wwPDB EM Validation Summary Report

Oct 19, 2026 – 03:18 PM JST

PDB ID	:	9XCR / pdb_00009xcr
EMDB ID	:	EMD-66741
Title	:	Cryo-EM structure of HalT (E643Q mutant), a peptidase-domain containing ABC transporter, incubated with ATP
Authors	:	Gan, B.K.; Luo, M.
Deposited on	:	2025-10-26
Resolution	:	3.82 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:

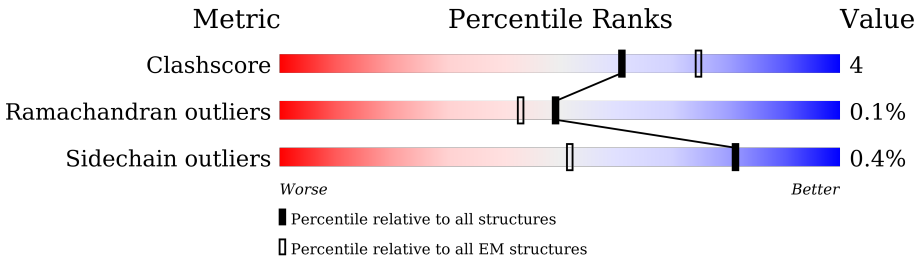
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

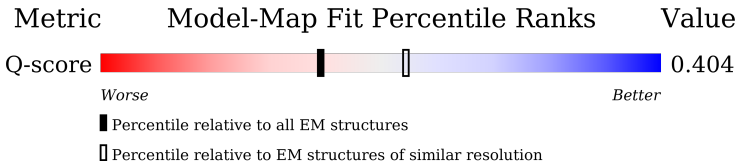
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.82 Å.

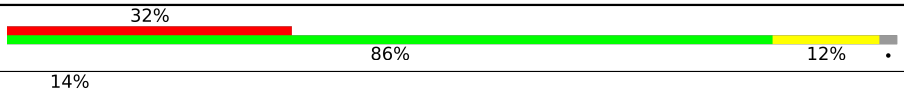
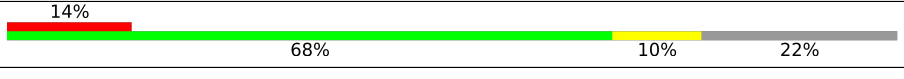
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





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	9152 (3.32 - 4.32)

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	724	
1	B	724	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10111 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.

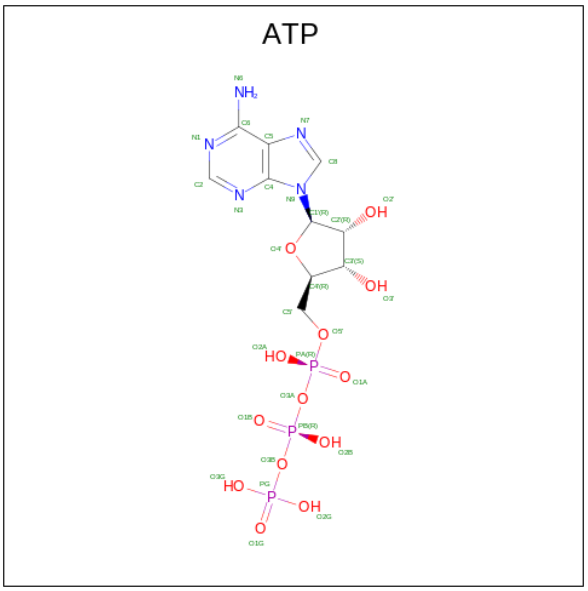
- Molecule 1 is a protein called Lantibiotic mersacidin transporter system.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	708	Total	C	N	O	S	0	0
			5651	3653	960	1009	29		
1	B	564	Total	C	N	O	S	0	0
			4396	2843	738	794	21		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	643	GLN	GLU	engineered mutation	UNP Q9KFM8
B	643	GLN	GLU	engineered mutation	UNP Q9KFM8

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			31	10	5	13	3	

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Mol	Chain	Residues	Atoms					AltConf
2	B	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

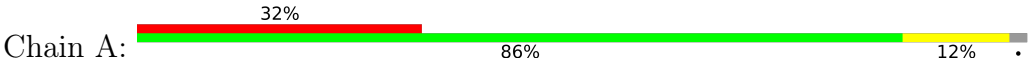
Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Mg	0
			1	1	
3	B	1	Total	Mg	0
			1	1	

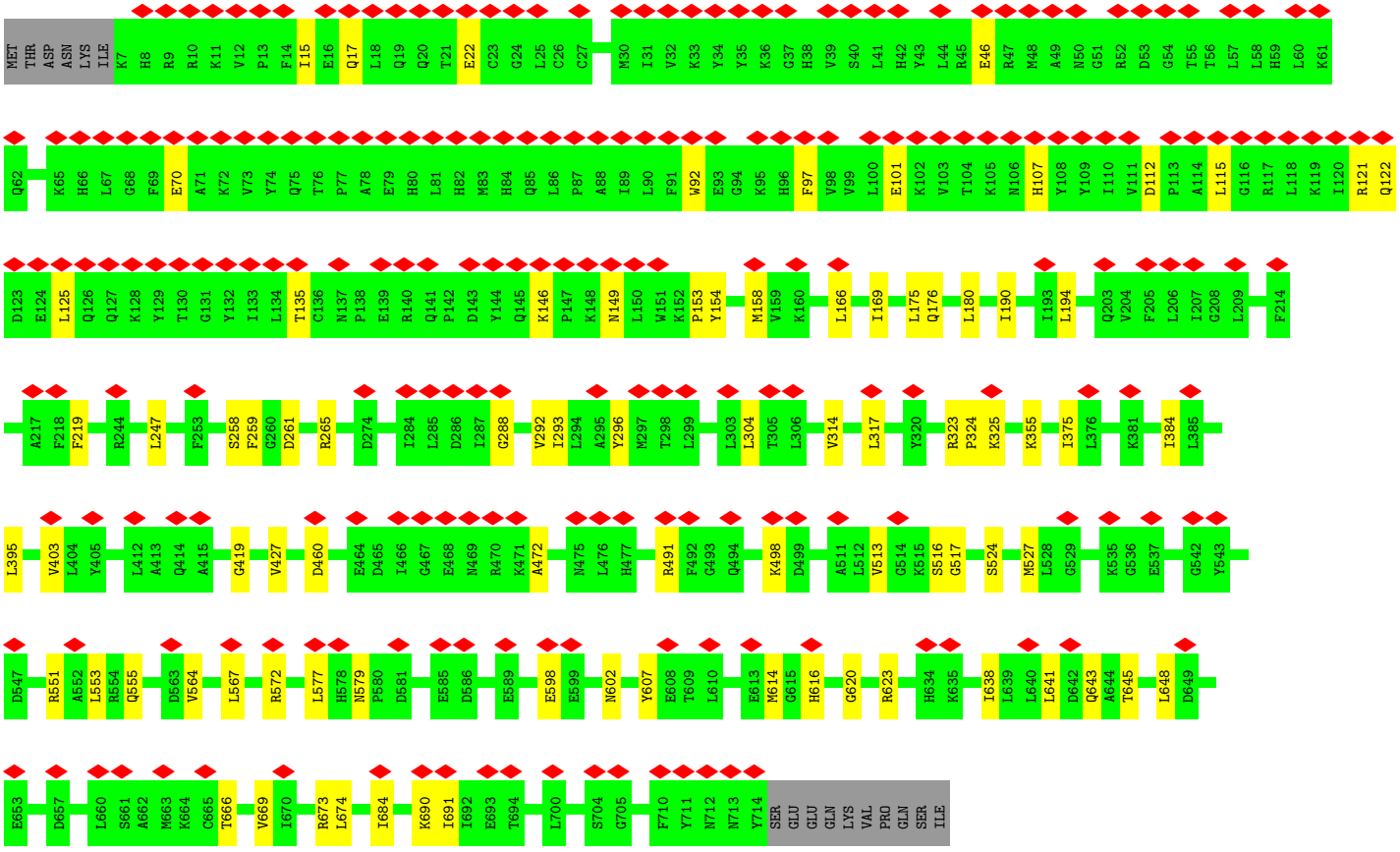
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Lantibiotic mersacidin transporter system

Chain A:

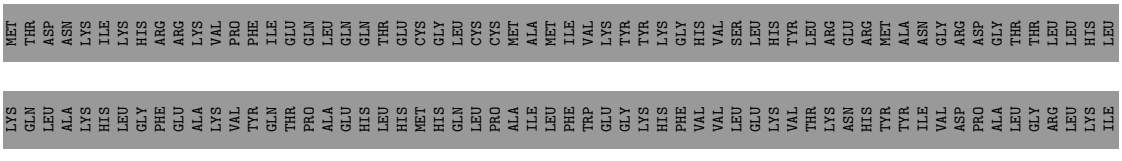


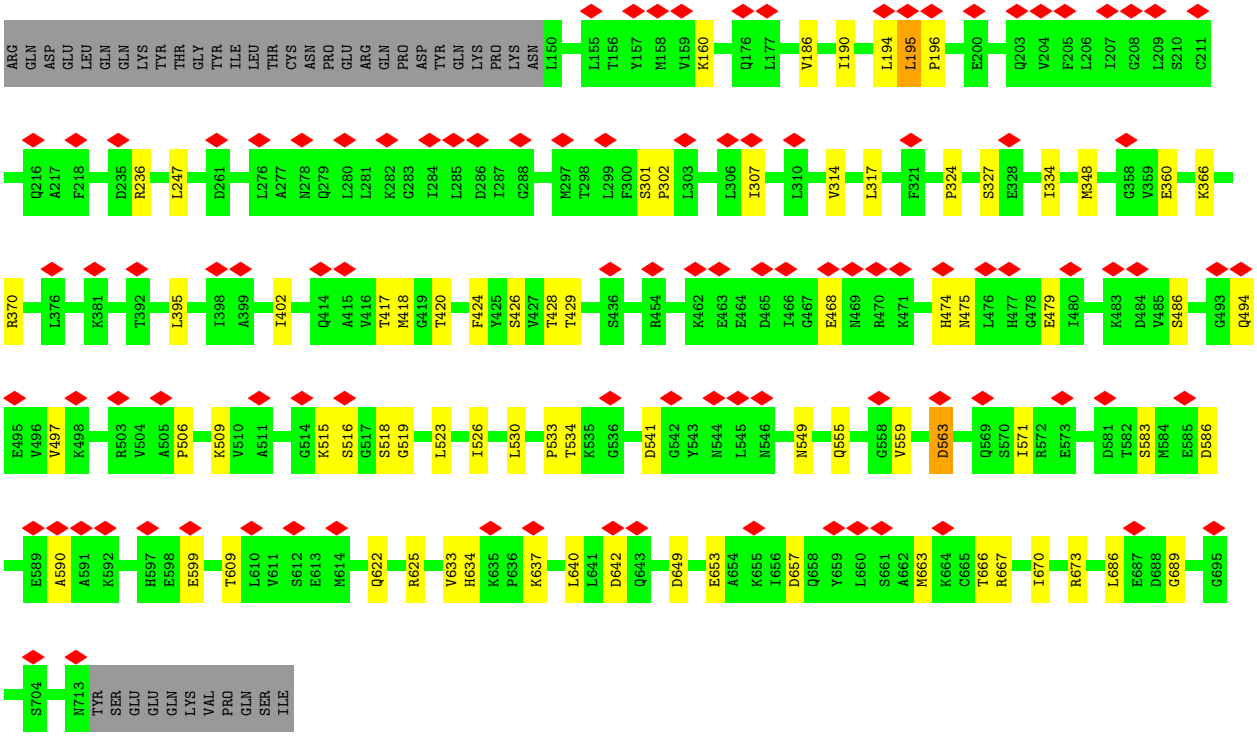


• Molecule 1: Lantibiotic mersacidin transporter system

Chain B:






ARG GLN ASP GLU LEU GLN GLN LYS TYR THR GLY TYR ILE LEU THR CYS ASN PRO GLU ARG GLN PRO ASP TYR GLN LYS PRO LYS ASN L150
L155 T156 Y157 M158 V159 K160 Q176 L177 V186 I190 L194 L195 P196 E200 Q203 V204 F205 L206 I207 G208 L209 S210 C211
Q216 A217 F218 D235 R236 L247 D261 L276 A277 N278 Q279 L280 L281 K282 G283 I284 L285 D286 I287 G288 M297 T298 L299 F300 S301 P302 L303 L306 I307 L310 V314 L317 F321 P324 S327 E328 I334 M348 G358 V359 E360 K366
R370 L376 K381 T392 L395 I398 A399 I402 Q414 A415 V416 T417 M418 G419 T420 F424 Y425 S426 V427 T428 T429 S436 R454 K462 E463 E464 D465 I466 G467 E468 N469 R470 K471 H474 N475 L476 H477 G478 E479 I480 K483 D484 V485 S486 G493 Q494
E495 V496 V497 K498 R503 V504 A505 P506 K509 V510 A511 G514 K515 S516 G517 S518 G519 L523 I526 L530 P533 T534 K535 G536 D541 G542 Y543 N544 L545 N546 N549 Q555 G558 V559 D563 Q569 S570 I571 R572 E573 D581 T582 S583 M584 E585 D586
E589 A590 A591 K592 H597 E598 E599 T609 L610 V611 S612 E613 M614 Q622 R625 V633 H634 K635 P636 K637 L640 L641 D642 Q643 D649 E653 A654 K655 I656 D657 Q658 Y659 L660 S661 A662 M663 K664 C665 T666 R667 I670 R673 L686 E687 D688 G689 G695
S704 N713 TYR SER GLU GLU GLN LYS VAL PRO GLN SER ILE

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	34916	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 ($e^-/Å^2$)	39.883	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.421	Depositor
Minimum map value	-1.354	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.060	Depositor
Recommended contour level	0.529	Depositor
Map size (Å)	282.88, 282.88, 282.88	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.105, 1.105, 1.105	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.30	2/5765 (0.0%)	0.62	4/7804 (0.1%)
1	B	0.19	0/4473	0.54	2/6061 (0.0%)
All	All	0.26	2/10238 (0.0%)	0.58	6/13865 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	153	PRO	CG-CD	-15.30	0.98	1.50
1	A	153	PRO	N-CD	7.66	1.58	1.47

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	153	PRO	N-CD-CG	-19.05	74.62	103.20
1	A	153	PRO	CA-CB-CG	-11.89	81.90	104.50
1	A	153	PRO	CA-N-CD	-10.37	97.48	112.00
1	A	153	PRO	CB-CG-CD	7.98	131.65	106.10
1	B	348	MET	CB-CG-SD	5.08	127.93	112.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5651	0	5779	52	0
1	B	4396	0	4480	45	0
2	A	31	0	12	1	0
2	B	31	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	10111	0	10283	90	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 90 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:A:673:ARG:HD2	1:B:673:ARG:HD3	1.80	0.62
1:A:564:VAL:HG21	1:A:623:ARG:HD3	1.83	0.60
1:A:614:MET:SD	1:A:616:HIS:ND1	2.75	0.60
1:A:684:ILE:HD11	1:A:691:ILE:HD12	1.85	0.59
1:B:468:GLU:O	1:B:549:ASN:ND2	2.36	0.59

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	706/724 (98%)	629 (89%)	76 (11%)	1 (0%)	48 79
1	B	562/724 (78%)	525 (93%)	37 (7%)	0	100 100
All	All	1268/1448 (88%)	1154 (91%)	113 (9%)	1 (0%)	49 79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	472	ALA

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	617/641 (96%)	615 (100%)	2 (0%)	86 85
1	B	473/641 (74%)	471 (100%)	2 (0%)	84 83
All	All	1090/1282 (85%)	1086 (100%)	4 (0%)	81 83

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

Mol	Chain	Res	Type
1	A	15	ILE
1	A	317	LEU
1	B	186	VAL
1	B	563	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	182	ASN
1	B	475	ASN
1	B	203	GLN
1	B	595	GLN
1	B	369	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ATP	B	801	3	29,33,33	0.31	0	44,52,52	0.44	1 (2%)
2	ATP	A	801	3	29,33,33	0.29	0	44,52,52	0.45	1 (2%)

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
2	ATP	B	801	3	-	6/22/38/38	0/3/3/3
2	ATP	A	801	3	-	7/22/38/38	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	801	ATP	PB-O3B-PG	2.04	139.83	132.83
2	B	801	ATP	PB-O3B-PG	2.01	139.73	132.83

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	ATP	PB-O3B-PG-O3G

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Mol	Chain	Res	Type	Atoms
2	A	801	ATP	C2'-C1'-N9-C8
2	A	801	ATP	O4'-C4'-C5'-O5'
2	B	801	ATP	O4'-C4'-C5'-O5'
2	A	801	ATP	C3'-C4'-C5'-O5'

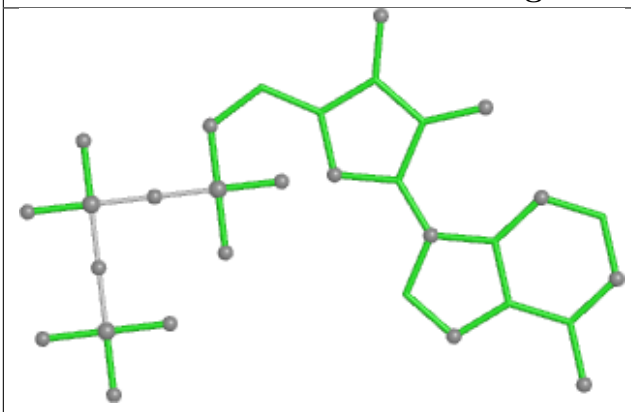
There are no ring outliers.

1 monomer is involved in 1 short contact:

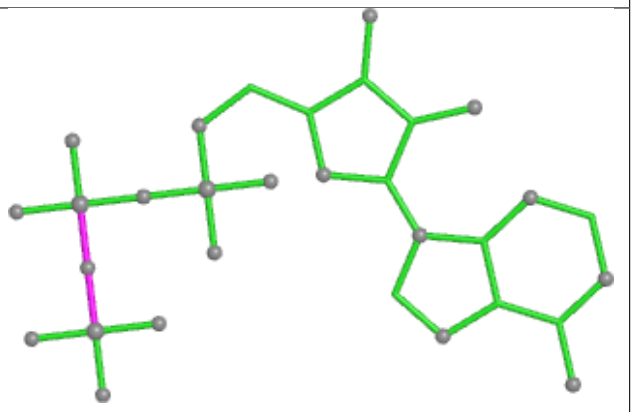
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	ATP	1	0

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

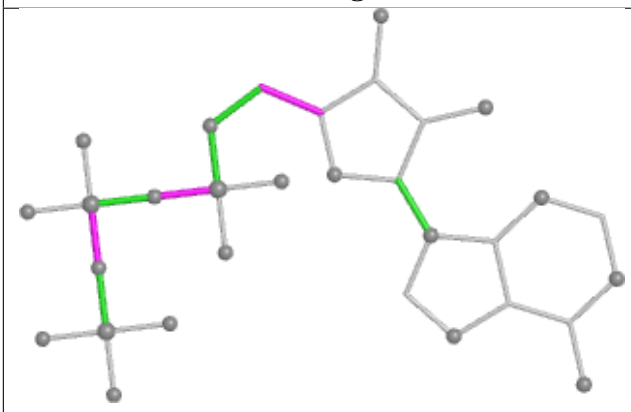
Ligand ATP B 801



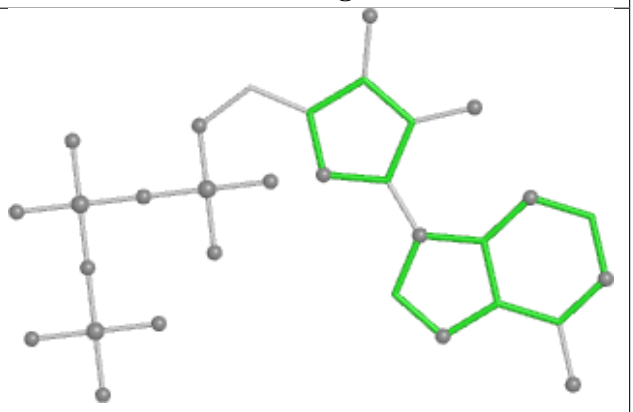
Bond lengths



Bond angles

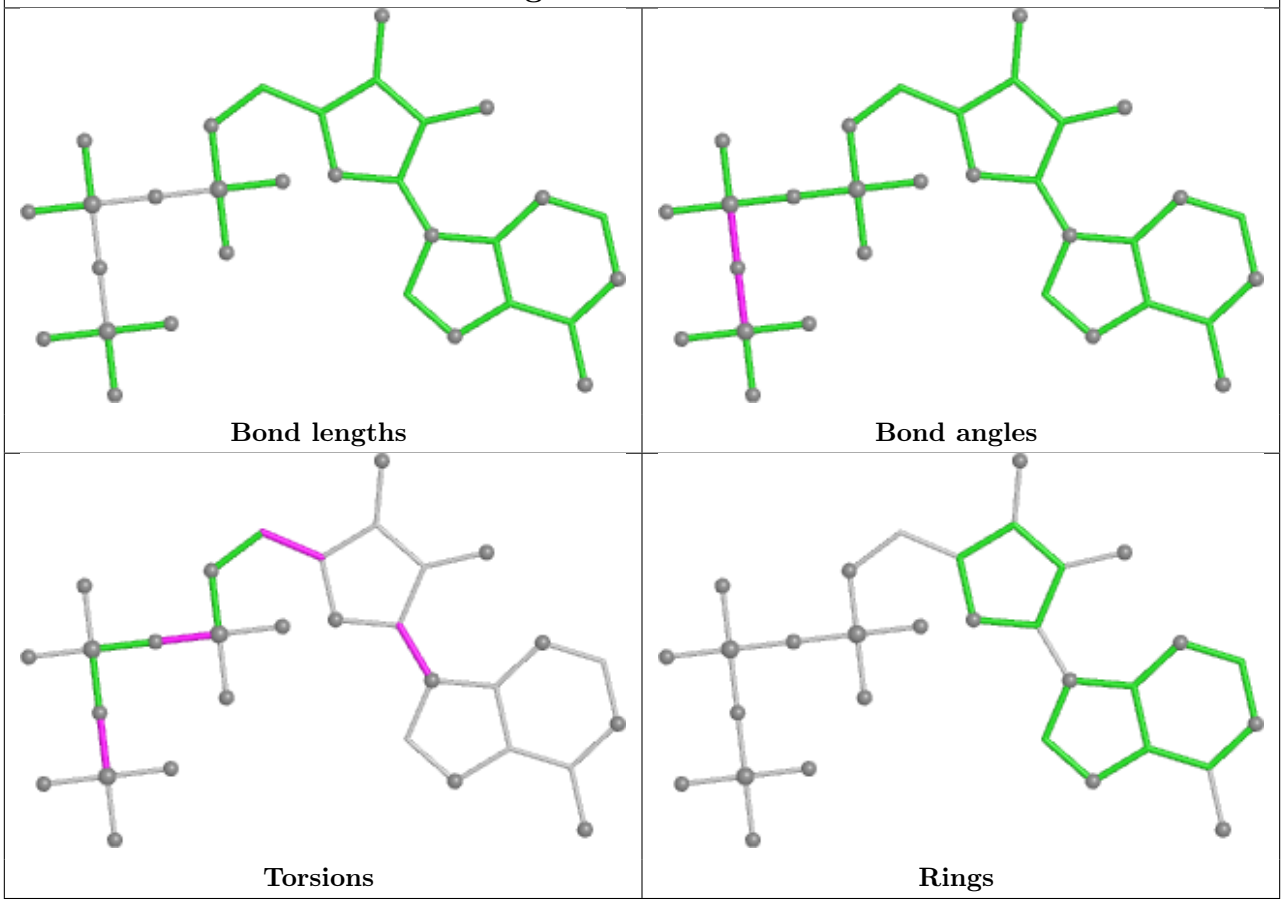


Torsions



Rings

Ligand ATP A 801



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.

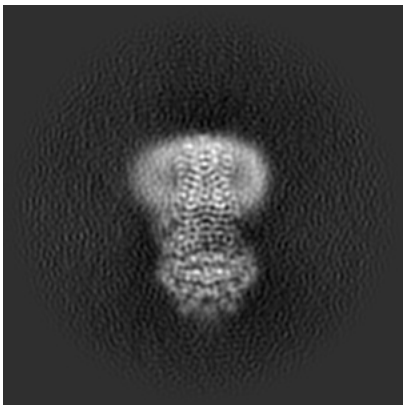
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-66741. These allow visual inspection of the internal detail of the map and identification of artifacts.

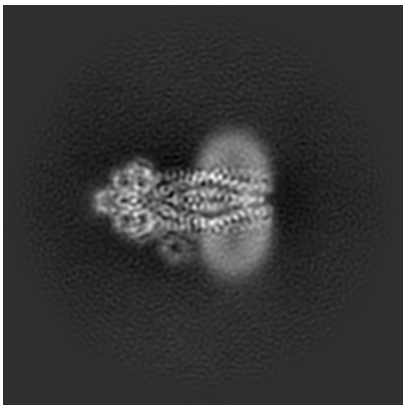
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

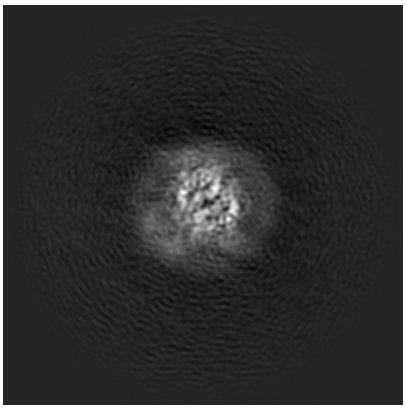
6.1.1 Primary map



X

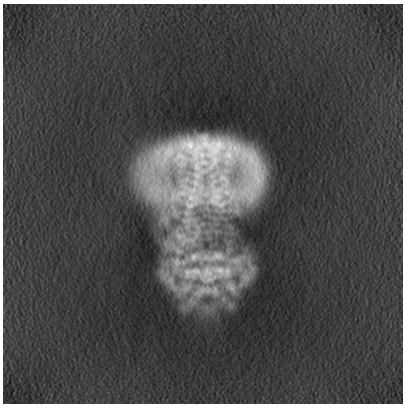


Y

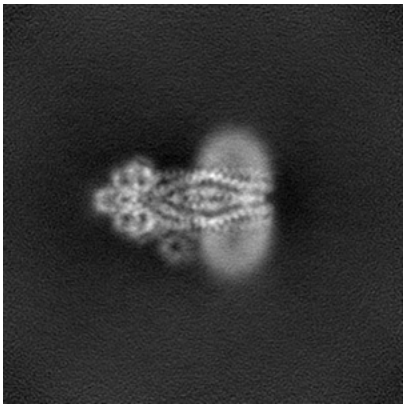


Z

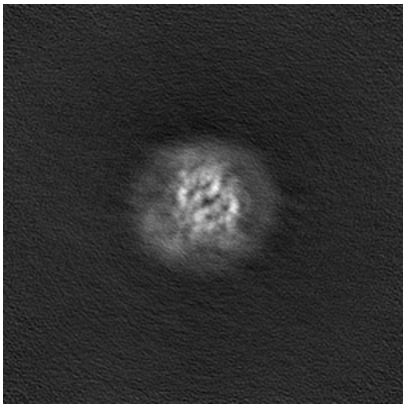
6.1.2 Raw map



X



Y

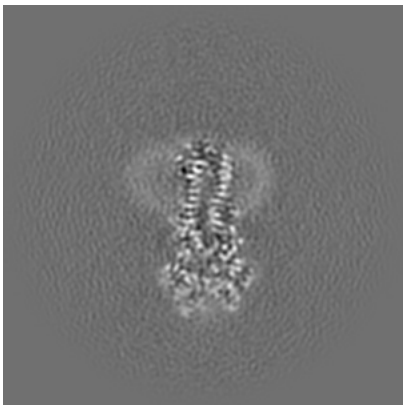


Z

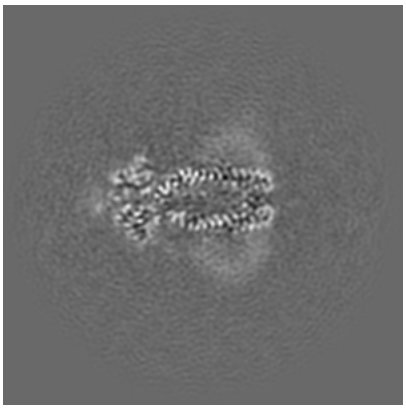
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

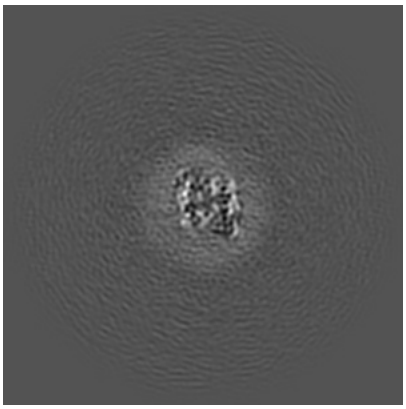
6.2.1 Primary map



X Index: 128

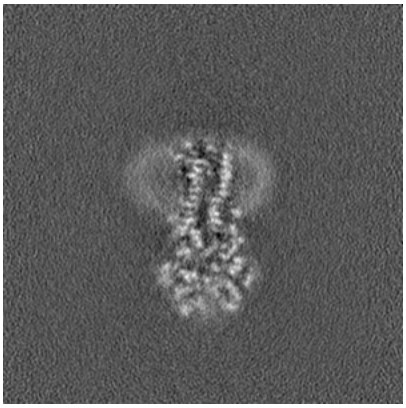


Y Index: 128

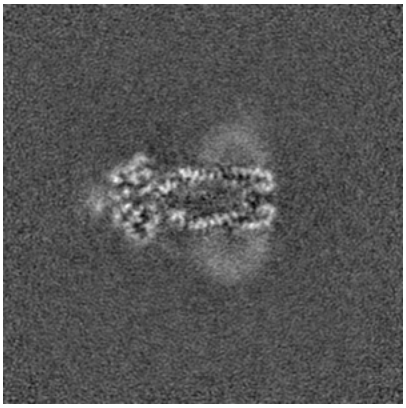


Z Index: 128

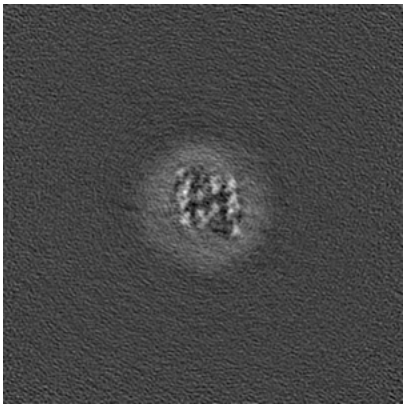
6.2.2 Raw map



X Index: 128



Y Index: 128

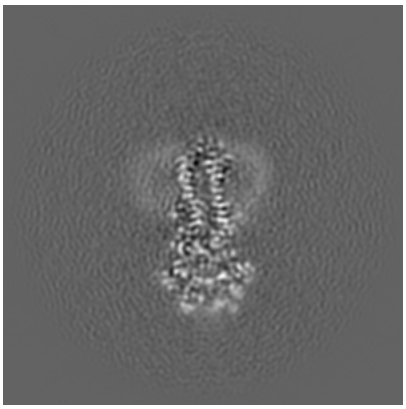


Z Index: 128

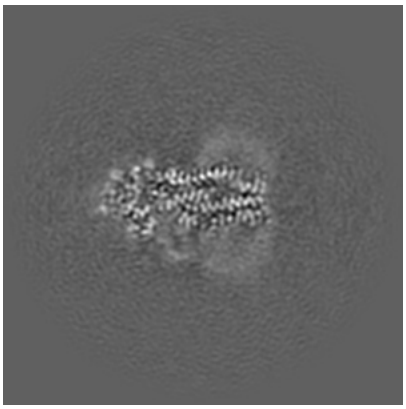
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

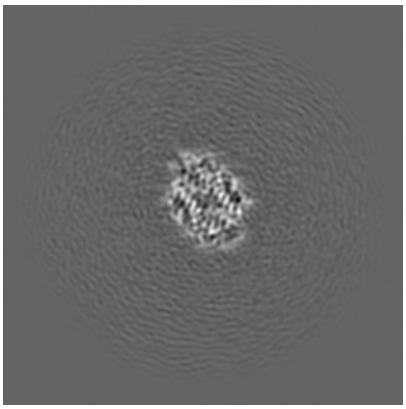
6.3.1 Primary map



X Index: 134

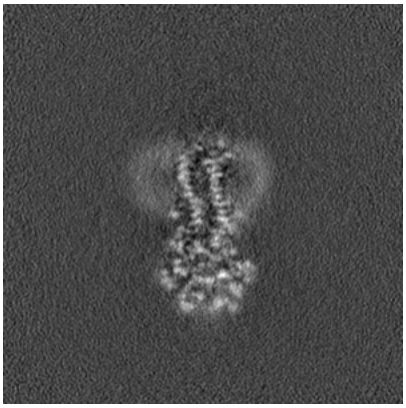


Y Index: 123

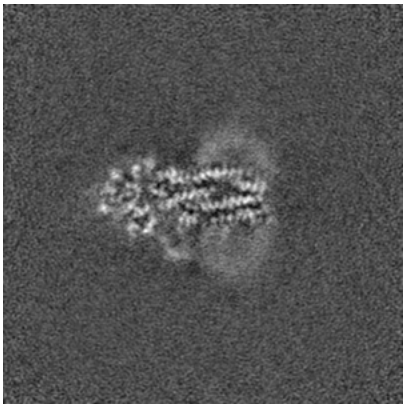


Z Index: 85

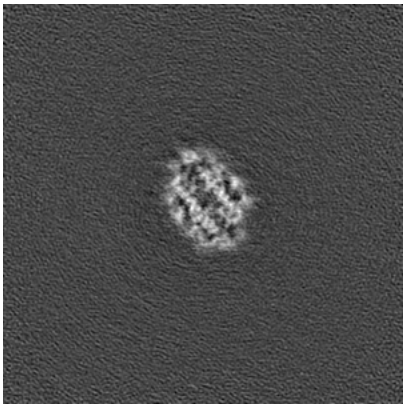
6.3.2 Raw map



X Index: 134



Y Index: 123

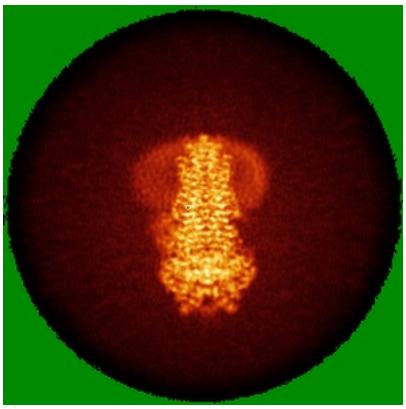


Z Index: 84

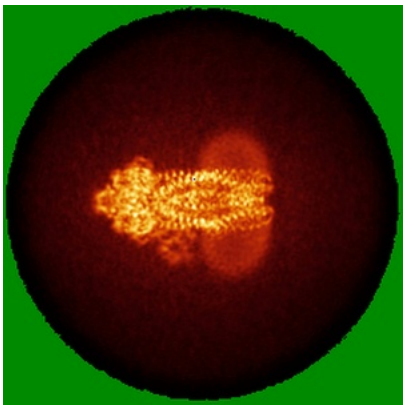
The images above show the largest variance slices of the map in three orthogonal directions.

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

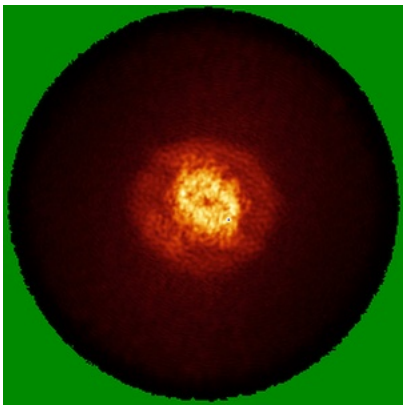
6.4.1 Primary map



X

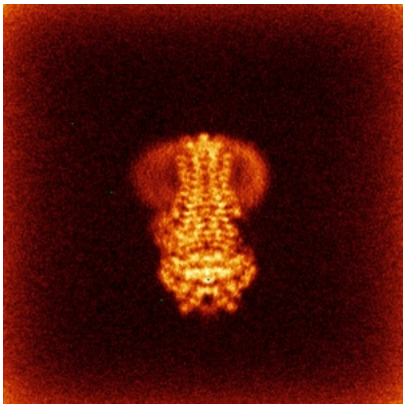


Y

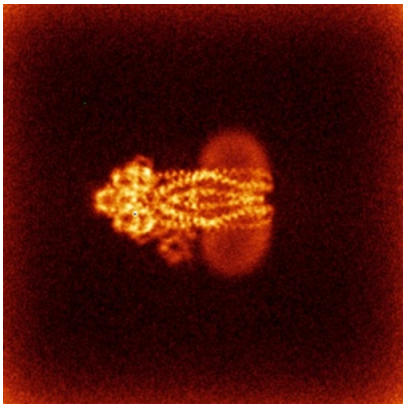


Z

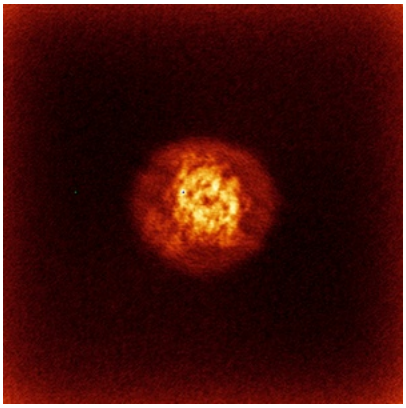
6.4.2 Raw map



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 0.529. 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.

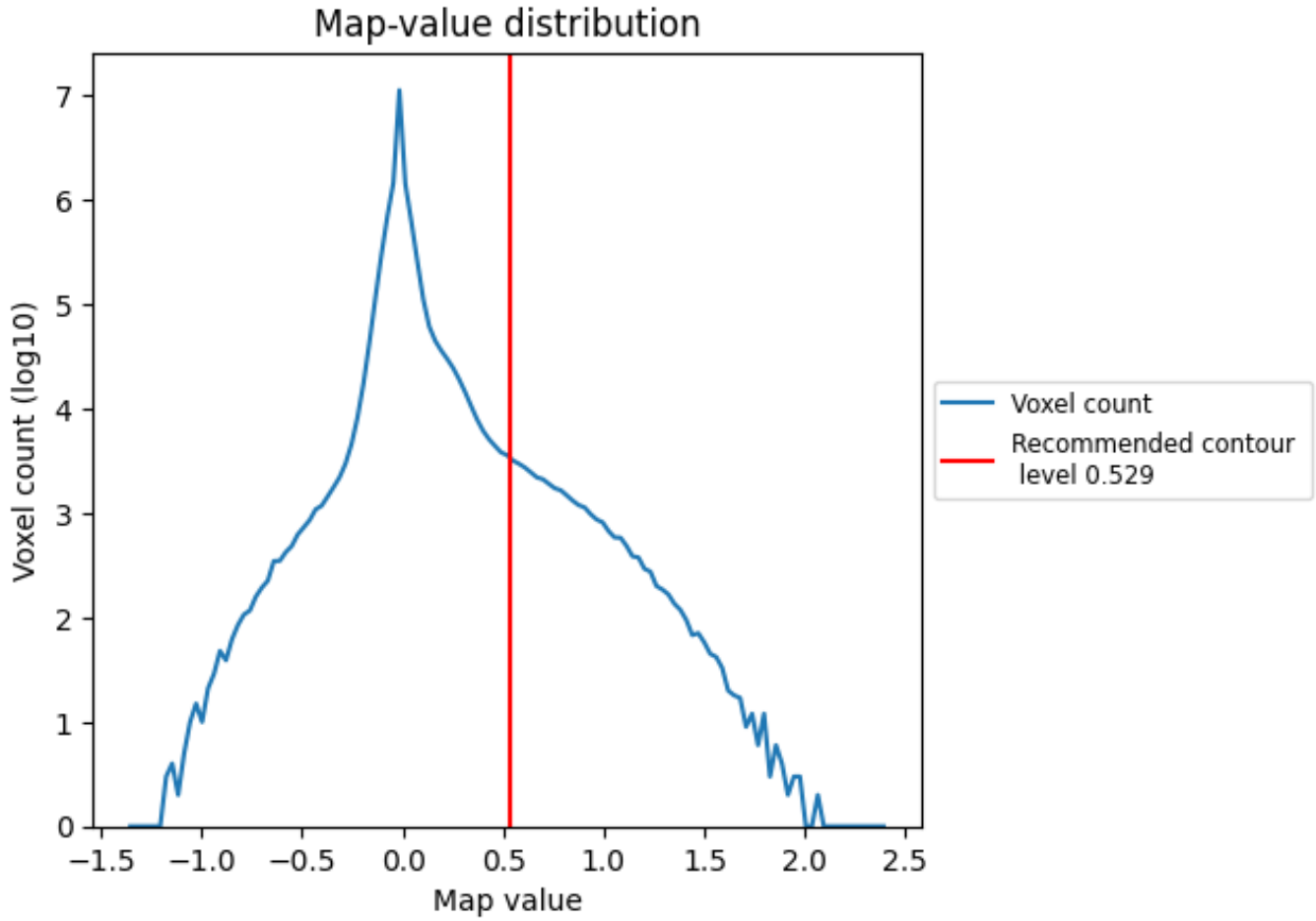
6.6 Mask visualisation (i)

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

7 Map analysis

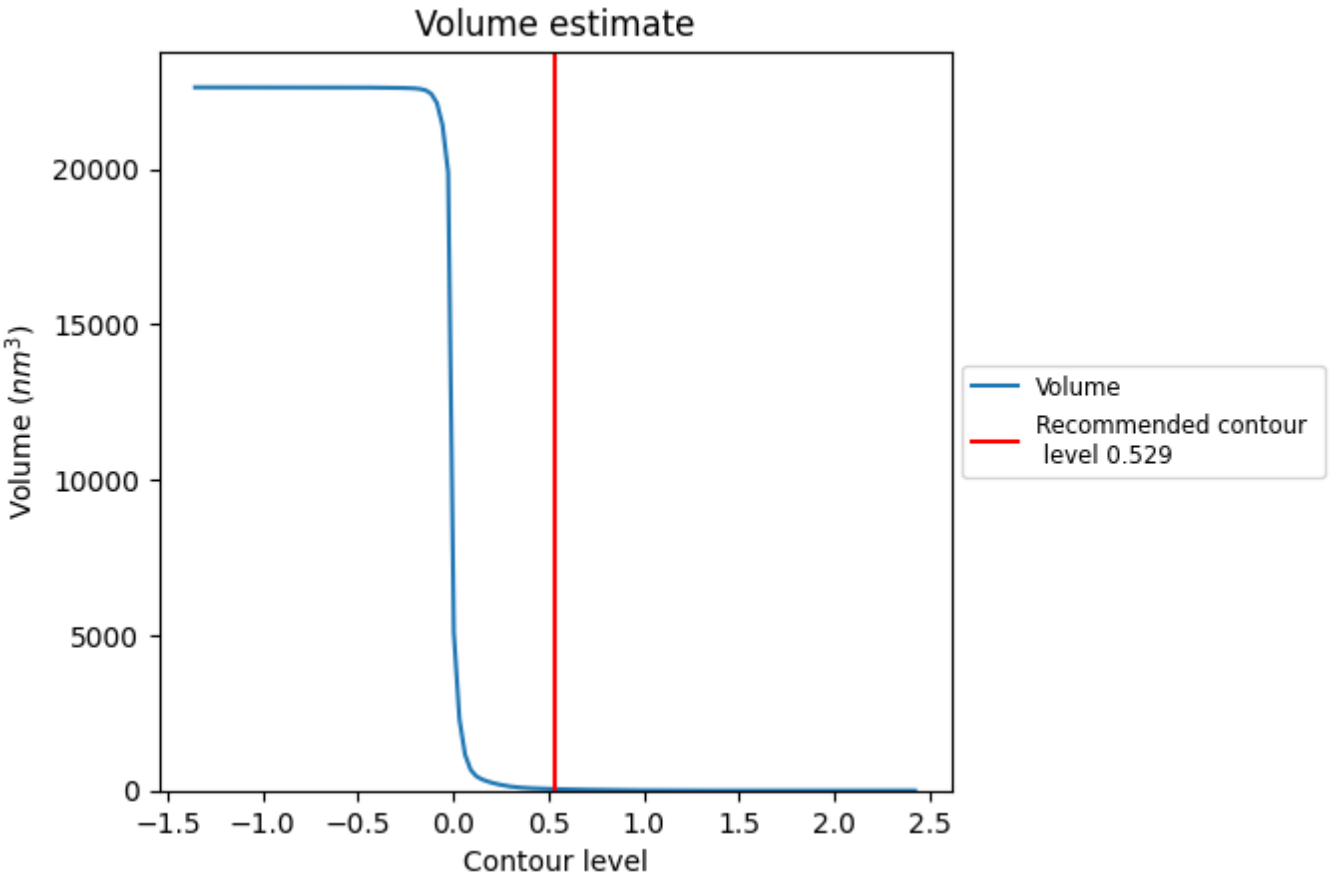
This section contains the results of statistical analysis of the map.

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.

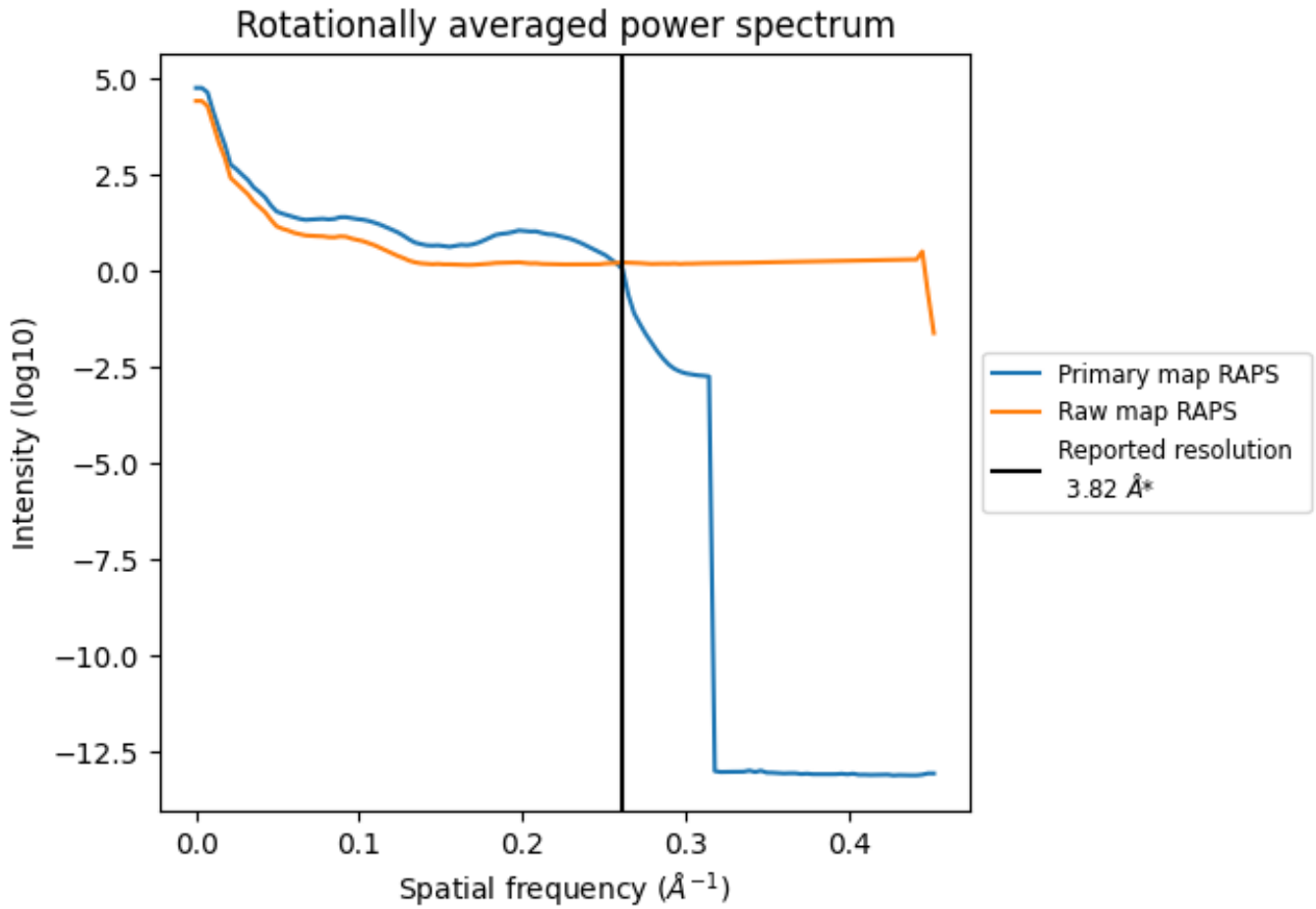
7.2 Volume estimate (i)



The volume at the recommended contour level is 49 nm^3; this corresponds to an approximate mass of 44 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)

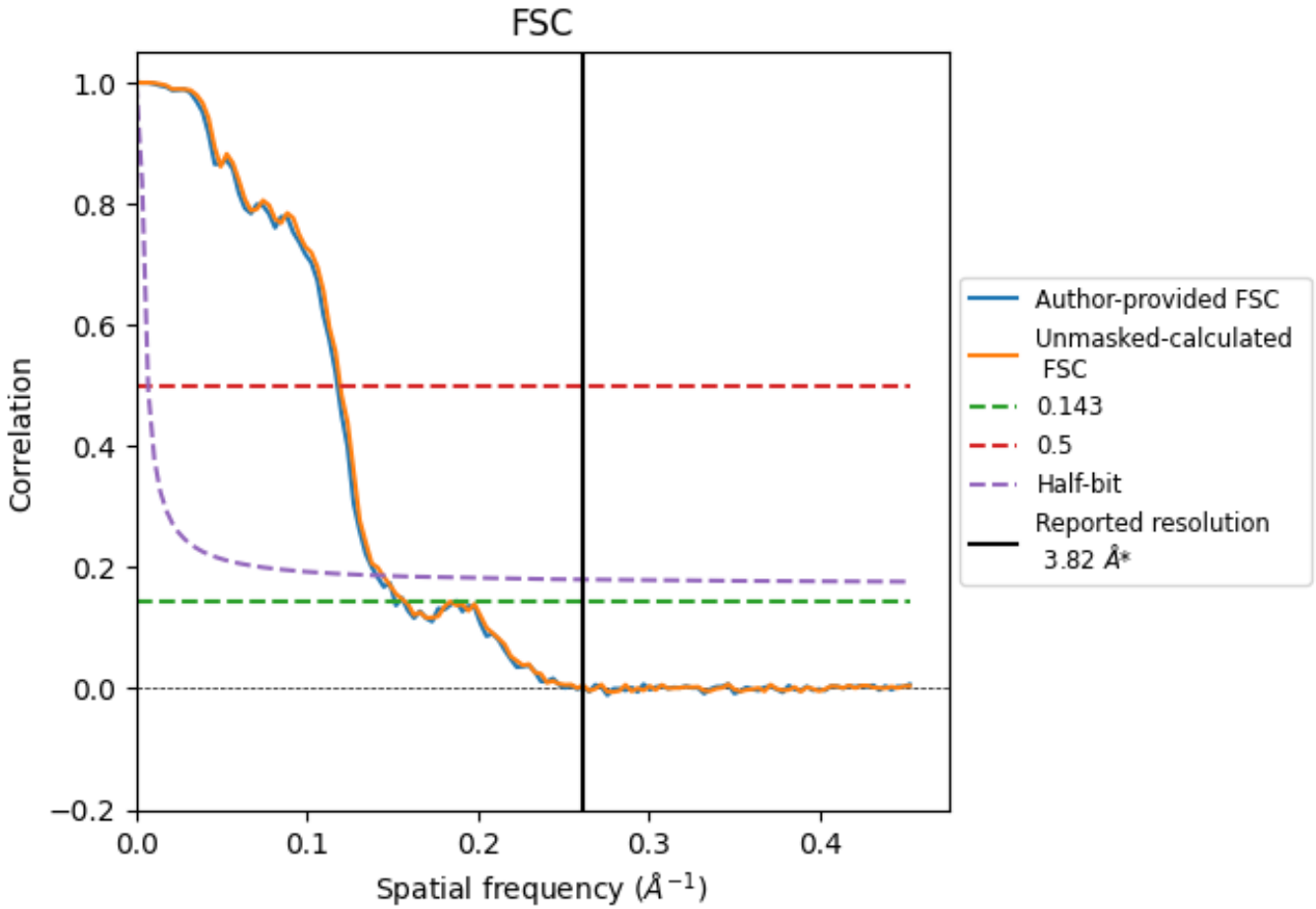


*Reported resolution corresponds to spatial frequency of 0.262 $Å^{-1}$

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 0.262 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.82	-	-
Author-provided FSC curve	6.61	8.50	7.10
Unmasked-calculated*	6.35	8.38	6.92

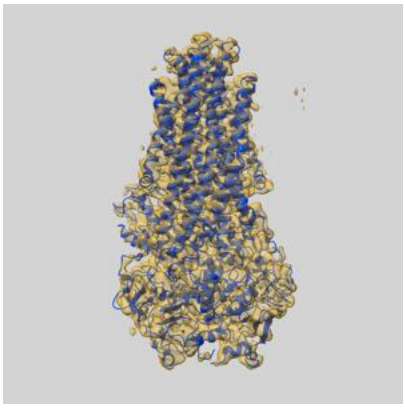
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 6.61 differs from the reported value 3.82 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.35 differs from the reported value 3.82 by more than 10 %

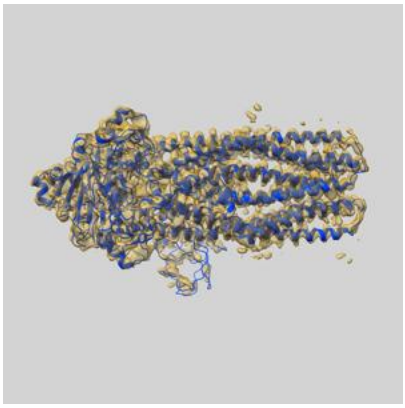
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-66741 and PDB model 9XCR. Per-residue inclusion information can be found in section 3 on page 5.

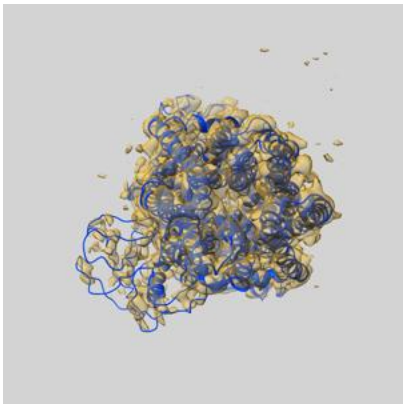
9.1 Map-model overlay



X



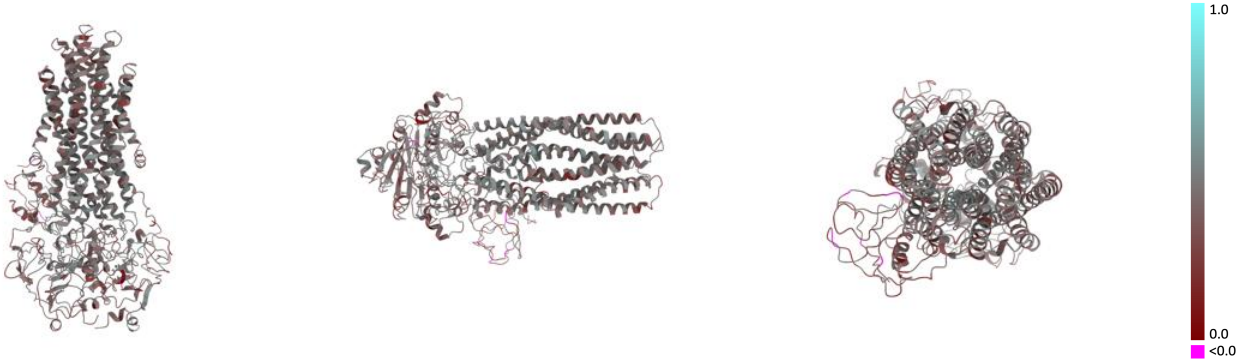
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.529 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.

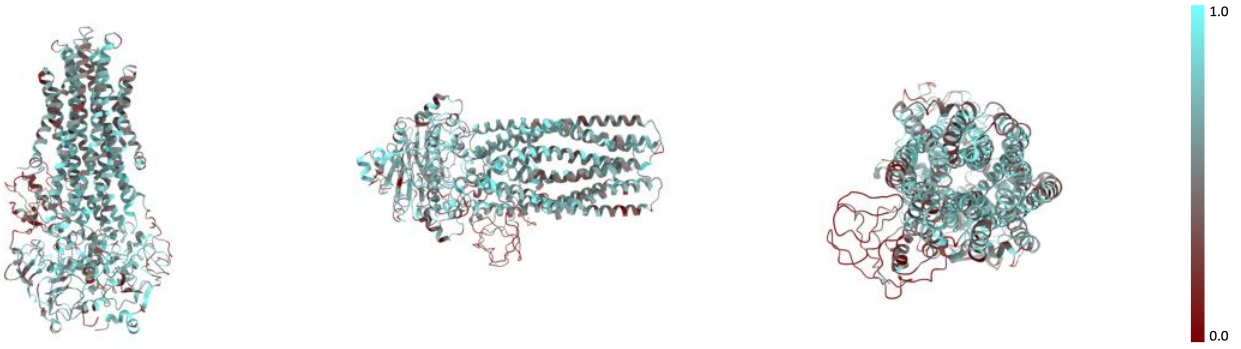
9.2 Q-score mapped to coordinate model



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.

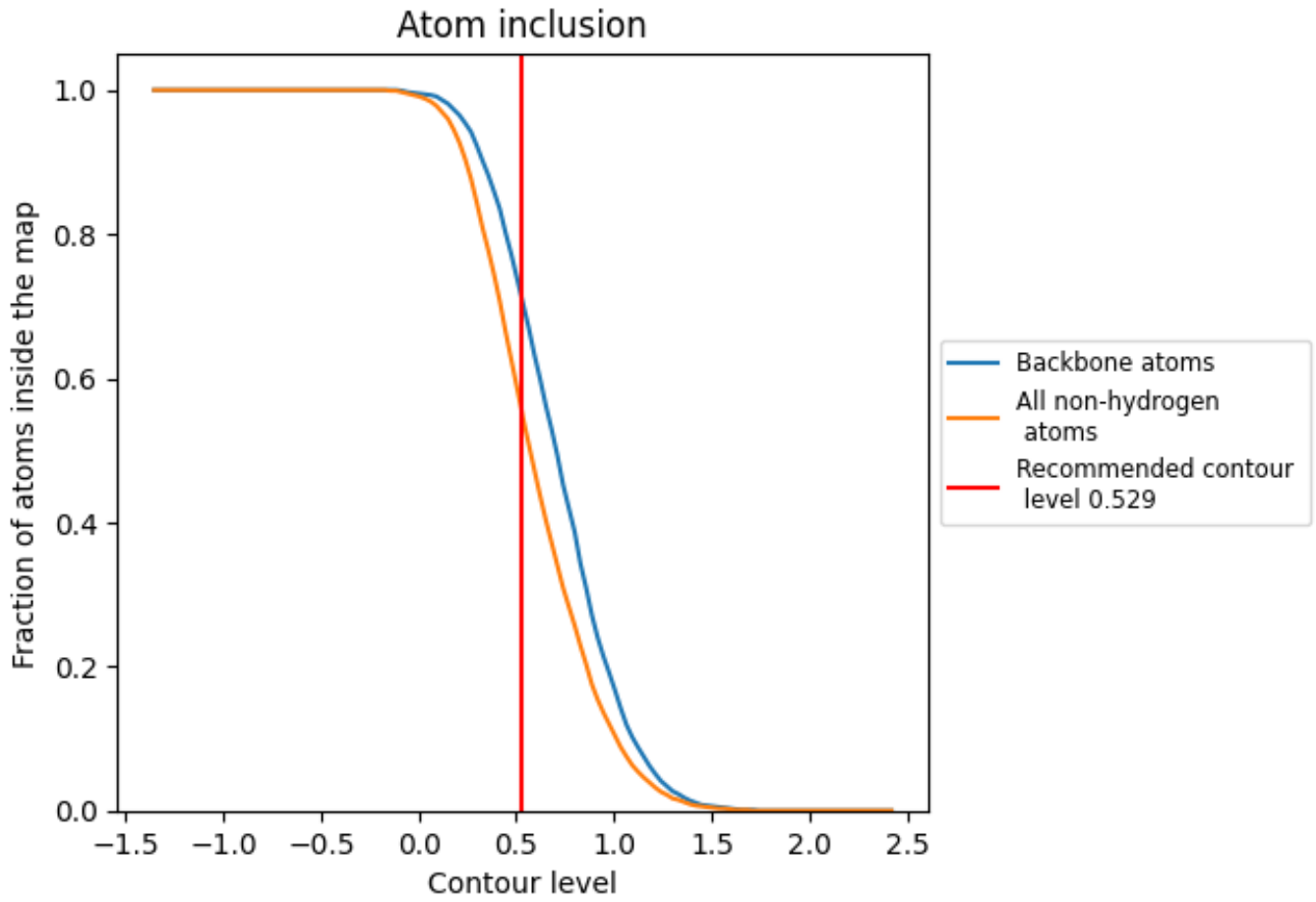
9.3 Atom inclusion mapped to coordinate model



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 (0.529).

9.4 Atom inclusion (i)



At the recommended contour level, 71% of all backbone atoms, 55% 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 (0.529) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.5530	0.4040
A	0.5090	0.3920
B	0.6080	0.4180