wwPDB EM Validation Summary Report

May 27, 2026 – 12:28 PM JST

PDB ID	:	22BD / pdb_000022bd
EMDB ID	:	EMD-68146
Title	:	ICA-1103811 bound KCNQ2/3 heteromer with 2:2 stoichiometry
Authors	:	Lu, F.; Fan, X.; Huang, J.
Deposited on	:	2026-01-05
Resolution	:	3.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

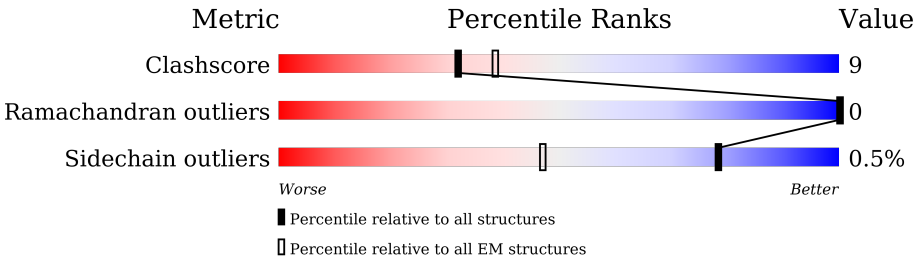
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

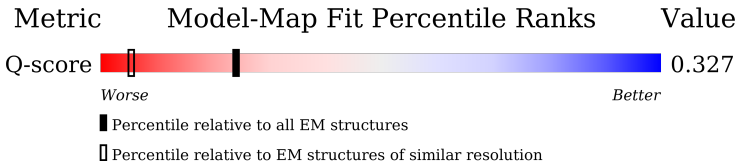
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

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 <=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	872	23% 6% 72%
1	C	872	5% 23% 5% 71%
2	B	872	10% 22% 6% 71%
2	D	872	12% 23% 5% 71%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8123 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 Potassium voltage-gated channel subfamily KQT member 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	248	Total	C	N	O	S	0	0
			2016	1339	339	329	9		
1	C	249	Total	C	N	O	S	0	0
			2027	1345	343	330	9		

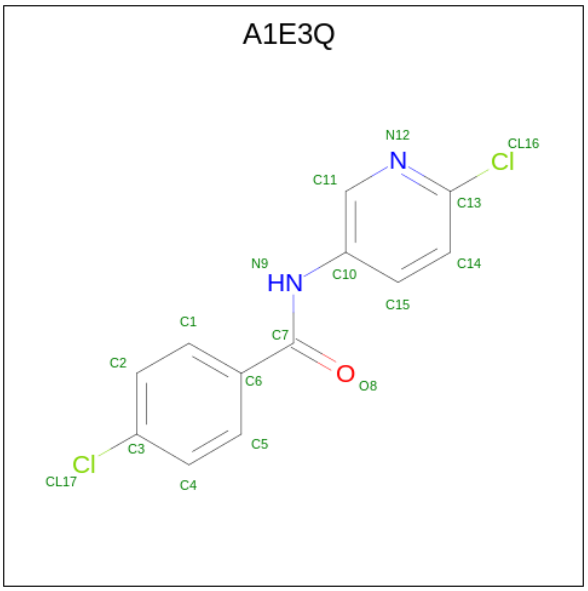
- Molecule 2 is a protein called Potassium voltage-gated channel subfamily KQT member 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	251	Total	C	N	O	S	0	0
			2021	1341	337	333	10		
2	B	251	Total	C	N	O	S	0	0
			2021	1341	337	333	10		

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
3	A	3	Total	K	0
			3	3	
3	C	1	Total	K	0
			1	1	

- Molecule 4 is 4-chloranyl- {N}-(6-chloranylpyridin-3-yl)benzamide (CCD ID: A1E3Q) (formula: $C_{12}H_8Cl_2N_2O$) (labeled as "Ligand of Interest" by depositor).



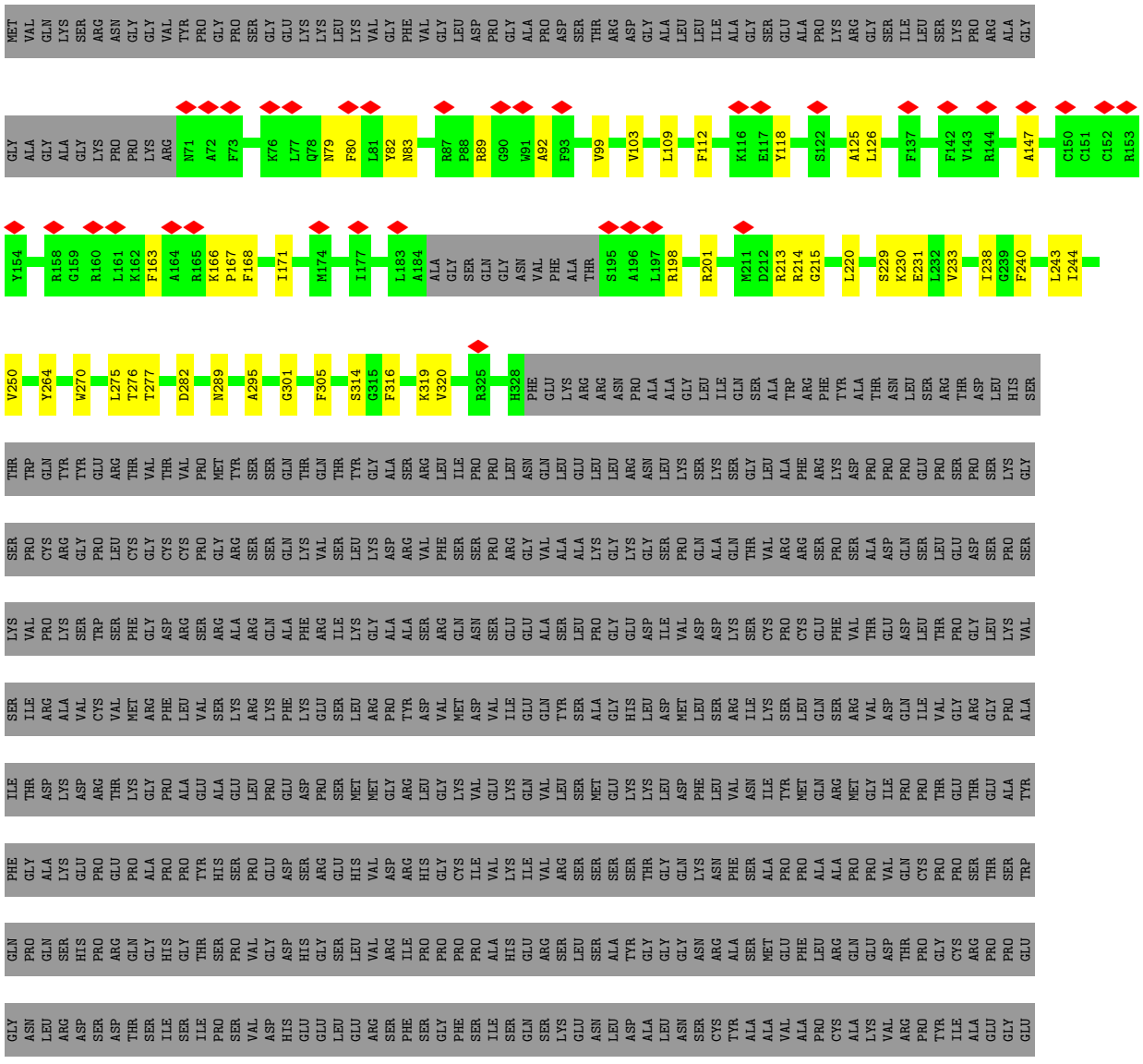
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	Cl	N	O	0
			17	12	2	2	1	
4	C	1	Total	C	Cl	N	O	0
			17	12	2	2	1	

3 Residue-property plots (i)

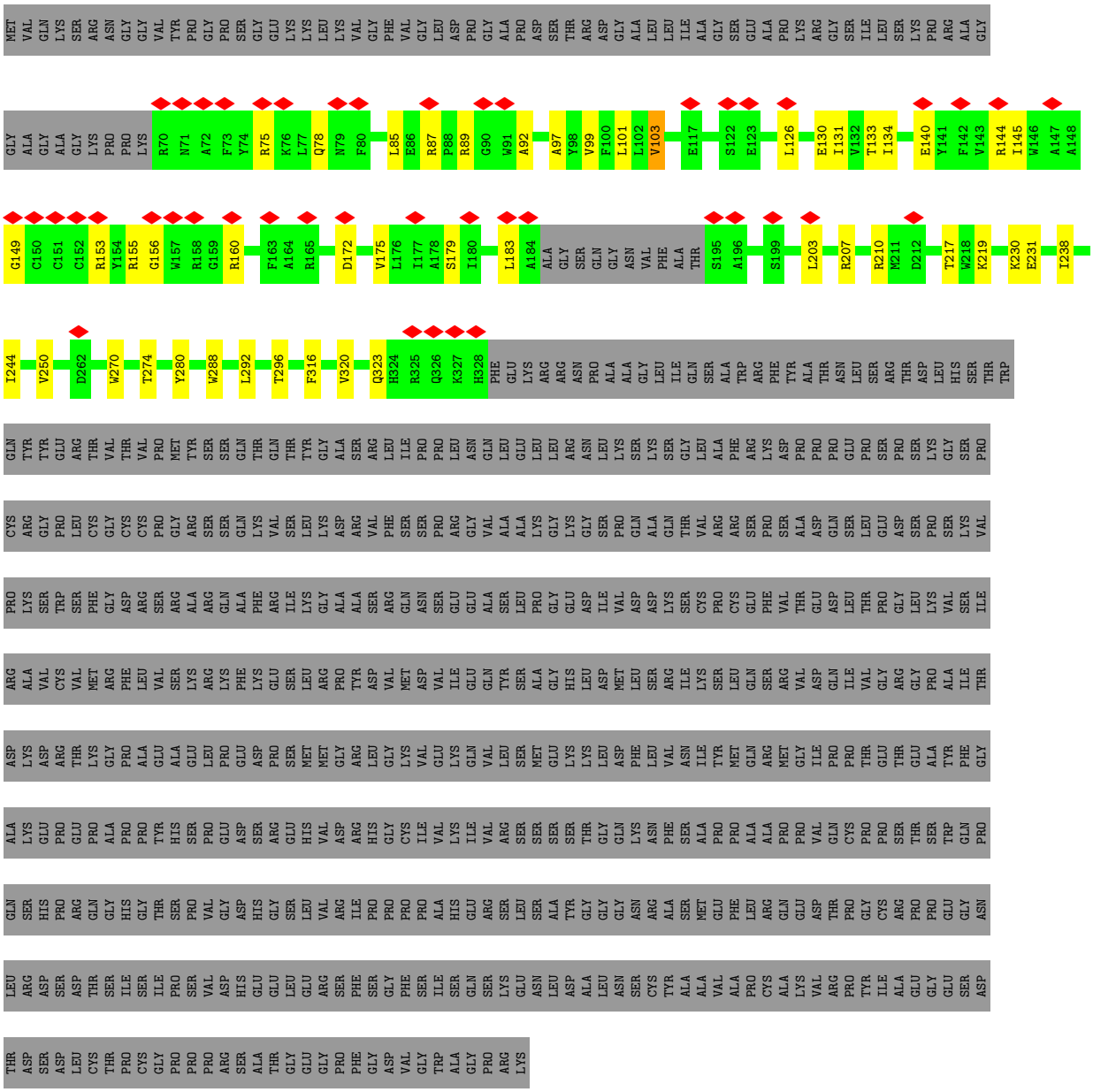
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Potassium voltage-gated channel subfamily KQT member 2

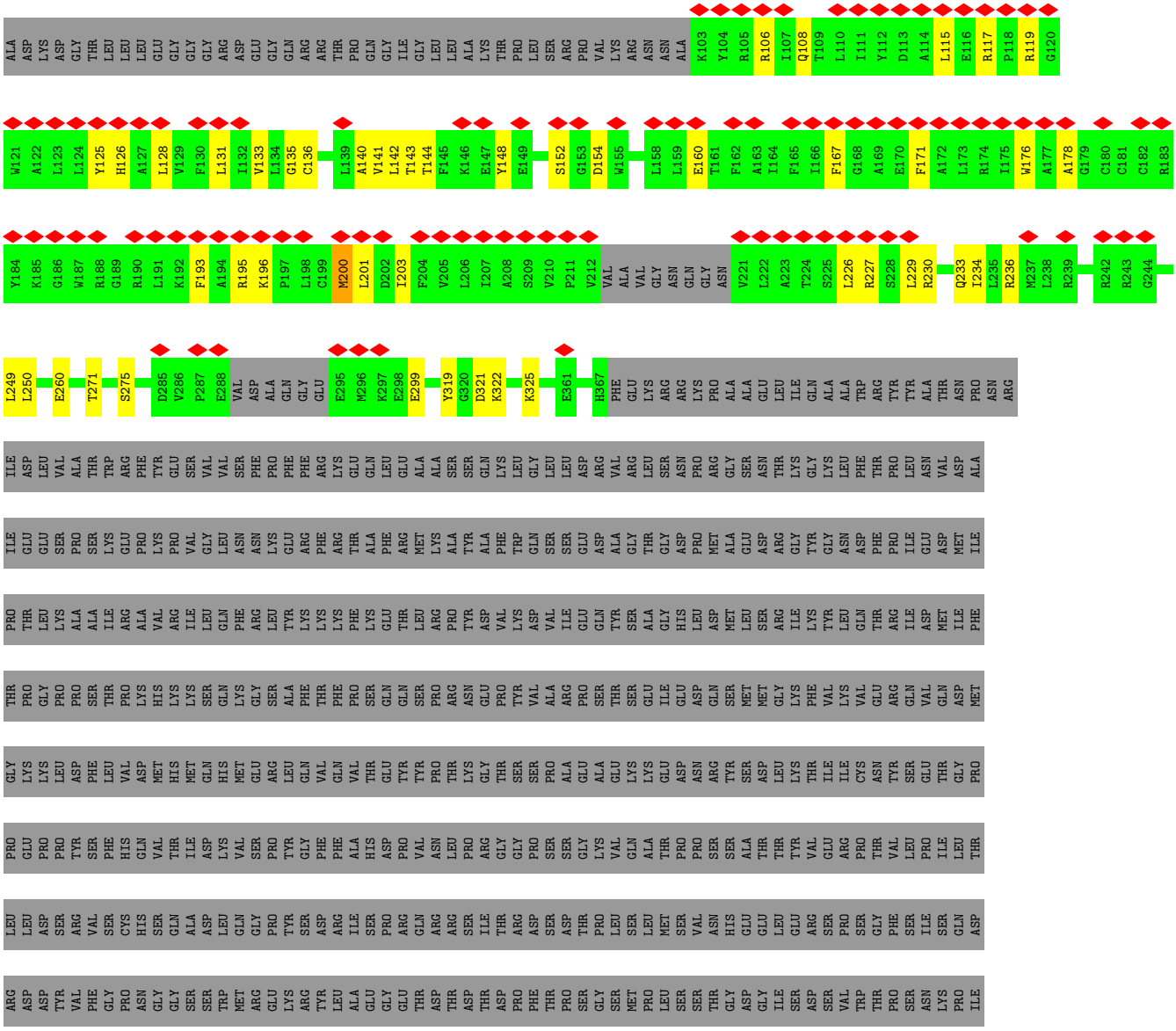
Chain A:



• Molecule 1: Potassium voltage-gated channel subfamily KQT member 2

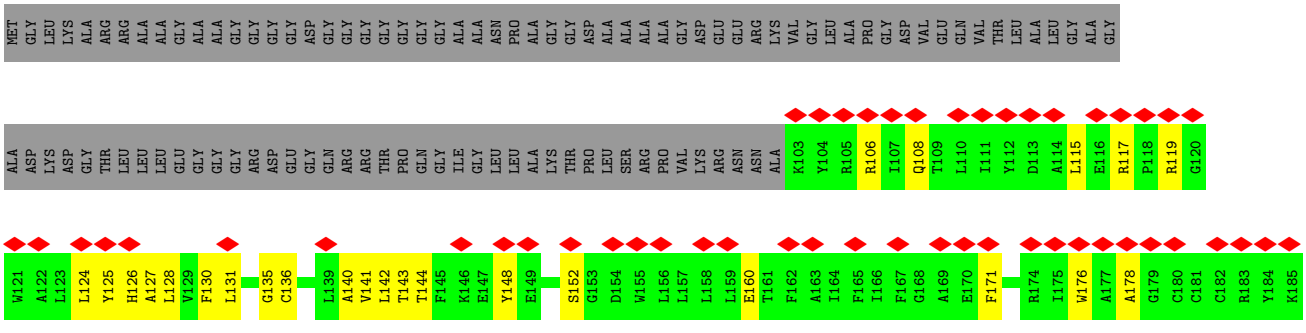


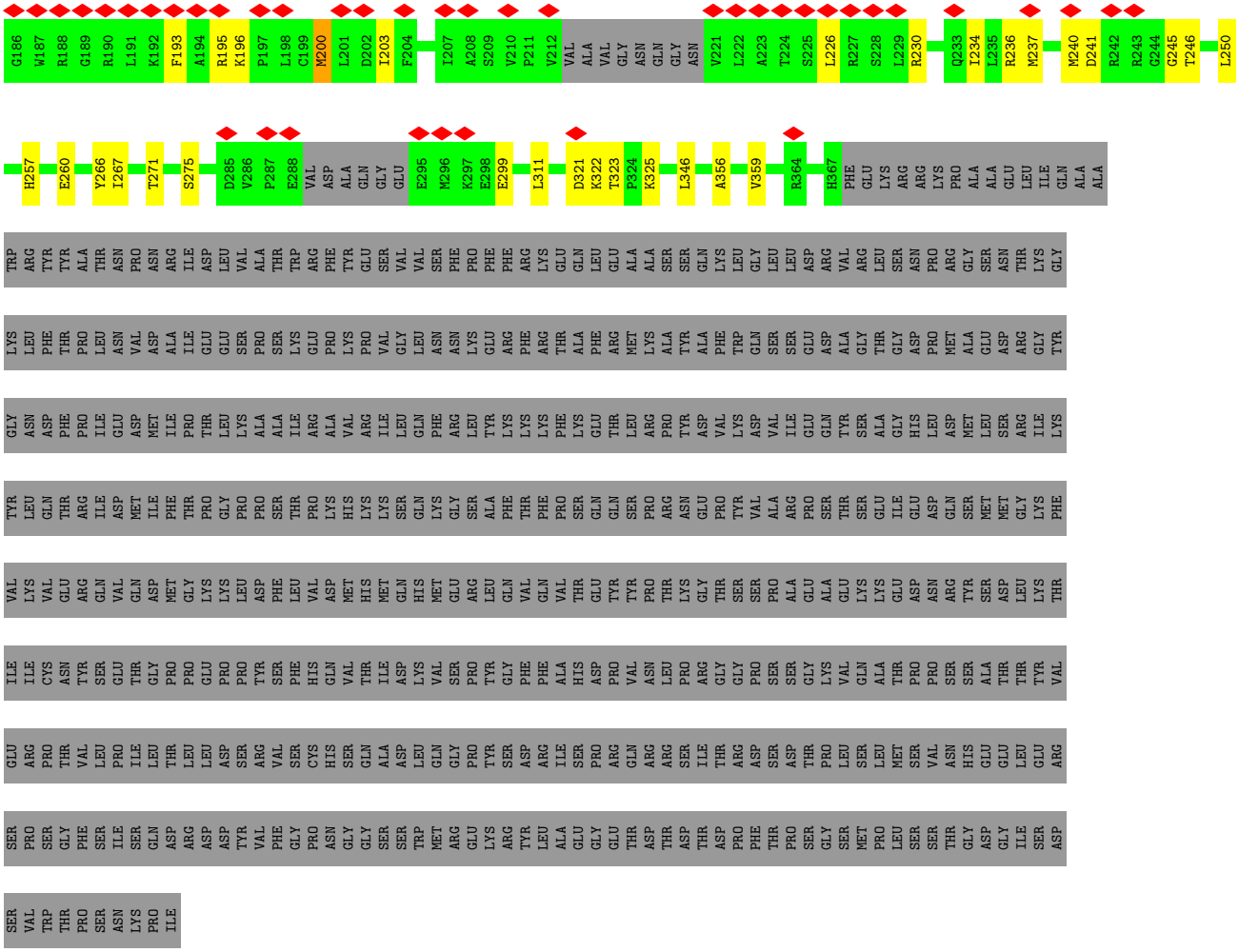
• Molecule 2: Potassium voltage-gated channel subfamily KQT member 3



• Molecule 2: Potassium voltage-gated channel subfamily KQT member 3

Chain B:




G186 W187 R188 G189 R190 L191 K192 F193 A194 R195 K196 P197 L198 C199 M200 L201 D202 I203 F204 I207 A208 S209 V210 P211 V212 VAL ALA VAL GLY ASN GLN GLY ASN V221 L222 A223 T224 S225 L226 R227 S228 L229 R230 Q233 I234 L235 R236 M237 M240 D241 R242 R243 G244 G245 T246 L250
H257 E260 Y266 I267 T271 S275 D285 V286 P287 E288 VAL ASP ALA GLN GLY GLU E295 M296 K297 E298 E299 L311 D321 K322 T323 P324 K325 L346 A356 V359 R364 H367 PHE GLU LYS ARG ARG LYS PRO ALA ALA GLU LEU ILE GLN ALA ALA
TRP ARG TYR TYR ALA THR ASN PRO ASN ARG ILE ASP LEU VAL ALA THR TRP ARG PHE TYR GLU SER VAL VAL SER PHE PRO PHE PHE ARG LYS GLU GLN LEU GLU ALA ALA SER SER GLN LYS LEU GLY LEU LEU ASP ARG VAL ARG LEU ARG GLY LEU SER ASN PRO ARG GLY SER ASN THR LYS GLY
LYS LEU PHE THR PRO LEU ASN VAL ASP ALA ILE GLU GLU SER PRO SER LYS GLU PRO LYS PRO VAL GLY LEU ASN ASN LYS GLU ARG PHE ARG THR ALA PHE ARG MET LYS ALA TYR ALA PHE TRP GLN SER SER GLU ASP ALA GLY THR GLY GLY ASP PRO MET ALA GLU ASP ARG GLY TYR
GLY ASN ASP PHE PRO ILE GLU ASP MET ILE PRO THR LEU LYS ALA ALA ILE ARG ALA VAL ARG ILE LEU GLN PHE ARG LEU TYR LYS LYS LYS PHE LYS GLU THR LEU ARG PRO TYR ASP VAL LYS ASP VAL ILE GLU GLN TYR SER ALA GLY HIS LEU ASP MET LEU SER ARG ILE LYS
TYR LEU GLN THR ARG ILE ASP MET ILE PHE THR PRO GLY PRO PRO SER THR PRO LYS HIS LYS LYS SER GLN LYS GLY SER ALA PHE THR PHE PRO SER GLN GLN SER PRO ARG ASN GLU PRO TYR VAL ALA ARG PRO SER THR SER GLU ILE GLU ASP GLN SER MET MET GLY LYS PHE
VAL LYS VAL GLU ARG GLN VAL GLN ASP MET GLY LYS LYS LEU ASP PHE LEU VAL ASP MET HIS MET GLN HIS MET GLU ARG LEU GLN VAL GLN VAL THR GLU TYR TYR PRO THR LYS GLY THR SER SER PRO ALA GLU ALA GLU LYS LYS GLU ASP ASN ARG TYR SER ASP LEU LYS THR
ILE ILE CYS ASN TYR SER GLU THR GLY PRO PRO GLU PRO PRO TYR SER PHE HIS GLN VAL THR ILE ASP LYS VAL SER PRO TYR GLY PHE PHE ALA HIS ASP PRO VAL ASN LEU PRO ARG GLY GLY PRO SER SER GLY LYS VAL GLN ALA THR PRO PRO SER SER ALA THR THR TYR VAL
GLU ARG PRO THR VAL LEU PRO ILE LEU LEU THR LEU LEU ASP SER SER ARG VAL SER CYS HIS SER GLN ALA ASP LEU GLN GLY PRO TYR SER ASP ARG ILE SER PRO ARG GLN ARG ARG SER ILE THR ARG ASP SER ASP THR PRO LEU SER LEU MET SER VAL ASN HIS GLU GLU LEU GLU ARG
SER PRO SER GLY PHE SER ILE SER GLN ASP ARG ASP ASP TYR VAL PHE GLY PRO ASN GLY GLY SER SER TRP MET ARG GLU LYS ARG TYR LEU ALA GLU GLY GLU THR ASP THR ASP THR ASP PRO PHE THR PRO SER GLY SER MET PRO LEU SER SER THR GLY ASP GLY ILE SER ASP
SER VAL TRP THR PRO SER ASN LYS PRO ILE

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	118562	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.699	Depositor
Minimum map value	-0.395	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	262.08, 262.08, 262.08	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.93599993, 0.93599993, 0.93599993	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1E3Q, K

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	0.15	0/2071	0.37	0/2805
1	C	0.13	0/2082	0.34	0/2819
2	B	0.13	0/2070	0.35	0/2801
2	D	0.13	0/2070	0.34	0/2801
All	All	0.13	0/8293	0.35	0/11226

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	2016	0	2053	41	0
1	C	2027	0	2066	44	0
2	B	2021	0	2101	54	0
2	D	2021	0	2101	33	0
3	A	3	0	0	0	0
3	C	1	0	0	0	0
4	A	17	0	0	0	0
4	C	17	0	0	0	0
All	All	8123	0	8321	142	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 9.

The worst 5 of 142 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:217:THR:CG2	2:B:267:ILE:HD11	1.79	1.12
1:C:217:THR:HG22	2:B:267:ILE:HD11	1.33	1.07
1:A:231:GLU:OE2	2:B:359:VAL:HG22	1.71	0.89
1:C:217:THR:CG2	2:B:267:ILE:CD1	2.51	0.87
1:C:217:THR:HG21	2:B:266:TYR:HD2	1.45	0.81

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	244/872 (28%)	242 (99%)	2 (1%)	0	100	100
1	C	245/872 (28%)	244 (100%)	1 (0%)	0	100	100
2	B	245/872 (28%)	242 (99%)	3 (1%)	0	100	100
2	D	245/872 (28%)	242 (99%)	3 (1%)	0	100	100
All	All	979/3488 (28%)	970 (99%)	9 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	207/728 (28%)	207 (100%)	0	100	100
1	C	208/728 (29%)	207 (100%)	1 (0%)	81	89
2	B	209/725 (29%)	208 (100%)	1 (0%)	81	89
2	D	209/725 (29%)	207 (99%)	2 (1%)	68	84
All	All	833/2906 (29%)	829 (100%)	4 (0%)	78	89

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

Mol	Chain	Res	Type
1	C	103	VAL
2	D	200	MET
2	D	201	LEU
2	B	200	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	326	GLN
1	C	71	ASN
1	C	78	GLN
1	C	323	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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	$\#\|Z\| > 2$
4	A1E3Q	A	904	-	18,18,18	0.14	0	24,24,24	0.25	0
4	A1E3Q	C	902	-	18,18,18	0.12	0	24,24,24	0.27	0

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
4	A1E3Q	A	904	-	-	0/8/8/8	0/2/2/2
4	A1E3Q	C	902	-	-	0/8/8/8	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

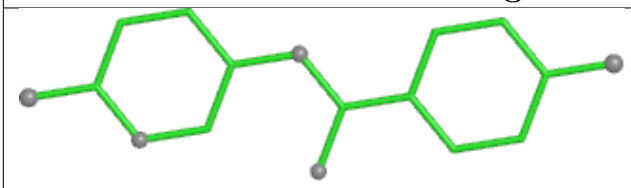
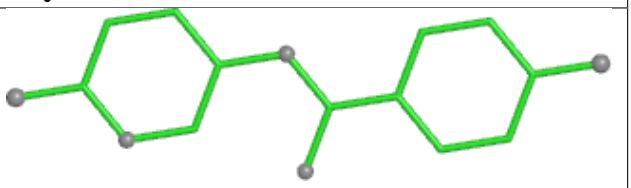
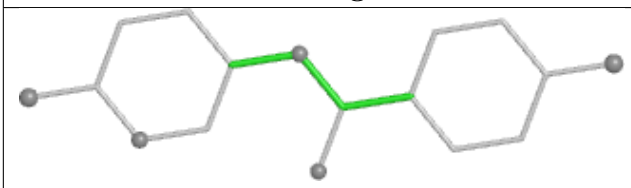
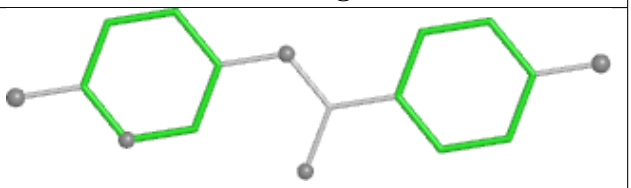
There are no chirality outliers.

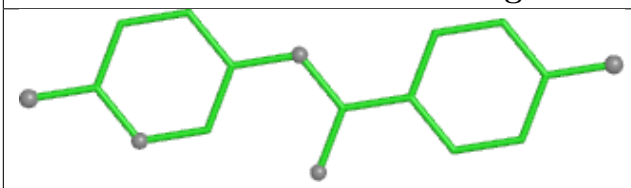
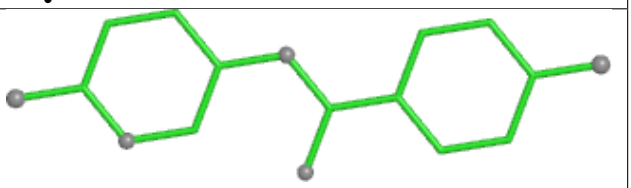
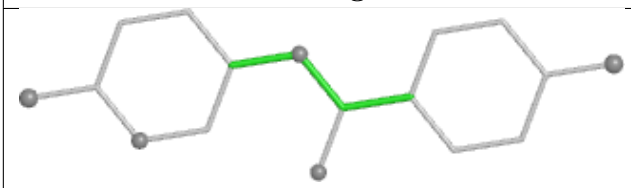
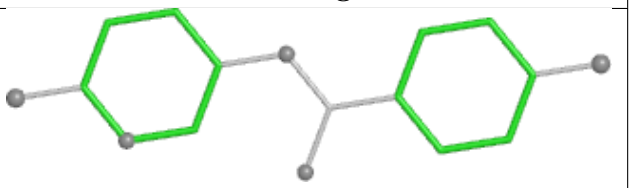
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand A1E3Q A 904	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand A1E3Q C 902	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

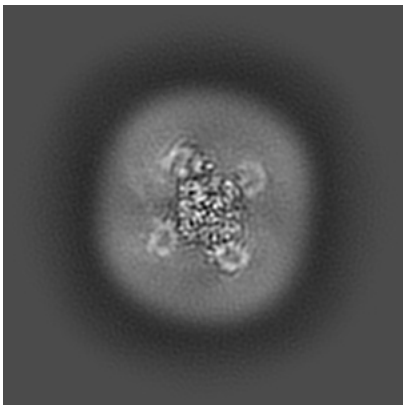
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-68146. These allow visual inspection of the internal detail of the map and identification of artifacts.

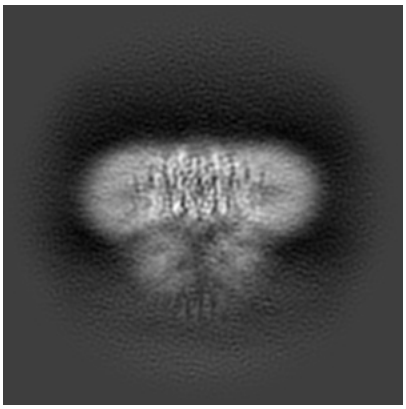
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

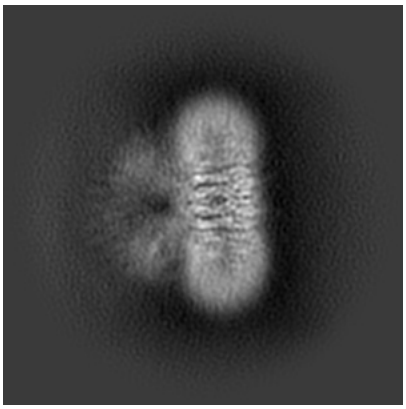
6.1.1 Primary map



X

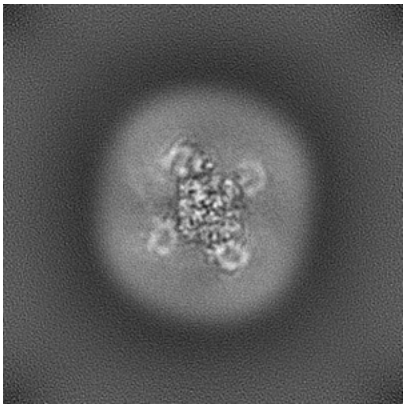


Y

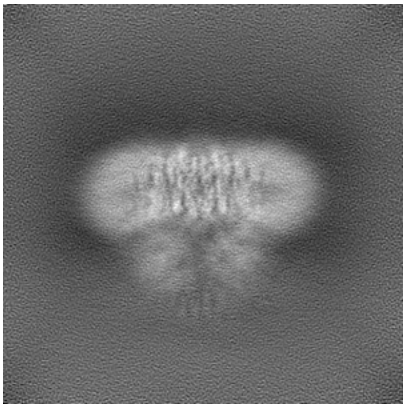


Z

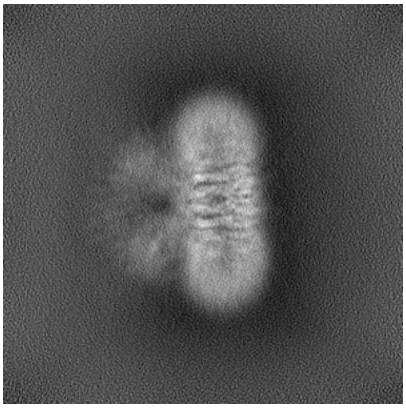
6.1.2 Raw map



X



Y

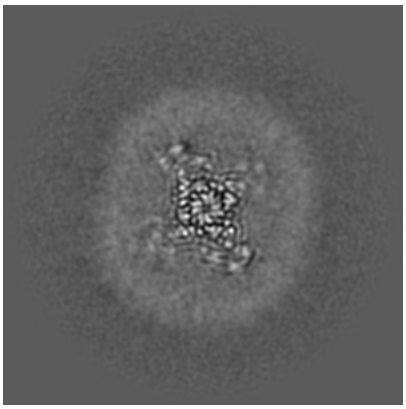


Z

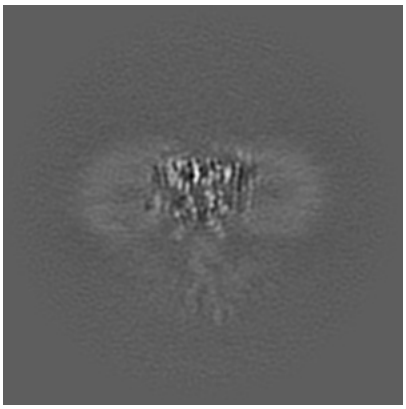
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

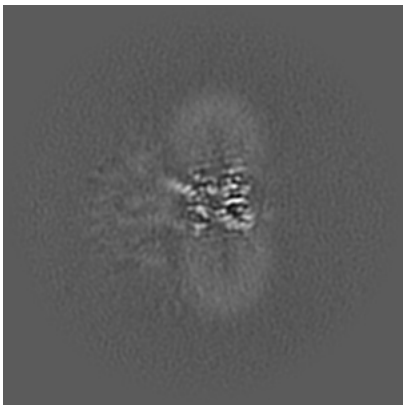
6.2.1 Primary map



X Index: 140

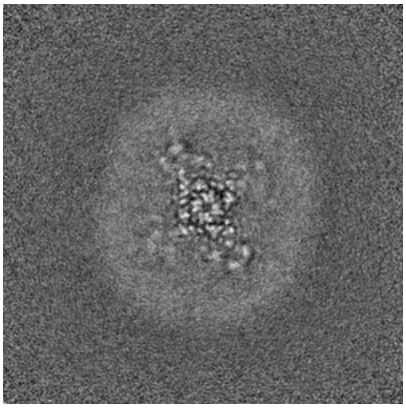


Y Index: 140

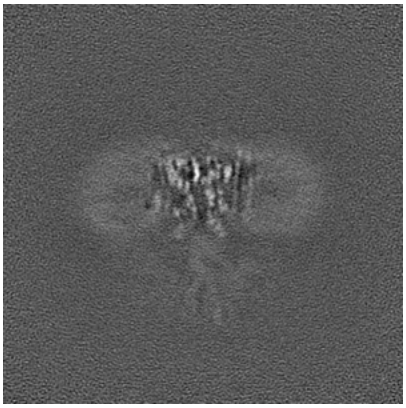


Z Index: 140

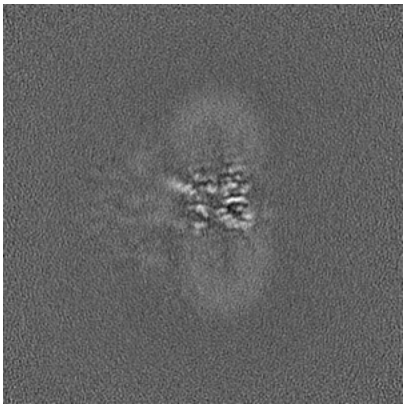
6.2.2 Raw map



X Index: 140



Y Index: 140

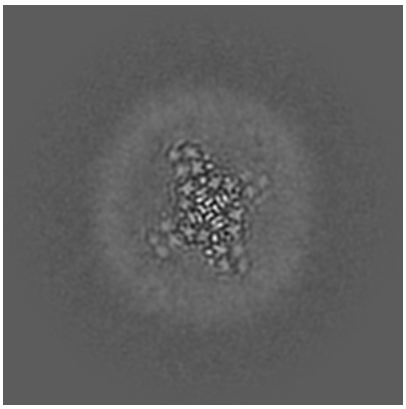


Z Index: 140

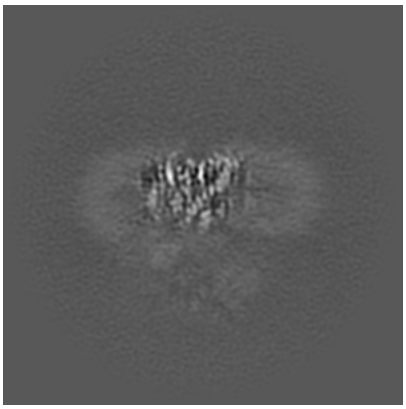
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

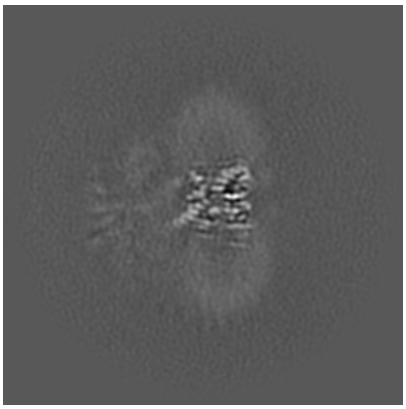
6.3.1 Primary map



X Index: 160

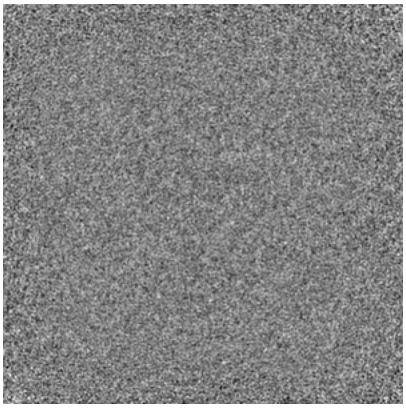


Y Index: 148

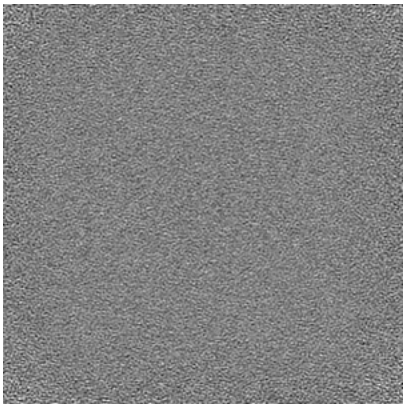


Z Index: 133

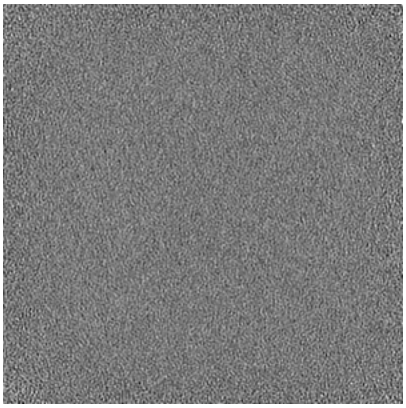
6.3.2 Raw map



X Index: 0



Y Index: 0

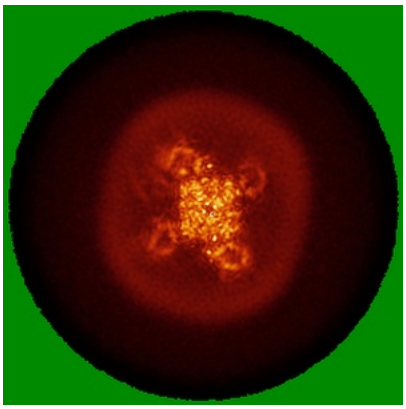


Z Index: 279

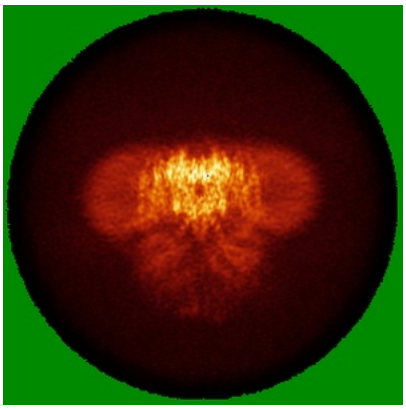
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

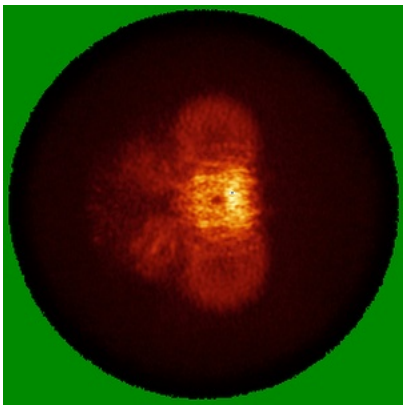
6.4.1 Primary map



X

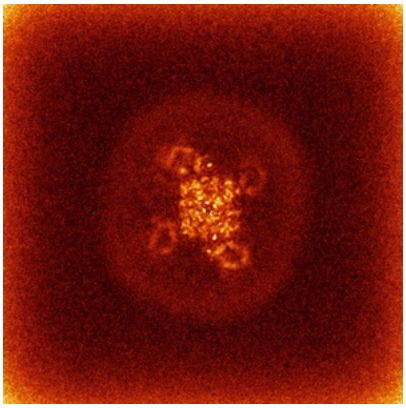


Y

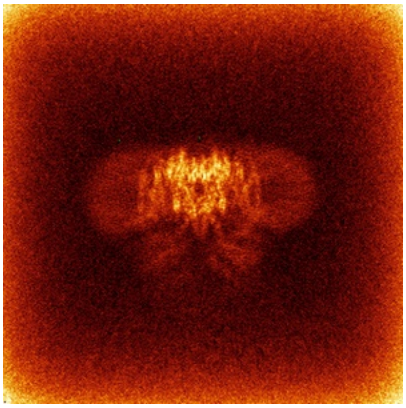


Z

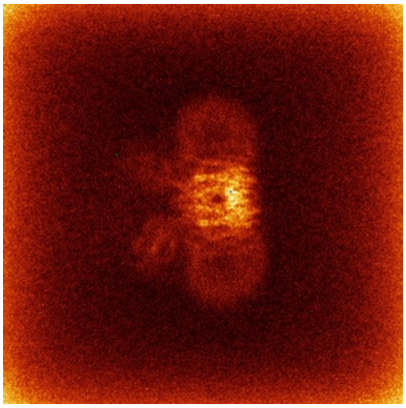
6.4.2 Raw map



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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. 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

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

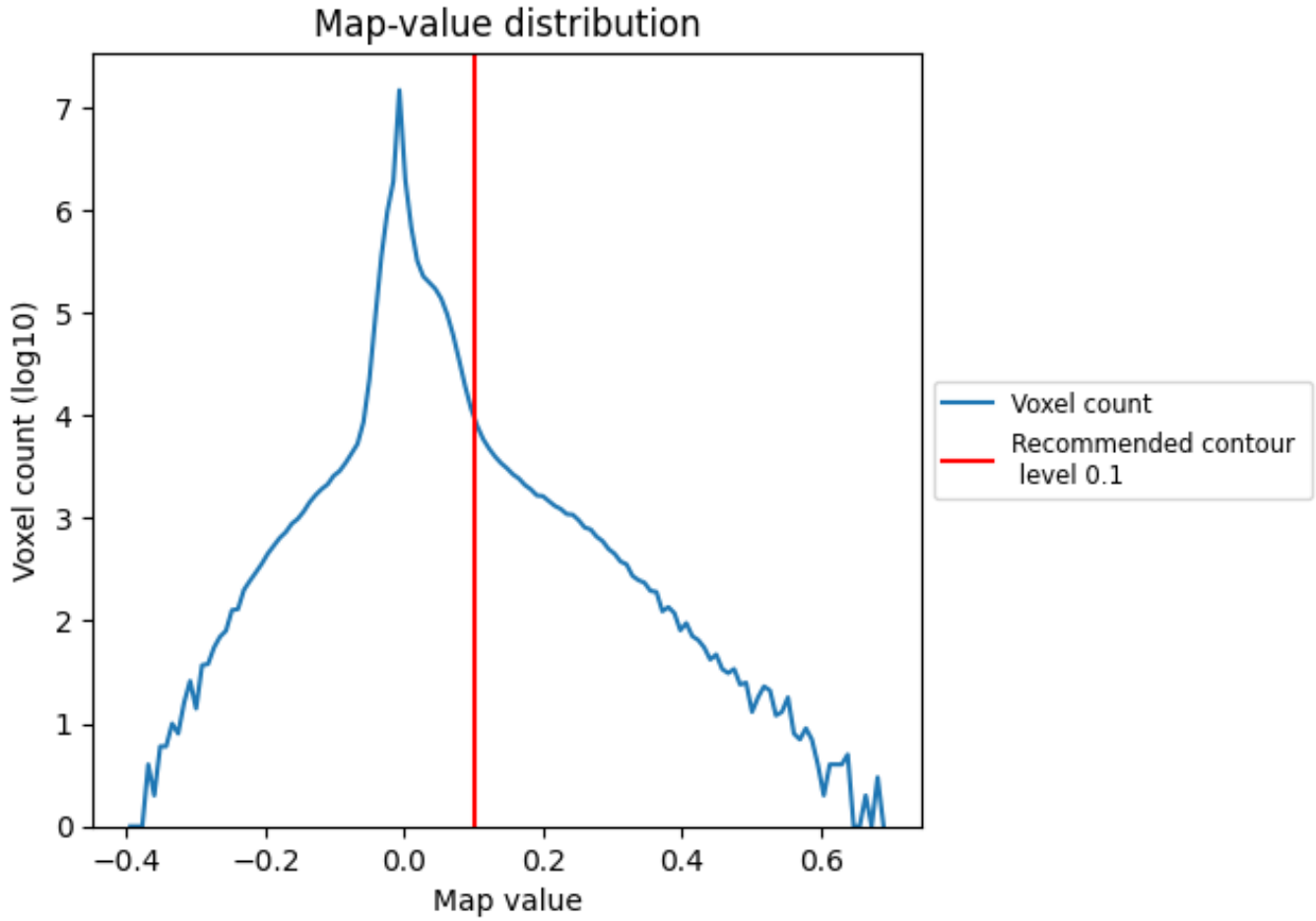
6.6 Mask visualisation (i)

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

7 Map analysis

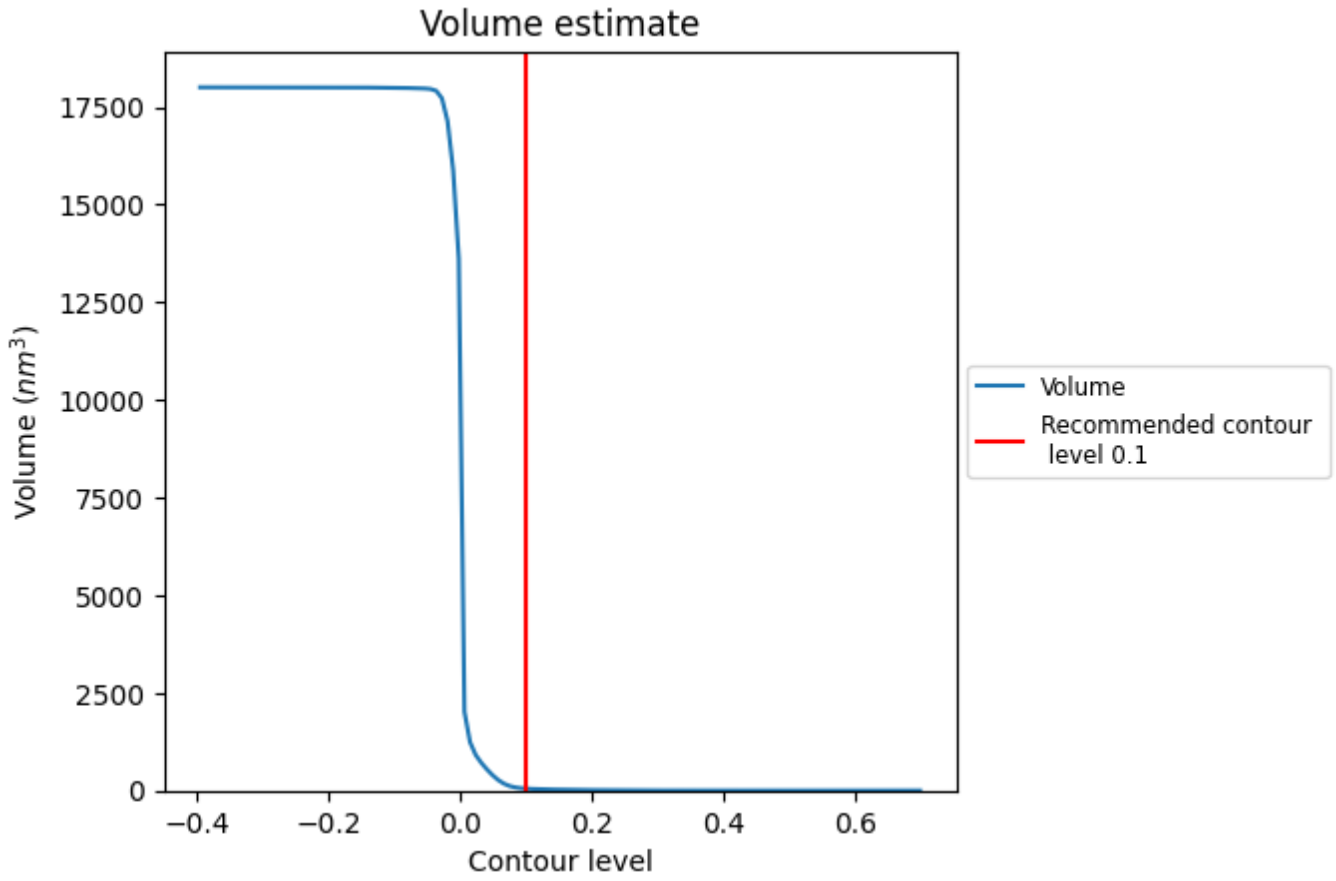
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

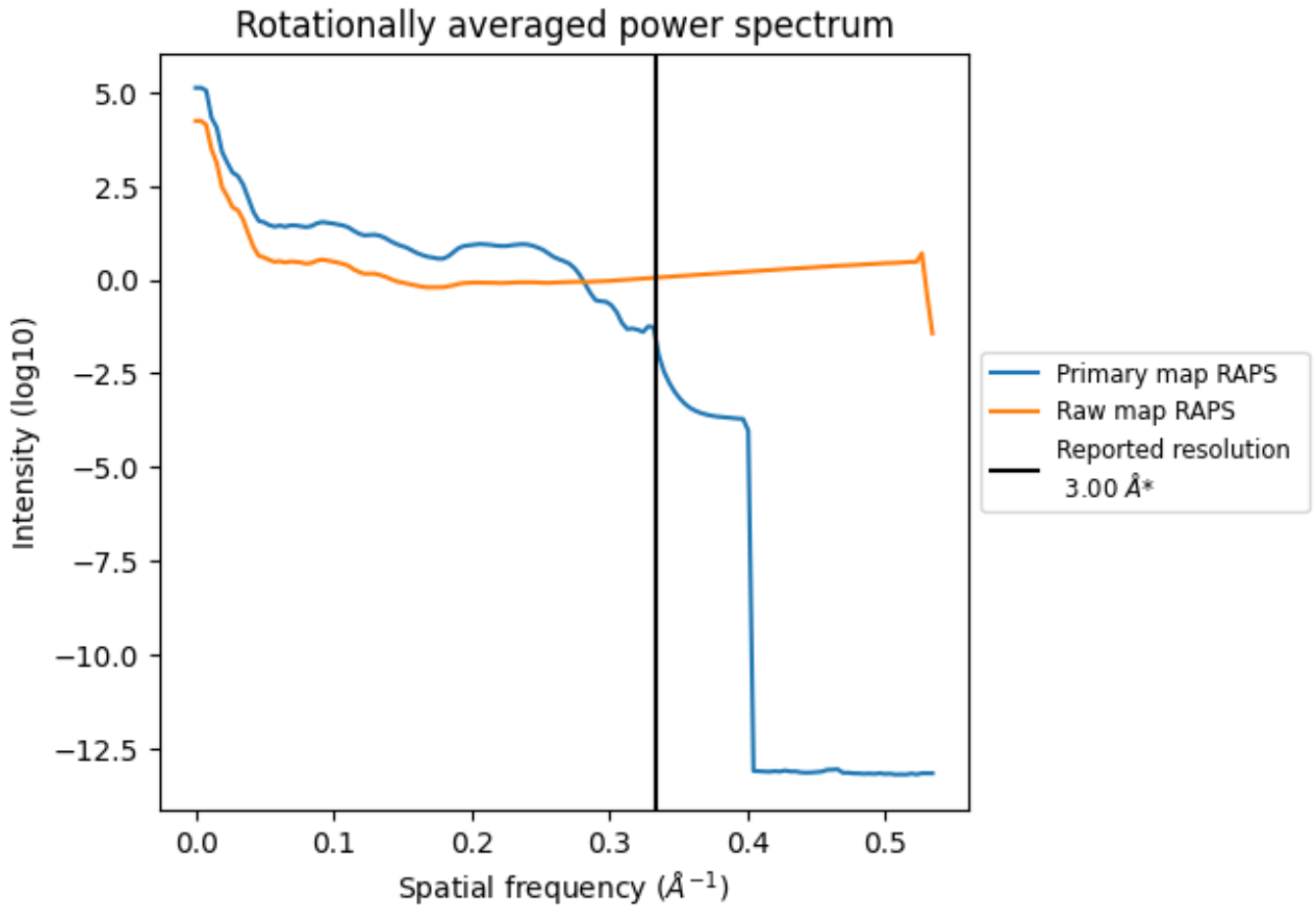
7.2 Volume estimate (i)



The volume at the recommended contour level is 50 nm^3; this corresponds to an approximate mass of 46 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)

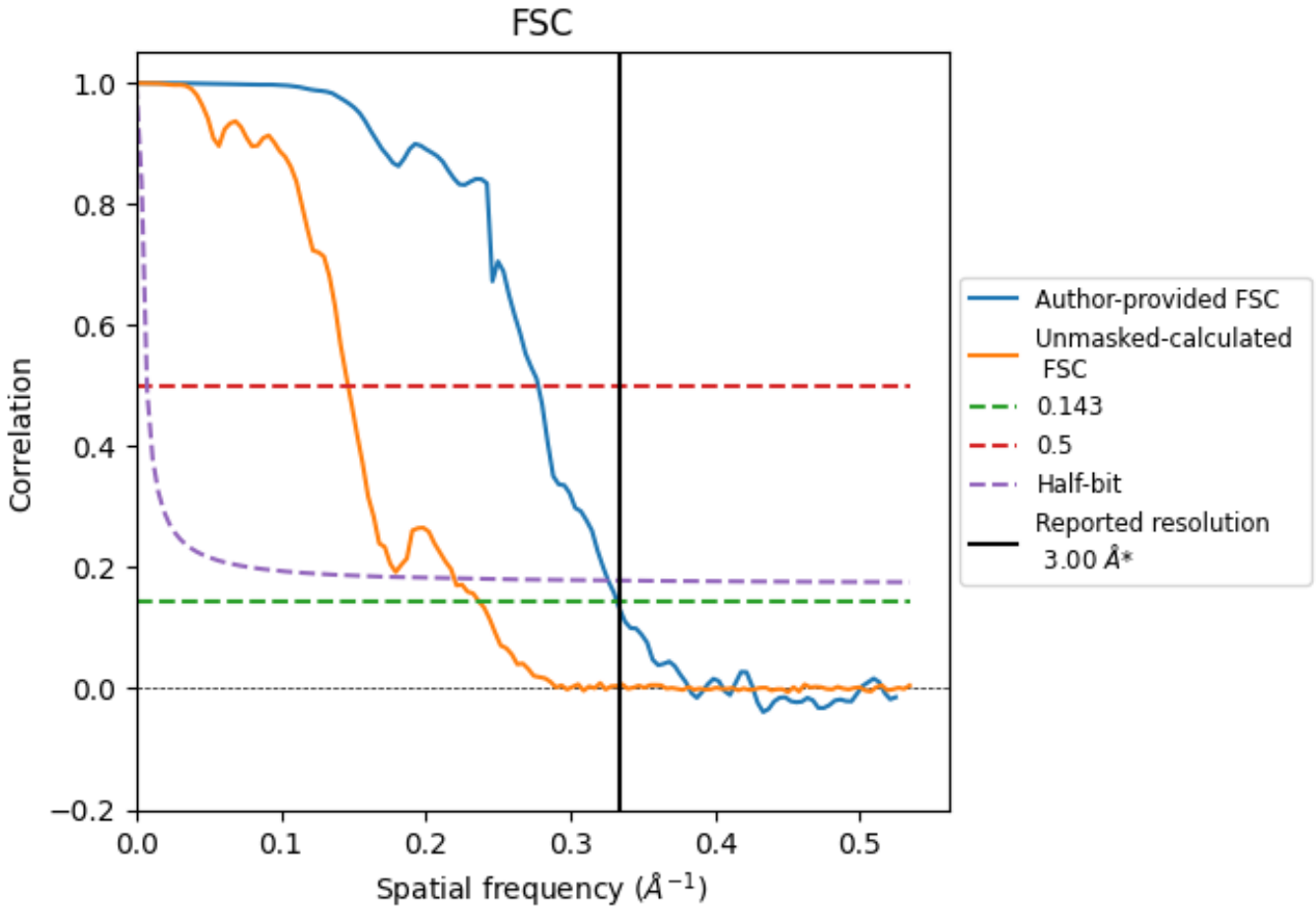


*Reported resolution corresponds to spatial frequency of 0.333 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8.2 Resolution estimates (i)

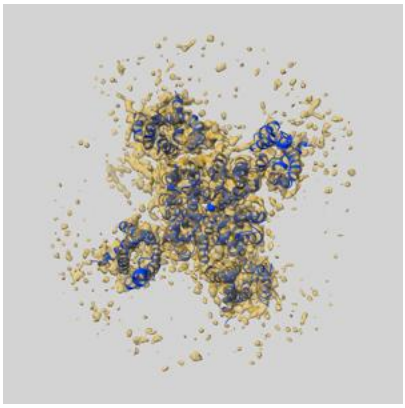
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.01	3.60	3.07
Unmasked-calculated*	4.22	6.83	4.55

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.22 differs from the reported value 3.0 by more than 10 %

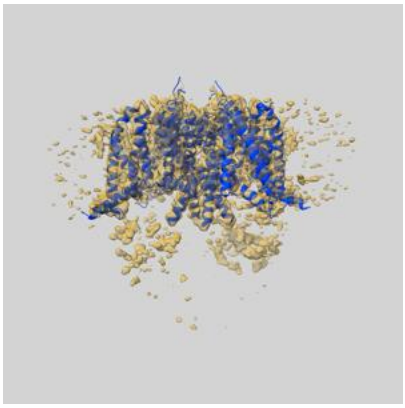
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-68146 and PDB model 22BD. Per-residue inclusion information can be found in section 3 on page 5.

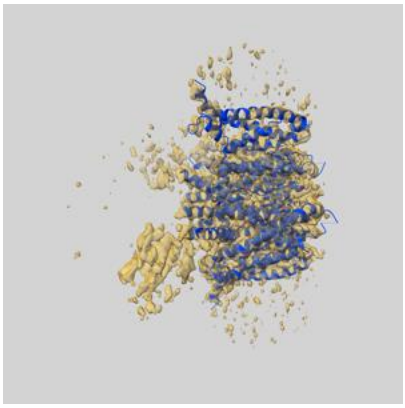
9.1 Map-model overlay



X



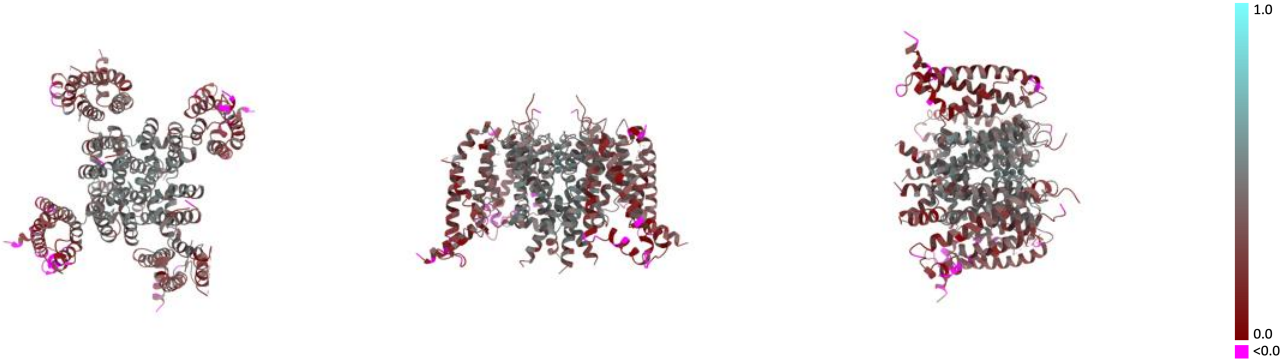
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 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.

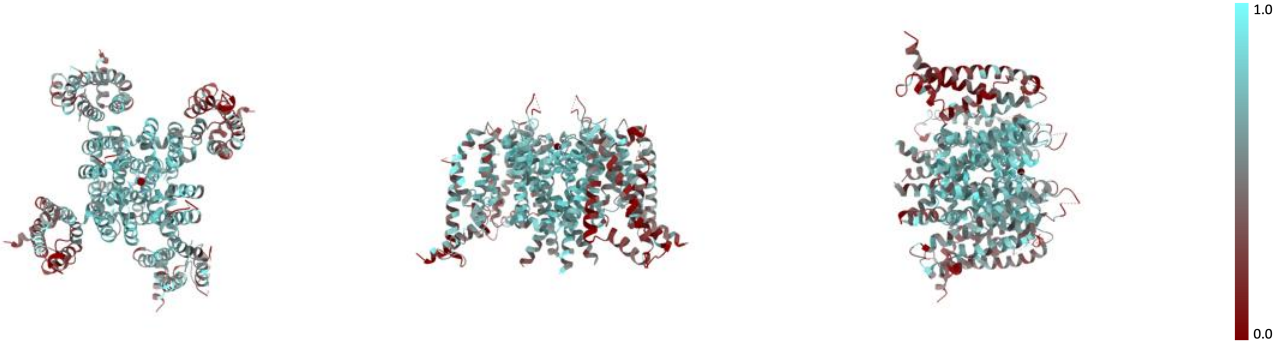
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

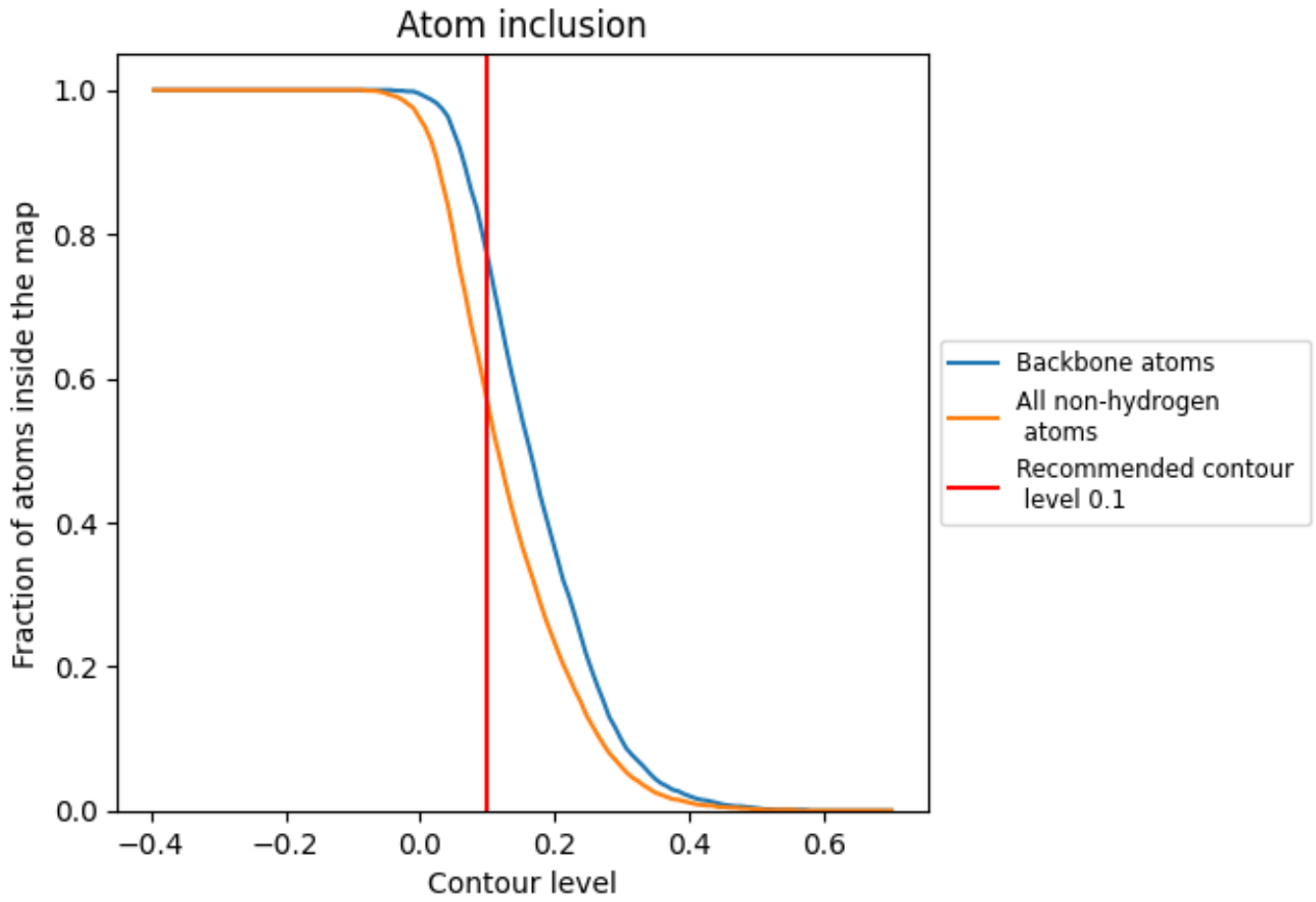
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 56% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5640	0.3270
A	0.6330	0.3500
B	0.5090	0.2950
C	0.6300	0.3560
D	0.4840	0.3050