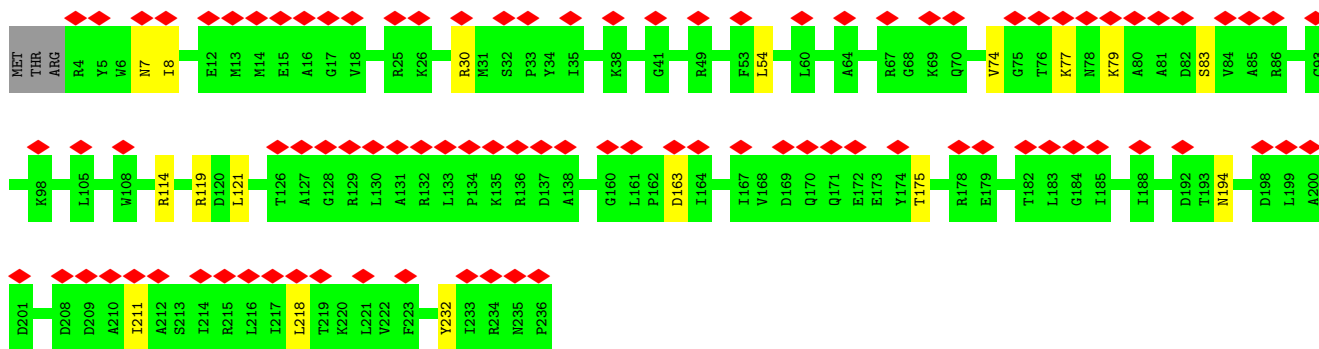
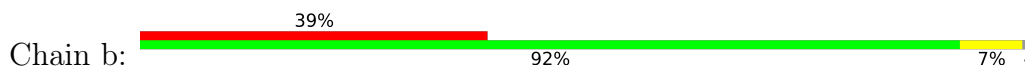


- Molecule 3: 16S ribosomal RNA



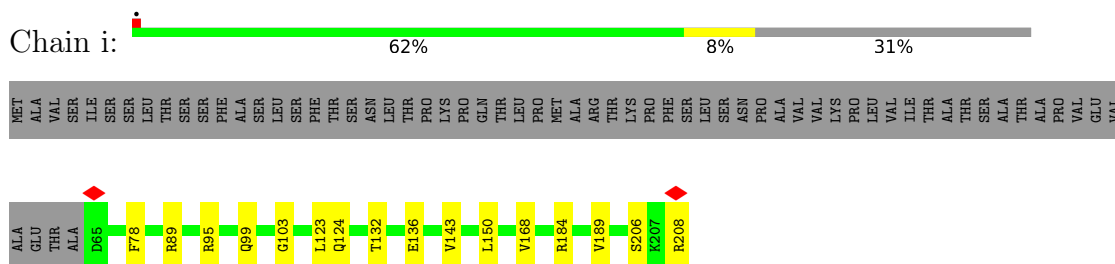


• Molecule 4: 30S ribosomal protein S2, chloroplastic

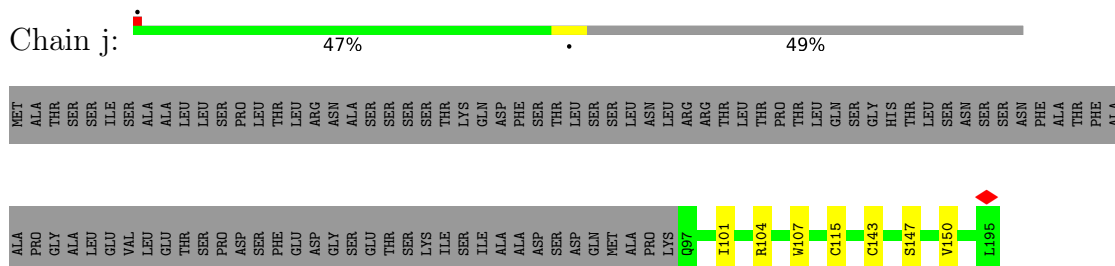


• Molecule 5: 30S ribosomal protein S3, chloroplastic

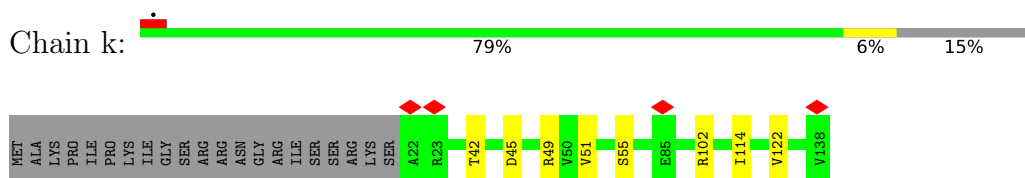
• Molecule 11: plastid ribosomal protein uS9c



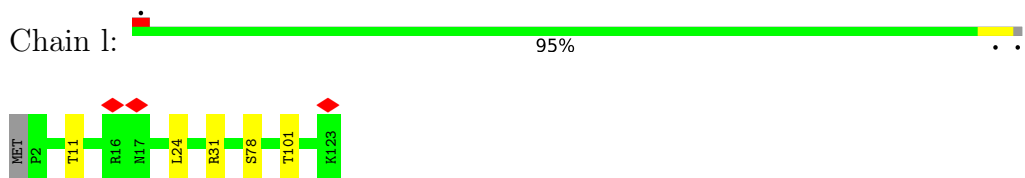
• Molecule 12: plastid ribosomal protein uS10c



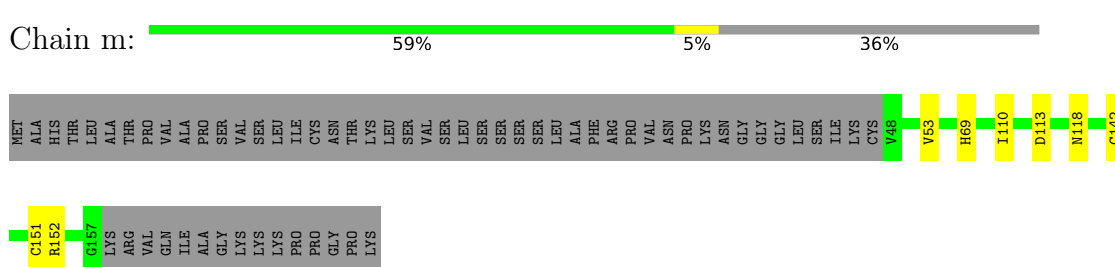
• Molecule 13: 30S ribosomal protein S11, chloroplastic



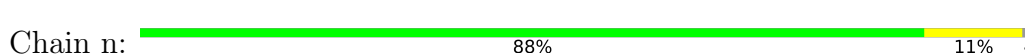
• Molecule 14: 30S ribosomal protein S12, chloroplastic



• Molecule 15: plastid ribosomal protein uS13c

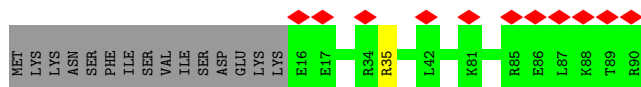
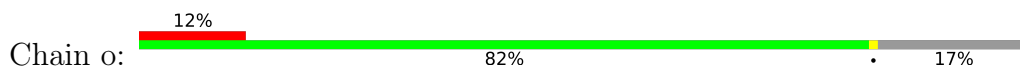


• Molecule 16: 30S ribosomal protein S14, chloroplastic

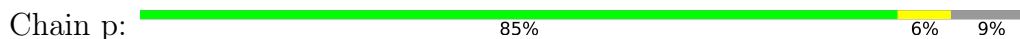




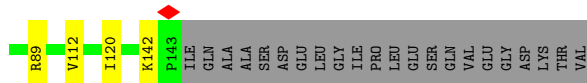
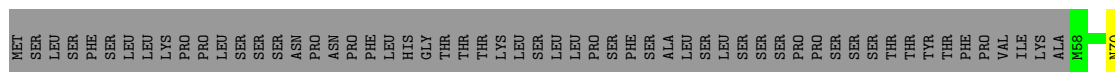
- Molecule 17: 30S ribosomal protein S15, chloroplastic



- Molecule 18: 30S ribosomal protein S16, chloroplastic



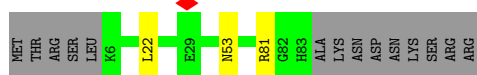
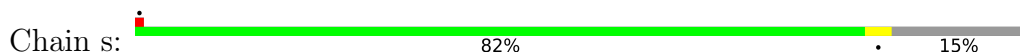
- Molecule 19: plastid ribosomal protein uS17c



- Molecule 20: 30S ribosomal protein S18, chloroplastic

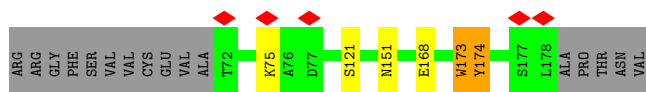


- Molecule 21: 30S ribosomal protein S19 alpha, chloroplastic

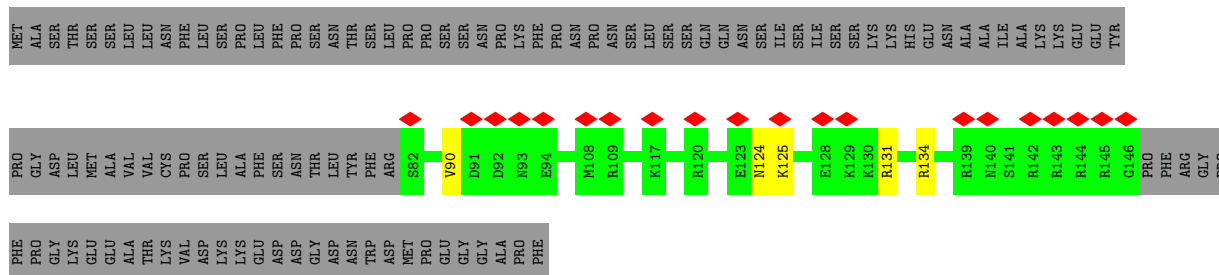


- Molecule 22: plastid ribosomal protein bS20c

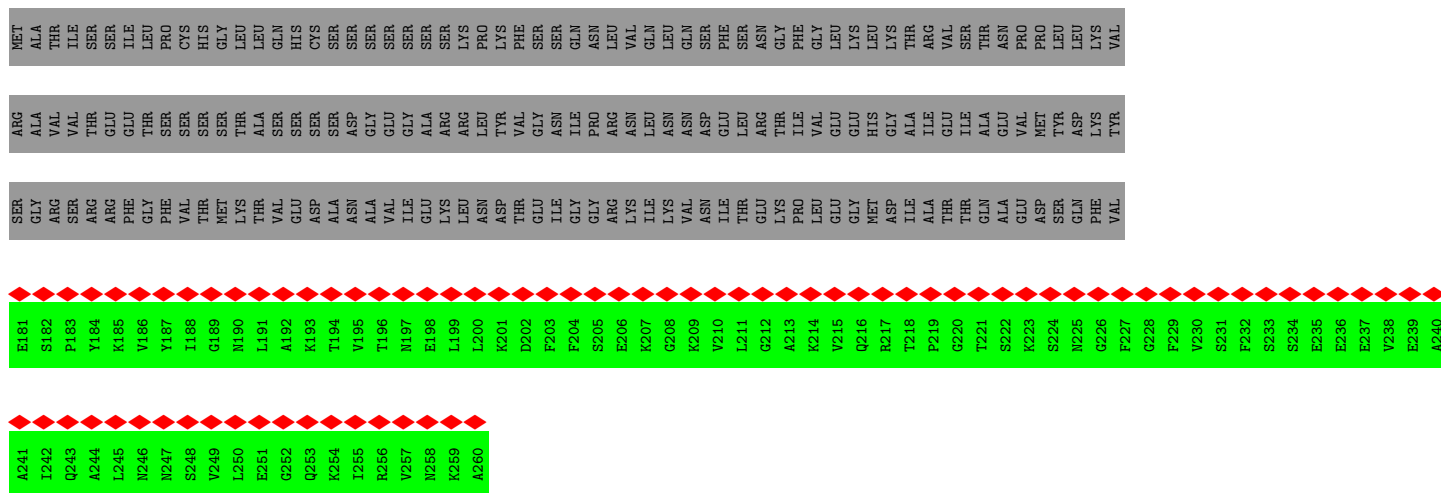




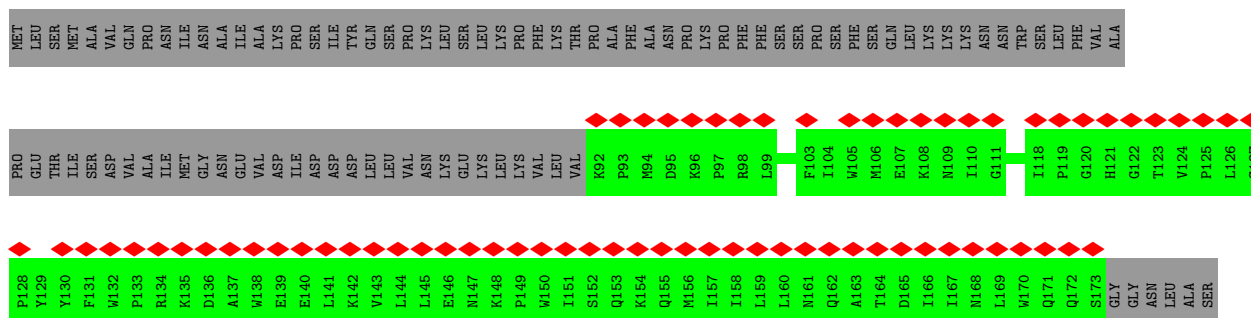
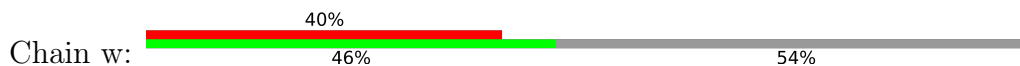
• Molecule 23: plastid ribosomal protein bS21c



• Molecule 24: 30S ribosomal protein 2, chloroplastic



• Molecule 25: 30S ribosomal protein 3, chloroplastic



• Molecule 26: 30S ribosomal protein S31, chloroplastic

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	127031	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)	800	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.345	Depositor
Minimum map value	-0.104	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	444.8, 444.8, 444.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.39	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.34	0/99	0.47	0/128
3	a	0.74	15/35687 (0.0%)	1.16	92/55680 (0.2%)
4	b	0.44	0/1878	0.60	0/2538
5	c	0.52	0/1763	0.70	1/2370 (0.0%)
6	d	0.46	0/1661	0.66	1/2230 (0.0%)
7	e	0.57	0/1345	0.70	0/1817
8	f	0.43	0/929	0.61	0/1255
9	g	0.39	0/1226	0.59	0/1641
10	h	0.48	0/1094	0.68	0/1467
11	i	0.52	0/1138	0.76	2/1526 (0.1%)
12	j	0.55	0/822	0.66	0/1111
13	k	0.43	0/896	0.64	0/1206
14	l	0.52	0/975	0.68	0/1312
15	m	0.46	0/912	0.67	0/1219
16	n	0.50	0/836	0.66	0/1116
17	o	0.40	0/642	0.53	0/852
18	p	0.46	0/674	0.70	0/902
19	q	0.44	0/707	0.62	0/949
20	r	0.45	0/494	0.67	0/660
21	s	0.51	0/646	0.77	0/870
22	t	0.49	0/862	0.68	0/1151
23	u	0.39	0/572	0.53	0/754
24	v	0.58	0/621	0.49	0/833
25	w	0.58	0/707	0.55	0/962
26	x	0.67	1/317 (0.3%)	0.80	0/418
27	y	0.45	0/930	0.65	0/1243
All	All	0.66	16/58433 (0.0%)	1.01	96/86210 (0.1%)

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
4	b	0	1
5	c	0	1
7	e	0	1
22	t	0	2
All	All	0	5

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	a	1152	A	C6-N6	-8.63	1.27	1.33
3	a	1006	G	N3-C4	-7.76	1.30	1.35
3	a	400	U	C4-C5	7.69	1.50	1.43
3	a	1152	A	N7-C5	-7.68	1.34	1.39
3	a	714	A	N9-C4	-7.31	1.33	1.37

The worst 5 of 96 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	a	1152	A	C5-C6-N1	21.25	128.32	117.70
3	a	1152	A	C6-N1-C2	-20.10	106.54	118.60
3	a	1006	G	C5-C6-N1	-16.13	103.43	111.50
3	a	1152	A	N1-C2-N3	15.45	137.03	129.30
3	a	1006	G	N7-C8-N9	-15.28	105.46	113.10

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	b	74	VAL	Peptide
5	c	103	LEU	Peptide
7	e	144	LYS	Peptide
22	t	173	TRP	Peptide
22	t	75	LYS	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	0	98	0	99	0	0
2	8	870	0	184	1	0
3	a	31868	0	16048	0	0
4	b	1844	0	1887	0	0
5	c	1736	0	1819	0	0
6	d	1633	0	1730	0	0
7	e	1331	0	1312	0	0
8	f	911	0	923	0	0
9	g	1210	0	1284	0	0
10	h	1079	0	1137	0	0
11	i	1119	0	1181	0	0
12	j	805	0	849	0	0
13	k	882	0	928	0	0
14	l	959	0	1035	0	0
15	m	904	0	943	0	0
16	n	820	0	858	0	0
17	o	635	0	686	0	0
18	p	664	0	703	0	0
19	q	693	0	729	0	0
20	r	490	0	532	0	0
21	s	631	0	661	0	0
22	t	853	0	915	0	0
23	u	568	0	576	0	0
24	v	613	0	621	0	0
25	w	686	0	706	0	0
26	x	309	0	323	0	0
27	y	919	0	958	0	0
28	a	182	0	0	0	0
28	k	1	0	0	0	0
28	l	1	0	0	0	0
28	x	1	0	0	0	0
All	All	55315	0	39627	1	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 11.

All (1) 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)
2:8:1131:UNK:CB	2:8:1219:UNK:HA	2.51	0.40

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	
1	0	9/130 (7%)	8 (89%)	1 (11%)	0	100	100
4	b	231/236 (98%)	220 (95%)	11 (5%)	0	100	100
5	c	214/218 (98%)	200 (94%)	14 (6%)	0	100	100
6	d	197/201 (98%)	181 (92%)	16 (8%)	0	100	100
7	e	185/308 (60%)	181 (98%)	4 (2%)	0	100	100
8	f	111/211 (53%)	106 (96%)	4 (4%)	1 (1%)	17	56
9	g	152/155 (98%)	146 (96%)	6 (4%)	0	100	100
10	h	131/134 (98%)	125 (95%)	4 (3%)	2 (2%)	10	46
11	i	142/208 (68%)	136 (96%)	6 (4%)	0	100	100
12	j	97/195 (50%)	92 (95%)	4 (4%)	1 (1%)	15	54
13	k	115/138 (83%)	107 (93%)	8 (7%)	0	100	100
14	l	120/123 (98%)	113 (94%)	7 (6%)	0	100	100
15	m	108/172 (63%)	97 (90%)	10 (9%)	1 (1%)	17	56
16	n	97/100 (97%)	93 (96%)	4 (4%)	0	100	100
17	o	73/90 (81%)	73 (100%)	0	0	100	100
18	p	78/88 (89%)	72 (92%)	6 (8%)	0	100	100
19	q	84/165 (51%)	78 (93%)	6 (7%)	0	100	100
20	r	58/101 (57%)	55 (95%)	3 (5%)	0	100	100
21	s	76/92 (83%)	74 (97%)	2 (3%)	0	100	100
22	t	105/183 (57%)	100 (95%)	4 (4%)	1 (1%)	15	54
23	u	63/180 (35%)	61 (97%)	2 (3%)	0	100	100
24	v	78/260 (30%)	76 (97%)	2 (3%)	0	100	100
25	w	80/179 (45%)	78 (98%)	2 (2%)	0	100	100
26	x	38/101 (38%)	37 (97%)	1 (3%)	0	100	100
27	y	114/302 (38%)	105 (92%)	8 (7%)	1 (1%)	17	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2756/4270 (64%)	2614 (95%)	135 (5%)	7 (0%)	44	74

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	h	68	ASN
12	j	150	VAL
15	m	53	VAL
22	t	174	TYR
10	h	69	LYS

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	10/117 (8%)	10 (100%)	0	100	100
4	b	198/201 (98%)	182 (92%)	16 (8%)	11	42
5	c	186/188 (99%)	171 (92%)	15 (8%)	11	42
6	d	178/180 (99%)	167 (94%)	11 (6%)	18	52
7	e	121/255 (48%)	113 (93%)	8 (7%)	16	50
8	f	100/186 (54%)	96 (96%)	4 (4%)	31	64
9	g	125/126 (99%)	120 (96%)	5 (4%)	31	64
10	h	116/117 (99%)	108 (93%)	8 (7%)	15	48
11	i	114/169 (68%)	100 (88%)	14 (12%)	4	25
12	j	91/173 (53%)	85 (93%)	6 (7%)	16	50
13	k	91/109 (84%)	83 (91%)	8 (9%)	10	40
14	l	105/106 (99%)	100 (95%)	5 (5%)	25	59
15	m	99/151 (66%)	92 (93%)	7 (7%)	14	47
16	n	89/90 (99%)	78 (88%)	11 (12%)	4	25
17	o	70/85 (82%)	69 (99%)	1 (1%)	67	84
18	p	71/79 (90%)	66 (93%)	5 (7%)	15	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	q	77/149 (52%)	72 (94%)	5 (6%)	17	50
20	r	56/96 (58%)	53 (95%)	3 (5%)	22	56
21	s	68/81 (84%)	65 (96%)	3 (4%)	28	62
22	t	89/156 (57%)	84 (94%)	5 (6%)	21	55
23	u	59/160 (37%)	54 (92%)	5 (8%)	10	41
24	v	67/225 (30%)	67 (100%)	0	100	100
25	w	76/162 (47%)	76 (100%)	0	100	100
26	x	30/85 (35%)	30 (100%)	0	100	100
27	y	104/275 (38%)	102 (98%)	2 (2%)	57	79
All	All	2390/3721 (64%)	2243 (94%)	147 (6%)	22	52

5 of 147 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	n	68	ARG
23	u	131	ARG
18	p	22	ILE
20	r	31	ARG
7	e	270	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
20	r	23	GLN
24	v	258	ASN
20	r	79	ASN
21	s	69	HIS
25	w	168	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	a	1483/1491 (99%)	389 (26%)	0

5 of 389 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	a	2	C
3	a	3	U
3	a	5	A
3	a	6	U
3	a	7	G

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 185 ligands modelled in this entry, 185 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
2	8	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	8	1068:UNK	C	1101:UNK	N	66.30
1	8	1143:UNK	C	1201:UNK	N	11.98

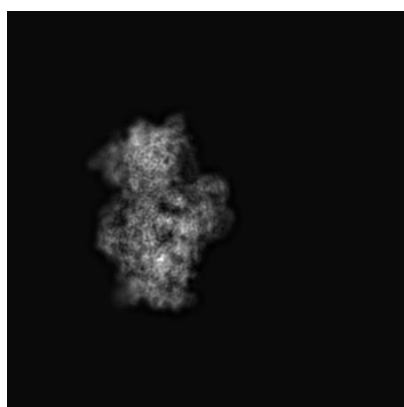
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3532. These allow visual inspection of the internal detail of the map and identification of artifacts.

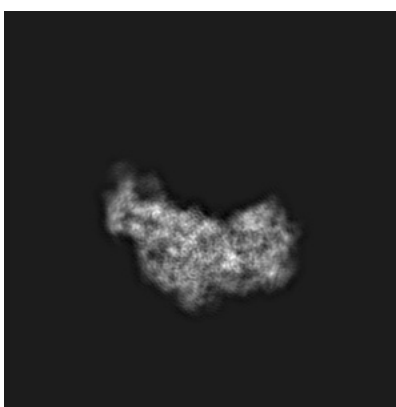
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

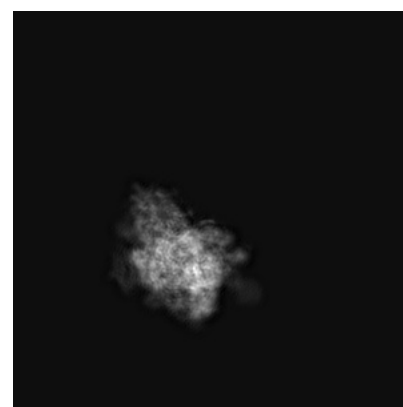
6.1.1 Primary map



X



Y

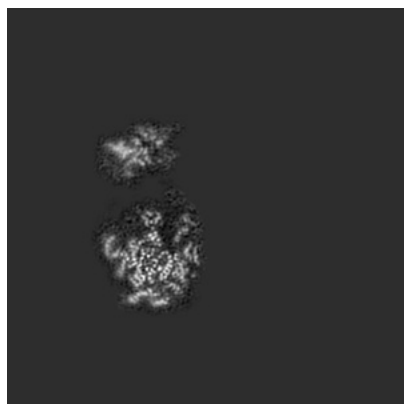


Z

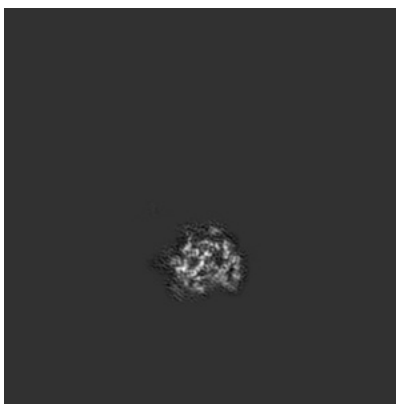
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

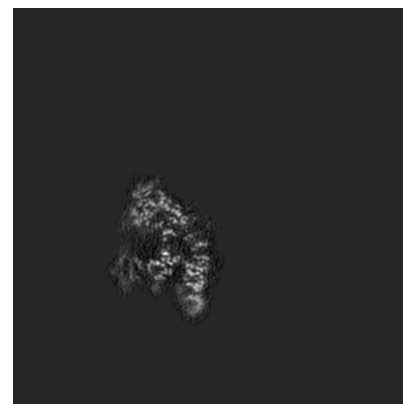
6.2.1 Primary map



X Index: 160



Y Index: 160

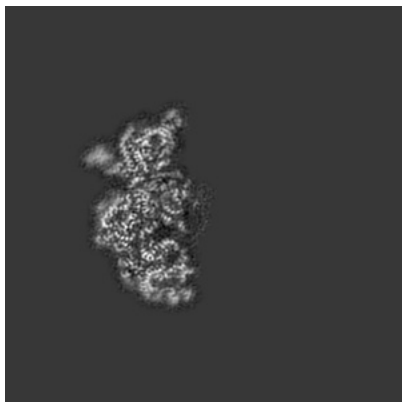


Z Index: 160

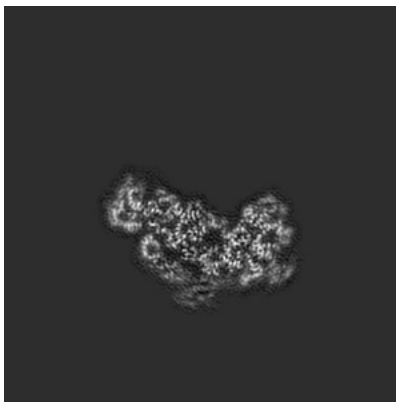
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

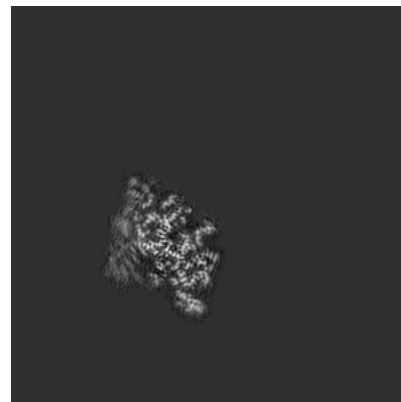
6.3.1 Primary map



X Index: 145



Y Index: 114



Z Index: 151

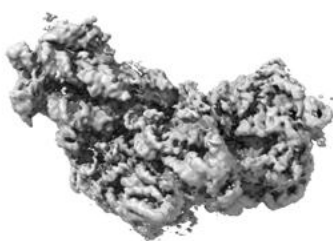
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

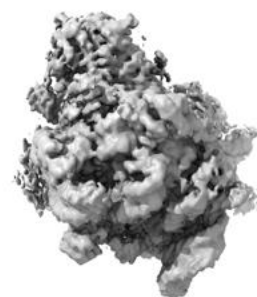
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

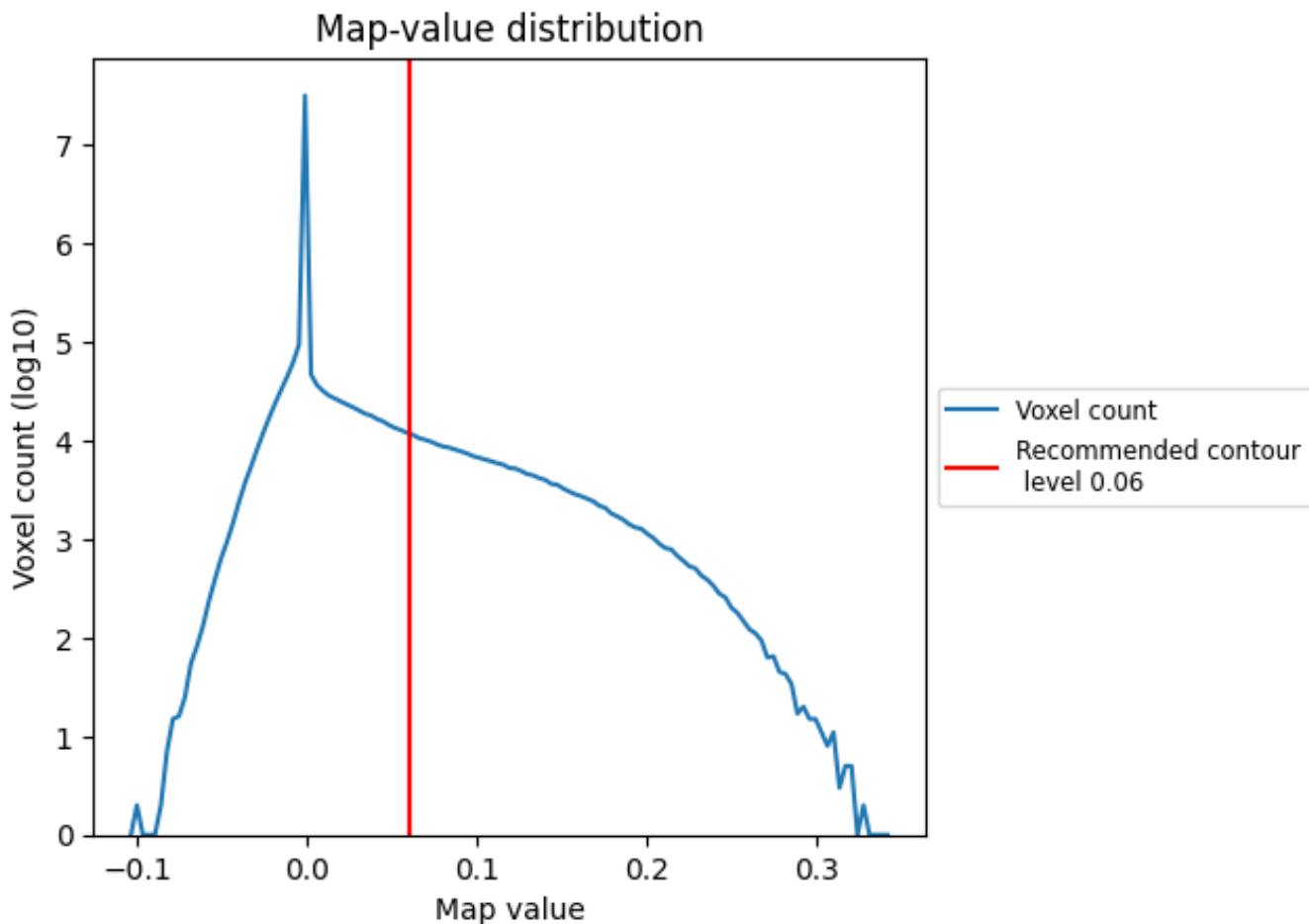
6.5 Mask visualisation

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

7 Map analysis [i](#)

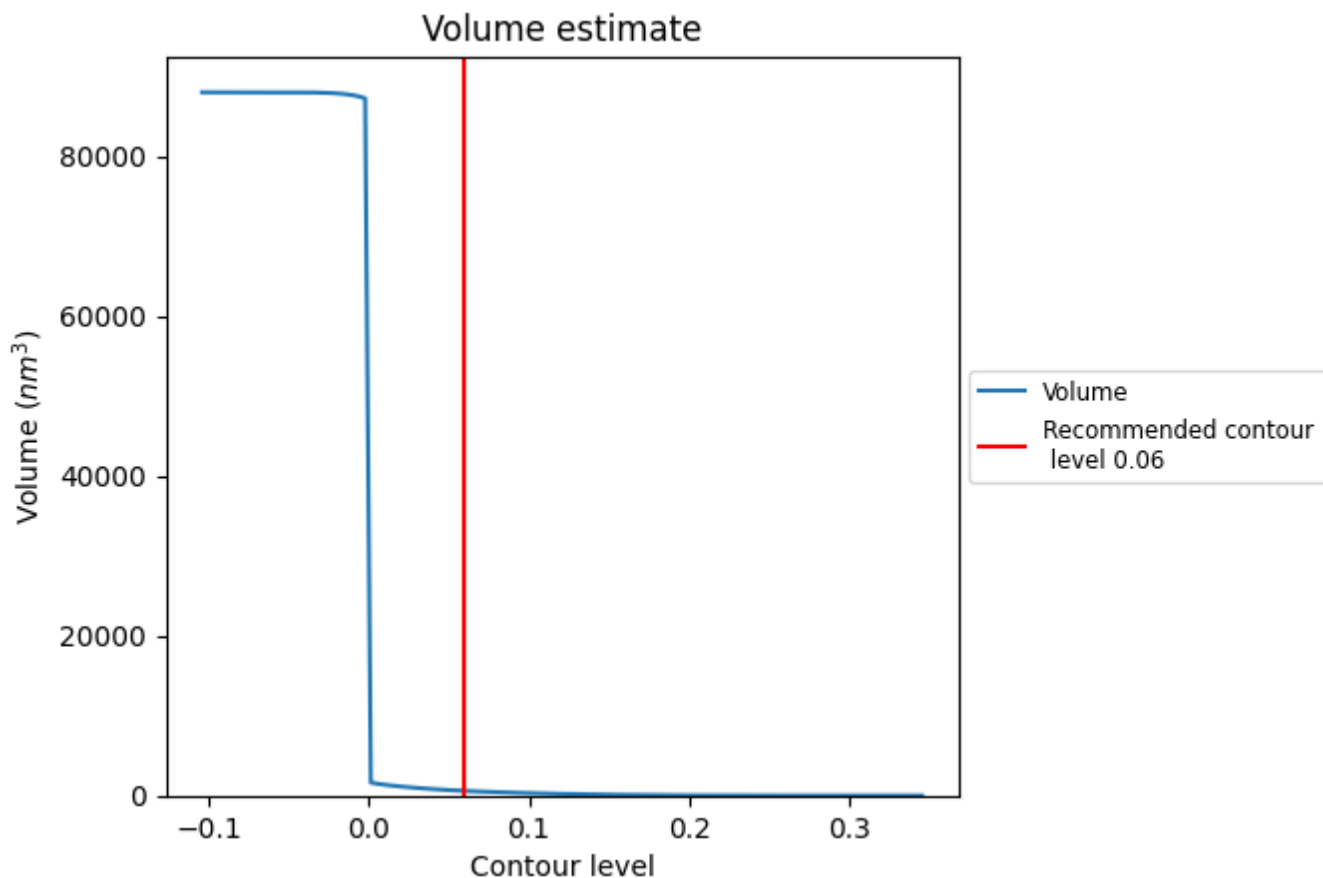
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

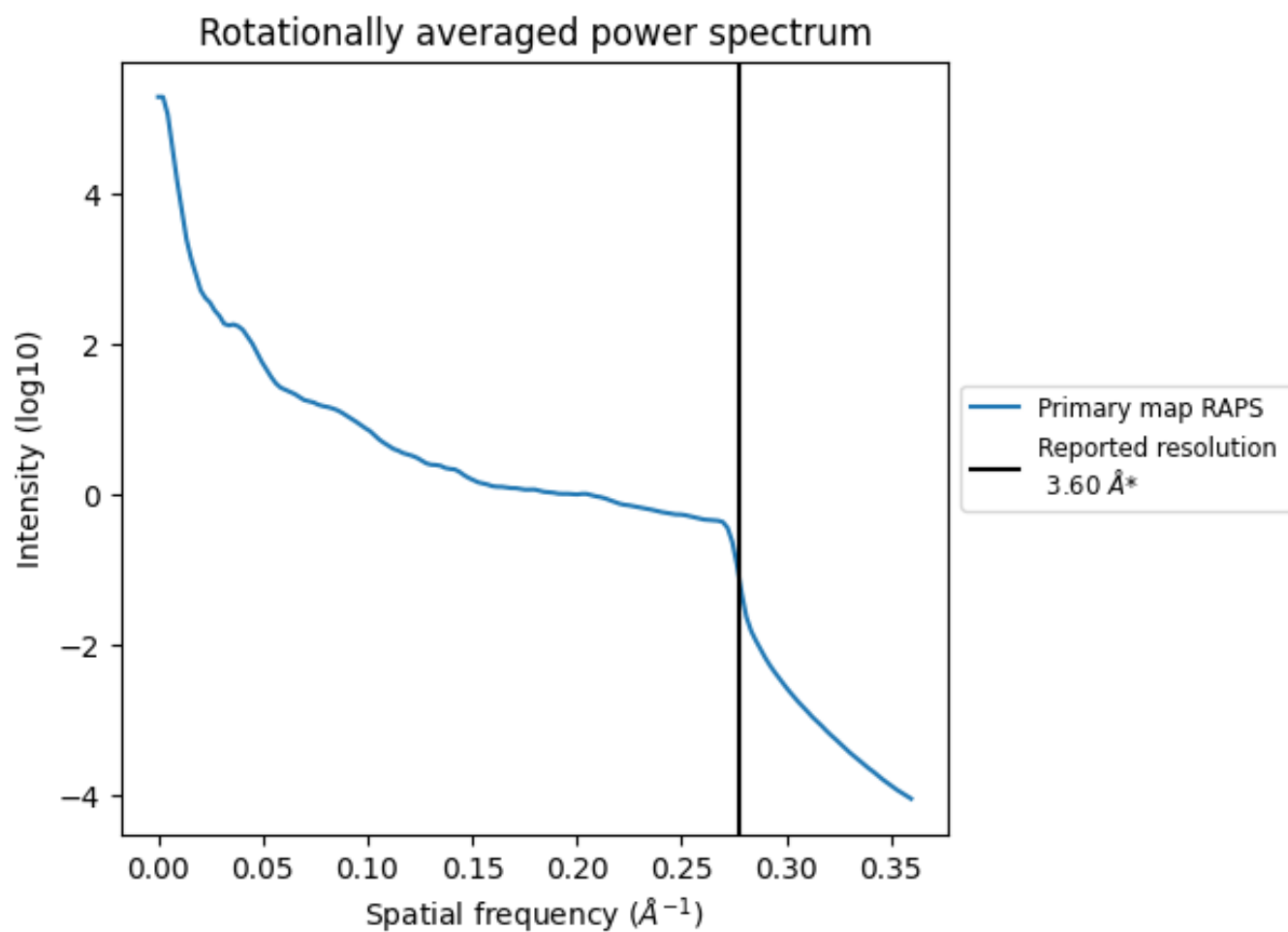
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 585 nm³; this corresponds to an approximate mass of 529 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

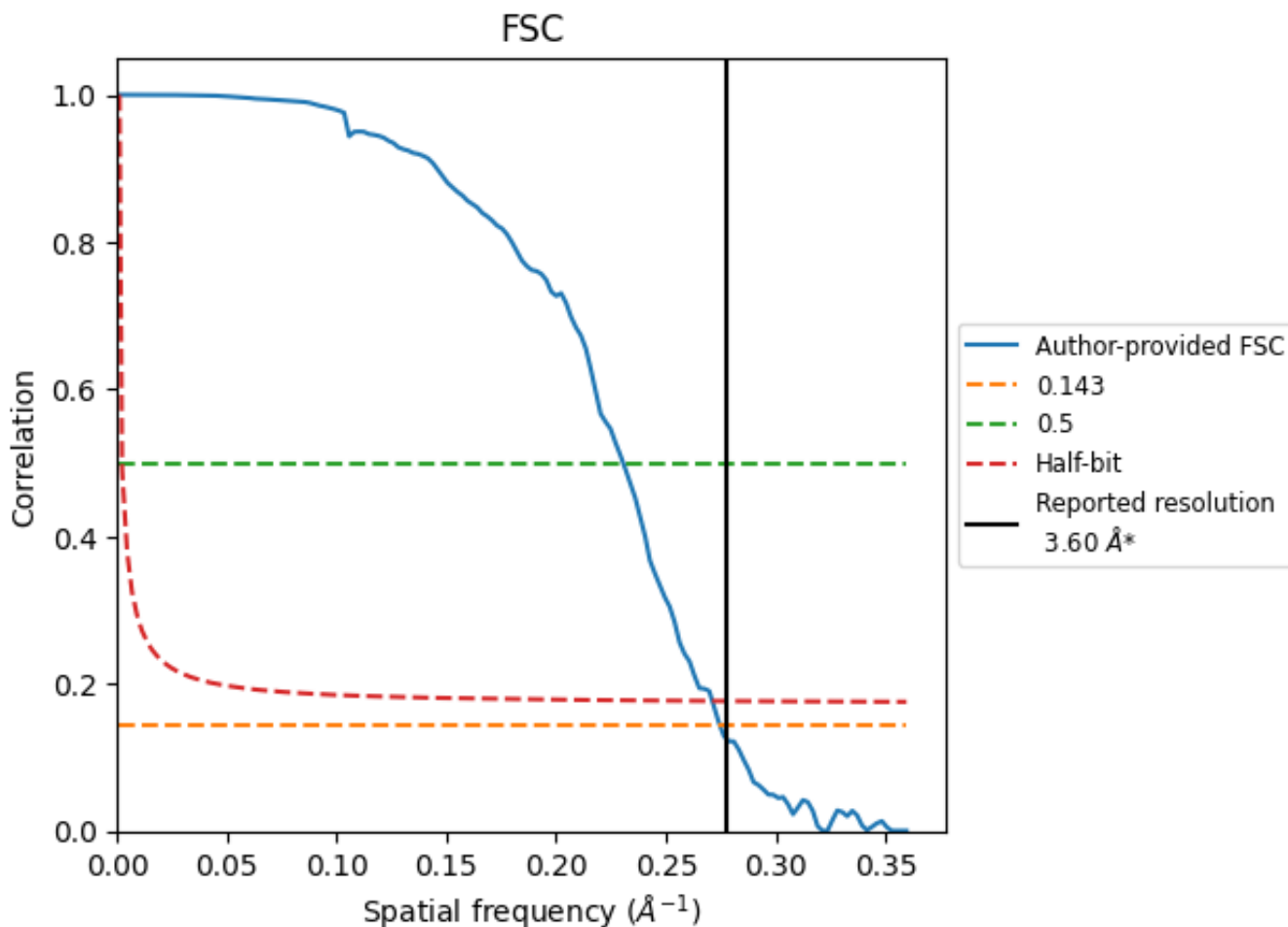


*Reported resolution corresponds to spatial frequency of 0.278\AA^{-1}

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 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

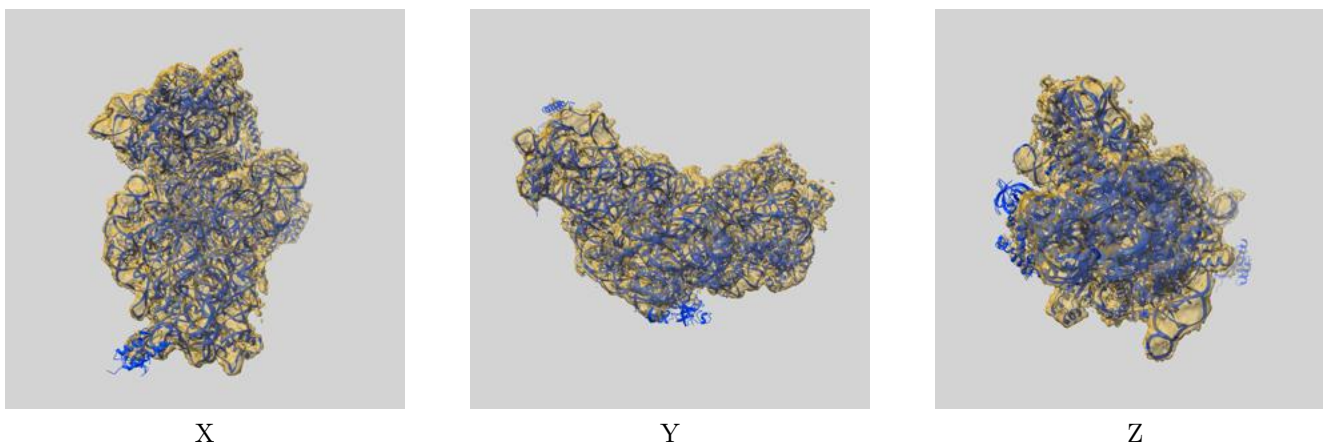
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.64	4.34	3.69
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

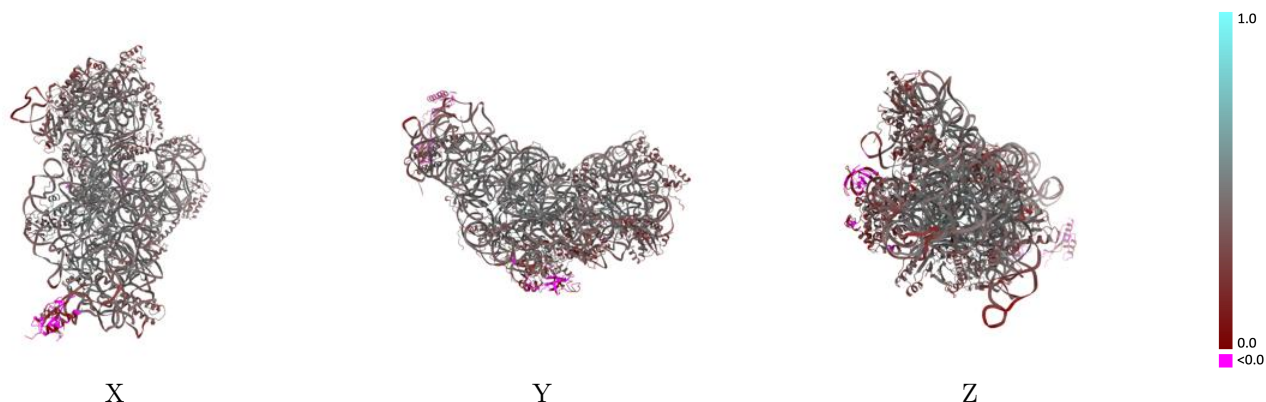
This section contains information regarding the fit between EMDB map EMD-3532 and PDB model 5MMJ. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



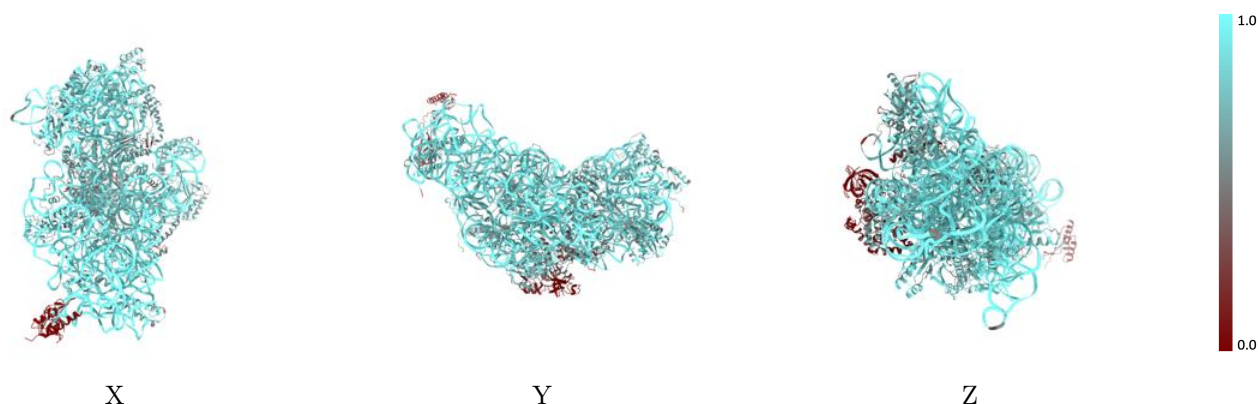
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



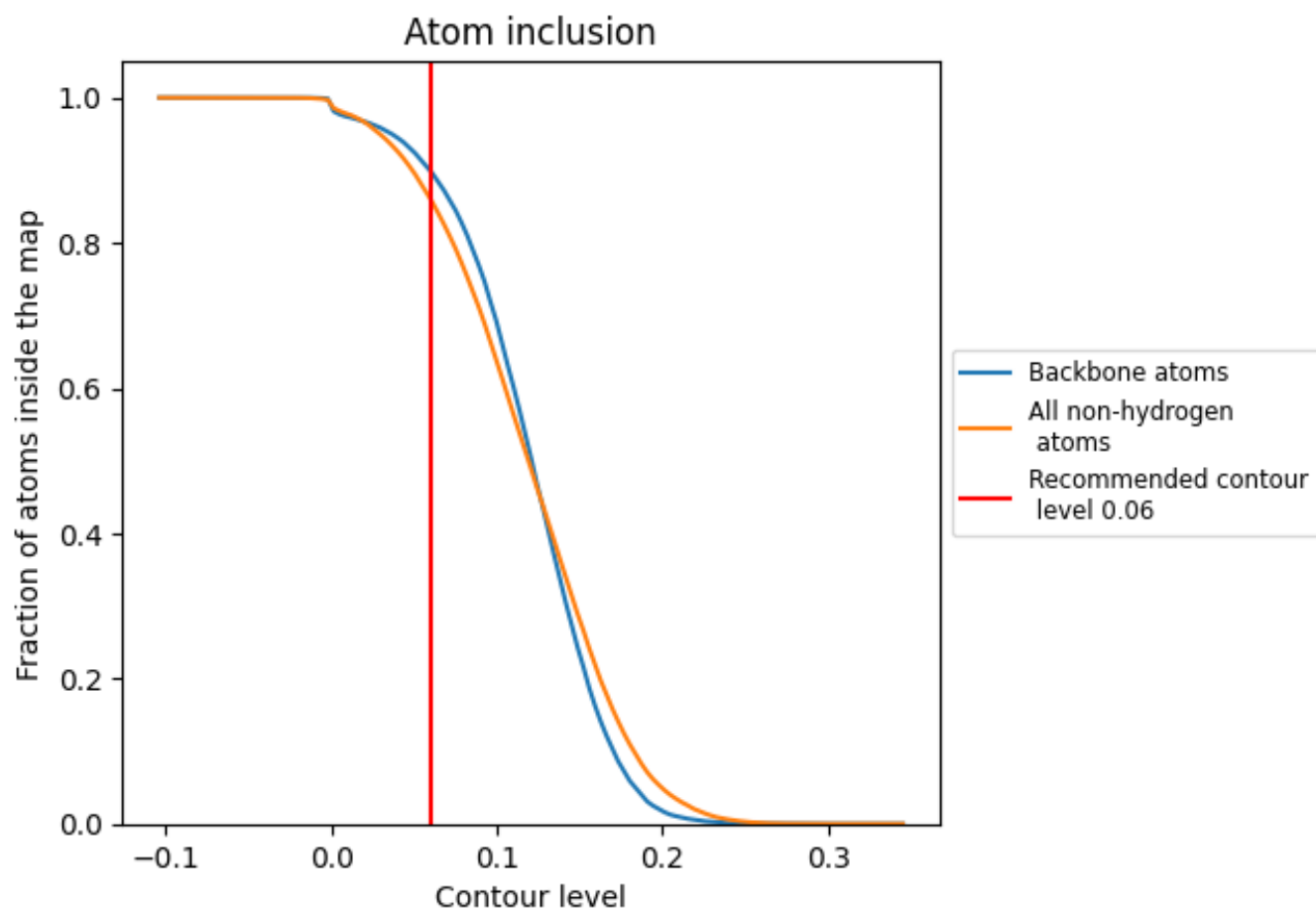
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).

























































9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 86% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8599	 0.3950
0	 0.6421	 0.2470
8	 0.0943	 0.0930
a	 0.9807	 0.4280
b	 0.4579	 0.3130
c	 0.8096	 0.4040
d	 0.8170	 0.4100
e	 0.7623	 0.4270
f	 0.7125	 0.3380
g	 0.6863	 0.3480
h	 0.7806	 0.3960
i	 0.8411	 0.3800
j	 0.8475	 0.4080
k	 0.7923	 0.3660
l	 0.8095	 0.4650
m	 0.8111	 0.3590
n	 0.8675	 0.4030
o	 0.6270	 0.3540
p	 0.8578	 0.4120
q	 0.8412	 0.4330
r	 0.7886	 0.3640
s	 0.8546	 0.3840
t	 0.8180	 0.3740
u	 0.5410	 0.3250
v	 0.0000	 -0.0400
w	 0.1363	 0.0400
x	 0.8667	 0.4060
y	 0.6506	 0.3690

