



## wwPDB EM Validation Summary Report ⓘ

May 2, 2026 – 07:16 am BST

PDB ID : 9I0H / pdb\_00009i0h  
EMDB ID : EMD-52558  
Title : CryoEM structure of transit-GmNifEN  
Authors : Paya Tormo, L.; Nguyen, T.Q.; Fyfe, C.; Basbous, H.; Dobrzynska, K.; Echavarri-Erasun, C.; Martin, L.; Caserta, G.; Legrand, P.; Thorn, A.; Amara, P.; Schoehn, G.; Cherrier, M.V.; Rubio, L.M.; Nicolet, Y.  
Deposited on : 2025-01-15  
Resolution : 2.62 Å(reported)  
Based on initial model : .

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.dev132  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
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) : 2.49

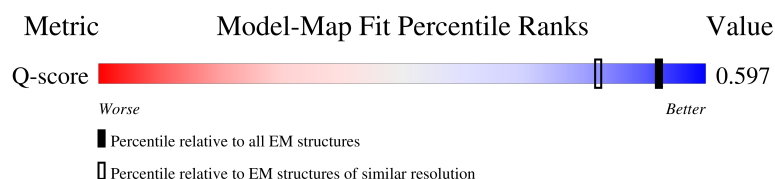
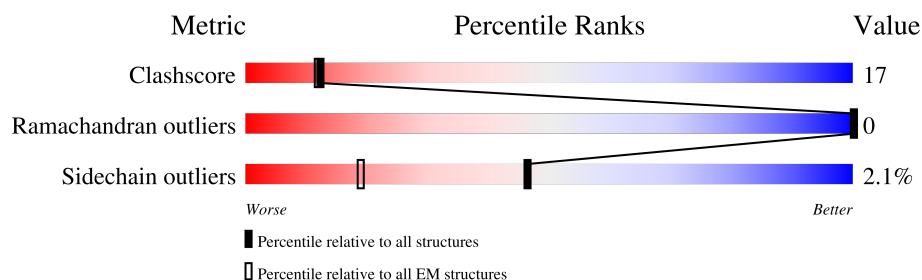
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.62 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	8810 ( 2.12 - 3.12 )

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	919	 59% 26% • 15%
1	B	919	 59% 26% • 15%

## 2 Entry composition [i](#)

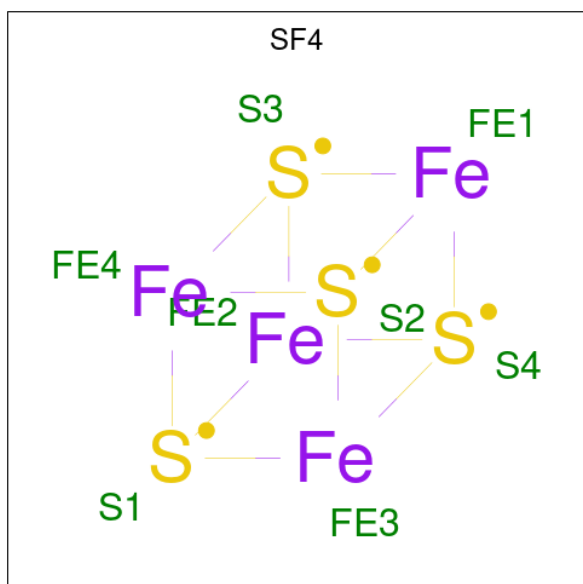
There are 4 unique types of molecules in this entry. The entry contains 12046 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Nitrogenase iron-molybdenum cofactor biosynthesis protein NifE.

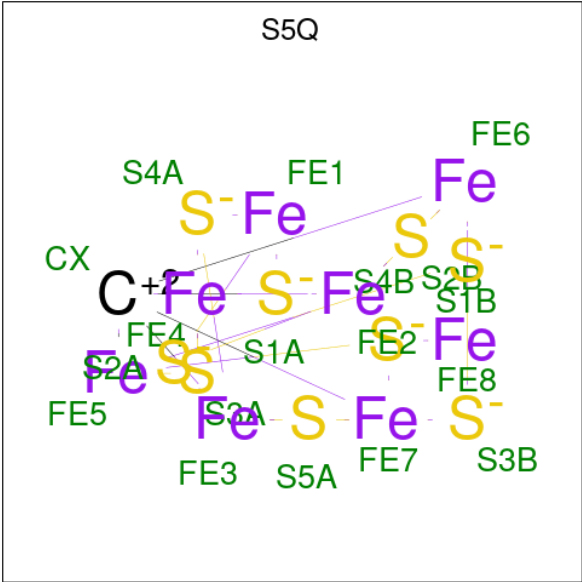
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	783	Total	C	N	O	S	0	0
			5994	3808	1044	1105	37		
1	B	783	Total	C	N	O	S	0	0
			5994	3808	1044	1105	37		

- Molecule 2 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total	Fe	S	0
			8	4	4	
2	B	1	Total	Fe	S	0
			8	4	4	

- Molecule 3 is FeFe cofactor (CCD ID: S5Q) (formula:  $\text{CFe}_8\text{S}_9$ ).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	Fe	S	0
			18	1	8	9	
3	B	1	Total	C	Fe	S	0
			18	1	8	9	

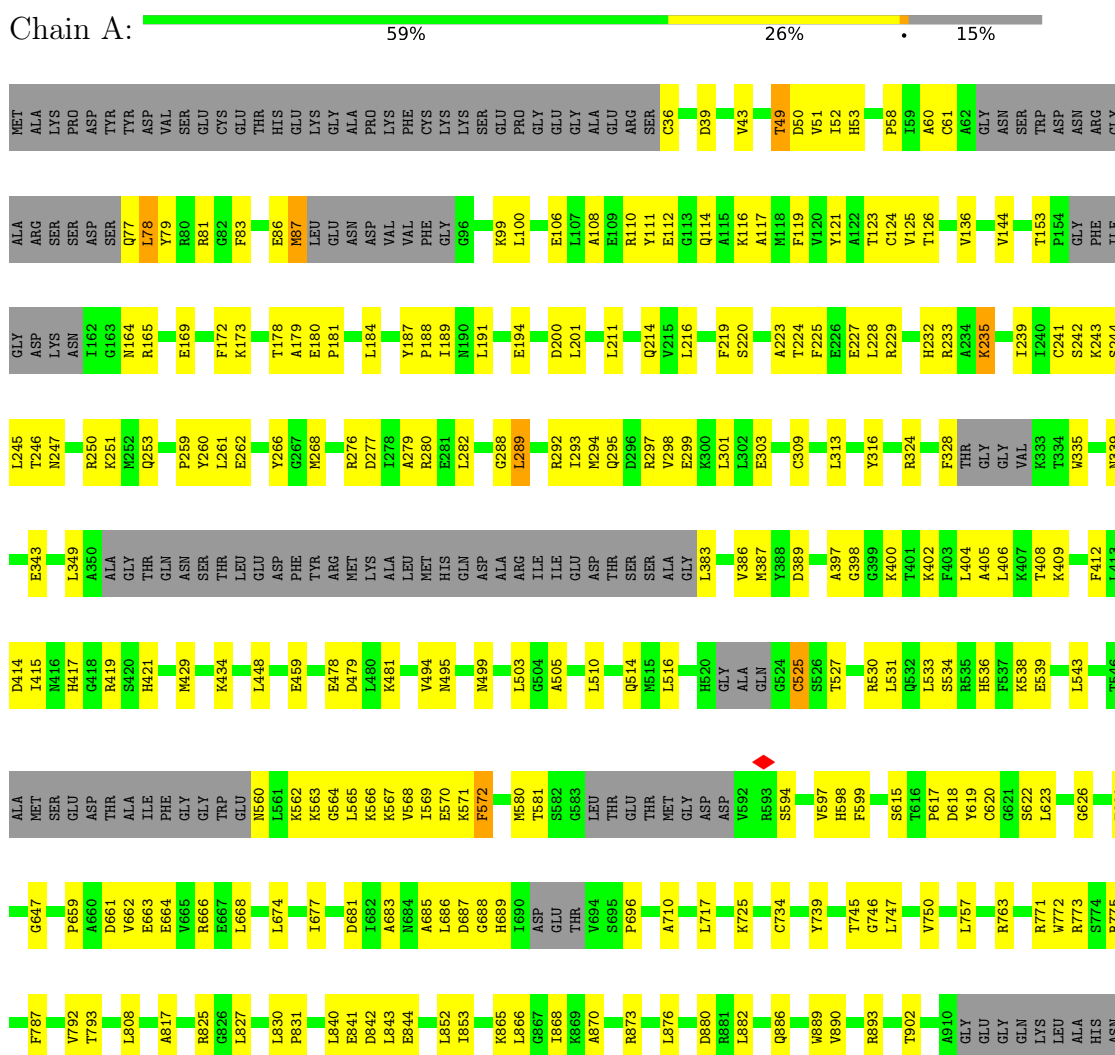
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		AltConf
4	A	3	Total	O	0
			3	3	
4	B	3	Total	O	0
			3	3	

### 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: Nitrogenase iron-molybdenum cofactor biosynthesis protein NifE



- Molecule 1: Nitrogenase iron-molybdenum cofactor biosynthesis protein NifE



V792	G647	MET	F412	N339	L245	GLY	ALA	MET
T793	P659	SER	L413	E343	T246	ASP	ARG	ALA
L808	A660	GLU	D414		N247	LYS	SER	LYS
A817	D661	THR	I415			ASN	ASP	PRO
R825	V662	ALA	H416	L349	R250	I162	SER	TYR
R825	E663	ILE	G418	A350	K251	G163	ASP	TYR
L830	E664	PHE	R419	ALA	Q252	N164	ASP	ASP
P831	V665	GLY	S420	GLY	Q253	R165	ASP	ASP
P831	E666	GLY	H421	THR	R254		L78	VAL
	E667	TRP		GLN	Y255	E169	R80	VAL
	L668	GLU	M429	ASN	Y256	V170	R81	GLU
D839		M560		SER	P259	L171	G82	CYS
L840	L674	L561	K434	THR	Y260	F172	F83	GLY
E841		K562	E459	LEU	L261	K173		THR
D842	I677	K563		GLU	E262		E86	HIS
L843		G564		ASP		T178	M87	HIS
E844	D631	G565	E478	PHE	Y266	A179	LEU	LYS
	L682	K566	D479	TYR	G267	E180	GLU	GLY
L852	A683	K567	L480	ARG	M268	P181	ASN	ALA
L853	H694	V568	K481	MET		L184	ASP	PRO
K865	A685	I569	V494	LYS	R276		LYS	LYS
L866	L686	E570	N495	ALA	D277	Y187	VAL	PHE
G867	D687	K571		LEU	I278	P188	PHE	CYS
I868	G688	F572	M499	MET	A279	I189	GLY	LYS
R869	H689			HIS	R280		SER	LYS
A870	I690	M580	L503	GLN	E281	H190	GLU	GLU
R873	ASP	T581	G504	ASP	L282	L191	L100	PRO
	THR	G582	A505	ALA		E194	E106	GLY
L876	V694	LEU	L510	ARG	L289	D200	L107	GLY
D880	S695	THR		ILE	R292	L201	A108	GLY
R881	P696	GLU	Q514	GLU	I293		E109	ALA
L882	A710	THR	M515	ASP	M294	M204	R110	GLU
	L717	MET	L516	THR	Q295		Y111	ARG
Q886		GLY		SER	D296	L211	E112	SER
		ASP	H520	SER	R297		Q113	C36
		ASP	GLY	ALA	V298	Q214	Q114	
		V592	ALA	GLY	E299	V215	A115	D39
		S594	L383	LYS	R300	L216	K116	
					L301		A117	V43
						A223	M118	
					E303	T224	F119	T49
					C309	F225	V120	D50
						E227	Y121	V51
						R229	A122	I52
							T123	H53
							V125	
							T126	P58
							V136	I59
							K143	A60
							K235	C61
							V144	A62
							T153	GLY
							F154	ASN
							PHE	ASP
							ILE	ASN
								ARG
								GLY

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	370821	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 ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	18.157	Depositor
Minimum map value	-0.129	Depositor
Average map value	-0.032	Depositor
Map value standard deviation	0.484	Depositor
Recommended contour level	0.75	Depositor
Map size (Å)	276.87, 276.87, 276.87	wwPDB
Map dimensions	330, 330, 330	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.839, 0.839, 0.839	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: S5Q, SF4

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	0.29	0/6100	0.51	4/8252 (0.0%)
1	B	0.29	0/6100	0.51	4/8252 (0.0%)
All	All	0.29	0/12200	0.51	8/16504 (0.0%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	289	LEU	N-CA-C	-7.26	102.55	111.33
1	B	289	LEU	N-CA-C	-7.26	102.55	111.33
1	A	617	PRO	N-CA-C	6.69	122.33	113.57
1	B	617	PRO	N-CA-C	6.69	122.33	113.57
1	A	78	LEU	N-CA-C	-5.36	106.44	112.87

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	5994	0	6074	210	0
1	B	5994	0	6074	214	0
2	A	8	0	0	0	0
2	B	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	18	0	0	0	0
3	B	18	0	0	0	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
All	All	12046	0	12148	411	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 17.

The worst 5 of 411 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:494:VAL:CG1	1:B:83:PHE:CD2	2.46	0.98
1:A:83:PHE:CD2	1:B:494:VAL:CG1	2.46	0.97
1:A:494:VAL:HG11	1:B:83:PHE:CD2	2.07	0.89
1:A:83:PHE:CD2	1:B:494:VAL:HG11	2.07	0.89
1:A:494:VAL:HG12	1:B:83:PHE:CD2	2.08	0.88

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	763/919 (83%)	737 (97%)	26 (3%)	0	100	100
1	B	763/919 (83%)	737 (97%)	26 (3%)	0	100	100
All	All	1526/1838 (83%)	1474 (97%)	52 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	626/732 (86%)	613 (98%)	13 (2%)	47	72
1	B	626/732 (86%)	613 (98%)	13 (2%)	47	72
All	All	1252/1464 (86%)	1226 (98%)	26 (2%)	46	72

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	49	THR
1	B	116	LYS
1	B	572	PHE
1	B	87	MET
1	B	124	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	339	ASN
1	B	385	GLN
1	B	885	HIS
1	B	495	ASN
1	B	858	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

4 ligands are modelled in this entry.

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
3	S5Q	A	1002	1	18,30,30	2.55	10 (55%)	-		
2	SF4	A	1001	1	0,12,12	-	-	-		
2	SF4	B	1001	1	0,12,12	-	-	-		
3	S5Q	B	1002	1	18,30,30	2.55	10 (55%)	-		

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	SF4	A	1001	1	-	-	0/6/5/5
2	SF4	B	1001	1	-	-	0/6/5/5

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1002	S5Q	S3A-FE4	-4.27	2.14	2.24
3	B	1002	S5Q	S3A-FE4	-4.27	2.14	2.24
3	A	1002	S5Q	S4A-FE4	-4.23	2.22	2.32
3	B	1002	S5Q	S4A-FE4	-4.23	2.22	2.32
3	A	1002	S5Q	S3B-FE6	-3.94	2.22	2.32

There are no bond angle outliers.

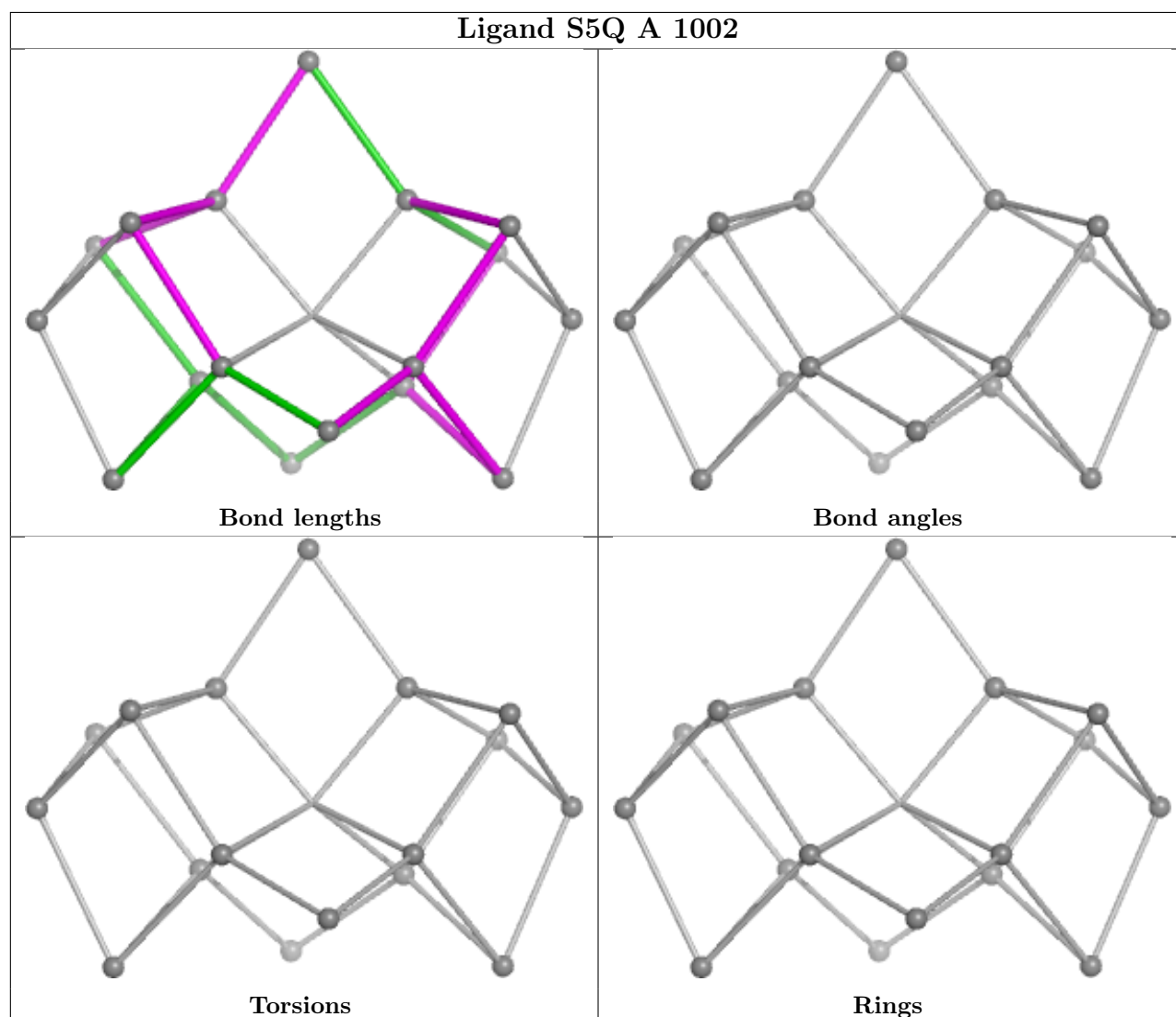
There are no chirality outliers.

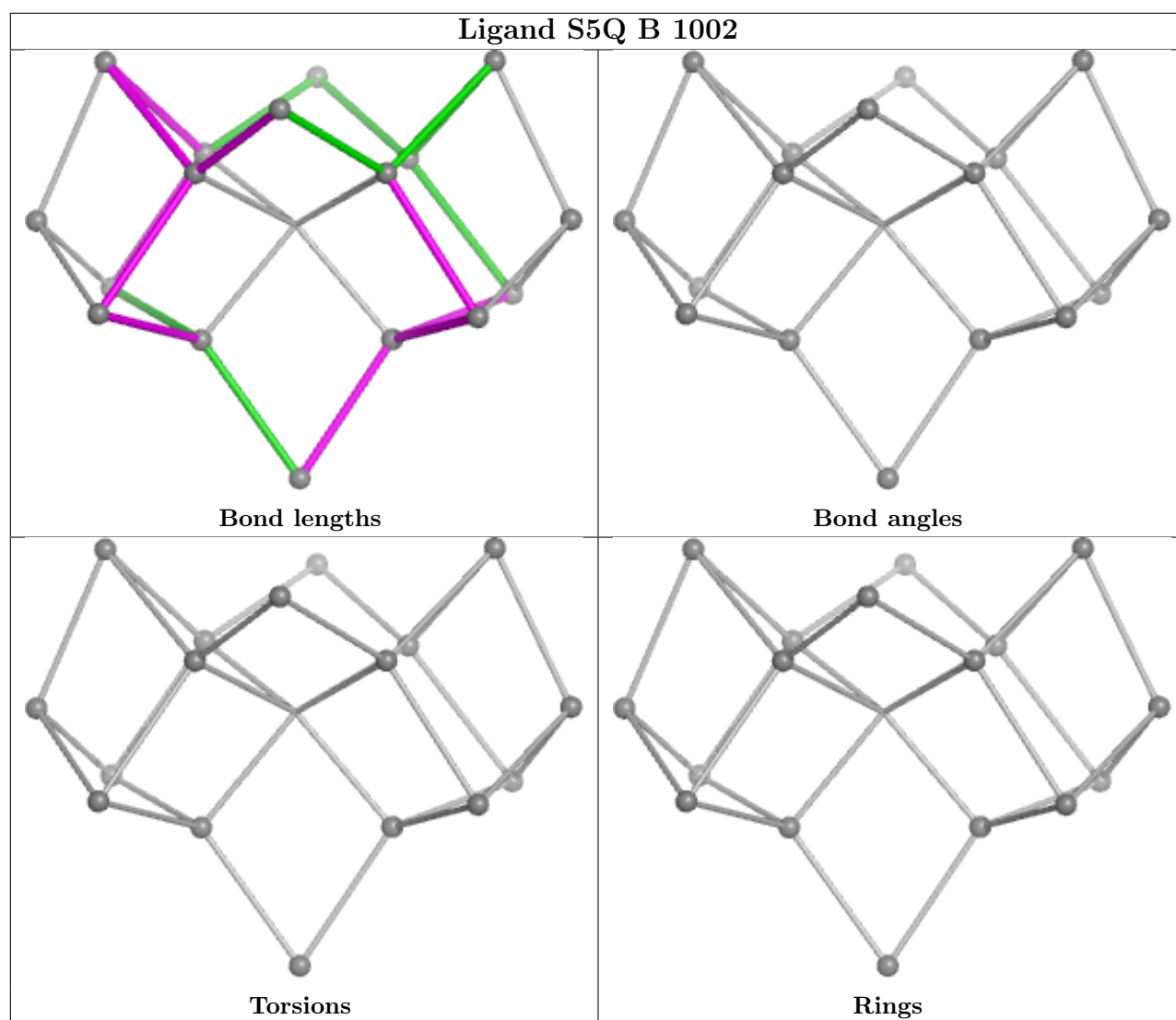
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

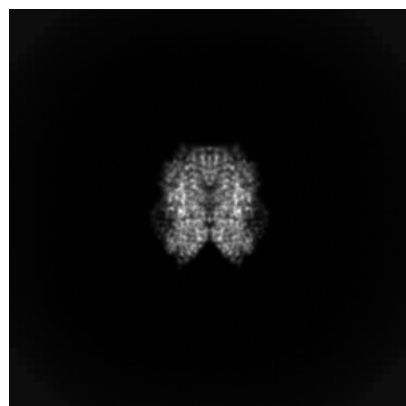
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52558. These allow visual inspection of the internal detail of the map and identification of artifacts.

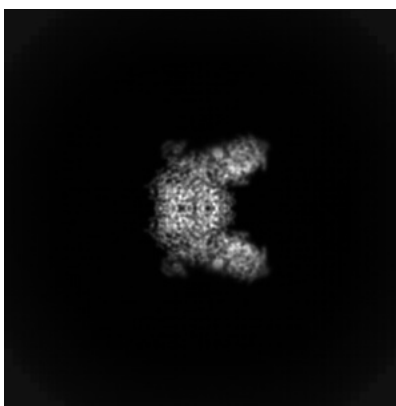
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

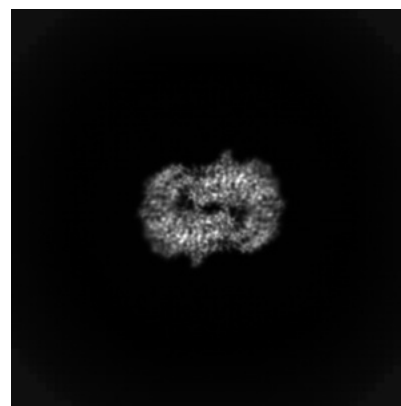
#### 6.1.1 Primary map



X

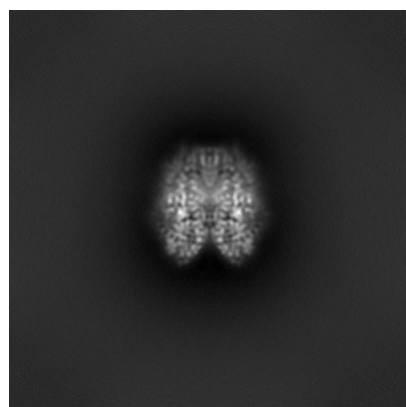


Y

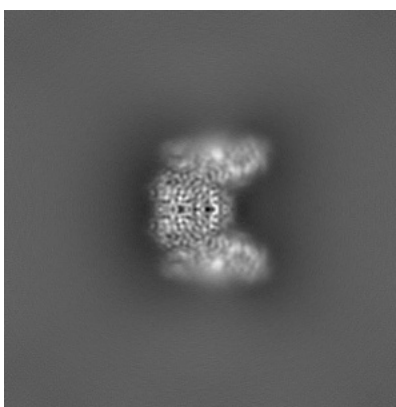


Z

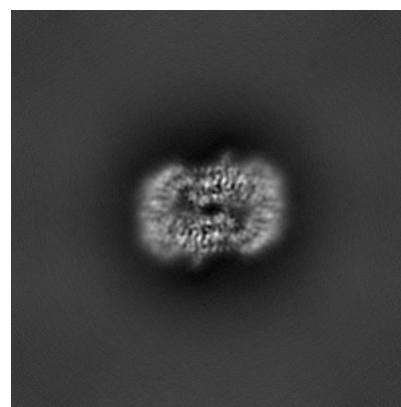
#### 6.1.2 Raw map



X



Y

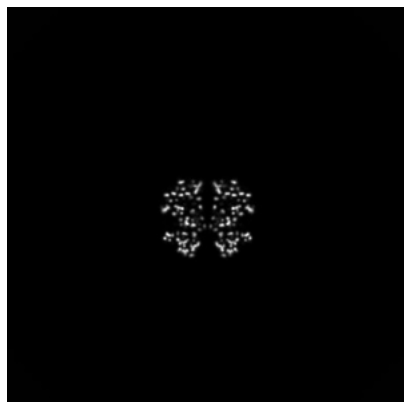


Z

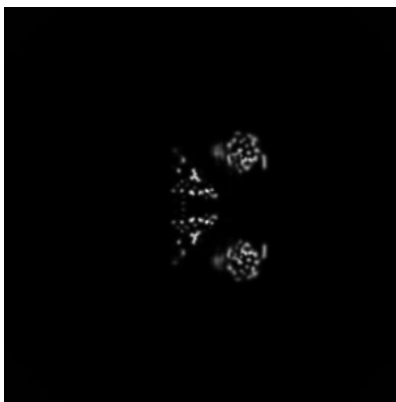
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

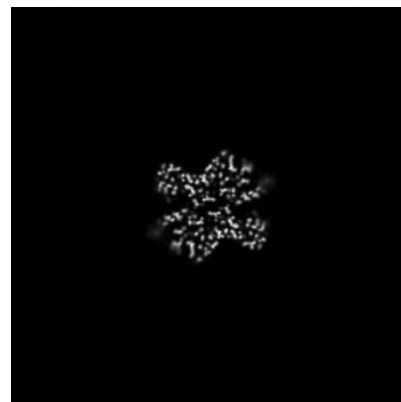
### 6.2.1 Primary map



X Index: 165

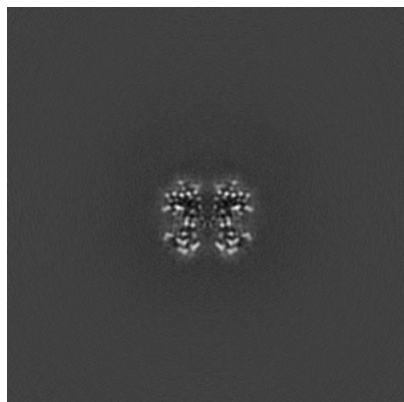


Y Index: 165

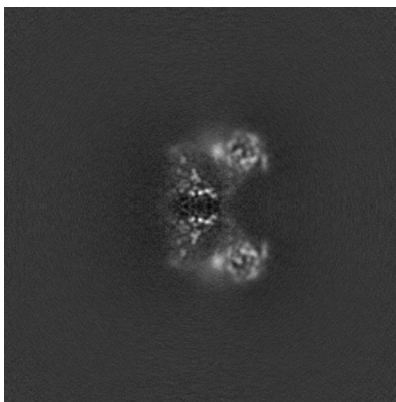


Z Index: 165

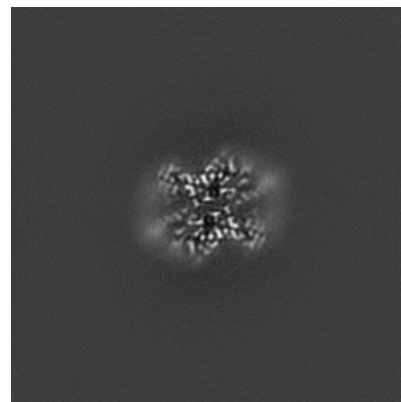
### 6.2.2 Raw map



X Index: 165



Y Index: 165

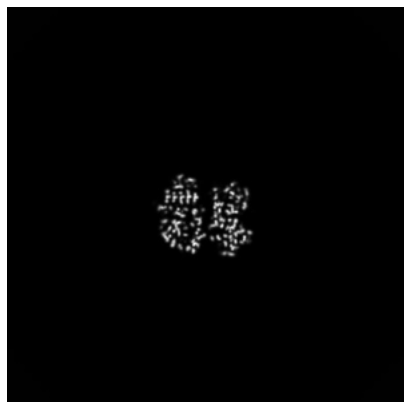


Z Index: 165

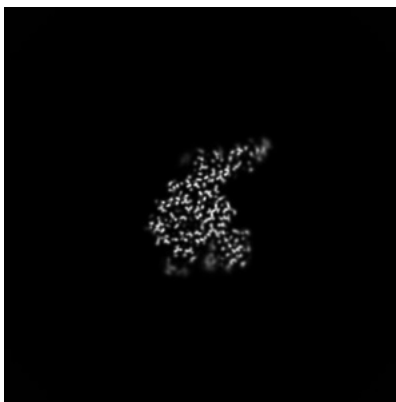
The images above show central slices of the map in three orthogonal directions.

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

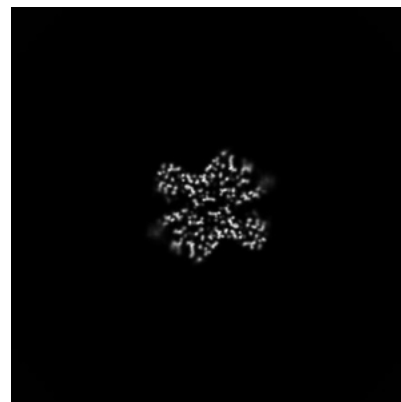
### 6.3.1 Primary map



X Index: 161

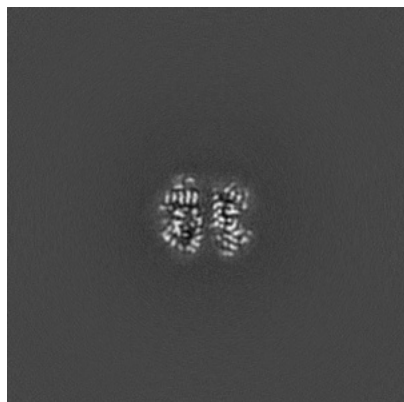


Y Index: 143

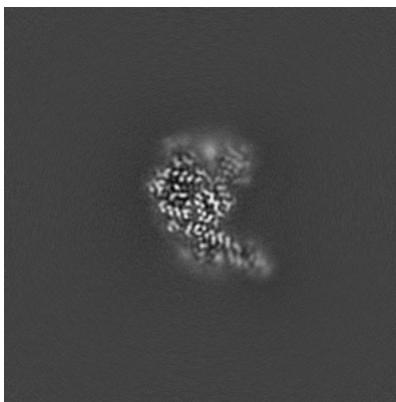


Z Index: 165

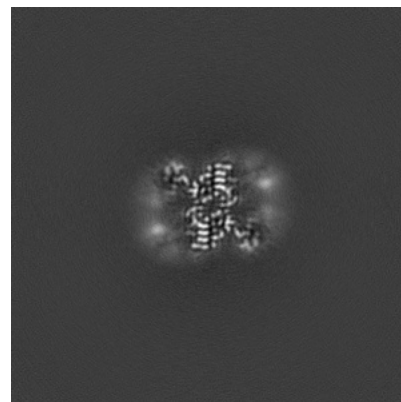
### 6.3.2 Raw map



X Index: 161



Y Index: 187



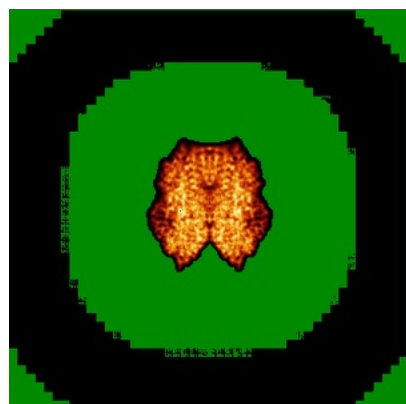
Z Index: 171

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

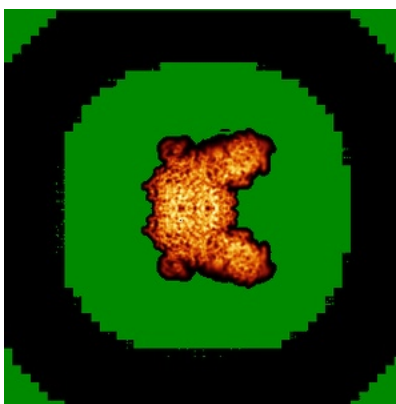


## 6.4 Orthogonal standard-deviation projections (False-color) ⓘ

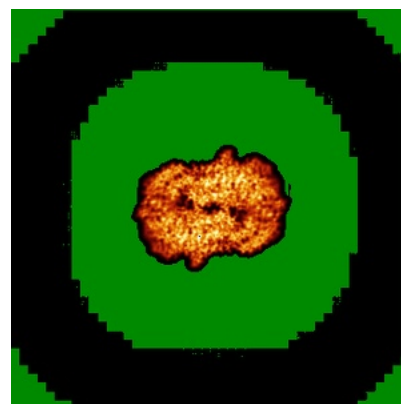
### 6.4.1 Primary map



X

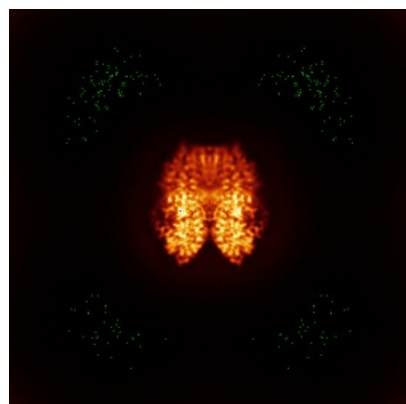


Y

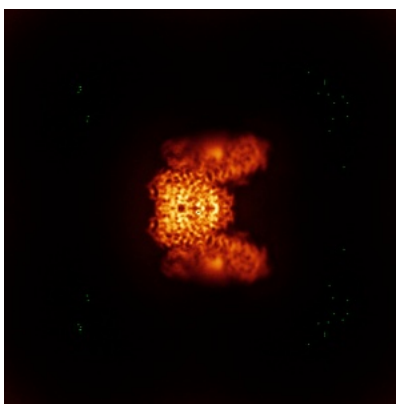


Z

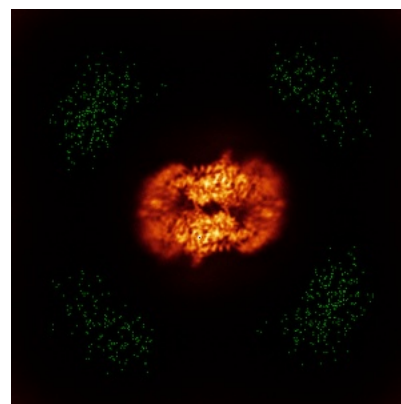
### 6.4.2 Raw map



X



Y

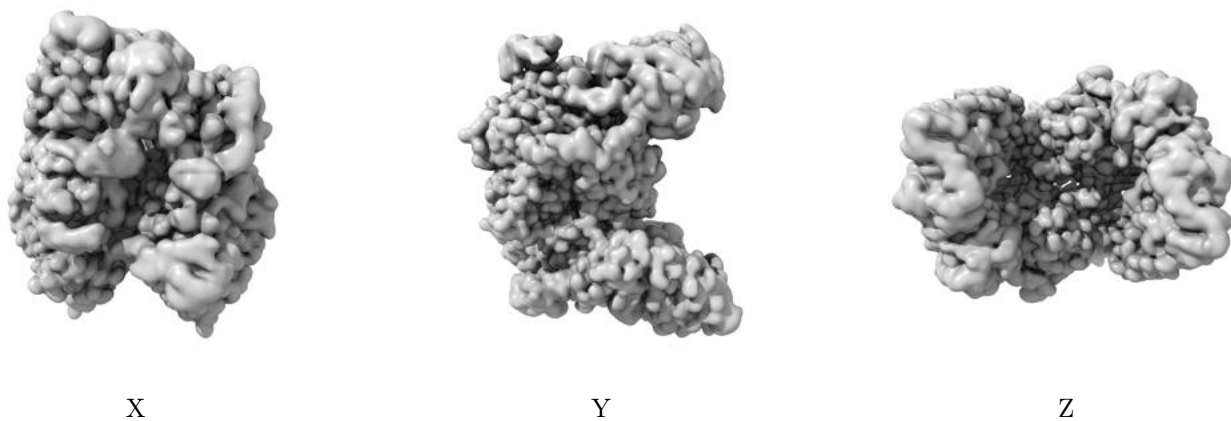


Z

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.

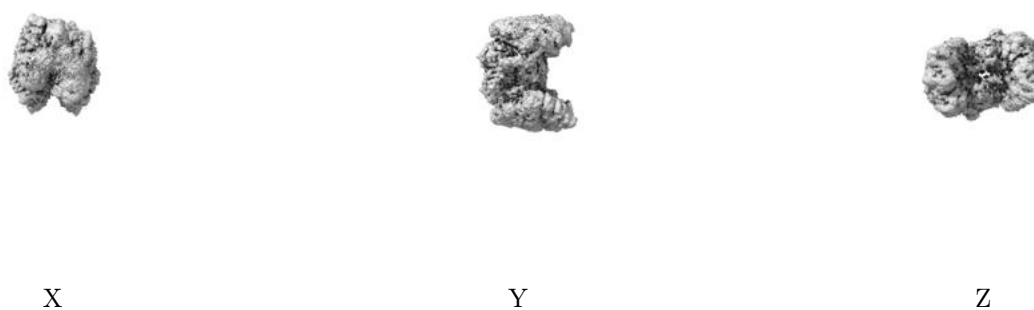
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.75. 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.

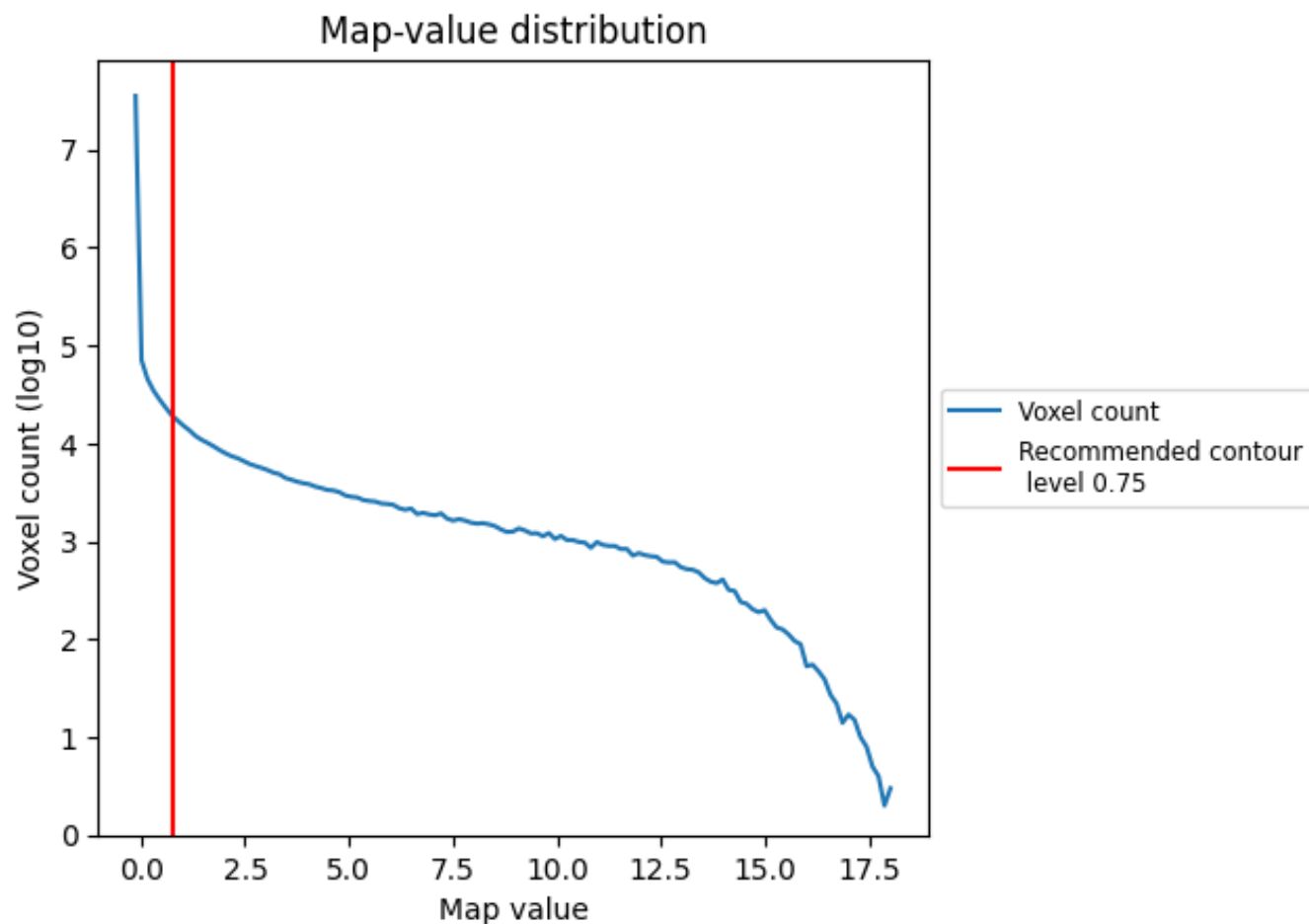
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

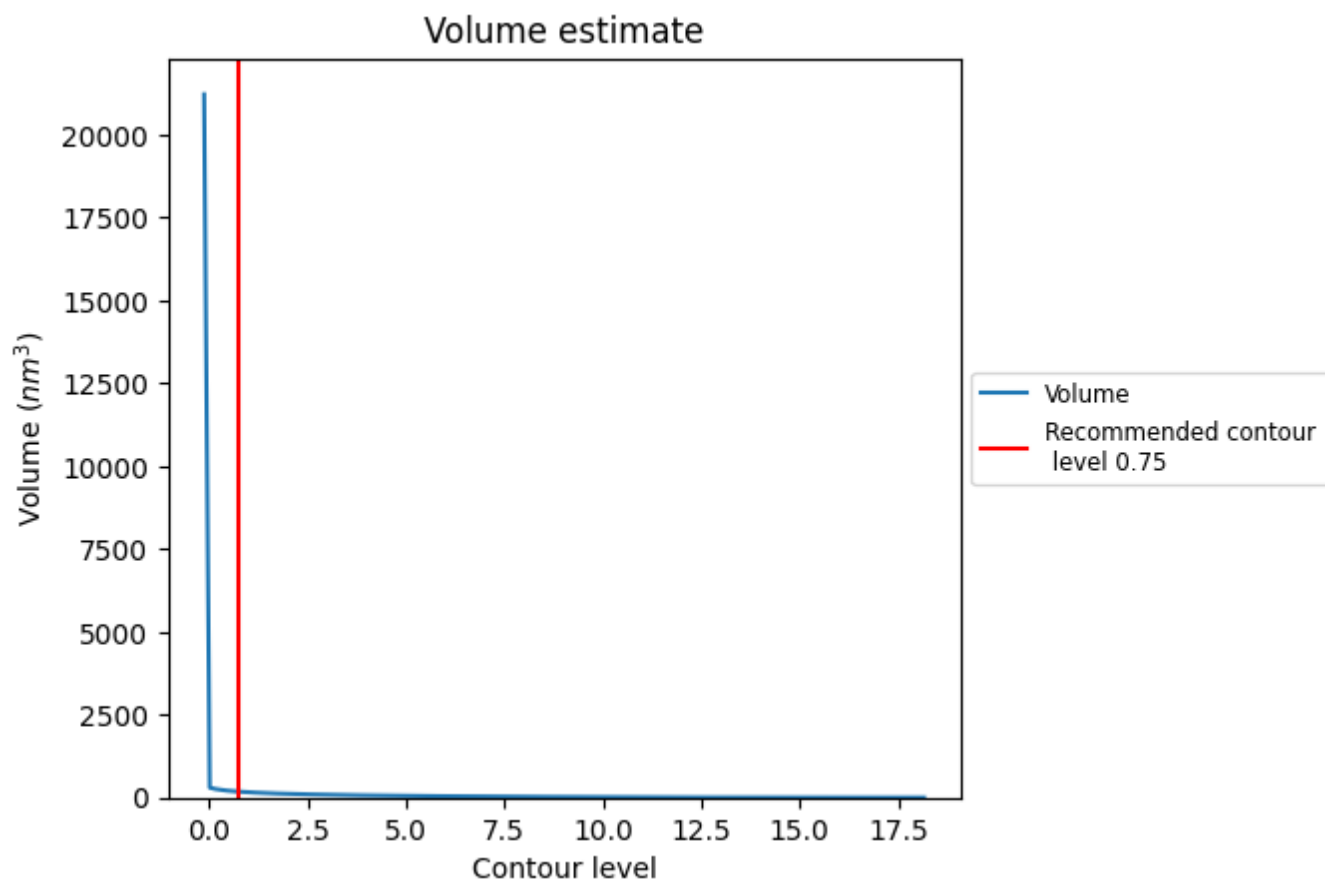
This section contains the results of statistical analysis of the map.

### 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.

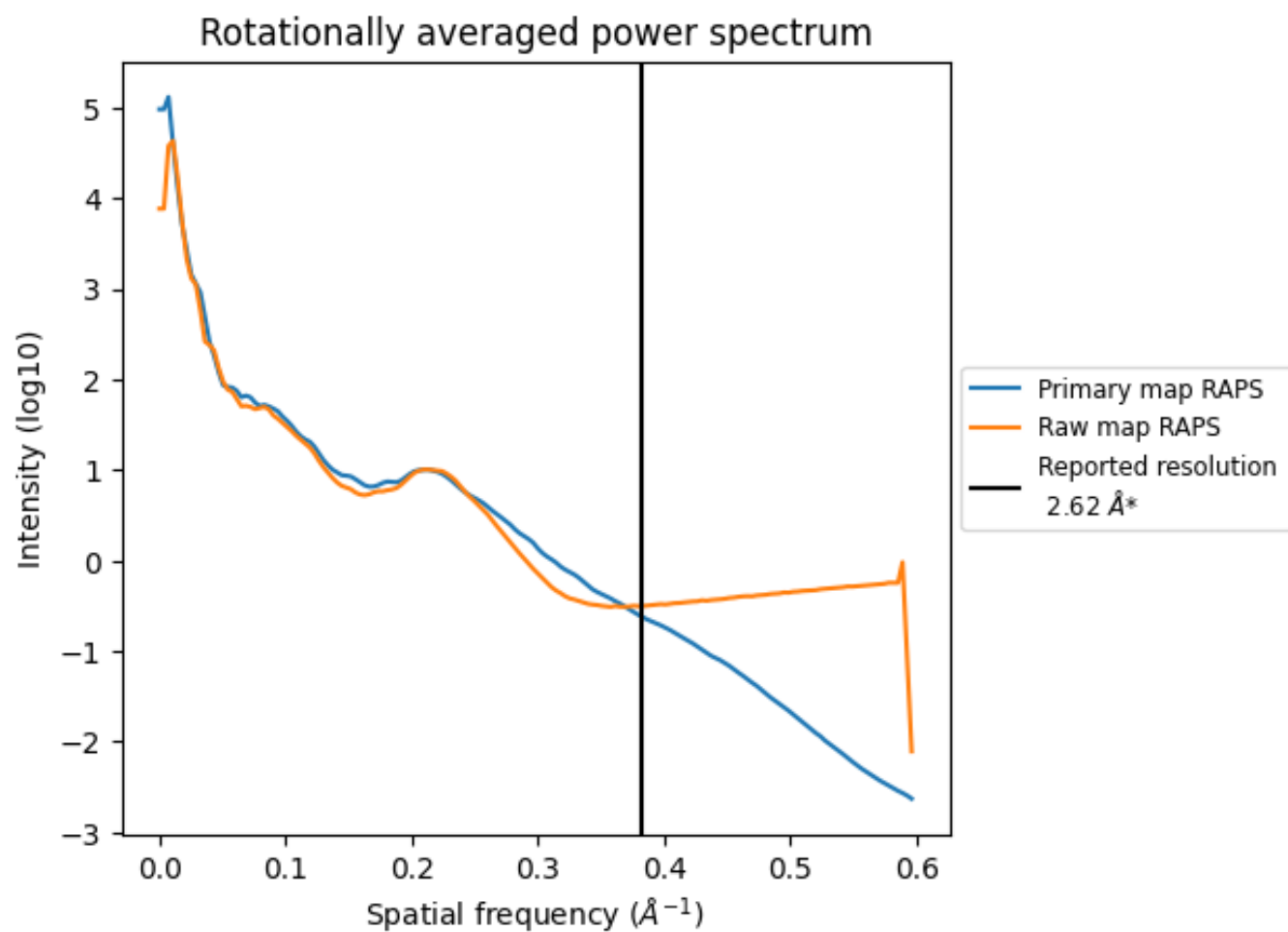
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 179  $\text{nm}^3$ ; this corresponds to an approximate mass of 162 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 ⓘ

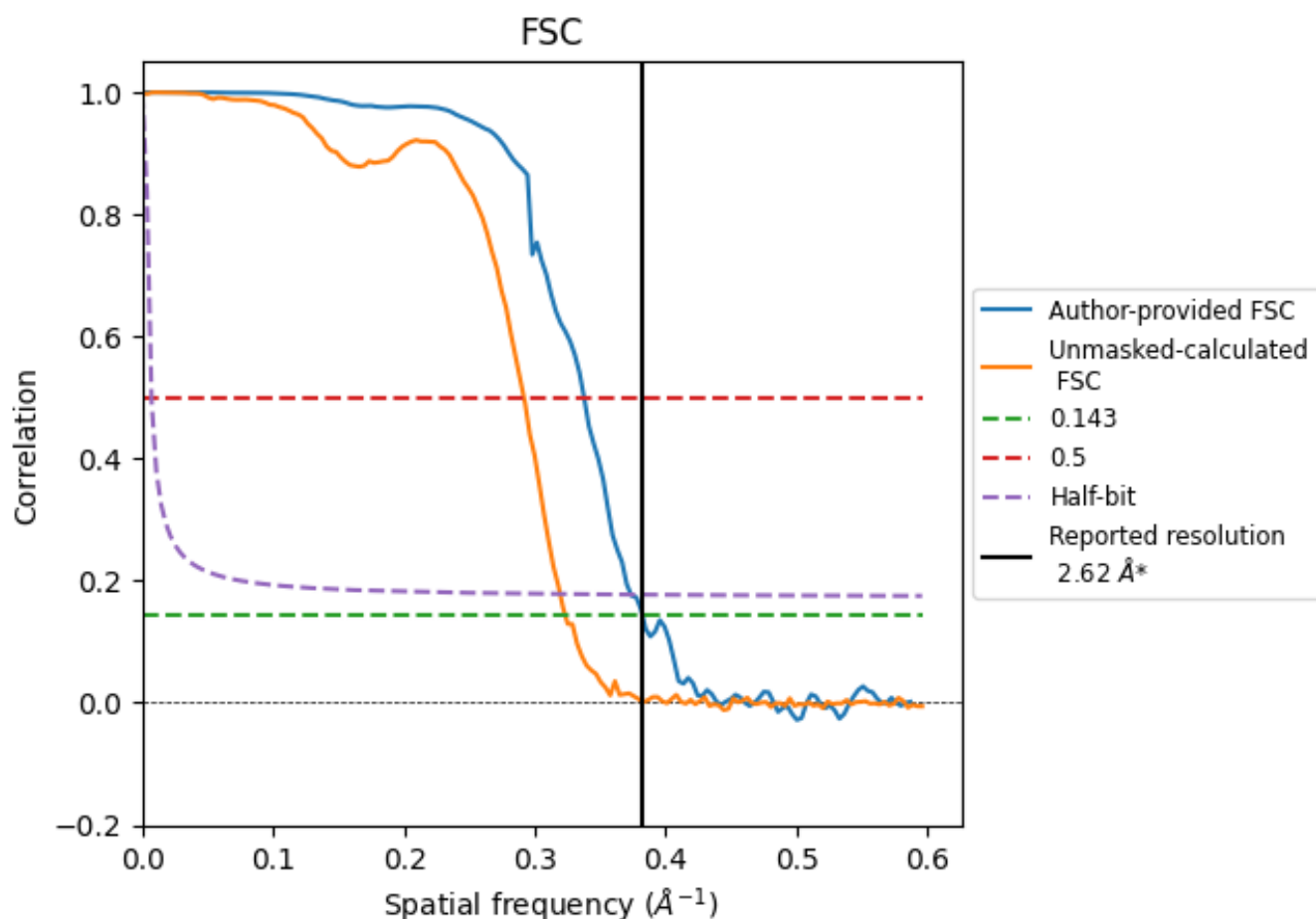


\*Reported resolution corresponds to spatial frequency of  $0.382 \text{ \AA}^{-1}$

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

## 8.2 Resolution estimates [i](#)

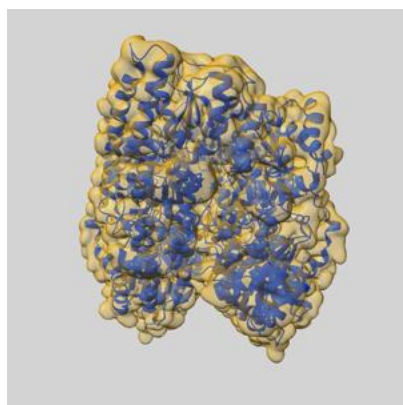
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.62	-	-
Author-provided FSC curve	2.62	2.96	2.68
Unmasked-calculated*	3.09	3.43	3.13

\*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 3.09 differs from the reported value 2.62 by more than 10 %

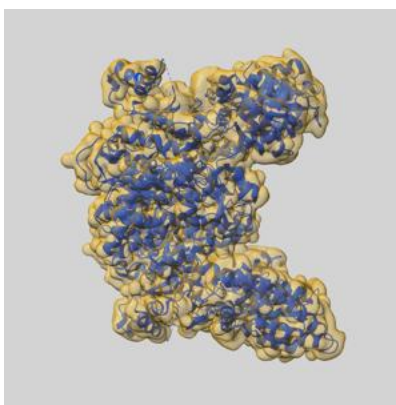
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52558 and PDB model 9I0H. Per-residue inclusion information can be found in section 3 on page 5.

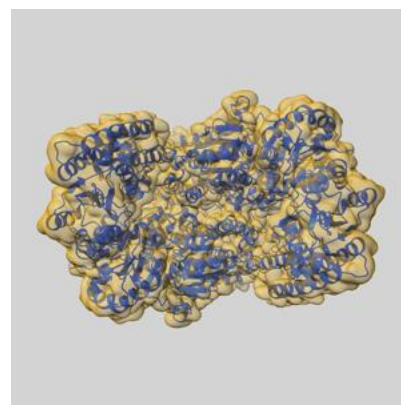
### 9.1 Map-model overlay [i](#)



X



Y

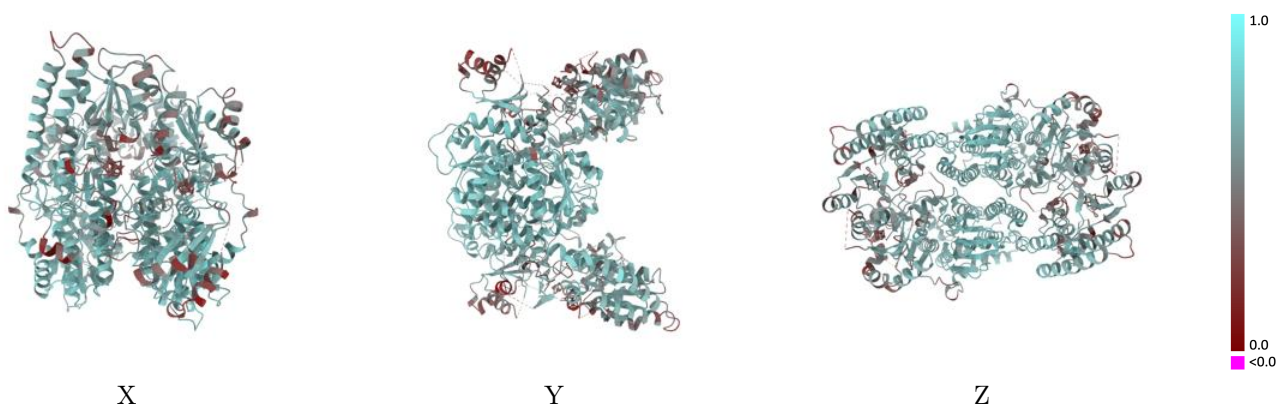


Z

The images above show the 3D surface view of the map at the recommended contour level 0.75 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.

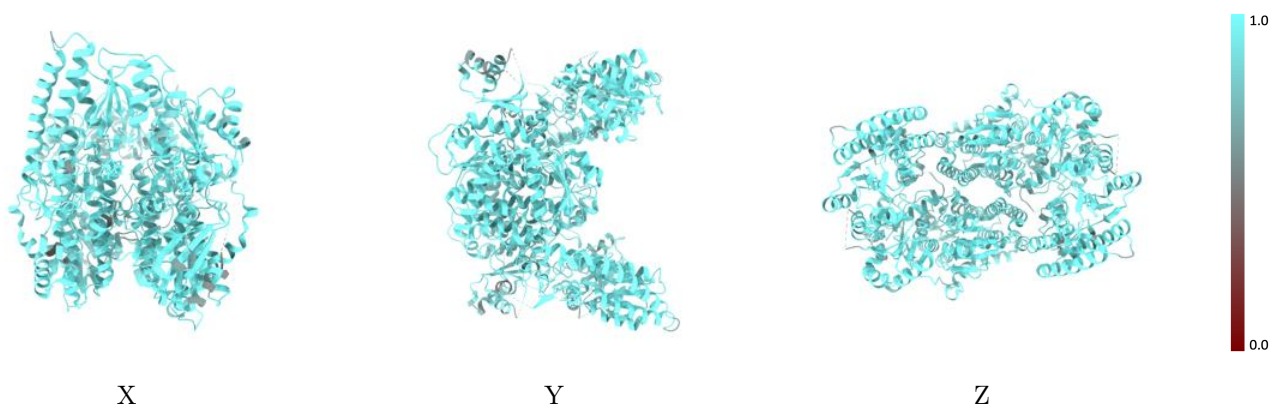


## 9.2 Q-score mapped to coordinate model [i](#)



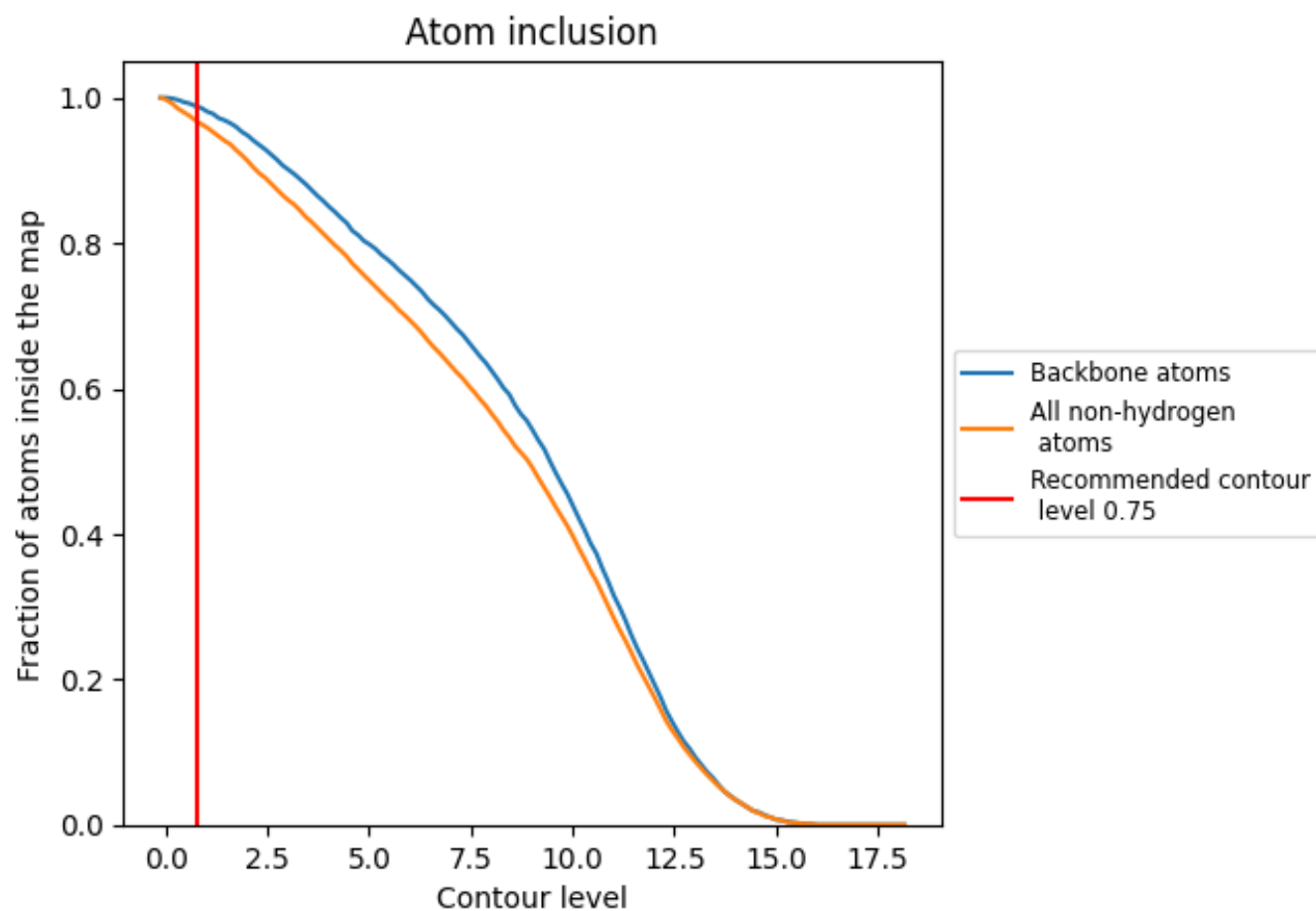
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.75).

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 99% of all backbone atoms, 97% 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 (0.75) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9680	<div></div> 0.5970
A	<div></div> 0.9690	<div></div> 0.5980
B	<div></div> 0.9710	<div></div> 0.5970

