



## wwPDB EM Validation Summary Report ⓘ

Jun 10, 2026 – 02:35 PM EDT

PDB ID : 12RP / pdb\_000012rp  
EMDB ID : EMD-76713  
Title : Local refinement of RBDA, RBDC, and NTDB of SARS-CoV-2 BA.3.2.1 spike with K852A mutation, closed conformation  
Authors : Wang, Y.; Hu, Y.; Xie, X.  
Deposited on : 2026-04-15  
Resolution : 2.78 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](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 : 2022.3.0, CSD as543be (2022)  
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

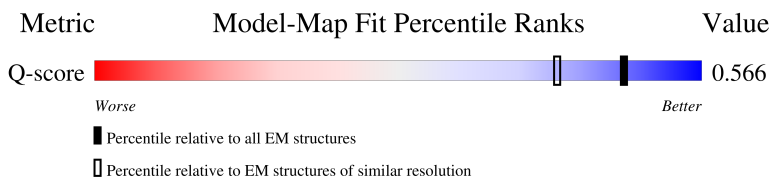
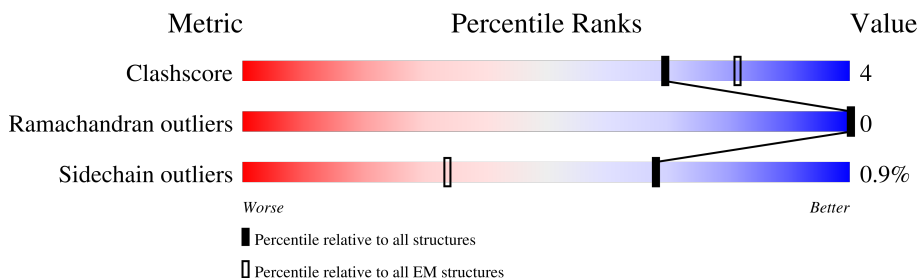
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.78 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	10754 ( 2.28 - 3.28 )

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	1271	
1	B	1271	
1	C	1271	

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 4903 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 SARS-CoV-2 BA.3.2.1 spike with K852A mutation.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	195	Total	C	N	O	S	0	0
			1590	1035	262	285	8		
1	C	189	Total	C	N	O	S	0	0
			1548	1007	253	281	7		
1	B	211	Total	C	N	O	S	0	0
			1709	1118	278	310	3		

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
2	B	1	14	8	1	5	0

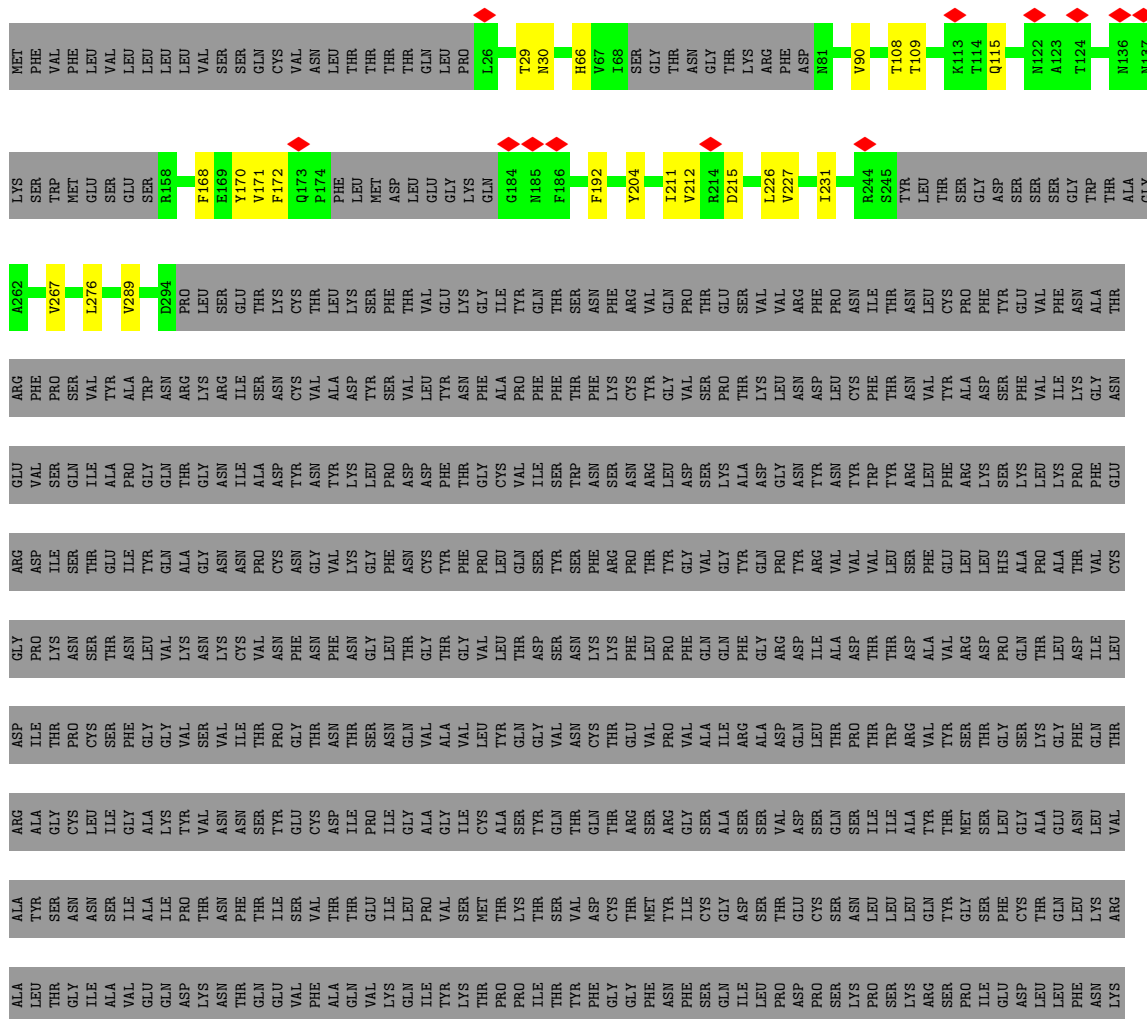




[illegible]

- Molecule 1: SARS-CoV-2 BA.3.2.1 spike with K852A mutation.

Chain B:  15% 83%



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



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	656342	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 ( $e^-/\text{\AA}^2$ )	41	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.747	Depositor
Minimum map value	-0.347	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.15	Depositor
Map size ( $\text{\AA}$ )	346.112, 346.112, 346.112	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.832, 0.832, 0.832	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: NAG

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	0.21	0/1641	0.34	0/2233
1	B	0.17	0/1754	0.35	0/2385
1	C	0.14	0/1599	0.29	0/2177
All	All	0.18	0/4994	0.33	0/6795

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1590	0	1511	11	0
1	B	1709	0	1662	14	0
1	C	1548	0	1460	10	0
2	A	14	0	13	0	0
2	B	28	0	26	0	0
2	C	14	0	13	0	0
All	All	4903	0	4685	34	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 4.

The worst 5 of 34 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:B:170:TYR:CE1	1:B:172:PHE:HB3	2.35	0.61
1:A:422:ASN:HD21	1:A:453:TYR:HB2	1.65	0.60
1:C:421:TYR:HB3	1:C:454:ARG:HG2	1.84	0.59
1:B:226:LEU:HG	1:B:227:VAL:HG23	1.84	0.59
1:B:276:LEU:HB3	1:B:289:VAL:HG22	1.85	0.57

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	189/1271 (15%)	179 (95%)	10 (5%)	0	100	100
1	B	201/1271 (16%)	191 (95%)	10 (5%)	0	100	100
1	C	187/1271 (15%)	181 (97%)	6 (3%)	0	100	100
All	All	577/3813 (15%)	551 (96%)	26 (4%)	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	175/1105 (16%)	173 (99%)	2 (1%)	65	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	190/1105 (17%)	189 (100%)	1 (0%)	81	92
1	C	169/1105 (15%)	167 (99%)	2 (1%)	63	84
All	All	534/3315 (16%)	529 (99%)	5 (1%)	68	87

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	333	THR
1	A	489	TYR
1	C	368	LEU
1	C	382	VAL
1	B	66	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	360	ASN
1	A	409	GLN
1	A	439	ASN
1	C	409	GLN
1	B	188	ASN

### 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](#)

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	$\# Z  > 2$
2	NAG	B	1301	1	14,14,15	0.71	0	17,19,21	1.14	1 (5%)
2	NAG	B	1302	1	14,14,15	0.72	0	17,19,21	0.86	0
2	NAG	C	1301	1	14,14,15	0.73	0	17,19,21	0.77	0
2	NAG	A	1301	1	14,14,15	0.39	0	17,19,21	0.40	0

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	NAG	B	1301	1	-	3/6/23/26	0/1/1/1
2	NAG	B	1302	1	-	1/6/23/26	0/1/1/1
2	NAG	C	1301	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1301	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1301	NAG	C2-N2-C7	2.99	126.91	122.90

There are no chirality outliers.

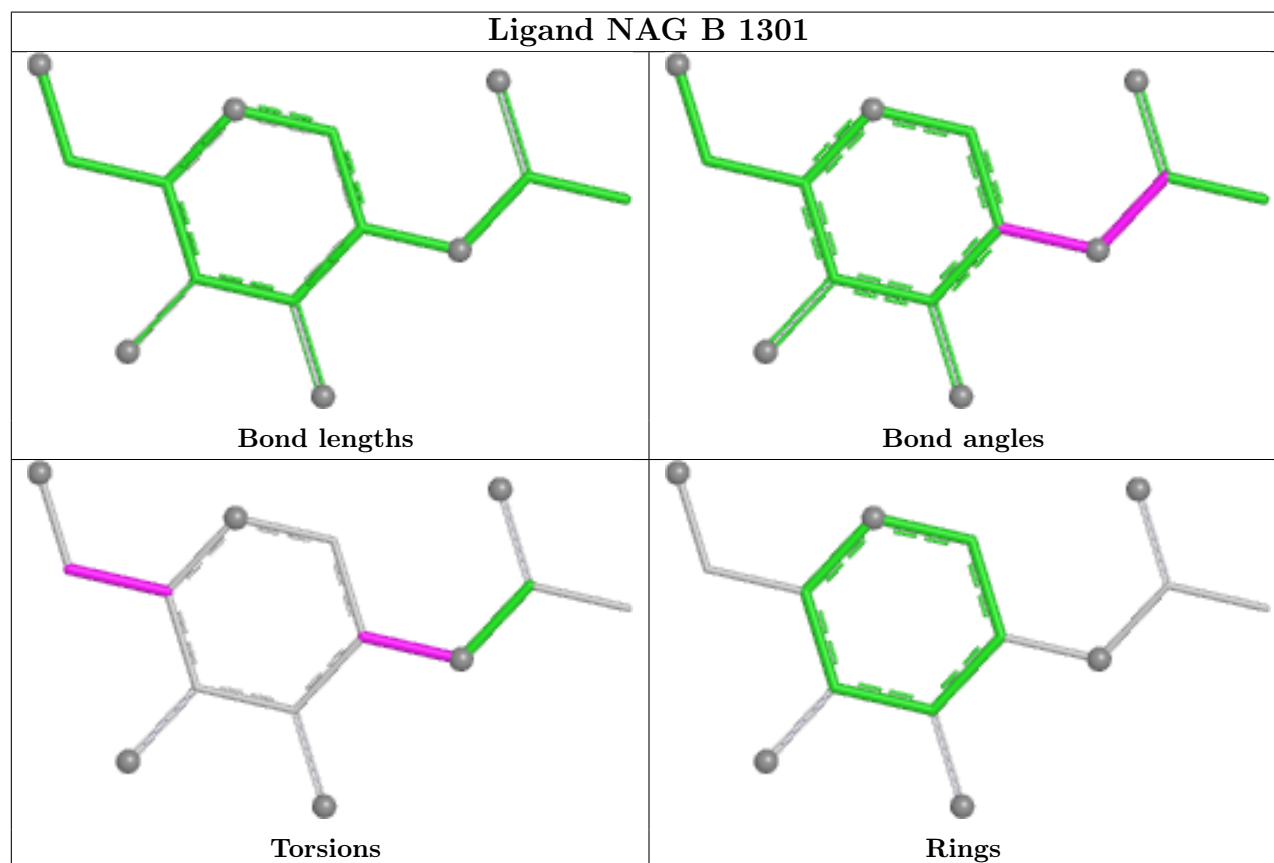
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1301	NAG	O5-C5-C6-O6
2	B	1302	NAG	O5-C5-C6-O6
2	B	1301	NAG	C1-C2-N2-C7
2	B	1301	NAG	C3-C2-N2-C7

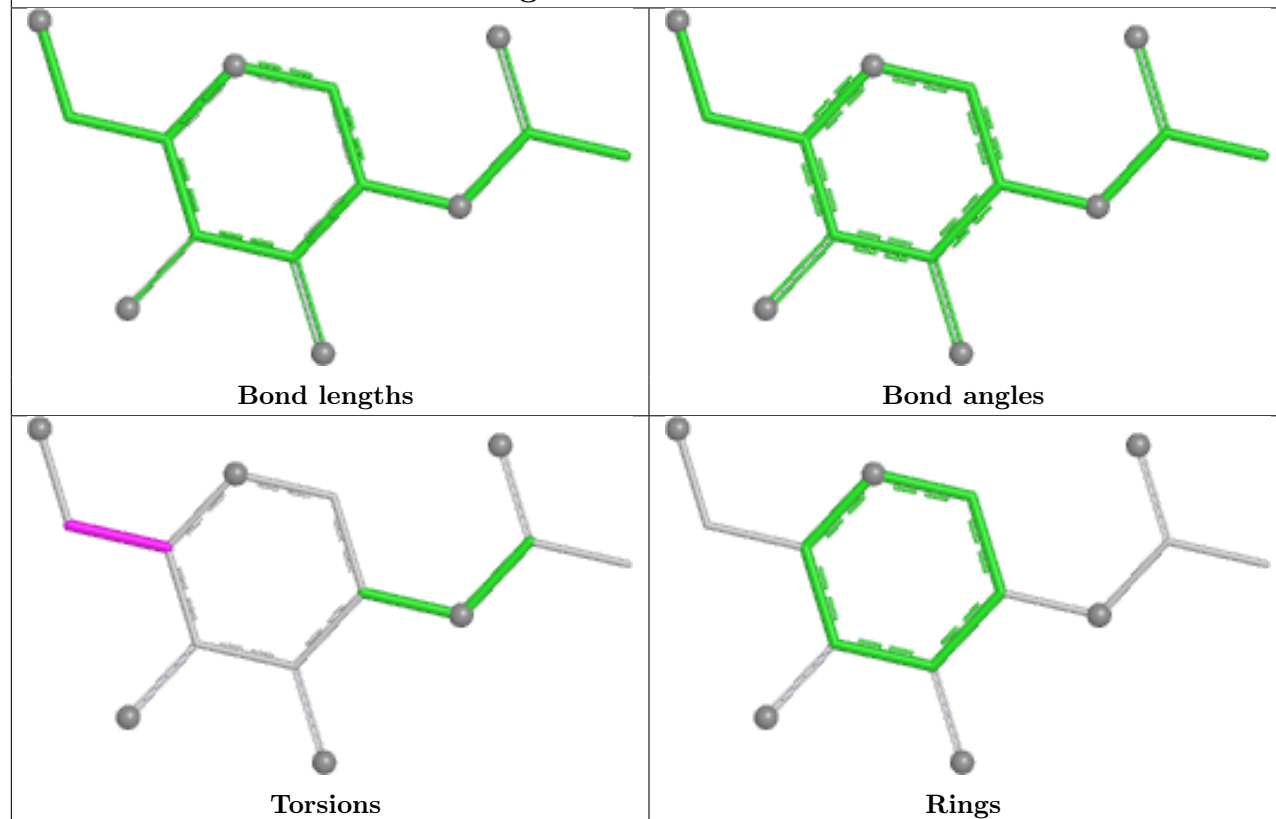
There are no ring outliers.

No monomer is involved in short contacts.

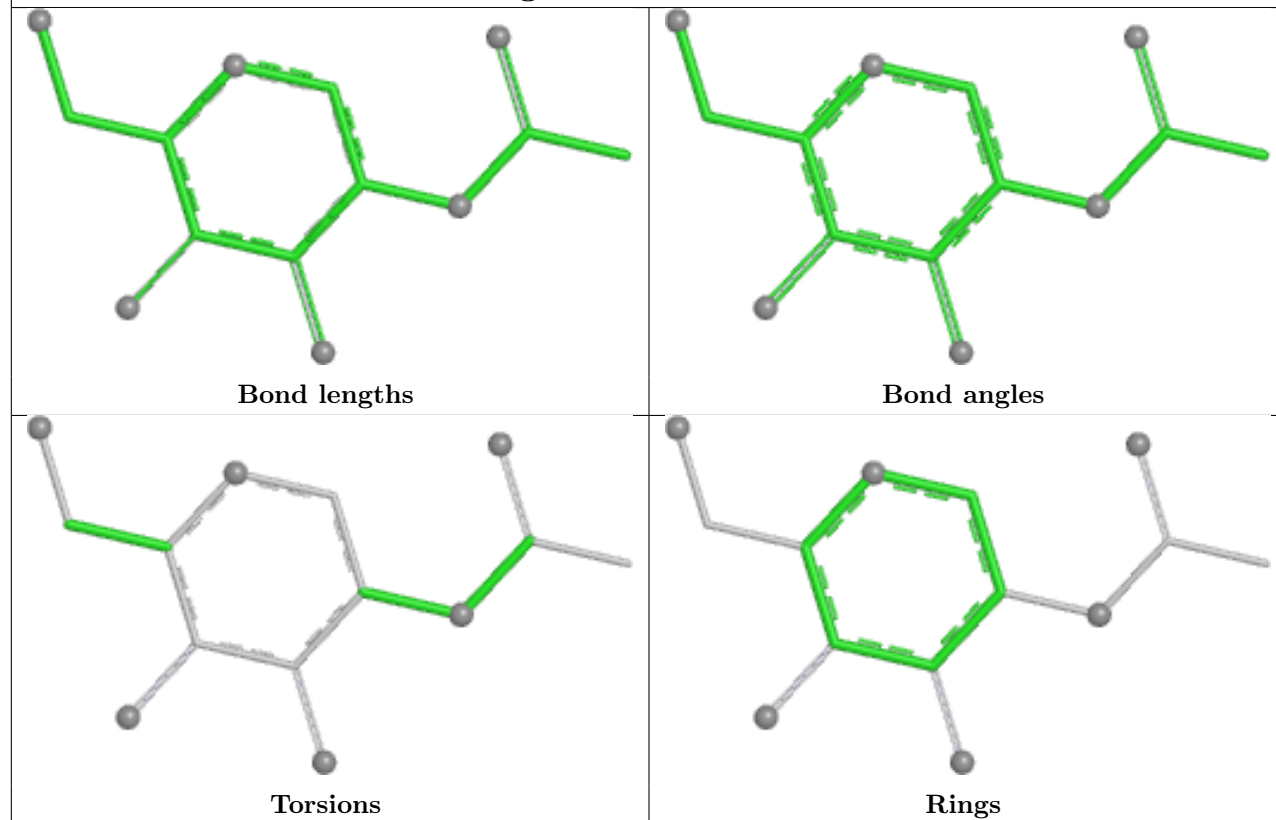
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

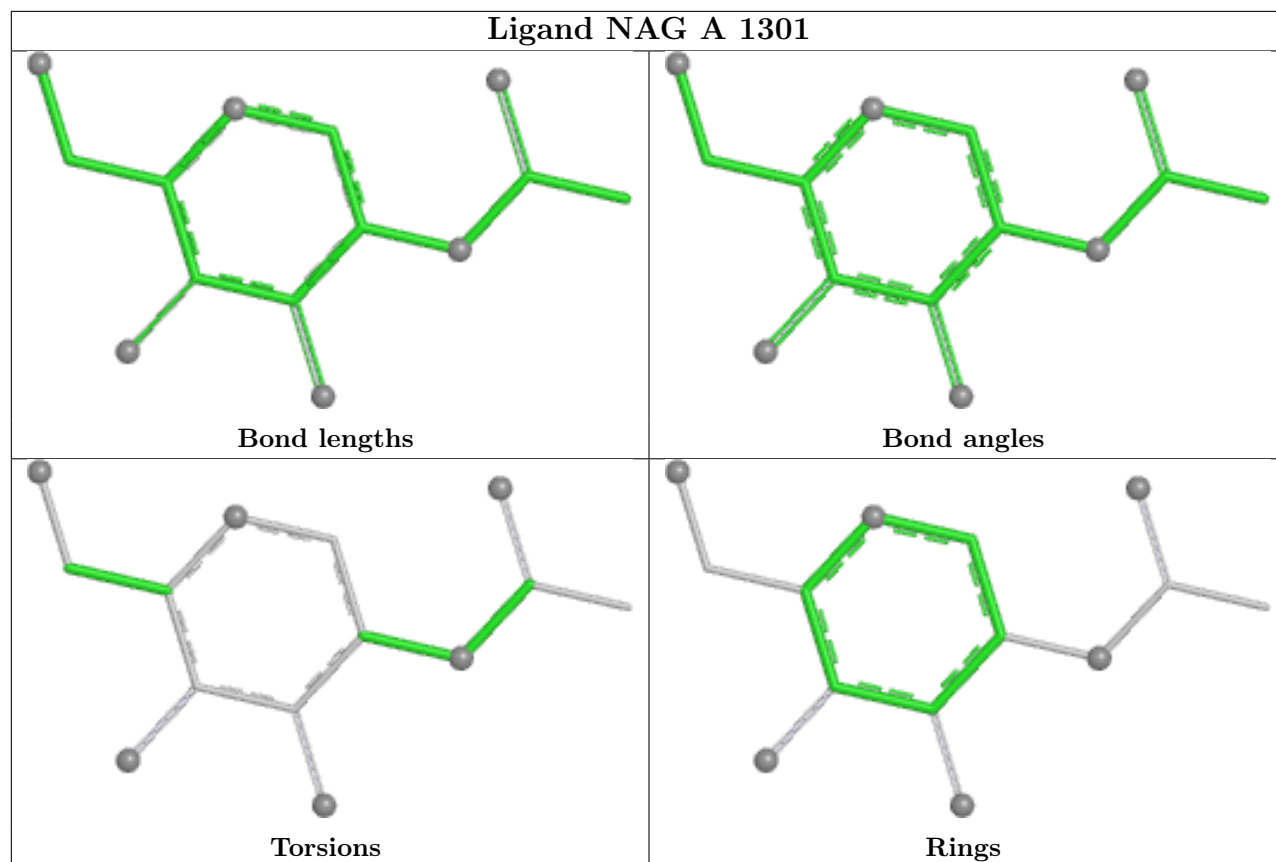


## Ligand NAG B 1302



## Ligand NAG C 1301





## 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.



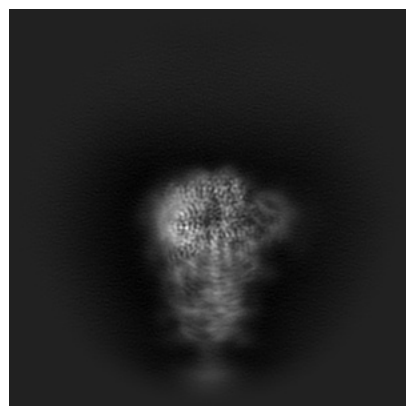
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-76713. These allow visual inspection of the internal detail of the map and identification of artifacts.

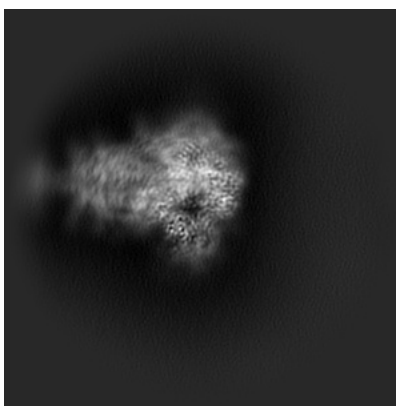
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

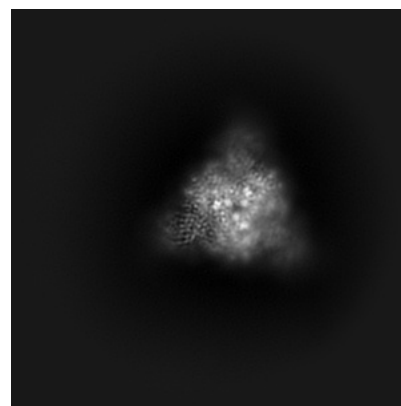
#### 6.1.1 Primary map



X

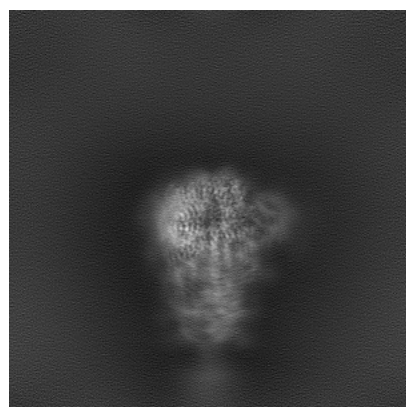


Y

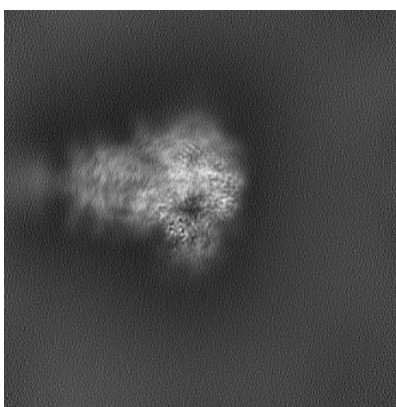


Z

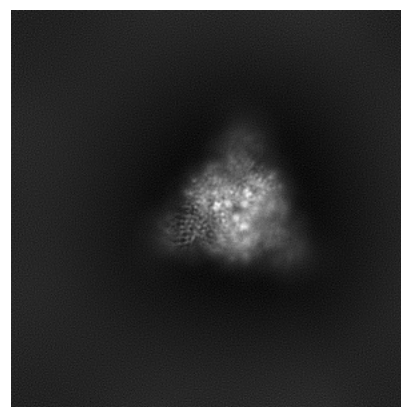
#### 6.1.2 Raw map



X



Y

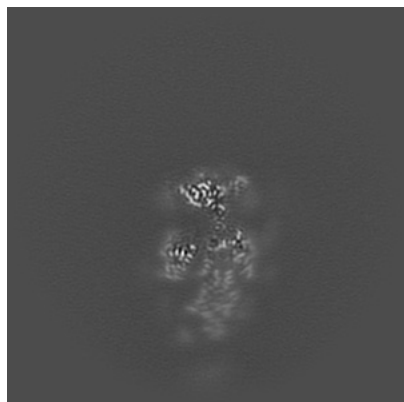


Z

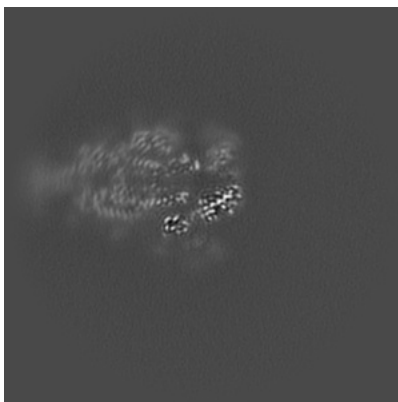
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

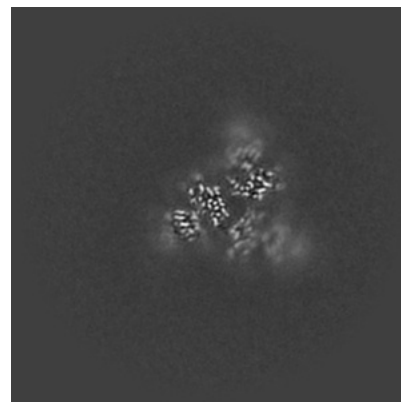
### 6.2.1 Primary map



X Index: 208

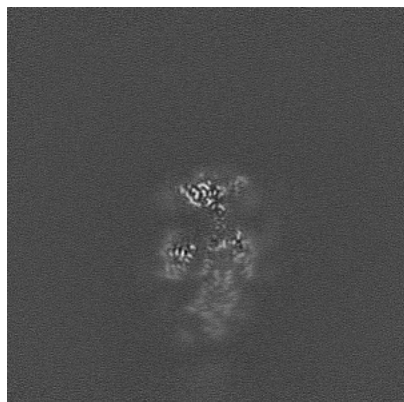


Y Index: 208

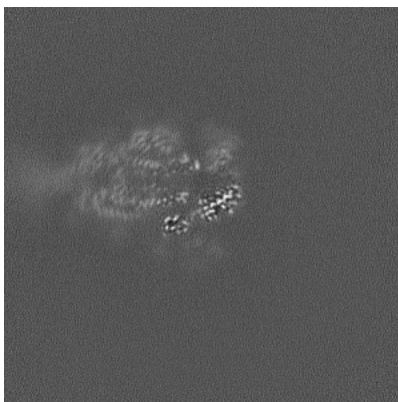


Z Index: 208

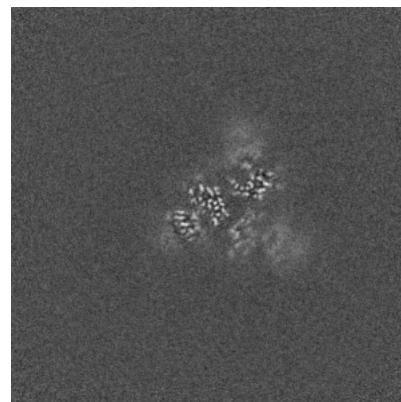
### 6.2.2 Raw map



X Index: 208



Y Index: 208

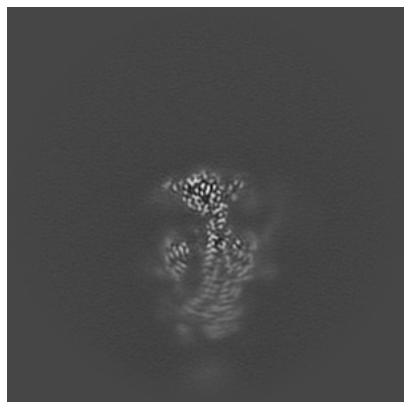


Z Index: 208

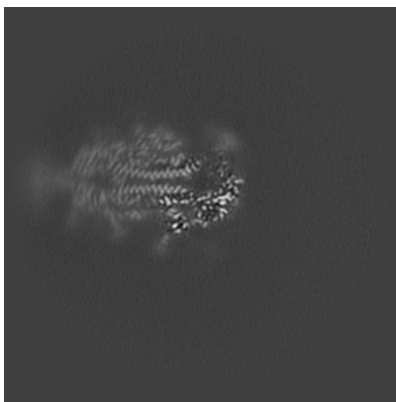
The images above show central slices of the map in three orthogonal directions.

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

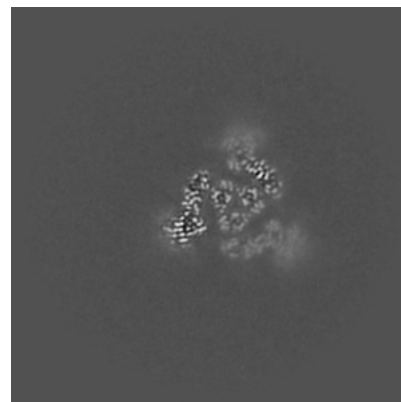
### 6.3.1 Primary map



X Index: 214

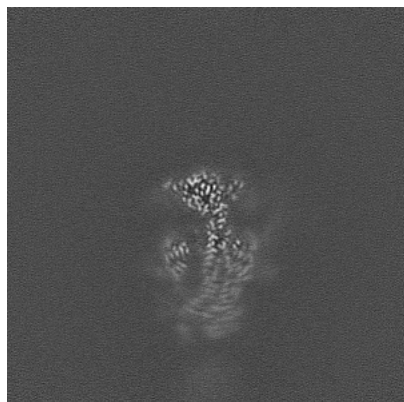


Y Index: 214

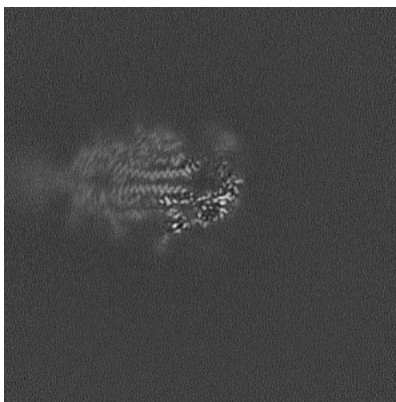


Z Index: 187

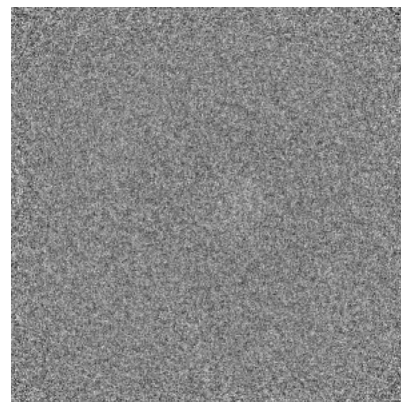
### 6.3.2 Raw map



X Index: 214



Y Index: 214

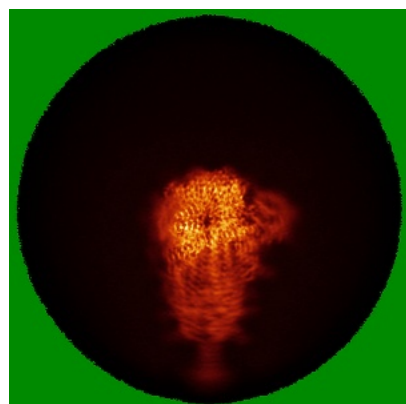


Z Index: 415

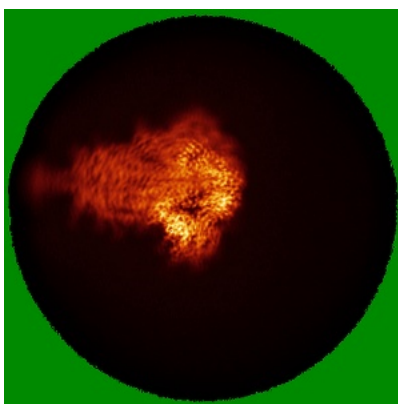
The images above show the largest variance slices of the map in three orthogonal directions.

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

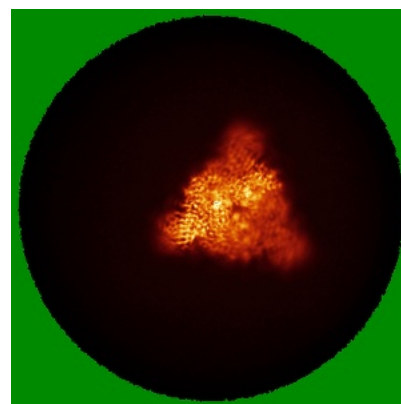
### 6.4.1 Primary map



X

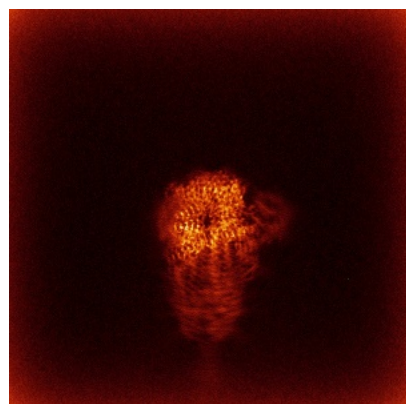


Y

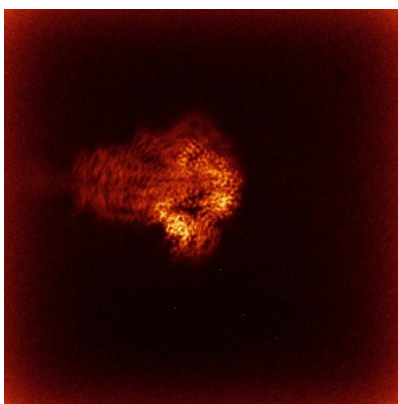


Z

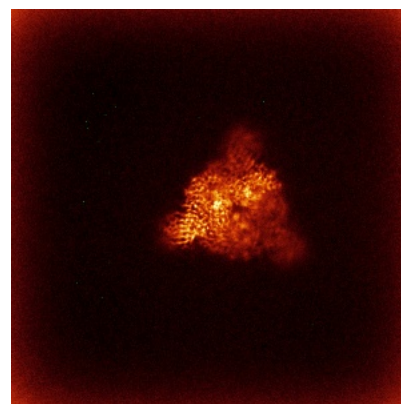
### 6.4.2 Raw map



X



Y



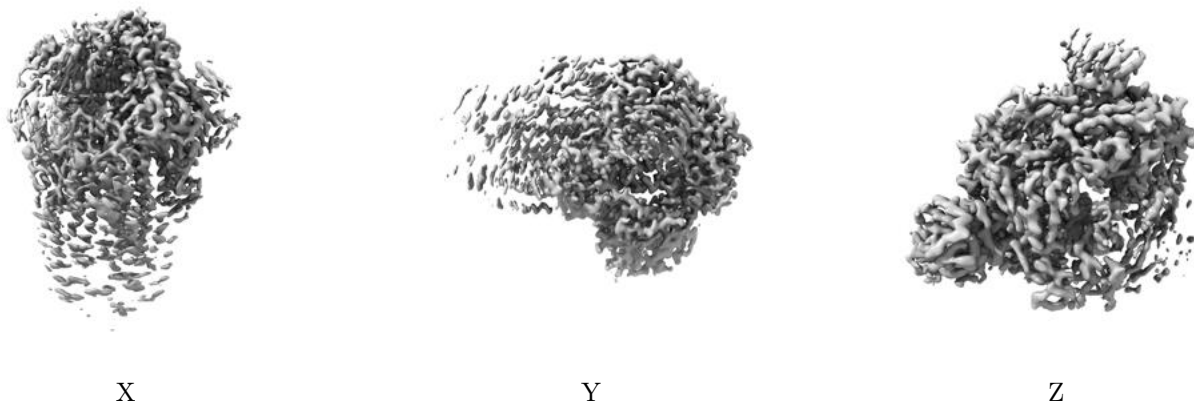
Z

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.



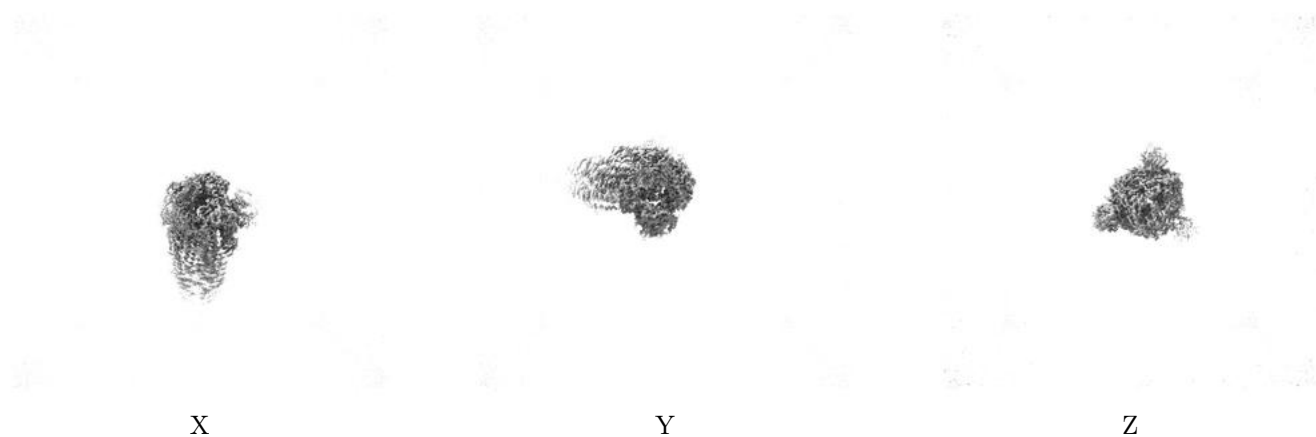
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. 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.

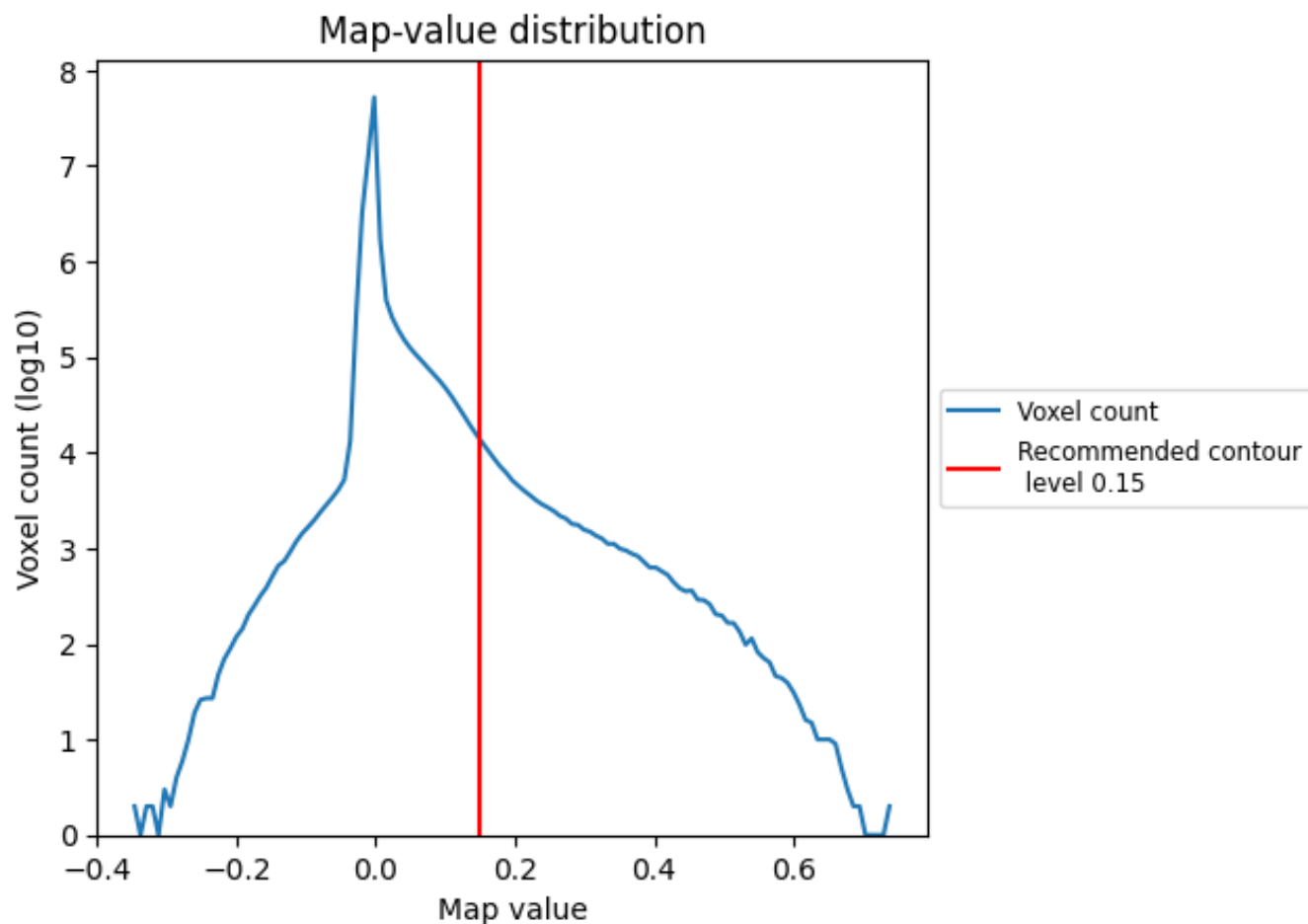
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

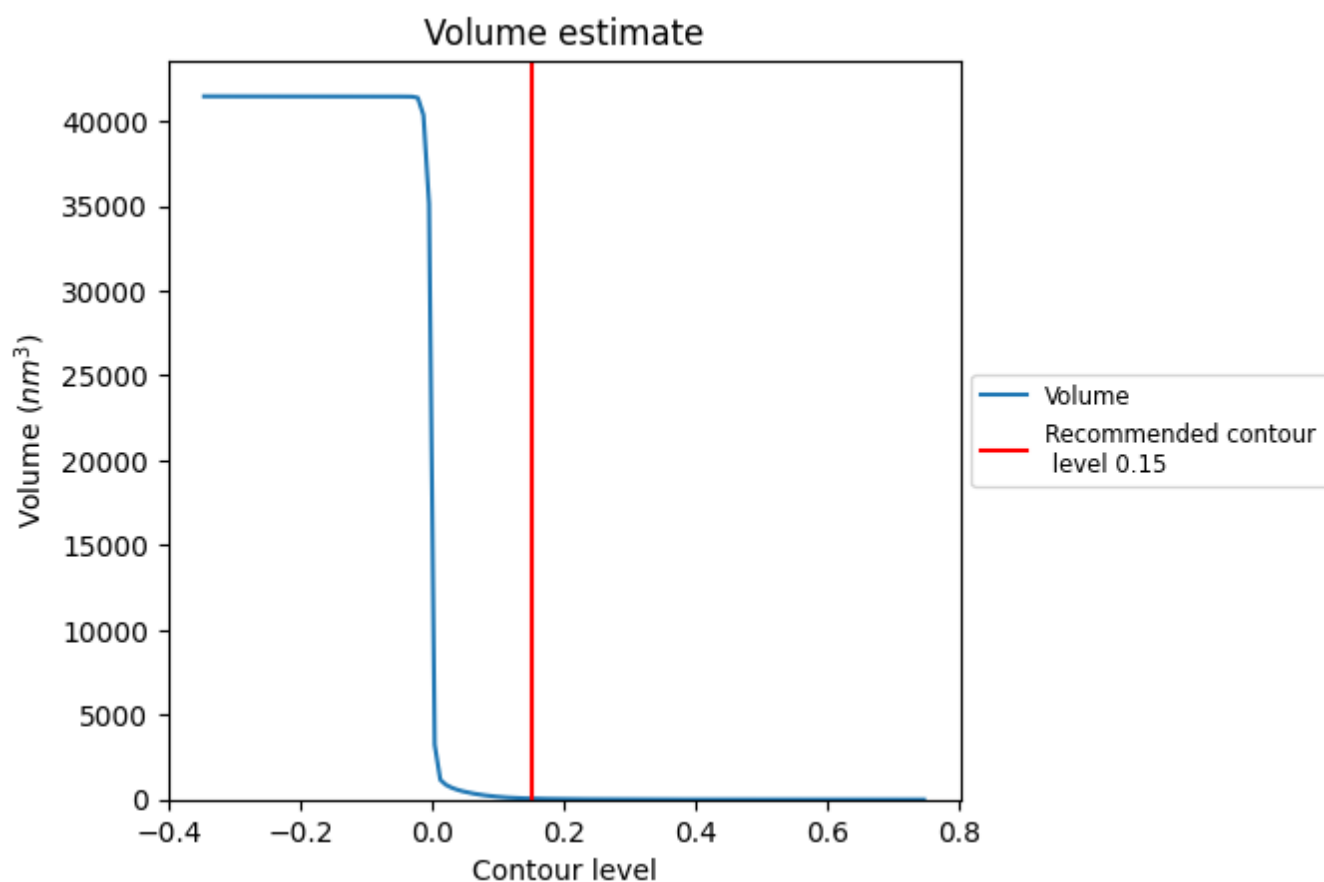
This section contains the results of statistical analysis of the map.

### 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.

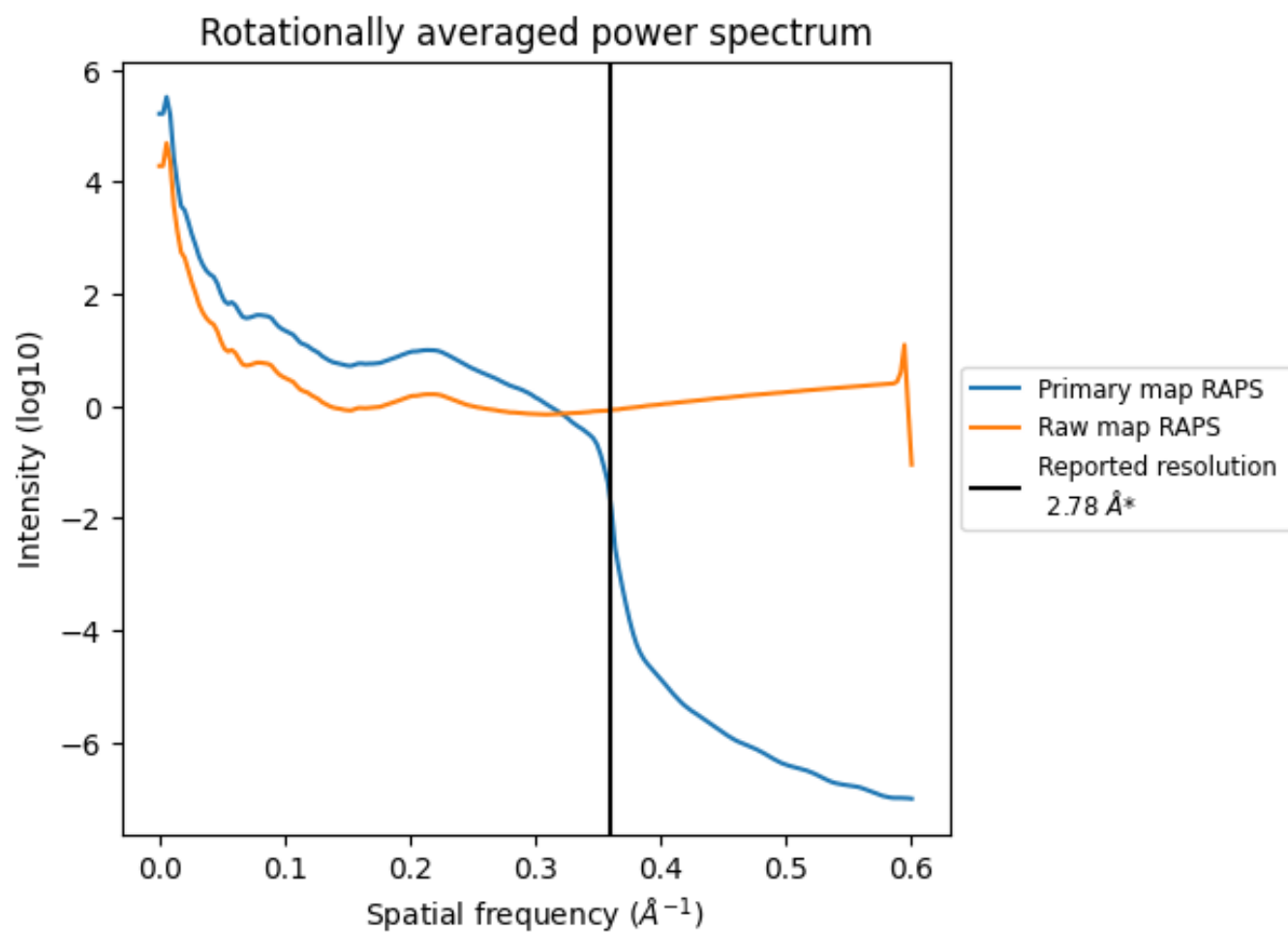
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 60  $\text{nm}^3$ ; this corresponds to an approximate mass of 55 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 ⓘ



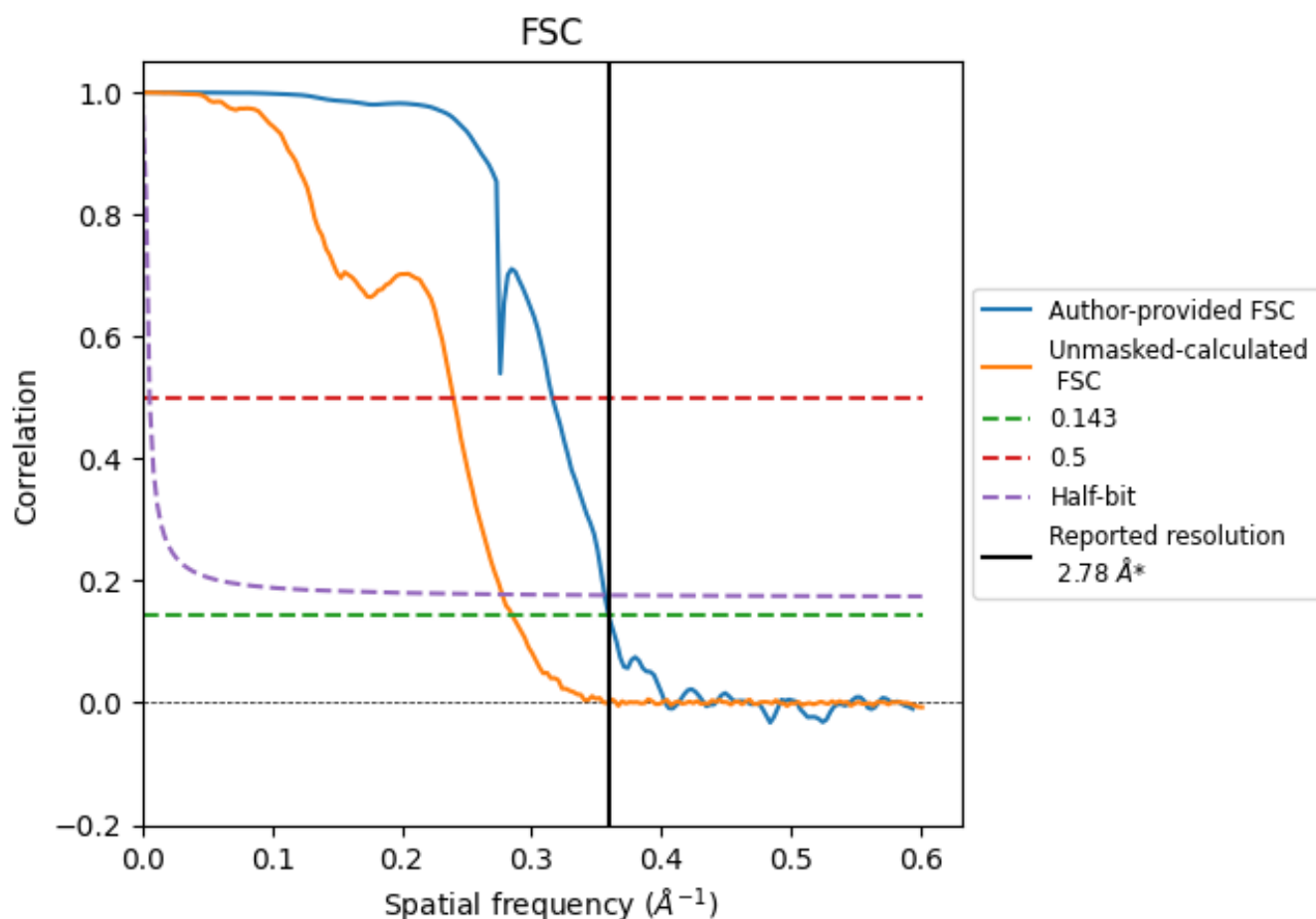
\*Reported resolution corresponds to spatial frequency of 0.360 Å<sup>-1</sup>



## 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  $0.360 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

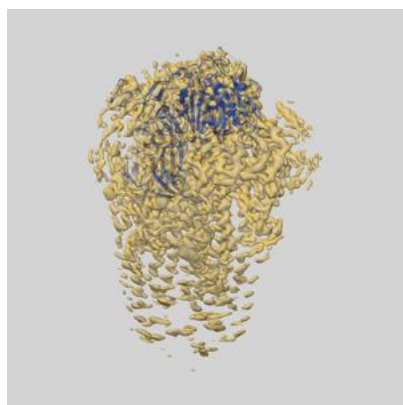
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.78	-	-
Author-provided FSC curve	2.78	3.16	2.81
Unmasked-calculated*	3.51	4.17	3.61

\*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 3.51 differs from the reported value 2.78 by more than 10 %

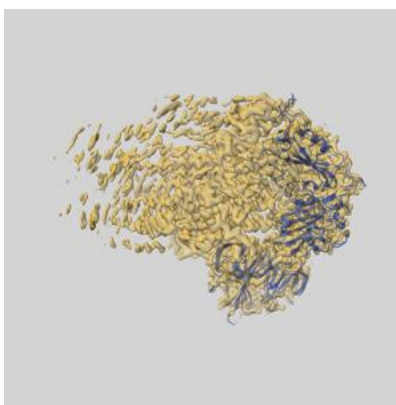
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-76713 and PDB model 12RP. Per-residue inclusion information can be found in section [3](#) on page [5](#).

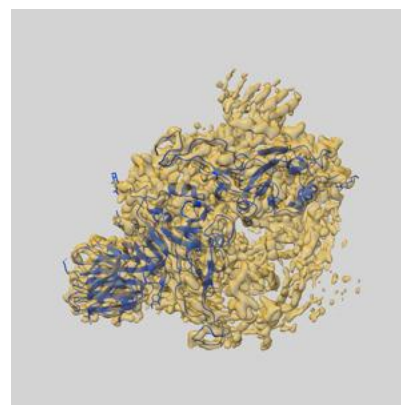
### 9.1 Map-model overlay [i](#)



X



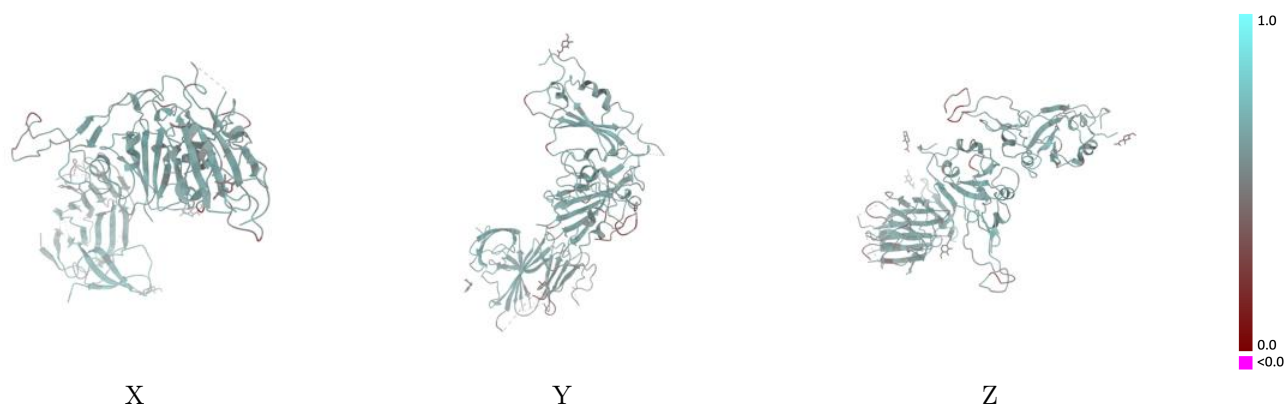
Y



Z

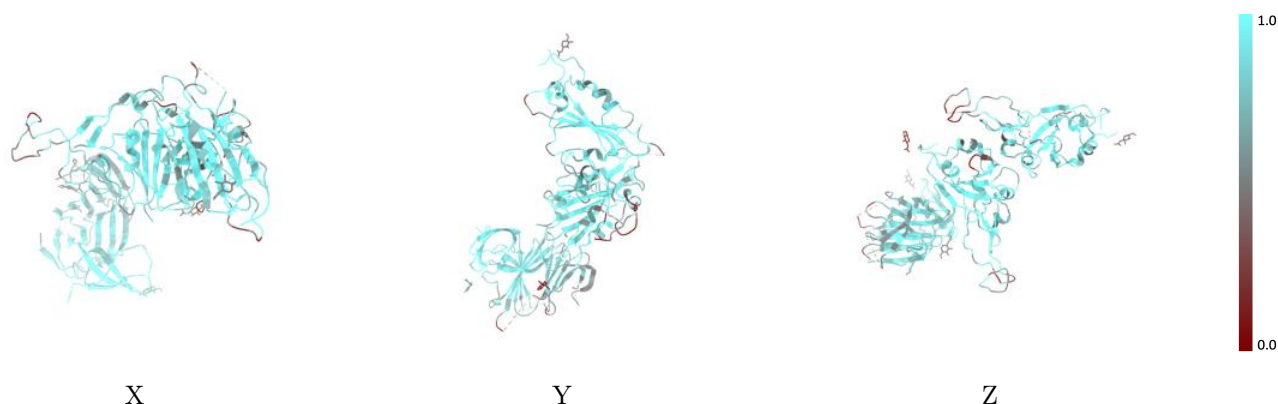
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



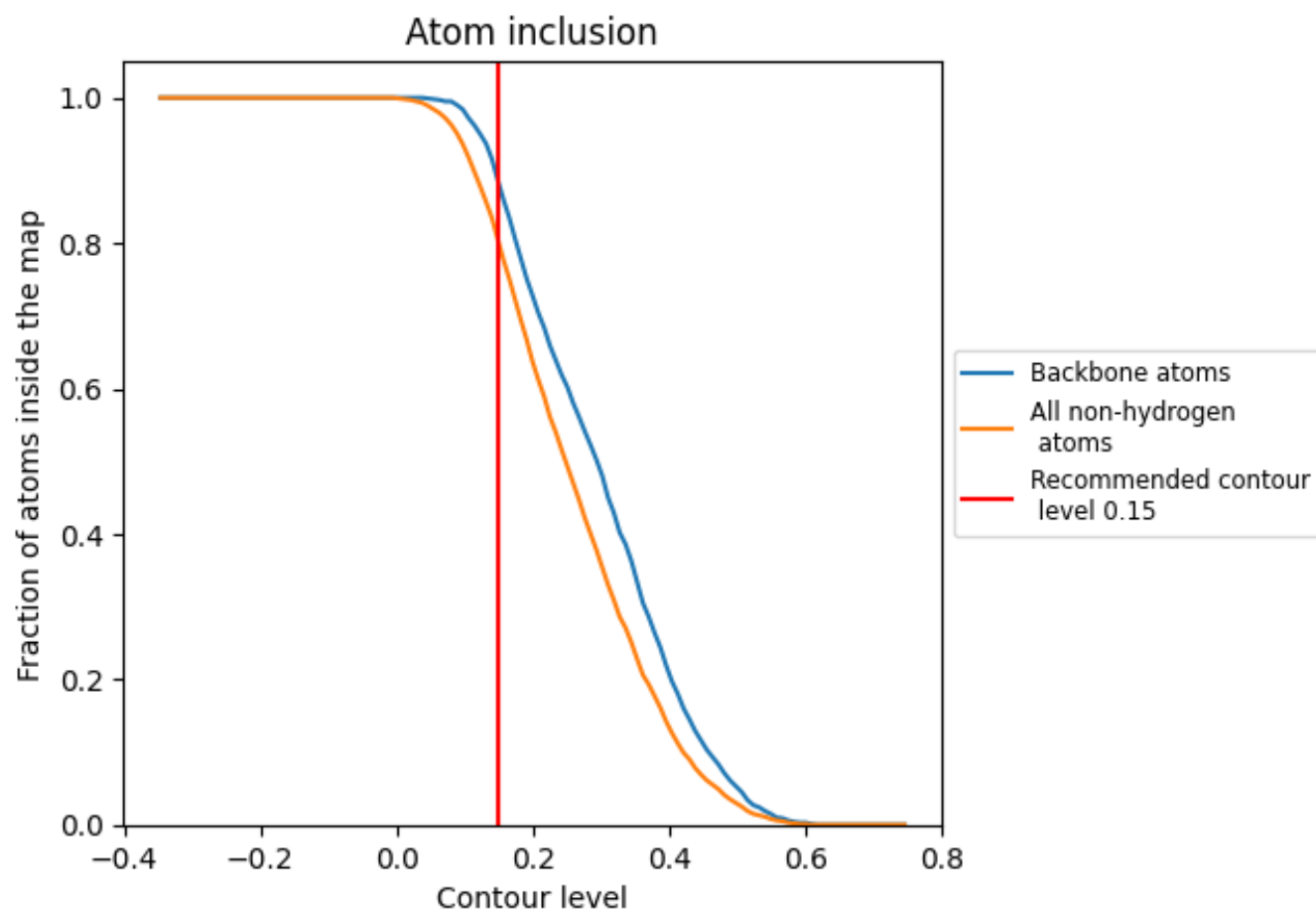
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 80% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8010	<div></div> 0.5660
A	<div></div> 0.7860	<div></div> 0.5590
B	<div></div> 0.7940	<div></div> 0.5640
C	<div></div> 0.8230	<div></div> 0.5750

