



wwPDB EM Validation Summary Report ⓘ

Nov 11, 2024 – 05:40 AM EST

PDB ID : 7TYK
EMDB ID : EMD-26183
Title : Cryo-EM Structure of insulin receptor-related receptor (IRR) in apo-state captured at pH 7. The 3D refinement was applied with C2 symmetry
Authors : Wang, L.W.; Hall, C.; Li, J.; Choi, E.; Bai, X.C.
Deposited on : 2022-02-13
Resolution : 3.50 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.dev113
MolProbity : 4.02b-467
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) : 2.39

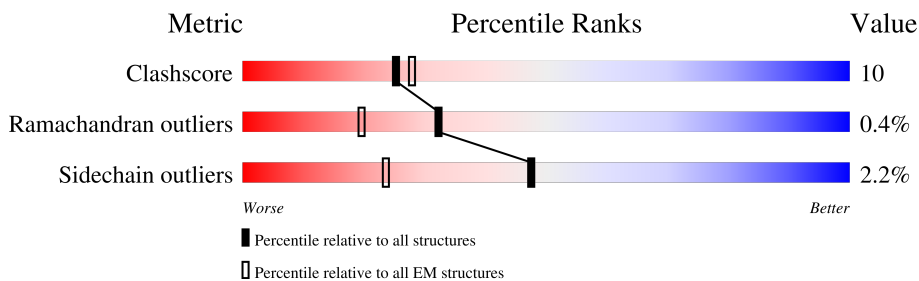
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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	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 ≥ 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	1297	<div> <div>8%</div> <div>47%</div> <div>14%</div> <div>38%</div> </div>
1	B	1297	<div> <div>8%</div> <div>47%</div> <div>15%</div> <div>38%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12698 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.

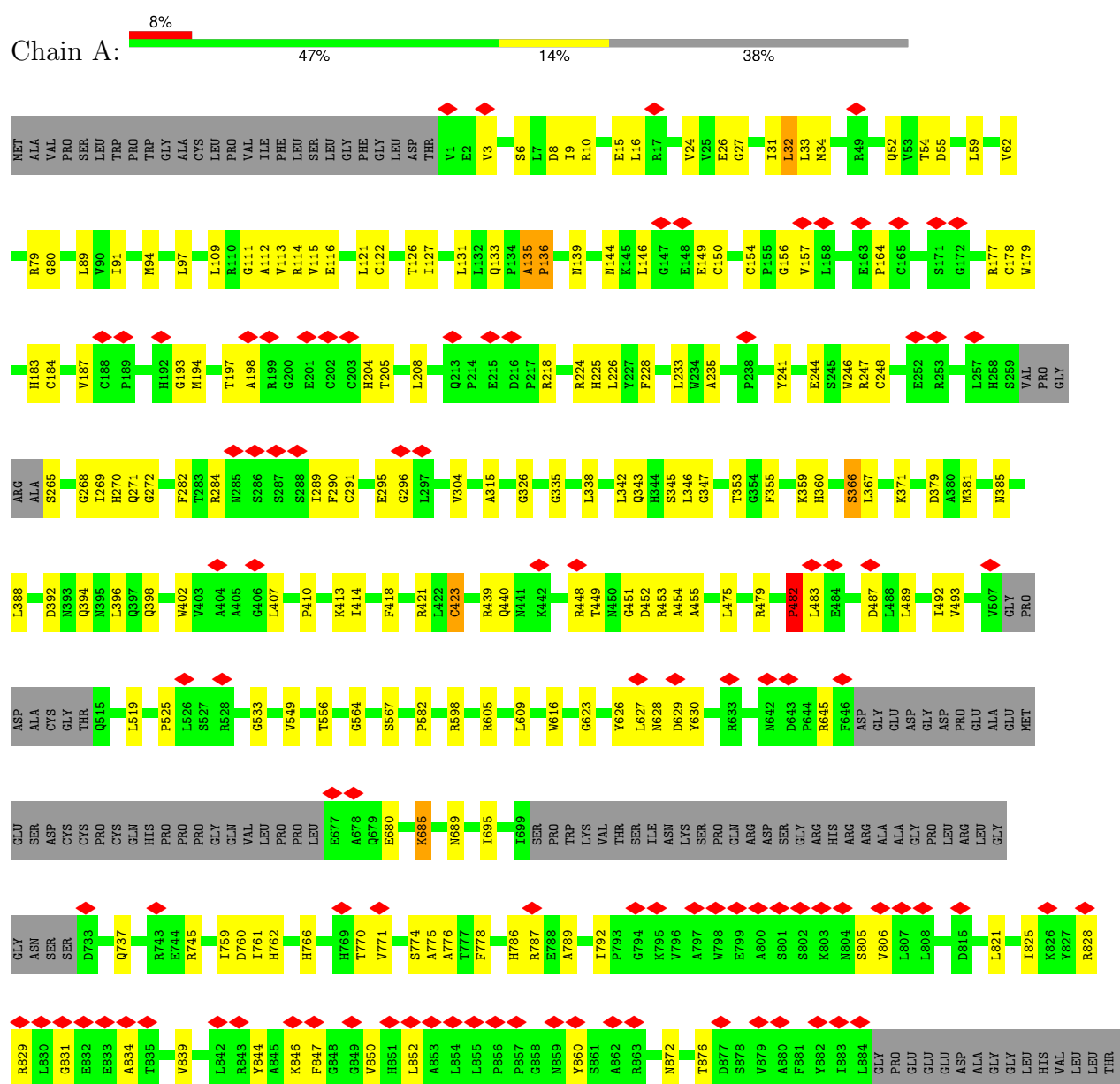
- Molecule 1 is a protein called Insulin receptor-related protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	809	Total	C	N	O	S	0	0
			6349	4017	1130	1163	39		
1	B	809	Total	C	N	O	S	0	0
			6349	4017	1130	1163	39		

3 Residue-property plots

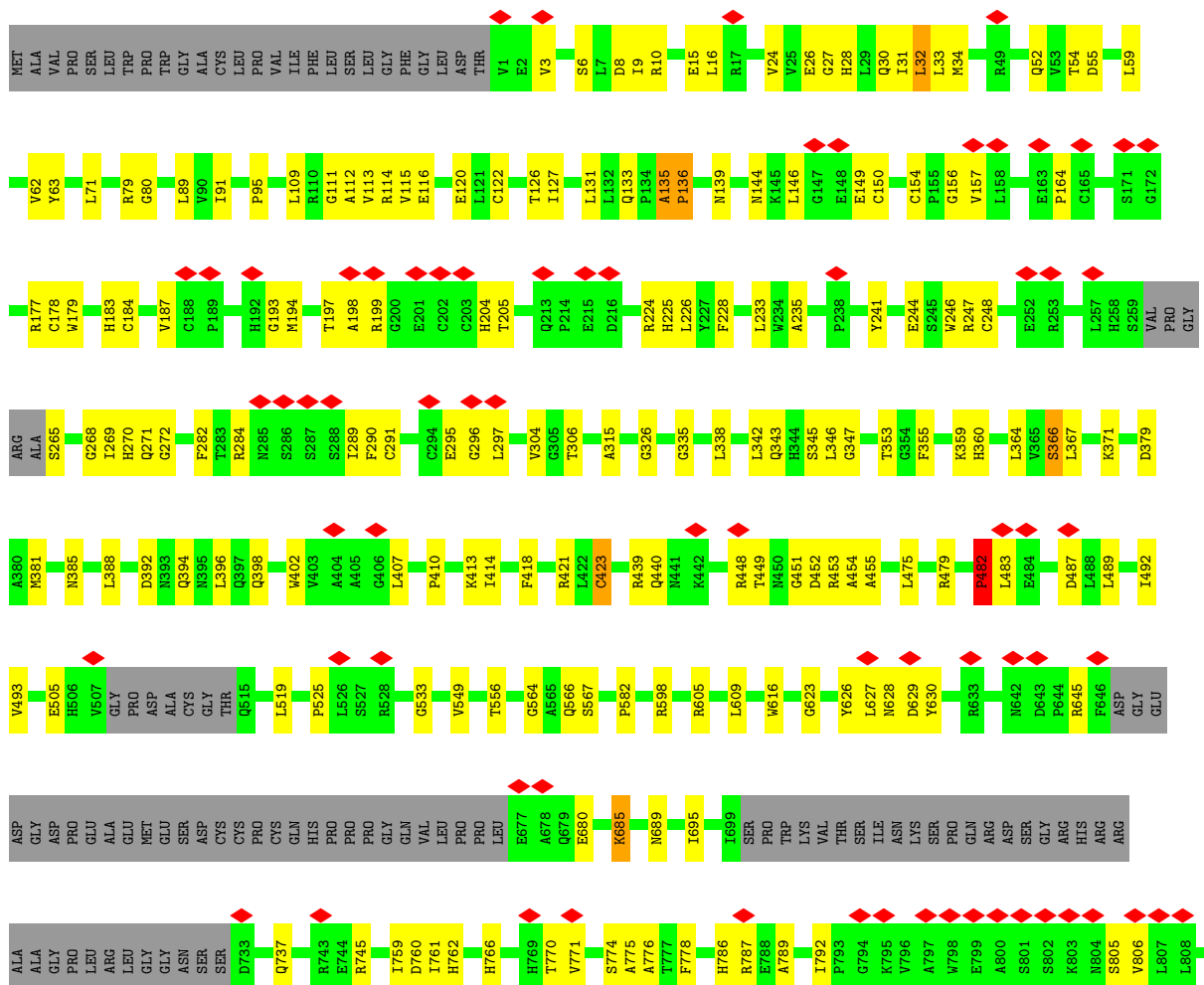
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Insulin receptor-related protein



ASP	ARG	GLY	ALA	GLY	ALA	GLY	GLN	THR
CYS	CYS	ILE	ASN	ILE	ASN	VAL	GLY	PRO
SER	TRP	THR	ASN	THR	VAL	VAL	SER	GLY
PRO	GLN	THR	PHE	THR	LYS	GLN	PHE	GLY
ASN	ASN	HIS	VAL	GLY	VAL	GLY	MET	THR
PRO	PRO	SER	HIS	SER	ARG	GLN	VAL	LEU
GLY	ARG	ASP	ARG	ASP	ARG	PRO	THR	LEU
PRO	LEU	VAL	ASP	VAL	ASN	THR	GLY	LEU
GLY	ARG	TRP	LEU	TRP	LEU	LEU	GLY	ILE
HIS	SER	PHE	ALA	THR	ALA	VAL	ALA	ALA
	THR	GLY	ARG	SER	ARG	ILE	ARG	ALA
	THR	VAL	ASN	GLU	ASN	MET	GLY	LEU
	HIS	VAL	CYS	VAL	CYS	GLY	LEU	GLY
	ILE	LEU	MET	THR	MET	MET	GLU	PHE
	LEU	TRP	VAL	SER	VAL	THR	ALA	THR
	ASP	GLU	SER	GLY	GLN	ARG	GLY	TYR
	SER	ILE	GLN	ILE	ASP	ASP	GLY	GLY
	ILE	VAL	PHE	THR	PHE	LEU	GLY	LYS
	GLN	THR	THR	THR	THR	LYS	THR	ARG
	GLU	LEU	VAL	VAL	VAL	SER	PRO	ASN
	GLU	ALA	ILE	LYS	LYS	HIS	VAL	ARG
	LEU	GLU	ILE	LEU	LEU	LEU	ALA	THR
	ARG	GLN	GLN	GLN	THR	GLY	ASN	VAL
	PRO	PRO	ASN	GLU	ARG	ARG	GLU	ASN
	SER	SER	ARG	THR	THR	GLY	LEU	PRO
	PHE	GLU	ASP	GLU	ASP	GLY	ALA	GLU
	LEU	VAL	VAL	GLN	VAL	ASN	SER	TYR
	TYR	THR	THR	VAL	GLY	ASN	PRO	PHE
	SER	LEU	GLU	THR	GLY	PRO	ARG	SER
	PRO	LYS	THR	THR	GLY	GLY	GLU	ALA
	GLU	PHE	ASP	VAL	TYR	PRO	ILE	ASP
	CYS	VAL	TYR	THR	GLN	GLY	GLU	ASP
	ARG	MET	TYR	GLN	GLY	GLY	GLY	MET
	GLY	ASP	ARG	ASP	LYS	ALA	PHE	TYR
	ALA	GLY	LYS	GLY	GLY	LEU	LEU	VAL
	ARG	VAL	GLY	GLY	GLY	LEU	LYS	PRO
	GLY	VAL	ARG	VAL	GLY	GLY	ASP	GLY
	GLY	LEU	LYS	LYS	GLY	ALA	GLU	ARG
	LEU	GLU	SER	GLY	GLY	MET	SER	TRP
	PRO	GLU	LEU	ILE	ILE	VAL	VAL	GLY
	THR	LEU	LEU	GLN	GLN	MET	PRO	VAL
	THR	GLU	PRO	MET	GLN	LYS	LYS	PRO
	ASP	GLN	ALA	ALA	ALA	HIS	CYS	ILE
	SER	GLN	PRO	ALA	ALA	SER	THR	SER
	THR	LEU	PRO	ASP	PRO	HIS	ILE	ILE
	SER	GLN	ARG	GLY	GLY	VAL	VAL	ARG
	SER	GLU	SER	MET	GLY	VAL	ARG	GLY
	PRO	LEU	LYS	TYR	THR	LEU	LEU	GLY

- Molecule 1: Insulin receptor-related protein



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	129384	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.204	Depositor
Minimum map value	-0.139	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	259.2, 259.2, 259.2	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.44	3/6500 (0.0%)	0.70	9/8836 (0.1%)
1	B	0.44	3/6500 (0.0%)	0.70	9/8836 (0.1%)
All	All	0.44	6/13000 (0.0%)	0.70	18/17672 (0.1%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	136	PRO	CB-CG	19.69	2.48	1.50
1	B	136	PRO	CB-CG	19.68	2.48	1.50
1	B	136	PRO	CG-CD	-17.33	0.93	1.50
1	A	136	PRO	CG-CD	-17.32	0.93	1.50
1	A	482	PRO	CG-CD	-10.88	1.14	1.50

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	136	PRO	CB-CG-CD	-27.30	0.01	106.50
1	A	136	PRO	CB-CG-CD	-27.30	0.03	106.50
1	A	482	PRO	N-CD-CG	-17.31	77.23	103.20
1	B	482	PRO	N-CD-CG	-17.29	77.26	103.20
1	B	482	PRO	CA-CB-CG	-15.49	74.57	104.00

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	6349	0	6230	132	0
1	B	6349	0	6230	130	0
All	All	12698	0	12460	257	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 10.

The worst 5 of 257 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:136:PRO:CG	1:A:136:PRO:N	1.83	1.37
1:B:136:PRO:N	1:B:136:PRO:CG	1.83	1.36
1:A:136:PRO:CD	1:A:136:PRO:HG3	1.70	1.11
1:B:136:PRO:CG	1:B:136:PRO:HD2	1.59	1.10
1:A:136:PRO:CG	1:A:136:PRO:HD3	1.59	1.09

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	799/1297 (62%)	728 (91%)	68 (8%)	3 (0%)	30	64
1	B	799/1297 (62%)	728 (91%)	68 (8%)	3 (0%)	30	64
All	All	1598/2594 (62%)	1456 (91%)	136 (8%)	6 (0%)	32	64

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	157	VAL
1	B	157	VAL
1	A	453	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	453	ARG
1	A	483	LEU

5.3.2 Protein sidechains ⓘ

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	689/1097 (63%)	674 (98%)	15 (2%)	47	70
1	B	689/1097 (63%)	673 (98%)	16 (2%)	45	69
All	All	1378/2194 (63%)	1347 (98%)	31 (2%)	47	70

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	872	ASN
1	B	685	LYS
1	B	122	CYS
1	B	844	TYR
1	B	482	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	343	GLN
1	B	762	HIS
1	A	343	GLN
1	B	133	GLN
1	B	139	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

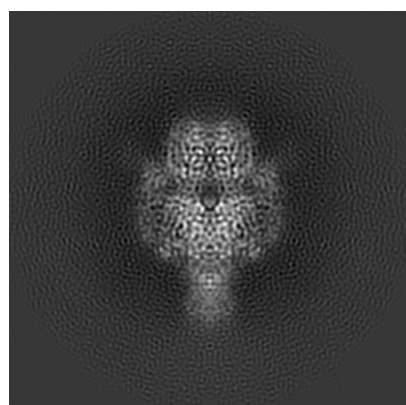
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26183. These allow visual inspection of the internal detail of the map and identification of artifacts.

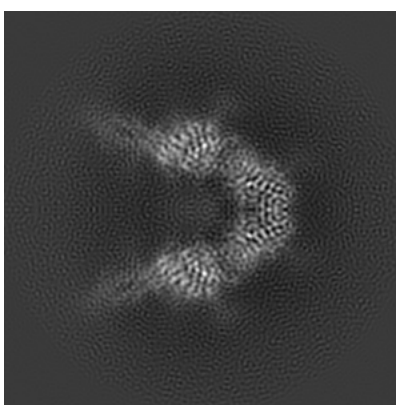
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

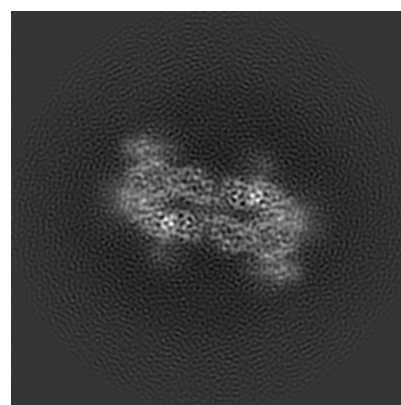
6.1.1 Primary map



X



Y

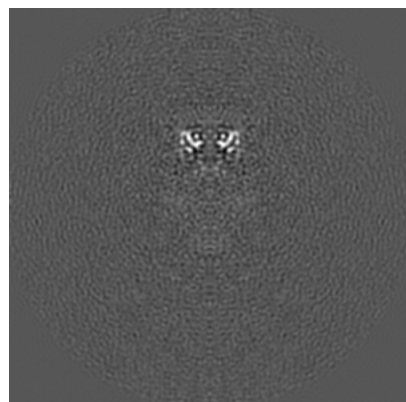


Z

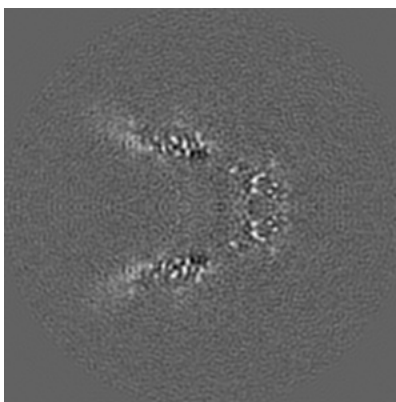
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

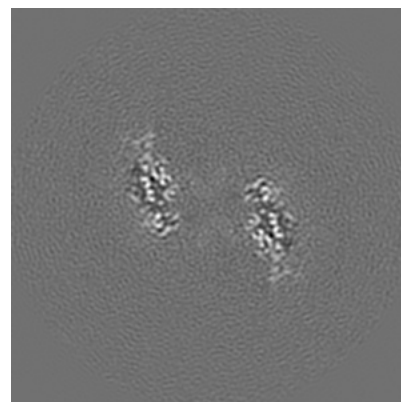
6.2.1 Primary map



X Index: 120



Y Index: 120

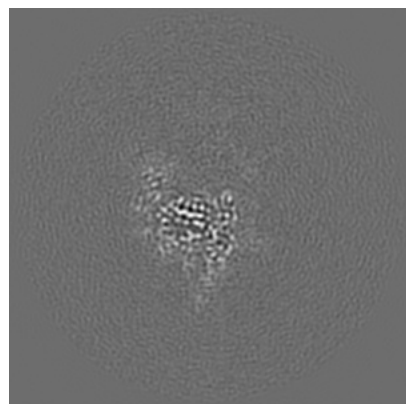


Z Index: 120

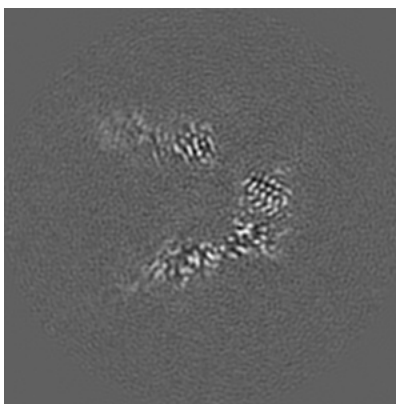
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

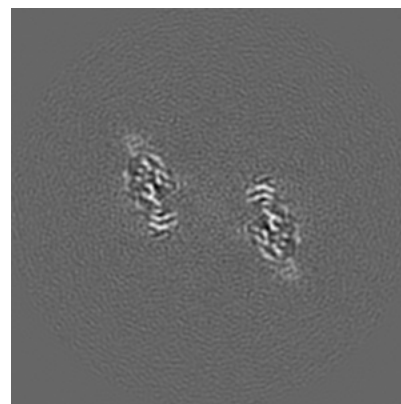
6.3.1 Primary map



X Index: 156



Y Index: 113

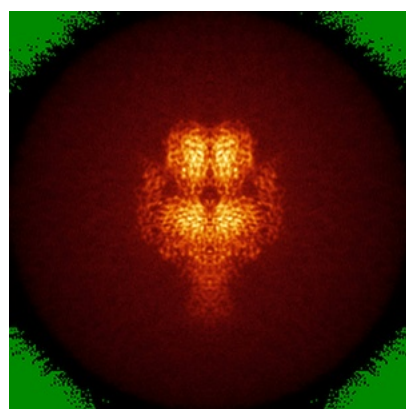


Z Index: 115

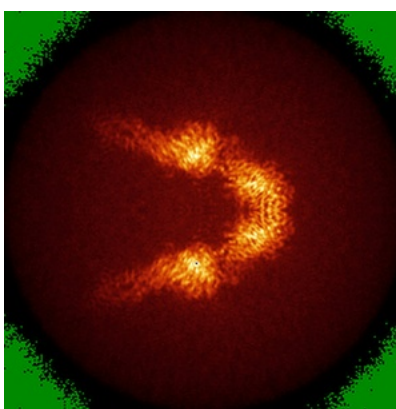
The images above show the largest variance slices of the map in three orthogonal directions.

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

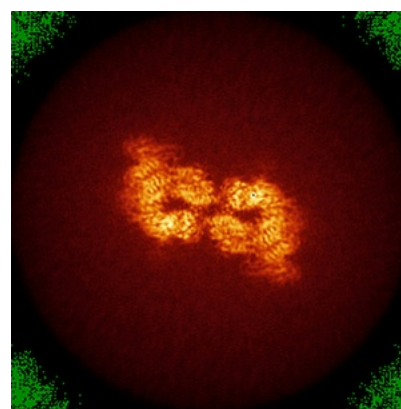
6.4.1 Primary map



X



Y

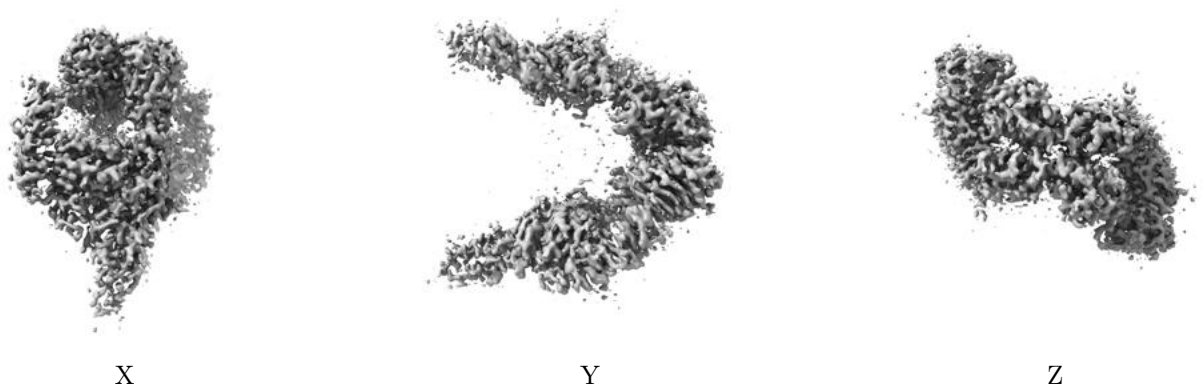


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

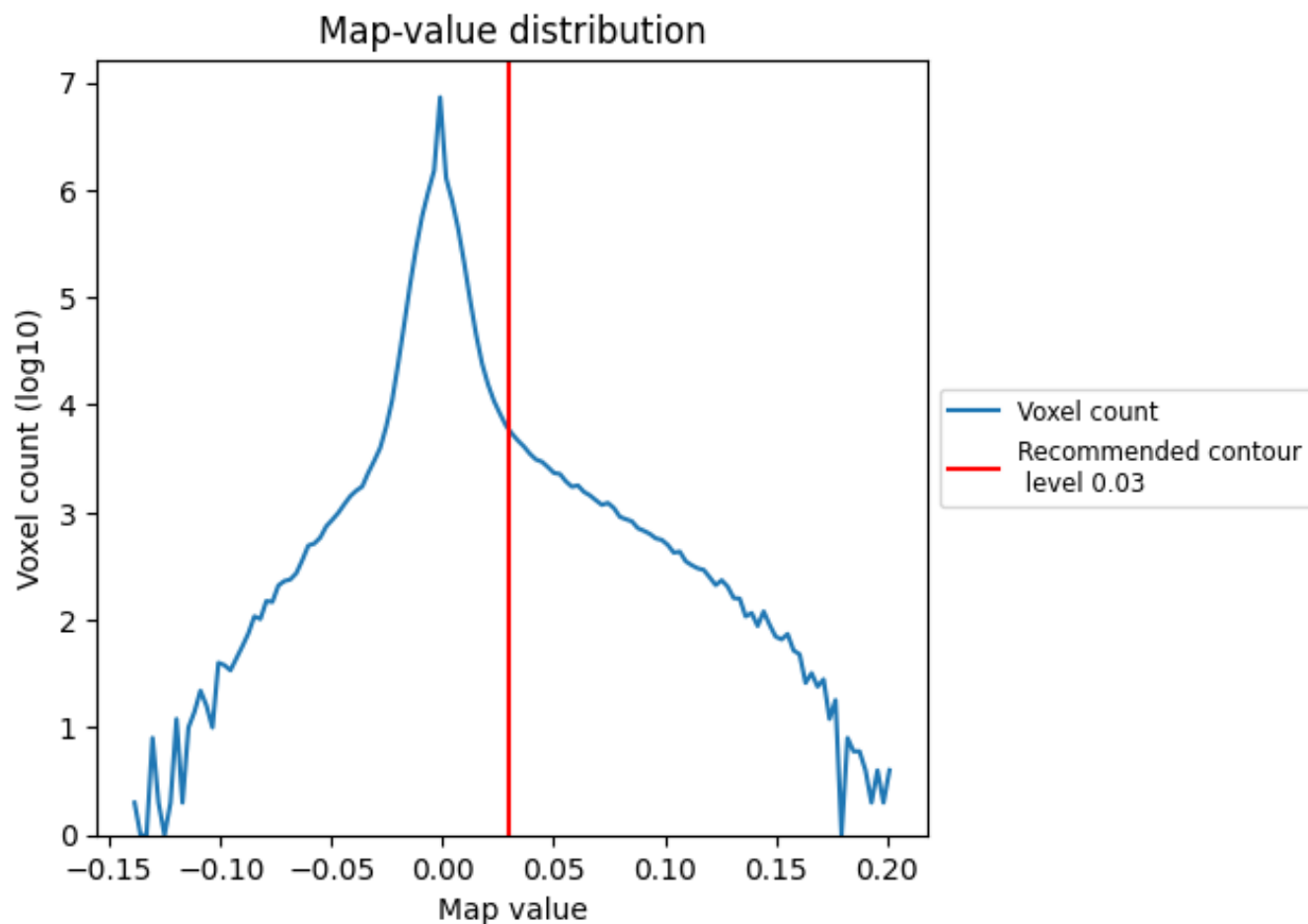
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

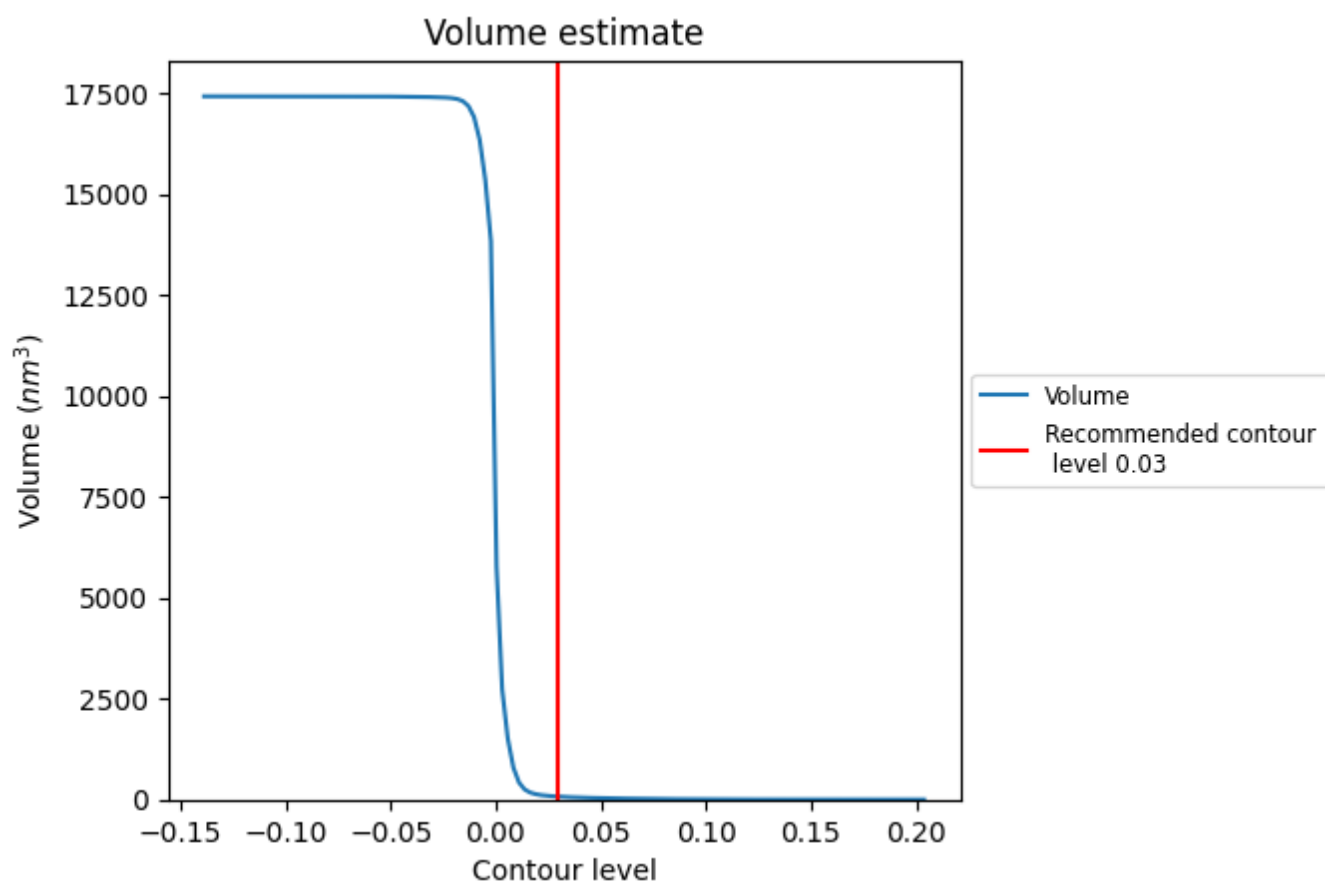
This section contains the results of statistical analysis of the map.

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.

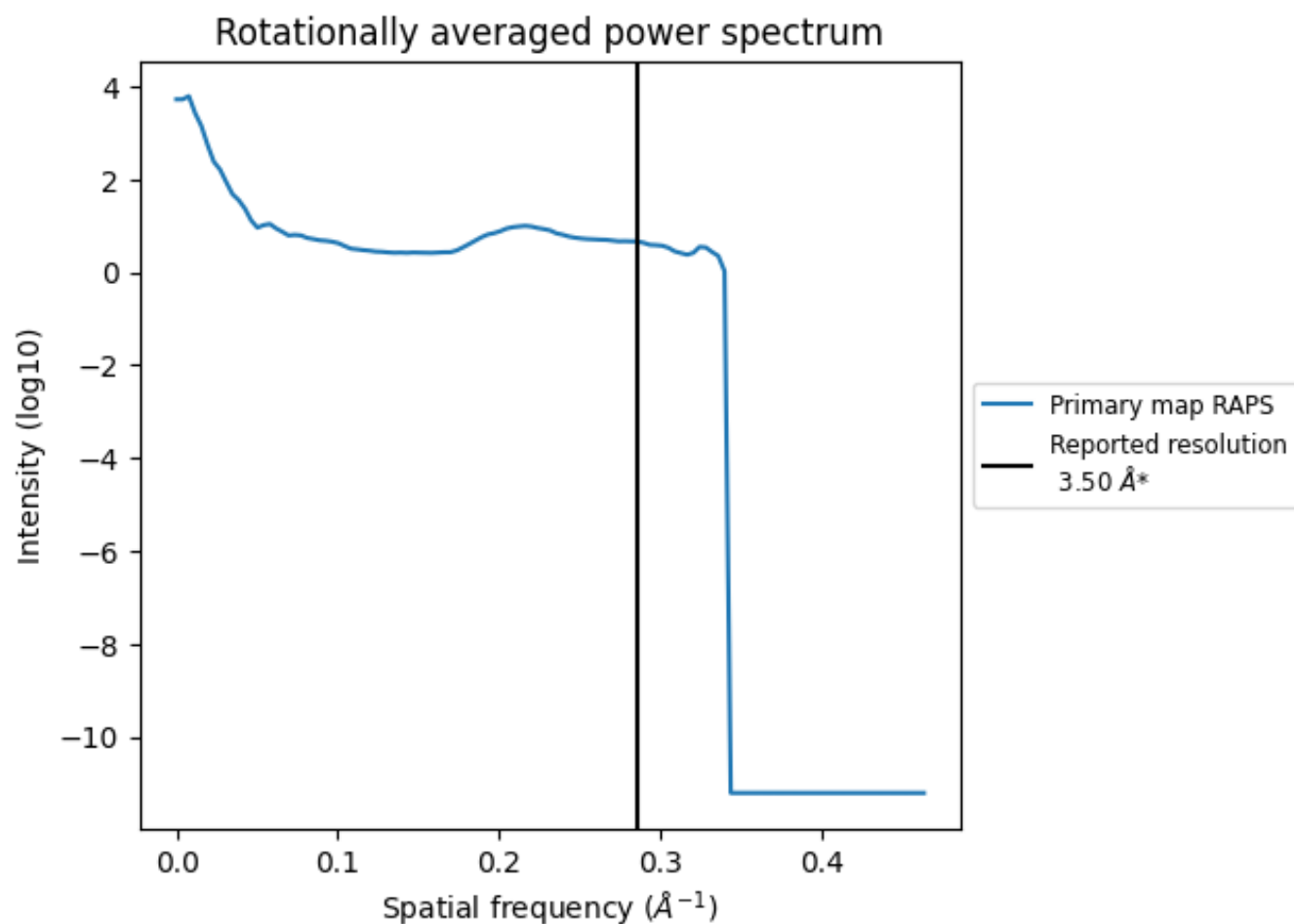
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 73 nm^3 ; this corresponds to an approximate mass of 66 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 ⓘ



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

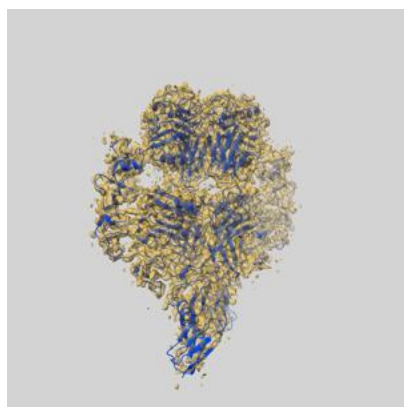
8 Fourier-Shell correlation

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

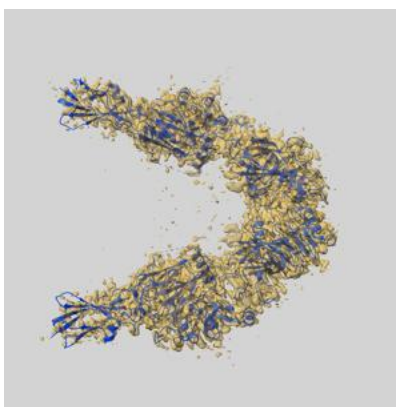
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-26183 and PDB model 7TYK. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

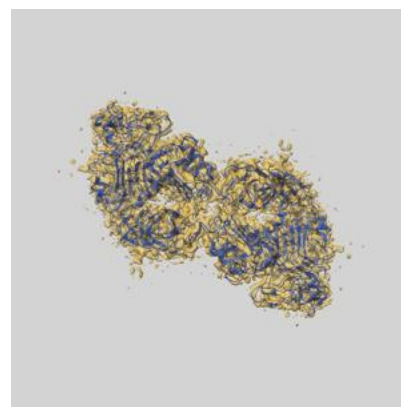
9.1 Map-model overlay [i](#)



X



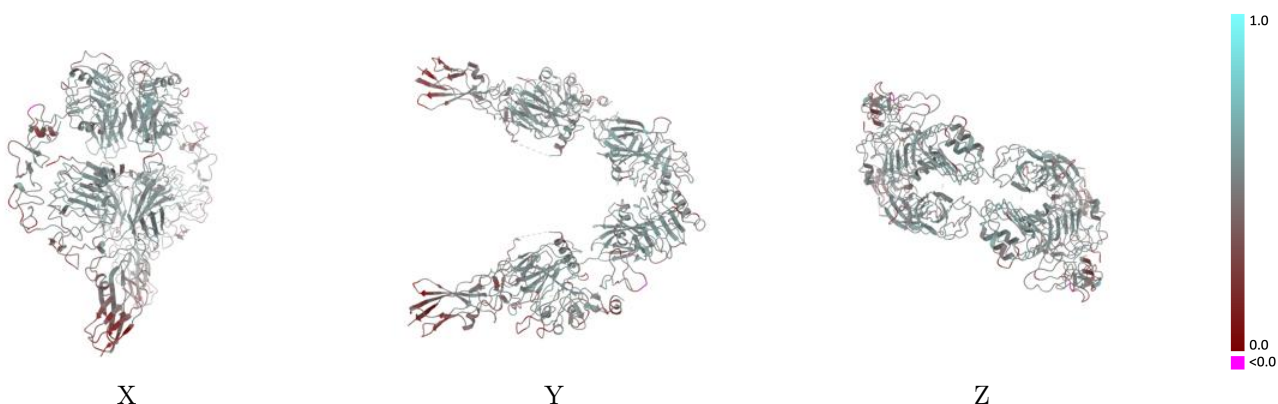
Y



Z

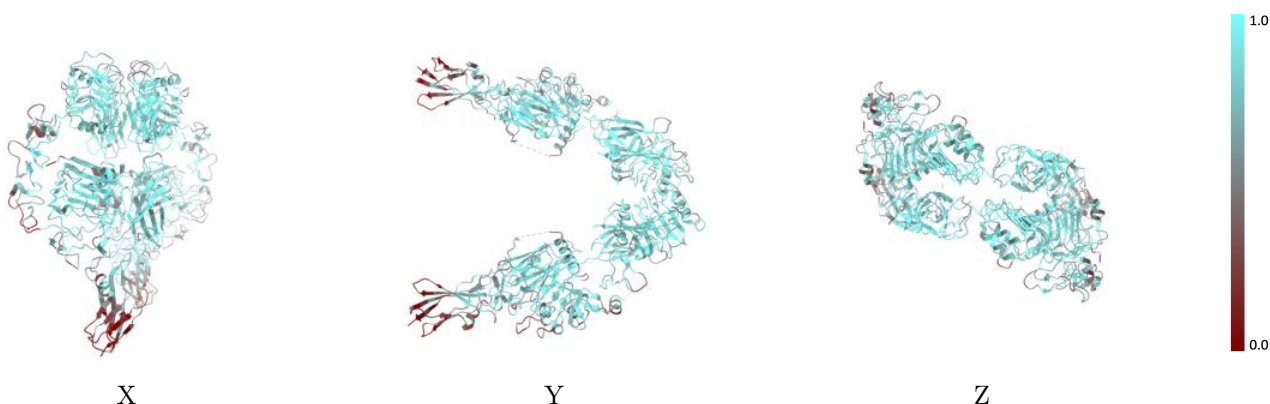
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



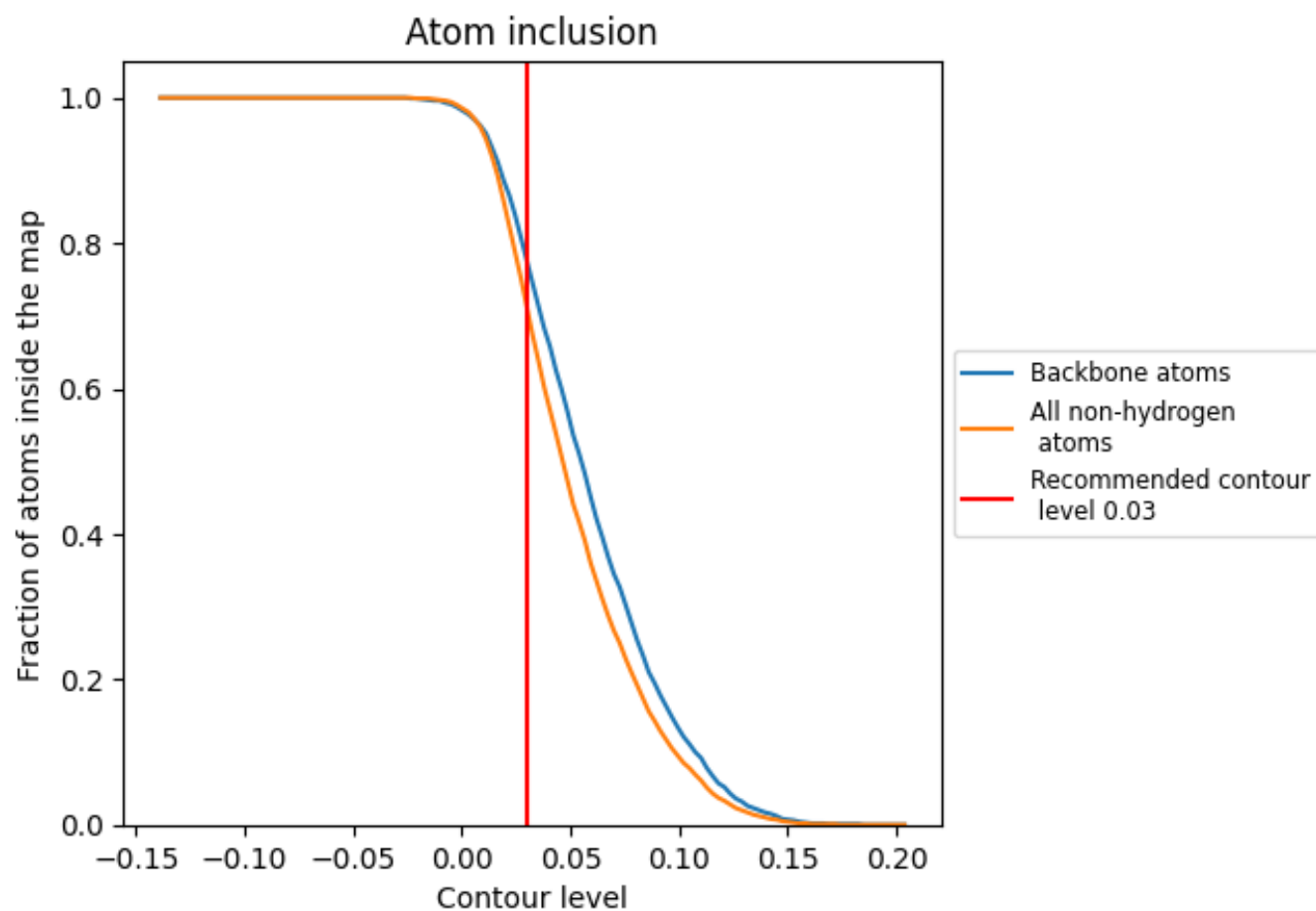
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 71% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7120	<div></div> 0.4790
A	<div></div> 0.7120	<div></div> 0.4780
B	<div></div> 0.7130	<div></div> 0.4790

