



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 05:11 AM UTC

PDB ID : 8GZP / pdb_00008gzp
EMDB ID : EMD-34400
Title : Cryo-EM structure of the NS5-SLA complex
Authors : Osawa, T.; Ehara, H.; Sekine, S.
Deposited on : 2022-09-27
Resolution : 3.60 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

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:

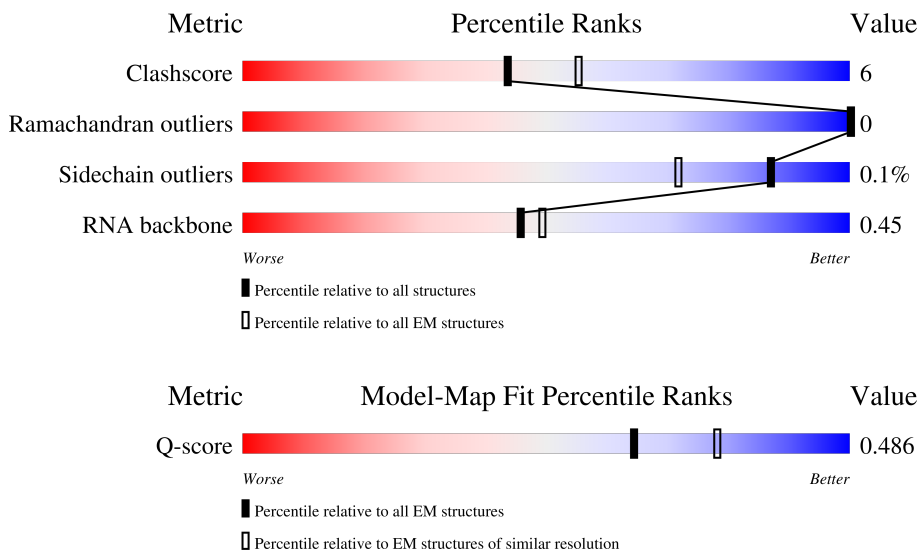
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.60 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	-
RNA backbone	8273	3508	-
Q-score	-	25397	12797 (3.10 - 4.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	908	
2	S	168	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8237 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 Genome polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	854	Total	C	N	O	S	0	0
			6778	4290	1232	1213	43		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	expression tag	UNP Q5I3C1
A	-6	PRO	-	expression tag	UNP Q5I3C1
A	-5	SER	-	expression tag	UNP Q5I3C1
A	-4	SER	-	expression tag	UNP Q5I3C1
A	-3	GLY	-	expression tag	UNP Q5I3C1
A	-2	SER	-	expression tag	UNP Q5I3C1
A	-1	SER	-	expression tag	UNP Q5I3C1
A	0	GLY	-	expression tag	UNP Q5I3C1

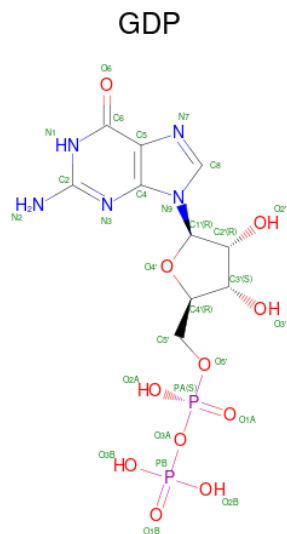
- Molecule 2 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	S	67	Total	C	N	O	P	0	0
			1428	639	256	466	67		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	2	Total	Zn	0
			2	2	

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	S	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	S	1	Total 1	Mg 1	0

- Molecule 1: Genome polypotein

TLE TRP	D663	C449	S221	GLY
	P692	M454	V234	PRO
	Q695	LYS	L238	SER
	K719	ARG	L239	GLY
	L724	LYS	F242	SER
	L724	LYS	T250	GLY
	C728	LEU	D256	THR
	G736	GLU	L257	GLY
	I740	PHE	R262	GLN
	G743	LYS	E267	GLY
	A744	ALA	N297	E7
	G745	GLY	T313	K29
	W746	SER	GLY	K30
	A757	E484	SER	T34
	M761	W496	SER	R38
	Y766	N501	SER	A54
	R769	S504	SER	V77
	L774	L511	T336	L94
	P789	M529	M340	V100
	R792	T553	A341	E111
	W795	M556	M342	V114
	E834	I567	THR	P115
	R871	K575	ASP	M116
	L880	R581	T345	Y119
	D881	R594	R352	V124
	P884	K595	E366	P137
	M885	M614	P367	C140
	K887	V627	K371	D141
	F889	L655	L380	T142
	R890	L655	P390	L143
	LYS	W646	A406	W171
	GLU	P636	ALA	Q176
	GLU	W646	MET	P184
	GLU	L655	GLY	V189
	SER	L655	ALA	H192
	GLU	M658	VAL	H215
	GLY	A859	PHE	
	ALA	I660	THR	
			E414	
			C446	

- Molecule 2: RNA

Category	Item	Value
GDP	A1	100
	G2	100
	U3	100
	U4	100
	G5	100
	A8	100
	G9	100
	U10	100
	C11	100
	U14	100
GDP	G15	100
	U16	100
	G17	100
	G18	100
	A19	100
	C20	100
	C21	100
	G22	100
	A23	100
	C24	100
GDP	A25	100
	A31	100
	G32	100
	U33	100
	U34	100
	U40	100
	C41	100
	G42	100
	G43	100
	A44	100
GDP	A45	100
	G46	100
	C47	100
	U	100
	U49	100
	G50	100
	C51	100
	U52	100
	U53	100
	A54	100
GDP	C55	100
	C56	100
	A57	100
	C58	100
	A59	100
	G60	100
	U61	100
	U62	100
	C63	100
	U64	100
GDP	A65	100
	A66	100
	C67	100
	A68	100
	G	100

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	82059	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 ($e^-/\text{\AA}^2$)	55.46	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.076	Depositor
Minimum map value	-0.040	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.011	Depositor
Map size (Å)	198.84, 198.84, 198.84	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8285, 0.8285, 0.8285	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: GDP, ZN, MG

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	0.46	0/6947	0.43	0/9414
2	S	0.26	0/1596	0.39	0/2482
All	All	0.43	0/8543	0.42	0/11896

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	6778	0	6593	58	0
2	S	1428	0	722	46	0
3	A	2	0	0	0	0
4	S	28	0	12	0	0
5	S	1	0	0	0	0
All	All	8237	0	7327	101	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 6.

The worst 5 of 101 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:CYS:SG	1:A:449:CYS:HB2	2.11	0.90
2:S:17:G:H21	2:S:54:A:H62	1.32	0.74
2:S:45:A:H2'	2:S:46:G:H8	1.55	0.72
2:S:10:U:H3	2:S:62:U:H3	1.41	0.67
1:A:728:CYS:SG	1:A:769:ARG:NH1	2.69	0.66

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	844/908 (93%)	794 (94%)	50 (6%)	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	706/788 (90%)	705 (100%)	1 (0%)	88	87

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	192	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	547	HIS
1	A	613	ASN
1	A	621	GLN
1	A	876	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	S	66/168 (39%)	15 (22%)	4 (6%)

5 of 15 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	S	5	G
2	S	19	A
2	S	20	C
2	S	34	U
2	S	50	G

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	S	19	A
2	S	49	U
2	S	60	G
2	S	61	U

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

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
4	GDP	S	201	2,5	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)

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
4	GDP	S	201	2,5	-	3/16/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	S	201	GDP	C5-C4	2.88	1.46	1.38
4	S	201	GDP	C6-N1	-2.62	1.34	1.38
4	S	201	GDP	C5-N7	-2.32	1.34	1.39

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	S	201	GDP	C5-C4-N3	-5.93	118.95	128.39
4	S	201	GDP	C2-N3-C4	5.02	120.94	112.30
4	S	201	GDP	N9-C4-N3	4.42	134.80	125.95
4	S	201	GDP	C6-C5-N7	3.15	136.02	130.29
4	S	201	GDP	O6-C6-C5	-2.38	120.25	126.53

There are no chirality outliers.

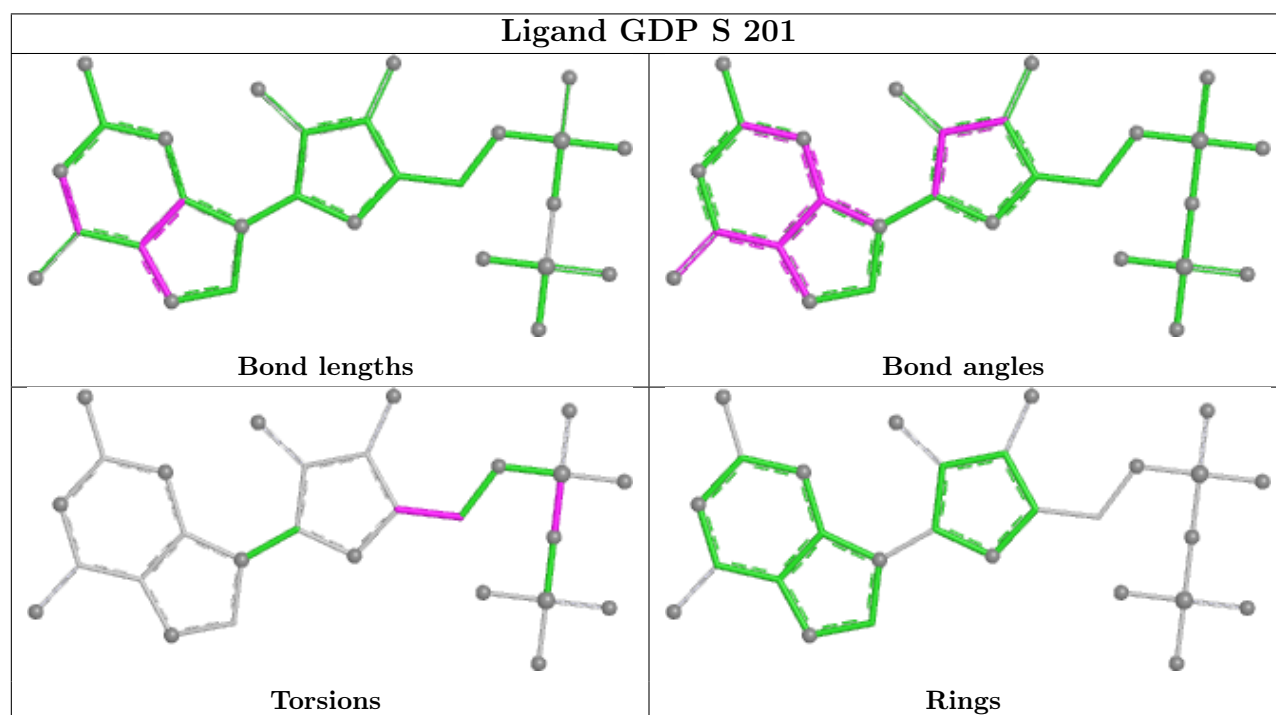
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	S	201	GDP	O4'-C4'-C5'-O5'
4	S	201	GDP	PB-O3A-PA-O2A
4	S	201	GDP	PB-O3A-PA-O1A

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

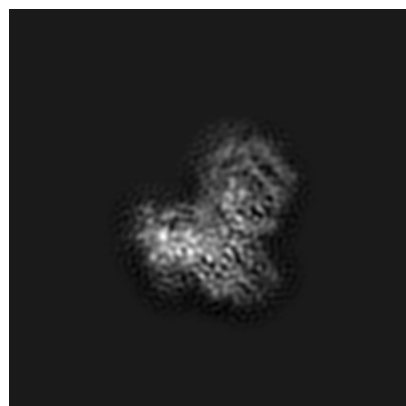
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34400. These allow visual inspection of the internal detail of the map and identification of artifacts.

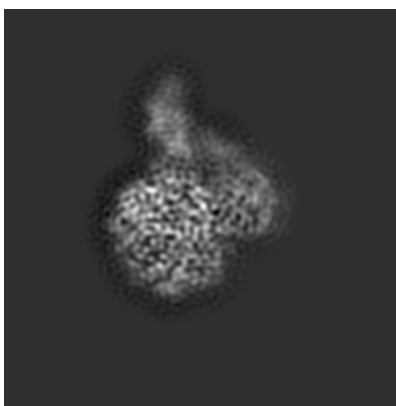
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

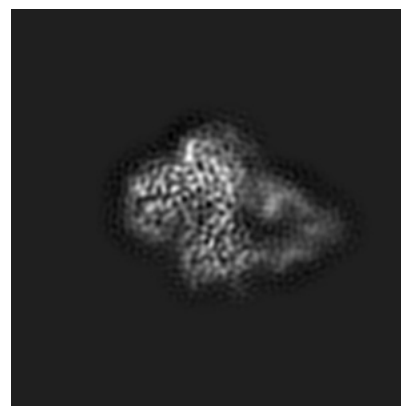
6.1.1 Primary map



X

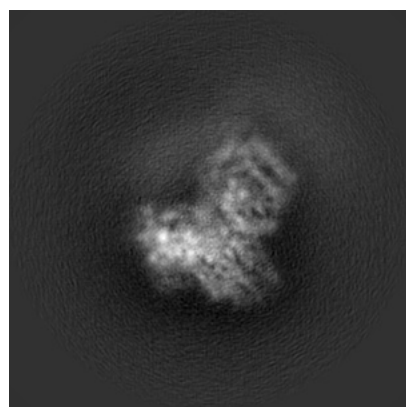


Y

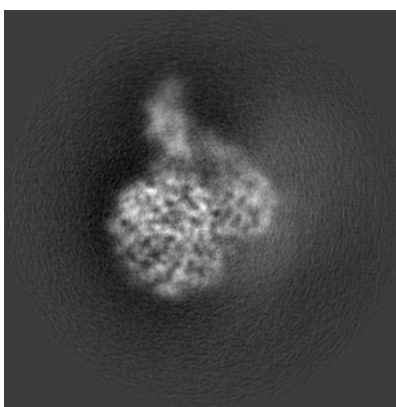


Z

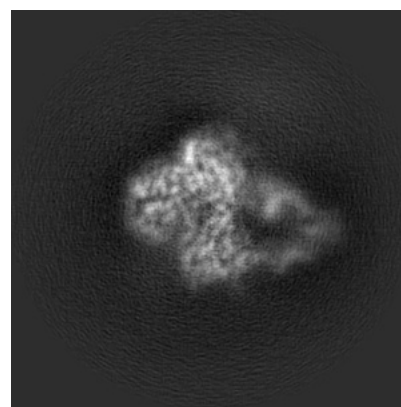
6.1.2 Raw map



X



Y

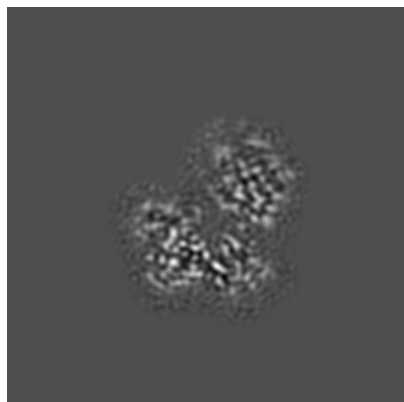


Z

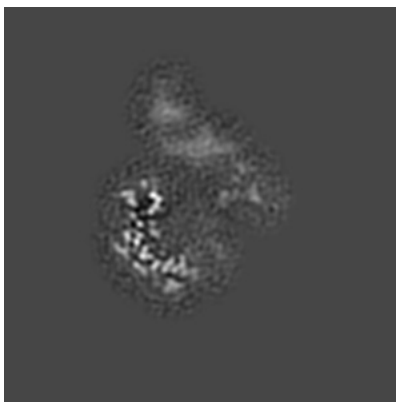
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

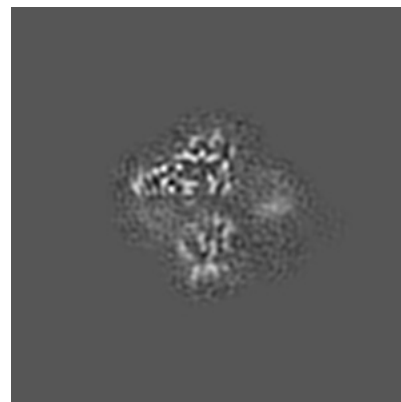
6.2.1 Primary map



X Index: 120

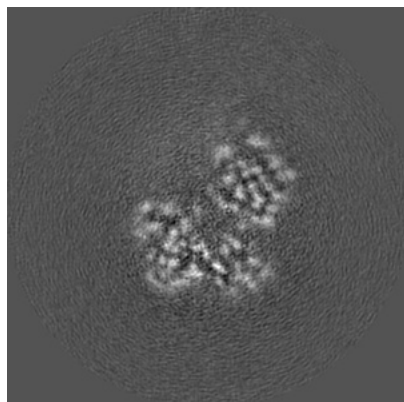


Y Index: 120

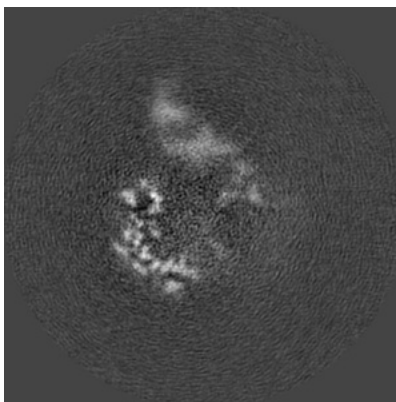


Z Index: 120

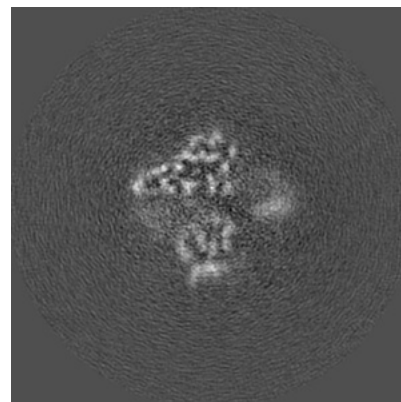
6.2.2 Raw map



X Index: 120



Y Index: 120

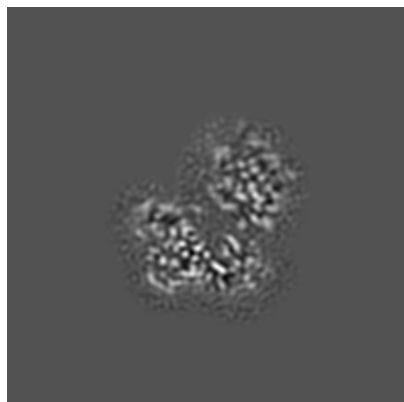


Z Index: 120

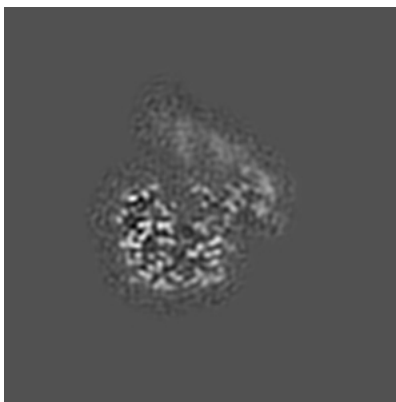
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

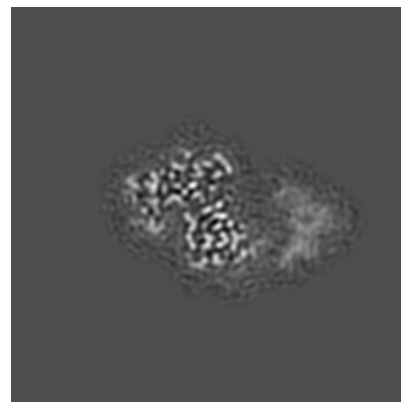
6.3.1 Primary map



X Index: 121

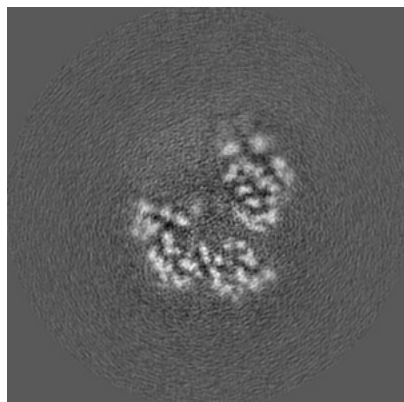


Y Index: 132

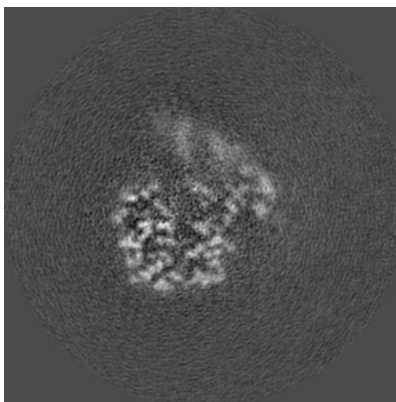


Z Index: 93

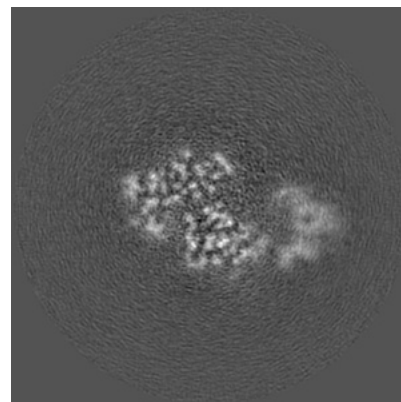
6.3.2 Raw map



X Index: 117



Y Index: 132

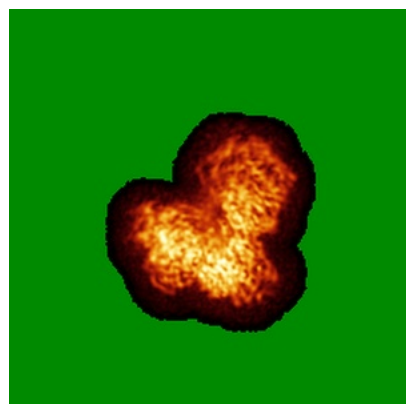


Z Index: 94

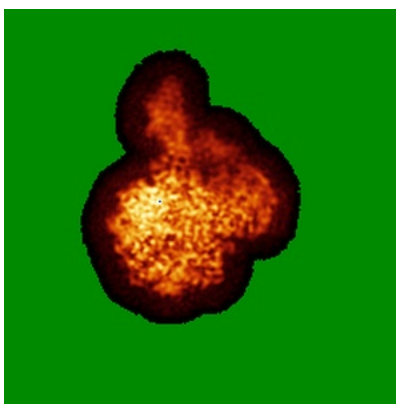
The images above show the largest variance slices of the map in three orthogonal directions.

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

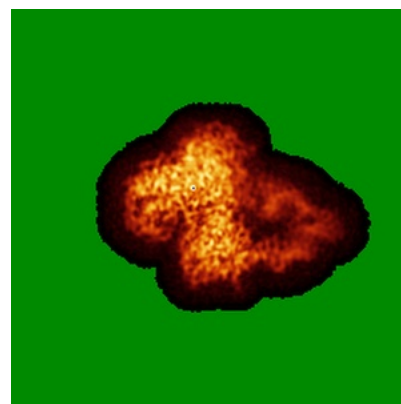
6.4.1 Primary map



X

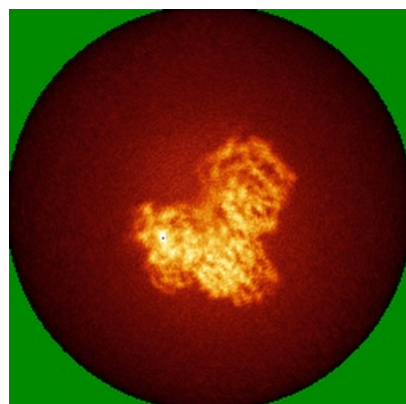


Y

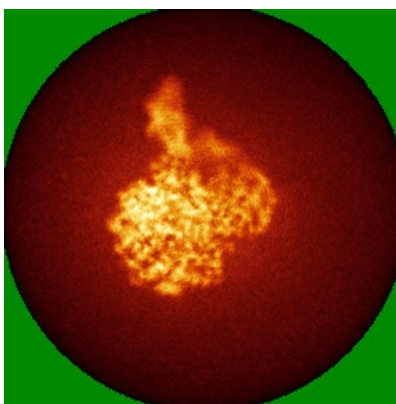


Z

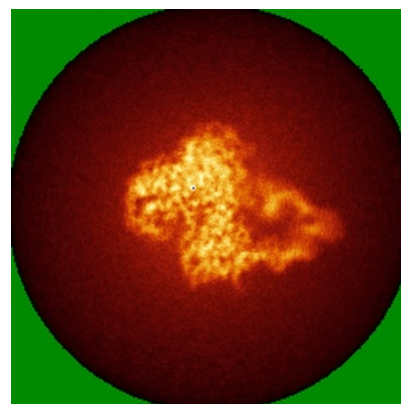
6.4.2 Raw map



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](#)

This section was not generated.

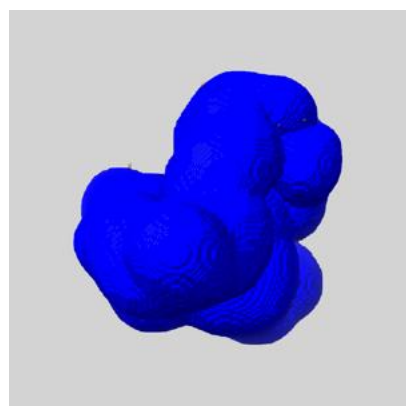
6.6 Mask visualisation [i](#)

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

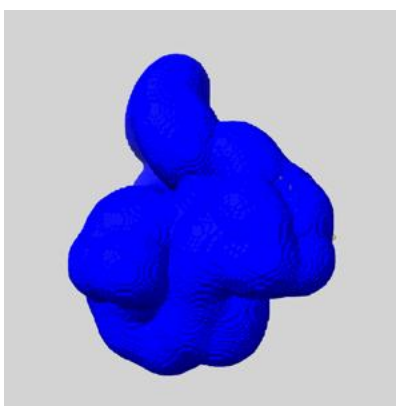
A mask typically either:

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

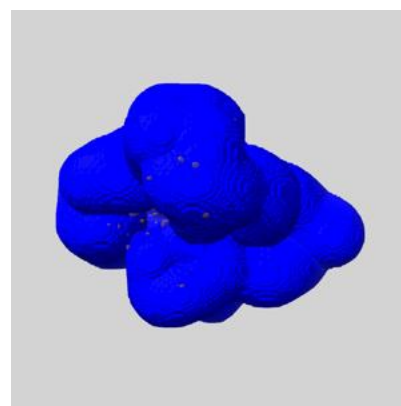
6.6.1 emd_34400_msk_1.map [i](#)



X



Y

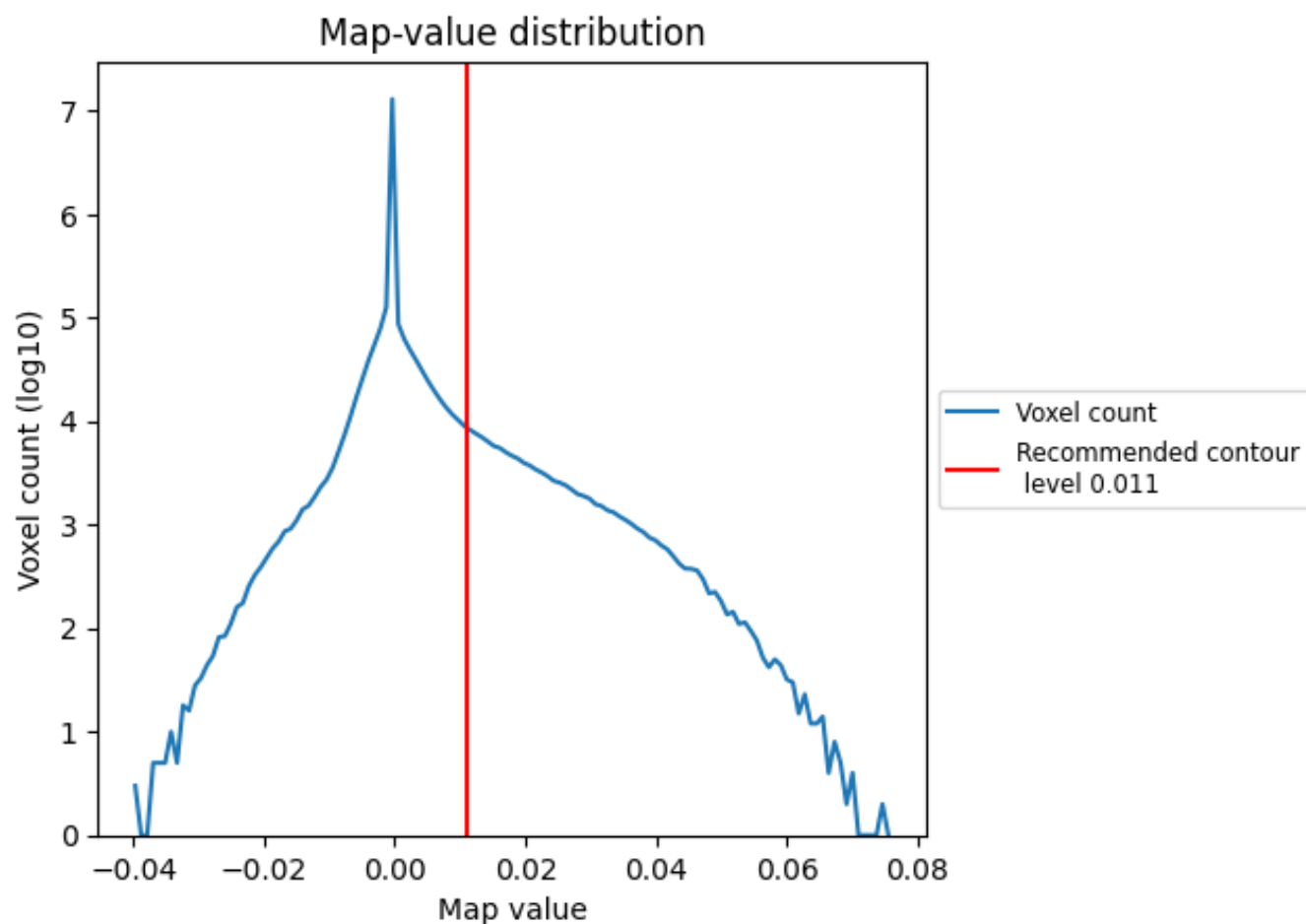


Z

7 Map analysis [i](#)

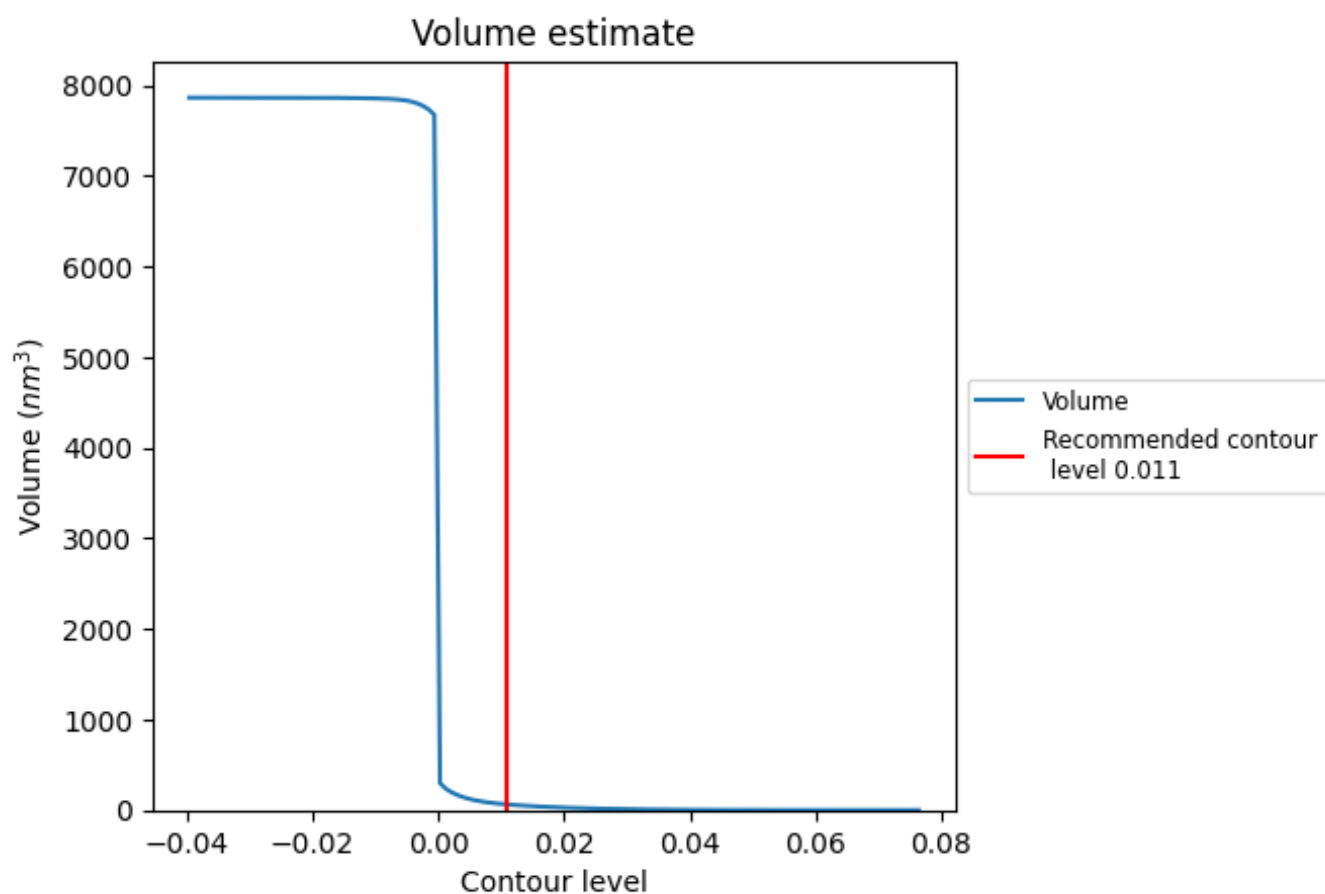
This section contains the results of statistical analysis of the map.

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.

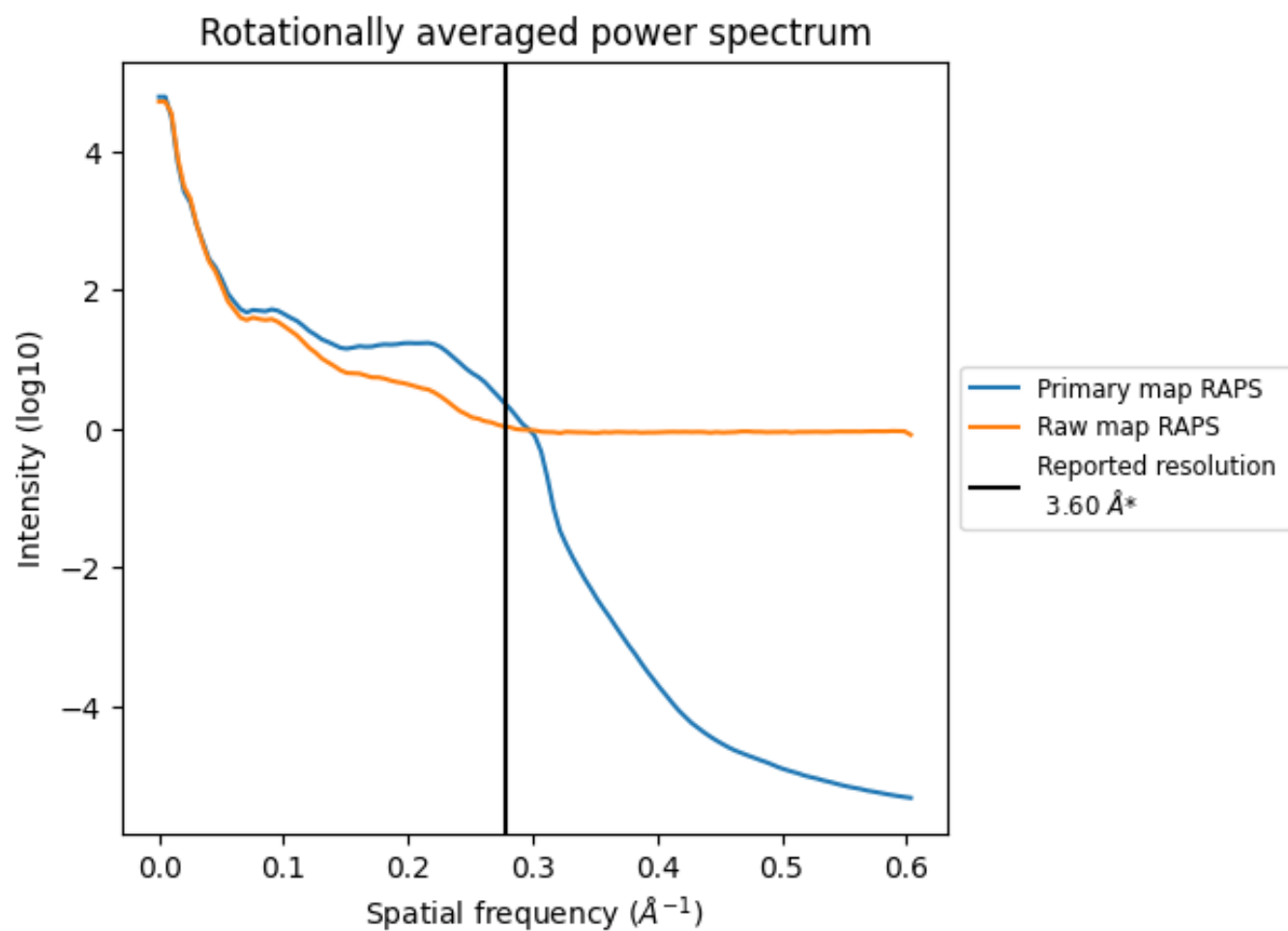
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 62 nm³; this corresponds to an approximate mass of 56 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](#)

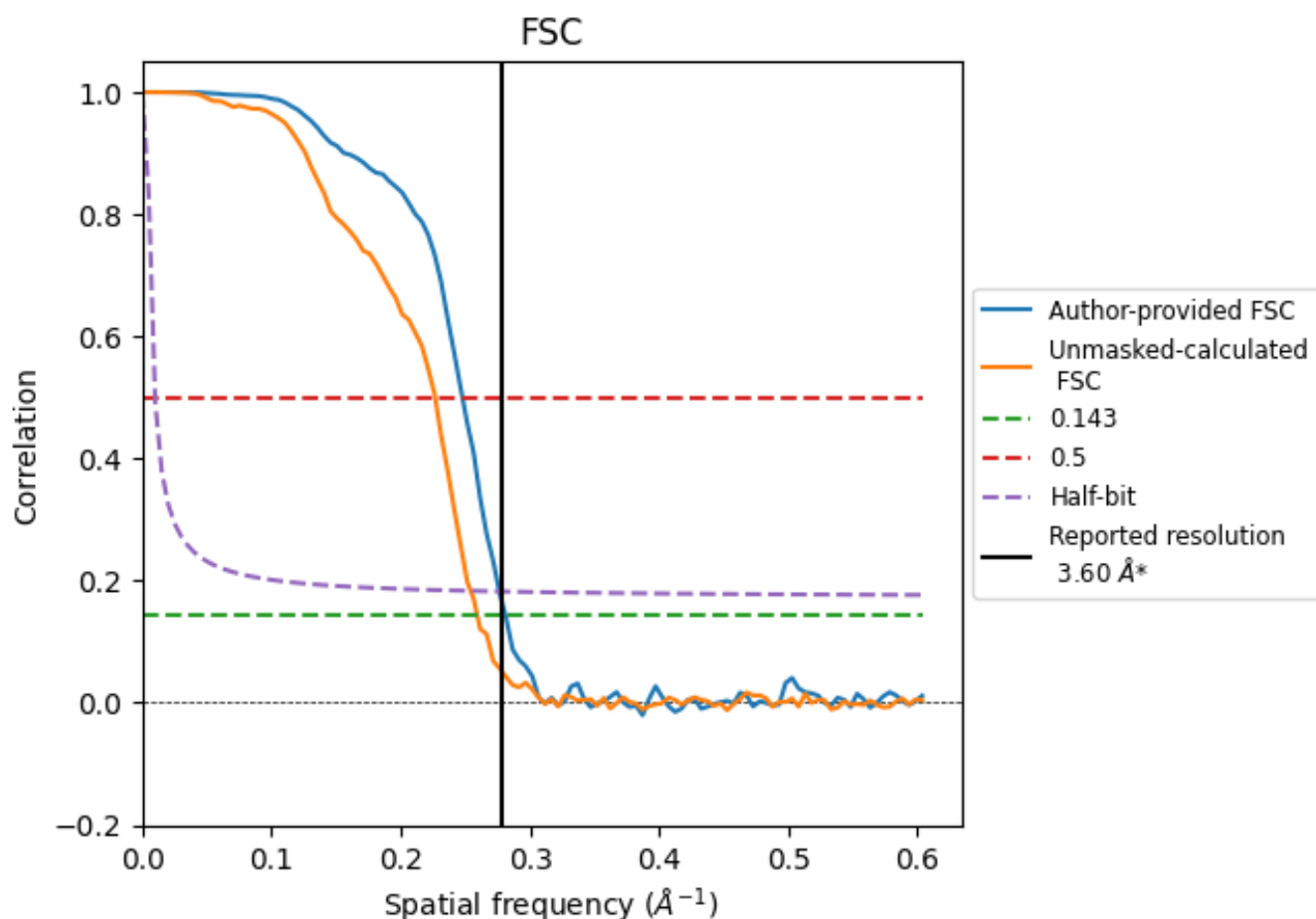


*Reported resolution corresponds to spatial frequency of $0.278 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.56	4.04	3.62
Unmasked-calculated*	3.86	4.41	3.94

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

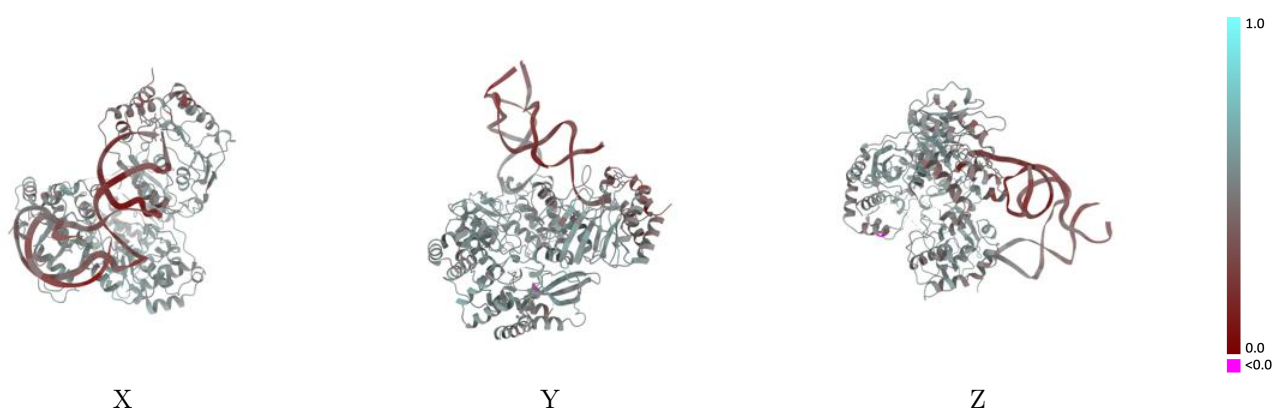
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-34400 and PDB model 8GZP. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)

This section was not generated.

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

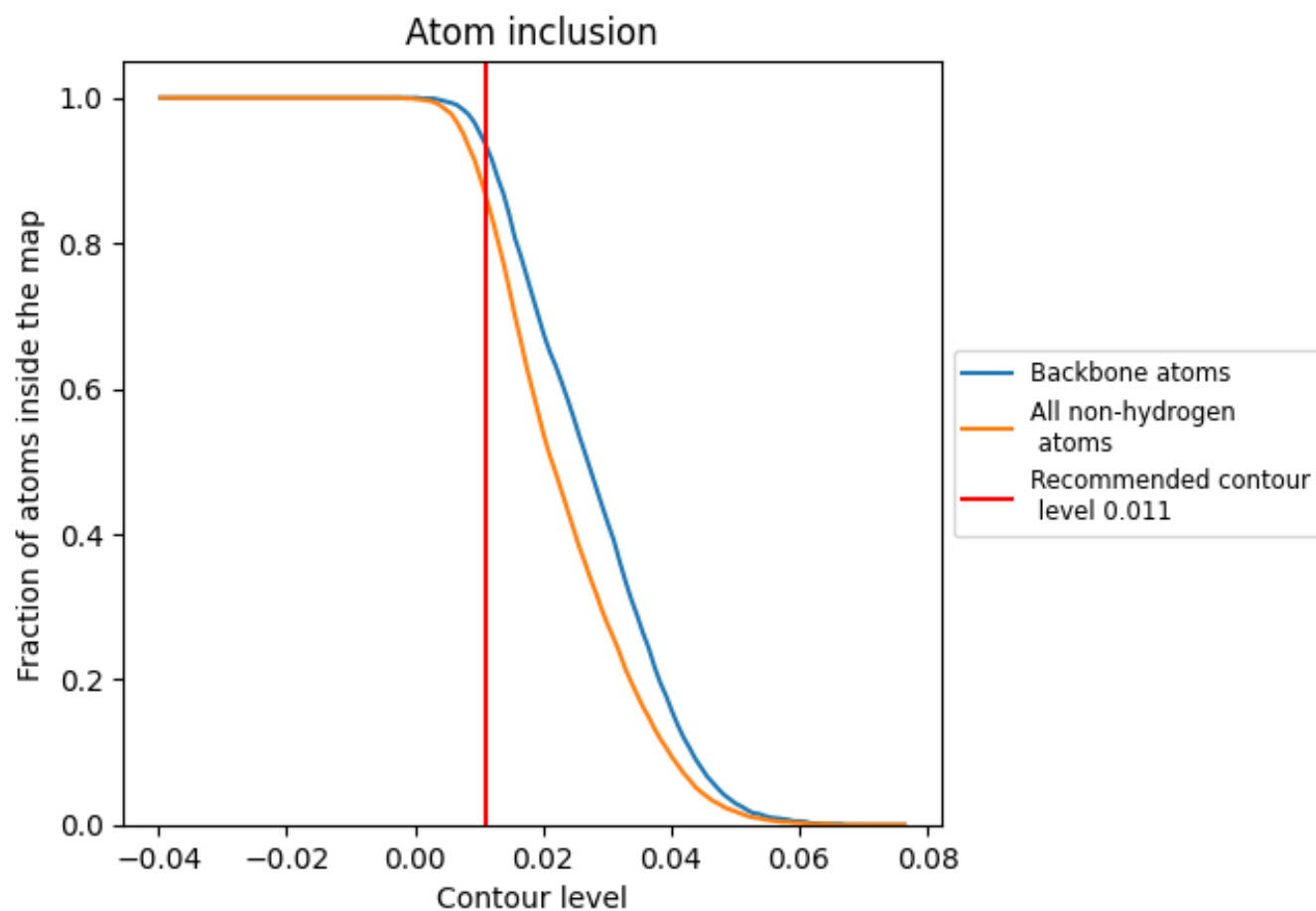


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 87% 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 (0.011) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8680	0.4860
A	0.8810	0.5210
S	0.8050	0.3230

