wwPDB EM Validation Summary Report (i)

Oct 10, 2026 – 10:17 am BST

PDB ID	:	32AJ / pdb_000032aj
EMDB ID	:	EMD-58749
Title	:	SARS-CoV2 KP.3 with fab JN.1-9 local refinement
Authors	:	Duyvesteyn, H.M.E.; Ren, J.
Deposited on	:	2026-07-01
Resolution	:	3.20 Å(reported)
Based on initial models	:	8CIM, .

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 (i) 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 (1)) were used in the production of this report:

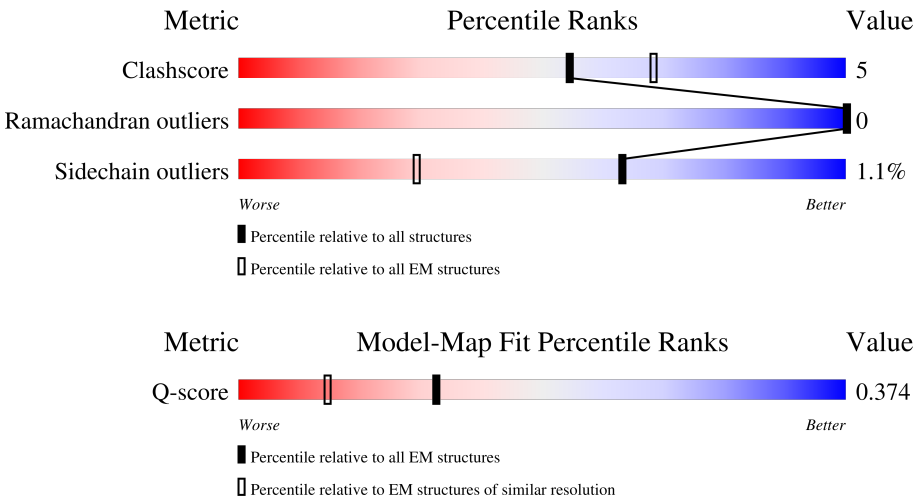
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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	15020 (2.70 - 3.70)

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 <=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	H	121	21% 79% 20%
2	L	112	12% 86% 12%
3	A	1284	13% 85%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3291 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 JN.1-9 fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	H	120	939	602	152	183	2	0	0

- Molecule 2 is a protein called IG c20_light_IGLV1-40_IGLJ2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	L	110	796	495	136	163	2	0	0

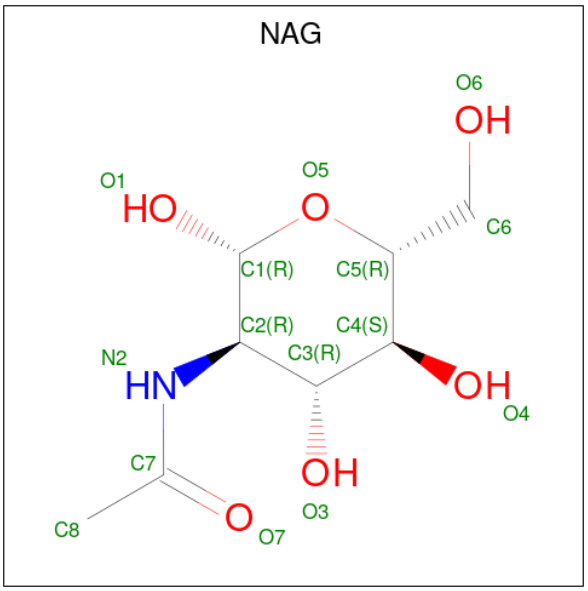
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	4	VAL	LEU	conflict	UNP A0A5C2GP18
L	25	GLY	SER	conflict	UNP A0A5C2GP18
L	99	ALA	GLY	conflict	UNP A0A5C2GP18

- Molecule 3 is a protein called Receptor binding domain from SARS-CoV-2 KP.3 variant.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	A	192	1542	995	258	281	8	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



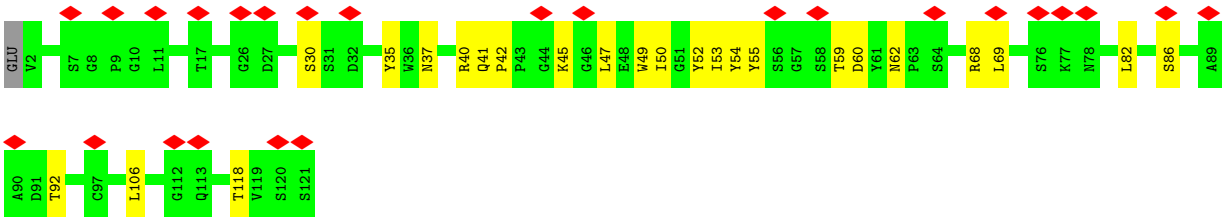
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	A	1	14	8	1	5	0

3 Residue-property plots (i)

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.

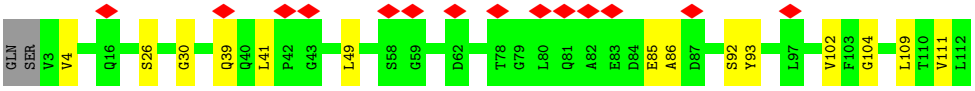
- Molecule 1: JN.1-9 fab heavy chain

Chain H:



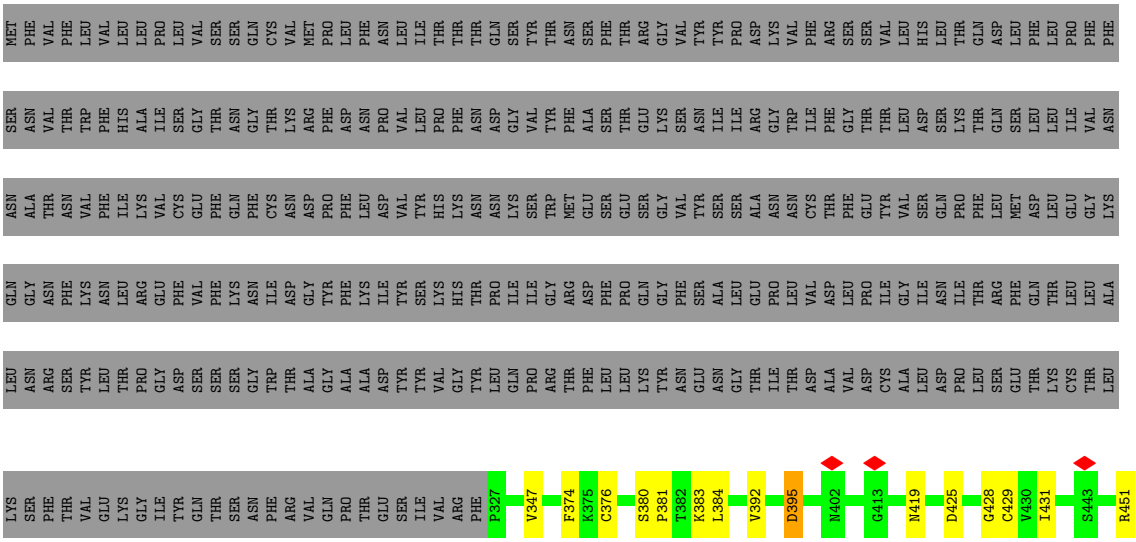
- Molecule 2: IG c20_light_IGLV1-40_IGLJ2

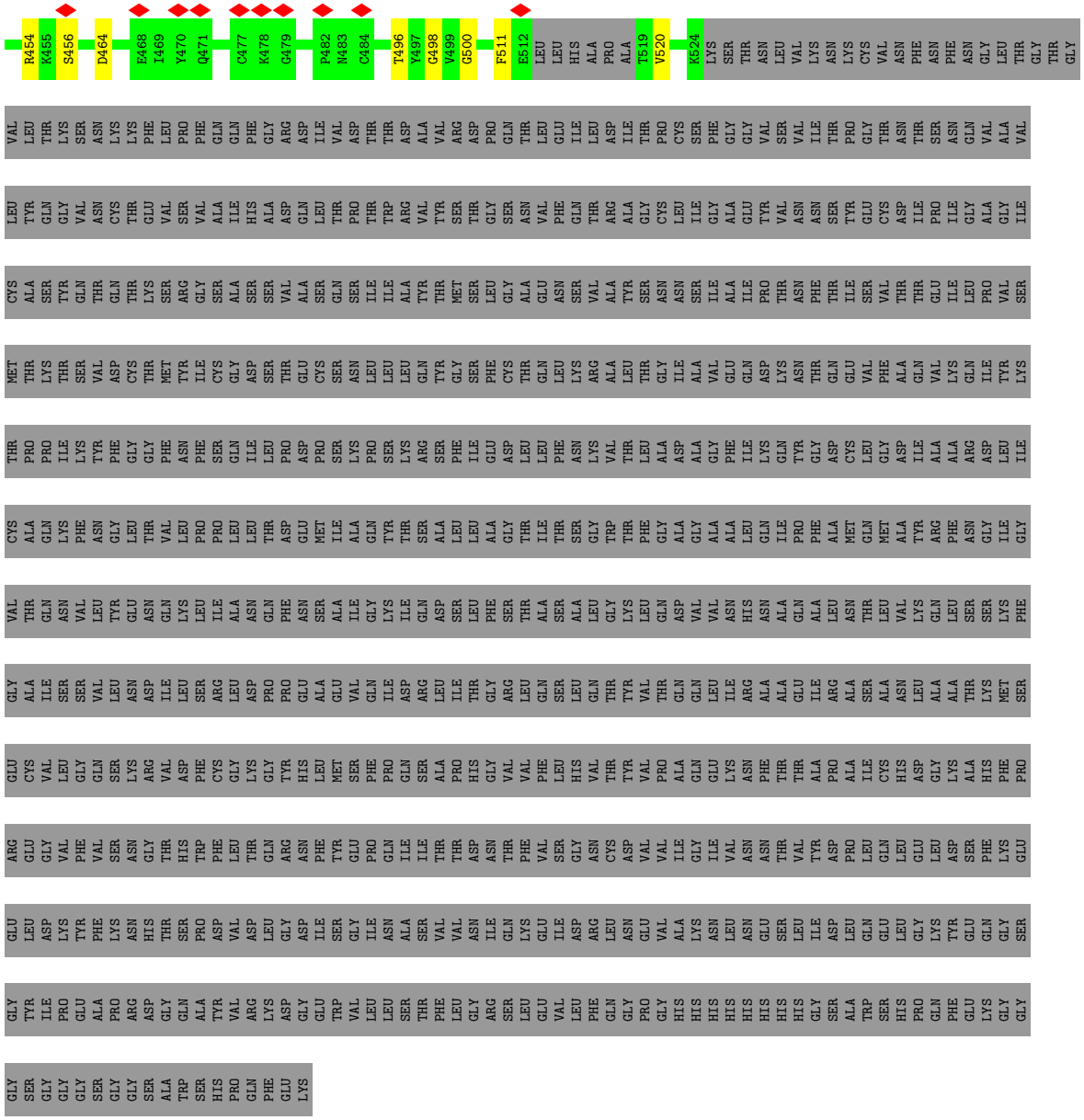
Chain L:



- Molecule 3: Receptor binding domain from SARS-CoV-2 KP.3 variant

Chain A:




R454 K455 S456 D464 E468 I469 Y470 Q471 C477 K478 G479 P482 N483 C484 T496 Y497 G498 V499 G500 F511 E512 T519 V520 K524
VAL LEU THR LYS SER ASN LYS LYS PHE LEU PRO PHE GLN GLN PHE GLY ARG ASP ILE VAL ASP THR THR ASP ALA VAL ARG ASP PRO GLN THR LEU GLU ILE LEU ASP ILE THR PRO CYS SER PHE GLY GLY VAL SER VAL ILE THR PRO GLY THR ASN THR SER ASN GLN VAL ALA VAL
LEU TYR GLN GLY VAL ASN CYS THR GLU VAL SER VAL ALA ILE HIS ALA ASP GLN LEU THR PRO THR TRP ARG VAL TYR SER THR GLY SER ASN VAL PHE GLN THR ARG ALA GLY CYS LEU ILE GLY ALA GLU TYR VAL ASN ASN SER TYR GLU CYS ASP ILE PRO ILE GLY ALA GLY ILE
CYS ALA SER TYR GLN THR LYS SER ARG GLY SER ALA SER SER VAL ALA SER GLN SER ILE ILE ALA TYR THR MET SER LEU GLY ALA GLU ASN SER VAL ALA TYR SER ASN ASN SER ILE ALA ILE PRO THR ASN PHE THR ILE SER VAL THR THR GLU ILE LEU PRO VAL SER
MET THR LYS THR SER VAL ASP CYS THR MET TYR ILE CYS GLY ASP SER THR GLU CYS SER ASN LEU LEU LEU GLN TYR GLY SER PHE CYS THR GLN LEU LYS ARG ALA LEU THR GLY ILE ALA VAL GLU GLN ASP LYS ASN THR GLN GLU VAL PHE ALA GLN VAL LYS GLN ILE TYR LYS
THR PRO PRO ILE LYS TYR PHE GLY GLY PHE PHE ASN PHE SER GLN ILE LEU PRO ASP PRO SER LYS PRO SER LYS ARG SER PHE ILE ILE GLU ASP LEU LEU PHE ASN LYS VAL THR LEU ALA ASP ALA GLY PHE ILE LYS GLN TYR GLY ASP CYS LEU GLY ASP ILE ALA ARG ASP LEU ILE
CYS ALA GLN LYS PHE ASN GLY LEU THR VAL LEU PRO PRO LEU LEU THR ASP GLU MET ILE ALA GLN TYR THR SER ALA LEU LEU ALA GLY THR ILE THR SER GLY GLY TRP THR PHE GLY ALA GLY ALA ALA LEU GLN ILE PRO PHE ALA MET GLN MET ALA TYR ARG PHE ASN GLY LEU GLY
VAL THR GLN ASN VAL LEU TYR GLU ASN GLN LYS LEU ILE ALA ASN GLN PHE ASN SER ALA ILE GLY ILE GLN ASP SER LEU PHE SER THR ALA SER ALA LEU GLY LYS LEU GLN ASP VAL VAL ASN HIS ASN ALA GLN ALA LEU ASN THR LEU VAL LYS GLN LEU SER SER LYS PHE
GLY ALA ILE SER SER VAL LEU ASN ASP ILE LEU SER ARG LEU ASP PRO PRO GLU ALA GLU VAL GLN ILE ASP ARG ARG LEU ILE ILE THR GLY ARG LEU GLN SER LEU GLN THR TYR VAL THR GLN GLN LEU ILE ARG ALA SER ALA ASN LEU ALA GLU ILE ARG ALA THR LYS MET SER
GLU CYS VAL LEU GLY GLN SER LYS ARG VAL ASP PHE CYS GLY LYS GLY TYR HIS LEU MET SER PHE PRO GLN SER ALA PRO HIS HIS GLY VAL VAL PHE LEU HIS VAL THR TYR VAL PRO ALA GLN GLU LYS ASN PHE THR THR ALA PRO ALA ILE CYS HIS ASP GLY LYS ALA HIS PHE PRO
ARG GLU GLY VAL PHE VAL SER ASN GLY THR HIS TRP PHE LEU THR GLN ARG ASN PHE TYR GLU PRO GLN ILE ILE THR THR ASP ASN THR PHE VAL SER GLY ASN CYS ASP VAL VAL ILE GLY ILE VAL ASN ASN THR VAL TYR ASP PRO LEU GLN GLU LEU GLU LEU ASP SER PHE LYS GLU
GLU LEU ASP LYS TYR PHE LYS ASN HIS THR SER PRO ASP VAL ASP LEU GLY ASP ILE SER GLY ILE ASN ALA SER VAL VAL ASN ILE GLN LYS GLU ILE ASP ARG LEU ASN GLU VAL ALA LYS ASN LEU ASN GLU SER LEU ILE ASP PRO LEU GLN GLU LEU GLY LYS TYR GLU GLN GLY SER
GLY TYR ILE PRO GLU ALA PRO ARG ASP GLY GLN ALA TYR VAL ARG LYS ASP GLY GLU TRP VAL LEU LEU SER THR PHE LEU GLY ARG SER LEU GLU VAL LEU PHE GLN GLY PRO GLY HIS HIS HIS HIS HIS HIS HIS HIS GLY SER ALA TRP SER HIS PRO GLN PHE GLU LYS GLY GLY
GLY SER GLY GLY GLY SER GLY GLY SER ALA TRP SER HIS PRO GLN PHE GLU LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	108638	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Cryosparc patch CTF correction	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50.0	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.713	Depositor
Minimum map value	-0.543	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.0853	Depositor
Map size (Å)	328.635, 328.635, 328.635	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.7303, 0.7303, 0.7303	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	H	0.09	0/966	0.23	0/1323
2	L	0.09	0/814	0.25	0/1110
3	A	0.10	0/1591	0.24	0/2162
All	All	0.09	0/3371	0.24	0/4595

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	H	939	0	903	13	0
2	L	796	0	762	7	0
3	A	1542	0	1462	16	0
4	A	14	0	13	0	0
All	All	3291	0	3140	33	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 5.

The worst 5 of 33 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:H:49:TRP:O	1:H:62:ASN:ND2	2.31	0.61
3:A:395:ASP:N	3:A:395:ASP:OD1	2.37	0.58
3:A:374:PHE:HE2	3:A:381:PRO:HB3	1.71	0.56
3:A:380:SER:HB3	3:A:383:LYS:HB2	1.85	0.56
2:L:39:GLN:HB2	2:L:49:LEU:HD22	1.87	0.56

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	H	118/121 (98%)	117 (99%)	1 (1%)	0	100	100
2	L	108/112 (96%)	106 (98%)	2 (2%)	0	100	100
3	A	188/1284 (15%)	178 (95%)	10 (5%)	0	100	100
All	All	414/1517 (27%)	401 (97%)	13 (3%)	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	H	105/106 (99%)	103 (98%)	2 (2%)	50	73
2	L	87/89 (98%)	86 (99%)	1 (1%)	65	79
3	A	168/1111 (15%)	167 (99%)	1 (1%)	78	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	360/1306 (28%)	356 (99%)	4 (1%)	63 79

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	37	ASN
1	H	82	LEU
2	L	102	VAL
3	A	395	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	445	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)

1 ligand is 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	$\#\|Z\| > 2$
4	NAG	A	1301	3	14,14,15	0.29	0	17,19,21	0.46	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
4	NAG	A	1301	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

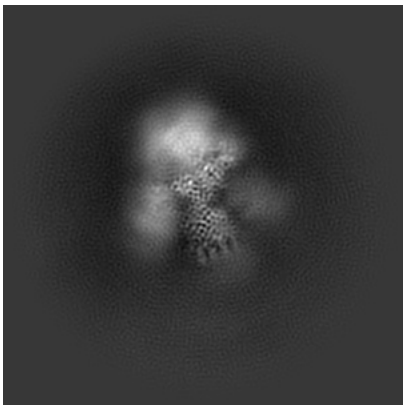
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-58749. These allow visual inspection of the internal detail of the map and identification of artifacts.

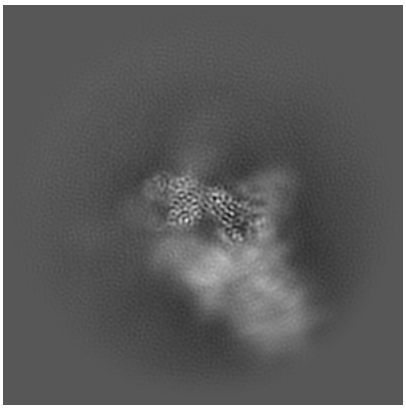
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

6.1.1 Primary map



X



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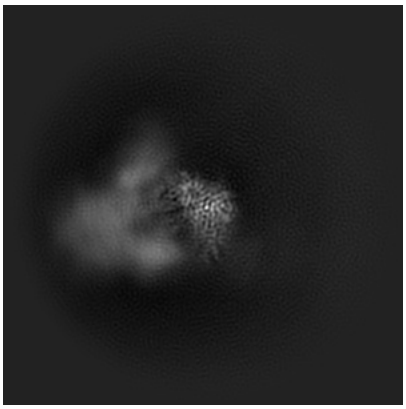
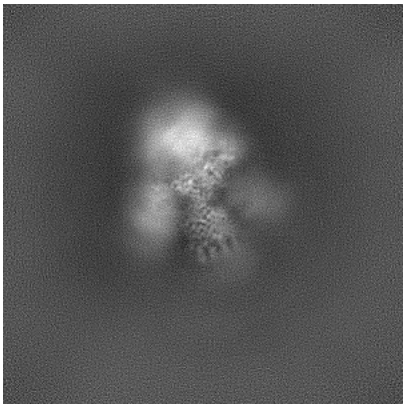


Z

6.1.2 Raw map



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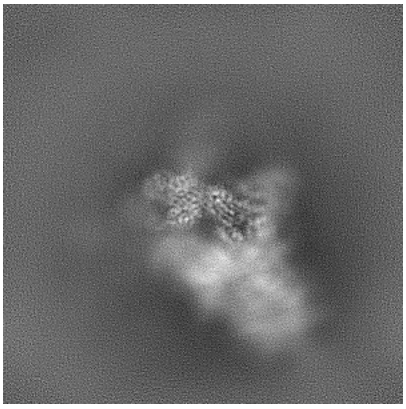

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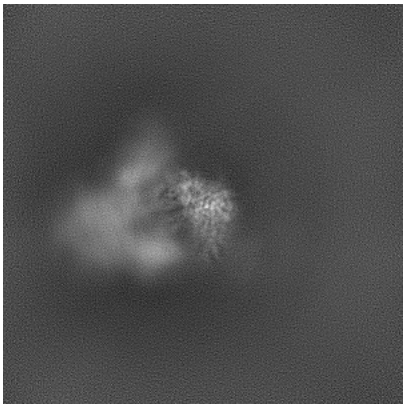
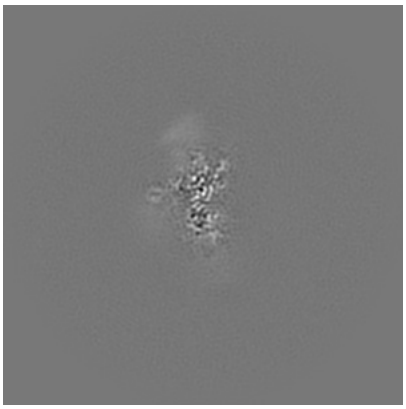


Z

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

6.2 Central slices (i)

6.2.1 Primary map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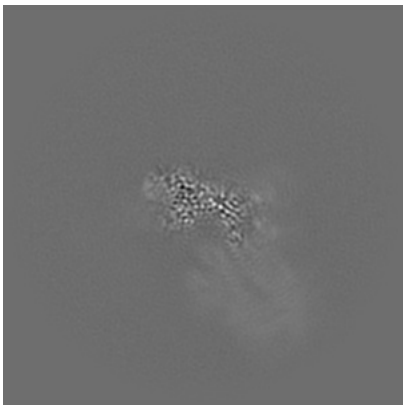
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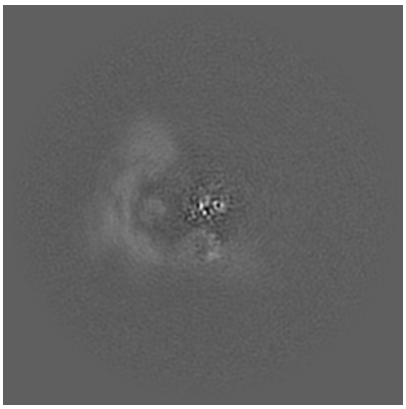
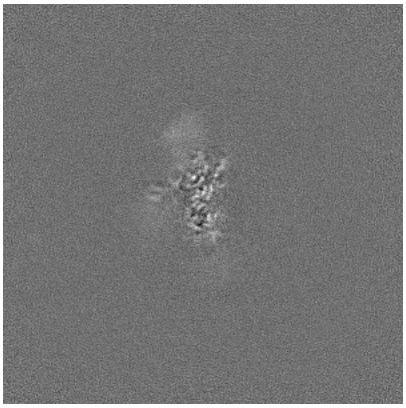
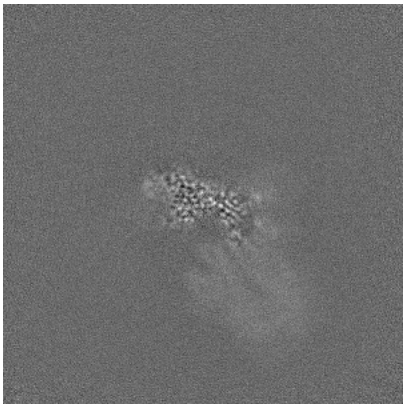

Z Index: 225

6.2.2 Raw map


X Index: 225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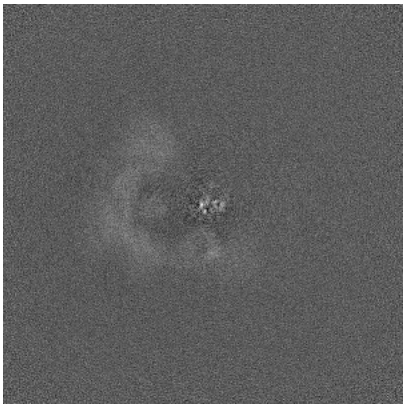
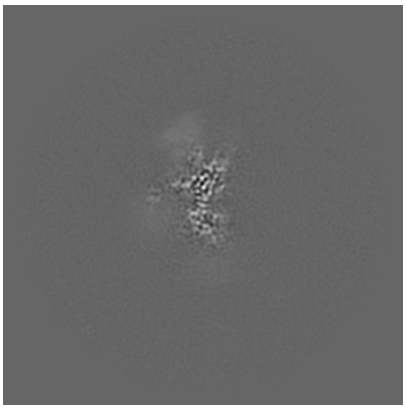

Z Index: 225

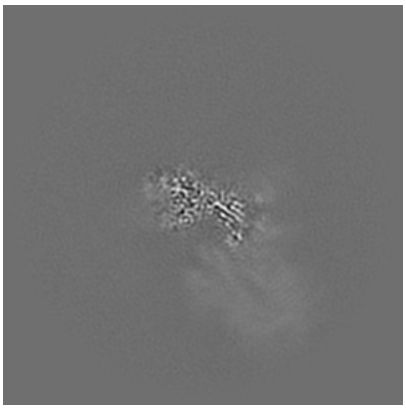
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

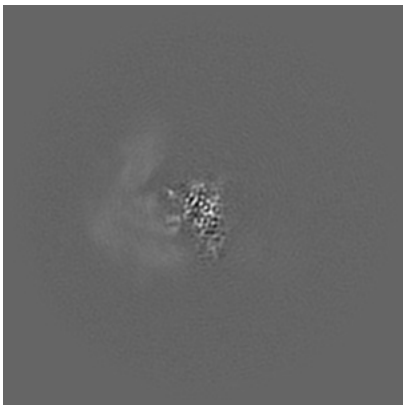
6.3.1 Primary map



X Index: 223

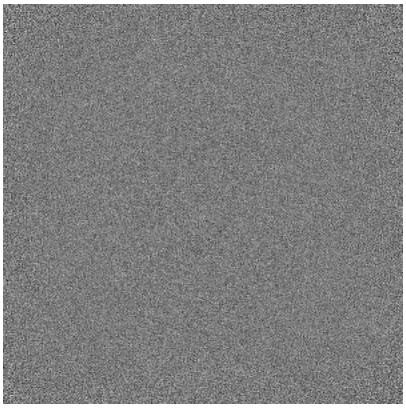


Y Index: 227

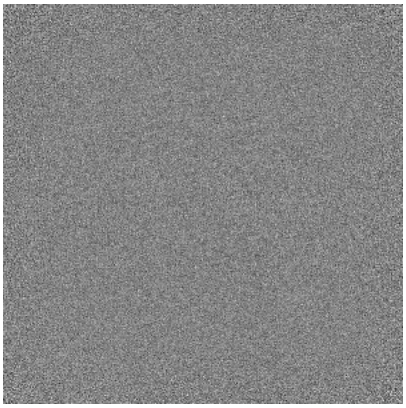


Z Index: 246

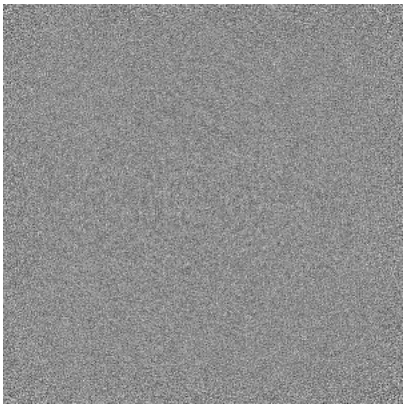
6.3.2 Raw map



X Index: 0



Y Index: 0

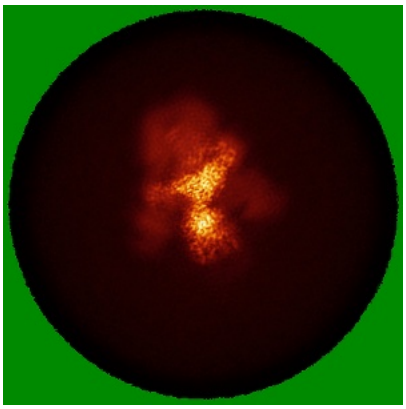


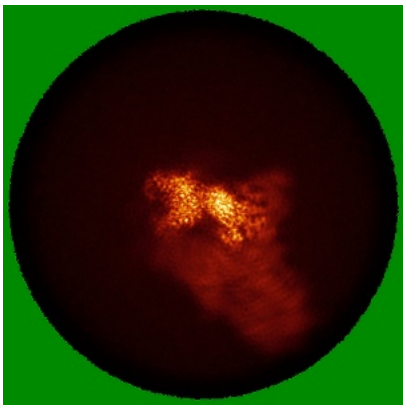
Z Index: 0

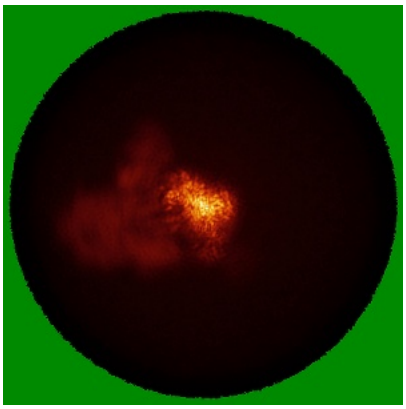
The images above show the largest variance slices of the map in three orthogonal directions.

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

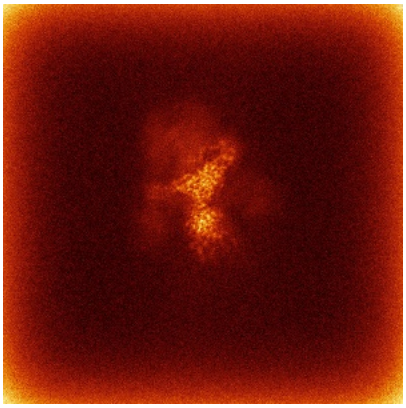
6.4.1 Primary map

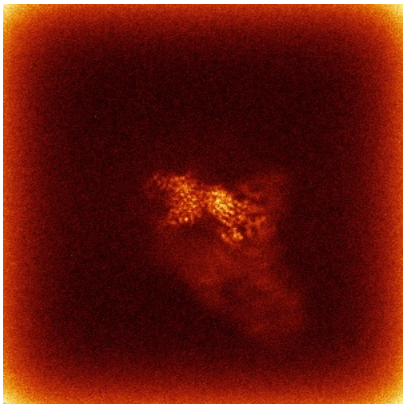

X

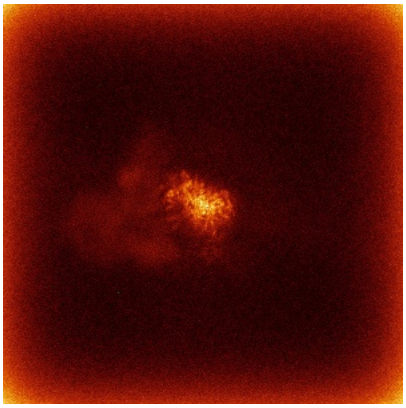

Y


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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0853. 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.

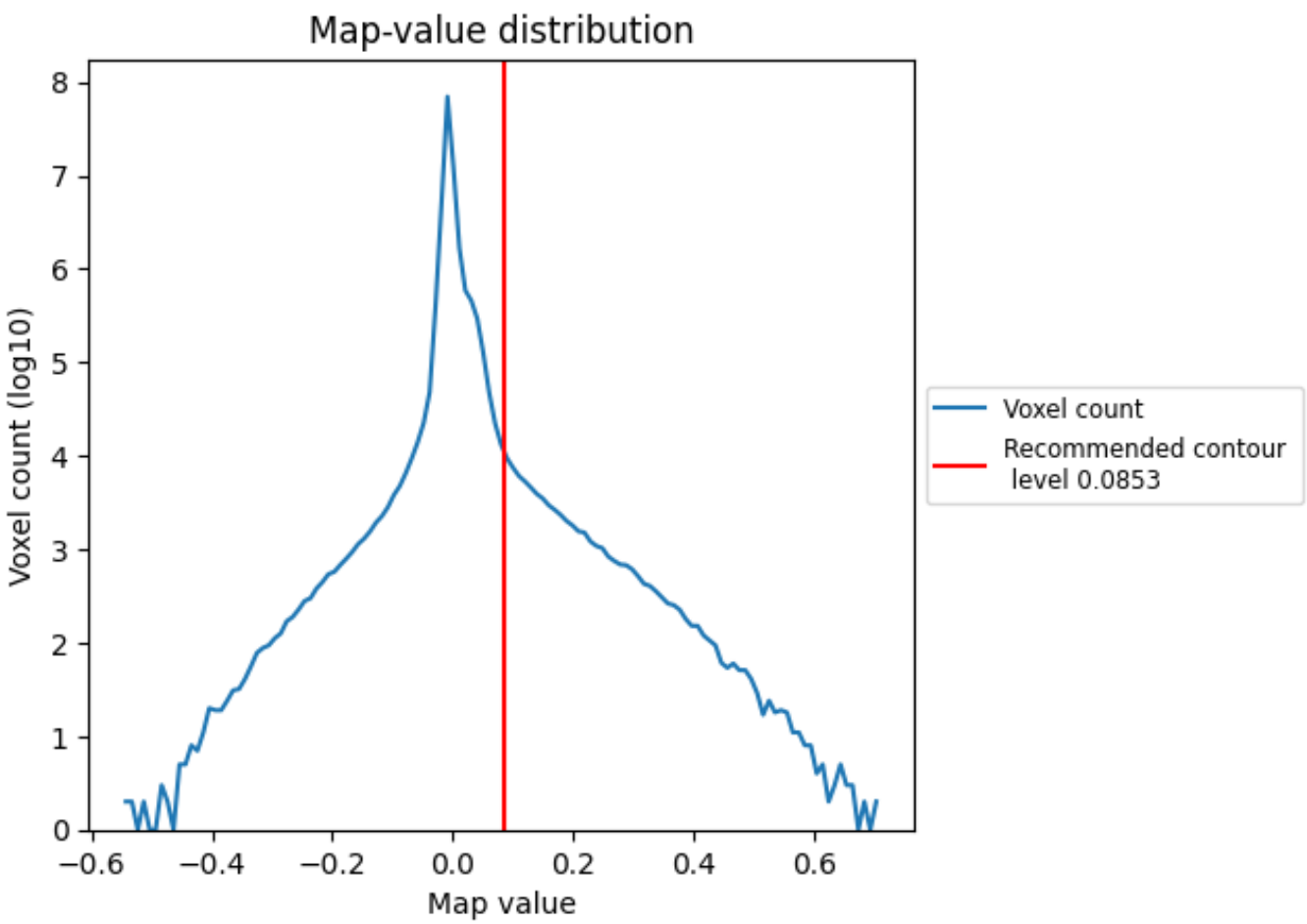
6.6 Mask visualisation (i)

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

7 Map analysis (i)

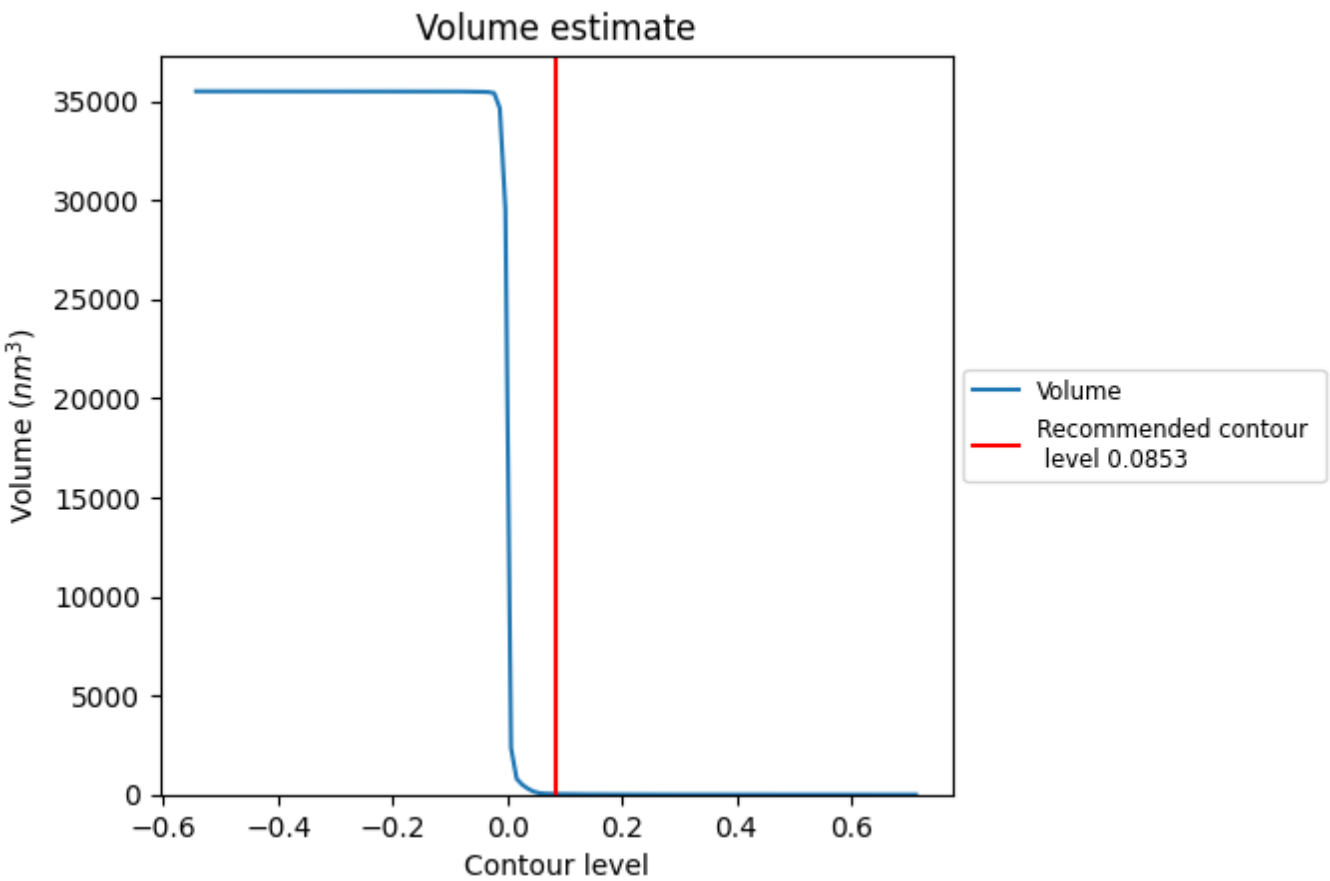
This section contains the results of statistical analysis of the map.

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.

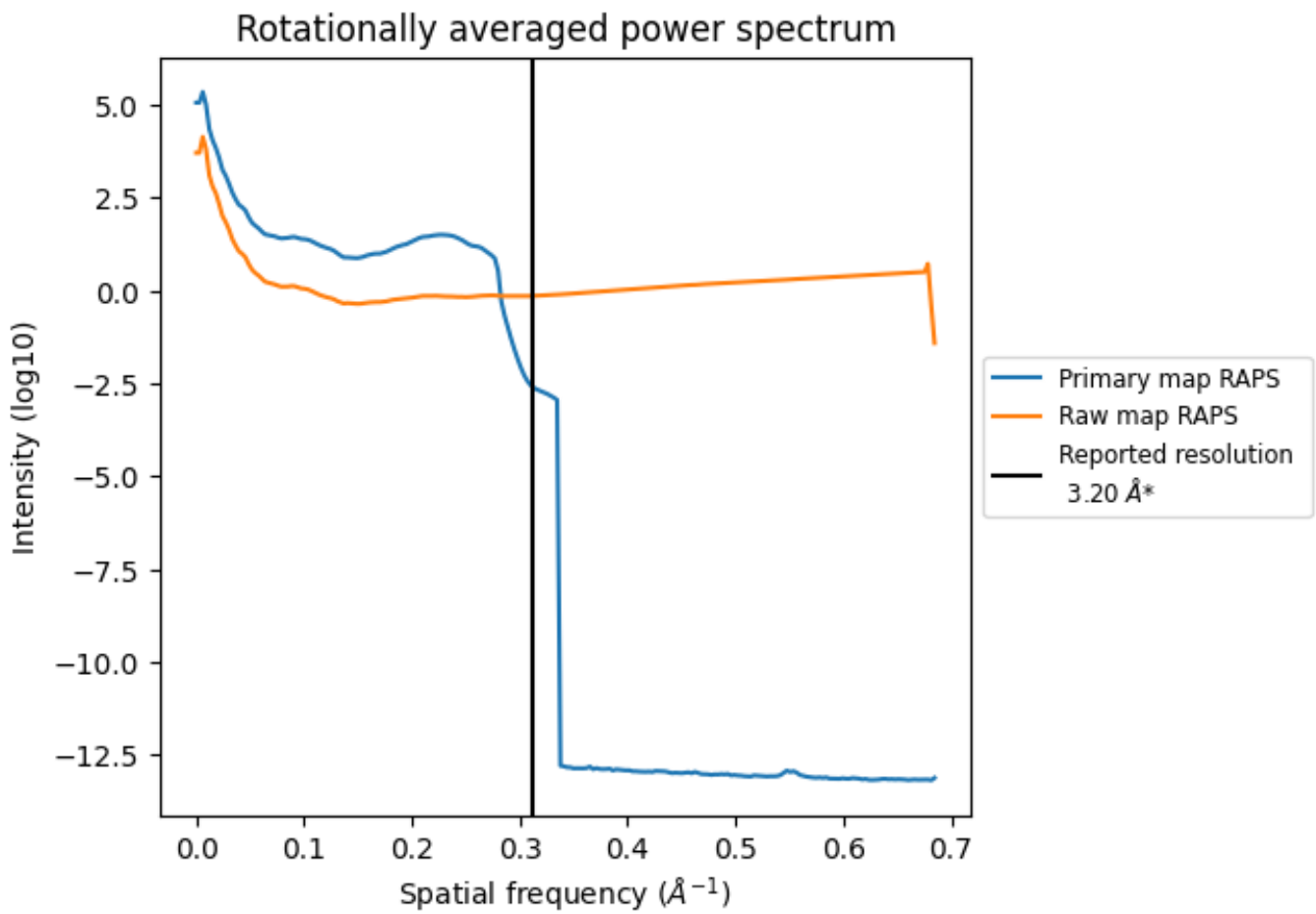
7.2 Volume estimate (i)



The volume at the recommended contour level is 28 nm^3; this corresponds to an approximate mass of 25 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)

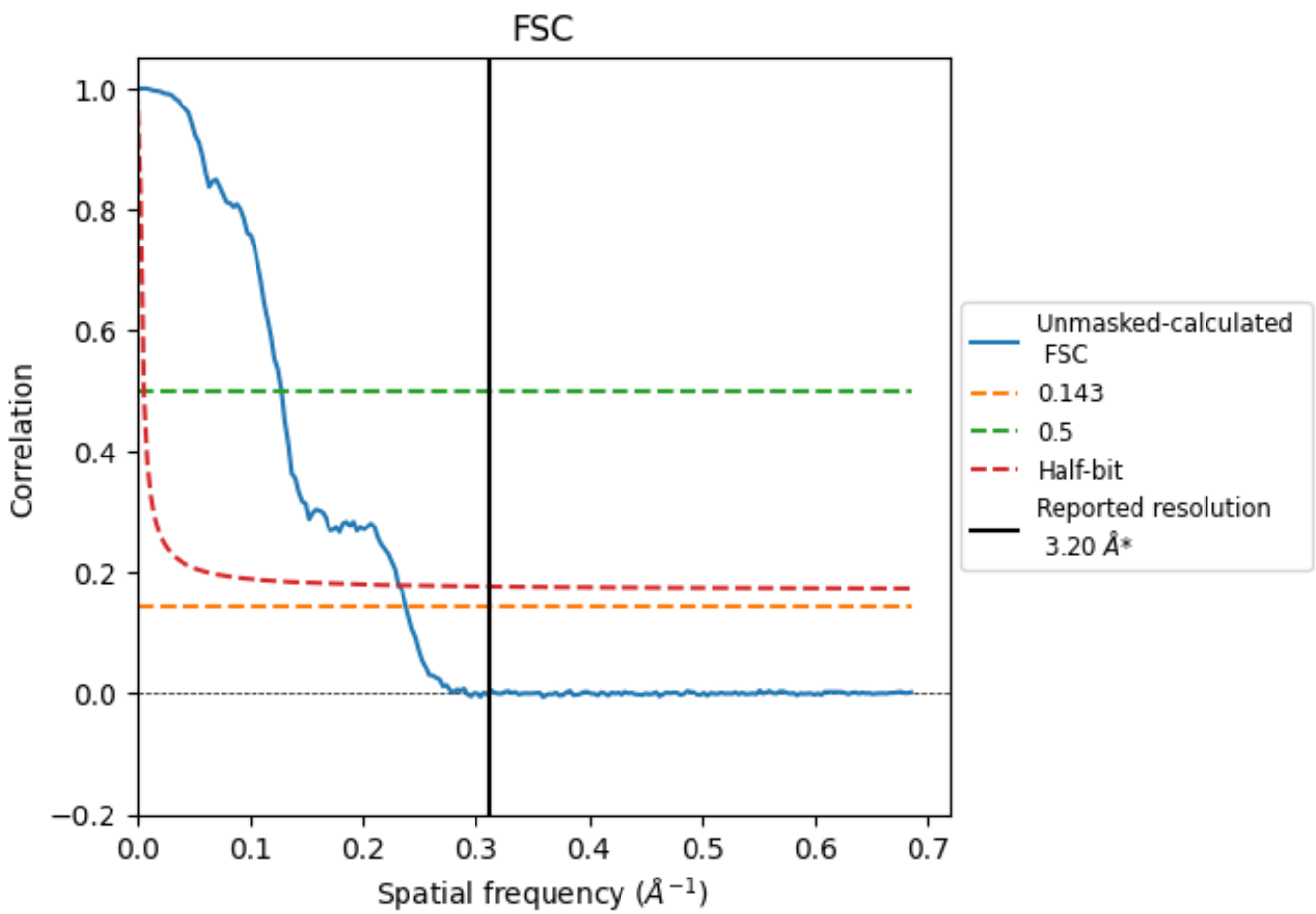


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

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 0.312 Å^{-1}

8.2 Resolution estimates (i)

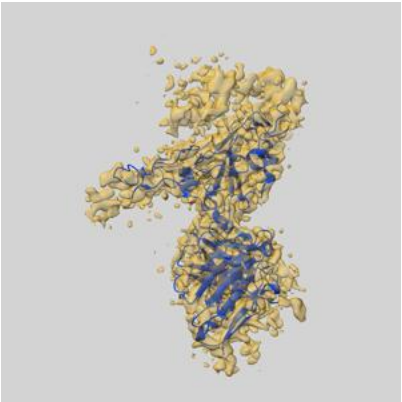
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.20	7.82	4.33

*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 4.20 differs from the reported value 3.2 by more than 10 %

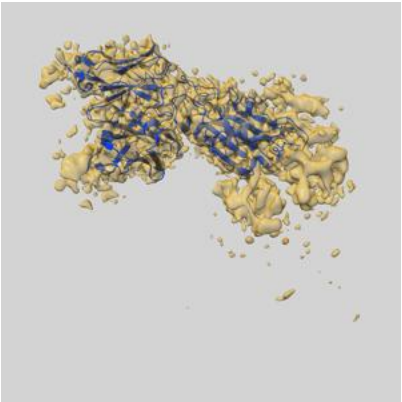
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-58749 and PDB model 32AJ. Per-residue inclusion information can be found in section 3 on page 5.

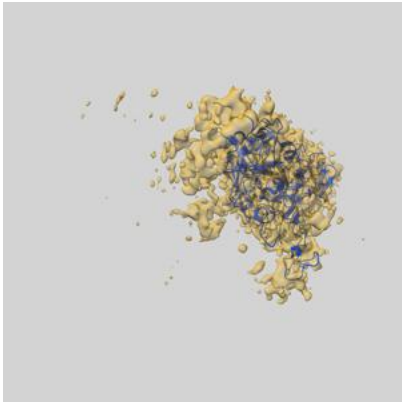
9.1 Map-model overlay (i)



X



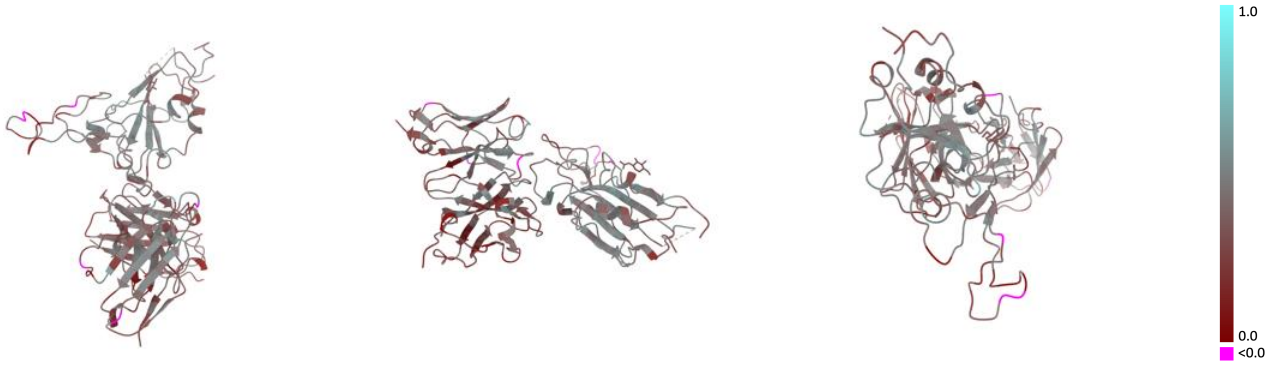
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0853 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.

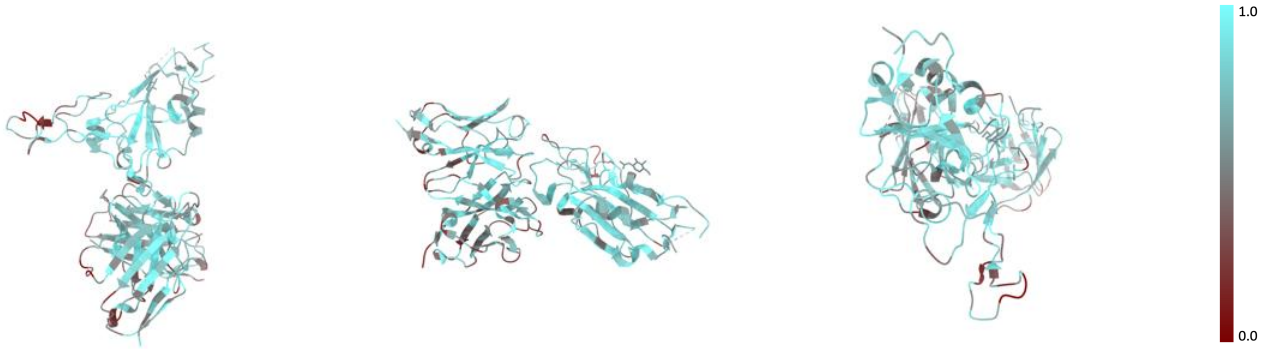
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

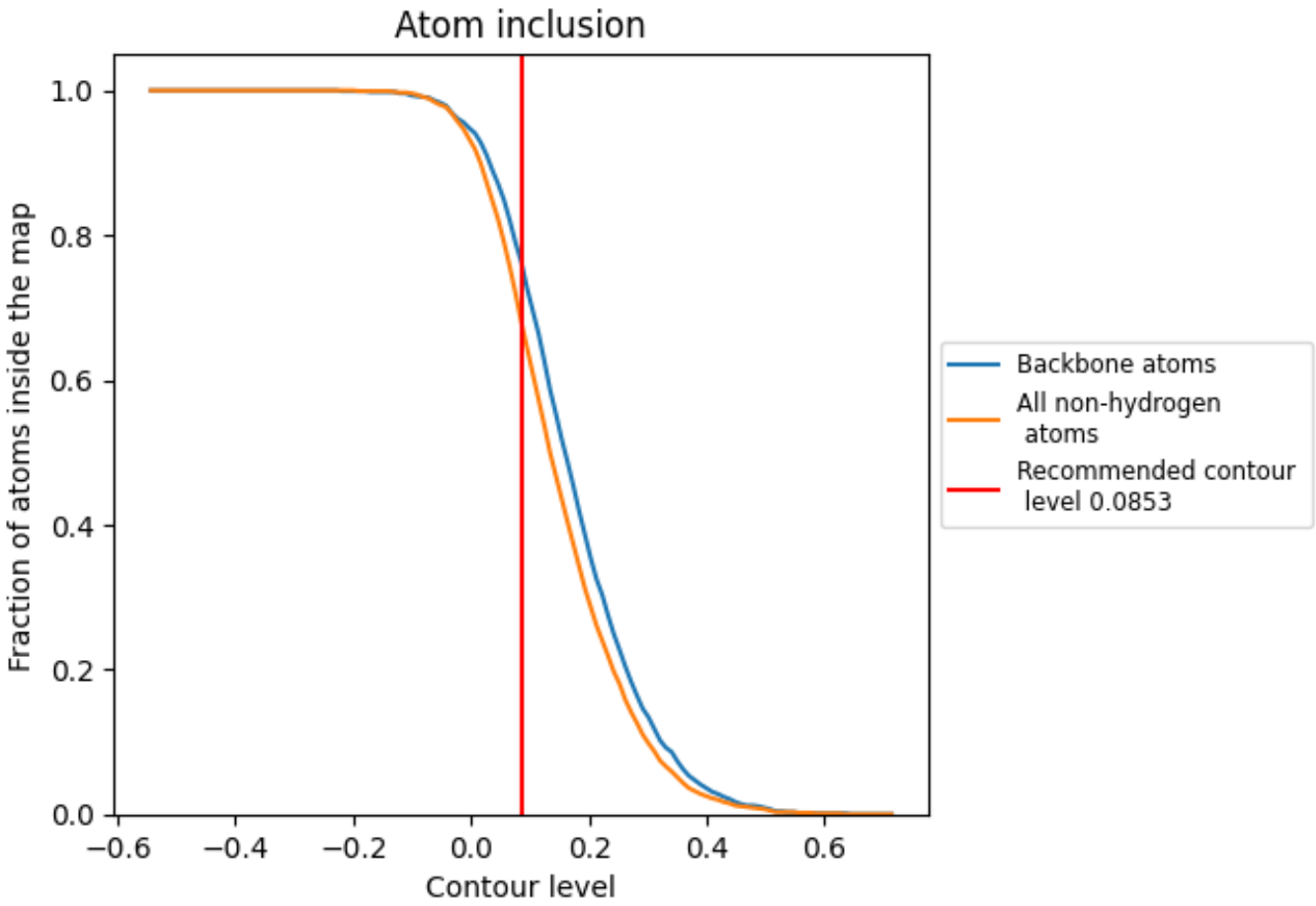
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.0853).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0853) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6800	0.3740
A	0.7160	0.4100
H	0.6260	0.3160
L	0.6730	0.3730