



## wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 02:25 PM UTC

PDB ID : 8DRA / pdb\_00008dra  
EMDB ID : EMD-27675  
Title : LRRC8A:C conformation 2 (oblong) LRR mask  
Authors : Kern, D.M.; Brohawn, S.G.  
Deposited on : 2022-07-20  
Resolution : 3.98 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:

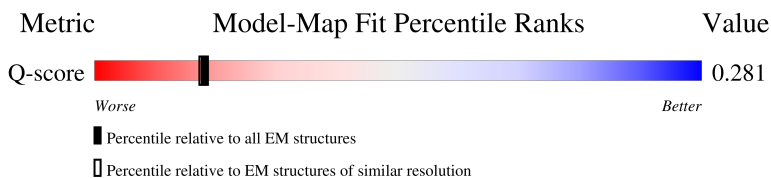
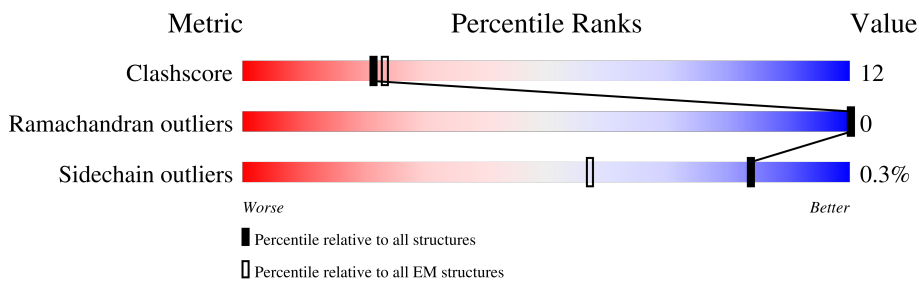
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : 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 3.98 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	7512 ( 3.48 - 4.48 )

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	911	 5% 32% 12% 55%
1	B	911	 26% 32% 13% 55%
2	F	813	 17% 34% 15% 50%

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 9899 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 Volume-regulated anion channel subunit LRRC8A,Soluble cytochrome b562.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	407	3321	2135	583	595	8	0	0
1	B	407	3321	2135	583	595	8	0	0

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	TRP	-	linker	UNP Q80WG5
A	-19	ALA	-	linker	UNP Q80WG5
A	-18	ALA	-	linker	UNP Q80WG5
A	-17	SER	-	linker	UNP Q80WG5
A	-16	SER	-	linker	UNP Q80WG5
A	-9	TRP	MET	conflict	UNP P0ABE7
A	86	ILE	HIS	conflict	UNP P0ABE7
A	90	LEU	-	linker	UNP P0ABE7
A	811	SER	-	expression tag	UNP Q80WG5
A	812	ASN	-	expression tag	UNP Q80WG5
A	813	SER	-	expression tag	UNP Q80WG5
A	814	LEU	-	expression tag	UNP Q80WG5
A	815	GLU	-	expression tag	UNP Q80WG5
A	816	VAL	-	expression tag	UNP Q80WG5
A	817	LEU	-	expression tag	UNP Q80WG5
A	818	PHE	-	expression tag	UNP Q80WG5
A	819	GLN	-	expression tag	UNP Q80WG5
B	-20	TRP	-	linker	UNP Q80WG5
B	-19	ALA	-	linker	UNP Q80WG5
B	-18	ALA	-	linker	UNP Q80WG5
B	-17	SER	-	linker	UNP Q80WG5
B	-16	SER	-	linker	UNP Q80WG5
B	-9	TRP	MET	conflict	UNP P0ABE7
B	86	ILE	HIS	conflict	UNP P0ABE7
B	90	LEU	-	linker	UNP P0ABE7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	811	SER	-	expression tag	UNP Q80WG5
B	812	ASN	-	expression tag	UNP Q80WG5
B	813	SER	-	expression tag	UNP Q80WG5
B	814	LEU	-	expression tag	UNP Q80WG5
B	815	GLU	-	expression tag	UNP Q80WG5
B	816	VAL	-	expression tag	UNP Q80WG5
B	817	LEU	-	expression tag	UNP Q80WG5
B	818	PHE	-	expression tag	UNP Q80WG5
B	819	GLN	-	expression tag	UNP Q80WG5

- Molecule 2 is a protein called Volume-regulated anion channel subunit LRRC8C.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	F	404	3257	2099	547	595	16	0	0

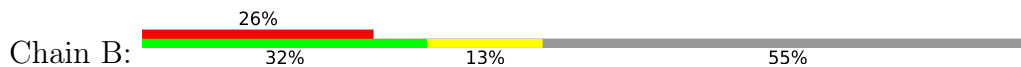
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	804	SER	-	expression tag	UNP Q8R502
F	805	ASN	-	expression tag	UNP Q8R502
F	806	SER	-	expression tag	UNP Q8R502
F	807	GLU	-	expression tag	UNP Q8R502
F	808	ASN	-	expression tag	UNP Q8R502
F	809	LEU	-	expression tag	UNP Q8R502
F	810	TYR	-	expression tag	UNP Q8R502
F	811	PHE	-	expression tag	UNP Q8R502
F	812	GLN	-	expression tag	UNP Q8R502
F	813	GLY	-	expression tag	UNP Q8R502

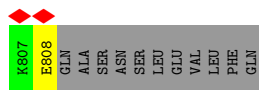




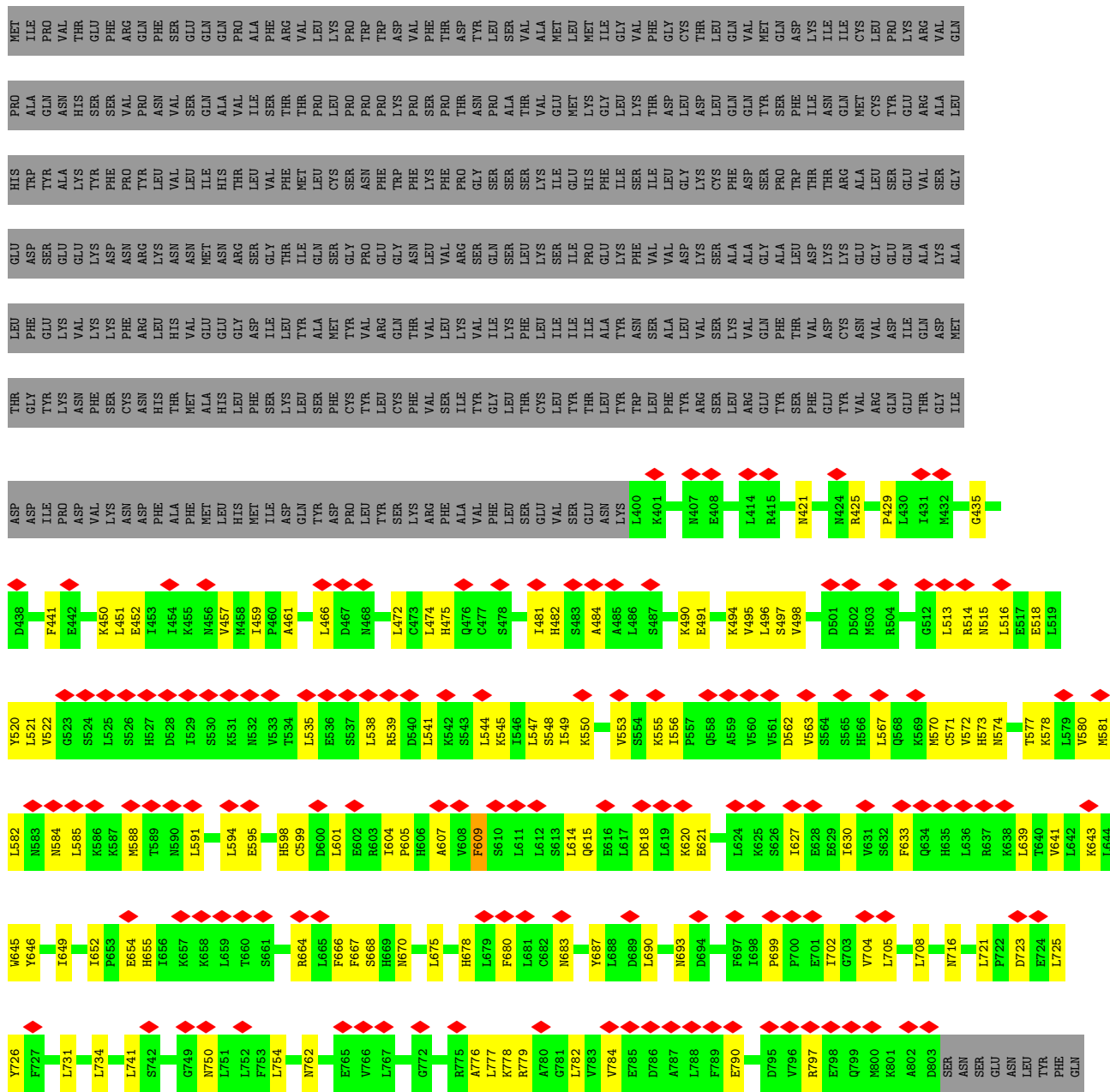
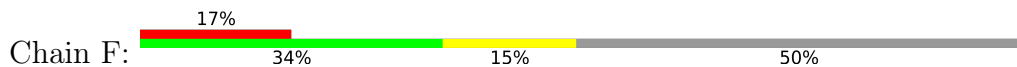
• Molecule 1: Volume-regulated anion channel subunit LRRC8A,Soluble cytochrome b562



MET	ILE	PRO	VAL	THR	GLU	LEU	ARG	LEU	ASP	THR	TYR	PHE	ALA	ASP	THR	GLN	PRO	ALA	GLN	ALA	ALA	ASN	SER	SER	LEU	GLU	VAL	VAL	PHE	GLN																												
THR	LYS	ASP	THR	CYS	ASN	ASP	SER	ASP	PHE	ARG	GLY	ALA	TRP	ALA	THR	ALA	GLN	PRO	ALA	TYR	SER	ALA	ALA	ASN	SER	LEU	GLU	VAL	VAL	THR	THR																											
PRO	PRO	LYS	LEU	GLU	ASP	LYS	SER	PRO	PRO	ASP	GLY	LEU	GLU	GLY	THR	GLN	VAL	ASP	ASP	GLY	GLN	GLN	GLN	GLN	LEU	LEU	VAL	VAL	THR	LYS																												
TYR	LEU	ASP	THR	GLY	PRO	THR	GLY	ILE	ILE	TYR	TYR	TYR	ASP	ASP	ASP	ASP	ASP	HIS	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ARG																											
THR	SER	SER	LYS	LEU	GLU	HIS	PHE	VAL	VAL	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	CYS	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	THR																												
VAL	PRO	MET	GLN	GLY	THR	LYS	SER	ALA	SER	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	THR																												
ILE	ILE	LYS	VAL	ILE	LYS	PHE	ALA	ALA	SER	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR																												
VAL	ILE	PHE	TYR	GLY	LEU	ILE	CYS	VAL	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR																												
ARG	PHE	ALA	VAL	PHE	LEU	SER	GLU	SER	LEU	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	THR																												
L476	Y477	H478	I483	E484	A485	P486	A487	L488	A489	E493	M494	L495	R496	A497	L498	H499	F502	T503	D504	K422	N423	A424	Q425	D426	K427	H431	L432	F433	M434	D440	T441	V442	F443	D444	V450	L451	K452	L453	E454	L455	I461	P462	I465	A466	Q467	L468	E473	L474	W475									
K547	R550	L551	K552	S553	N554	L555	S556	K557	L558	P559	Q560	V561	V562	T563	D564	G566	V567	H568	L569	L572	N575	N576	E577	G578	T579	K580	L581	I582	V583	L584	N585	S586	L587	K588	K589	M590	V591	L593	T594	E595	L596	E597	L598	I599	R600	C601	D602	I606	P607	H608	S609	I610	F611					
S612	L613	H614	M615	L616	Q617	E618	I619	D620	L621	K622	D623	I629	E630	E631	I632	L633	S634	F635	Q636	H637	L638	H639	R640	L641	T642	C643	L644	K645	L646	M647	H650	I651	A652	Y653	L658	L661	T662	N663	L664	E665	R666	L667	Y668	L669	N670	R671	K676	I677	P678	T679	Q680	L681	F682	Y683				
C684	R685	R688	V689	L690	D691	L692	S693	H694	L697	T698	R699	L700	F701	A702	D703	I704	G705	L706	L707	Q708	N709	L710	Q711	N712	L713	A714	W715	N718	R719	I720	E721	A722	L723	P724	P725	E726	L727	F728	Q729	C730	R731	K732	L733	R734	A735	L736	H737	L738	G739	N740	N741	V742	L743	Q744	S745	L746		
P747	S748	R749	V750	G751	E752	L753	T754	N755	L756	T757	Q758	L759	E760	L761	R762	G763	N764	R765	L766	E767	C768	L769	P770	W771	E772	L773	G774	E775	C776	P777	L778	L779	K780	R781	S782	G783	L784	V785	V786	E787	E788	D789	L790	F791	S792	T793	L794	P795	P796	E797	V798	K799	E800	H801	L802	R804	A805	P806



• Molecule 2: Volume-regulated anion channel subunit LRRC8C



GLY

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	126955	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.587	Depositor
Minimum map value	-2.413	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.045	Depositor
Recommended contour level	0.45	Depositor
Map size (Å)	435.968, 435.968, 435.968	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.048, 1.048, 1.048	Depositor

## 5 Model quality [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.15	0/3378	0.40	0/4580
1	B	0.15	0/3378	0.44	0/4580
2	F	0.16	0/3315	0.43	0/4482
All	All	0.16	0/10071	0.42	0/13642

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	3321	0	3491	73	0
1	B	3321	0	3491	85	0
2	F	3257	0	3405	82	0
All	All	9899	0	10387	237	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

The worst 5 of 237 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:476:LEU:HD12	1:B:476:LEU:O	1.64	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:582:LEU:HB3	2:F:607:ALA:HB2	1.67	0.77
1:B:620:ASP:HA	1:B:645:LYS:HB2	1.69	0.74
2:F:585:LEU:HB3	2:F:607:ALA:HB1	1.71	0.71
1:B:725:PRO:HA	1:B:728:PHE:HB2	1.73	0.71

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	405/911 (44%)	387 (96%)	18 (4%)	0	100	100
1	B	405/911 (44%)	376 (93%)	29 (7%)	0	100	100
2	F	402/813 (49%)	383 (95%)	19 (5%)	0	100	100
All	All	1212/2635 (46%)	1146 (95%)	66 (5%)	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	378/830 (46%)	377 (100%)	1 (0%)	86	85
1	B	378/830 (46%)	377 (100%)	1 (0%)	86	85
2	F	382/756 (50%)	381 (100%)	1 (0%)	86	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1138/2416 (47%)	1135 (100%)	3 (0%)	84 85

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	750	VAL
1	B	733	LEU
2	F	609	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	558	GLN
2	F	799	GLN
2	F	762	ASN
2	F	402	GLN
2	F	515	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](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

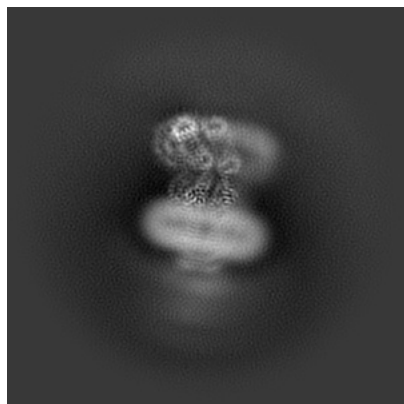
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27675. These allow visual inspection of the internal detail of the map and identification of artifacts.

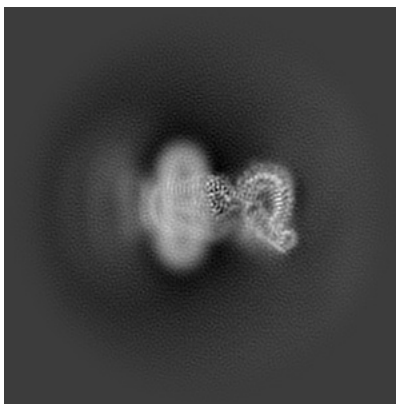
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

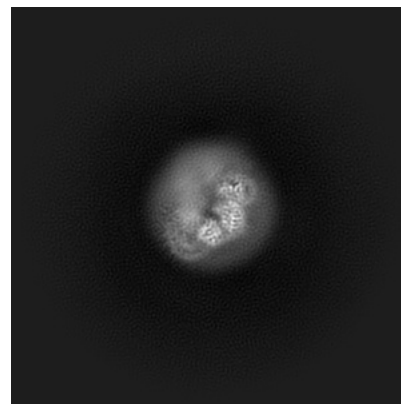
#### 6.1.1 Primary map



X

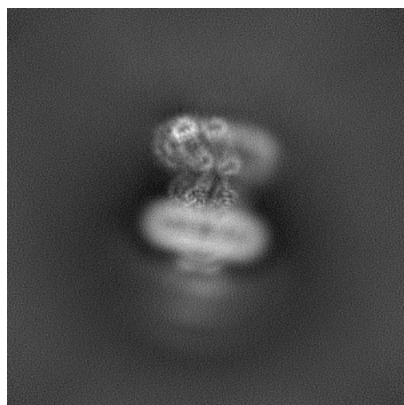


Y

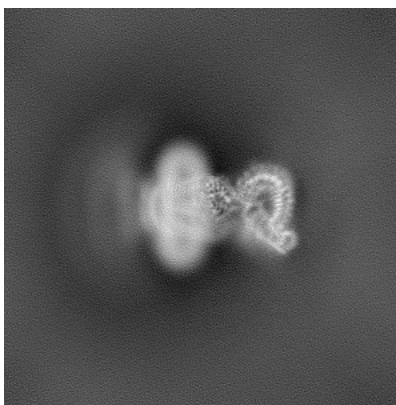


Z

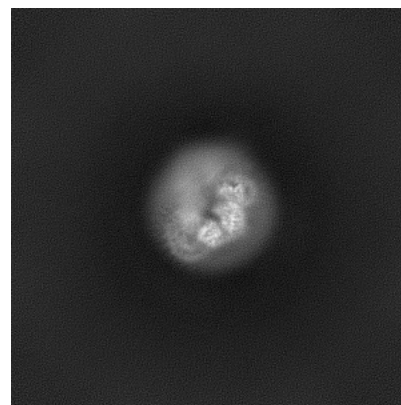
#### 6.1.2 Raw map



X



Y

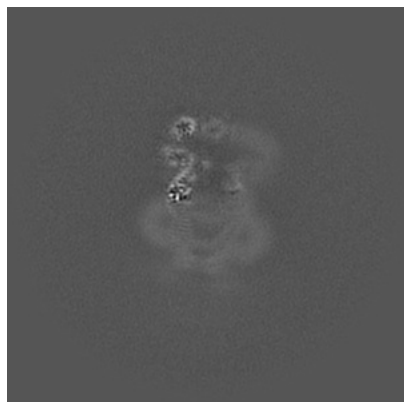


Z

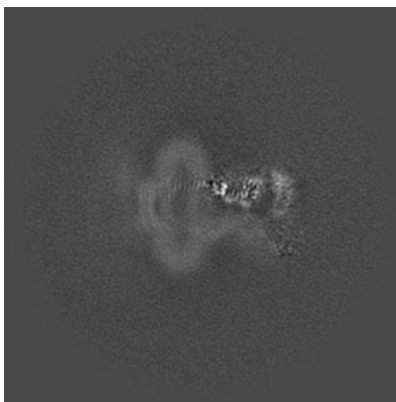
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

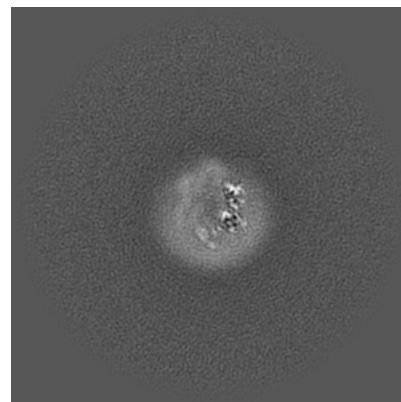
### 6.2.1 Primary map



X Index: 208

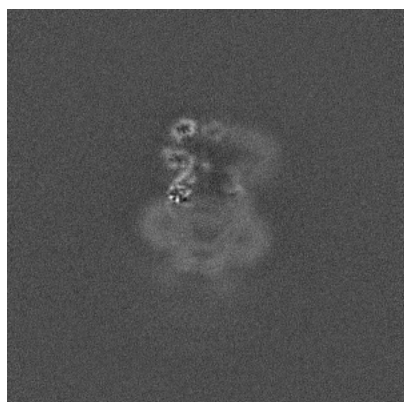


Y Index: 208

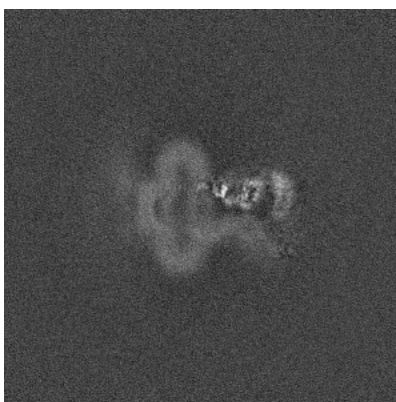


Z Index: 208

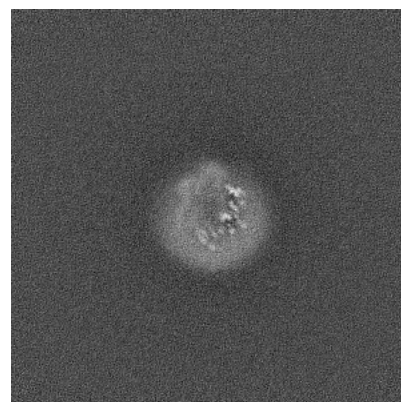
### 6.2.2 Raw map



X Index: 208



Y Index: 208

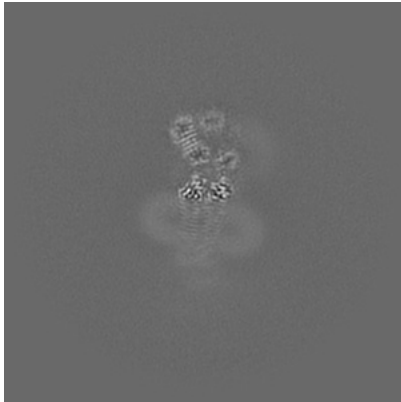


Z Index: 208

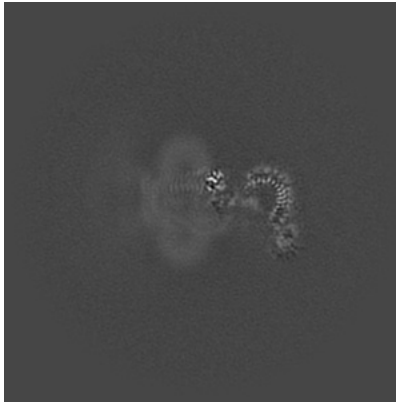
The images above show central slices of the map in three orthogonal directions.

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

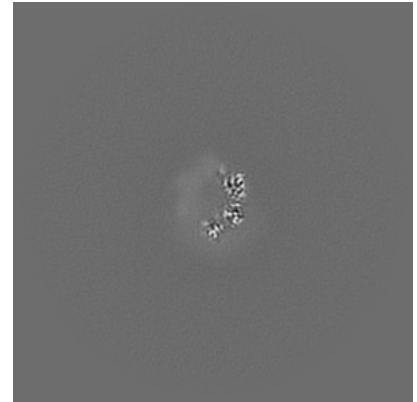
### 6.3.1 Primary map



X Index: 229

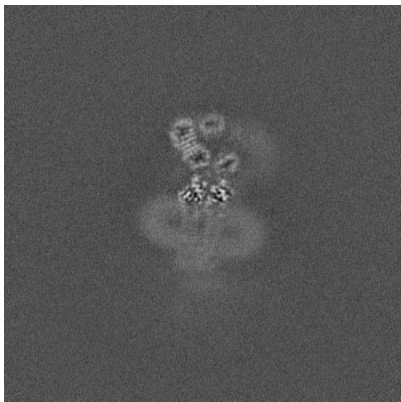


Y Index: 191

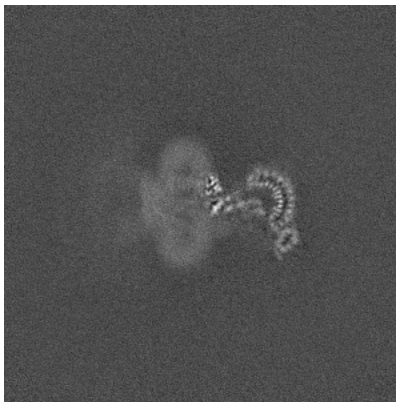


Z Index: 216

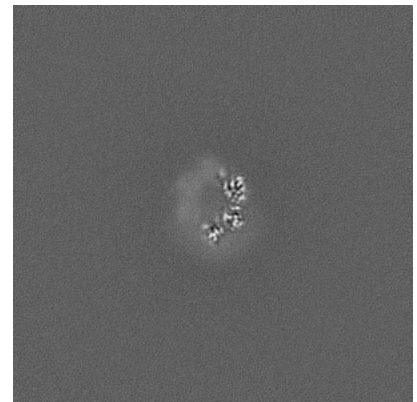
### 6.3.2 Raw map



X Index: 229



Y Index: 187

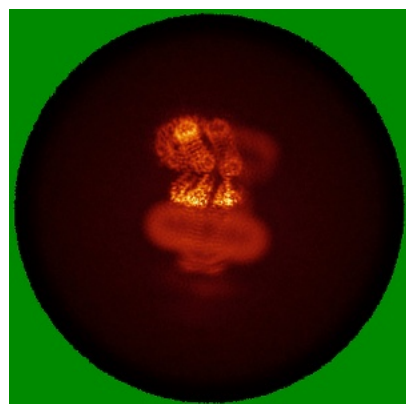


Z Index: 216

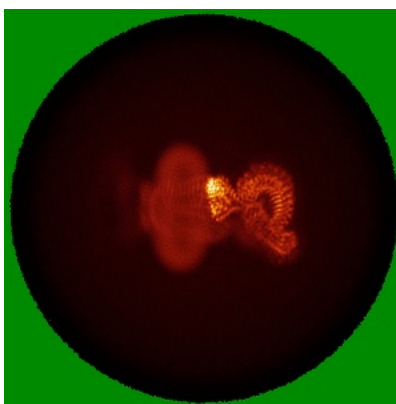
The images above show the largest variance slices of the map in three orthogonal directions.

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

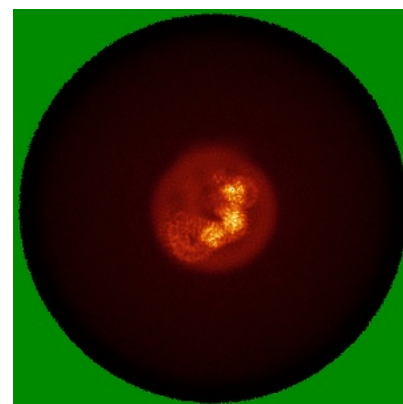
### 6.4.1 Primary map



X

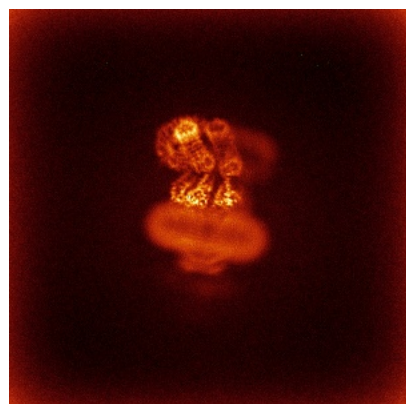


Y

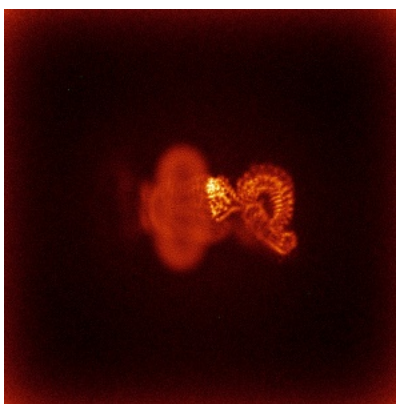


Z

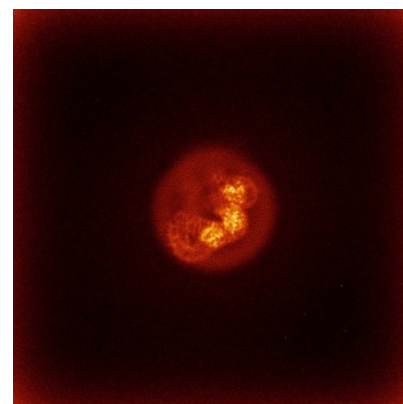
### 6.4.2 Raw map



X



Y



Z

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

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

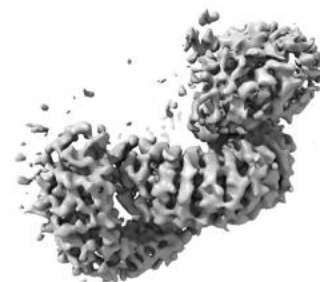
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.45. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



X



Y



Z

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

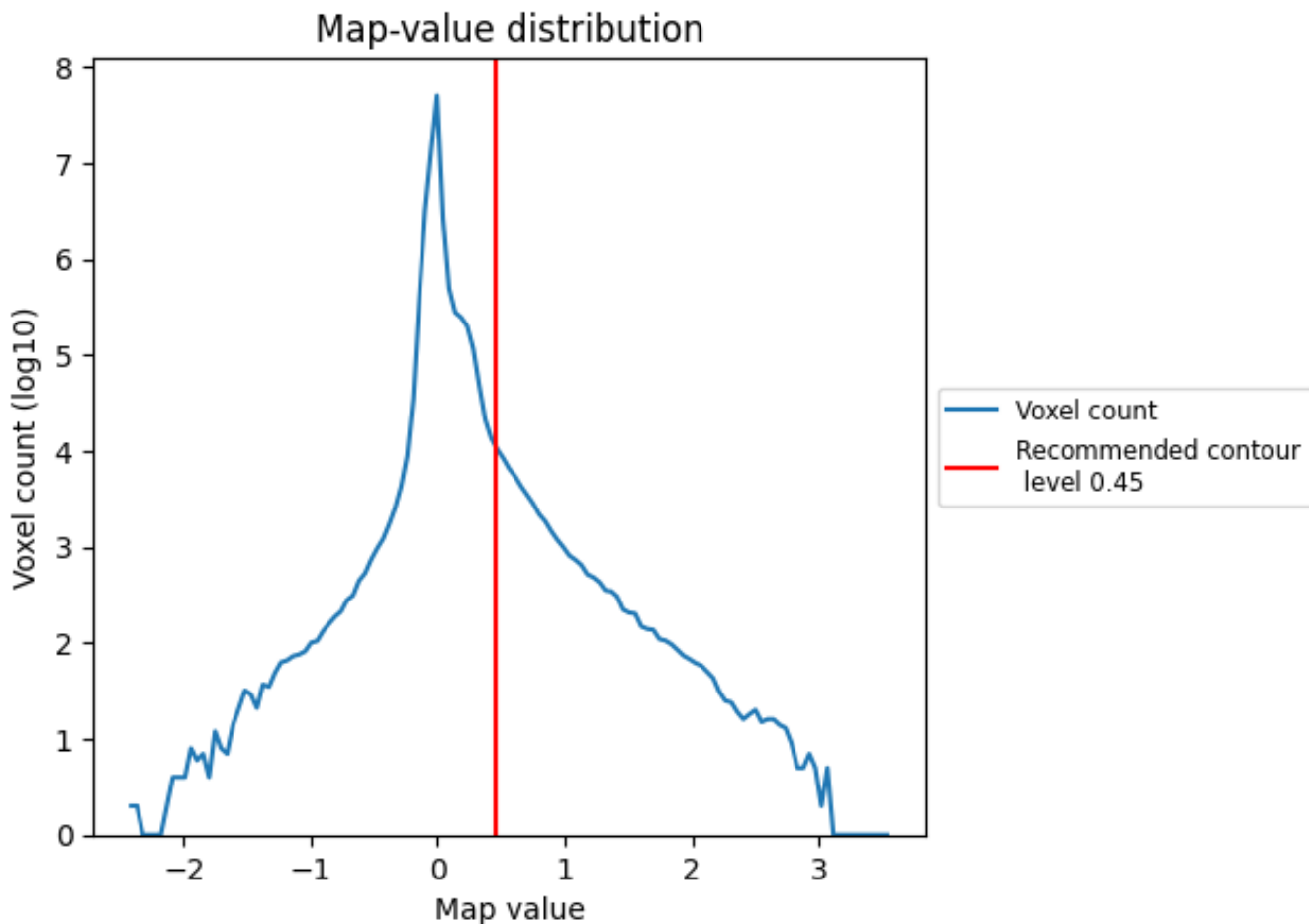
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

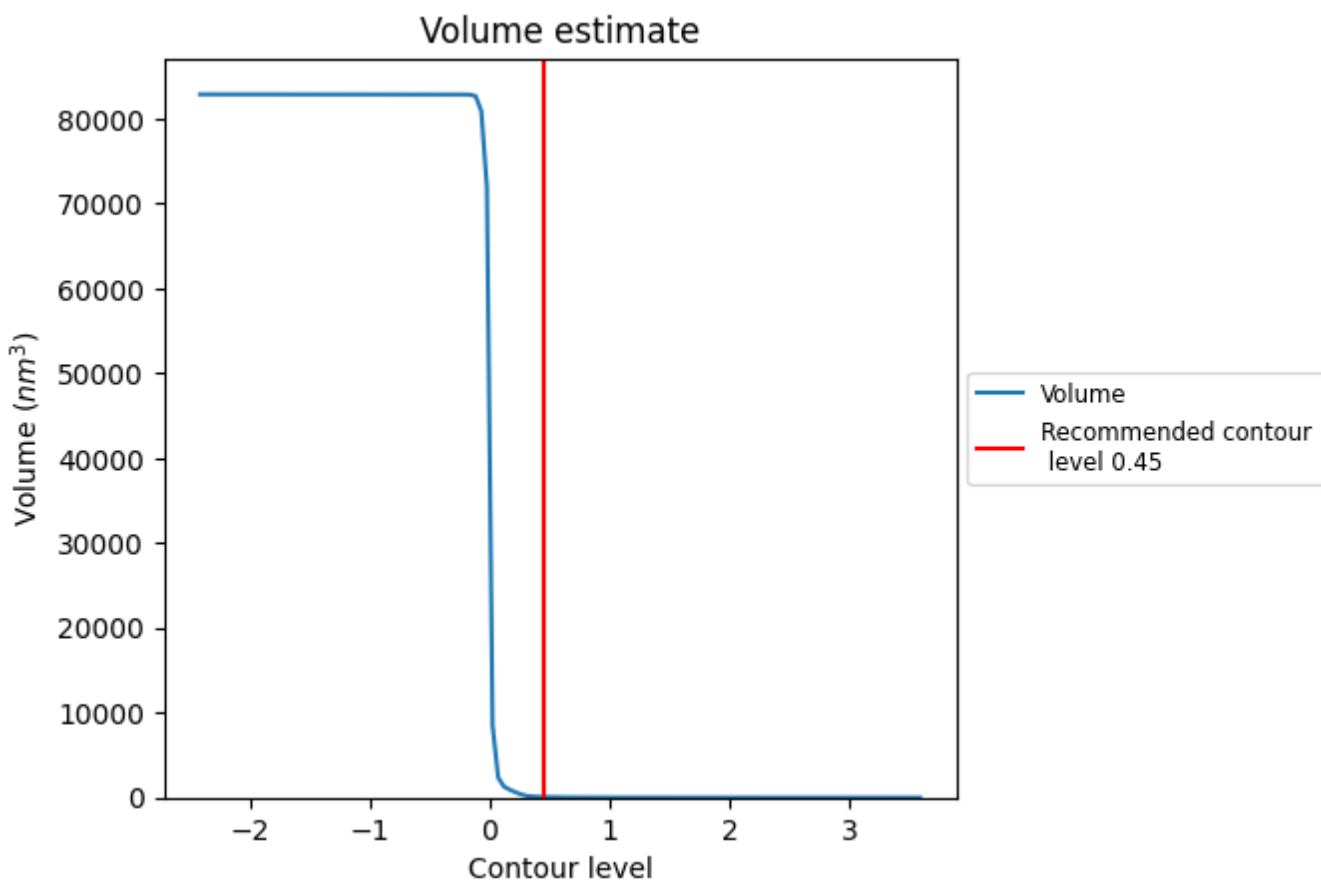
This section contains the results of statistical analysis of the map.

### 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.

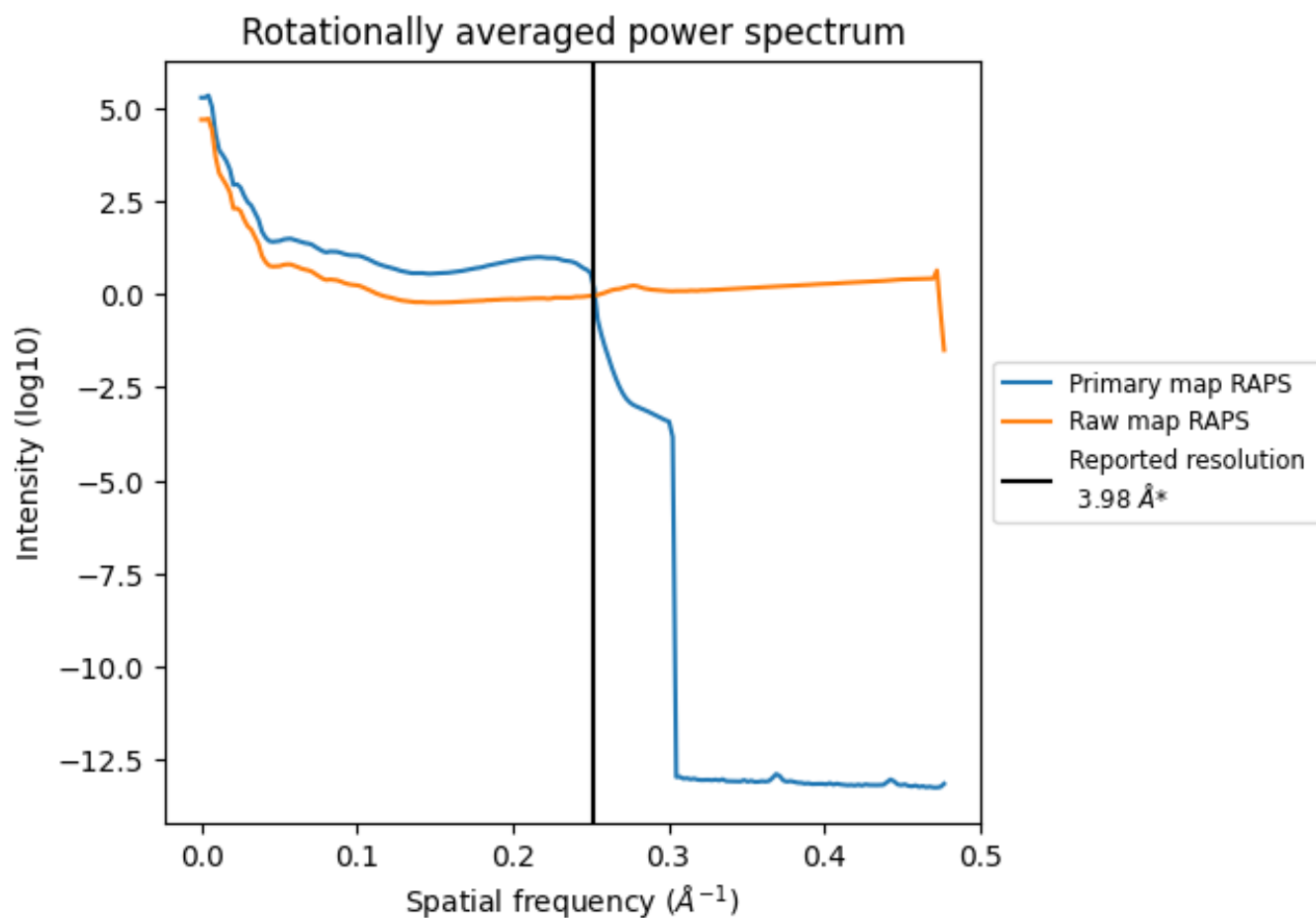
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 70 nm<sup>3</sup>; this corresponds to an approximate mass of 63 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum [i](#)

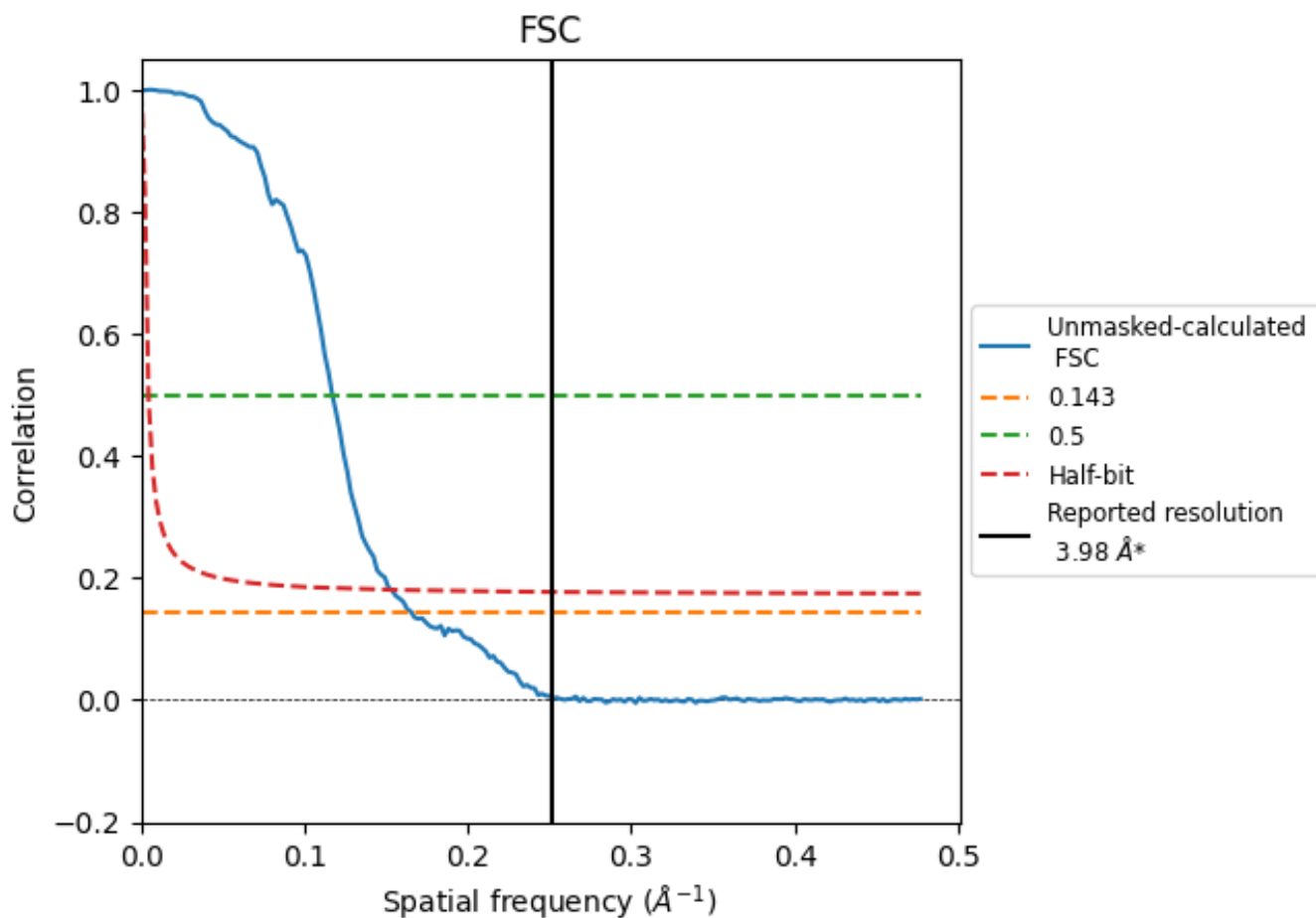


\*Reported resolution corresponds to spatial frequency of 0.251 Å<sup>-1</sup>

## 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 0.251 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

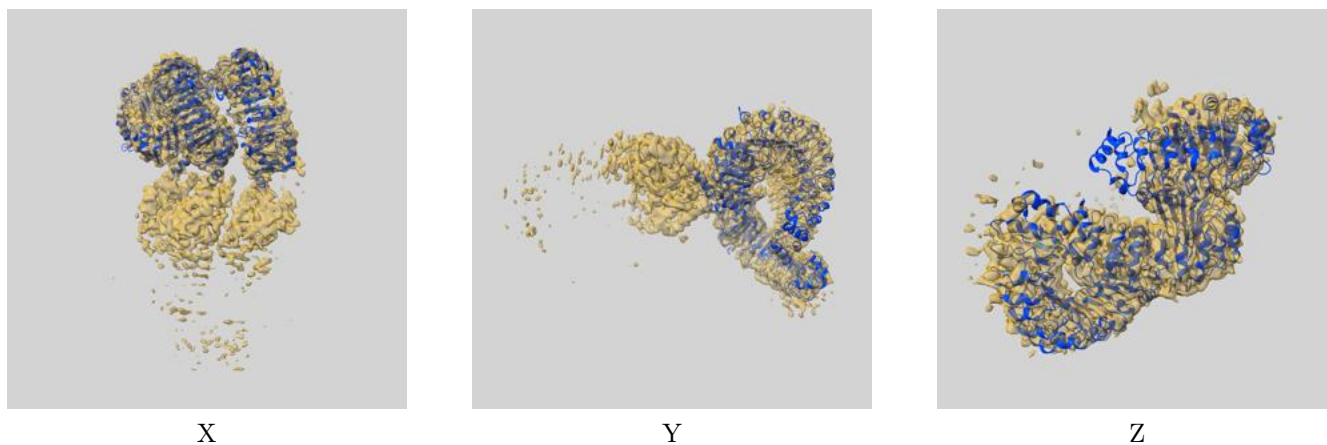
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.98	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.04	8.55	6.53

\*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 6.04 differs from the reported value 3.98 by more than 10 %

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

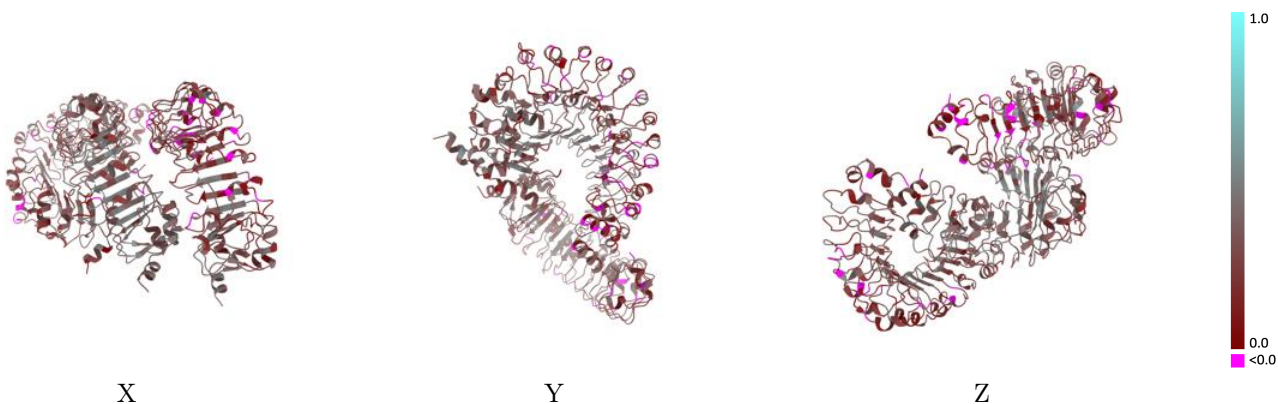
This section contains information regarding the fit between EMDB map EMD-27675 and PDB model 8DRA. Per-residue inclusion information can be found in section [3](#) on page [5](#).

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



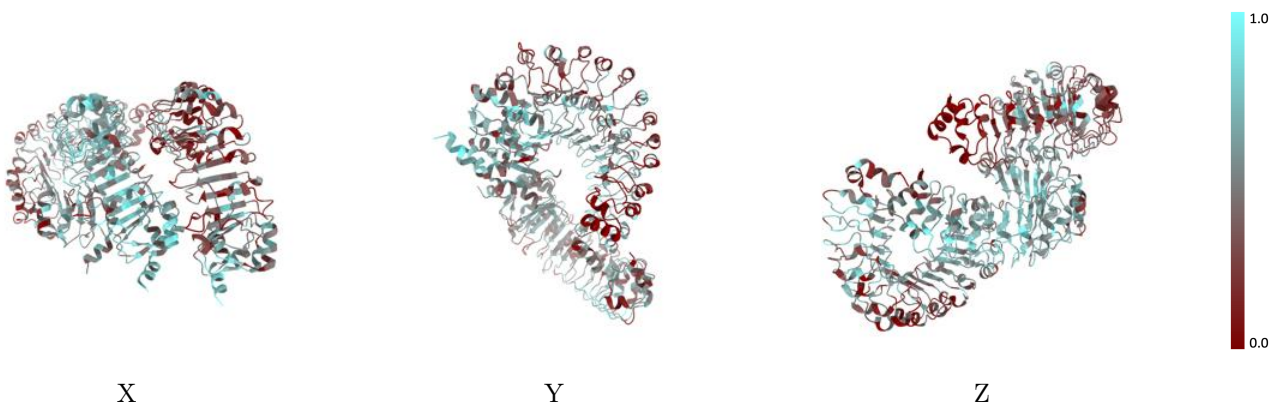
The images above show the 3D surface view of the map at the recommended contour level 0.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



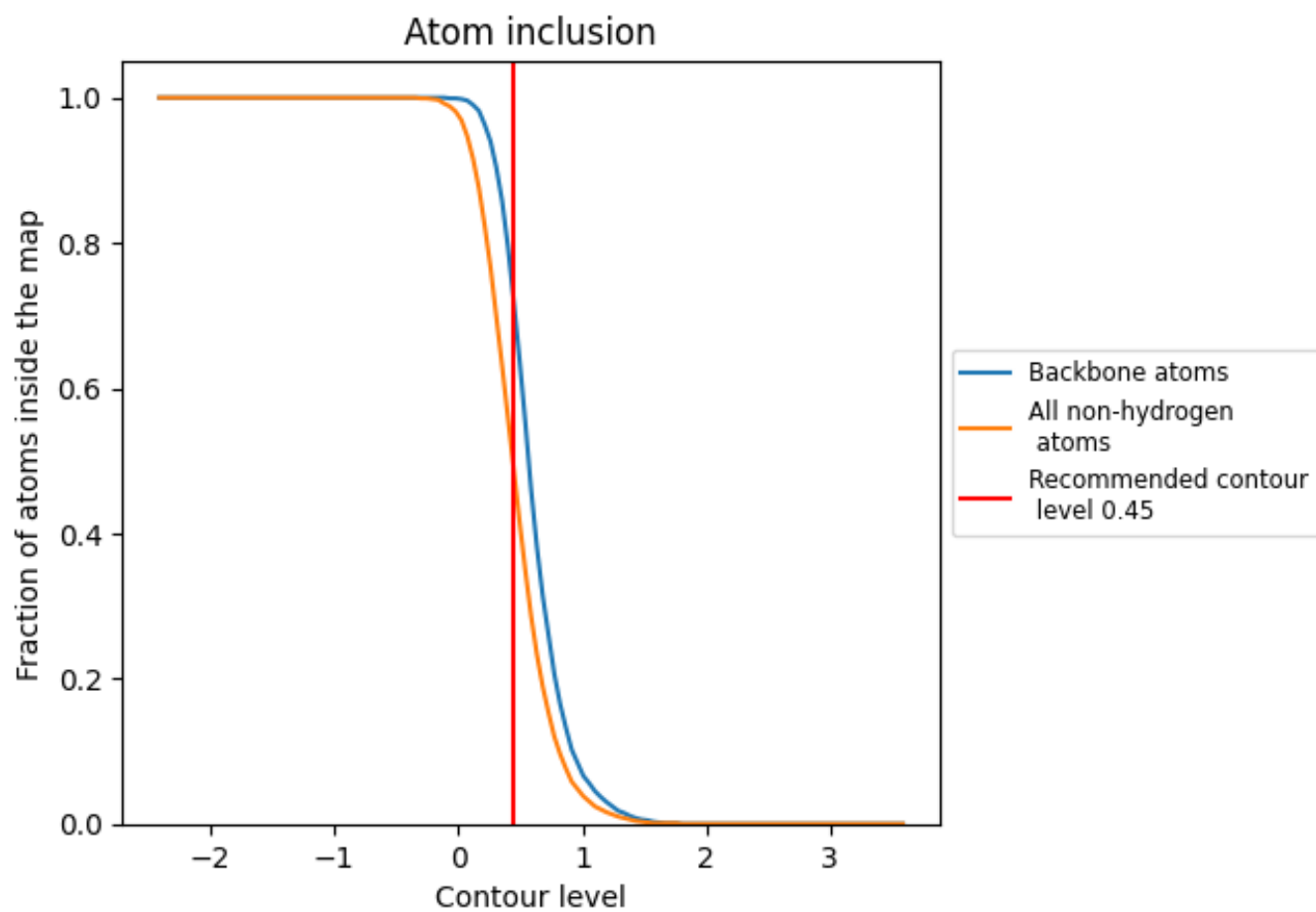
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.45).









## 9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 48% 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 (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4800	 0.2810
A	 0.6280	 0.3540
B	 0.3480	 0.2280
F	 0.4630	 0.2600

