



wwPDB EM Validation Summary Report ⓘ

Jun 5, 2023 – 04:31 pm BST

PDB ID : 7ND2
EMDB ID : EMD-12273
Title : Cryo-EM structure of the human FERRY complex
Authors : Quentin, D.; Klink, B.U.; Raunser, S.
Deposited on : 2021-01-29
Resolution : 4.00 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.dev50
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) : 2.33

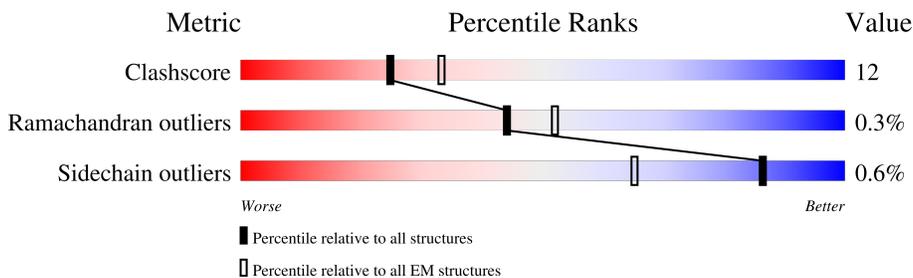
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 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
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	784	19% (Upper red bar) 28% (Red), 13% (Orange), 58% (Green), 2% (Yellow), 0% (Grey)
1	B	784	18% (Upper red bar) 28% (Red), 14% (Orange), 58% (Green), 0% (Yellow), 0% (Grey)
2	C	356	22% (Upper red bar) 74% (Green), 24% (Yellow), 2% (Grey)
2	D	356	22% (Upper red bar) 72% (Green), 26% (Yellow), 2% (Grey)
3	E	227	84% (Upper red bar) 62% (Green), 30% (Yellow), 7% (Grey)
3	F	227	81% (Upper red bar) 70% (Green), 19% (Yellow), 7% (Grey)
3	G	227	82% (Upper red bar) 63% (Green), 29% (Yellow), 7% (Grey)
3	H	227	81% (Upper red bar) 70% (Green), 20% (Yellow), 7% (Grey)

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 16824 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 Protein phosphatase 1 regulatory subunit 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	330	Total	C	N	O	S	0	0
			2565	1633	437	483	12		
1	B	330	Total	C	N	O	S	0	0
			2565	1633	437	483	12		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	MET	-	initiating methionine	UNP Q6ZMI0
A	-2	ALA	-	expression tag	UNP Q6ZMI0
A	-1	ALA	-	expression tag	UNP Q6ZMI0
A	0	ALA	-	expression tag	UNP Q6ZMI0
B	-3	MET	-	initiating methionine	UNP Q6ZMI0
B	-2	ALA	-	expression tag	UNP Q6ZMI0
B	-1	ALA	-	expression tag	UNP Q6ZMI0
B	0	ALA	-	expression tag	UNP Q6ZMI0

- Molecule 2 is a protein called Quinone oxidoreductase-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	352	Total	C	N	O	S	0	0
			2721	1734	464	511	12		
2	D	352	Total	C	N	O	S	0	0
			2721	1734	464	511	12		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	MET	-	initiating methionine	UNP O95825
C	-5	SER	-	expression tag	UNP O95825
C	-4	HIS	-	expression tag	UNP O95825
C	-3	HIS	-	expression tag	UNP O95825
C	-2	HIS	-	expression tag	UNP O95825

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	HIS	-	expression tag	UNP O95825
C	0	HIS	-	expression tag	UNP O95825
C	1	HIS	-	expression tag	UNP O95825
D	-6	MET	-	initiating methionine	UNP O95825
D	-5	SER	-	expression tag	UNP O95825
D	-4	HIS	-	expression tag	UNP O95825
D	-3	HIS	-	expression tag	UNP O95825
D	-2	HIS	-	expression tag	UNP O95825
D	-1	HIS	-	expression tag	UNP O95825
D	0	HIS	-	expression tag	UNP O95825
D	1	HIS	-	expression tag	UNP O95825

- Molecule 3 is a protein called Glutamine amidotransferase-like class 1 domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	210	Total	C	N	O	S	1	0
			1563	984	273	295	11		
3	F	210	Total	C	N	O	S	1	0
			1563	984	273	295	11		
3	H	210	Total	C	N	O	S	1	0
			1563	984	273	295	11		
3	G	210	Total	C	N	O	S	1	0
			1563	984	273	295	11		

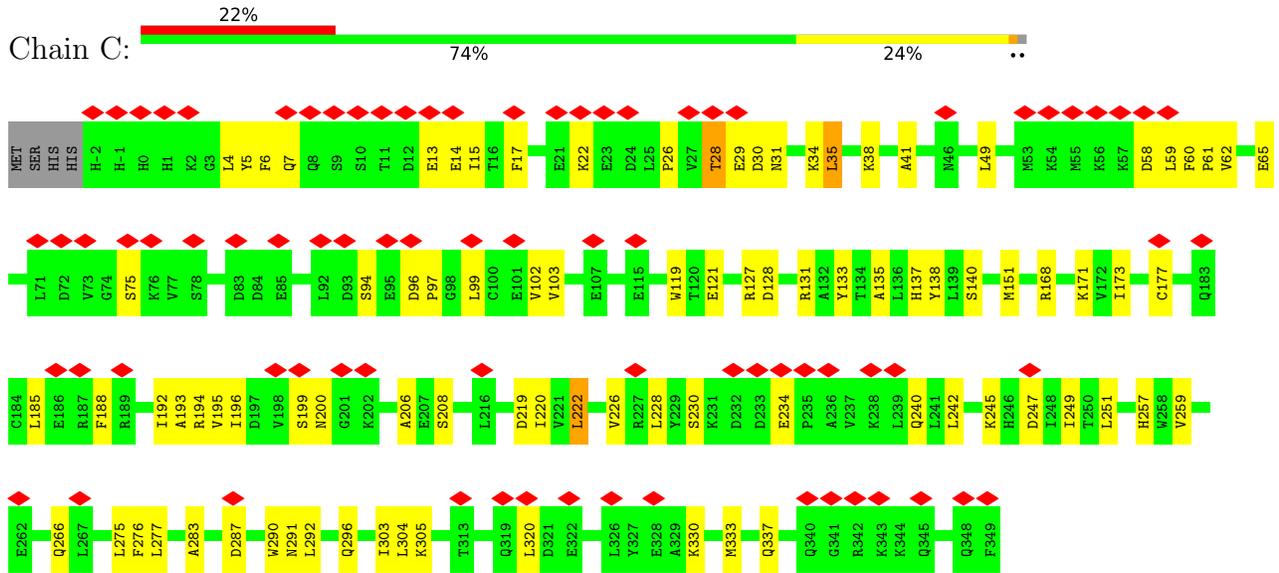
There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-6	MET	-	initiating methionine	UNP Q8NB37
E	-5	SER	-	expression tag	UNP Q8NB37
E	-4	HIS	-	expression tag	UNP Q8NB37
E	-3	HIS	-	expression tag	UNP Q8NB37
E	-2	HIS	-	expression tag	UNP Q8NB37
E	-1	HIS	-	expression tag	UNP Q8NB37
E	0	HIS	-	expression tag	UNP Q8NB37
E	1	HIS	-	expression tag	UNP Q8NB37
F	-6	MET	-	initiating methionine	UNP Q8NB37
F	-5	SER	-	expression tag	UNP Q8NB37
F	-4	HIS	-	expression tag	UNP Q8NB37
F	-3	HIS	-	expression tag	UNP Q8NB37
F	-2	HIS	-	expression tag	UNP Q8NB37
F	-1	HIS	-	expression tag	UNP Q8NB37

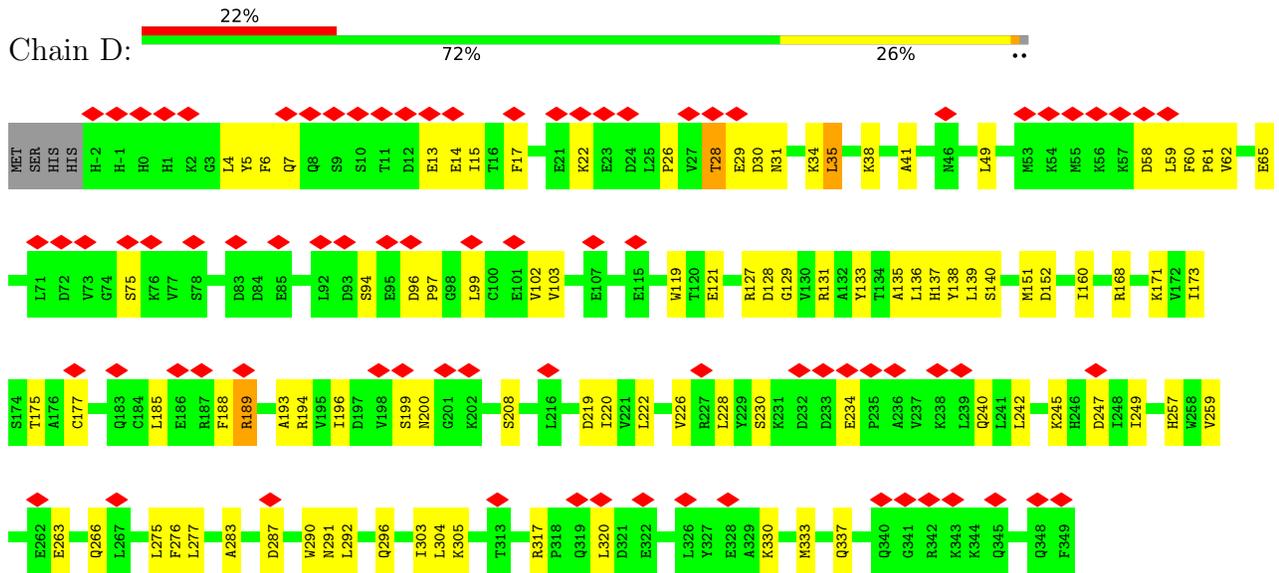
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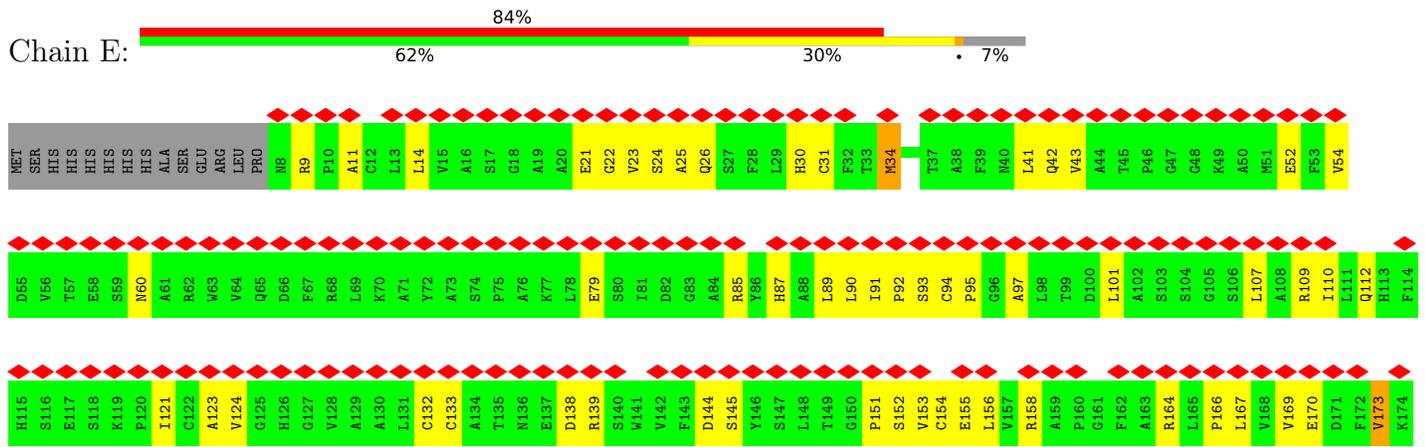
Chain	Residue	Modelled	Actual	Comment	Reference
F	0	HIS	-	expression tag	UNP Q8NB37
F	1	HIS	-	expression tag	UNP Q8NB37
H	-6	MET	-	initiating methionine	UNP Q8NB37
H	-5	SER	-	expression tag	UNP Q8NB37
H	-4	HIS	-	expression tag	UNP Q8NB37
H	-3	HIS	-	expression tag	UNP Q8NB37
H	-2	HIS	-	expression tag	UNP Q8NB37
H	-1	HIS	-	expression tag	UNP Q8NB37
H	0	HIS	-	expression tag	UNP Q8NB37
H	1	HIS	-	expression tag	UNP Q8NB37
G	-6	MET	-	initiating methionine	UNP Q8NB37
G	-5	SER	-	expression tag	UNP Q8NB37
G	-4	HIS	-	expression tag	UNP Q8NB37
G	-3	HIS	-	expression tag	UNP Q8NB37
G	-2	HIS	-	expression tag	UNP Q8NB37
G	-1	HIS	-	expression tag	UNP Q8NB37
G	0	HIS	-	expression tag	UNP Q8NB37
G	1	HIS	-	expression tag	UNP Q8NB37



• Molecule 2: Quinone oxidoreductase-like protein 1



• Molecule 3: Glutamine amidotransferase-like class 1 domain-containing protein 1



H115	S116	E117	S118	K119	P120	I121	C122	A123	V124	G125	H126	G127	V128	A129	A130	L131	C132	C133	A134	T135	N136	E137	D138	R139	S140	W141	V142	F143	D144	S145	Y146	S147	L148	T149	G150	P151	S152	V153	C154	E155	L156	V157	R158	A159	P160	G161	F162	A163	R164	L165	P166	L167	V168	V169	E170	D171	F172	V173	K174
D175	S176	G177	A178	C179	F180	S181	A182	S183	E184	P185	D186	A187	V190	V191	L192	D193	R194	H195	L196	V197	T198	G199	Q200	N201	A202	S203	S204	T205	V209	Q210	N211	L212	L213	F214	L215	C216	G217	SER	ARG	LYS																			

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	18300	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	75.8	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.049	Depositor
Minimum map value	-0.026	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.011	Depositor
Map size (\AA)	285.12003, 285.12003, 285.12003	wwPDB
Map dimensions	264, 264, 264	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	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	0.50	0/2609	0.84	7/3532 (0.2%)
1	B	0.52	0/2609	0.83	4/3532 (0.1%)
2	C	0.62	0/2774	0.87	5/3760 (0.1%)
2	D	0.62	0/2774	0.88	5/3760 (0.1%)
3	E	0.45	0/1599	0.92	6/2179 (0.3%)
3	F	0.42	0/1599	0.85	6/2179 (0.3%)
3	G	0.51	1/1599 (0.1%)	0.97	8/2179 (0.4%)
3	H	0.40	0/1599	0.85	5/2179 (0.2%)
All	All	0.53	1/17162 (0.0%)	0.87	46/23300 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	F	0	1
3	H	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	92	PRO	CG-CD	-8.80	1.21	1.50

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	92	PRO	N-CD-CG	-10.27	87.80	103.20
3	F	165	LEU	CA-CB-CG	9.50	137.16	115.30
3	H	165	LEU	CA-CB-CG	9.15	136.34	115.30
1	A	424	LEU	CA-CB-CG	8.74	135.40	115.30
3	E	21	GLU	CA-CB-CG	8.28	131.62	113.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	F	70	LYS	Peptide
3	H	70	LYS	Peptide

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	2565	0	2564	79	0
1	B	2565	0	2564	81	0
2	C	2721	0	2727	56	0
2	D	2721	0	2727	61	0
3	E	1563	0	1526	41	0
3	F	1563	0	1526	33	0
3	G	1563	0	1526	36	0
3	H	1563	0	1526	32	0
All	All	16824	0	16686	391	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 12.

The worst 5 of 391 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:412:PRO:HD2	1:A:511:PRO:HG3	1.71	0.73
1:B:412:PRO:HD2	1:B:511:PRO:HG3	1.73	0.70
3:H:59:SER:O	3:H:62:ARG:NH1	2.25	0.70
1:B:420:TYR:HA	1:B:423:VAL:HB	1.73	0.69
3:E:154:CYS:SG	3:E:155:GLU:N	2.67	0.67

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	326/784 (42%)	313 (96%)	13 (4%)	0	100	100
1	B	326/784 (42%)	313 (96%)	13 (4%)	0	100	100
2	C	350/356 (98%)	333 (95%)	15 (4%)	2 (1%)	25	63
2	D	350/356 (98%)	332 (95%)	16 (5%)	2 (1%)	25	63
3	E	209/227 (92%)	194 (93%)	15 (7%)	0	100	100
3	F	209/227 (92%)	198 (95%)	10 (5%)	1 (0%)	29	67
3	G	209/227 (92%)	193 (92%)	15 (7%)	1 (0%)	29	67
3	H	209/227 (92%)	196 (94%)	12 (6%)	1 (0%)	29	67
All	All	2188/3188 (69%)	2072 (95%)	109 (5%)	7 (0%)	44	75

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	29	GLU
3	F	152	SER
2	D	29	GLU
3	H	152	SER
3	G	20	ALA

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	278/694 (40%)	278 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	278/694 (40%)	277 (100%)	1 (0%)	91	94
2	C	298/310 (96%)	298 (100%)	0	100	100
2	D	298/310 (96%)	298 (100%)	0	100	100
3	E	168/183 (92%)	165 (98%)	3 (2%)	59	77
3	F	168/183 (92%)	163 (97%)	5 (3%)	41	64
3	G	168/183 (92%)	166 (99%)	2 (1%)	71	84
3	H	168/183 (92%)	164 (98%)	4 (2%)	49	69
All	All	1824/2740 (67%)	1809 (99%)	15 (1%)	86	89

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	F	195[B]	HIS
3	G	195[A]	HIS
1	B	419	ASN
3	G	195[B]	HIS
3	H	195[A]	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	297	GLN
1	B	419	ASN
3	G	60	ASN
3	G	26	GLN
3	E	42	GLN

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.

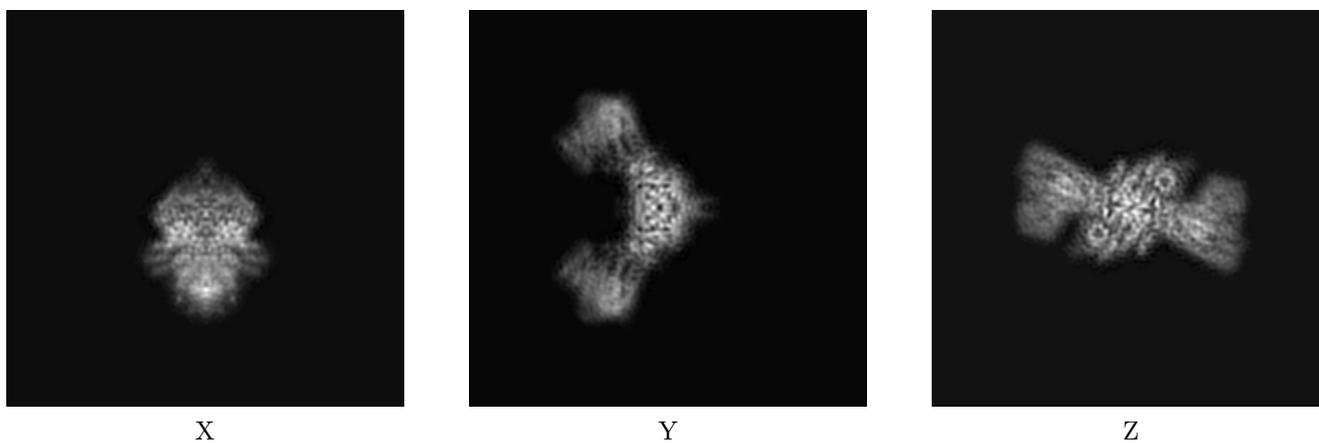
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12273. 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](#)

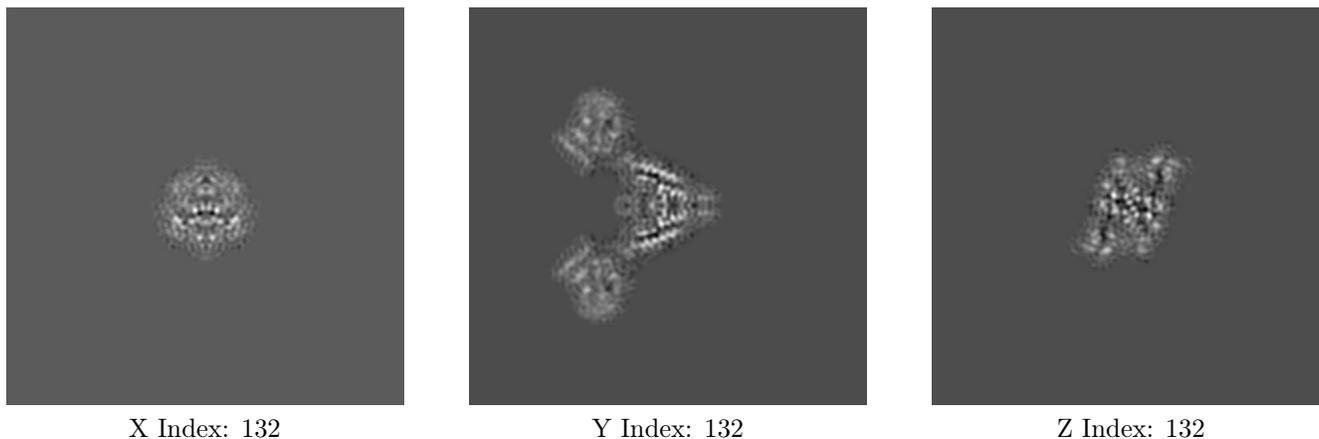
6.1.1 Primary map



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

6.2 Central slices [i](#)

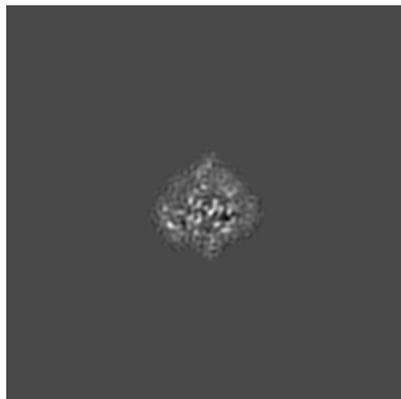
6.2.1 Primary map



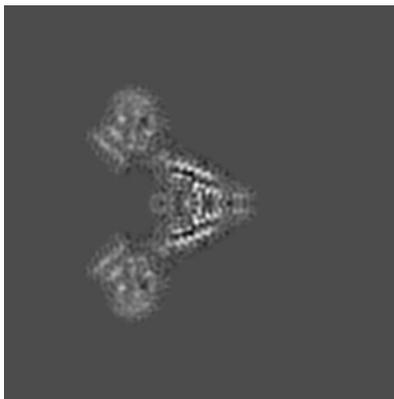
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

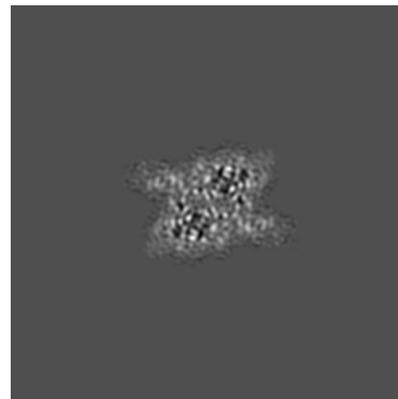
6.3.1 Primary map



X Index: 128



Y Index: 132

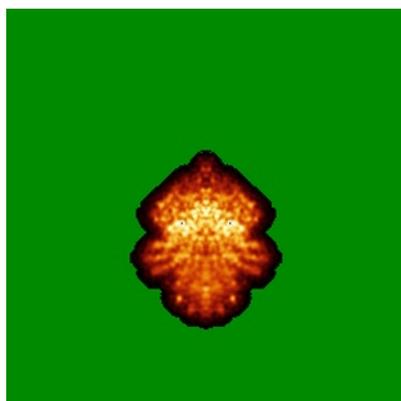


Z Index: 119

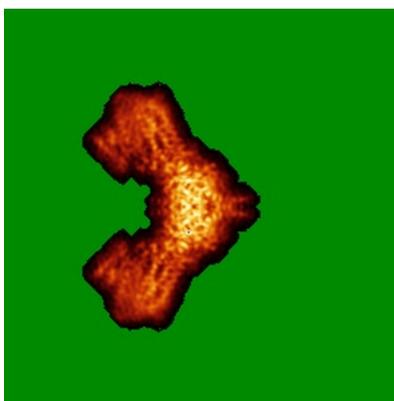
The images above show the largest variance slices of the map in three orthogonal directions.

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

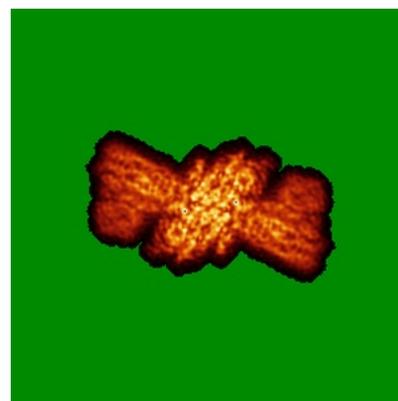
6.4.1 Primary map



X



Y

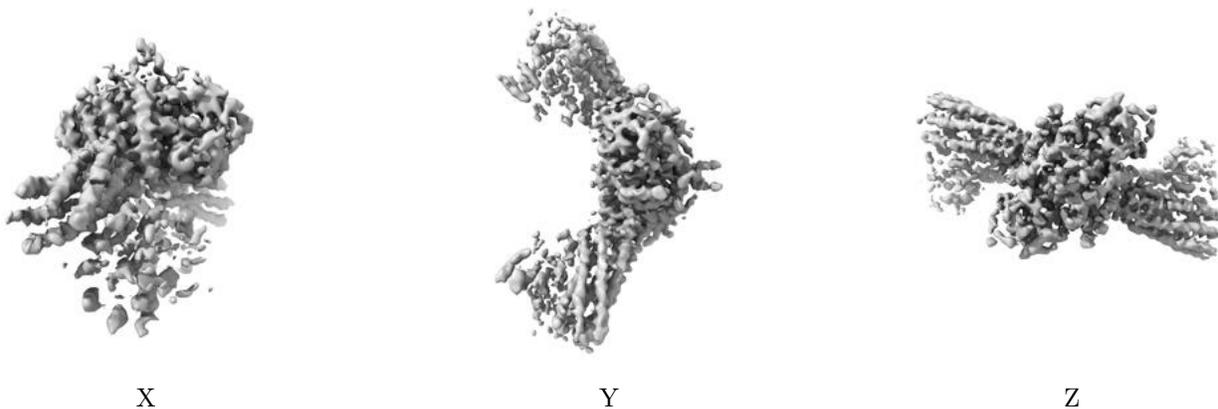


Z

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

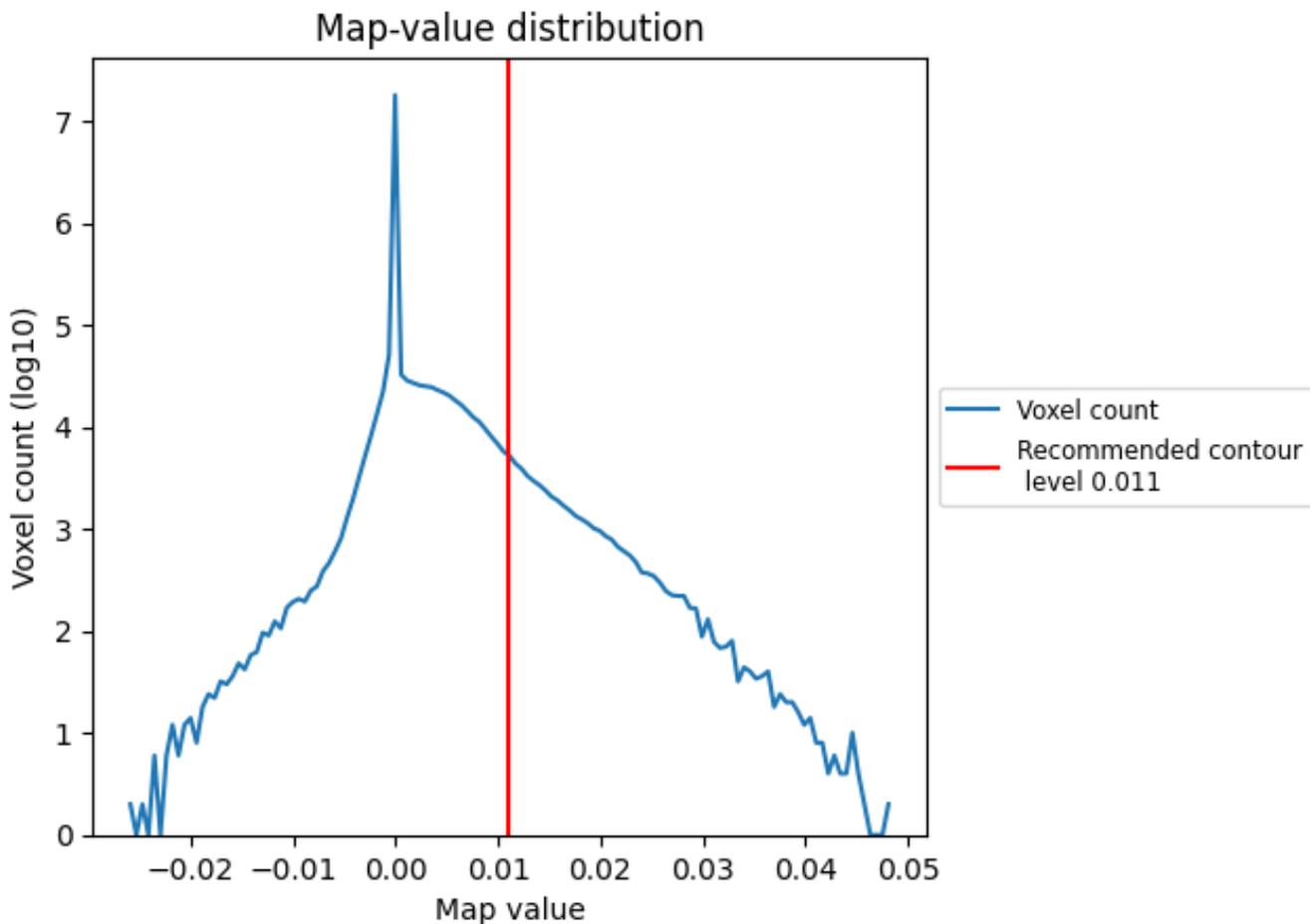
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

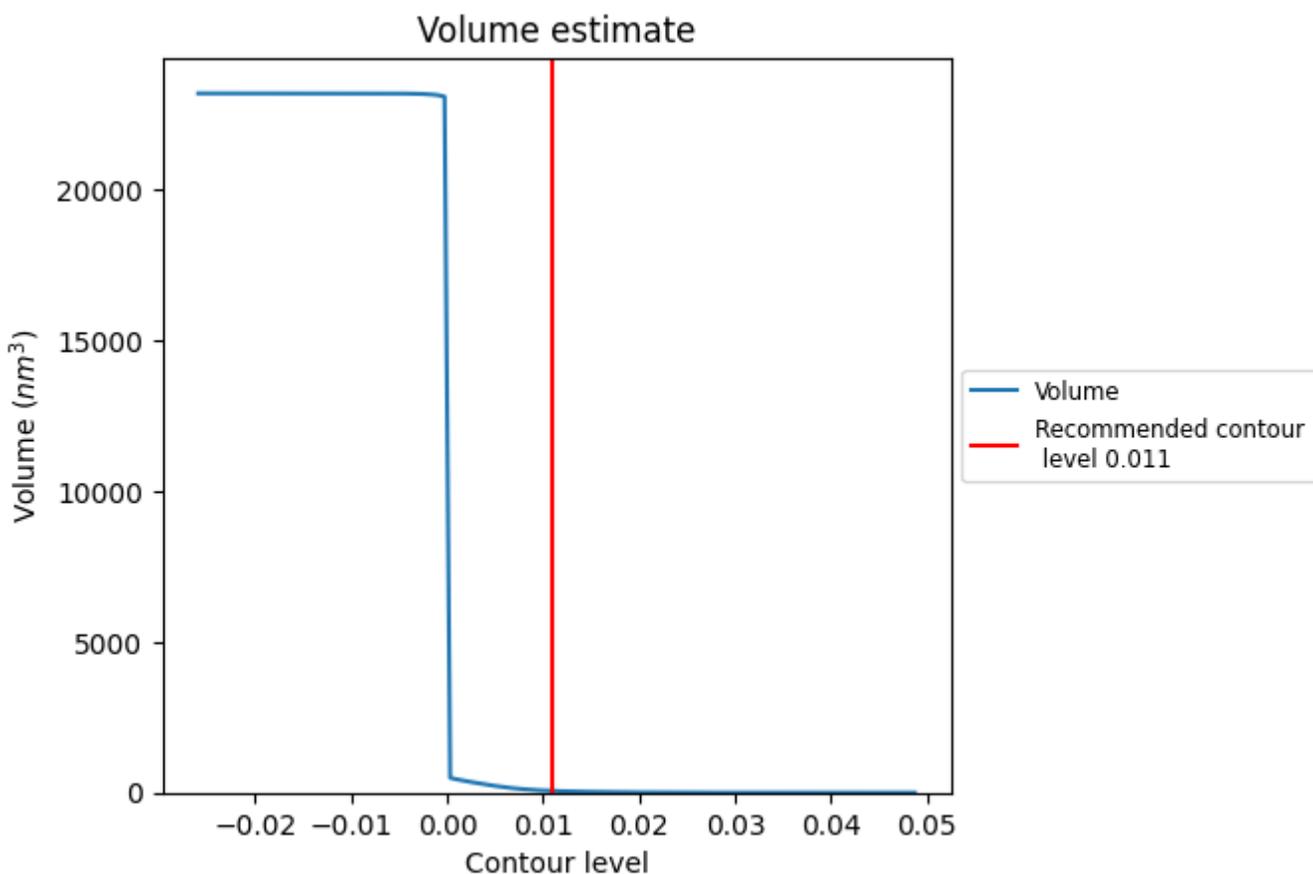
This section contains the results of statistical analysis of the map.

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.

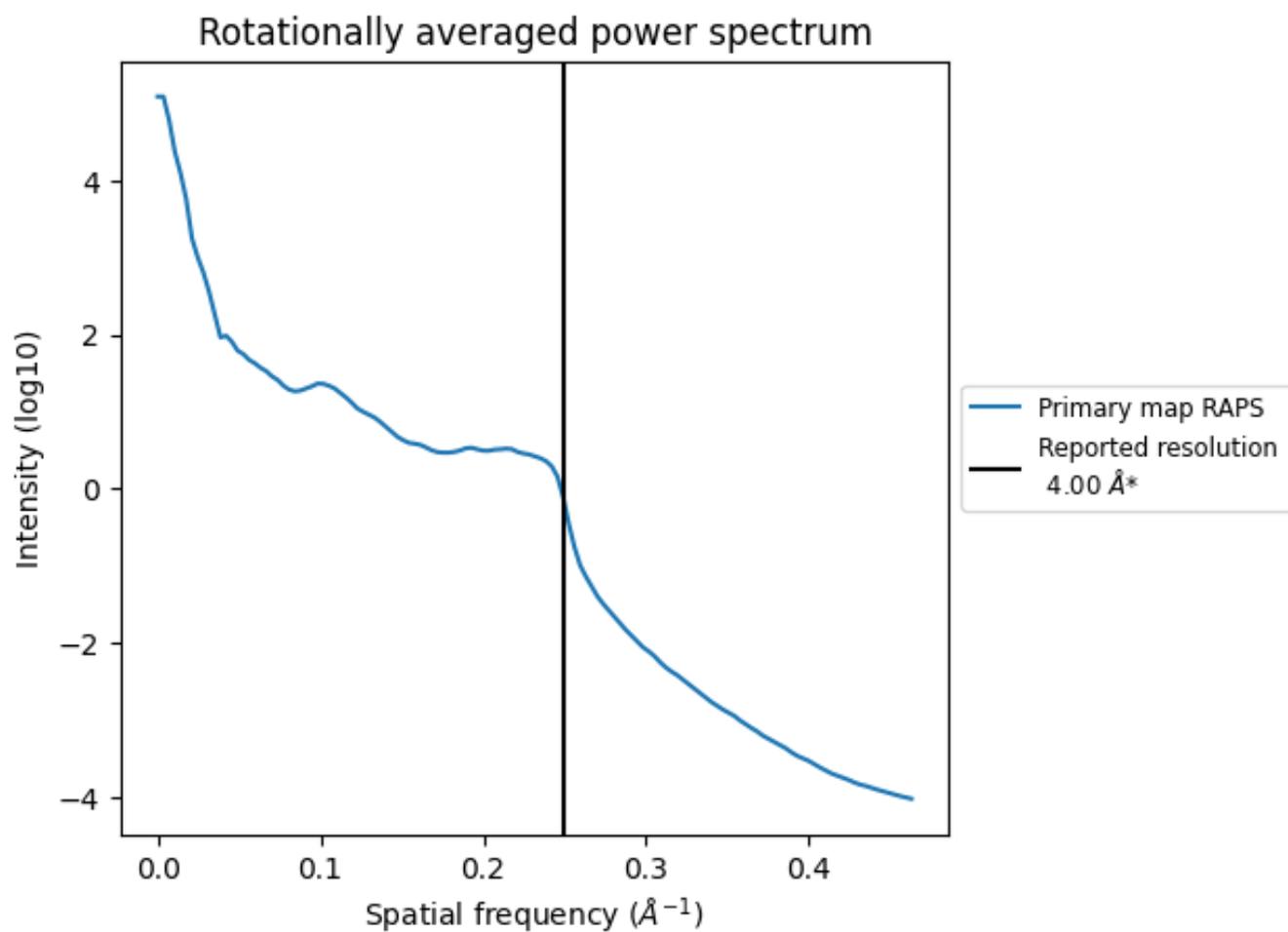
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 58 nm³; this corresponds to an approximate mass of 53 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 0.250\AA^{-1}

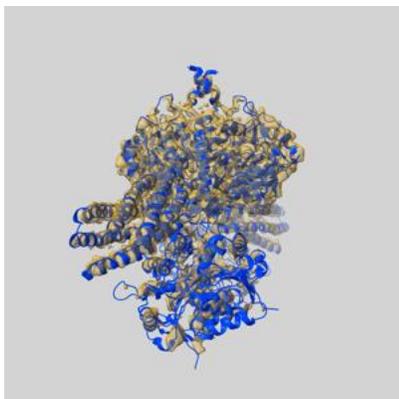
8 Fourier-Shell correlation

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

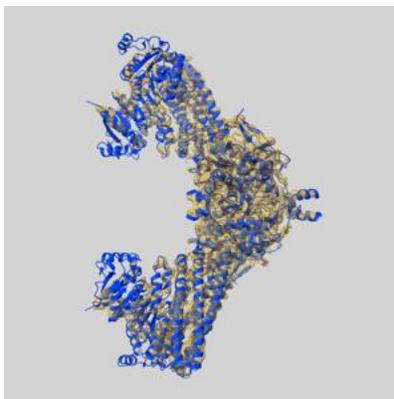
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12273 and PDB model 7ND2. Per-residue inclusion information can be found in section 3 on page 6.

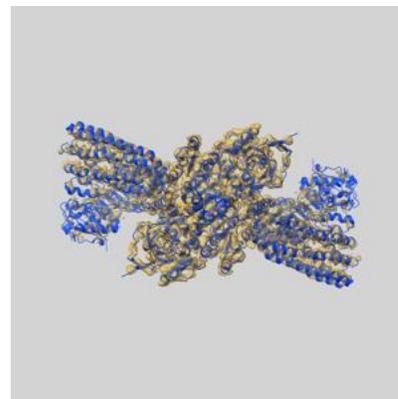
9.1 Map-model overlay [i](#)



X



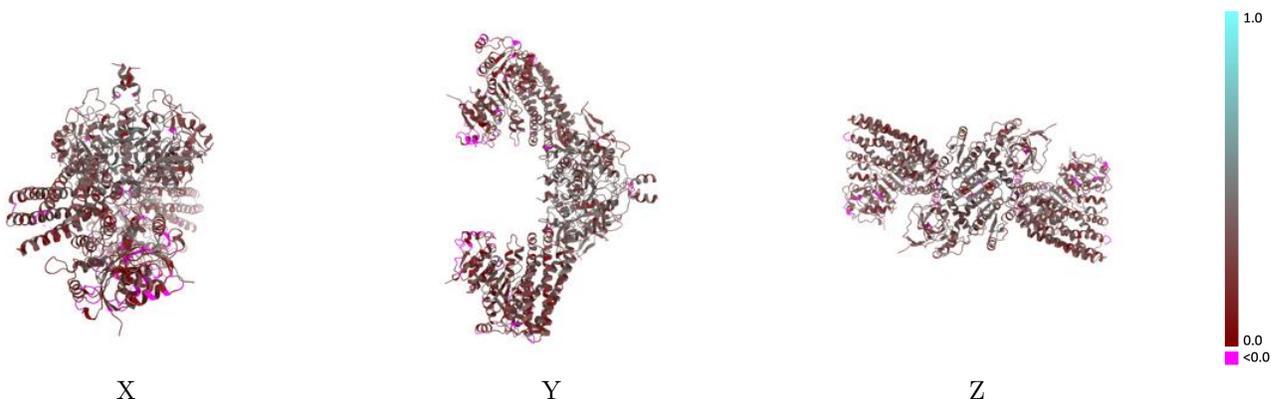
Y



Z

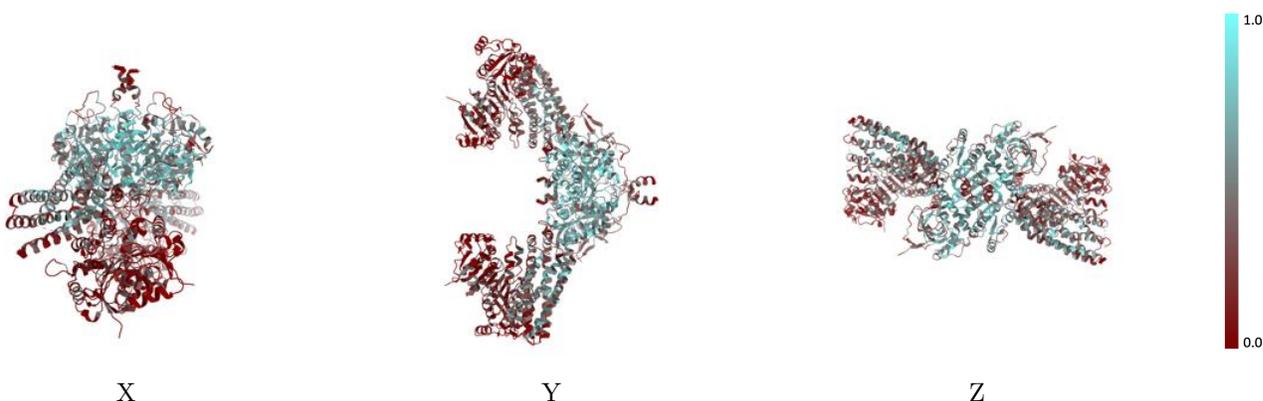
The images above show the 3D surface view of the map at the recommended contour level 0.011 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



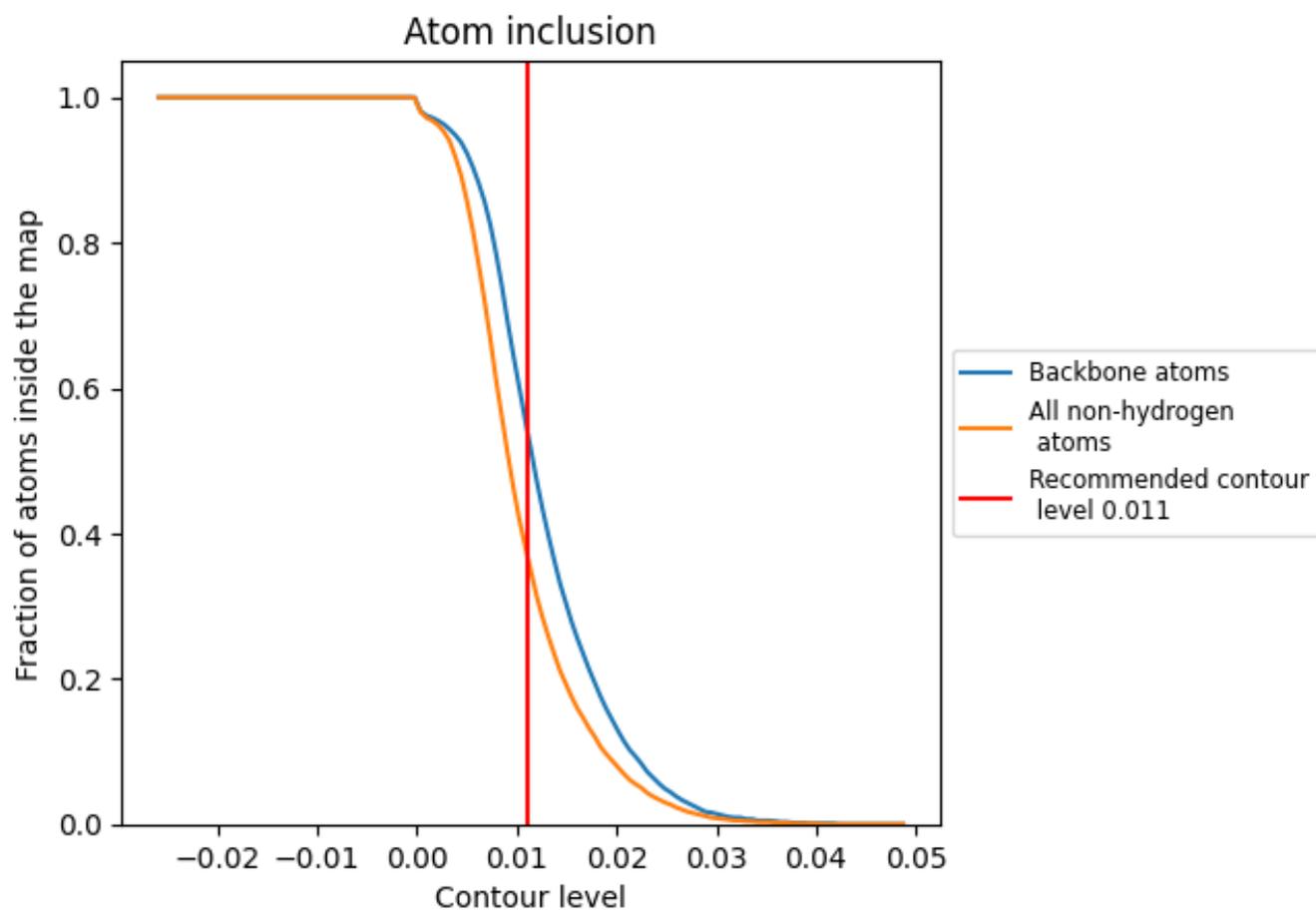
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.011).

9.4 Atom inclusion [i](#)



At the recommended contour level, 54% of all backbone atoms, 37% 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 (0.011) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3720	 0.2850
A	 0.4360	 0.2990
B	 0.4390	 0.3020
C	 0.5740	 0.3540
D	 0.5730	 0.3530
E	 0.1410	 0.2010
F	 0.1410	 0.2240
G	 0.1440	 0.2020
H	 0.1420	 0.2230

