wwPDB EM Validation Summary Report

Nov 12, 2026 – 03:36 pm GMT

PDB ID	:	9TIB / pdb_00009tib
EMDB ID	:	EMD-55949
Title	:	Cryo-EM structure of the y LAT1/CD98hc heteromeric complex
Authors	:	Aparicio, D.; Martinez, M.; Llorca, O.; Palacin, M.
Deposited on	:	2025-12-05
Resolution	:	3.50 Å(reported)
Based on initial model	:	.

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:

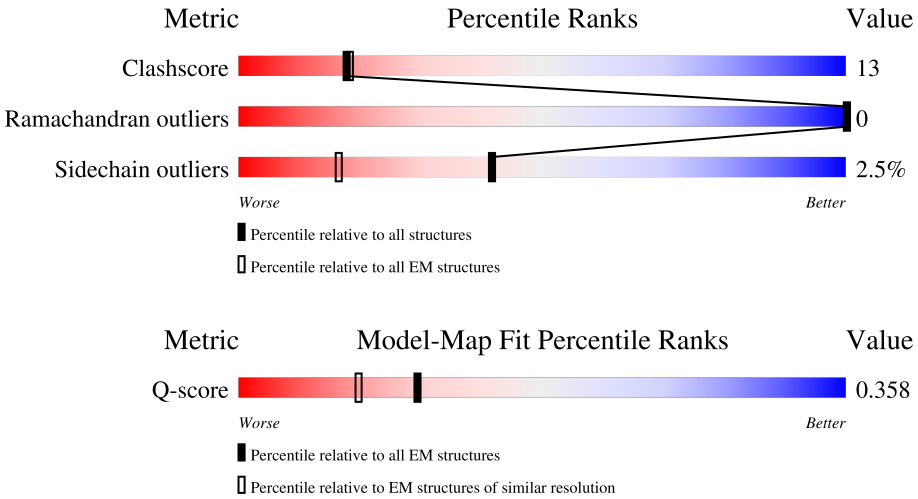
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & 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 3.50 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	13950 (3.00 - 4.00)

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	B	511	14% 66% 23% 10%
2	C	630	31% 48% 24% 28%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7105 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 Y+L amino acid transporter 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	458	3556	2374	555	609	18	1	0

- Molecule 2 is a protein called 4F2 cell-surface antigen heavy chain.

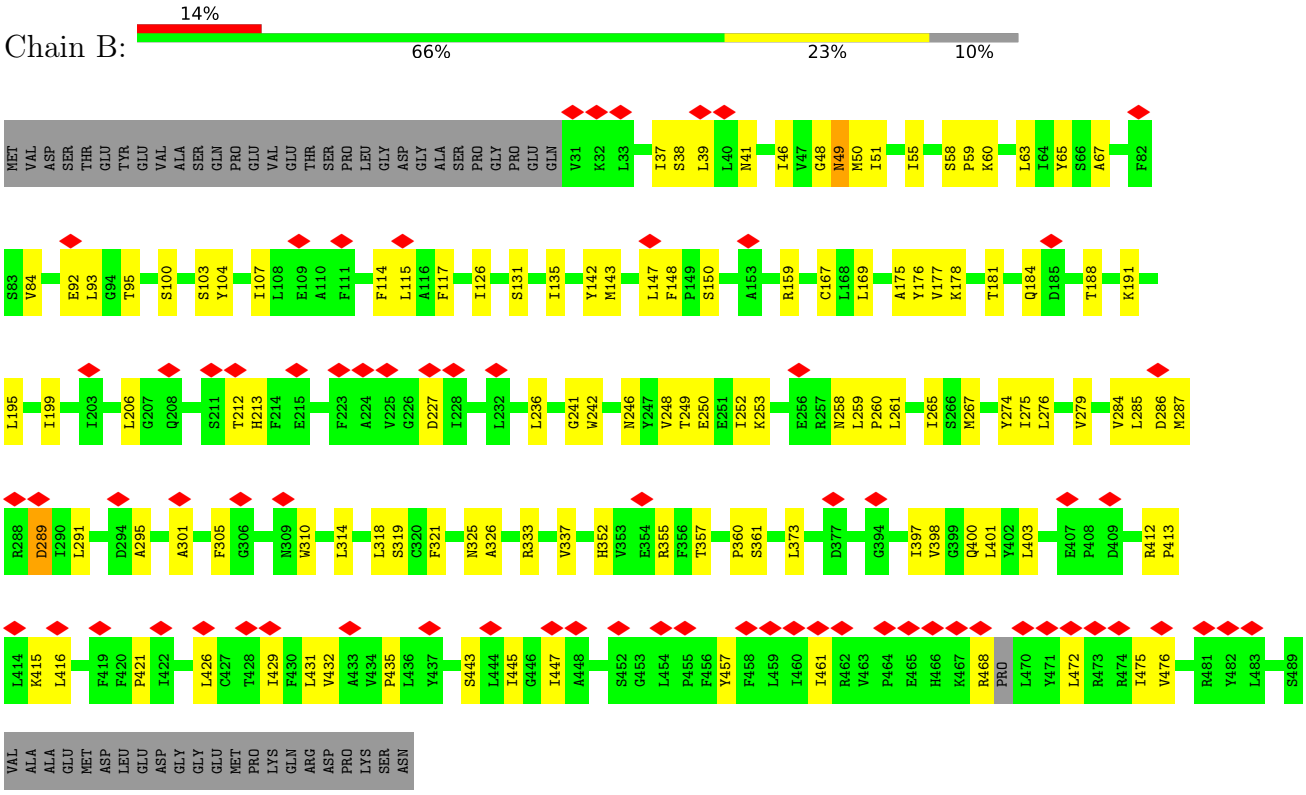
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	454	3549	2275	607	660	7	0	0

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.

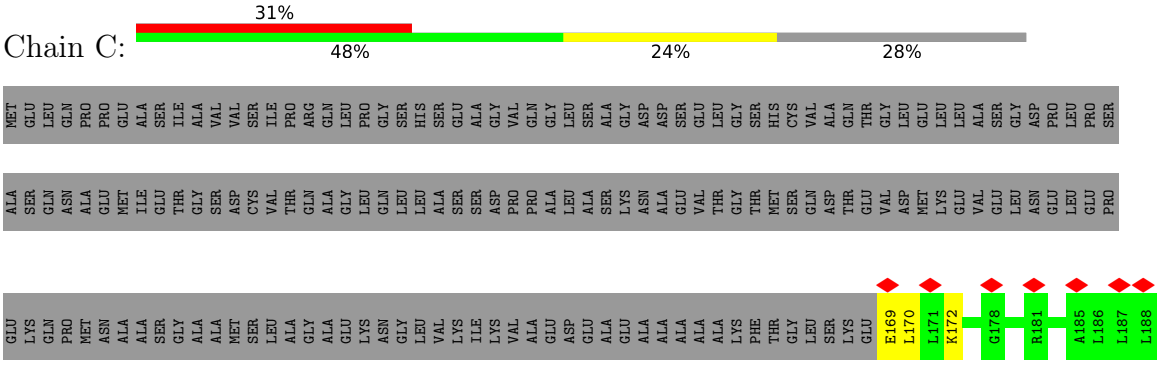
• Molecule 1: Y+L amino acid transporter 1

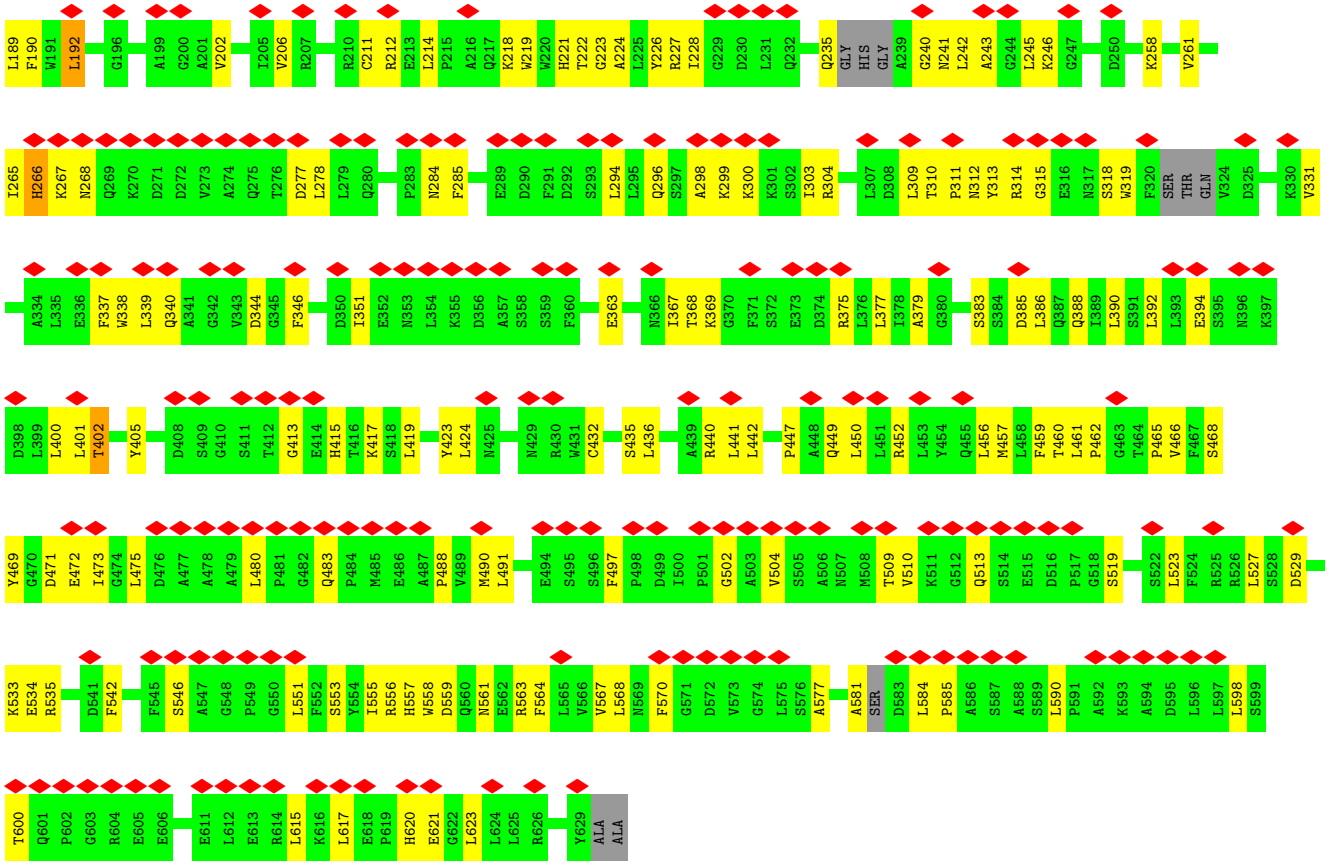
Chain B:



• Molecule 2: 4F2 cell-surface antigen heavy chain

Chain C:




L189 F190 W191 L192 G196 A199 G200 A201 V202 I205 V206 R207 R210 C211 R212 E213 L214 P215 A216 Q217 K218 W219 W220 H221 T222 G223 A224 L225 Y226 R227 I228 G229 D230 L231 Q232 Q235 GLY HIS GLY A239 G240 N241 L242 A243 G244 L245 K246 G247 D250 K258 V261
I265 H266 K267 N268 Q269 K270 D271 D272 V273 A274 Q275 T276 D277 L278 L279 Q280 P283 N284 F285 E289 D290 F291 D292 S293 L294 L295 Q296 S297 A298 K299 K300 K301 S302 I303 R304 L307 D308 L309 T310 P311 N312 Y313 R314 G315 E316 N317 S318 W319 F320 SER THR GLN V324 D325 K330 V331
A334 L335 E336 F337 W338 L339 Q340 A341 G342 V343 D344 G345 F346 D350 I351 E352 N353 L354 K355 D356 A357 S358 S359 F360 E363 N366 I367 T368 K369 G370 F371 S372 E373 D374 R375 L376 L377 I378 A379 G380 S383 S384 D385 L386 Q387 Q388 I389 L390 S391 L392 L393 E394 S395 N396 K397
D398 L399 L400 L401 T402 Y405 D408 S409 G410 S411 T412 G413 E414 H415 T416 K417 S418 L419 Y423 L424 N425 N429 R430 W431 C432 S435 L436 A439 R440 L441 L442 P447 A448 Q449 L450 L451 R452 L453 Y454 Q455 L456 M457 L458 F459 T460 L461 P462 G463 T464 P465 V466 F467 S468
Y469 G470 D471 E472 I473 G474 L475 D476 A477 A478 A479 L480 P481 G482 Q483 P484 M485 E486 A487 P488 V489 M490 L491 E494 S495 S496 F497 P498 D499 I500 P501 G502 A503 V504 S505 A506 N507 M508 T509 V510 K511 G512 Q513 S514 E515 D516 P517 G518 S519 S522 L523 F524 R525 R526 L527 S528 D529
K533 E534 R535 D541 F542 F545 S546 A547 G548 P549 G550 L551 F552 S553 Y554 I555 R556 H557 W558 D559 Q560 N561 E562 R563 F564 L565 V566 V567 L568 N569 F570 G571 D572 V573 G574 L575 S576 A577 A581 SER D583 L584 P585 A586 S587 A588 S589 L590 P591 A592 K593 A594 D595 L596 L597 L598 S599
T600 Q601 P602 G603 R604 E605 E606 E611 L612 E613 R614 L615 K616 L617 E618 P619 H620 E621 G622 L623 L624 L625 R626 Y629 ALA ALA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	175245	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 ($e^-/Å^2$)	43.1	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	2.085	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.229	Depositor
Map size (Å)	210.8928, 210.8928, 210.8928	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8238, 0.8238, 0.8238	Depositor

5 Model quality

5.1 Standard geometry

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	B	0.15	0/3651	0.39	0/4978
2	C	0.13	0/3629	0.35	0/4922
All	All	0.14	0/7280	0.37	0/9900

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	B	3556	0	3649	83	0
2	C	3549	0	3541	111	0
All	All	7105	0	7190	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 13.

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)
1:B:49:ASN:C	1:B:49:ASN:HD22	1.77	0.92
2:C:242:LEU:HA	2:C:245:LEU:HB2	1.60	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:385:ASP:HB3	2:C:388:GLN:HE22	1.47	0.80
2:C:227:ARG:HA	2:C:261:VAL:HB	1.68	0.74
2:C:227:ARG:HG2	2:C:468:SER:HA	1.73	0.69

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	B	455/511 (89%)	430 (94%)	25 (6%)	0	100	100
2	C	446/630 (71%)	431 (97%)	15 (3%)	0	100	100
All	All	901/1141 (79%)	861 (96%)	40 (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	B	381/428 (89%)	375 (98%)	6 (2%)	55	70
2	C	381/514 (74%)	368 (97%)	13 (3%)	32	57
All	All	762/942 (81%)	743 (98%)	19 (2%)	42	63

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	424	LEU
2	C	551	LEU
2	C	559	ASP
2	C	490	MET
2	C	202	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	208	GLN
2	C	232	GLN
2	C	415	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.

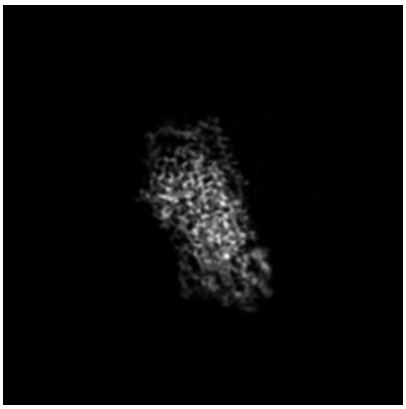
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-55949. These allow visual inspection of the internal detail of the map and identification of artifacts.

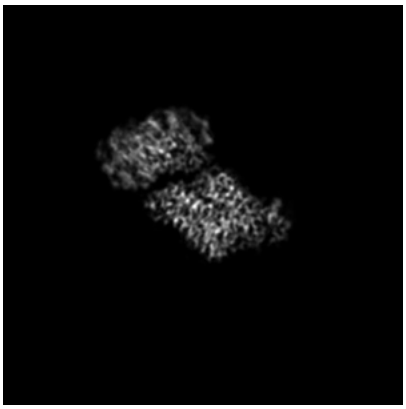
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

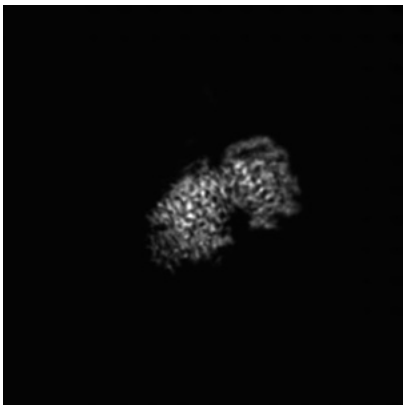
6.1.1 Primary map



X

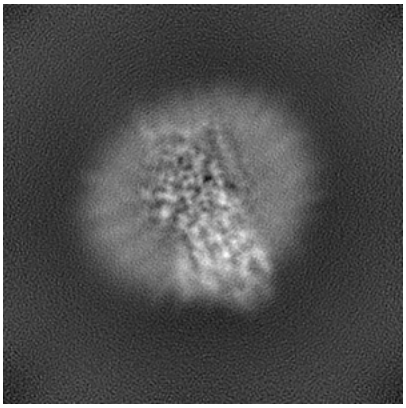


Y

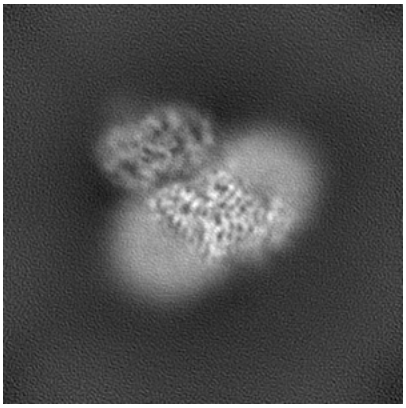


Z

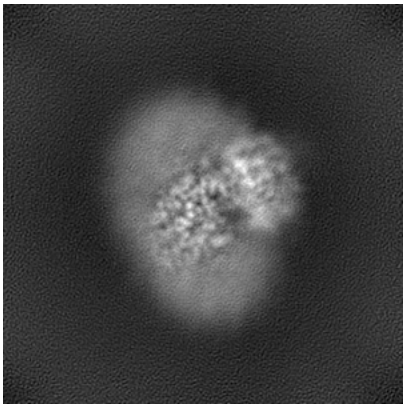
6.1.2 Raw map



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: 128

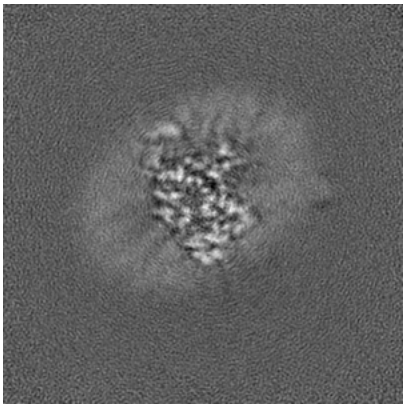


Y Index: 128

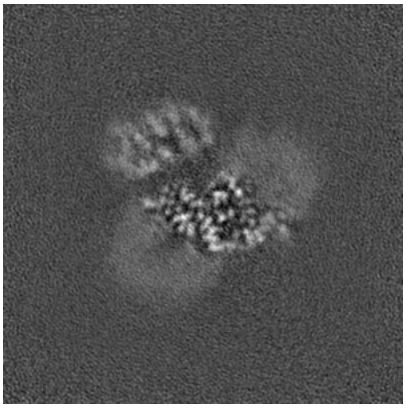


Z Index: 128

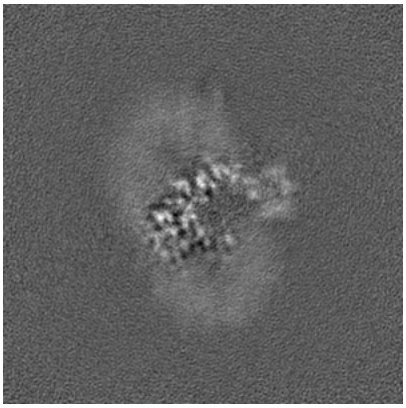
6.2.2 Raw map



X Index: 128



Y Index: 128

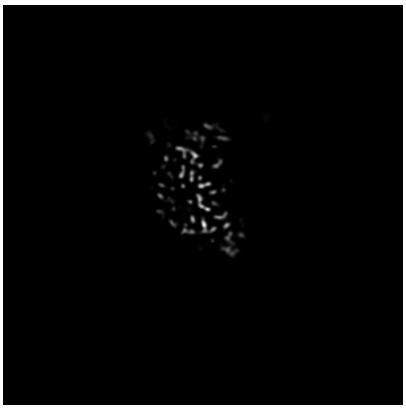


Z Index: 128

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

6.3 Largest variance slices (i)

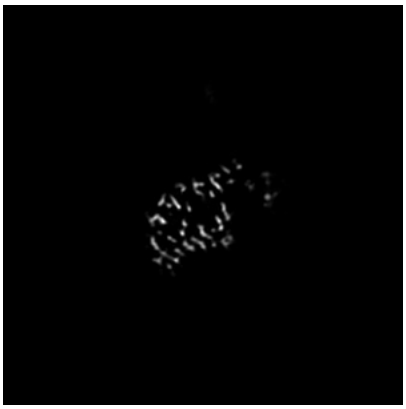
6.3.1 Primary map



X Index: 119

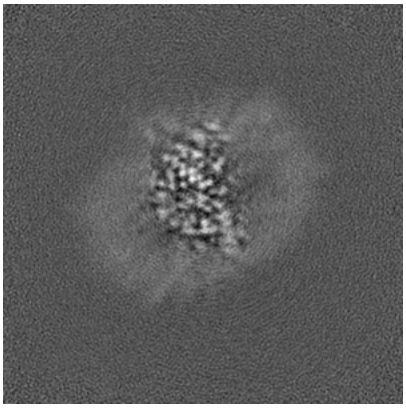


Y Index: 142

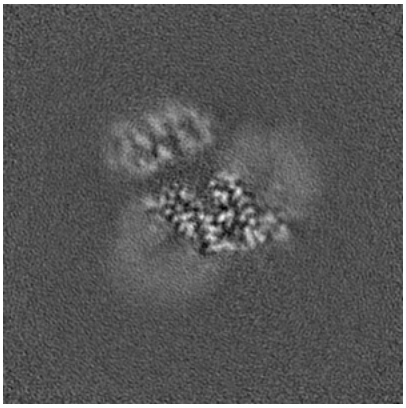


Z Index: 133

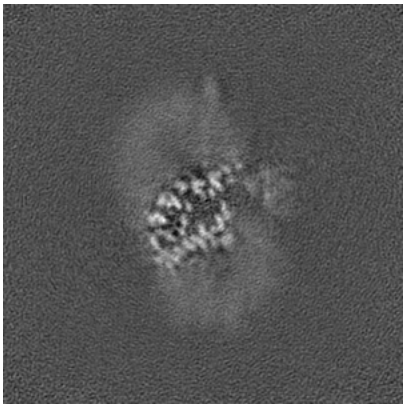
6.3.2 Raw map



X Index: 118



Y Index: 127

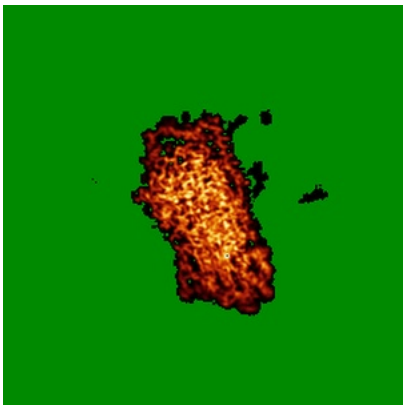


Z Index: 133

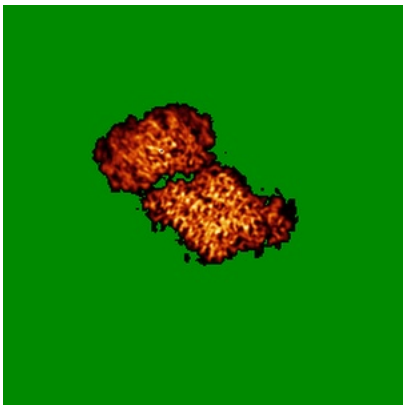
The images above show the largest variance slices of the map in three orthogonal directions.

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

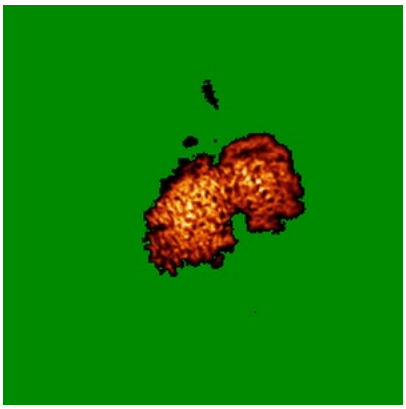
6.4.1 Primary map



X

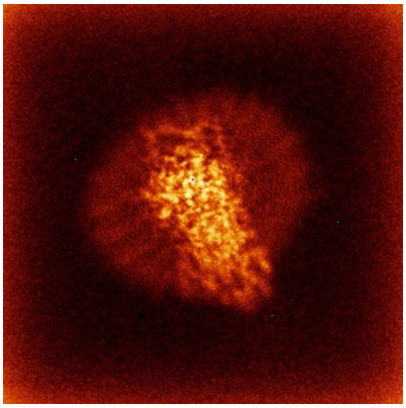


Y

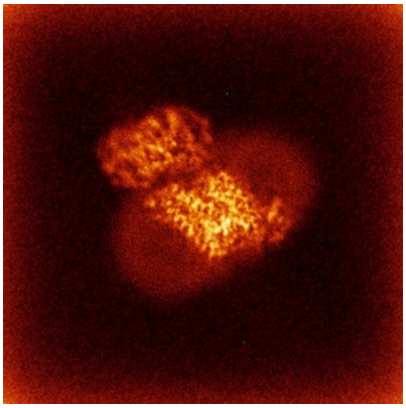


Z

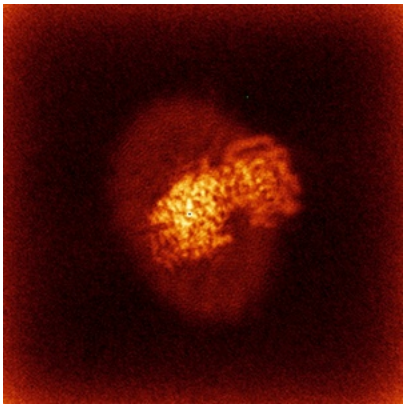
6.4.2 Raw map



X



Y

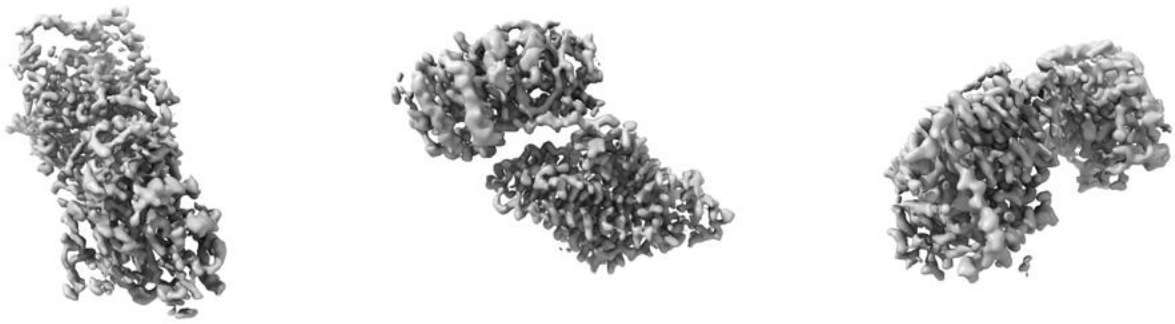


Z

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 0.229. 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.

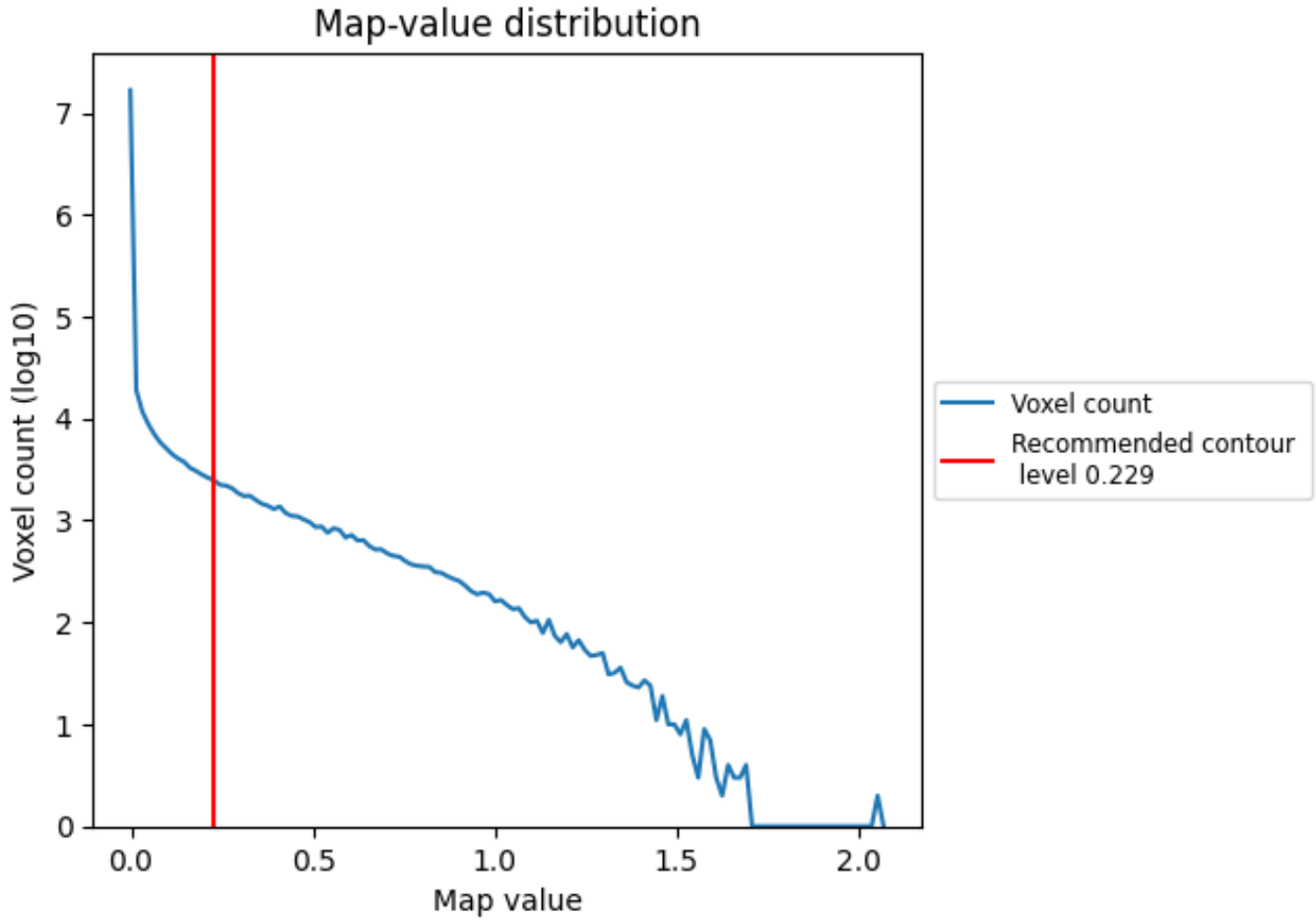
6.6 Mask visualisation (i)

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

7 Map analysis

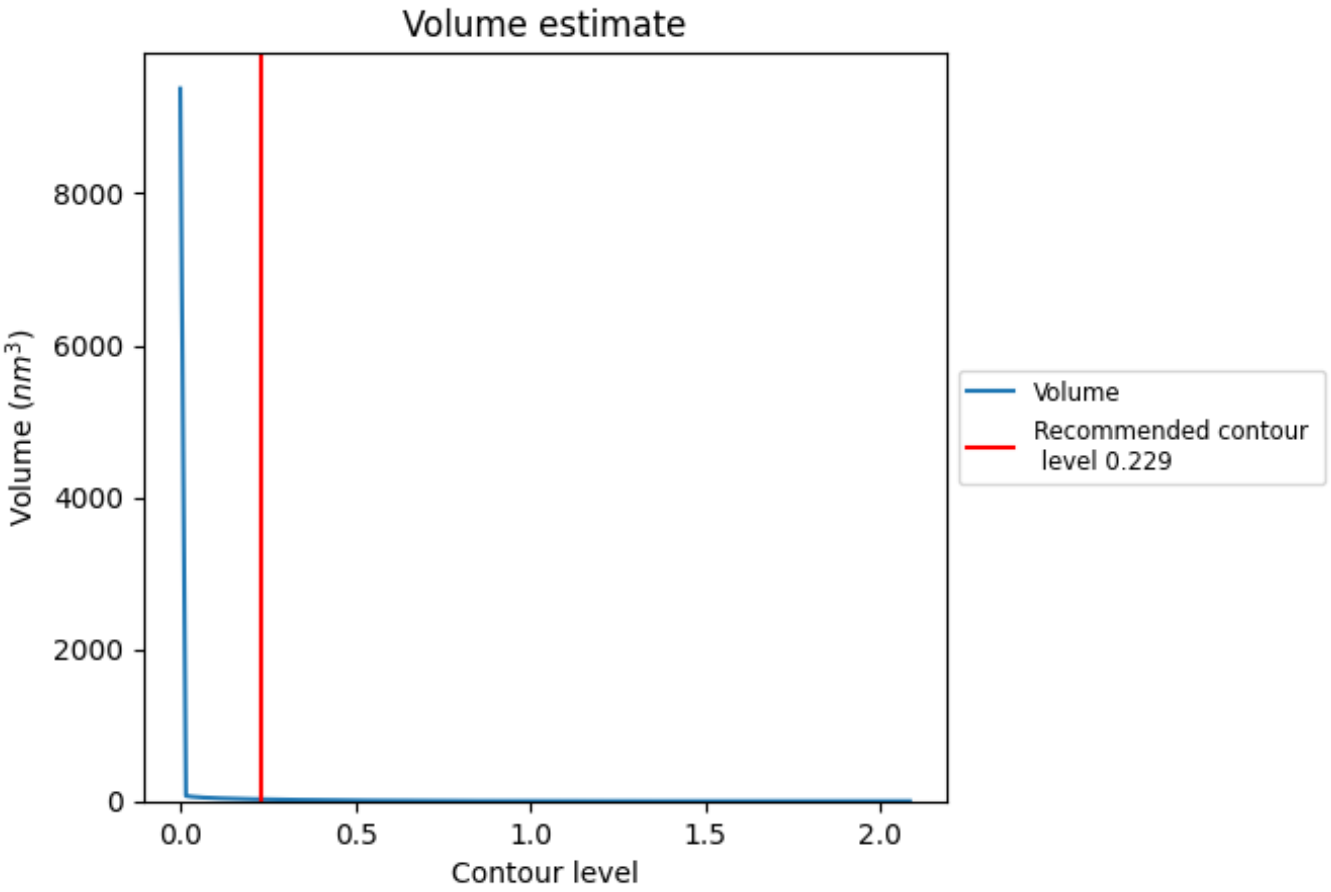
This section contains the results of statistical analysis of the map.

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.

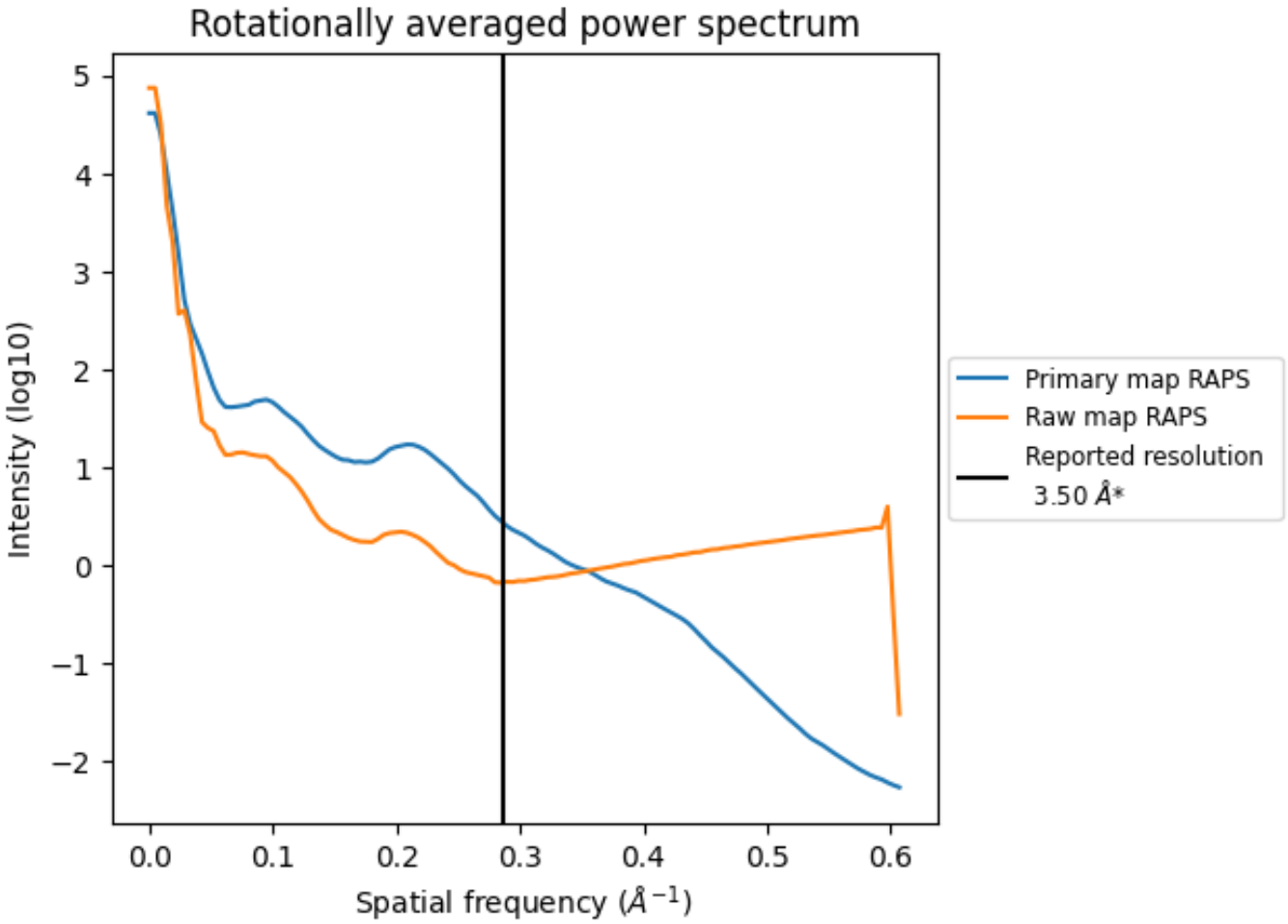
7.2 Volume estimate (i)



The volume at the recommended contour level is 24 nm^3; this corresponds to an approximate mass of 22 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)

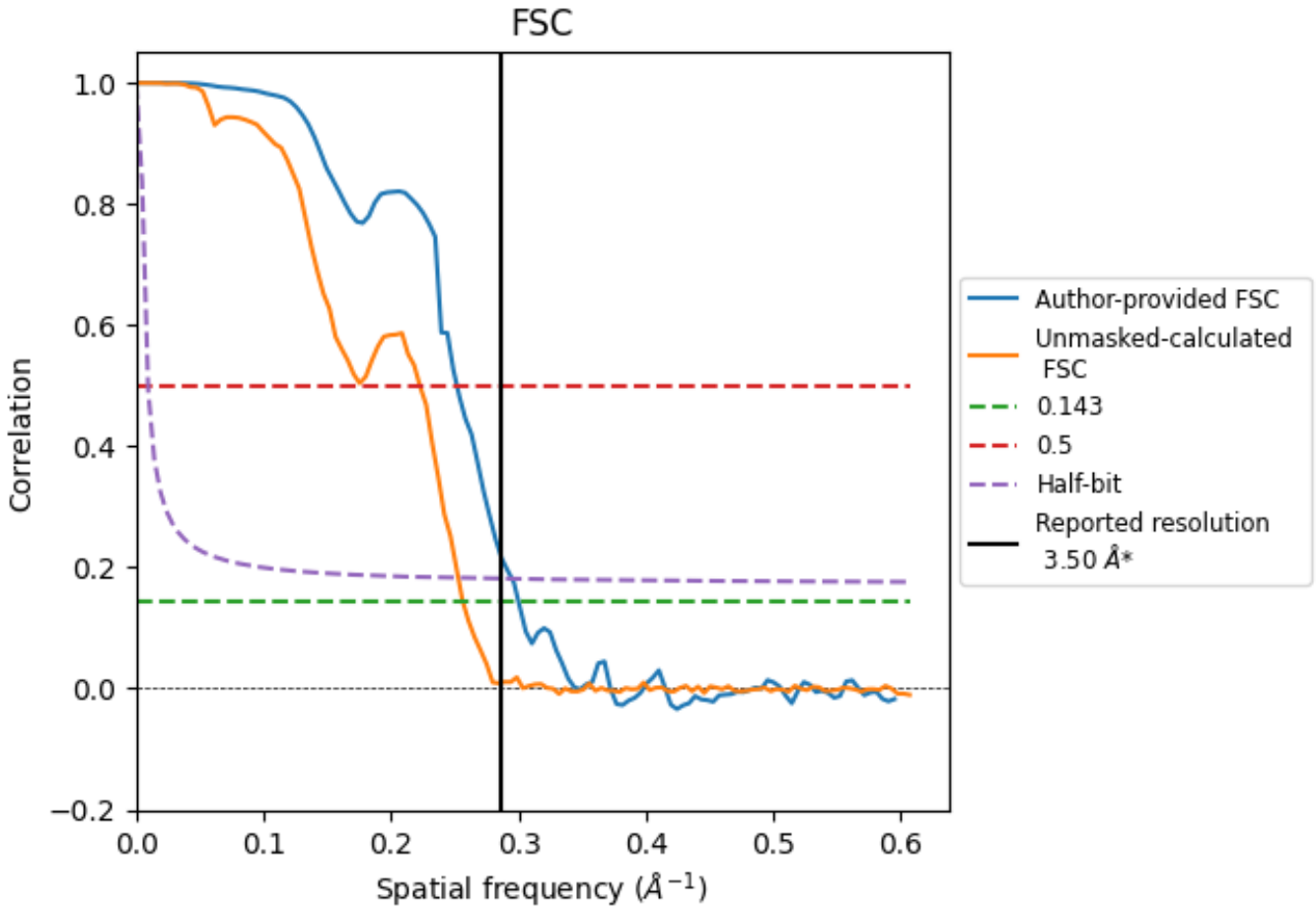


*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

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 0.286 Å^{-1}

8.2 Resolution estimates (i)

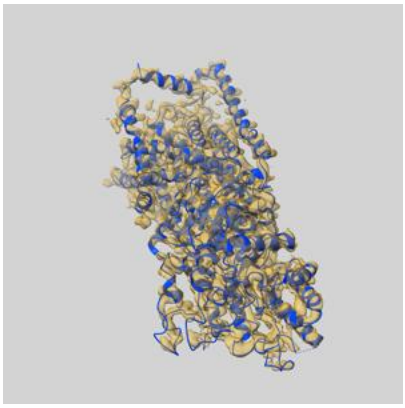
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.33	3.97	3.39
Unmasked-calculated*	3.90	4.49	3.96

*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 3.90 differs from the reported value 3.5 by more than 10 %

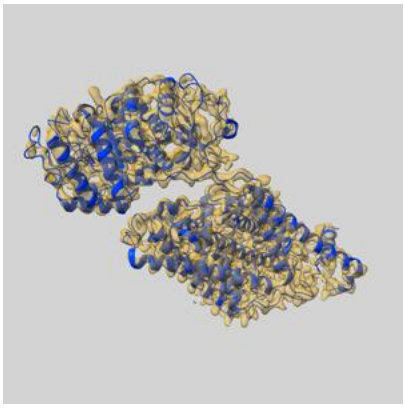
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-55949 and PDB model 9TIB. Per-residue inclusion information can be found in section 3 on page 4.

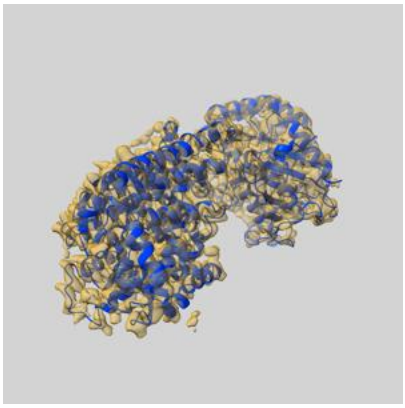
9.1 Map-model overlay



X



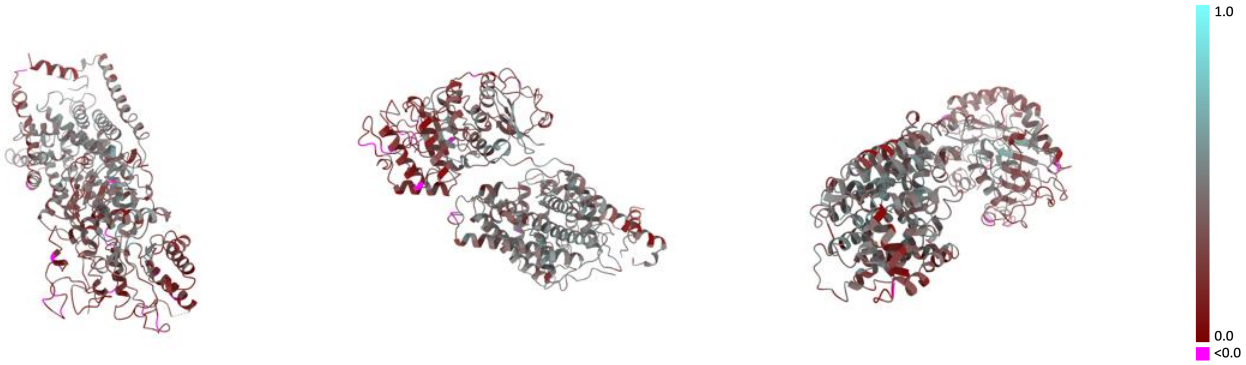
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.229 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.

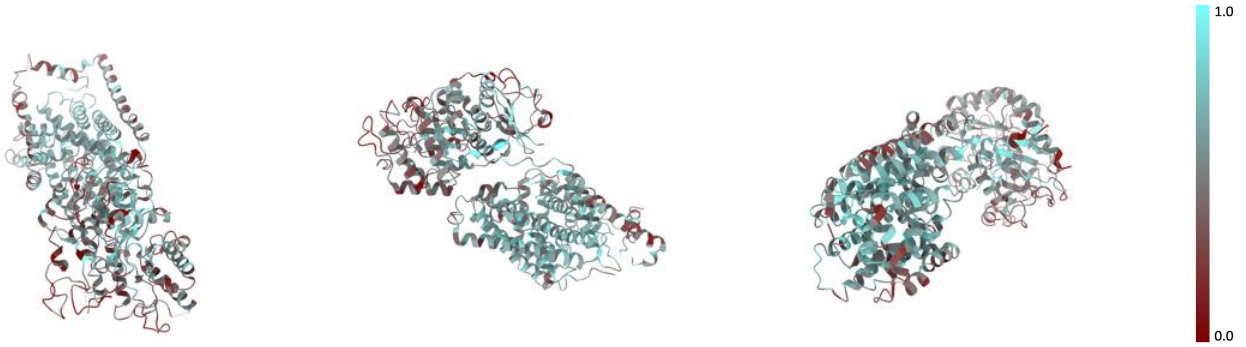
9.2 Q-score mapped to coordinate model (i)



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.

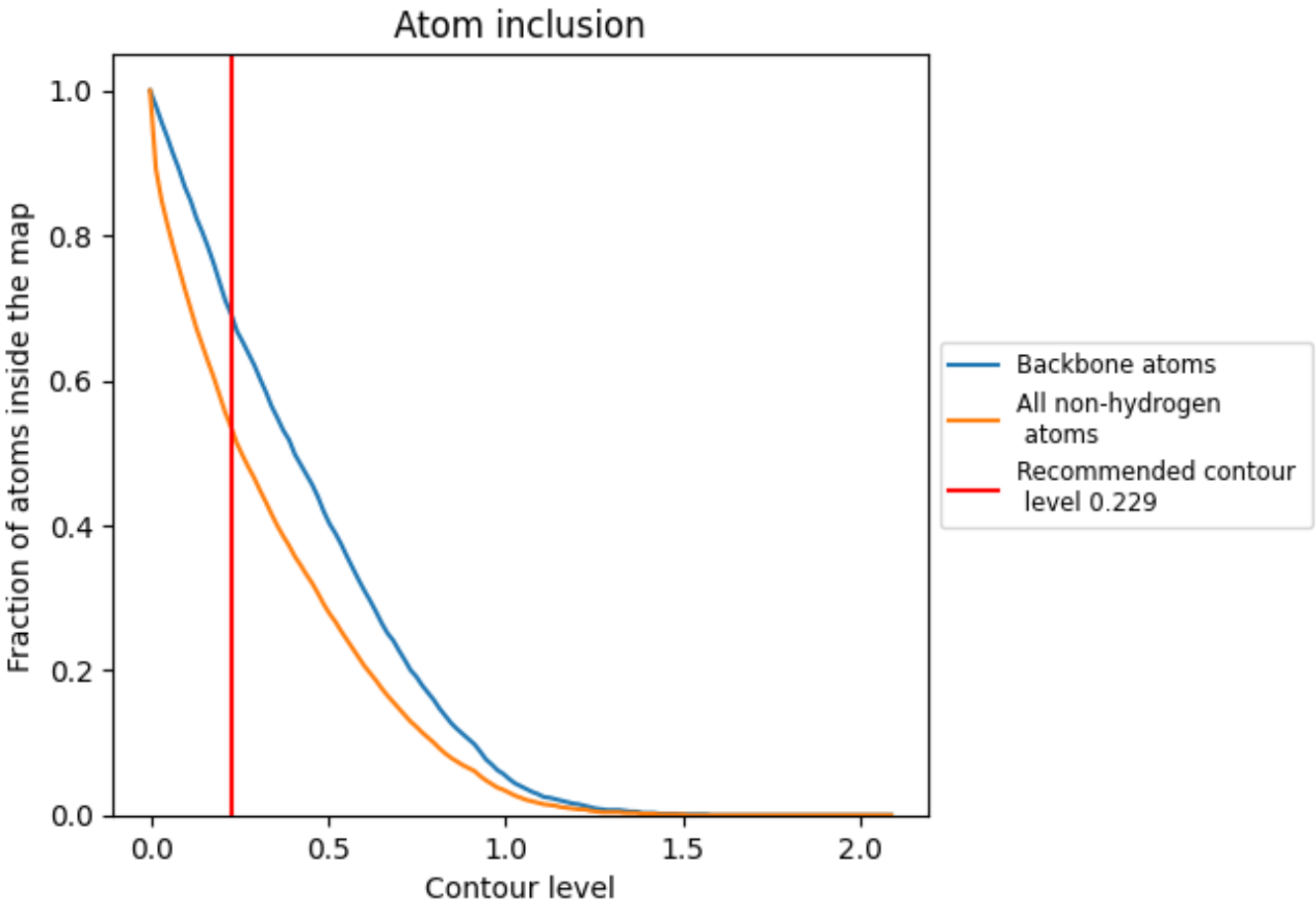
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.229).

9.4 Atom inclusion (i)



At the recommended contour level, 69% of all backbone atoms, 53% 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 (0.229) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.5320	0.3580
B	0.6030	0.4070
C	0.4610	0.3090