



## wwPDB EM Validation Summary Report ⓘ

Oct 12, 2024 – 01:24 PM EDT

PDB ID : 5KK2  
EMDB ID : EMD-8256  
Title : Architecture of fully occupied GluA2 AMPA receptor - TARP complex elucidated by single particle cryo-electron microscopy  
Authors : Zhao, Y.; Chen, S.; Yoshioka, C.; Bacongus, I.; Gouaux, E.  
Deposited on : 2016-06-20  
Resolution : 7.30 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev113  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

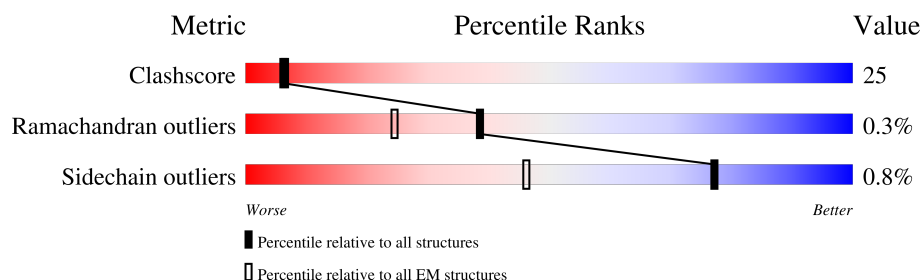
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 7.30 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	889	
1	B	889	
1	C	889	
1	D	889	
2	E	323	
2	F	323	
2	G	323	
2	H	323	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14639 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 Glutamate receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	408	Total	C	N	O	S	0	0
			2831	1822	453	538	18		
1	B	406	Total	C	N	O	S	0	0
			2810	1801	452	540	17		
1	C	406	Total	C	N	O	S	0	0
			2819	1812	452	536	19		
1	D	407	Total	C	N	O	S	0	0
			2829	1819	456	536	18		

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	586	ARG	GLN	variant	UNP P19491
A	848	ASP	-	insertion	UNP P19491
A	849	TYR	-	insertion	UNP P19491
A	850	LYS	-	insertion	UNP P19491
A	851	ASP	-	insertion	UNP P19491
A	852	ASP	-	insertion	UNP P19491
A	853	ASP	-	insertion	UNP P19491
A	854	ASP	TYR	conflict	UNP P19491
B	586	ARG	GLN	variant	UNP P19491
B	848	ASP	-	insertion	UNP P19491
B	849	TYR	-	insertion	UNP P19491
B	850	LYS	-	insertion	UNP P19491
B	851	ASP	-	insertion	UNP P19491
B	852	ASP	-	insertion	UNP P19491
B	853	ASP	-	insertion	UNP P19491
B	854	ASP	TYR	conflict	UNP P19491
C	586	ARG	GLN	variant	UNP P19491
C	848	ASP	-	insertion	UNP P19491
C	849	TYR	-	insertion	UNP P19491
C	850	LYS	-	insertion	UNP P19491
C	851	ASP	-	insertion	UNP P19491
C	852	ASP	-	insertion	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
C	853	ASP	-	insertion	UNP P19491
C	854	ASP	TYR	conflict	UNP P19491
D	586	ARG	GLN	variant	UNP P19491
D	848	ASP	-	insertion	UNP P19491
D	849	TYR	-	insertion	UNP P19491
D	850	LYS	-	insertion	UNP P19491
D	851	ASP	-	insertion	UNP P19491
D	852	ASP	-	insertion	UNP P19491
D	853	ASP	-	insertion	UNP P19491
D	854	ASP	TYR	conflict	UNP P19491

- Molecule 2 is a protein called Voltage-dependent calcium channel gamma-2 subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	E	173	Total	C	N	O	0	0
			850	504	173	173		
2	F	167	Total	C	N	O	0	0
			820	486	167	167		
2	G	174	Total	C	N	O	0	0
			855	507	174	174		
2	H	168	Total	C	N	O	0	0
			825	489	168	168		



- Molecule 1: Glutamate receptor 2

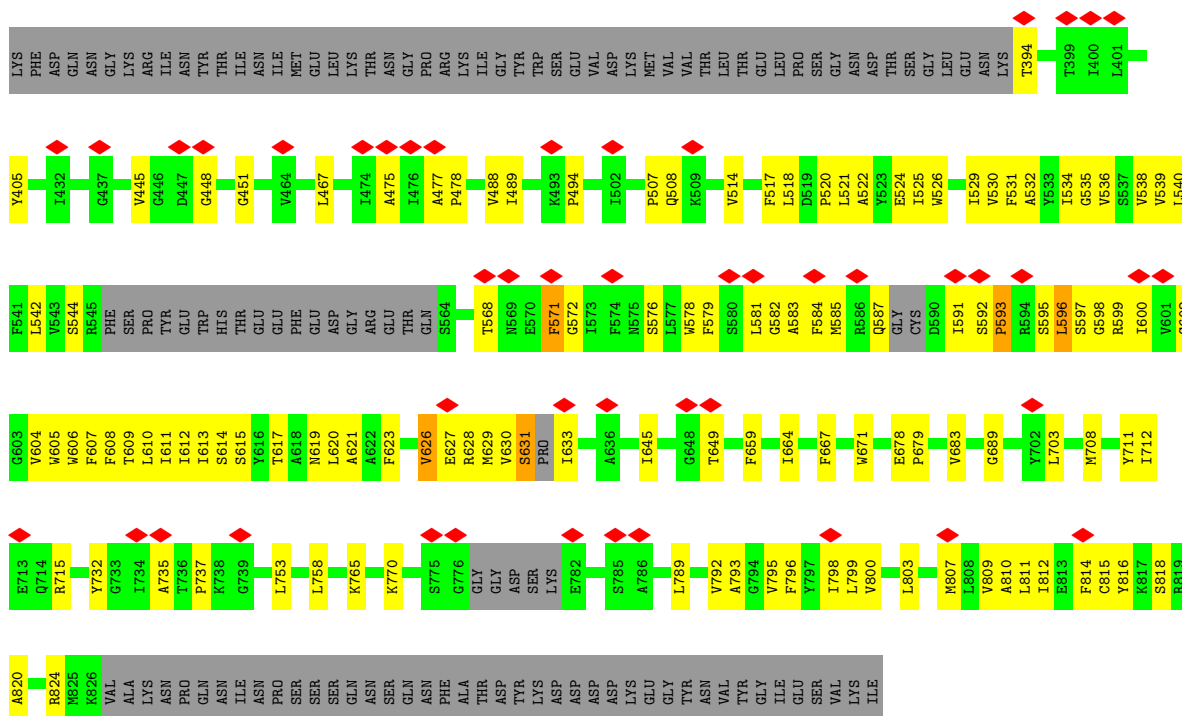
TYR	ASP	ALA	ALA	VAL	GLN	MET	THR	GLU	ALA	ALA	ARG	ASN	LEU	ARG	GLN	LYS	ARG	ILE	GLU	ILE	SER	ARG	GLY	ASP	CYS	LEU	ALA	ASN	PRO	VAL	ALA	VAL	PRO	TRP	GLY	GLN	GLY	VAL	GLU	ILE	GLU	ARG	ALA	LEU	LYS	VAL	GLN	VAL	VAL	GLU	GLY	SER	ASN	THR	ILE
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S818	R819	A820	R824	M825	K826	VAL	ALA	ALA	LYS	ASN	PRO	GLN	ASN	ILE	ASN	PRO	SER	SER	SER	GLN	ASN	GLN	ASN	PHE	ALA	ALA	THR	TYR	LYS	ASP	ASP	ASP	ASP	LYS	GLU	GLY	TYR	ASN	VAL	TYR	GLY	ILE	GLU	SER	VAL	LYS	TYR
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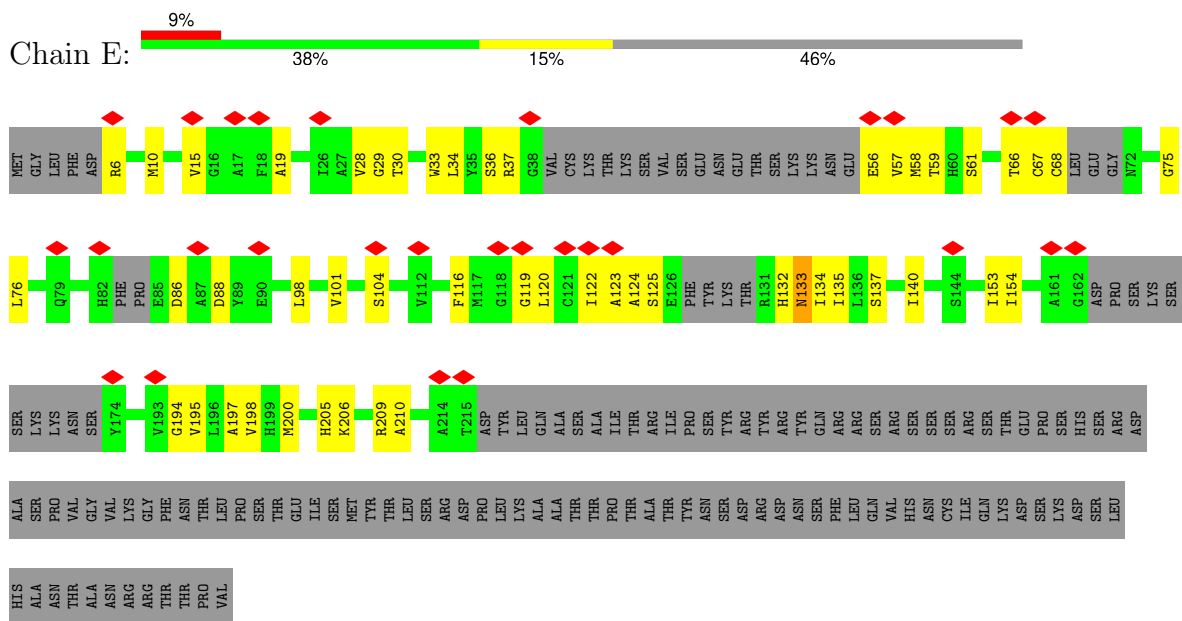
- Molecule 1: Glutamate receptor 2

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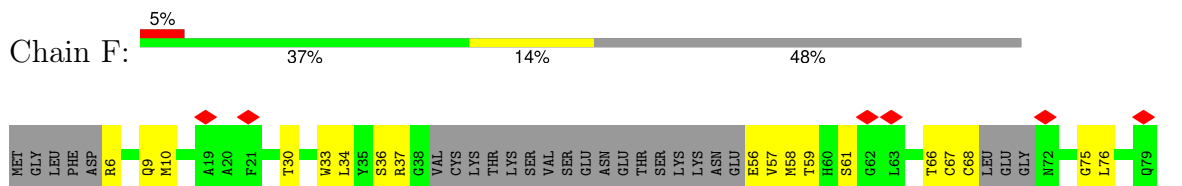




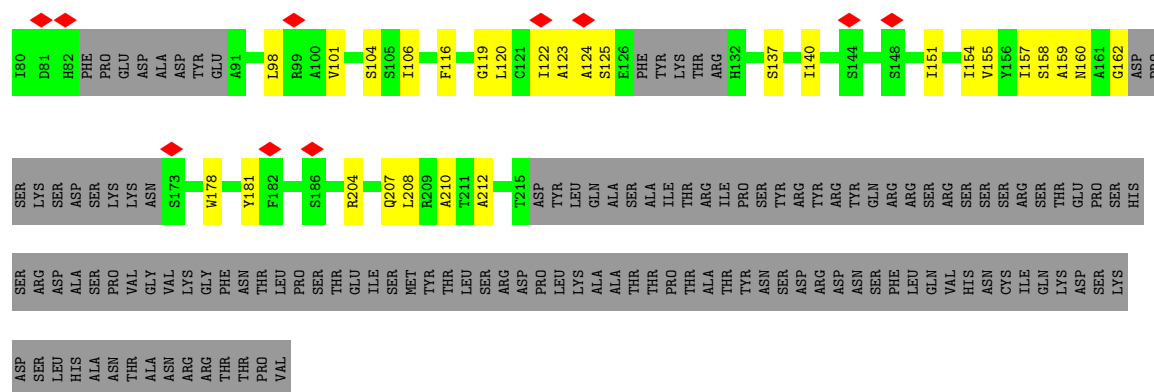
- Molecule 2: Voltage-dependent calcium channel gamma-2 subunit



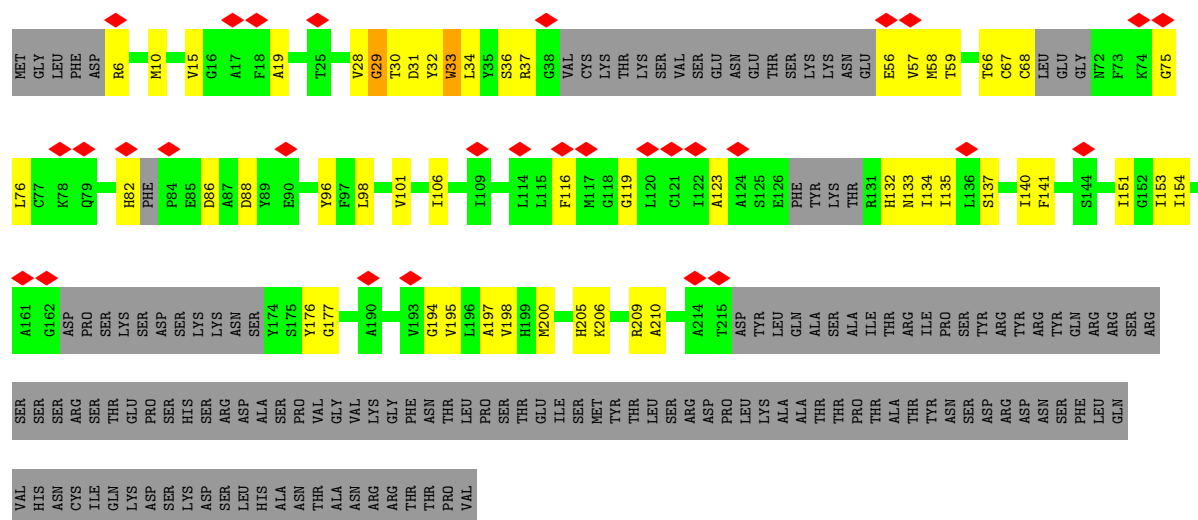
- Molecule 2: Voltage-dependent calcium channel gamma-2 subunit



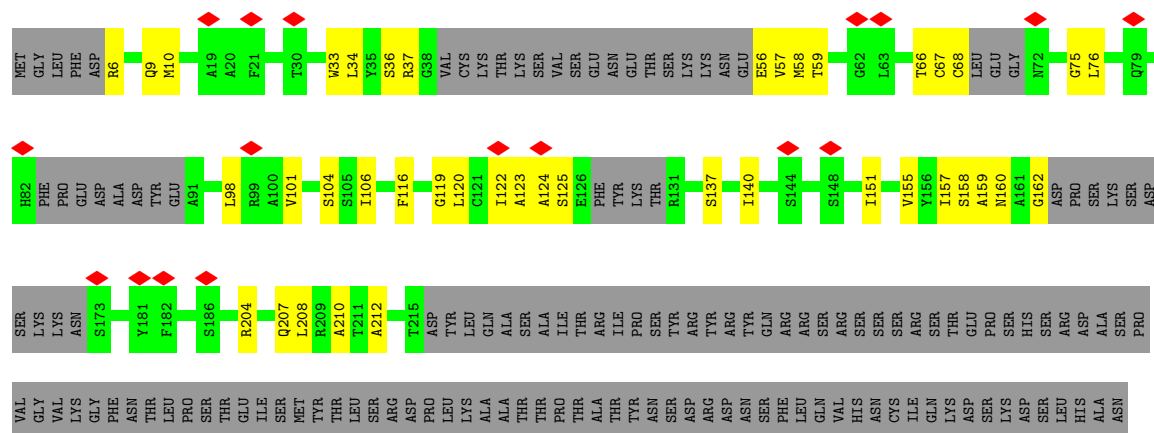




• Molecule 2: Voltage-dependent calcium channel gamma-2 subunit



• Molecule 2: Voltage-dependent calcium channel gamma-2 subunit



THR  
ALA  
ASN  
ARG  
THR  
THR  
PRO  
VAL

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	26297	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 ( $e^-/\text{\AA}^2$ )	55	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	0.095	Depositor
Minimum map value	-0.045	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.034	Depositor
Map size (Å)	405.0, 405.0, 405.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	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	0.33	0/2879	0.53	1/3933 (0.0%)
1	B	0.33	0/2857	0.53	2/3906 (0.1%)
1	C	0.32	0/2866	0.54	2/3913 (0.1%)
1	D	0.34	0/2877	0.56	4/3930 (0.1%)
2	E	0.39	0/844	0.66	2/1163 (0.2%)
2	F	0.39	0/814	0.65	2/1121 (0.2%)
2	G	0.37	0/849	0.72	2/1170 (0.2%)
2	H	0.39	0/819	0.65	2/1128 (0.2%)
All	All	0.34	0/14805	0.57	17/20264 (0.1%)

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	2
1	B	0	1
1	C	0	3
1	D	0	1
2	E	0	1
2	F	0	1
2	G	0	1
2	H	0	1
All	All	0	11

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	29	GLY	N-CA-C	-11.01	85.56	113.10
1	D	571	PHE	CB-CA-C	-10.68	89.03	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	451	GLY	N-CA-C	-9.20	90.10	113.10
1	B	451	GLY	N-CA-C	-9.16	90.19	113.10
1	C	451	GLY	N-CA-C	-8.78	91.16	113.10

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	515	PHE	Peptide
1	A	593	PRO	Peptide
1	B	593	PRO	Peptide
1	C	505	LYS	Mainchain
1	C	515	PHE	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	2831	0	2571	152	0
1	B	2810	0	2535	163	0
1	C	2819	0	2569	149	0
1	D	2829	0	2573	144	0
2	E	850	0	417	38	0
2	F	820	0	402	34	0
2	G	855	0	419	41	0
2	H	825	0	404	27	0
All	All	14639	0	11890	674	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 25.

The worst 5 of 674 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:D:583:ALA:HB1	1:D:605:TRP:NE1	1.48	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:631:SER:C	1:A:633:ILE:CD1	2.05	1.24
1:B:544:SER:O	1:B:568:THR:CB	1.89	1.19
1:D:814:PHE:O	1:D:818:SER:OG	1.60	1.18
1:B:814:PHE:O	1:B:818:SER:OG	1.60	1.15

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	398/889 (45%)	350 (88%)	47 (12%)	1 (0%)	37	73
1	B	396/889 (44%)	357 (90%)	37 (9%)	2 (0%)	25	64
1	C	396/889 (44%)	348 (88%)	48 (12%)	0	100	100
1	D	397/889 (45%)	358 (90%)	37 (9%)	2 (0%)	25	64
2	E	161/323 (50%)	136 (84%)	24 (15%)	1 (1%)	22	60
2	F	155/323 (48%)	131 (84%)	24 (16%)	0	100	100
2	G	162/323 (50%)	137 (85%)	25 (15%)	0	100	100
2	H	156/323 (48%)	134 (86%)	22 (14%)	0	100	100
All	All	2221/4848 (46%)	1951 (88%)	264 (12%)	6 (0%)	38	73

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	571	PHE
1	A	783	LYS
1	B	507	PRO
2	E	133	ASN
1	B	626	VAL

### 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	258/761 (34%)	255 (99%)	3 (1%)	67	78
1	B	255/761 (34%)	254 (100%)	1 (0%)	89	91
1	C	258/761 (34%)	256 (99%)	2 (1%)	79	85
1	D	258/761 (34%)	256 (99%)	2 (1%)	79	85
All	All	1029/3044 (34%)	1021 (99%)	8 (1%)	77	85

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	631	SER
1	D	394	THR
1	C	394	THR
1	B	394	THR
1	C	635	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 oligosaccharides 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.



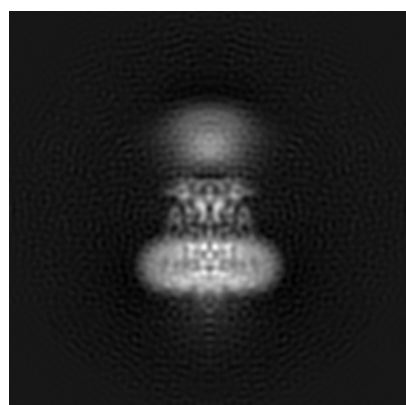
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8256. These allow visual inspection of the internal detail of the map and identification of artifacts.

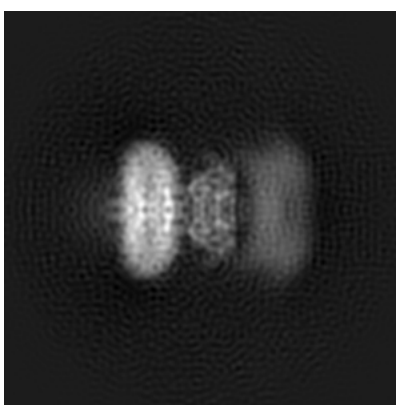
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

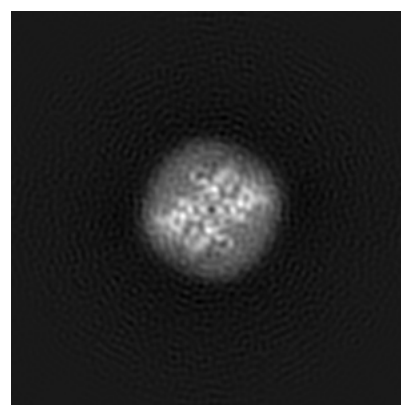
#### 6.1.1 Primary map



X



Y

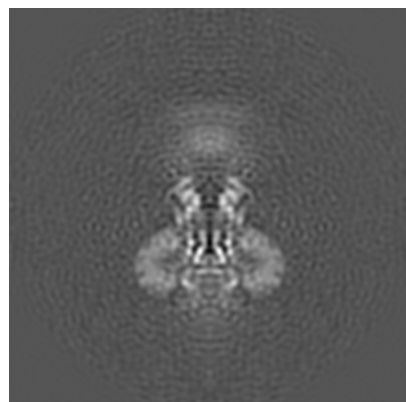


Z

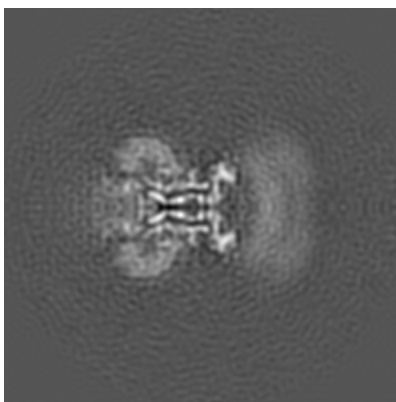
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

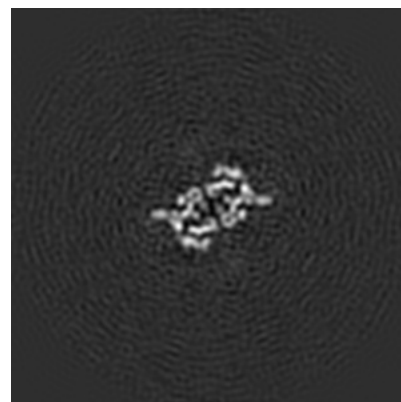
#### 6.2.1 Primary map



X Index: 150



Y Index: 150

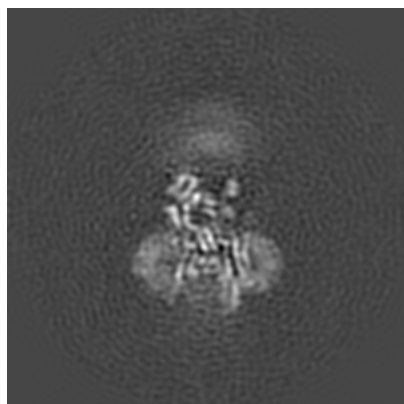


Z Index: 150

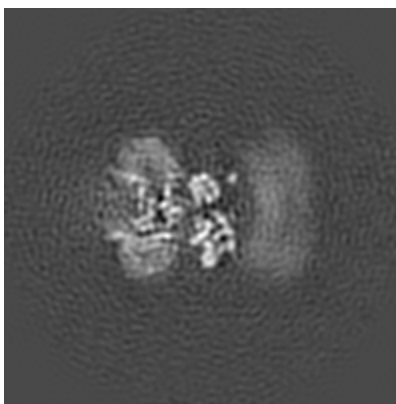
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

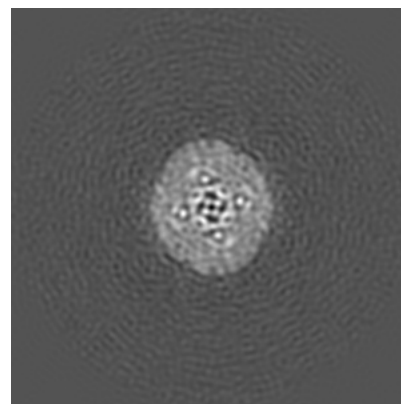
### 6.3.1 Primary map



X Index: 146



Y Index: 145

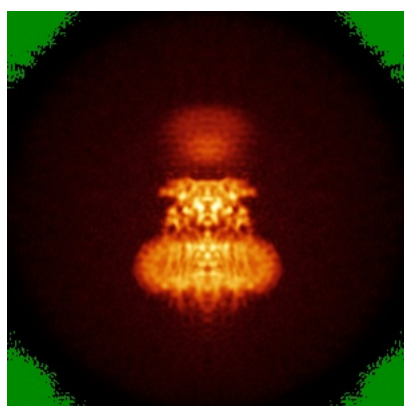


Z Index: 122

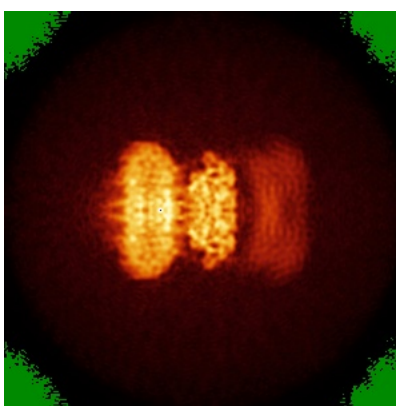
The images above show the largest variance slices of the map in three orthogonal directions.

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

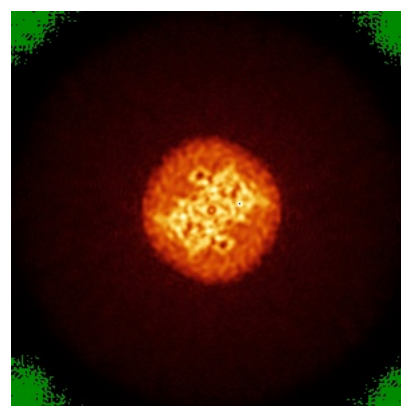
### 6.4.1 Primary map



X



Y

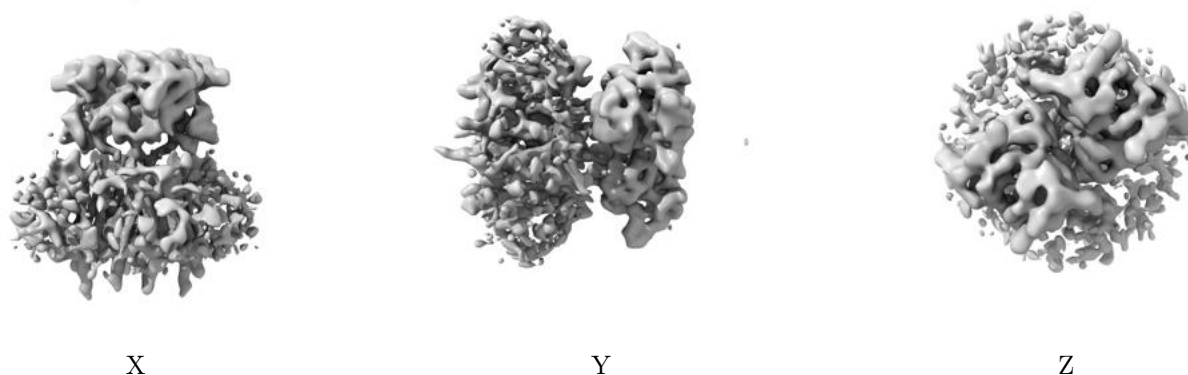


Z

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 0.034. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

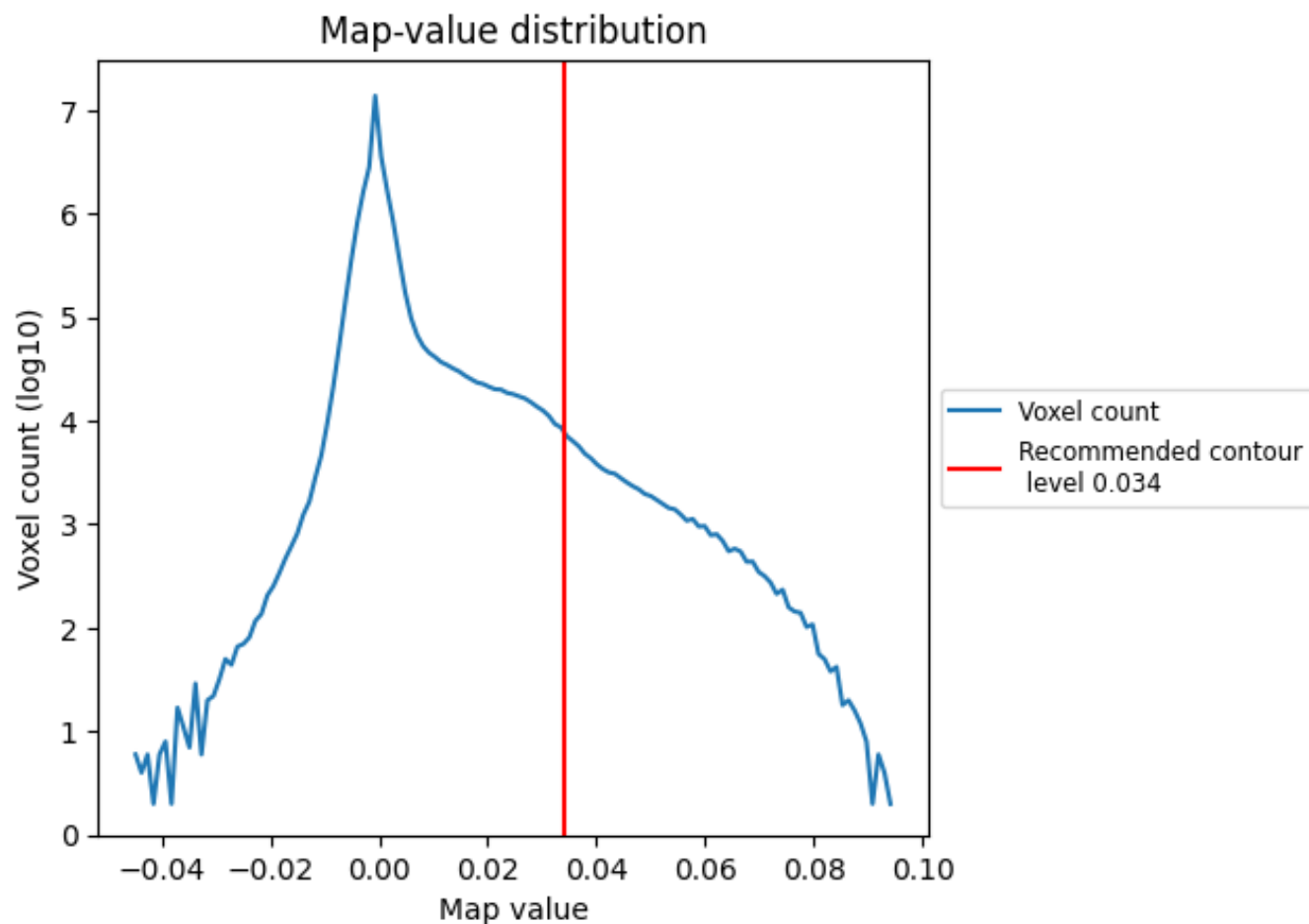
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

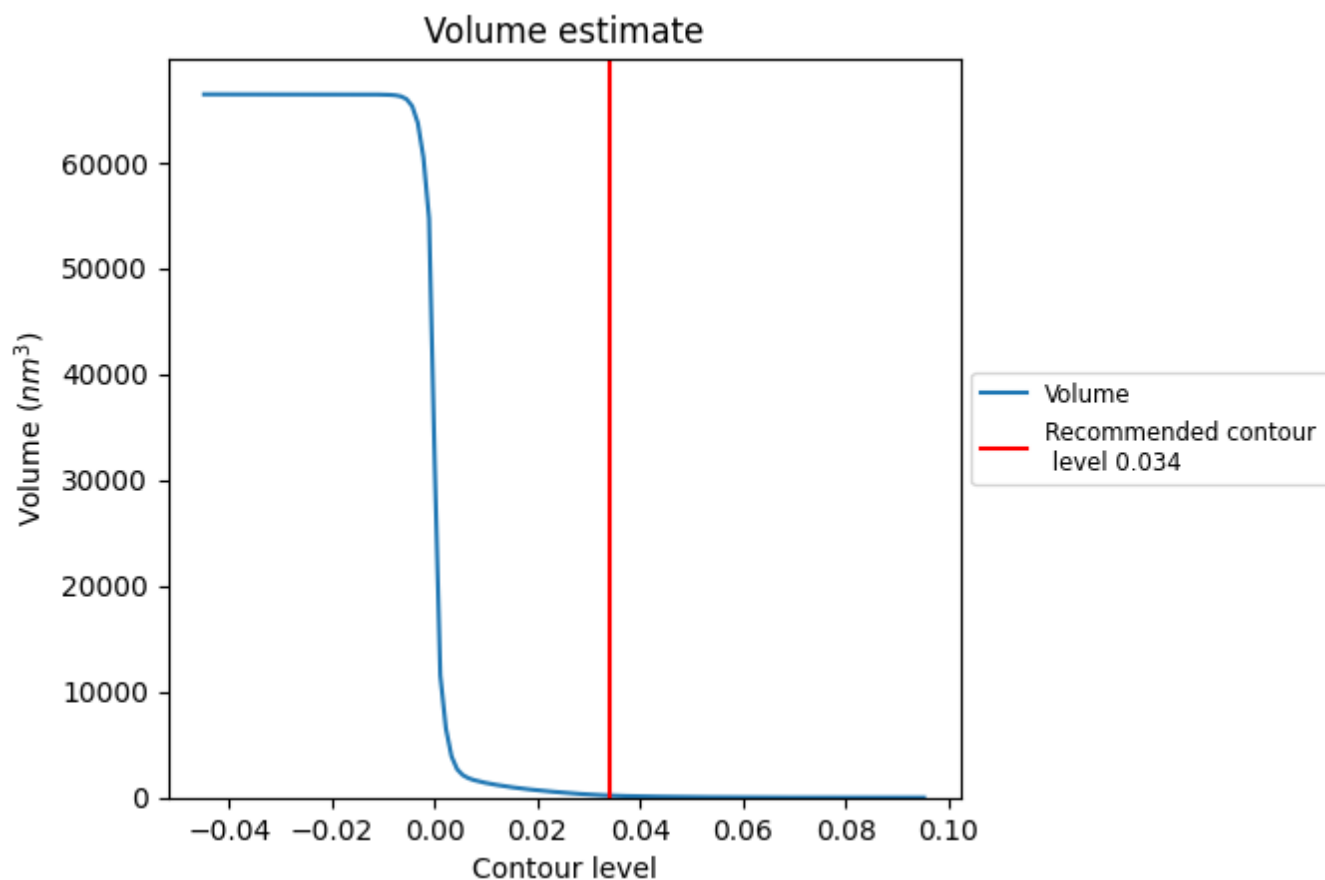
This section contains the results of statistical analysis of the map.

### 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.

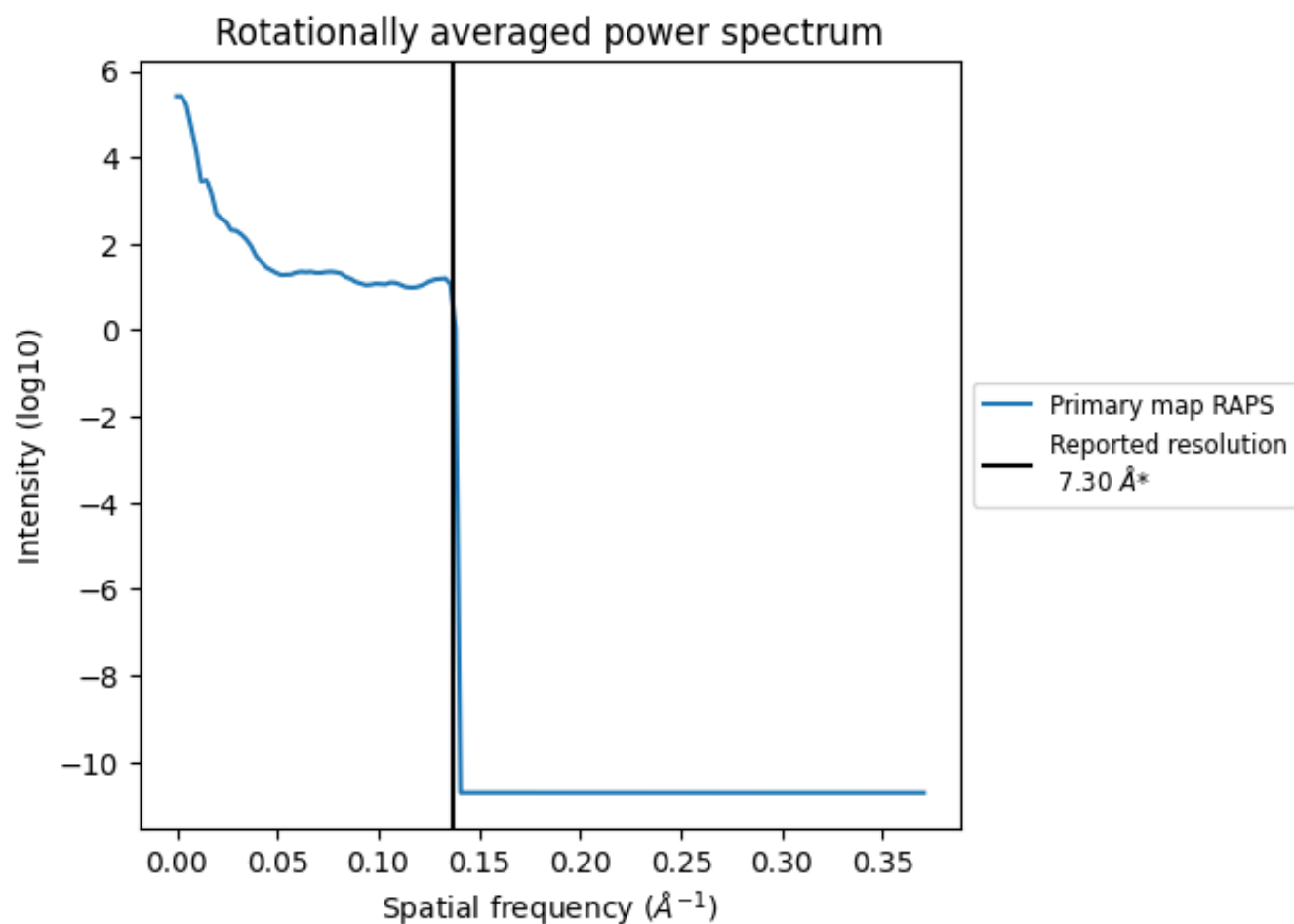
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 193 nm<sup>3</sup>; this corresponds to an approximate mass of 174 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 0.137  $\text{\AA}^{-1}$

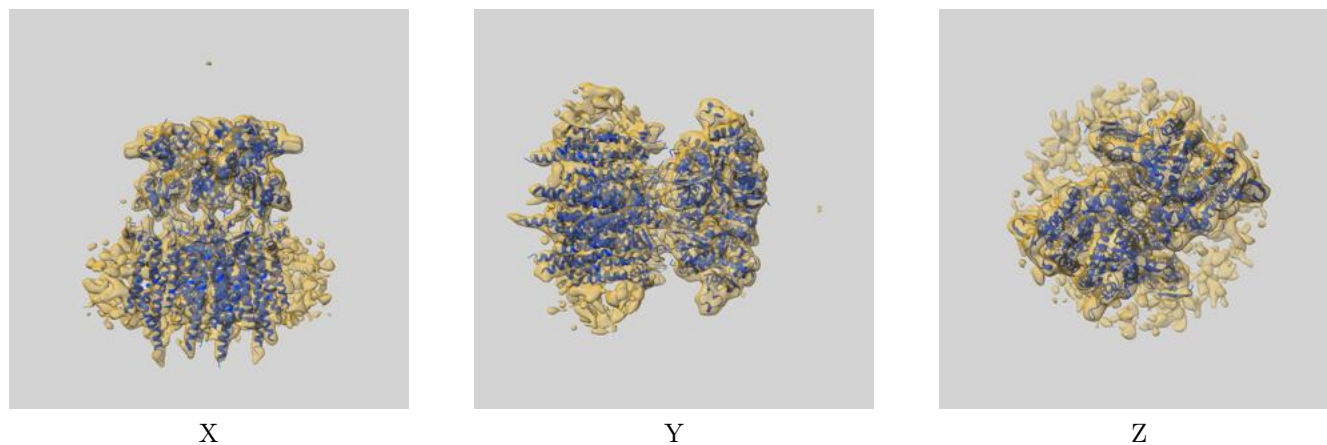
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8256 and PDB model 5KK2. Per-residue inclusion information can be found in section 3 on page 5.

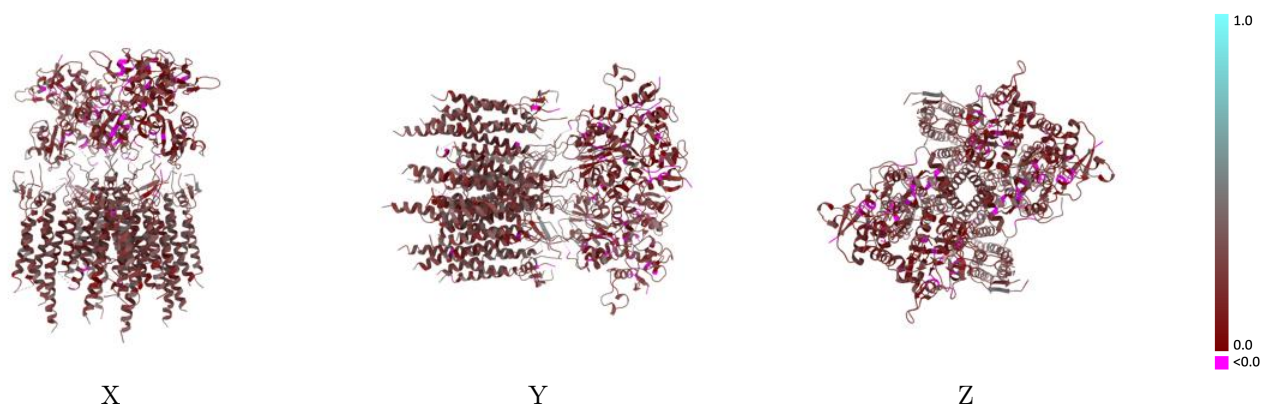
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.034 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.

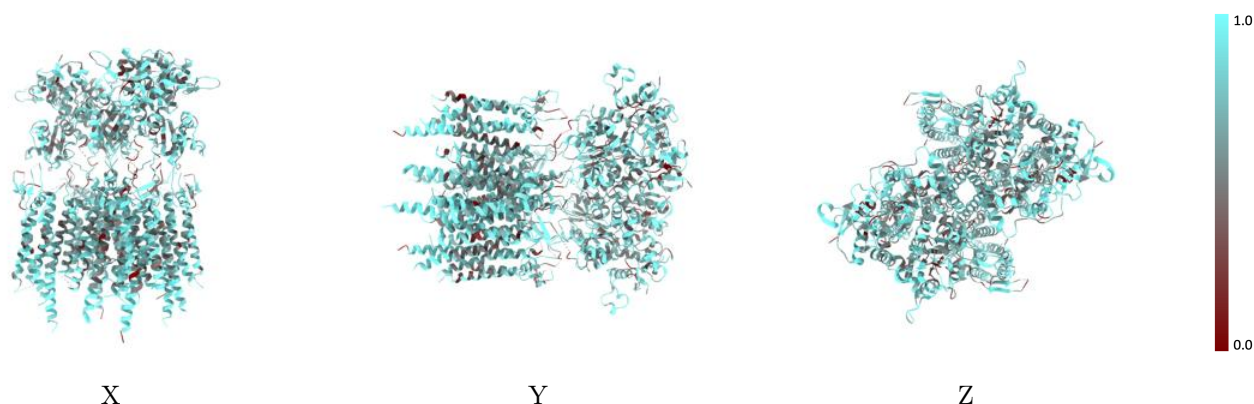


## 9.2 Q-score mapped to coordinate model [i](#)



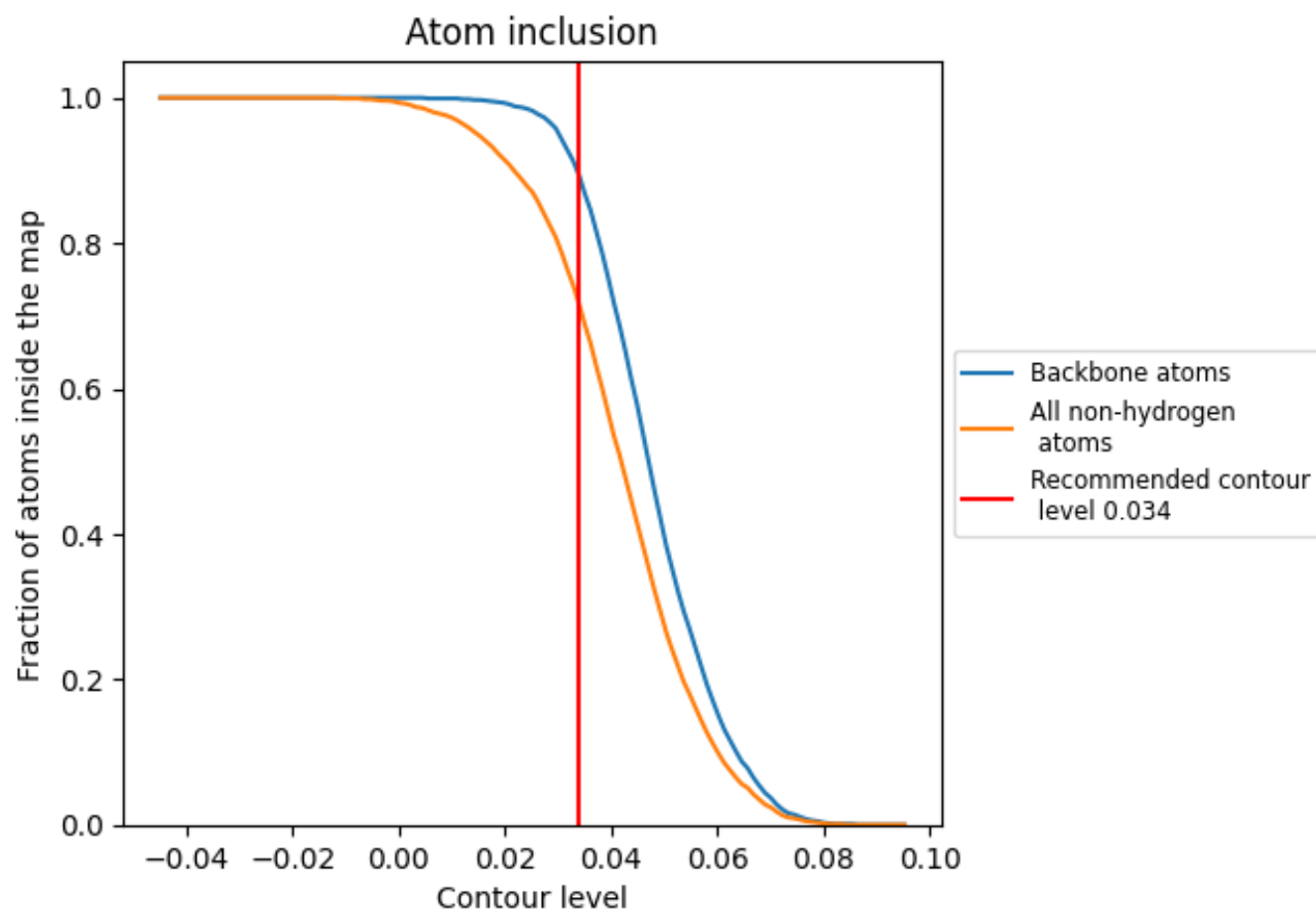
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.034).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 72% 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 (0.034) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7160	<div></div> 0.2070
A	<div></div> 0.7060	<div></div> 0.1900
B	<div></div> 0.6840	<div></div> 0.1880
C	<div></div> 0.7090	<div></div> 0.1890
D	<div></div> 0.6840	<div></div> 0.1860
E	<div></div> 0.7630	<div></div> 0.2710
F	<div></div> 0.8120	<div></div> 0.2750
G	<div></div> 0.7570	<div></div> 0.2620
H	<div></div> 0.8120	<div></div> 0.2730

