



# wwPDB EM Validation Summary Report ⓘ

Aug 27, 2024 – 04:37 PM JST

PDB ID : 8JGJ  
EMDB ID : EMD-36236  
Title : Cryo-EM structure of mClC-3 with ATP  
Authors : Wan, Y.Z.Q.; Yang, F.  
Deposited on : 2023-05-20  
Resolution : 3.30 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev112  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.38.2

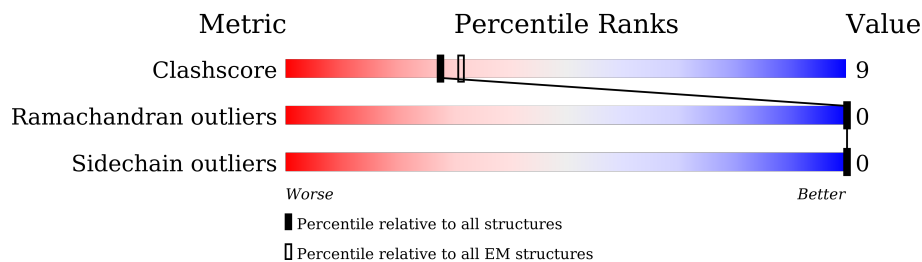
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.30 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	818	
1	B	818	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	A	904	-	-	X	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 21692 atoms, of which 10874 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.

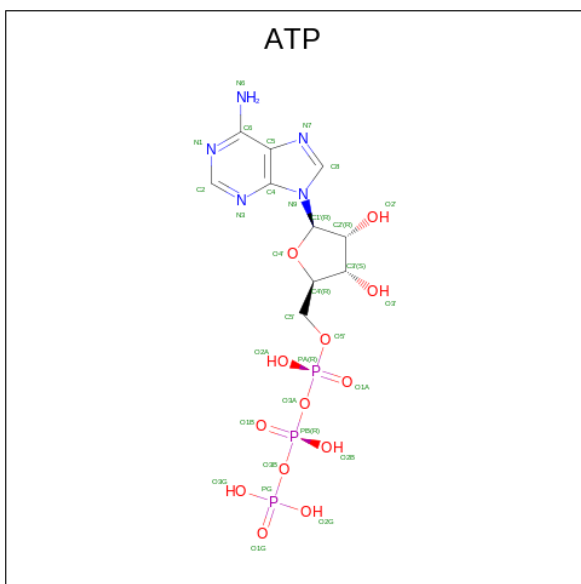
- Molecule 1 is a protein called H(+)/Cl(-) exchange transporter 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	684	10798	3520	5425	885	932	36	0	0
1	B	684	10798	3520	5425	885	932	36	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	790	ARG	ILE	engineered mutation	UNP P51791
A	791	LEU	VAL	engineered mutation	UNP P51791
B	790	ARG	ILE	engineered mutation	UNP P51791
B	791	LEU	VAL	engineered mutation	UNP P51791

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



Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
2	A	1	43	10	12	5	13	3	0
2	B	1	43	10	12	5	13	3	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Cl	
3	A	3	3	3	0
3	B	3	3	3	0

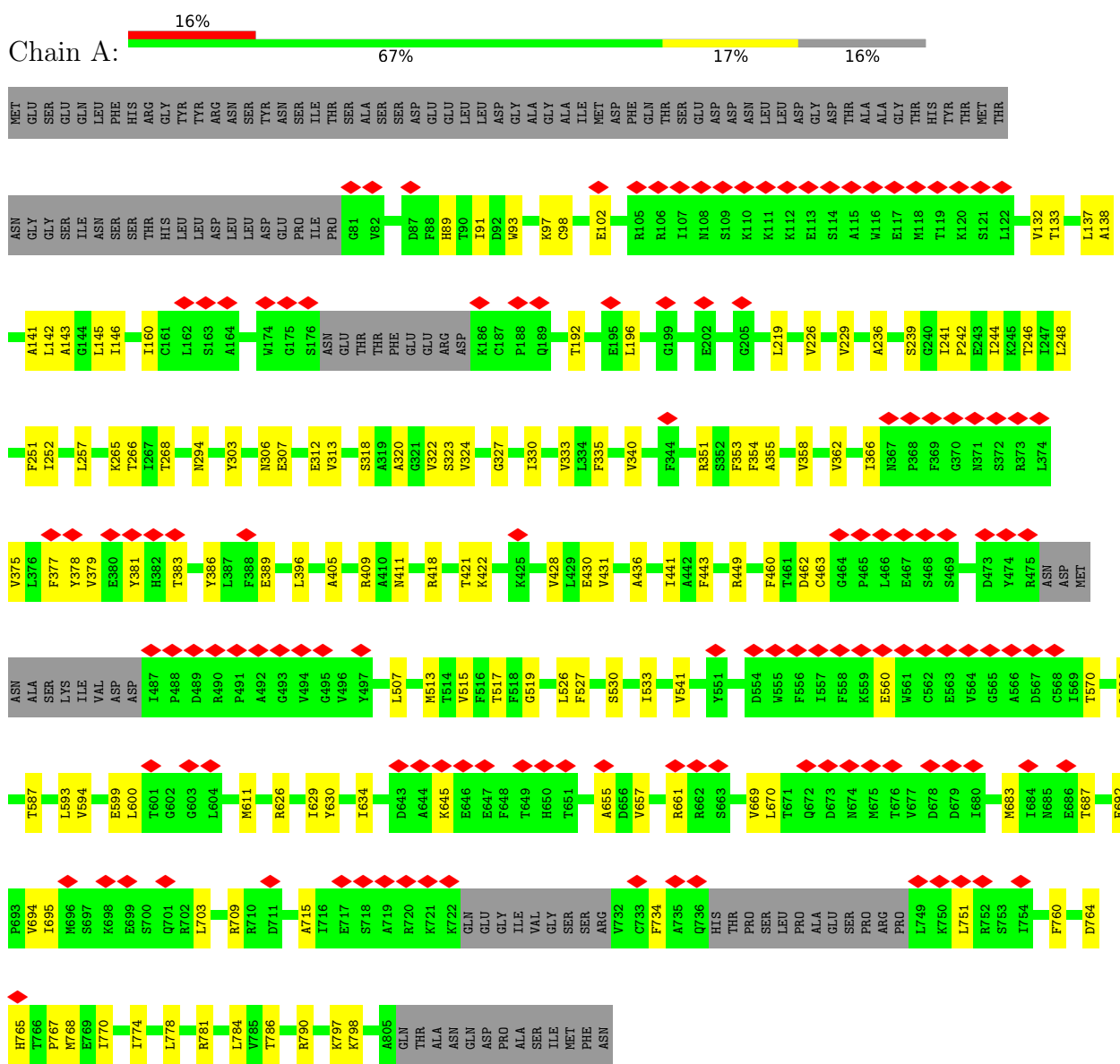
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
4	A	2	2	2	0
4	B	2	2	2	0

### 3 Residue-property plots

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: H(+)/Cl(-) exchange transporter 3



- Molecule 1: H(+)/Cl(-) exchange transporter 3



MET	GLU	SER	GLU	GLN	LEU	PHE	HIS	ARG	GLY	TYR	TVR	ASP	ARG	ASN	SER	TYR	ASN	SER	PRO	ILE	THR	SER	ALA	ALA	GLY	ALA	ALA	MET	ASP	PHE	GLN	THR	SER	GLU	ASP	ASP	ASN	LEU	LEU	ASP	GLY	ASP	THR	ALA	ALA	GLY	THR	HIS	THR	THR	THR	THR																																
ASN	GLY	GLY	SER	ILE	ASN	SER	THR	HIS	LEU	LEU	ASN	LEU	LEU	LEU	LEU	ASP	THR	PHE	GLU	PRO	ILE	PRO	G81	V82	D87	I91	D92	W93	K97	C98	E102	R105	R106	I107	N108	S109	K110	K111	K112	E113	S114	A115	W116	E117	M118	T119	K120	S121	L122	V132	L137	A138	L142	A143																														
I160	C161	L162	S163	A164	W174	G175	S176	GLU	THR	THR	ASP	K186	C187	P188	Q189	E195	L196	E202	C205	L219	V226	V229	A236	S239	G240	I241	P242	E243	I244	R245	T246	L247	L248	F251	L252	L257	K265	T268	E282	L285	V288	Y303	N306	E307	V313	L314	S318	A319	A320	G321	V322	S323	V324	C327	V333	L334	F335	V340	F344	F353	F354	A355	V358	V362	I366	N367	P368	F369	G370	N371	S372	R373	L374	V375	L376	F377	Y378	V379	E380	Y381	H382	T383	L387	F388
E389	L390	F393	L394	L395	L396	M411	R418	T421	K422	K425	V428	L429	E430	V431	A436	T441	F460	T461	D462	C463	G464	P465	F466	E467	S468	S469	D473	Y474	R475	ASN	ASP	MET	ASN	ALA	SER	LYS	ILE	VAL	ASP	I487	P488	D489	R490	P491	A492	G493	V494	G495																																				
V496	Y497	S498	L503	L507	M513	T514	V515	F516	T517	F518	G519	I520	K521	V522	L526	F527	I528	I533	I536	V541	Y551	D554	M555	F556	F557	F558	K559	E560	M561	C562	E563	V564	A566	D567	G568	M576	L583	T587	L593	V594	L600	T601	G602	G603																																								
P609	L610	M611	R626	I629	Y630	I634	D643	A644	K645	E646	E647	F648	T649	H650	T651	T652	L653	A654	A655	D656	V657	R661	R662	S663	D672	D673	M674	M675	T676	V677	D678	D679	I680	E681	M682	M683	I684	M685	F686	T687	I695	M696	S697	F698	E699	S700	Q701	R702	L703	V704																																		
R709	R710	D711	A715	I716	E717	S718	A719	R720	K721	K722	GLN	GLU	GLY	ALA	ASN	ILE	VAL	GLY	SER	SER	ALA	ARG	V732	C733	F734	A735	Q736	HIS	THR	PRO	SER	LEU	PRO	ALA	ALA	GLU	SER	PRO	ARG	PRO	L749	K750	L751	R752	S753	I754	F760	D764	H765	T766	F767	M768	E769	I770	I774	L778	L778	R781																										
L784	V785	T786	R790	I794	I795	T796	K797	K798	K805	GLN	THR	THR	ALA	ASN	GLN	ASP	PRO	SER	SER	ALA	SER	ILE	MET	PHE	ASN																																																											

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	97275	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	52	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.330	Depositor
Minimum map value	-0.807	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.167	Depositor
Map size (Å)	238.08, 238.08, 238.08	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.93, 0.93, 0.93	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, 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	0.27	0/5512	0.47	0/7481
1	B	0.27	0/5512	0.47	0/7481
All	All	0.27	0/11024	0.47	0/14962

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	A	5373	5425	5436	107	0
1	B	5373	5425	5436	103	0
2	A	31	12	12	1	0
2	B	31	12	12	1	0
3	A	3	0	0	2	0
3	B	3	0	0	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
All	All	10818	10874	10896	206	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 9.



The worst 5 of 206 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:248:LEU:HD12	1:A:340:VAL:HG12	1.55	0.89
1:B:626:ARG:O	1:B:645:LYS:NZ	2.10	0.84
1:A:626:ARG:O	1:A:645:LYS:NZ	2.10	0.83
1:A:381:TYR:OH	1:A:460:PHE:O	1.99	0.81
1:B:248:LEU:HD12	1:B:340:VAL:HG12	1.64	0.79

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	674/818 (82%)	662 (98%)	12 (2%)	0	100	100
1	B	674/818 (82%)	661 (98%)	13 (2%)	0	100	100
All	All	1348/1636 (82%)	1323 (98%)	25 (2%)	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	A	568/684 (83%)	568 (100%)	0	100	100

*Continued on next page...*

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	568/684 (83%)	568 (100%)	0	100	100
All	All	1136/1368 (83%)	1136 (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. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	787	HIS
1	B	787	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](#)

Of 8 ligands modelled in this entry, 6 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	901	-	26,33,33	0.61	0	31,52,52	1.06	2 (6%)
2	ATP	A	901	-	26,33,33	0.61	0	31,52,52	1.07	2 (6%)

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	901	-	-	8/18/38/38	0/3/3/3
2	ATP	A	901	-	-	6/18/38/38	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	ATP	C5-C6-N6	2.31	123.86	120.35
2	A	901	ATP	C5-C6-N6	2.30	123.84	120.35
2	A	901	ATP	PB-O3B-PG	2.03	139.78	132.83
2	B	901	ATP	PB-O3B-PG	2.02	139.76	132.83

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	ATP	PB-O3B-PG-O2G
2	B	901	ATP	PB-O3B-PG-O2G
2	B	901	ATP	PB-O3B-PG-O3G
2	B	901	ATP	C5'-O5'-PA-O1A
2	B	901	ATP	C5'-O5'-PA-O2A

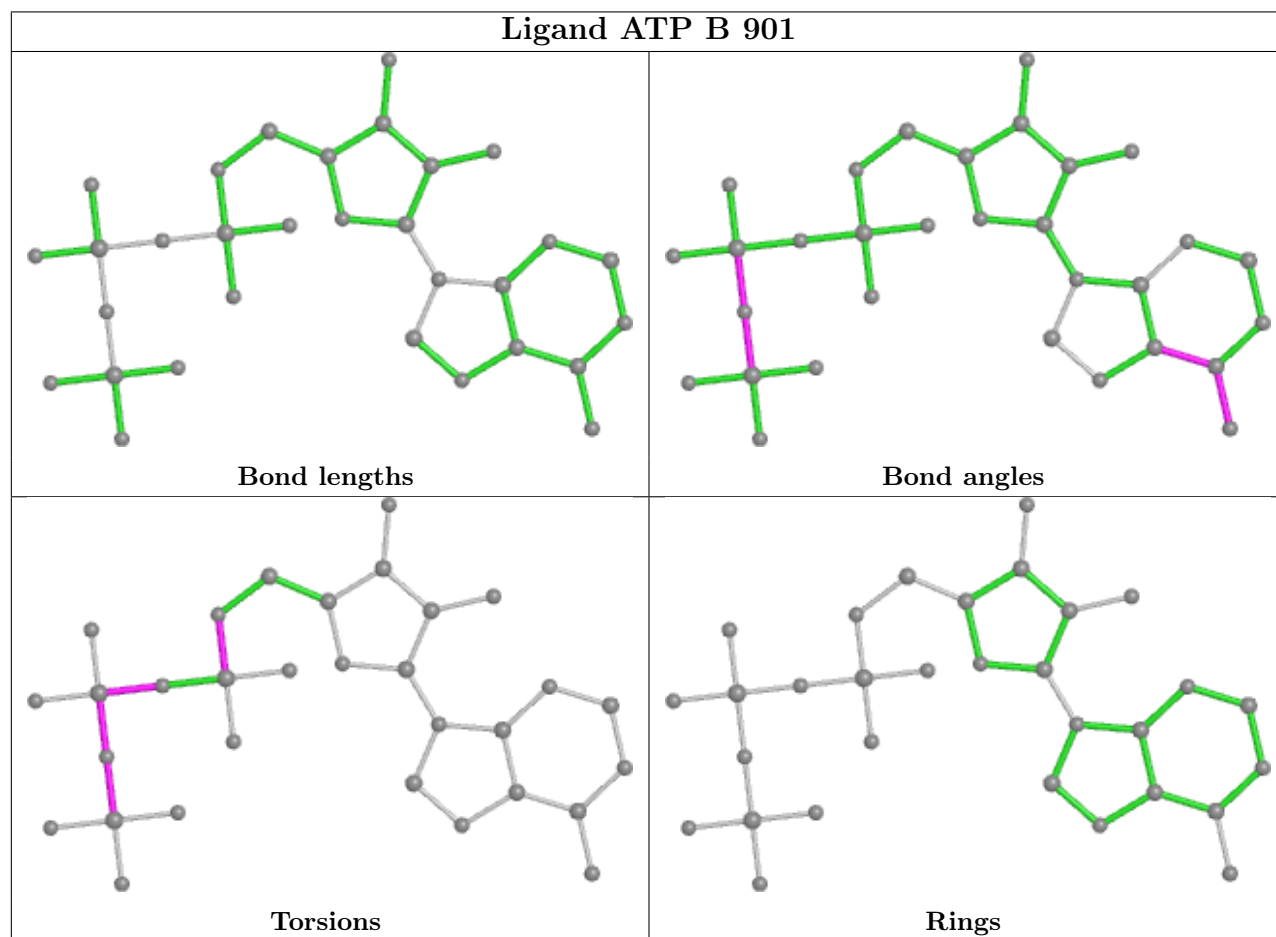
There are no ring outliers.

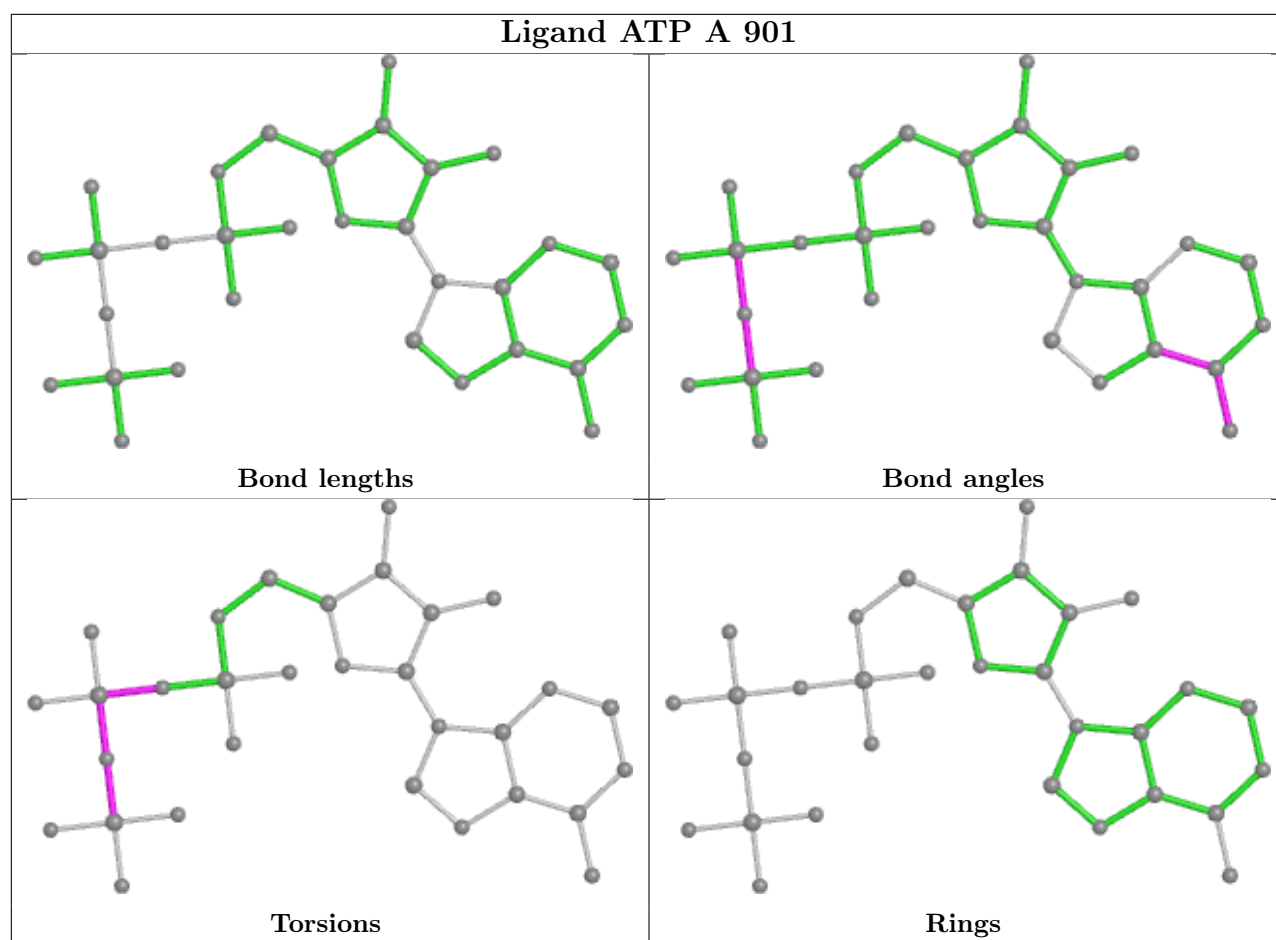
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	901	ATP	1	0
2	A	901	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 than 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.





## 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.

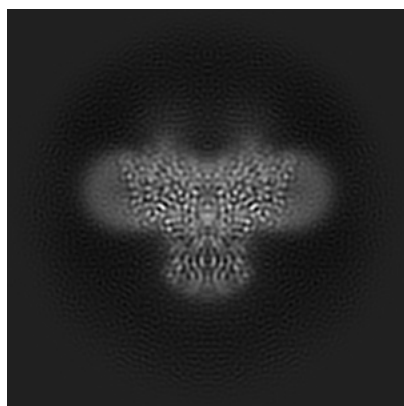
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36236. These allow visual inspection of the internal detail of the map and identification of artifacts.

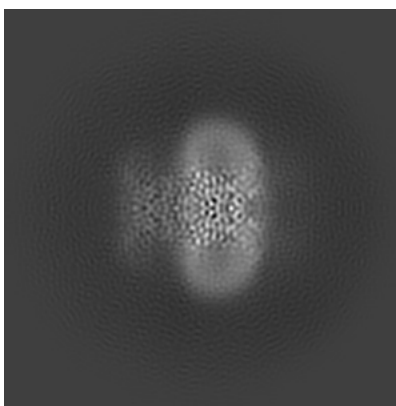
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

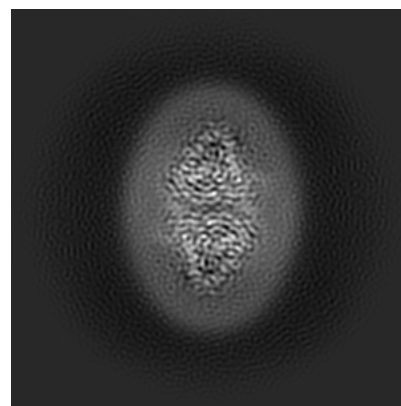
#### 6.1.1 Primary map



X

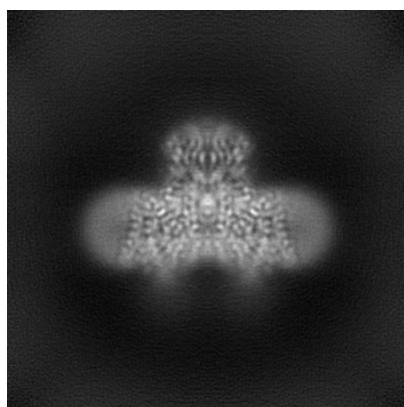


Y

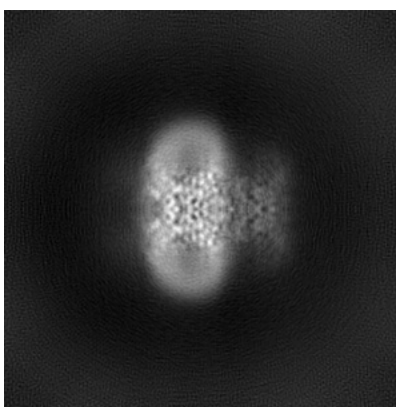


Z

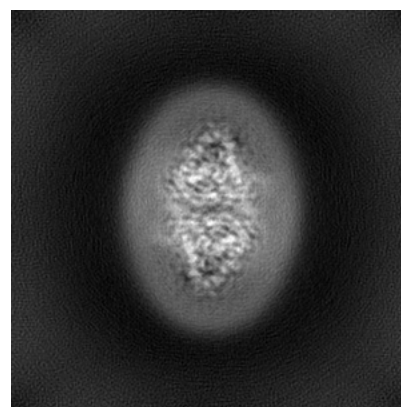
#### 6.1.2 Raw map



X



Y

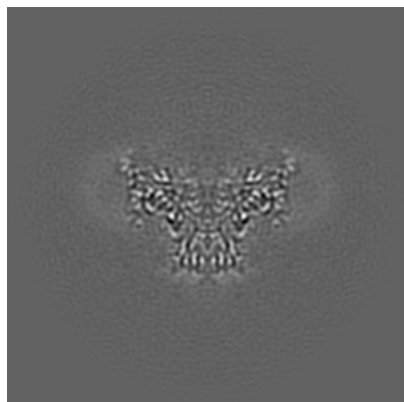


Z

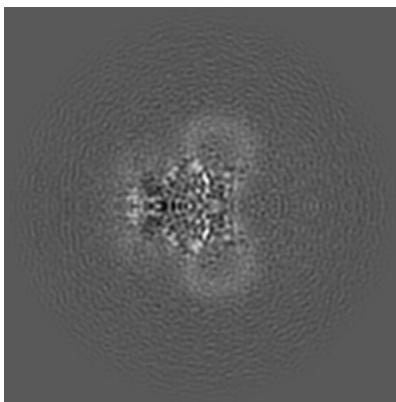
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

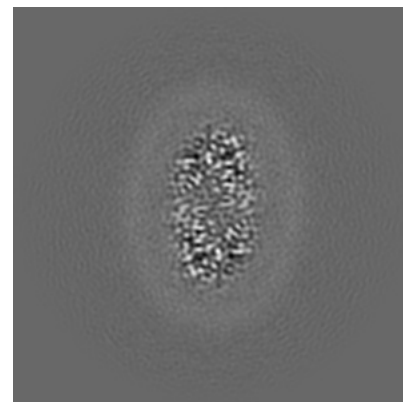
### 6.2.1 Primary map



X Index: 128

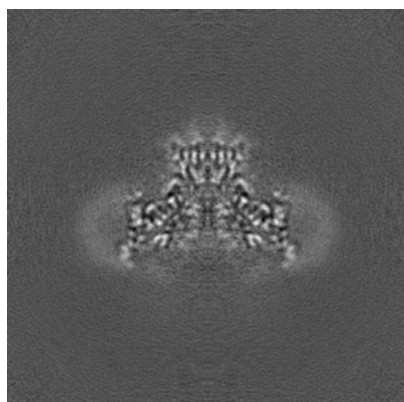


Y Index: 128

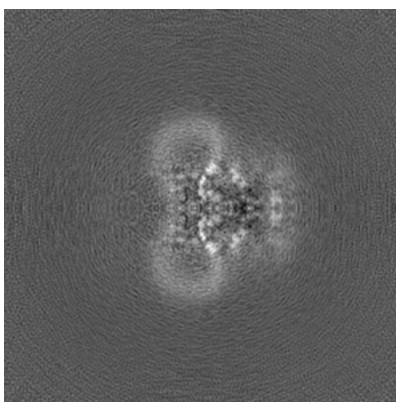


Z Index: 128

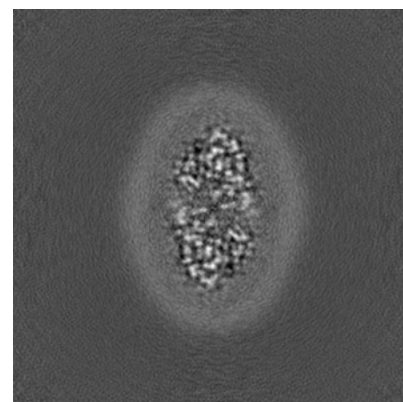
### 6.2.2 Raw map



X Index: 128



Y Index: 128



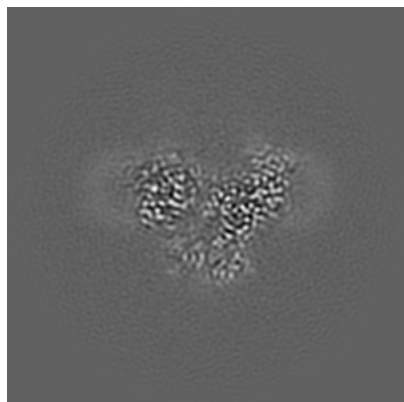
Z Index: 128

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

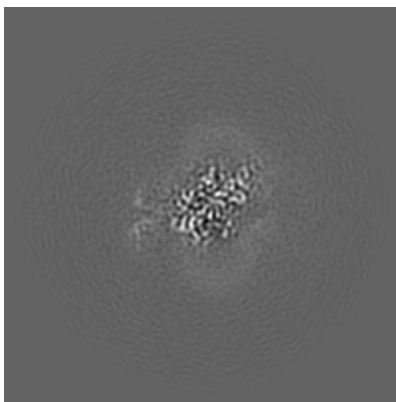


## 6.3 Largest variance slices [i](#)

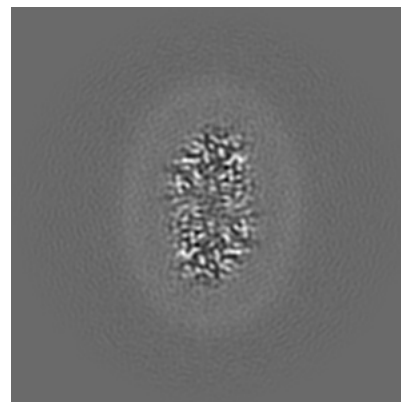
### 6.3.1 Primary map



X Index: 138

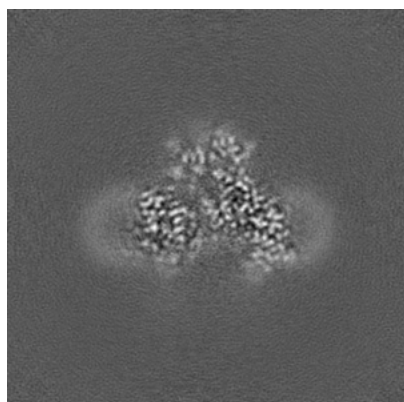


Y Index: 103

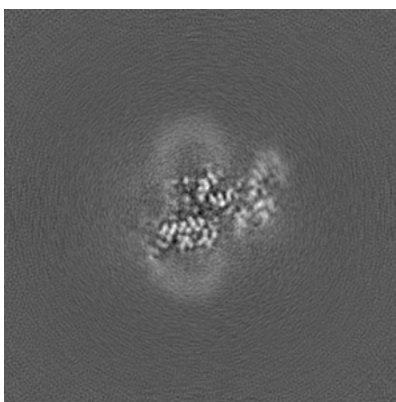


Z Index: 129

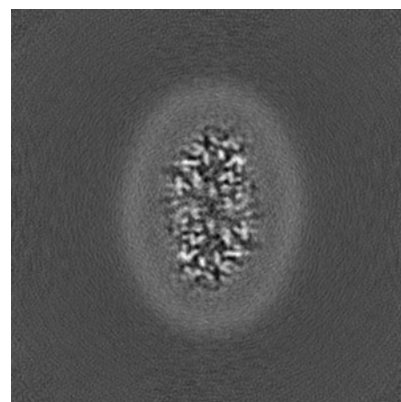
### 6.3.2 Raw map



X Index: 138



Y Index: 147



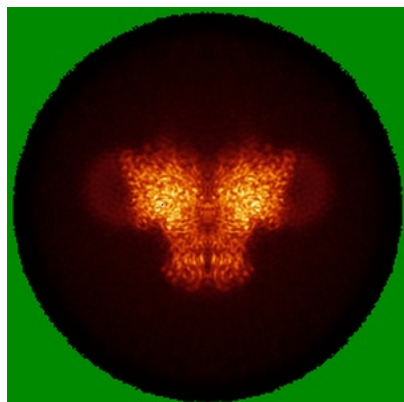
Z Index: 126

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

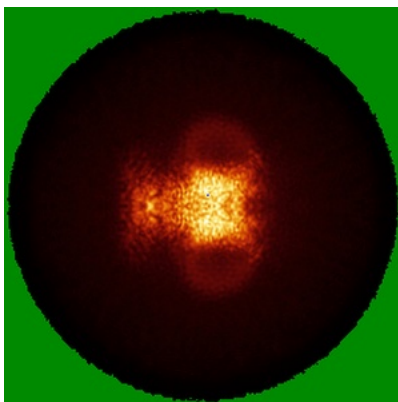


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

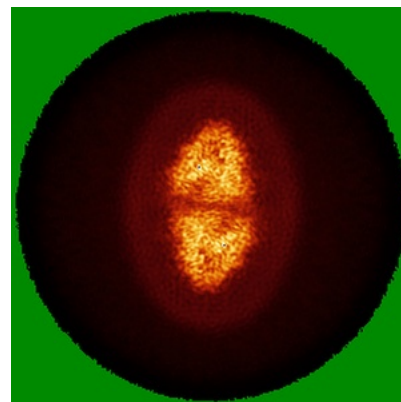
### 6.4.1 Primary map



X

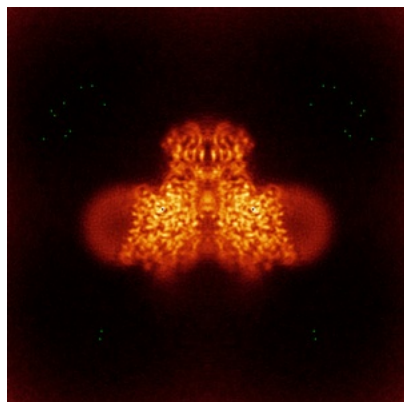


Y

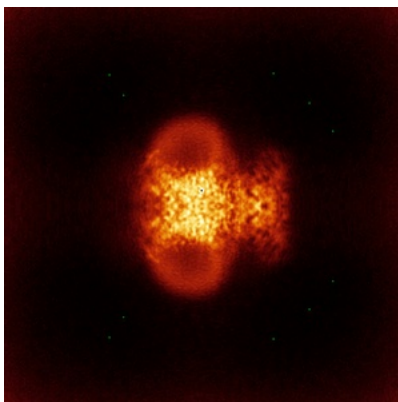


Z

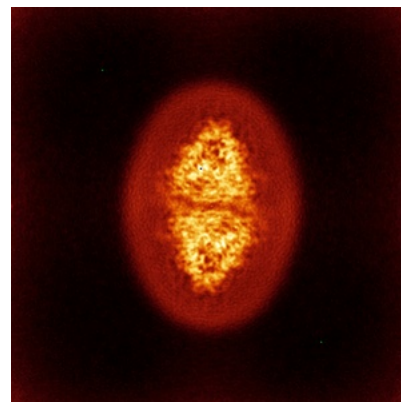
### 6.4.2 Raw map



X



Y

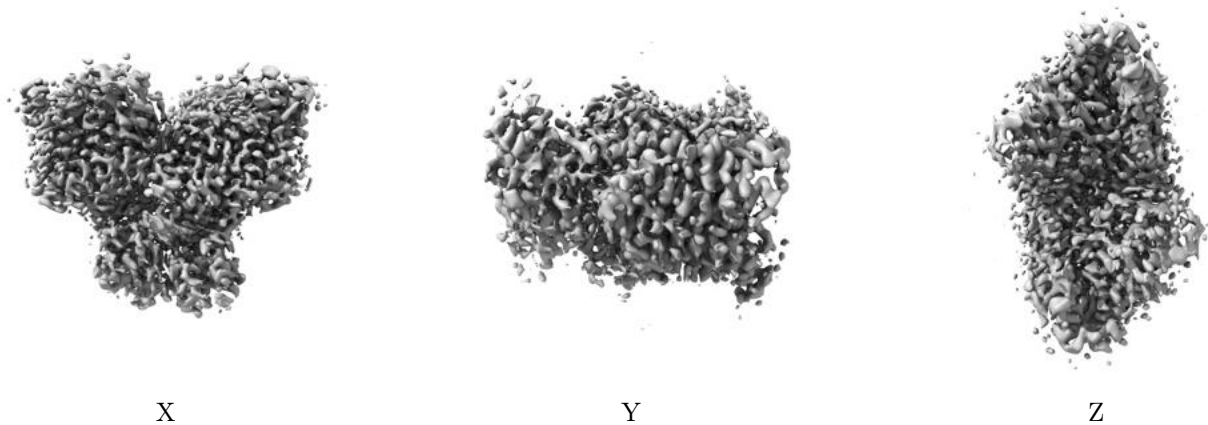


Z

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.

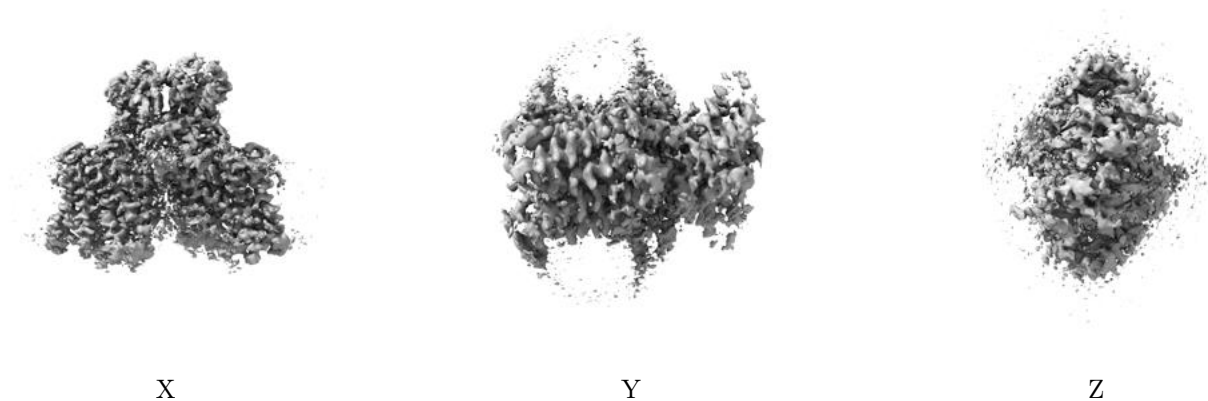
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.167. 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



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.

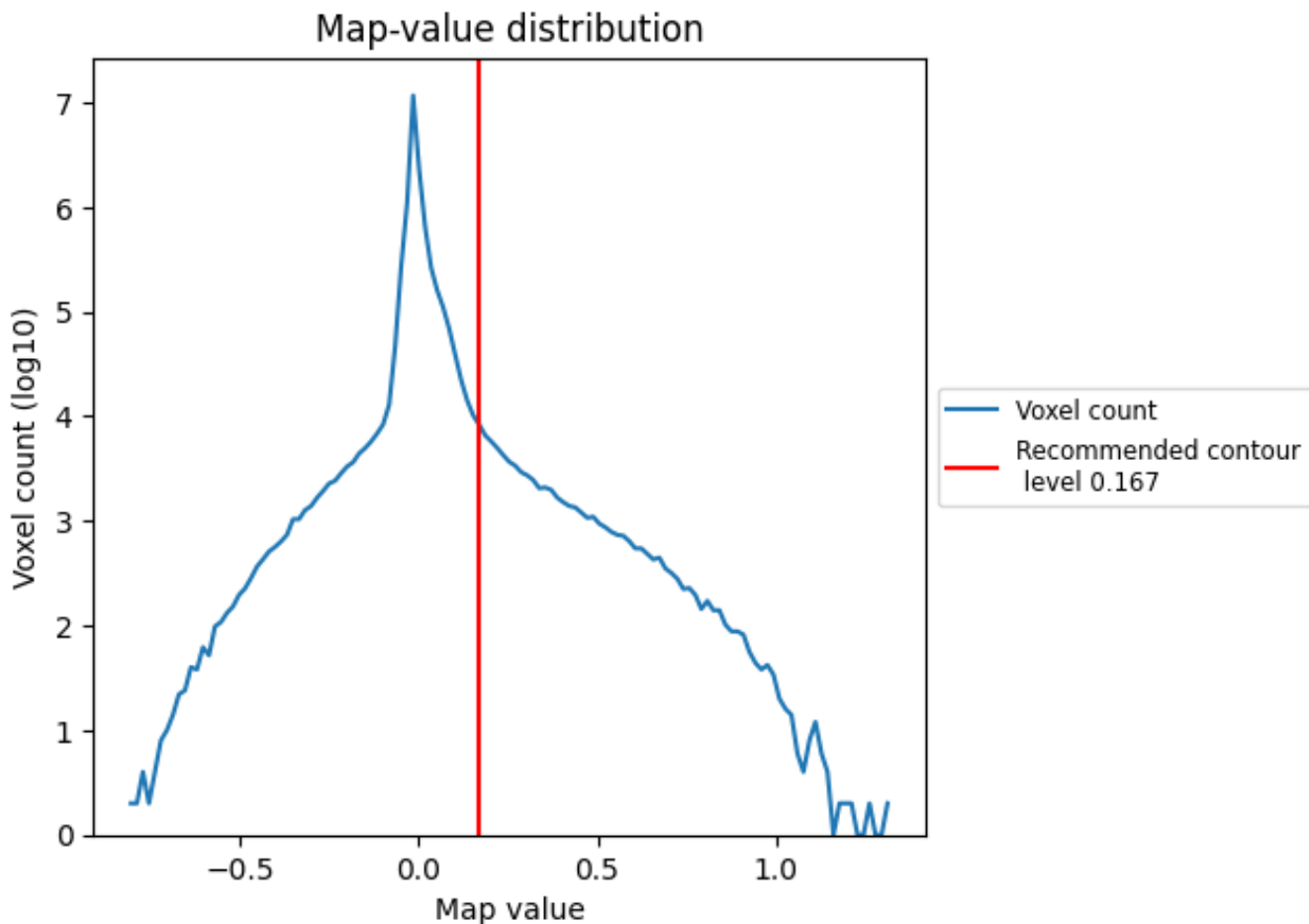
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

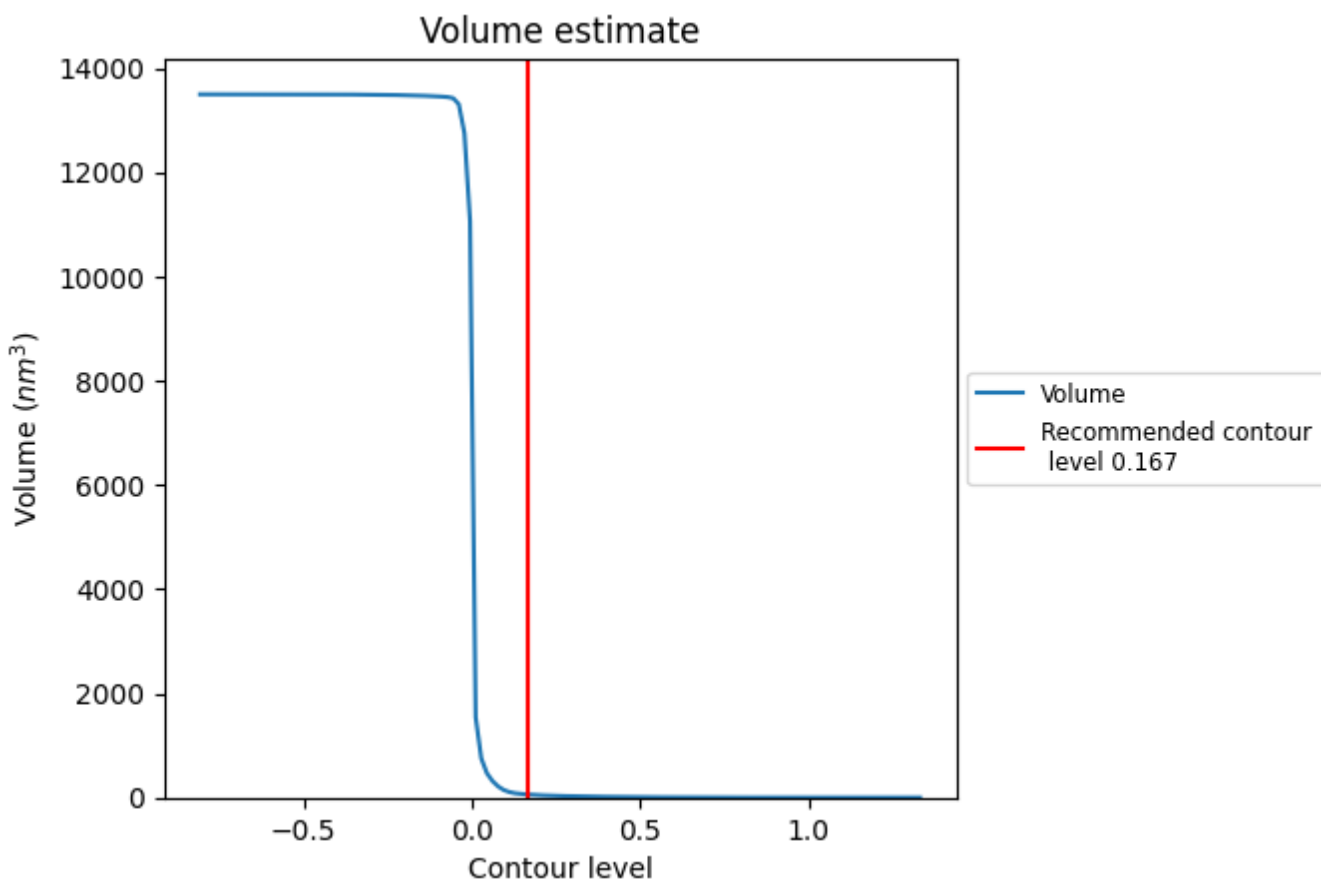
This section contains the results of statistical analysis of the map.

### 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.

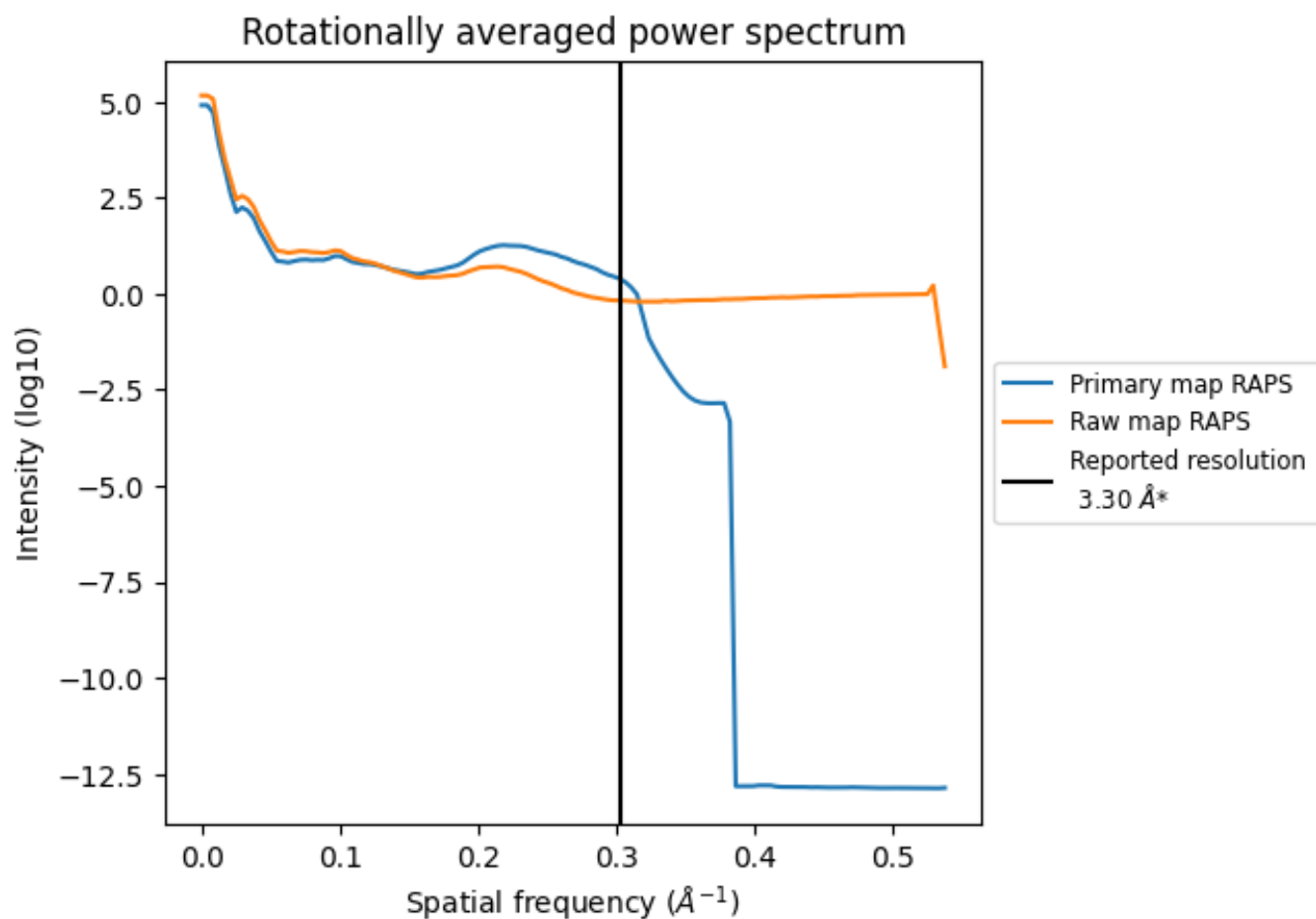
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 58 nm<sup>3</sup>; this corresponds to an approximate mass of 52 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](#)

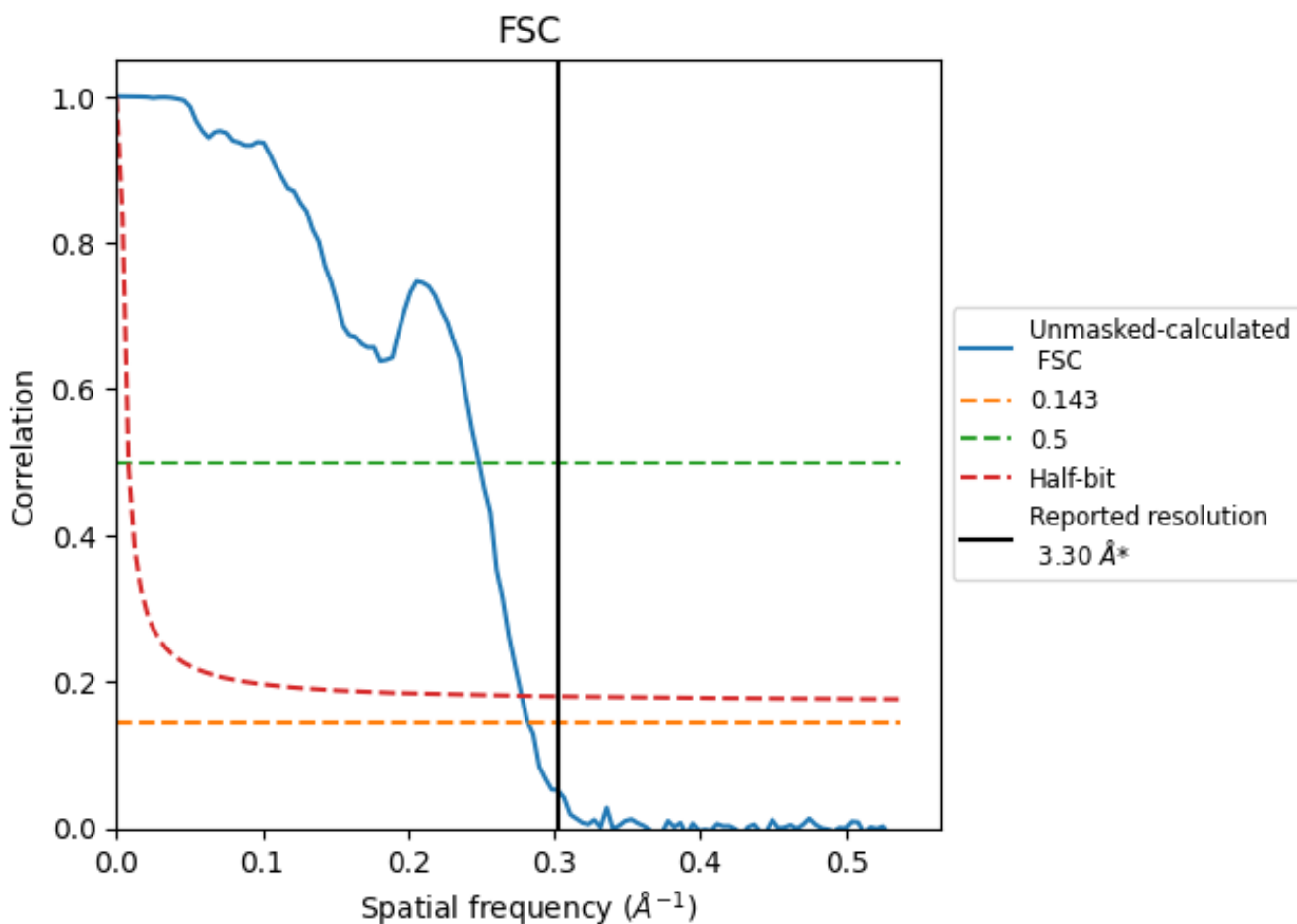


\*Reported resolution corresponds to spatial frequency of 0.303 Å<sup>-1</sup>

## 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  $0.303 \text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

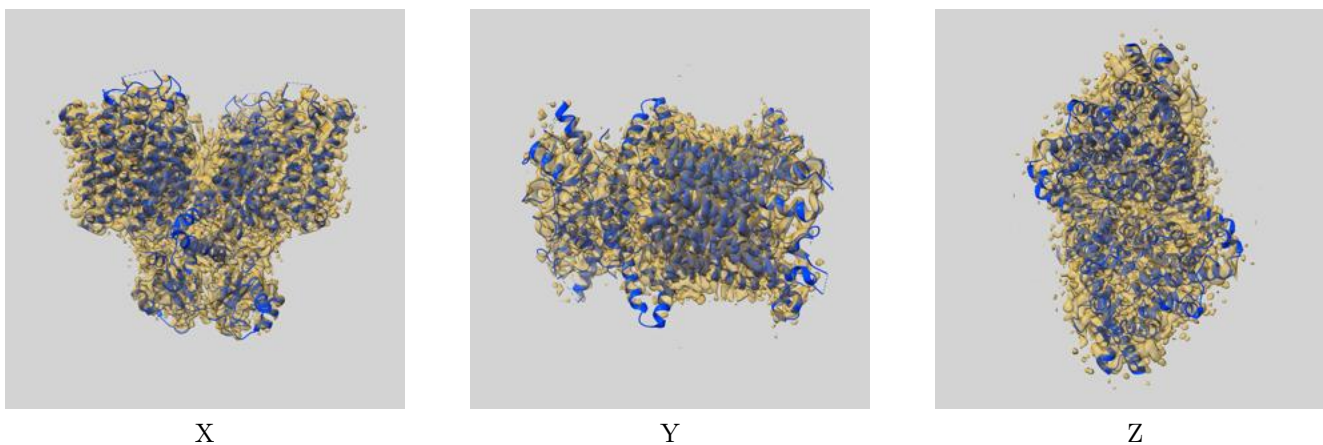
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.54	4.02	3.60

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-36236 and PDB model 8JGJ. Per-residue inclusion information can be found in section 3 on page 5.

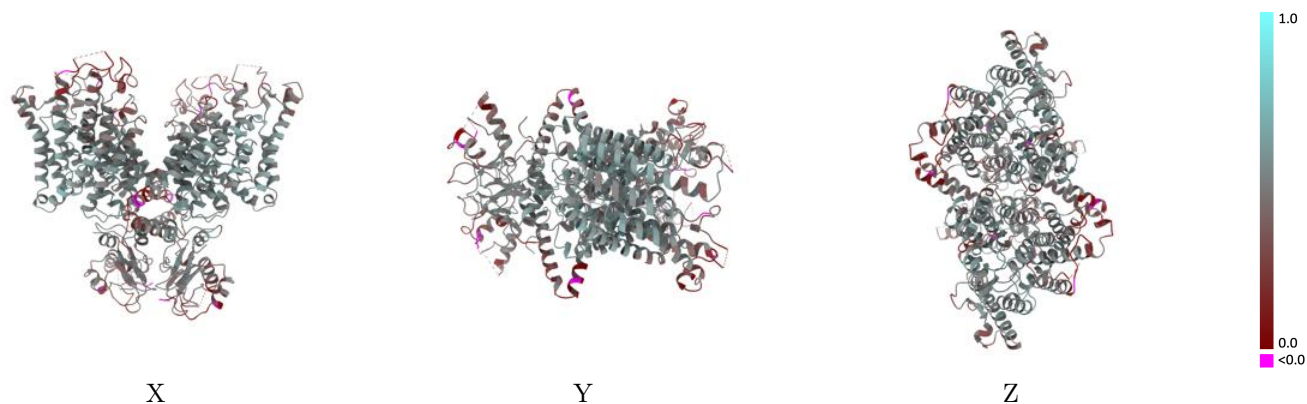
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.167 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

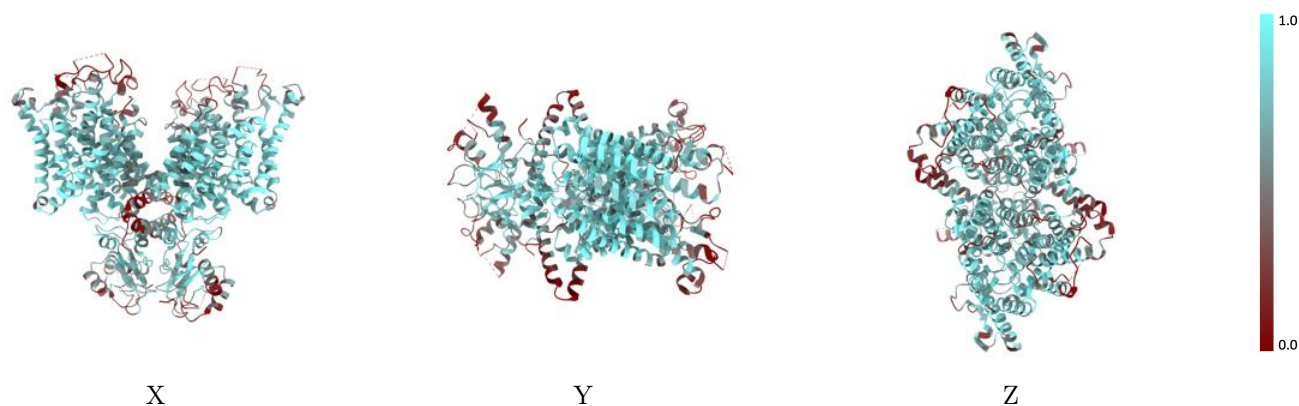


## 9.2 Q-score mapped to coordinate model [i](#)



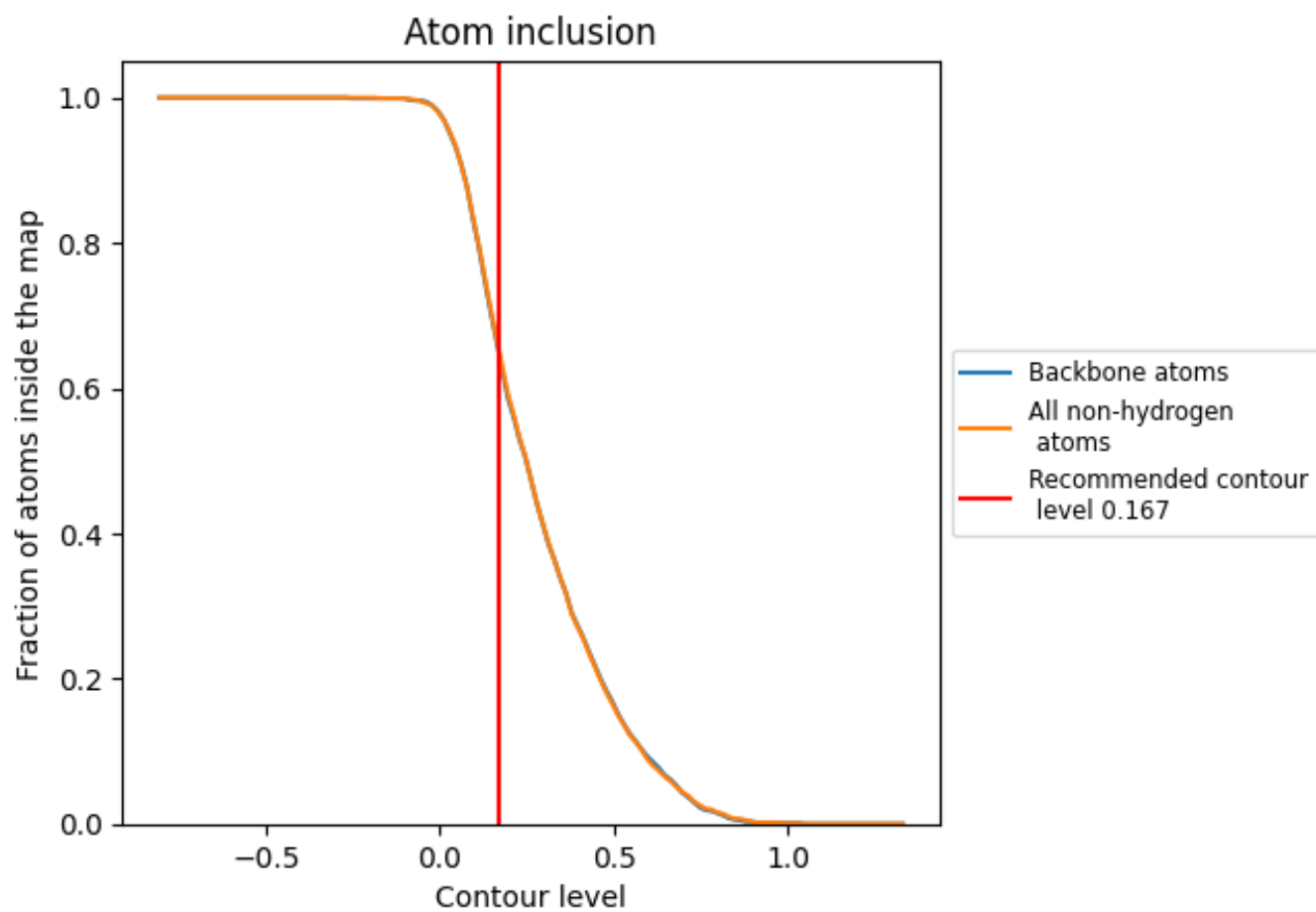
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.167).







## 9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 66% 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 (0.167) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6570	 0.4540
A	 0.6670	 0.4540
B	 0.6690	 0.4550

