wwPDB EM Validation Summary Report (i)

Oct 20, 2026 – 04:18 PM EDT

PDB ID	:	12HR / pdb_000012hr
EMDB ID	:	EMD-76442
Title	:	structure of human GluD1 with calcium
Authors	:	Mondal, A.K.; Twomey, E.C.
Deposited on	:	2026-04-06
Resolution	:	5.86 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:

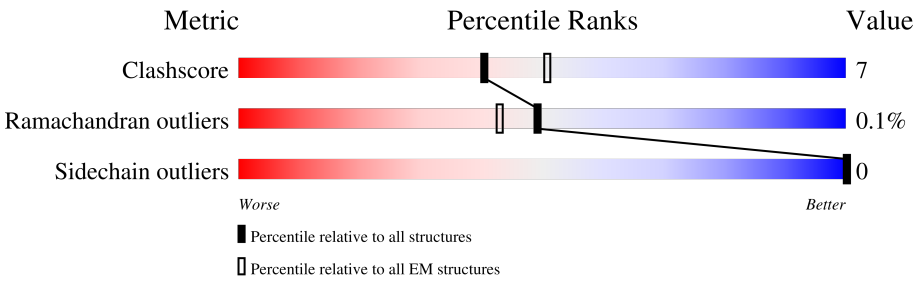
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

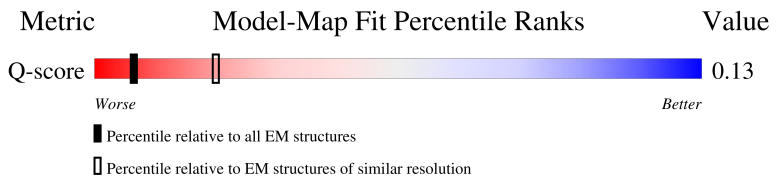
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 5.86 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	479 (5.36 - 6.36)

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	1009	24% 66% 14% 19%
1	B	1009	16% 67% 14% 19%
1	C	1009	24% 68% 13% 19%
1	D	1009	16% 68% 13% 19%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 51245 atoms, of which 25541 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, delta-1.

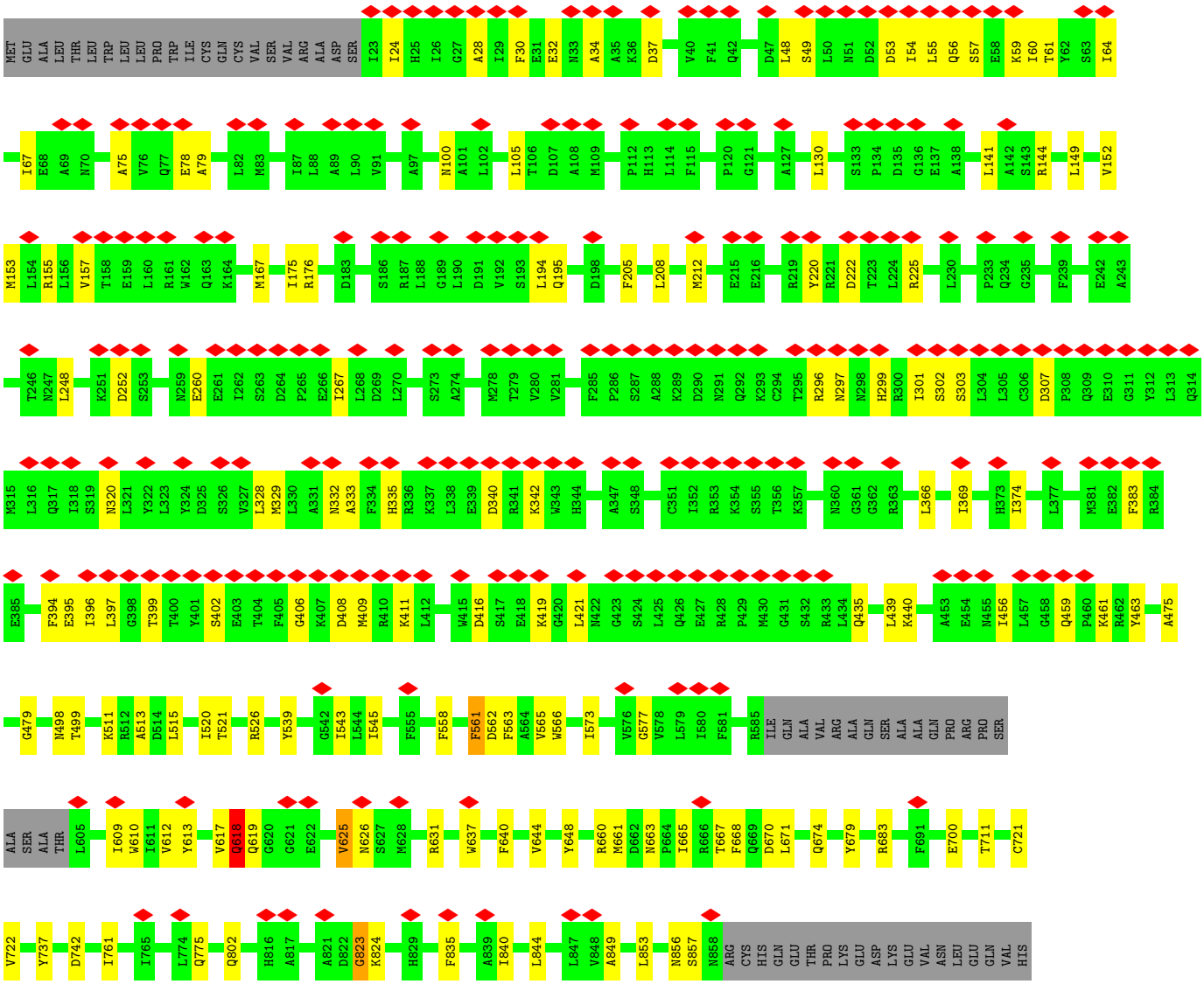
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	817	12812	4085	6386	1103	1203	35	0	0
1	B	817	12811	4085	6385	1103	1203	35	0	0
1	C	817	12811	4085	6385	1103	1203	35	0	0
1	D	817	12811	4085	6385	1103	1203	35	0	0

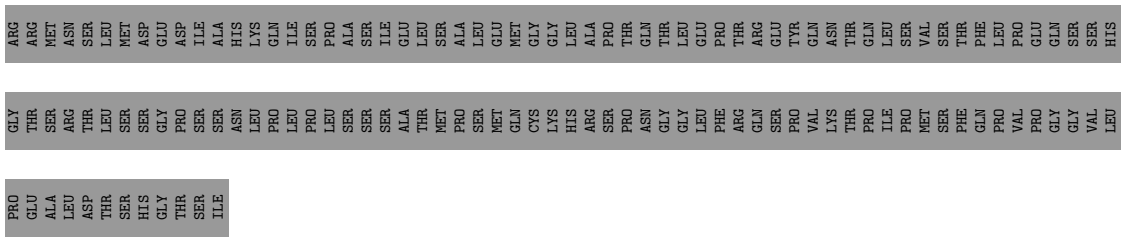
3 Residue-property plots (i)

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: Glutamate receptor ionotropic, delta-1

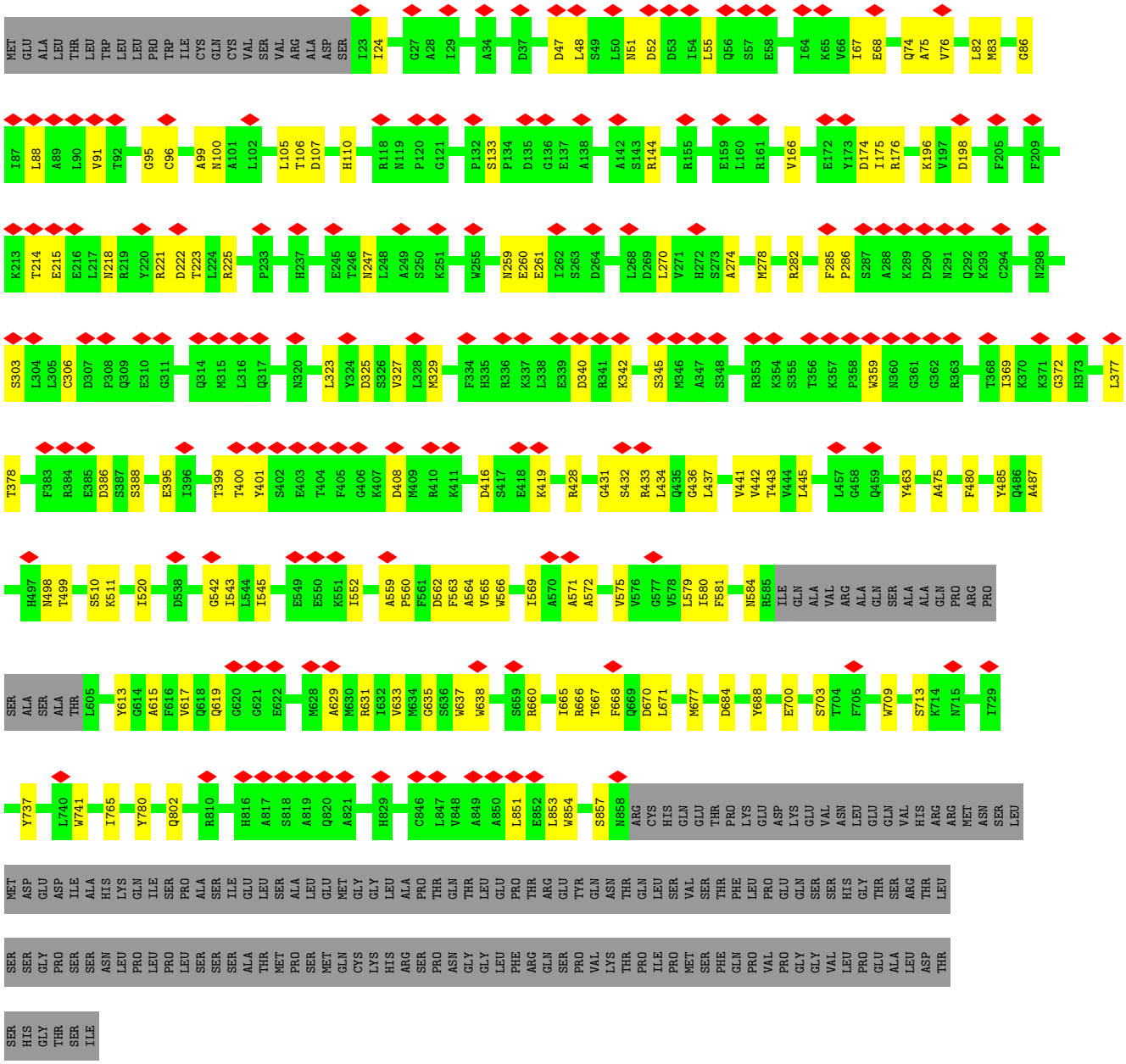
Chain A:





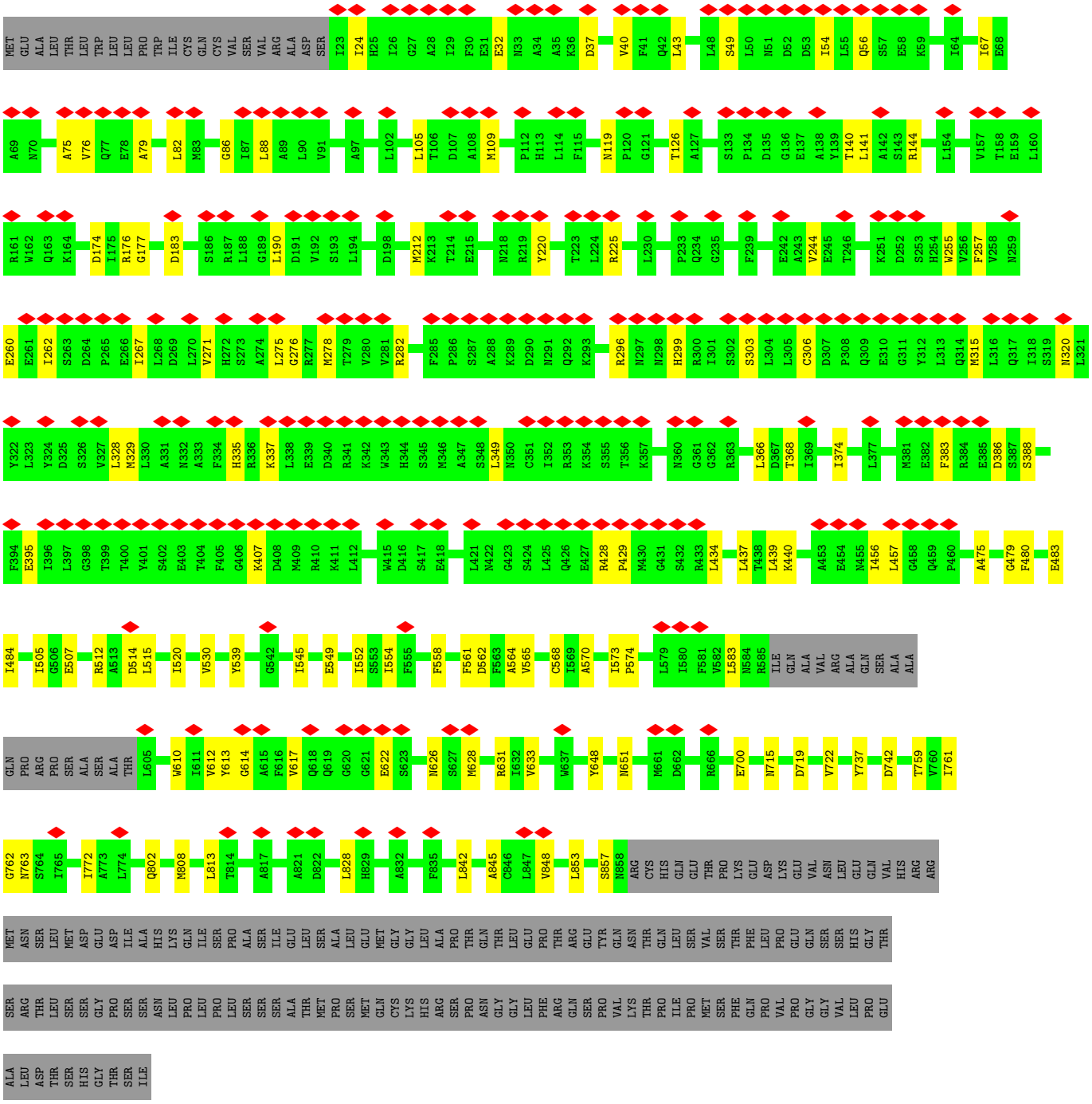
- Molecule 1: Glutamate receptor ionotropic, delta-1

Chain B:



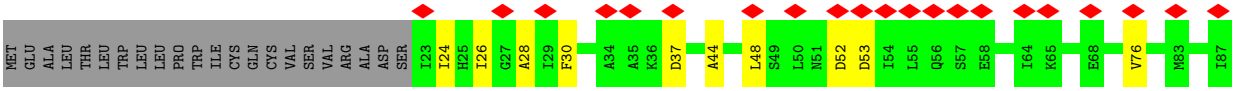
- Molecule 1: Glutamate receptor ionotropic, delta-1

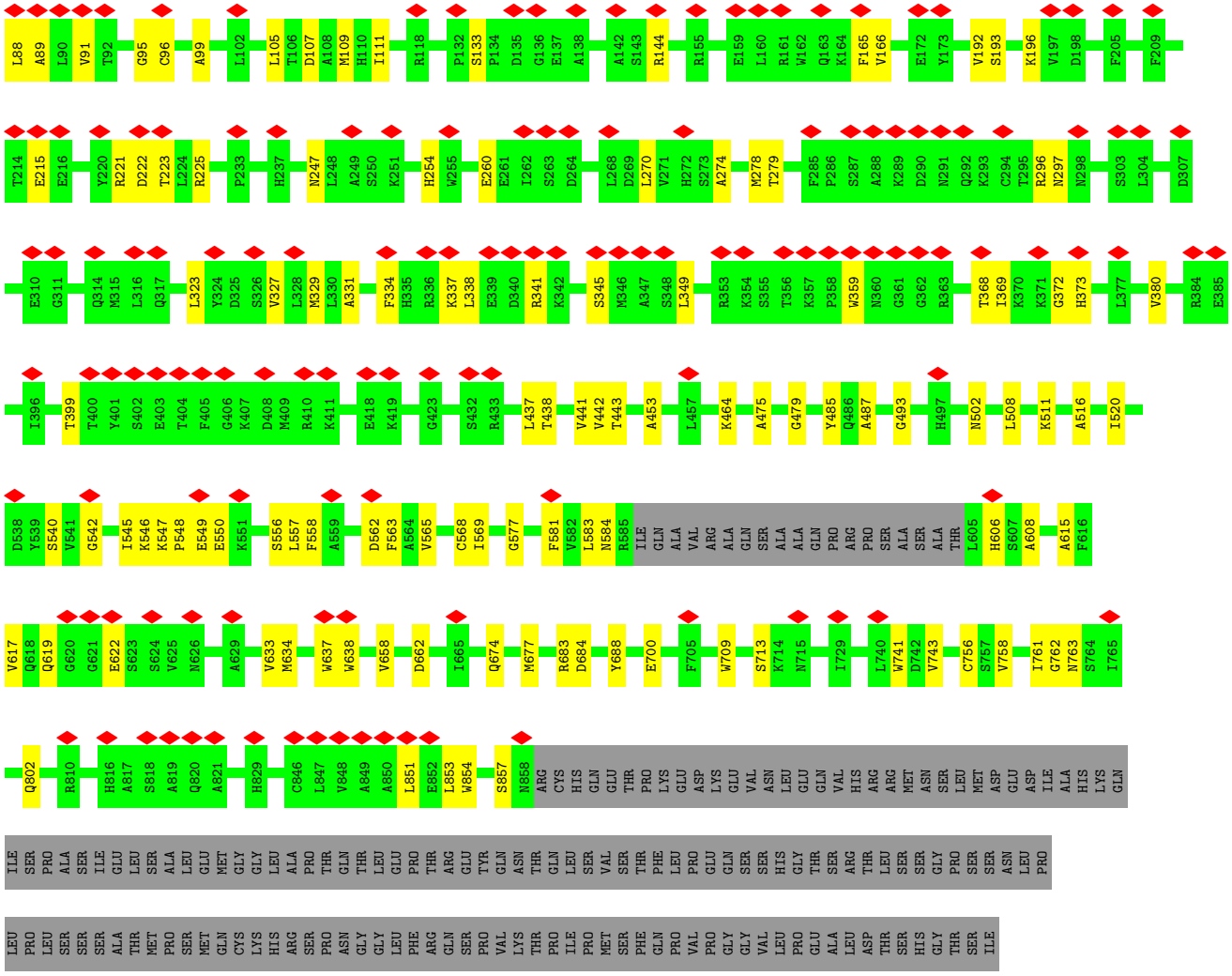
Chain C:



- Molecule 1: Glutamate receptor ionotropic, delta-1

Chain D:




L88 A89 L90 V91 T92 G95 C96 A99 L102 L105 T106 D107 A108 M109 H110 I111 R118 P132 S133 P134 D135 G136 E137 A138 A142 S143 R144 R155 E159 L160 R161 W162 Q163 K164 F165 V166 E172 Y173 V192 S193 K196 V197 D198 F205 F209
T214 E215 E216 Y220 R221 D222 T223 L224 R225 P233 H237 N247 L248 A249 S250 K251 H254 W255 E260 E261 I262 S263 D264 L268 D269 L270 V271 H272 S273 A274 M278 T279 F285 P286 S287 A288 K289 D290 N291 Q292 K293 C294 T295 R296 N297 N298 S303 L304 D307
E310 G311 Q314 M315 L316 Q317 L323 Y324 D325 S326 V327 L328 M329 L330 A331 F334 H335 R336 K337 L338 E339 D340 R341 K342 S345 M346 A347 S348 L349 R353 K354 S355 T356 K357 P358 W359 N360 G361 G362 R363 T368 I369 K370 K371 G372 H373 L377 V380 R384 E385
I396 T399 T400 Y401 S402 E403 T404 F405 G406 K407 D408 M409 R410 K411 E418 K419 G423 S432 R433 L437 T438 V441 V442 T443 A453 L457 K464 A475 G479 Y485 Q486 A487 G493 H497 N502 L508 K511 A516 I520
D538 Y539 S540 V541 G542 I545 K546 K547 P548 E549 E550 K551 S556 L557 F558 A559 D562 F563 A564 V565 C568 I569 G577 F581 V582 L583 N584 R585 ILE GLN ALA VAL ARG ALA GLN SER ALA ALA GLN PRO ARG PRO SER ALA SER ALA THR L605 H606 S607 A608 A615 F616
V617 Q618 Q619 G620 G621 E622 S623 S624 V625 N626 A629 V633 M634 W637 W638 V658 D662 I665 Q674 M677 R683 D684 Y688 E700 F705 W709 S713 K714 N715 I729 L740 W741 D742 V743 C756 S757 V758 I761 G762 N763 S764 I765
Q802 R810 H816 A817 S818 A819 Q820 A821 H829 C846 L847 V848 A849 A850 L851 E852 L853 W854 S857 N858 ARG CYS HIS GLN GLU THR PRO LYS GLU ASP LYS GLU VAL ASN LEU GLU GLN VAL HIS ARG ARG MET ASN SER LEU MET ASP GLU ASP ILE ALA HIS LYS GLN
ILE SER PRO ALA SER ILE GLU LEU SER ALA LEU GLU MET GLY GLY LEU ALA PRO THR GLN THR LEU GLU PRO THR ARG GLU TYR GLN ASN THR GLN LEU SER VAL SER THR PHE LEU PRO GLU GLN SER SER HIS GLY THR SER ARG THR LEU SER SER GLY PRO SER SER ASN LEU PRO
LEU PRO LEU SER SER ALA THR MET PRO SER MET GLN CYS LYS HIS ARG SER PRO ASN GLY GLY LEU PHE ARG GLN SER PRO VAL LYS THR PRO ILE PRO MET SER PHE GLN PRO VAL PRO GLY GLY VAL LEU PRO GLU ALA LEU ASP THR SER HIS GLY THR SER ILE

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	194885	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.314	Depositor
Minimum map value	-0.140	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	409.2, 409.2, 409.2	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.93, 0.93, 0.93	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	0.15	0/6562	0.35	0/8892
1	B	0.14	0/6562	0.35	0/8892
1	C	0.15	0/6562	0.35	0/8892
1	D	0.14	0/6562	0.35	0/8892
All	All	0.14	0/26248	0.35	0/35568

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	561	PHE	Peptide
1	A	618	GLN	Peptide
1	A	823	GLY	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	6426	6386	6383	99	0
1	B	6426	6385	6383	107	0
1	C	6426	6385	6383	87	0
1	D	6426	6385	6383	84	0
All	All	25704	25541	25532	356	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 7.

The worst 5 of 356 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:666:ARG:N	1:B:670:ASP:OD2	2.00	0.95
1:A:511:LYS:NZ	1:A:775:GLN:OE1	2.03	0.90
1:A:24:ILE:O	1:A:61:THR:OG1	1.97	0.83
1:D:562:ASP:OD1	1:D:563:PHE:N	2.11	0.82
1:A:332:ASN:OD1	1:A:333:ALA:N	2.13	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	813/1009 (81%)	756 (93%)	55 (7%)	2 (0%)	43 77
1	B	813/1009 (81%)	759 (93%)	54 (7%)	0	100 100
1	C	813/1009 (81%)	760 (94%)	53 (6%)	0	100 100
1	D	813/1009 (81%)	749 (92%)	63 (8%)	1 (0%)	48 83
All	All	3252/4036 (81%)	3024 (93%)	225 (7%)	3 (0%)	49 83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	618	GLN
1	A	625	VAL
1	D	556	SER

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	703/872 (81%)	703 (100%)	0	100	100
1	B	703/872 (81%)	703 (100%)	0	100	100
1	C	703/872 (81%)	703 (100%)	0	100	100
1	D	703/872 (81%)	703 (100%)	0	100	100
All	All	2812/3488 (81%)	2812 (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 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	100	ASN
1	D	344	HIS
1	D	720	ASN
1	D	498	ASN
1	D	606	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Map visualisation (i)

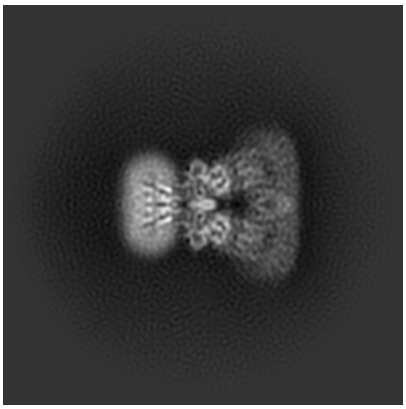
This section contains visualisations of the EMDB entry EMD-76442. These allow visual inspection of the internal detail of the map and identification of artifacts.

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.

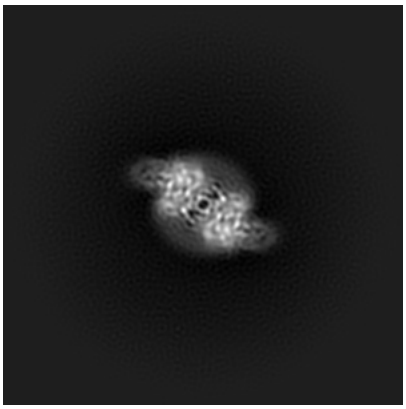
6.1 Orthogonal projections (i)

6.1.1 Primary map

X

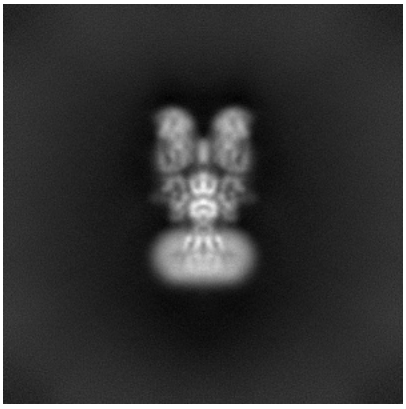


Y

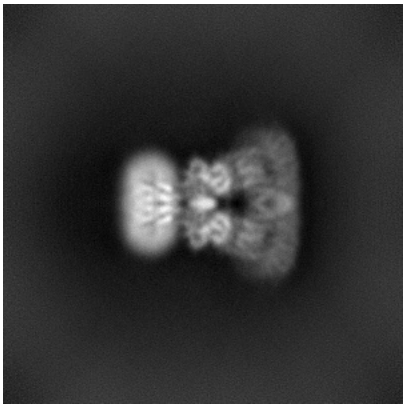


Z

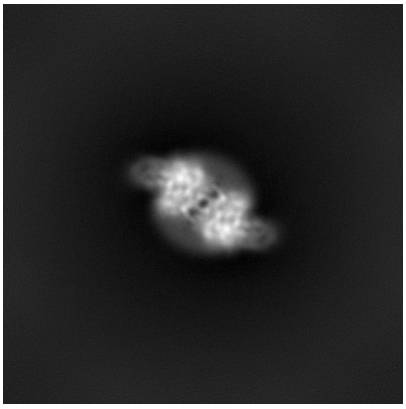
6.1.2 Raw map



X



Y

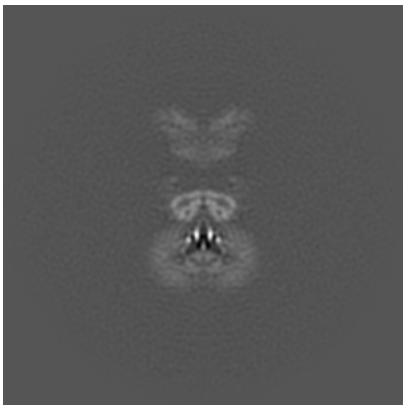


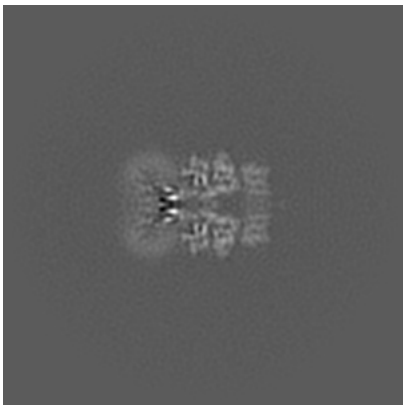
Z

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

6.2 Central slices (i)

6.2.1 Primary map


X Index: 220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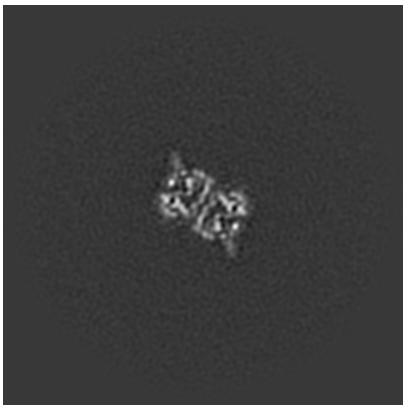
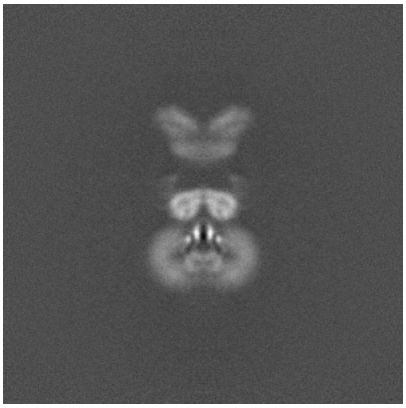

Z Index: 220

6.2.2 Raw map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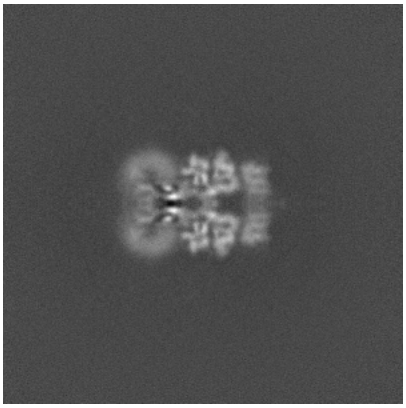
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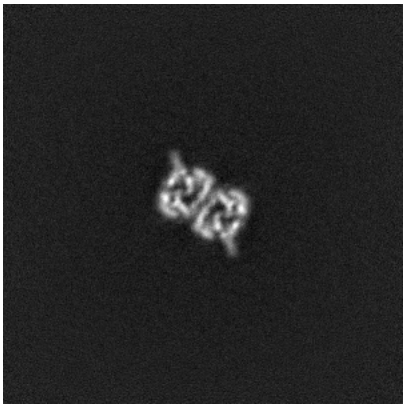
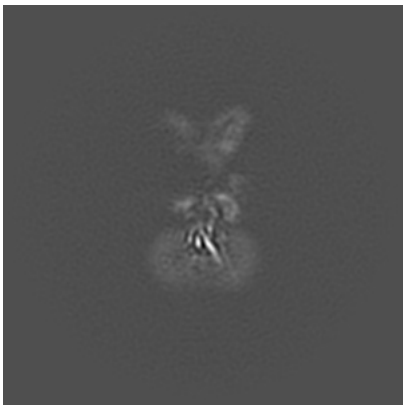

Z Index: 220

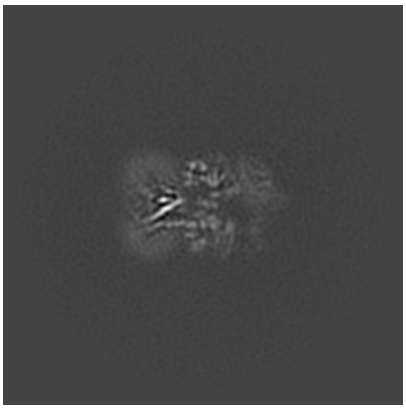
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

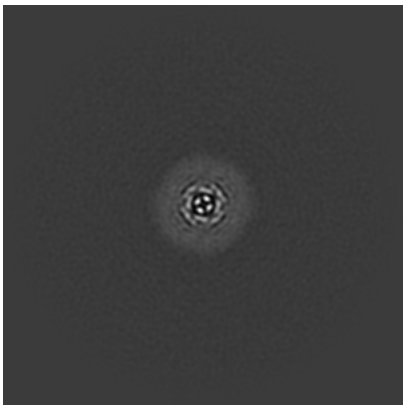
6.3.1 Primary map



X Index: 215

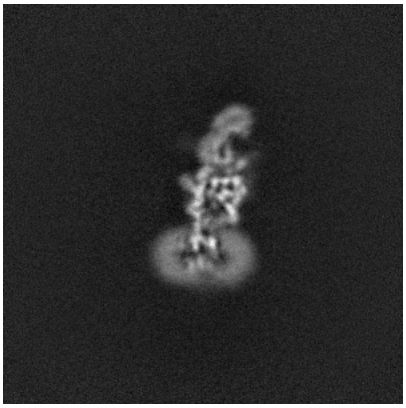


Y Index: 214

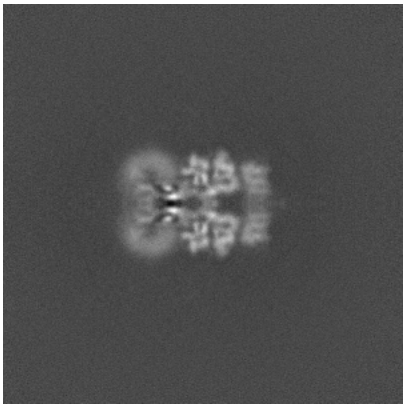


Z Index: 181

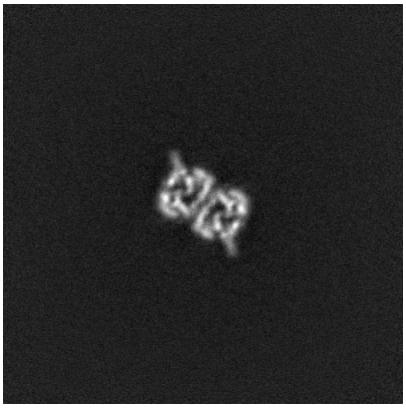
6.3.2 Raw map



X Index: 200



Y Index: 220

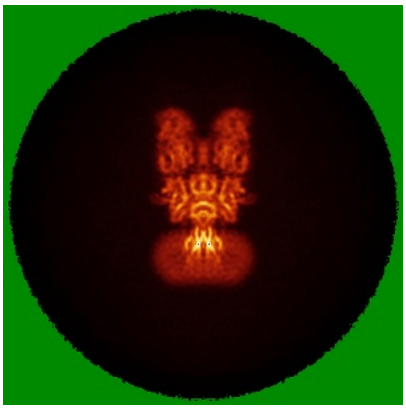


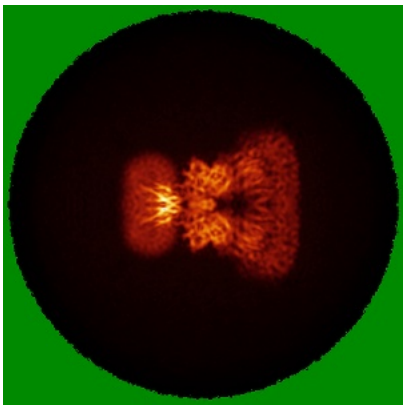
Z Index: 220

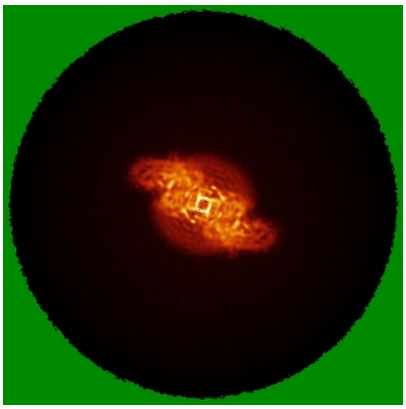
The images above show the largest variance slices of the map in three orthogonal directions.

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

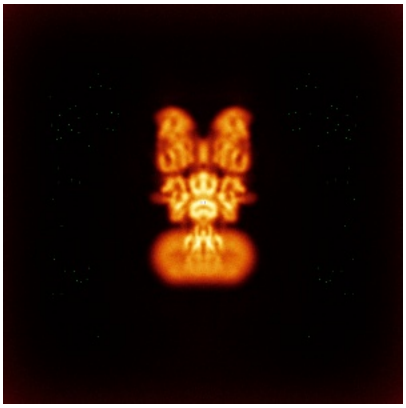
6.4.1 Primary map

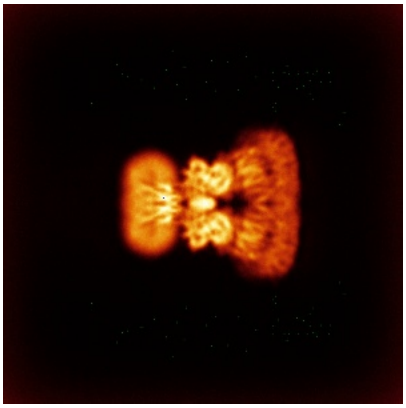

X

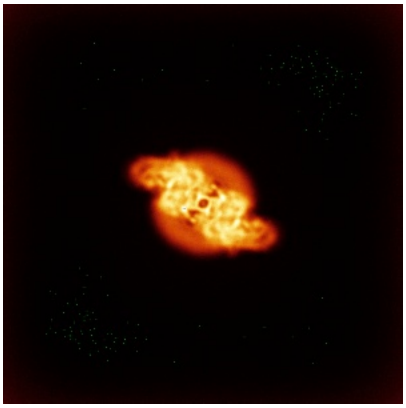

Y


Z

6.4.2 Raw map


X

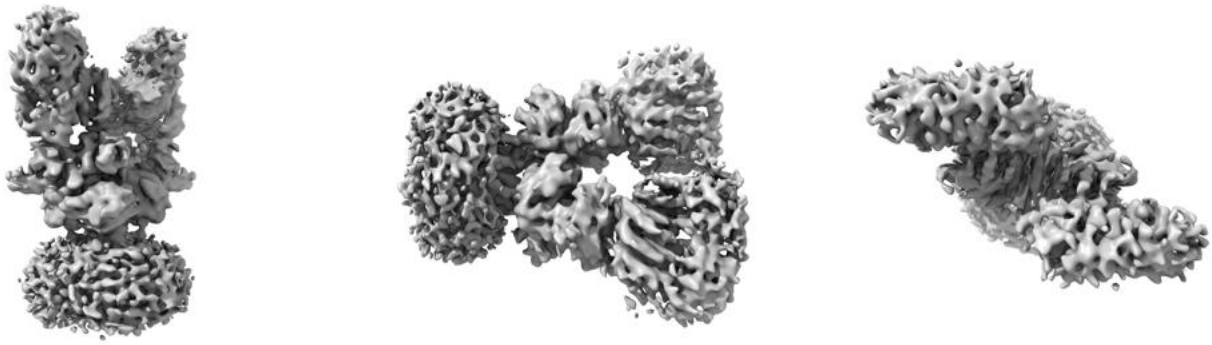

Y


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)

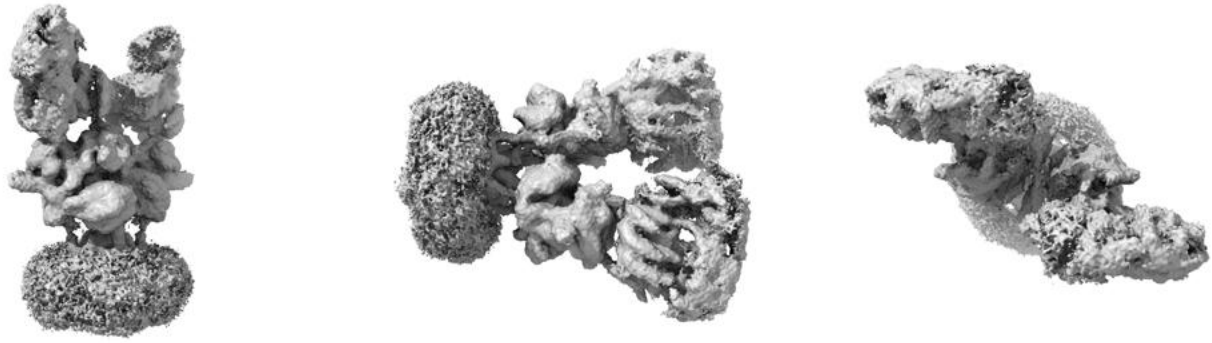
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. 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.

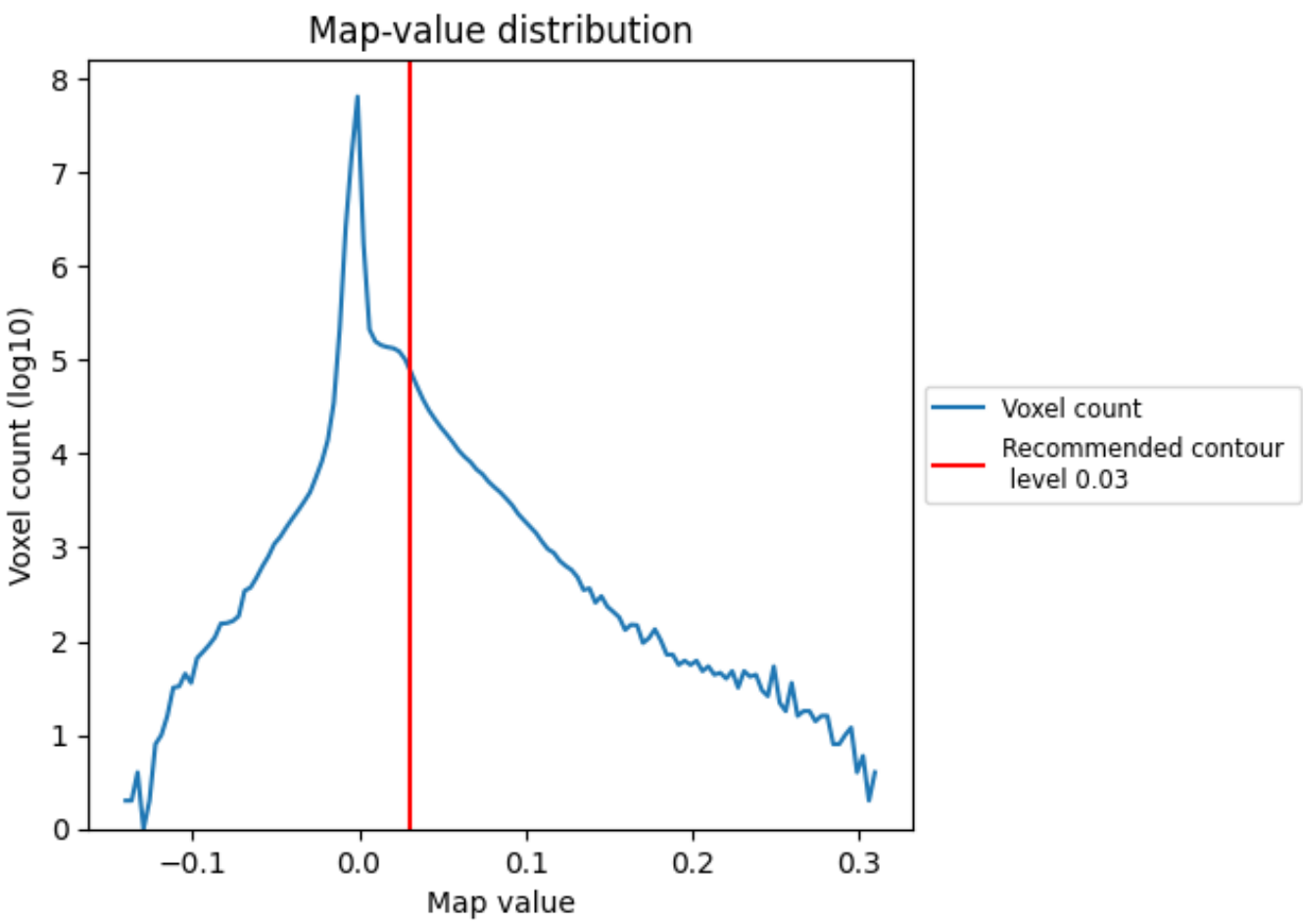
6.6 Mask visualisation (i)

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

7 Map analysis (i)

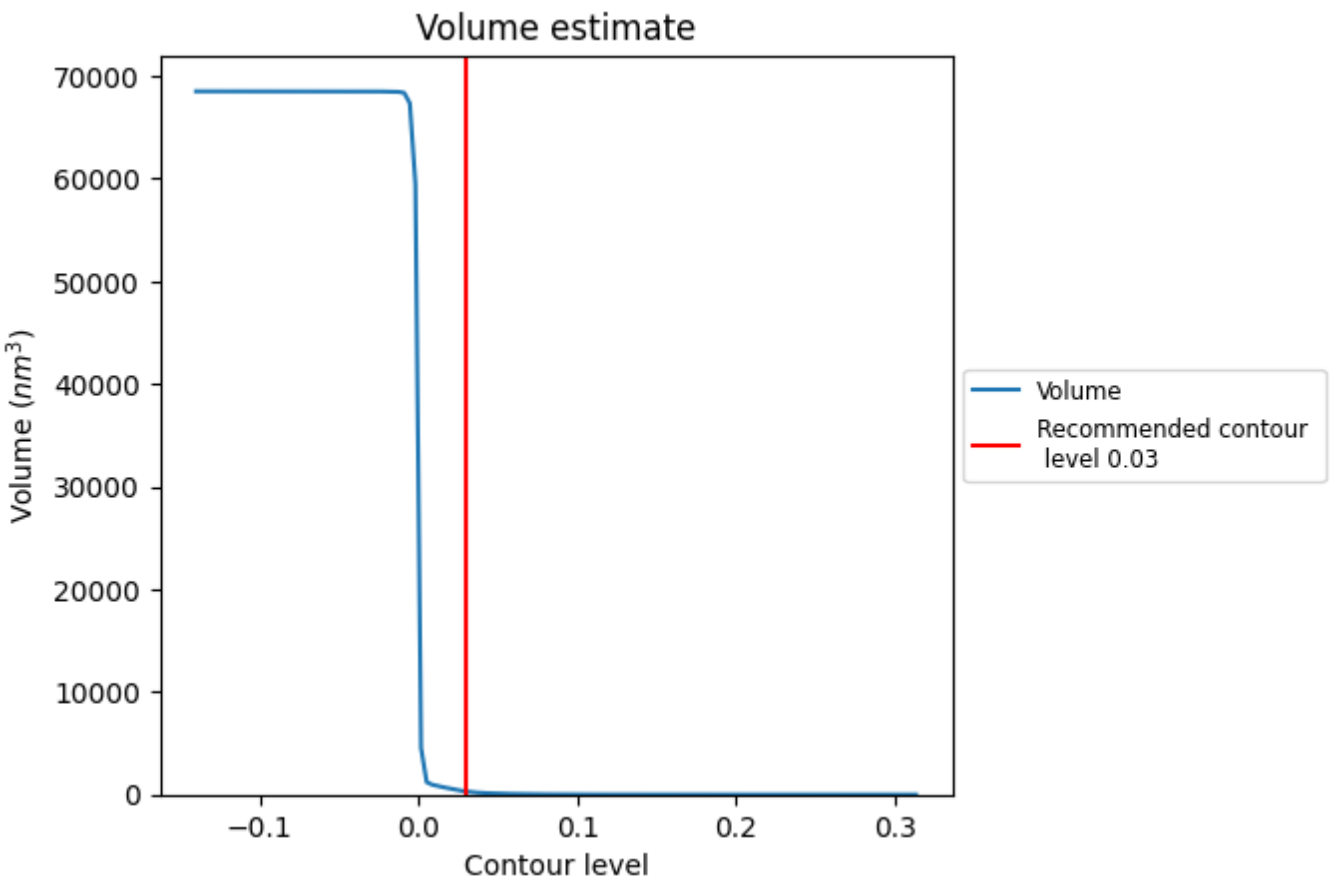
This section contains the results of statistical analysis of the map.

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.

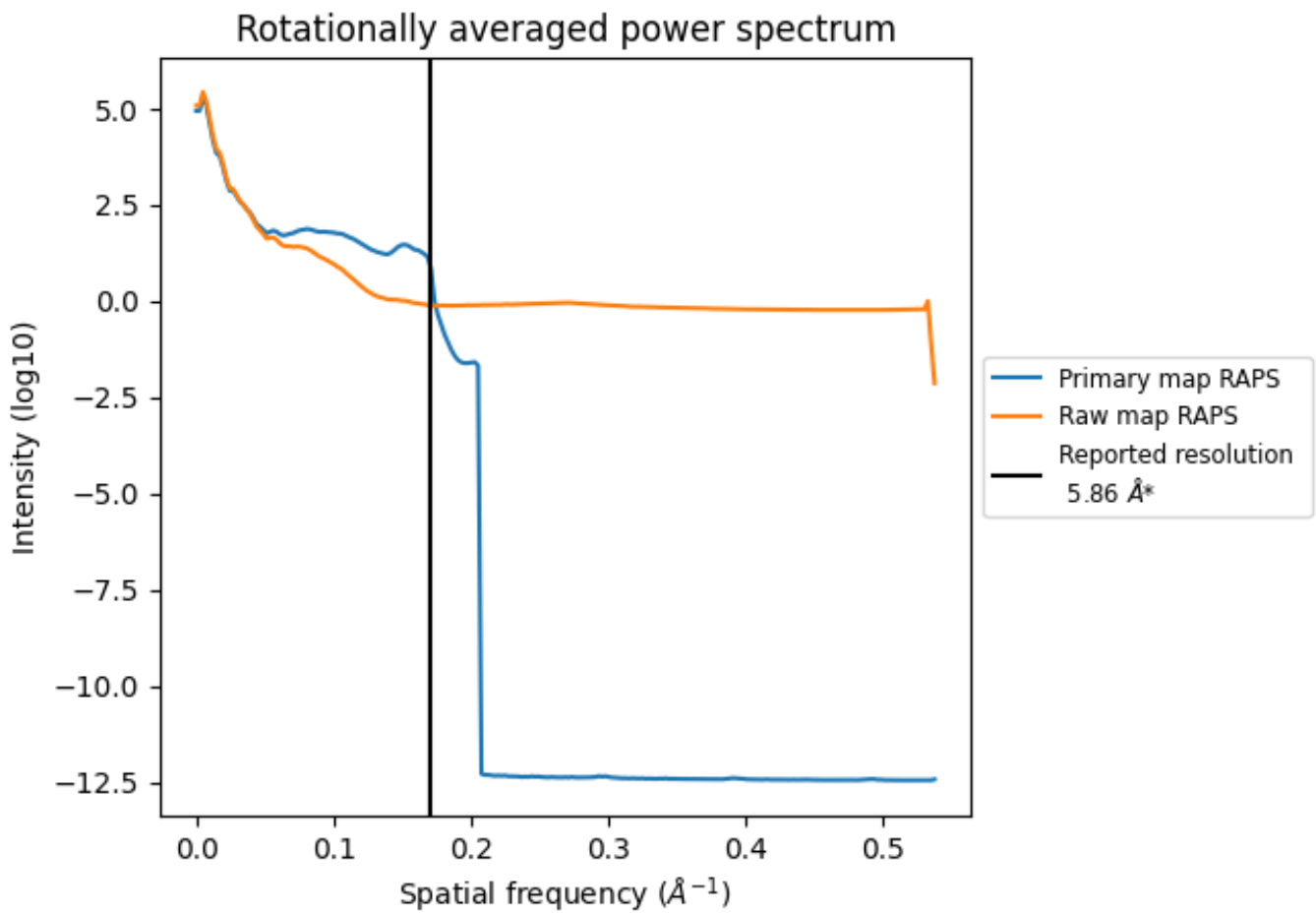
7.2 Volume estimate (i)



The volume at the recommended contour level is 301 nm^3; this corresponds to an approximate mass of 272 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)

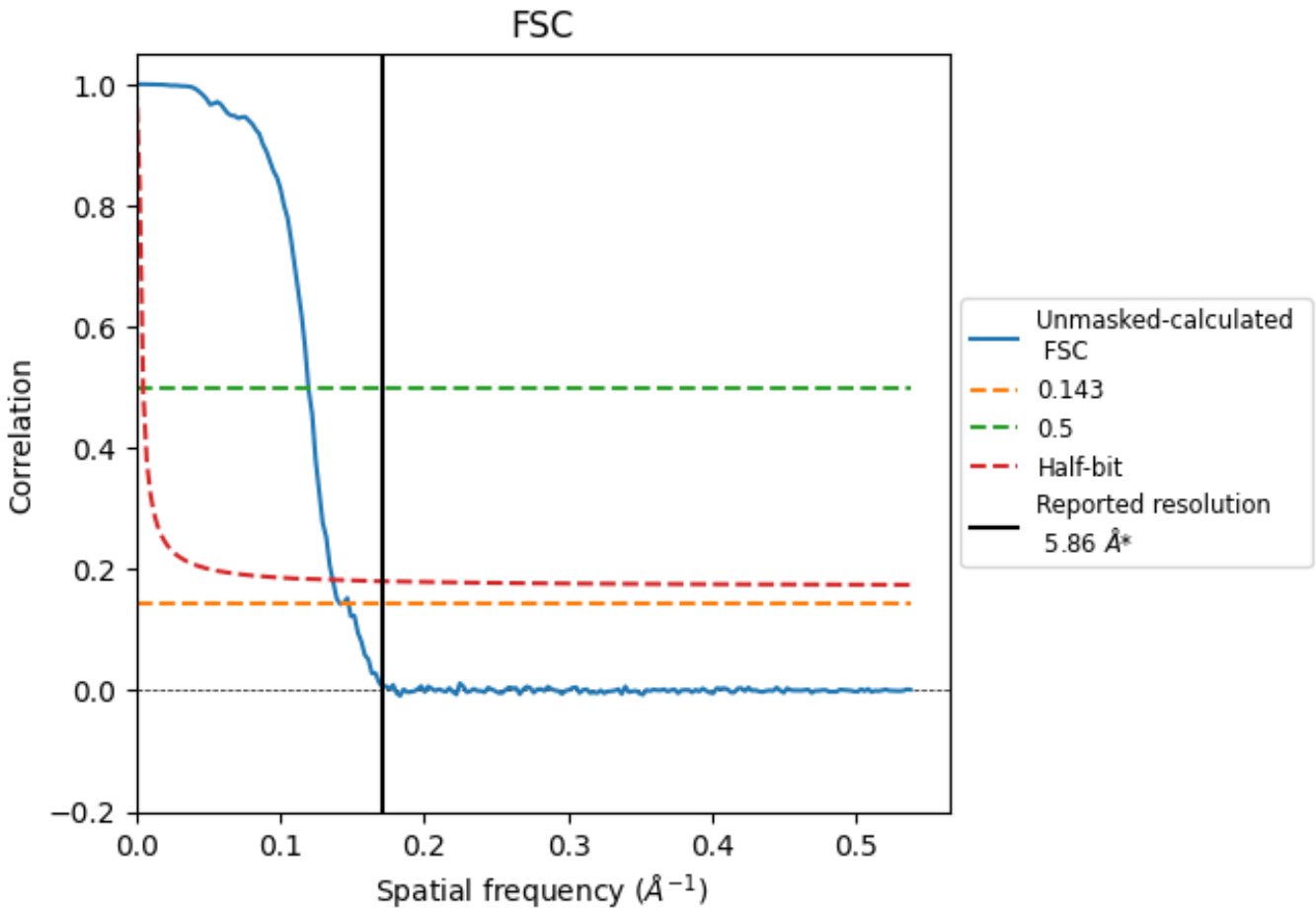


*Reported resolution corresponds to spatial frequency of 0.171 Å^{-1}

8 Fourier-Shell correlation (i)

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 (i)



*Reported resolution corresponds to spatial frequency of 0.171 Å^{-1}

8.2 Resolution estimates (i)

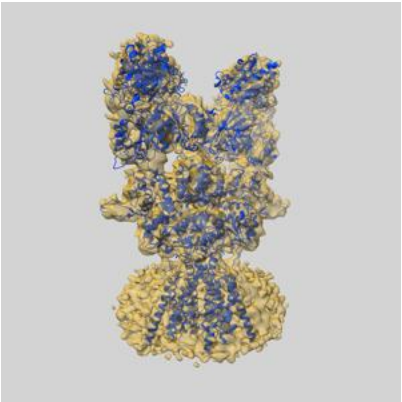
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.86	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.07	8.36	7.33

*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 7.07 differs from the reported value 5.86 by more than 10 %

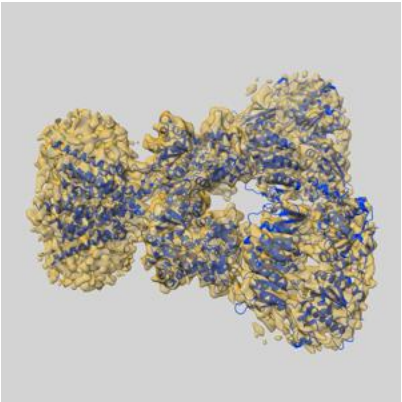
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-76442 and PDB model 12HR. Per-residue inclusion information can be found in section 3 on page 4.

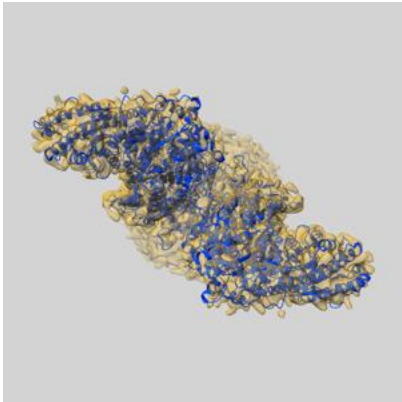
9.1 Map-model overlay (i)



X



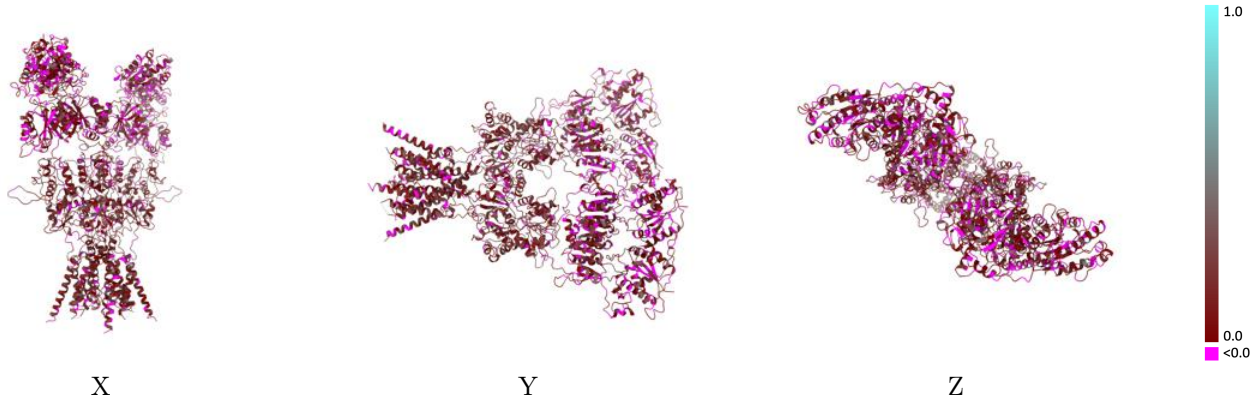
Y



Z

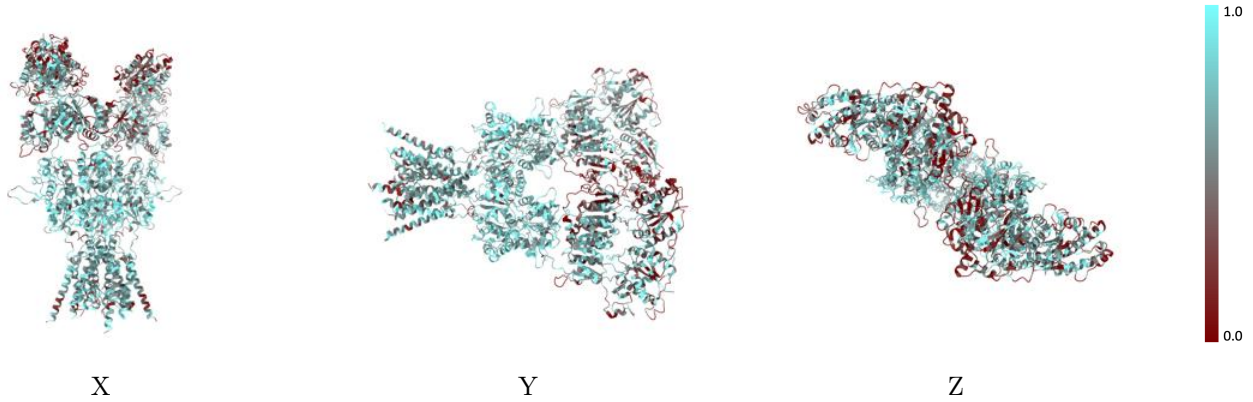
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



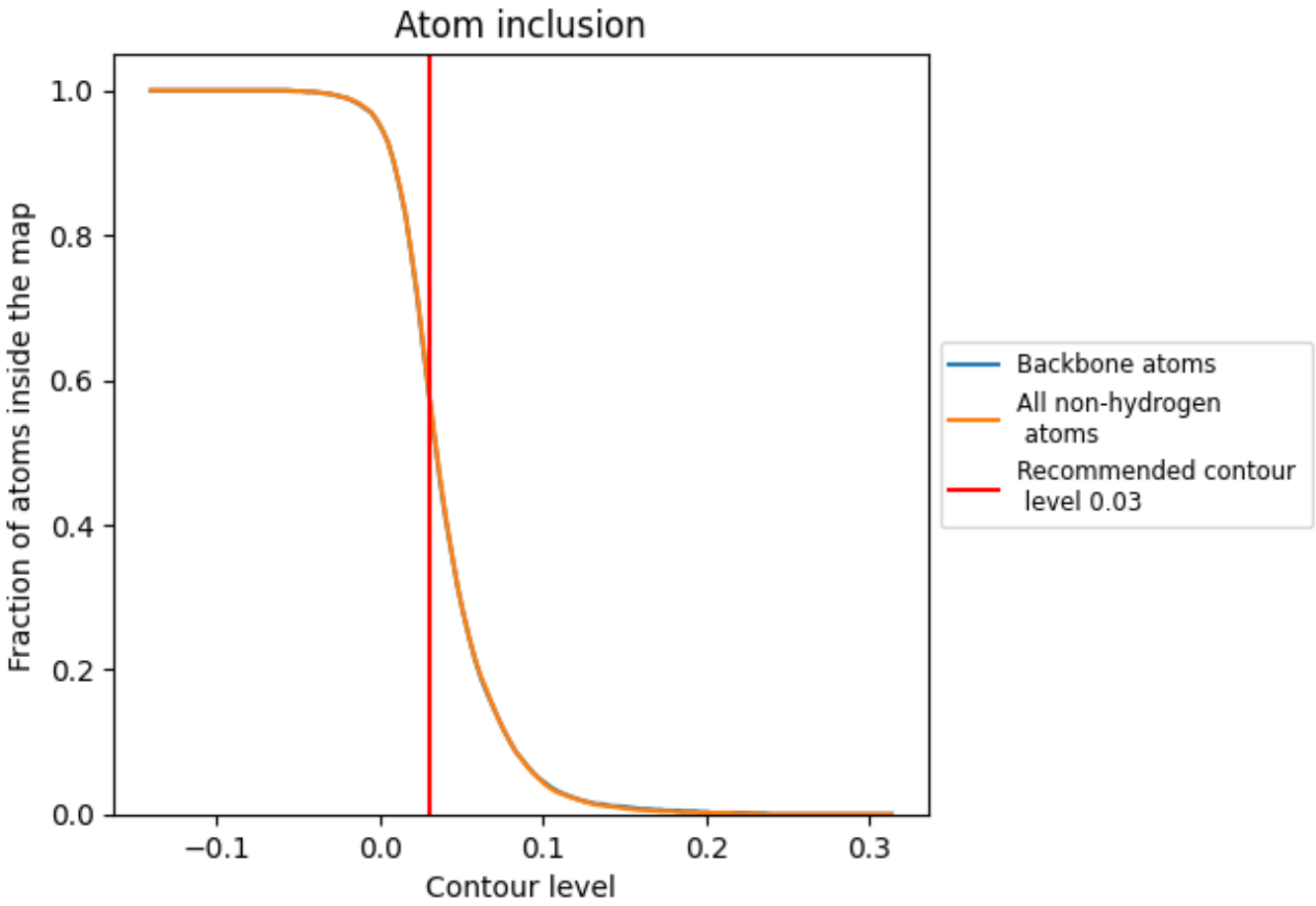
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion (i)



At the recommended contour level, 58% of all backbone atoms, 58% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5850	0.1300
A	0.5610	0.1240
B	0.6270	0.1360
C	0.5580	0.1240
D	0.6270	0.1360