



wwPDB EM Validation Summary Report ⓘ

Feb 13, 2024 – 06:10 PM EST

PDB ID : 3IXZ
EMDB ID : EMD-5104
Title : Pig gastric H⁺/K⁺-ATPase complexed with aluminium fluoride
Authors : Abe, K.; Tani, K.; Nishizawa, T.; Fujiyoshi, Y.
Deposited on : 2009-03-09
Resolution : 6.50 Å (reported)
Based on initial model : 3B8E

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.dev70
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

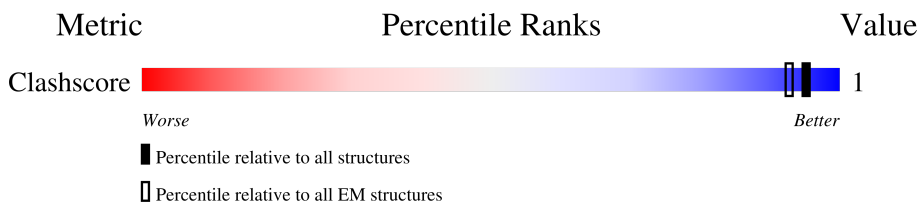
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON CRYSTALLOGRAPHY

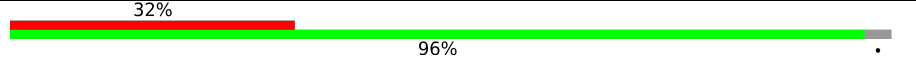

The reported resolution of this entry is 6.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297

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 $\leq 5\%$. 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	1034	
2	B	290	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 1044 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 Potassium-transporting ATPase alpha.

Mol	Chain	Residues	Atoms		AltConf	Trace
1	A	998	Total 998	C 998	0	998

- Molecule 2 is a protein called Potassium-transporting ATPase subunit beta.

Mol	Chain	Residues	Atoms		AltConf	Trace
2	B	46	Total 46	C 46	0	46

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: Potassium-transporting ATPase alpha



- Molecule 2: Potassium-transporting ATPase subunit beta



MET	ALA	ALA	LEU	GLN	GLU	LYS	SER	GLN	ARG	MET	GLU	GLU	PHE	GLN	ARG	TYR	CYS	TRP	ASN	PRO	ASP	THR	THR	GLY	GLN	MET	LEU	GLY	ARG	I33	G53	I54	F55	A56	L57	C58	I59	Y60	V61	L62	M63	R64	T65	I66	D67	P68	Y69	T70	P71	D72	Y73	Q74	D75	Q76	L77	K78													
SER	PRO	GLY	VAL	THR	LEU	ARG	PRO	ASN	ASP	VAL	TYR	GLY	GLU	ILE	ASP	TYR	ASN	VAL	VAL	ASN	ASP	ASP	THR	THR	THR	PRO	GLY	ALA	ALA	HIS	THR	LEU	LEU	GLY	ALA	ALA	HIS	GLY	GLU	HIS	ARG	PHE	LEU	PRO	ALA	ALA	GLY	GLY	VAL	ALA	VAL	GLY	SER	ILE	LEU	ASN	CYS	PRO	GLY	THR	SER	ASN	THR	LYS	TYR	PRO	PHE	ARG	VAL
GLN	GLU	SER	PHE	LEU	ALA	PRO	ASN	HIS	THR	VAL	TYR	PHE	GLY	CYS	LEU	PHE	THR	ALA	ASP	MET	LEU	ASN	GLN	VAL	ASN	ASN	GLY	CYS	THR	GLY	ARG	PRO	ASP	ALA	THR	PHE	GLY	TYR	THR	LEU	ALA	ALA	GLY	LEU	LEU	ILE	LEU	ASN	PRO	CYS	GLY	THR	SER	ASN	THR	ALA	PRO	PHE	ARG										
VAL	ASP	CYS	ALA	PHE	LEU	ASP	GLN	PRO	ARG	ASP	GLY	PRO	PRO	LEU	GLN	VAL	GLU	TYR	PHE	PRO	PRO	ALA	ALA	LYS	LYS	ALA	GLN	PRO	HIS	TYR	PHE	PRO	TYR	TYR	TYR	ASN	ASN	PRO	LEU	VAL	VAL	ALA	ALA	LYS	LEU	LEU	ASN	ASN	VAL	VAL	PRO	ARG	ASN	ARG	ASP	VAL													
VAL	ILE	VAL	CYS	LYS	ILE	LEU	ALA	GLU	HIS	VAL	SER	PHE	ASP	ASN	PRO	HIS	ASP	PRO	TYR	GLU	GLY	LYS	VAL	GLU	PHE	LYS	LEU	LYS	ILE	ILE	GLN	LYS																																					

4 Experimental information

Property	Value	Source
EM reconstruction method	CRYSTALLOGRAPHY	Depositor
Imposed symmetry	2D CRYSTAL, a =Not provided Å, b =Not provided Å, c =Not provided Å, γ =Not provided°, space group=Not provided	Depositor
Number of images used	Not provided	
Resolution determination method	Not provided	
CTF correction method	Each images were CTF corrected.	Depositor
Microscope	JEOL KYOTO-3000SFF	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	25	Depositor
Minimum defocus (nm)	3480	Depositor
Maximum defocus (nm)	390	Depositor
Magnification	59100	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	0.010	Depositor
Minimum map value	-0.008	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0015	Depositor
Map size (Å)	140.40027, 108.999794, 319.99966	wwPDB
Map dimensions	145, 69, 53	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.06471, 2.09615, 2.22222	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	998	0	0	1	0
2	B	46	0	0	0	0
All	All	1044	0	0	1	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 1.

All (1) 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:902:HIS:CA	1:A:912:GLY:CA	2.93	0.46

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5104. These allow visual inspection of the internal detail of the map and identification of artifacts.

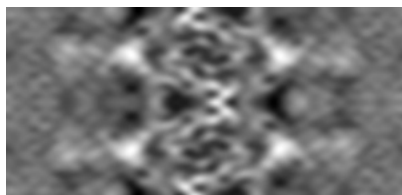
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

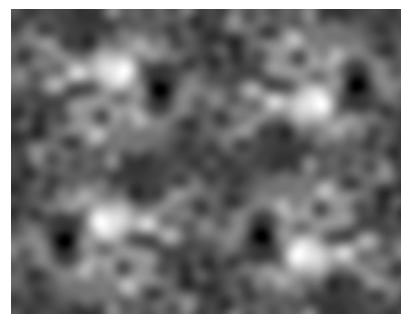
6.1.1 Primary map



X



Y



Z

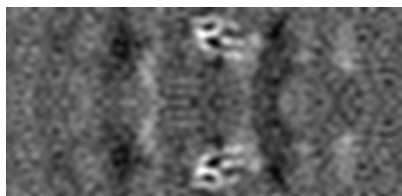
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 34



Y Index: 26

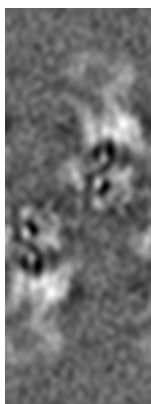


Z Index: 72

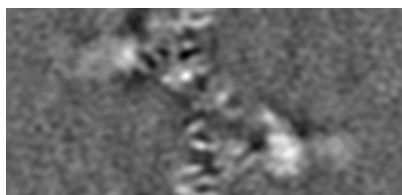
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

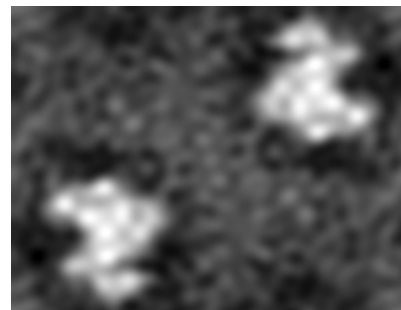
6.3.1 Primary map



X Index: 17



Y Index: 42

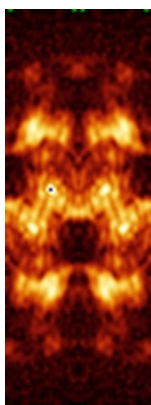


Z Index: 44

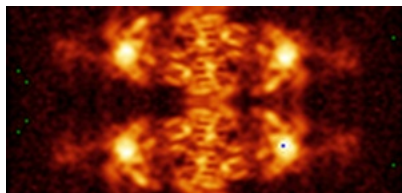
The images above show the largest variance slices of the map in three orthogonal directions.

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

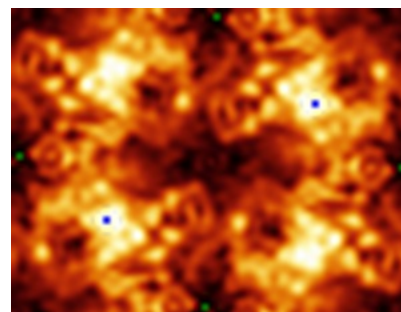
6.4.1 Primary map



X



Y



Z

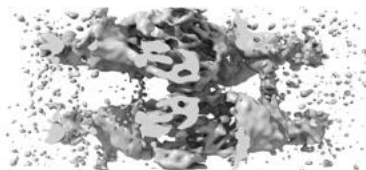
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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 0.0015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

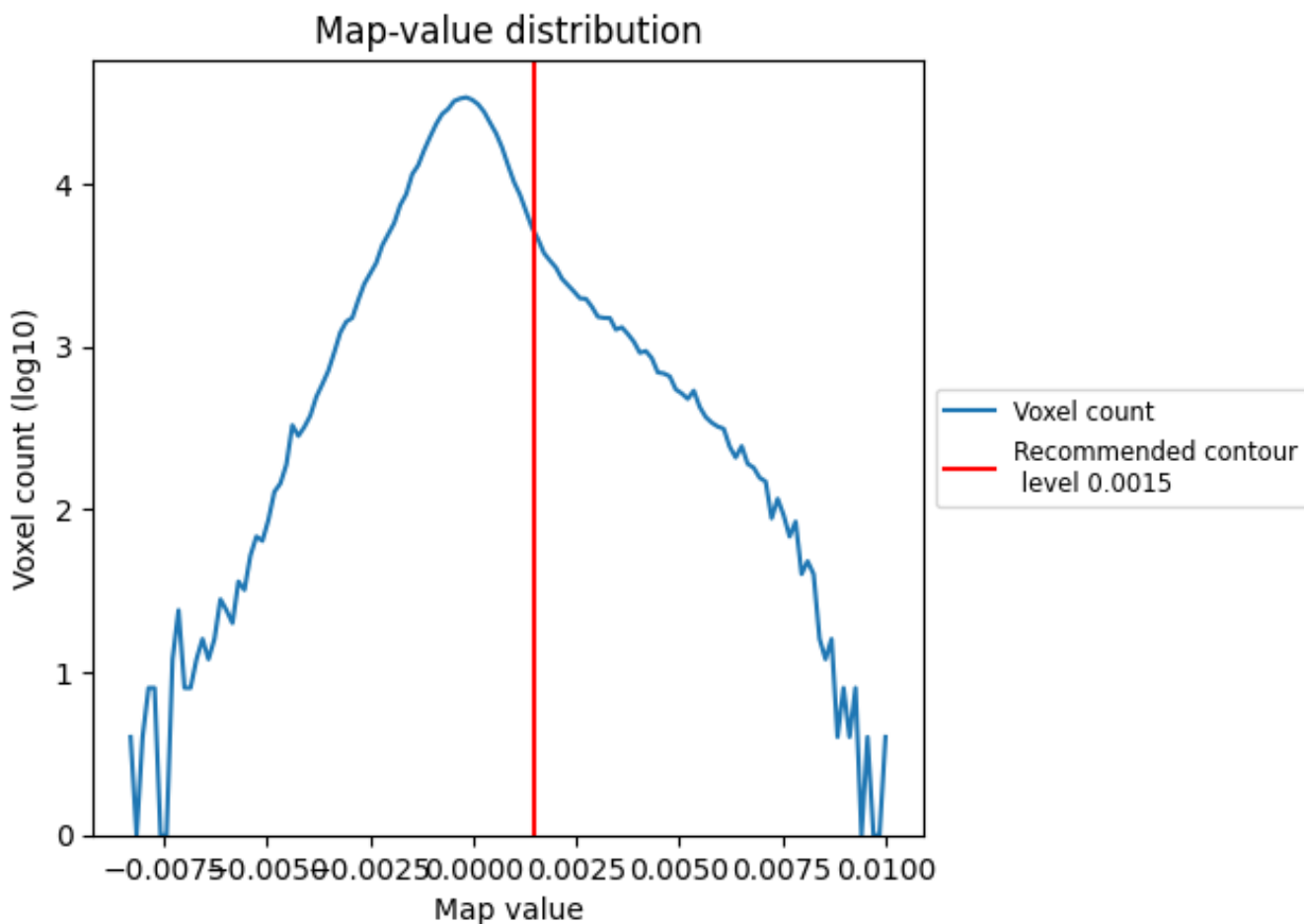
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

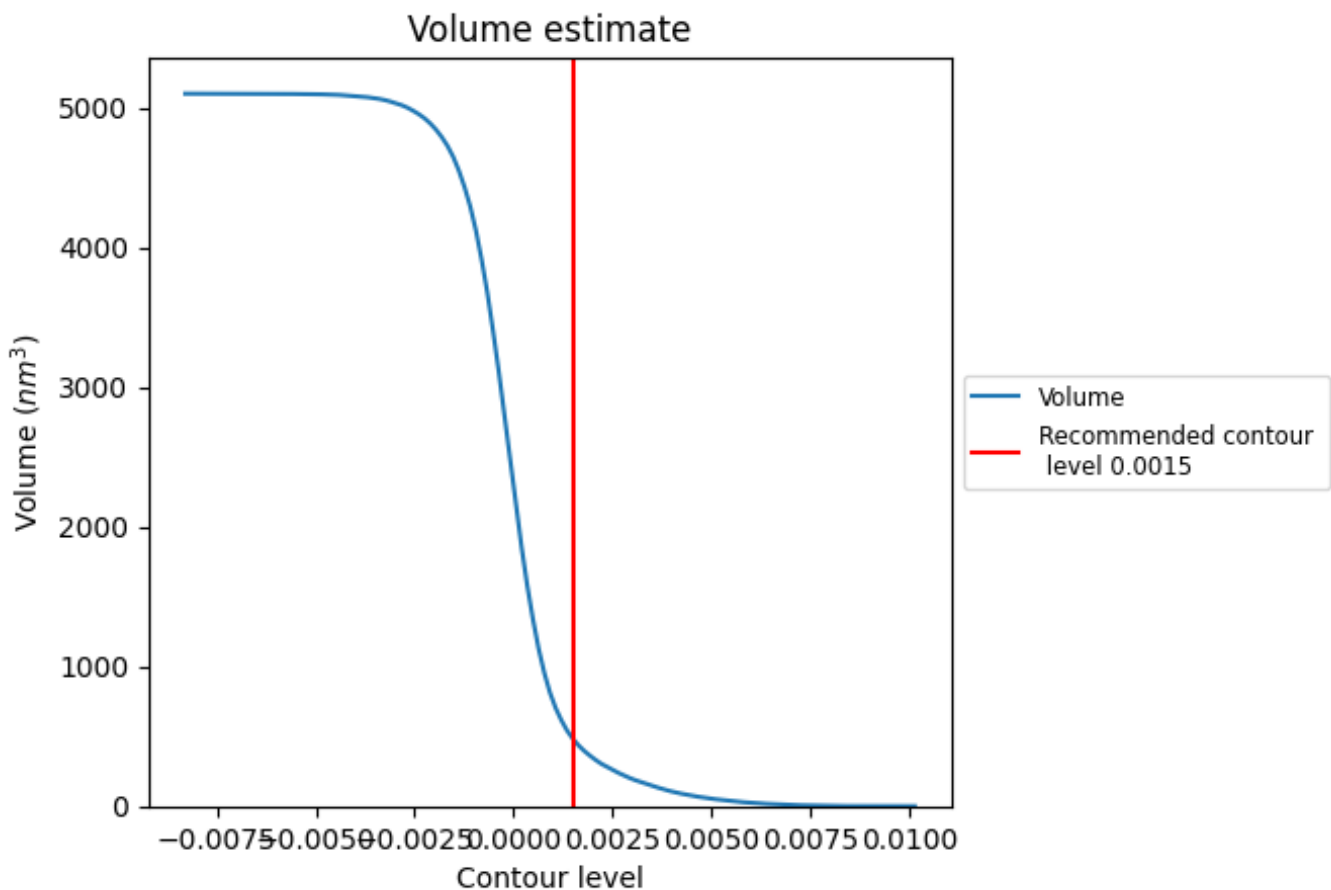
This section contains the results of statistical analysis of the map.

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 483 nm^3 ; this corresponds to an approximate mass of 436 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](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

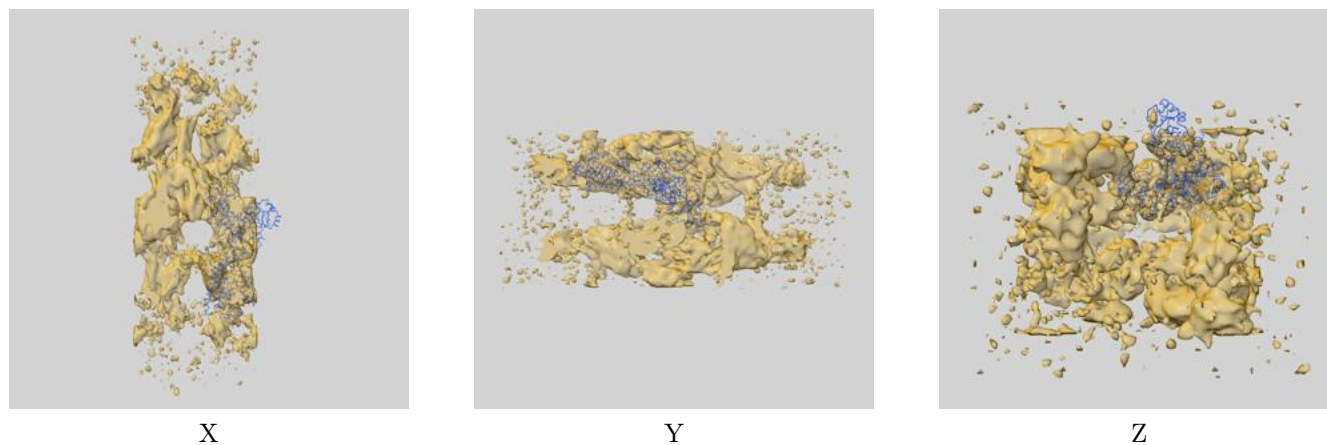
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

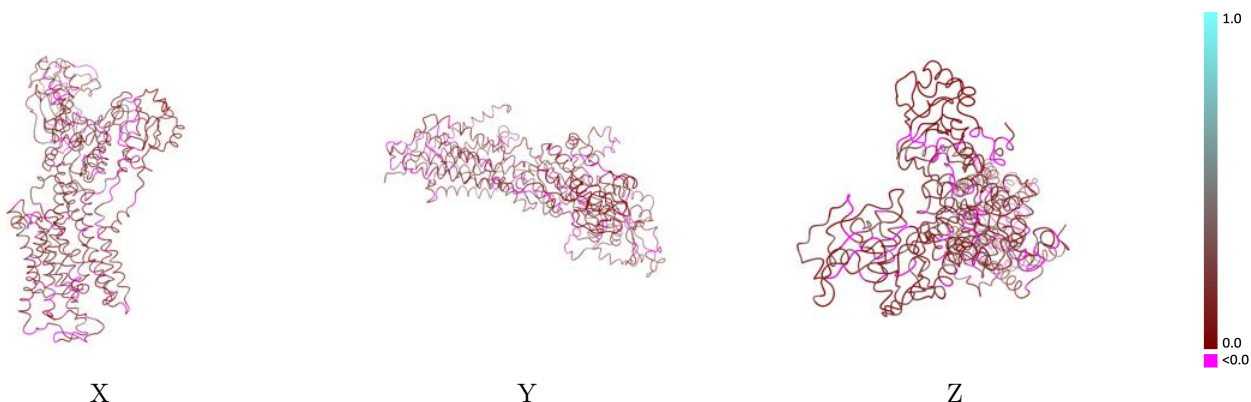
This section contains information regarding the fit between EMDB map EMD-5104 and PDB model 3IXZ. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay [i](#)



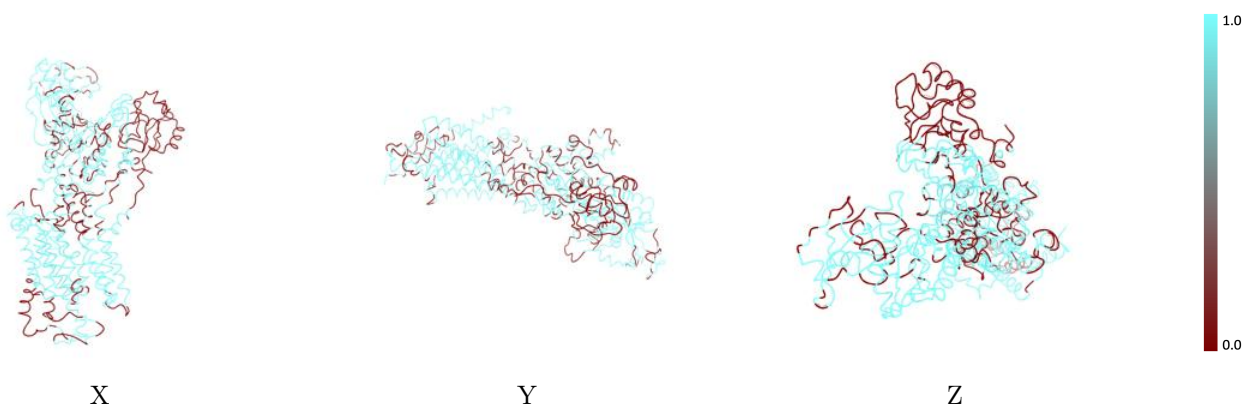
The images above show the 3D surface view of the map at the recommended contour level 0.0015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



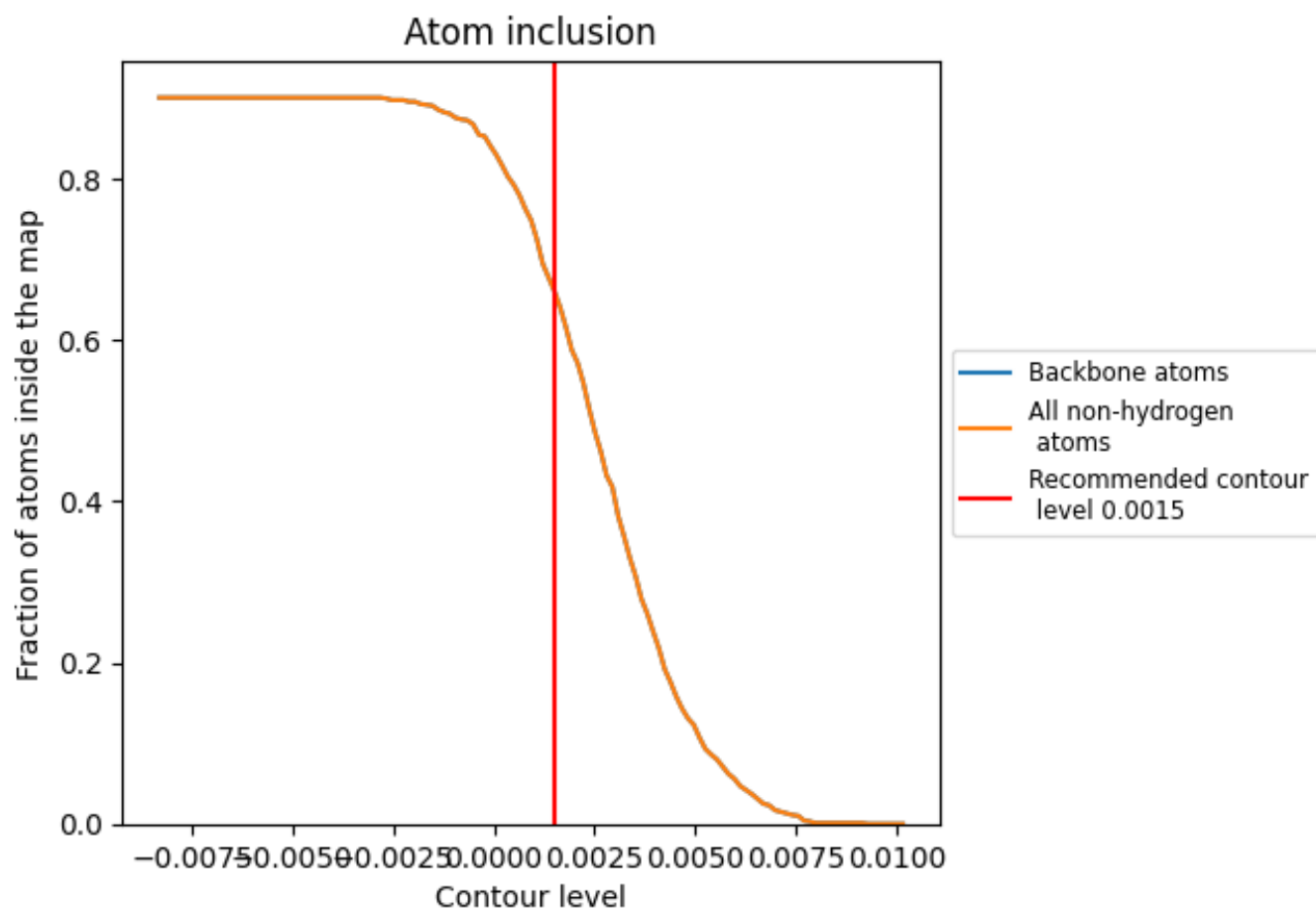
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0015).







9.4 Atom inclusion [i](#)



At the recommended contour level, 66% 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 (0.0015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6610	 0.1060
A	 0.6660	 0.1070
B	 0.5430	 0.0990

