wwPDB EM Validation Summary Report (i)

Mar 19, 2024 – 06:29 PM JST

PDB ID	:	6IJZ
EMDB ID	:	EMD-9682
Title	:	Structure of a plant cation channel
Authors	:	Sun, L.; Wang, J.; Liu, X.
Deposited on	:	2018-10-12
Resolution	:	3.68 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 (i)) were used in the production of this report:

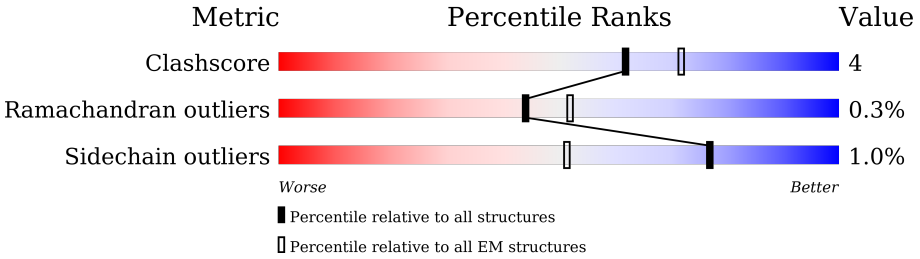
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.68 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 <=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	771	26% 76% 12% • 11%
1	B	771	27% 77% 11% • 11%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 10964 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 Calcium permeable stress-gated cation channel 1.

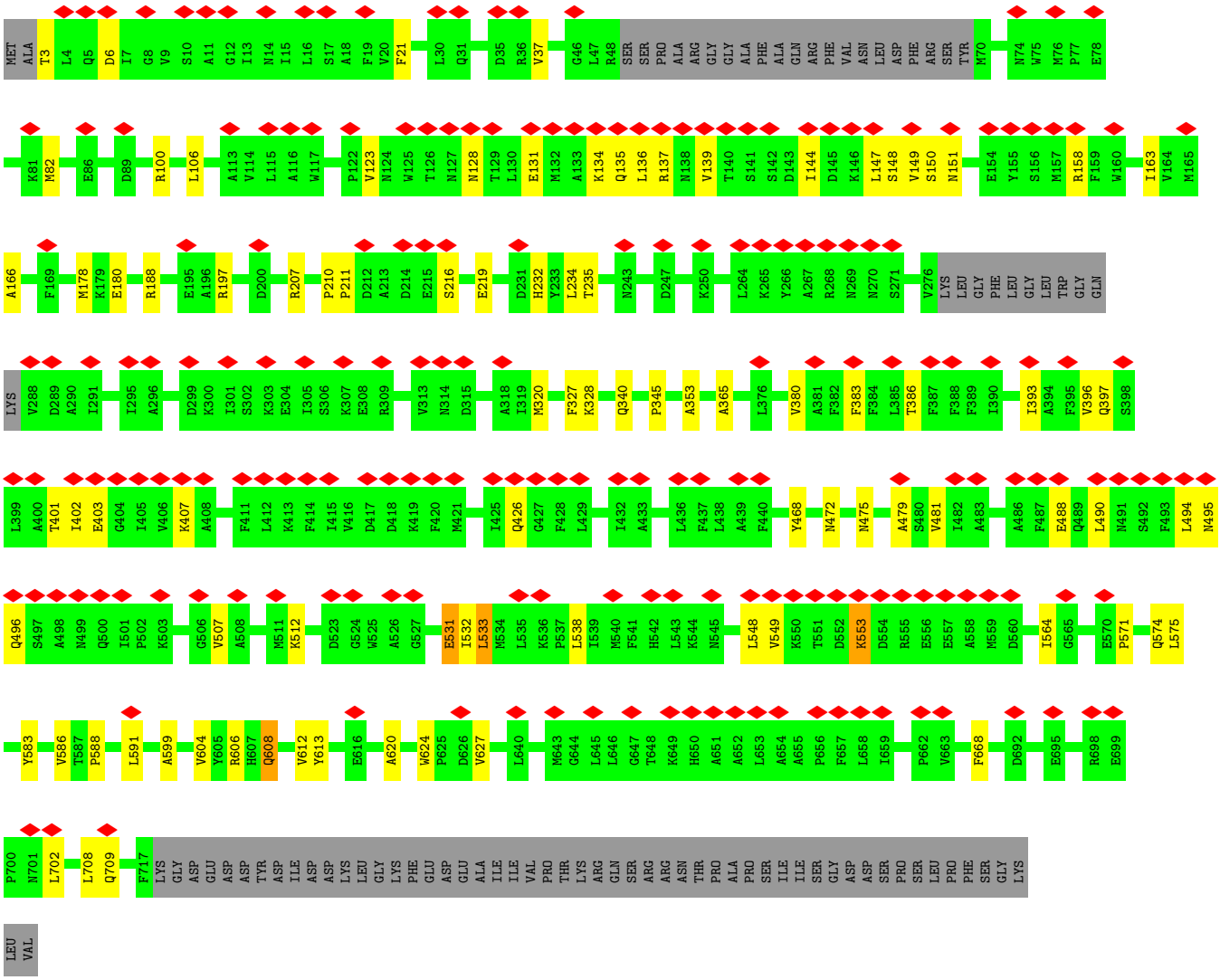
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	683	5482	3632	889	936	25	0	0
1	B	683	5482	3632	889	936	25	0	0

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: Calcium permeable stress-gated cation channel 1

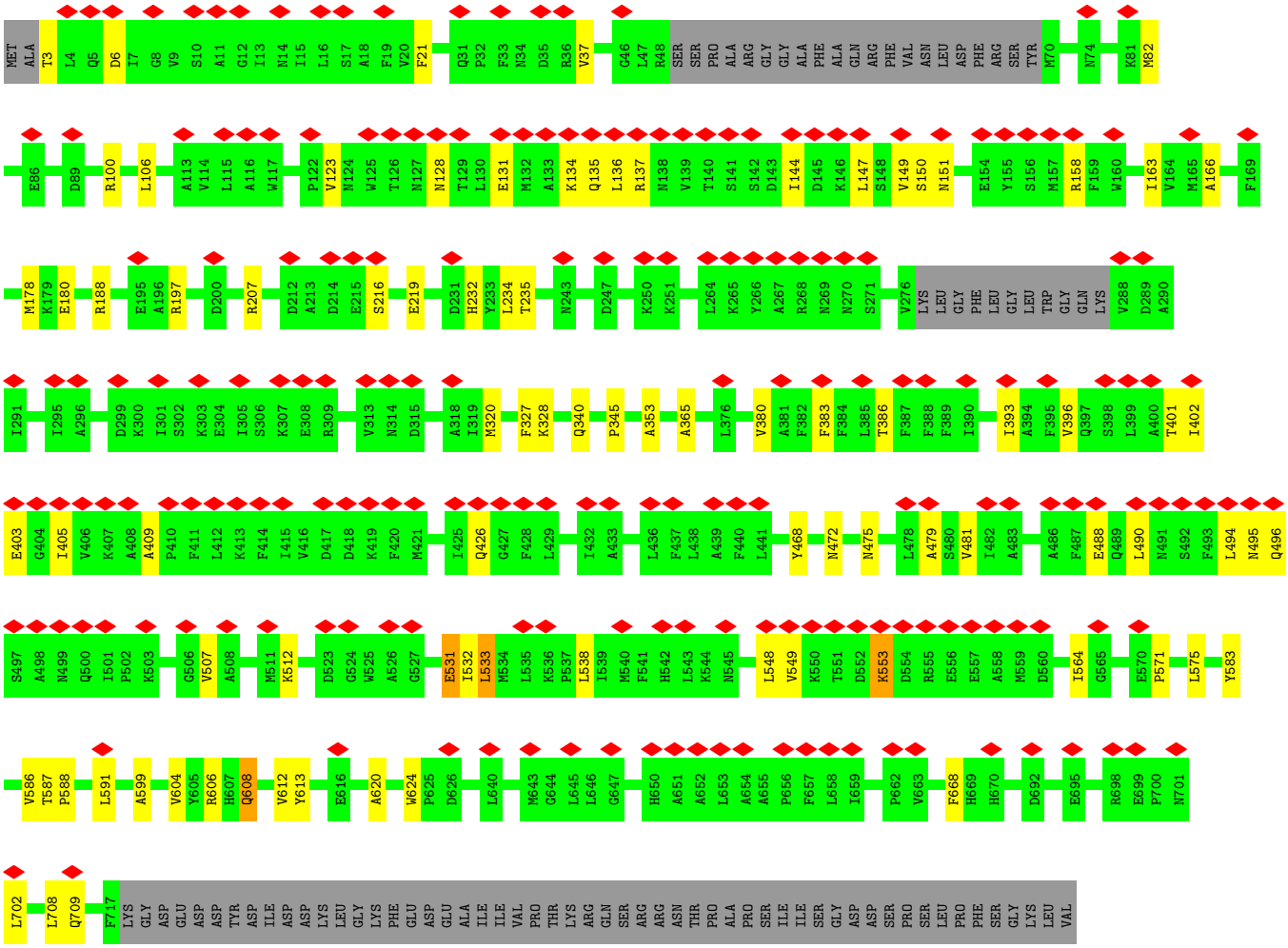
Chain A:



- Molecule 1: Calcium permeable stress-gated cation channel 1

Chain B:

27%
77%
11%
11%


MET ALA T3 L4 Q5 D6 I7 G8 V9 S10 A11 G12 I13 N14 I15 L16 S17 A18 F19 V20 F21 Q31 P32 F33 N34 D35 R36 V37 G46 L47 R48 SER SER PRO ALA ARG GLY GLY ALA PHE ALA GLN ARG PHE VAL ASN LEU ASP PHE ARG SER TYR M70 M74 K81 M82
E86 D89 R100 L106 A113 V114 L115 A116 W117 P122 V123 N124 W125 T126 N127 N128 T129 L130 E131 M132 A133 K134 Q135 L136 R137 N138 V139 T140 S141 S142 D143 I144 D145 K146 L147 S148 V149 S150 N151 E154 Y155 S156 M157 R158 F159 W160 I163 V164 M165 A166 F169
M178 K179 E180 R188 E195 A196 R197 D200 R207 D212 A213 D214 E215 S216 E219 D231 H232 Y233 L234 T235 N243 D247 K250 K251 L264 K265 Y266 A267 R268 N269 N270 S271 V276 LYS LEU GLY PHE LEU GLY LEU TRP GLY GLN LYS V288 D289 A290
I291 I295 A296 D299 K300 I301 S302 K303 E304 I305 S306 K307 E308 R309 V313 N314 D315 A318 I319 M320 F327 K328 Q340 P345 A353 A365 L376 V380 A381 F382 F383 F384 L385 T386 F387 F388 F389 I390 I393 A394 F395 V396 Q397 S398 L399 A400 T401 I402
E403 G404 I405 V406 K407 A408 A409 P410 F411 L412 K413 F414 I415 V416 D417 D418 K419 F420 M421 I425 Q426 G427 F428 L429 I432 A433 L436 F437 L438 A439 F440 L441 Y468 N472 N475 L478 A479 S480 V481 I482 A483 A486 F487 F488 Q489 L490 N491 S492 F493 L494 N495 Q496
S497 A498 N499 Q500 I501 P502 K503 G506 V507 A508 M511 K512 D523 G524 W525 A526 G527 E531 I532 L533 M534 L535 K536 P537 L538 I539 M540 F541 H542 L543 K544 N545 L548 V549 K550 T551 D552 K553 D554 R555 E556 E557 A558 M559 D560 I564 G565 E570 P571 L575 Y583
V586 T587 P588 L591 A599 V604 Y605 R606 H607 Q608 V612 Y613 E616 A620 W624 P625 D626 L640 M643 G644 L645 L646 G647 H650 A651 A652 L653 A654 A655 P656 F657 L658 I659 P662 V663 F668 H669 H670 D692 E695 R698 E699 P700 N701
L702 L708 Q709 F717 LYS GLY ASP GLU ASP ASP TYR ASP ILE ASP ASP LYS LEU GLY LYS PHE GLU ASP GLU ALA ILE ILE VAL PRO THR LYS ARG GLN SER ARG ARG ASN THR PRO ALA PRO SER ILE ILE SER GLY ASP ASP SER PRO PRO SER LEU PRO PHE SER GLY LYS LEU VAL

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	271802	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 ($e^-/Å^2$)	50	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	0.421	Depositor
Minimum map value	-0.266	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	261.4, 261.4, 261.4	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3069999, 1.3069999, 1.3069999	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	0.40	1/5636 (0.0%)	0.60	1/7674 (0.0%)
1	B	0.40	1/5636 (0.0%)	0.60	1/7674 (0.0%)
All	All	0.40	2/11272 (0.0%)	0.60	2/15348 (0.0%)

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	3
1	B	0	3
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	624	TRP	CB-CG	-5.20	1.40	1.50
1	B	624	TRP	CB-CG	-5.18	1.41	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	708	LEU	CA-CB-CG	5.09	127.02	115.30
1	B	708	LEU	CA-CB-CG	5.09	127.00	115.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	134	LYS	Peptide
1	A	135	GLN	Peptide

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Mol	Chain	Res	Type	Group
1	A	353	ALA	Peptide
1	B	134	LYS	Peptide
1	B	135	GLN	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	5482	0	5526	50	0
1	B	5482	0	5526	49	0
All	All	10964	0	11052	99	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 4.

The worst 5 of 99 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:B:612:VAL:O	1:B:613:TYR:CD1	2.00	1.15
1:A:612:VAL:O	1:A:613:TYR:CD1	2.00	1.13
1:B:144:ILE:HG12	1:B:147:LEU:HD12	1.78	0.65
1:A:144:ILE:HG12	1:A:147:LEU:HD12	1.78	0.64
1:B:320:MET:HG3	1:B:365:ALA:HA	1.83	0.61

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	677/771 (88%)	601 (89%)	74 (11%)	2 (0%)	41	74
1	B	677/771 (88%)	601 (89%)	74 (11%)	2 (0%)	41	74
All	All	1354/1542 (88%)	1202 (89%)	148 (11%)	4 (0%)	44	74

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	207	ARG
1	B	207	ARG
1	A	149	VAL
1	B	149	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	580/666 (87%)	574 (99%)	6 (1%)	76	86
1	B	580/666 (87%)	574 (99%)	6 (1%)	76	86
All	All	1160/1332 (87%)	1148 (99%)	12 (1%)	77	86

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	531	GLU
1	B	533	LEU
1	B	608	GLN
1	B	549	VAL
1	A	549	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	607	HIS
1	B	495	ASN

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Mol	Chain	Res	Type
1	B	162	HIS
1	B	426	GLN
1	A	608	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

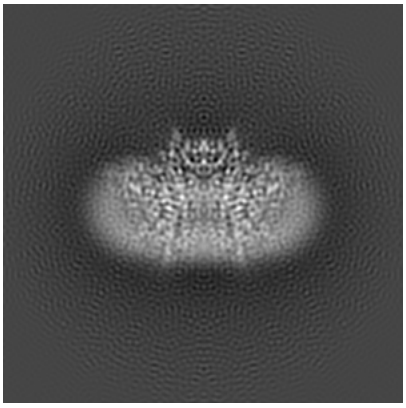
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-9682. These allow visual inspection of the internal detail of the map and identification of artifacts.

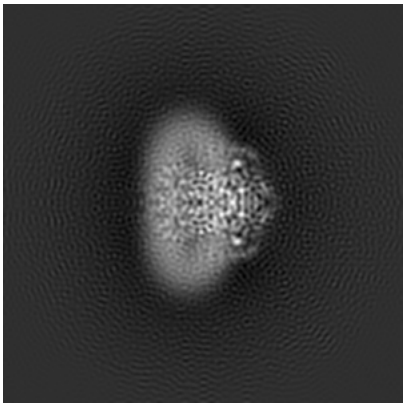
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

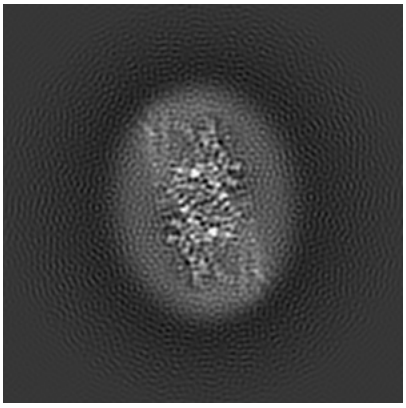
6.1.1 Primary map



X



Y

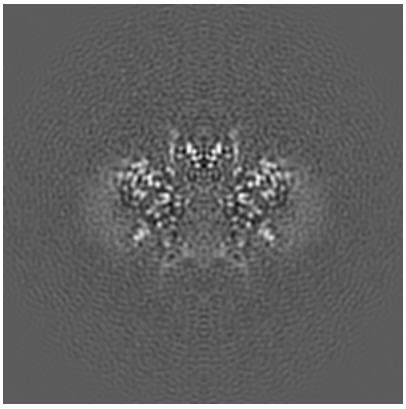


Z

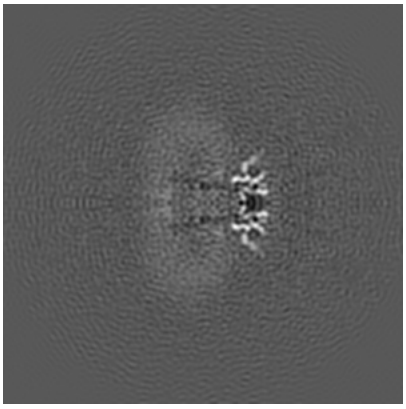
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

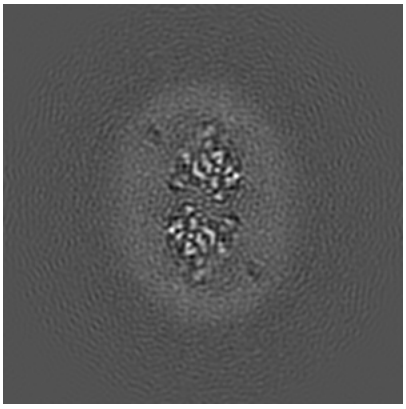
6.2.1 Primary map



X Index: 100



Y Index: 100

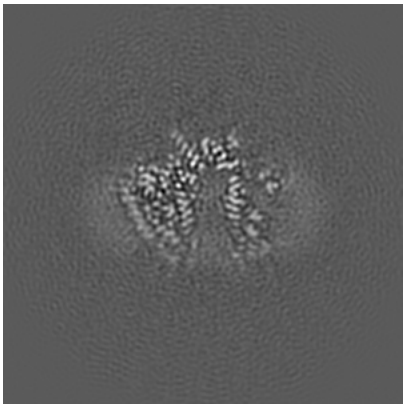


Z Index: 100

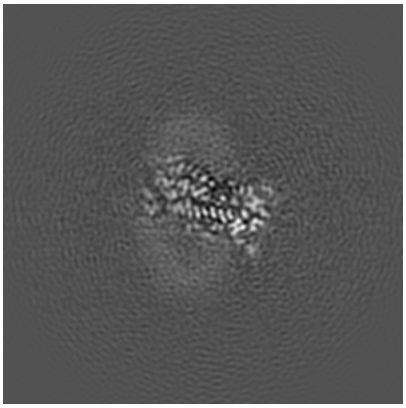
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

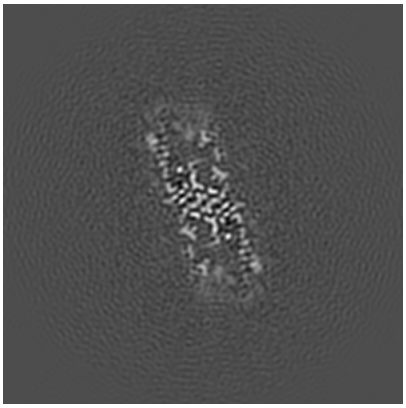
6.3.1 Primary map



X Index: 95



Y Index: 116

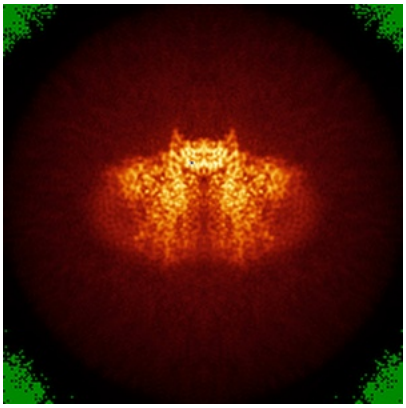


Z Index: 119

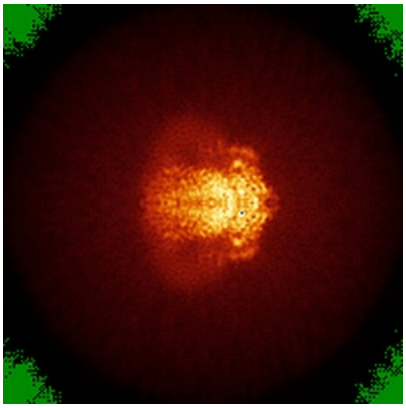
The images above show the largest variance slices of the map in three orthogonal directions.

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

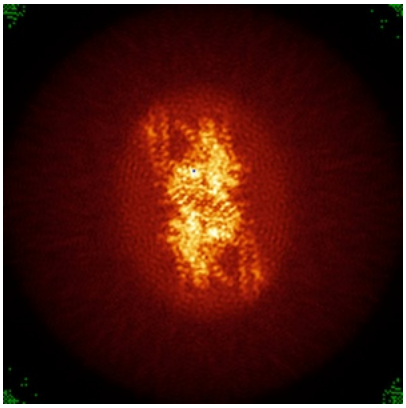
6.4.1 Primary map



X



Y

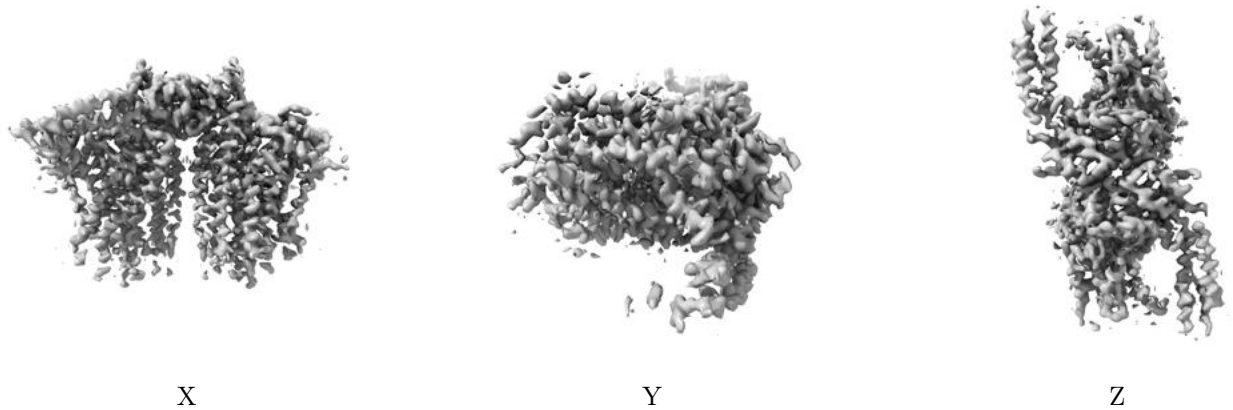


Z

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



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.

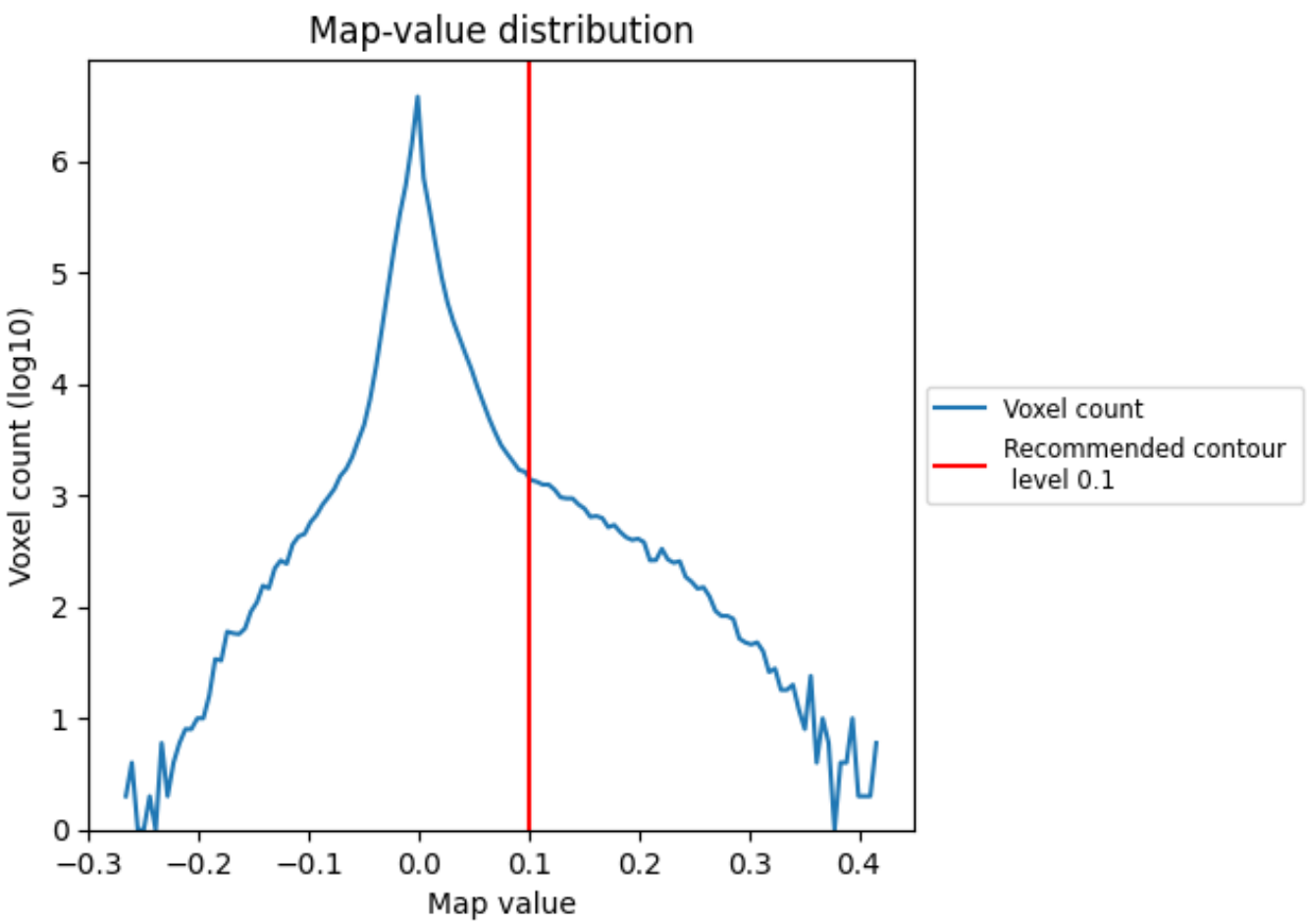
6.6 Mask visualisation (i)

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

7 Map analysis (i)

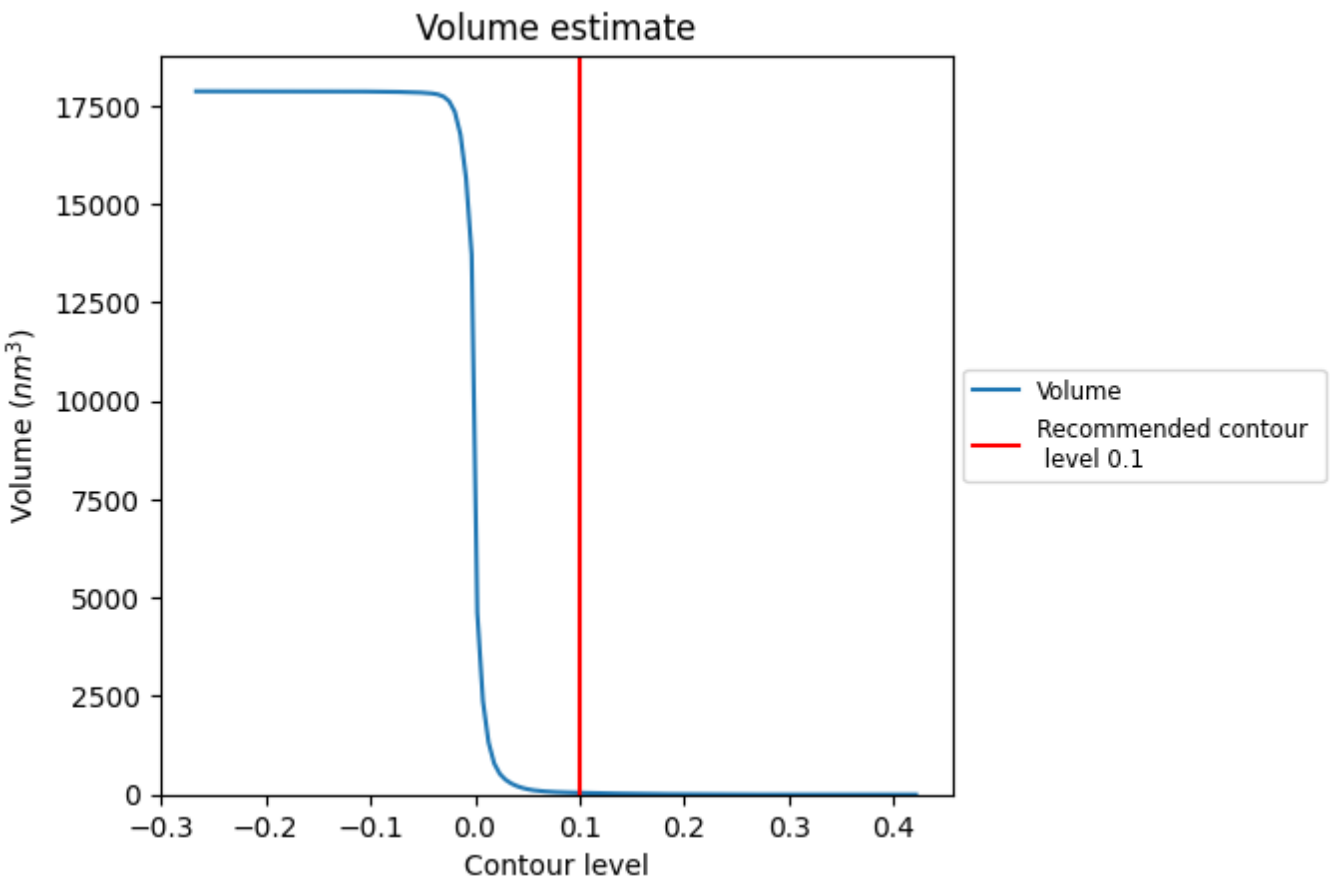
This section contains the results of statistical analysis of the map.

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.

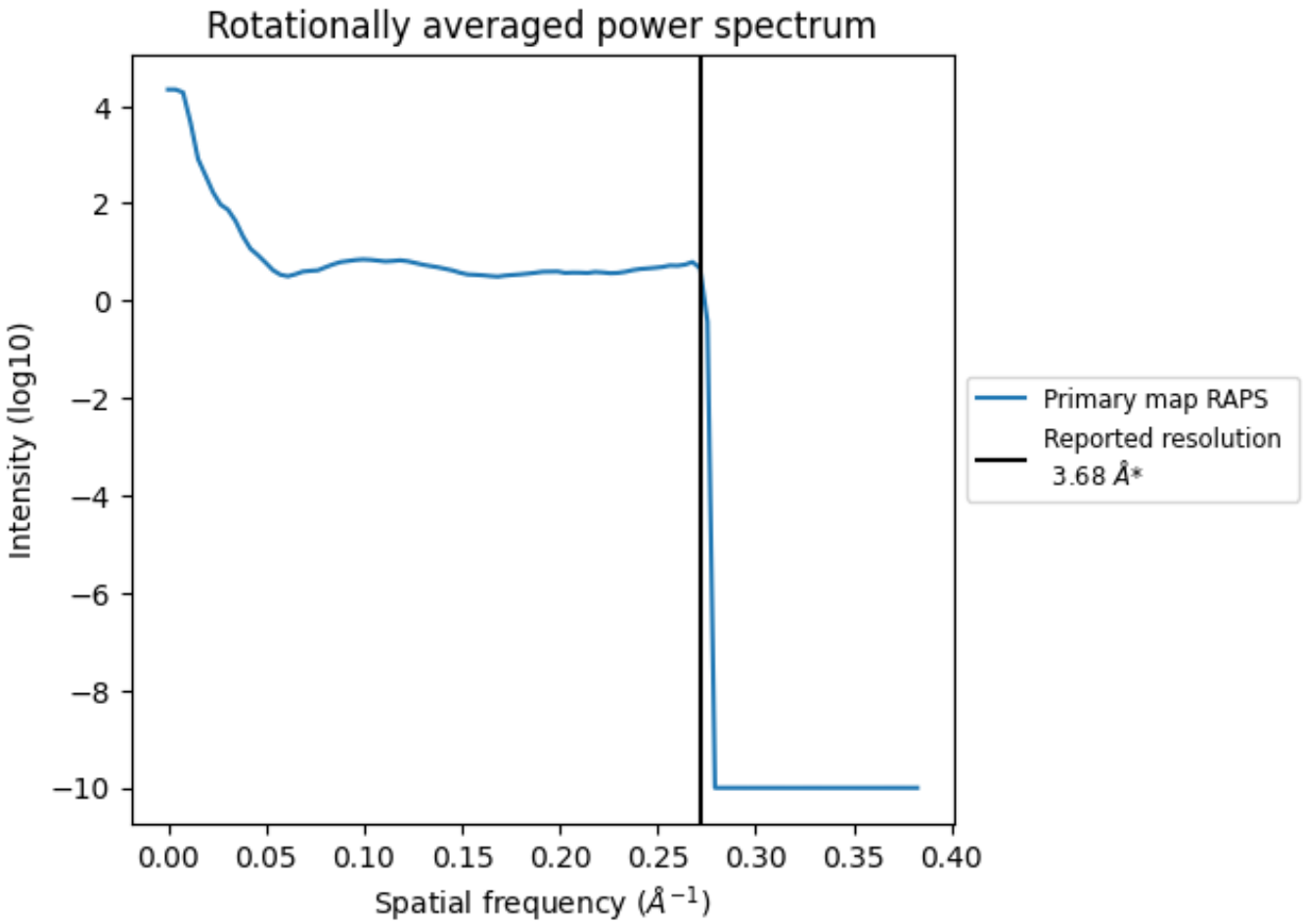
7.2 Volume estimate (i)



The volume at the recommended contour level is 44 nm^3; this corresponds to an approximate mass of 39 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 0.272 Å^{-1}

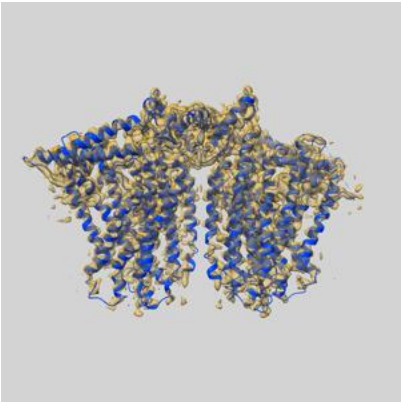
8 Fourier-Shell correlation (i)

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

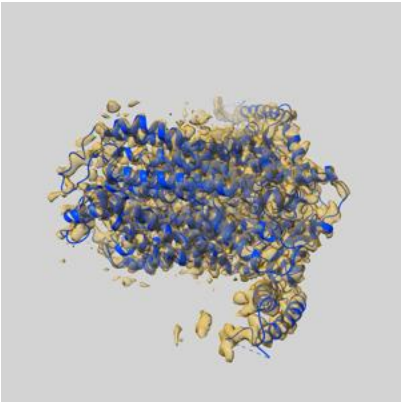
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-9682 and PDB model 6IJZ. Per-residue inclusion information can be found in section 3 on page 4.

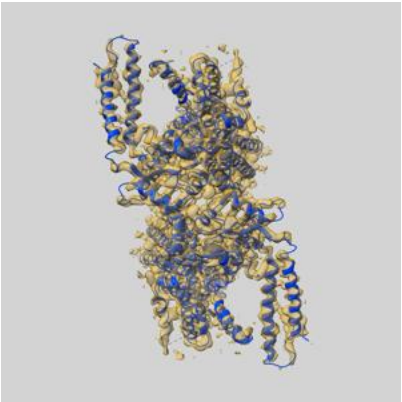
9.1 Map-model overlay (i)



X



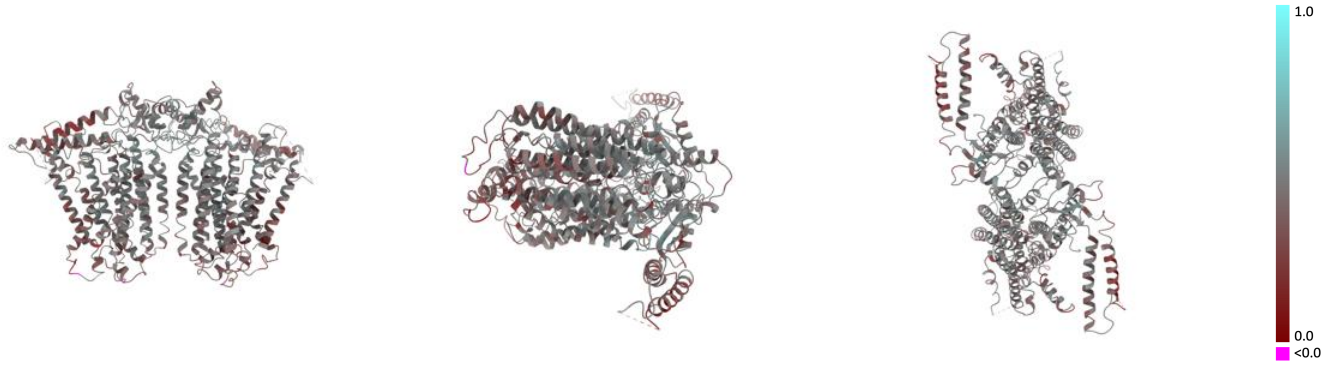
Y



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.

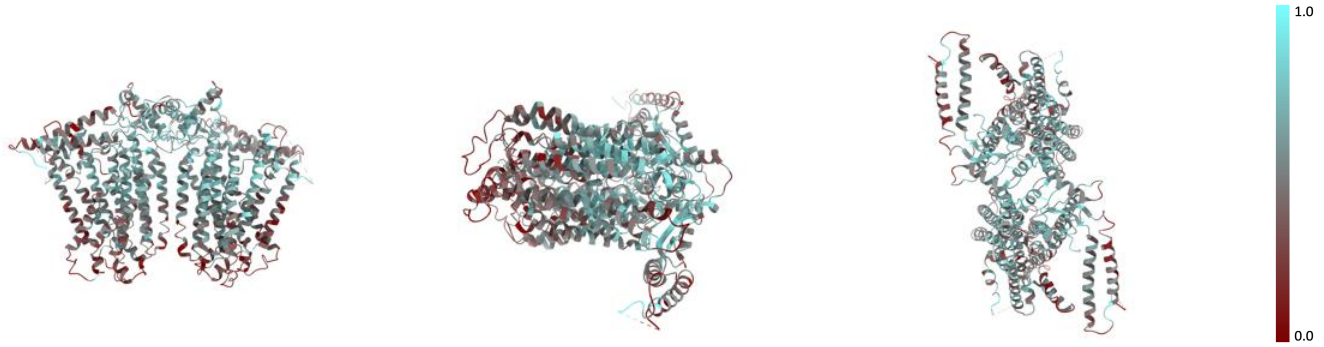
9.2 Q-score mapped to coordinate model (i)



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.

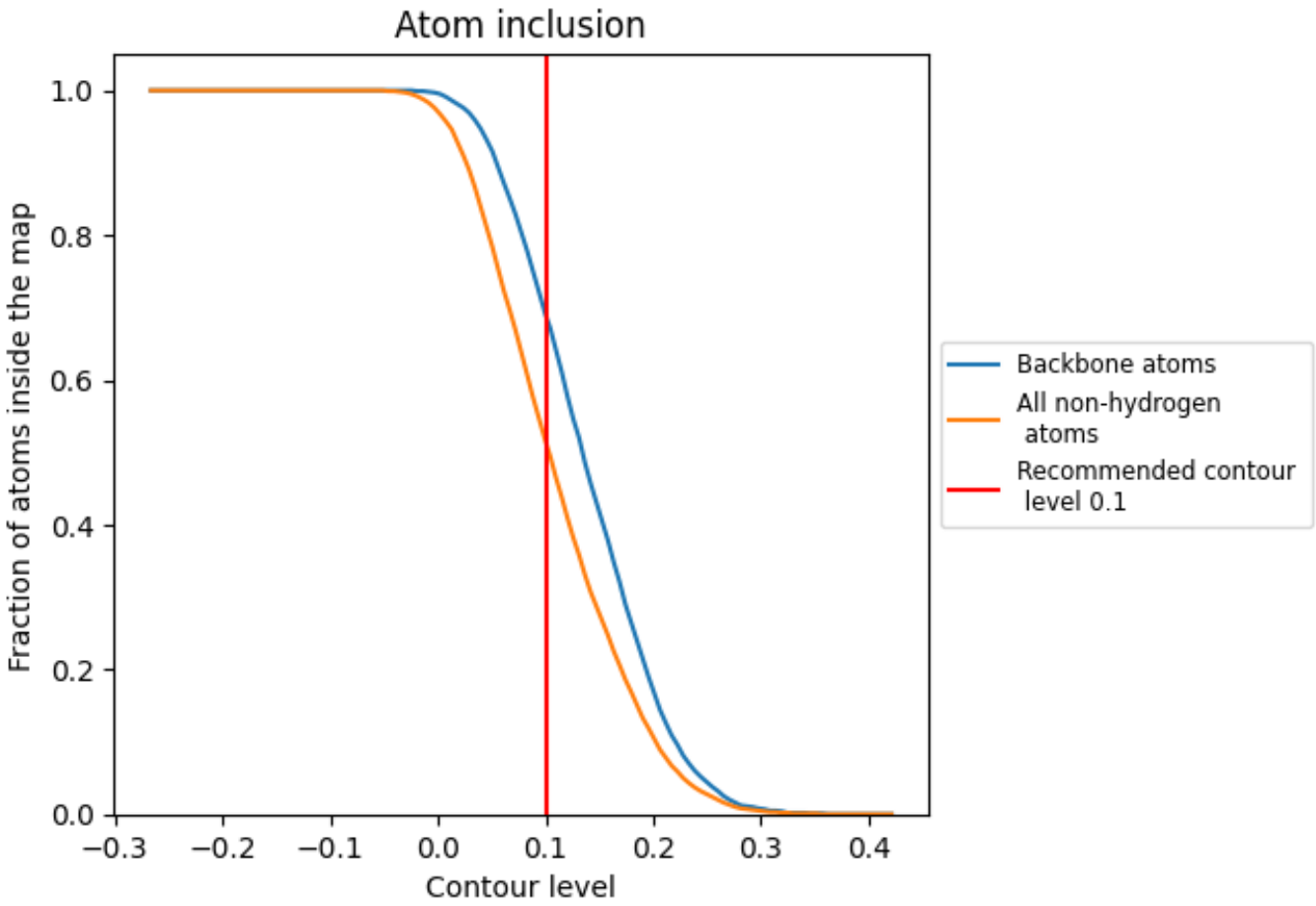
9.3 Atom inclusion mapped to coordinate model (i)



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, 69% of all backbone atoms, 52% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5150	0.4330
A	0.5150	0.4330
B	0.5150	0.4330