



wwPDB EM Validation Summary Report ⓘ

Nov 7, 2024 – 11:33 AM EST

PDB ID : 5VOU
EMDB ID : EMD-8722
Title : Structure of AMPA receptor-TARP complex
Authors : Chen, S.; Zhao, Y.; Wang, Y.S.; Shekhar, M.; Tajkhorshid, E.; Gouaux, E.
Deposited on : 2017-05-03
Resolution : 6.40 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

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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.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

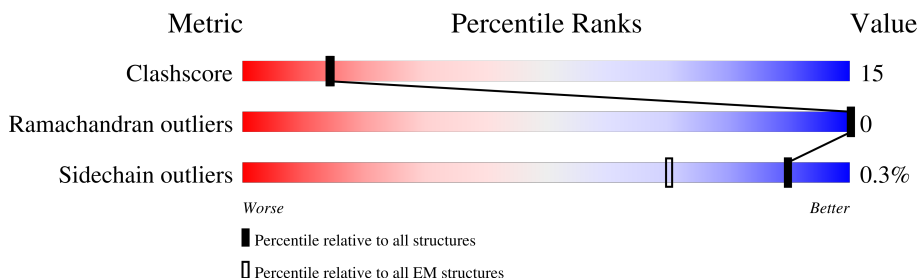
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.40 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 ≥ 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 16668 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	409	Total	C	N	O	S	0	0
			3104	2011	497	575	21		
1	D	410	Total	C	N	O	S	0	0
			3074	1987	499	571	17		
1	C	409	Total	C	N	O	S	0	0
			3104	2011	497	575	21		
1	B	410	Total	C	N	O	S	0	0
			3074	1987	499	571	17		

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	586	ARG	GLN	conflict	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
D	586	ARG	GLN	conflict	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
C	586	ARG	GLN	conflict	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

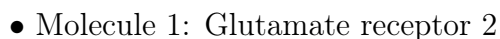
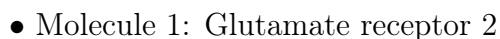
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Chain	Residue	Modelled	Actual	Comment	Reference
C	853	ASP	-	insertion	UNP P19491
C	854	ASP	TYR	conflict	UNP P19491
B	586	ARG	GLN	conflict	UNP P19491
B	848	ASP	-	insertion	UNP P19491
B	849	TYR	-	insertion	UNP P19491
B	850	LYS	-	insertion	UNP P19491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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	169	Total	C	N	O	S	0	0
			1007	645	173	186	3		
2	H	175	Total	C	N	O	S	0	0
			1149	750	183	209	7		
2	G	169	Total	C	N	O	S	0	0
			1007	645	173	186	3		
2	F	175	Total	C	N	O	S	0	0
			1149	750	183	209	7		



- Molecule 1: Glutamate receptor 2

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

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	84500	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 ($e^-/\text{\AA}^2$)	54	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	0.285	Depositor
Minimum map value	-0.117	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.075	Depositor
Map size (Å)	430.0, 430.0, 430.0	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.72, 1.72, 1.72	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	0.26	0/3170	0.40	0/4291
1	B	0.26	0/3138	0.42	0/4252
1	C	0.26	0/3170	0.40	0/4291
1	D	0.26	0/3138	0.42	0/4252
2	E	0.26	0/1021	0.38	0/1401
2	F	0.25	0/1169	0.40	0/1601
2	G	0.26	0/1021	0.38	0/1401
2	H	0.25	0/1169	0.40	0/1601
All	All	0.26	0/16996	0.40	0/23090

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	3104	0	3047	103	0
1	B	3074	0	2995	98	0
1	C	3104	0	3047	102	0
1	D	3074	0	2995	104	0
2	E	1007	0	718	22	0
2	F	1149	0	981	34	0
2	G	1007	0	718	21	0
2	H	1149	0	981	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	16668	0	15482	487	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 15.

The worst 5 of 487 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:754:ASN:OD1	1:C:759:LEU:HD11	1.32	1.27
1:A:754:ASN:OD1	1:A:759:LEU:HD11	1.31	1.27
1:C:754:ASN:OD1	1:C:759:LEU:CD1	1.82	1.27
1:A:754:ASN:OD1	1:A:759:LEU:CD1	1.81	1.26
1:C:753:LEU:CD2	1:C:758:LEU:HD12	1.72	1.17

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	403/889 (45%)	383 (95%)	20 (5%)	0	100	100
1	B	404/889 (45%)	385 (95%)	19 (5%)	0	100	100
1	C	403/889 (45%)	384 (95%)	19 (5%)	0	100	100
1	D	404/889 (45%)	385 (95%)	19 (5%)	0	100	100
2	E	159/323 (49%)	151 (95%)	8 (5%)	0	100	100
2	F	167/323 (52%)	146 (87%)	21 (13%)	0	100	100
2	G	159/323 (49%)	151 (95%)	8 (5%)	0	100	100
2	H	167/323 (52%)	147 (88%)	20 (12%)	0	100	100
All	All	2266/4848 (47%)	2132 (94%)	134 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	321/761 (42%)	320 (100%)	1 (0%)	91	92
1	B	312/761 (41%)	311 (100%)	1 (0%)	91	92
1	C	321/761 (42%)	320 (100%)	1 (0%)	91	92
1	D	312/761 (41%)	311 (100%)	1 (0%)	91	92
2	E	50/275 (18%)	50 (100%)	0	100	100
2	F	87/275 (32%)	87 (100%)	0	100	100
2	G	50/275 (18%)	50 (100%)	0	100	100
2	H	87/275 (32%)	87 (100%)	0	100	100
All	All	1540/4144 (37%)	1536 (100%)	4 (0%)	90	92

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	407	MET
1	D	407	MET
1	C	407	MET
1	B	407	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	764	ASN
2	F	199	HIS
2	H	199	HIS
2	H	205	HIS
1	C	709	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 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.

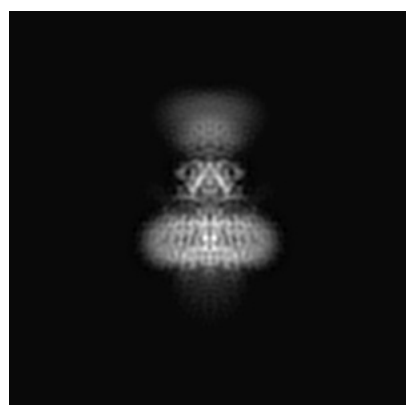
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8722. These allow visual inspection of the internal detail of the map and identification of artifacts.

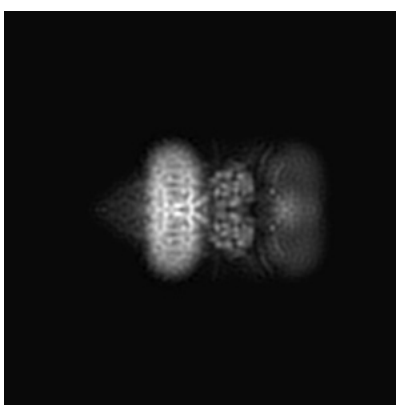
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

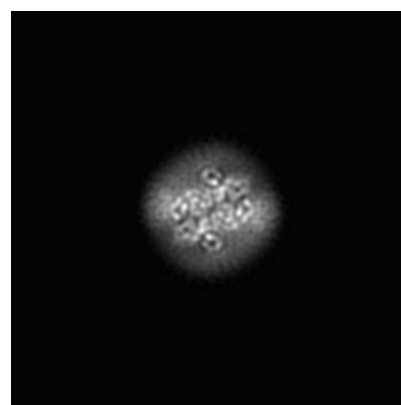
6.1.1 Primary map



X



Y

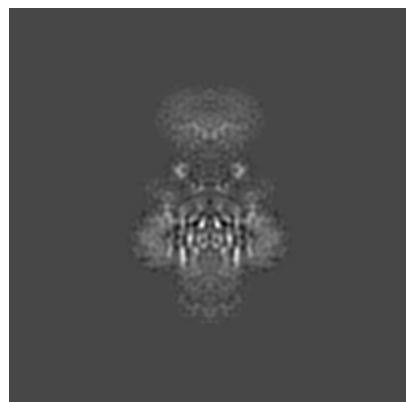


Z

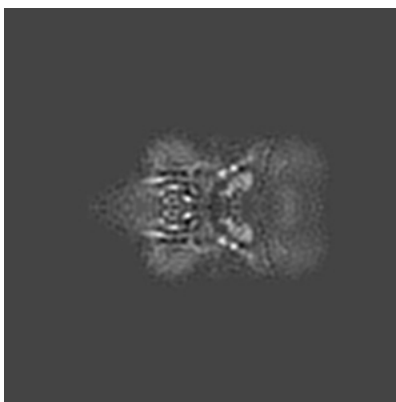
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

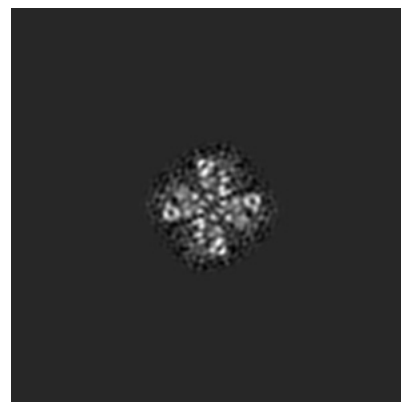
6.2.1 Primary map



X Index: 125



Y Index: 125



Z Index: 125

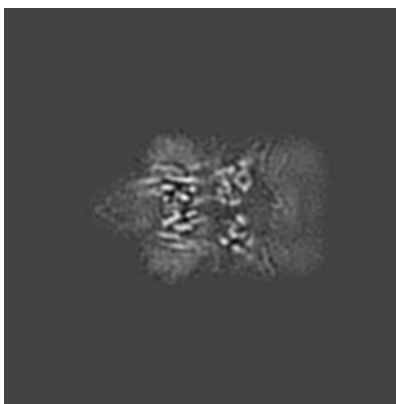
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

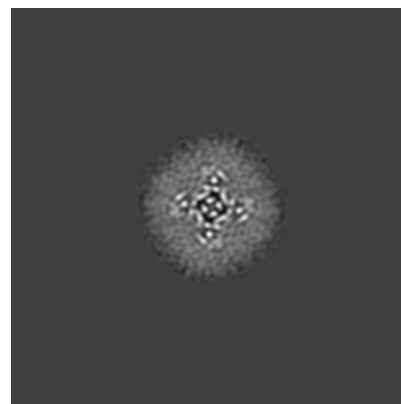
6.3.1 Primary map



X Index: 122



Y Index: 123

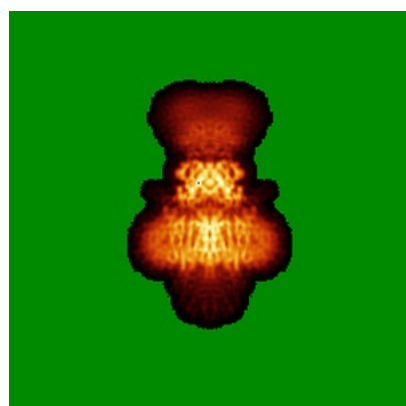


Z Index: 116

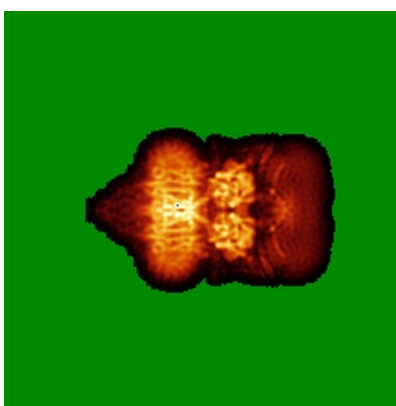
The images above show the largest variance slices of the map in three orthogonal directions.

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

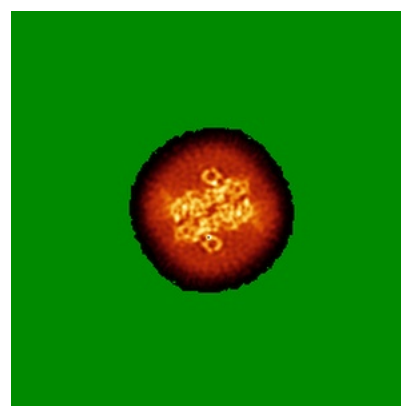
6.4.1 Primary map



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

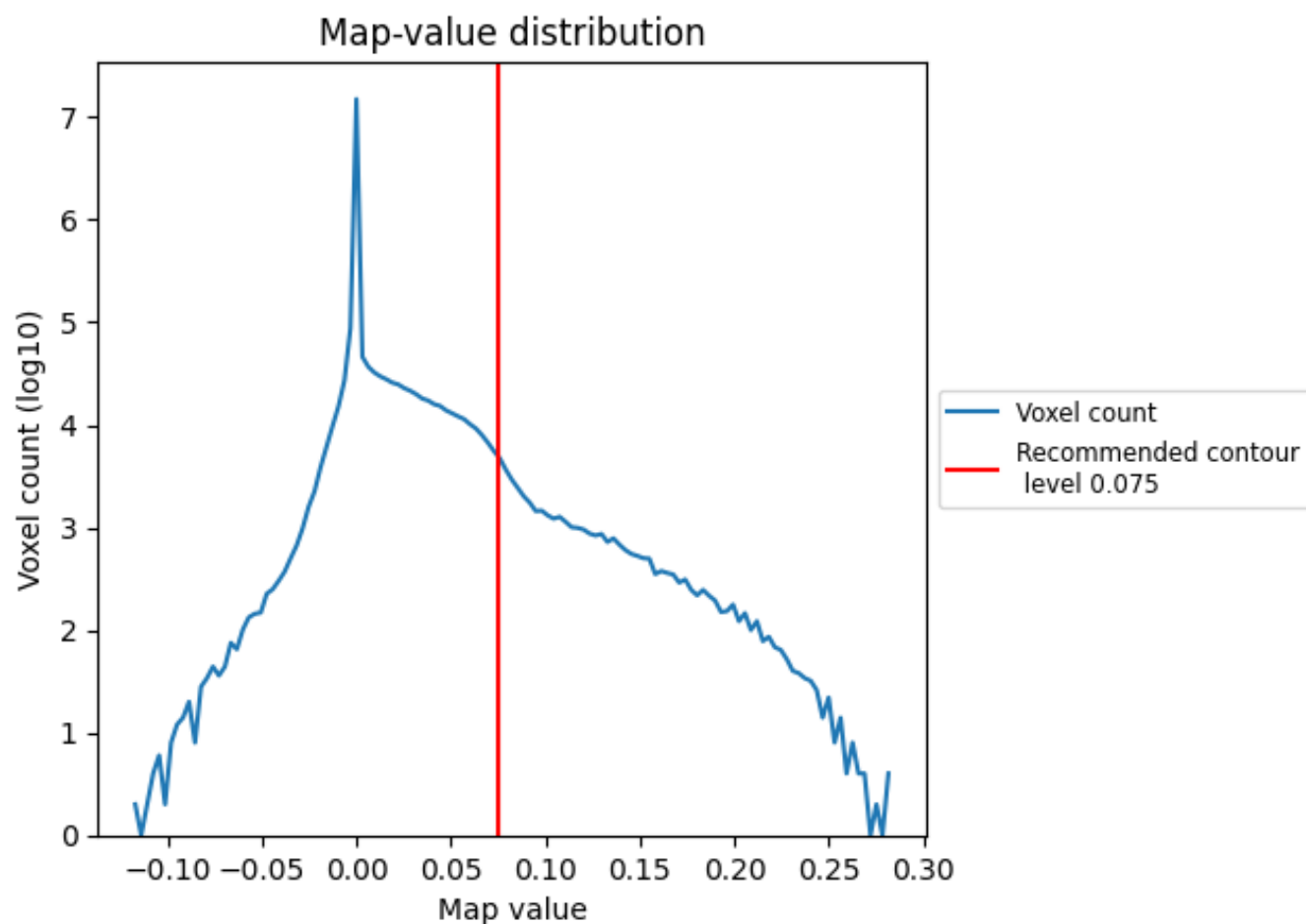
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

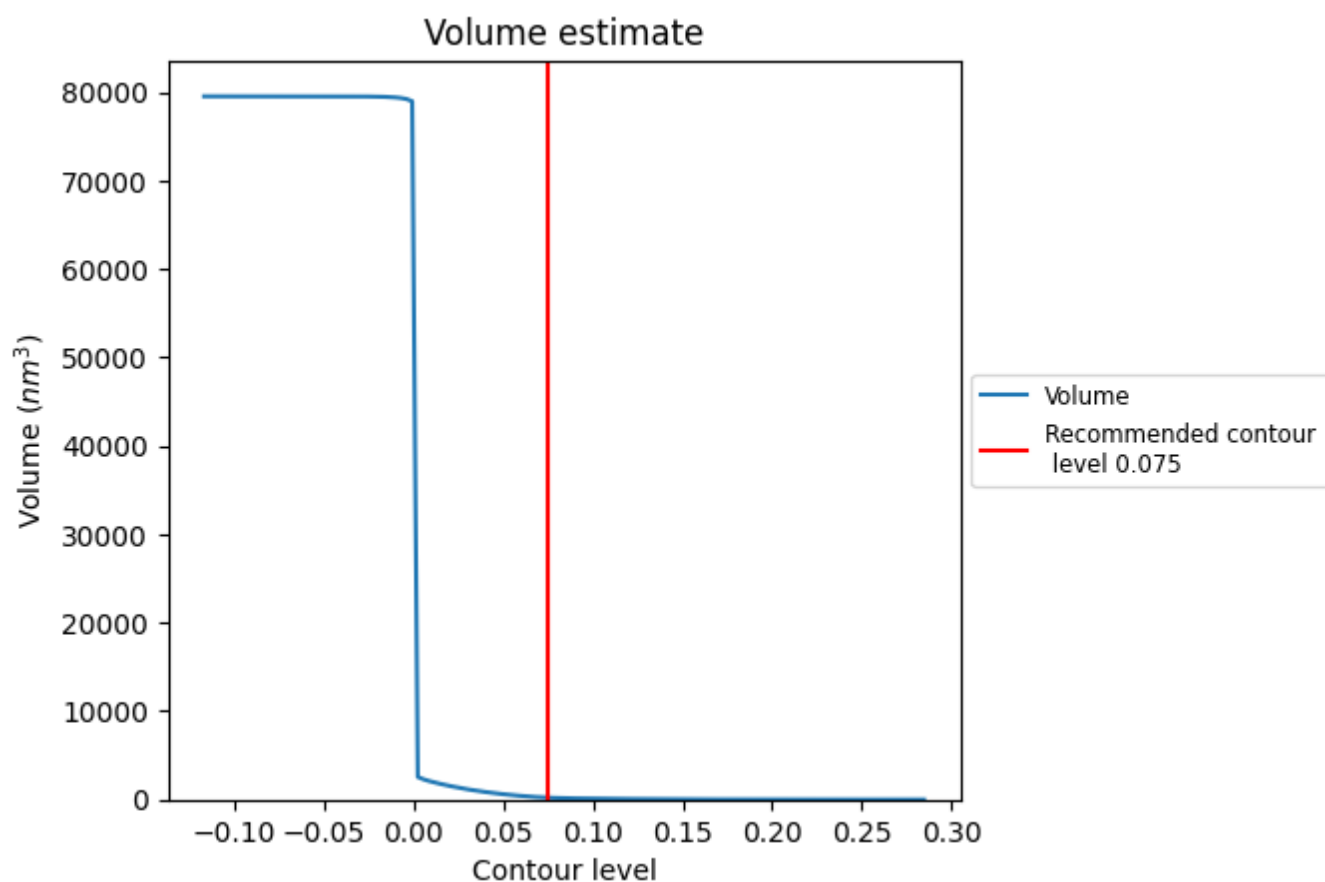
This section contains the results of statistical analysis of the map.

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.

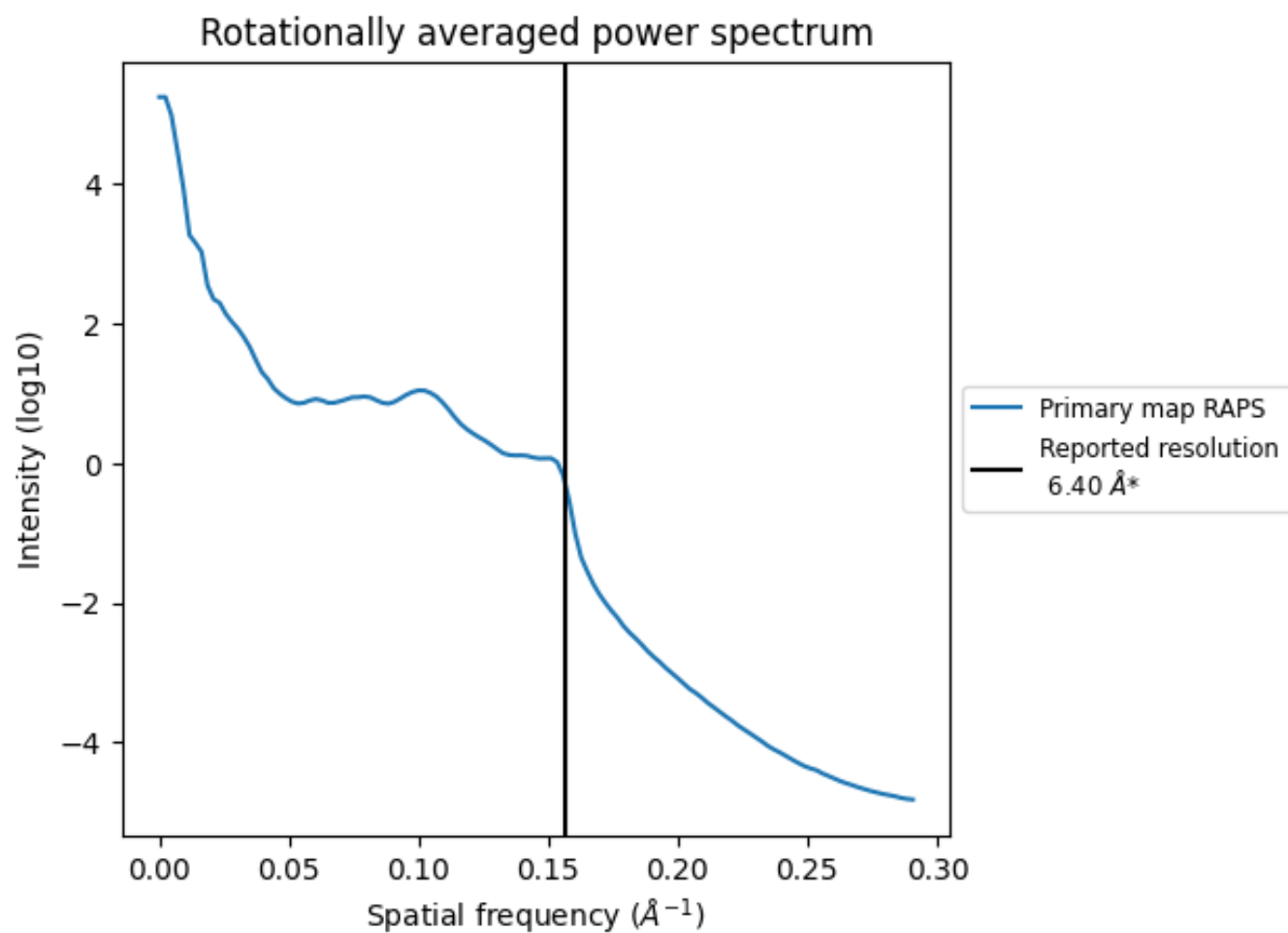
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 214 nm³; this corresponds to an approximate mass of 193 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 0.156 Å⁻¹

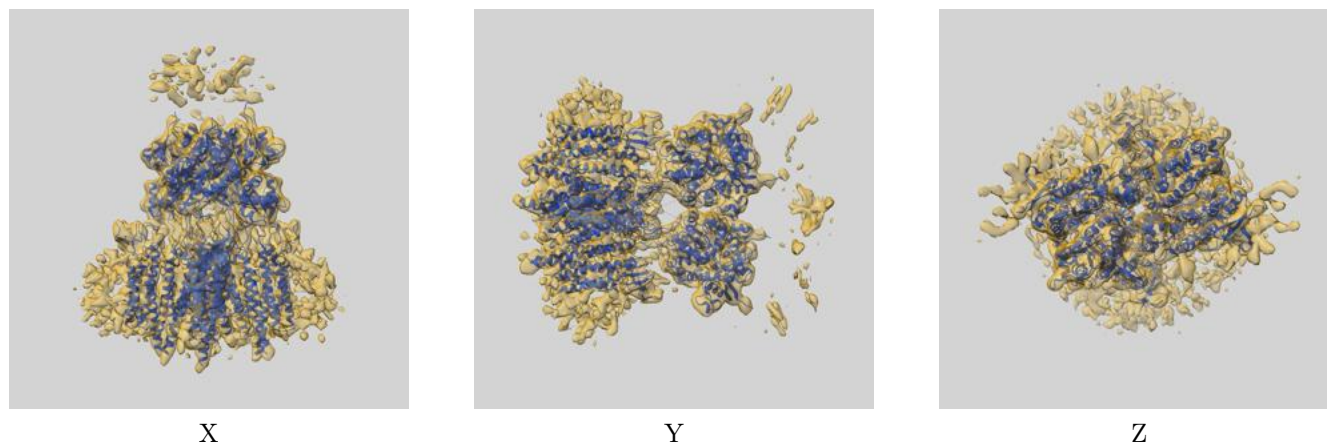
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

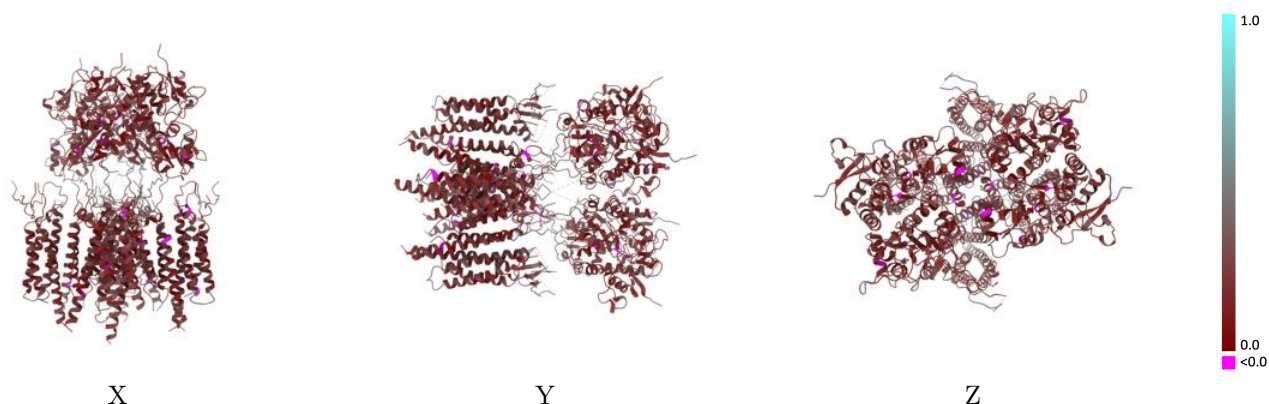
This section contains information regarding the fit between EMDB map EMD-8722 and PDB model 5VOU. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



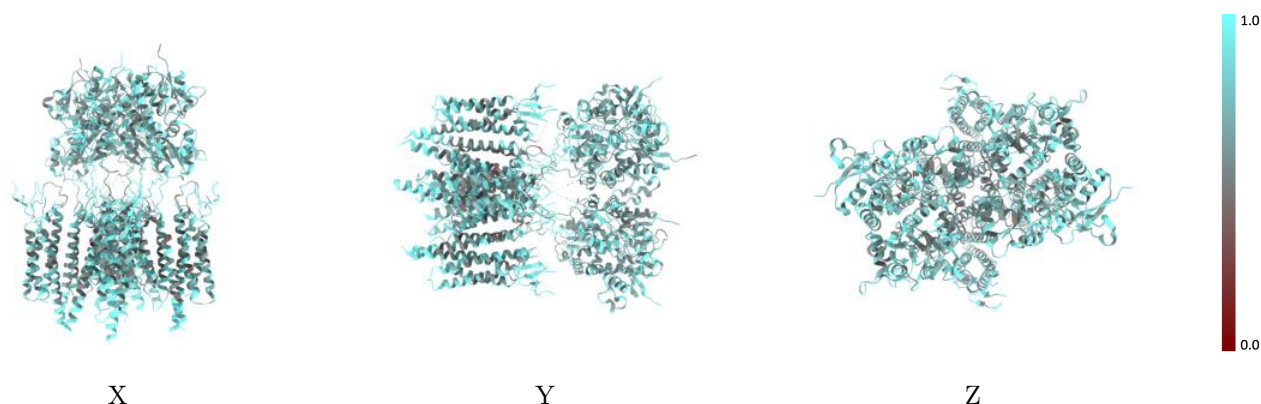
The images above show the 3D surface view of the map at the recommended contour level 0.075 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



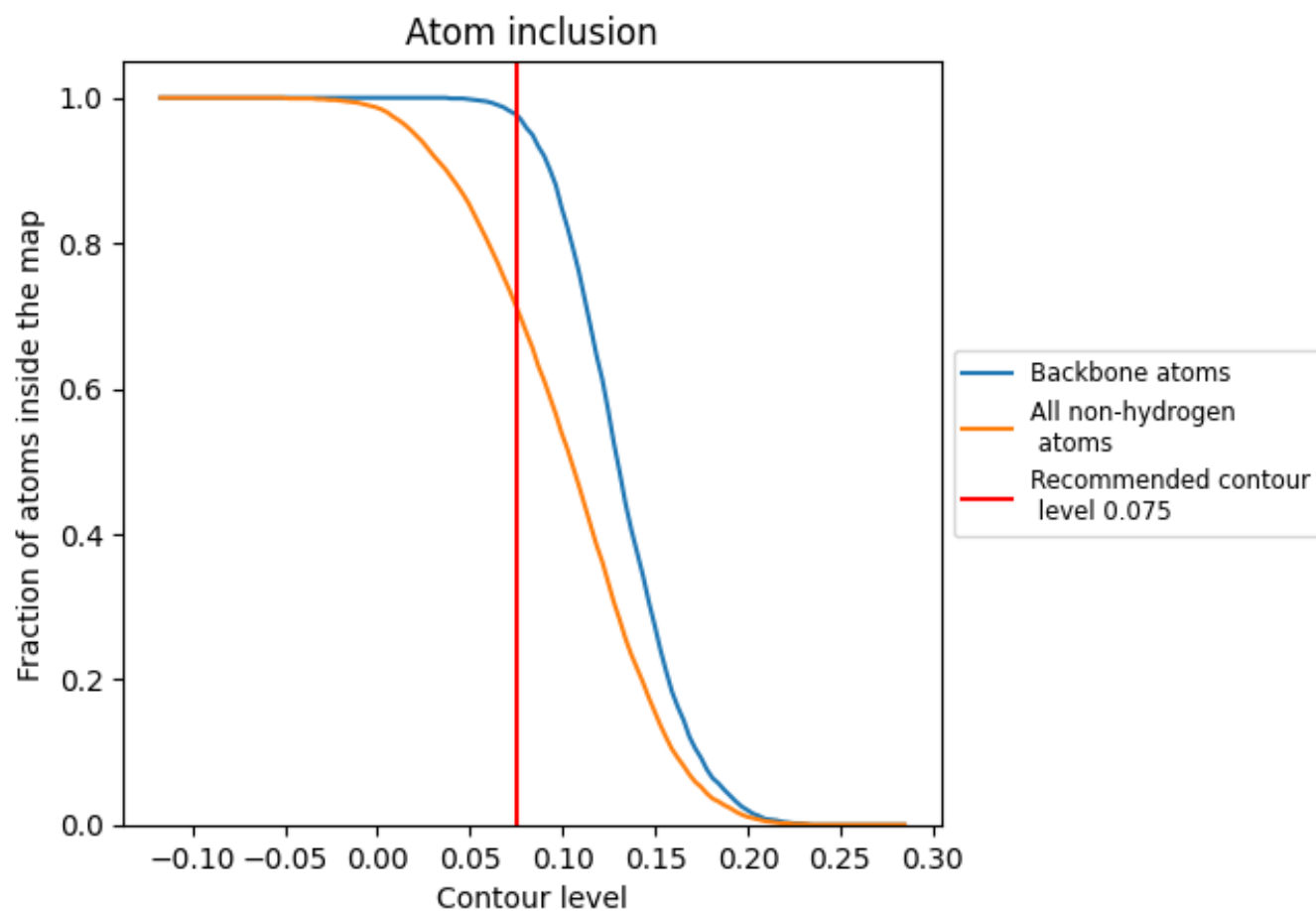
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.075).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 71% 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 (0.075) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7130	<div></div> 0.2160
A	<div></div> 0.6950	<div></div> 0.2090
B	<div></div> 0.7050	<div></div> 0.2120
C	<div></div> 0.6940	<div></div> 0.2100
D	<div></div> 0.7040	<div></div> 0.2120
E	<div></div> 0.7800	<div></div> 0.2460
F	<div></div> 0.7260	<div></div> 0.2210
G	<div></div> 0.7810	<div></div> 0.2460
H	<div></div> 0.7250	<div></div> 0.2180

1.0

0.0

<0.0