wwPDB EM Validation Summary Report (i)

Nov 9, 2026 – 02:13 PM JST

PDB ID	:	9XW2 / pdb_00009xw2
EMDB ID	:	EMD-67320
Title	:	Cryo-EM structure of PI3Kalpha E542K mutation in complex with RLY-2608
Authors	:	Liu, X.; Chen, Y.; Li, G.; Chen, A.; Zhou, Q.; Wang, M.-W.
Deposited on	:	2025-11-27
Resolution	:	2.89 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:

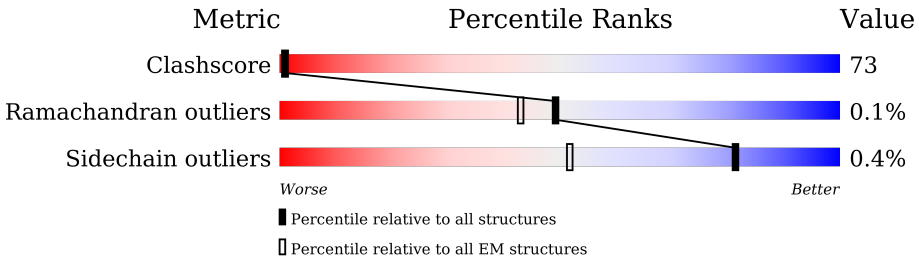
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using 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

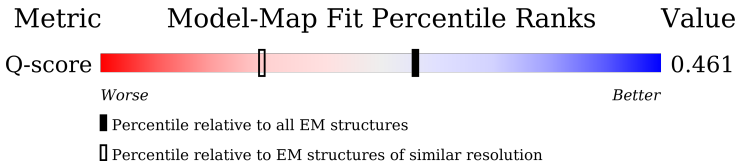
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.89 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	12148 (2.39 - 3.39)

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	1096	20% 22% 56% 22%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7057 atoms, of which 14 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 Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit alpha isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	859	Total	C	N	O	S	0	0
			7000	4478	1197	1264	61		

There are 29 discrepancies between the modelled and reference sequences:

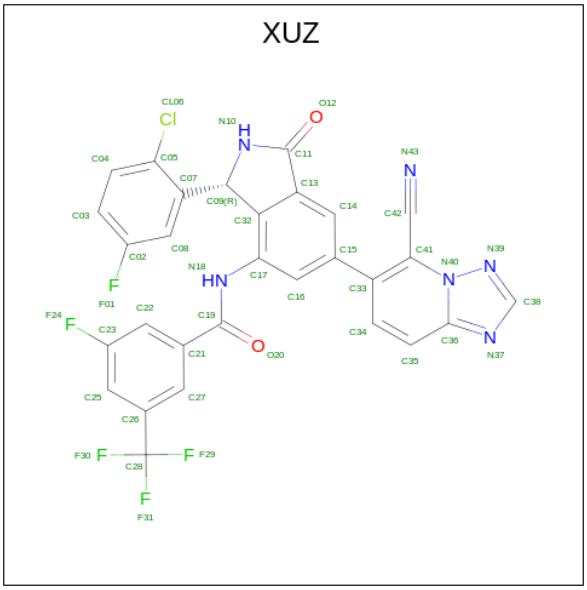
Chain	Residue	Modelled	Actual	Comment	Reference
B	-27	MET	-	initiating methionine	UNP P42336
B	-26	SER	-	expression tag	UNP P42336
B	-25	TYR	-	expression tag	UNP P42336
B	-24	TYR	-	expression tag	UNP P42336
B	-23	HIS	-	expression tag	UNP P42336
B	-22	HIS	-	expression tag	UNP P42336
B	-21	HIS	-	expression tag	UNP P42336
B	-20	HIS	-	expression tag	UNP P42336
B	-19	HIS	-	expression tag	UNP P42336
B	-18	HIS	-	expression tag	UNP P42336
B	-17	ASP	-	expression tag	UNP P42336
B	-16	TYR	-	expression tag	UNP P42336
B	-15	ASP	-	expression tag	UNP P42336
B	-14	ILE	-	expression tag	UNP P42336
B	-13	PRO	-	expression tag	UNP P42336
B	-12	THR	-	expression tag	UNP P42336
B	-11	THR	-	expression tag	UNP P42336
B	-10	GLU	-	expression tag	UNP P42336
B	-9	ASN	-	expression tag	UNP P42336
B	-8	LEU	-	expression tag	UNP P42336
B	-7	TYR	-	expression tag	UNP P42336
B	-6	PHE	-	expression tag	UNP P42336
B	-5	GLN	-	expression tag	UNP P42336
B	-4	GLY	-	expression tag	UNP P42336
B	-3	ALA	-	expression tag	UNP P42336
B	-2	MET	-	expression tag	UNP P42336
B	-1	GLY	-	expression tag	UNP P42336

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	SER	-	expression tag	UNP P42336
B	542	LYS	GLU	engineered mutation	UNP P42336

- Molecule 2 is N-{(3R,6M)-3-(2-chloro-5-fluorophenyl)-6-[(4S)-5-cyano[1,2,4]triazolo[1,5-a]pyridin-6-yl]-1-oxo-2,3-dihydro-1H-isoindol-4-yl}-3-fluoro-5-(trifluoromethyl)benzamide (CCD ID: XUZ) (formula: $C_{29}H_{14}ClF_5N_6O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							AltConf
			Total	C	Cl	F	H	N	O	
2	B	1	57	29	1	5	14	6	2	0

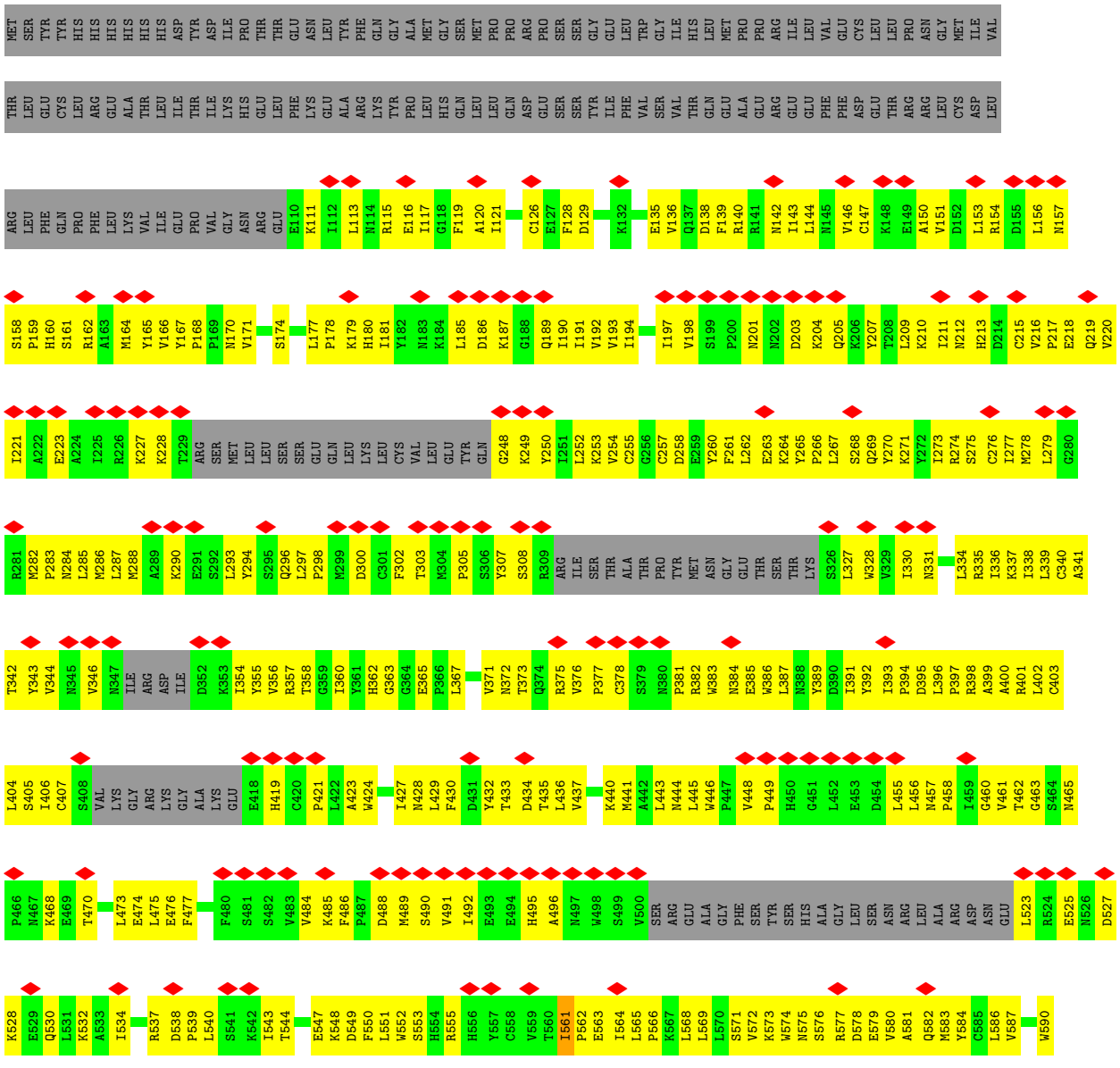
3 Residue-property plots (i)

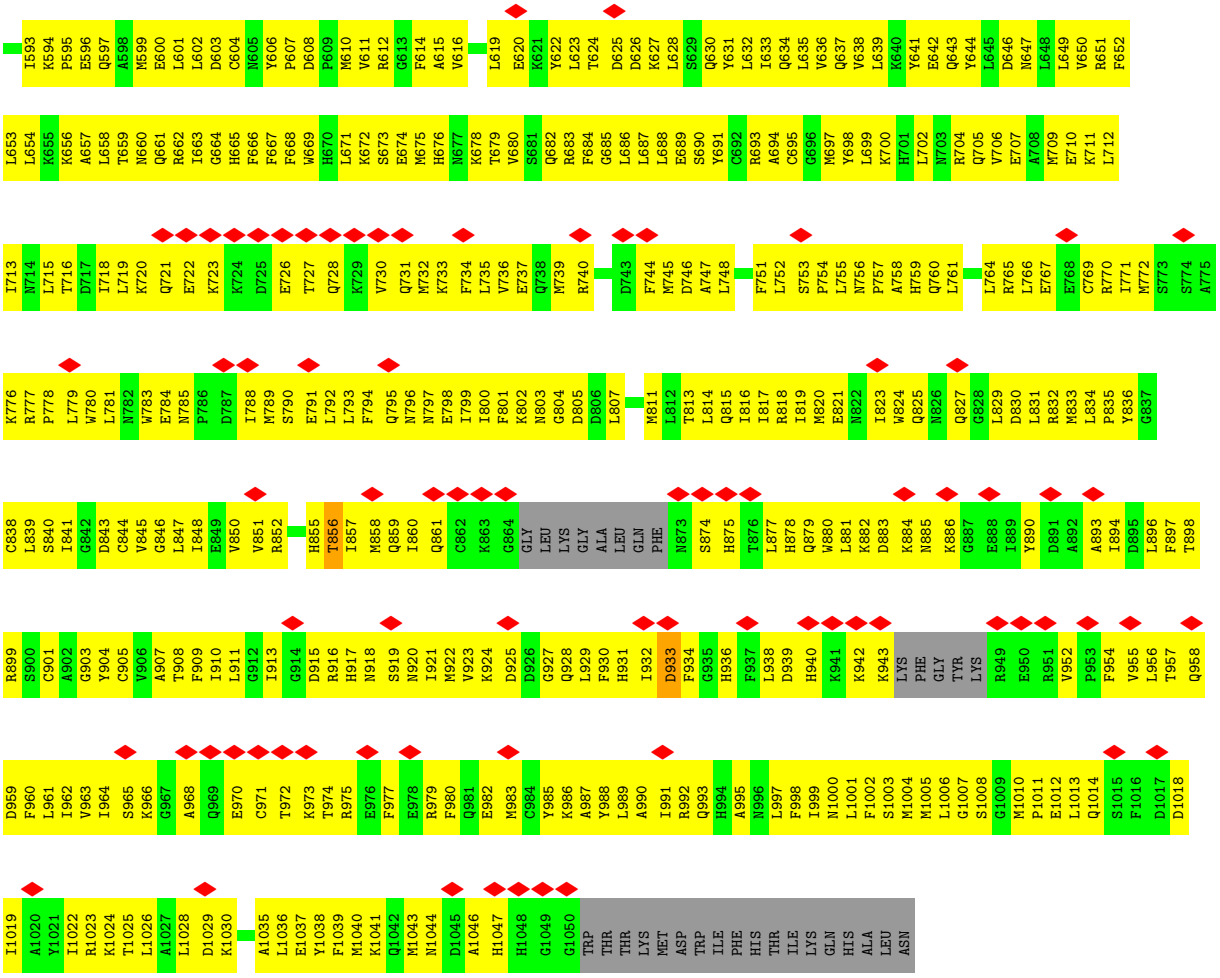
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit alpha isoform

Chain B:






I593 K594 P595 E596 Q597 A598 M599 E600 L601 L602 D603 C604 N605 Y606 P607 D608 P609 M610 V611 R612 G613 F614 A615 V616 L619 E620 K621 Y622 L623 T624 D625 D626 K627 L628 S629 Q630 Y631 L632 I633 Q634 L635 V636 Q637 V638 L639 K640 Y641 E642 Q643 Y644 L645 D646 N647 L648 L649 V650 R651 F652
L653 L654 K655 K656 A657 L658 T659 N660 Q661 R662 I663 G664 H665 F666 F667 F668 W669 H670 L671 K672 S673 E674 M675 H676 N677 K678 T679 V680 S681 Q682 R683 F684 G685 L686 L687 L688 E689 S690 Y691 C692 R693 A694 C695 G696 M697 Y698 L699 K700 H701 L702 N703 R704 Q705 V706 E707 A708 M709 E710 K711 L712
I713 N714 L715 T716 D717 I718 L719 K720 Q721 E722 K723 K724 D725 E726 T727 Q728 K729 V730 Q731 M732 K733 F734 L735 V736 E737 Q738 M739 R740 D743 F744 M745 D746 A747 L748 F751 L752 S753 P754 L755 N756 P757 A758 H759 Q760 L761 L764 R765 L766 E767 E768 C769 R770 I771 M772 S773 S774 A775
K776 R777 P778 L779 W780 L781 N782 W783 E784 N785 P786 D787 I788 M789 S790 E791 L792 L793 F794 Q795 N796 N797 E798 I799 I800 F801 K802 N803 G804 D805 D806 L807 H811 L812 T813 L814 Q815 I816 I817 R818 I819 M820 E821 N822 I823 W824 Q825 N826 Q827 G828 L829 D830 L831 R832 M833 L834 P835 Y836 G837
C838 L839 S840 I841 G842 D843 C844 V845 G846 L847 I848 E849 V850 V851 R852 H855 T856 I857 M858 Q859 I860 Q861 C862 K863 G864 GLY LEU LYS GLY ALA LEU GLN PHE N873 S874 H875 T876 L877 H878 Q879 W880 L881 K882 D883 K884 N885 K886 G887 E888 I889 Y890 D891 A892 A893 I894 D895 L896 F897 T898
R899 S900 C901 A902 G903 Y904 C905 V906 A907 T908 F909 I910 L911 G912 I913 G914 D915 R916 H917 N918 S919 N920 I921 M922 V923 K924 D925 D926 G927 Q928 L929 F930 H931 I932 D933 F934 G935 H936 F937 L938 D939 H940 K941 K942 K943 LYS PHE GLY TYR LYS R949 E950 R951 V952 P953 F954 V955 L956 T957 Q958
D959 F960 L961 I962 V963 I964 S965 K966 G967 A968 Q969 E970 C971 T972 K973 T974 R975 E976 F977 E978 R979 F980 Q981 E982 M983 C984 Y985 K986 A987 Y988 L989 A990 I991 R992 Q993 H994 A995 N996 L997 F998 I999 N1000 L1001 F1002 S1003 M1004 M1005 L1006 G1007 S1008 G1009 M1010 P1011 E1012 L1013 Q1014 S1015 F1016 D1017 D1018
I1019 A1020 Y1021 I1022 R1023 K1024 T1025 L1026 A1027 L1028 D1029 K1030 A1035 L1036 E1037 Y1038 F1039 M1040 K1041 Q1042 M1043 N1044 D1045 A1046 H1047 H1048 G1049 G1050 TRP THR THR LYS MET ASP TRP ILE PHE HIS THR ILE LYS GLN HIS ALA LEU ASN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	5674855	Depositor
Resolution determination method	FSC 1/2 BIT CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	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	1.335	Depositor
Minimum map value	-0.886	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.164	Depositor
Map size (Å)	210.944, 210.944, 210.944	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.824, 0.824, 0.824	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.11	0/7156	0.27	2/9669 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	561	ILE	CA-C-N	-6.80	112.77	119.64
1	B	561	ILE	C-N-CA	-6.80	112.77	119.64

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	7000	0	6978	1029	0
2	B	43	14	0	5	0
All	All	7043	14	6978	1029	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 73.

The worst 5 of 1029 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:705:GLN:NE2	1:B:752:LEU:O	1.56	1.38
1:B:680:VAL:HG13	1:B:683:ARG:CG	1.58	1.31
1:B:427:ILE:HG12	1:B:443:LEU:CD1	1.65	1.25
1:B:427:ILE:CG1	1:B:443:LEU:CD1	2.16	1.24
1:B:382:ARG:HH22	1:B:384:ASN:ND2	1.36	1.23

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	843/1096 (77%)	812 (96%)	30 (4%)	1 (0%)	48 77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	933	ASP

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	782/999 (78%)	779 (100%)	3 (0%)	84 94

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	563	GLU
1	B	564	ILE
1	B	856	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	853	ASN
1	B	920	ASN
1	B	1014	GLN
1	B	969	GLN
1	B	885	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)

1 ligand is 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	$\#\|Z\| > 2$
2	XUZ	B	1101	-	46,48,48	2.76	10 (21%)	61,73,73	1.98	14 (22%)

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	XUZ	B	1101	-	-	4/22/36/36	0/6/6/6

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1101	XUZ	C11-N10	12.05	1.44	1.35
2	B	1101	XUZ	C15-C33	-6.58	1.39	1.48
2	B	1101	XUZ	C36-N40	-6.48	1.30	1.39
2	B	1101	XUZ	C42-C41	6.20	1.53	1.43
2	B	1101	XUZ	C19-N18	4.02	1.46	1.35

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1101	XUZ	C38-N39-N40	7.10	107.46	100.84
2	B	1101	XUZ	F29-C28-C26	-5.58	100.68	112.93
2	B	1101	XUZ	N39-C38-N37	-4.99	107.94	116.74
2	B	1101	XUZ	C36-N40-N39	-4.37	107.18	112.25
2	B	1101	XUZ	C25-C26-C28	4.35	125.46	119.58

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1101	XUZ	C08-C07-C09-N10
2	B	1101	XUZ	C16-C17-N18-C19
2	B	1101	XUZ	C32-C17-N18-C19
2	B	1101	XUZ	C05-C07-C09-N10

There are no ring outliers.

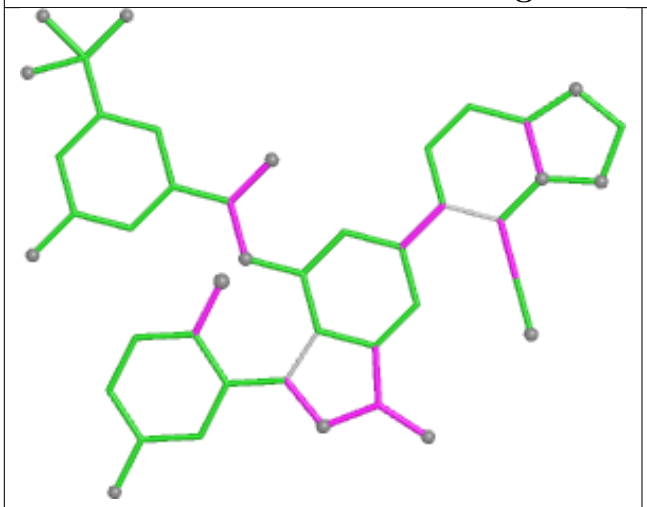
1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1101	XUZ	5	0

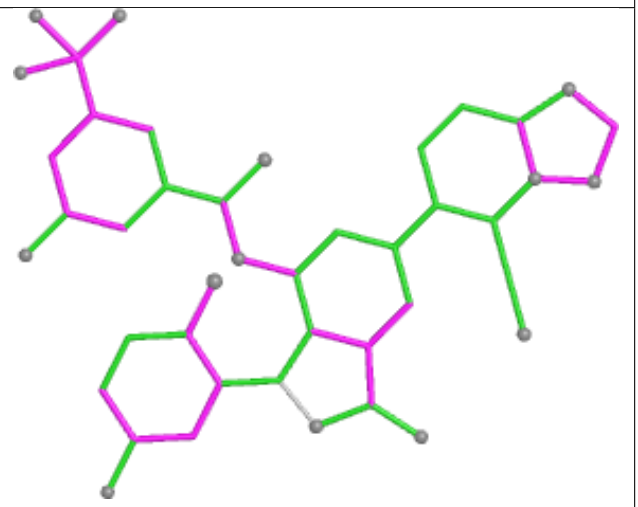
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

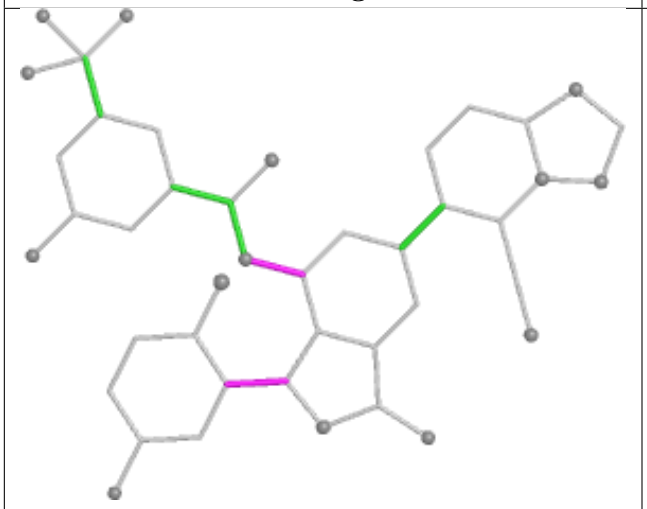
Ligand XUZ B 1101



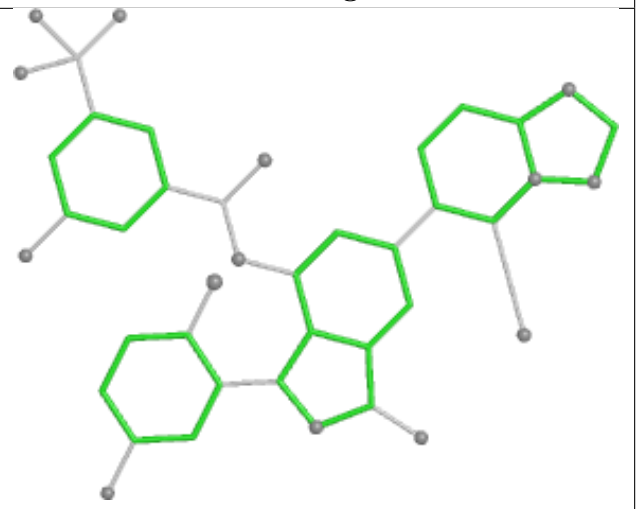
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

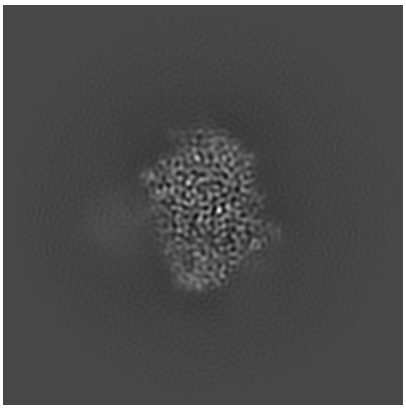
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-67320. These allow visual inspection of the internal detail of the map and identification of artifacts.

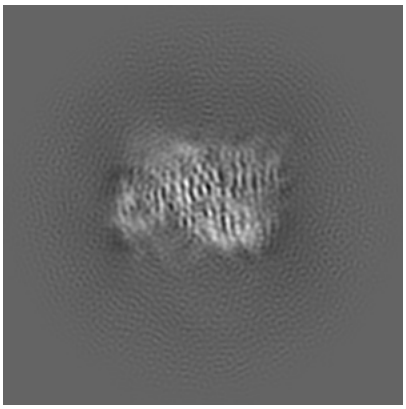
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

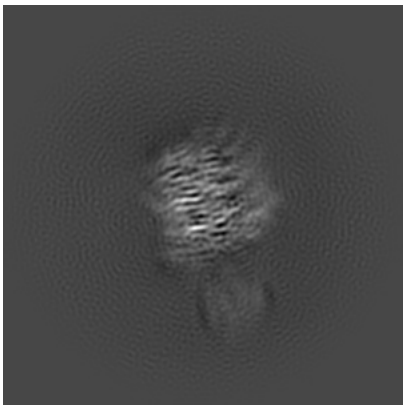
6.1.1 Primary map



X

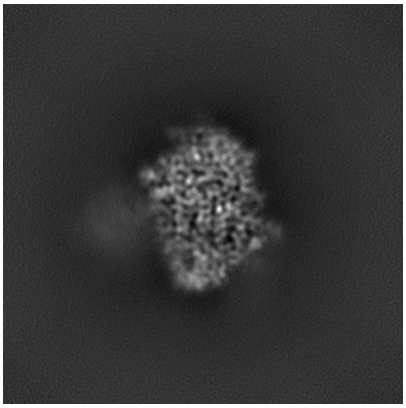


Y

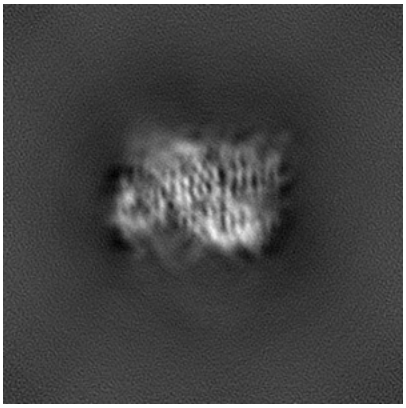


Z

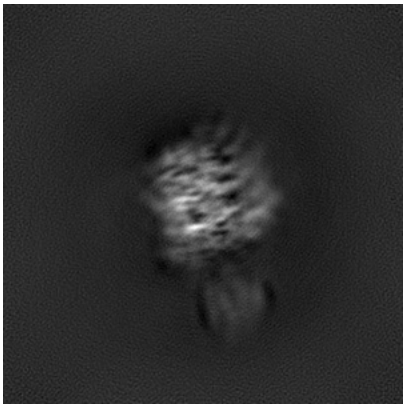
6.1.2 Raw map



X



Y

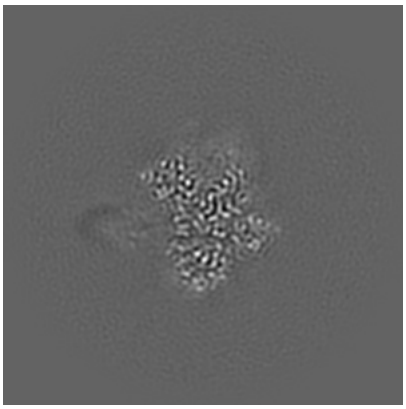


Z

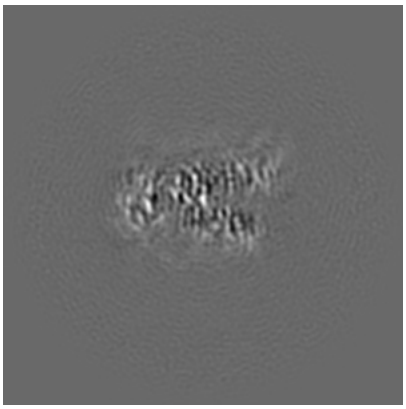
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

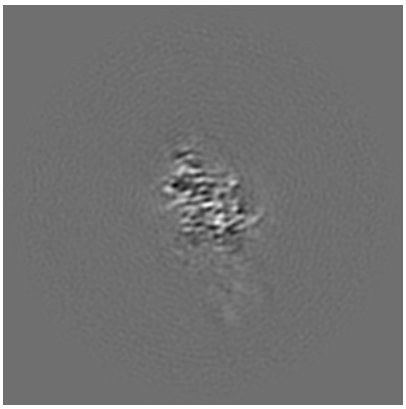
6.2.1 Primary map



X Index: 128

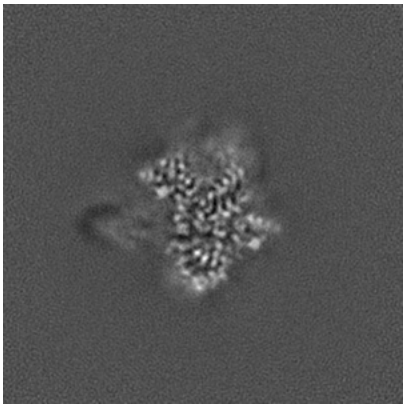


Y Index: 128

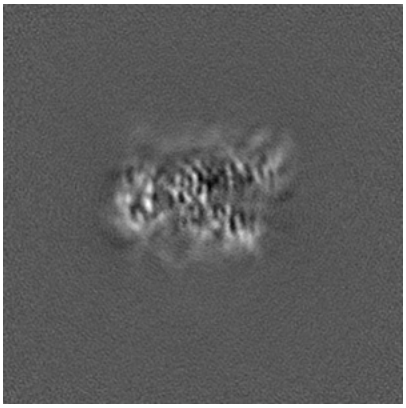


Z Index: 128

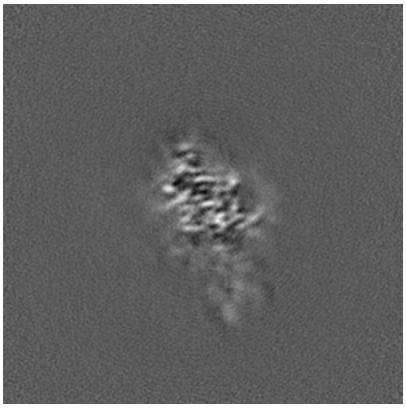
6.2.2 Raw map



X Index: 128



Y Index: 128

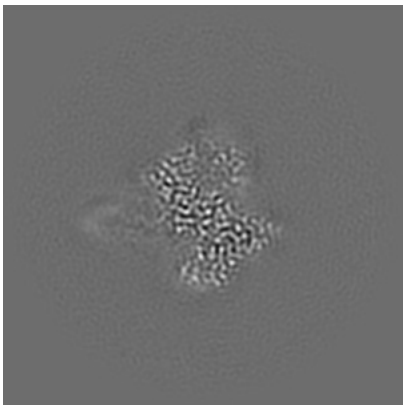


Z Index: 128

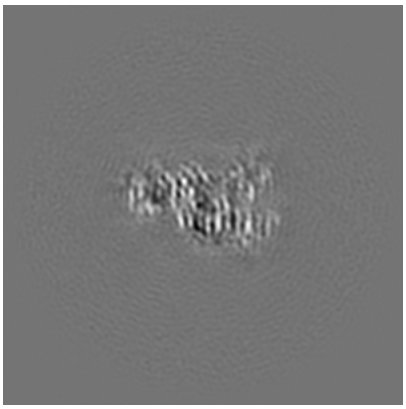
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

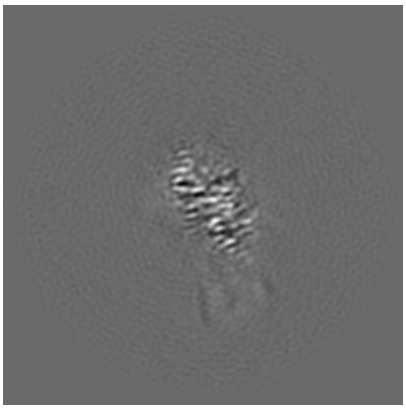
6.3.1 Primary map



X Index: 134

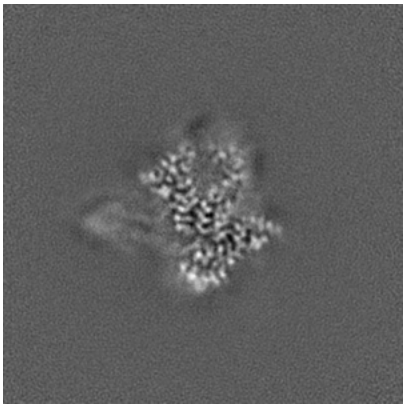


Y Index: 141

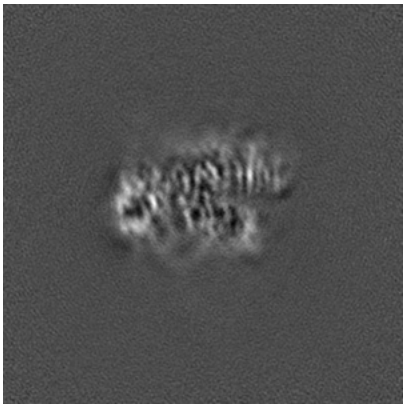


Z Index: 123

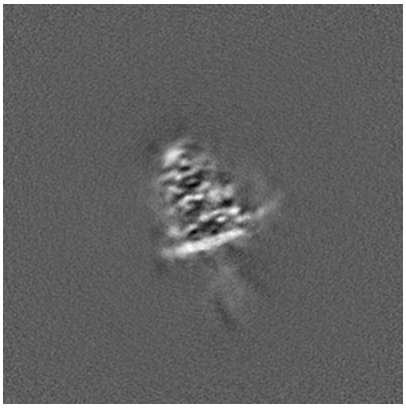
6.3.2 Raw map



X Index: 132



Y Index: 124

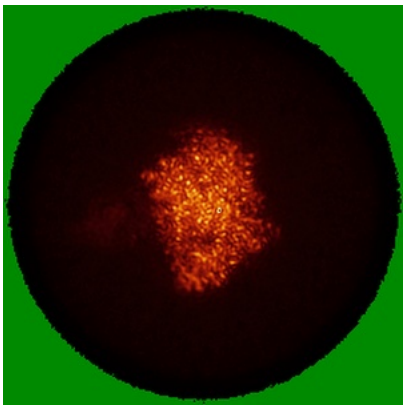


Z Index: 135

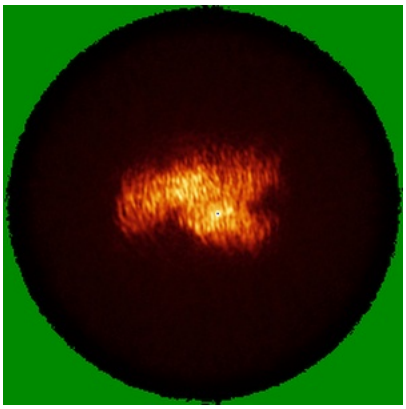
The images above show the largest variance slices of the map in three orthogonal directions.

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

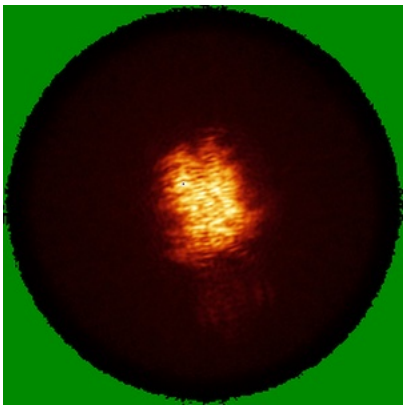
6.4.1 Primary map



X

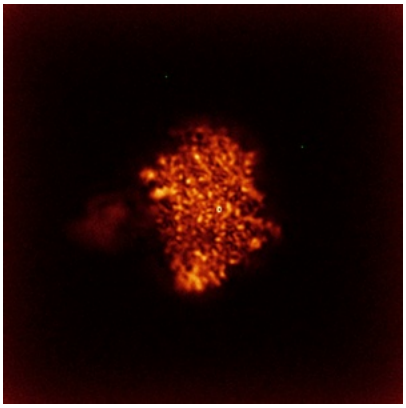


Y

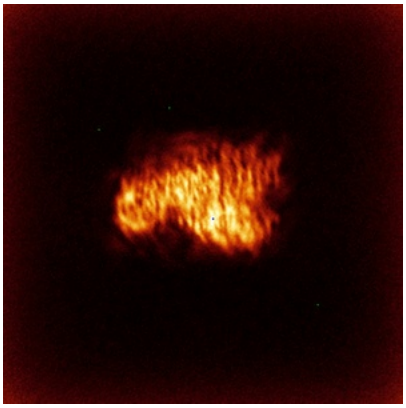


Z

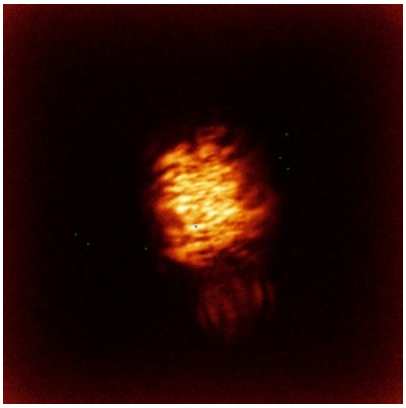
6.4.2 Raw map



X



Y

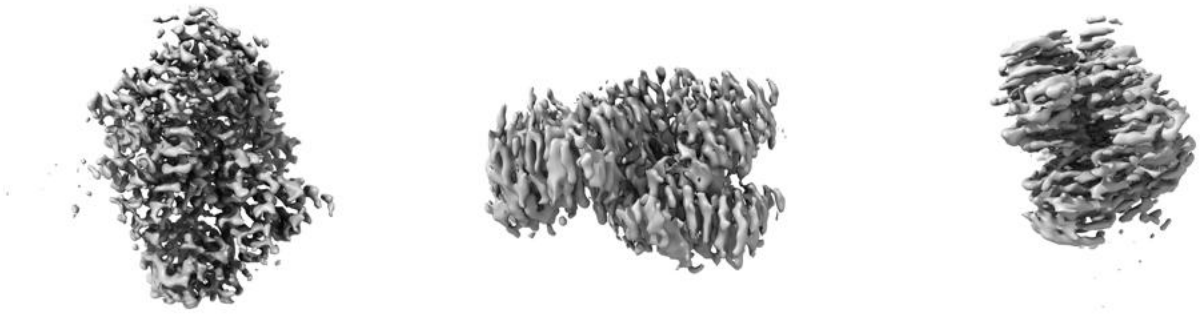


Z

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 0.164. 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.

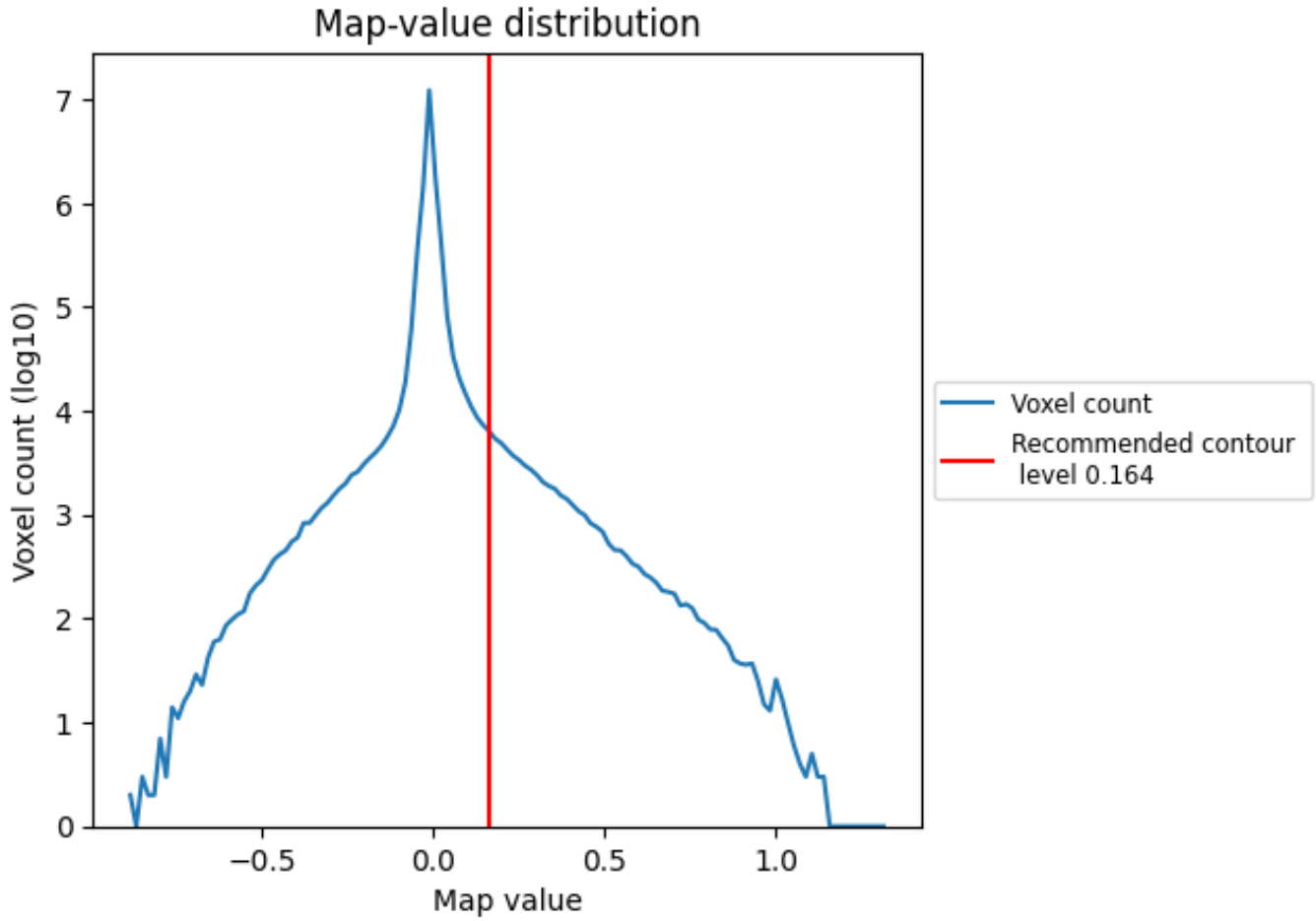
6.6 Mask visualisation (i)

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

7 Map analysis

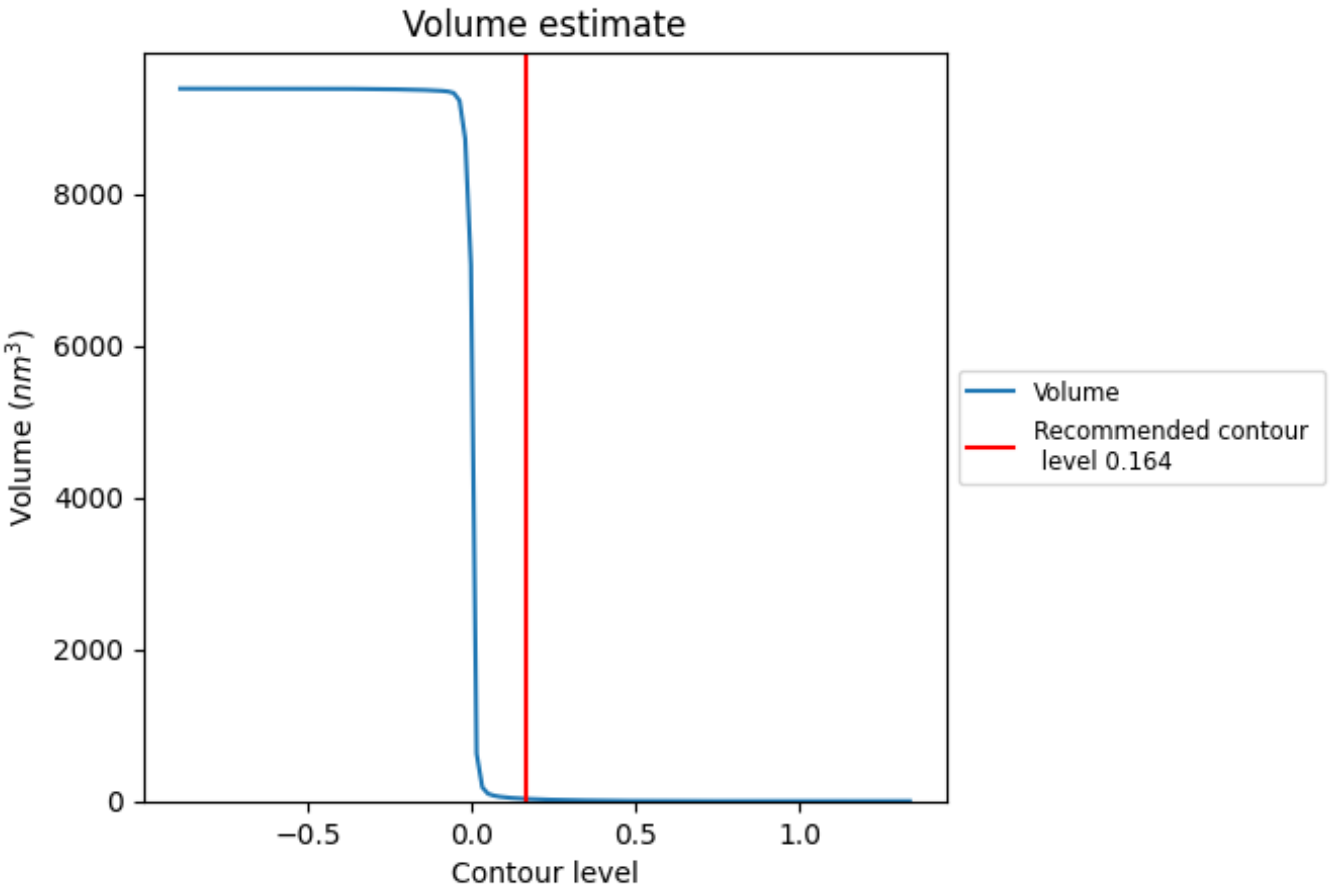
This section contains the results of statistical analysis of the map.

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.

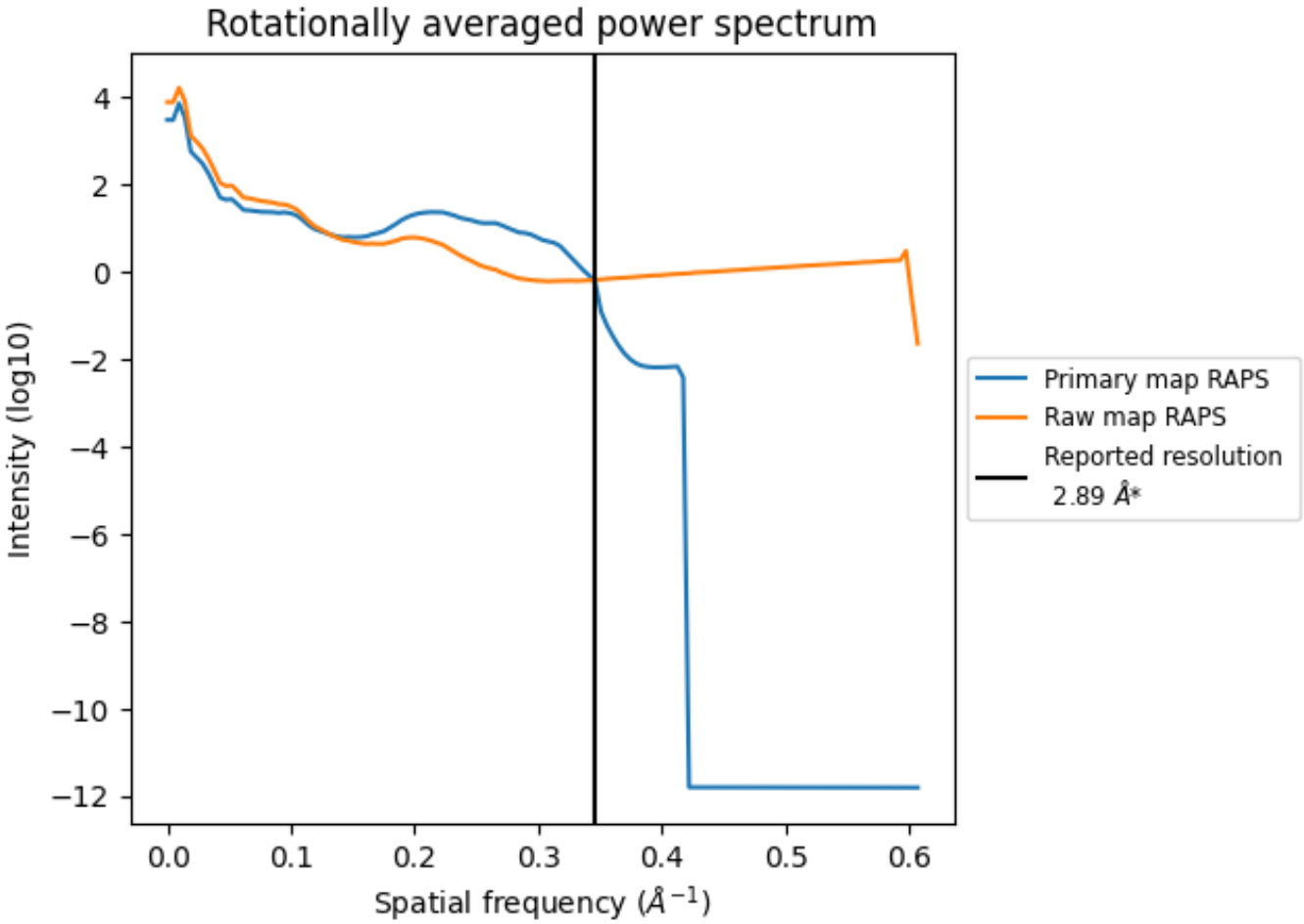
7.2 Volume estimate (i)



The volume at the recommended contour level is 31 nm^3; this corresponds to an approximate mass of 28 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)

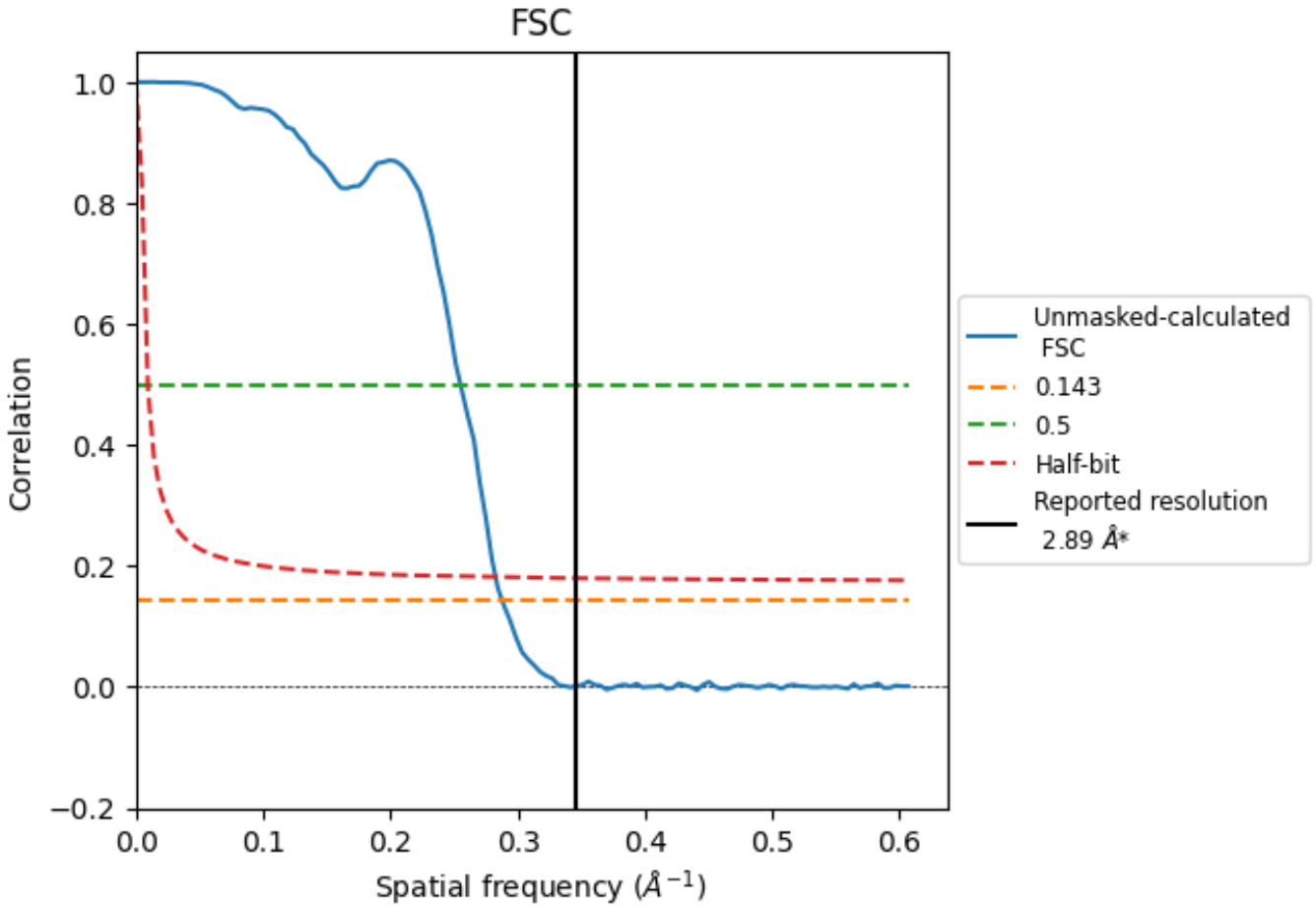


*Reported resolution corresponds to spatial frequency of 0.346 Å^{-1}

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 0.346 Å^{-1}

8.2 Resolution estimates (i)

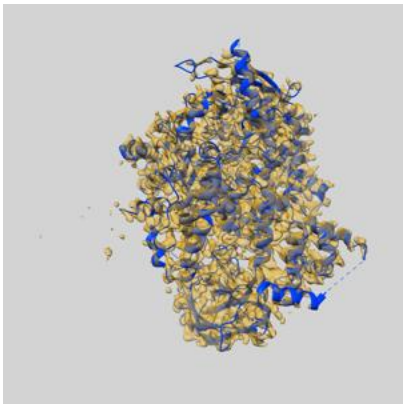
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	2.89
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.48	3.92	3.54

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 1/2 BIT CUT-OFF 3.54 differs from the reported value 2.89 by more than 10 %

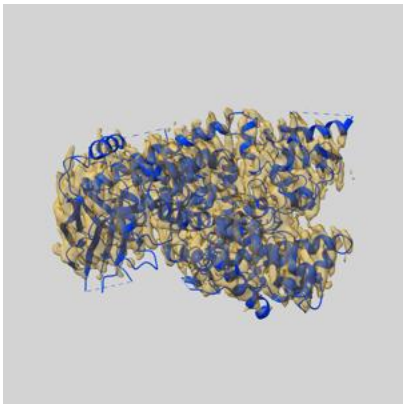
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-67320 and PDB model 9XW2. Per-residue inclusion information can be found in section 3 on page 5.

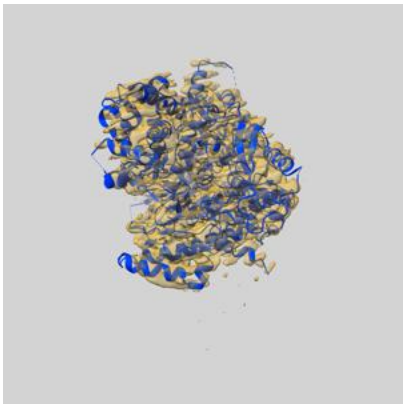
9.1 Map-model overlay



X



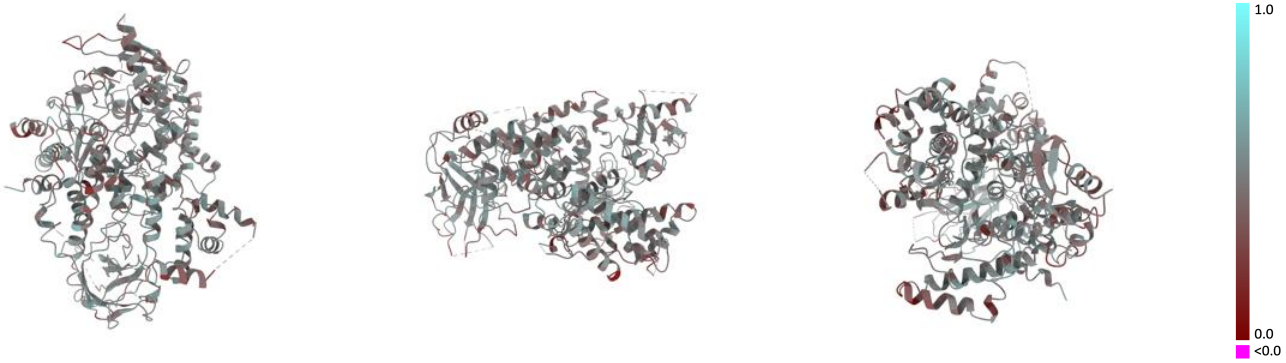
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.164 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.

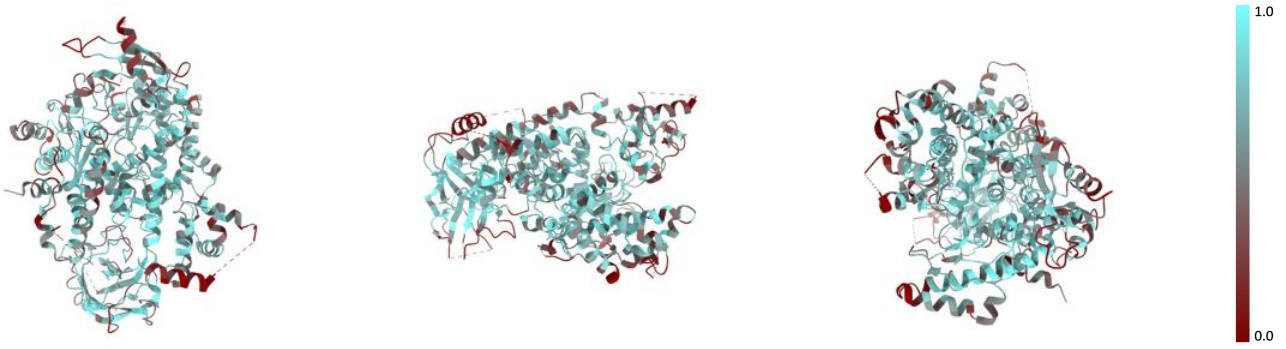
9.2 Q-score mapped to coordinate model



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.

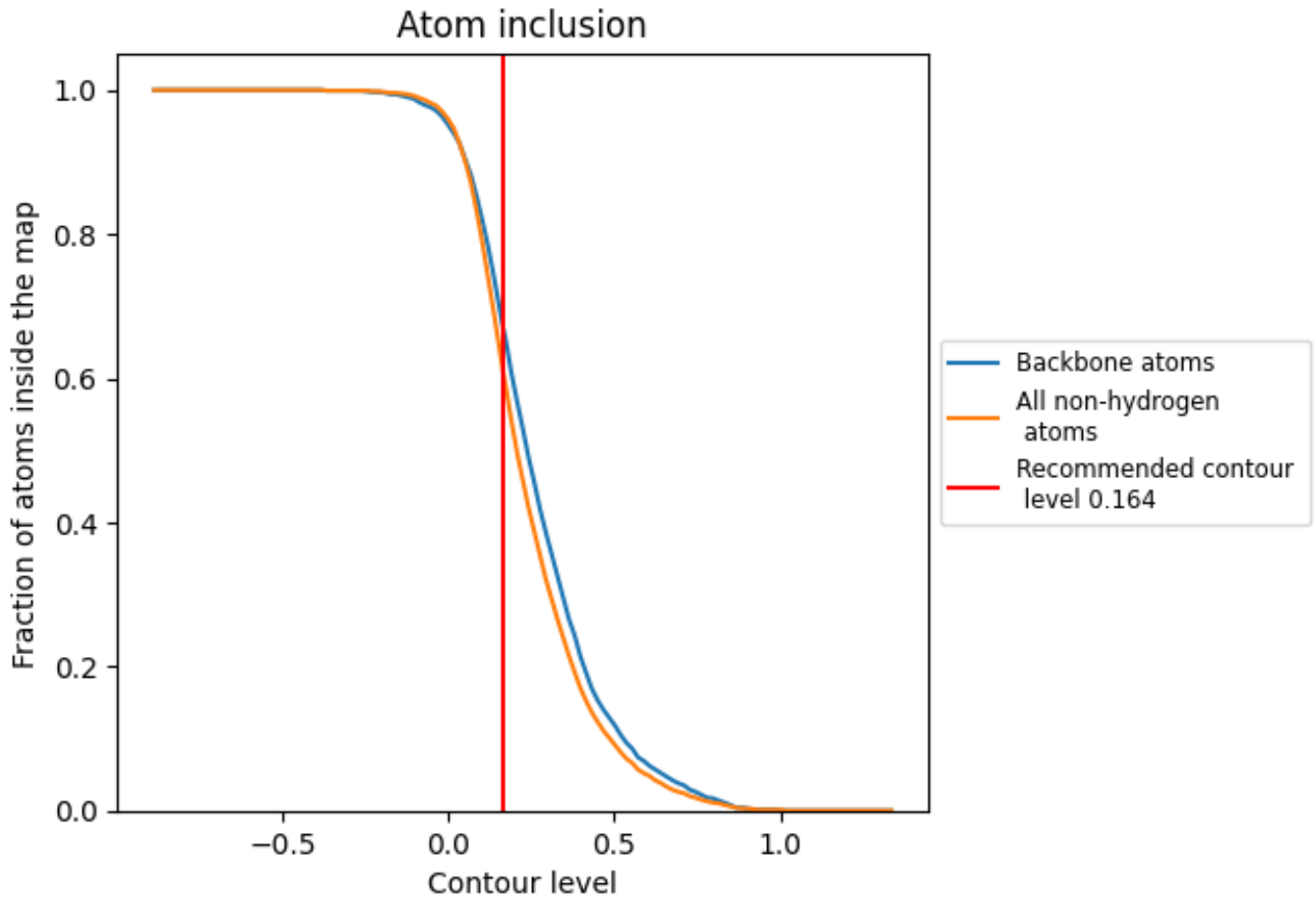
9.3 Atom inclusion mapped to coordinate model



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 (0.164).

9.4 Atom inclusion (i)



At the recommended contour level, 67% of all backbone atoms, 61% 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 (0.164) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.6110	0.4610
B	0.6110	0.4610