



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2024 – 08:05 AM JST

PDB ID : 6LYP
EMDB ID : EMD-30017
Title : Cryo-EM structure of AtMSL1 wild type
Authors : Sun, L.
Deposited on : 2020-02-15
Resolution : 3.30 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.dev70
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

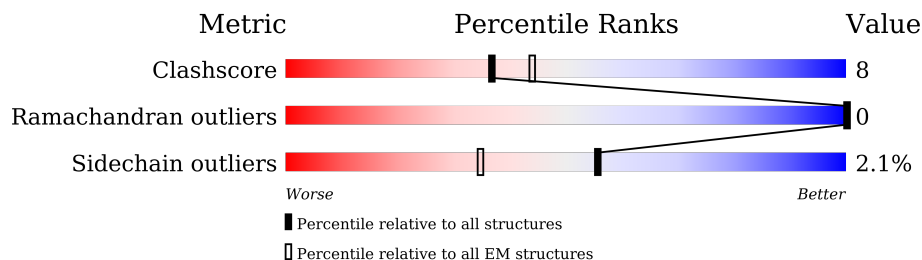
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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

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	497	
1	B	497	
1	C	497	
1	D	497	
1	E	497	
1	F	497	
1	G	497	

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 15169 atoms, of which 0 are hydrogens and 0 are deuteriums.

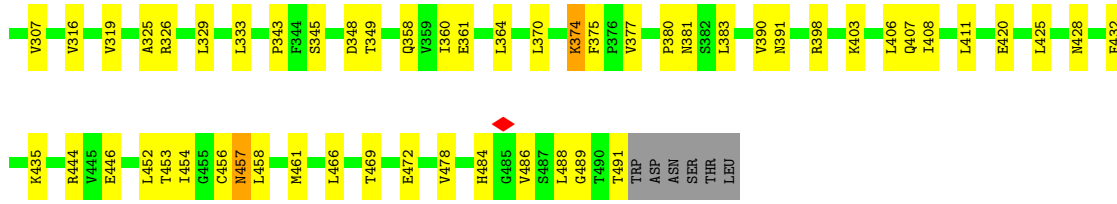
In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Mechanosensitive ion channel protein 1, mitochondrial.

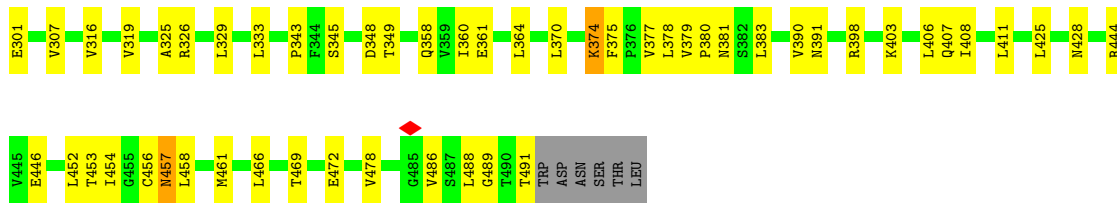
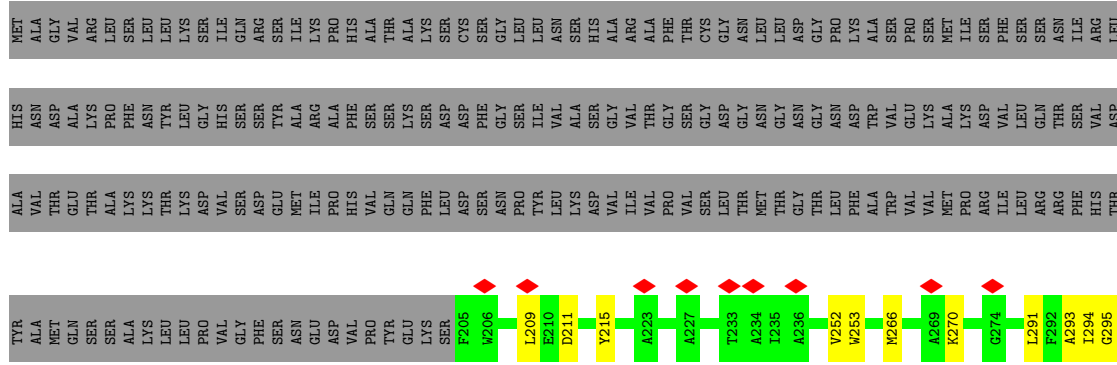
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	287	2167	1392	364	399	12	0	0
1	B	287	2167	1392	364	399	12	0	0
1	C	287	2167	1392	364	399	12	0	0
1	D	287	2167	1392	364	399	12	0	0
1	E	287	2167	1392	364	399	12	0	0
1	F	287	2167	1392	364	399	12	0	0
1	G	287	2167	1392	364	399	12	0	0

There are 14 discrepancies between the modelled and reference sequences:

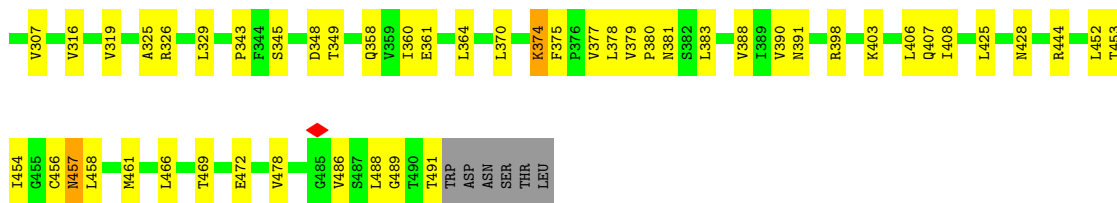
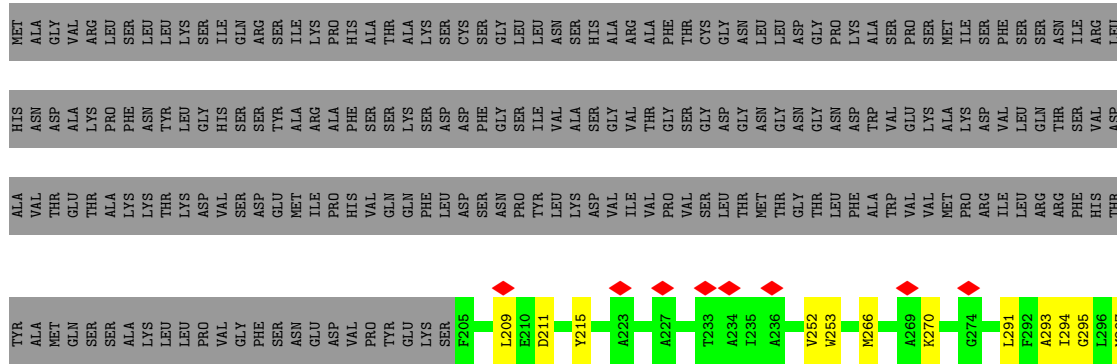
Chain	Residue	Modelled	Actual	Comment	Reference
A	234	ALA	ILE	engineered mutation	UNP Q8VZL4
A	235	ILE	ALA	engineered mutation	UNP Q8VZL4
B	234	ALA	ILE	engineered mutation	UNP Q8VZL4
B	235	ILE	ALA	engineered mutation	UNP Q8VZL4
C	234	ALA	ILE	engineered mutation	UNP Q8VZL4
C	235	ILE	ALA	engineered mutation	UNP Q8VZL4
D	234	ALA	ILE	engineered mutation	UNP Q8VZL4
D	235	ILE	ALA	engineered mutation	UNP Q8VZL4
E	234	ALA	ILE	engineered mutation	UNP Q8VZL4
E	235	ILE	ALA	engineered mutation	UNP Q8VZL4
F	234	ALA	ILE	engineered mutation	UNP Q8VZL4
F	235	ILE	ALA	engineered mutation	UNP Q8VZL4
G	234	ALA	ILE	engineered mutation	UNP Q8VZL4
G	235	ILE	ALA	engineered mutation	UNP Q8VZL4



● Molecule 1: Mechanosensitive ion channel protein 1, mitochondrial



● Molecule 1: Mechanosensitive ion channel protein 1, mitochondrial



HIS ASN
VAL THR ASP ALA
LYS PRO PHE ASN
TYR LYS ASP GLY HIS SER
SER ASP TYR MET ALA ARG
ALA PRO HIS PHE SER
SER GLN LYS PHE SER
LEU ASP LEU ASP ASP
PHE ASP PHE

ALA VAL THR
GLN THR LYS
ALA LYS THR
LEU LYS ASP
VAL HIS SER
ASP MET ASP
GLU ILE ARG
SER PRO HIS
VAL VAL SER
GLN LYS PHE
SER LEU ASP
ASP SER PHE
SER ASN PRO
GLY TYR ILE
LEU TYR LEU
VAL LYS ASP
SER ASP VAL
GLY VAL ILE
VAL THR VAL
GLY PRO GLY
SER VAL SER
GLY SER GLY
ASP LEU ASP
GLY THR MET
ASN THR THR
GLY ASN ASN
GLY THR THR
LEU LEU PHE
ASP TRP ALA
TRP VAL VAL
GLU VAL VAL
LYS MET ALA
ALA PRO LYS
ASP ARG ASP
VAL ILE VAL
LEU LEU LEU
GLN ARG ARG
THR ARG THR
VAL HIS VAL
ASP THR ASP

TYR
ALA MET GLN SER ALA LYS LEU PRO VAL GLY PHE SER ASN ASP PRO VAL ILE THR VAL SER GLY ASP GLY THR MET ASN THR THR ASN ASN GLY THR LEU PHE TRP ALA TRP VAL VAL VAL MET VAL PRO LYS ARG ASP ILE VAL LEU LEU ARG ARG THR HIS VAL ASP

V316 V319 A325 R326 L329 L333 P343 F344 S345 D348 T349 Q358 V359 I360 E361 L364 L370 K374 F375 P376 V377 L378 V379 P380 N381 S382 L383 N391 R398 K403 L406 Q407 I408 L411 I414 I417 E420 L425 N428

R444 V445 E446 L452 T453 I454 G455 C456 N457 L458 M461 L466 Y467 M468 T469 Q470 Q471 E472 V478 H484 G485 V486 S487 L488 G489 T490 T491 TRP ASP ASN SER THR LEU

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C7	Depositor
Number of particles used	251528	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.454	Depositor
Minimum map value	-0.302	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.019	Depositor
Map size (Å)	249.59999, 249.59999, 249.59999	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	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	0.48	1/2201 (0.0%)	0.73	1/2979 (0.0%)
1	B	0.48	1/2201 (0.0%)	0.73	1/2979 (0.0%)
1	C	0.48	1/2201 (0.0%)	0.73	1/2979 (0.0%)
1	D	0.48	1/2201 (0.0%)	0.73	1/2979 (0.0%)
1	E	0.48	1/2201 (0.0%)	0.73	1/2979 (0.0%)
1	F	0.48	1/2201 (0.0%)	0.73	1/2979 (0.0%)
1	G	0.48	1/2201 (0.0%)	0.73	1/2979 (0.0%)
All	All	0.48	7/15407 (0.0%)	0.73	7/20853 (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
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
All	All	0	7

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	375	PHE	C-N	-7.02	1.21	1.34
1	A	375	PHE	C-N	-6.98	1.21	1.34
1	E	375	PHE	C-N	-6.97	1.21	1.34
1	C	375	PHE	C-N	-6.97	1.21	1.34
1	F	375	PHE	C-N	-6.97	1.21	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	374	LYS	C-N-CA	5.43	135.28	121.70
1	D	374	LYS	C-N-CA	5.42	135.26	121.70
1	F	374	LYS	C-N-CA	5.42	135.25	121.70
1	E	374	LYS	C-N-CA	5.41	135.23	121.70
1	G	374	LYS	C-N-CA	5.40	135.21	121.70

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	253	TRP	Peptide
1	B	253	TRP	Peptide
1	C	253	TRP	Peptide
1	D	253	TRP	Peptide
1	E	253	TRP	Peptide

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	2167	0	2251	38	0
1	B	2167	0	2251	41	0
1	C	2167	0	2251	41	0
1	D	2167	0	2251	38	0
1	E	2167	0	2251	41	0
1	F	2167	0	2251	50	0
1	G	2167	0	2251	44	0
All	All	15169	0	15757	255	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 8.

The worst 5 of 255 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:F:211:ASP:O	1:F:215:TYR:HB2	1.77	0.84
1:C:211:ASP:O	1:C:215:TYR:HB2	1.77	0.84
1:A:211:ASP:O	1:A:215:TYR:HB2	1.77	0.83
1:G:211:ASP:O	1:G:215:TYR:HB2	1.77	0.83
1:D:211:ASP:O	1:D:215:TYR:HB2	1.77	0.83

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	285/497 (57%)	257 (90%)	28 (10%)	0	100	100
1	B	285/497 (57%)	257 (90%)	28 (10%)	0	100	100
1	C	285/497 (57%)	258 (90%)	27 (10%)	0	100	100
1	D	285/497 (57%)	257 (90%)	28 (10%)	0	100	100
1	E	285/497 (57%)	257 (90%)	28 (10%)	0	100	100
1	F	285/497 (57%)	257 (90%)	28 (10%)	0	100	100
1	G	285/497 (57%)	257 (90%)	28 (10%)	0	100	100
All	All	1995/3479 (57%)	1800 (90%)	195 (10%)	0	100	100

There are no Ramachandran outliers to report.

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	234/417 (56%)	229 (98%)	5 (2%)	53	75
1	B	234/417 (56%)	229 (98%)	5 (2%)	53	75
1	C	234/417 (56%)	229 (98%)	5 (2%)	53	75
1	D	234/417 (56%)	229 (98%)	5 (2%)	53	75
1	E	234/417 (56%)	229 (98%)	5 (2%)	53	75
1	F	234/417 (56%)	229 (98%)	5 (2%)	53	75
1	G	234/417 (56%)	229 (98%)	5 (2%)	53	75
All	All	1638/2919 (56%)	1603 (98%)	35 (2%)	56	75

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	444	ARG
1	F	457	ASN
1	G	428	ASN
1	C	428	ASN
1	C	329	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	428	ASN
1	E	428	ASN
1	G	428	ASN
1	F	428	ASN
1	G	358	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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](#)

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.

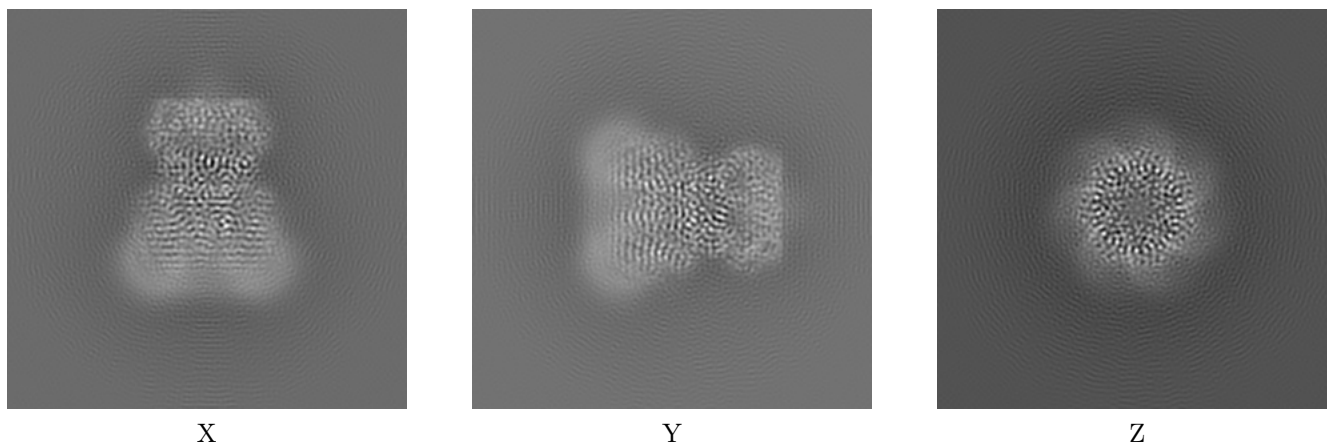
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30017. These allow visual inspection of the internal detail of the map and identification of artifacts.

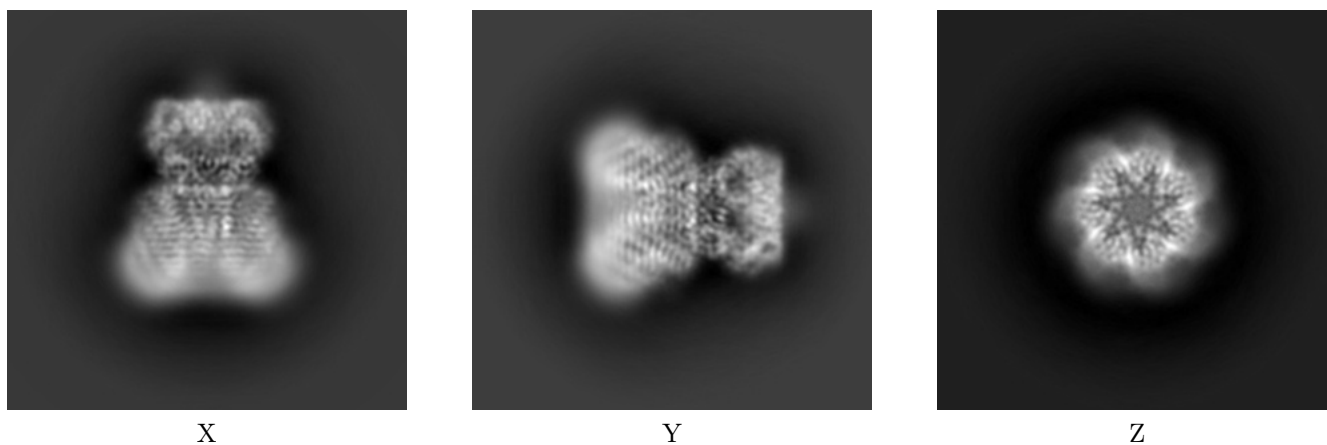
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



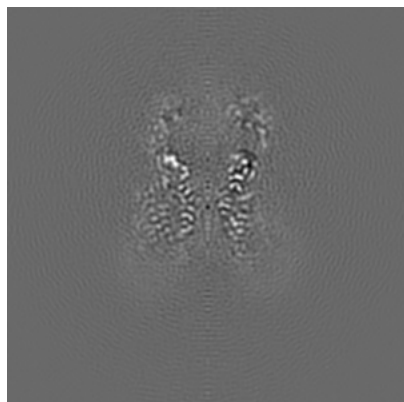
6.1.2 Raw map



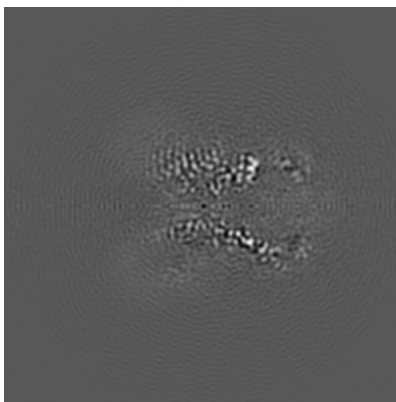
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

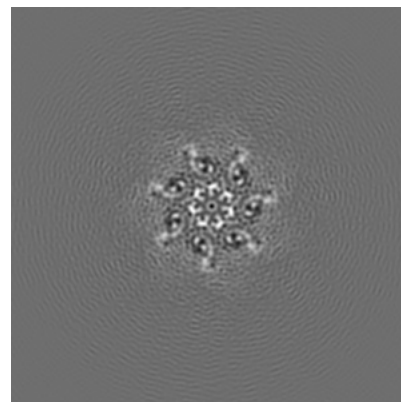
6.2.1 Primary map



X Index: 120

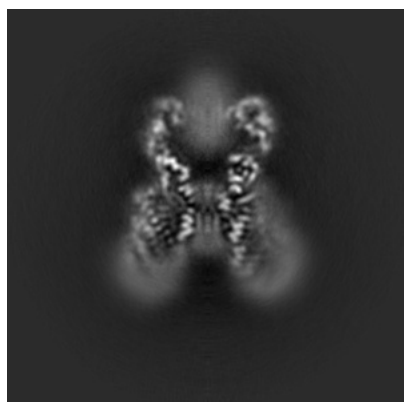


Y Index: 120

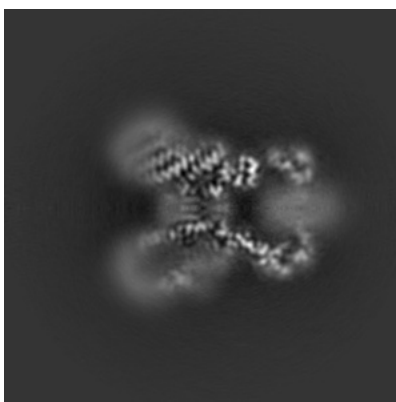


Z Index: 120

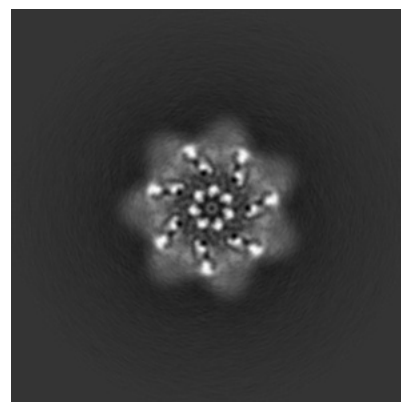
6.2.2 Raw map



X Index: 120



Y Index: 120

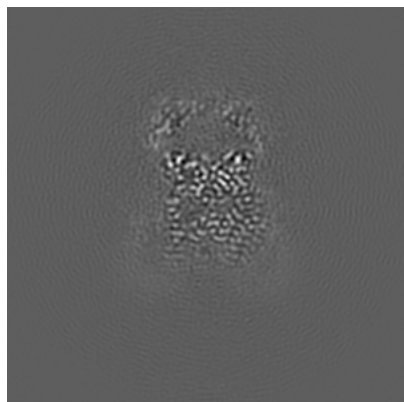


Z Index: 120

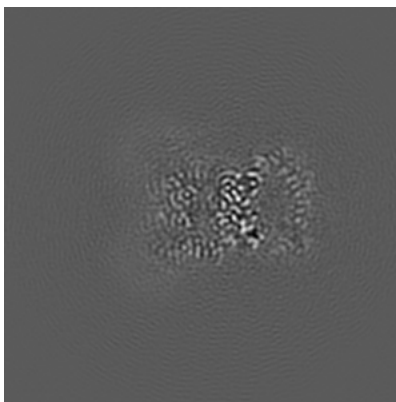
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

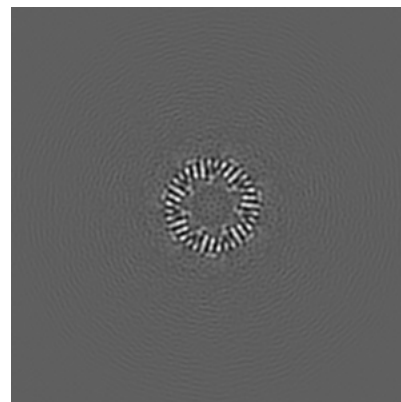
6.3.1 Primary map



X Index: 134

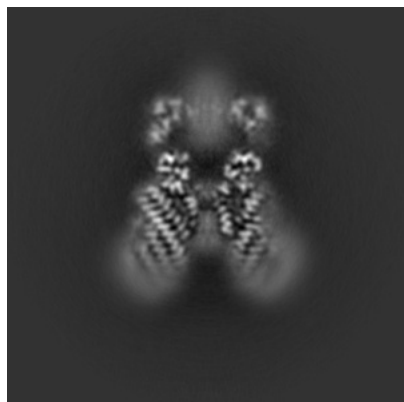


Y Index: 104

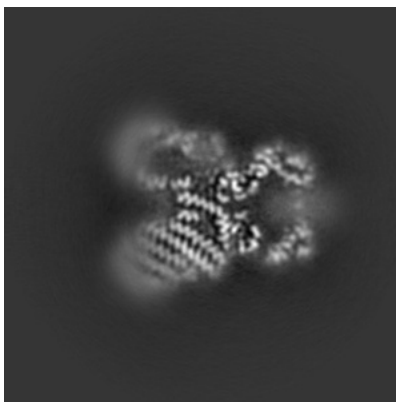


Z Index: 149

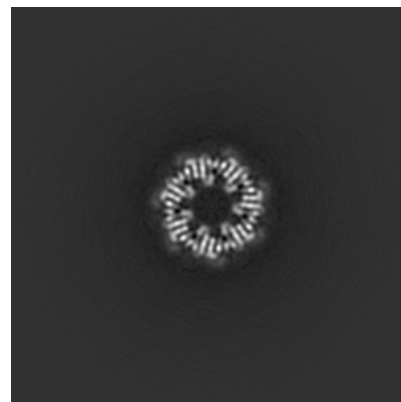
6.3.2 Raw map



X Index: 115



Y Index: 131

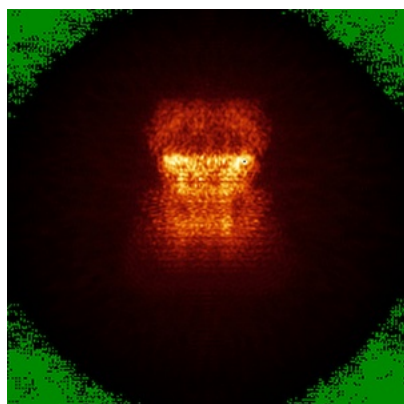


Z Index: 149

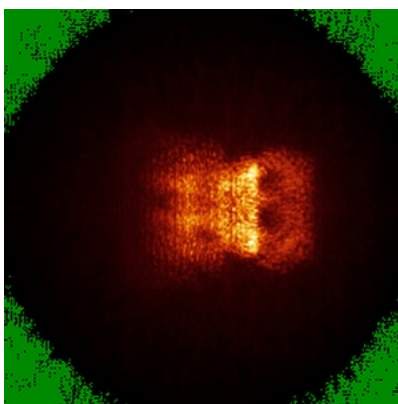
The images above show the largest variance slices of the map in three orthogonal directions.

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

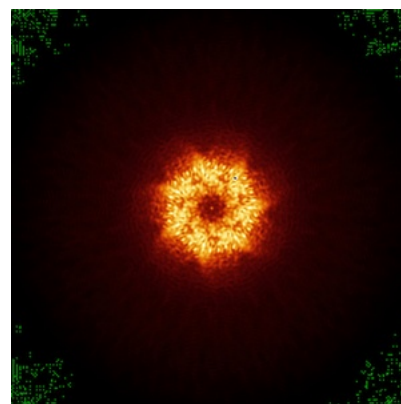
6.4.1 Primary map



X

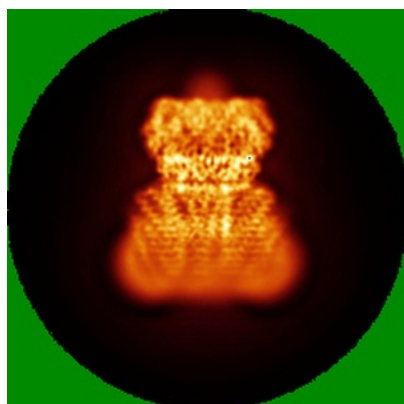


Y

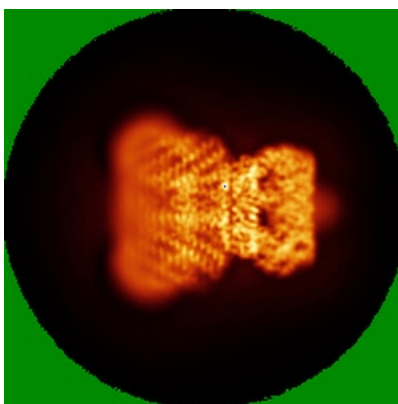


Z

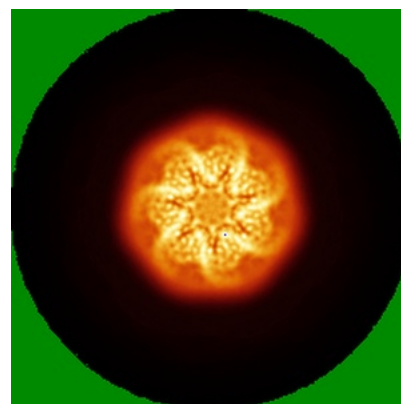
6.4.2 Raw map



X



Y

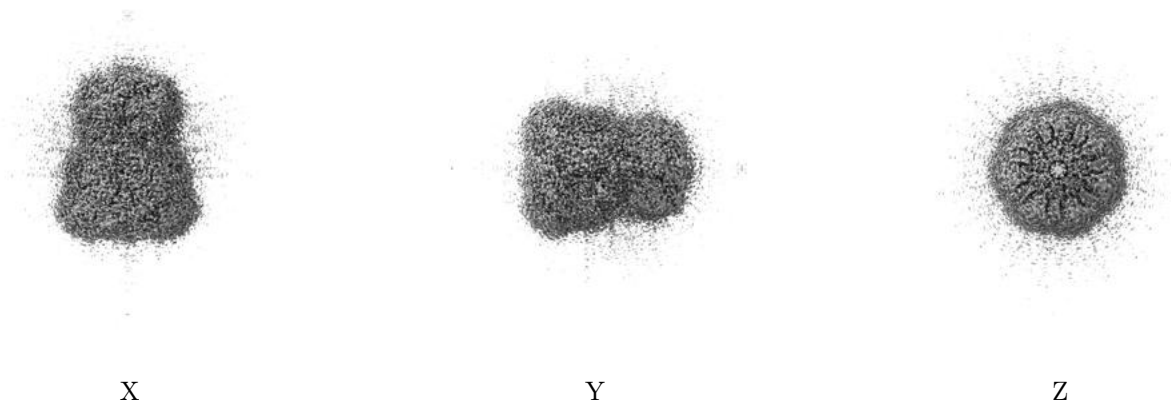


Z

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.

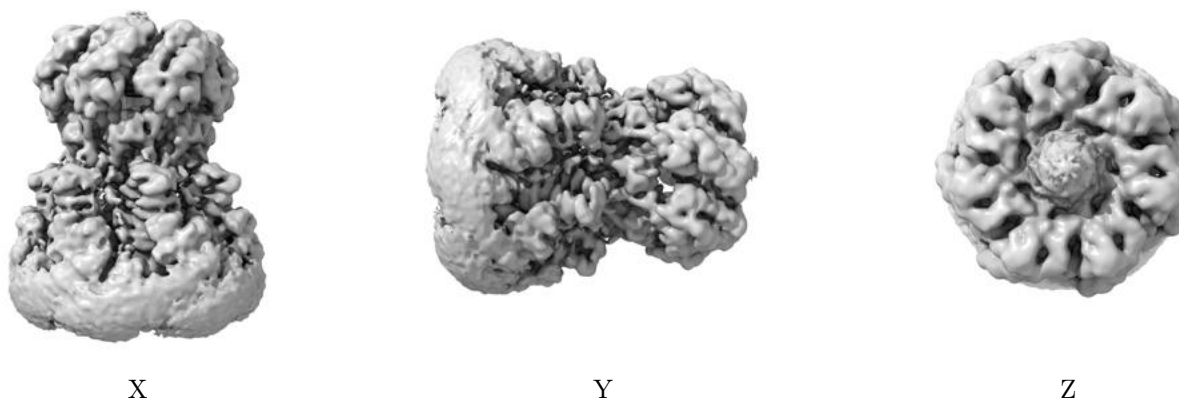
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.019. 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.

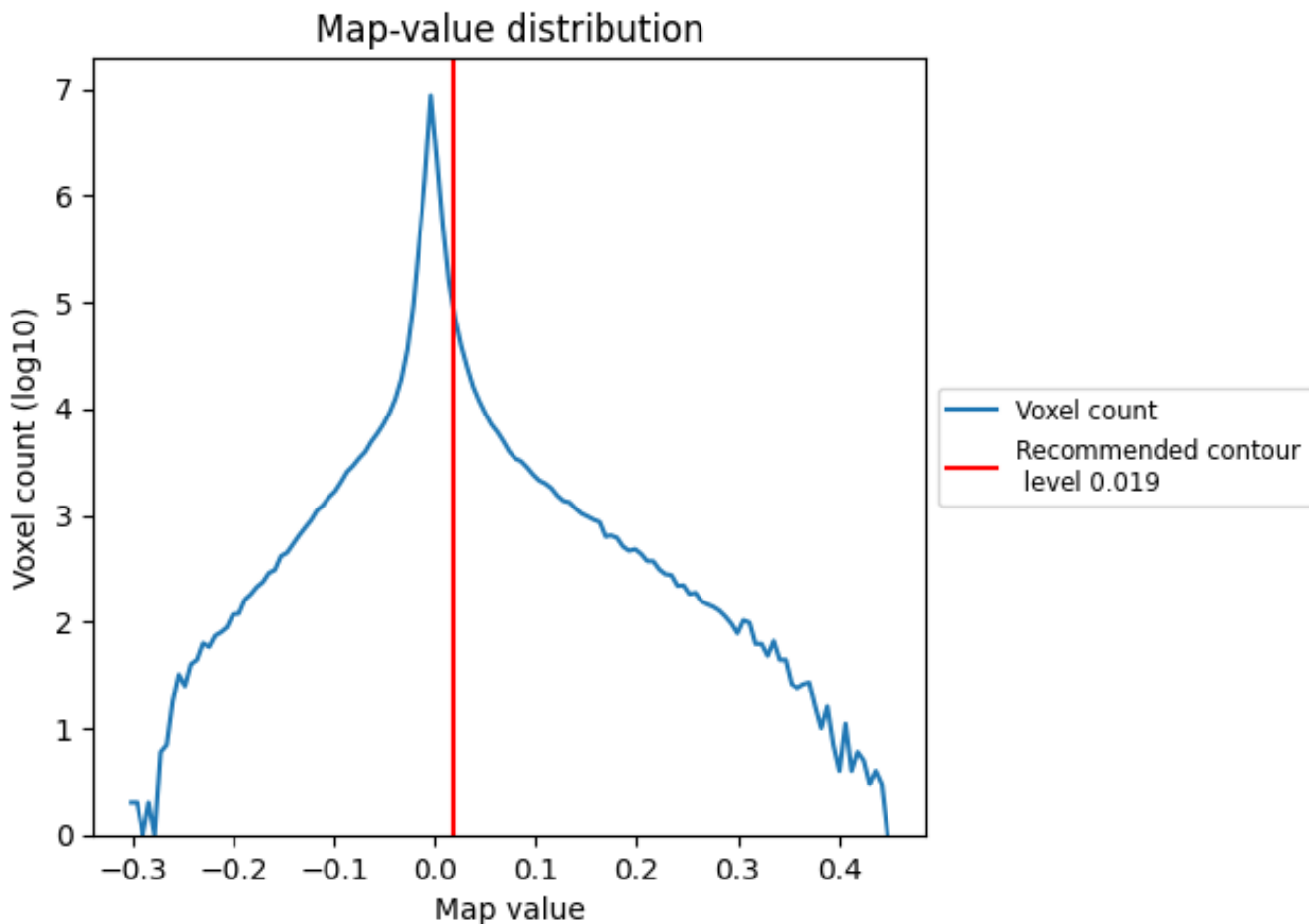
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

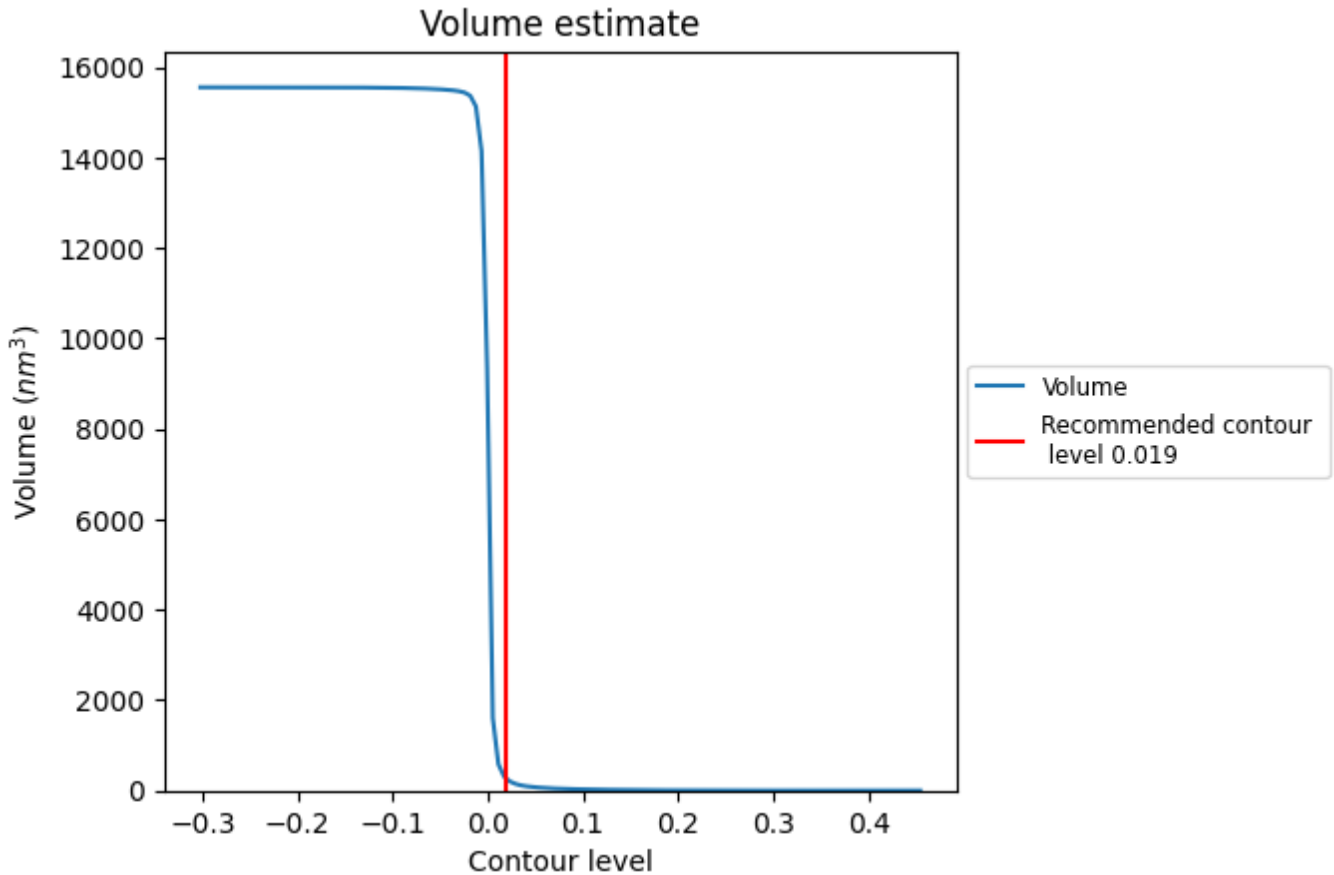
This section contains the results of statistical analysis of the map.

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.

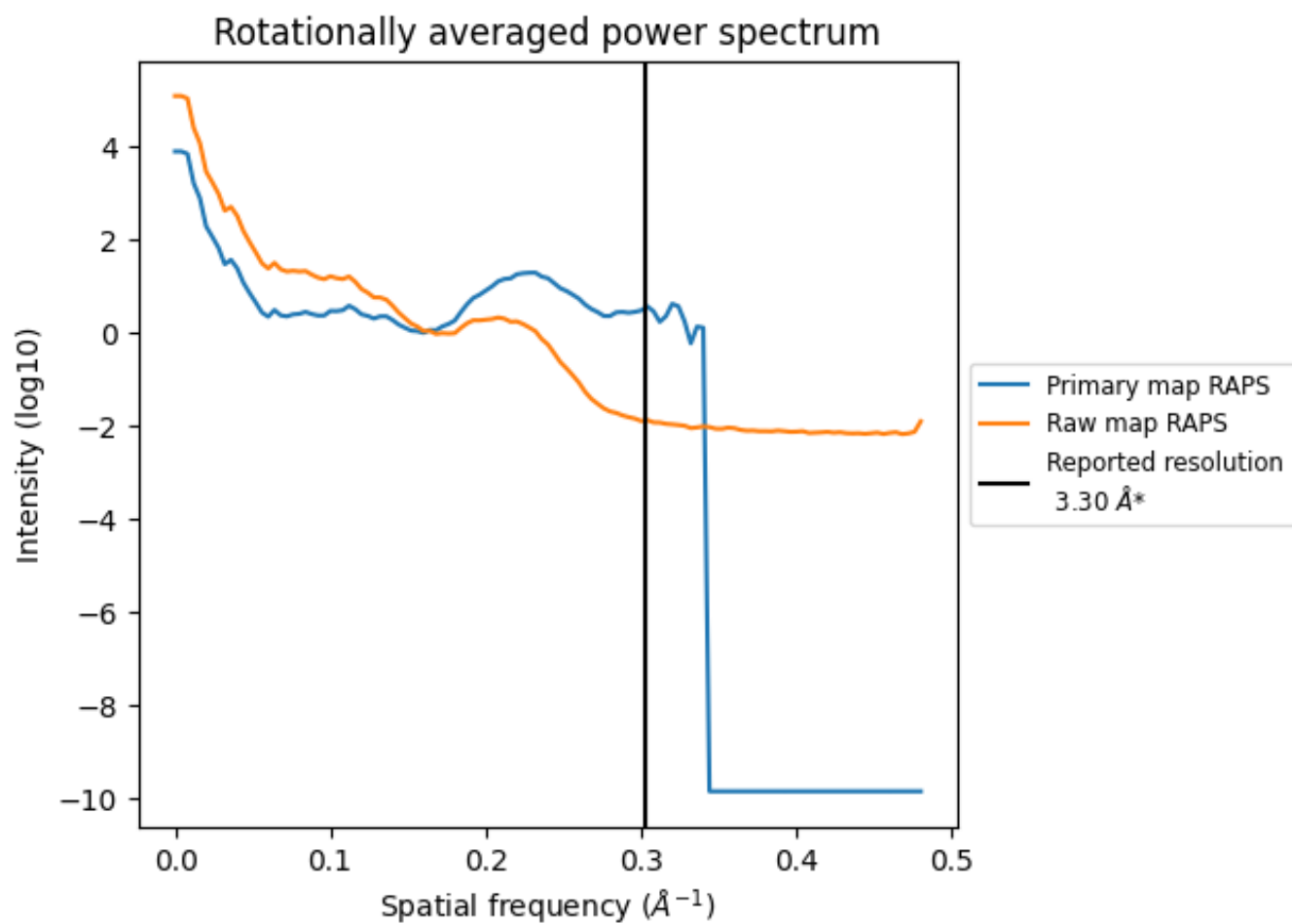
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 277 nm³; this corresponds to an approximate mass of 250 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](#)

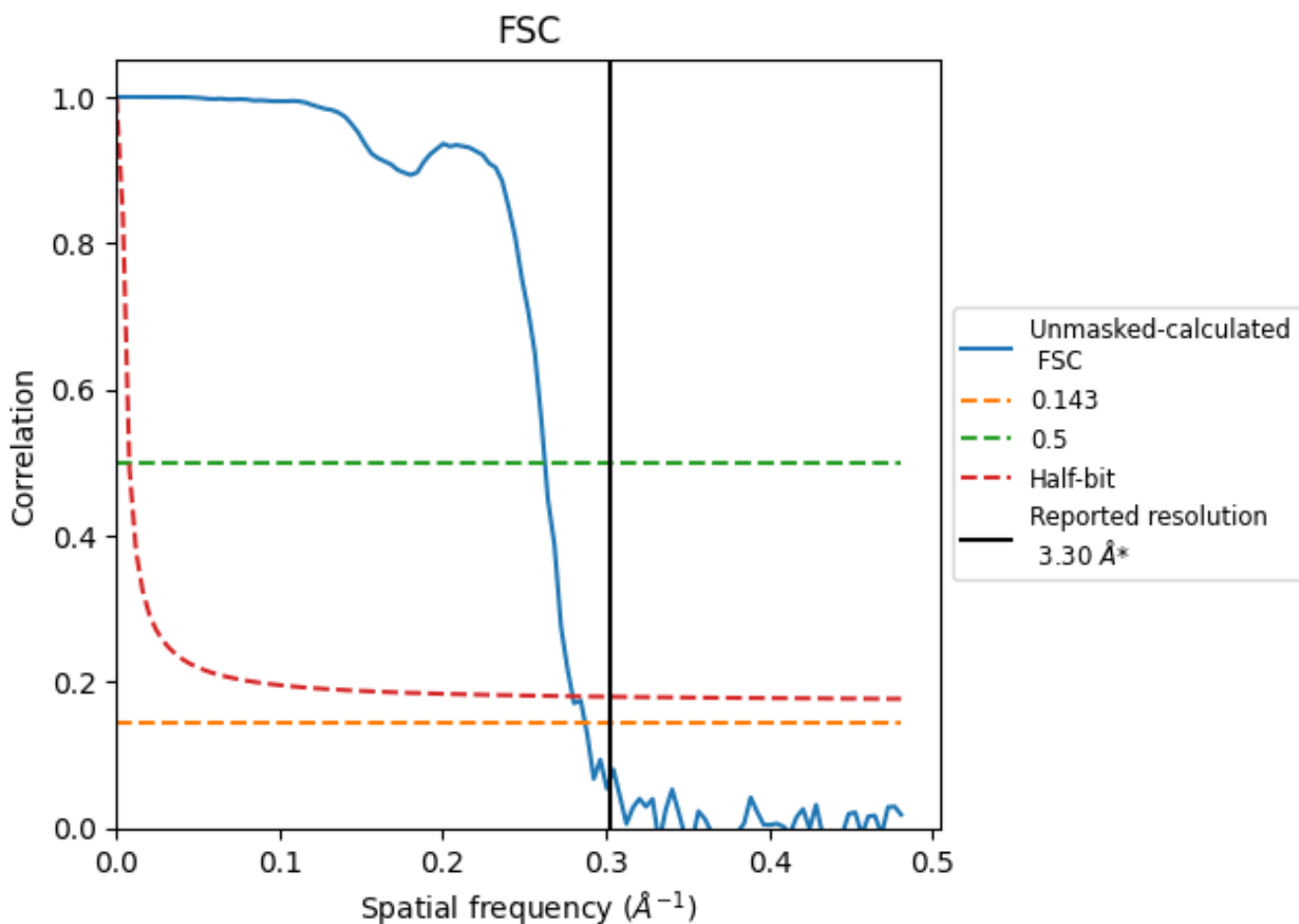


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 \AA^{-1}

8.2 Resolution estimates [i](#)

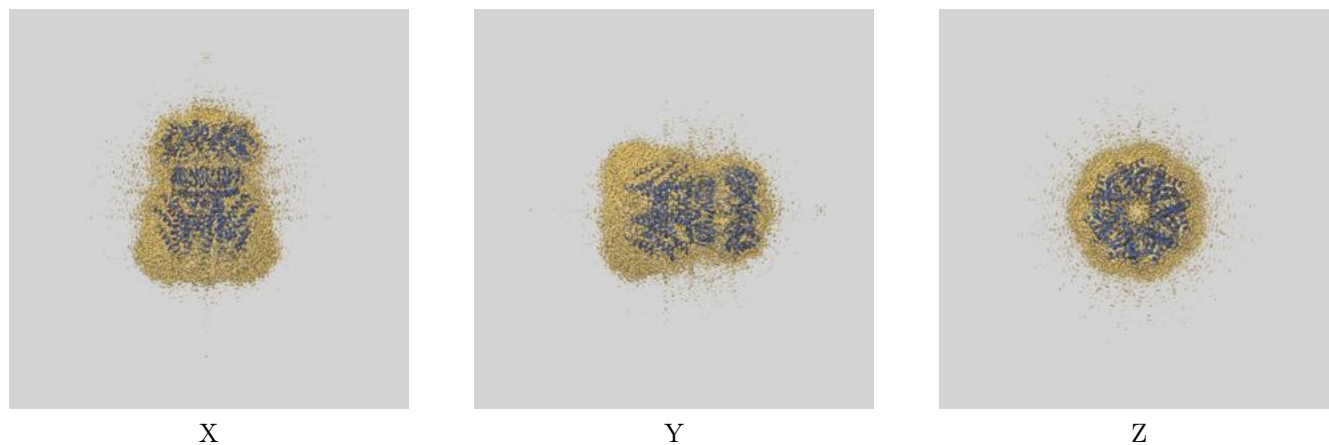
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.48	3.81	3.58

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

9 Map-model fit [i](#)

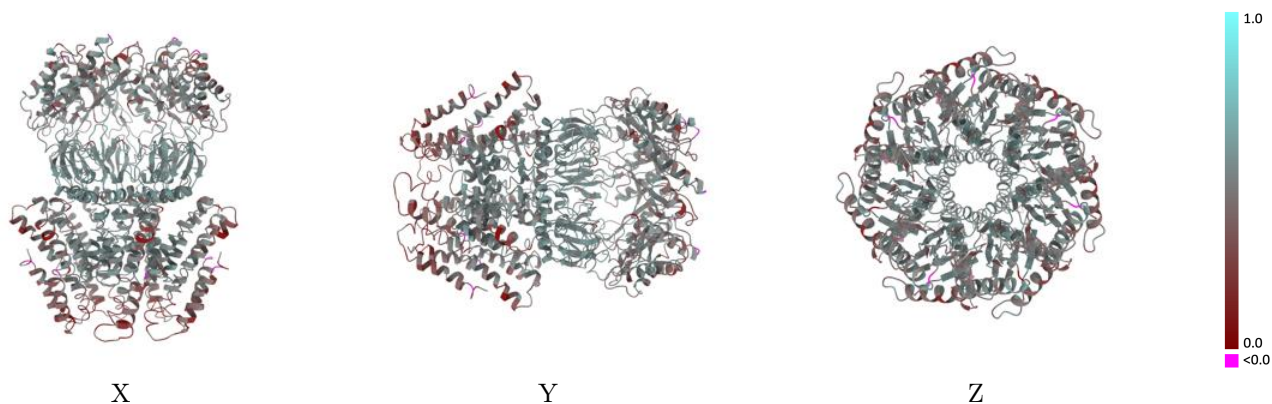
This section contains information regarding the fit between EMDB map EMD-30017 and PDB model 6LYP. Per-residue inclusion information can be found in section [3](#) on page [4](#).

9.1 Map-model overlay [i](#)



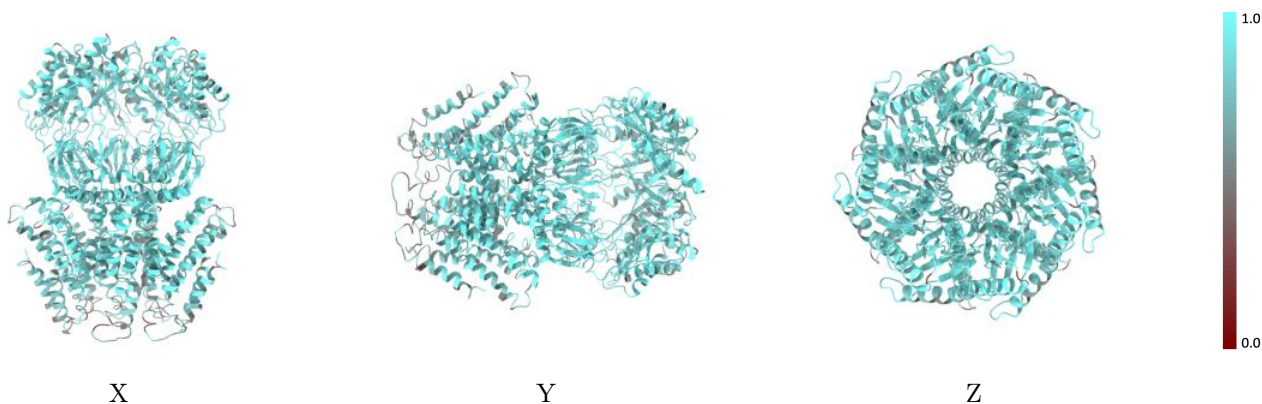
The images above show the 3D surface view of the map at the recommended contour level 0.019 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



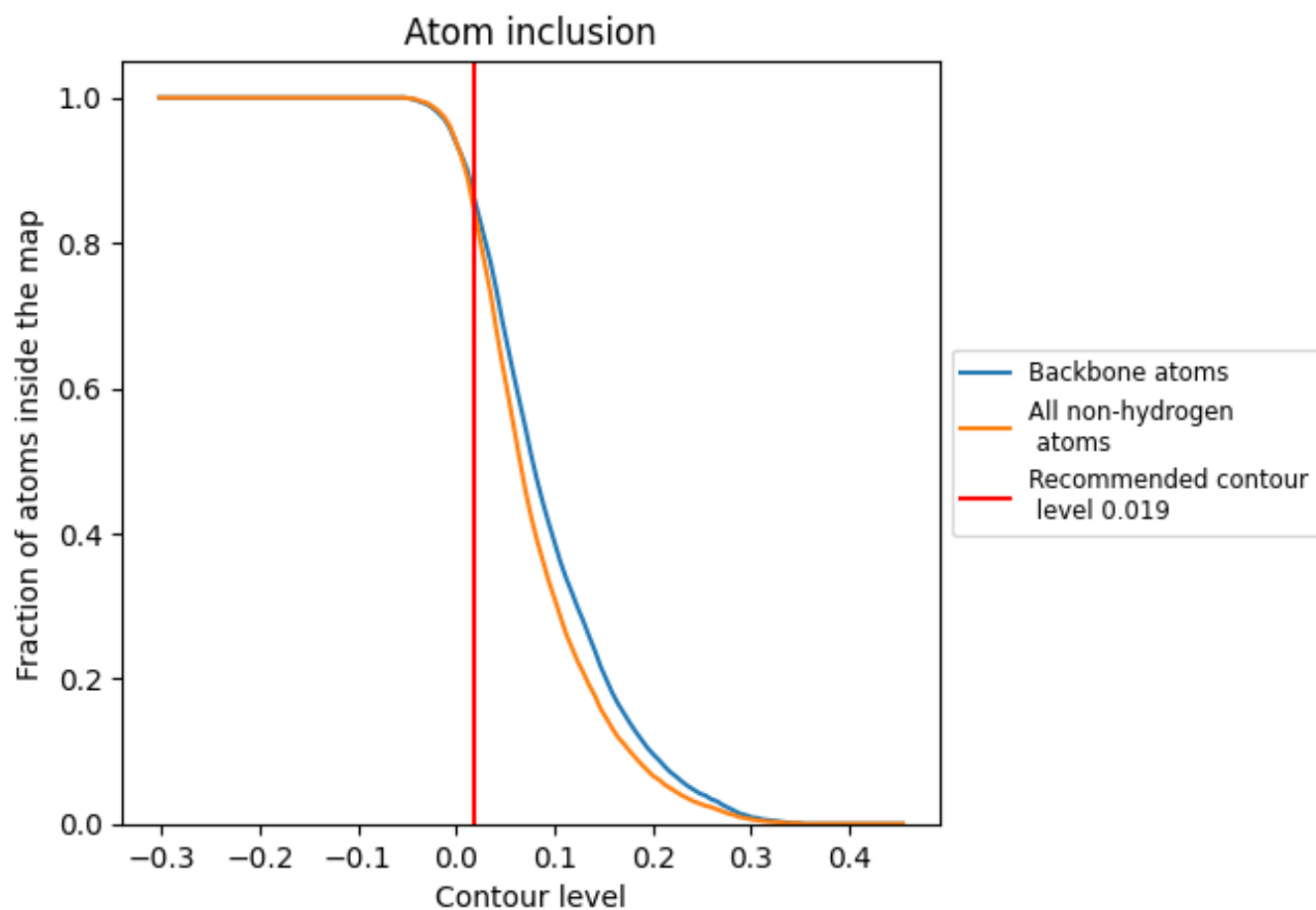
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.019).

















9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 84% 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 (0.019) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8410	 0.4550
A	 0.8420	 0.4560
B	 0.8380	 0.4570
C	 0.8390	 0.4540
D	 0.8390	 0.4530
E	 0.8420	 0.4560
F	 0.8450	 0.4540
G	 0.8410	 0.4570

