Full wwPDB EM Validation Report

Nov 9, 2026 – 02:11 PM EST

PDB ID	:	9OJ9 / pdb_00009oj9
EMDB ID	:	EMD-70531
Title	:	CryoEM Structure of MHC-IGRP228 in Complex with FAb 1
Authors	:	Jaremko, M.J.; Fischmann, T.
Deposited on	:	2025-05-07
Resolution	:	2.50 Å(reported)

This is a Full wwPDB EM Validation 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:

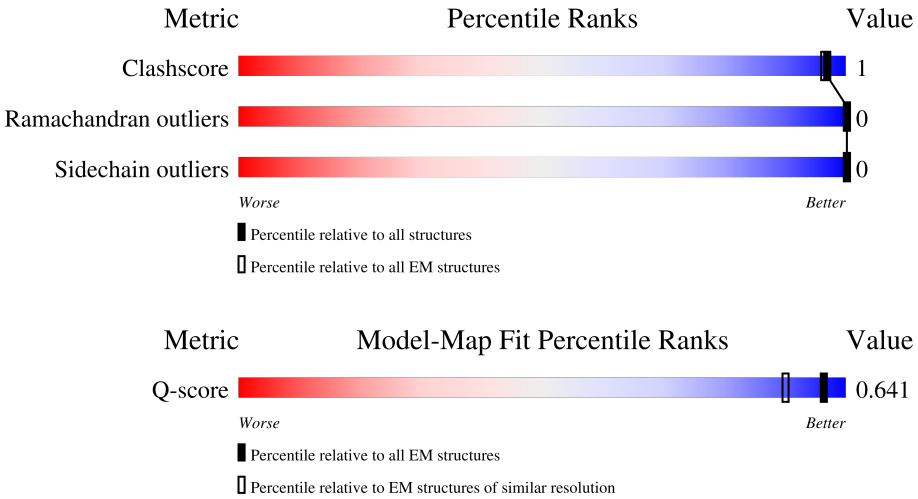
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 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.



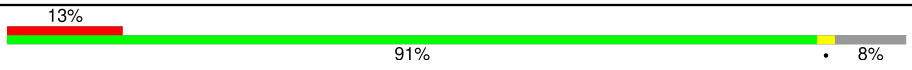
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7115 (2.00 - 3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	276	15% 97%
2	B	100	7% 100%
3	C	9	100%
4	D	214	16% 97%

Continued on next page...

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Mol	Chain	Length	Quality of chain
5	E	233	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12582 atoms, of which 6160 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 MHC class I antigen, A-2 alpha chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	275	Total	C	H	N	O	S	0	0
			4340	1403	2094	409	425	9		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A5B8RNS7

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	100	Total	C	H	N	O	S	0	0
			1640	533	803	141	159	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called Glucose-6-phosphatase 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	9	Total	C	H	N	O	0	0
			156	51	80	11	14		

- Molecule 4 is a protein called FAb 1 Light Chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	213	Total	C	H	N	O	S	0	0
			3246	1029	1602	281	330	4		

- Molecule 5 is a protein called FAb 1 Heavy Chain.

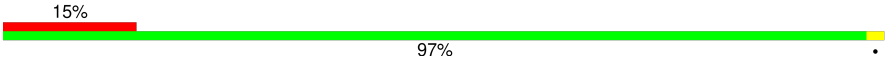
Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	215	Total	C	H	N	O	S	0	0
			3200	1025	1581	268	318	8		

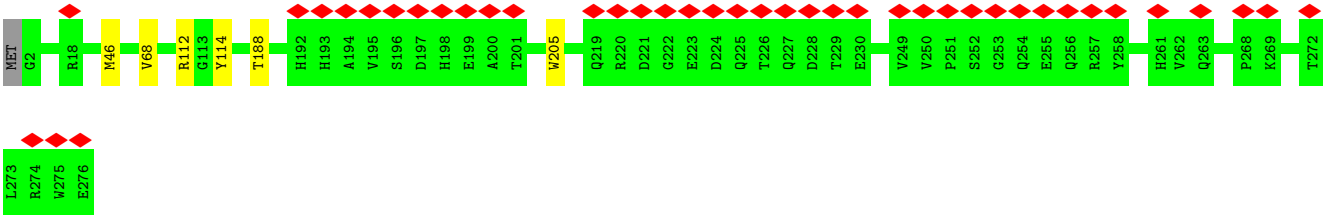
3 Residue-property plots (i)

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: MHC class I antigen, A-2 alpha chain

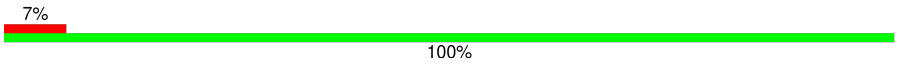
Chain A:

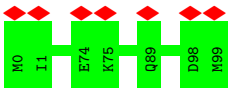




• Molecule 2: Beta-2-microglobulin

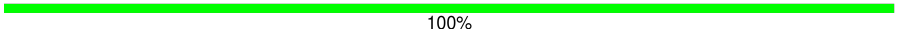
Chain B:





• Molecule 3: Glucose-6-phosphatase 2

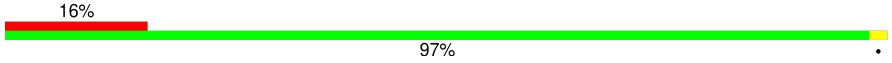
Chain C:

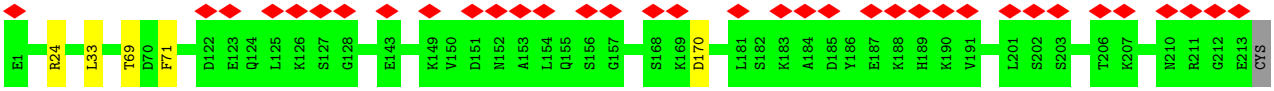


There are no outlier residues recorded for this chain.

• Molecule 4: FAb 1 Light Chain

Chain D:

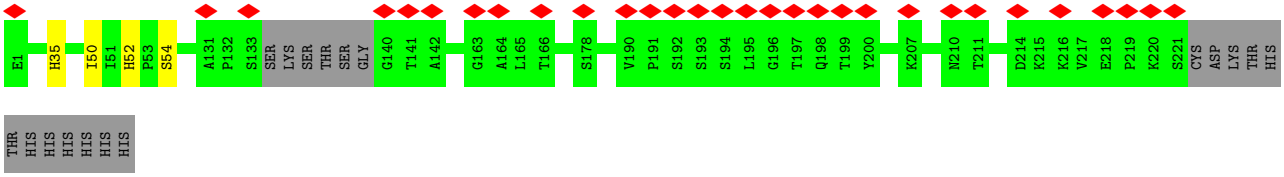




• Molecule 5: FAb 1 Heavy Chain

Chain E:




E1
H35
I50
I51
H52
P53
S54
A131
P132
S133
SER
LYS
SER
THR
SER
GLY
G140
T141
A142
G163
A164
L165
T166
S178
V190
P191
S192
S193
S194
L195
G196
T197
Q198
T199
Y200
K207
N210
T211
D214
K215
K216
V217
E218
P219
K220
S221
CYS
ASP
LYS
THR
HIS
THR
HIS
HIS
HIS
HIS
HIS
HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1310945	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50.52	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	2.510	Depositor
Minimum map value	-1.556	Depositor
Average map value	0.013	Depositor
Map value standard deviation	0.159	Depositor
Recommended contour level	0.382	Depositor
Map size (Å)	76.728, 85.068, 163.464	wwPDB
Map dimensions	196, 102, 92	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.834, 0.834, 0.83400005	Depositor

5 Model quality

5.1 Standard geometry

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	0.31	0/2311	0.50	0/3137
2	B	0.30	0/860	0.47	0/1162
3	C	0.33	0/77	0.38	0/104
4	D	0.29	0/1681	0.49	0/2286
5	E	0.28	0/1660	0.49	0/2261
All	All	0.30	0/6589	0.49	0/8950

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	2246	2094	2093	3	0
2	B	837	803	803	0	0
3	C	76	80	80	0	0
4	D	1644	1602	1602	3	0
5	E	1619	1581	1580	3	0
All	All	6422	6160	6158	9	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 (9) 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:46:MET:HE1	1:A:68:VAL:HG11	1.92	0.51
4:D:33:LEU:HD22	4:D:71:PHE:CG	2.48	0.49
5:E:35:HIS:CE1	5:E:50:ILE:HD12	2.52	0.43
4:D:170:ASP:OD1	4:D:170:ASP:C	2.61	0.43
5:E:52:HIS:HD2	5:E:54:SER:HB3	1.84	0.43
1:A:112:ARG:HD2	1:A:114:TYR:OH	2.20	0.42
4:D:24:ARG:HA	4:D:69:THR:O	2.19	0.42
5:E:52:HIS:CD2	5:E:54:SER:HB3	2.54	0.42
1:A:188:THR:HA	1:A:205:TRP:O	2.21	0.41

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	273/276 (99%)	269 (98%)	4 (2%)	0	100	100
2	B	98/100 (98%)	98 (100%)	0	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
4	D	211/214 (99%)	206 (98%)	5 (2%)	0	100	100
5	E	211/233 (91%)	210 (100%)	1 (0%)	0	100	100
All	All	800/832 (96%)	790 (99%)	10 (1%)	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	231/232 (100%)	231 (100%)	0	100	100
2	B	95/95 (100%)	95 (100%)	0	100	100
3	C	9/9 (100%)	9 (100%)	0	100	100
4	D	185/186 (100%)	185 (100%)	0	100	100
5	E	182/199 (92%)	182 (100%)	0	100	100
All	All	702/721 (97%)	702 (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 (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	189	HIS
1	A	193	HIS
2	B	13	HIS
4	D	38	GLN
4	D	100	GLN
4	D	189	HIS
5	E	39	GLN
5	E	52	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)

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.

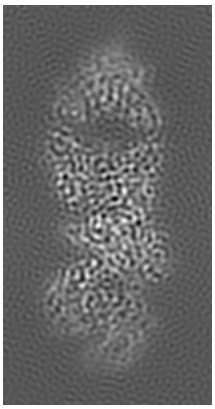
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-70531. These allow visual inspection of the internal detail of the map and identification of artifacts.

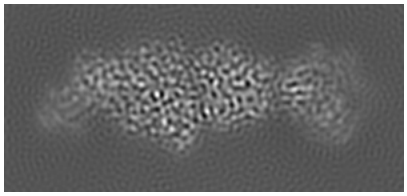
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

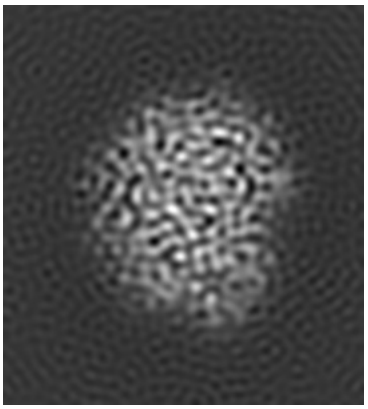
6.1.1 Primary map



X

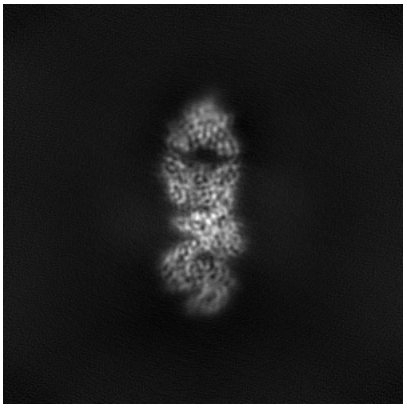


Y

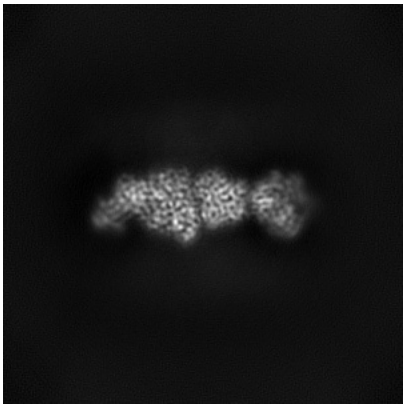


Z

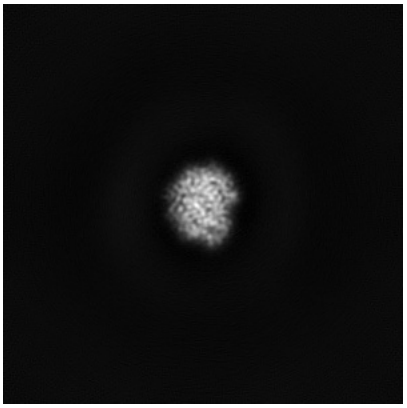
6.1.2 Raw map



X



Y

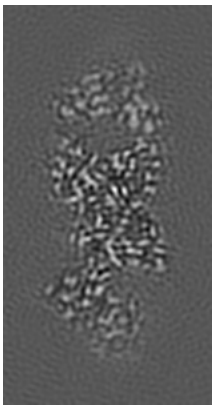


Z

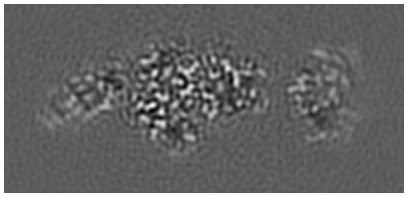
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

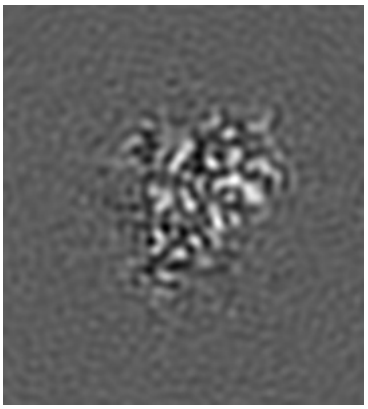
6.2.1 Primary map



X Index: 46

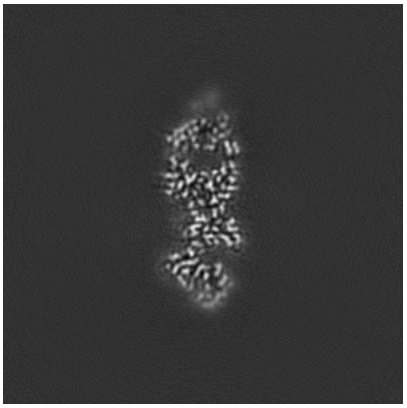


Y Index: 51

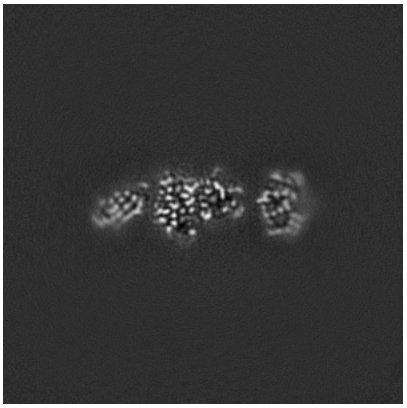


Z Index: 98

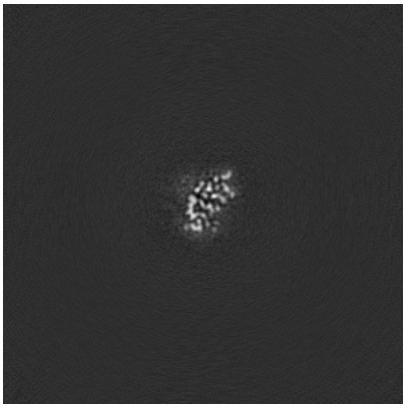
6.2.2 Raw map



X Index: 150



Y Index: 150

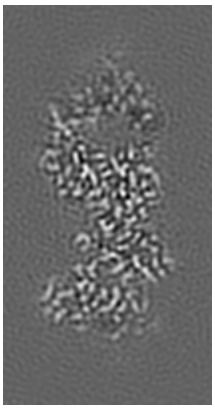


Z Index: 150

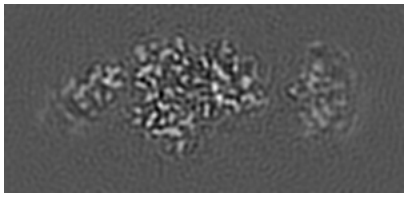
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

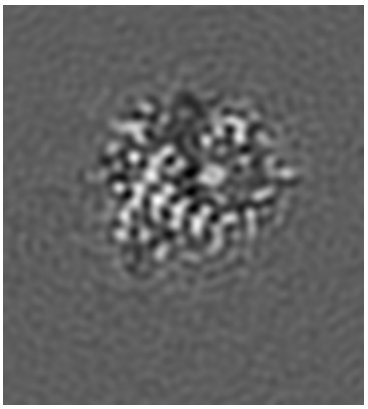
6.3.1 Primary map



X Index: 53

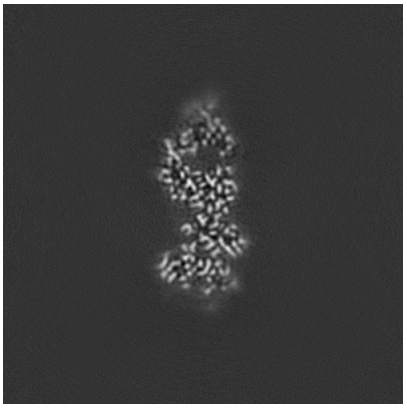


Y Index: 54

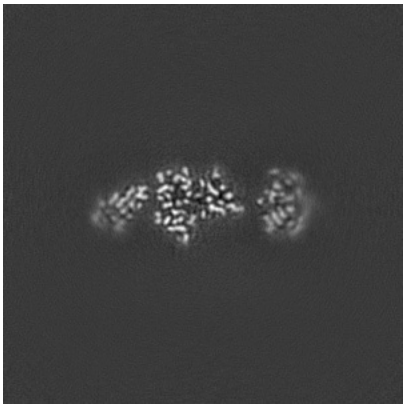


Z Index: 77

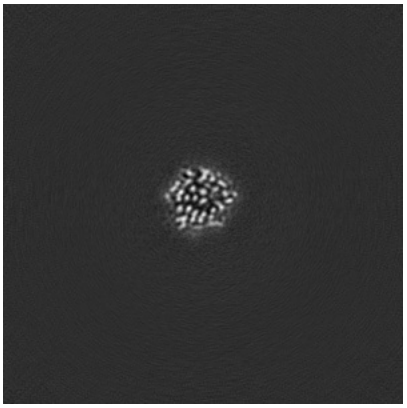
6.3.2 Raw map



X Index: 155



Y Index: 153

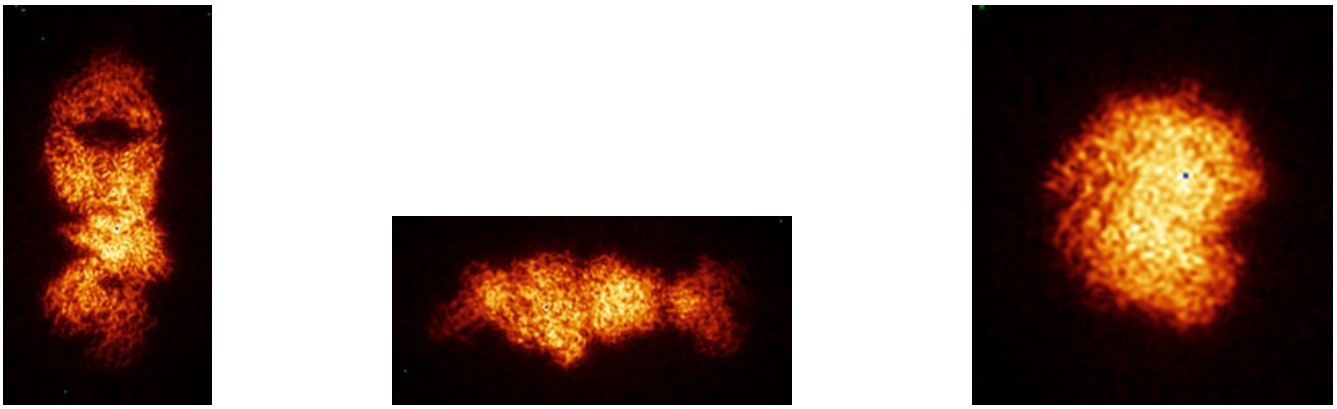


Z Index: 131

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

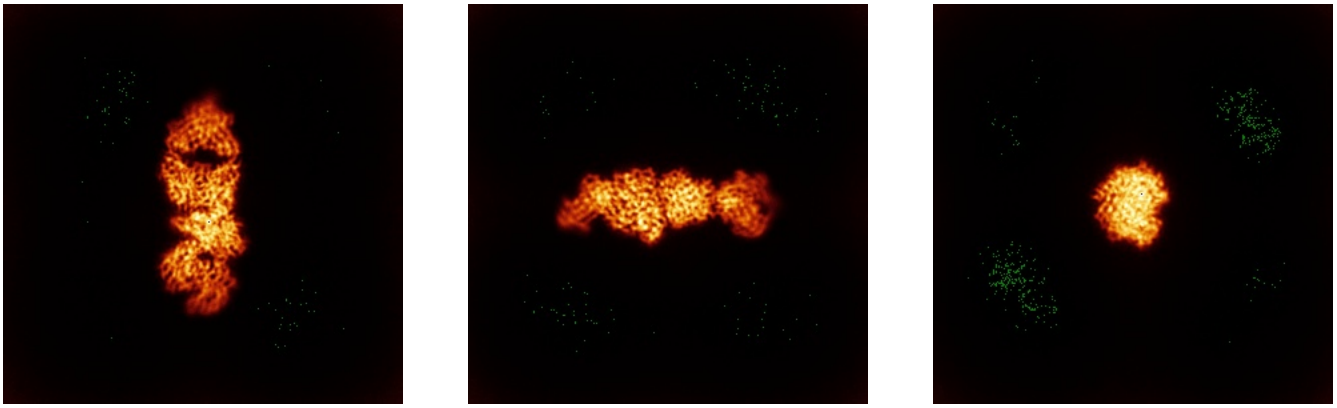
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



X Y Z

6.4.2 Raw map

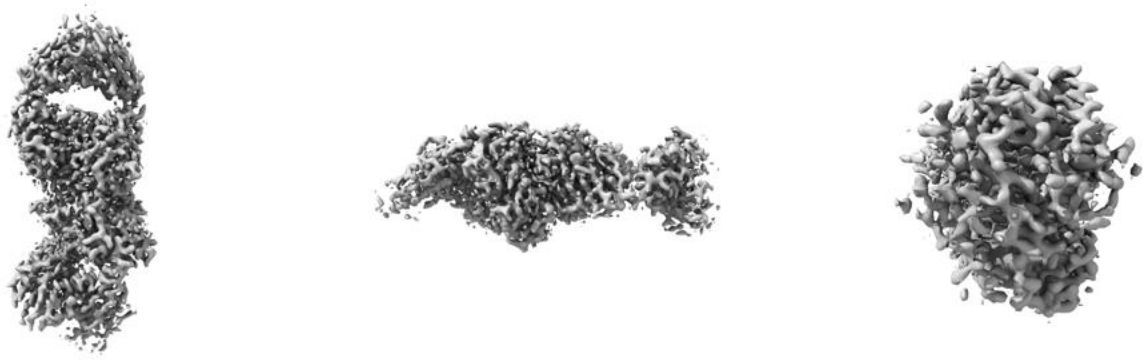


X Y Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.382. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

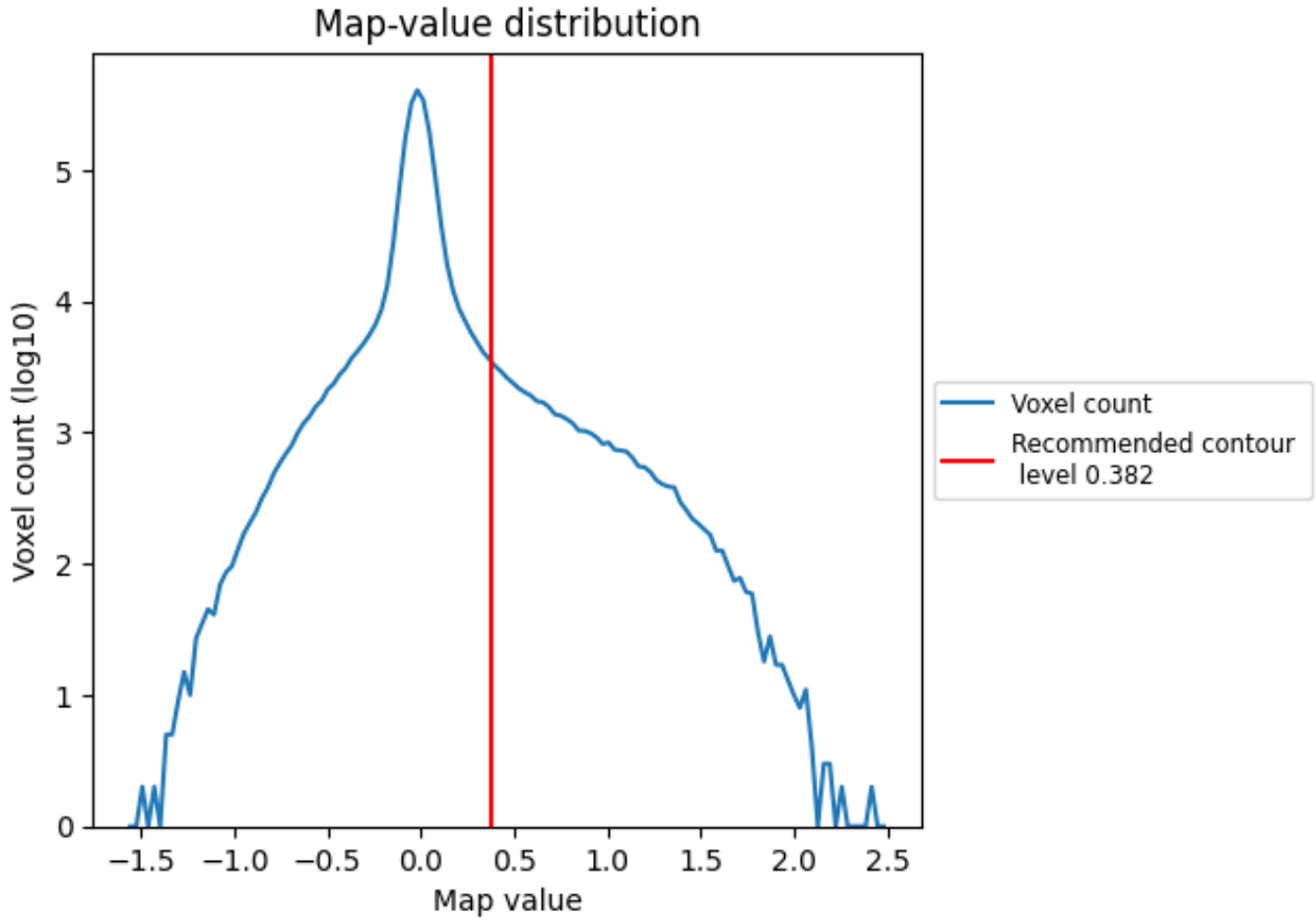
6.6 Mask visualisation (i)

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

7 Map analysis

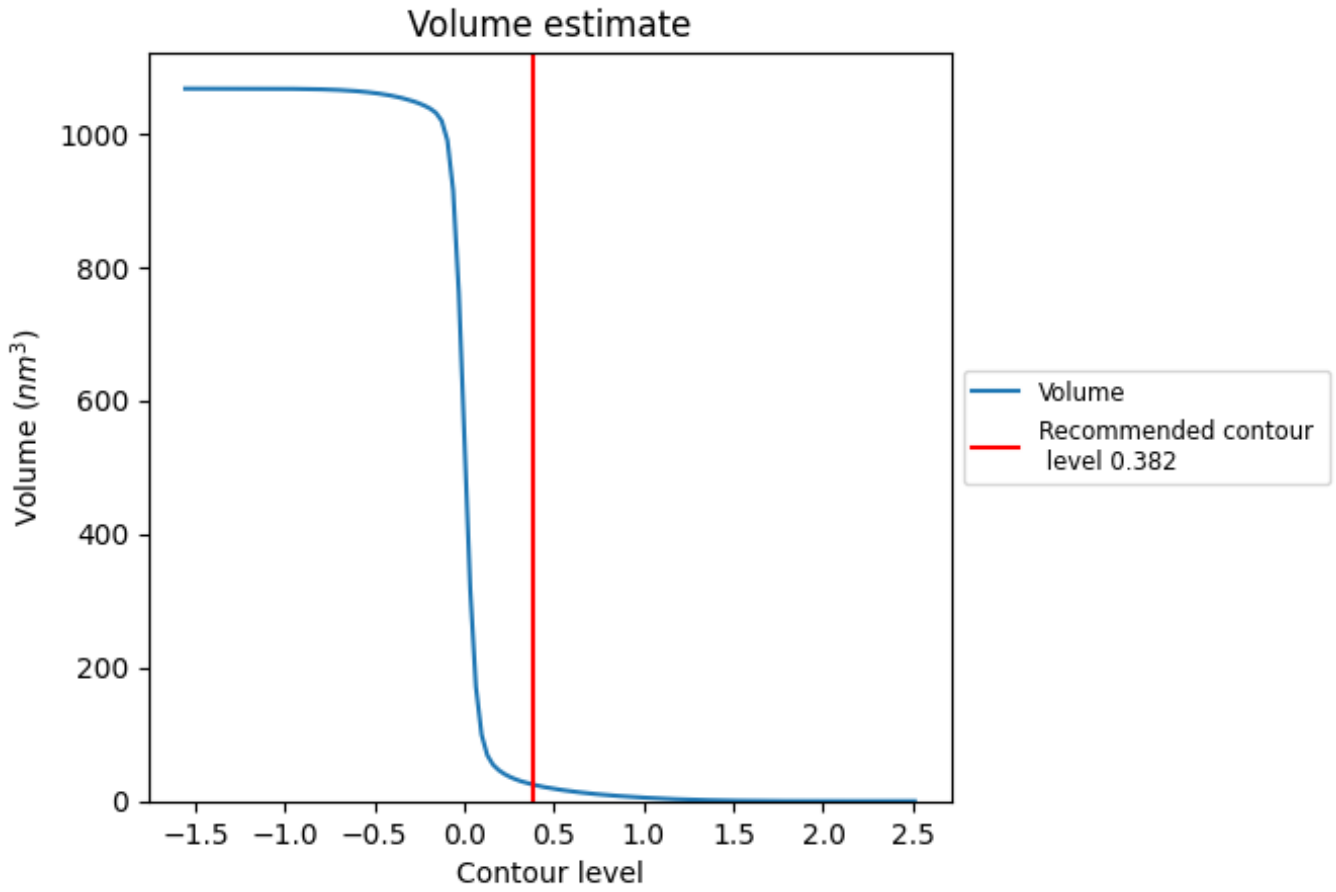
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate (i)



The volume at the recommended contour level is 25 nm^3; this corresponds to an approximate mass of 22 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.

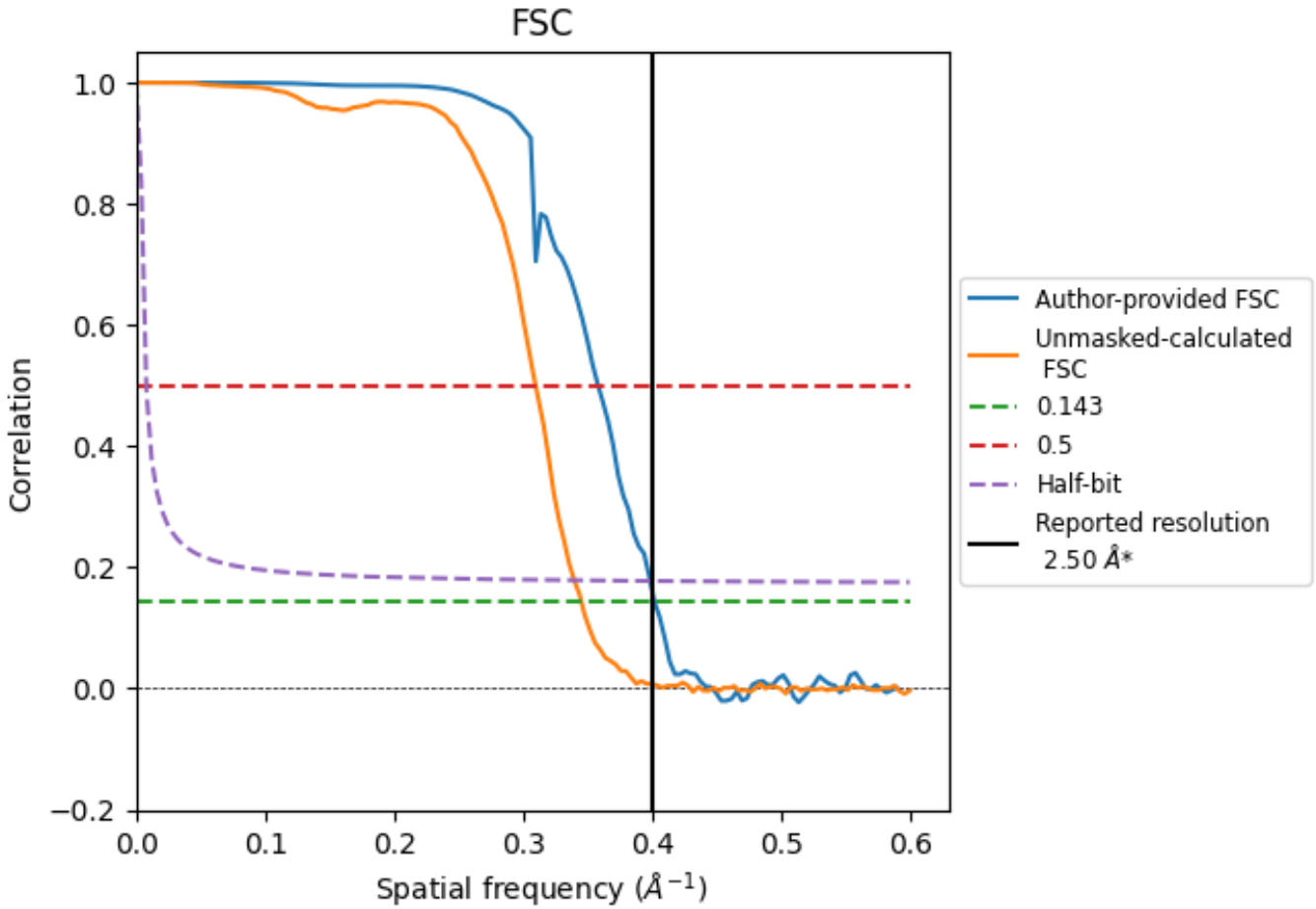
7.3 Rotationally averaged power spectrum (i)

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

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.400 Å^{-1}

8.2 Resolution estimates (i)

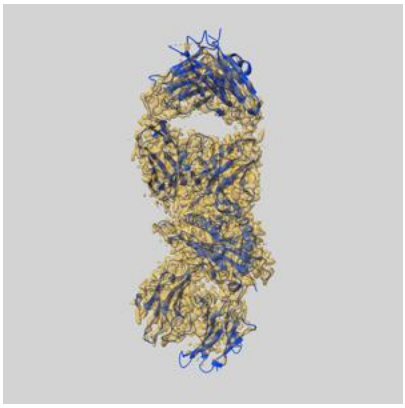
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.49	2.79	2.51
Unmasked-calculated*	2.90	3.23	2.94

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.90 differs from the reported value 2.5 by more than 10 %

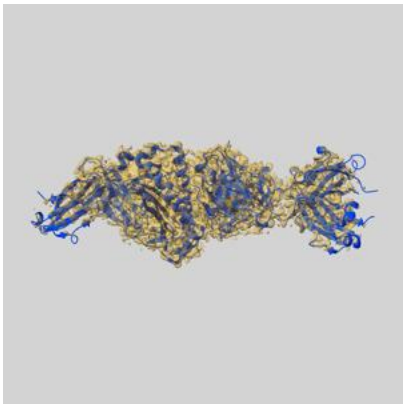
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-70531 and PDB model 9OJ9. Per-residue inclusion information can be found in section 3 on page 6.

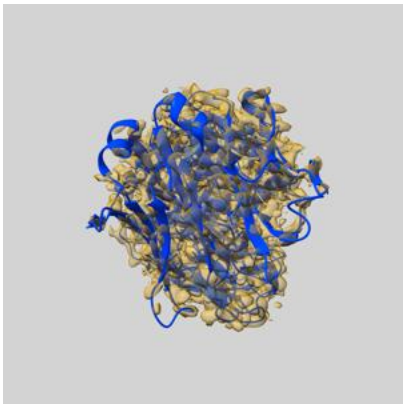
9.1 Map-model overlay



X



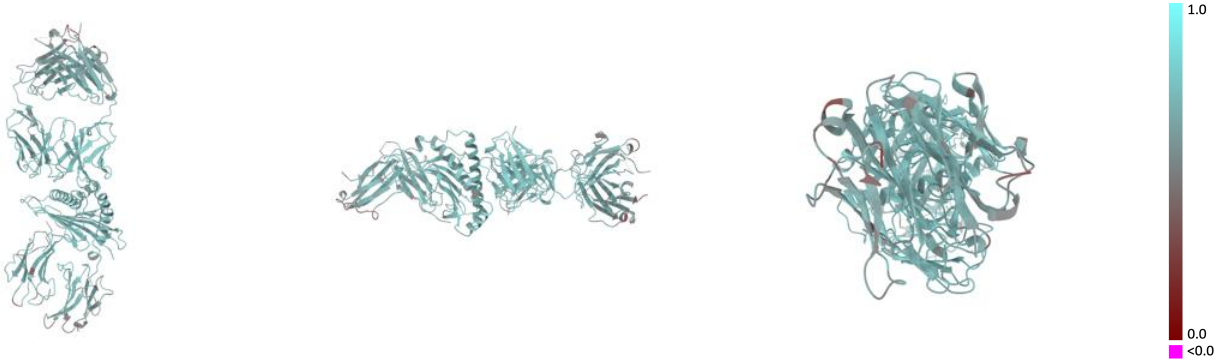
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.382 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.

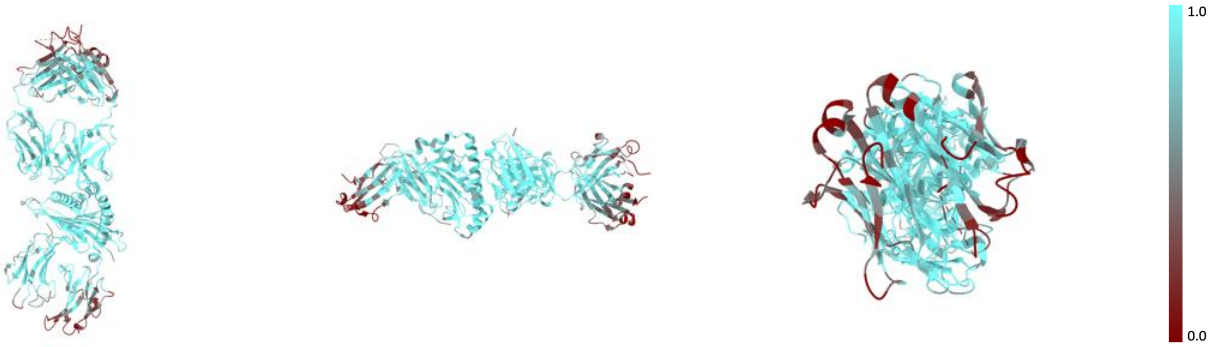
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

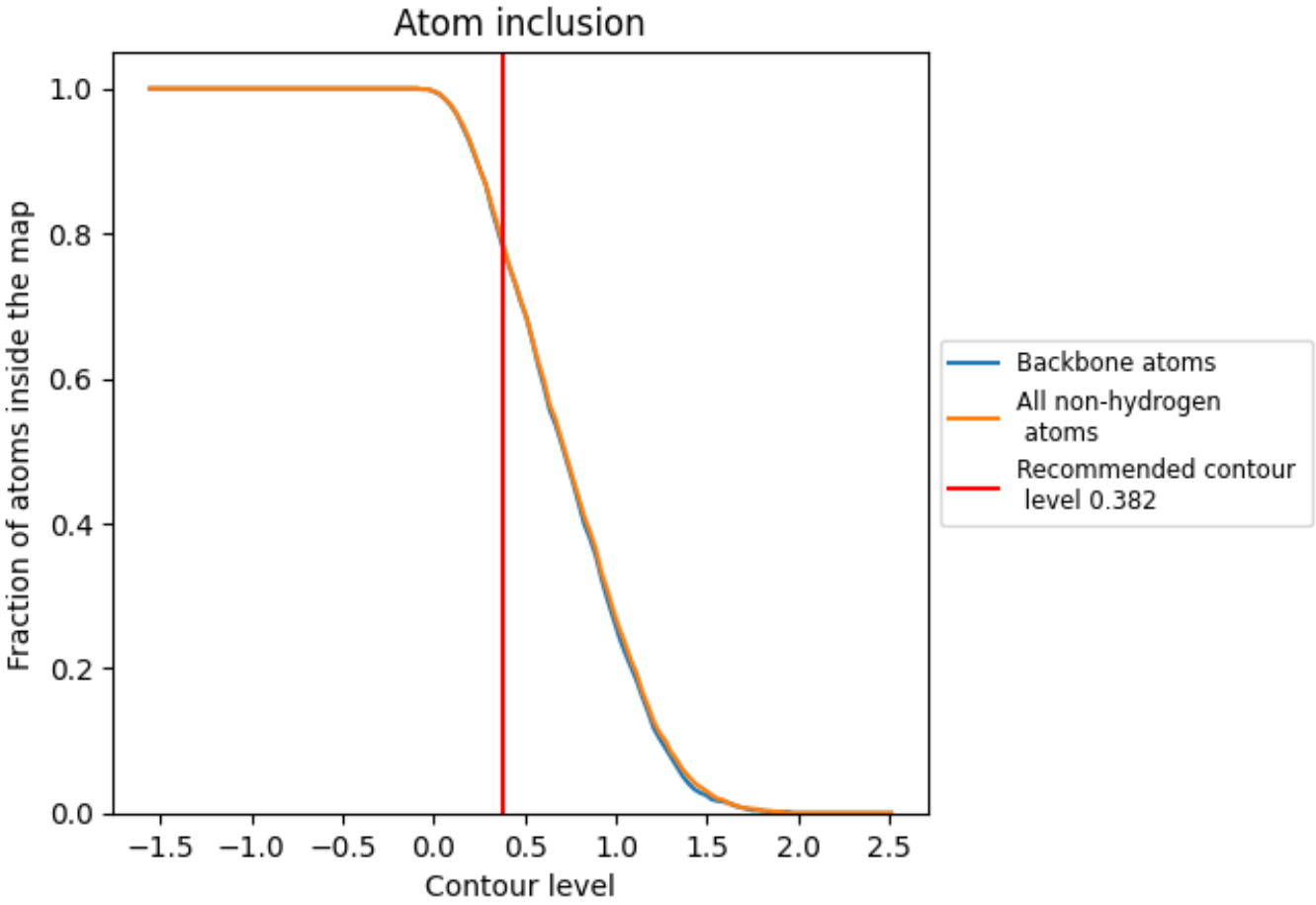
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.382).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 78% 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 (0.382) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.7840	0.6410
A	0.7830	0.6430
B	0.8210	0.6320
C	0.9870	0.6920
D	0.7410	0.6300
E	0.8030	0.6530