



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 11:32 PM UTC

PDB ID : 6YPU / pdb_00006ypu
EMDB ID : EMD-10869
Title : Acinetobacter baumannii ribosome-amikacin complex - 30S subunit body
Authors : Nicholson, D.; Edwards, T.A.; O'Neill, A.J.; Ranson, N.A.
Deposited on : 2020-04-16
Resolution : 2.90 Å(reported)
Based on initial models : 5AFI, 5MDZ

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:

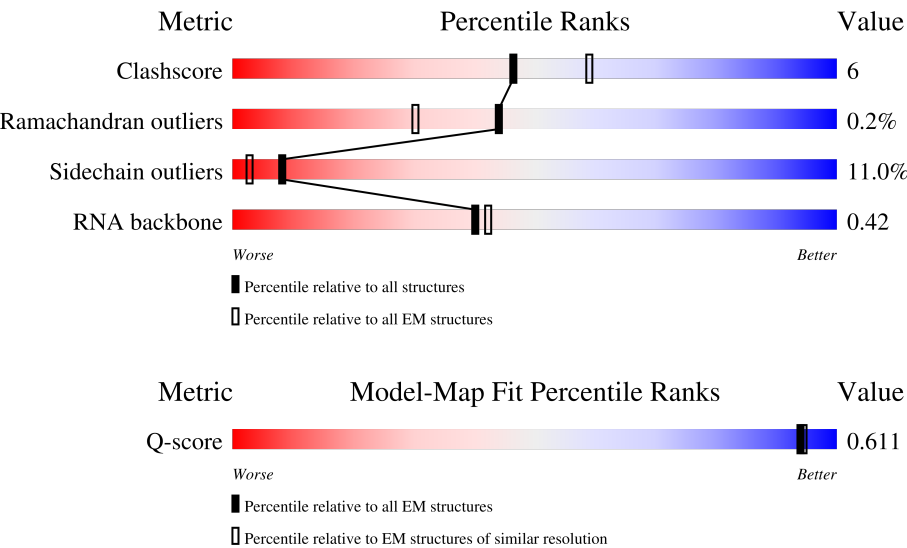
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

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

The reported resolution of this entry is 2.90 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	13054 (2.40 - 3.40)

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	2	1544	38%16%•42%
1	4	1544	6%•91%
2	c	250	49%85%•12%

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Mol	Chain	Length	Quality of chain
3	e	208	
4	f	165	
5	g	127	
6	i	131	
7	l	128	
8	m	124	
9	p	89	
10	q	83	
11	r	85	
12	s	75	
13	u	88	
14	v	71	

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 33322 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	2	894	Total	C	N	O	P	0	0
			19228	8575	3556	6203	894		
1	4	146	Total	C	N	O	P	0	0
			3129	1395	572	1016	146		

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	c	219	Total	C	N	O	0	0
			1079	641	219	219		

- Molecule 3 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	e	207	Total	C	N	O	S	0	0
			1592	991	306	293	2		

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	f	155	Total	C	N	O	S	0	0
			1129	700	217	207	5		

- Molecule 5 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	g	103	Total	C	N	O	S	0	0
			858	540	156	158	4		

- Molecule 6 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	i	130	Total	C	N	O	S	0	0
			984	615	177	186	6		

- Molecule 7 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	l	114	Total	C	N	O	S	0	0
			836	521	161	153	1		

- Molecule 8 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	m	122	Total	C	N	O	S	0	0
			945	580	193	167	5		

- Molecule 9 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	p	88	Total	C	N	O	S	0	0
			704	434	144	125	1		

- Molecule 10 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	q	80	Total	C	N	O	S	0	0
			632	396	126	109	1		

- Molecule 11 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	r	79	Total	C	N	O	S	0	0
			621	390	116	114	1		

- Molecule 12 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	s	53	Total	C	N	O	0	0
			434	277	76	81		

- Molecule 13 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	u	86	Total	C	N	O	S	0	0
			663	409	139	113	2		

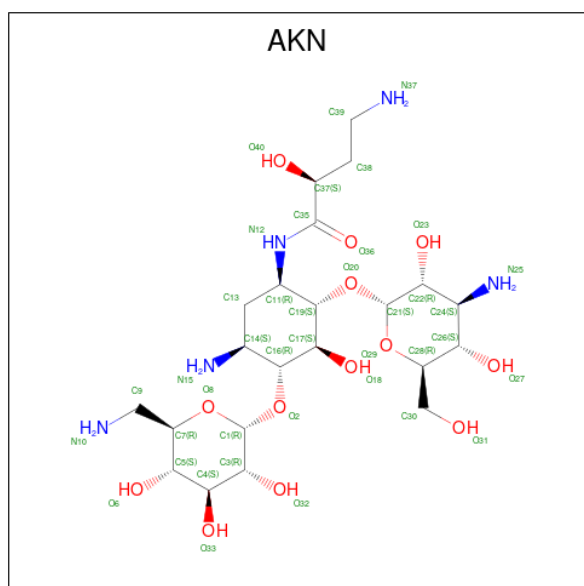
- Molecule 14 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	v	60	Total	C	N	O	0	0
			389	242	78	69		

- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
15	2	53	Total	Mg	0
			53	53	
15	4	6	Total	Mg	0
			6	6	

- Molecule 16 is (2S)-N-[(1R,2S,3S,4R,5S)-4-[(2R,3R,4S,5S,6R)-6-(aminomethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-5-azanyl-2-[(2S,3R,4S,5S,6R)-4-azanyl-6-(hydroxymethyl)-3,5-bis(oxidanyl)oxan-2-yl]oxy-3-oxidanyl-cyclohexyl]-4-azanyl-2-oxidanyl-butanamide (CCD ID: AKN) (formula: C₂₂H₄₃N₅O₁₃) (labeled as "Ligand of Interest" by depositor).

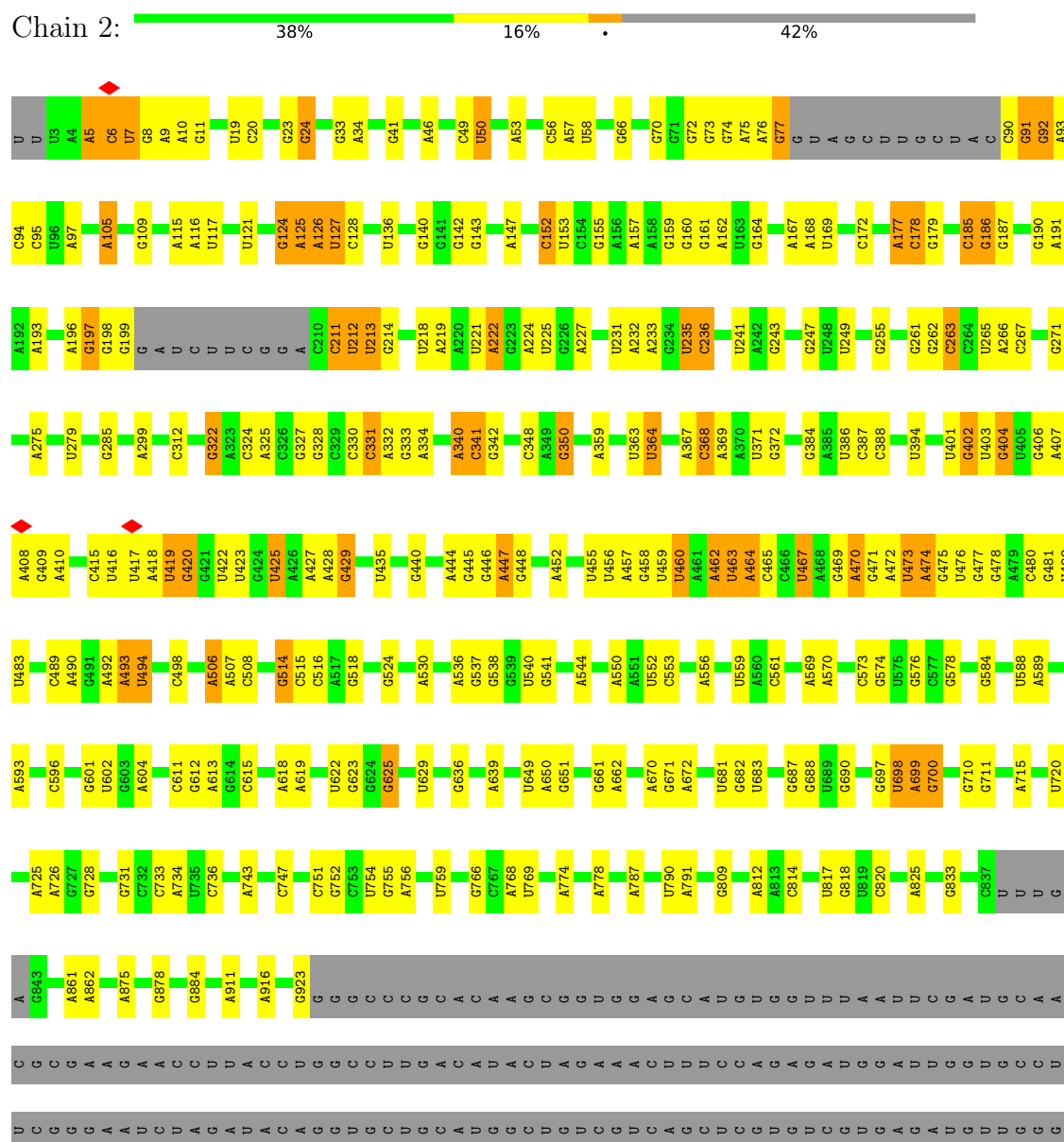


Mol	Chain	Residues	Atoms				AltConf
16	4	1	Total	C	N	O	0
			40	22	5	13	

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



U U A A G G U C C C G G C A A C G A G G C C A A A C C C U U U U U C C U U A C U D G C C A G C A U U U C C G A A G G G A A C C U D

U A A G G A U A C C U G C C A G U U G A C A A A C C U D G G A G G A A A G G C G G G G A C C G A A G G U C C A U U C C A U D G G C C C

C U U A C G C C C A G G C C U A A C A A C G G U C G C U D A C C A A A U G G U C G G U A C C A A A C G G U U U G C U A C C A C A G C G C A

U G U G A A U G C U U A A A A A A A A C C G A U C G G A A A G U C G G G A A U U G G A A G U C U U G C A A C U C G C A C U C C C A

U G A A A U C C G G A A U C C G C U A A A U C C G G A U C A A A U G C C G C G G G U U A A C G G U U C C C G G G C C

U U G U A C A A C A C C G C C C G U C A A C C C G A U D G G G A G A U U U G U C C A C C A A G U U A G C U A A C C U

G C A A A G A G G G C G G U U A A C C A C G G U G A U G G C C C G A U G A A C U G G G G U G A A G U U C C U A A C A A G G U A G C

C G U A G G G A A C C U G C G G G C C U G A U C C A C C U C C C U U A A C C G A A

• Molecule 1: 16S ribosomal RNA

Chain 4:  6%  91%

U U A A C C U G A A A G A G U U U U G A U C A A A G G G C U U A C C U A A C C G A A U G A A C A A U G C

A A G U C G A C C G G G G G A A A G G U A A G C U U G C U A C C G A A C C U A A G C G G C G G A C G G A U U A A U G C C U

U A G G A A U C U U G C C U A U U A A G G U G A G G G G A C A A C A A U C C G A A A G G A A C C U A A C C G G A A C G G U

C C U A C G G G A G A A G C A A G G A A G G A A U C C G G A C C U U C G G A C C U U A A U G A A U G A A C C G G A A U

U A G C C U A C U U G G G U A A A G G C C A A C C A A C G C G A A U C C U G G A A G C G G G U C U U A A G G A A U

G A U C C G C C A A C A A C U G G G A A C U A G A A C C G A A C C A A C C U A A C C A A C C U A A C C U G G A A

U A U U G G A C A A U G G G G A A C C C U C G A U C C A G C C A A U G C C G C G G U G G A A G G A A C C U U G

G U U G U A A A G G C A C U U U A A A G C C G A G G G A A G C U U U U A C U U A A C C U A A G A A G U G G A A C

G U U A C U C G C A A G A A A A G A C C G G C A A C G G U A C C U U G C C A G C U A A G C C A A C A A G G G U

G C G A G C C U U A A U C G G A A U U A C C U U G G C C G U U A A C C G G G C C U U A A A A U C C G G A U

G U G A A A U C C C A A C A G C U U U A A C U U G G A A C C U U G C A A U C C A A G G C U A A G A A U G G G A

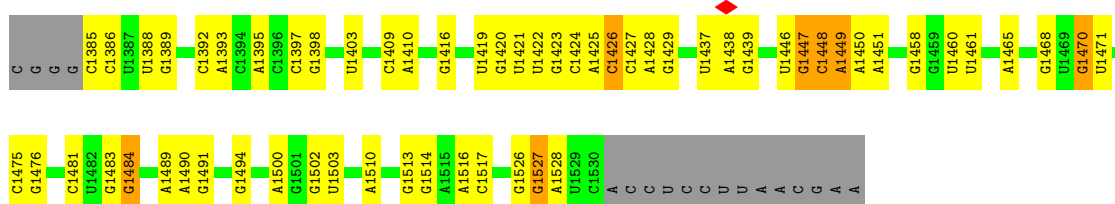
G A G G A U G G U A A A A U C C C A G G U G G U A A C C G G U G A A U G C C A A U C C U G G A A C C G G A U

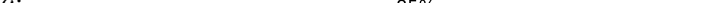
G G C G A A G G C A A G C C A U C C U G G C C U U G A A C C U G A A C C U G A A A G C C A A U G G G A A C

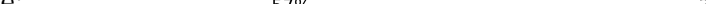
A G G A U A G A A U A C C C U G G U A G U C C A A C C G A A A C C U U A C C U A G C C U U A G C C C U U U

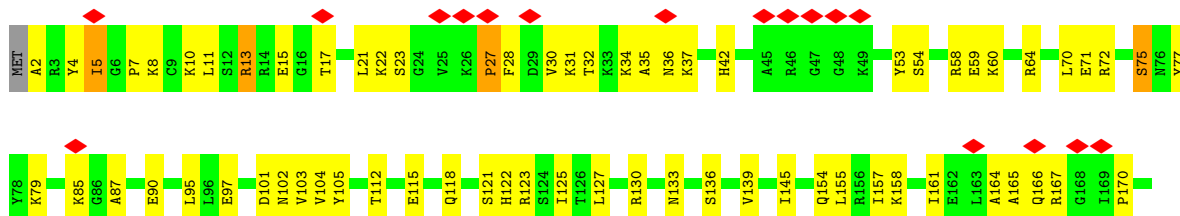
G A G G C U U A G A U G G C G C A A A C C G G C A A A A G A A C C G C C U U G G G A A C C A A G A

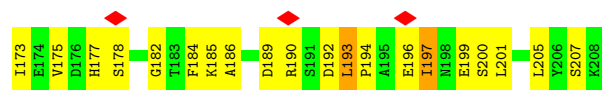
C U A A A C U C A A A A U G A A A U U G A C G G G C C C C C C C C A C A A G C C G G U U G G C A C C U U U G



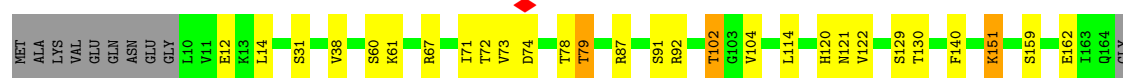
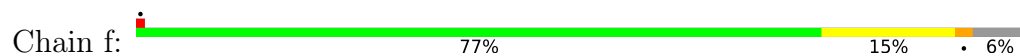
Chain c:  49% 85% 12%

Chain e:  10% 57% 39%

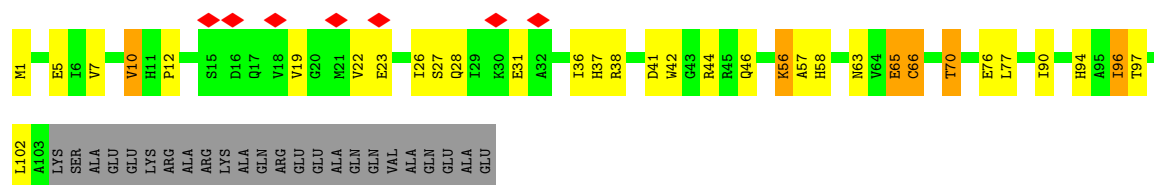




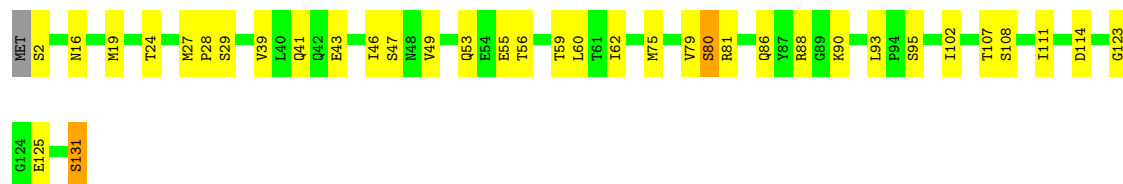
• Molecule 4: 30S ribosomal protein S5



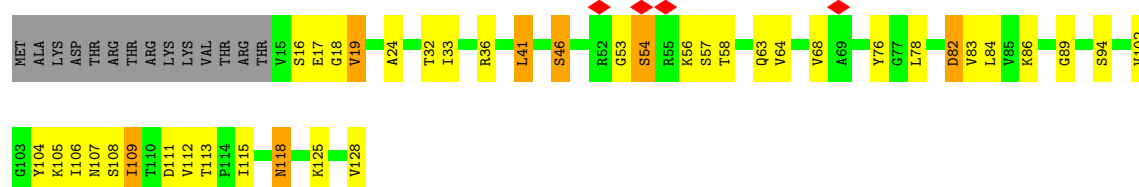
• Molecule 5: 30S ribosomal protein S6



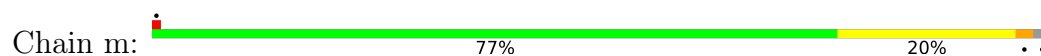
• Molecule 6: 30S ribosomal protein S8



• Molecule 7: 30S ribosomal protein S11

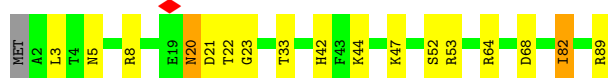


• Molecule 8: 30S ribosomal protein S12



- Molecule 9: 30S ribosomal protein S15

Chain p:  80% 17% ..



- Molecule 10: 30S ribosomal protein S16

Chain q:  80% 17% .



- Molecule 11: 30S ribosomal protein S17

Chain r:  65% 27% . 7%



- Molecule 12: 30S ribosomal protein S18

Chain s:  48% 23% 29%



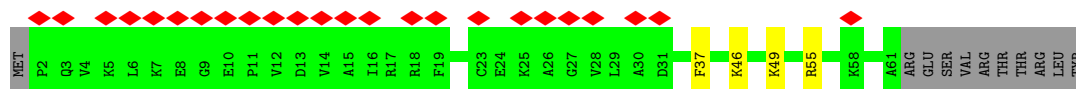
- Molecule 13: 30S ribosomal protein S20

Chain u:  80% 18% .



- Molecule 14: 30S ribosomal protein S21

Chain v:  34% 79% 6% 15%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	51958	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 ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.223	Depositor
Minimum map value	-0.125	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	428.00003, 428.00003, 428.00003	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AKN, 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	2	0.65	0/21541	0.50	0/33605
1	4	0.57	0/3501	0.47	0/5459
2	c	0.19	0/1078	0.43	0/1498
3	e	0.39	0/1612	0.55	1/2162 (0.0%)
4	f	0.45	0/1141	0.51	0/1537
5	g	0.36	0/873	0.49	0/1178
6	i	0.50	0/992	0.50	0/1331
7	l	0.35	0/852	0.49	0/1155
8	m	0.52	0/958	0.57	0/1284
9	p	0.51	0/714	0.58	0/958
10	q	0.54	0/643	0.59	0/862
11	r	0.43	0/628	0.61	0/847
12	s	0.49	0/440	0.45	0/594
13	u	0.52	0/669	0.53	0/892
14	v	0.30	0/392	0.48	0/528
All	All	0.59	0/36034	0.50	1/53890 (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
8	m	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	e	53	TYR	N-CA-C	-6.20	106.68	114.56

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	m	101	SER	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	2	19228	0	9654	137	0
1	4	3129	0	1579	32	0
2	c	1079	0	518	3	0
3	e	1592	0	1611	51	0
4	f	1129	0	1174	10	0
5	g	858	0	855	22	0
6	i	984	0	1047	20	0
7	l	836	0	850	19	0
8	m	945	0	998	13	0
9	p	704	0	712	11	0
10	q	632	0	646	7	0
11	r	621	0	665	12	0
12	s	434	0	453	7	0
13	u	663	0	715	10	0
14	v	389	0	318	2	0
15	2	53	0	0	0	0
15	4	6	0	0	0	0
16	4	40	0	43	0	0
All	All	33322	0	21838	332	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 332 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)
1:2:74:G:H1	1:2:93:A:N6	1.51	1.06
1:2:152:C:O2	1:2:161:G:N2	1.93	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:152:C:N3	1:2:161:G:N1	2.16	0.93
1:2:76:A:H2	1:2:91:G:H1	1.14	0.92
1:2:331:C:HO2'	1:2:332:A:H8	1.14	0.89

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	c	217/250 (87%)	195 (90%)	21 (10%)	1 (0%)	24	54
3	e	205/208 (99%)	163 (80%)	40 (20%)	2 (1%)	12	39
4	f	153/165 (93%)	147 (96%)	6 (4%)	0	100	100
5	g	101/127 (80%)	94 (93%)	7 (7%)	0	100	100
6	i	128/131 (98%)	118 (92%)	10 (8%)	0	100	100
7	l	112/128 (88%)	102 (91%)	10 (9%)	0	100	100
8	m	120/124 (97%)	111 (92%)	9 (8%)	0	100	100
9	p	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
10	q	78/83 (94%)	70 (90%)	8 (10%)	0	100	100
11	r	77/85 (91%)	69 (90%)	8 (10%)	0	100	100
12	s	51/75 (68%)	49 (96%)	2 (4%)	0	100	100
13	u	84/88 (96%)	83 (99%)	1 (1%)	0	100	100
14	v	58/71 (82%)	51 (88%)	7 (12%)	0	100	100
All	All	1470/1624 (90%)	1331 (90%)	136 (9%)	3 (0%)	44	72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	e	27	PRO
3	e	28	PHE
2	c	157	GLY

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	e	158/171 (92%)	136 (86%)	22 (14%)	3	11
4	f	113/120 (94%)	97 (86%)	16 (14%)	3	11
5	g	93/111 (84%)	83 (89%)	10 (11%)	6	21
6	i	108/109 (99%)	100 (93%)	8 (7%)	13	38
7	l	85/98 (87%)	67 (79%)	18 (21%)	1	4
8	m	104/106 (98%)	93 (89%)	11 (11%)	6	22
9	p	71/72 (99%)	65 (92%)	6 (8%)	10	31
10	q	62/63 (98%)	58 (94%)	4 (6%)	15	44
11	r	71/76 (93%)	66 (93%)	5 (7%)	14	40
12	s	47/66 (71%)	40 (85%)	7 (15%)	3	10
13	u	65/67 (97%)	64 (98%)	1 (2%)	57	84
14	v	21/62 (34%)	19 (90%)	2 (10%)	8	26
All	All	998/1121 (89%)	888 (89%)	110 (11%)	8	20

5 of 110 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	l	19	VAL
7	l	113	THR
14	v	55	ARG
11	r	49	ASP
7	l	33	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
6	i	53	GLN
13	u	68	HIS
7	l	118	ASN
13	u	75	HIS
13	u	3	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	890/1544 (57%)	183 (20%)	4 (0%)
1	4	145/1544 (9%)	30 (20%)	1 (0%)
All	All	1035/3088 (33%)	213 (20%)	5 (0%)

5 of 213 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	5	A
1	2	6	C
1	2	7	U
1	2	8	G
1	2	9	A

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	91	G
1	2	125	A
1	2	177	A
1	2	186	G
1	4	1490	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

Of 60 ligands modelled in this entry, 59 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
16	AKN	4	1607	-	41,42,42	1.98	9 (21%)	55,61,61	1.42	10 (18%)

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
16	AKN	4	1607	-	-	9/23/83/83	0/3/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	4	1607	AKN	C26-C24	-6.45	1.45	1.53
16	4	1607	AKN	C35-N12	6.30	1.47	1.34
16	4	1607	AKN	C22-C24	-4.29	1.48	1.53
16	4	1607	AKN	C24-N25	3.18	1.52	1.47
16	4	1607	AKN	O36-C35	-2.86	1.17	1.23

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	4	1607	AKN	C13-C11-N12	-4.55	103.82	110.78
16	4	1607	AKN	C19-C17-C16	3.01	115.22	109.11
16	4	1607	AKN	C39-C38-C37	-2.62	108.93	112.52
16	4	1607	AKN	C4-C5-C7	-2.46	105.77	110.23
16	4	1607	AKN	C5-C4-C3	-2.42	106.58	110.83

There are no chirality outliers.

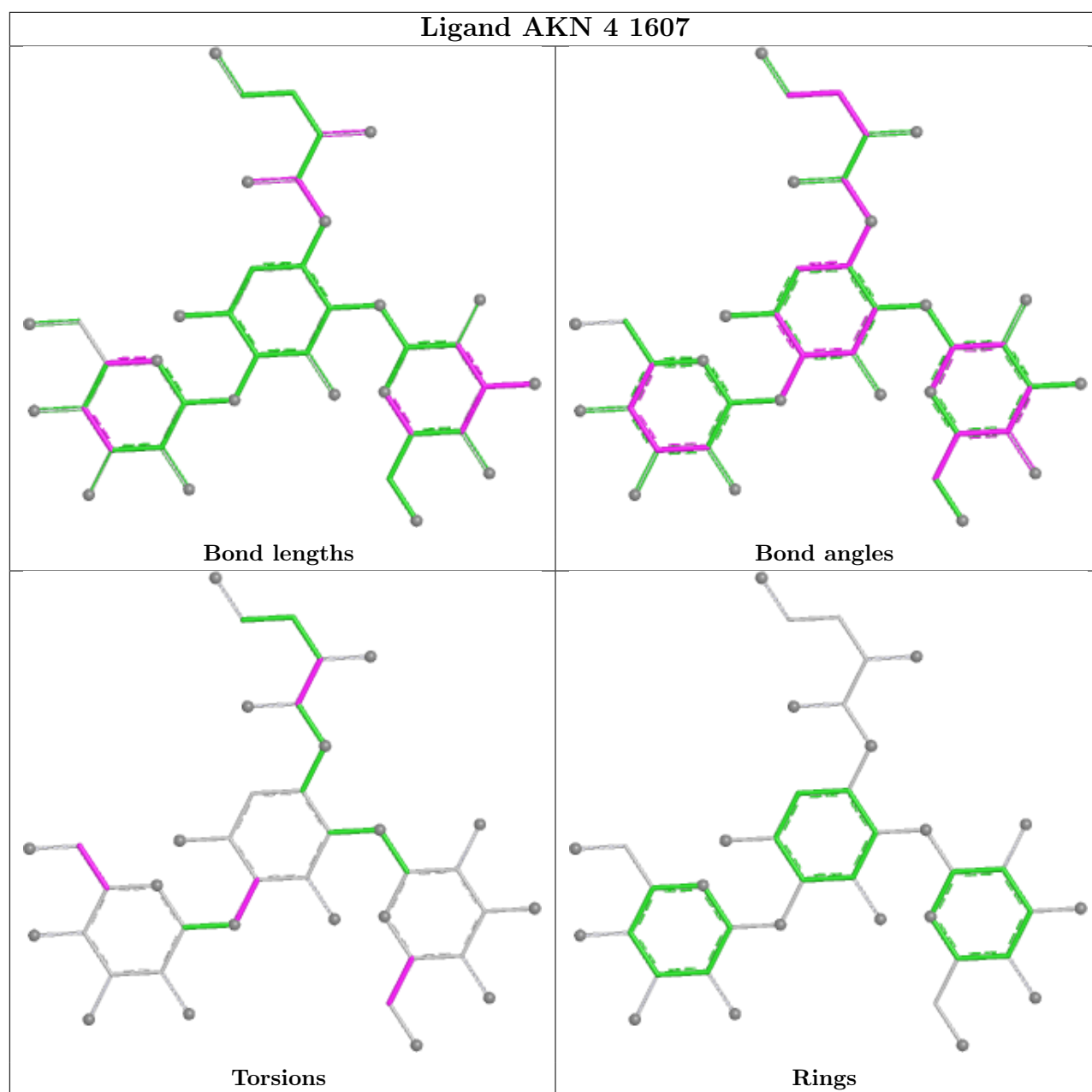
5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	4	1607	AKN	C5-C7-C9-N10
16	4	1607	AKN	O8-C7-C9-N10
16	4	1607	AKN	N12-C35-C37-O40
16	4	1607	AKN	O36-C35-C37-O40
16	4	1607	AKN	O29-C28-C30-O31

There are no ring outliers.

No monomer is involved in short contacts.

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.

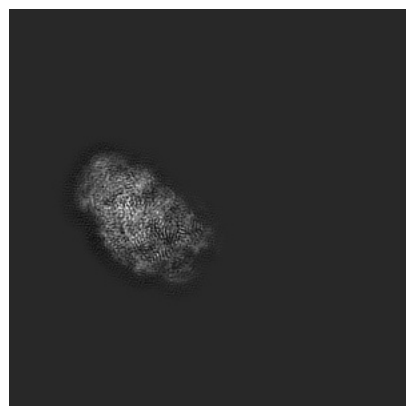
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10869. These allow visual inspection of the internal detail of the map and identification of artifacts.

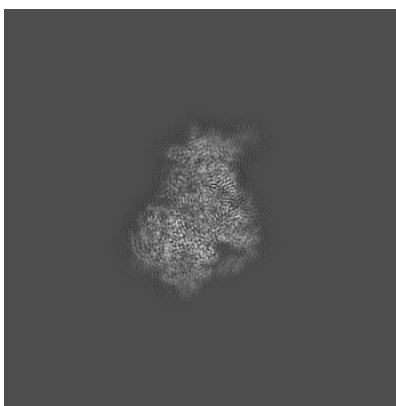
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

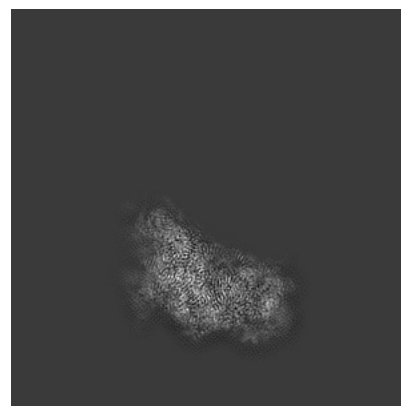
6.1.1 Primary map



X

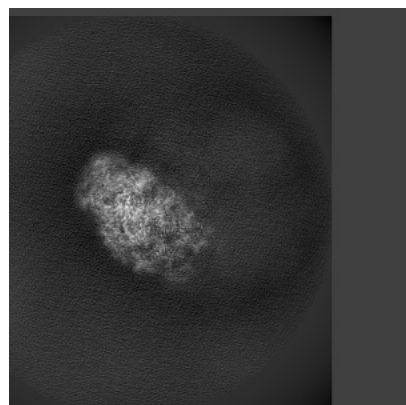


Y

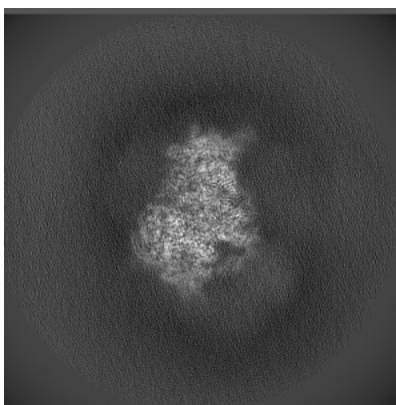


Z

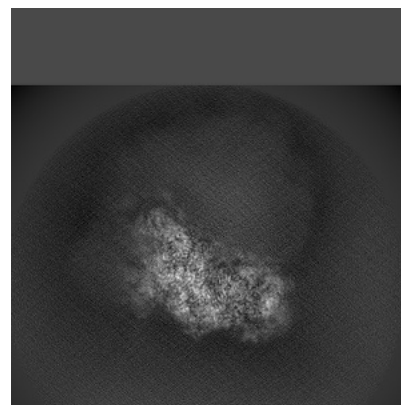
6.1.2 Raw map



X



Y

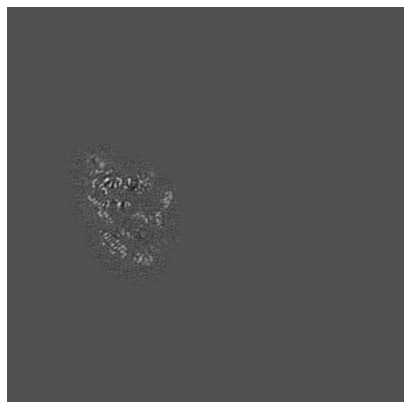


Z

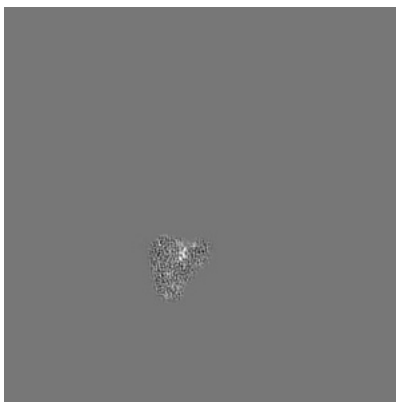
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

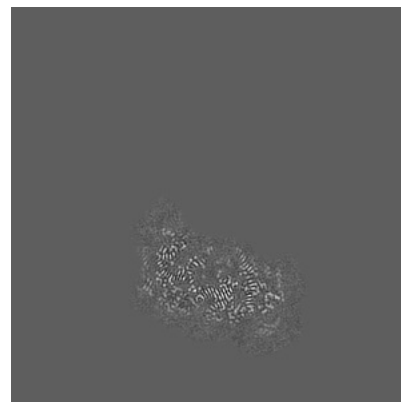
6.2.1 Primary map



X Index: 200

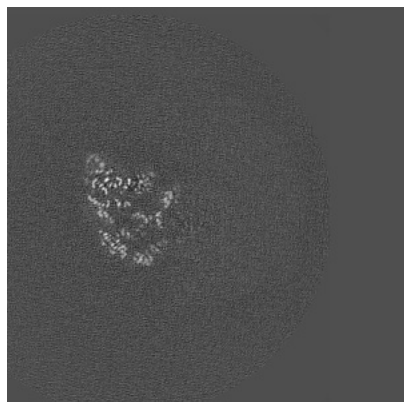


Y Index: 200

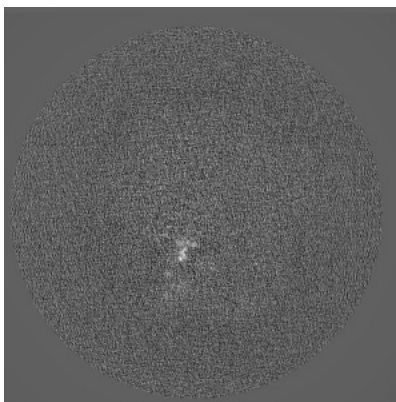


Z Index: 200

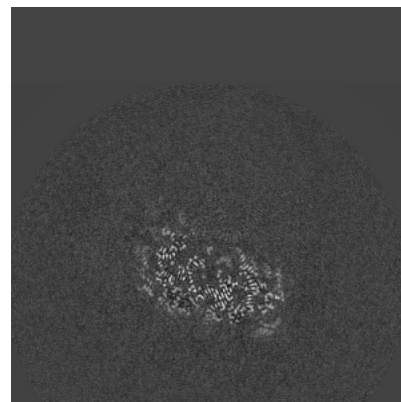
6.2.2 Raw map



X Index: 200



Y Index: 200

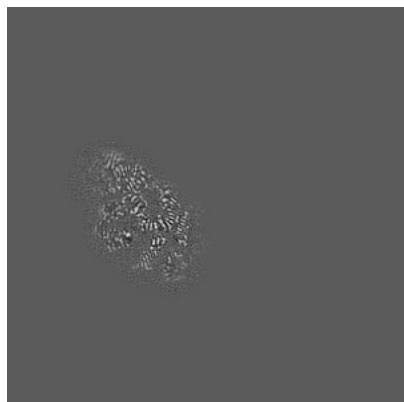


Z Index: 200

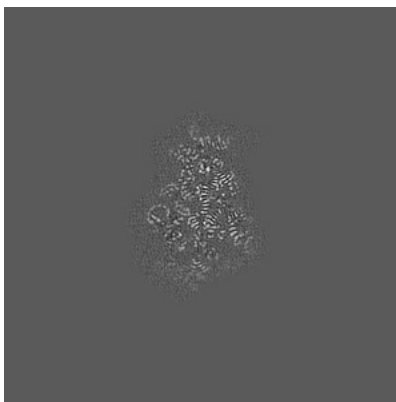
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

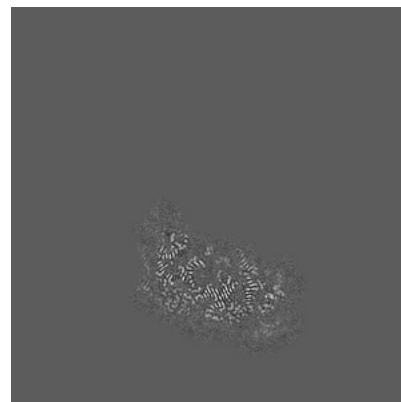
6.3.1 Primary map



X Index: 170

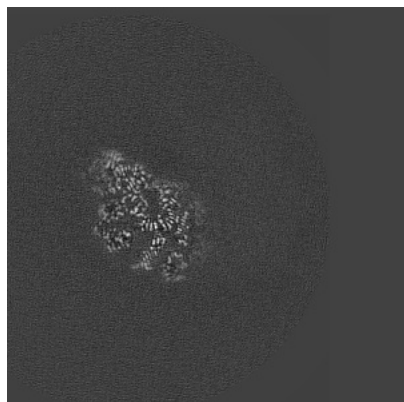


Y Index: 116

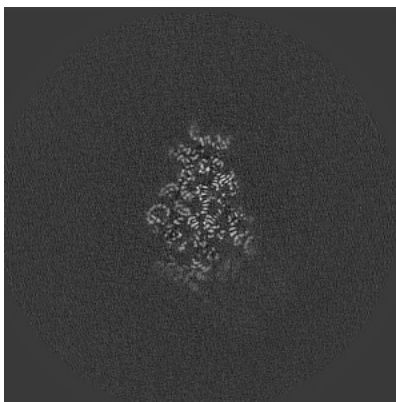


Z Index: 201

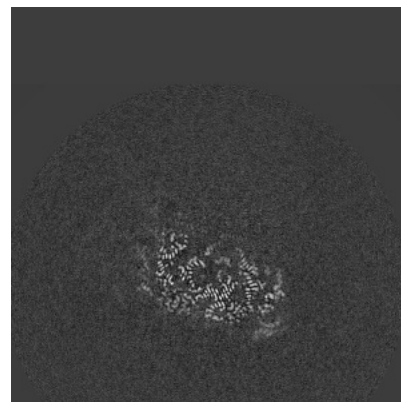
6.3.2 Raw map



X Index: 170



Y Index: 116

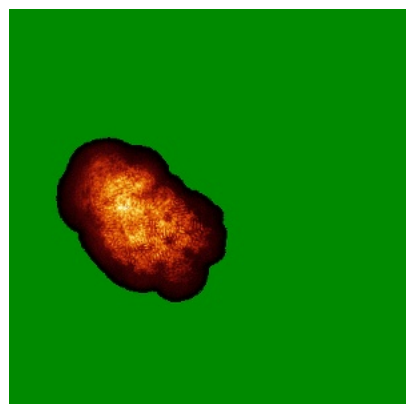


Z Index: 201

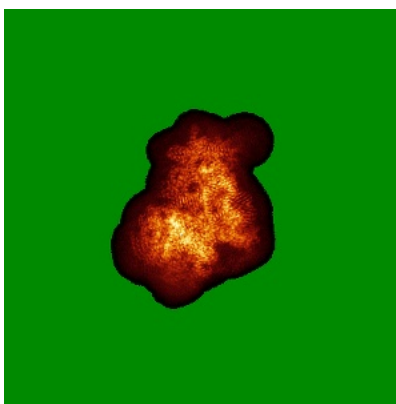
The images above show the largest variance slices of the map in three orthogonal directions.

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

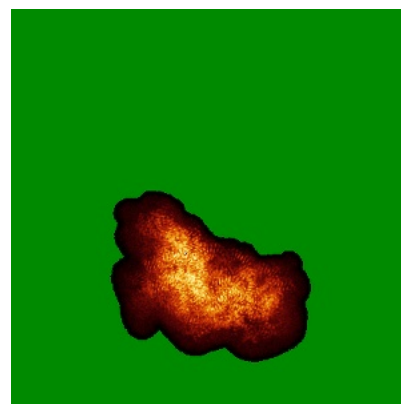
6.4.1 Primary map



X

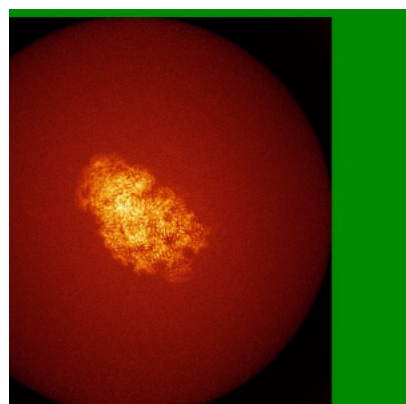


Y

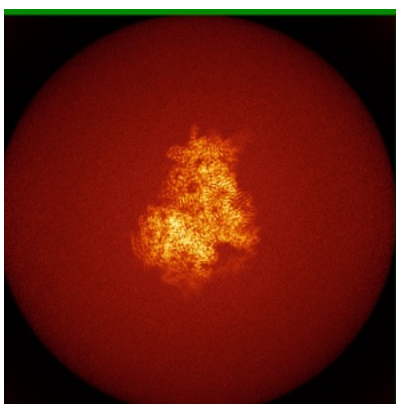


Z

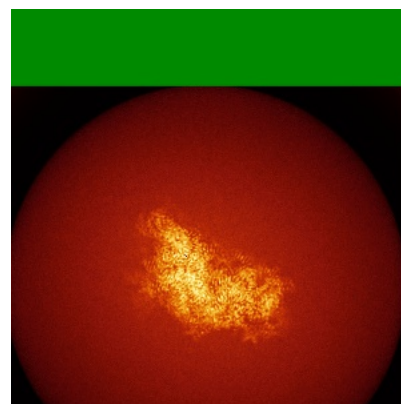
6.4.2 Raw map



X



Y

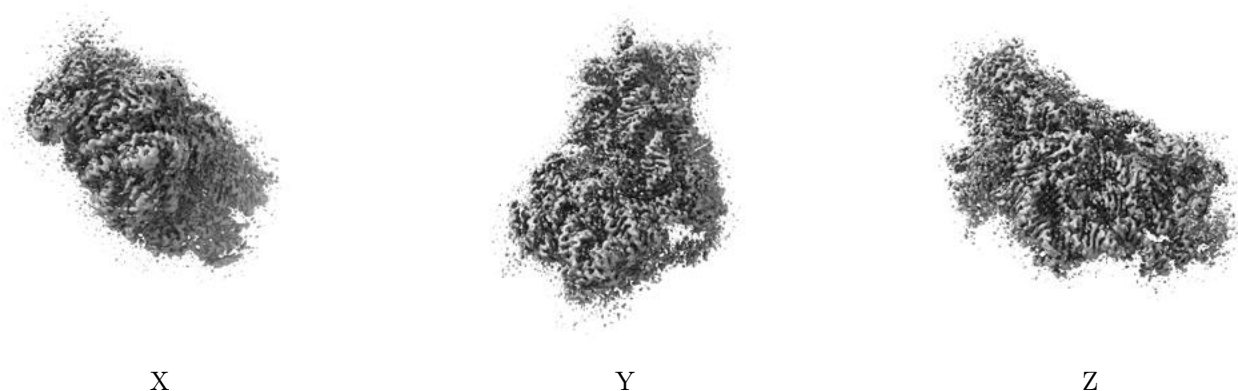


Z

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.

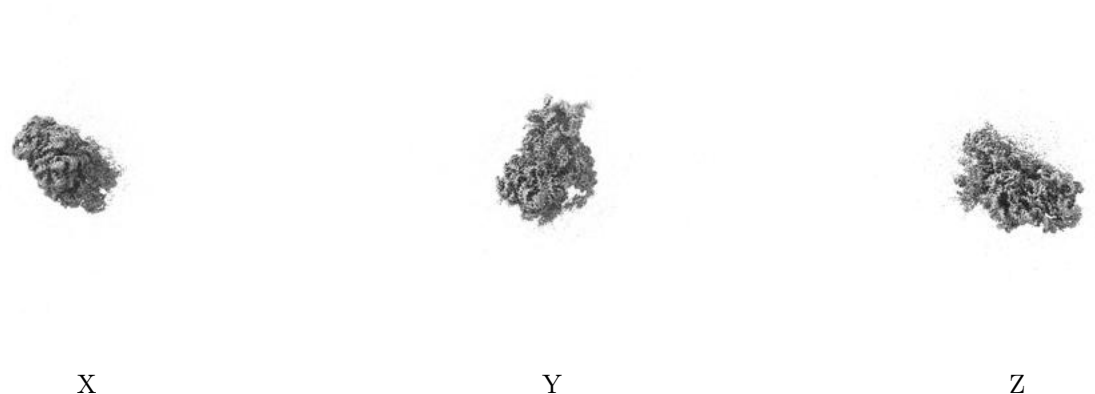
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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



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.

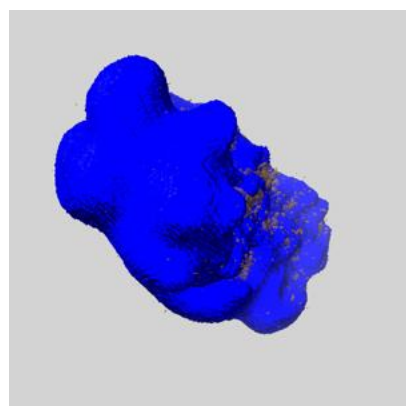
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

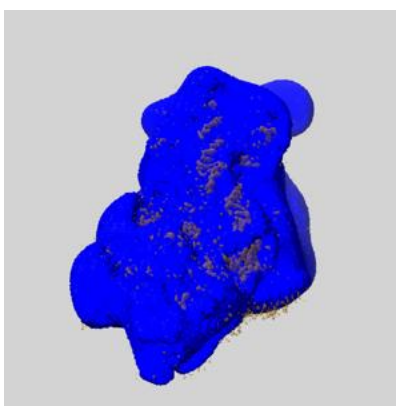
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

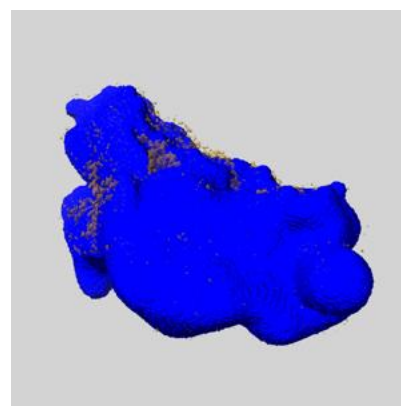
6.6.1 emd_10869_msk_1.map [i](#)



X



Y

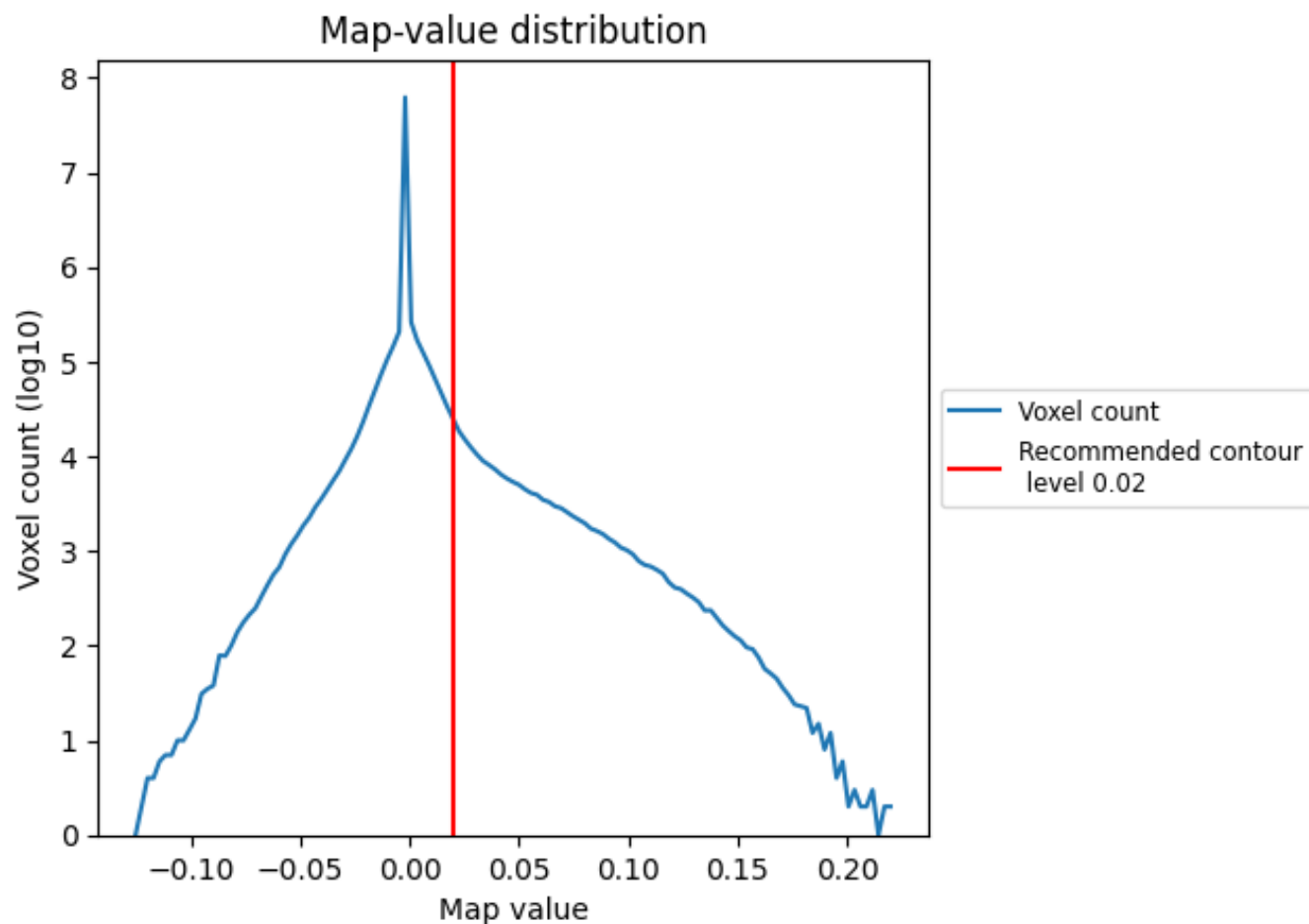


Z

7 Map analysis [i](#)

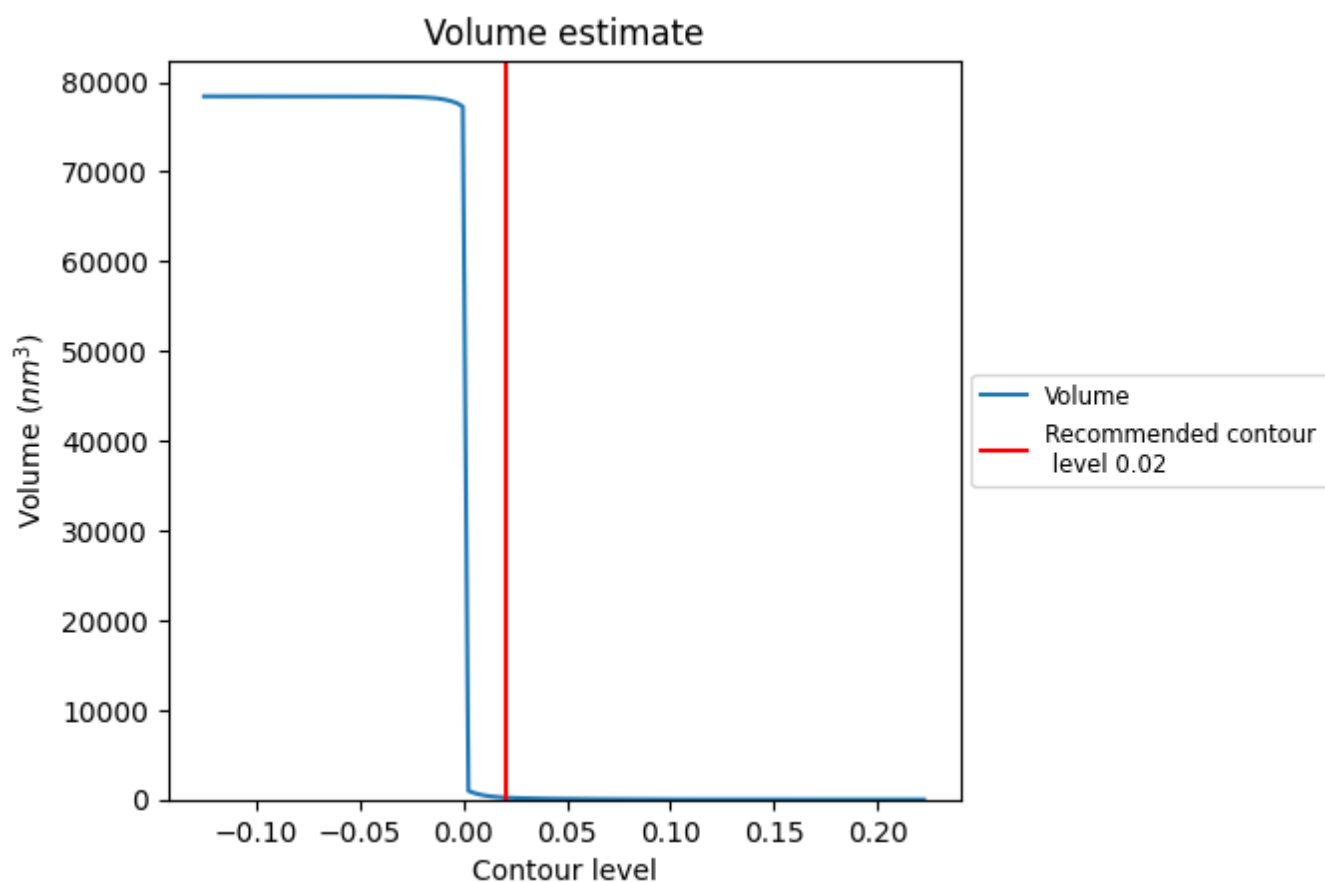
This section contains the results of statistical analysis of the map.

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.

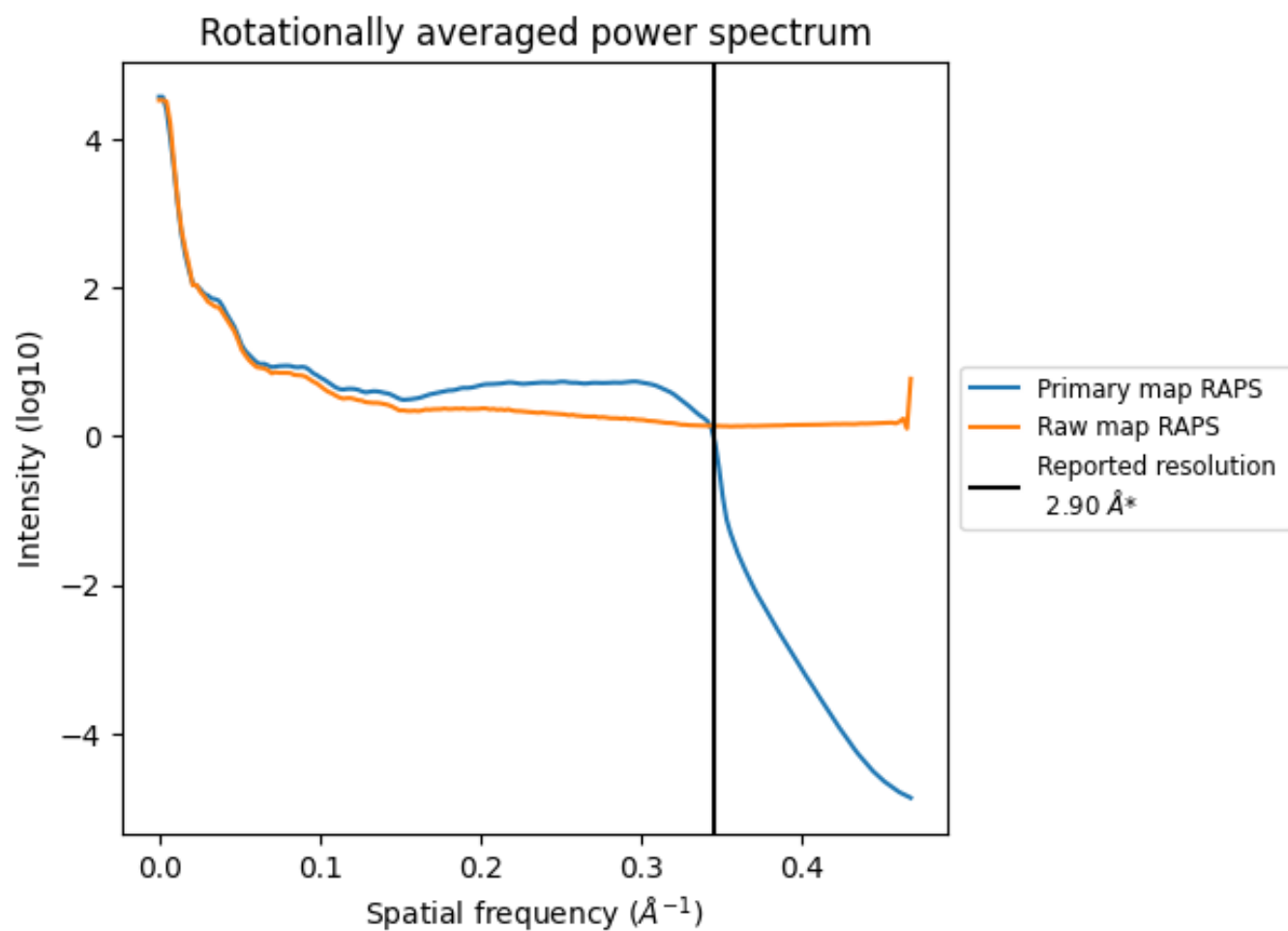
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 220 nm^3 ; this corresponds to an approximate mass of 198 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 ⓘ

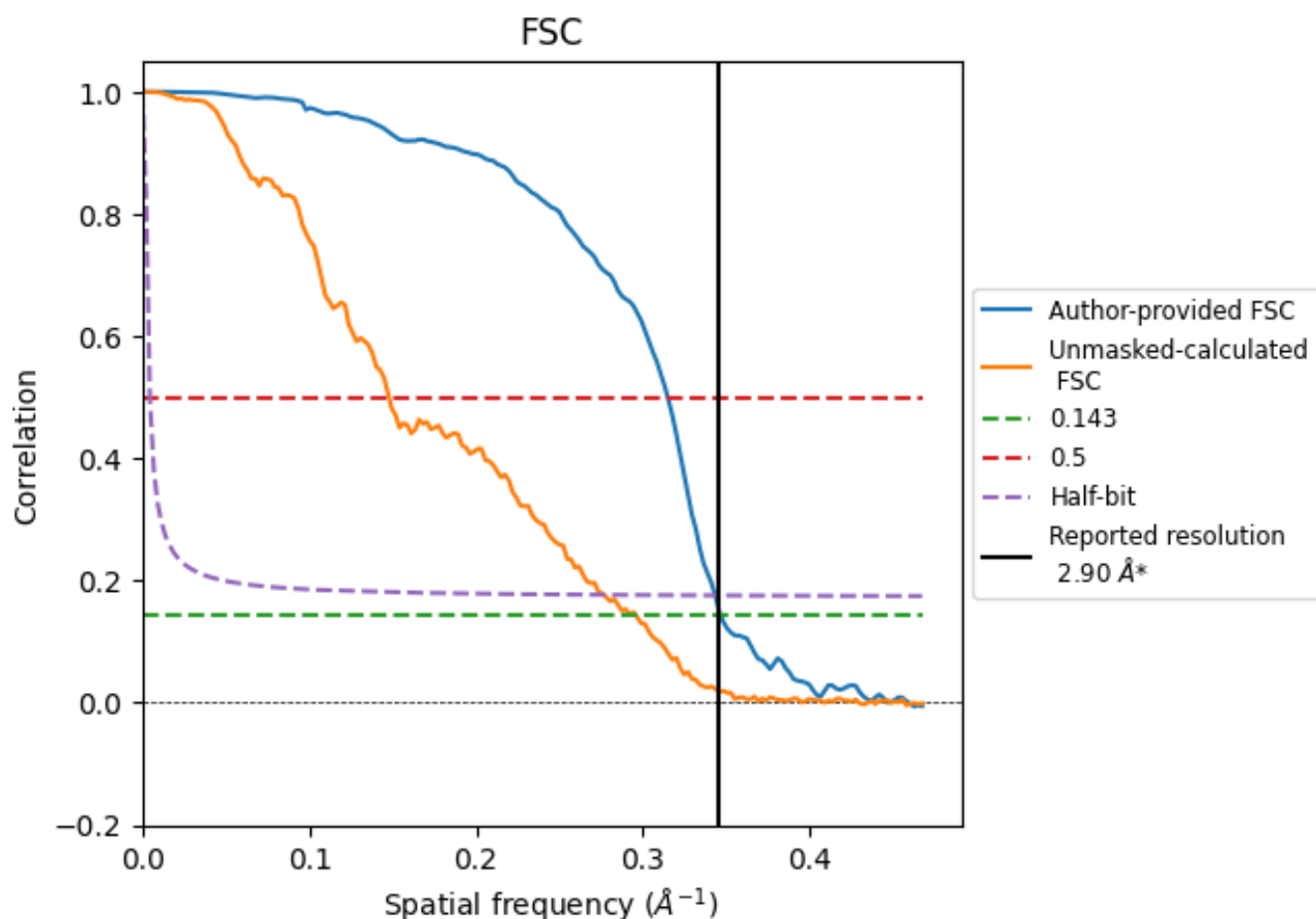


*Reported resolution corresponds to spatial frequency of $0.345 \text{ \AA}^{-1}$

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 0.345 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

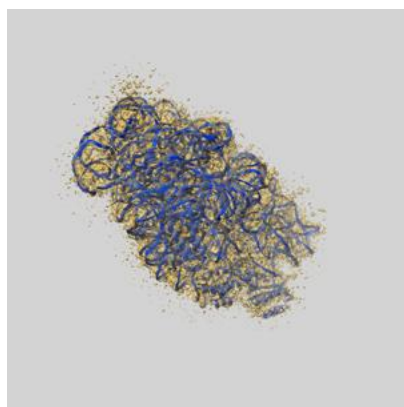
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.89	3.18	2.91
Unmasked-calculated*	3.38	6.76	3.62

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.38 differs from the reported value 2.9 by more than 10 %

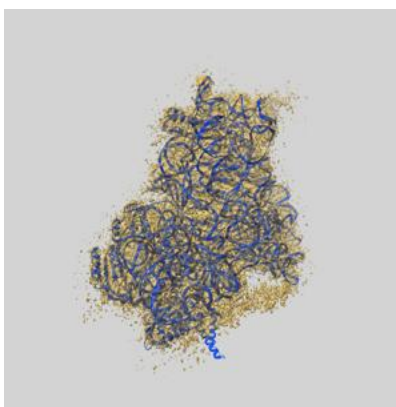
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10869 and PDB model 6YPU. Per-residue inclusion information can be found in section [3](#) on page [7](#).

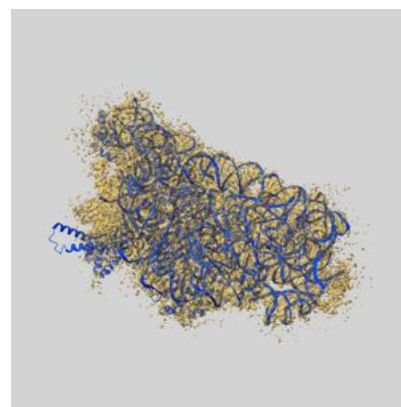
9.1 Map-model overlay [i](#)



X



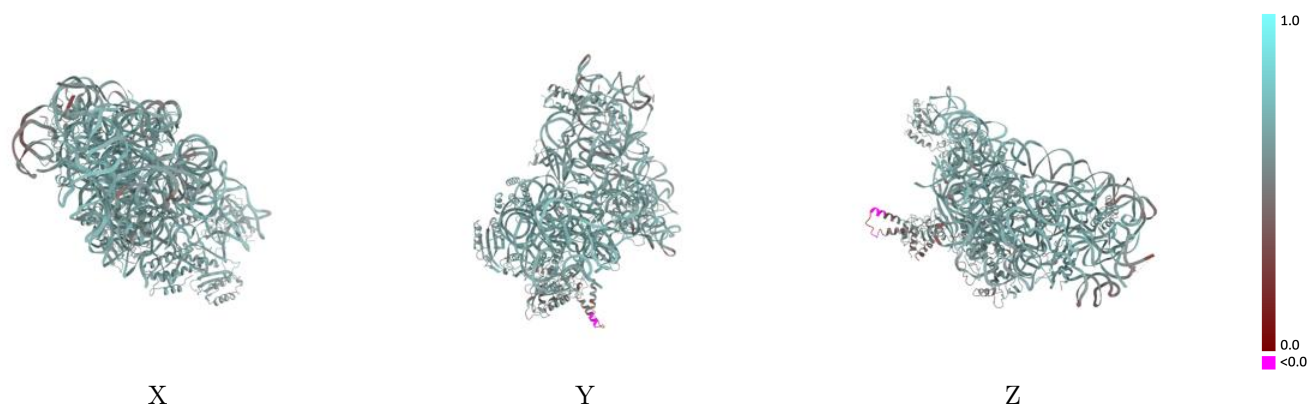
Y



Z

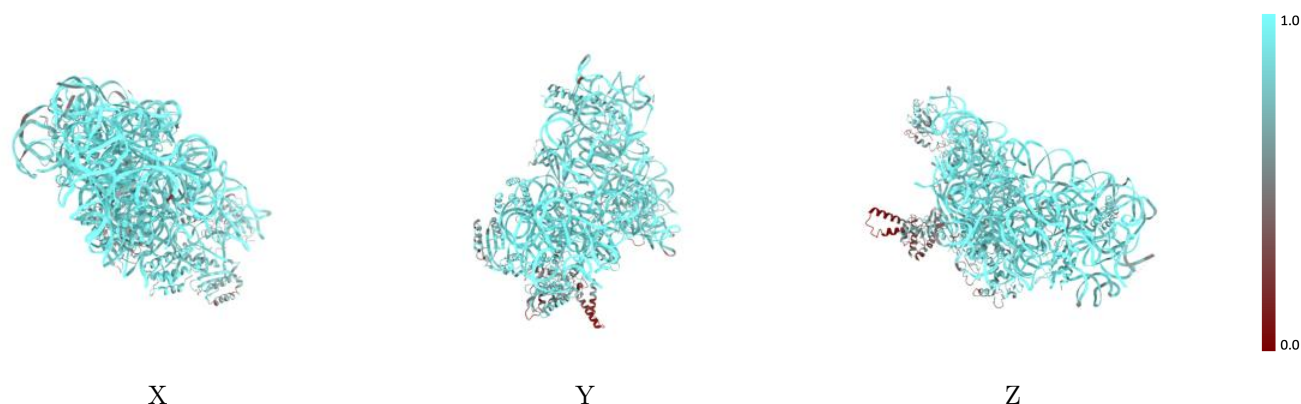
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



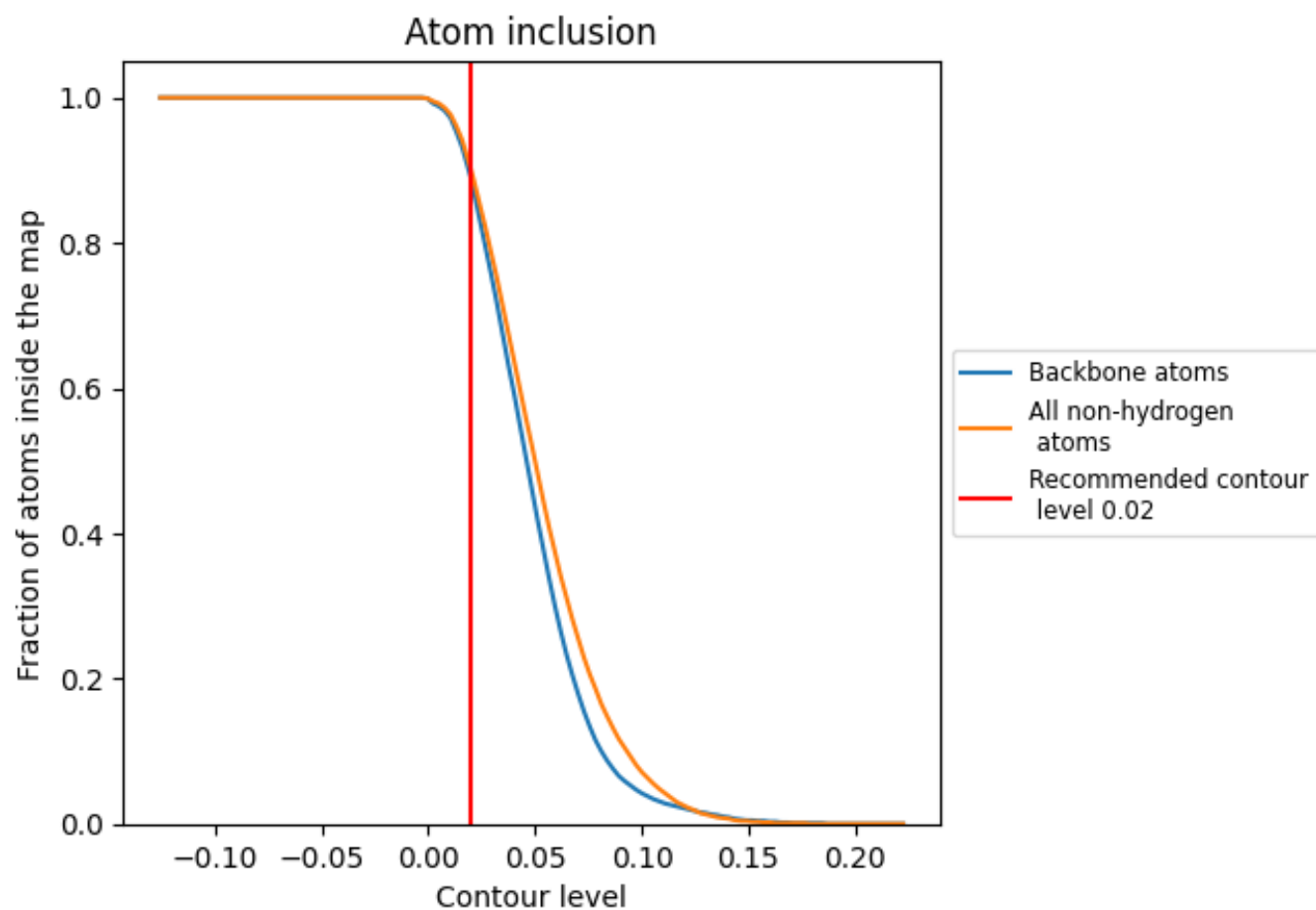
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 90% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9020	0.6110
2	0.9610	0.6260
4	0.9250	0.6020
c	0.3990	0.4520
e	0.7570	0.5570
f	0.8930	0.6210
g	0.7340	0.5800
i	0.9020	0.6240
l	0.7580	0.5740
m	0.9040	0.6290
p	0.8930	0.6190
q	0.9260	0.6320
r	0.8340	0.5880
s	0.8690	0.6130
u	0.9060	0.6230
v	0.6010	0.5730

1.0

0.0

<0.0