



wwPDB EM Validation Summary Report ⓘ

Mar 7, 2026 – 12:52 AM UTC

PDB ID : 9ARL / pdb_00009arl
EMDB ID : EMD-43786
Title : CryoEM structure of BoNT-NTNH-OrfX2 complex from Clostridium botulinum strain A1-ST7B, major class
Authors : Gao, L.
Deposited on : 2024-02-23
Resolution : 4.00 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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

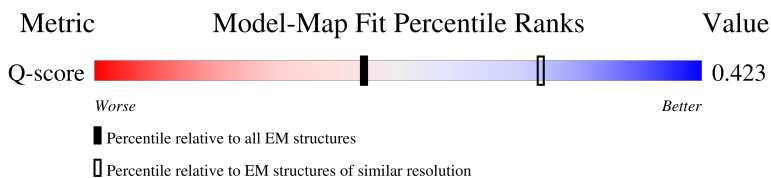
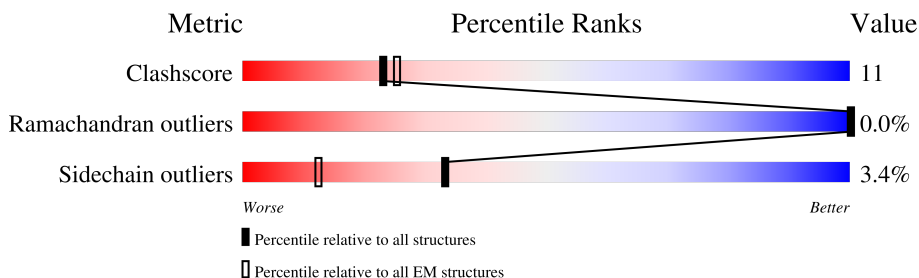
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7587 (3.50 - 4.50)

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

Mol	Chain	Length	Quality of chain
1	A	1296	
2	B	1161	
3	C	750	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24054 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 Botulinum neurotoxin type A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1275	Total	C	N	O	S	0	0
			10336	6634	1704	1965	33		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	224	GLN	GLU	engineered mutation	UNP P0DPI1
A	363	ALA	ARG	engineered mutation	UNP P0DPI1
A	366	PHE	TYR	engineered mutation	UNP P0DPI1

- Molecule 2 is a protein called NtnH.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1147	Total	C	N	O	S	0	0
			9349	6013	1485	1820	31		

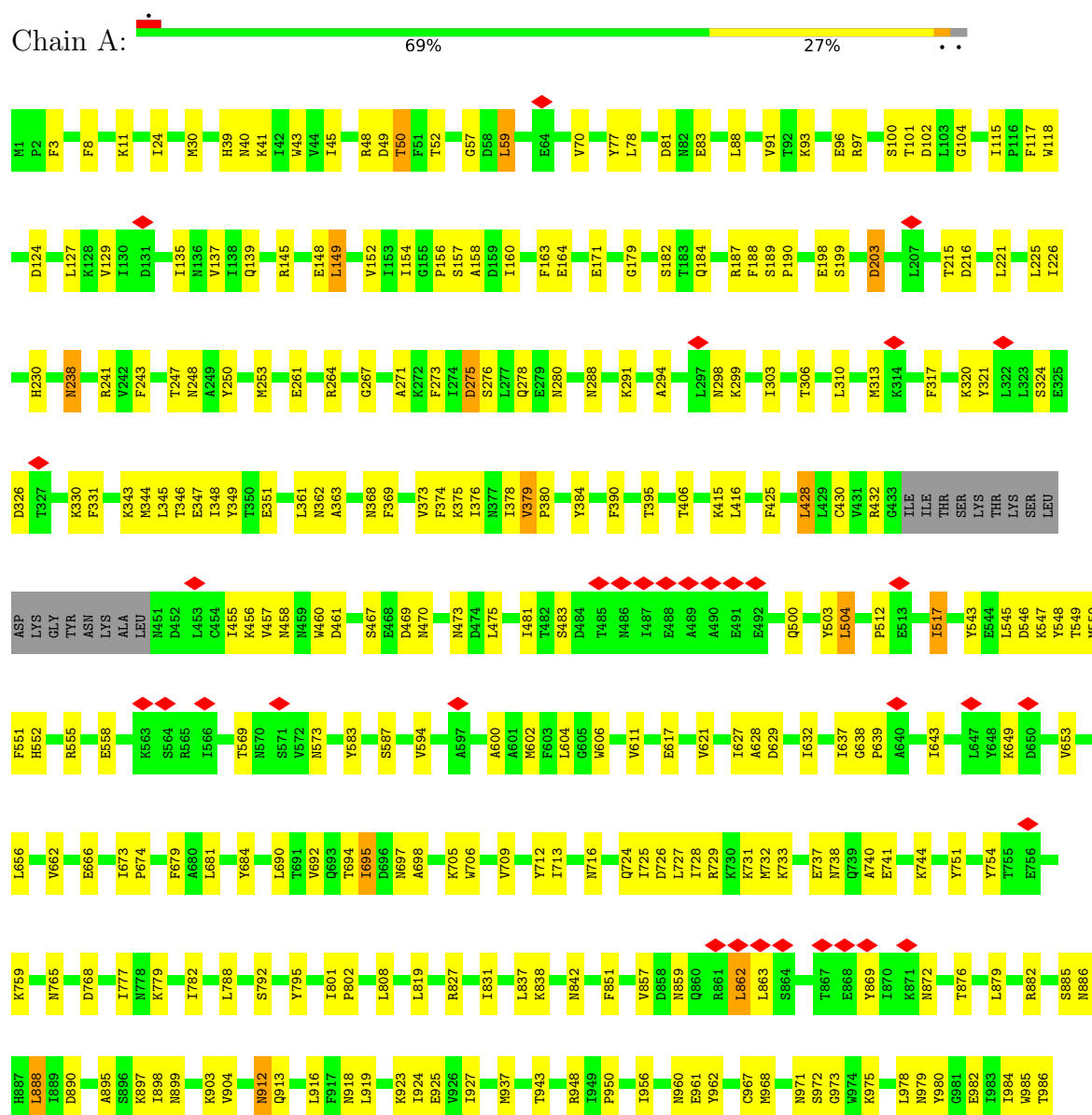
- Molecule 3 is a protein called OrfX2.

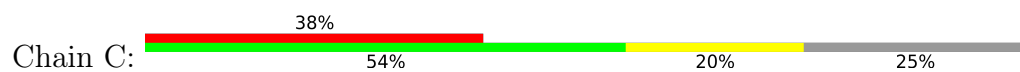
Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	561	Total	C	N	O	S	0	0
			4369	2766	735	861	7		

3 Residue-property plots [i](#)

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: Botulinum neurotoxin type A





MET
ASN
GLY
SER
LEU
LYS
PRO
PHE
ILE
TYR
LYS
TYR
ASP
ASN
ILE
TRP
GLU
LYS
THR
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TYR
LEU
LYS
ASN
MET
THR
LYS
PHE
GLY
ALA
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ASP
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G168
D169
L170
S171
L172
L173
G174
F183
M186
N187

LYS
ASP
ASN
SER
SER
LYS
ILE
SER
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ASN
ASP
ILE
LEU
LEU
ASP
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TYR
TYR
ASN
LYS
LEU
LEU
ASP
LYS
P236
Y242
D243
S251
E25A
L258
L259
D262
L263
F266
D267
S268
L272
N273
T276
G277
E278
N279
D280
G281
K282
Q283
F284
N285
L286
T290
ASN
ASP
ASP
LYS
LYS

L190
R207
T212
D218
T223
G225
A226
D227
G228
R229
W230
I231
R232
P236
Y242
D243
S251
E25A
L258
L259
D262
L263
F266
D267
S268
L272
N273
T276
G277
E278
N279
D280
G281
K282
Q283
F284
N285
L286
T290
ASN
ASP
ASP
LYS
LYS

R297
V298
L299
I300
T301
T302
Y303
G310
D316
K317
D318
I332
E336
Q337
I338
F339
A340
Y341
I342
L343
L344
D345
E346
T347
A348
K349
I350
P351
E352
Y353
Q354
W355
L356
K357
P358
T359
Q360
I361
S362
Y363
S367
A371
N372
D373
E374
P375
D376
L377
I381
A384
V388

E389
N390
N391
T392
N393
S394
T395
P396
S397
H398
V400
D401
M402
R403
R404
L405
Q406
D407
T408
A413
I416
S417
F418
P419
L420
F421
I422
E423
M424
F425
L426
K427
Q428
A429
L430
L431
S432
S433
Q434
F435
I436
S437
V438
D439
D440
I441
V442
A443
D444
I445
M446
T447
L448
T449
I450
T451
M452

M453
K454
Q455
I456
I457
F458
Q459
K460
V461
E462
M463
S464
D465
Q466
K467
N468
V469
D470
S471
S472
L473
K474
P475
G476
K477
L478
K479
L480
S481
L482
Q483
N484
M485
L486
I487
V488
L489
E490
L491
F492
D493
L494
T495
W496
E497
Q498
Q499
R500
G501
V502
T503
G504
H505
F506
D507
R508
R509
Q510
E511
Y512

E513
I514
A515
L516
K519
S520
G521
I526
L527
K528
V529
H530
D531
E532
P533
E534
I535
E536
Y537
Y538
V539
E540
E541
A542
Q543
W544
K545
T546
N547
E548
D549
M550
I551
V552
S553
A554
V555
V556
G557
T558
V559
F560
S561
M562
S567
M568
K569
L570
A571
G572
S573
A574
L575
S576
K577
G579

K580
L581
I582
R583
S584
K585
A586
T587
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Y596
I597
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R618
I619
N620
R621
R622
N623
S624
S625
I626
A627
A628
E629
R632
L633
I634
S635
N636
N637
G638
T639
T640

S641
I642
Q643
T644
L645
G646
D647
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K650
K651
P652
M653
S654
T655
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I659
A660
I661
G662
A663
K664
K665
I666
A667
G668
T669
A670
V671
V676
G677
LEU
GLY
MET
N681
F682
I687
I690
M693
E694
N695
N696
D697
Y698
S699
A700
I701
P702
Q709
I710
C711
I712
G713

D719
LYS
ASP
SER
GLU
L724
T727
L741
GLU
LYS
ASN
ASN
LYS
THR
ASP
ASN
LYS

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	135181	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.407	Depositor
Minimum map value	-0.223	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.05	Depositor
Map size ($\text{\AA}$)	403.456, 403.456, 403.456	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.788, 0.788, 0.788	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.16	0/10556	0.29	0/14298
2	B	0.17	0/9549	0.28	0/12956
3	C	0.09	0/4443	0.25	0/6008
All	All	0.16	0/24548	0.28	0/33262

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10336	0	10182	235	0
2	B	9349	0	9070	204	0
3	C	4369	0	4292	98	0
All	All	24054	0	23544	526	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.

The worst 5 of 526 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:B:848:LEU:O	2:B:979:PRO:HA	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1239:LEU:HD12	1:A:1247:ILE:HD11	1.63	0.79
3:C:533:PRO:HD2	3:C:602:VAL:HG11	1.65	0.78
1:A:1117:TYR:HD1	1:A:1278:LEU:HD11	1.53	0.73
1:A:1278:LEU:HD12	1:A:1278:LEU:C	2.13	0.73

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	
1	A	1269/1296 (98%)	1226 (97%)	42 (3%)	1 (0%)	48	81
2	B	1139/1161 (98%)	1084 (95%)	55 (5%)	0	100	100
3	C	553/750 (74%)	547 (99%)	6 (1%)	0	100	100
All	All	2961/3207 (92%)	2857 (96%)	103 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1278	LEU

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	A	1147/1177 (98%)	1100 (96%)	47 (4%)	27	49
2	B	1055/1093 (96%)	1015 (96%)	40 (4%)	29	51
3	C	474/667 (71%)	470 (99%)	4 (1%)	73	77
All	All	2676/2937 (91%)	2585 (97%)	91 (3%)	33	55

5 of 91 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	243	LEU
2	B	637	LEU
2	B	326	HIS
2	B	452	VAL
2	B	800	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	895	ASN
3	C	498	GLN
2	B	1149	ASN
3	C	331	ASN
2	B	80	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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 ⓘ

There are no ligands in this entry.

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.

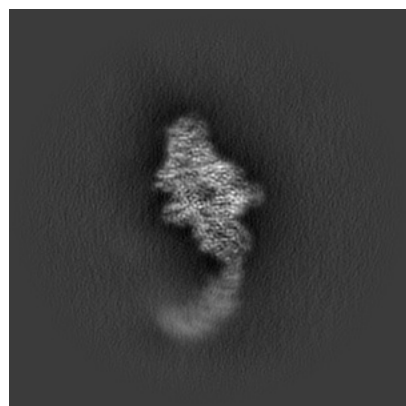
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43786. These allow visual inspection of the internal detail of the map and identification of artifacts.

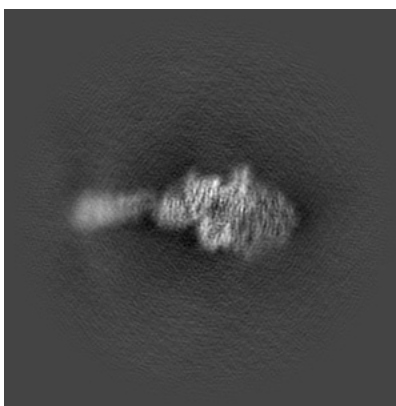
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

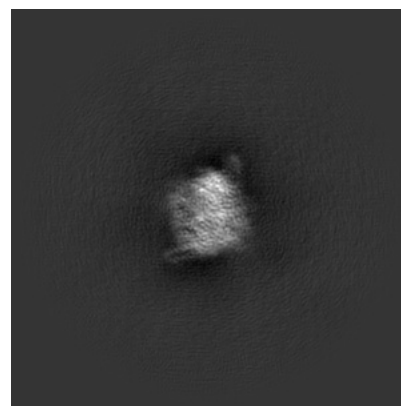
6.1.1 Primary map



X

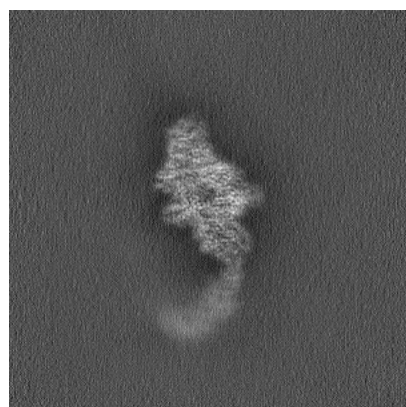


Y

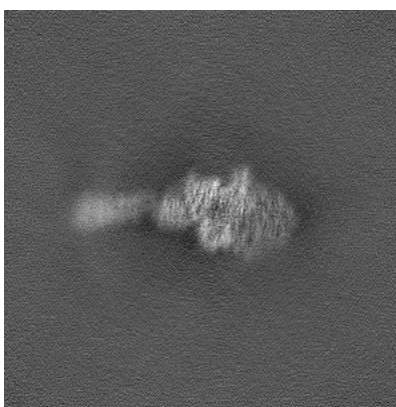


Z

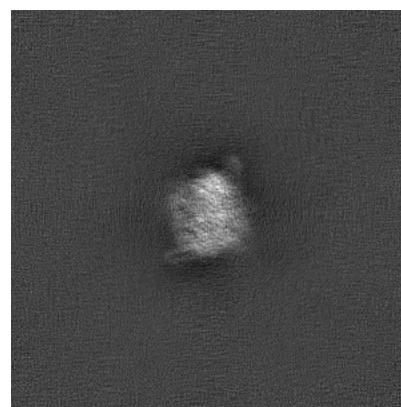
6.1.2 Raw map



X



Y

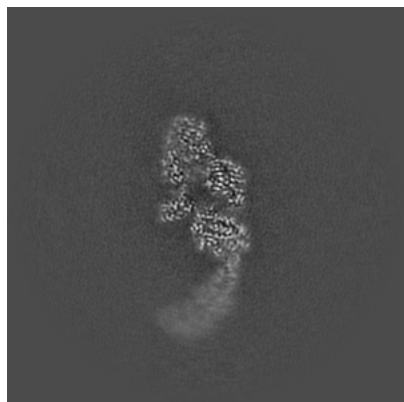


Z

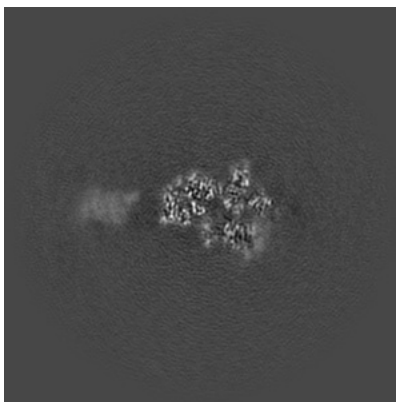
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

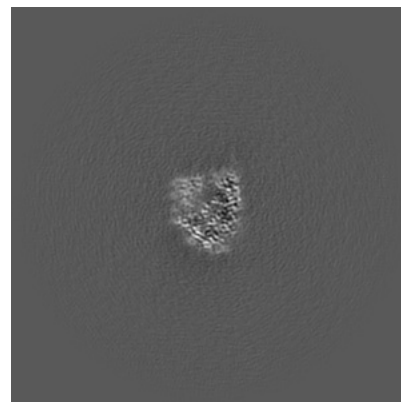
6.2.1 Primary map



X Index: 256



Y Index: 256

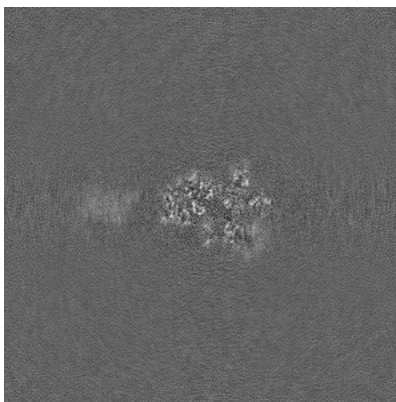


Z Index: 256

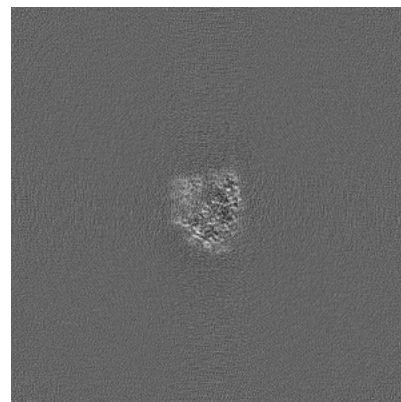
6.2.2 Raw map



X Index: 256



Y Index: 256



Z Index: 256

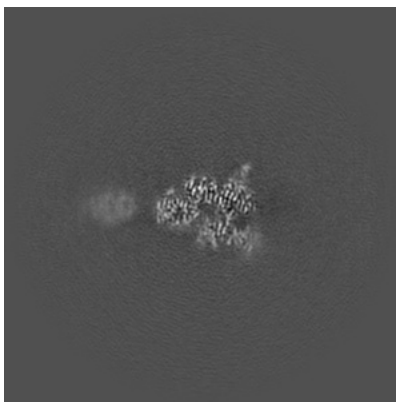
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

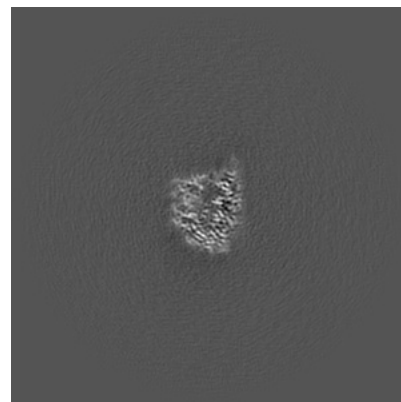
6.3.1 Primary map



X Index: 255



Y Index: 266

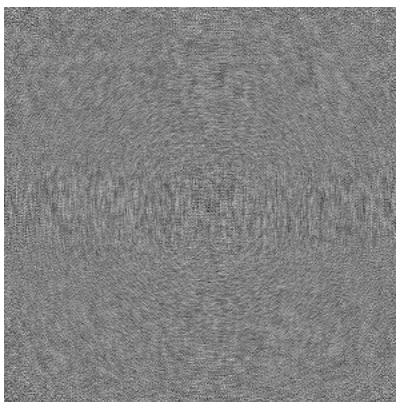


Z Index: 258

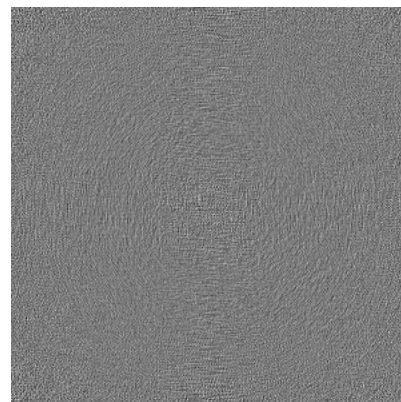
6.3.2 Raw map



X Index: 255



Y Index: 0

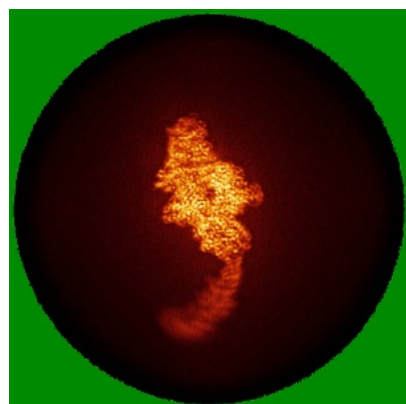


Z Index: 511

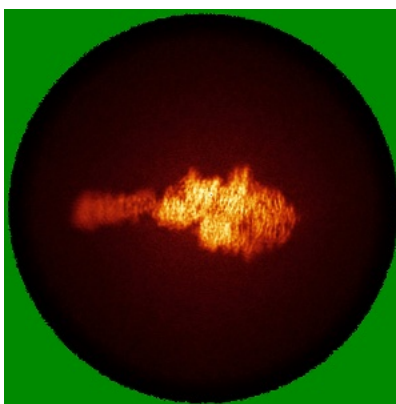
The images above show the largest variance slices of the map in three orthogonal directions.

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

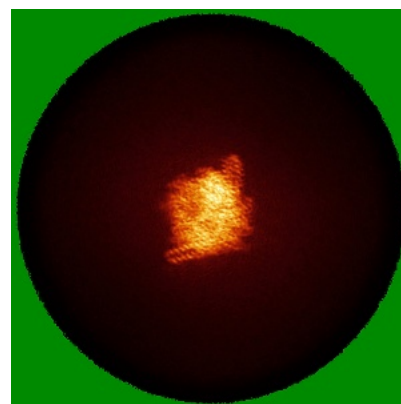
6.4.1 Primary map



X

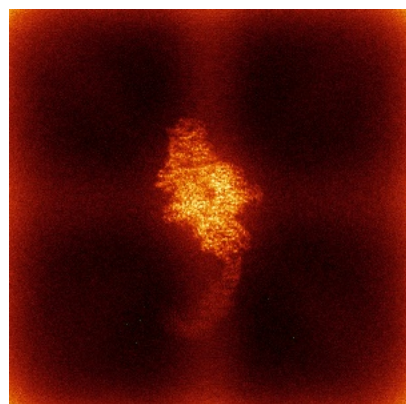


Y

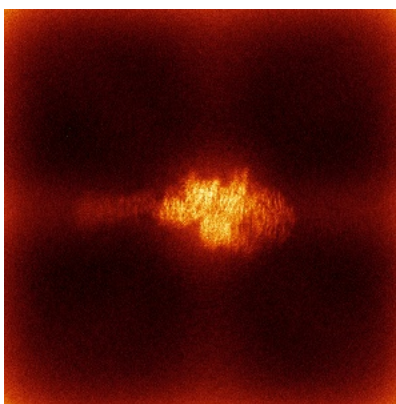


Z

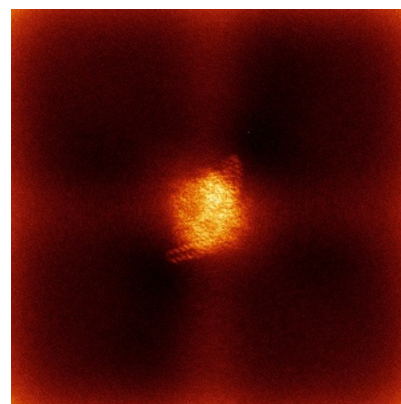
6.4.2 Raw map



X



Y

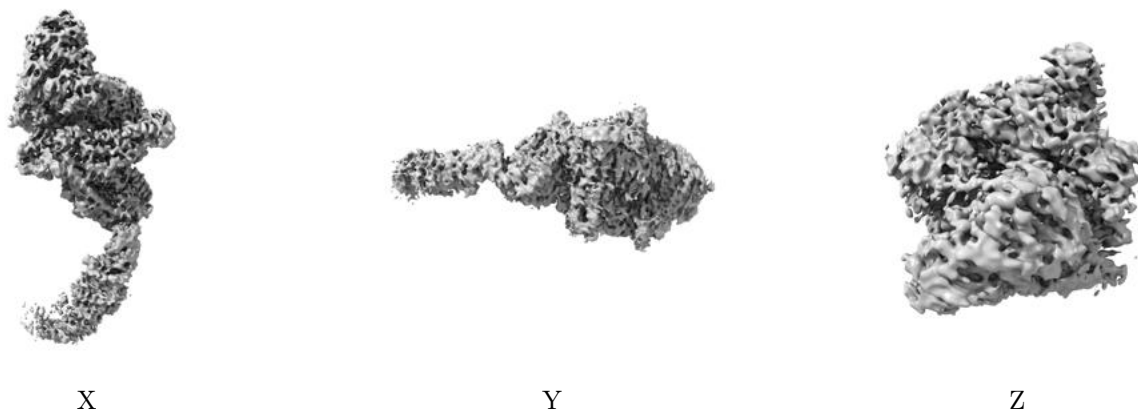


Z

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.

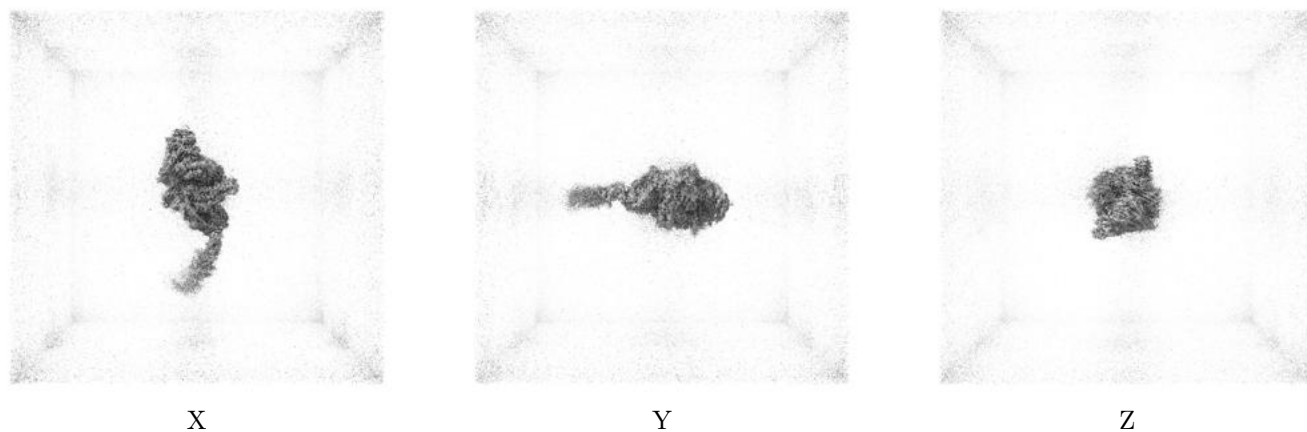
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. 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.

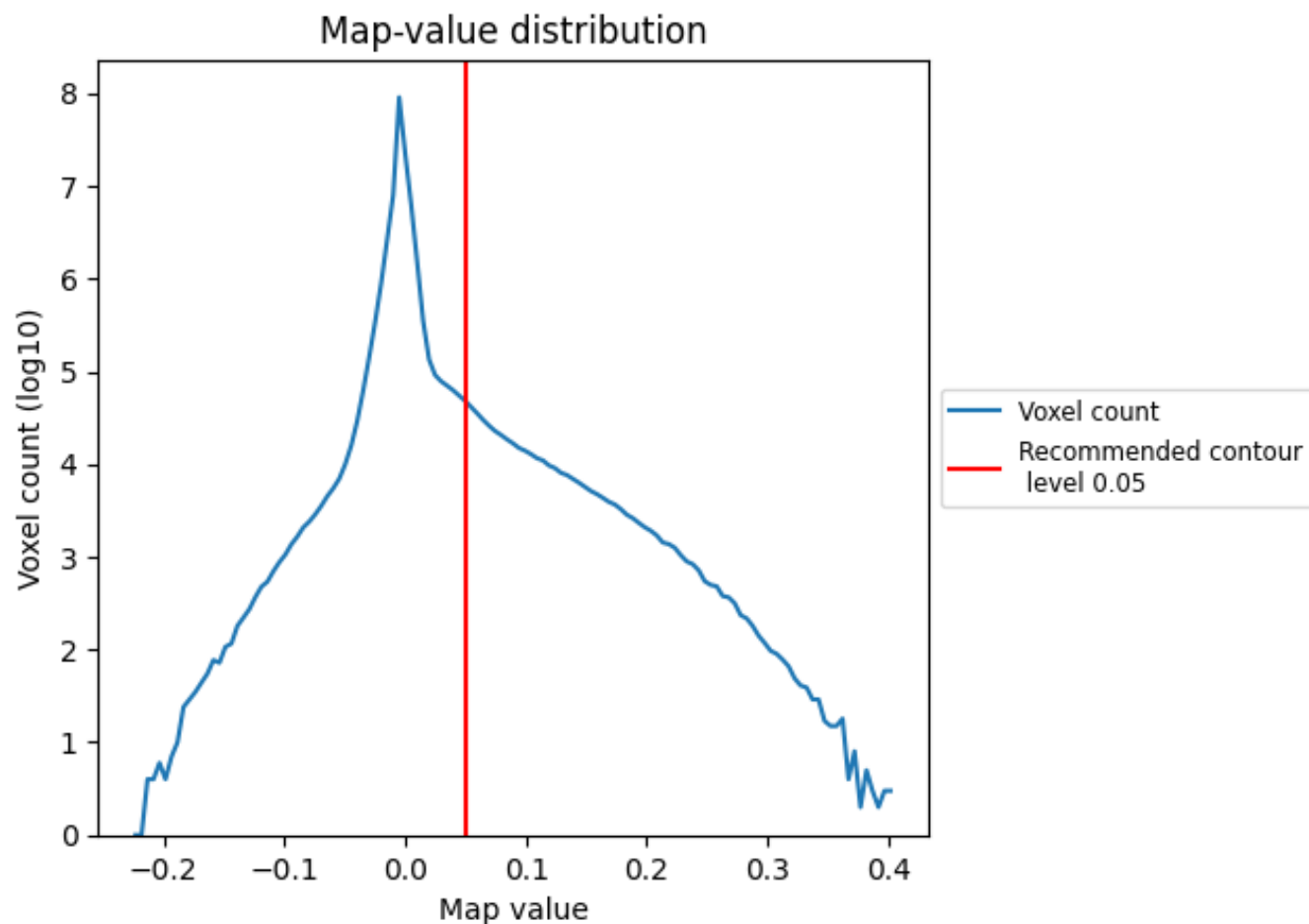
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

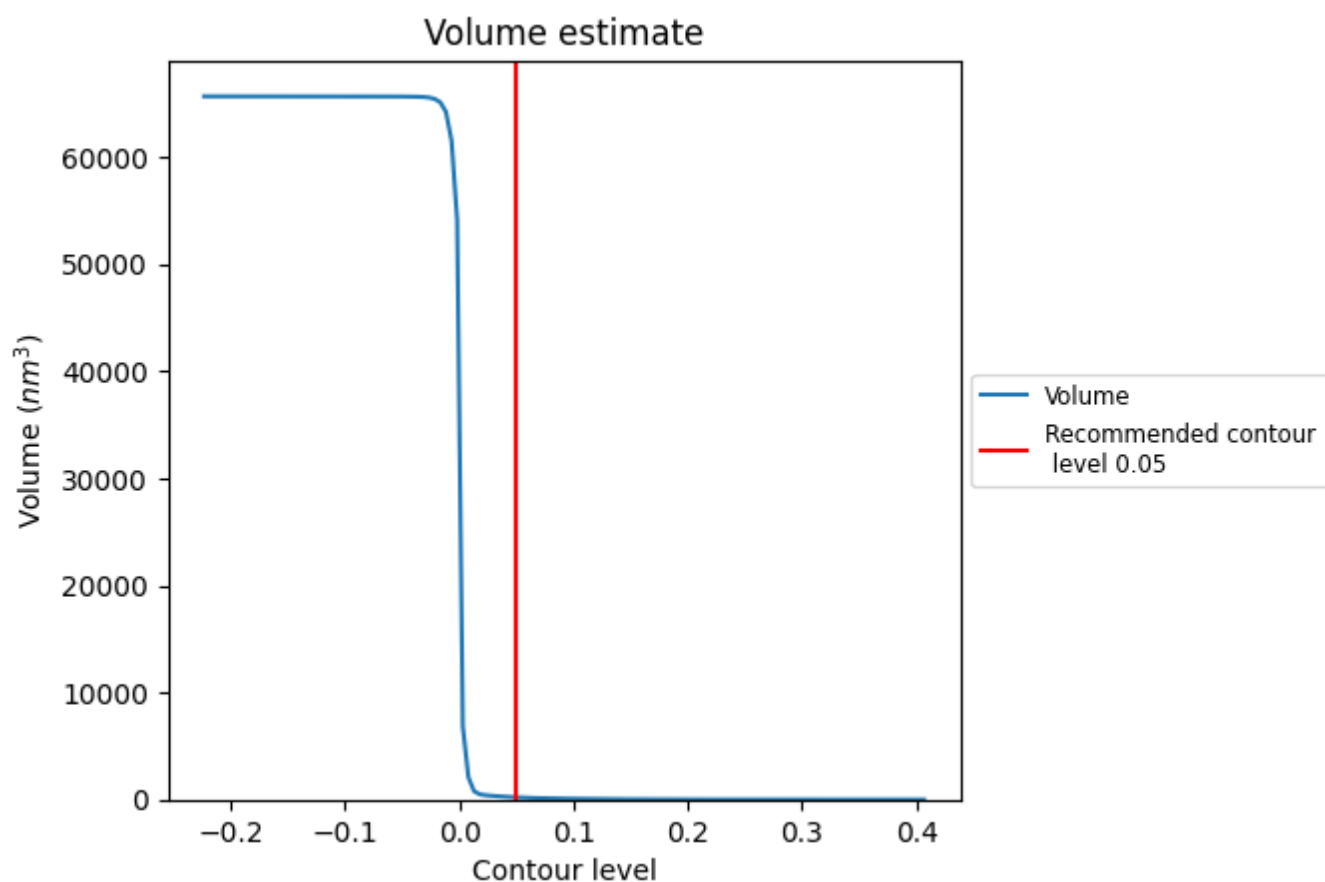
This section contains the results of statistical analysis of the map.

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.

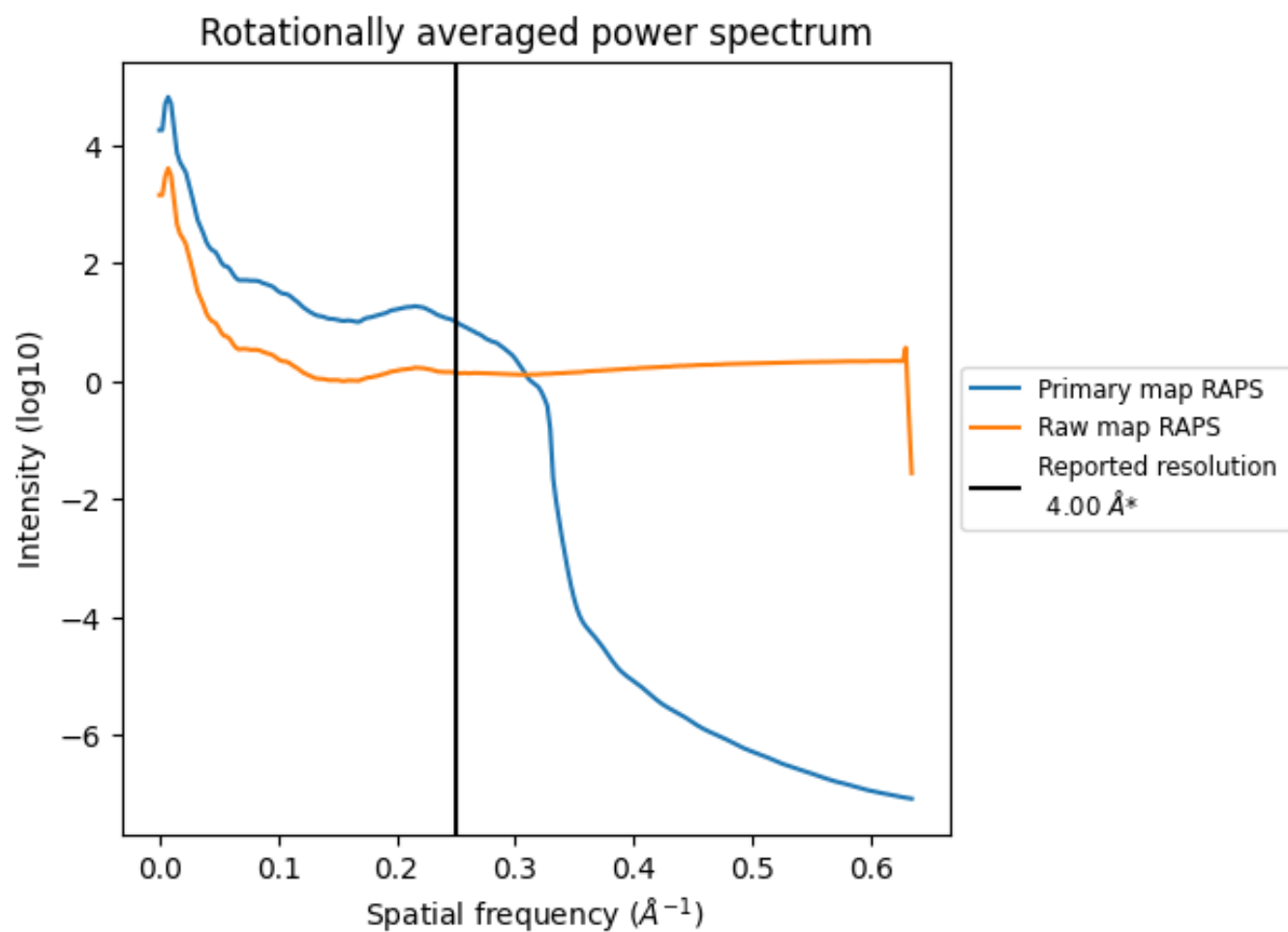
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 208 nm^3 ; this corresponds to an approximate mass of 188 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 ⓘ

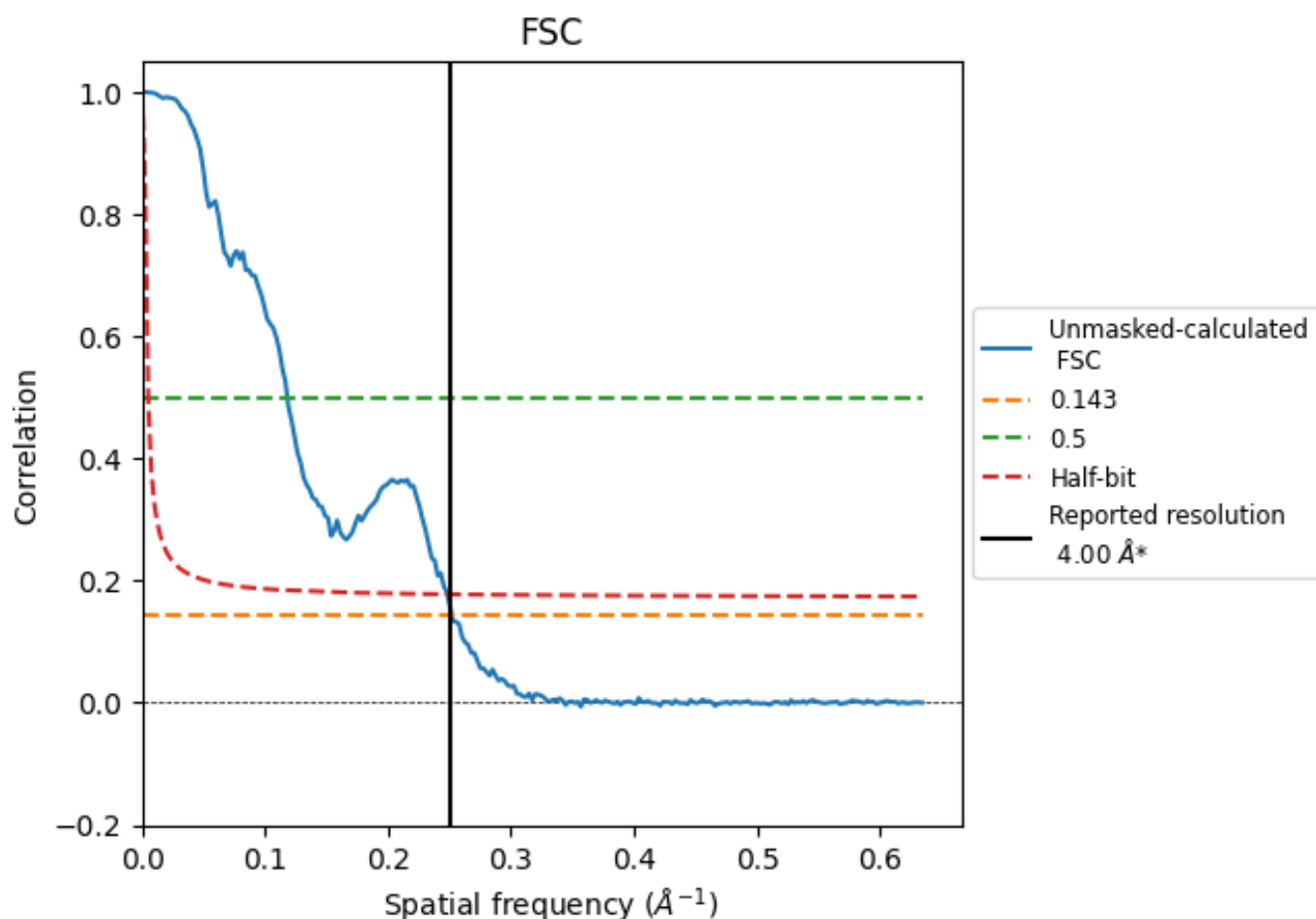


*Reported resolution corresponds to spatial frequency of $0.250 \text{ \AA}^{-1}$

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 0.250 Å⁻¹

8.2 Resolution estimates [i](#)

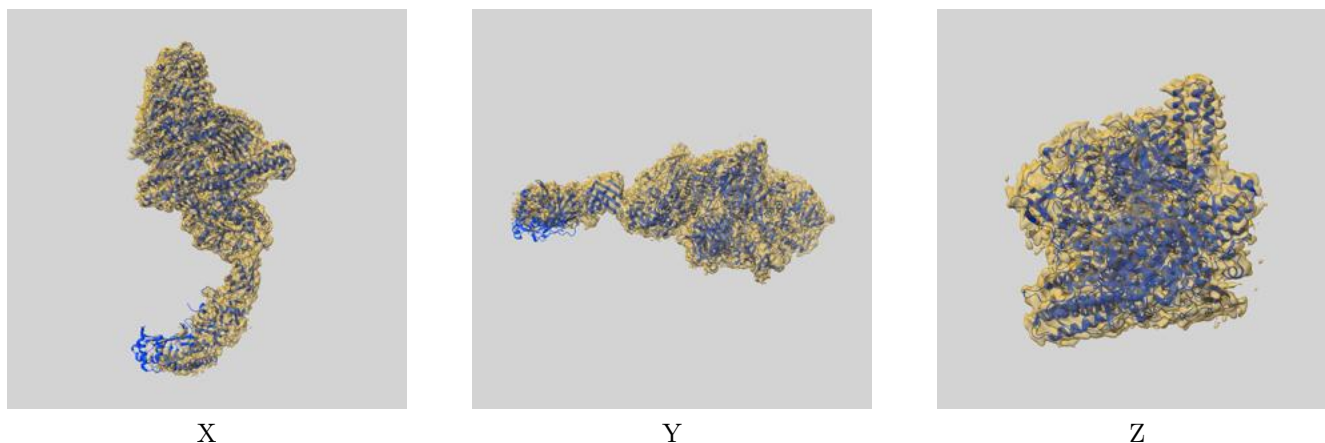
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.97	8.47	4.03

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

9 Map-model fit [i](#)

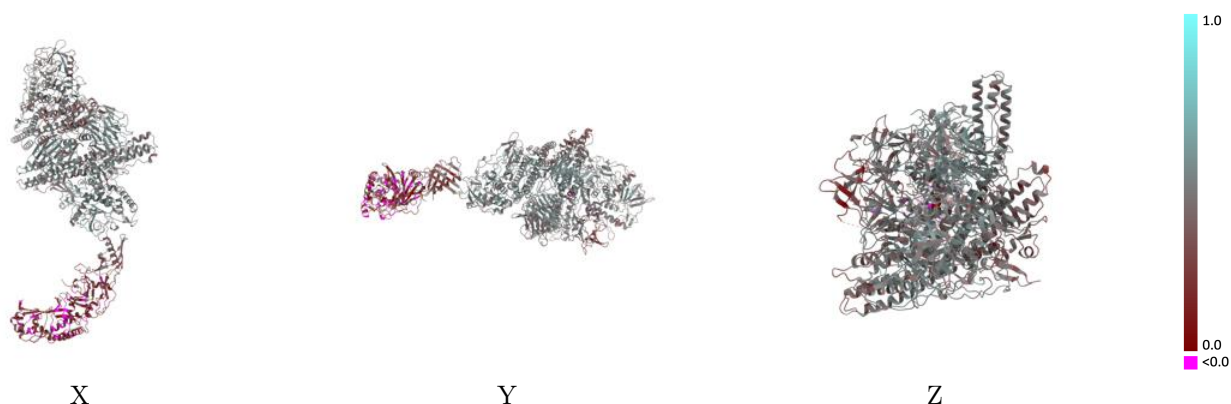
This section contains information regarding the fit between EMDB map EMD-43786 and PDB model 9ARL. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



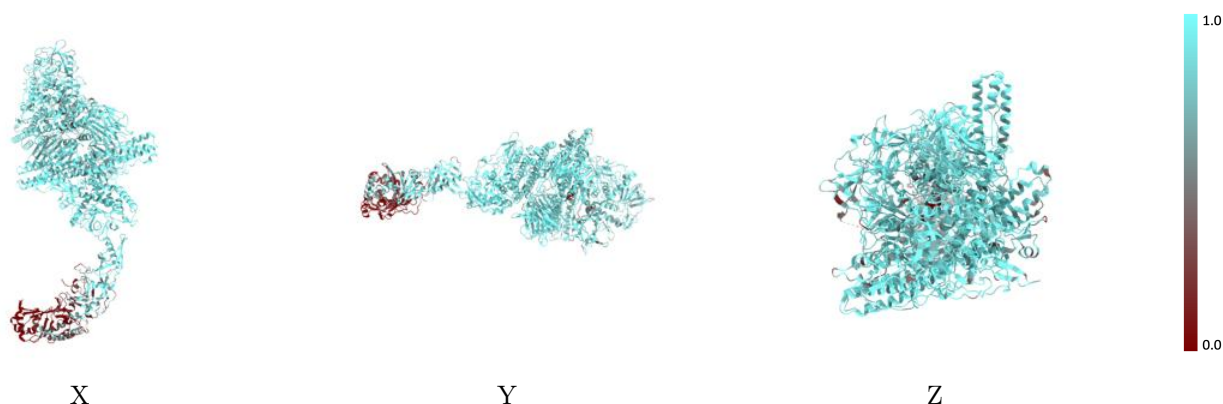
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



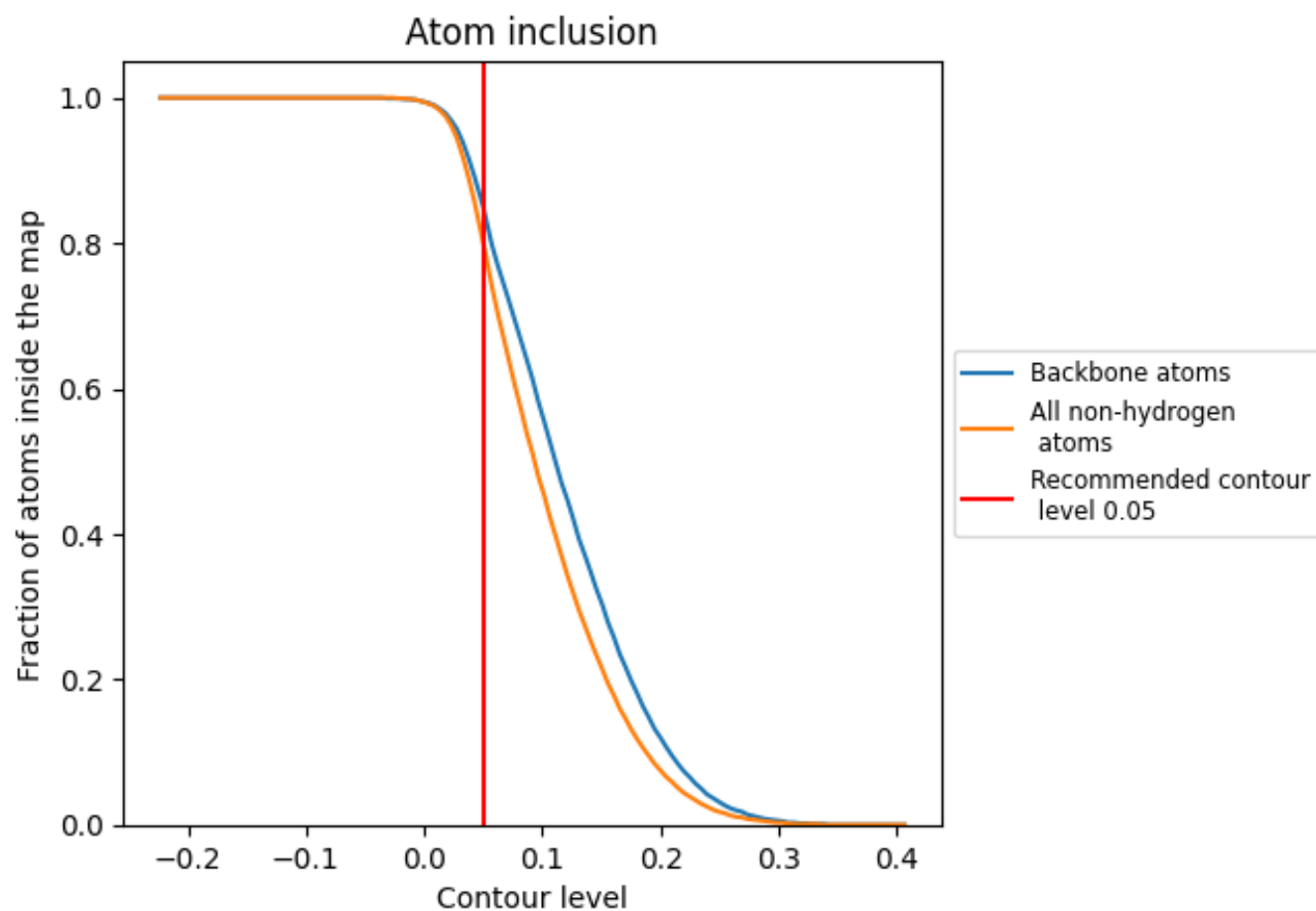
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 80% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8010	0.4230
A	0.8680	0.4640
B	0.9040	0.4810
C	0.4250	0.2000

