



wwPDB EM Validation Summary Report ⓘ

Jul 26, 2023 – 08:16 PM JST

PDB ID : 7YFM
EMDB ID : EMD-33793
Title : Structure of GluN1b-GluN2D NMDA receptor in complex with agonists glycine and glutamate.
Authors : Zhang, J.L.; Zhu, S.J.; Zhang, M.
Deposited on : 2022-07-08
Resolution : 5.10 Å (reported)
Based on initial model : 6WI1

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.dev50
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.34

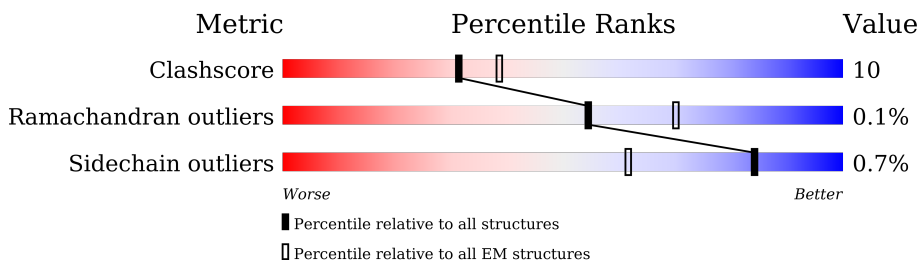
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.10 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	868	
1	C	868	
2	B	891	
2	D	891	

2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 18836 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 Isoform 6 of Glutamate receptor ionotropic, NMDA 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	663	Total	C	N	O	S	0	0
			5010	3169	875	941	25		
1	C	663	Total	C	N	O	S	0	0
			5010	3169	875	941	25		

- Molecule 2 is a protein called Glutamate receptor ionotropic, NMDA 2D.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	596	Total	C	N	O	S	0	0
			4408	2821	749	823	15		
2	D	596	Total	C	N	O	S	0	0
			4408	2821	749	823	15		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	880	ALA	-	expression tag	UNP O15399
B	881	ALA	-	expression tag	UNP O15399
B	882	SER	-	expression tag	UNP O15399
B	883	ALA	-	expression tag	UNP O15399
B	884	TRP	-	expression tag	UNP O15399
B	885	SER	-	expression tag	UNP O15399
B	886	HIS	-	expression tag	UNP O15399
B	887	PRO	-	expression tag	UNP O15399
B	888	GLN	-	expression tag	UNP O15399
B	889	PHE	-	expression tag	UNP O15399
B	890	GLU	-	expression tag	UNP O15399
B	891	LYS	-	expression tag	UNP O15399
D	880	ALA	-	expression tag	UNP O15399
D	881	ALA	-	expression tag	UNP O15399
D	882	SER	-	expression tag	UNP O15399
D	883	ALA	-	expression tag	UNP O15399
D	884	TRP	-	expression tag	UNP O15399

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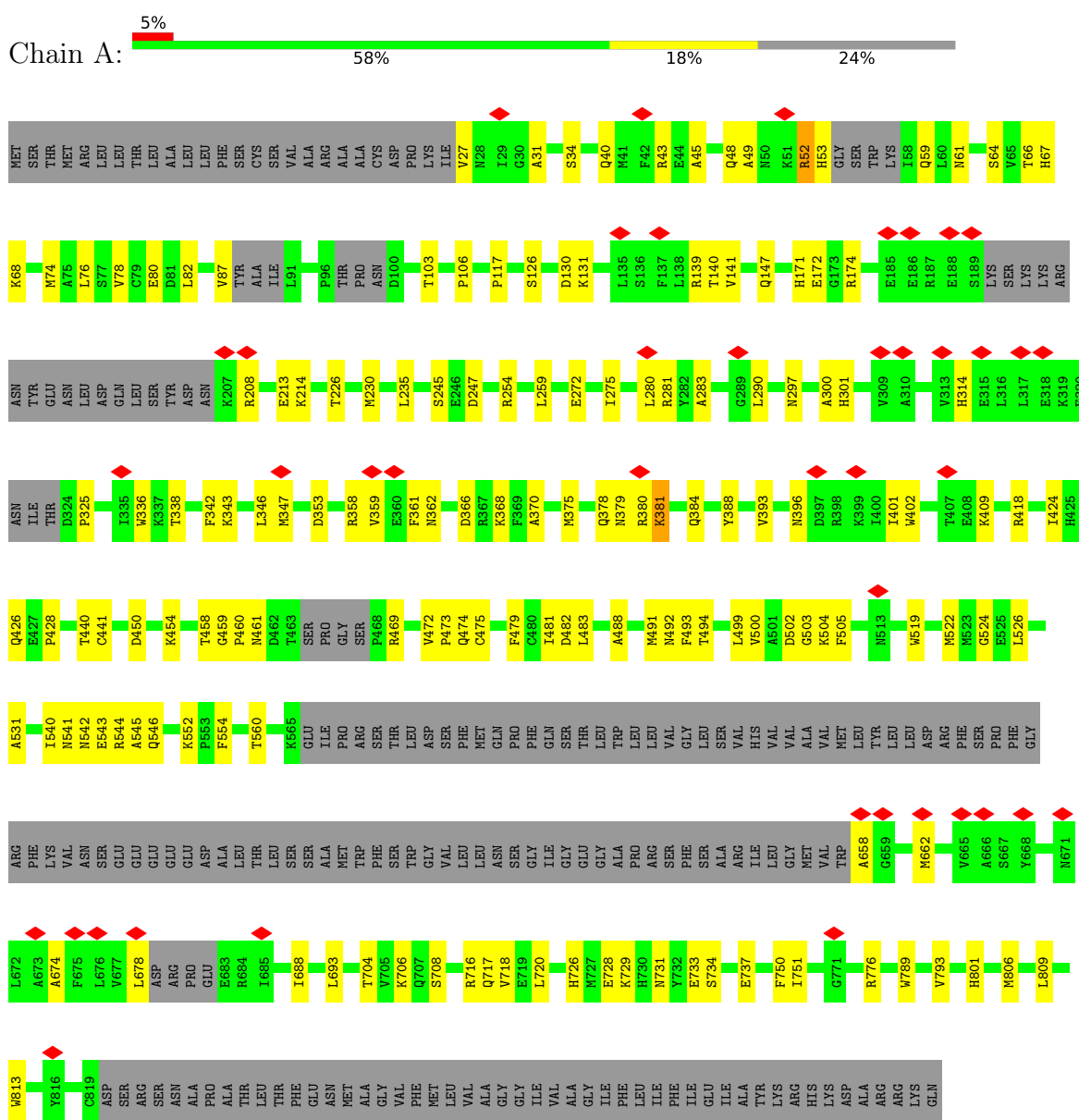
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Chain	Residue	Modelled	Actual	Comment	Reference
D	885	SER	-	expression tag	UNP O15399
D	886	HIS	-	expression tag	UNP O15399
D	887	PRO	-	expression tag	UNP O15399
D	888	GLN	-	expression tag	UNP O15399
D	889	PHE	-	expression tag	UNP O15399
D	890	GLU	-	expression tag	UNP O15399
D	891	LYS	-	expression tag	UNP O15399

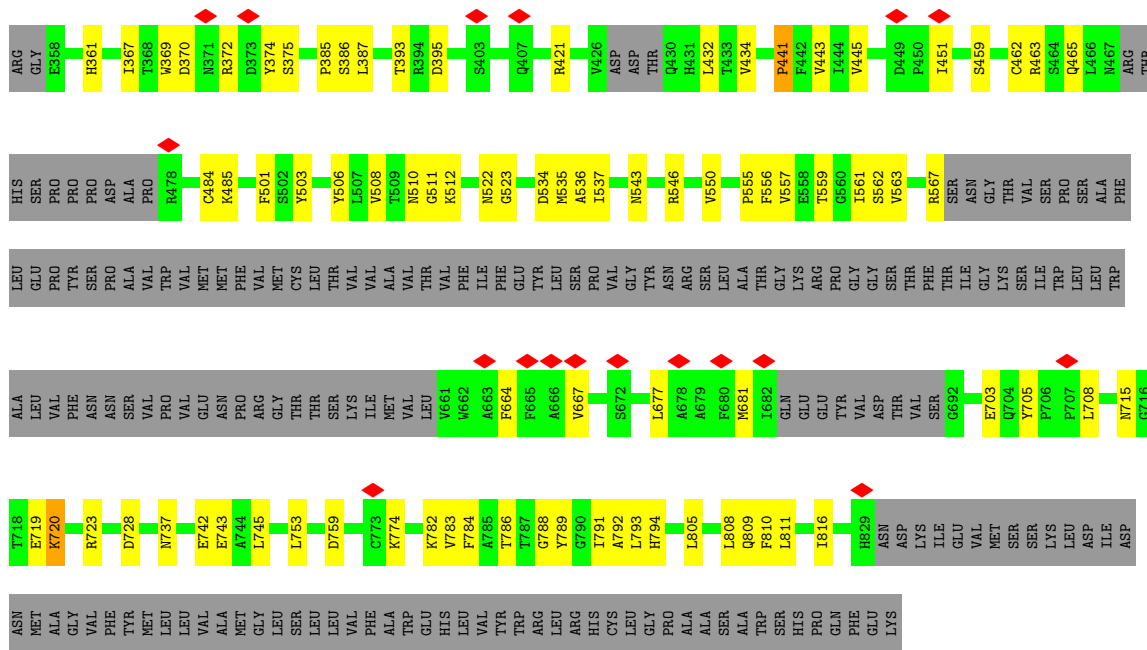
3 Residue-property plots i

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.

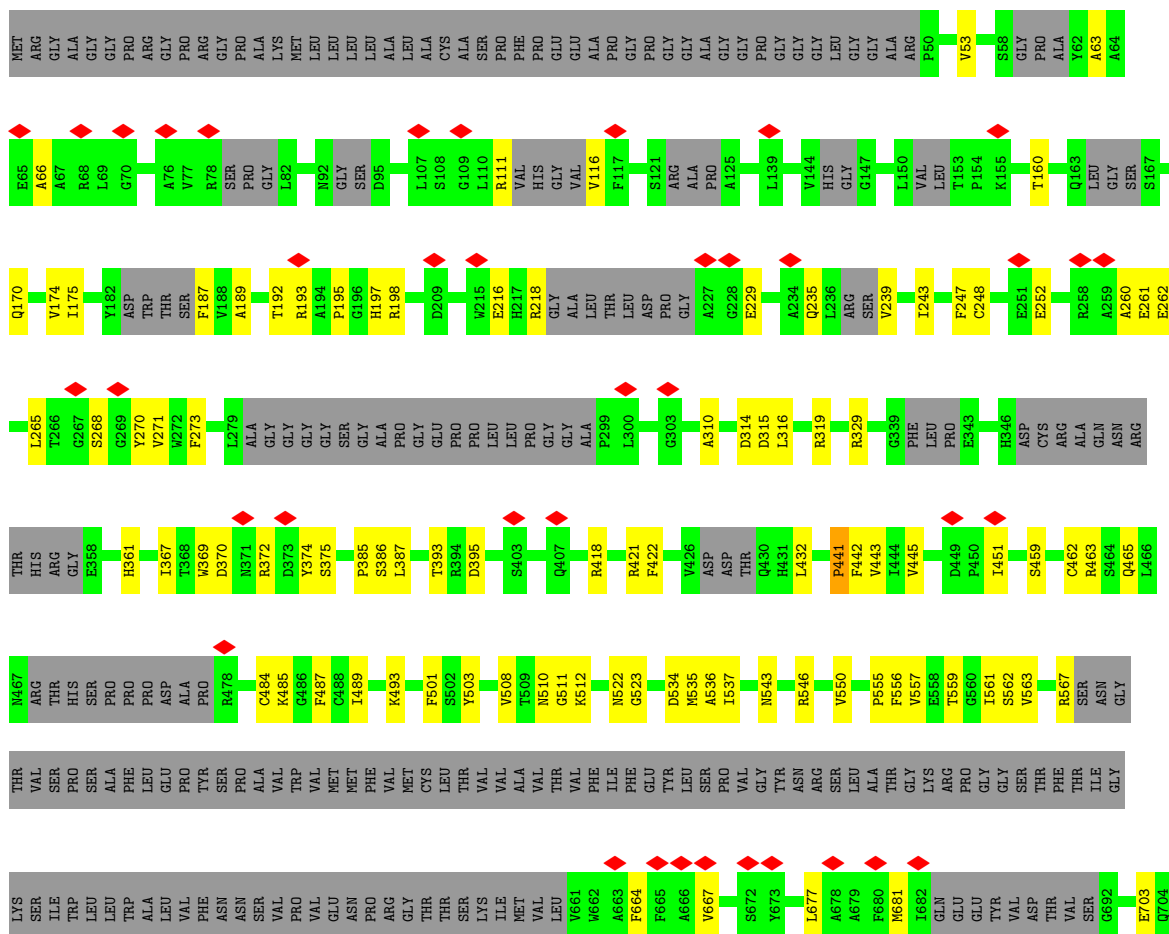
- Molecule 1: Isoform 6 of Glutamate receptor ionotropic, NMDA 1



- Molecule 1: Isoform 6 of Glutamate receptor ionotropic, NMDA 1



● Molecule 2: Glutamate receptor ionotropic, NMDA 2D



Y705	P706	P707	L708	N715	G716	S717	T718	E719	K720	R723	D728	N737	E742	E743	A744	L745	L753	D759	C773	K774	K782	V783	F784	A785	T786	T787	G788	Y789	G790	I791	A792	L793	H794	L805	L808	Q809	F810	L811	I816	H829	ASN	ASP	LYS	ILE	GLU	VAL				
MET	SER	SER	LYS	LEU	ASP	ILE	ASP	ASN	MET	ALA	GLY	VAL	PHE	TYR	MET	LEU	LEU	VAL	ALA	ALA	TRP	GLU	HIS	LEU	VAL	VAL	TRP	TRP	ARG	LEU	ANG	HIS	CYS	LEU	GLY	PRO	ALA	ALA	SER	SER	ALA	TRP	SER	HIS	PRO	PRO	GLN	PHE	GLU	LYS

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	98449	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	DIRECT ELECTRON DE-10 (5k x 4k)	Depositor
Maximum map value	0.025	Depositor
Minimum map value	-0.011	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0066	Depositor
Map size (\AA)	232.4, 232.4, 232.4	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

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	0.25	0/5110	0.52	0/6928
1	C	0.25	0/5110	0.52	0/6928
2	B	0.25	0/4488	0.50	0/6097
2	D	0.25	0/4488	0.50	0/6097
All	All	0.25	0/19196	0.51	0/26050

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

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	5010	0	4732	101	0
1	C	5010	0	4732	96	0
2	B	4408	0	4162	78	0
2	D	4408	0	4162	83	0
All	All	18836	0	17788	350	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 10.

The worst 5 of 350 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:D:261:GLU:OE2	2:D:265:LEU:N	2.16	0.78
1:A:459:GLY:HA3	1:A:499:LEU:H	1.49	0.78
1:C:459:GLY:HA3	1:C:499:LEU:H	1.49	0.76
2:B:261:GLU:OE2	2:B:265:LEU:N	2.16	0.76
1:A:280:LEU:HD23	1:A:281:ARG:HG3	1.70	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	645/868 (74%)	597 (93%)	48 (7%)	0	100	100
1	C	645/868 (74%)	596 (92%)	49 (8%)	0	100	100
2	B	558/891 (63%)	513 (92%)	44 (8%)	1 (0%)	47	81
2	D	558/891 (63%)	513 (92%)	44 (8%)	1 (0%)	47	81
All	All	2406/3518 (68%)	2219 (92%)	185 (8%)	2 (0%)	54	85

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	441	PRO
2	D	441	PRO

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	504/750 (67%)	500 (99%)	4 (1%)	81	89
1	C	504/750 (67%)	500 (99%)	4 (1%)	81	89
2	B	431/720 (60%)	428 (99%)	3 (1%)	84	90
2	D	431/720 (60%)	428 (99%)	3 (1%)	84	90
All	All	1870/2940 (64%)	1856 (99%)	14 (1%)	84	90

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	52	ARG
1	C	208	ARG
2	D	782	LYS
2	D	111	ARG
2	D	720	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	707	GLN
2	D	361	HIS
1	A	707	GLN
1	A	542	ASN
2	D	522	ASN

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.

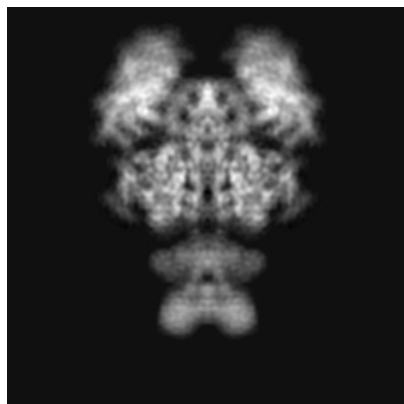
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33793. These allow visual inspection of the internal detail of the map and identification of artifacts.

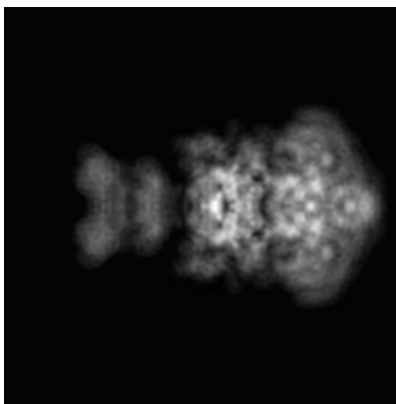
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

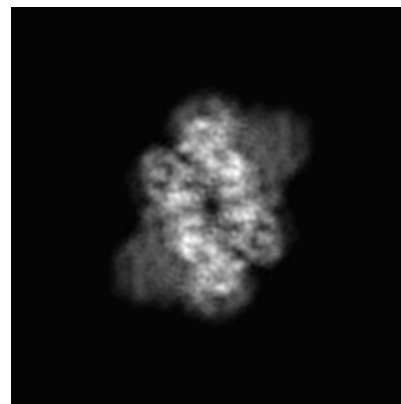
6.1.1 Primary map



X

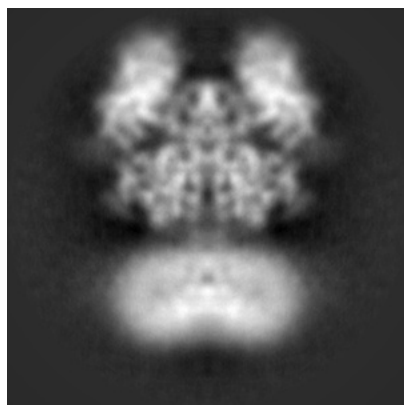


Y

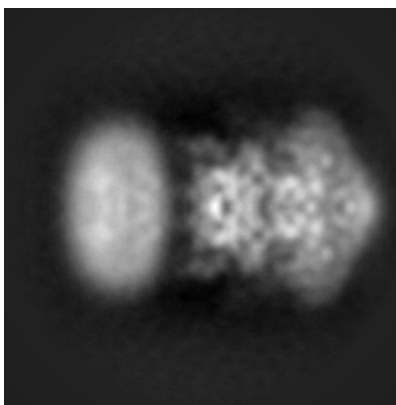


Z

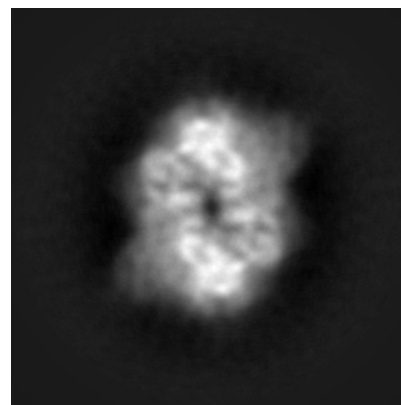
6.1.2 Raw map



X



Y

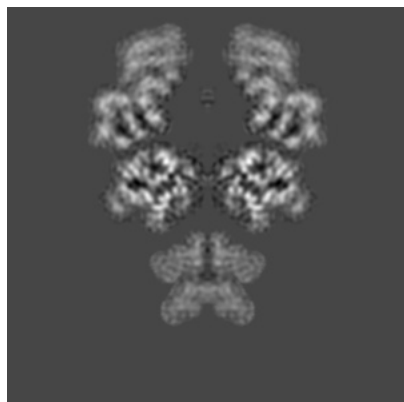


Z

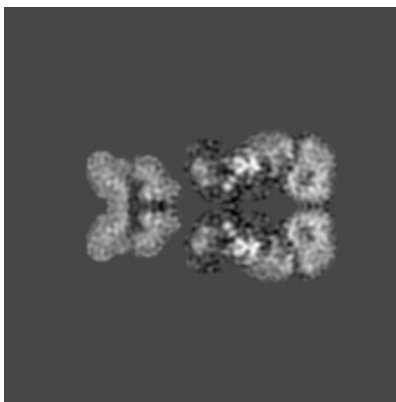
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

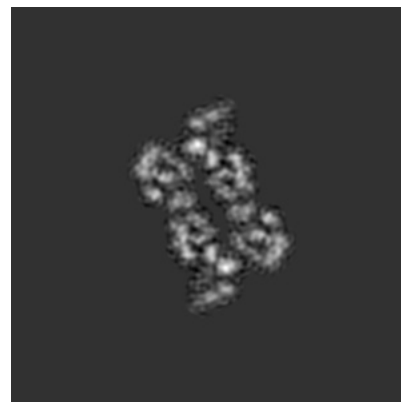
6.2.1 Primary map



X Index: 140

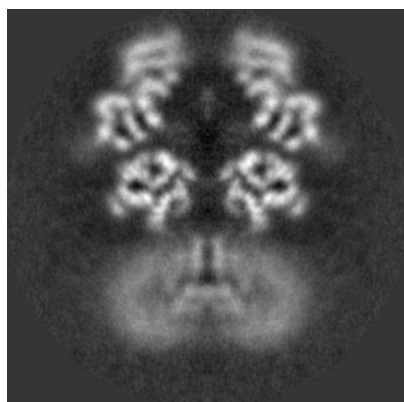


Y Index: 140

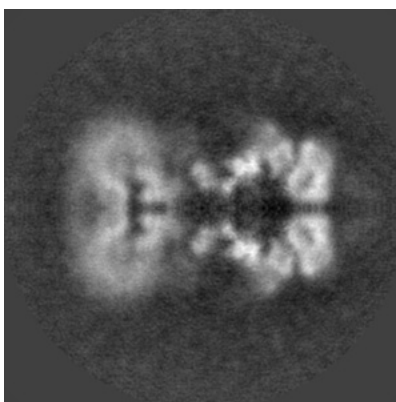


Z Index: 140

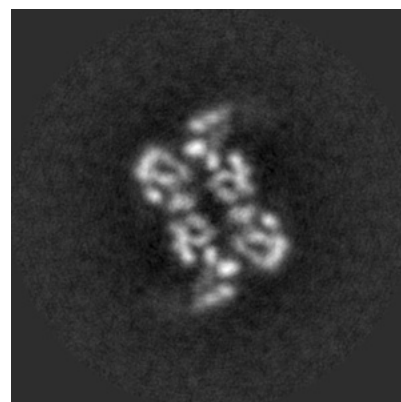
6.2.2 Raw map



X Index: 140



Y Index: 140

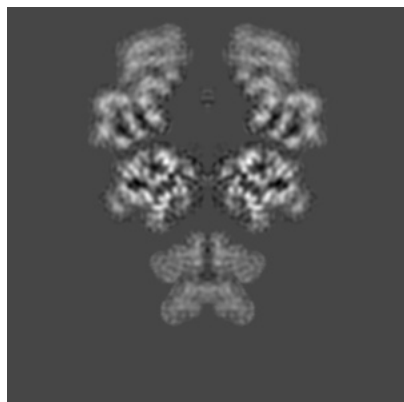


Z Index: 140

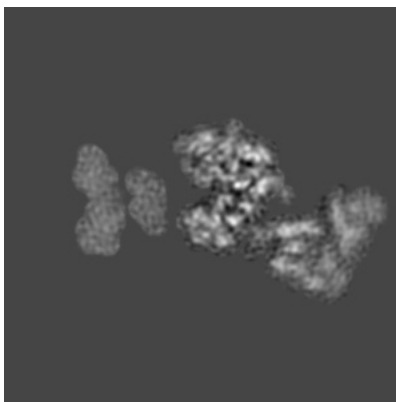
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

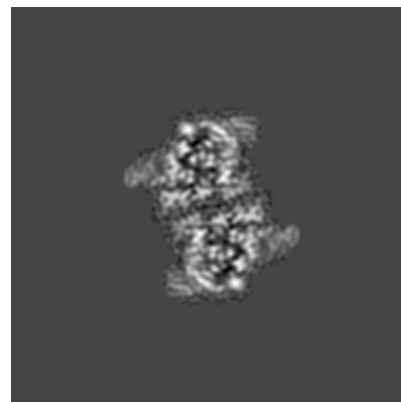
6.3.1 Primary map



X Index: 140

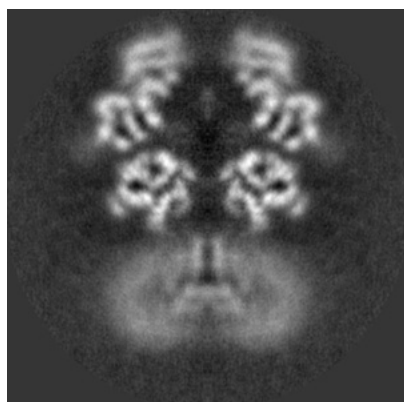


Y Index: 116

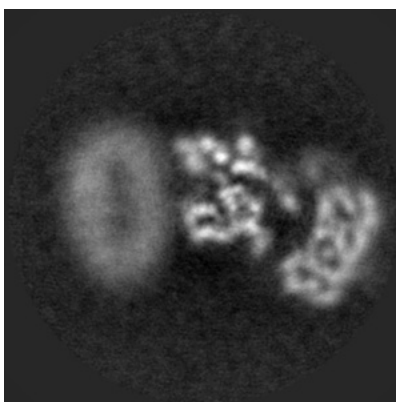


Z Index: 161

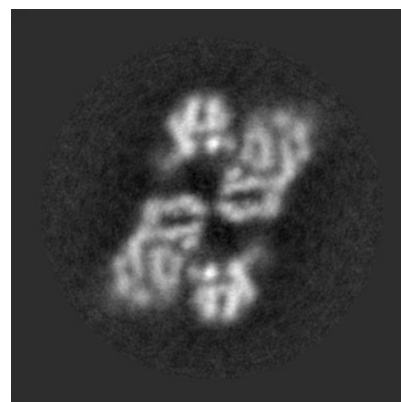
6.3.2 Raw map



X Index: 140



Y Index: 107

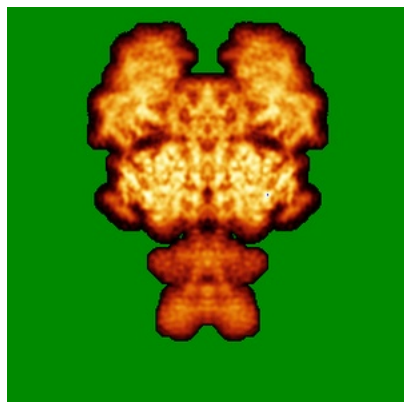


Z Index: 215

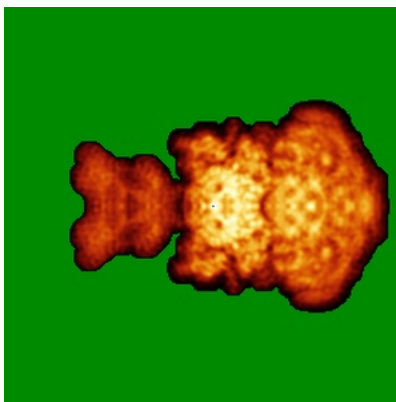
The images above show the largest variance slices of the map in three orthogonal directions.

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

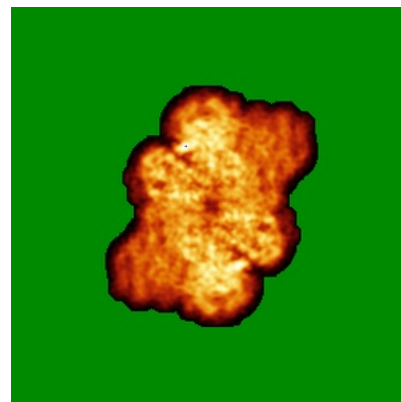
6.4.1 Primary map



X

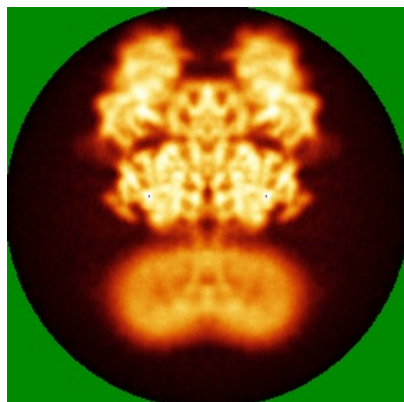


Y

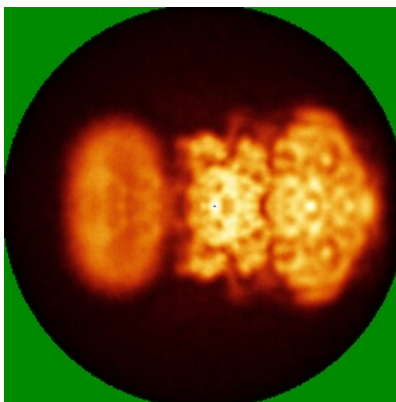


Z

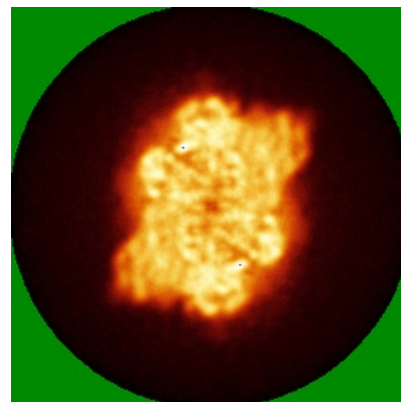
6.4.2 Raw map



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.

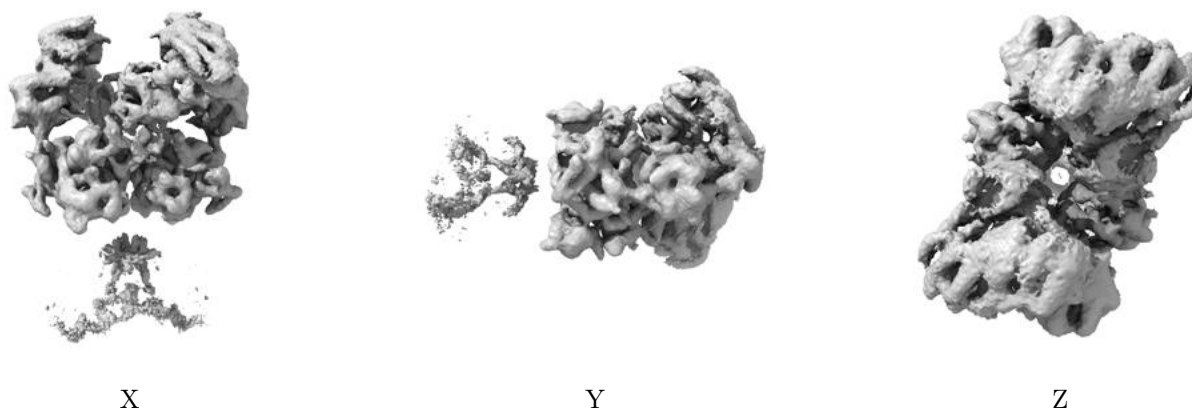
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0066. 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.

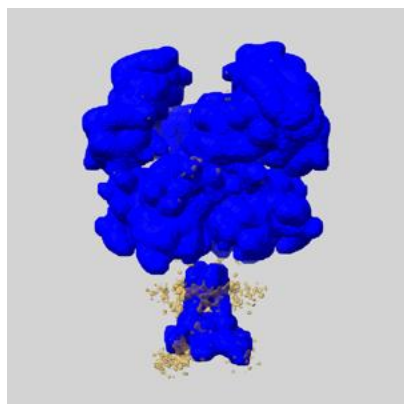
6.6 Mask visualisation [i](#)

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

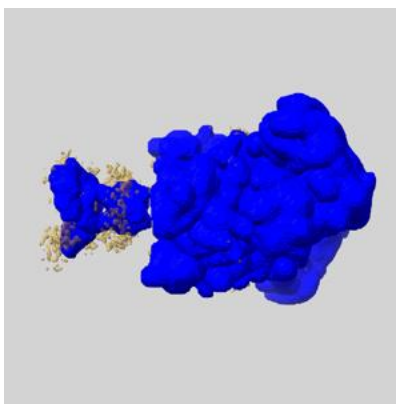
A mask typically either:

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

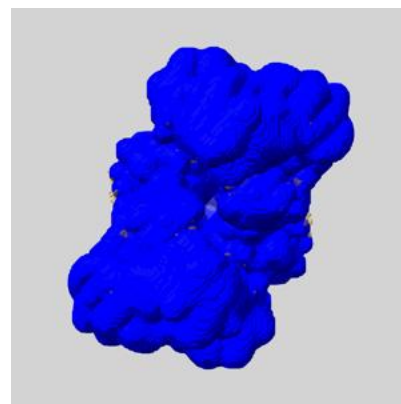
6.6.1 emd_33793_msk_1.map [i](#)



X



Y

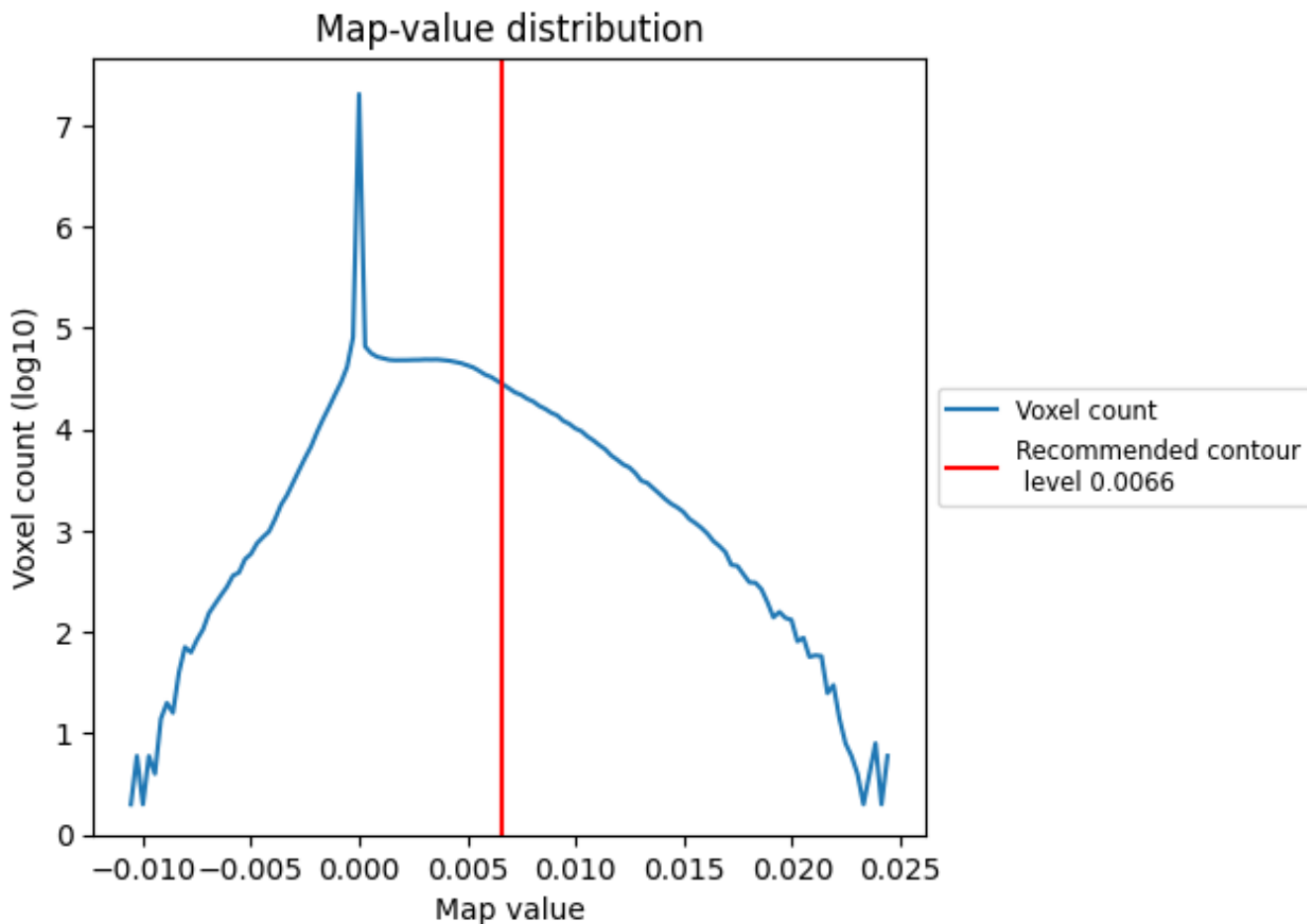


Z

7 Map analysis [i](#)

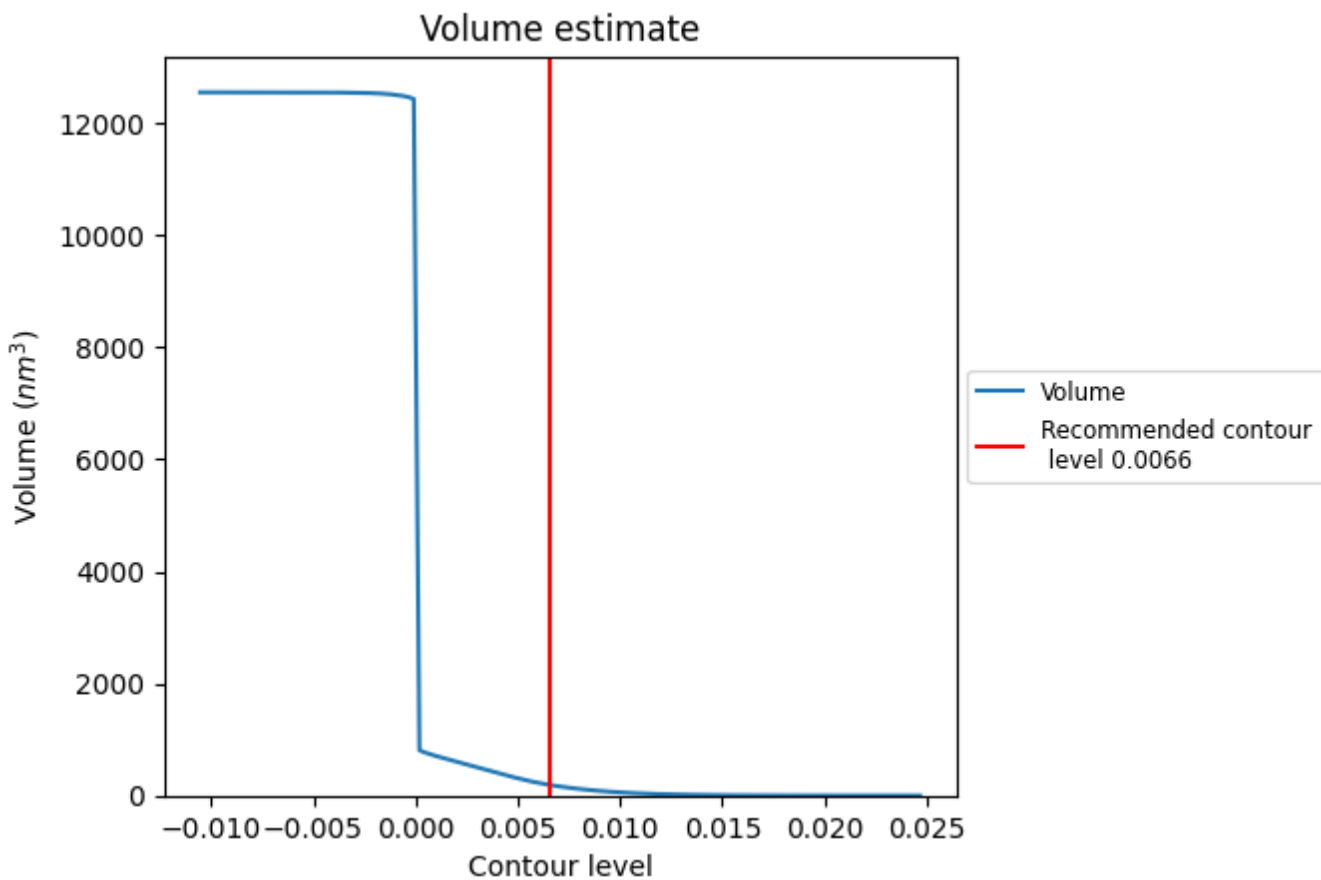
This section contains the results of statistical analysis of the map.

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.

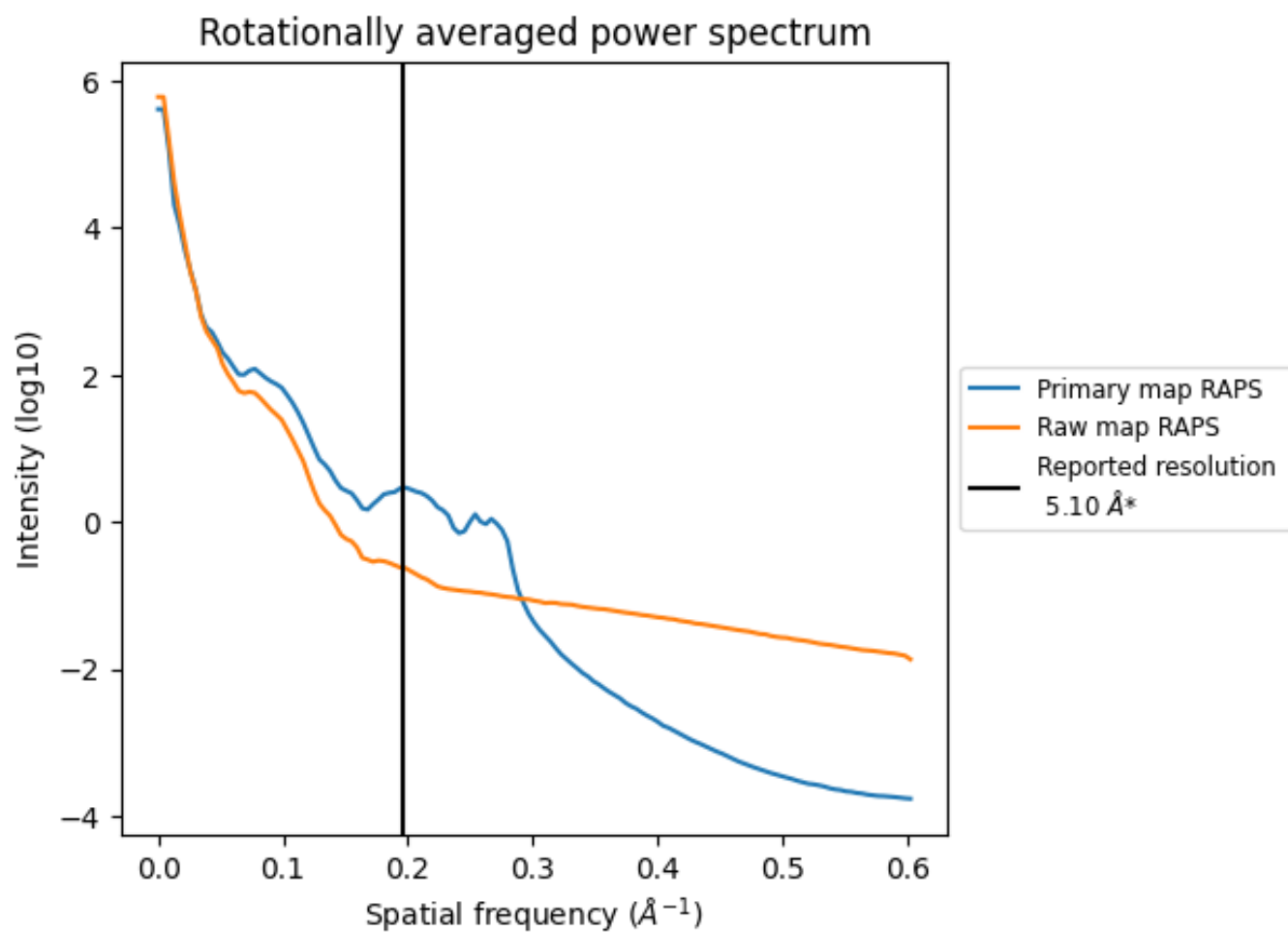
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 188 nm³; this corresponds to an approximate mass of 169 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 [\(i\)](#)

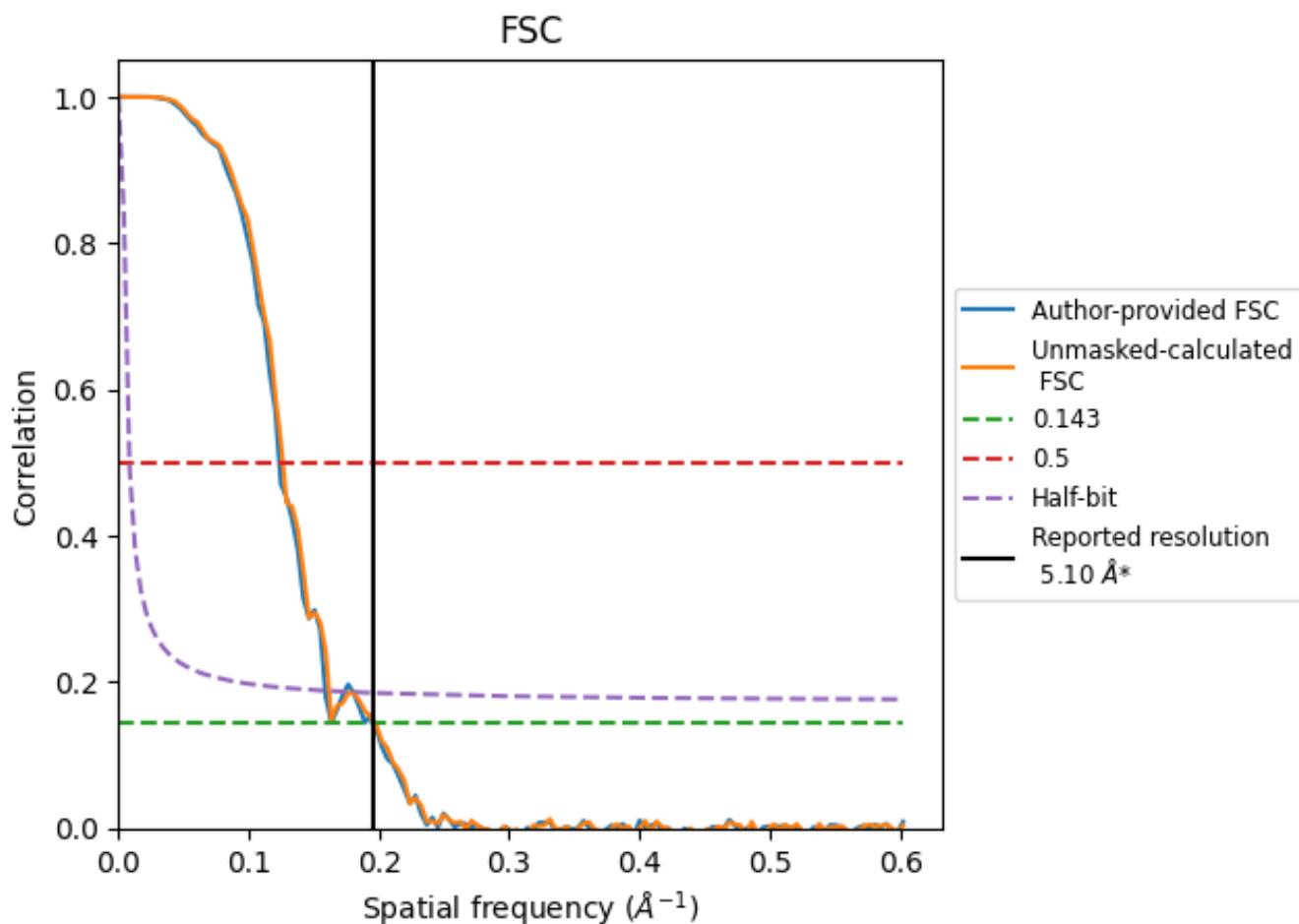


*Reported resolution corresponds to spatial frequency of 0.196 Å⁻¹

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 0.196 Å⁻¹

8.2 Resolution estimates [i](#)

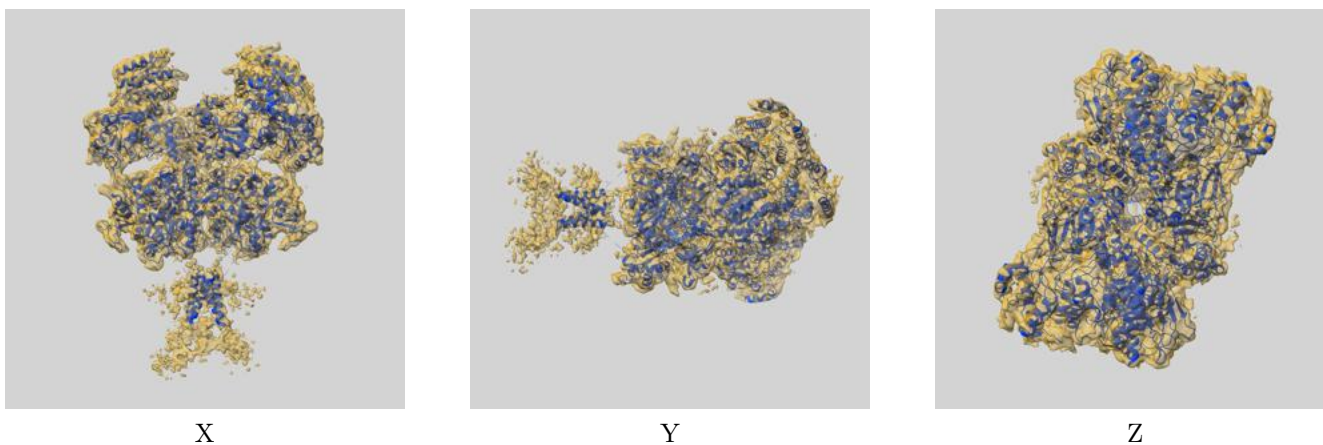
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.10	-	-
Author-provided FSC curve	5.10	8.10	6.30
Unmasked-calculated*	5.07	7.92	6.18

*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-33793 and PDB model 7YFM. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



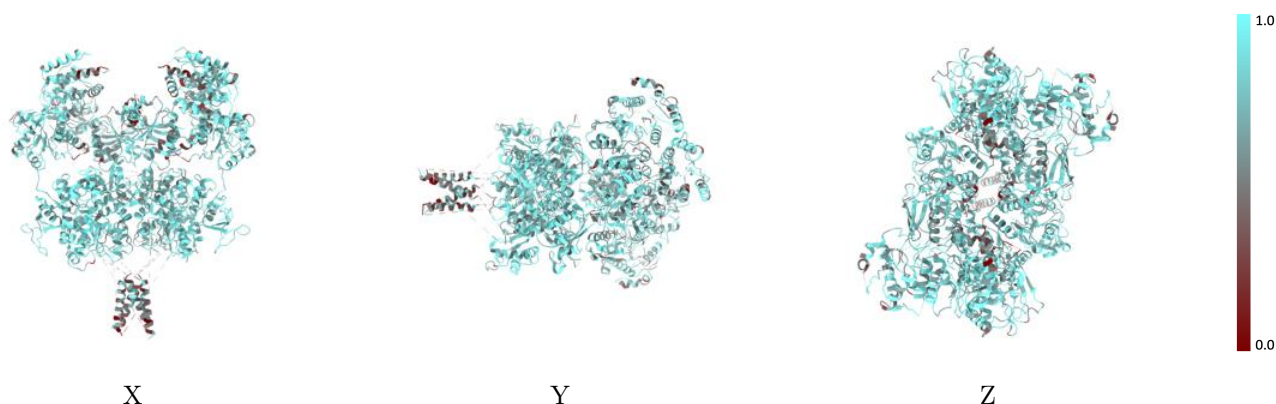
The images above show the 3D surface view of the map at the recommended contour level 0.0066 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



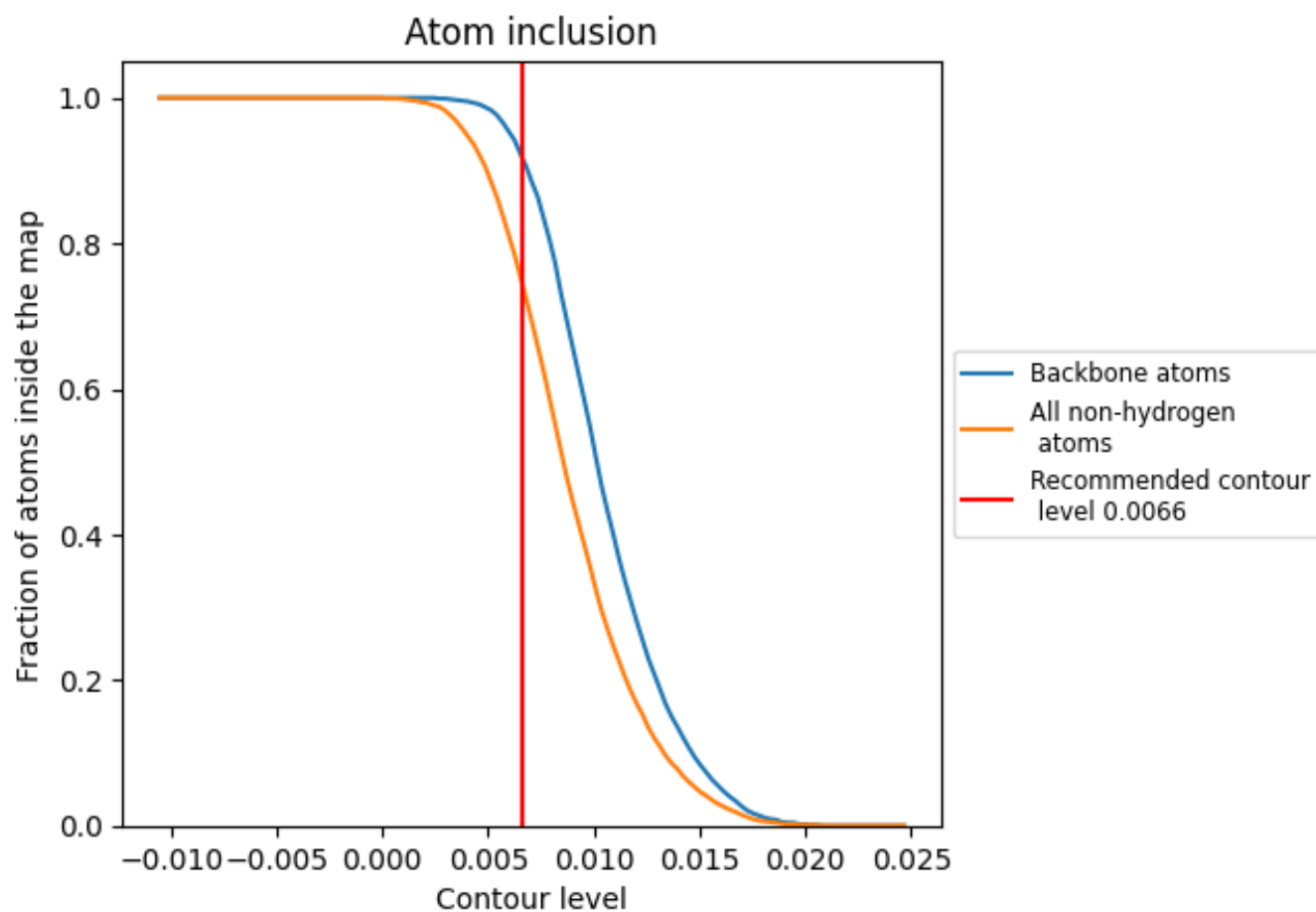
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0066).











9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 75% 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 (0.0066) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7460	 0.3090
A	 0.7550	 0.3080
B	 0.7350	 0.3100
C	 0.7550	 0.3080
D	 0.7370	 0.3090

