



wwPDB EM Validation Summary Report ⓘ

Dec 10, 2022 – 10:09 am GMT

PDB ID : 4UQQ
EMDB ID : EMD-2685
Title : Electron density map of GluK2 desensitized state in complex with 2S,4R-4-methylglutamate
Authors : Meyerson, J.R.; Kumar, J.; Chittori, S.; Rao, P.; Pierson, J.; Bartesaghi, A.; Mayer, M.L.; Subramaniam, S.
Deposited on : 2014-06-24
Resolution : 7.60 Å (reported)
Based on initial models : 3KG2, 3G3F, 3H6G

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.dev43
Mogul : 1.8.4, CSD as541be (2020)
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) : 2.31.3

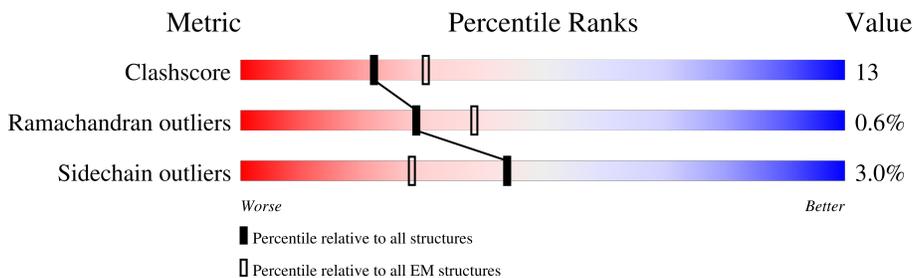
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.60 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	882	
1	B	882	
1	C	882	
1	D	882	

2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 22081 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 IONOTROPIC, KAINATE 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	693	5523	3545	922	1025	31	0	0
1	B	688	5498	3530	918	1020	30	0	0
1	C	693	5523	3545	922	1025	31	0	0
1	D	688	5497	3529	918	1020	30	0	0

There are 36 discrepancies between the modelled and reference sequences:

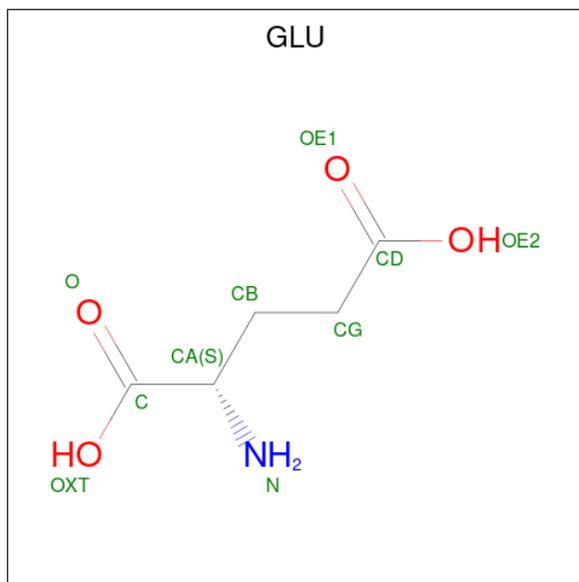
Chain	Residue	Modelled	Actual	Comment	Reference
A	878	GLY	-	expression tag	UNP P42260
A	879	LEU	-	expression tag	UNP P42260
A	880	VAL	-	expression tag	UNP P42260
A	881	PRO	-	expression tag	UNP P42260
A	882	ARG	-	expression tag	UNP P42260
A	536	VAL	ILE	variant	UNP P42260
A	540	CYS	TYR	variant	UNP P42260
A	545	VAL	CYS	engineered mutation	UNP P42260
A	564	SER	CYS	engineered mutation	UNP P42260
B	878	GLY	-	expression tag	UNP P42260
B	879	LEU	-	expression tag	UNP P42260
B	880	VAL	-	expression tag	UNP P42260
B	881	PRO	-	expression tag	UNP P42260
B	882	ARG	-	expression tag	UNP P42260
B	536	VAL	ILE	variant	UNP P42260
B	540	CYS	TYR	variant	UNP P42260
B	545	VAL	CYS	engineered mutation	UNP P42260
B	564	SER	CYS	engineered mutation	UNP P42260
C	878	GLY	-	expression tag	UNP P42260
C	879	LEU	-	expression tag	UNP P42260
C	880	VAL	-	expression tag	UNP P42260
C	881	PRO	-	expression tag	UNP P42260

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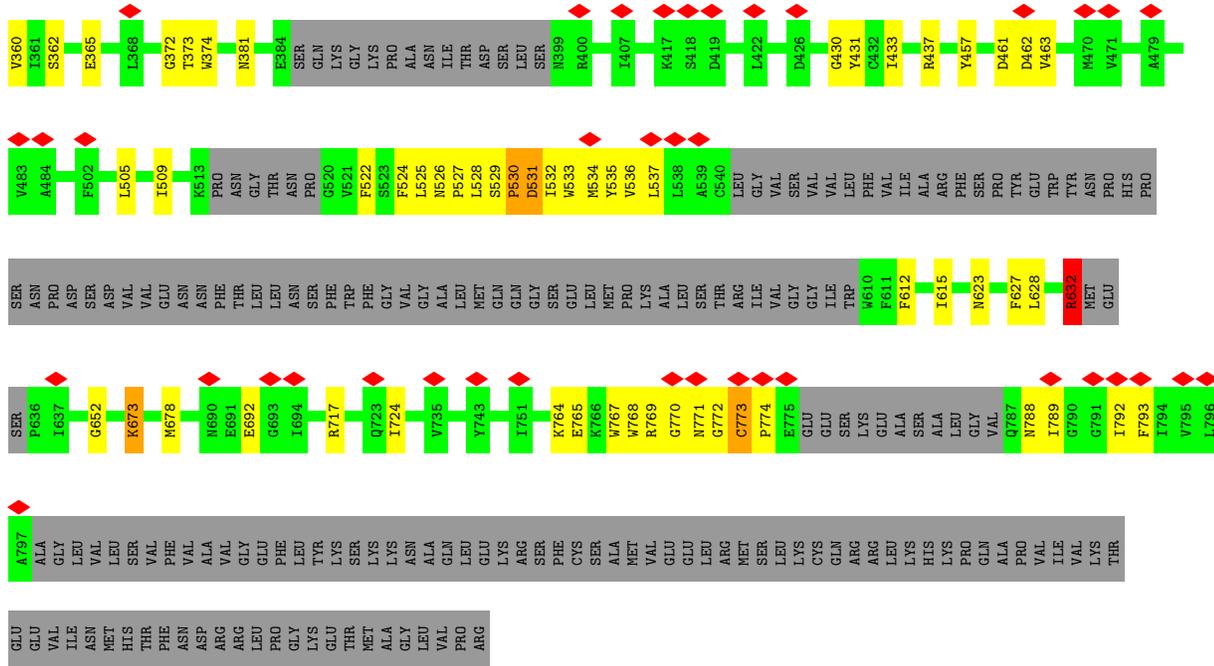
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Chain	Residue	Modelled	Actual	Comment	Reference
C	882	ARG	-	expression tag	UNP P42260
C	536	VAL	ILE	variant	UNP P42260
C	540	CYS	TYR	variant	UNP P42260
C	545	VAL	CYS	engineered mutation	UNP P42260
C	564	SER	CYS	engineered mutation	UNP P42260
D	878	GLY	-	expression tag	UNP P42260
D	879	LEU	-	expression tag	UNP P42260
D	880	VAL	-	expression tag	UNP P42260
D	881	PRO	-	expression tag	UNP P42260
D	882	ARG	-	expression tag	UNP P42260
D	536	VAL	ILE	variant	UNP P42260
D	540	CYS	TYR	variant	UNP P42260
D	545	VAL	CYS	engineered mutation	UNP P42260
D	564	SER	CYS	engineered mutation	UNP P42260

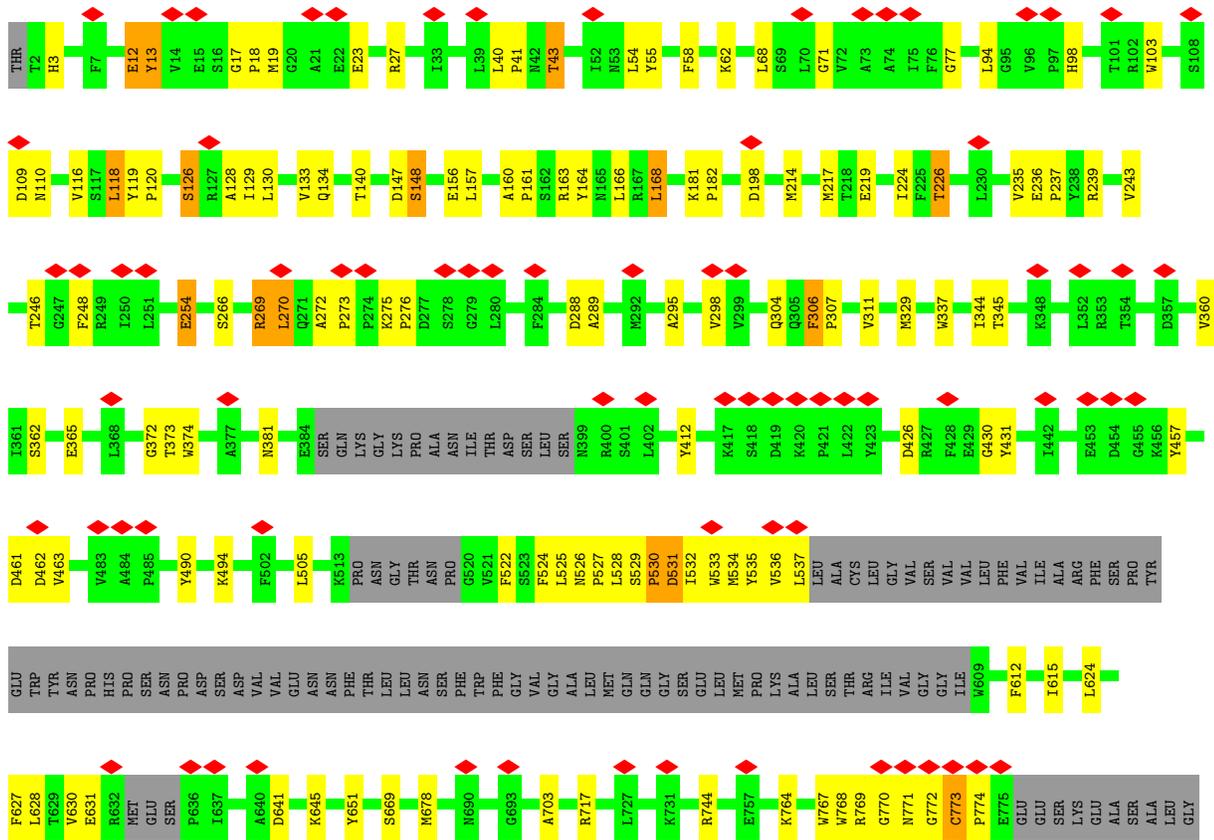
- Molecule 2 is GLUTAMIC ACID (three-letter code: GLU) (formula: C₅H₉NO₄).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
2	A	1	10	5	1	4	0
2	B	1	10	5	1	4	0
2	C	1	10	5	1	4	0
2	D	1	10	5	1	4	0



• Molecule 1: GLUTAMATE RECEPTOR IONOTROPIC, KAINATE 2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	21360	Depositor
Resolution determination method	Not provided	
CTF correction method	EACH PARTICLE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	47000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.480	Depositor
Minimum map value	-0.277	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.121	Depositor
Map size (\AA)	281.2, 281.2, 281.2	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.406, 1.406, 1.406	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.56	2/5642 (0.0%)	0.68	5/7628 (0.1%)
1	B	0.59	1/5619 (0.0%)	0.70	4/7597 (0.1%)
1	C	0.56	2/5642 (0.0%)	0.69	5/7628 (0.1%)
1	D	0.59	1/5617 (0.0%)	0.70	4/7593 (0.1%)
All	All	0.58	6/22520 (0.0%)	0.69	18/30446 (0.1%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	457	TYR	CE2-CZ	-6.43	1.30	1.38
1	D	457	TYR	CE2-CZ	-6.41	1.30	1.38
1	C	692	GLU	CB-CG	5.71	1.63	1.52
1	A	692	GLU	CB-CG	5.69	1.62	1.52
1	A	457	TYR	CE2-CZ	-5.23	1.31	1.38

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	632	ARG	NE-CZ-NH2	-13.83	113.39	120.30
1	A	632	ARG	NE-CZ-NH2	-12.54	114.03	120.30
1	C	632	ARG	NE-CZ-NH1	11.76	126.18	120.30
1	A	632	ARG	NE-CZ-NH1	11.31	125.96	120.30
1	C	530	PRO	CA-N-CD	-8.46	99.65	111.50

There are no chirality outliers.

There are no planarity outliers.

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	5523	0	5507	156	0
1	B	5498	0	5471	153	0
1	C	5523	0	5507	150	0
1	D	5497	0	5467	148	0
2	A	10	0	5	0	0
2	B	10	0	5	0	0
2	C	10	0	5	0	0
2	D	10	0	5	0	0
All	All	22081	0	21972	563	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 13.

The worst 5 of 563 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:A:764:LYS:O	1:A:768:TRP:HB2	1.39	1.19
1:A:530:PRO:HD2	1:A:531:ASP:H	1.05	1.14
1:C:530:PRO:HD2	1:C:531:ASP:H	1.06	1.12
1:C:764:LYS:O	1:C:768:TRP:HB2	1.47	1.12
1:B:530:PRO:HD2	1:B:531:ASP:H	1.06	1.11

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	681/882 (77%)	647 (95%)	30 (4%)	4 (1%)	25 66
1	B	676/882 (77%)	643 (95%)	30 (4%)	3 (0%)	34 72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	681/882 (77%)	645 (95%)	31 (5%)	5 (1%)	22 63
1	D	676/882 (77%)	642 (95%)	30 (4%)	4 (1%)	25 66
All	All	2714/3528 (77%)	2577 (95%)	121 (4%)	16 (1%)	29 66

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	771	ASN
1	A	276	PRO
1	A	773	CYS
1	B	276	PRO
1	B	773	CYS

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	604/769 (78%)	586 (97%)	18 (3%)	41 63
1	B	601/769 (78%)	583 (97%)	18 (3%)	41 63
1	C	604/769 (78%)	585 (97%)	19 (3%)	40 62
1	D	601/769 (78%)	583 (97%)	18 (3%)	41 63
All	All	2410/3076 (78%)	2337 (97%)	73 (3%)	44 63

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	43	THR
1	D	505	LEU
1	D	126	SER
1	D	269	ARG
1	B	163	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	623	ASN
1	C	106	GLN
1	D	304	GLN
1	D	106	GLN
1	D	110	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](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLU	B	999	-	8,9,9	1.23	1 (12%)	10,11,11	1.14	1 (10%)
2	GLU	C	999	-	8,9,9	1.15	0	10,11,11	1.49	2 (20%)
2	GLU	D	999	-	8,9,9	1.24	1 (12%)	10,11,11	1.14	1 (10%)
2	GLU	A	999	-	8,9,9	1.16	0	10,11,11	1.49	2 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLU	B	999	-	-	0/9/9/9	-
2	GLU	C	999	-	-	2/9/9/9	-
2	GLU	D	999	-	-	0/9/9/9	-
2	GLU	A	999	-	-	2/9/9/9	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	999	GLU	OXT-C	-2.01	1.24	1.30
2	D	999	GLU	OXT-C	-2.01	1.24	1.30

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	999	GLU	OXT-C-CA	2.50	121.89	113.38
2	C	999	GLU	OXT-C-CA	2.48	121.84	113.38
2	C	999	GLU	OE1-CD-CG	-2.29	115.74	123.08
2	A	999	GLU	OE1-CD-CG	-2.28	115.76	123.08
2	B	999	GLU	OE2-CD-CG	2.25	121.26	114.03

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	999	GLU	OXT-C-CA-CB
2	C	999	GLU	O-C-CA-CB
2	C	999	GLU	OXT-C-CA-CB
2	A	999	GLU	O-C-CA-CB

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.

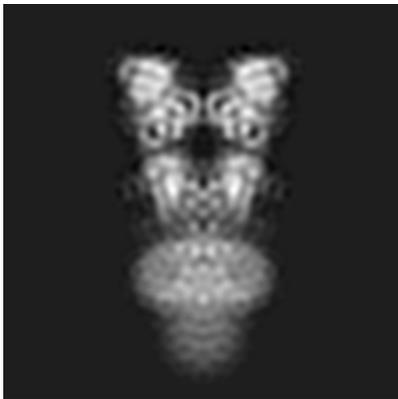
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2685. These allow visual inspection of the internal detail of the map and identification of artifacts.

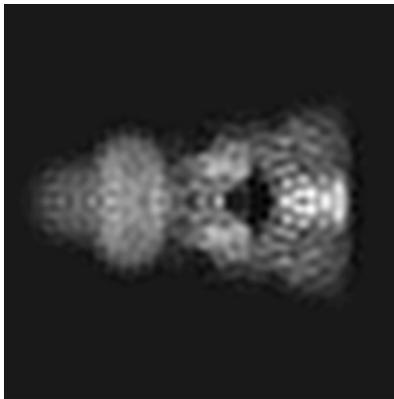
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

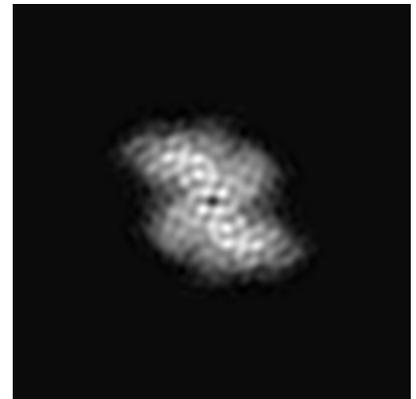
6.1.1 Primary map



X



Y



Z

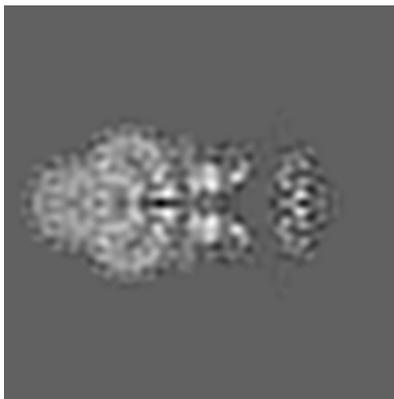
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 100



Y Index: 100

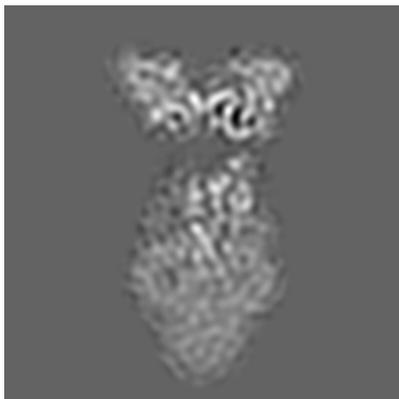


Z Index: 100

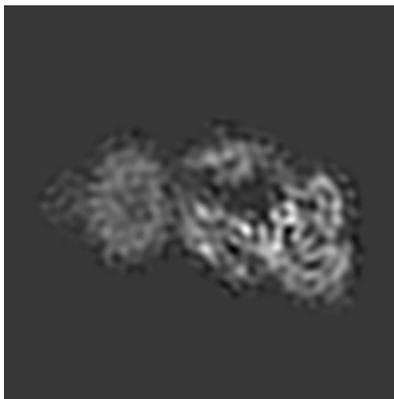
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

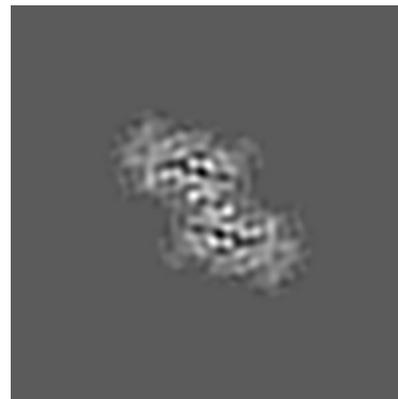
6.3.1 Primary map



X Index: 95



Y Index: 121

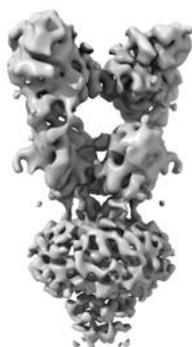


Z Index: 142

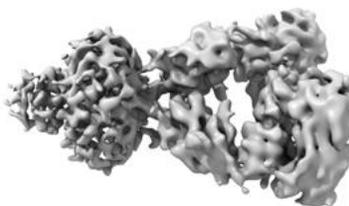
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

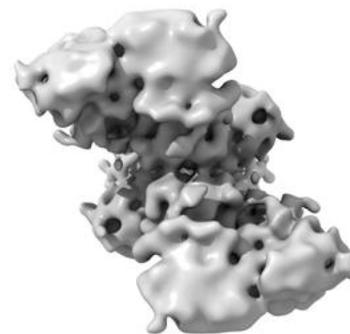
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.121. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

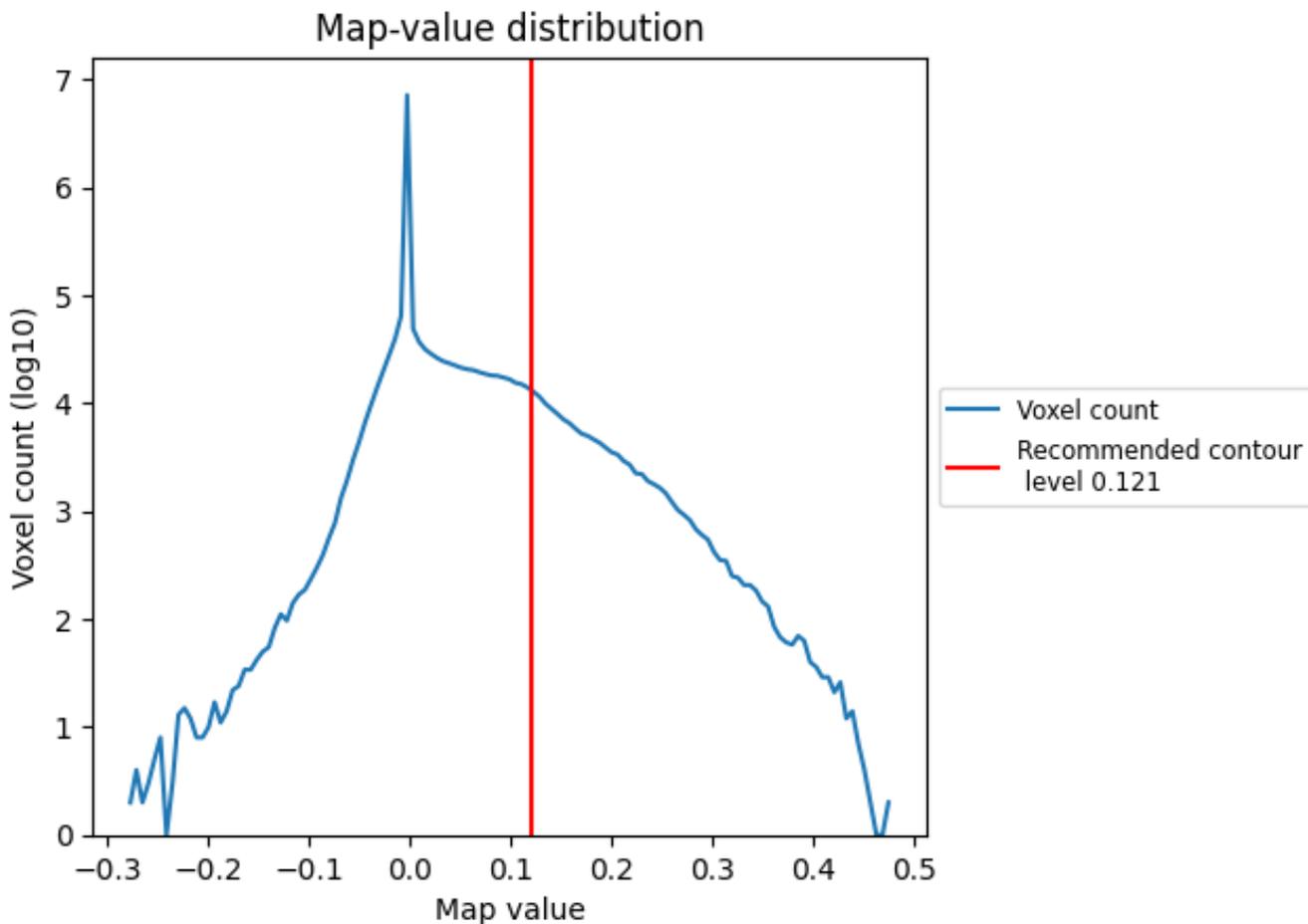
6.5 Mask visualisation

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

7 Map analysis [i](#)

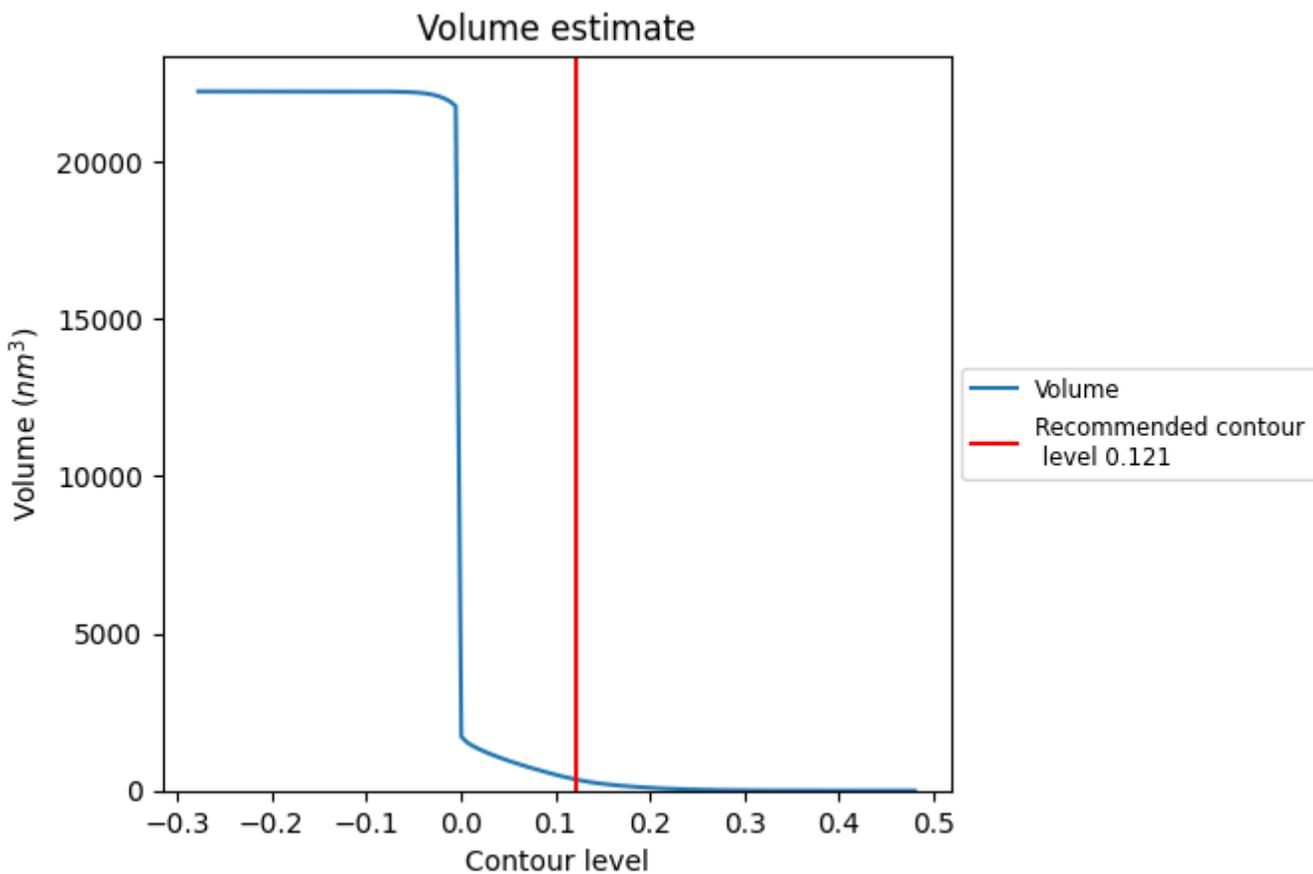
This section contains the results of statistical analysis of the map.

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.

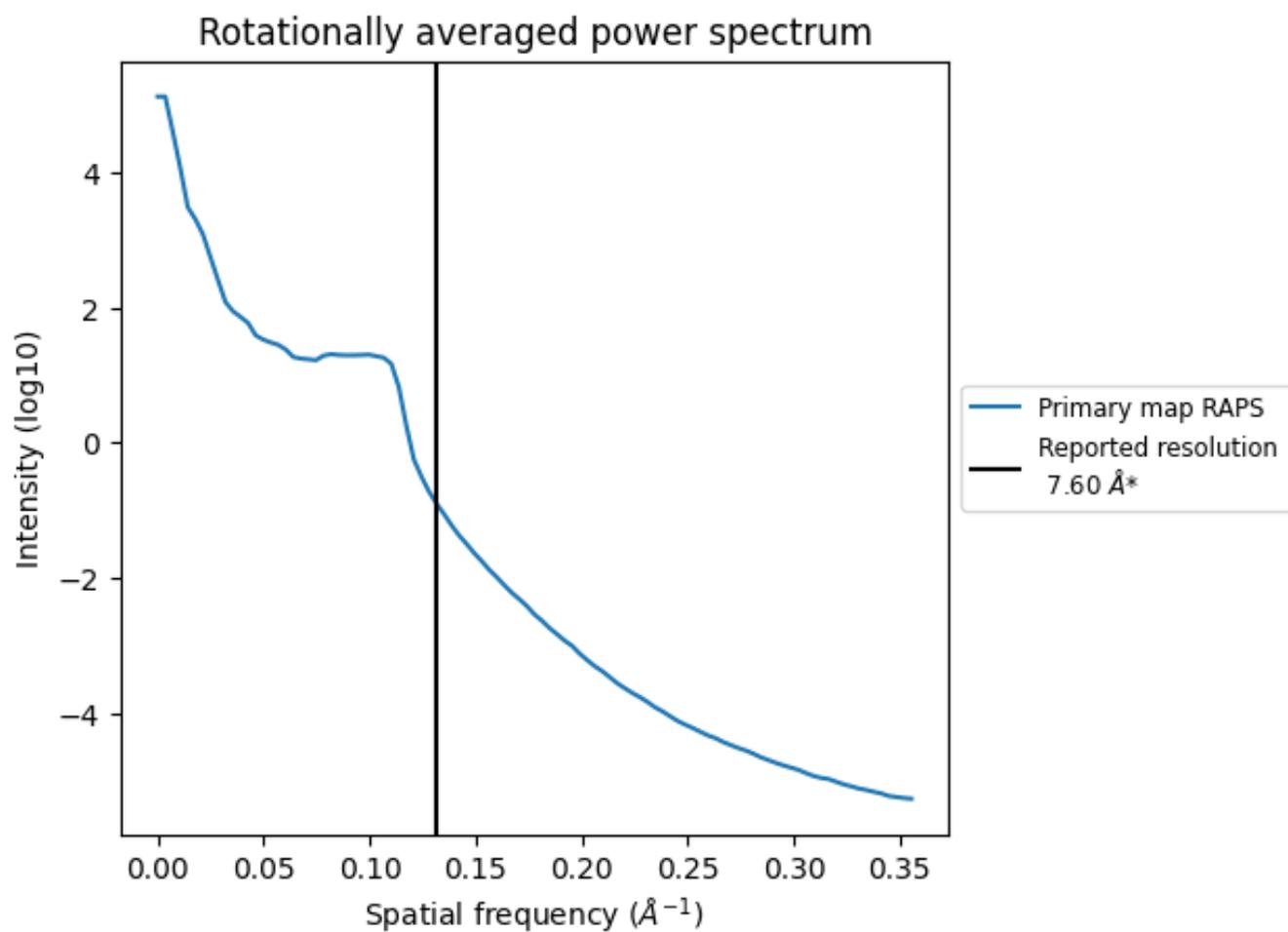
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 359 nm³; this corresponds to an approximate mass of 325 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 0.132\AA^{-1}

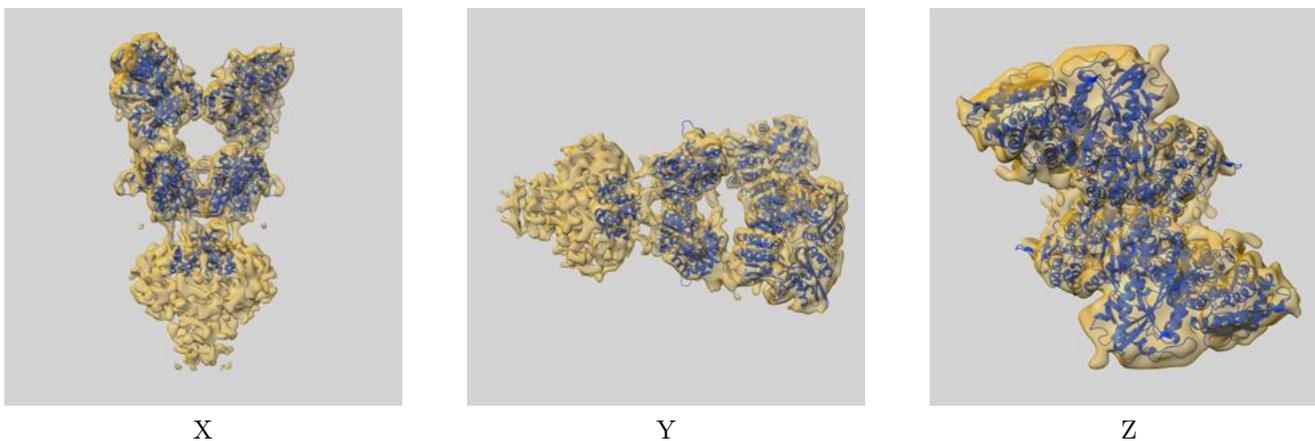
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

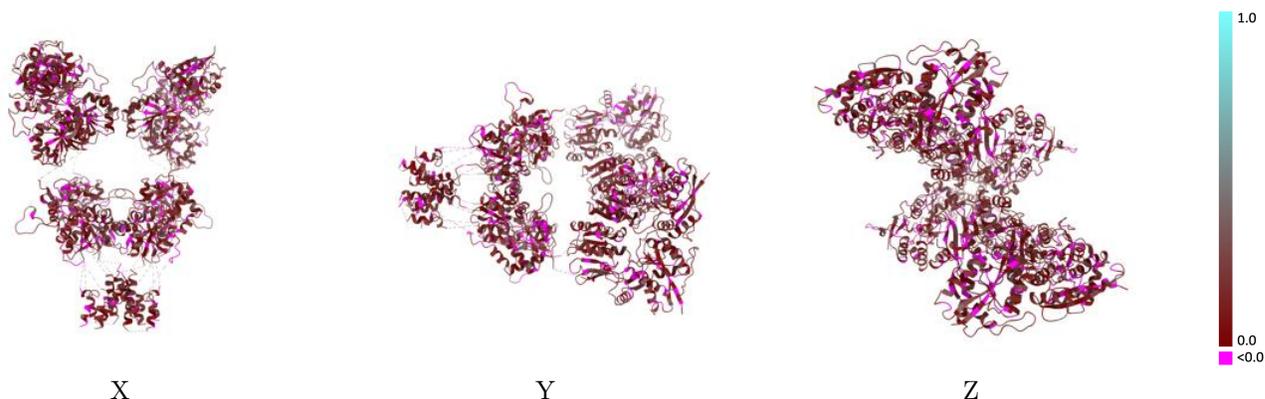
This section contains information regarding the fit between EMDB map EMD-2685 and PDB model 4UQQ. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



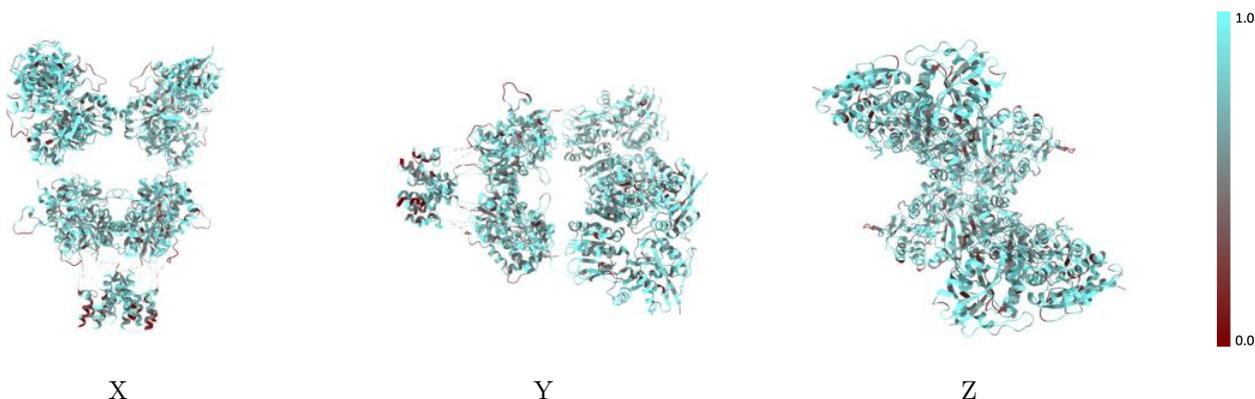
The images above show the 3D surface view of the map at the recommended contour level 0.121 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



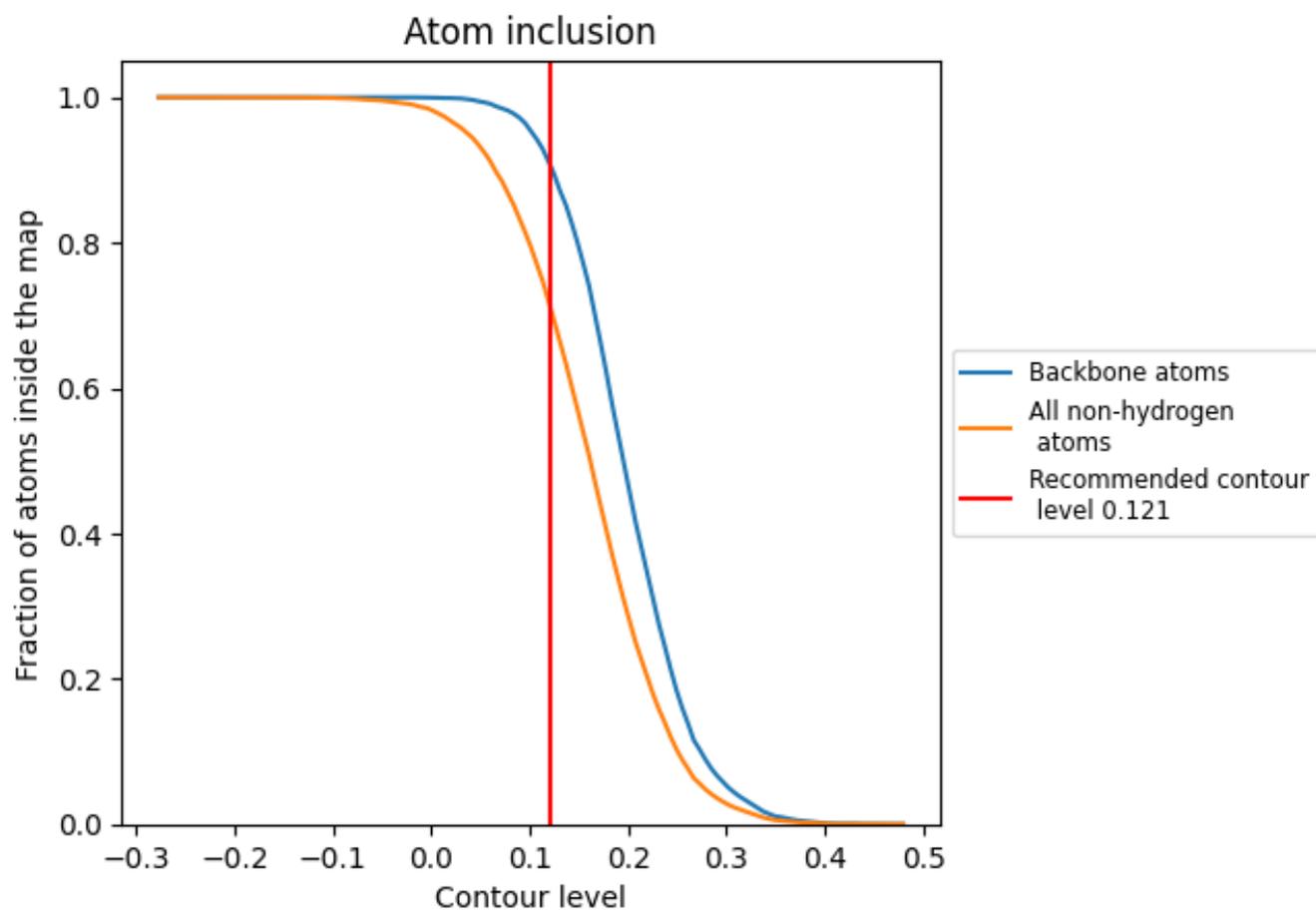
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.121).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.121) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7109	 0.1320
A	 0.7143	 0.1340
B	 0.7079	 0.1310
C	 0.7141	 0.1340
D	 0.7075	 0.1300

