



## wwPDB EM Validation Summary Report ⓘ

Jul 14, 2024 – 08:32 pm BST

PDB ID : 8AVV  
EMDB ID : EMD-15684  
Title : Cryo-EM structure of DrBphP photosensory module in Pr state  
Authors : Wahlgren, W.Y.; Takala, H.; Westenhoff, S.  
Deposited on : 2022-08-27  
Resolution : 3.40 Å(reported)  
Based on initial model : 4Q0J

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>.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev92  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

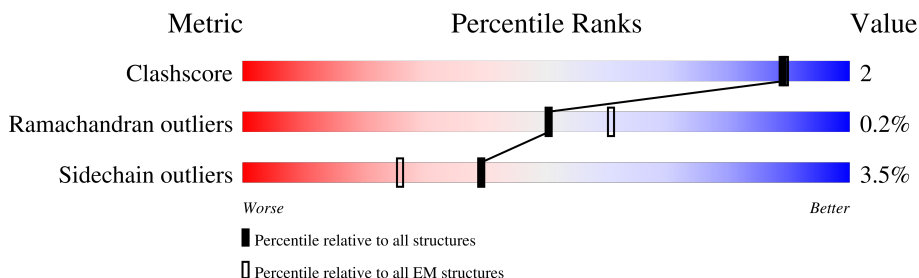
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.40 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  $\geq 3$ , 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	938	
1	B	938	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7794 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 Bacteriophytochrome,Response regulator.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	504	Total	C	N	O	S	0	0
			3849	2443	684	711	11		
1	B	506	Total	C	N	O	S	0	0
			3859	2449	686	713	11		

There are 68 discrepancies between the modelled and reference sequences:

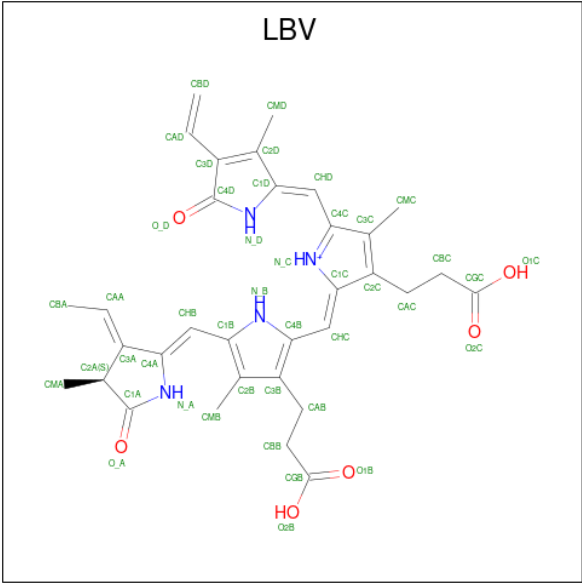
Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP Q9RZA4
A	-12	ALA	-	expression tag	UNP Q9RZA4
A	-11	SER	-	expression tag	UNP Q9RZA4
A	-10	MET	-	expression tag	UNP Q9RZA4
A	-9	THR	-	expression tag	UNP Q9RZA4
A	-8	GLY	-	expression tag	UNP Q9RZA4
A	-7	GLY	-	expression tag	UNP Q9RZA4
A	-6	GLN	-	expression tag	UNP Q9RZA4
A	-5	GLN	-	expression tag	UNP Q9RZA4
A	-4	MET	-	expression tag	UNP Q9RZA4
A	-3	GLY	-	expression tag	UNP Q9RZA4
A	-2	ARG	-	expression tag	UNP Q9RZA4
A	-1	GLY	-	expression tag	UNP Q9RZA4
A	0	SER	-	expression tag	UNP Q9RZA4
A	756	ALA	-	linker	UNP Q9RZA4
A	757	SER	-	linker	UNP Q9RZA4
A	758	SER	-	linker	UNP Q9RZA4
A	759	ALA	-	linker	UNP Q9RZA4
A	760	GLY	-	linker	UNP Q9RZA4
A	761	GLY	-	linker	UNP Q9RZA4
A	762	SER	-	linker	UNP Q9RZA4
A	763	ALA	-	linker	UNP Q9RZA4
A	764	GLY	-	linker	UNP Q9RZA4
A	765	SER	-	linker	UNP Q9RZA4
A	766	ALA	-	linker	UNP Q9RZA4
A	767	GLY	-	linker	UNP Q9RZA4

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	917	LEU	-	expression tag	UNP Q9RZA5
A	918	GLU	-	expression tag	UNP Q9RZA5
A	919	HIS	-	expression tag	UNP Q9RZA5
A	920	HIS	-	expression tag	UNP Q9RZA5
A	921	HIS	-	expression tag	UNP Q9RZA5
A	922	HIS	-	expression tag	UNP Q9RZA5
A	923	HIS	-	expression tag	UNP Q9RZA5
A	924	HIS	-	expression tag	UNP Q9RZA5
B	-13	MET	-	initiating methionine	UNP Q9RZA4
B	-12	ALA	-	expression tag	UNP Q9RZA4
B	-11	SER	-	expression tag	UNP Q9RZA4
B	-10	MET	-	expression tag	UNP Q9RZA4
B	-9	THR	-	expression tag	UNP Q9RZA4
B	-8	GLY	-	expression tag	UNP Q9RZA4
B	-7	GLY	-	expression tag	UNP Q9RZA4
B	-6	GLN	-	expression tag	UNP Q9RZA4
B	-5	GLN	-	expression tag	UNP Q9RZA4
B	-4	MET	-	expression tag	UNP Q9RZA4
B	-3	GLY	-	expression tag	UNP Q9RZA4
B	-2	ARG	-	expression tag	UNP Q9RZA4
B	-1	GLY	-	expression tag	UNP Q9RZA4
B	0	SER	-	expression tag	UNP Q9RZA4
B	756	ALA	-	linker	UNP Q9RZA4
B	757	SER	-	linker	UNP Q9RZA4
B	758	SER	-	linker	UNP Q9RZA4
B	759	ALA	-	linker	UNP Q9RZA4
B	760	GLY	-	linker	UNP Q9RZA4
B	761	GLY	-	linker	UNP Q9RZA4
B	762	SER	-	linker	UNP Q9RZA4
B	763	ALA	-	linker	UNP Q9RZA4
B	764	GLY	-	linker	UNP Q9RZA4
B	765	SER	-	linker	UNP Q9RZA4
B	766	ALA	-	linker	UNP Q9RZA4
B	767	GLY	-	linker	UNP Q9RZA4
B	917	LEU	-	expression tag	UNP Q9RZA5
B	918	GLU	-	expression tag	UNP Q9RZA5
B	919	HIS	-	expression tag	UNP Q9RZA5
B	920	HIS	-	expression tag	UNP Q9RZA5
B	921	HIS	-	expression tag	UNP Q9RZA5
B	922	HIS	-	expression tag	UNP Q9RZA5
B	923	HIS	-	expression tag	UNP Q9RZA5
B	924	HIS	-	expression tag	UNP Q9RZA5

- Molecule 2 is 3-[2-[(Z)-[3-(2-carboxyethyl)-5-[(Z)-(4-ethenyl-3-methyl-5-oxidanylidene-pyrrol-2-ylidene)methyl]-4-methyl-pyrrol-1-ium -2-ylidene]methyl]-5-[(Z)-[(3E)-3-ethylidene-4-methyl-5-oxidanylidene-pyrrolidin-2-ylidene]methyl]-4-methyl-1H-pyrrol-3- yl]propanoic acid (three-letter code: LBV) (formula: C<sub>33</sub>H<sub>37</sub>N<sub>4</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).

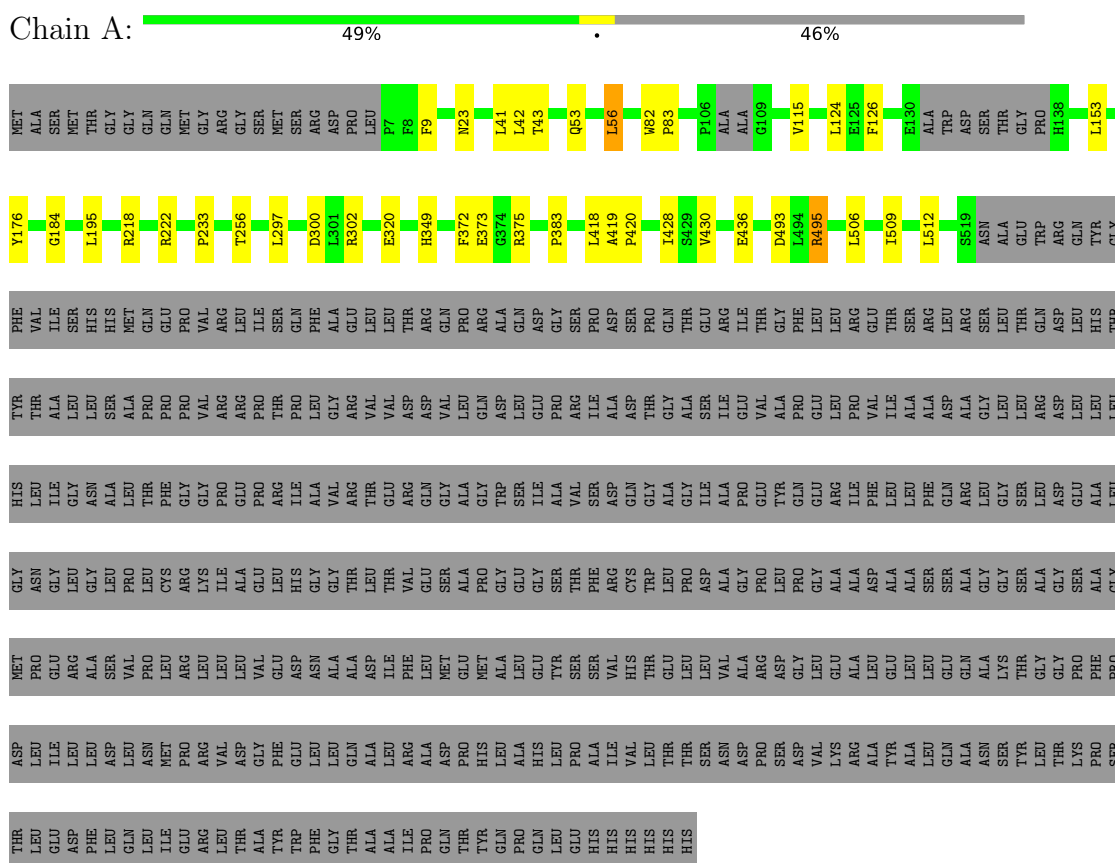


Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			43	33	4	6	
2	B	1	Total	C	N	O	0
			43	33	4	6	

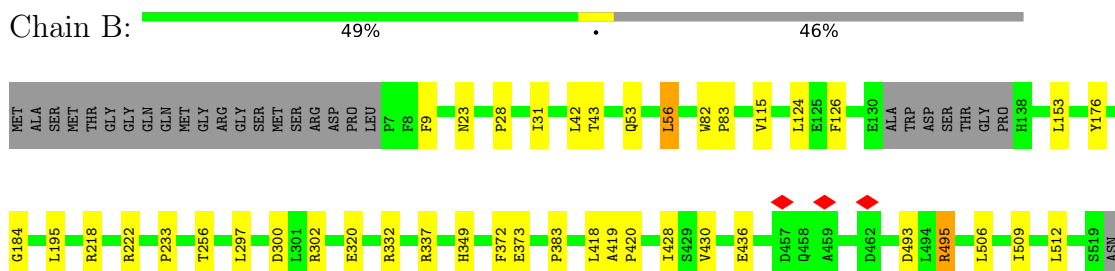
### 3 Residue-property plots

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: Bacteriophytochrome,Response regulator



- Molecule 1: Bacteriophytochrome,Response regulator



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

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	117296	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	48.3	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.507	Depositor
Minimum map value	-0.890	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.09	Depositor
Map size ( $\text{\AA}$ )	386.0416, 386.0416, 386.0416	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.8617, 0.8617, 0.8617	Depositor



## 5 Model quality

### 5.1 Standard geometry

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

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	0.28	0/3946	0.59	0/5396
1	B	0.28	0/3957	0.59	0/5413
All	All	0.28	0/7903	0.59	0/10809

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	3849	0	3820	14	0
1	B	3859	0	3831	15	0
2	A	43	0	35	0	0
2	B	43	0	35	0	0
All	All	7794	0	7721	28	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 2.

The worst 5 of 28 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:43:THR:OG1	1:B:53:GLN:HB2	2.12	0.50
1:A:43:THR:OG1	1:A:53:GLN:HB2	2.11	0.50
1:B:115:VAL:HG22	1:B:124:LEU:HG	1.93	0.50
1:A:383:PRO:HB3	1:A:418:LEU:HD22	1.95	0.48
1:A:372:PHE:HA	1:A:436:GLU:HG2	1.96	0.48

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	498/938 (53%)	474 (95%)	23 (5%)	1 (0%)	47	78
1	B	502/938 (54%)	477 (95%)	24 (5%)	1 (0%)	47	78
All	All	1000/1876 (53%)	951 (95%)	47 (5%)	2 (0%)	50	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	373	GLU
1	B	373	GLU

### 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.

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	398/746 (53%)	384 (96%)	14 (4%)	36 65
1	B	398/746 (53%)	384 (96%)	14 (4%)	36 65
All	All	796/1492 (53%)	768 (96%)	28 (4%)	39 65

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	56	LEU
1	B	512	LEU
1	B	222	ARG
1	B	493	ASP
1	B	218	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	349	HIS
1	B	317	GLN
1	B	72	GLN
1	A	349	HIS
1	B	315	GLN

### 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 ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

2 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	LBV	A	1000	-	42,46,46	1.08	3 (7%)	47,67,67	1.24	5 (10%)
2	LBV	B	1000	-	42,46,46	1.10	3 (7%)	47,67,67	1.31	3 (6%)

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	LBV	A	1000	-	-	8/26/74/74	0/4/4/4
2	LBV	B	1000	-	-	9/26/74/74	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1000	LBV	C3D-C2D	3.28	1.43	1.37
2	B	1000	LBV	C3D-C2D	3.16	1.43	1.37
2	B	1000	LBV	C4A-C3A	-3.01	1.39	1.45
2	A	1000	LBV	CAD-C3D	-2.62	1.40	1.47
2	A	1000	LBV	C4A-C3A	-2.58	1.40	1.45

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1000	LBV	C4B-CHC-C1C	4.38	134.04	128.81
2	A	1000	LBV	C4B-CHC-C1C	3.46	132.95	128.81
2	B	1000	LBV	CMD-C2D-C1D	3.12	128.06	124.17
2	A	1000	LBV	CMD-C2D-C1D	2.94	127.83	124.17
2	B	1000	LBV	CAA-C3A-C4A	-2.70	123.10	126.36

There are no chirality outliers.

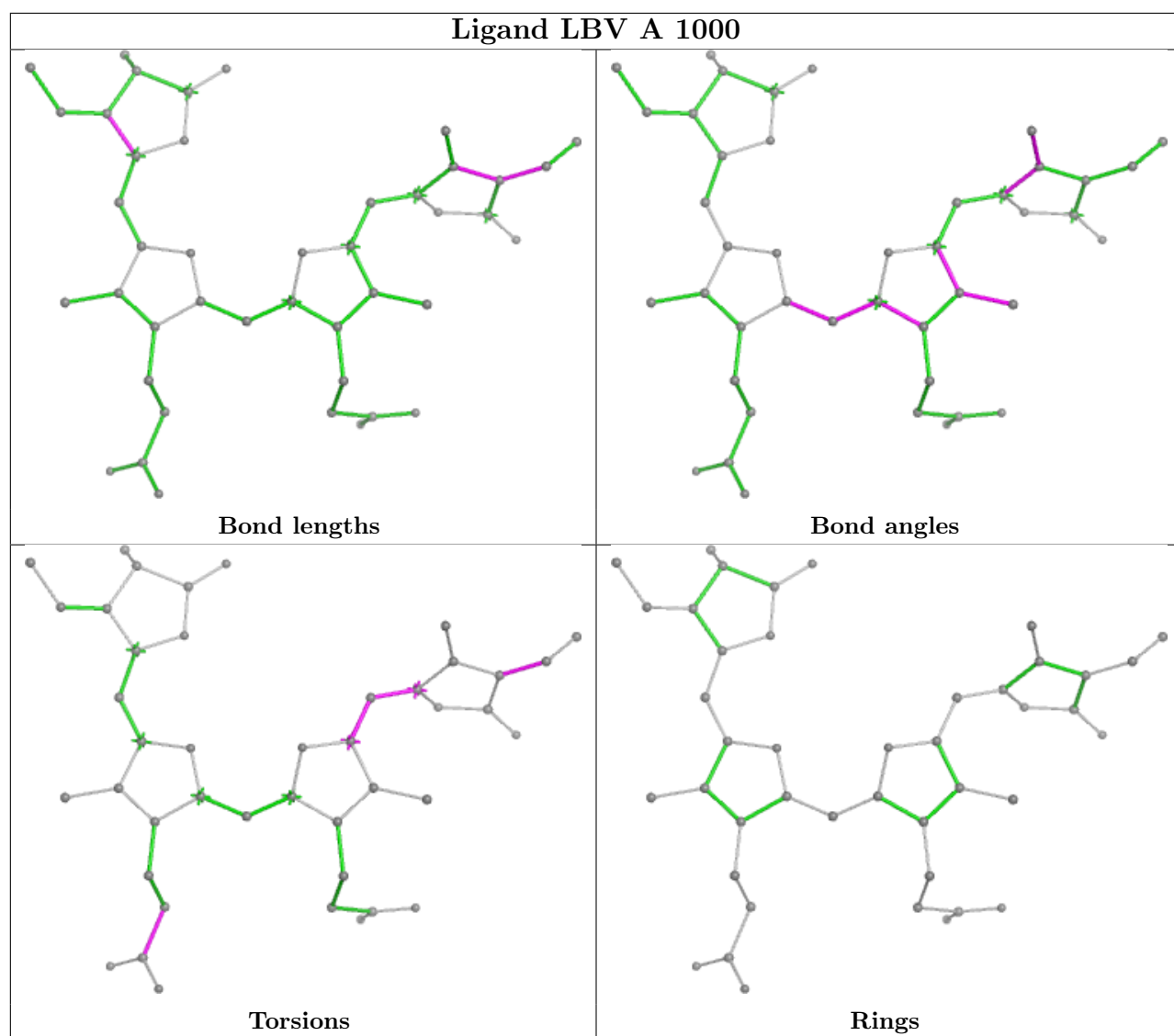
5 of 17 torsion outliers are listed below:

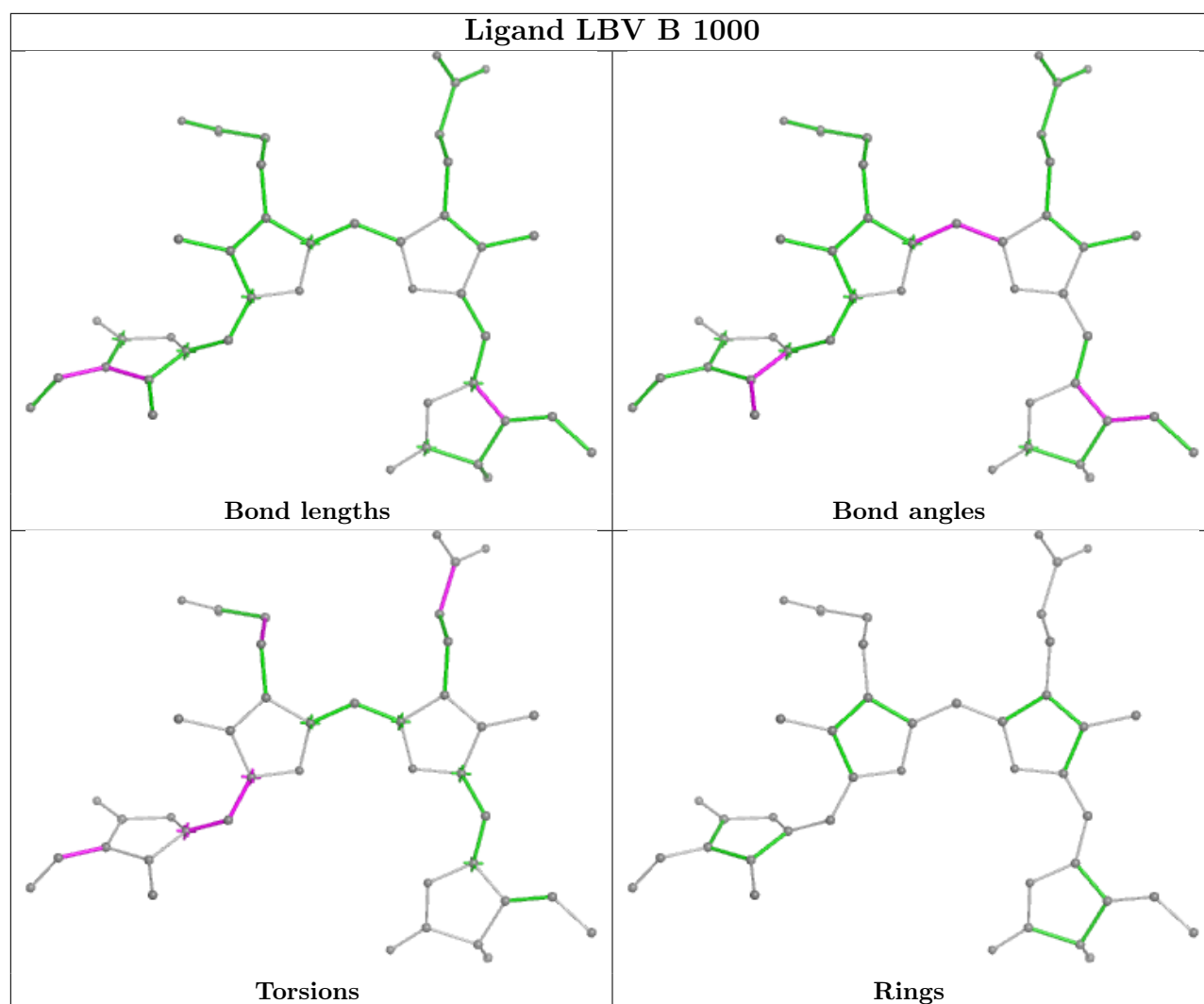
Mol	Chain	Res	Type	Atoms
2	A	1000	LBV	C2D-C1D-CHD-C4C
2	A	1000	LBV	D-N-C1D-CHD-C4C
2	A	1000	LBV	C2D-C3D-CAD-CBD
2	A	1000	LBV	C4D-C3D-CAD-CBD
2	B	1000	LBV	C2D-C1D-CHD-C4C

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.

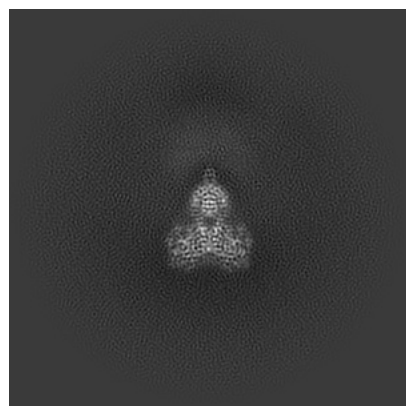
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15684. These allow visual inspection of the internal detail of the map and identification of artifacts.

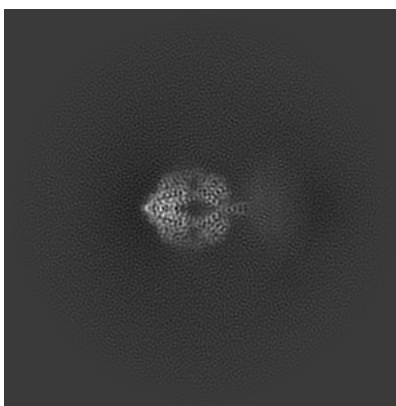
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

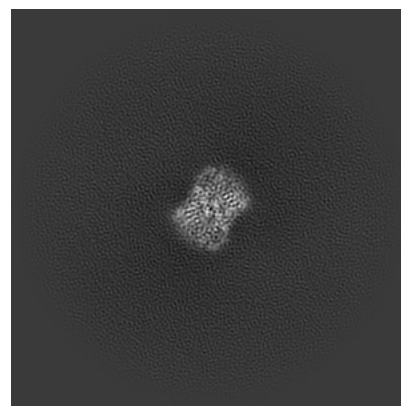
#### 6.1.1 Primary map



X

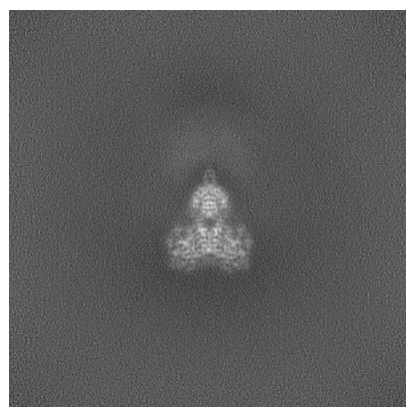


Y

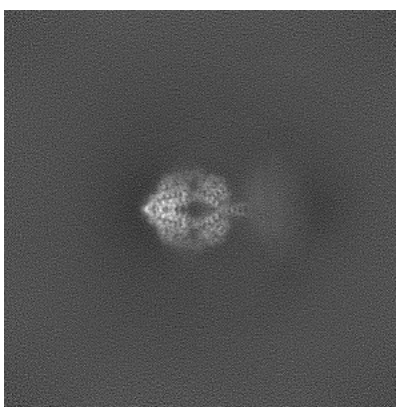


Z

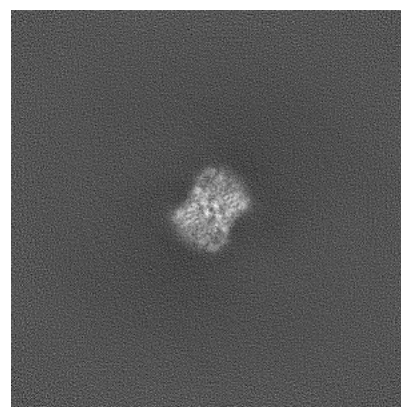
#### 6.1.2 Raw map



X



Y



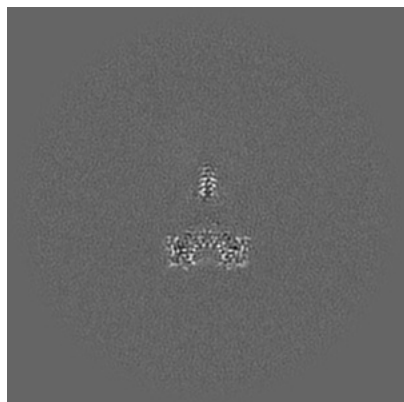
Z

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

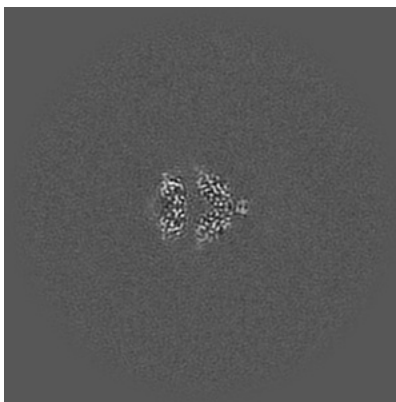


## 6.2 Central slices [i](#)

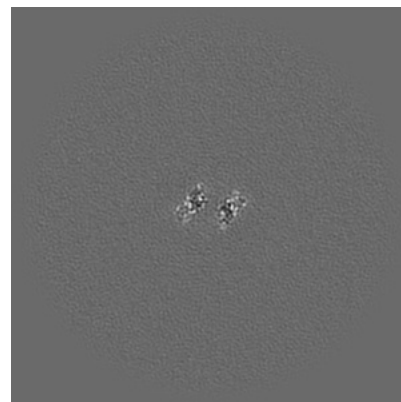
### 6.2.1 Primary map



X Index: 224

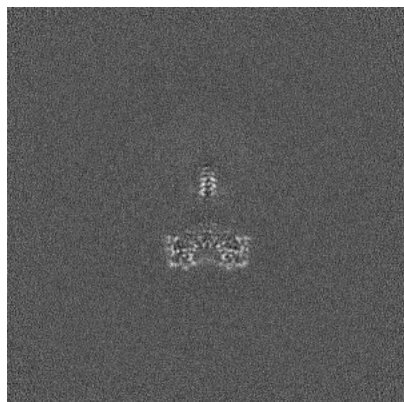


Y Index: 224

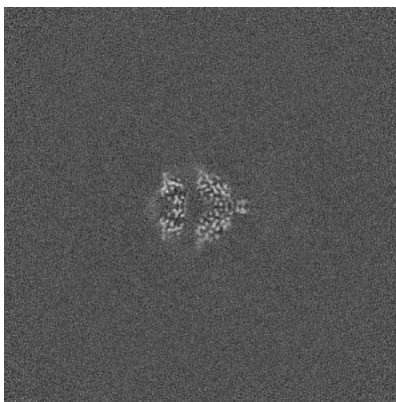


Z Index: 224

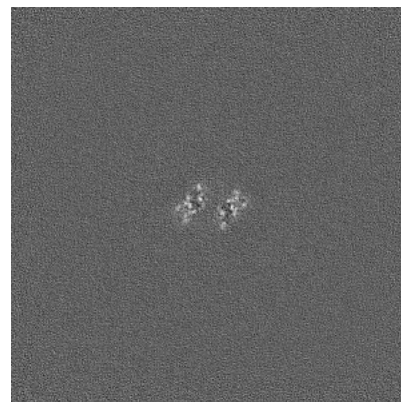
### 6.2.2 Raw map



X Index: 224



Y Index: 224

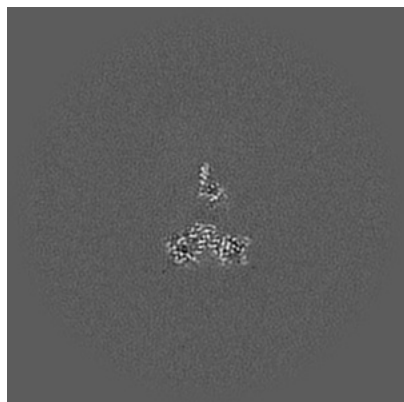


Z Index: 224

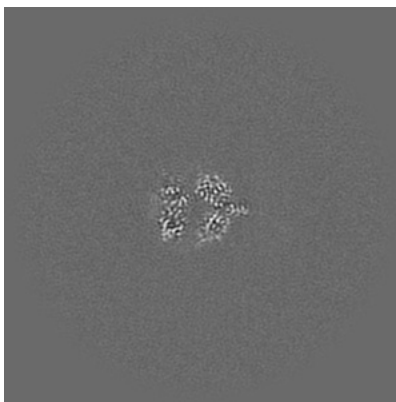
The images above show central slices of the map in three orthogonal directions.

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

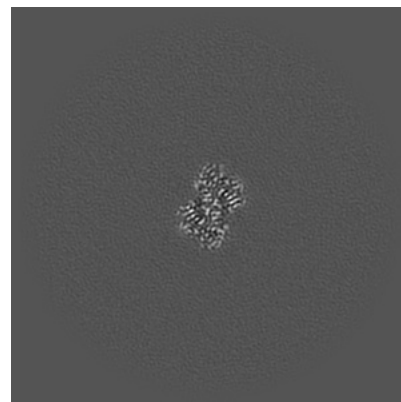
### 6.3.1 Primary map



X Index: 219

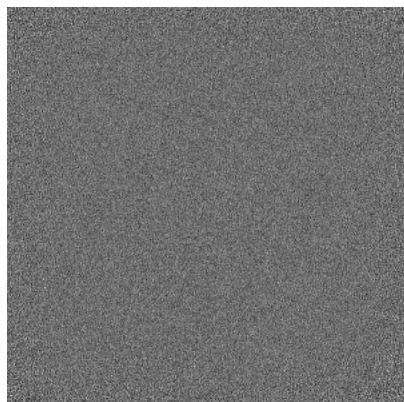


Y Index: 222

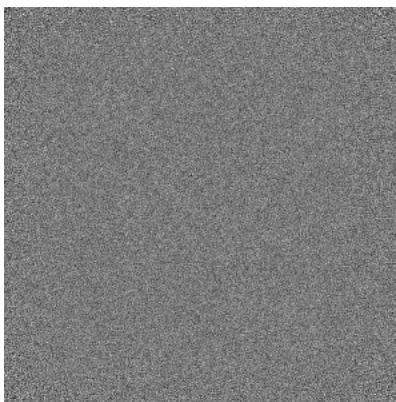


Z Index: 185

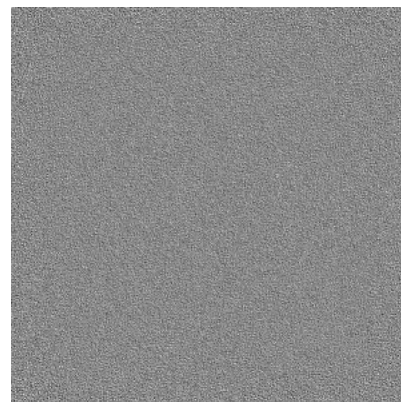
### 6.3.2 Raw map



X Index: 0



Y Index: 0

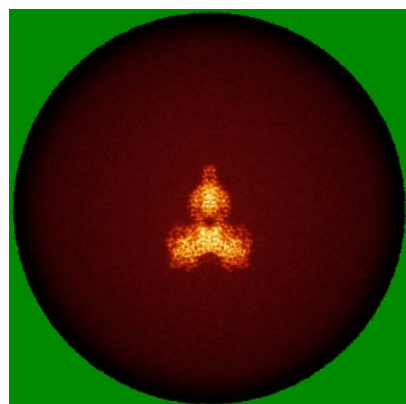


Z Index: 0

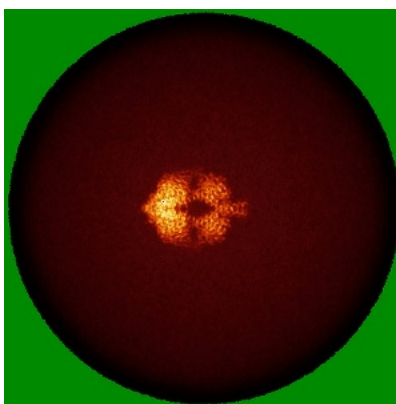
The images above show the largest variance slices of the map in three orthogonal directions.

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

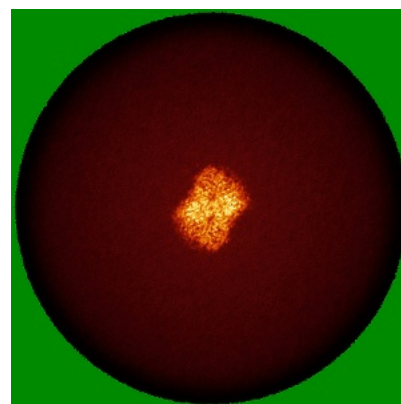
### 6.4.1 Primary map



X

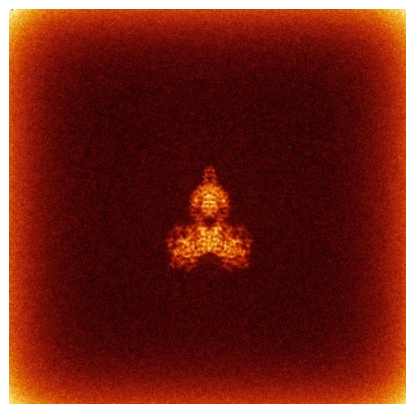


Y

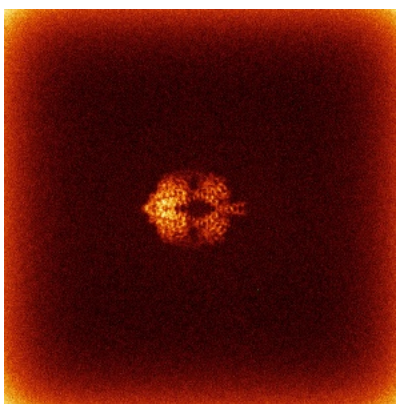


Z

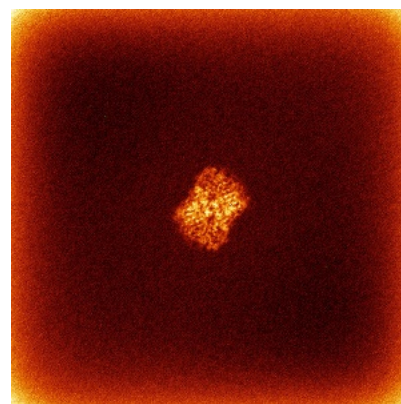
### 6.4.2 Raw map



X



Y

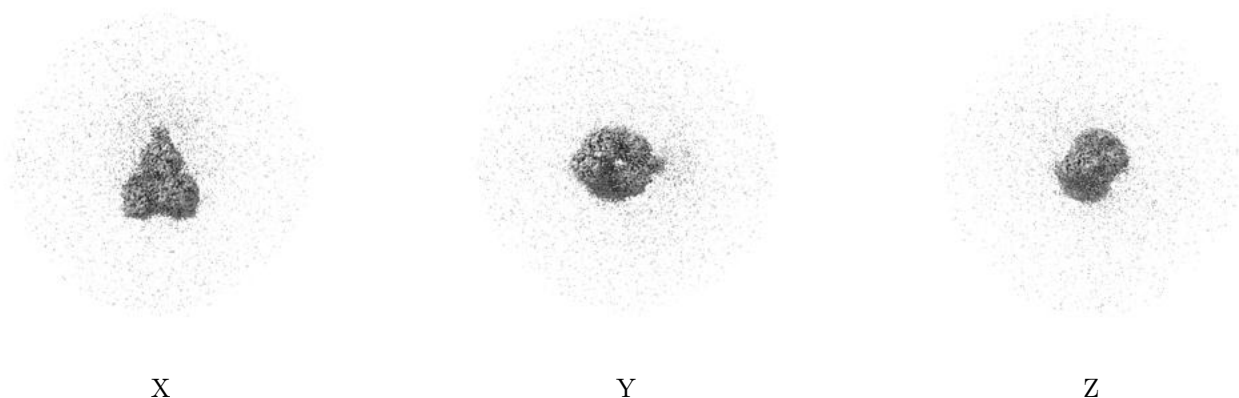


Z

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.

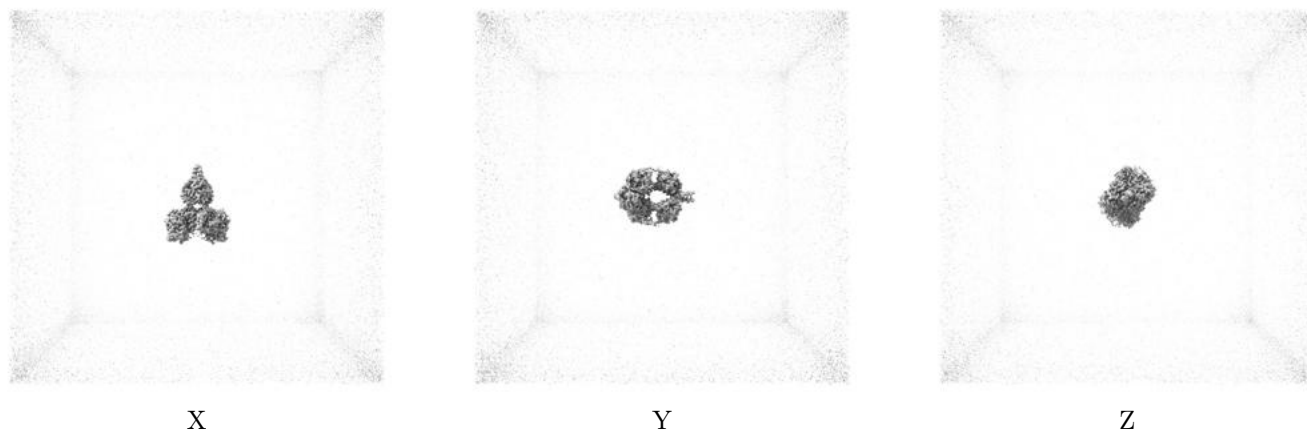
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.09. 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.



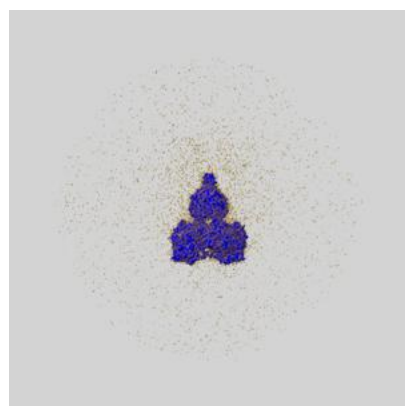
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

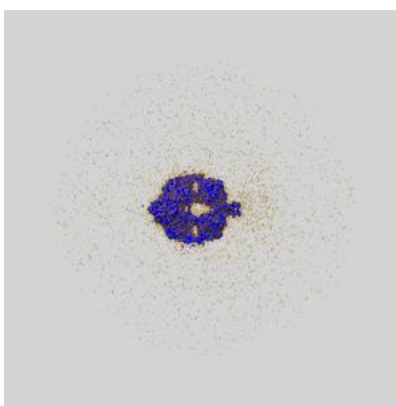
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

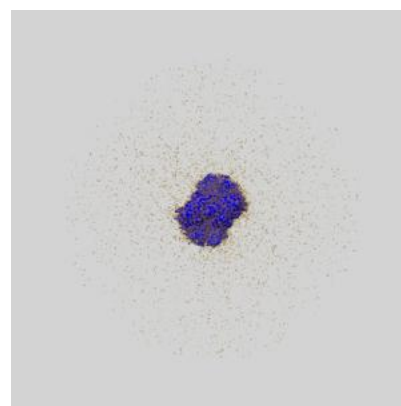
### 6.6.1 emd\_15684\_msk\_1.map [i](#)



X



Y

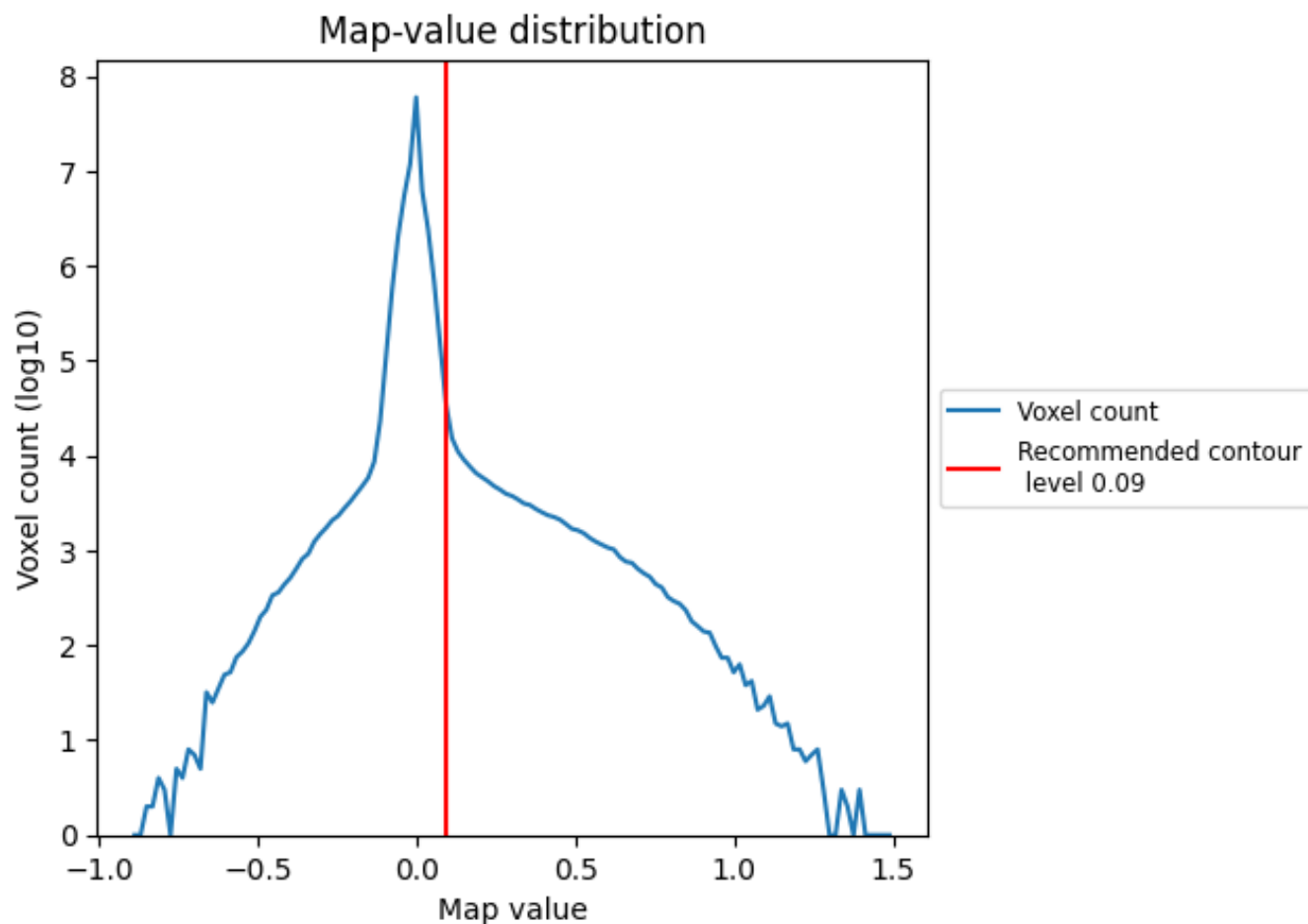


Z

## 7 Map analysis [i](#)

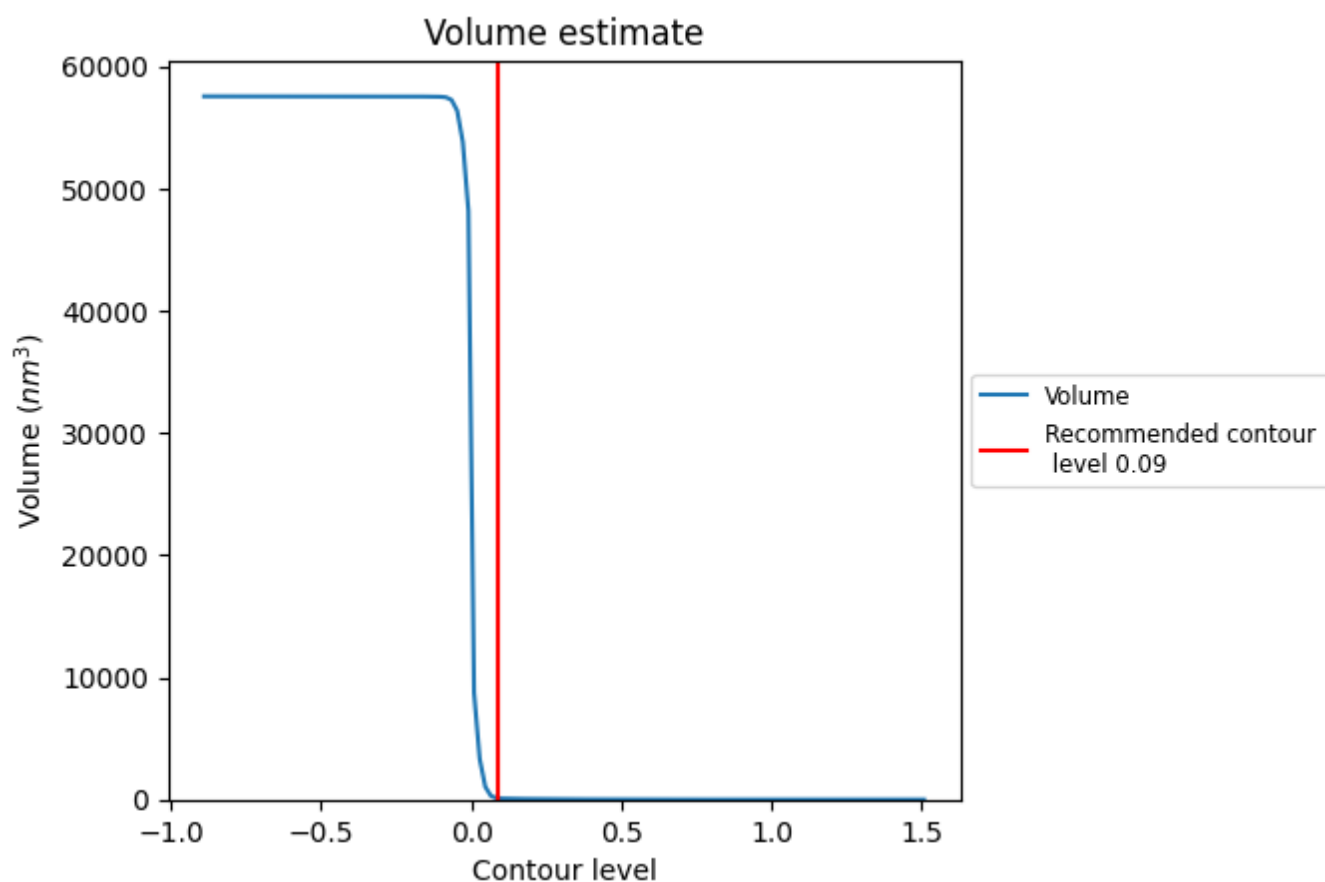
This section contains the results of statistical analysis of the map.

### 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.

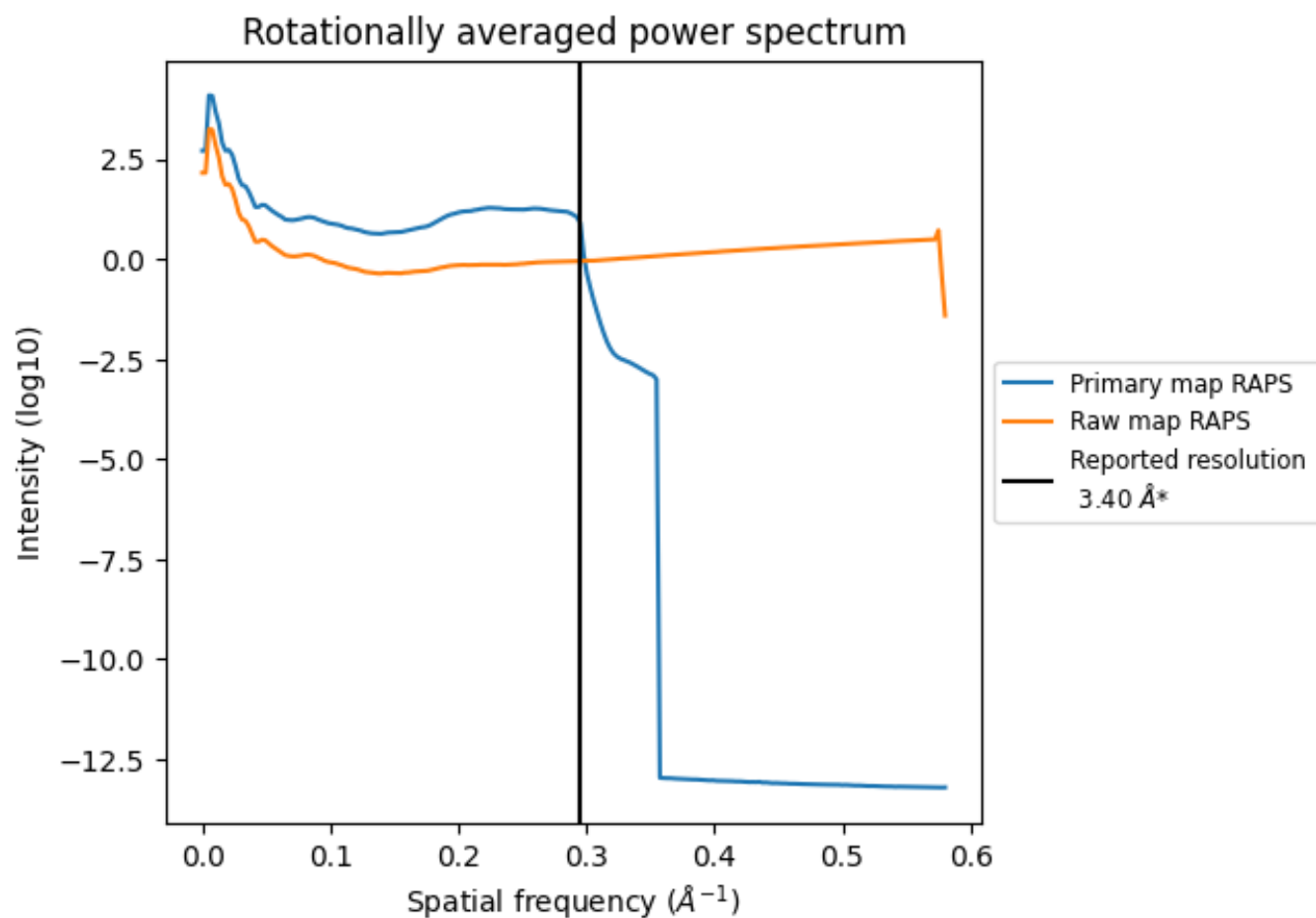
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 108 nm<sup>3</sup>; this corresponds to an approximate mass of 98 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 ⓘ



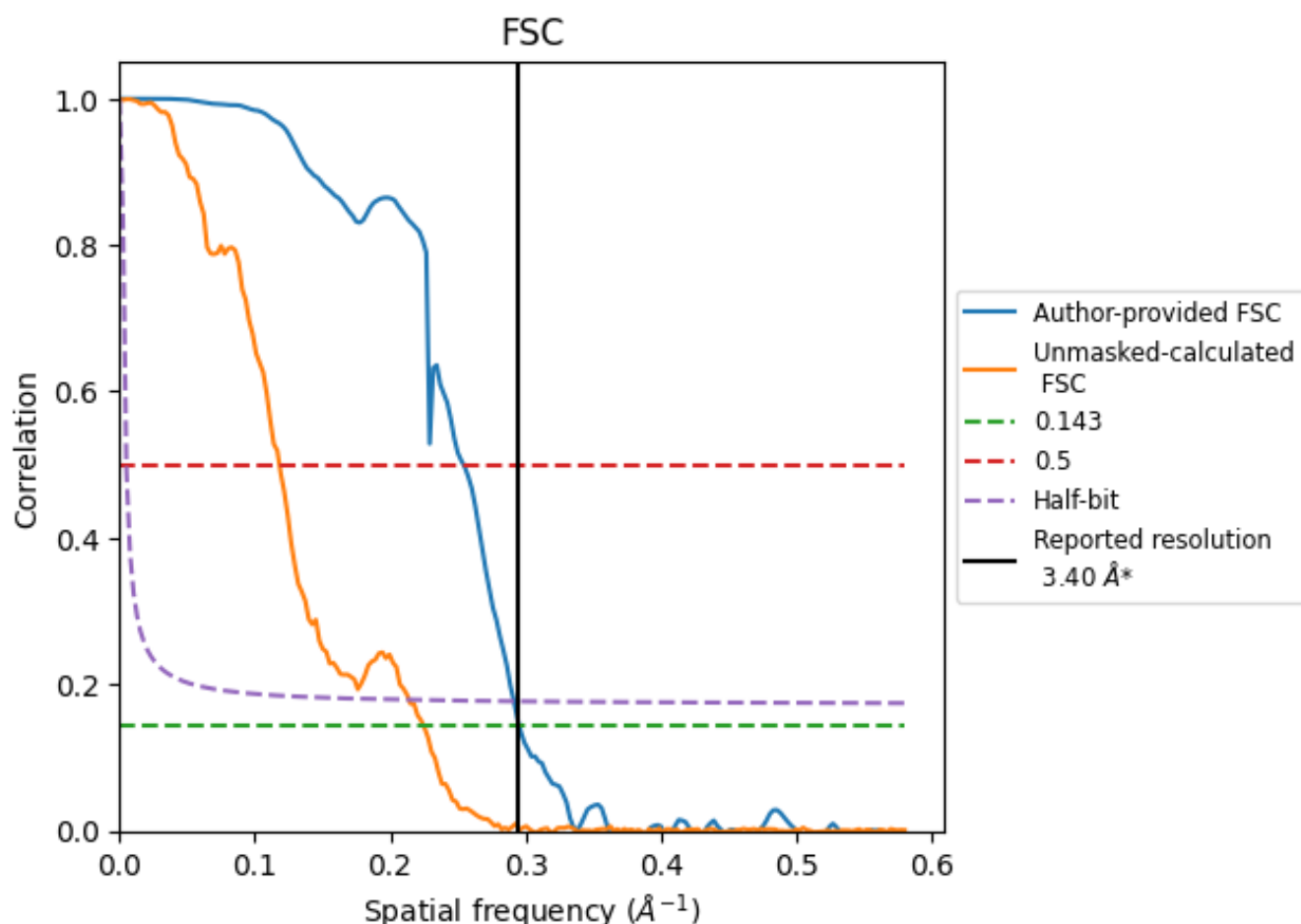
\*Reported resolution corresponds to spatial frequency of 0.294 Å<sup>-1</sup>



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

## 8.2 Resolution estimates [i](#)

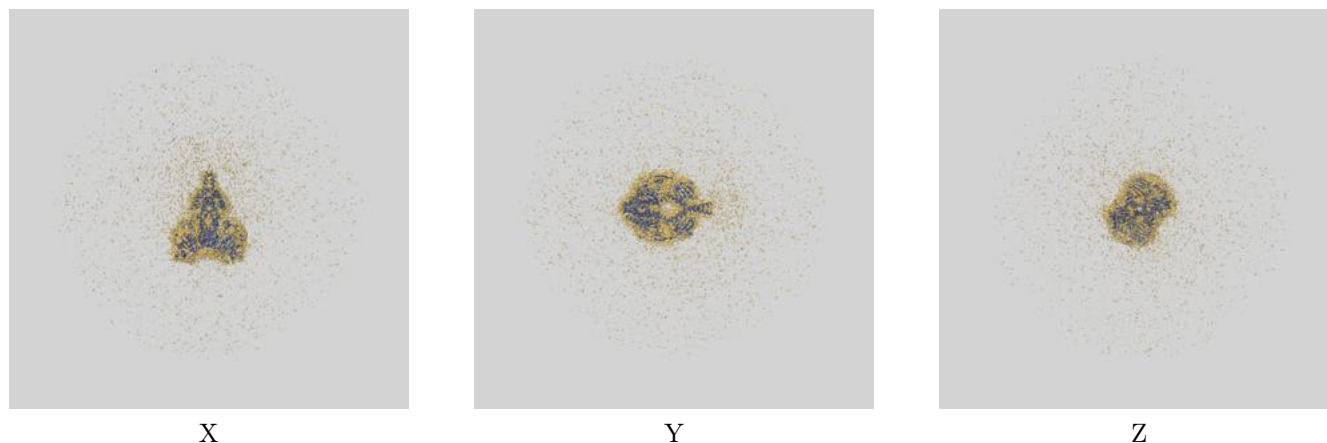
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.39	3.94	3.43
Unmasked-calculated*	4.45	8.47	4.68

\*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 4.45 differs from the reported value 3.4 by more than 10 %

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

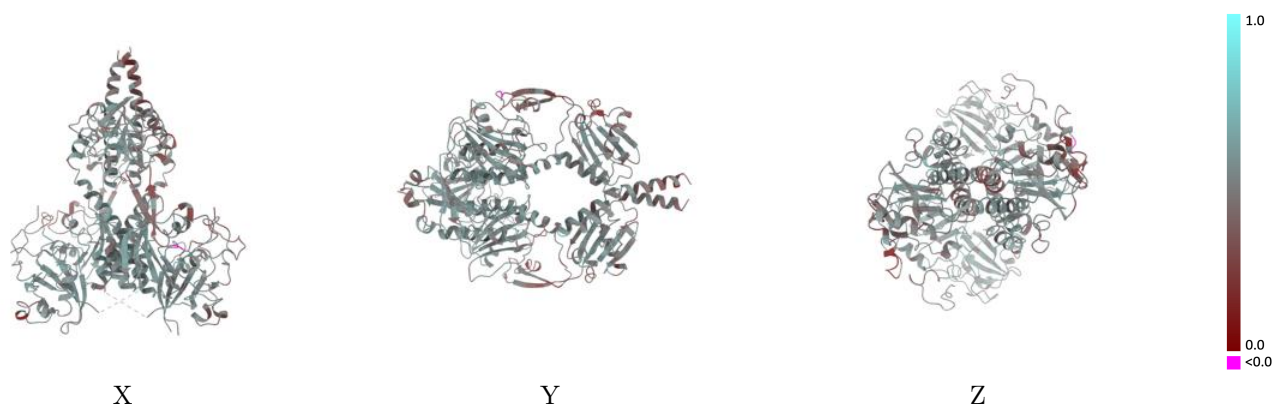
This section contains information regarding the fit between EMDB map EMD-15684 and PDB model 8AVV. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

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



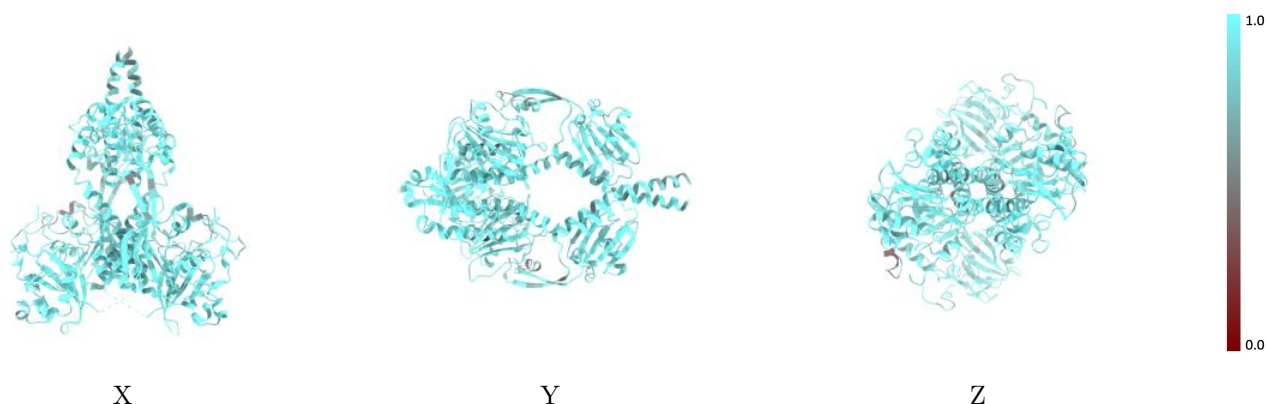
The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



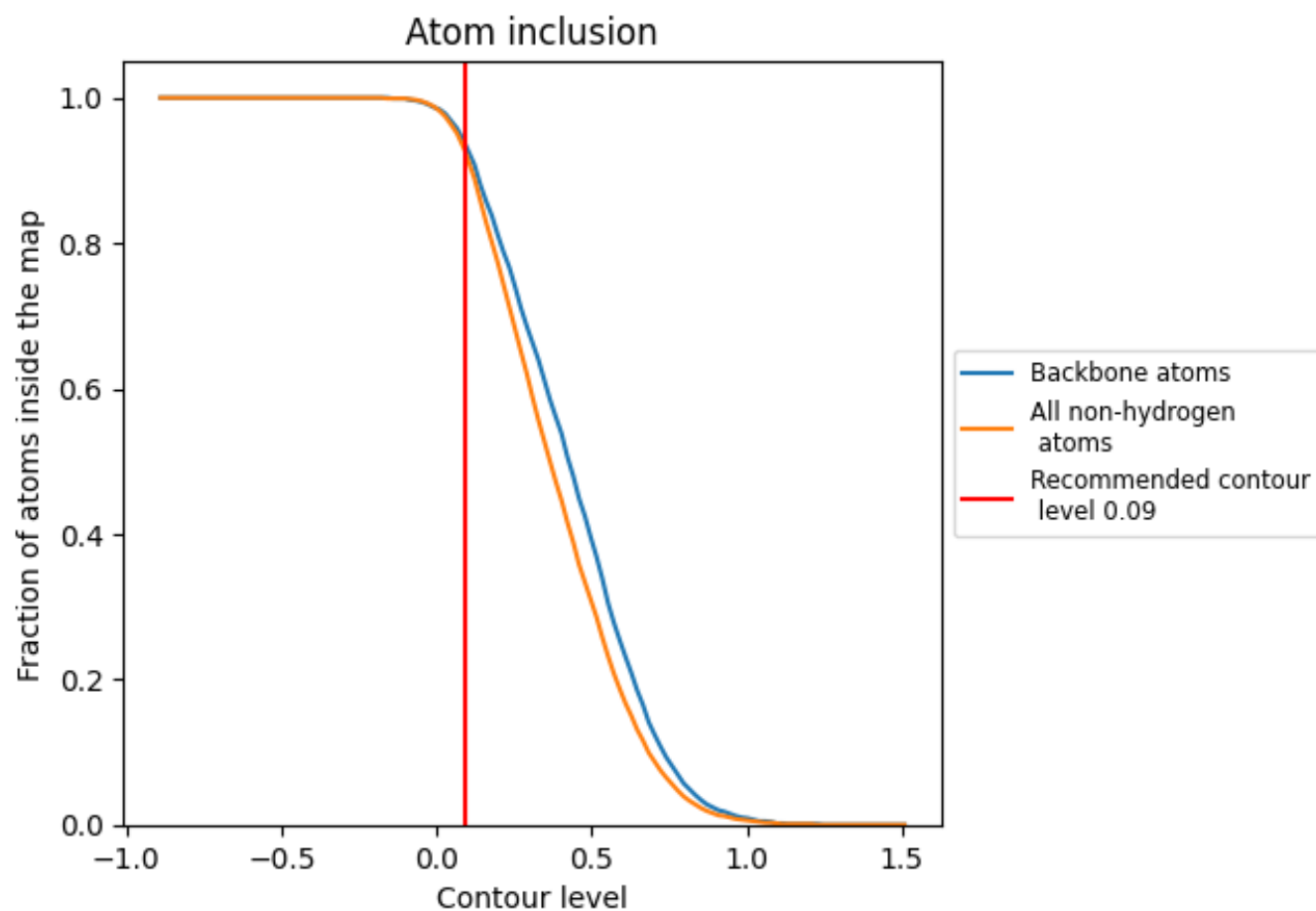
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.09).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 93% 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 (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9280	<div></div> 0.4960
A	<div></div> 0.9320	<div></div> 0.4970
B	<div></div> 0.9230	<div></div> 0.4940

