



wwPDB EM Validation Summary Report ⓘ

Aug 3, 2026 – 09:52 PM JST

PDB ID : 21LT / pdb_000021lt
EMDB ID : EMD-67804
Title : Cryo-EM structure of the setmelanotide-bound human melanocortin receptor 4 (MC4R)-Gq complex
Authors : Feng, W.B.; Zhou, Q.T.; Wang, M.W.
Deposited on : 2025-12-17
Resolution : 3.11 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 ⓘ 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.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
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) : 2.50

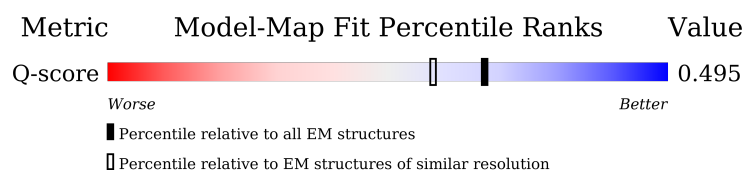
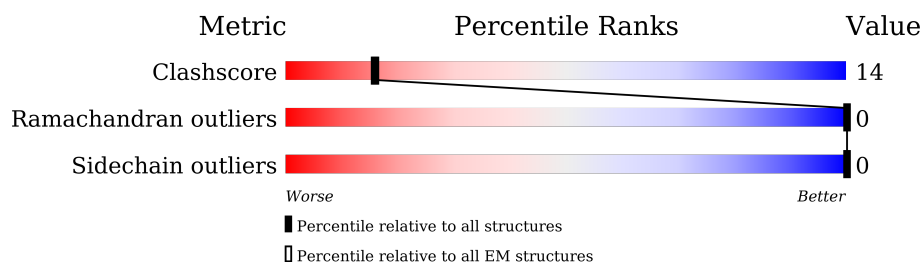
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.11 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	14465 (2.61 - 3.61)

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	P	8	75% 25%
2	R	505	33% 19% 49%
3	A	361	48% 17% 35%
4	B	371	66% 25% 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	G	71	8% 61% 10% 30%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6748 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 Setmelanotide.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	P	8	Total	C	N	O	S	0	0
			74	47	17	8	2		

- Molecule 2 is a protein called Melanocortin receptor 4,LgBiT subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	R	260	Total	C	N	O	S	0	0
			2007	1336	311	337	23		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	333	GLY	-	linker	UNP P32245
R	334	SER	-	linker	UNP P32245
R	335	SER	-	linker	UNP P32245
R	336	GLY	-	linker	UNP P32245
R	337	GLY	-	linker	UNP P32245
R	338	GLY	-	linker	UNP P32245
R	339	GLY	-	linker	UNP P32245
R	340	SER	-	linker	UNP P32245
R	341	GLY	-	linker	UNP P32245
R	342	GLY	-	linker	UNP P32245
R	343	GLY	-	linker	UNP P32245
R	344	GLY	-	linker	UNP P32245
R	345	SER	-	linker	UNP P32245
R	346	SER	-	linker	UNP P32245
R	347	GLY	-	linker	UNP P32245

- Molecule 3 is a protein called G subunit q (Gi1-Gq chimeric).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	235	Total	C	N	O	S	0	0
			1887	1198	337	344	8		

- Molecule 4 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1, HiBiT.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	336	Total	C	N	O	S	0	0
			2452	1527	431	475	19		

There are 21 discrepancies between the modelled and reference sequences:

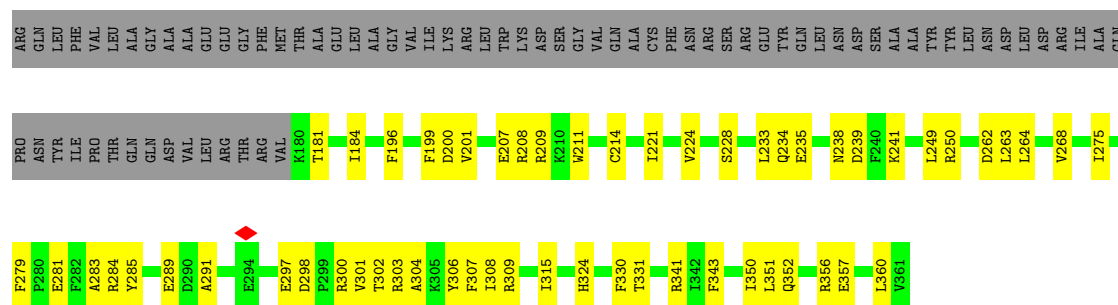
Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	MET	-	initiating methionine	UNP P54311
B	-3	GLY	-	expression tag	UNP P54311
B	-2	SER	-	expression tag	UNP P54311
B	-1	LEU	-	expression tag	UNP P54311
B	0	LEU	-	expression tag	UNP P54311
B	1	GLN	-	expression tag	UNP P54311
B	341	GLY	-	linker	UNP P54311
B	342	SER	-	linker	UNP P54311
B	343	SER	-	linker	UNP P54311
B	344	GLY	-	linker	UNP P54311
B	345	GLY	-	linker	UNP P54311
B	346	GLY	-	linker	UNP P54311
B	347	GLY	-	linker	UNP P54311
B	348	SER	-	linker	UNP P54311
B	349	GLY	-	linker	UNP P54311
B	350	GLY	-	linker	UNP P54311
B	351	GLY	-	linker	UNP P54311
B	352	GLY	-	linker	UNP P54311
B	353	SER	-	linker	UNP P54311
B	354	SER	-	linker	UNP P54311
B	355	GLY	-	linker	UNP P54311

- Molecule 5 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

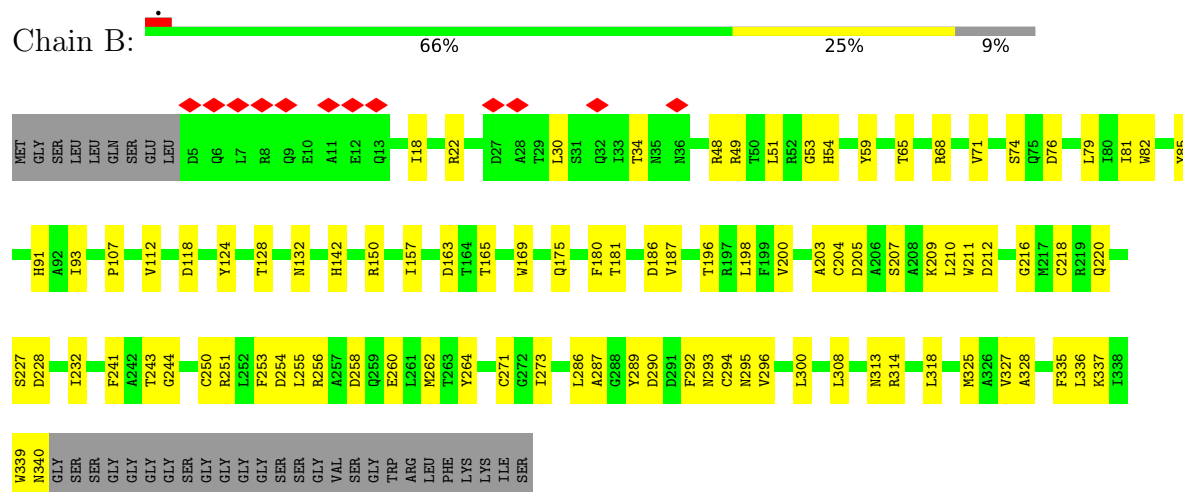
Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	50	Total	C	N	O	S	0	0
			327	204	56	65	2		

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

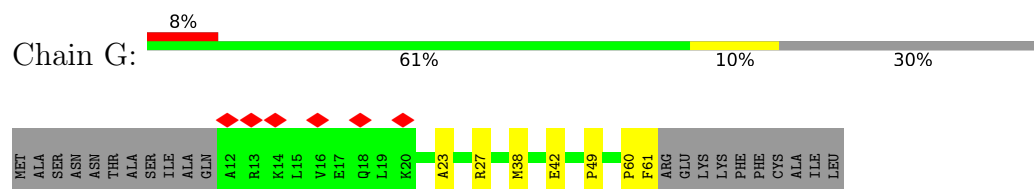
Mol	Chain	Residues	Atoms		AltConf
6	R	1	Total 1	Ca 1	0



- Molecule 4: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1, HiBiT



- Molecule 5: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	58767	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 ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.777	Depositor
Minimum map value	-0.548	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.1	Depositor
Map size ($\text{\AA}$)	263.68, 263.68, 263.68	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.03, 1.03, 1.03	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DPN, CA, DAL

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	P	0.40	0/58	0.52	0/73
2	R	0.44	0/2048	0.53	0/2792
3	A	0.29	0/1923	0.41	0/2595
4	B	0.29	0/2499	0.44	0/3409
5	G	0.15	0/333	0.31	0/460
All	All	0.34	0/6861	0.46	0/9329

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 [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	P	74	0	65	6	0
2	R	2007	0	2059	80	0
3	A	1887	0	1846	40	0
4	B	2452	0	2260	76	0
5	G	327	0	267	8	0
6	R	1	0	0	0	0
All	All	6748	0	6497	191	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 14.

The worst 5 of 191 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)
2:R:74:ASN:HD21	4:B:335:PHE:HZ	1.12	0.91
4:B:30:LEU:HD22	4:B:262:MET:HE1	1.69	0.73
3:A:184:ILE:HD11	3:A:199:PHE:HB3	1.71	0.72
3:A:234:GLN:O	3:A:238:ASN:ND2	2.22	0.72
2:R:198:ILE:HG21	2:R:266:ILE:HD11	1.72	0.72

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	P	4/8 (50%)	4 (100%)	0	0	100	100
2	R	254/505 (50%)	240 (94%)	14 (6%)	0	100	100
3	A	231/361 (64%)	224 (97%)	7 (3%)	0	100	100
4	B	334/371 (90%)	318 (95%)	16 (5%)	0	100	100
5	G	48/71 (68%)	48 (100%)	0	0	100	100
All	All	871/1316 (66%)	834 (96%)	37 (4%)	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	P	6/6 (100%)	6 (100%)	0	100	100
2	R	224/438 (51%)	224 (100%)	0	100	100
3	A	199/316 (63%)	199 (100%)	0	100	100
4	B	244/302 (81%)	244 (100%)	0	100	100
5	G	25/58 (43%)	25 (100%)	0	100	100
All	All	698/1120 (62%)	698 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
2	R	294	ASN
3	A	352	GLN
4	B	340	ASN
4	B	239	ASN
2	R	222	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	DAL	P	3	1	3,4,5	0.57	0	2,4,6	0.84	0
1	DPN	P	5	1	10,11,12	0.90	0	10,13,15	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
1	DAL	P	3	1	-	0/0/2/4	-
1	DPN	P	5	1	-	3/5/6/8	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	P	5	DPN	O-C-CA-CB
1	P	5	DPN	CA-CB-CG-CD2
1	P	5	DPN	CA-CB-CG-CD1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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.

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.

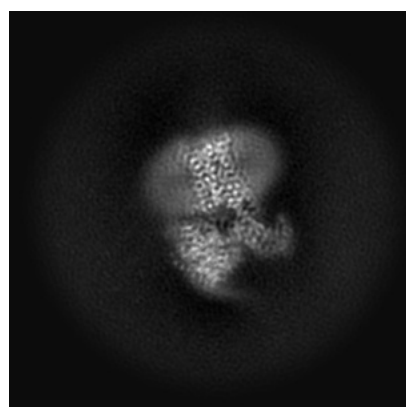
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-67804. These allow visual inspection of the internal detail of the map and identification of artifacts.

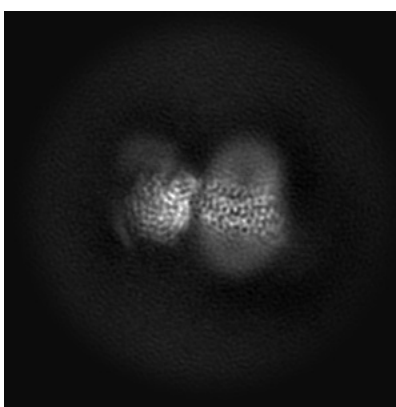
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

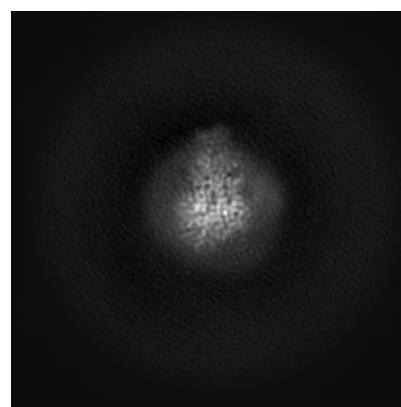
6.1.1 Primary map



X



Y

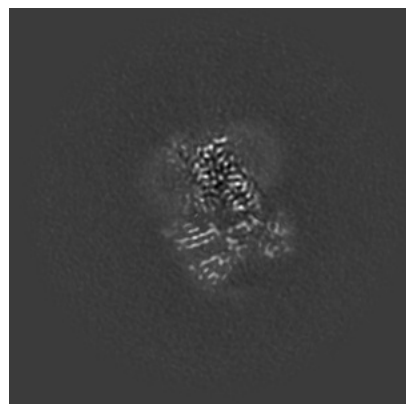


Z

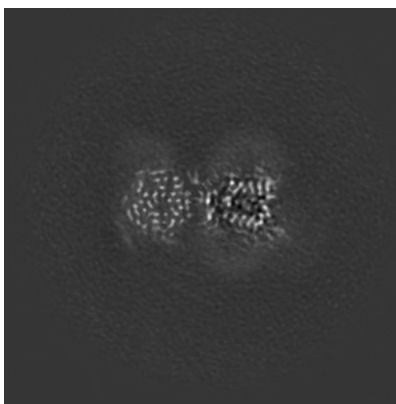
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

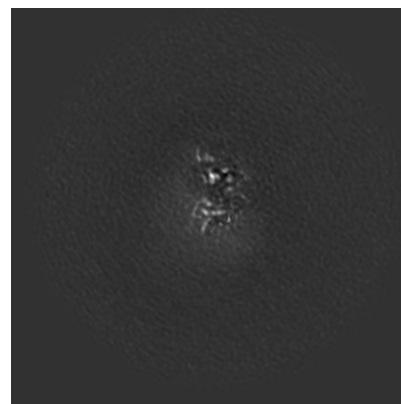
6.2.1 Primary map



X Index: 128



Y Index: 128

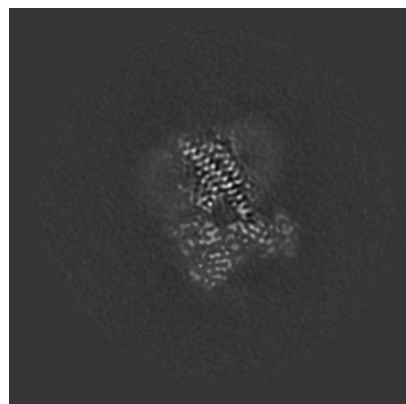


Z Index: 128

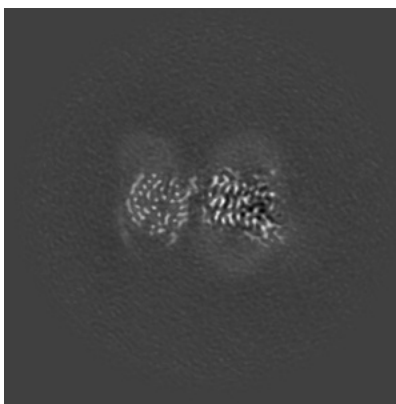
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

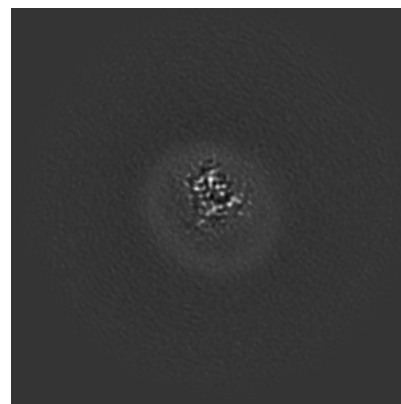
6.3.1 Primary map



X Index: 132



Y Index: 131

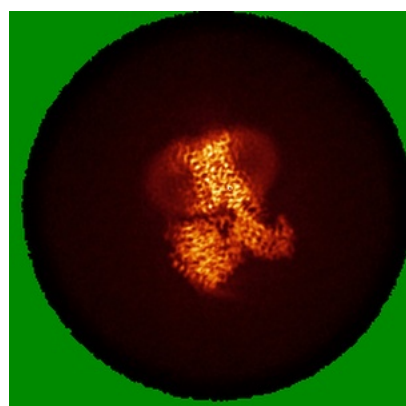


Z Index: 143

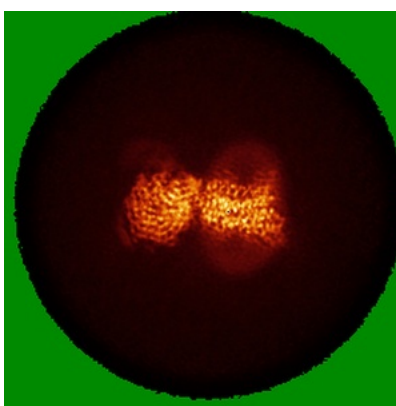
The images above show the largest variance slices of the map in three orthogonal directions.

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

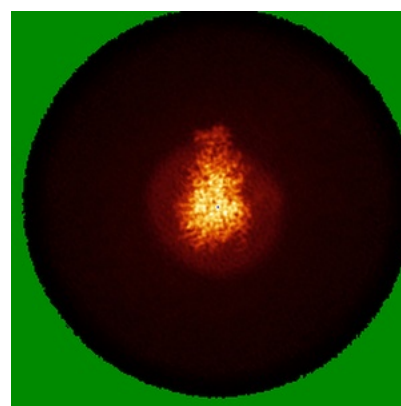
6.4.1 Primary map



X



Y

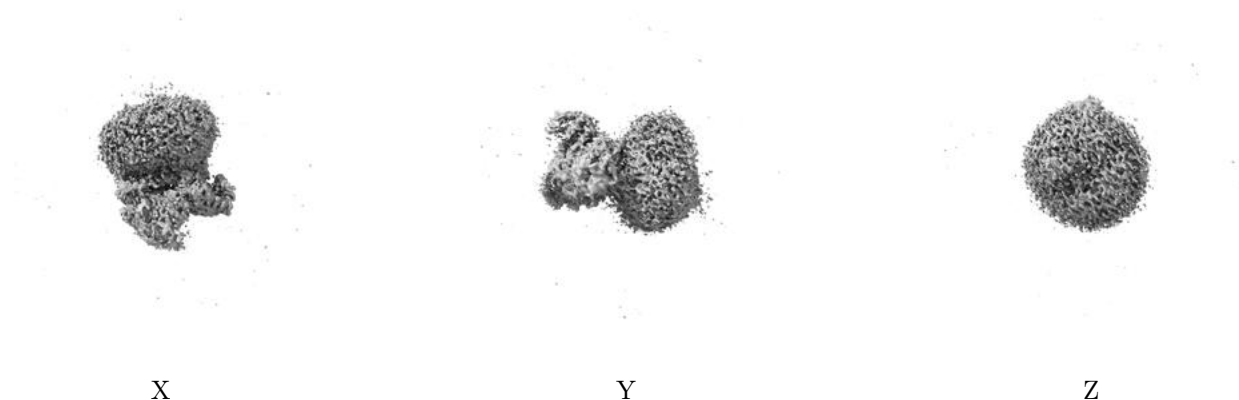


Z

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

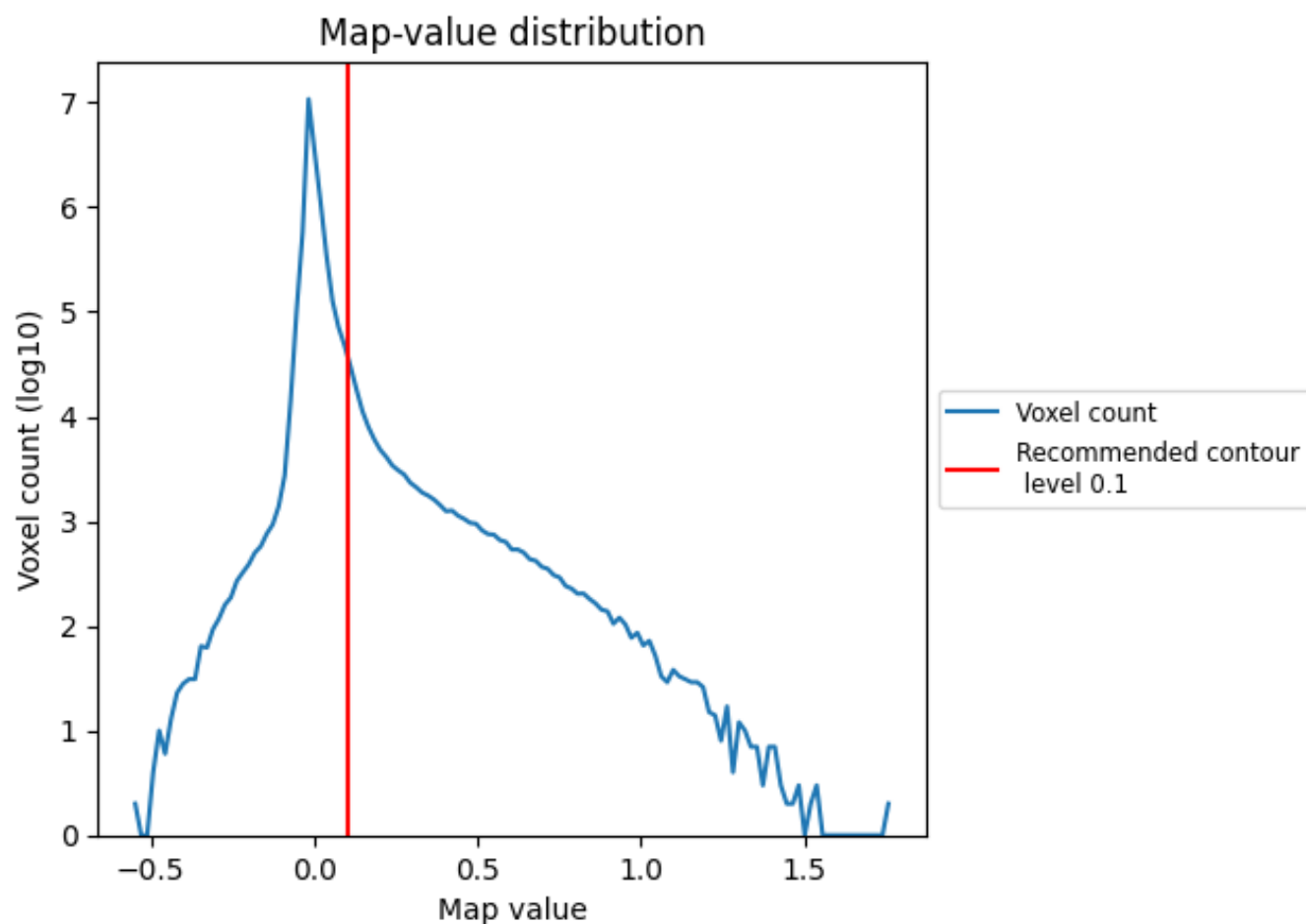
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

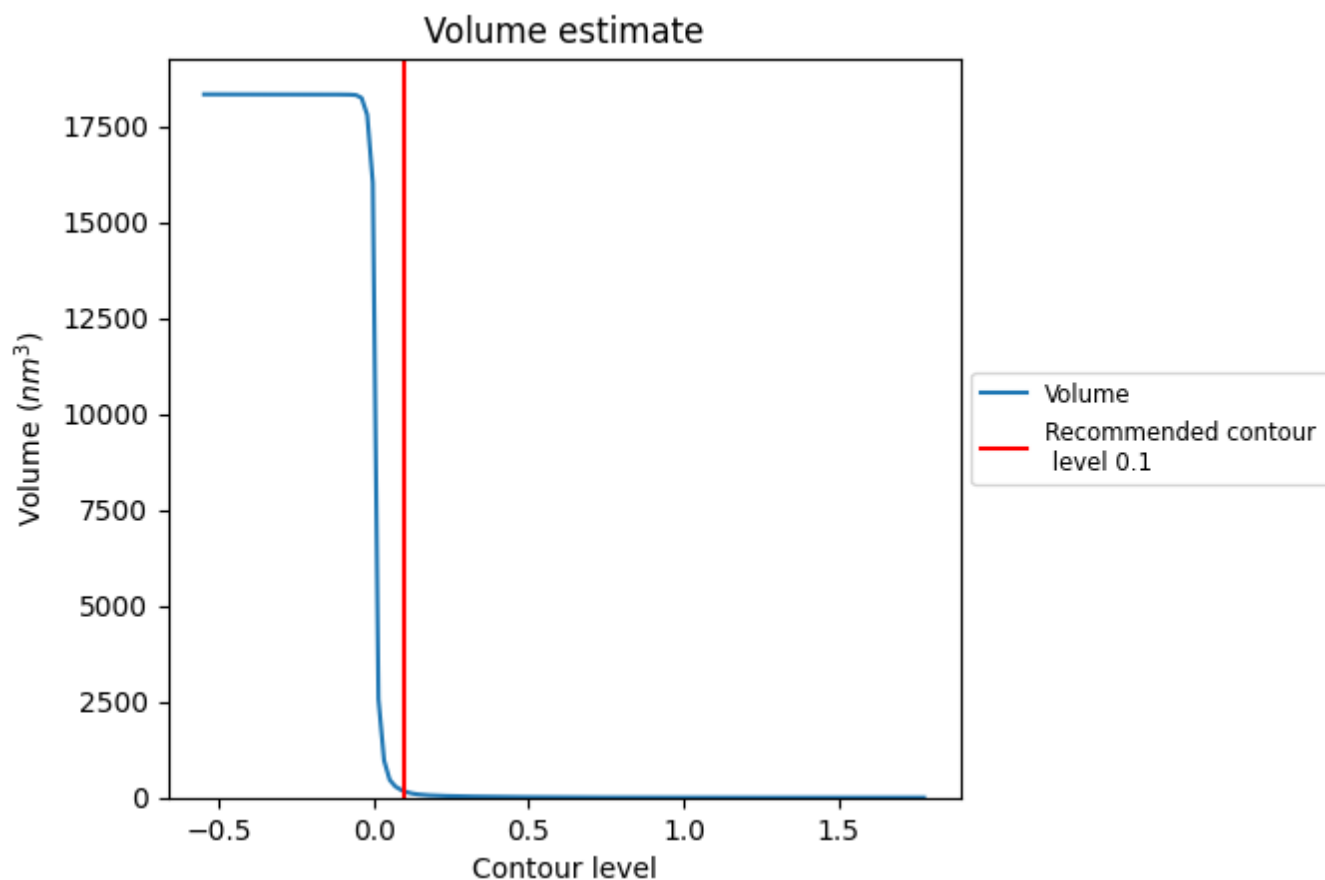
This section contains the results of statistical analysis of the map.

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.

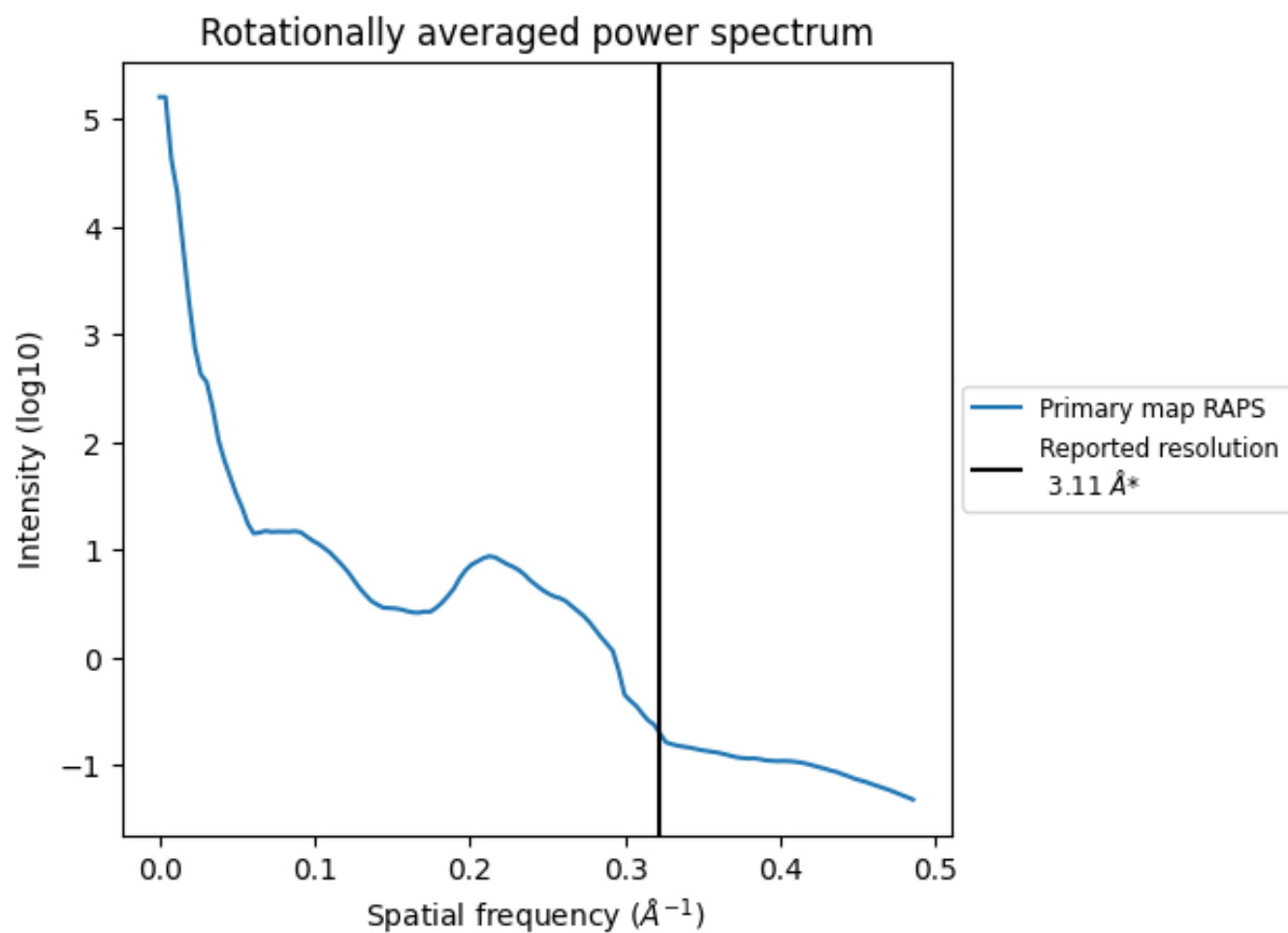
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 161 nm^3 ; this corresponds to an approximate mass of 146 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 0.322 Å⁻¹

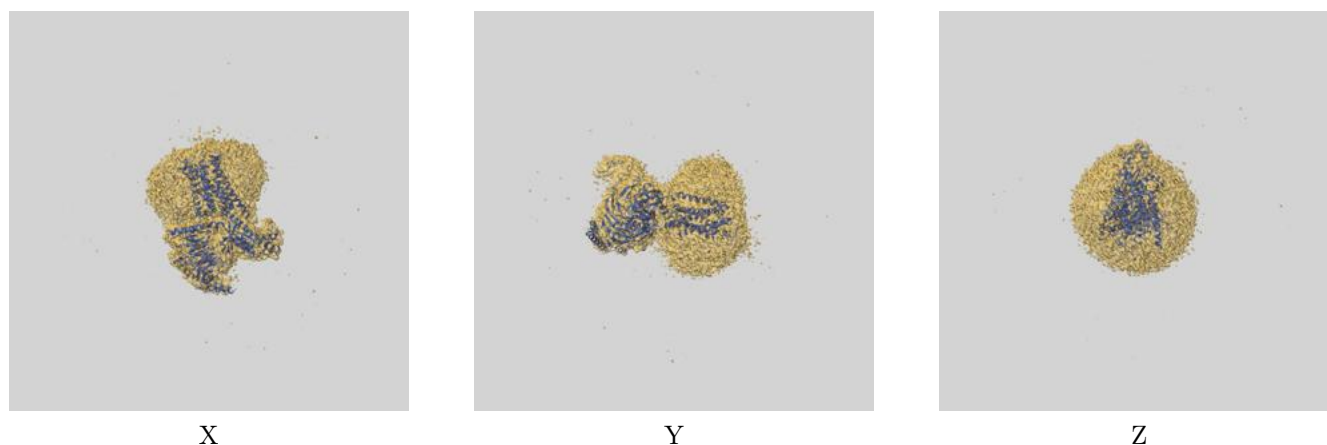
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

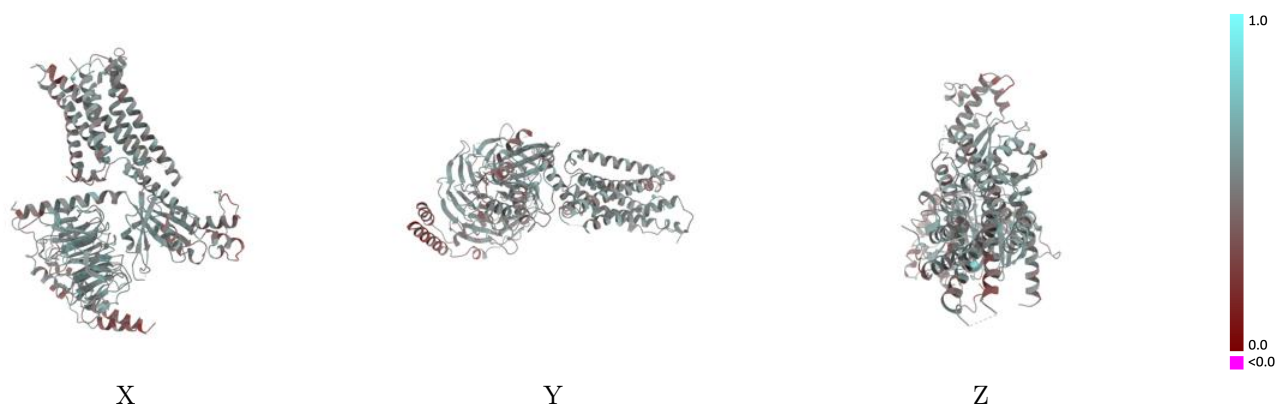
This section contains information regarding the fit between EMDB map EMD-67804 and PDB model 21LT. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



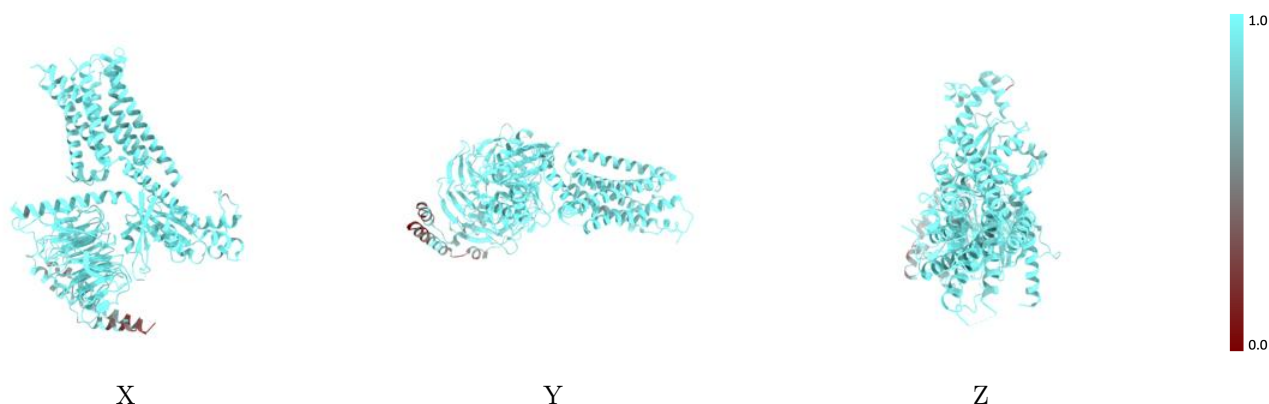
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



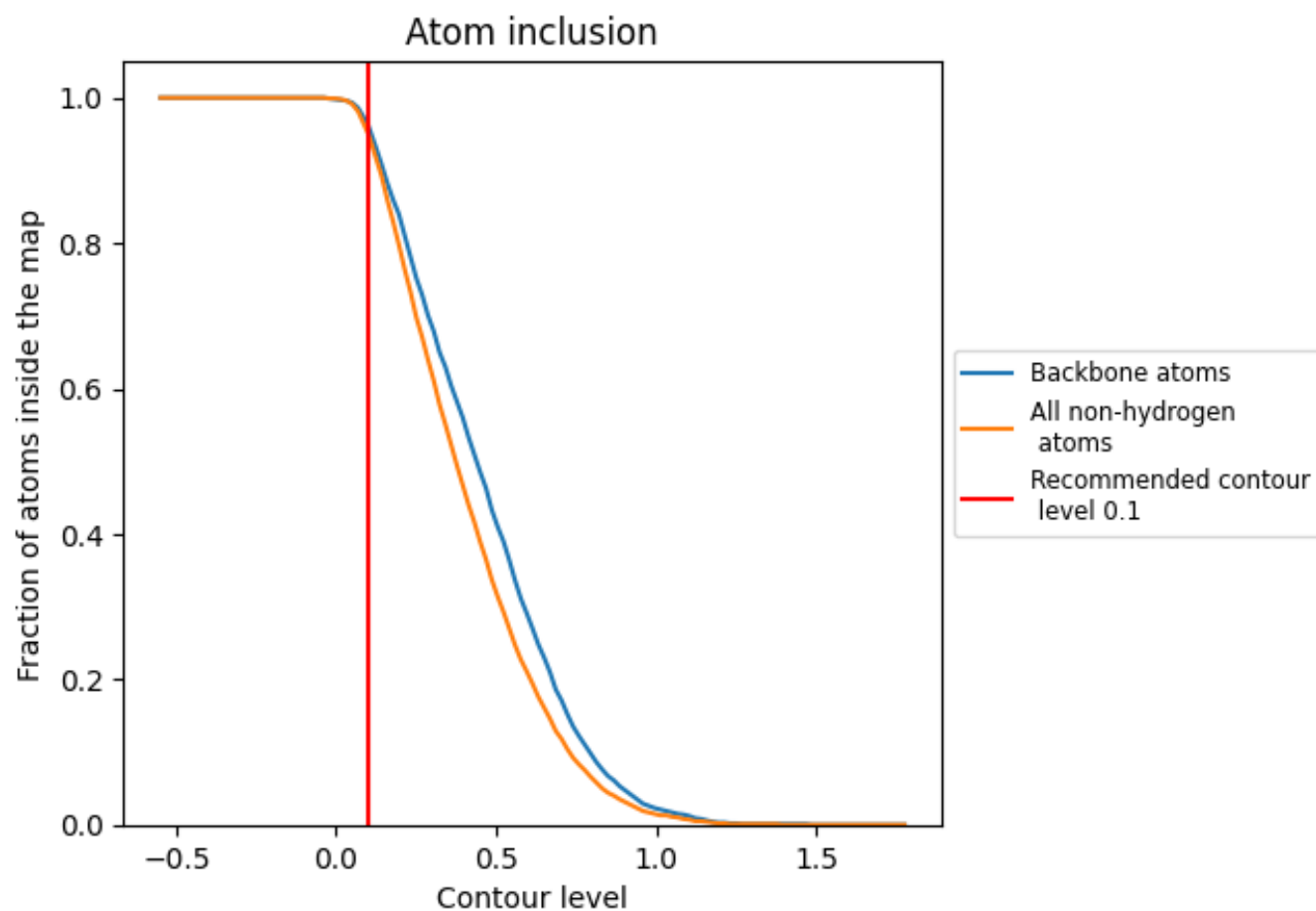
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 95% 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	0.9510	0.4950
A	0.9660	0.4960
B	0.9420	0.5050
G	0.8090	0.4180
P	1.0000	0.5340
R	0.9690	0.4940

