



wwPDB EM Validation Summary Report ⓘ

Jul 3, 2024 – 03:51 am BST

PDB ID : 7A2G
EMDB ID : EMD-11624
Title : Full-length structure of the substrate-free tyrosine hydroxylase (apo-TH).
Authors : Bueno-Carrasco, M.T.; Cuellar, J.; Santiago, C.; Flydal, M.I.; Martinez, A.; Valpuesta, J.M.
Deposited on : 2020-08-17
Resolution : 4.10 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.dev92
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)	:	2.37.1

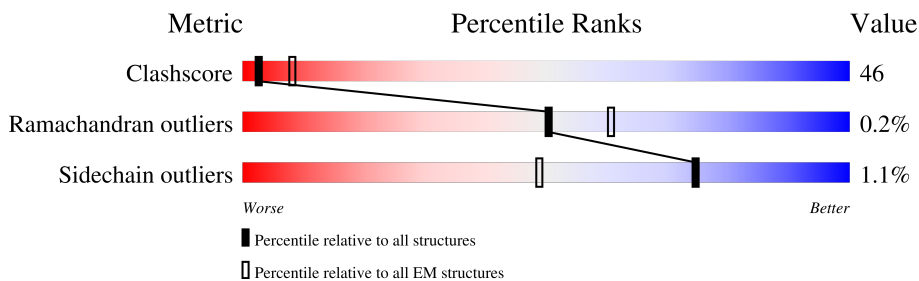
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 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	420	 31% 68%
1	B	420	 31% 68%
1	C	420	 32% 67%
1	D	420	 29% 69%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 13408 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 Tyrosine 3-monooxygenase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	420	Total	C	N	O	S	0	0
			3350	2130	586	624	10		
1	B	420	Total	C	N	O	S	0	0
			3350	2130	586	624	10		
1	C	420	Total	C	N	O	S	0	0
			3350	2130	586	624	10		
1	D	420	Total	C	N	O	S	0	0
			3350	2130	586	624	10		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	81	MET	VAL	conflict	UNP P07101
B	81	MET	VAL	conflict	UNP P07101
C	81	MET	VAL	conflict	UNP P07101
D	81	MET	VAL	conflict	UNP P07101

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Fe	0
			1	1	
2	B	1	Total	Fe	0
			1	1	
2	C	1	Total	Fe	0
			1	1	
2	D	1	Total	Fe	0
			1	1	

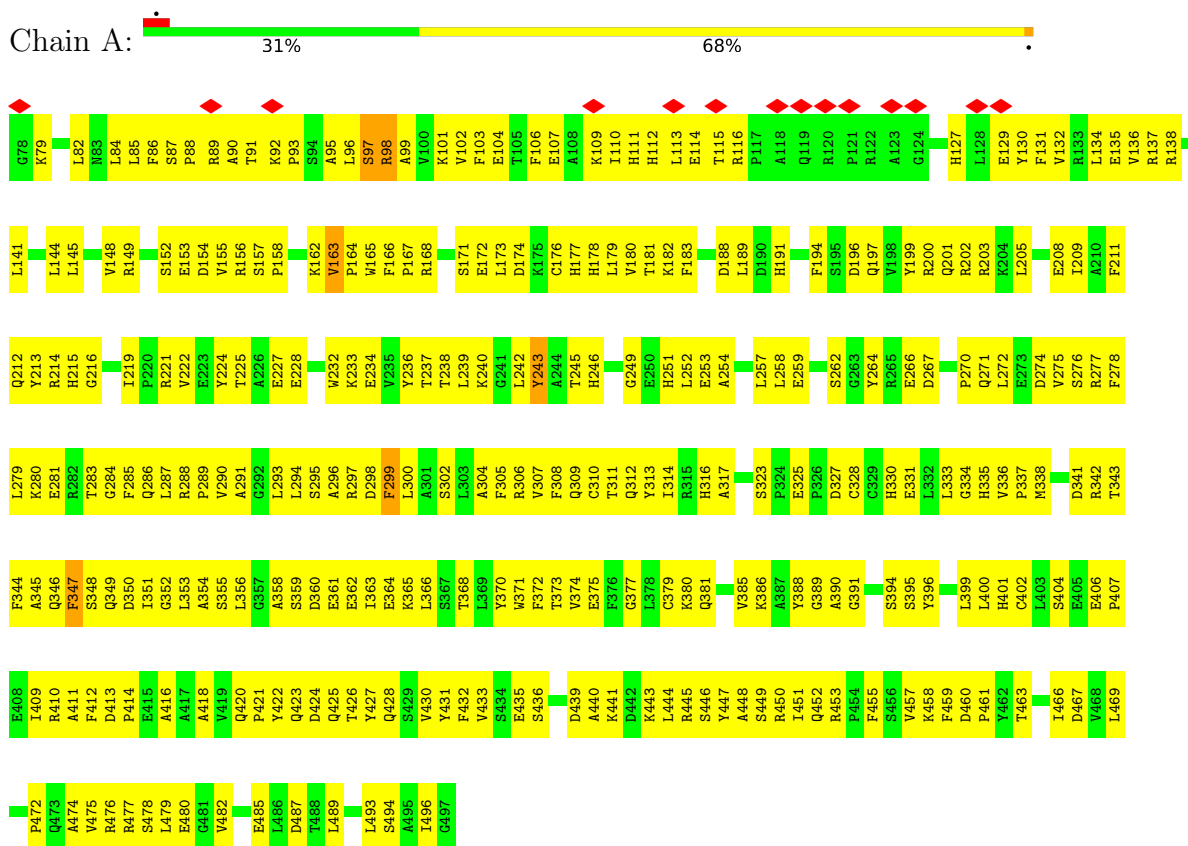
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total 1	O 1	0
3	B	1	Total 1	O 1	0
3	C	1	Total 1	O 1	0
3	D	1	Total 1	O 1	0

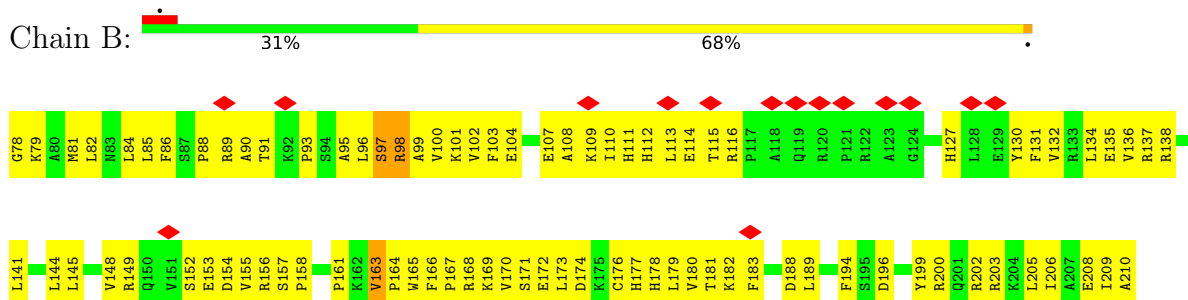
3 Residue-property plots

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: Tyrosine 3-monooxygenase

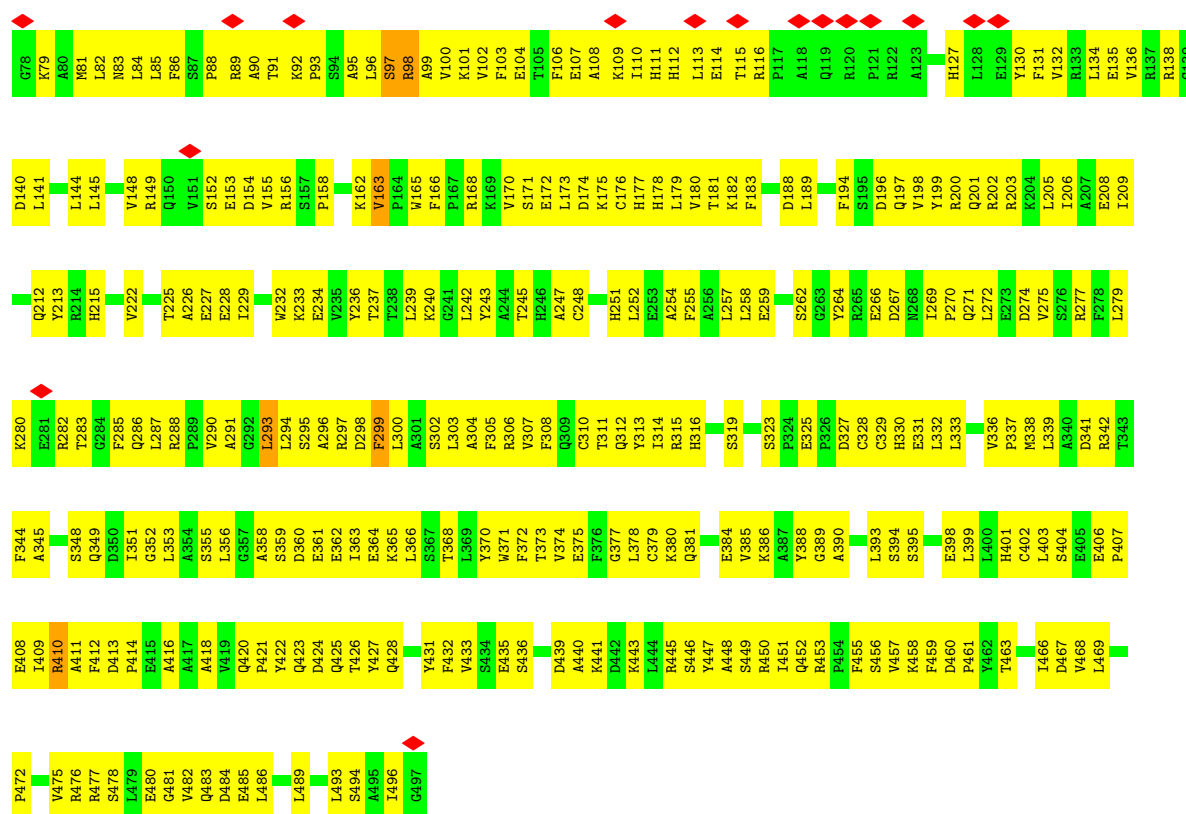
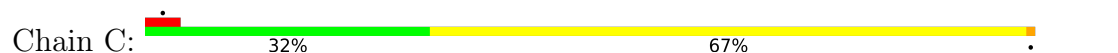


• Molecule 1: Tyrosine 3-monooxygenase

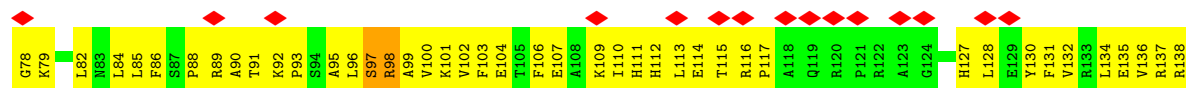




• Molecule 1: Tyrosine 3-monooxygenase



• Molecule 1: Tyrosine 3-monooxygenase



L141	H215	L279	A345	R410	P472
L144	G216	K280	Q346	A411	V475
L145	I219	E281	F347	F412	R476
V148	V222	R282	S348	D413	R477
R149	E223	T283	Q349	P414	S478
S152	Y224	G284	D350	E415	L479
E153	T225	F285	I351	A416	E480
D154	Y226	Q286	Q352	A417	G481
V155	A226	L287	L353	A418	V482
R156	E227	P288	A354	V419	Q420
S157	E228	V290	S355	P421	P422
P158	I229	L293	L356	Y422	Q423
V163	W232	L294	A358	Q424	Q425
P164	K233	S295	S359	D424	T426
V165	E234	A296	D360	Q428	Y427
F166	T237	R297	E361	Q429	S429
P167	T238	F299	E362	V430	V431
R168	L239	L300	I363	F432	F433
K169	K240	A301	E364	S367	S434
V170	G241	S302	K365	T368	E435
S171	L242	L303	L366	W371	D439
E172	Y243	A304	S367	F372	A440
L173	A244	F305	T368	E375	K441
D174	T245	R306	W371	F376	D442
H177	H246	V307	F372	G377	K443
H178	A247	F308	E375	L378	L444
L179	C248	Q309	G377	C379	R445
V180	G249	C310	L378	K380	S446
T181	E250	Q311	Q381	Y447	A448
K182	H251	Q312	V385	S449	R450
F183	E252	Y313	K386	R451	I451
D188	A254	I314	A387	Q452	R453
L189	F255	R315	Y388	P454	F455
F194	A256	H316	A388	F456	S456
S195	L257	A317	Y389	V457	K458
D196	L258	S323	G389	F459	D460
Y199	E259	P324	A390	P461	Y462
R200	R260	E325	G391	T463	T463
Q201	F261	F326	L392	L464	A465
R202	S262	C327	L393	L465	I466
R203	G263	D328	L400	S404	D467
K204	Y264	C329	H401	E405	V468
L205	R265	H330	C402	E406	L469
I206	E266	E331	L403	P407	D470
A207	D267	L332	L404	E408	S471
E208	N268	L333	E405	I409	
I209	L269	G334	E406		
A210	P270	H335	P407		
F211	Q271	V336	E408		
Q212	L272	P337	I409		
Y213	E273	M338			
E214	D274	D341			
	V275	R342			
	S276	T343			
	R277	F344			
	F278				

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	29418	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 ($e^-/\text{\AA}^2$)	39.6	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.735	Depositor
Minimum map value	-0.394	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.048	Depositor
Recommended contour level	0.129	Depositor
Map size (\AA)	188.99998, 188.99998, 188.99998	wwPDB
Map dimensions	180, 180, 180	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.05, 1.05, 1.05	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: FE

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	0.35	0/3435	0.48	0/4654
1	B	0.36	0/3435	0.48	0/4654
1	C	0.36	0/3435	0.48	0/4654
1	D	0.35	0/3435	0.48	0/4654
All	All	0.36	0/13740	0.48	0/18616

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	2
1	C	0	2
1	D	0	2
All	All	0	7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	163	VAL	Peptide
1	B	163	VAL	Peptide
1	B	293	LEU	Peptide
1	C	163	VAL	Peptide
1	C	293	LEU	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	A	3350	0	3278	318	0
1	B	3350	0	3278	326	0
1	C	3350	0	3278	324	0
1	D	3350	0	3278	337	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	13408	0	13112	1229	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 46.

The worst 5 of 1229 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:C:111:HIS:HB2	1:D:114:GLU:H	1.19	1.03
1:A:109:LYS:HB2	1:B:115:THR:H	1.31	0.95
1:A:310:CYS:SG	1:A:312:GLN:NE2	2.41	0.93
1:C:115:THR:H	1:D:109:LYS:HB2	1.34	0.92
1:A:111:HIS:HB2	1:B:114:GLU:H	1.36	0.90

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	A	418/420 (100%)	351 (84%)	66 (16%)	1 (0%)	47	80
1	B	418/420 (100%)	351 (84%)	66 (16%)	1 (0%)	47	80
1	C	418/420 (100%)	349 (84%)	68 (16%)	1 (0%)	47	80
1	D	418/420 (100%)	344 (82%)	73 (18%)	1 (0%)	47	80
All	All	1672/1680 (100%)	1395 (83%)	273 (16%)	4 (0%)	50	80

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	97	SER
1	B	97	SER
1	C	97	SER
1	D	97	SER

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	
1	A	357/357 (100%)	353 (99%)	4 (1%)	73	84
1	B	357/357 (100%)	354 (99%)	3 (1%)	81	88
1	C	357/357 (100%)	354 (99%)	3 (1%)	81	88
1	D	357/357 (100%)	352 (99%)	5 (1%)	67	80
All	All	1428/1428 (100%)	1413 (99%)	15 (1%)	74	84

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	98	ARG
1	D	388	TYR
1	C	299	PHE
1	D	439	ASP

Continued on next page...

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Mol	Chain	Res	Type
1	D	267	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	111	HIS
1	D	346	GLN
1	D	312	GLN
1	D	381	GLN
1	B	271	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](#)

Of 4 ligands modelled in this entry, 4 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](#)

There are no chain breaks in this entry.

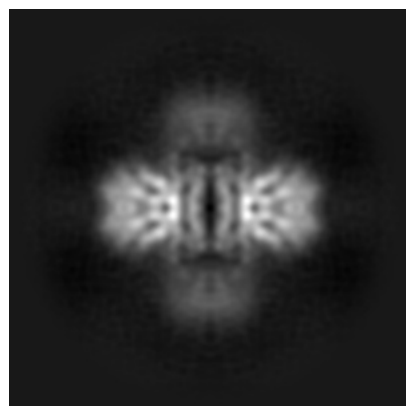
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11624. These allow visual inspection of the internal detail of the map and identification of artifacts.

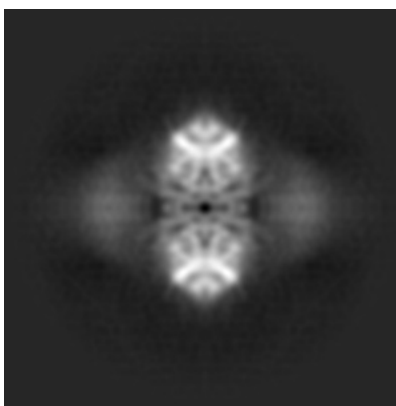
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

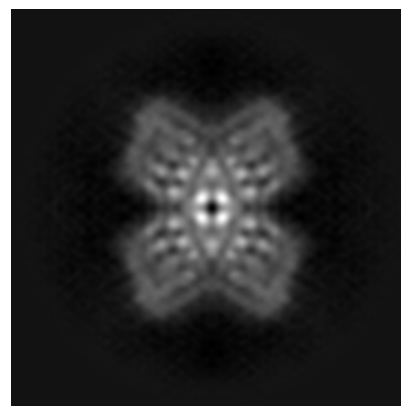
6.1.1 Primary map



X

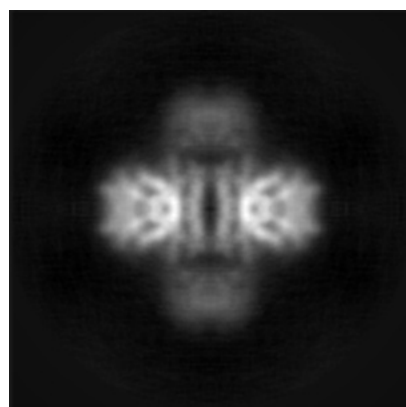


Y

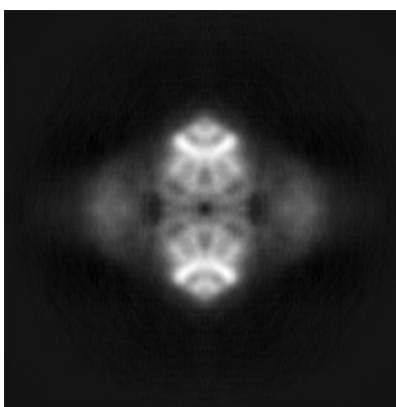


Z

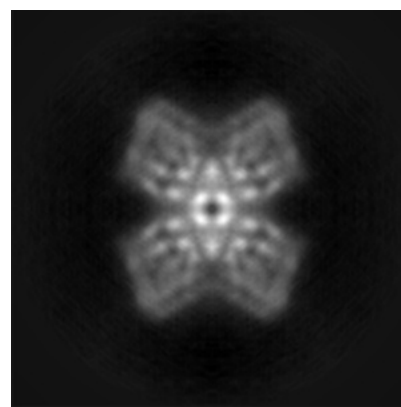
6.1.2 Raw map



X



Y

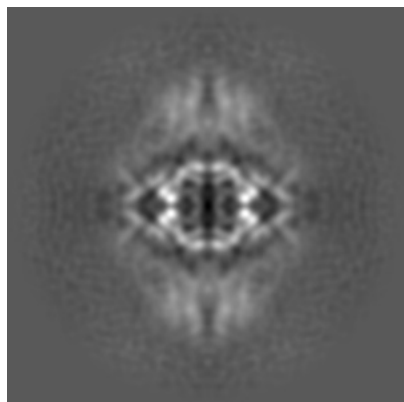


Z

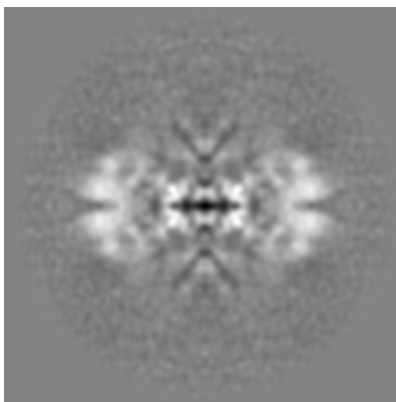
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

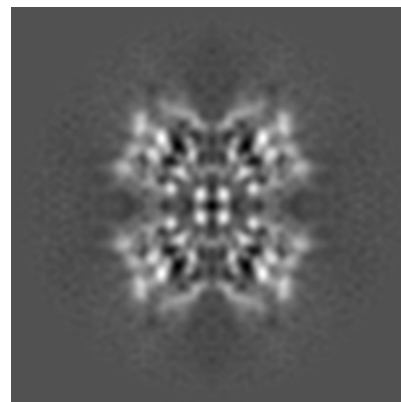
6.2.1 Primary map



X Index: 90

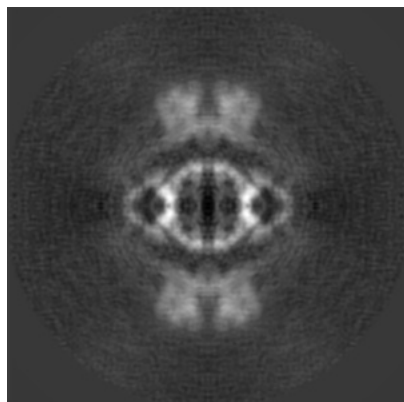


Y Index: 90

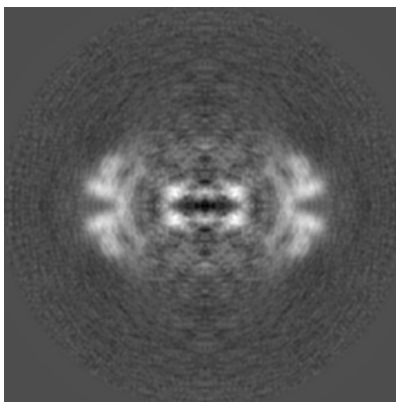


Z Index: 90

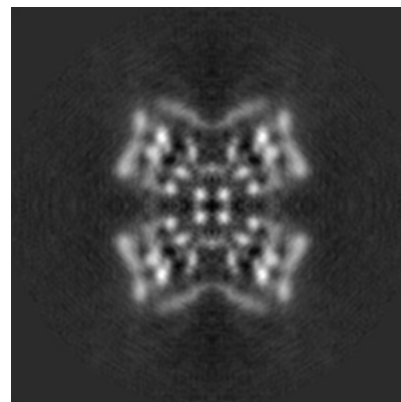
6.2.2 Raw map



X Index: 90



Y Index: 90

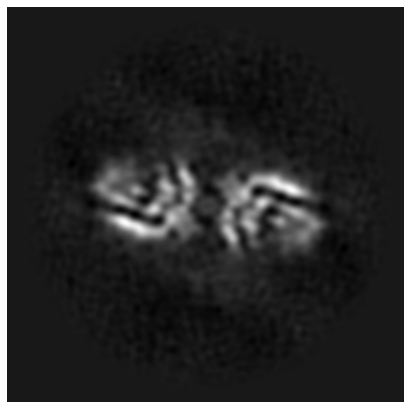


Z Index: 90

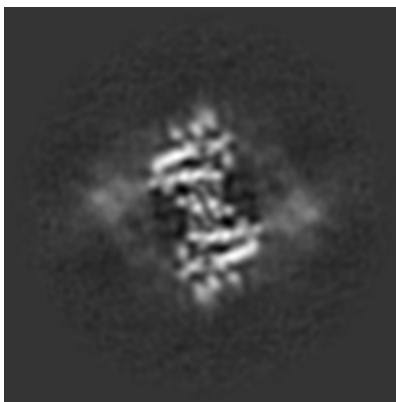
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

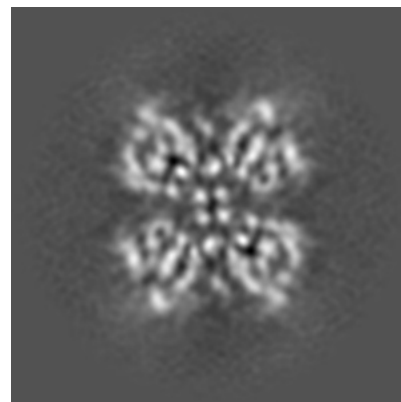
6.3.1 Primary map



X Index: 62

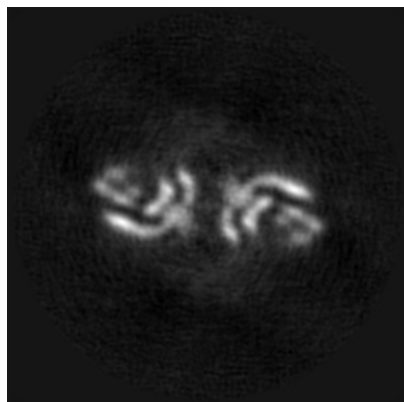


Y Index: 74

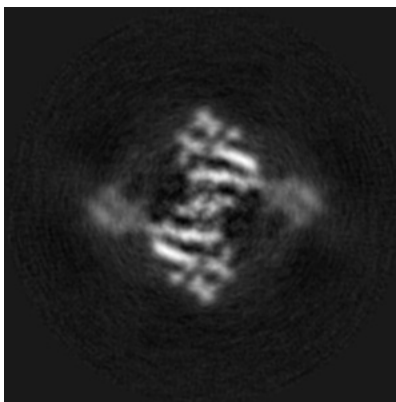


Z Index: 86

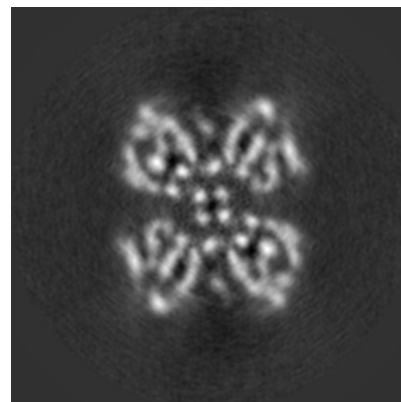
6.3.2 Raw map



X Index: 63



Y Index: 106

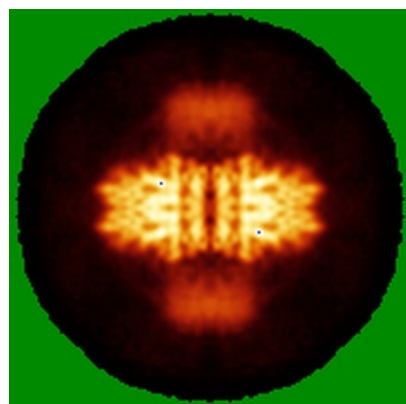


Z Index: 86

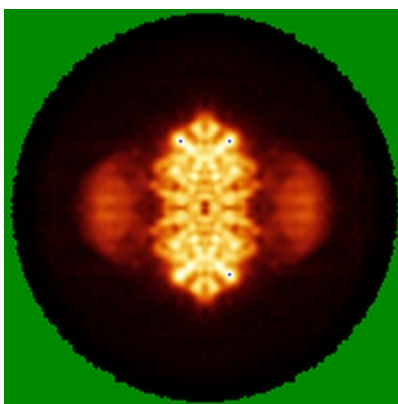
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

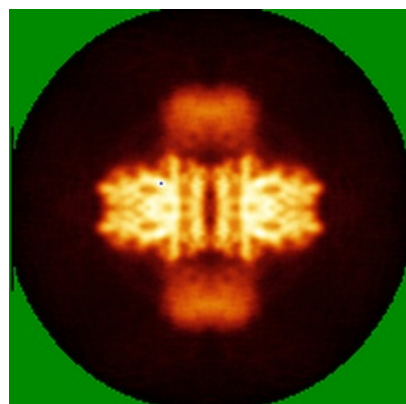


Y

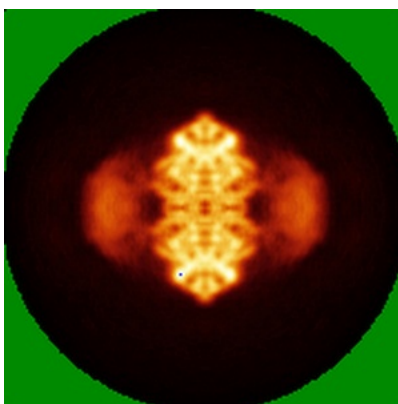


Z

6.4.2 Raw map



X



Y

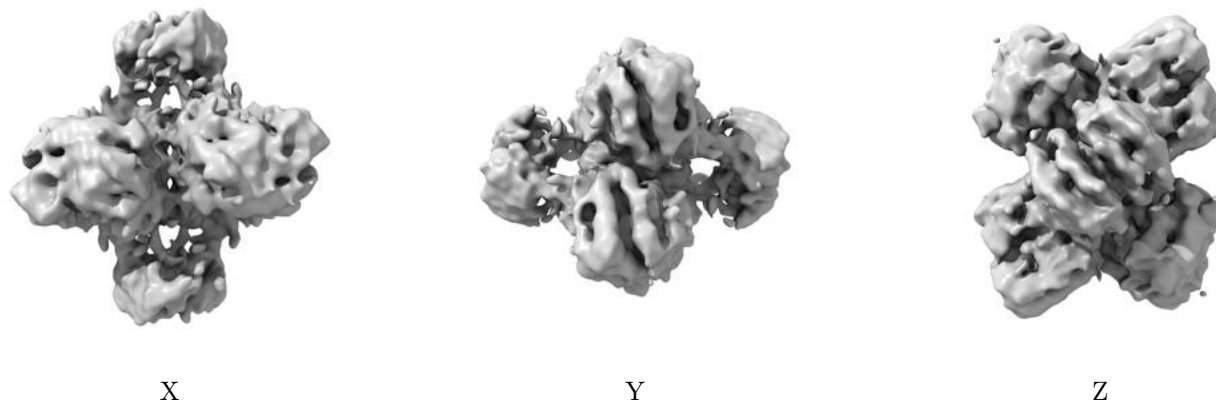


Z

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.

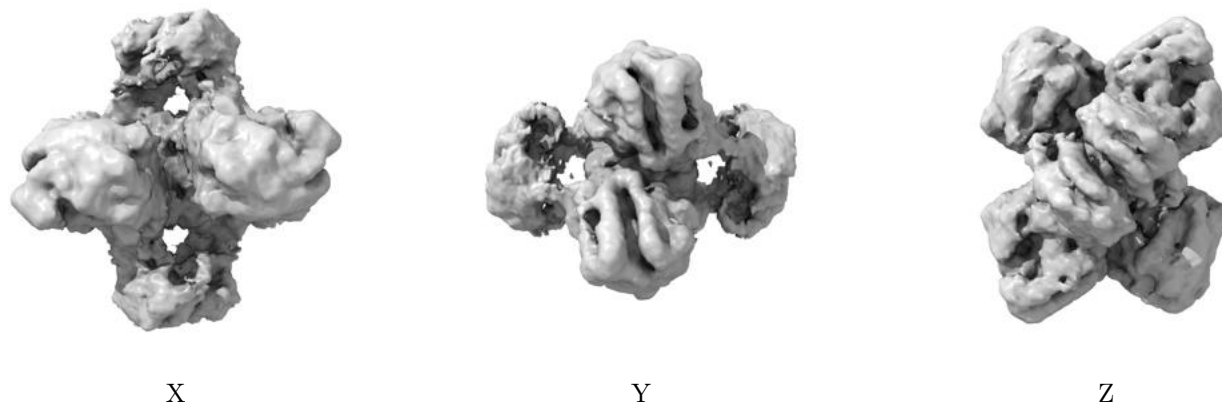
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.129. 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.

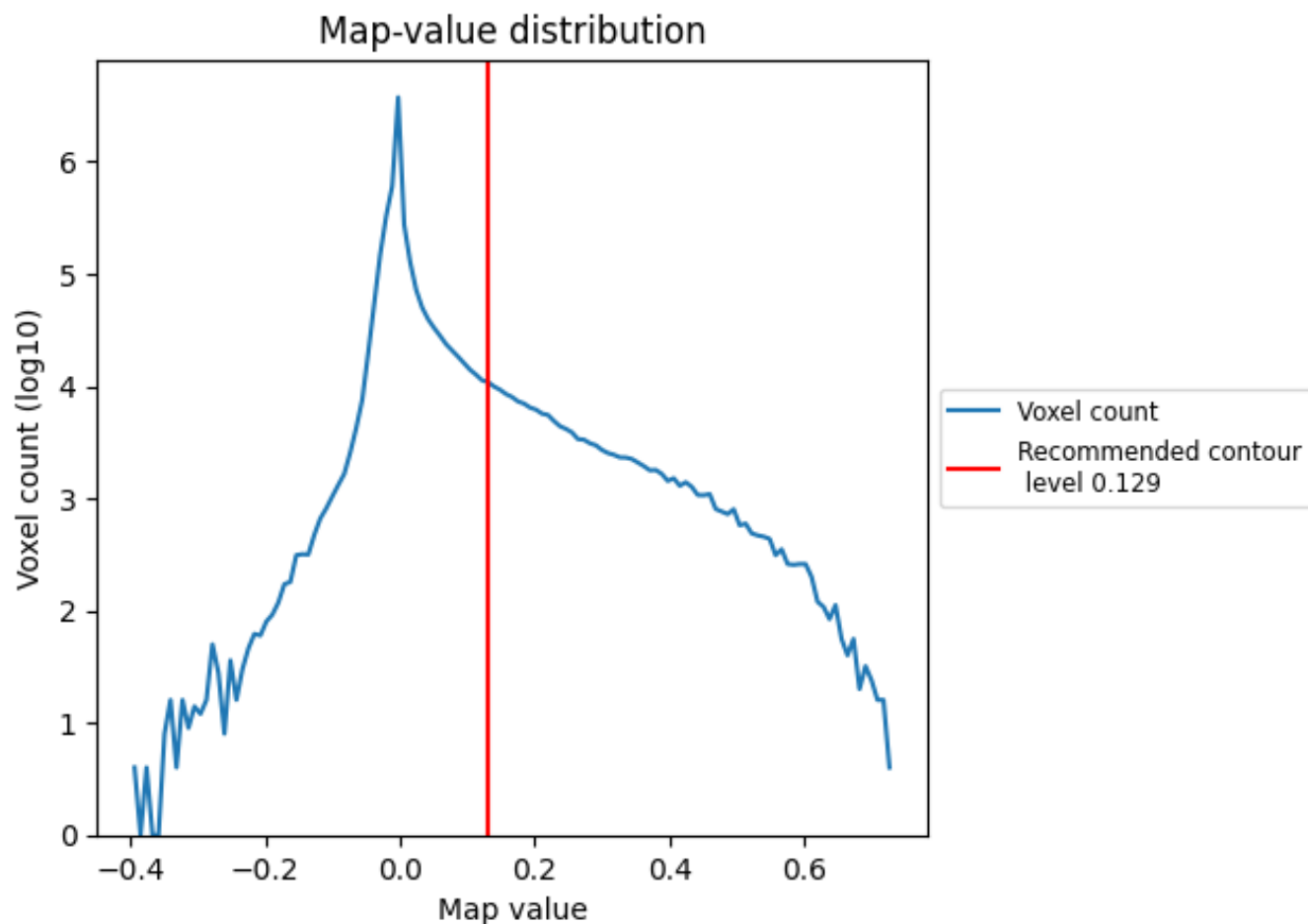
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

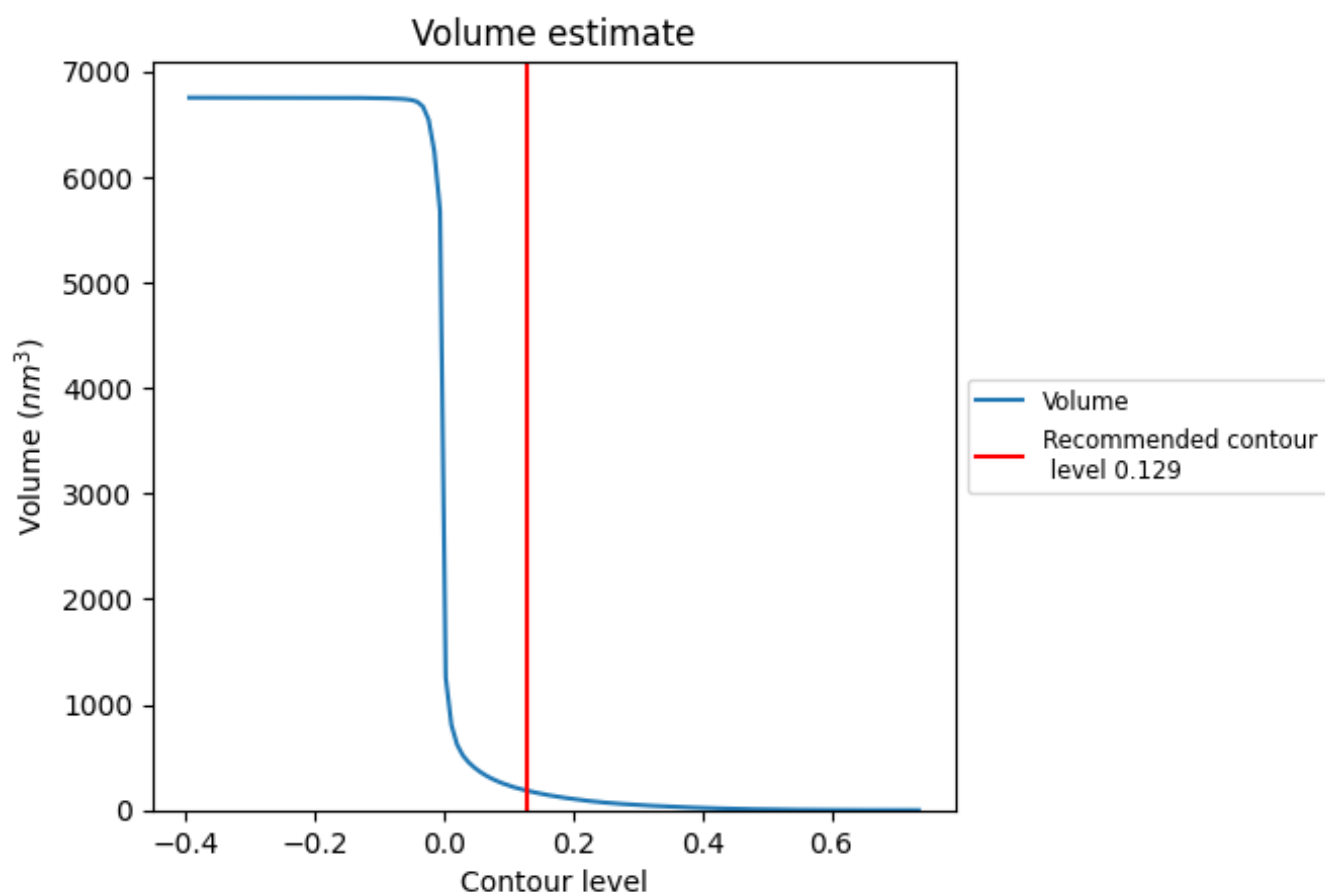
This section contains the results of statistical analysis of the map.

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.

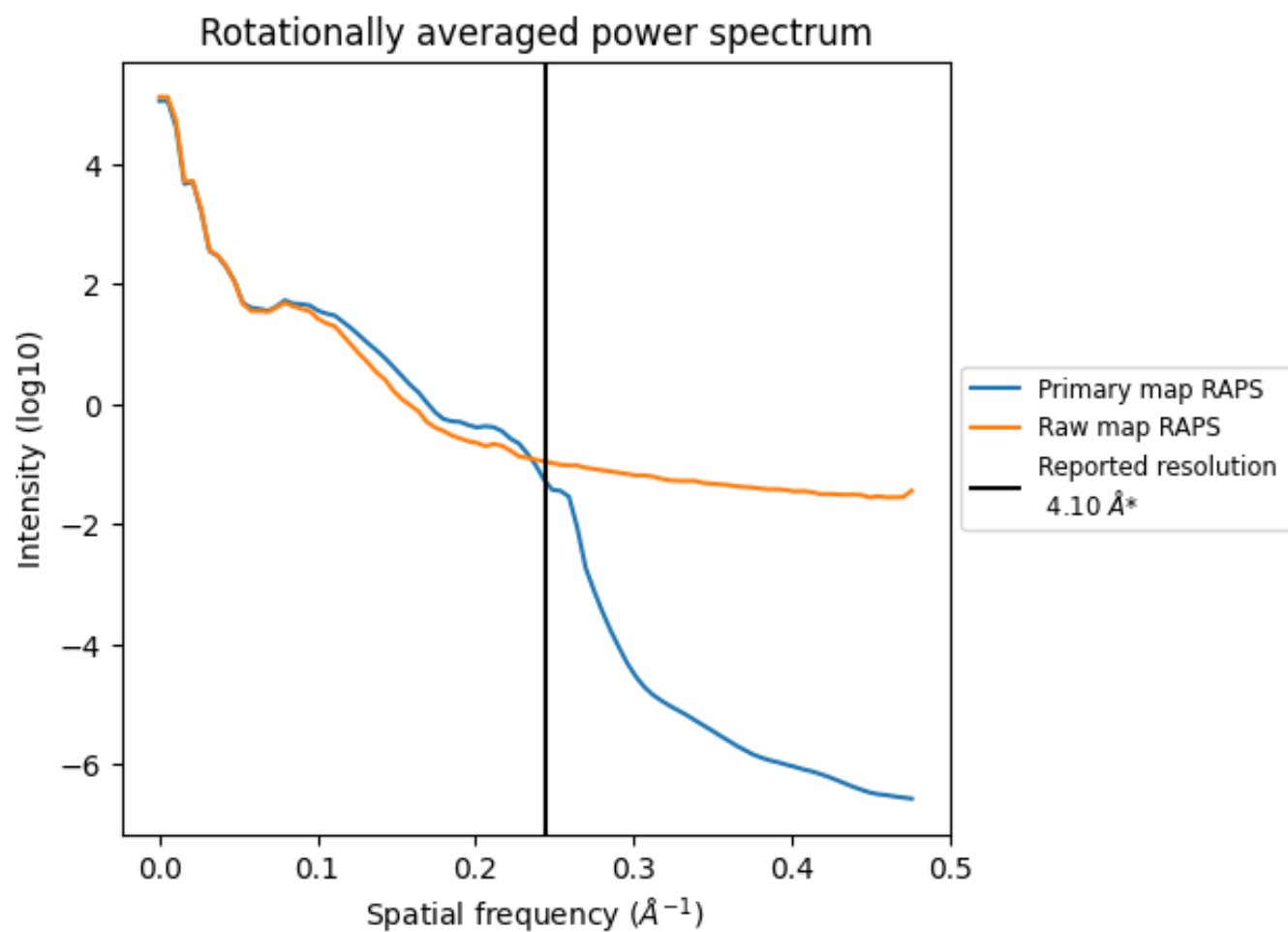
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 185 nm³; this corresponds to an approximate mass of 167 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 ⓘ

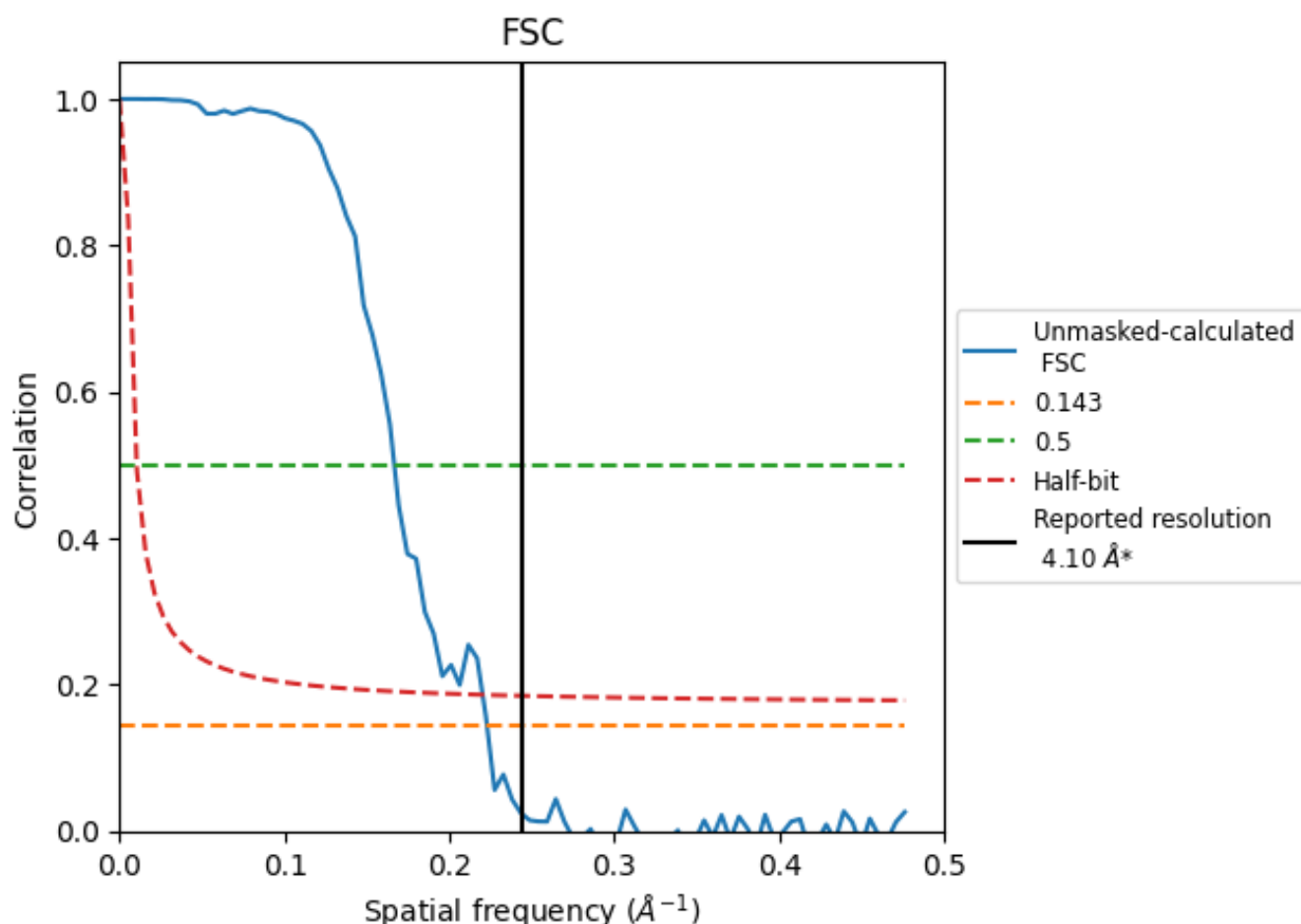


*Reported resolution corresponds to spatial frequency of 0.244 \AA^{-1}

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 0.244 Å⁻¹

8.2 Resolution estimates [i](#)

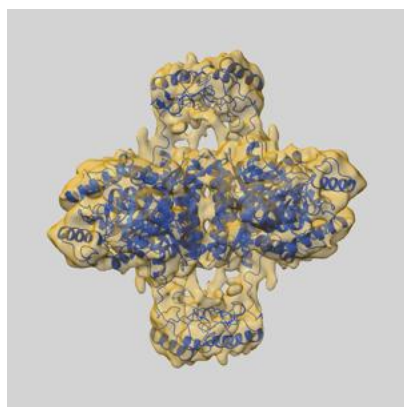
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.49	6.00	4.54

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

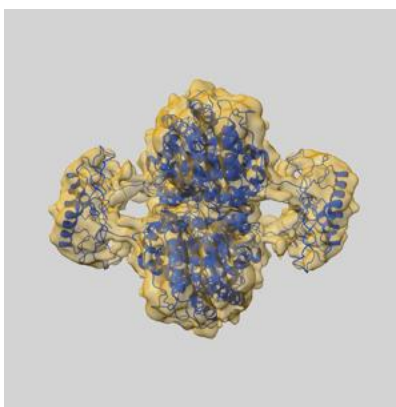
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11624 and PDB model 7A2G. Per-residue inclusion information can be found in section [3](#) on page [5](#).

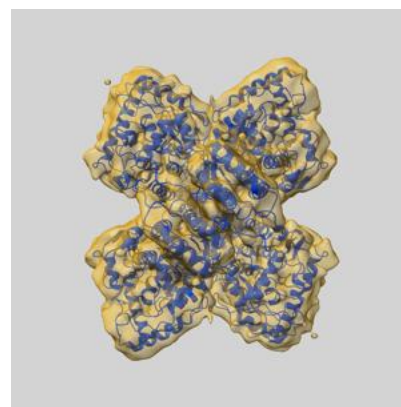
9.1 Map-model overlay [i](#)



X



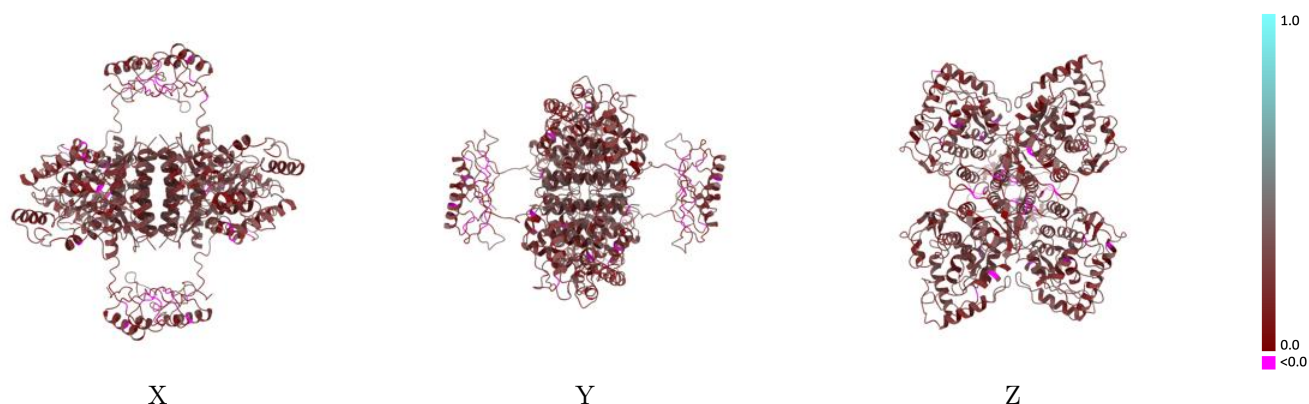
Y



Z

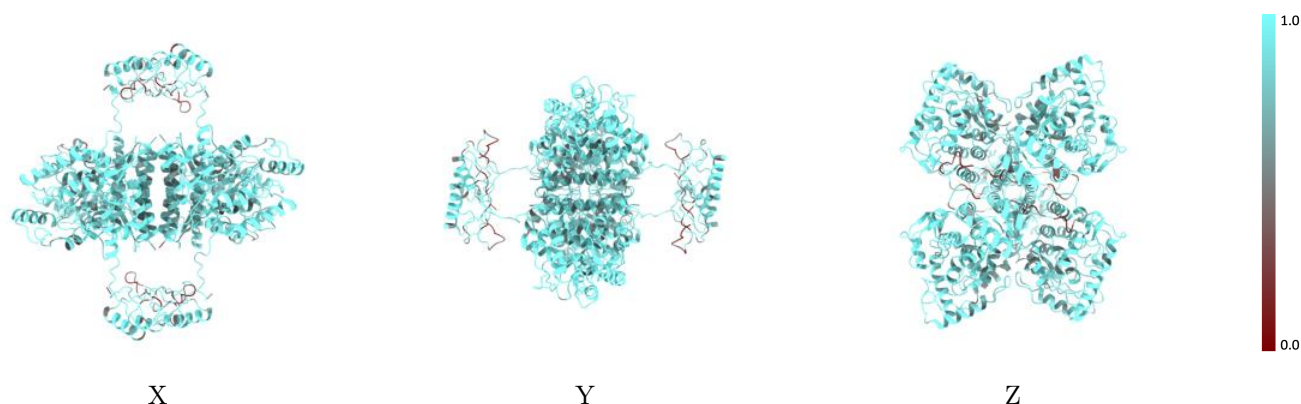
The images above show the 3D surface view of the map at the recommended contour level 0.129 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



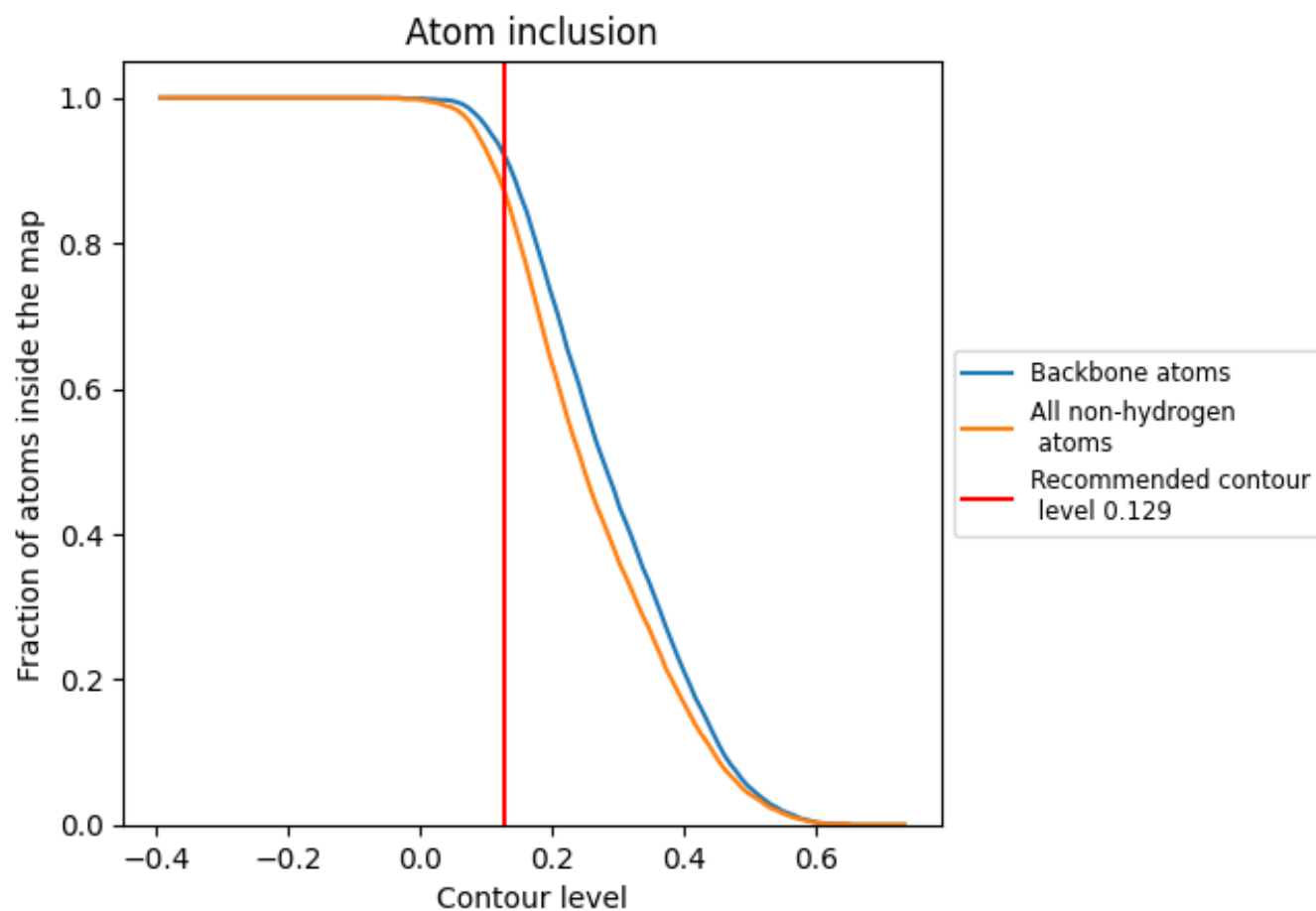
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.129).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 87% 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 (0.129) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8690	<div></div> 0.2340
A	<div></div> 0.8730	<div></div> 0.2350
B	<div></div> 0.8730	<div></div> 0.2330
C	<div></div> 0.8750	<div></div> 0.2350
D	<div></div> 0.8770	<div></div> 0.2340

