Full wwPDB EM Validation Report ⓘ

Apr 28, 2023 – 11:42 AM EDT

PDB ID	:	8SNR
EMDB ID	:	EMD-40632
Title	:	Nucleocapsid protein from SARS-CoV-2, flexible conformation 1
Deposited on	:	2023-04-27
Resolution	:	4.40 Å(reported)
Based on initial model	:	.

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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:

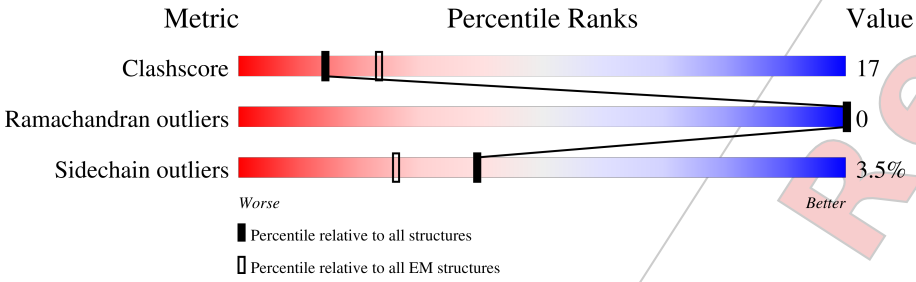
EMDB validation analysis	:	0.0.1.dev50
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

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 4.40 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 >=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	A	419	5% 68% 30%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 6375 atoms, of which 3161 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 Nucleoprotein.

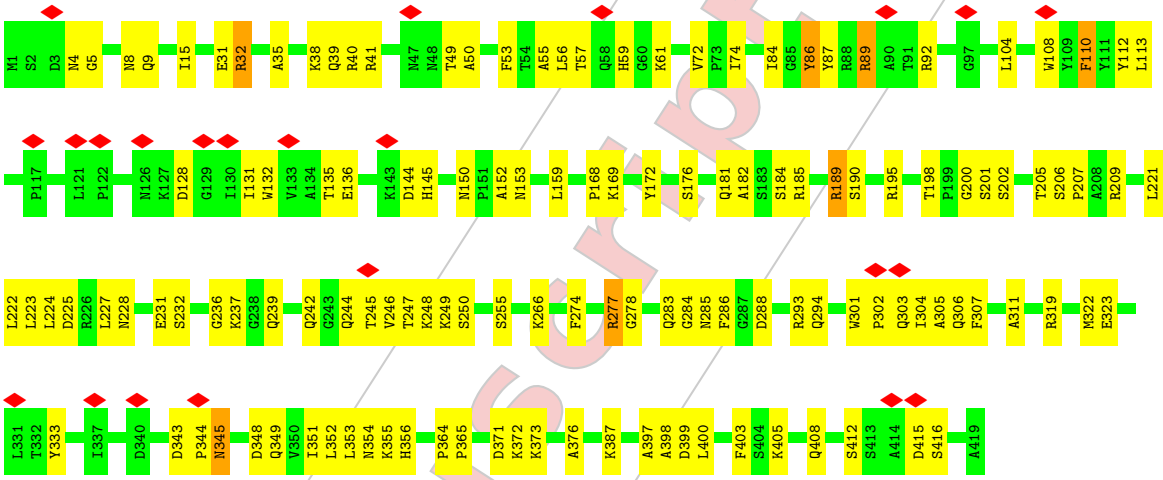
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	419	6375	1971	3161	607	629	7	0	0

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: Nucleoprotein

Chain A:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	20000	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS TALOS F200C	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	45000	Depositor
Image detector	DIRECT ELECTRON DE-12 (4k x 3k)	Depositor
Maximum map value	12.115	Depositor
Minimum map value	-1.173	Depositor
Average map value	0.047	Depositor
Map value standard deviation	0.984	Depositor
Recommended contour level	0.75	Depositor
Map size (Å)	94.35, 88.8, 96.200005	wwPDB
Map dimensions	51, 48, 52	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.85, 1.85, 1.8500001	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	0.27	0/3279	0.65	0/4422

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	245	THR	Peptide

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	3214	3161	3161	110	0
All	All	3214	3161	3161	110	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 17.

All (110) 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:31:GLU:OE1	1:A:35:ALA:CB	1.96	1.13
1:A:31:GLU:OE1	1:A:35:ALA:HB3	1.59	0.99
1:A:31:GLU:OE1	1:A:35:ALA:HB2	1.67	0.93
1:A:223:LEU:HD21	1:A:227:LEU:HD12	1.50	0.91
1:A:145:HIS:HB3	1:A:150:ASN:OD1	1.74	0.88
1:A:113:LEU:HD12	1:A:113:LEU:O	1.74	0.86
1:A:136:GLU:N	1:A:136:GLU:OE1	2.09	0.85
1:A:307:PHE:O	1:A:349:GLN:NE2	2.11	0.84
1:A:225:ASP:O	1:A:247:THR:HG21	1.81	0.80
1:A:408:GLN:O	1:A:408:GLN:NE2	2.22	0.72
1:A:74:ILE:O	1:A:74:ILE:HG22	1.93	0.69
1:A:266:LYS:O	1:A:311:ALA:HB3	1.95	0.66
1:A:319:ARG:O	1:A:333:TYR:OH	2.09	0.66
1:A:415:ASP:OD1	1:A:416:SER:N	2.32	0.62
1:A:201:SER:OG	1:A:205:THR:N	2.32	0.62
1:A:288:ASP:HA	1:A:352:LEU:HD22	1.82	0.61
1:A:113:LEU:O	1:A:113:LEU:CD1	2.49	0.60
1:A:306:GLN:OE1	1:A:319:ARG:NE	2.36	0.58
1:A:41:ARG:NH1	1:A:144:ASP:OD2	2.36	0.58
1:A:89:ARG:NE	1:A:128:ASP:O	2.30	0.58
1:A:239:GLN:N	1:A:239:GLN:OE1	2.37	0.58
1:A:242:GLN:O	1:A:244:GLN:NE2	2.37	0.57
1:A:56:LEU:HD23	1:A:108:TRP:CZ3	2.39	0.57
1:A:246:VAL:HG22	1:A:247:THR:H	1.70	0.57
1:A:152:ALA:O	1:A:153:ASN:ND2	2.37	0.56
1:A:322:MET:SD	1:A:322:MET:N	2.78	0.56
1:A:236:GLY:O	1:A:239:GLN:NE2	2.39	0.56
1:A:159:LEU:H	1:A:159:LEU:HD12	1.72	0.54
1:A:159:LEU:HD13	1:A:176:SER:HA	1.88	0.54
1:A:9:GLN:OE1	1:A:9:GLN:N	2.39	0.54
1:A:5:GLY:O	1:A:8:ASN:ND2	2.37	0.53
1:A:56:LEU:O	1:A:57:THR:OG1	2.22	0.53
1:A:351:ILE:O	1:A:354:ASN:OD1	2.28	0.52
1:A:189:ARG:HE	1:A:247:THR:HB	1.74	0.52
1:A:206:SER:N	1:A:207:PRO:CD	2.73	0.51
1:A:182:ALA:HA	1:A:249:LYS:H	1.76	0.51
1:A:184:SER:O	1:A:248:LYS:HB3	2.10	0.50
1:A:399:ASP:OD1	1:A:400:LEU:N	2.45	0.50
1:A:224:LEU:HD12	1:A:228:ASN:OD1	2.12	0.49
1:A:135:THR:HB	1:A:136:GLU:OE1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:ALA:HA	1:A:399:ASP:HB3	1.95	0.48
1:A:349:GLN:OE1	1:A:352:LEU:HD12	2.13	0.48
1:A:184:SER:CB	1:A:246:VAL:HG13	2.43	0.48
1:A:181:GLN:HB3	1:A:222:LEU:HD21	1.95	0.48
1:A:87:TYR:CG	1:A:131:ILE:O	2.67	0.48
1:A:185:ARG:O	1:A:248:LYS:N	2.46	0.48
1:A:364:PRO:HB2	1:A:365:PRO:HD3	1.96	0.48
1:A:283:GLN:NE2	1:A:323:GLU:OE1	2.47	0.47
1:A:303:GLN:NE2	1:A:345:ASN:OD1	2.46	0.47
1:A:354:ASN:OD1	1:A:355:LYS:N	2.47	0.47
1:A:249:LYS:HG2	1:A:250:SER:N	2.29	0.47
1:A:387:LYS:O	1:A:398:ALA:HB3	2.15	0.47
1:A:49:THR:HG22	1:A:50:ALA:N	2.30	0.47
1:A:184:SER:OG	1:A:185:ARG:N	2.46	0.47
1:A:223:LEU:O	1:A:223:LEU:HD23	2.15	0.47
1:A:198:THR:OG1	1:A:224:LEU:HA	2.15	0.46
1:A:15:ILE:HG13	1:A:15:ILE:O	2.16	0.46
1:A:224:LEU:O	1:A:228:ASN:HB2	2.16	0.46
1:A:144:ASP:O	1:A:144:ASP:OD1	2.32	0.46
1:A:184:SER:HG	1:A:185:ARG:H	1.63	0.46
1:A:4:ASN:HB2	1:A:8:ASN:ND2	2.31	0.46
1:A:86:TYR:CD1	1:A:87:TYR:N	2.83	0.46
1:A:195:ARG:HE	1:A:231:GLU:CD	2.20	0.45
1:A:293:ARG:HG3	1:A:294:GLN:H	1.80	0.45
1:A:349:GLN:O	1:A:353:LEU:HD13	2.17	0.45
1:A:371:ASP:OD1	1:A:372:LYS:N	2.50	0.45
1:A:184:SER:HB3	1:A:246:VAL:HG13	2.00	0.44
1:A:112:TYR:CG	1:A:136:GLU:OE2	2.71	0.44
1:A:278:GLY:O	1:A:284:GLY:HA2	2.17	0.44
1:A:412:SER:HA	1:A:416:SER:O	2.19	0.43
1:A:112:TYR:CB	1:A:136:GLU:OE2	2.66	0.43
1:A:181:GLN:O	1:A:222:LEU:HD11	2.17	0.43
1:A:348:ASP:O	1:A:352:LEU:HG	2.18	0.43
1:A:92:ARG:O	1:A:104:LEU:HD13	2.19	0.43
1:A:304:ILE:HD11	1:A:343:ASP:OD2	2.19	0.43
1:A:355:LYS:HA	1:A:405:LYS:HZ2	1.83	0.43
1:A:209:ARG:O	1:A:221:LEU:HB2	2.19	0.43
1:A:39:GLN:C	1:A:40:ARG:HE	2.22	0.42
1:A:74:ILE:O	1:A:74:ILE:CG2	2.64	0.42
1:A:32:ARG:O	1:A:32:ARG:HD3	2.19	0.42
1:A:38:LYS:O	1:A:40:ARG:NE	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:LYS:HG3	1:A:249:LYS:O	2.19	0.42
1:A:277:ARG:CZ	1:A:277:ARG:H	2.32	0.42
1:A:55:ALA:O	1:A:56:LEU:HD13	2.20	0.42
1:A:172:TYR:OH	1:A:200:GLY:O	2.34	0.42
1:A:209:ARG:O	1:A:255:SER:OG	2.25	0.42
1:A:354:ASN:OD1	1:A:354:ASN:C	2.57	0.42
1:A:301:TRP:N	1:A:302:PRO:CD	2.83	0.42
1:A:61:LYS:HE2	1:A:169:LYS:HB3	2.01	0.42
1:A:172:TYR:OH	1:A:201:SER:HA	2.20	0.42
1:A:190:SER:C	1:A:232:SER:HB3	2.41	0.41
1:A:225:ASP:HB3	1:A:248:LYS:O	2.20	0.41
1:A:84:ILE:O	1:A:84:ILE:HG22	2.20	0.41
1:A:304:ILE:CG2	1:A:305:ALA:N	2.83	0.41
1:A:72:VAL:HG23	1:A:74:ILE:HG13	2.03	0.41
1:A:364:PRO:CB	1:A:365:PRO:HD3	2.50	0.41
1:A:59:HIS:CD2	1:A:172:TYR:O	2.74	0.41
1:A:221:LEU:C	1:A:221:LEU:HD13	2.41	0.41
1:A:343:ASP:OD1	1:A:344:PRO:N	2.54	0.41
1:A:184:SER:O	1:A:248:LYS:CD	2.69	0.41
1:A:144:ASP:O	1:A:144:ASP:CG	2.60	0.40
1:A:168:PRO:O	1:A:202:SER:C	2.59	0.40
1:A:266:LYS:O	1:A:311:ALA:CB	2.68	0.40
1:A:181:GLN:NE2	1:A:248:LYS:HA	2.36	0.40
1:A:285:ASN:HB2	1:A:356:HIS:CB	2.51	0.40
1:A:225:ASP:O	1:A:247:THR:CG2	2.63	0.40
1:A:355:LYS:HA	1:A:405:LYS:NZ	2.37	0.40
1:A:373:LYS:HE3	1:A:397:ALA:HB3	2.03	0.40
1:A:110:PHE:CD1	1:A:110:PHE:C	2.94	0.40
1:A:236:GLY:C	1:A:237:LYS:HD3	2.41	0.40

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	417/419 (100%)	333 (80%)	84 (20%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	339/339 (100%)	327 (96%)	12 (4%)	36 60

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ARG
1	A	53	PHE
1	A	86	TYR
1	A	89	ARG
1	A	110	PHE
1	A	132	TRP
1	A	189	ARG
1	A	274	PHE
1	A	277	ARG
1	A	286	PHE
1	A	345	ASN
1	A	403	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

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 monosaccharides 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 (i)

There are no chain breaks in this entry.

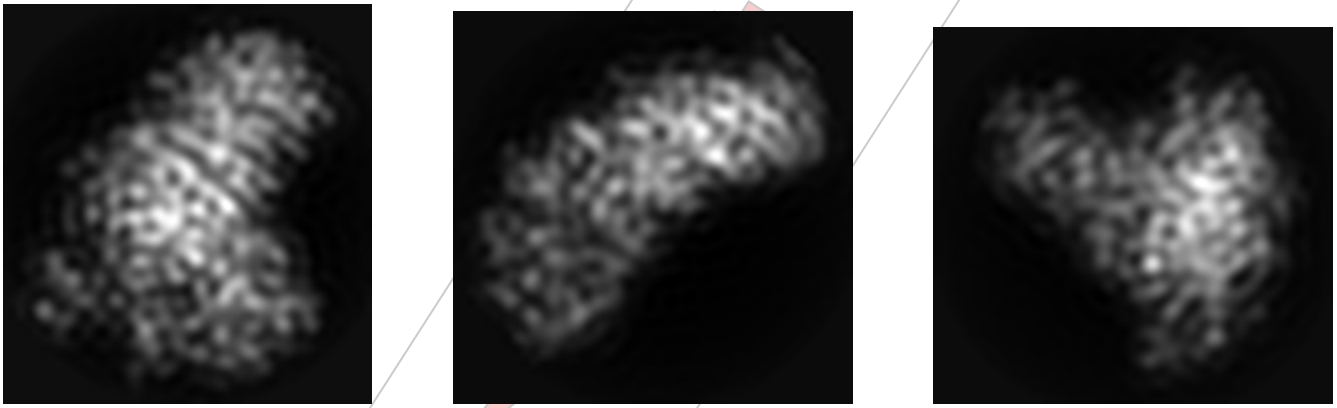
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-40632. 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.

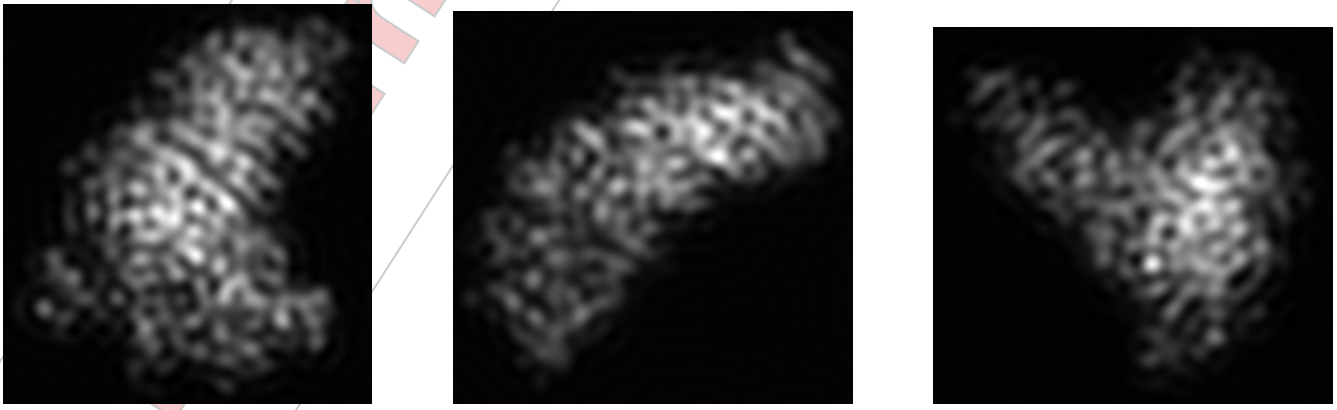
6.1 Orthogonal projections

6.1.1 Primary map



X Y Z

6.1.2 Raw map

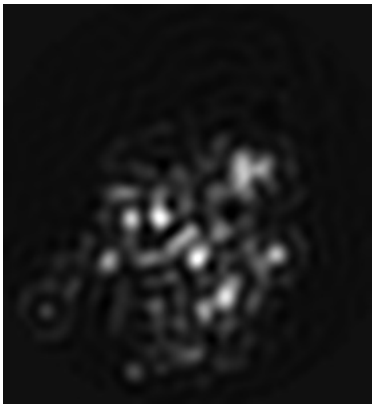


X Y Z

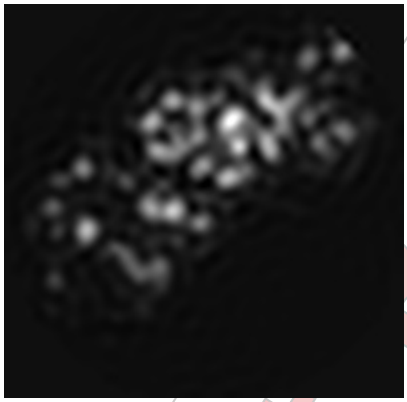
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

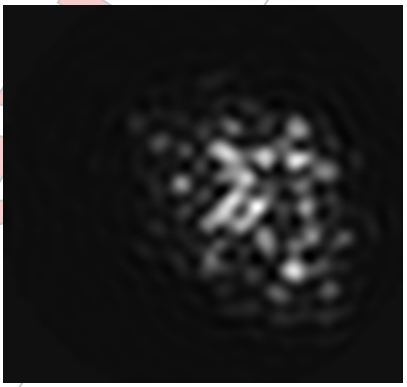
6.2.1 Primary map



X Index: 25

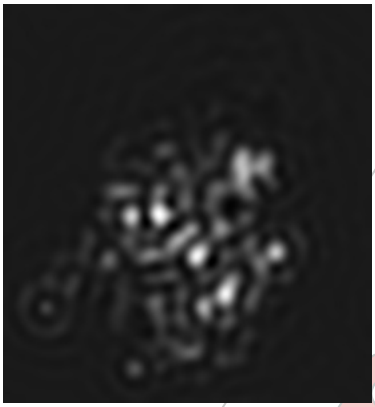


Y Index: 24

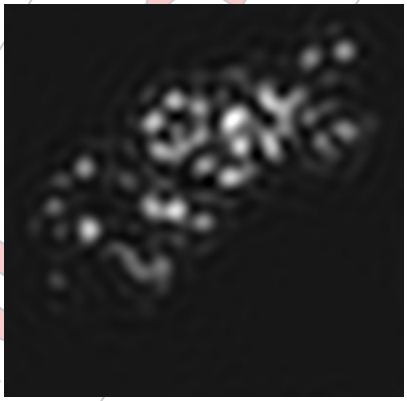


Z Index: 26

6.2.2 Raw map



X Index: 25



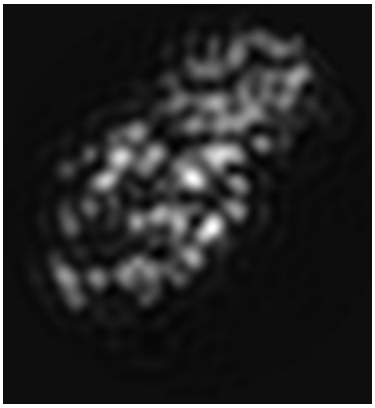
Y Index: 24

Z Index: 26

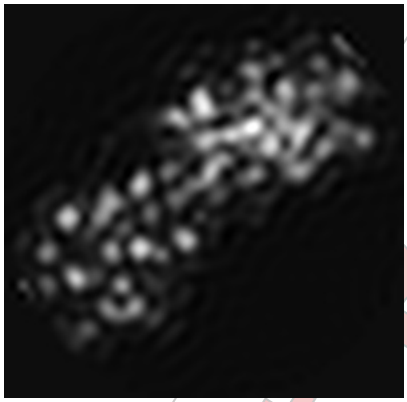
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

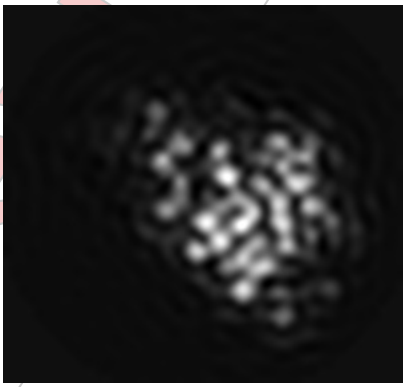
6.3.1 Primary map



X Index: 35

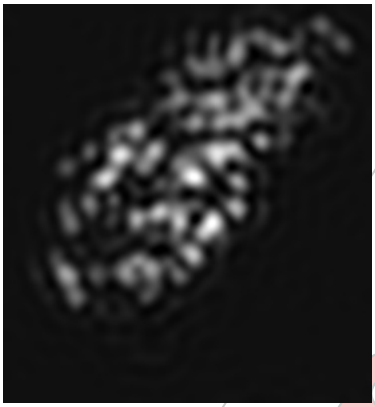


Y Index: 28

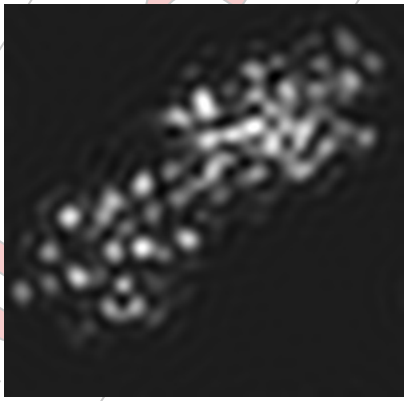


Z Index: 24

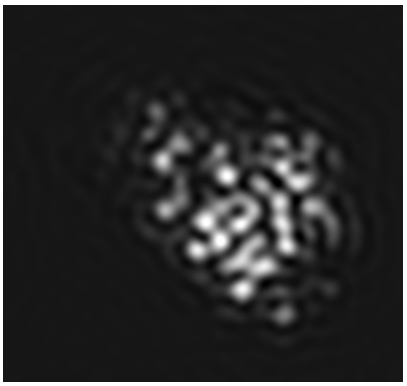
6.3.2 Raw map



X Index: 35



Y Index: 28

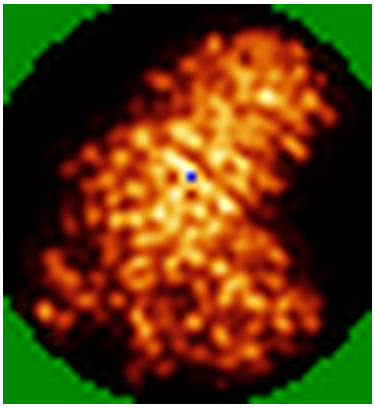


Z Index: 24

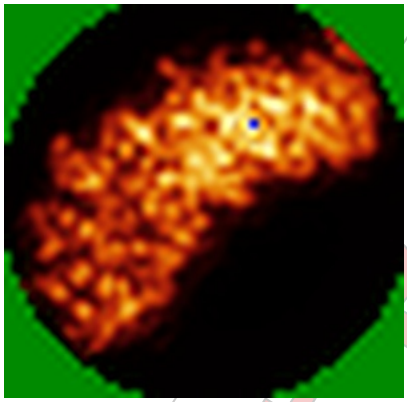
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color)

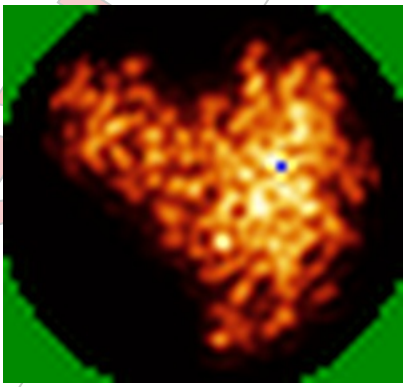
6.4.1 Primary map



X

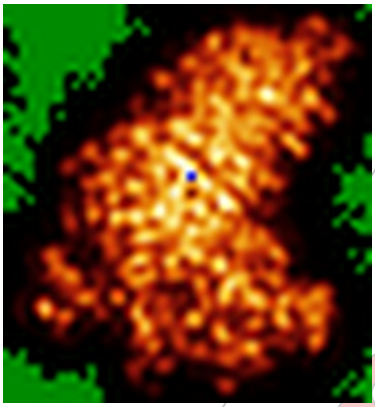


Y

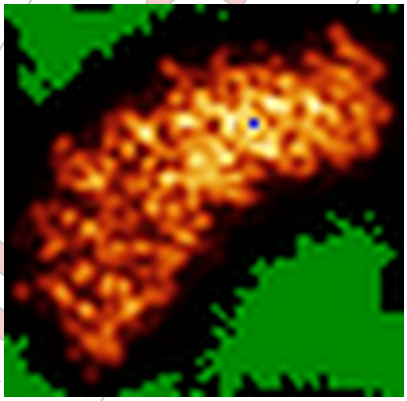


Z

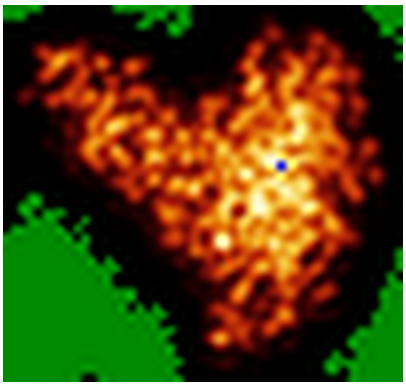
6.4.2 Raw map



X



Y

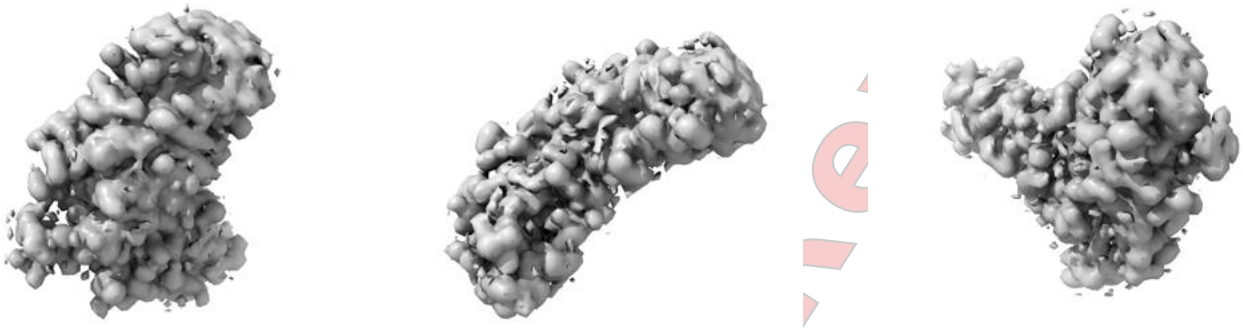


Z

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)

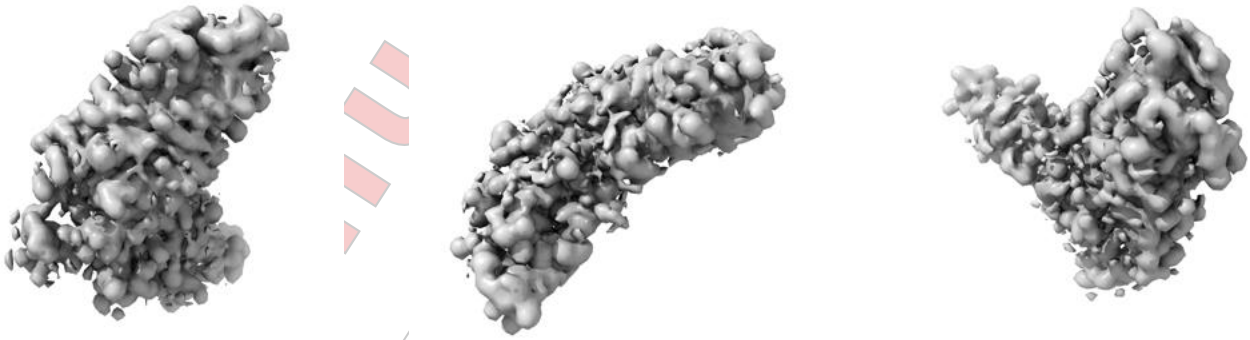
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.75. 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.

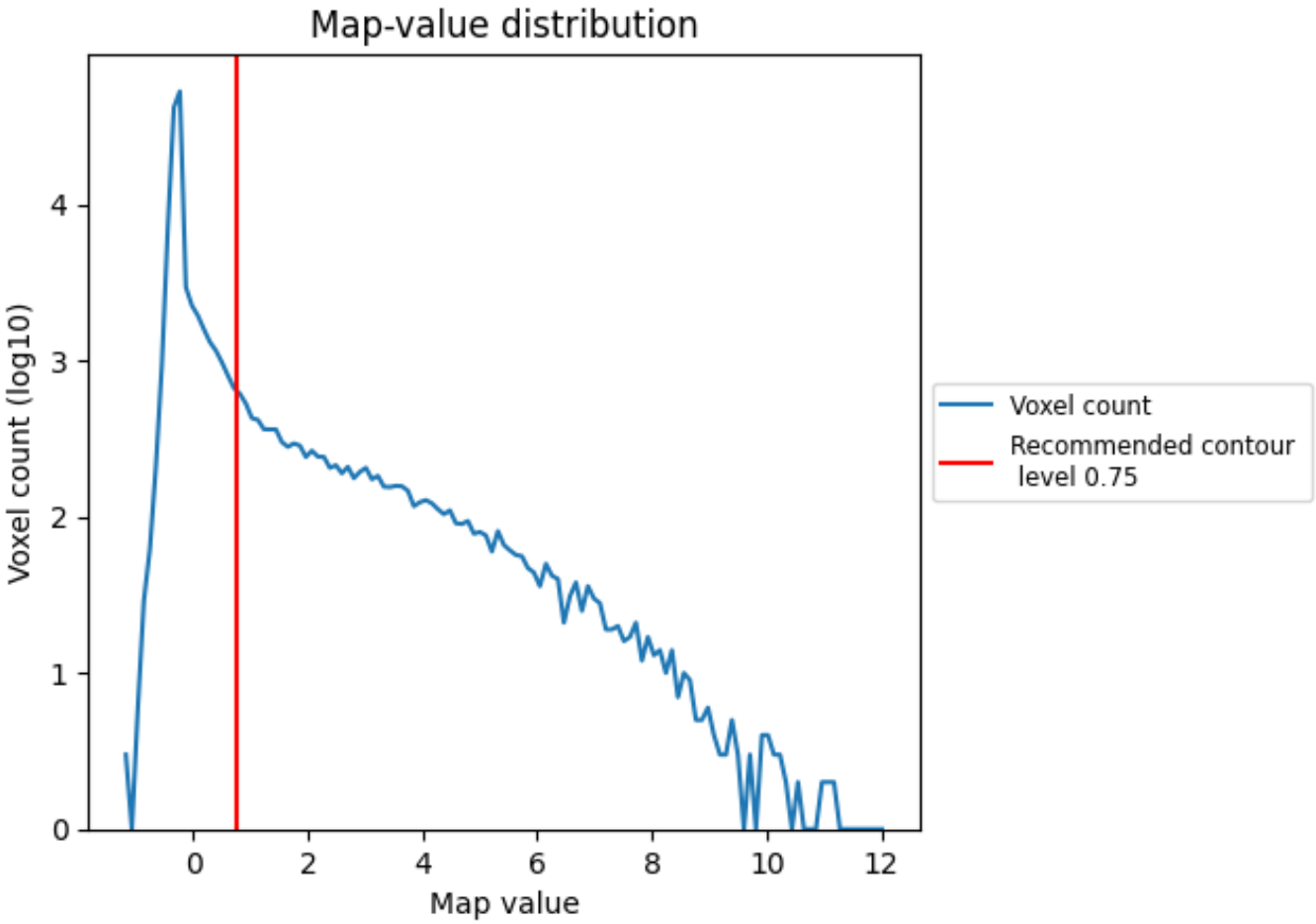
6.6 Mask visualisation (i)

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

7 Map analysis

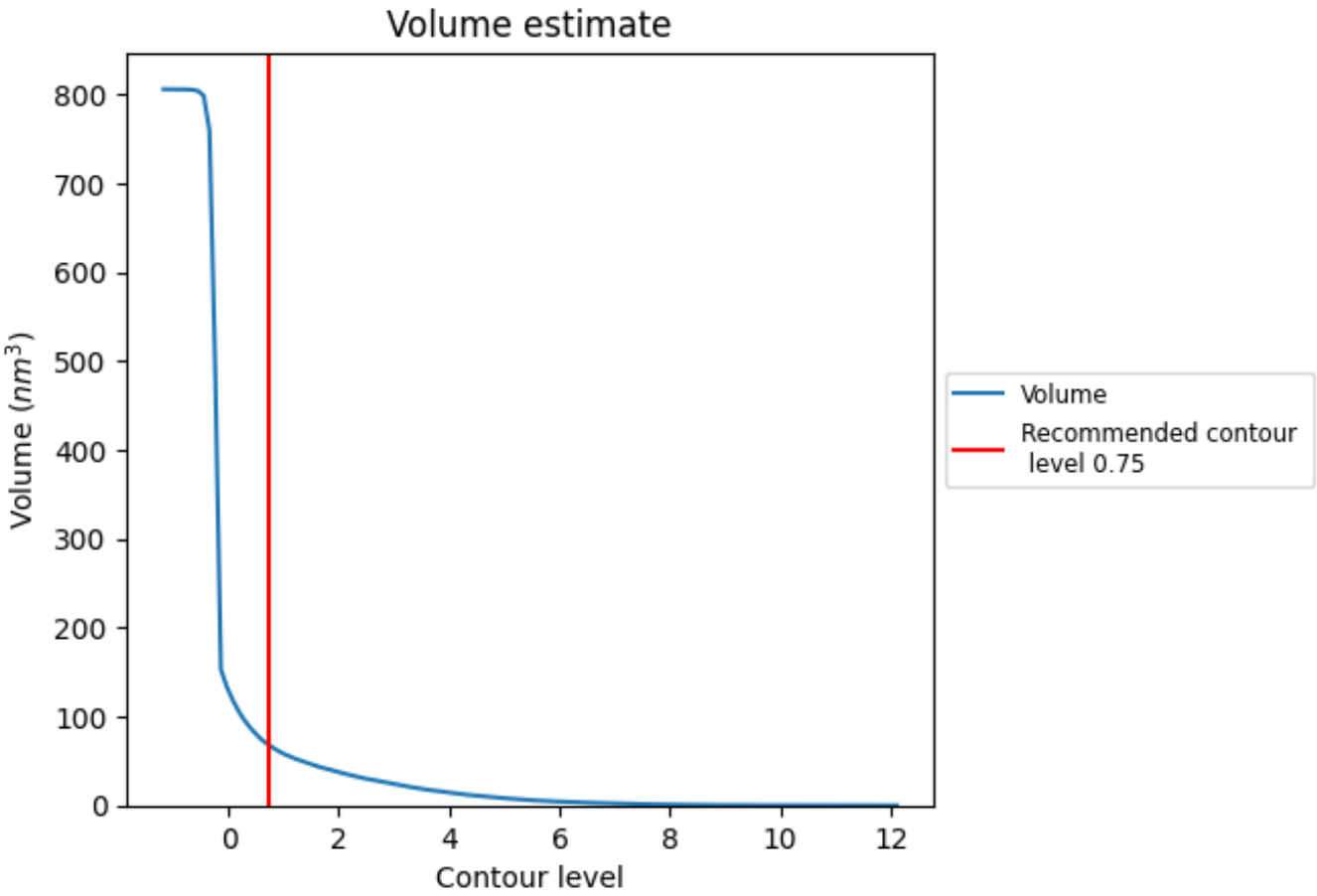
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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 67 nm^3; this corresponds to an approximate mass of 61 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.

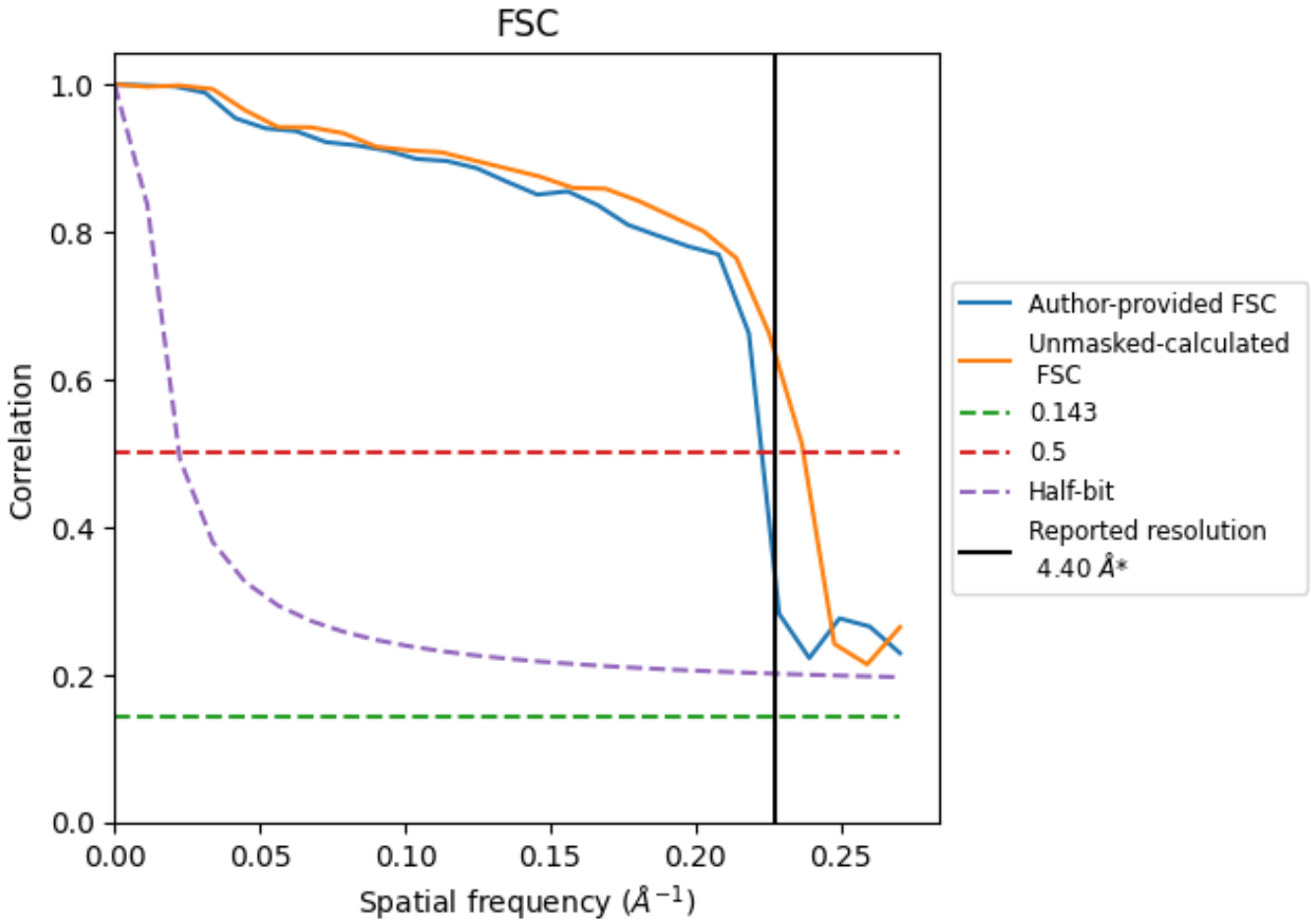
7.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.227 Å^{-1}

8.2 Resolution estimates (i)

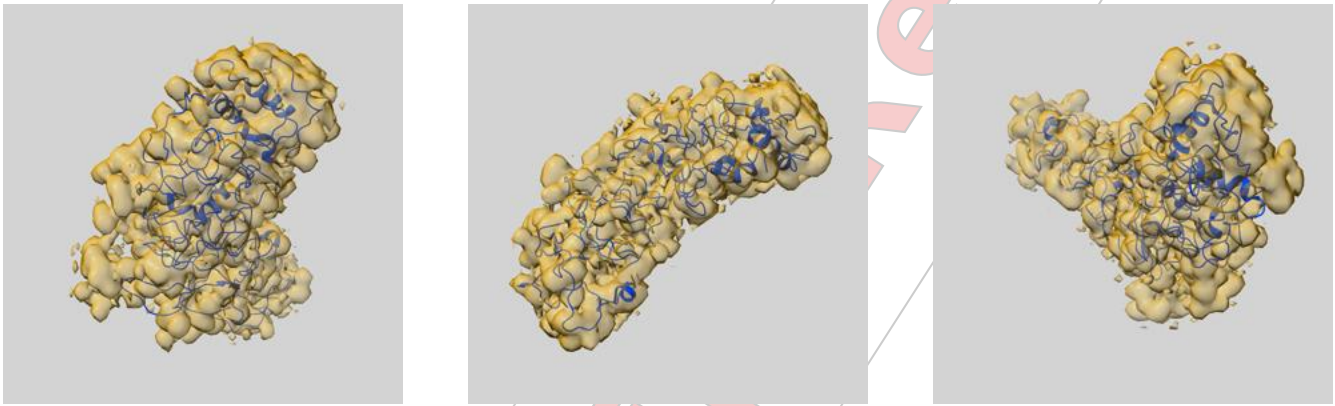
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	4.40	-
Author-provided FSC curve	-	4.49	-
Unmasked-calculated*	-	4.22	-

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

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-40632 and PDB model 8SNR. Per-residue inclusion information can be found in section 3 on page 4.

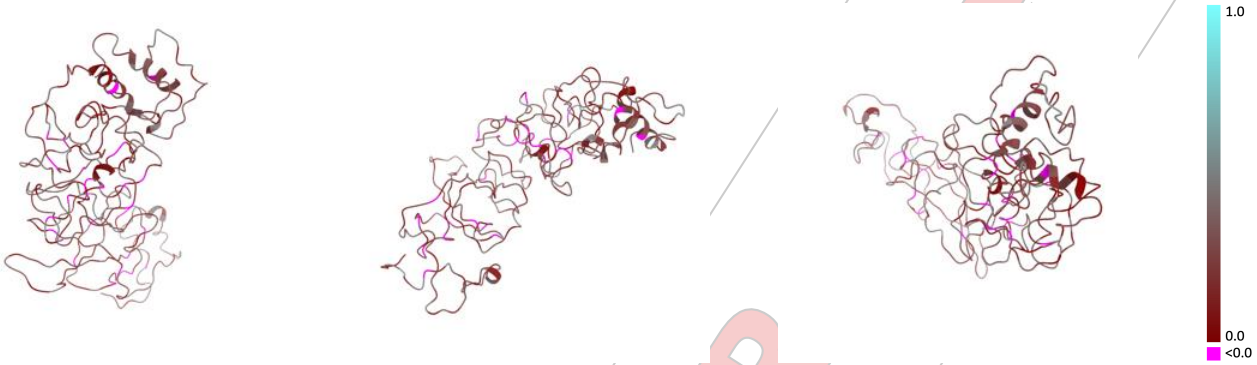
9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.75 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.

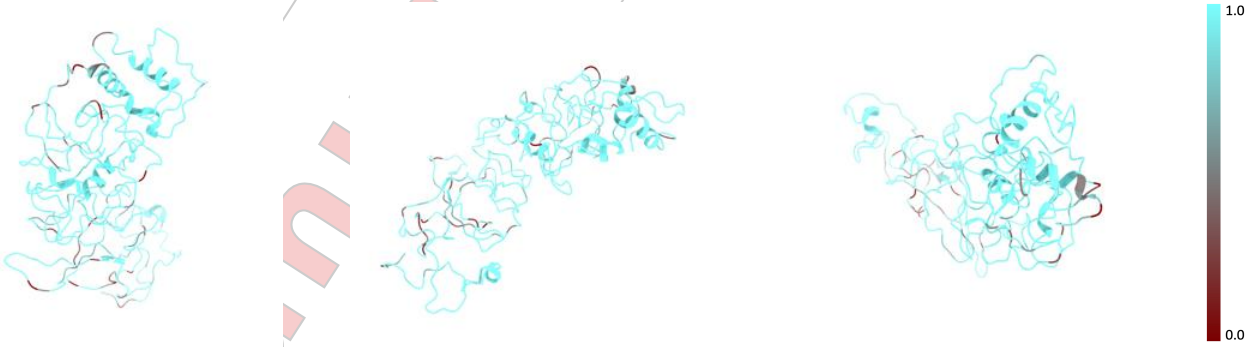
9.2 Q-score mapped to coordinate model



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.

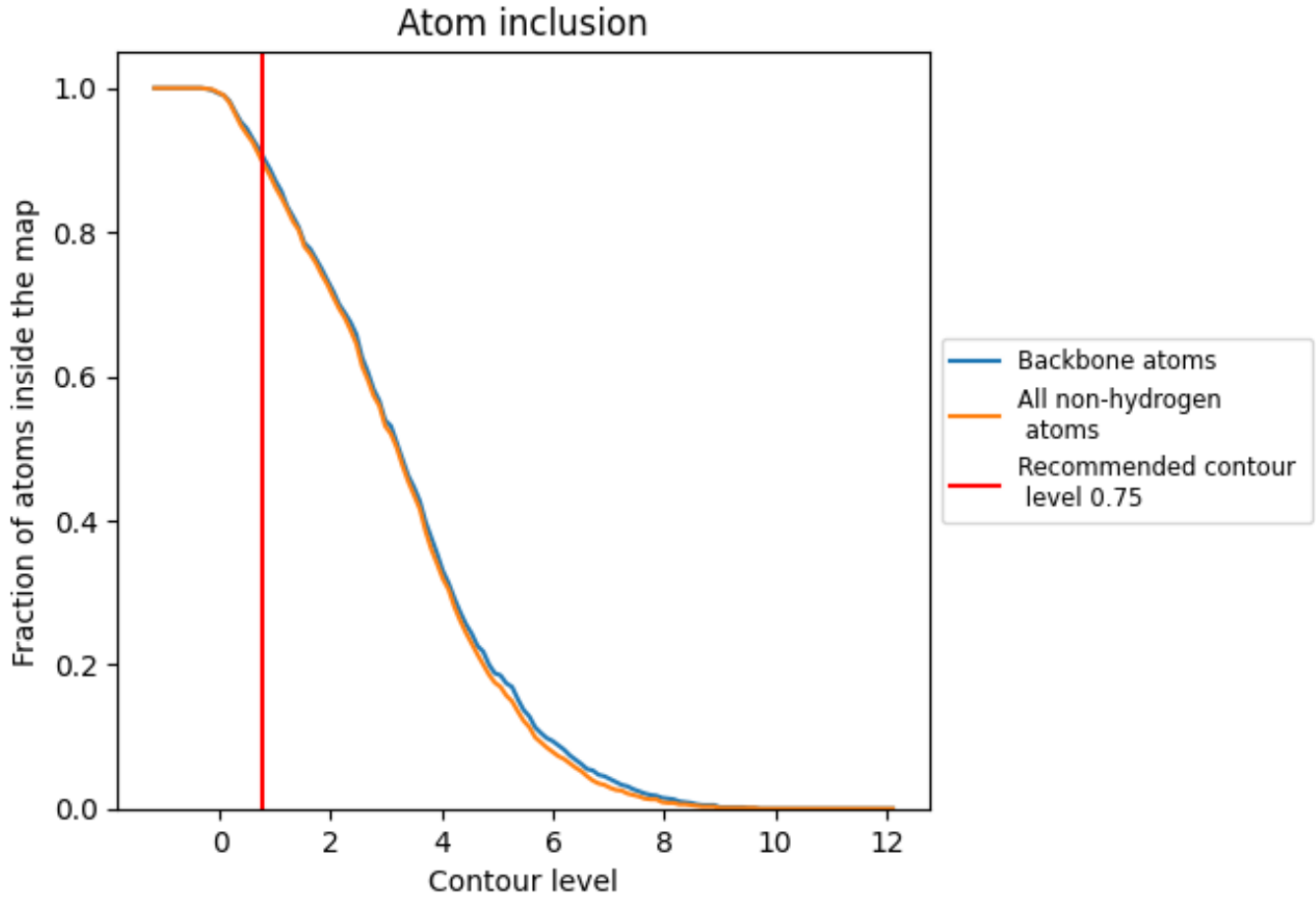
9.3 Atom inclusion mapped to coordinate model



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 (0.75).

9.4 Atom inclusion



At the recommended contour level, 91% of all backbone atoms, 90% 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 (0.75) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9010	0.2540
A	0.9020	0.2540

Full wwPDB EM Validation Report ⓘ

Apr 28, 2023 – 11:34 AM EDT

PDB ID	:	8SNS
EMDB ID	:	EMD-40633
Title	:	Nucleocapsid protein from SARS-CoV-2, flexible conformation 2
Deposited on	:	2023-04-27
Resolution	:	4.40 Å(reported)
Based on initial model	:	.

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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:

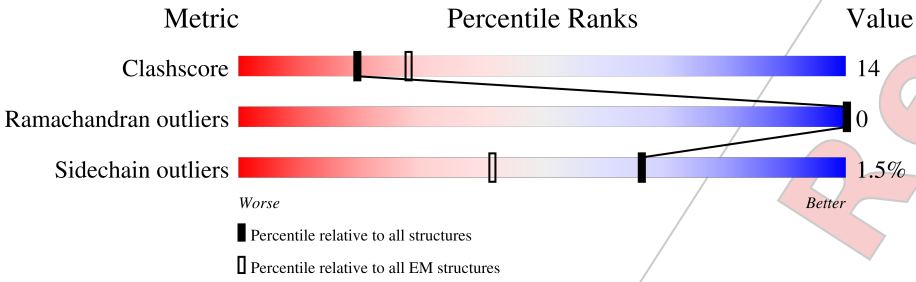
EMDB validation analysis	:	0.0.1.dev50
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

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 4.40 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 >=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	A	419	11% 70% 28%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6230 atoms, of which 3091 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 Nucleoprotein.

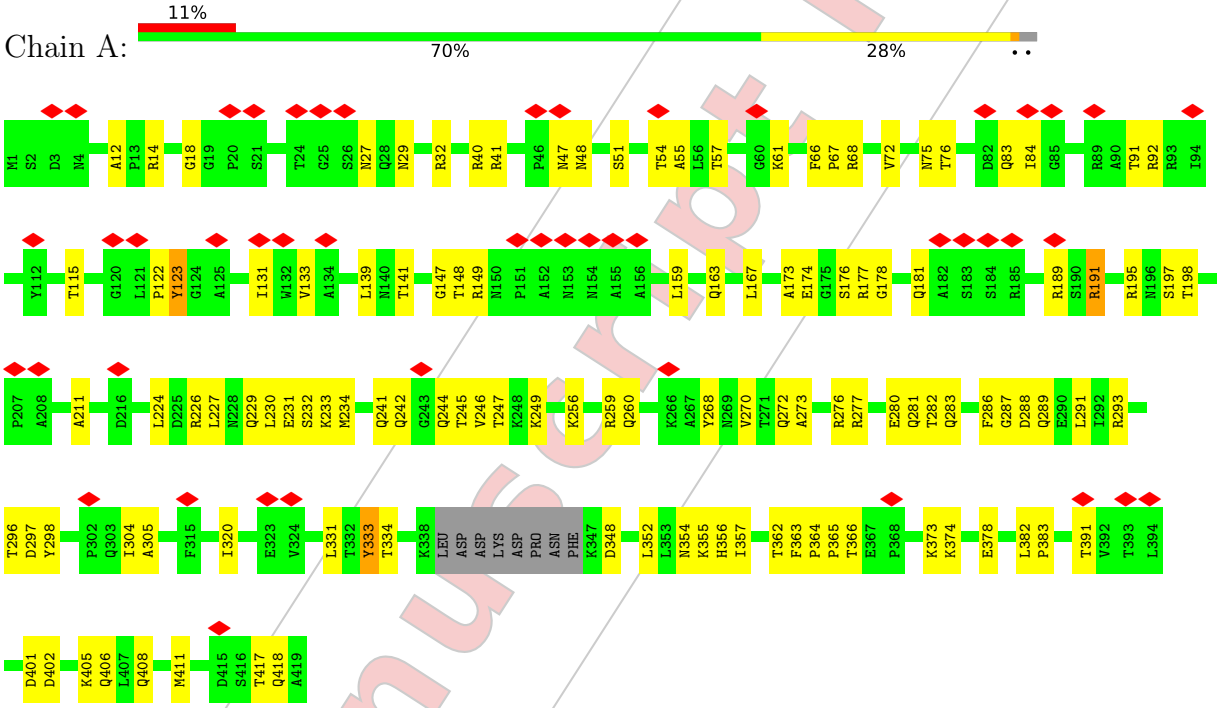
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	411	6230	1923	3091	596	613	7	0	1

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: Nucleoprotein

Chain A:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	20000	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS TALOS F200C	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	45000	Depositor
Image detector	DIRECT ELECTRON DE-12 (4k x 3k)	Depositor
Maximum map value	12.115	Depositor
Minimum map value	-1.173	Depositor
Average map value	0.047	Depositor
Map value standard deviation	0.984	Depositor
Recommended contour level	0.75	Depositor
Map size (Å)	94.35, 88.8, 96.200005	wwPDB
Map dimensions	51, 48, 52	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.85, 1.85, 1.8500001	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	0.39	2/3201 (0.1%)	0.62	3/4316 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	67	PRO	CG-CD	-14.36	1.03	1.50
1	A	67	PRO	N-CD	7.80	1.58	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	67	PRO	N-CD-CG	-14.73	81.10	103.20
1	A	67	PRO	CA-N-CD	-11.07	96.00	111.50
1	A	67	PRO	CA-CB-CG	-8.16	88.50	104.00

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	3139	3091	3089	87	0
All	All	3139	3091	3089	87	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 14.

All (87) 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:195:ARG:O	1:A:195:ARG:NE	2.08	0.85
1:A:277:ARG:NH2	1:A:287:GLY:O	2.11	0.84
1:A:66:PHE:O	1:A:68:ARG:NH2	2.11	0.84
1:A:91:THR:OG1	1:A:92:ARG:NH2	2.15	0.80
1:A:260:GLN:NE2	1:A:331:LEU:O	2.15	0.79
1:A:18:GLY:O	1:A:32:ARG:NH2	2.16	0.79
1:A:198:THR:O	1:A:259:ARG:NH1	2.17	0.77
1:A:378:GLU:OE2	1:A:406:GLN:NE2	2.19	0.76
1:A:198:THR:HG21	1:A:231:GLU:HB2	1.69	0.75
1:A:363:PHE:O	1:A:366:THR:OG1	2.05	0.74
1:A:354:ASN:O	1:A:408:GLN:NE2	2.21	0.73
1:A:231:GLU:OE2	1:A:283:GLN:NE2	2.22	0.72
1:A:41:ARG:NE	1:A:47:ASN:OD1	2.21	0.72
1:A:181:GLN:OE1	1:A:181:GLN:N	2.23	0.71
1:A:163:GLN:HG3	1:A:230:LEU:HD23	1.73	0.70
1:A:12:ALA:O	1:A:14:ARG:NE	2.25	0.69
1:A:191:ARG:NH2	1:A:230:LEU:O	2.24	0.69
1:A:241:GLN:N	1:A:241:GLN:OE1	2.29	0.65
1:A:373:LYS:NZ	1:A:402:ASP:OD2	2.30	0.65
1:A:277:ARG:NH2	1:A:286:PHE:O	2.30	0.63
1:A:320:ILE:HA	1:A:331:LEU:HD11	1.81	0.62
1:A:178:GLY:O	1:A:249:LYS:NZ	2.33	0.62
1:A:362:THR:OG1	1:A:405:LYS:NZ	2.33	0.61
1:A:197:SER:O	1:A:282:THR:HG21	2.02	0.60
1:A:181:GLN:O	1:A:249:LYS:NZ	2.32	0.59
1:A:224:LEU:HD13	1:A:256:LYS:HA	1.85	0.59
1:A:270:VAL:HG11	1:A:277:ARG:HD2	1.85	0.58
1:A:176:SER:OG	1:A:226:ARG:NH1	2.37	0.58
1:A:277:ARG:NH1	1:A:289:GLN:OE1	2.37	0.57
1:A:411:MET:SD	1:A:411:MET:N	2.78	0.57
1:A:27:ASN:OD1	1:A:29:ASN:ND2	2.37	0.57
1:A:242:GLN:OE1	1:A:276:ARG:NH2	2.38	0.56
1:A:167:LEU:HD12	1:A:173:ALA:HA	1.88	0.56
1:A:177:ARG:O	1:A:181:GLN:NE2	2.37	0.56
1:A:297:ASP:N	1:A:297:ASP:OD1	2.39	0.55
1:A:174:GLU:N	1:A:174:GLU:OE1	2.40	0.54
1:A:391:THR:HG23	1:A:391:THR:O	2.07	0.54
1:A:357:ILE:O	1:A:408:GLN:NE2	2.36	0.54
1:A:401:ASP:OD1	1:A:405:LYS:NZ	2.27	0.52
1:A:333:TYR:O	1:A:334:THR:OG1	2.26	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:VAL:HG21	1:A:83:GLN:HG2	1.91	0.51
1:A:61:LYS:O	1:A:61:LYS:HD3	2.11	0.51
1:A:282:THR:HG23	1:A:283:GLN:OE1	2.11	0.50
1:A:75:ASN:HD21	1:A:159:LEU:HD21	1.78	0.49
1:A:131:ILE:HG22	1:A:133:VAL:HG13	1.94	0.49
1:A:354:ASN:OD1	1:A:355:LYS:N	2.46	0.49
1:A:163:GLN:HG2	1:A:198:THR:HG22	1.94	0.48
1:A:76:THR:O	1:A:189:ARG:NH2	2.44	0.48
1:A:270:VAL:HA	1:A:273:ALA:HB3	1.95	0.48
1:A:57:THR:OG1	1:A:211:ALA:O	2.25	0.47
1:A:84:ILE:HD11	1:A:147:GLY:O	2.15	0.47
1:A:417:THR:HG22	1:A:418:GLN:HG2	1.97	0.47
1:A:232:SER:OG	1:A:246:VAL:HG21	2.15	0.46
1:A:280:GLU:OE1	1:A:282:THR:HG22	2.14	0.46
1:A:131:ILE:HD12	1:A:131:ILE:N	2.29	0.46
1:A:374:LYS:O	1:A:374:LYS:HG3	2.16	0.45
1:A:198:THR:HB	1:A:227:LEU:HB3	1.99	0.45
1:A:382:LEU:N	1:A:383:PRO:HD2	2.33	0.44
1:A:291:LEU:HD21	1:A:296:THR:HA	1.99	0.44
1:A:244:GLN:O	1:A:245:THR:OG1	2.28	0.44
1:A:123:TYR:C	1:A:123:TYR:CD1	2.91	0.44
1:A:286:PHE:CG	1:A:305:ALA:HA	2.52	0.44
1:A:198:THR:HG21	1:A:231:GLU:CB	2.44	0.44
1:A:75:ASN:ND2	1:A:83:GLN:OE1	2.51	0.43
1:A:320:ILE:HG13	1:A:331:LEU:HD21	1.99	0.43
1:A:40:ARG:HE	1:A:41:ARG:HH12	1.66	0.43
1:A:304:ILE:HD13	1:A:356:HIS:HB2	2.01	0.43
1:A:348:ASP:O	1:A:352:LEU:HD23	2.18	0.43
1:A:260:GLN:HG2	1:A:331:LEU:HD22	2.01	0.43
1:A:232:SER:OG	1:A:233:LYS:NZ	2.34	0.43
1:A:191:ARG:NE	1:A:234:MET:HA	2.34	0.42
1:A:247:THR:OG1	1:A:272:GLN:HG2	2.19	0.42
1:A:304:ILE:HD13	1:A:356:HIS:CG	2.55	0.42
1:A:51:SER:OG	1:A:149:ARG:NH1	2.42	0.42
1:A:289:GLN:O	1:A:293:ARG:HG2	2.19	0.42
1:A:139:LEU:CD2	1:A:141:THR:HG23	2.49	0.42
1:A:320:ILE:HG23	1:A:331:LEU:HD11	2.01	0.42
1:A:72:VAL:HG11	1:A:83:GLN:HG2	2.02	0.41
1:A:268:TYR:HE1	1:A:273:ALA:HB2	1.84	0.41
1:A:115:THR:OG1	1:A:122:PRO:O	2.29	0.41
1:A:48:ASN:CG	1:A:148:THR:HG1	2.12	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:LYS:HA	1:A:61:LYS:HE2	2.03	0.41
1:A:364:PRO:N	1:A:365:PRO:CD	2.84	0.41
1:A:352:LEU:O	1:A:356:HIS:ND1	2.42	0.41
1:A:54:THR:HG22	1:A:55:ALA:N	2.36	0.40
1:A:281:GLN:O	1:A:333:TYR:OH	2.21	0.40
1:A:229:GLN:HE21	1:A:249:LYS:HD3	1.86	0.40

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	407/419 (97%)	370 (91%)	37 (9%)	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	330/339 (97%)	325 (98%)	5 (2%)	65 80

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

Mol	Chain	Res	Type
1	A	123	TYR
1	A	191	ARG
1	A	288	ASP
1	A	298	TYR
1	A	333	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

There are no ligands in this entry.

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.

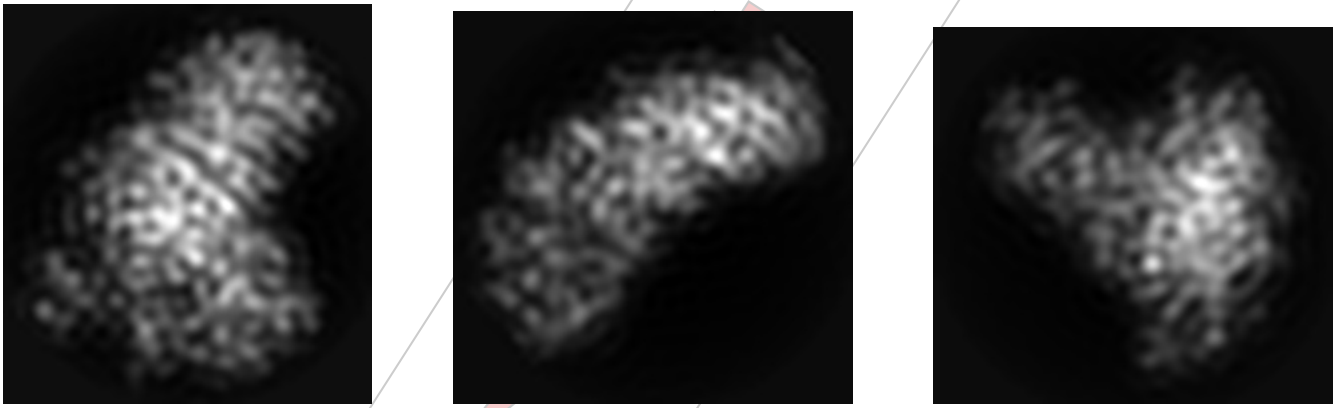
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-40633. 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.

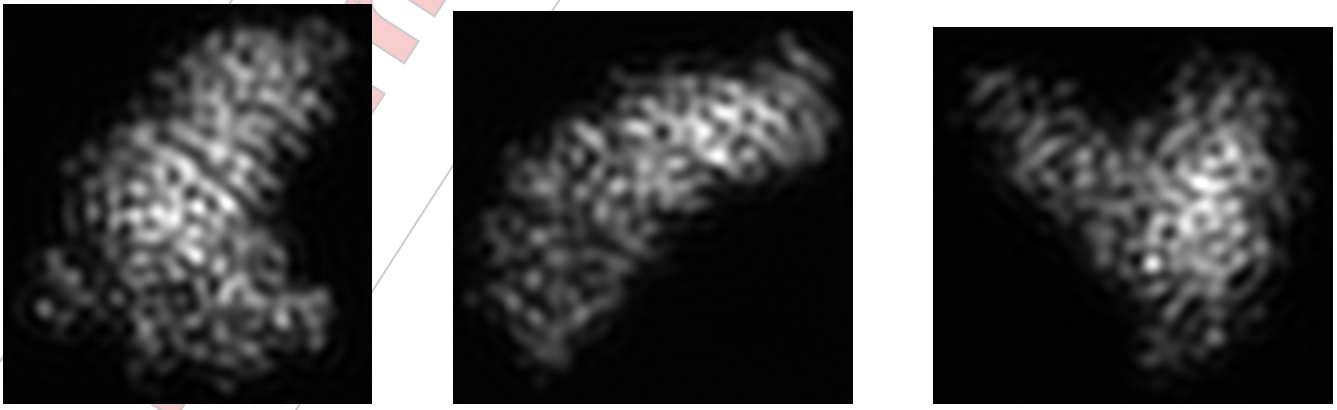
6.1 Orthogonal projections

6.1.1 Primary map



X Y Z

6.1.2 Raw map

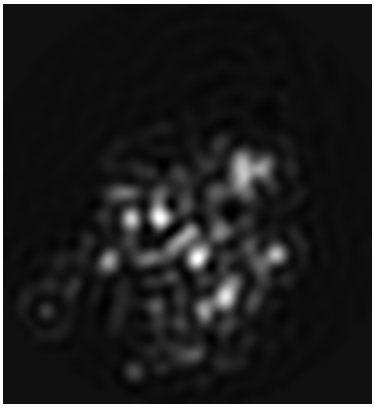


X Y Z

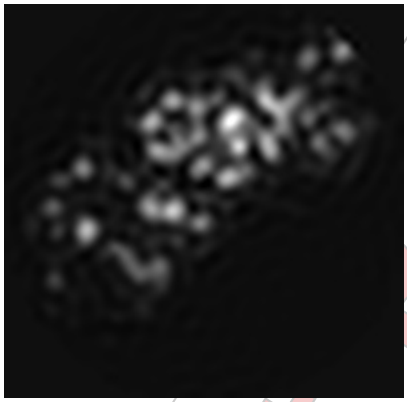
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

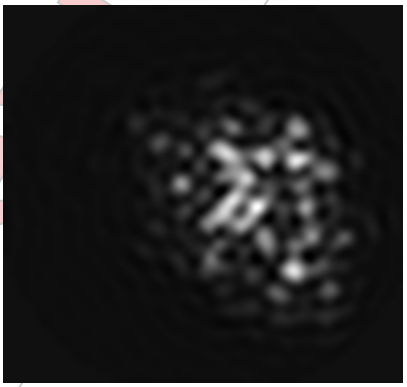
6.2.1 Primary map



X Index: 25

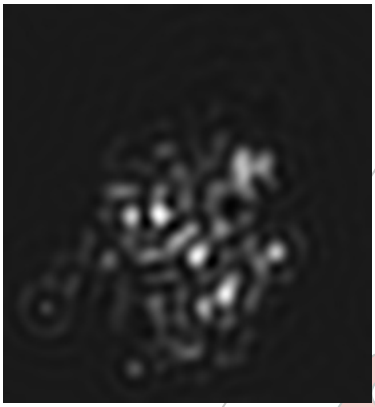


Y Index: 24

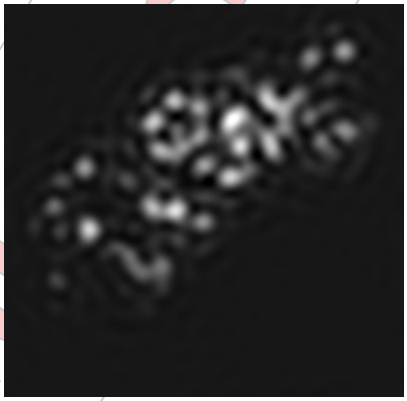


Z Index: 26

6.2.2 Raw map



X Index: 25



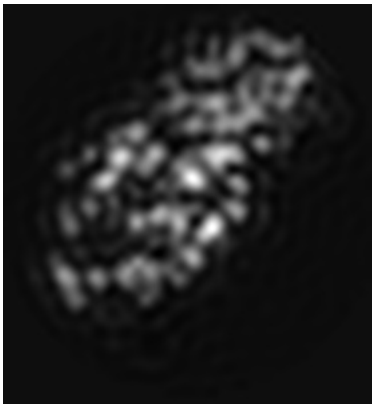
Y Index: 24

Z Index: 26

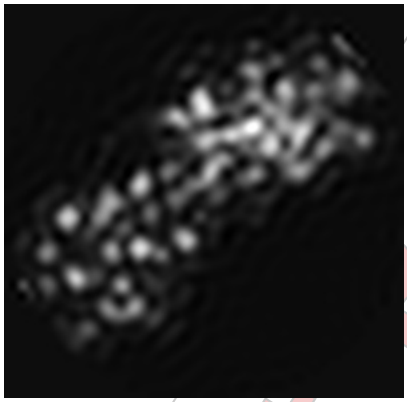
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

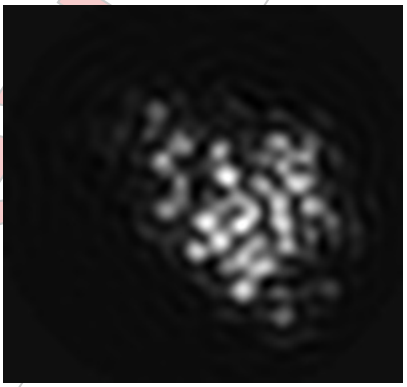
6.3.1 Primary map



X Index: 35

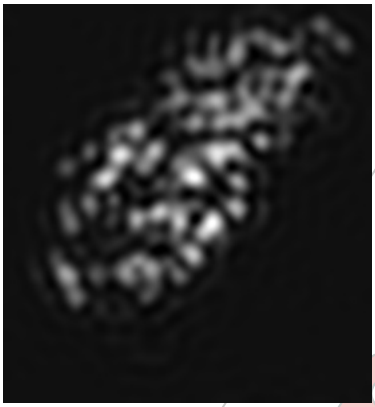


Y Index: 28

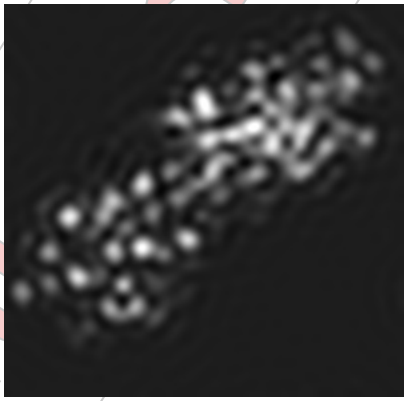


Z Index: 24

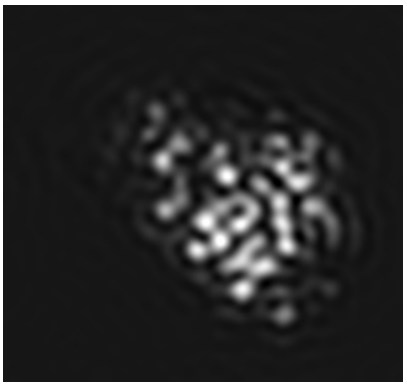
6.3.2 Raw map



X Index: 35



Y Index: 28

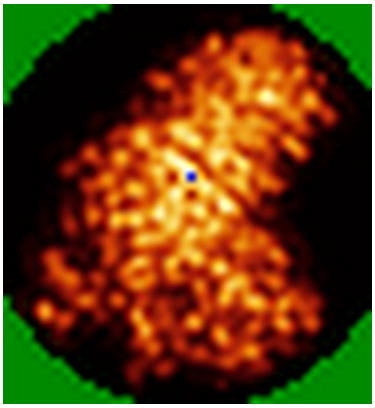


Z Index: 24

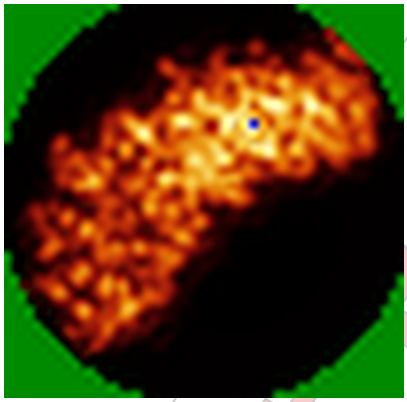
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color)

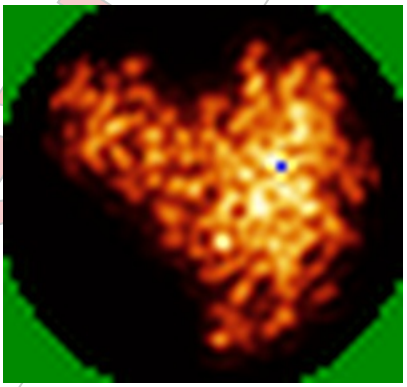
6.4.1 Primary map



X

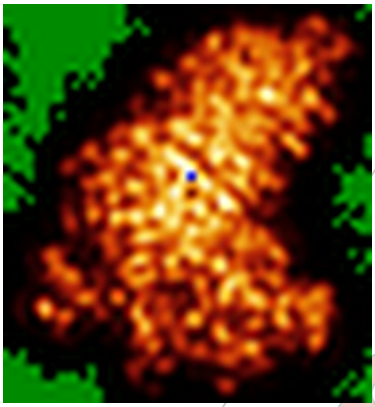


Y

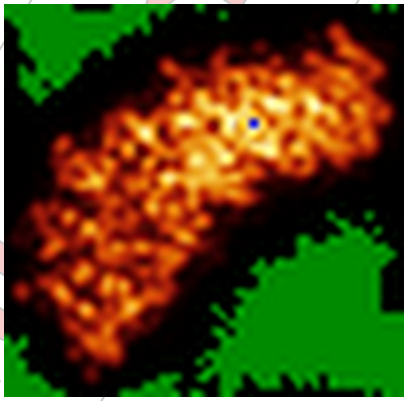


Z

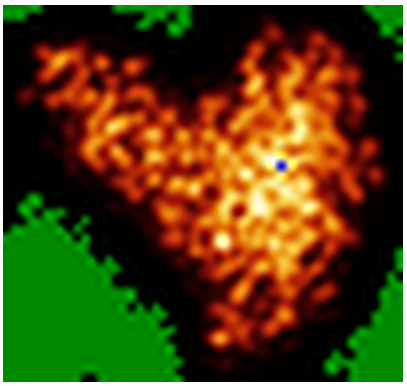
6.4.2 Raw map



X



Y

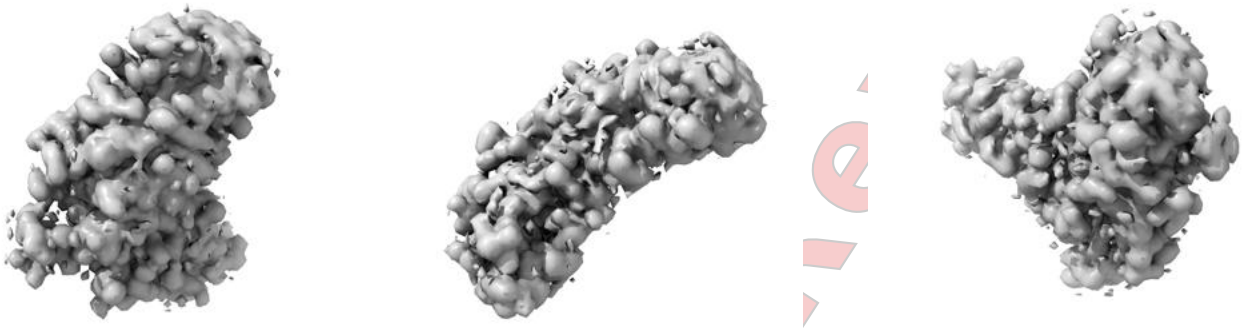


Z

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)

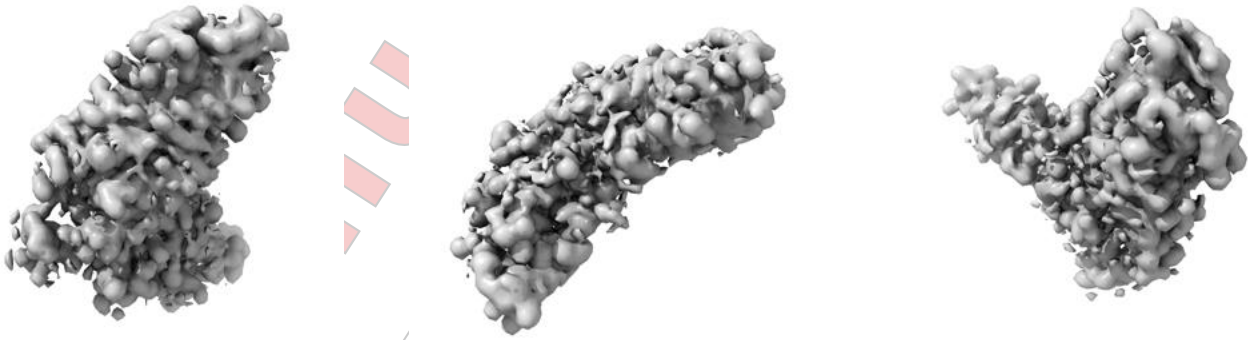
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.75. 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.

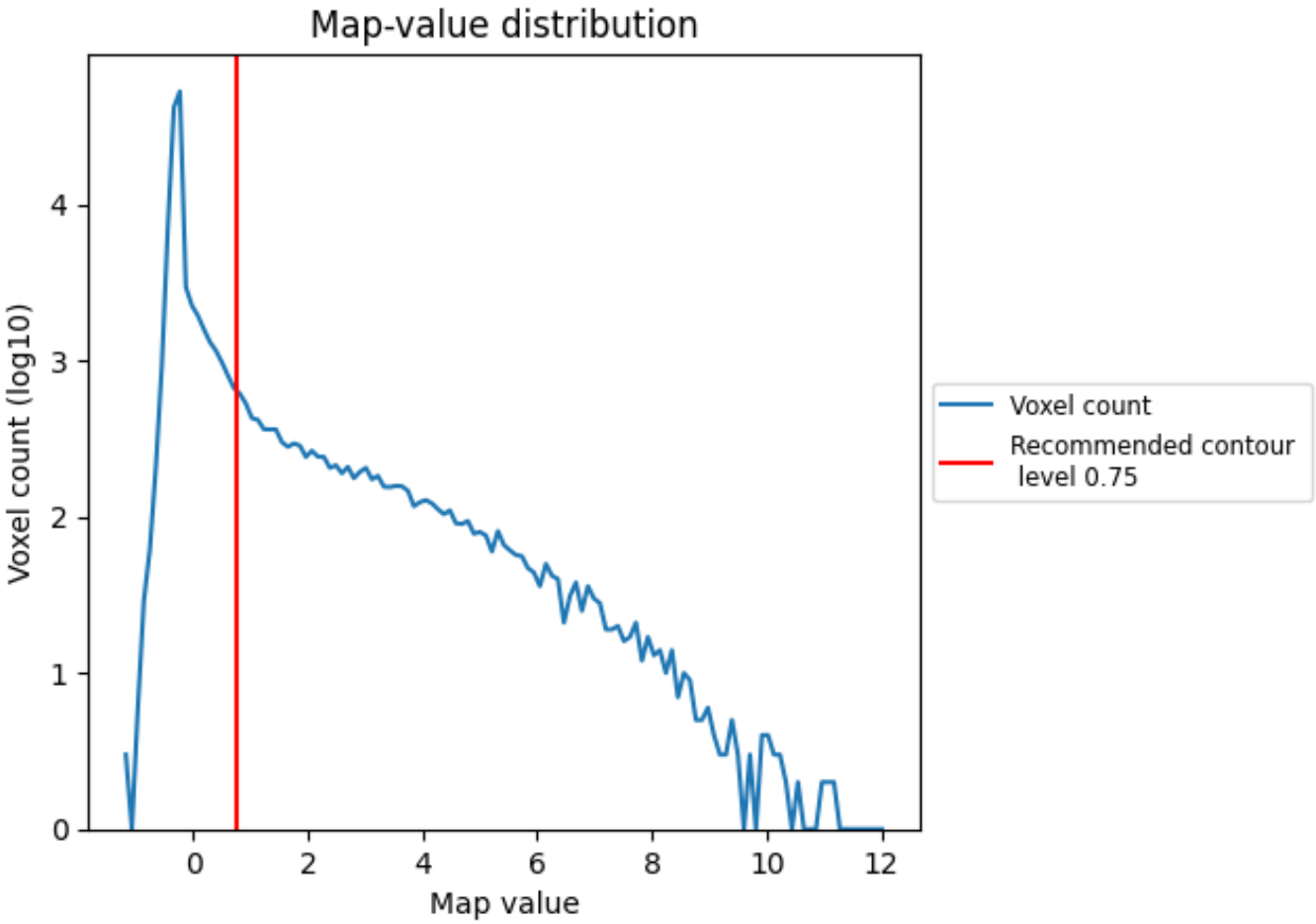
6.6 Mask visualisation (i)

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

7 Map analysis

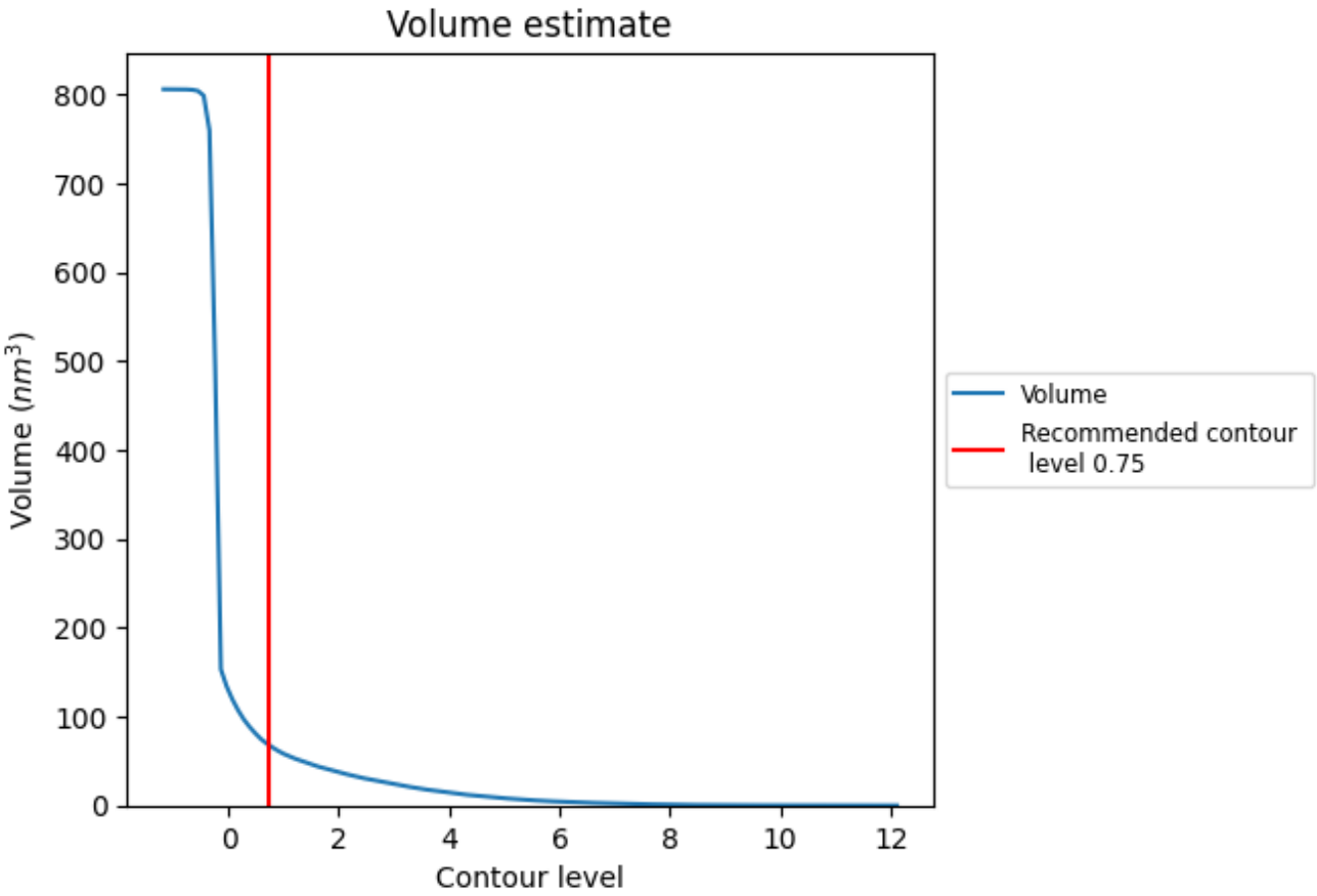
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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 67 nm^3; this corresponds to an approximate mass of 61 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.

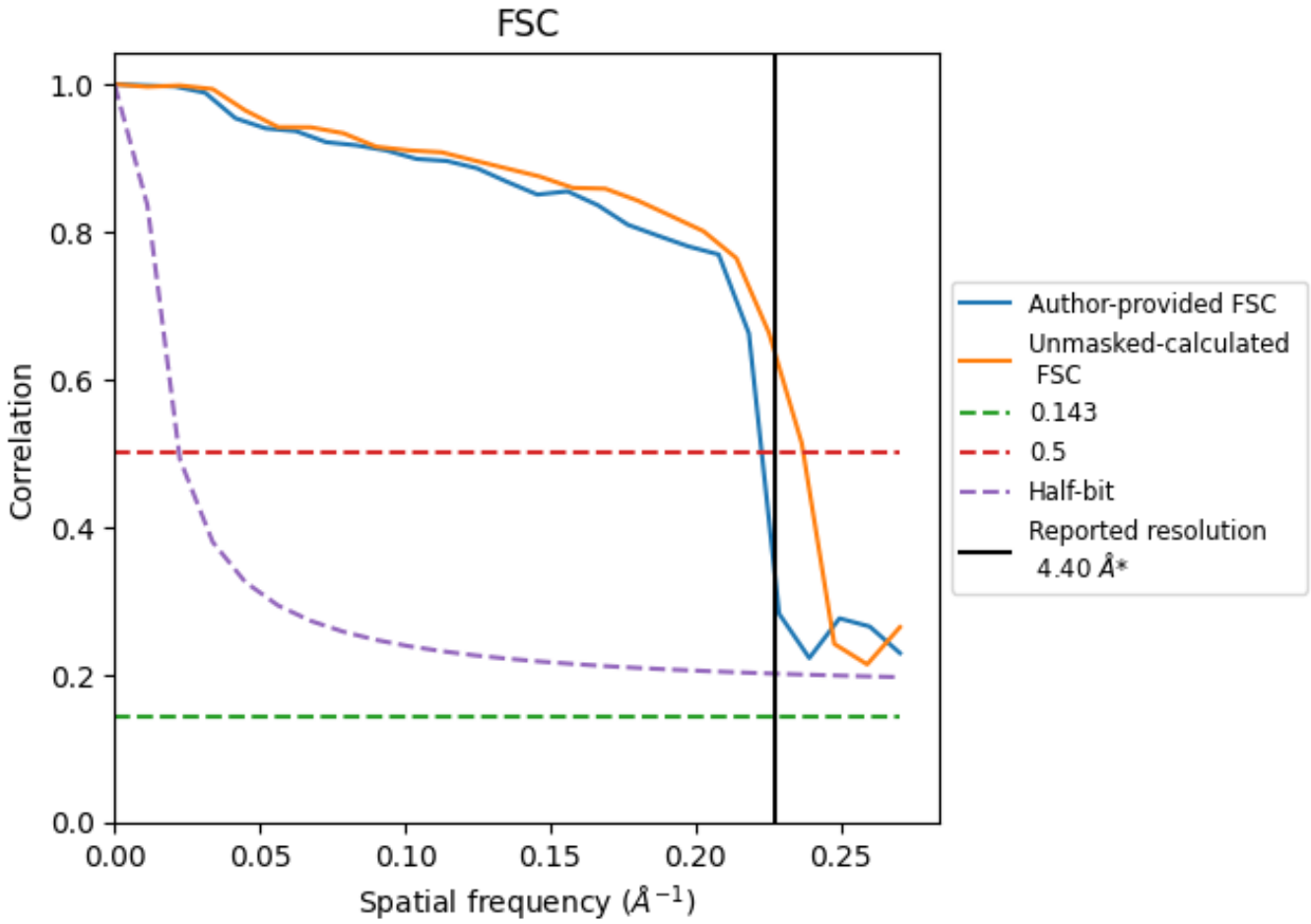
7.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.227 Å^{-1}

8.2 Resolution estimates (i)

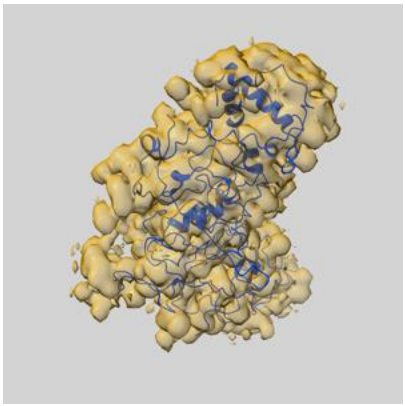
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	4.40	-
Author-provided FSC curve	-	4.49	-
Unmasked-calculated*	-	4.22	-

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

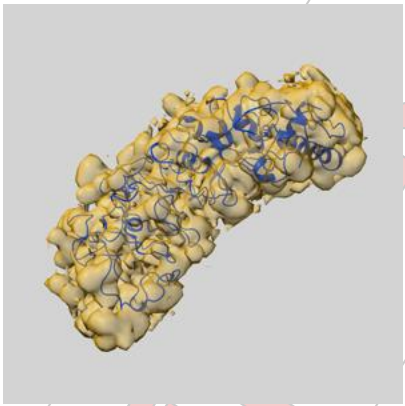
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-40633 and PDB model 8SNS. Per-residue inclusion information can be found in section 3 on page 4.

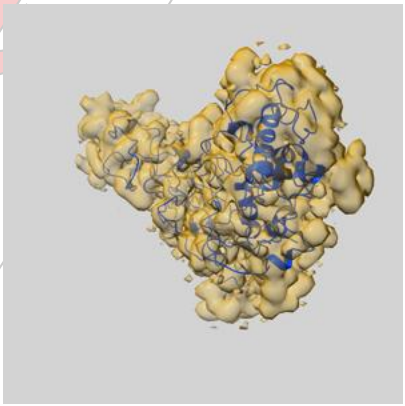
9.1 Map-model overlay



X



Y



Z

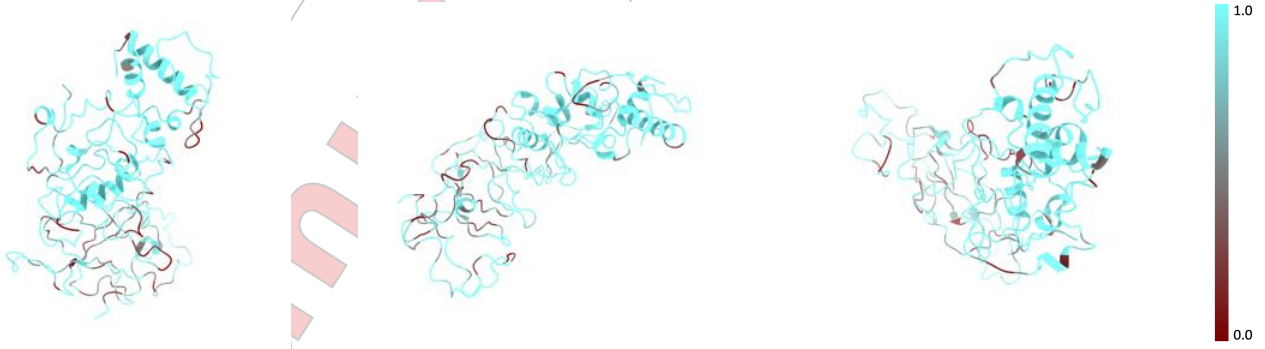
The images above show the 3D surface view of the map at the recommended contour level 0.75 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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.

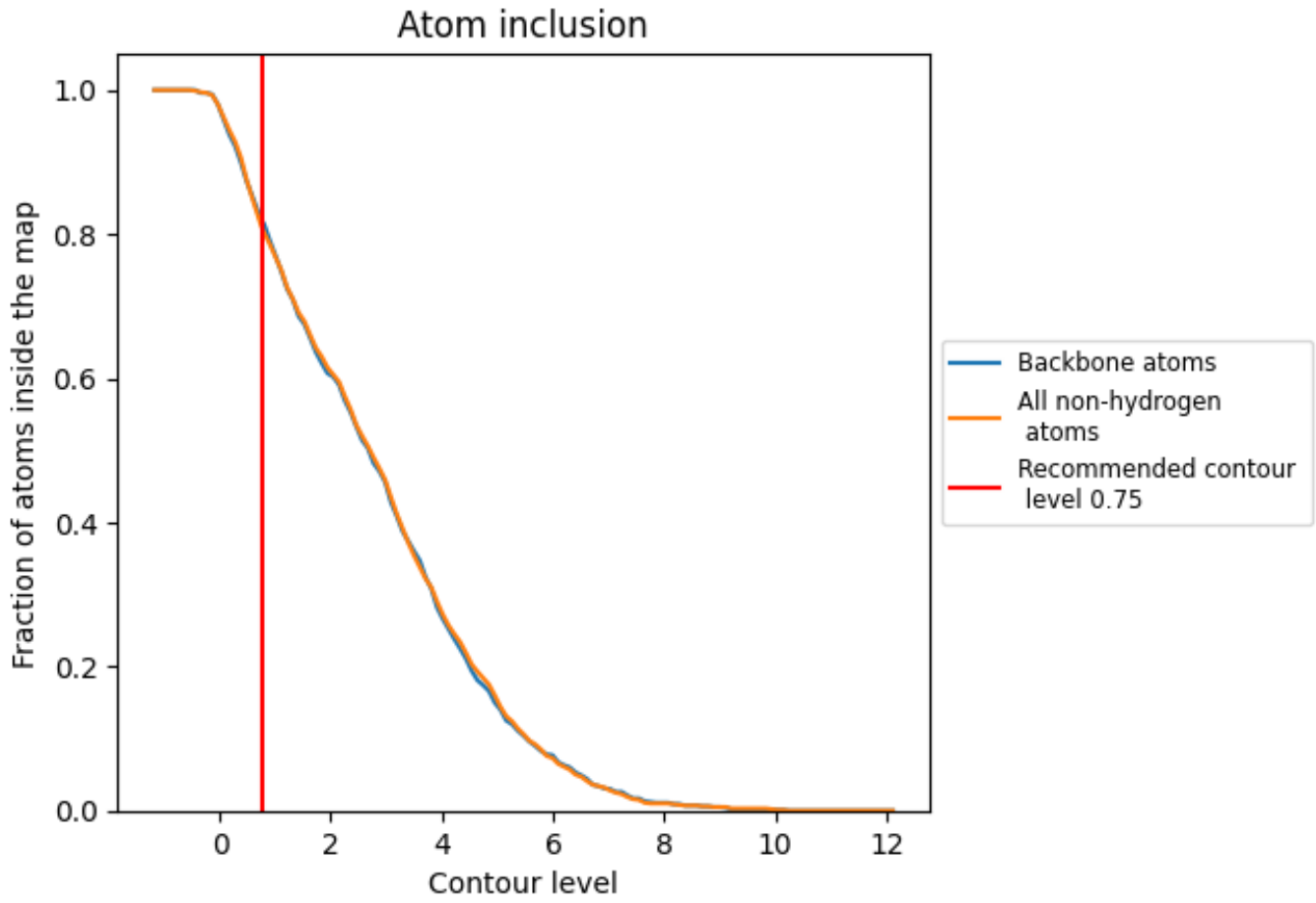
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.75).

9.4 Atom inclusion



At the recommended contour level, 82% of all backbone atoms, 81% 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 (0.75) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8110	0.1830
A	0.8200	0.1830

Full wwPDB EM Validation Report ⓘ

May 2, 2023 – 11:43 AM EDT

PDB ID	:	8SO4
EMDB ID	:	EMD-40647
Title	:	Nucleocapsid protein from SARS-CoV-2, flexible conformation 3
Deposited on	:	2023-04-28
Resolution	:	4.85 Å(reported)
Based on initial model	:	.

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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:

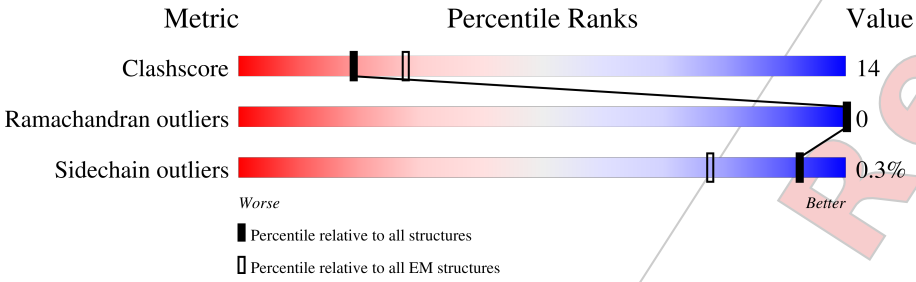
EMDB validation analysis	:	0.0.1.dev50
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

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 4.85 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 >=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	A	425	10% 68% 31%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 6373 atoms, of which 3159 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 Nucleoprotein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	419	6373	1971	3159	607	629	7	0	0

There are 6 discrepancies between the modelled and reference sequences:

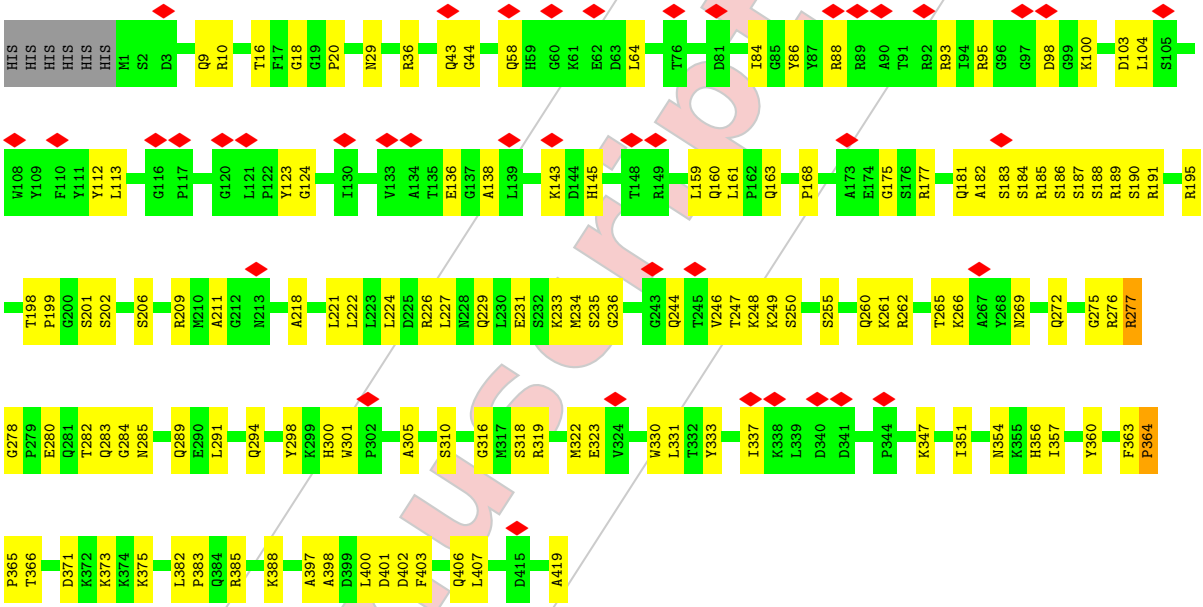
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP P0DTC9
A	-4	HIS	-	expression tag	UNP P0DTC9
A	-3	HIS	-	expression tag	UNP P0DTC9
A	-2	HIS	-	expression tag	UNP P0DTC9
A	-1	HIS	-	expression tag	UNP P0DTC9
A	0	HIS	-	expression tag	UNP P0DTC9

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: Nucleoprotein

Chain A:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	20000	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS TALOS F200C	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	45000	Depositor
Image detector	DIRECT ELECTRON DE-12 (4k x 3k)	Depositor
Maximum map value	12.115	Depositor
Minimum map value	-1.173	Depositor
Average map value	0.047	Depositor
Map value standard deviation	0.984	Depositor
Recommended contour level	0.922	Depositor
Map size (Å)	102.0, 96.0, 104.0	wwPDB
Map dimensions	51, 48, 52	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.0, 2.0, 2.0	Depositor

5 Model quality

5.1 Standard geometry

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	0.26	0/3279	0.60	1/4422 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	364	PRO	CA-N-CD	-9.99	97.51	111.50

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	3214	3159	3161	91	0
All	All	3214	3159	3161	91	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 14.

All (91) 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:357:ILE:HD12	1:A:419:ALA:HA	1.65	0.77
1:A:209:ARG:NH2	1:A:255:SER:OG	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:SER:H	1:A:248:LYS:HA	1.52	0.73
1:A:289:GLN:OE1	1:A:356:HIS:NE2	2.21	0.72
1:A:191:ARG:NH2	1:A:234:MET:SD	2.63	0.72
1:A:388:LYS:HA	1:A:397:ALA:HA	1.72	0.72
1:A:86:TYR:HB3	1:A:113:LEU:HD21	1.72	0.70
1:A:398:ALA:O	1:A:402:ASP:N	2.26	0.69
1:A:159:LEU:HG	1:A:160:GLN:H	1.56	0.68
1:A:58:GLN:HG2	1:A:64:LEU:HB2	1.74	0.67
1:A:161:LEU:HD21	1:A:199:PRO:HG2	1.75	0.67
1:A:277:ARG:NH1	1:A:291:LEU:O	2.29	0.65
1:A:181:GLN:HB3	1:A:222:LEU:HD11	1.79	0.64
1:A:184:SER:OG	1:A:246:VAL:O	2.14	0.64
1:A:269:ASN:ND2	1:A:272:GLN:OE1	2.30	0.63
1:A:185:ARG:NH2	1:A:188:SER:OG	2.32	0.63
1:A:9:GLN:HG2	1:A:10:ARG:H	1.63	0.62
1:A:319:ARG:O	1:A:333:TYR:OH	2.11	0.62
1:A:398:ALA:HB1	1:A:401:ASP:HB2	1.82	0.61
1:A:363:PHE:O	1:A:366:THR:OG1	2.18	0.60
1:A:43:GLN:HG3	1:A:44:GLY:H	1.68	0.59
1:A:385:ARG:HD2	1:A:388:LYS:HD2	1.84	0.58
1:A:278:GLY:O	1:A:284:GLY:HA2	2.04	0.58
1:A:318:SER:HB2	1:A:337:ILE:HG12	1.86	0.58
1:A:181:GLN:HG3	1:A:226:ARG:HE	1.68	0.58
1:A:185:ARG:NH1	1:A:294:GLN:O	2.37	0.57
1:A:322:MET:SD	1:A:322:MET:N	2.78	0.56
1:A:201:SER:HB2	1:A:206:SER:HB3	1.87	0.56
1:A:280:GLU:N	1:A:280:GLU:OE1	2.39	0.56
1:A:189:ARG:HG3	1:A:190:SER:H	1.72	0.54
1:A:191:ARG:HB3	1:A:235:SER:H	1.73	0.54
1:A:298:TYR:CE2	1:A:300:HIS:HB3	2.43	0.54
1:A:275:GLY:H	1:A:283:GLN:HG2	1.72	0.54
1:A:266:LYS:HB3	1:A:301:TRP:HE1	1.73	0.54
1:A:276:ARG:NH1	1:A:360:TYR:OH	2.32	0.53
1:A:351:ILE:HA	1:A:354:ASN:ND2	2.23	0.53
1:A:84:ILE:HG22	1:A:138:ALA:HB2	1.91	0.52
1:A:319:ARG:N	1:A:333:TYR:OH	2.36	0.52
1:A:88:ARG:NH1	1:A:123:TYR:O	2.43	0.52
1:A:175:GLY:O	1:A:177:ARG:NH1	2.41	0.51
1:A:16:THR:OG1	1:A:29:ASN:OD1	2.25	0.51
1:A:276:ARG:NH2	1:A:277:ARG:O	2.44	0.51
1:A:189:ARG:HG3	1:A:190:SER:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:ALA:HA	1:A:310:SER:HB3	1.93	0.50
1:A:143:LYS:HB3	1:A:145:HIS:CD2	2.48	0.49
1:A:186:SER:HB3	1:A:248:LYS:HG2	1.93	0.48
1:A:260:GLN:C	1:A:261:LYS:HD3	2.34	0.48
1:A:175:GLY:HA2	1:A:218:ALA:HB2	1.95	0.47
1:A:330:TRP:CG	1:A:331:LEU:N	2.81	0.47
1:A:364:PRO:HB2	1:A:365:PRO:HD3	1.95	0.47
1:A:168:PRO:HA	1:A:202:SER:HB2	1.96	0.47
1:A:100:LYS:HB2	1:A:103:ASP:OD1	2.15	0.47
1:A:88:ARG:HH12	1:A:124:GLY:HA2	1.78	0.46
1:A:363:PHE:CD2	1:A:365:PRO:HD2	2.50	0.46
1:A:93:ARG:CZ	1:A:95:ARG:HB2	2.46	0.46
1:A:190:SER:C	1:A:233:LYS:H	2.20	0.46
1:A:9:GLN:HG2	1:A:10:ARG:N	2.31	0.45
1:A:235:SER:OG	1:A:236:GLY:N	2.50	0.45
1:A:403:PHE:O	1:A:406:GLN:HG3	2.17	0.45
1:A:406:GLN:NE2	1:A:407:LEU:HD22	2.32	0.45
1:A:363:PHE:HB3	1:A:366:THR:HG23	1.98	0.45
1:A:161:LEU:O	1:A:163:GLN:N	2.43	0.44
1:A:182:ALA:HA	1:A:248:LYS:O	2.17	0.44
1:A:190:SER:HB2	1:A:235:SER:HB2	1.99	0.44
1:A:382:LEU:N	1:A:383:PRO:HD2	2.33	0.44
1:A:10:ARG:HH22	1:A:36:ARG:CZ	2.30	0.44
1:A:143:LYS:HB3	1:A:145:HIS:HD2	1.82	0.44
1:A:373:LYS:HG2	1:A:375:LYS:H	1.83	0.43
1:A:189:ARG:HB3	1:A:247:THR:HG23	2.01	0.43
1:A:282:THR:HA	1:A:323:GLU:HA	2.00	0.43
1:A:195:ARG:O	1:A:195:ARG:HG3	2.19	0.43
1:A:278:GLY:HA2	1:A:285:ASN:ND2	2.34	0.43
1:A:233:LYS:HE3	1:A:277:ARG:HH12	1.83	0.42
1:A:265:THR:C	1:A:266:LYS:HD3	2.40	0.42
1:A:112:TYR:CZ	1:A:136:GLU:HB2	2.54	0.42
1:A:198:THR:OG1	1:A:224:LEU:HA	2.19	0.42
1:A:249:LYS:HG2	1:A:250:SER:N	2.35	0.42
1:A:187:SER:HA	1:A:229:GLN:NE2	2.34	0.42
1:A:211:ALA:HB2	1:A:221:LEU:HD21	2.00	0.42
1:A:191:ARG:HG3	1:A:231:GLU:HA	2.02	0.41
1:A:262:ARG:HH11	1:A:316:GLY:HA3	1.85	0.41
1:A:189:ARG:O	1:A:244:GLN:HB2	2.21	0.41
1:A:277:ARG:HE	1:A:291:LEU:HB3	1.85	0.41
1:A:186:SER:HA	1:A:247:THR:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:ASP:H	1:A:104:LEU:HD22	1.86	0.41
1:A:371:ASP:OD2	1:A:400:LEU:HG	2.21	0.41
1:A:18:GLY:O	1:A:20:PRO:HD3	2.20	0.40
1:A:277:ARG:HD2	1:A:291:LEU:HD12	2.03	0.40
1:A:145:HIS:O	1:A:145:HIS:ND1	2.54	0.40
1:A:198:THR:H	1:A:227:LEU:HD13	1.86	0.40
1:A:347:LYS:NZ	1:A:351:ILE:HG21	2.37	0.40

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	417/425 (98%)	340 (82%)	77 (18%)	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	339/345 (98%)	338 (100%)	1 (0%)	92	95

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

Mol	Chain	Res	Type
1	A	277	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	269	ASN
1	A	272	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

There are no ligands in this entry.

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.

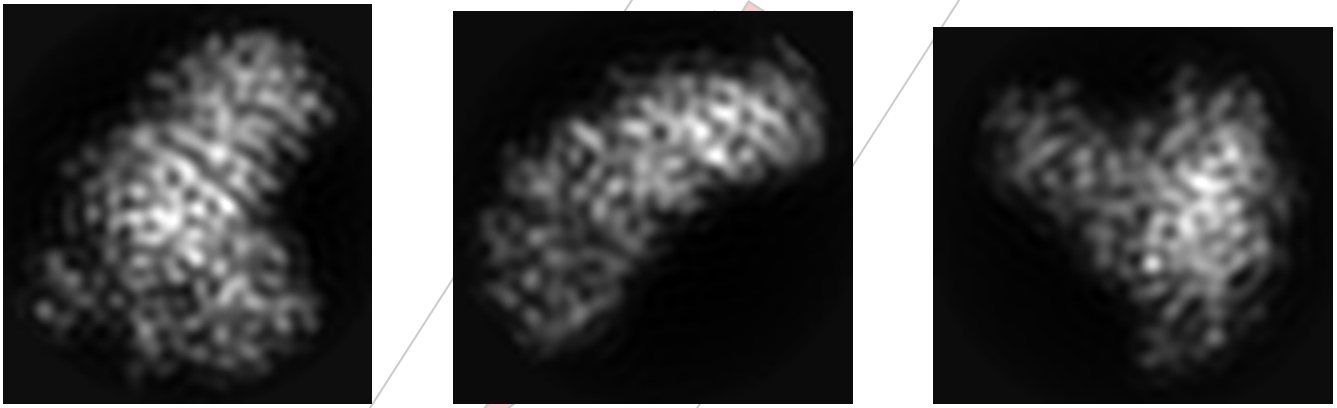
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-40647. 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.

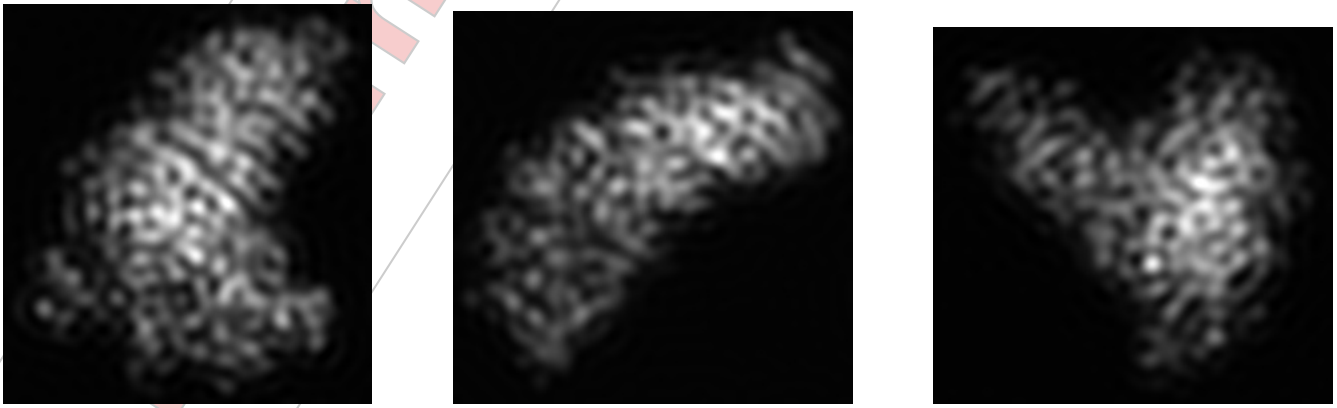
6.1 Orthogonal projections

6.1.1 Primary map



X Y Z

6.1.2 Raw map

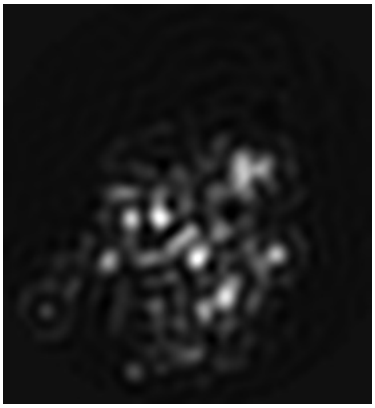


X Y Z

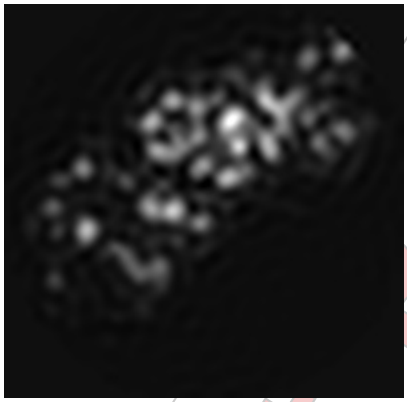
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

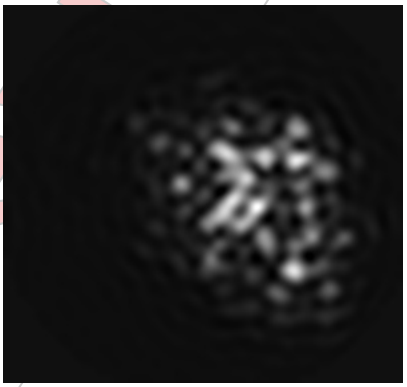
6.2.1 Primary map



X Index: 25

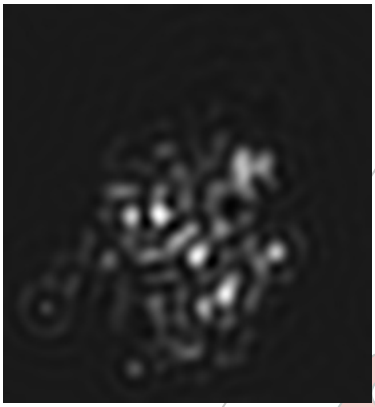


Y Index: 24

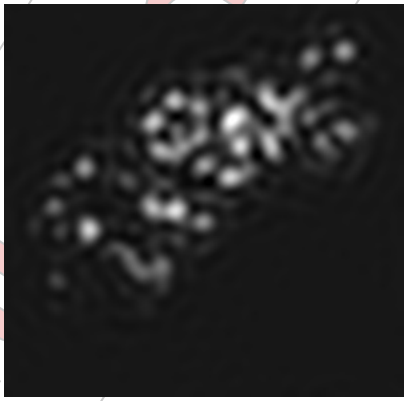


Z Index: 26

6.2.2 Raw map



X Index: 25



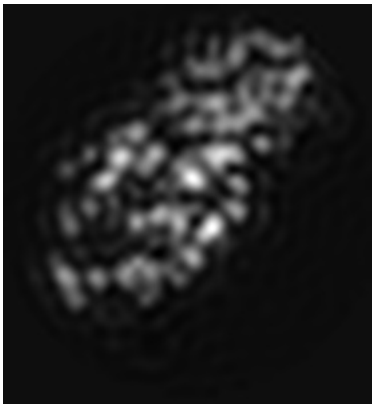
Y Index: 24

Z Index: 26

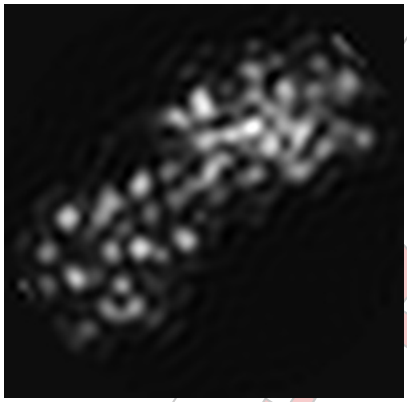
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

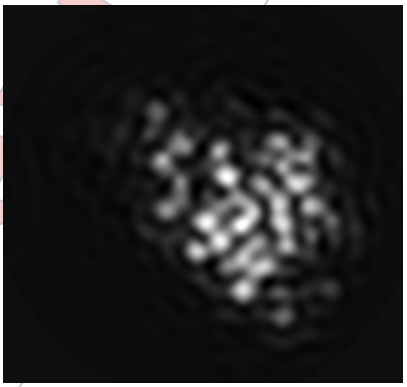
6.3.1 Primary map



X Index: 35

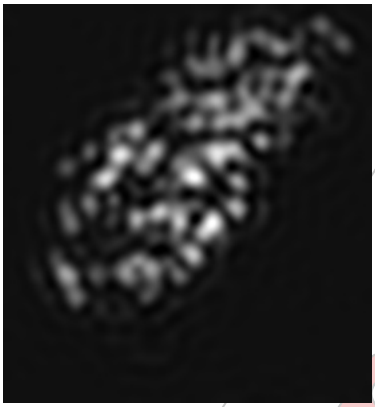


Y Index: 28

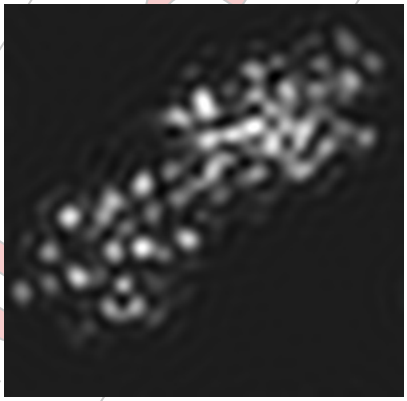


Z Index: 24

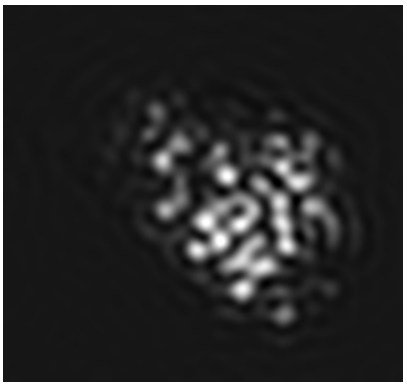
6.3.2 Raw map



X Index: 35



Y Index: 28

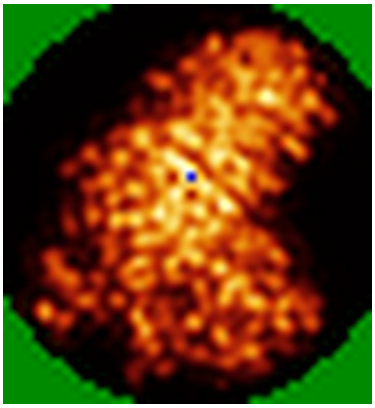


Z Index: 24

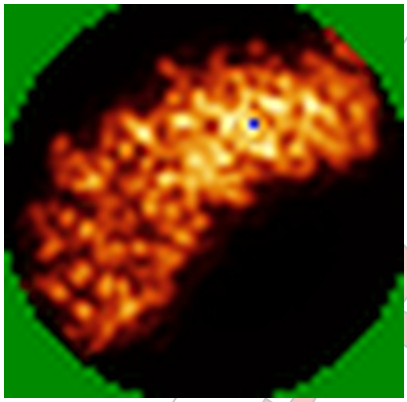
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color)

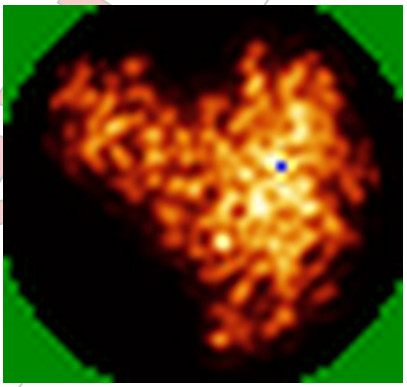
6.4.1 Primary map



X

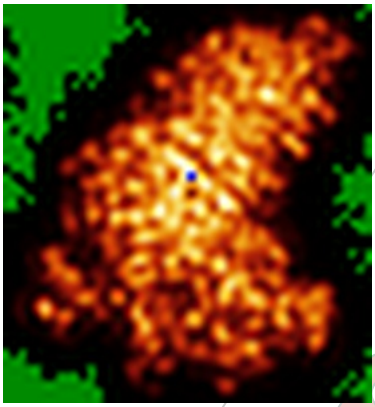


Y

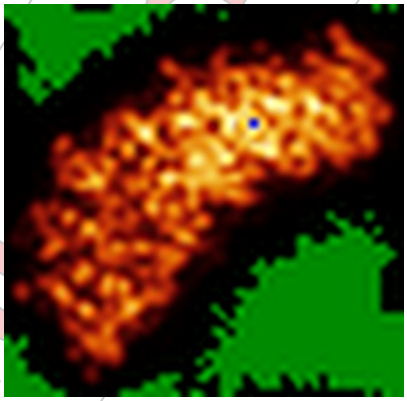


Z

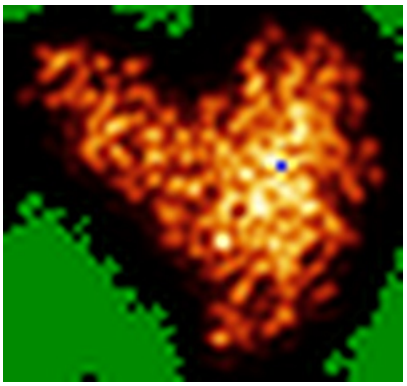
6.4.2 Raw map



X



Y

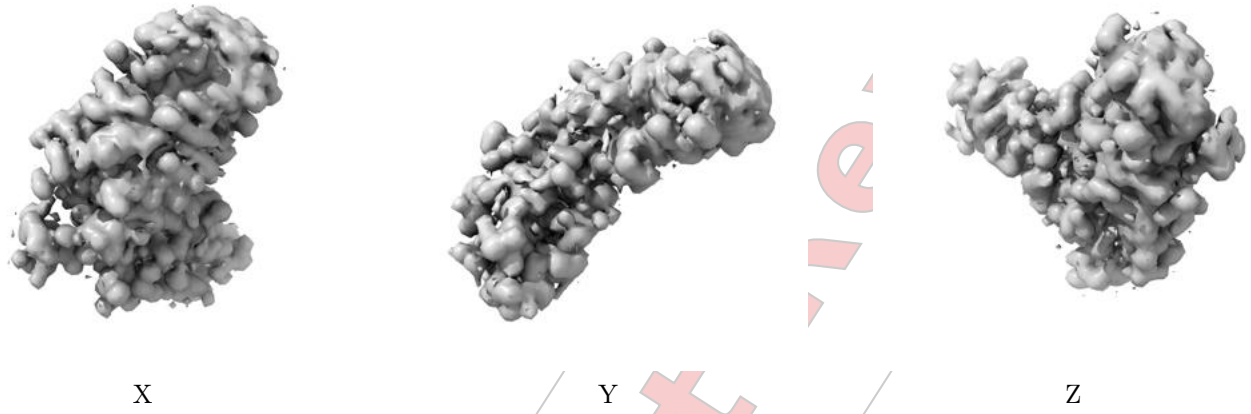


Z

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)

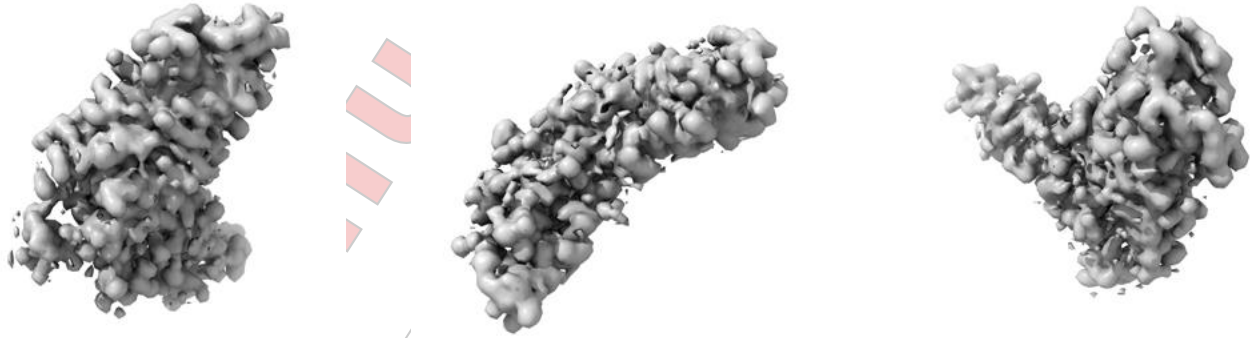
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.922. 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.

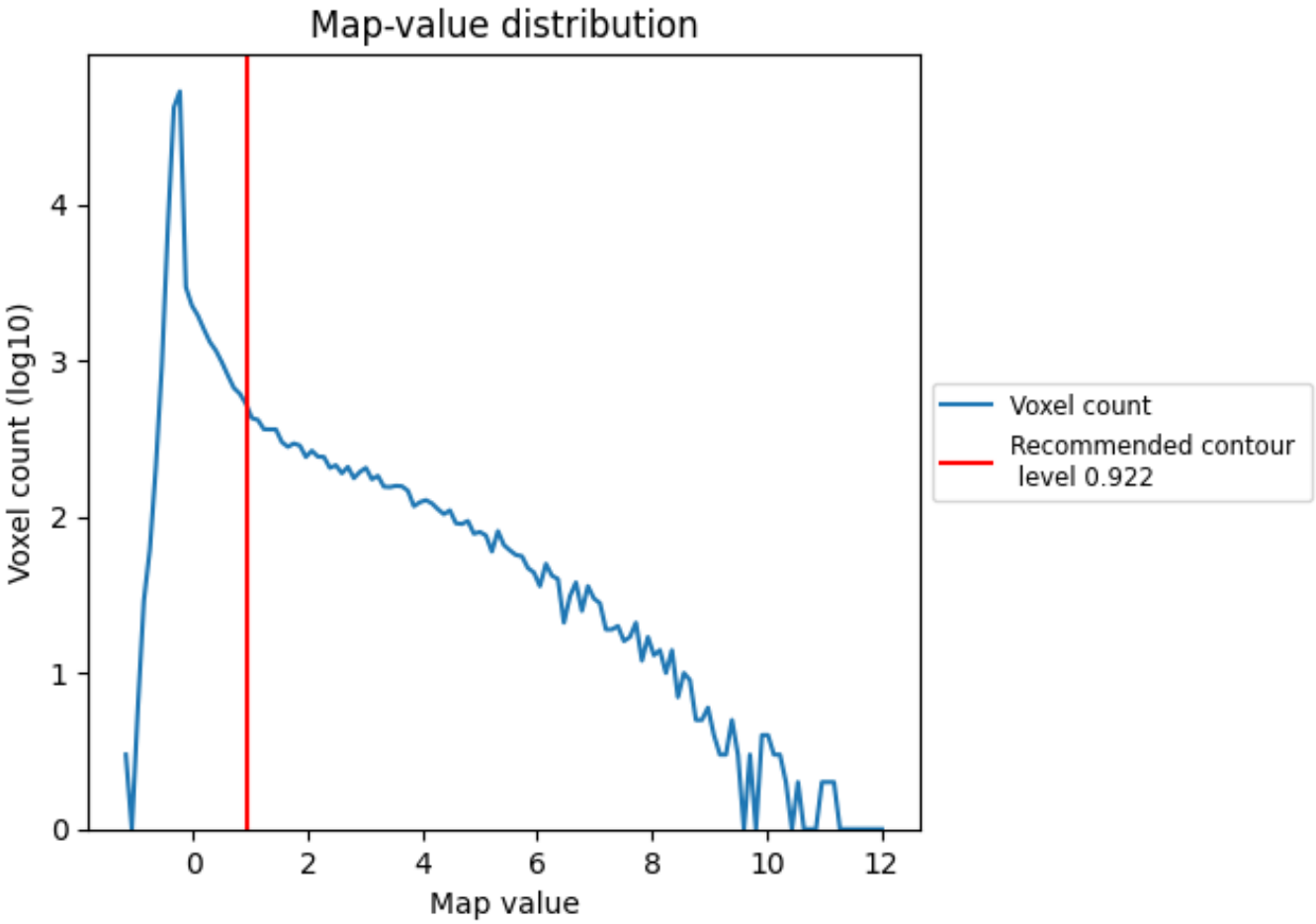
6.6 Mask visualisation (i)

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

7 Map analysis

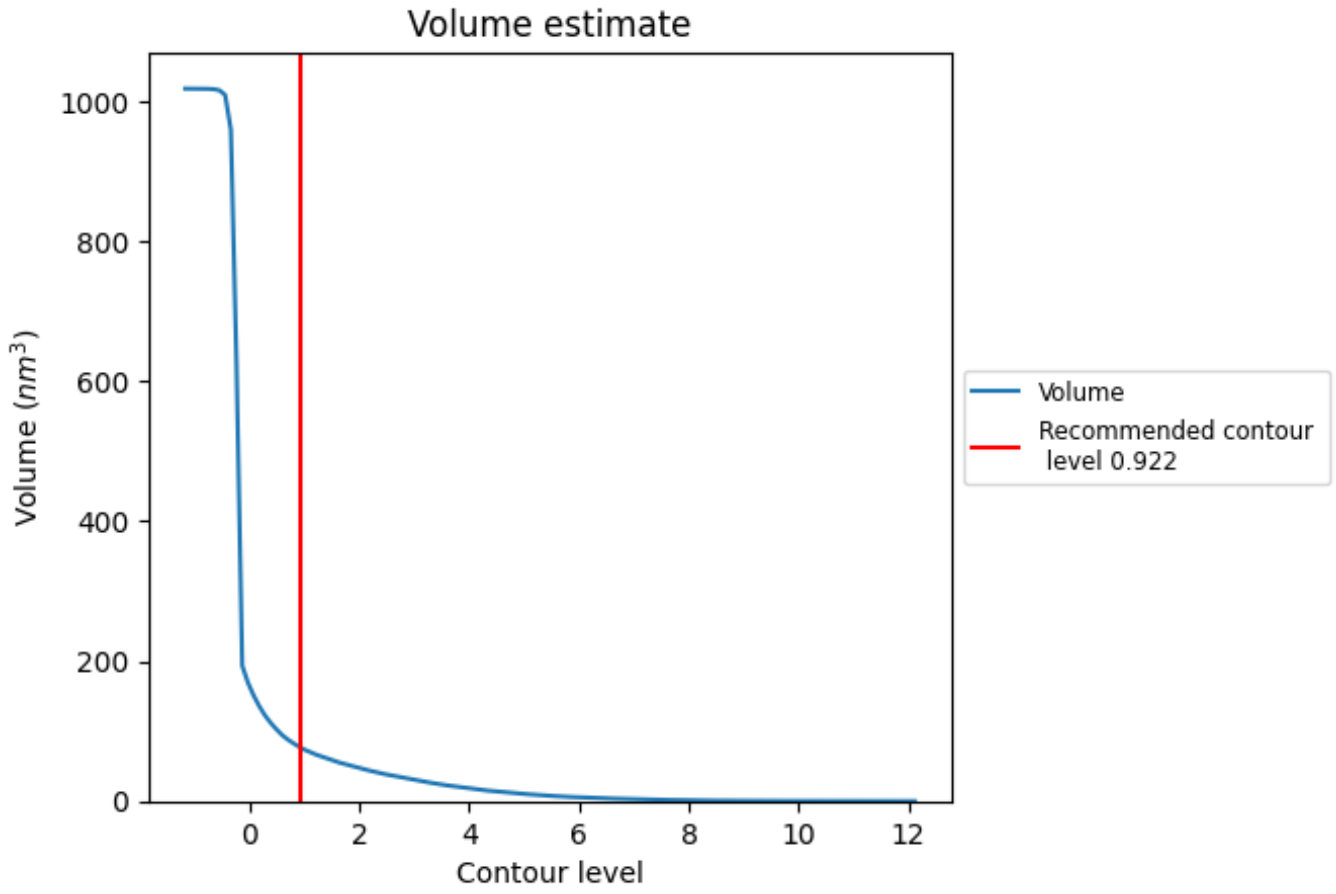
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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 77 nm^3; this corresponds to an approximate mass of 69 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.

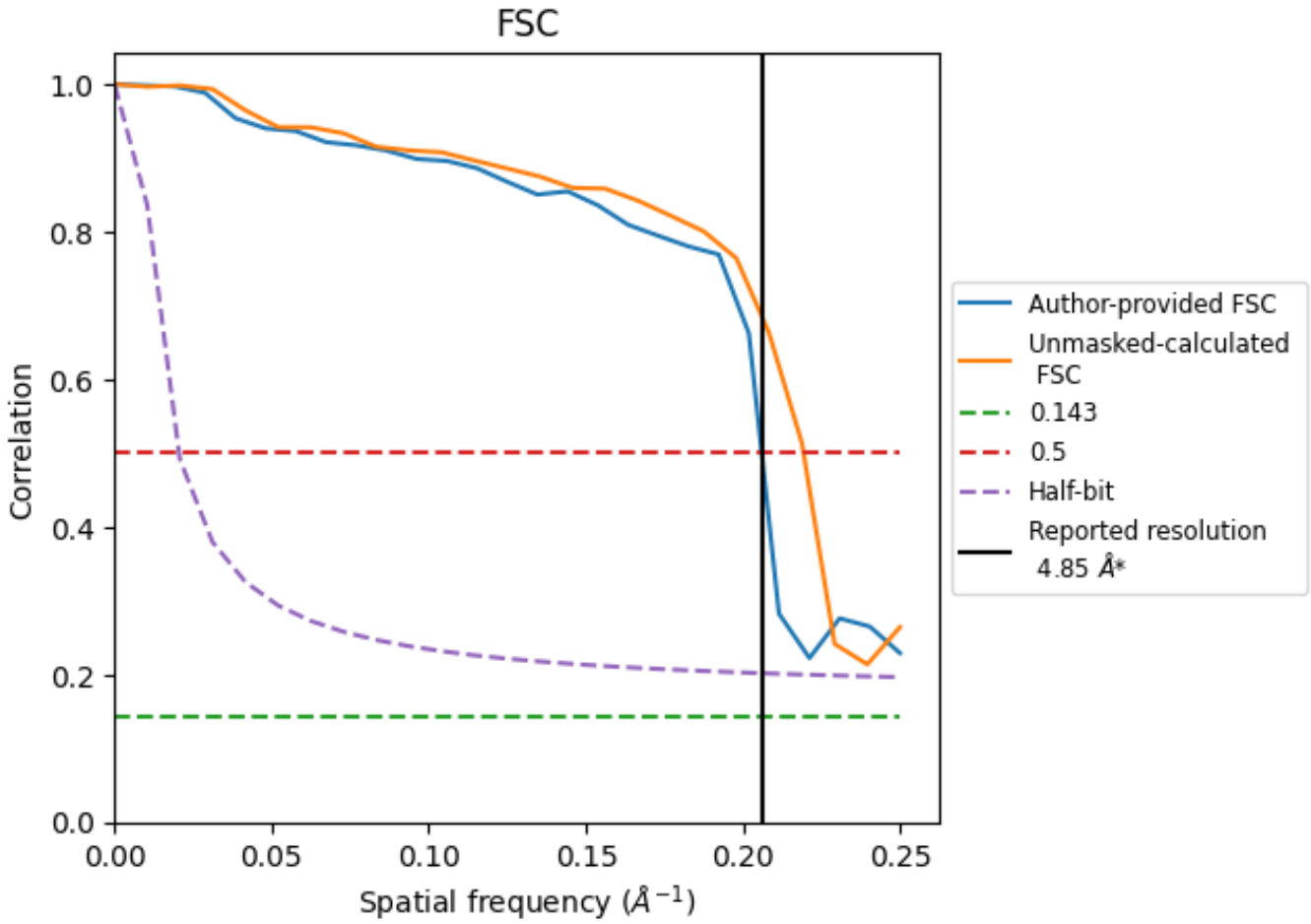
7.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.206 Å^{-1}

8.2 Resolution estimates (i)

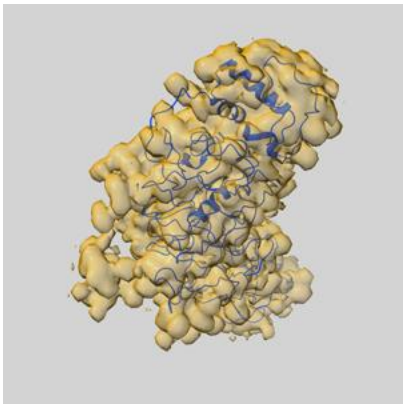
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	4.85	-
Author-provided FSC curve	-	4.85	-
Unmasked-calculated*	-	4.56	-

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

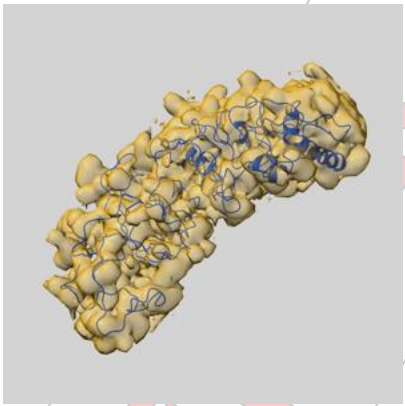
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-40647 and PDB model 8SO4. Per-residue inclusion information can be found in section 3 on page 4.

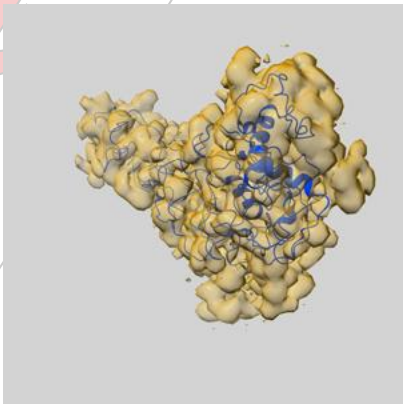
9.1 Map-model overlay



X



Y



Z

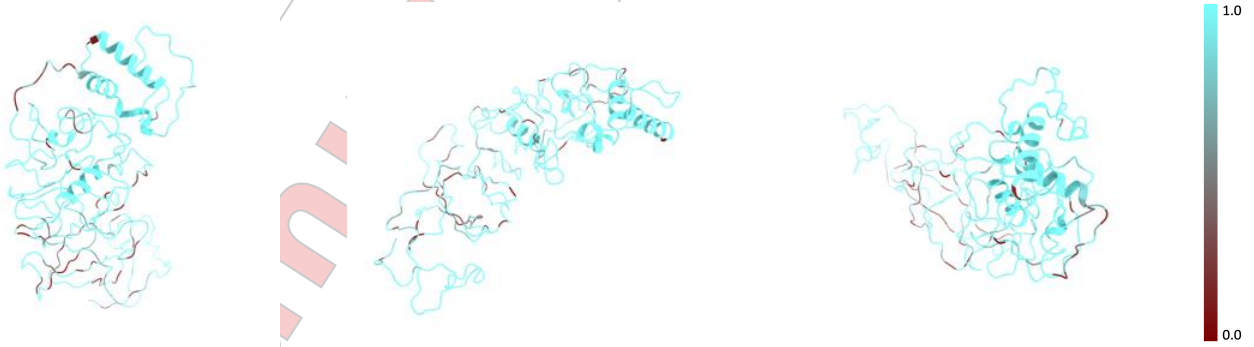
The images above show the 3D surface view of the map at the recommended contour level 0.922 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model

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.

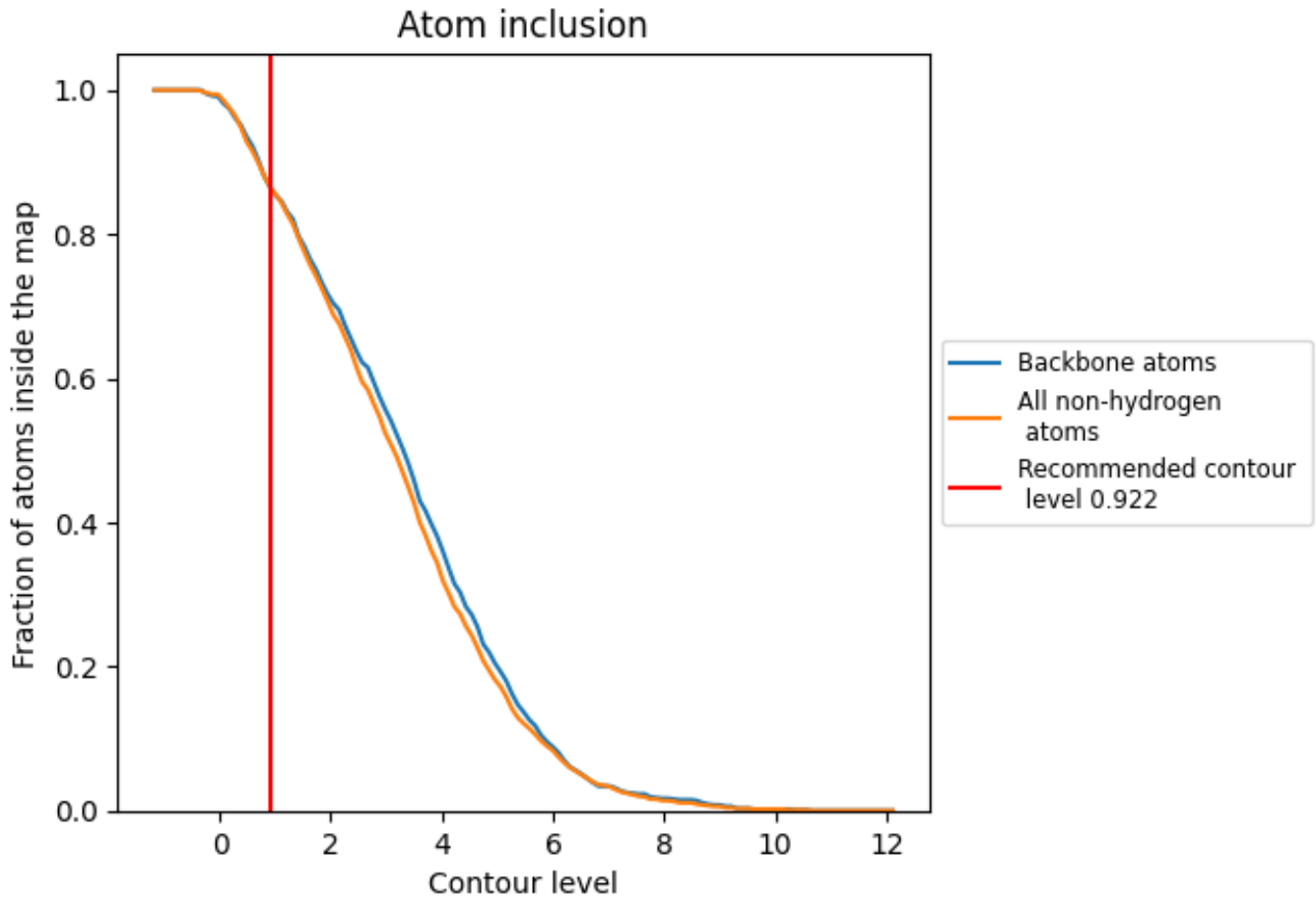
9.3 Atom inclusion mapped to coordinate model



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 (0.922).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 86% 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 (0.922) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8640	0.1920
A	0.8610	0.1920

Preliminary Full wwPDB EM Validation Report ⓘ

Jun 18, 2023 – 01:03 PM EDT

This wwPDB validation report is NOT for manuscript review

This is a Preliminary Full wwPDB EM Validation Report.

This report is produced by the standalone wwPDB validation server.
The structure in question has not been deposited to the wwPDB.
This report should not be submitted to journals.

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:

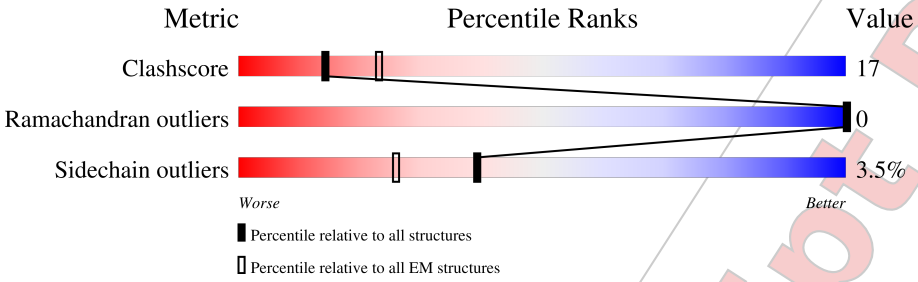
EMDB validation analysis	:	0.0.1.dev50
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

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 unknown.

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 >=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	A	419	10% 68% 30%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6375 atoms, of which 3161 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.

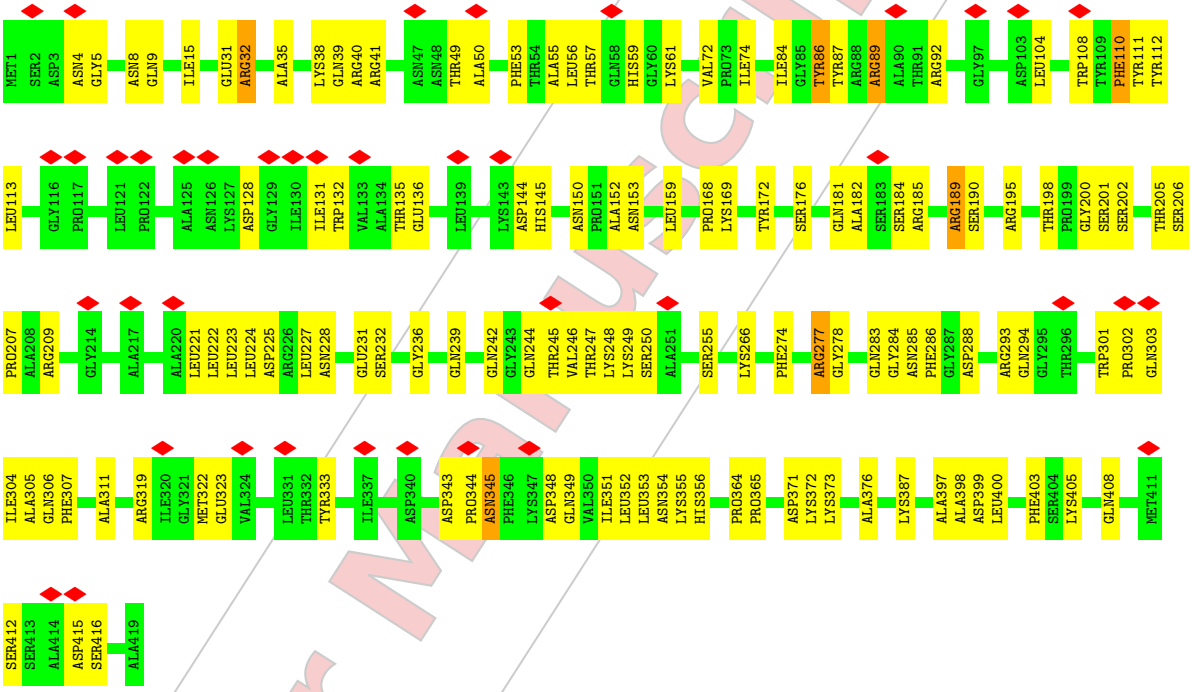
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	419	6375	1971	3161	607	629	7	0	0

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:

Chain A: 



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	Not provided	
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	Not provided	
Voltage (kV)	Not provided	
Electron dose ($e^-/Å^2$)	Not provided	
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	Not provided	
Maximum map value	14.788	Depositor
Minimum map value	-4.905	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	0.9	Depositor
Map size (Å)	94.86, 90.21, 97.65	wwPDB
Map dimensions	102, 97, 105	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.93, 0.93, 0.93	Depositor

5 Model quality

5.1 Standard geometry

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	0/3279	0.65	0/4422

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	245	THR	Peptide

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	3214	3161	3161	110	0
All	All	3214	3161	3161	110	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 17.

All (110) 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:31:GLU:OE1	1:A:35:ALA:CB	1.96	1.13
1:A:31:GLU:OE1	1:A:35:ALA:HB3	1.59	1.00
1:A:31:GLU:OE1	1:A:35:ALA:HB2	1.67	0.93
1:A:223:LEU:HD21	1:A:227:LEU:HD12	1.50	0.91
1:A:145:HIS:HB3	1:A:150:ASN:OD1	1.74	0.88
1:A:113:LEU:HD12	1:A:113:LEU:O	1.74	0.86
1:A:136:GLU:N	1:A:136:GLU:OE1	2.09	0.85
1:A:307:PHE:O	1:A:349:GLN:NE2	2.11	0.84
1:A:225:ASP:O	1:A:247:THR:HG21	1.81	0.80
1:A:408:GLN:O	1:A:408:GLN:NE2	2.22	0.72
1:A:74:ILE:O	1:A:74:ILE:HG22	1.93	0.69
1:A:266:LYS:O	1:A:311:ALA:HB3	1.95	0.66
1:A:319:ARG:O	1:A:333:TYR:OH	2.08	0.65
1:A:415:ASP:OD1	1:A:416:SER:N	2.32	0.62
1:A:201:SER:OG	1:A:205:THR:N	2.32	0.62
1:A:288:ASP:HA	1:A:352:LEU:HD22	1.82	0.61
1:A:113:LEU:O	1:A:113:LEU:CD1	2.49	0.60
1:A:306:GLN:OE1	1:A:319:ARG:NE	2.36	0.58
1:A:41:ARG:NH1	1:A:144:ASP:OD2	2.36	0.58
1:A:239:GLN:N	1:A:239:GLN:OE1	2.37	0.58
1:A:89:ARG:NE	1:A:128:ASP:O	2.30	0.58
1:A:242:GLN:O	1:A:244:GLN:NE2	2.37	0.57
1:A:56:LEU:HD23	1:A:108:TRP:CZ3	2.39	0.57
1:A:246:VAL:HG22	1:A:247:THR:H	1.70	0.57
1:A:322:MET:SD	1:A:322:MET:N	2.78	0.56
1:A:152:ALA:O	1:A:153:ASN:ND2	2.38	0.56
1:A:236:GLY:O	1:A:239:GLN:NE2	2.39	0.56
1:A:9:GLN:OE1	1:A:9:GLN:N	2.39	0.54
1:A:159:LEU:H	1:A:159:LEU:HD12	1.72	0.54
1:A:159:LEU:HD13	1:A:176:SER:HA	1.88	0.54
1:A:56:LEU:O	1:A:57:THR:OG1	2.22	0.54
1:A:5:GLY:O	1:A:8:ASN:ND2	2.37	0.53
1:A:351:ILE:O	1:A:354:ASN:OD1	2.28	0.52
1:A:189:ARG:HE	1:A:247:THR:HB	1.74	0.52
1:A:206:SER:N	1:A:207:PRO:CD	2.73	0.51
1:A:184:SER:O	1:A:248:LYS:HB3	2.10	0.51
1:A:182:ALA:HA	1:A:249:LYS:H	1.76	0.51
1:A:399:ASP:OD1	1:A:400:LEU:N	2.45	0.50
1:A:224:LEU:HD12	1:A:228:ASN:OD1	2.12	0.49
1:A:135:THR:HB	1:A:136:GLU:OE1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:GLN:OE1	1:A:352:LEU:HD12	2.13	0.48
1:A:376:ALA:HA	1:A:399:ASP:HB3	1.95	0.48
1:A:181:GLN:HB3	1:A:222:LEU:HD21	1.95	0.48
1:A:184:SER:CB	1:A:246:VAL:HG13	2.43	0.48
1:A:87:TYR:CG	1:A:131:ILE:O	2.67	0.48
1:A:185:ARG:O	1:A:248:LYS:N	2.46	0.48
1:A:364:PRO:HB2	1:A:365:PRO:HD3	1.96	0.48
1:A:303:GLN:NE2	1:A:345:ASN:OD1	2.46	0.47
1:A:249:LYS:HG2	1:A:250:SER:N	2.29	0.47
1:A:283:GLN:NE2	1:A:323:GLU:OE1	2.47	0.47
1:A:354:ASN:OD1	1:A:355:LYS:N	2.47	0.47
1:A:387:LYS:O	1:A:398:ALA:HB3	2.15	0.47
1:A:49:THR:HG22	1:A:50:ALA:N	2.30	0.47
1:A:184:SER:OG	1:A:185:ARG:N	2.46	0.47
1:A:198:THR:OG1	1:A:224:LEU:HA	2.15	0.46
1:A:223:LEU:O	1:A:223:LEU:HD23	2.15	0.46
1:A:15:ILE:HG13	1:A:15:ILE:O	2.16	0.46
1:A:224:LEU:O	1:A:228:ASN:HB2	2.16	0.46
1:A:144:ASP:O	1:A:144:ASP:OD1	2.32	0.46
1:A:4:ASN:HB2	1:A:8:ASN:ND2	2.31	0.46
1:A:86:TYR:CD1	1:A:87:TYR:N	2.83	0.46
1:A:195:ARG:HE	1:A:231:GLU:CD	2.20	0.45
1:A:293:ARG:HG3	1:A:294:GLN:H	1.80	0.45
1:A:349:GLN:O	1:A:353:LEU:HD13	2.17	0.45
1:A:371:ASP:OD1	1:A:372:LYS:N	2.50	0.45
1:A:112:TYR:CG	1:A:136:GLU:OE2	2.71	0.44
1:A:184:SER:HB3	1:A:246:VAL:HG13	2.00	0.44
1:A:86:TYR:OH	1:A:111:TYR:O	2.30	0.44
1:A:278:GLY:O	1:A:284:GLY:HA2	2.17	0.43
1:A:181:GLN:O	1:A:222:LEU:HD11	2.17	0.43
1:A:412:SER:HA	1:A:416:SER:O	2.19	0.43
1:A:112:TYR:CB	1:A:136:GLU:OE2	2.66	0.43
1:A:304:ILE:HD11	1:A:343:ASP:OD2	2.19	0.43
1:A:348:ASP:O	1:A:352:LEU:HG	2.18	0.43
1:A:92:ARG:O	1:A:104:LEU:HD13	2.19	0.43
1:A:184:SER:HG	1:A:185:ARG:H	1.65	0.43
1:A:355:LYS:HA	1:A:405:LYS:HZ2	1.83	0.43
1:A:209:ARG:O	1:A:221:LEU:HB2	2.19	0.43
1:A:39:GLN:C	1:A:40:ARG:HE	2.22	0.42
1:A:74:ILE:O	1:A:74:ILE:CG2	2.64	0.42
1:A:248:LYS:HG3	1:A:249:LYS:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:ARG:O	1:A:32:ARG:HD3	2.19	0.42
1:A:172:TYR:OH	1:A:200:GLY:O	2.34	0.42
1:A:277:ARG:CZ	1:A:277:ARG:H	2.33	0.42
1:A:354:ASN:OD1	1:A:354:ASN:C	2.57	0.42
1:A:38:LYS:O	1:A:40:ARG:NE	2.52	0.42
1:A:55:ALA:O	1:A:56:LEU:HD13	2.20	0.42
1:A:209:ARG:O	1:A:255:SER:OG	2.25	0.42
1:A:172:TYR:OH	1:A:201:SER:HA	2.20	0.42
1:A:301:TRP:N	1:A:302:PRO:CD	2.83	0.42
1:A:190:SER:C	1:A:232:SER:HB3	2.41	0.41
1:A:61:LYS:HE2	1:A:169:LYS:HB3	2.01	0.41
1:A:225:ASP:HB3	1:A:248:LYS:O	2.20	0.41
1:A:304:ILE:CG2	1:A:305:ALA:N	2.83	0.41
1:A:72:VAL:HG23	1:A:74:ILE:HG13	2.03	0.41
1:A:84:ILE:O	1:A:84:ILE:HG22	2.19	0.41
1:A:59:HIS:CD2	1:A:172:TYR:O	2.74	0.41
1:A:364:PRO:CB	1:A:365:PRO:HD3	2.50	0.41
1:A:184:SER:O	1:A:248:LYS:CD	2.69	0.41
1:A:221:LEU:C	1:A:221:LEU:HD13	2.41	0.41
1:A:343:ASP:OD1	1:A:344:PRO:N	2.54	0.41
1:A:144:ASP:O	1:A:144:ASP:CG	2.60	0.41
1:A:225:ASP:O	1:A:247:THR:CG2	2.63	0.40
1:A:285:ASN:HB2	1:A:356:HIS:CB	2.51	0.40
1:A:168:PRO:O	1:A:202:SER:C	2.59	0.40
1:A:181:GLN:NE2	1:A:248:LYS:HA	2.36	0.40
1:A:355:LYS:HA	1:A:405:LYS:NZ	2.37	0.40
1:A:373:LYS:HE3	1:A:397:ALA:HB3	2.03	0.40
1:A:110:PHE:CD1	1:A:110:PHE:C	2.94	0.40
1:A:189:ARG:HH11	1:A:247:THR:HG22	1.85	0.40

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	417/419 (100%)	332 (80%)	85 (20%)	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	339/339 (100%)	327 (96%)	12 (4%)	36 36

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ARG
1	A	53	PHE
1	A	86	TYR
1	A	89	ARG
1	A	110	PHE
1	A	132	TRP
1	A	189	ARG
1	A	274	PHE
1	A	277	ARG
1	A	286	PHE
1	A	345	ASN
1	A	403	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

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

There are no ligands in this entry.

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.

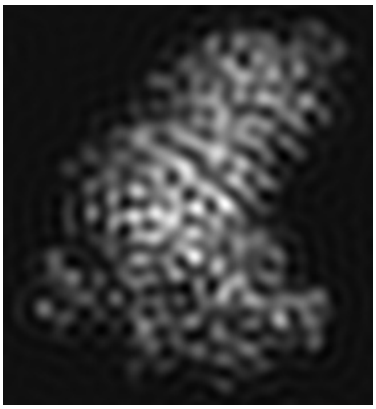
6 Map visualisation

This section contains visualisations of the EMDB entry D_9100078306. These allow visual inspection of the internal detail of the map and identification of artifacts.

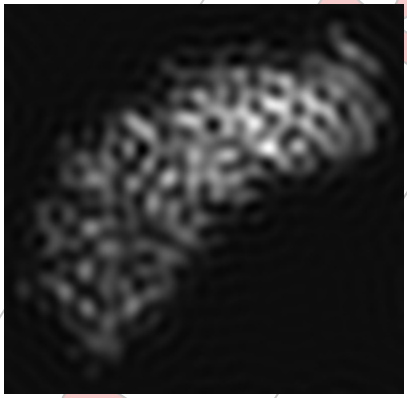
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

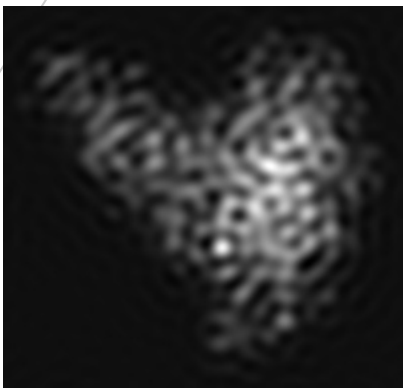
6.1.1 Primary map



X



Y



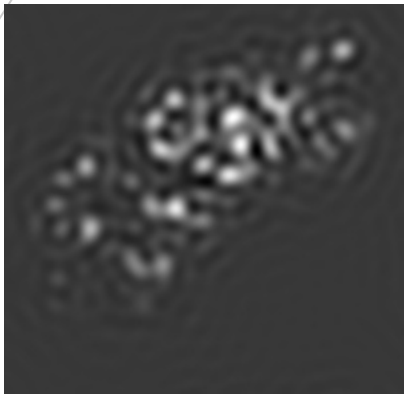
Z

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

6.2 Central slices

6.2.1 Primary map

X Index: 51



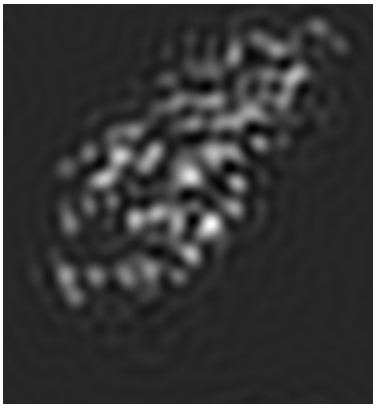
Y Index: 48

Z Index: 52

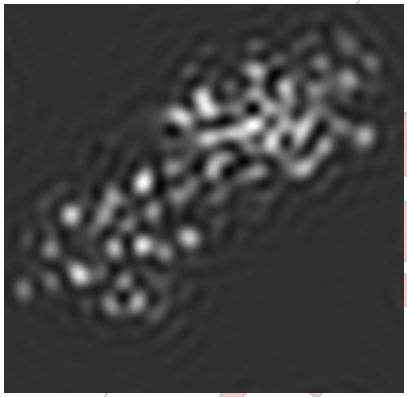
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

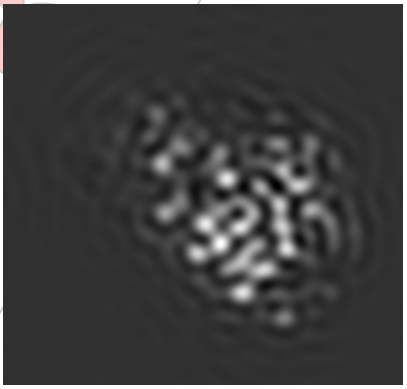
6.3.1 Primary map



X Index: 71



Y Index: 56

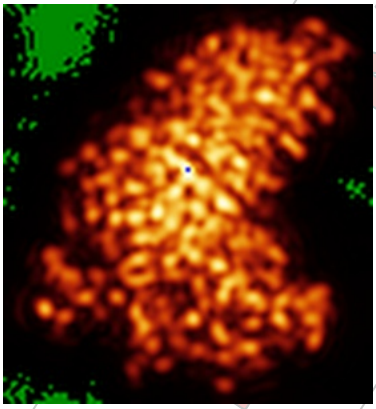


Z Index: 49

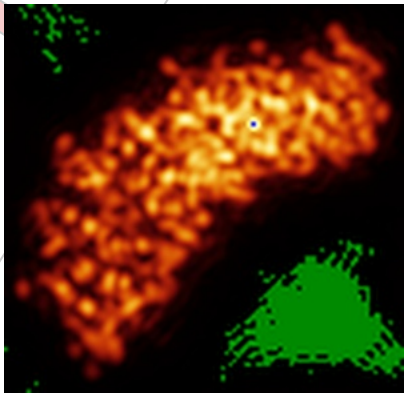
The images above show the largest variance slices of the map in three orthogonal directions.

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

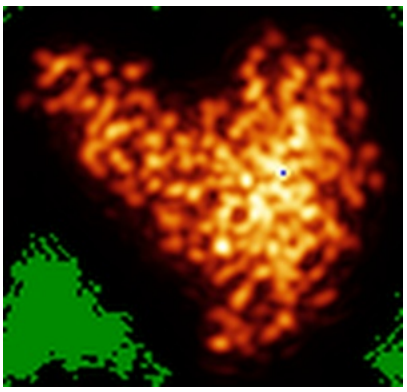
6.4.1 Primary map



X



Y

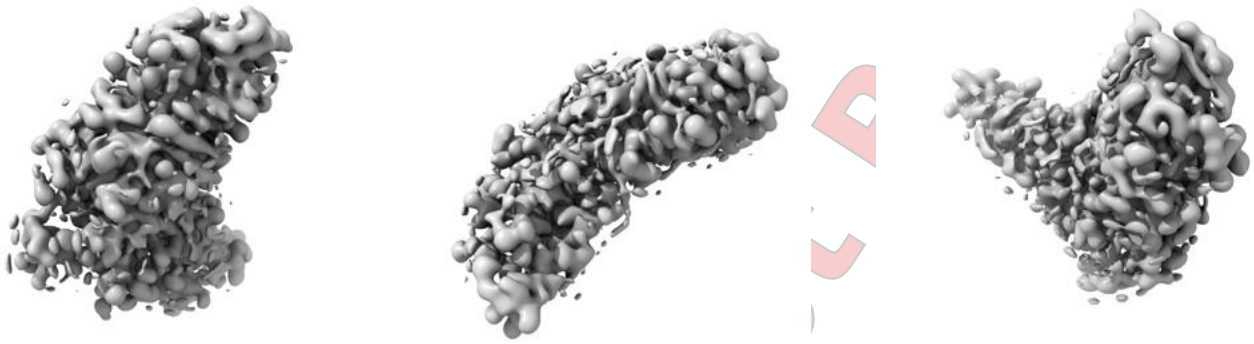


Z

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 0.9. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

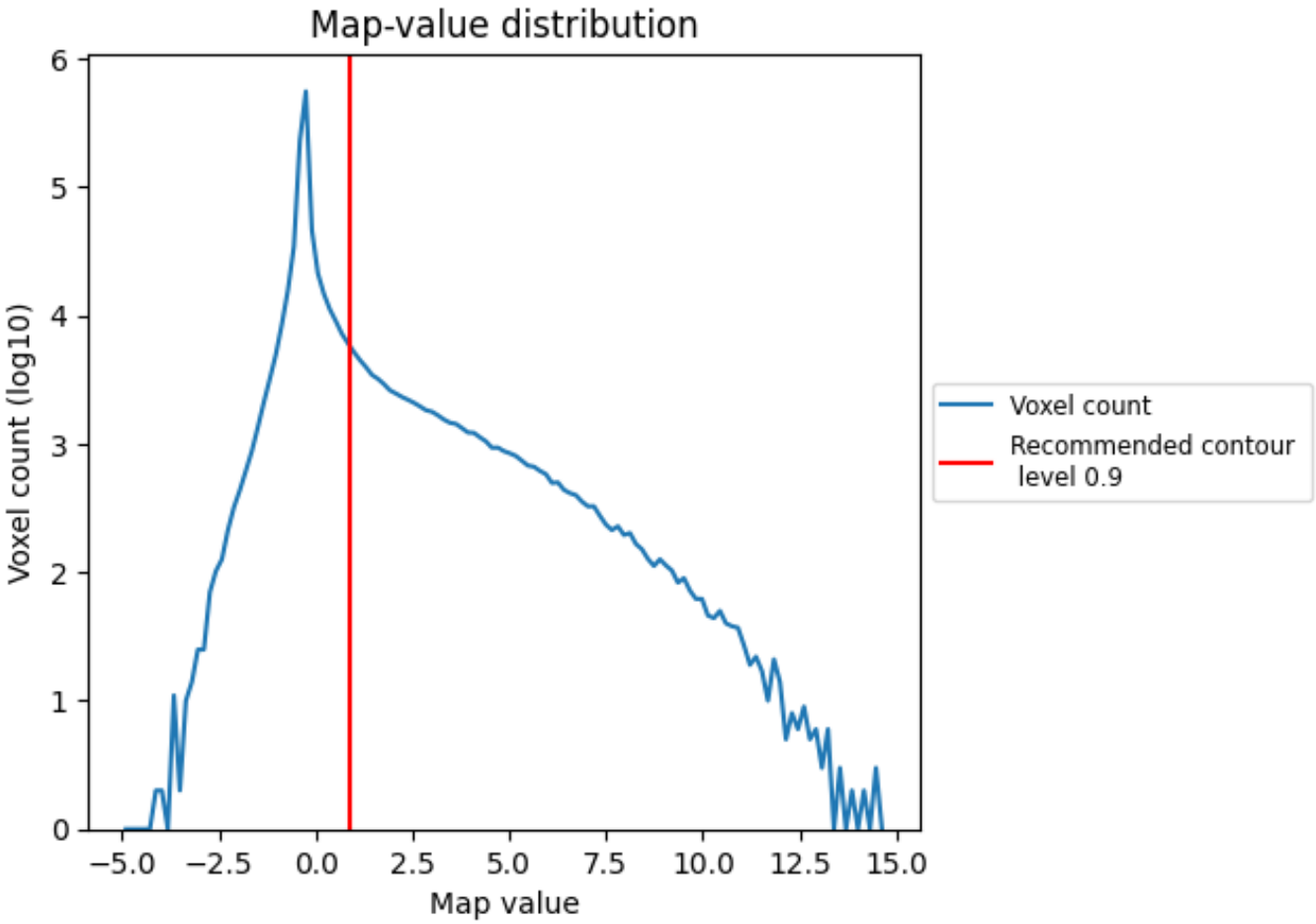
6.6 Mask visualisation (i)

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

7 Map analysis

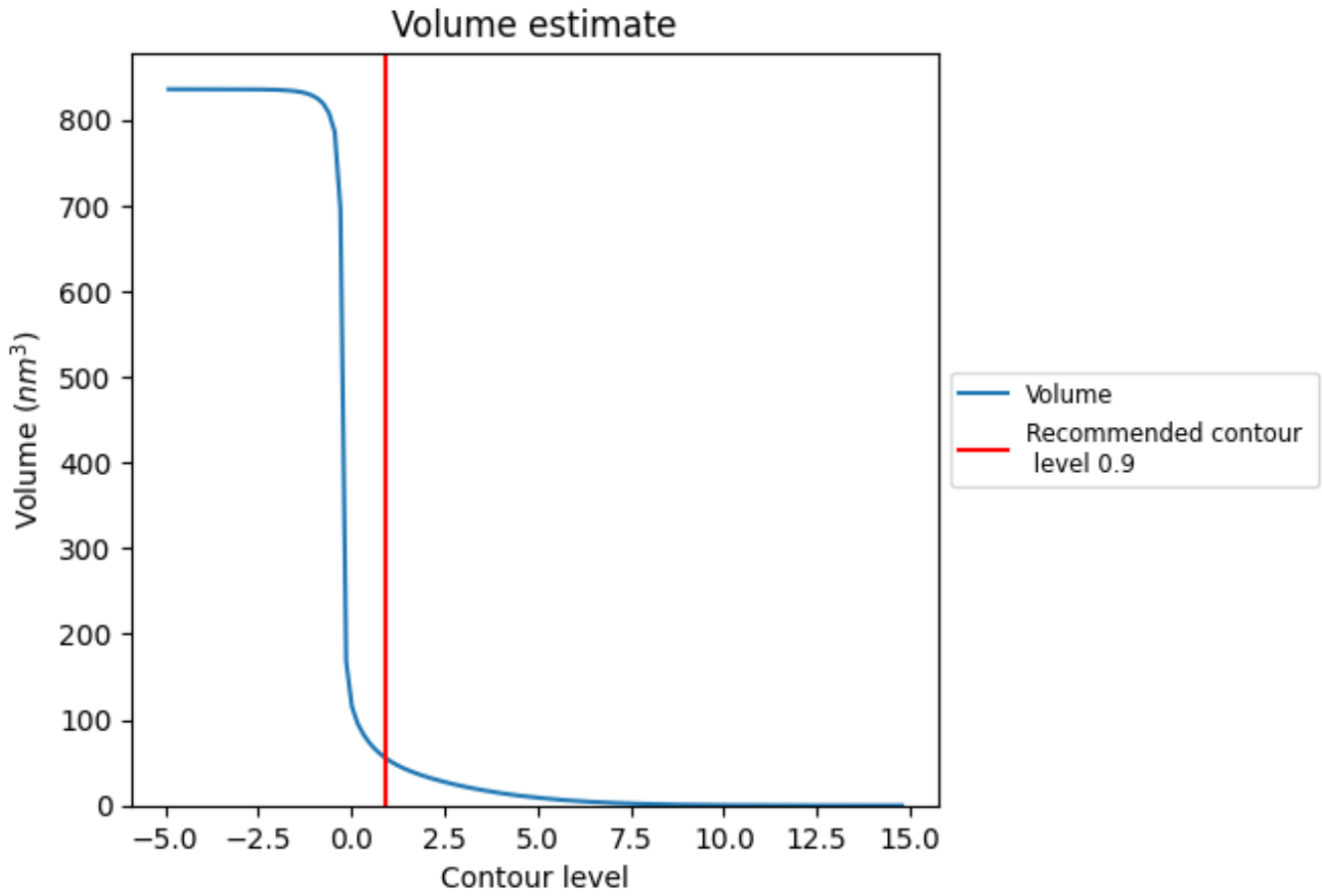
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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 56 nm^3; this corresponds to an approximate mass of 51 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)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

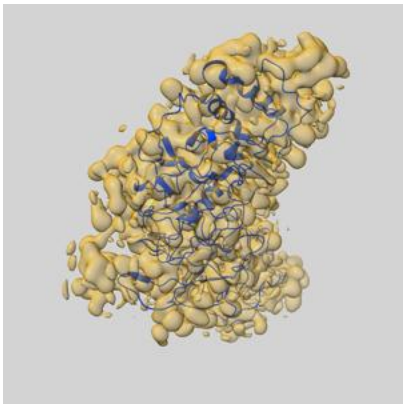
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

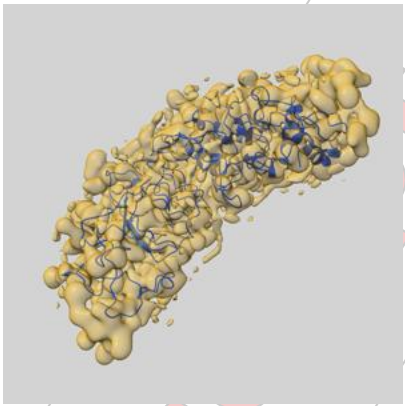
9 Map-model fit

This section contains information regarding the fit between EMDB map D_9100078306 and PDB model D_9100078306. Per-residue inclusion information can be found in section 3 on page 4.

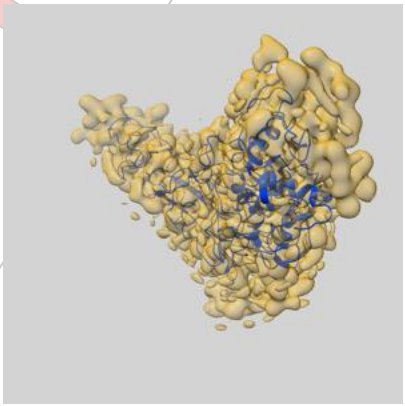
9.1 Map-model overlay



X



Y



Z

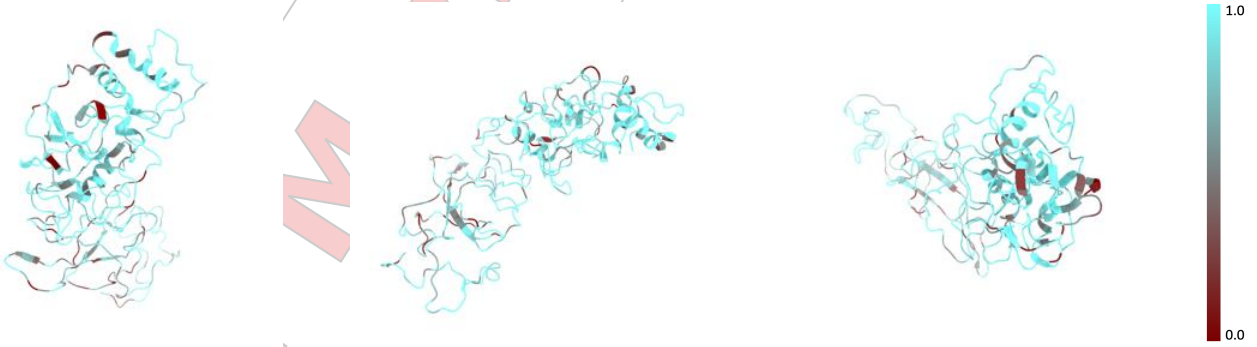
The images above show the 3D surface view of the map at the recommended contour level 0.9 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model

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.

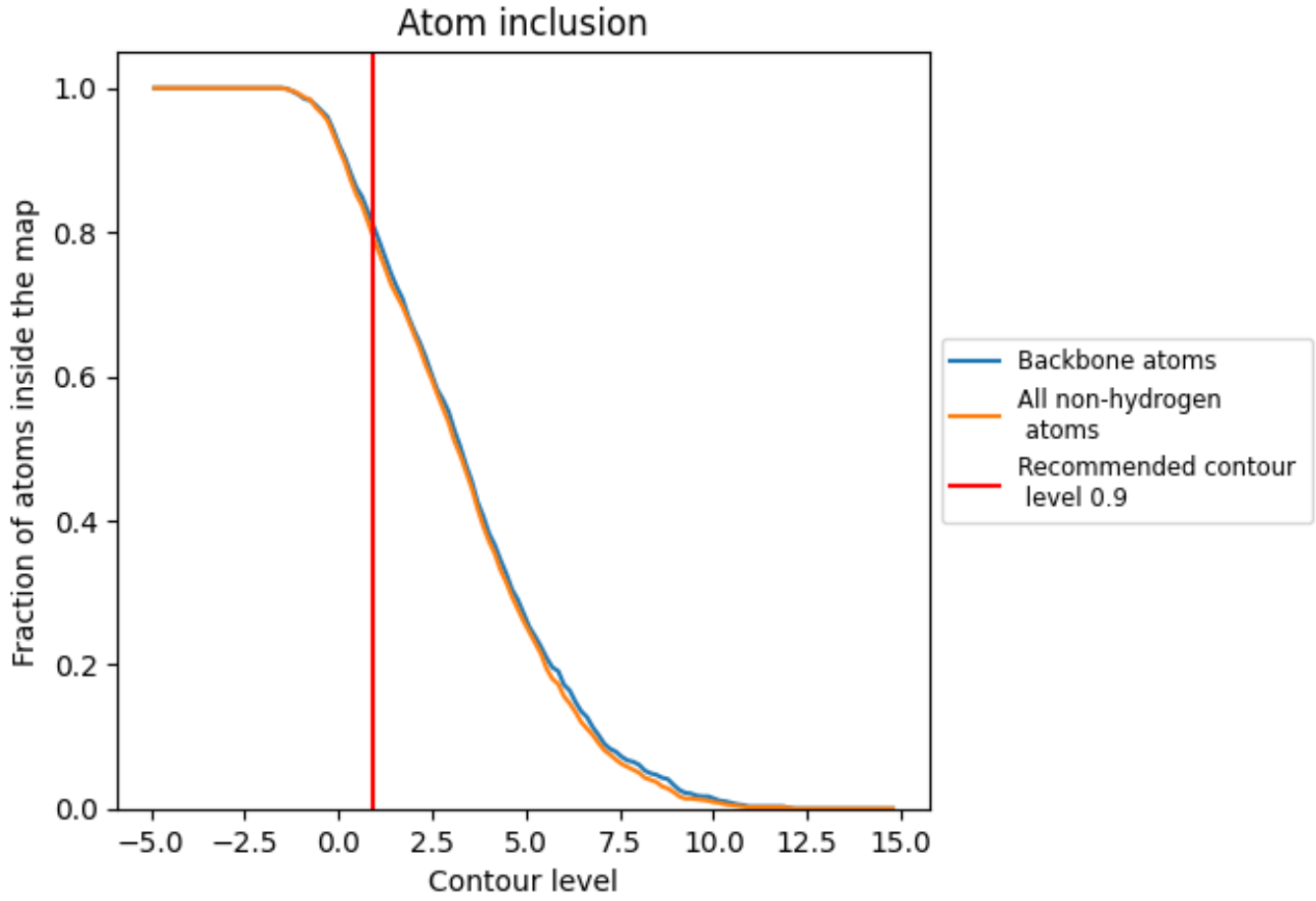
9.3 Atom inclusion mapped to coordinate model



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 (0.9).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 80% 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 (0.9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7980	0.2410
A	0.7940	0.2410

Full wwPDB EM Validation Report ⓘ

May 2, 2023 – 03:49 PM EDT

PDB ID	:	8SOF
EMDB ID	:	EMD-40656
Title	:	Nucleocapsid dimer from SARS-CoV-2, flexible conformation 1
Deposited on	:	2023-04-28
Resolution	:	5.40 Å(reported)
Based on initial model	:	.

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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:

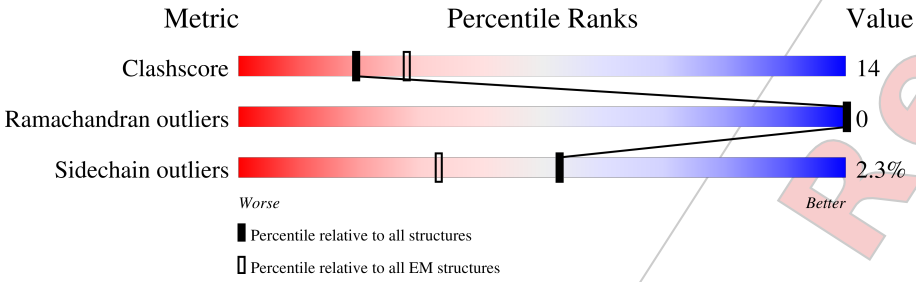
EMDB validation analysis	:	0.0.1.dev50
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

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 5.40 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 >=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	A	419	16% 74% 19% • 5%
1	B	419	26% 64% 24% 12%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 11608 atoms, of which 5746 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 Nucleoprotein.

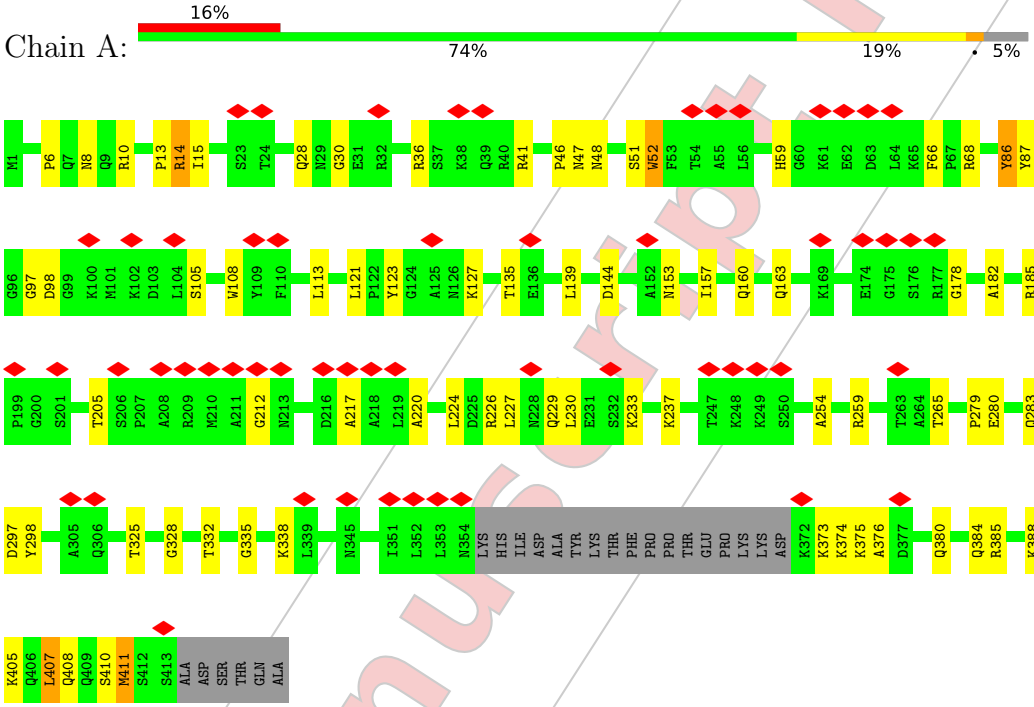
Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	396	Total	C	H	N	O	S	0	0
			6008	1856	2978	576	591	7		
1	B	368	Total	C	H	N	O	S	0	0
			5600	1733	2768	537	558	4		

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.

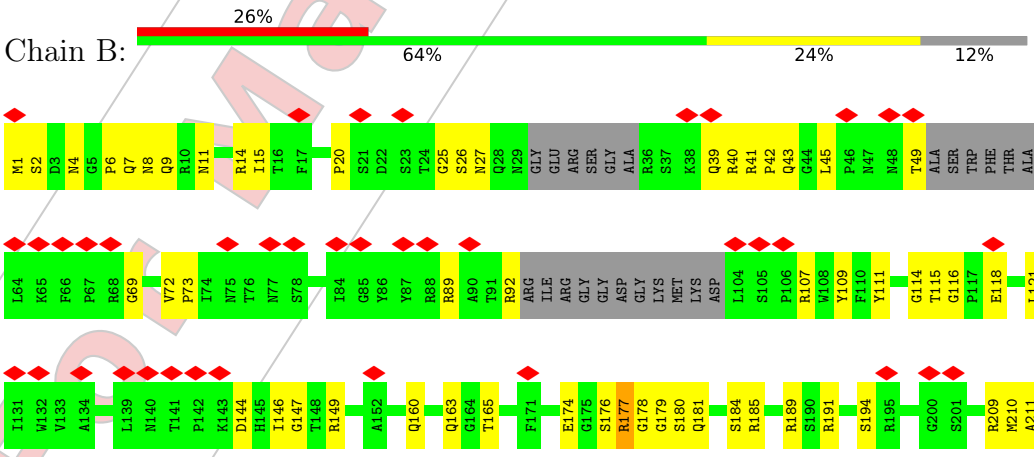
- Molecule 1: Nucleoprotein

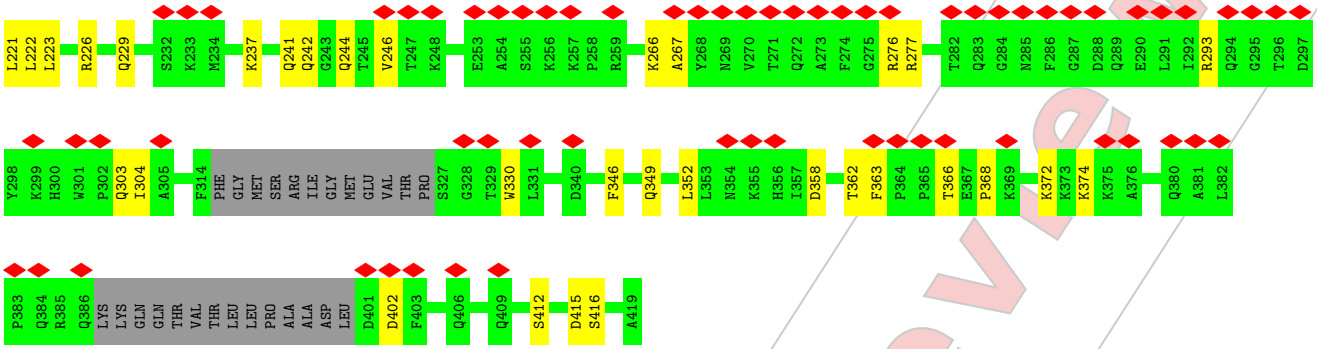
Chain A:



- Molecule 1: Nucleoprotein

Chain B:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	10000	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	29.300	Depositor
Minimum map value	-2.543	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	117.6, 107.799995, 127.4	wwPDB
Map dimensions	84, 77, 91	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	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	1.85	7/3088 (0.2%)	0.80	10/4161 (0.2%)
1	B	0.34	0/2886	0.63	1/3887 (0.0%)
All	All	1.35	7/5974 (0.1%)	0.73	11/8048 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	403	PHE	CE2-CZ	45.40	2.23	1.37
1	A	403	PHE	CE1-CZ	45.26	2.23	1.37
1	A	403	PHE	CD1-CE1	45.14	2.29	1.39
1	A	403	PHE	CD2-CE2	44.43	2.28	1.39
1	A	403	PHE	CG-CD1	28.60	1.81	1.38
1	A	403	PHE	CG-CD2	28.03	1.80	1.38
1	A	407	LEU	CB-CG	23.85	2.21	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	407	LEU	CA-CB-CG	21.90	165.67	115.30
1	A	407	LEU	CB-CG-CD2	13.43	133.83	111.00
1	A	279	PRO	CA-N-CD	-12.21	94.41	111.50
1	A	396	PRO	CA-N-CD	-11.57	95.30	111.50
1	A	407	LEU	CB-CG-CD1	11.27	130.16	111.00
1	A	279	PRO	N-CD-CG	-7.67	91.69	103.20
1	A	407	LEU	CD1-CG-CD2	-6.66	90.53	110.50
1	B	144	ASP	CB-CG-OD1	5.83	123.54	118.30
1	A	403	PHE	CB-CG-CD2	-5.65	116.85	120.80
1	A	403	PHE	CD1-CG-CD2	5.59	125.57	118.30
1	A	396	PRO	N-CD-CG	-5.54	94.89	103.20

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	3030	2978	2980	92	0
1	B	2832	2768	2763	71	0
All	All	5862	5746	5743	163	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 14.

All (163) 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:403:PHE:CD2	1:A:403:PHE:CG	1.80	1.65
1:A:403:PHE:CG	1:A:403:PHE:CD1	1.81	1.64
1:A:403:PHE:CD1	1:A:407:LEU:HB3	1.52	1.45
1:A:403:PHE:CZ	1:A:407:LEU:HG	1.53	1.44
1:A:403:PHE:CD2	1:A:407:LEU:HB2	1.56	1.41
1:A:403:PHE:CG	1:A:407:LEU:HB3	1.63	1.31
1:A:403:PHE:CE2	1:A:407:LEU:HB2	1.63	1.31
1:A:403:PHE:CZ	1:A:403:PHE:CE2	2.23	1.26
1:A:403:PHE:CZ	1:A:403:PHE:CE1	2.23	1.26
1:A:403:PHE:CE2	1:A:407:LEU:CB	2.20	1.24
1:A:403:PHE:CD2	1:A:407:LEU:CB	2.23	1.22
1:A:403:PHE:CD2	1:A:403:PHE:CE2	2.28	1.21
1:A:403:PHE:CD1	1:A:403:PHE:CE1	2.29	1.20
1:A:403:PHE:CD1	1:A:407:LEU:CB	2.25	1.19
1:A:403:PHE:CE1	1:A:407:LEU:CB	2.25	1.19
1:A:403:PHE:CZ	1:A:407:LEU:CB	2.26	1.18
1:A:407:LEU:CB	1:A:407:LEU:CG	2.21	1.17
1:A:407:LEU:HG	1:A:407:LEU:CB	1.79	1.12
1:A:403:PHE:CG	1:A:407:LEU:CB	2.32	1.11
1:A:403:PHE:CE2	1:A:407:LEU:HG	1.92	1.05
1:A:403:PHE:CZ	1:A:407:LEU:CG	2.47	0.97
1:A:403:PHE:CE1	1:A:407:LEU:CG	2.48	0.95
1:A:403:PHE:CE2	1:A:407:LEU:CG	2.52	0.91
1:A:403:PHE:CD1	1:A:407:LEU:CG	2.56	0.88
1:A:403:PHE:CD2	1:A:407:LEU:CG	2.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:PHE:CE1	1:A:407:LEU:HG	2.19	0.78
1:A:403:PHE:CG	1:A:407:LEU:CG	2.68	0.76
1:B:8:ASN:OD1	1:B:43:GLN:NE2	2.19	0.76
1:B:412:SER:O	1:B:416:SER:N	2.20	0.73
1:B:9:GLN:OE1	1:B:43:GLN:NE2	2.22	0.72
1:B:60:GLY:HA3	1:B:212:GLY:H	1.54	0.72
1:B:219:LEU:HA	1:B:223:LEU:HD13	1.72	0.71
1:A:376:ALA:HA	1:A:404:SER:HB2	1.72	0.70
1:A:403:PHE:CD2	1:A:407:LEU:HB3	2.25	0.70
1:A:13:PRO:HG2	1:A:15:ILE:HG12	1.74	0.70
1:A:293:ARG:HB2	1:A:384:GLN:HE21	1.56	0.70
1:B:15:ILE:HG12	1:B:26:SER:H	1.56	0.69
1:A:287:GLY:HA3	1:A:396:PRO:HD3	1.75	0.69
1:B:7:GLN:HG2	1:B:40:ARG:H	1.58	0.68
1:A:403:PHE:CE1	1:A:407:LEU:CD2	2.76	0.68
1:A:265:THR:HA	1:A:335:GLY:H	1.60	0.66
1:B:123:TYR:HB2	1:B:128:ASP:HB2	1.77	0.66
1:B:346:PHE:HA	1:B:349:GLN:HG3	1.77	0.66
1:A:10:ARG:HH22	1:A:113:LEU:H	1.43	0.65
1:A:403:PHE:CD2	1:A:407:LEU:CD1	2.78	0.65
1:B:60:GLY:O	1:B:214:GLY:N	2.30	0.65
1:A:292:ILE:HG22	1:A:293:ARG:HG3	1.78	0.64
1:A:66:PHE:HD2	1:A:135:THR:HG23	1.64	0.63
1:A:14:ARG:HD3	1:A:30:GLY:HA3	1.80	0.63
1:B:209:ARG:HH11	1:B:221:LEU:HD13	1.63	0.62
1:A:396:PRO:O	1:A:396:PRO:HD2	1.97	0.62
1:B:40:ARG:HG3	1:B:41:ARG:HG2	1.80	0.62
1:B:9:GLN:H	1:B:43:GLN:HE22	1.48	0.61
1:A:375:LYS:O	1:A:408:GLN:NE2	2.25	0.60
1:A:373:LYS:O	1:A:405:LYS:NZ	2.34	0.60
1:A:384:GLN:O	1:A:385:ARG:NH2	2.34	0.59
1:A:157:ILE:H	1:A:178:GLY:HA3	1.66	0.59
1:A:41:ARG:NH1	1:A:47:ASN:OD1	2.38	0.57
1:B:109:TYR:OH	1:B:181:GLN:OE1	2.23	0.57
1:A:10:ARG:NH1	1:A:86:TYR:OH	2.38	0.56
1:A:325:THR:OG1	1:A:328:GLY:O	2.23	0.56
1:B:89:ARG:HH12	1:B:127:LYS:HD2	1.69	0.56
1:A:6:PRO:HG3	1:A:46:PRO:HD3	1.86	0.56
1:B:293:ARG:NH2	1:B:368:PRO:O	2.36	0.55
1:B:147:GLY:O	1:B:149:ARG:NH2	2.40	0.55
1:A:205:THR:H	1:A:220:ALA:HB1	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:PHE:HB3	1:A:400:LEU:HB3	1.88	0.54
1:A:294:GLN:HG2	1:A:388:LYS:HB3	1.89	0.54
1:B:146:ILE:O	1:B:149:ARG:NH1	2.27	0.54
1:A:121:LEU:HD23	1:A:123:TYR:H	1.73	0.54
1:B:125:ALA:N	1:B:128:ASP:OD2	2.39	0.54
1:A:332:THR:HG22	1:A:338:LYS:HE3	1.88	0.54
1:A:160:GLN:HE21	1:A:229:GLN:HB3	1.73	0.54
1:B:189:ARG:NH2	1:B:241:GLN:OE1	2.37	0.54
1:A:97:GLY:HA3	1:A:217:ALA:H	1.72	0.54
1:A:294:GLN:NE2	1:A:385:ARG:O	2.34	0.54
1:B:177:ARG:HH21	1:B:178:GLY:N	2.06	0.54
1:A:403:PHE:CE1	1:A:407:LEU:HD23	2.43	0.53
1:A:51:SER:OG	1:A:52:TRP:N	2.41	0.52
1:B:9:GLN:OE1	1:B:9:GLN:N	2.41	0.52
1:B:163:GLN:HB3	1:B:194:SER:HA	1.91	0.52
1:A:144:ASP:OD1	1:A:185:ARG:NH2	2.42	0.52
1:B:191:ARG:NH2	1:B:241:GLN:OE1	2.42	0.52
1:A:404:SER:OG	1:A:405:LYS:N	2.43	0.52
1:B:177:ARG:HB3	1:B:180:SER:HB3	1.92	0.52
1:B:42:PRO:HG2	1:B:118:GLU:HA	1.90	0.52
1:B:49:THR:HG22	1:B:92:ARG:HG2	1.93	0.51
1:B:226:ARG:HD2	1:B:229:GLN:HE21	1.76	0.51
1:A:15:ILE:O	1:A:36:ARG:NE	2.43	0.51
1:B:43:GLN:HG3	1:B:114:GLY:H	1.76	0.51
1:A:407:LEU:O	1:A:410:SER:OG	2.24	0.51
1:A:163:GLN:HE22	1:A:233:LYS:HB2	1.76	0.50
1:A:227:LEU:HA	1:A:230:LEU:HG	1.93	0.50
1:A:68:ARG:HG2	1:A:139:LEU:H	1.77	0.50
1:A:403:PHE:CE1	1:A:407:LEU:C	2.85	0.50
1:B:174:GLU:N	1:B:174:GLU:OE1	2.44	0.50
1:A:98:ASP:HB2	1:A:212:GLY:HA2	1.93	0.49
1:B:69:GLY:O	1:B:165:THR:OG1	2.23	0.49
1:A:404:SER:O	1:A:408:GLN:HG2	2.13	0.49
1:B:14:ARG:HG3	1:B:20:PRO:HB3	1.94	0.48
1:B:372:LYS:NZ	1:B:374:LYS:H	2.11	0.48
1:A:224:LEU:HD23	1:A:227:LEU:HD21	1.95	0.48
1:B:58:GLN:HG2	1:B:210:MET:HG3	1.95	0.48
1:B:303:GLN:CD	1:B:304:ILE:H	2.17	0.48
1:B:160:GLN:OE1	1:B:226:ARG:NH1	2.46	0.47
1:A:160:GLN:HG2	1:A:229:GLN:HB3	1.96	0.47
1:B:8:ASN:N	1:B:11:ASN:OD1	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:GLY:HA2	1:A:400:LEU:HB2	1.96	0.47
1:A:403:PHE:CD2	1:A:403:PHE:CB	2.85	0.47
1:B:6:PRO:HD2	1:B:41:ARG:HD2	1.96	0.47
1:B:42:PRO:O	1:B:116:GLY:N	2.48	0.47
1:B:60:GLY:CA	1:B:212:GLY:H	2.23	0.47
1:B:184:SER:O	1:B:185:ARG:NH2	2.48	0.47
1:B:277:ARG:HD2	1:B:330:TRP:CD1	2.50	0.47
1:B:107:ARG:HH22	1:B:176:SER:HB2	1.80	0.46
1:B:181:GLN:O	1:B:185:ARG:NH2	2.46	0.46
1:A:254:ALA:HB1	1:A:259:ARG:HB2	1.97	0.46
1:A:403:PHE:CD1	1:A:407:LEU:CD2	2.99	0.46
1:B:25:GLY:O	1:B:27:ASN:ND2	2.49	0.46
1:A:153:ASN:HD21	1:A:182:ALA:HB3	1.80	0.45
1:B:415:ASP:OD1	1:B:416:SER:N	2.50	0.45
1:B:210:MET:SD	1:B:211:ALA:N	2.89	0.45
1:B:45:LEU:N	1:B:115:THR:O	2.50	0.45
1:B:177:ARG:O	1:B:181:GLN:N	2.39	0.45
1:A:403:PHE:CZ	1:A:407:LEU:CA	2.99	0.45
1:B:177:ARG:HH21	1:B:178:GLY:H	1.64	0.44
1:B:4:ASN:ND2	1:B:149:ARG:H	2.15	0.44
1:B:123:TYR:CZ	1:B:126:ASN:HA	2.52	0.44
1:A:287:GLY:HA3	1:A:396:PRO:CD	2.44	0.44
1:B:177:ARG:HD3	1:B:179:GLY:N	2.31	0.44
1:B:226:ARG:HD2	1:B:229:GLN:NE2	2.33	0.43
1:B:177:ARG:HD3	1:B:179:GLY:H	1.84	0.43
1:A:292:ILE:HG12	1:A:380:GLN:HA	1.99	0.43
1:A:88:ARG:HH12	1:A:127:LYS:HB3	1.84	0.43
1:A:87:TYR:HA	1:A:108:TRP:CD1	2.54	0.42
1:B:61:LYS:HD2	1:B:216:ASP:HA	2.00	0.42
1:B:374:LYS:NZ	1:B:402:ASP:OD2	2.46	0.42
1:B:363:PHE:HB3	1:B:366:THR:HG23	2.00	0.42
1:A:403:PHE:CD1	1:A:403:PHE:O	2.73	0.42
1:B:7:GLN:HG2	1:B:39:GLN:HA	2.02	0.42
1:A:374:LYS:HB3	1:A:405:LYS:HZ1	1.84	0.42
1:B:266:LYS:HG3	1:B:267:ALA:H	1.84	0.42
1:A:14:ARG:HG2	1:A:28:GLN:O	2.19	0.42
1:B:349:GLN:HA	1:B:352:LEU:HB2	2.01	0.42
1:B:244:GLN:HB3	1:B:246:VAL:HG23	2.01	0.42
1:A:97:GLY:HA3	1:A:217:ALA:HB3	2.01	0.42
1:A:403:PHE:CE1	1:A:407:LEU:CA	3.01	0.42
1:B:61:LYS:HB3	1:B:215:GLY:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:ARG:NH2	1:A:229:GLN:OE1	2.53	0.41
1:B:177:ARG:HD3	1:B:180:SER:H	1.85	0.41
1:A:59:HIS:HA	1:A:105:SER:HB2	2.02	0.41
1:A:280:GLU:HG3	1:A:283:GLN:HE22	1.84	0.41
1:B:121:LEU:HD13	1:B:123:TYR:CE1	2.55	0.41
1:B:242:GLN:HE22	1:B:244:GLN:HB2	1.85	0.41
1:B:358:ASP:OD1	1:B:362:THR:OG1	2.38	0.41
1:A:10:ARG:NH2	1:A:113:LEU:H	2.15	0.41
1:B:121:LEU:HD12	1:B:121:LEU:O	2.21	0.41
1:B:177:ARG:NH2	1:B:179:GLY:H	2.18	0.41
1:A:46:PRO:HG2	1:A:48:ASN:O	2.21	0.40
1:A:8:ASN:OD1	1:A:8:ASN:N	2.52	0.40
1:B:72:VAL:HA	1:B:73:PRO:HD3	1.96	0.40
1:A:407:LEU:O	1:A:411:MET:HG3	2.22	0.40
1:B:1:MET:HB3	1:B:2:SER:H	1.64	0.40

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	392/419 (94%)	330 (84%)	62 (16%)	0	100	100
1	B	356/419 (85%)	303 (85%)	53 (15%)	0	100	100
All	All	748/838 (89%)	633 (85%)	115 (15%)	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	318/339 (94%)	310 (98%)	8 (2%)	47	68
1	B	300/339 (88%)	294 (98%)	6 (2%)	55	73
All	All	618/678 (91%)	604 (98%)	14 (2%)	53	70

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	52	TRP
1	A	86	TYR
1	A	189	ARG
1	A	237	LYS
1	A	297	ASP
1	A	298	TYR
1	A	411	MET
1	B	111	TYR
1	B	177	ARG
1	B	219	LEU
1	B	222	LEU
1	B	237	LYS
1	B	276	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	27	ASN
1	B	229	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 (i)

There are no monosaccharides 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 (i)

There are no chain breaks in this entry.

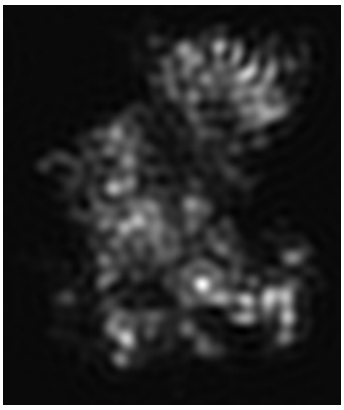
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-40656. These allow visual inspection of the internal detail of the map and identification of artifacts.

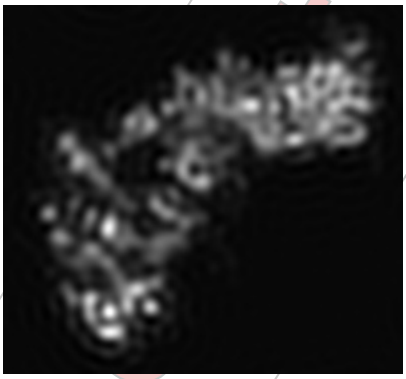
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

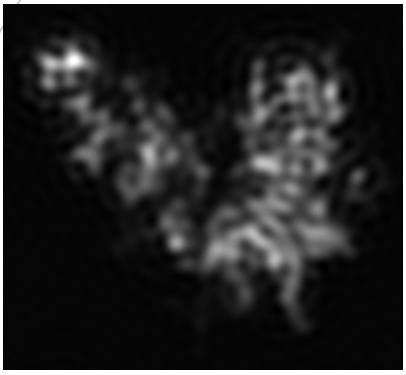
6.1.1 Primary map



X

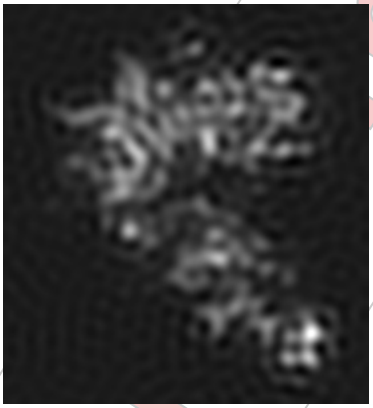


Y

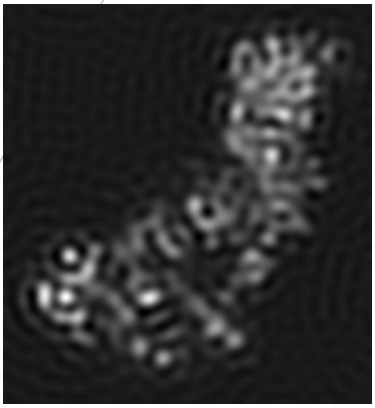


Z

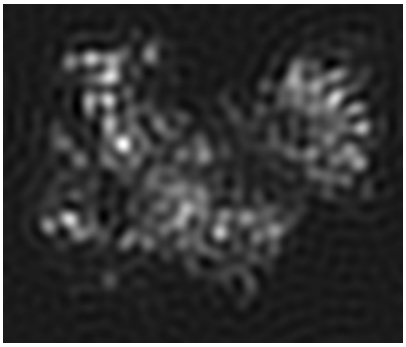
6.1.2 Raw map



X



Y

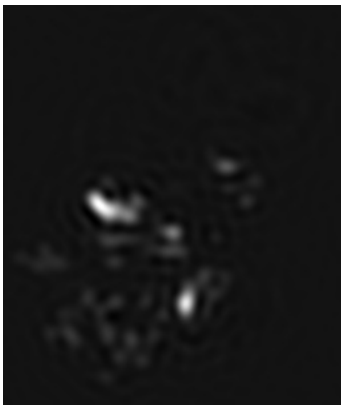


Z

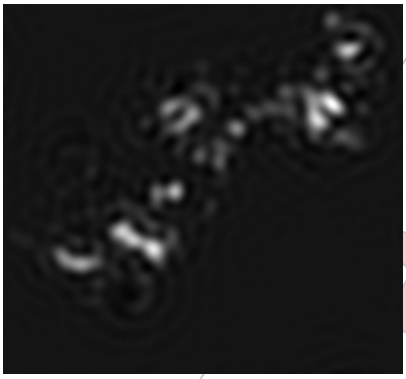
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

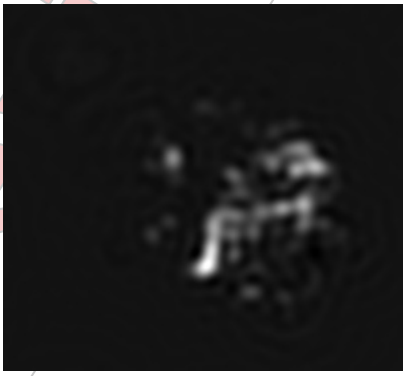
6.2.1 Primary map



X Index: 42

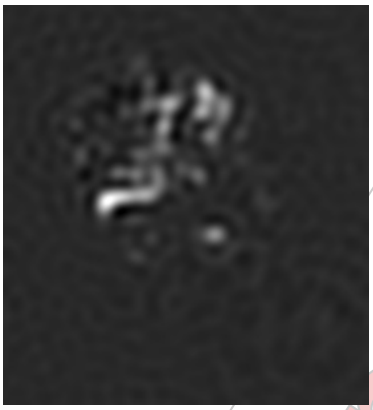


Y Index: 38

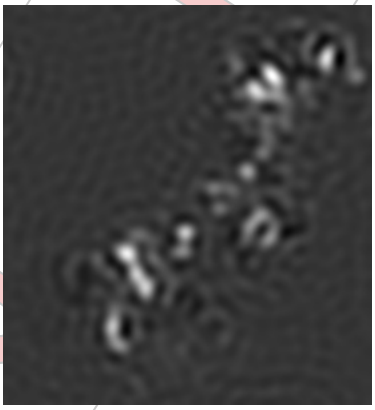


Z Index: 45

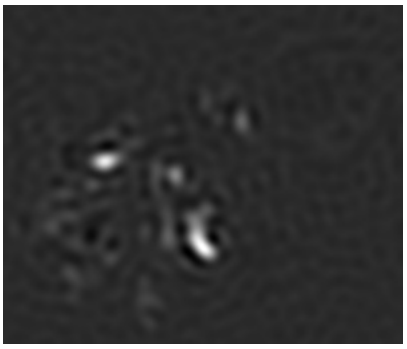
6.2.2 Raw map



X Index: 45



Y Index: 38

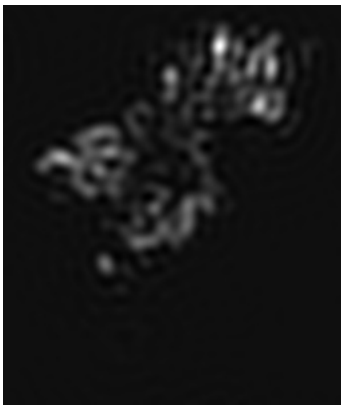


Z Index: 42

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

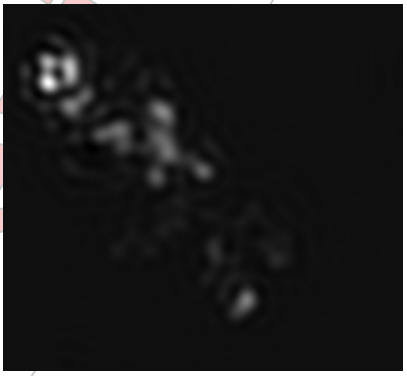
6.3 Largest variance slices (i)

6.3.1 Primary map



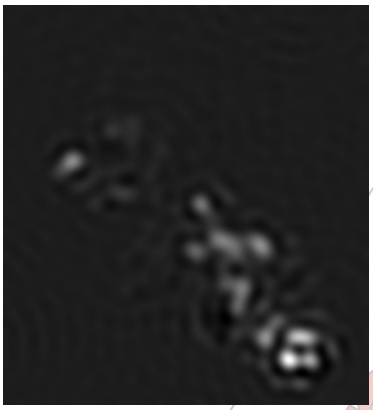
X Index: 61

Y Index: 64

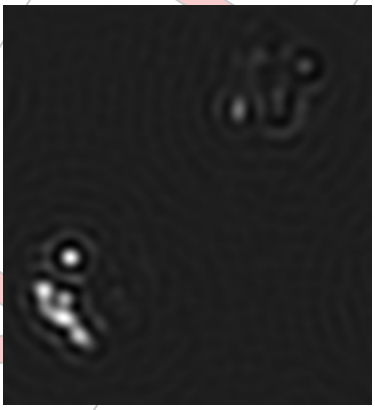


Z Index: 24

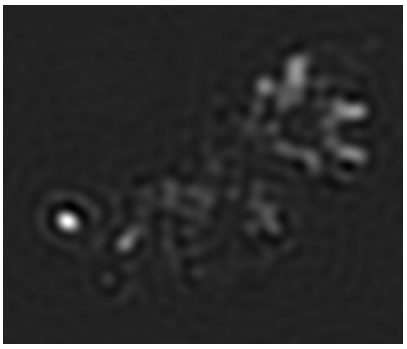
6.3.2 Raw map



X Index: 24



Y Index: 64

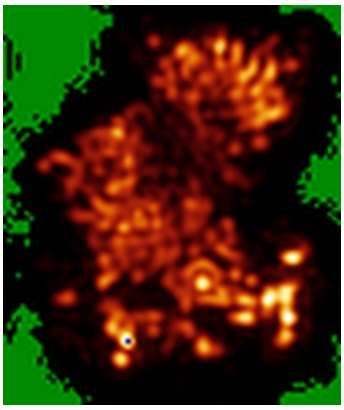


Z Index: 53

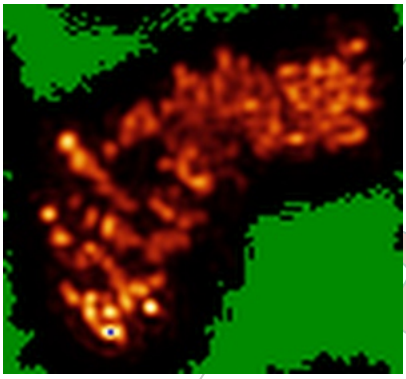
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color)

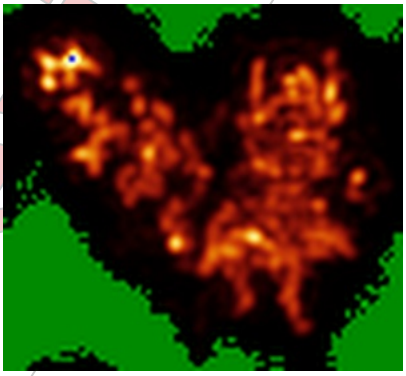
6.4.1 Primary map



X

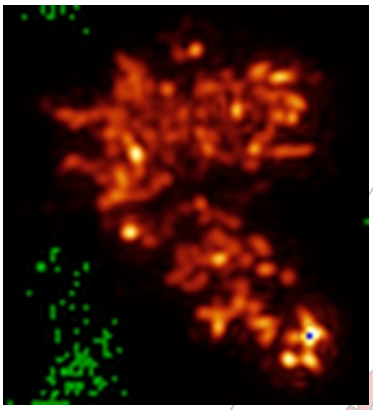


Y

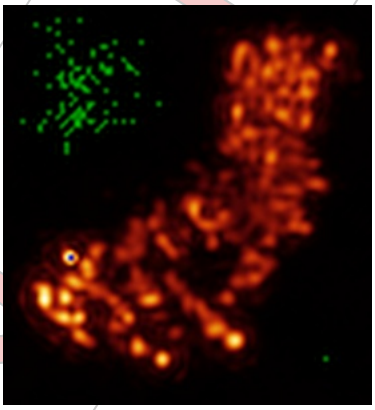


Z

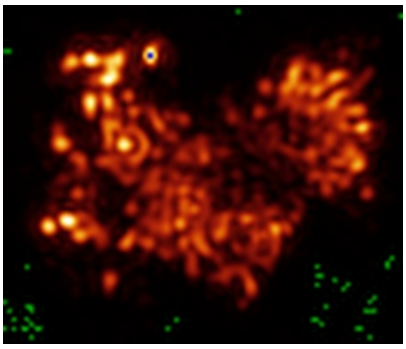
6.4.2 Raw map



X



Y

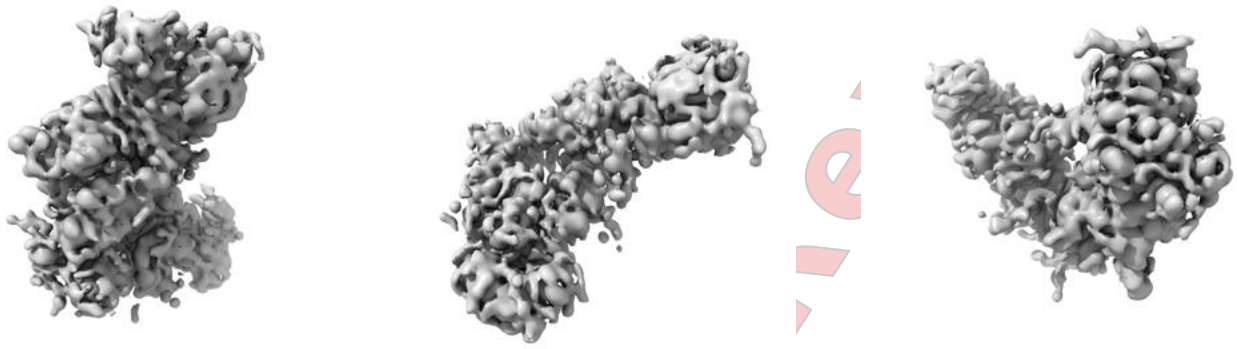


Z

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)

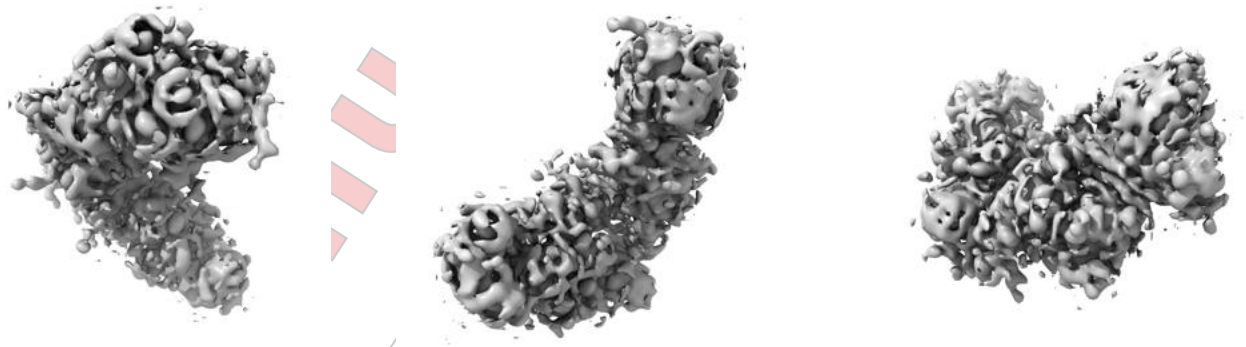
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.4. 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.

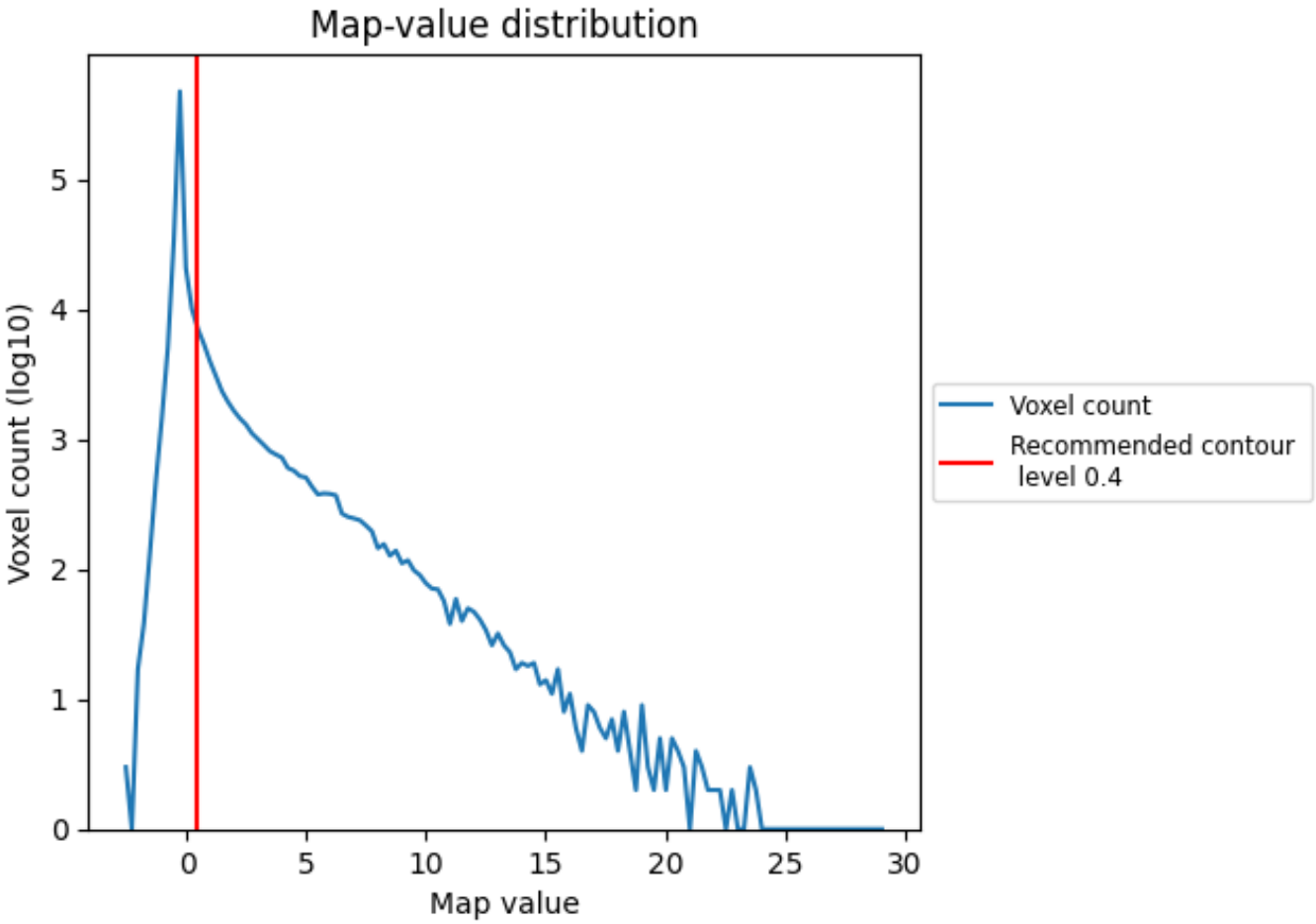
6.6 Mask visualisation (i)

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

7 Map analysis

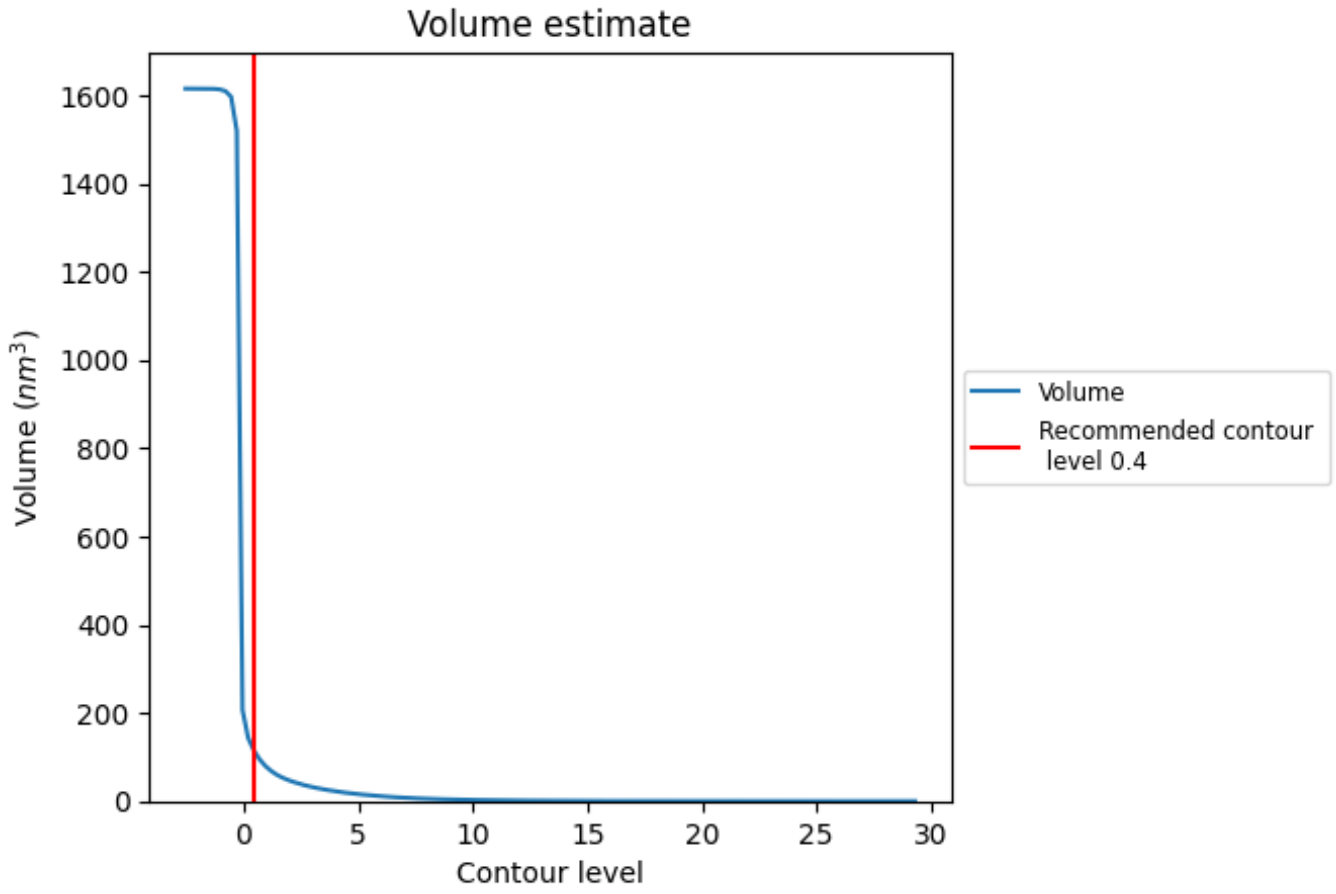
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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 119 nm^3; this corresponds to an approximate mass of 108 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.

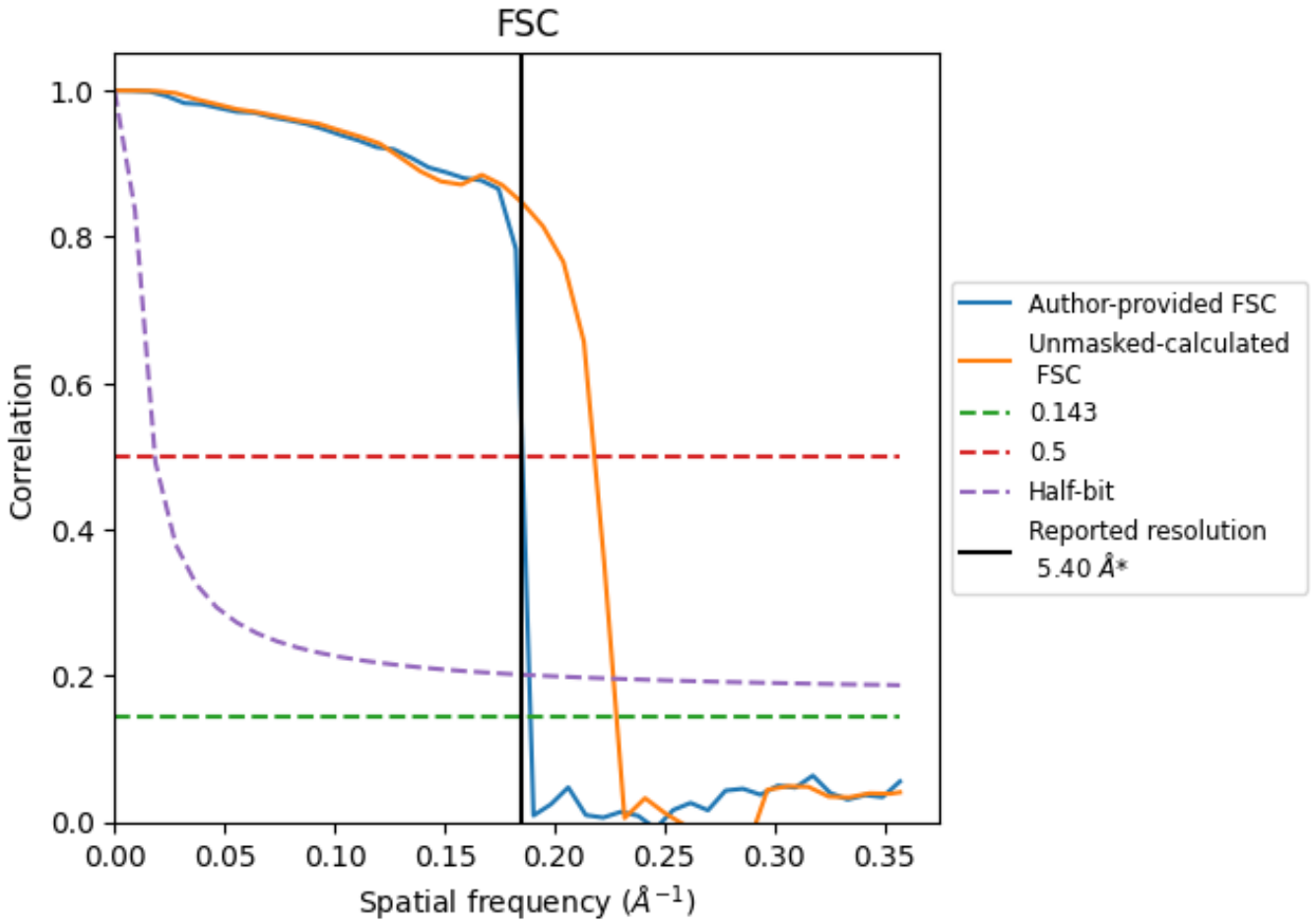
7.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.185 Å^{-1}

8.2 Resolution estimates (i)

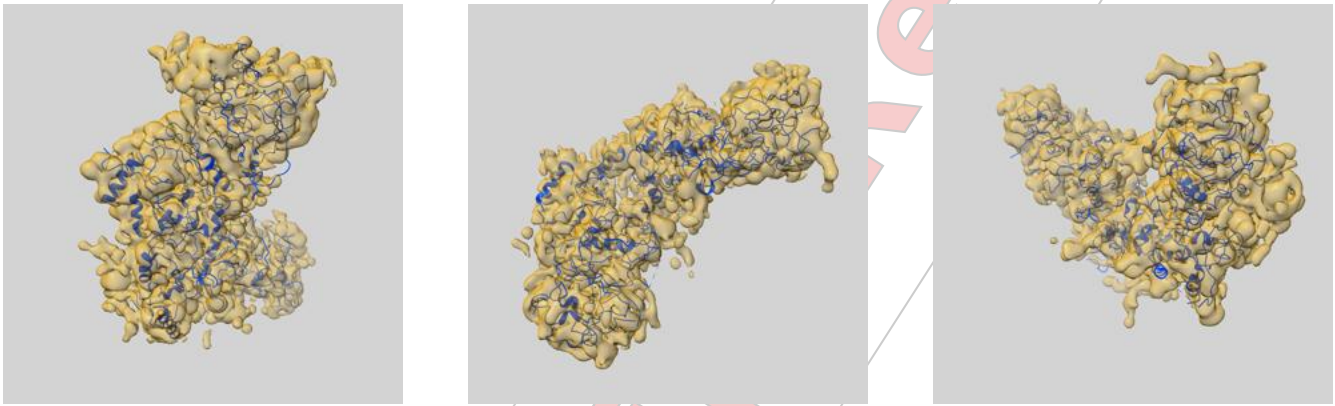
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	5.40	-
Author-provided FSC curve	5.29	5.39	5.30
Unmasked-calculated*	4.38	4.58	4.41

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.5 CUT-OFF 4.58 differs from the reported value 5.4 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-40656 and PDB model 8SOF. Per-residue inclusion information can be found in section 3 on page 4.

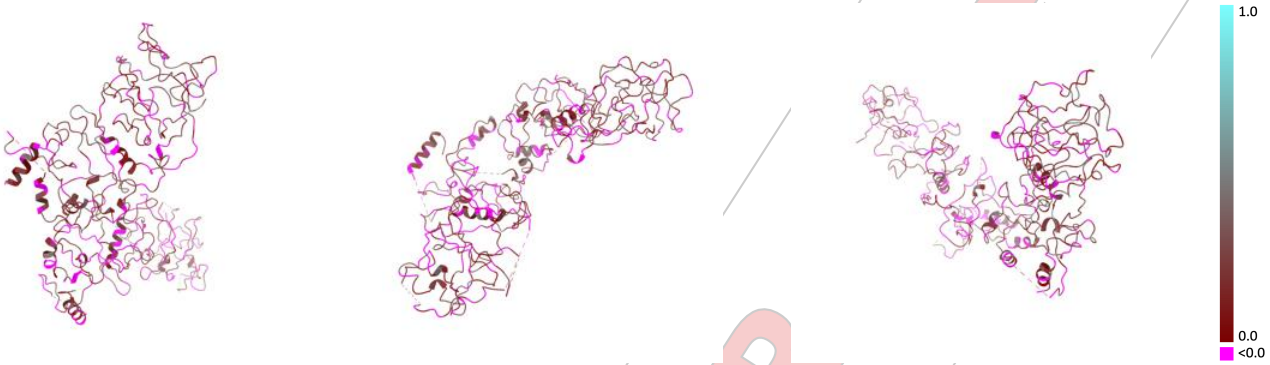
9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.4 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



X Y Z

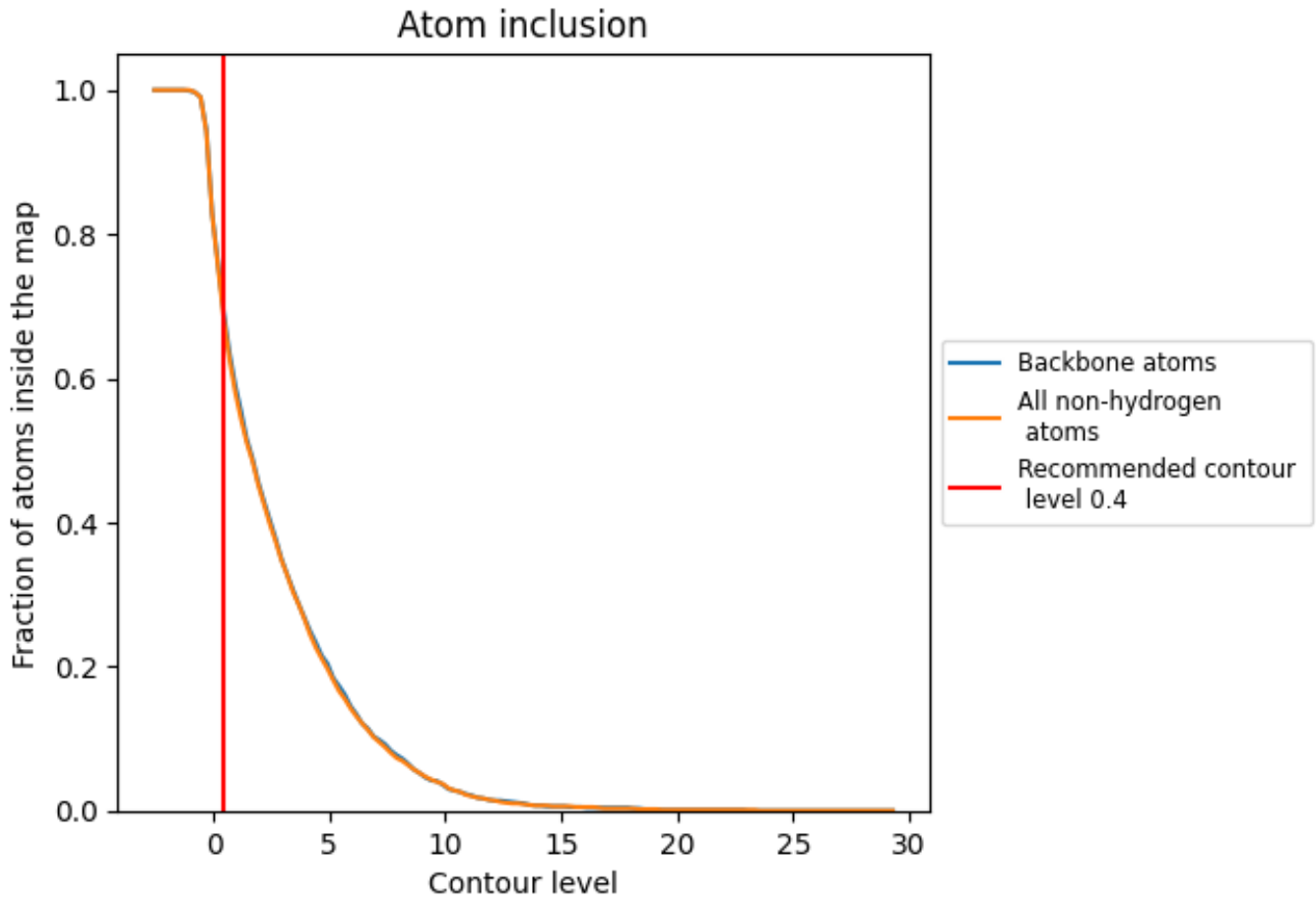
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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 (0.4).

9.4 Atom inclusion



At the recommended contour level, 70% of all backbone atoms, 70% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6950	0.1250
A	0.7730	0.1520
B	0.6290	0.0970

Full wwPDB EM Validation Report ⓘ

May 2, 2023 – 03:46 PM EDT

PDB ID	:	8SOH
EMDB ID	:	EMD-40657
Title	:	Nucleocapsid dimer from SARS-CoV-2, flexible conformation 2
Deposited on	:	2023-04-28
Resolution	:	5.40 Å(reported)
Based on initial model	:	.

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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:

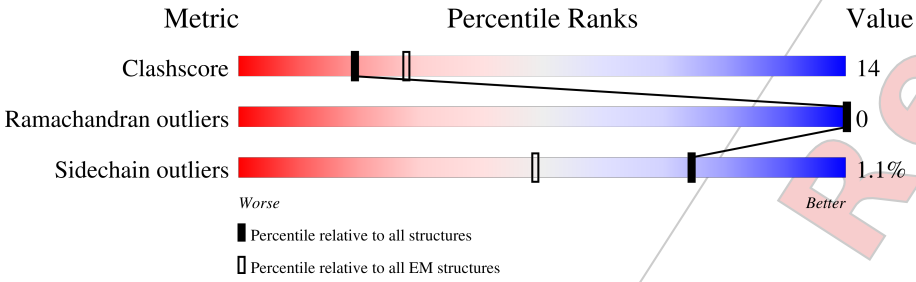
EMDB validation analysis	:	0.0.1.dev50
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

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 5.40 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 >=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	A	419	16% 72% 22% • 5%
1	B	419	26% 67% 20% 12%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11607 atoms, of which 5746 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 Nucleoprotein.

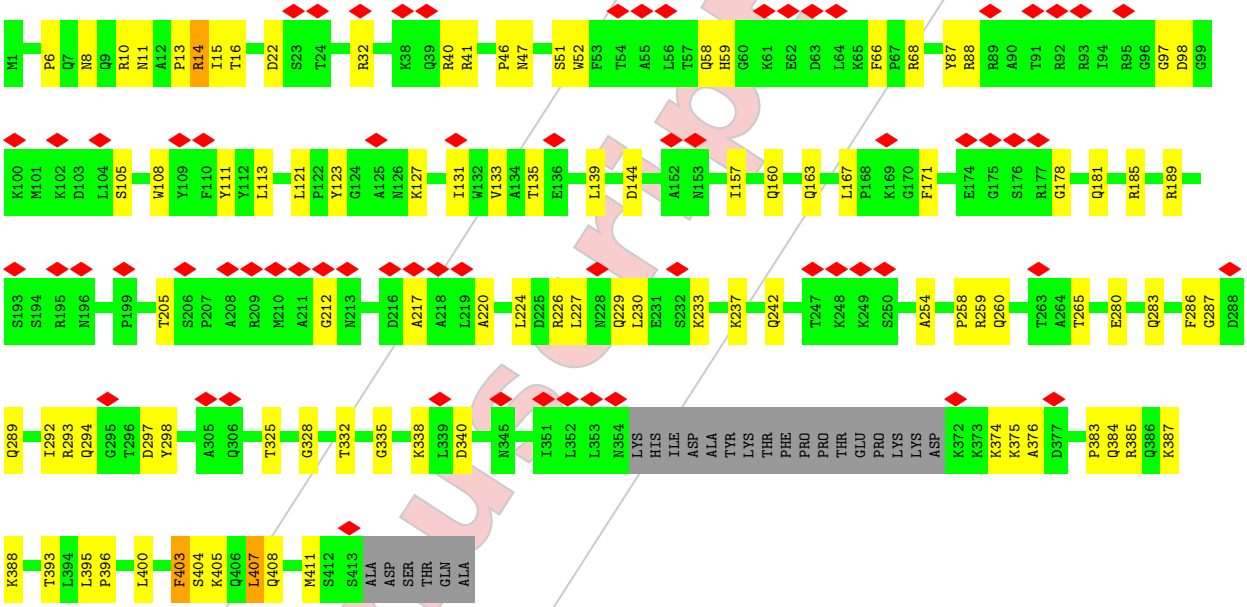
Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	396	Total	C	H	N	O	S	0	0
			6007	1856	2978	576	590	7		
1	B	368	Total	C	H	N	O	S	0	0
			5600	1733	2768	537	558	4		

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.

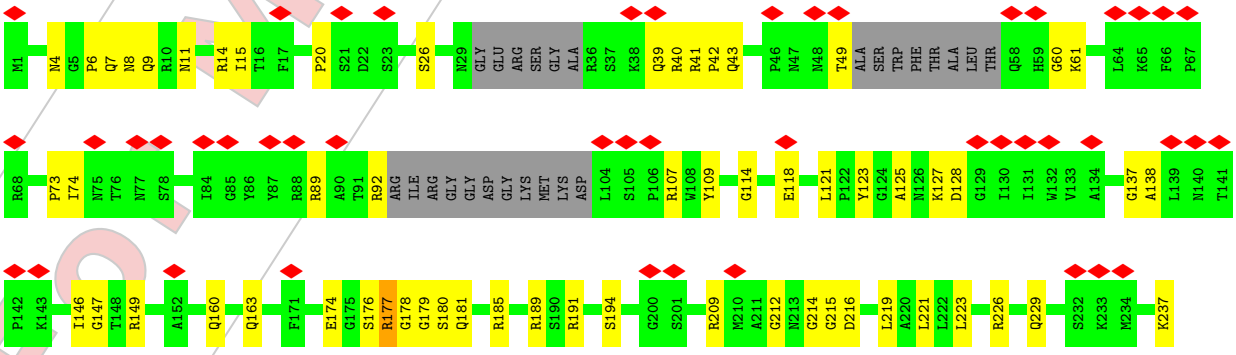
- Molecule 1: Nucleoprotein

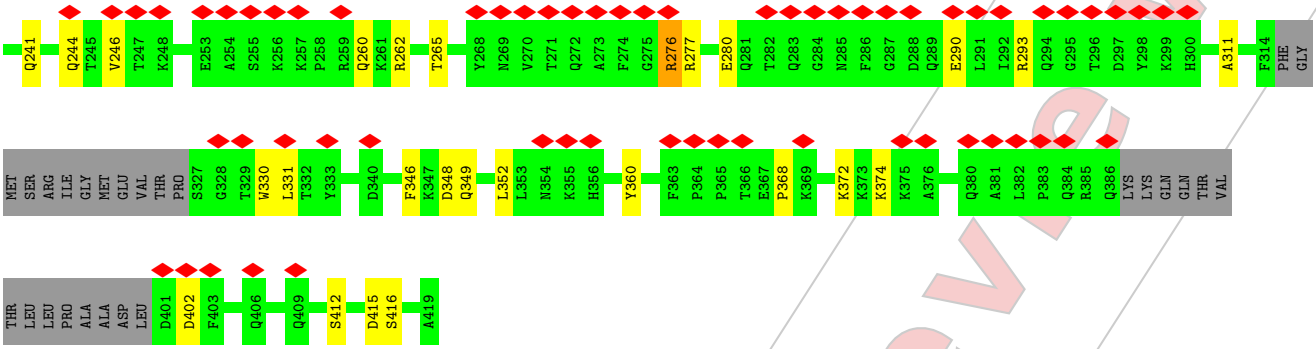
Chain A:



- Molecule 1: Nucleoprotein

Chain B:





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	10000	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	29.300	Depositor
Minimum map value	-2.543	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	117.6, 107.799995, 127.4	wwPDB
Map dimensions	84, 77, 91	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	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	1.85	7/3087 (0.2%)	0.73	7/4160 (0.2%)
1	B	0.31	0/2886	0.60	1/3887 (0.0%)
All	All	1.34	7/5973 (0.1%)	0.67	8/8047 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	403	PHE	CE1-CZ	46.86	2.26	1.37
1	A	403	PHE	CE2-CZ	45.88	2.24	1.37
1	A	403	PHE	CD2-CE2	43.95	2.27	1.39
1	A	403	PHE	CD1-CE1	42.84	2.25	1.39
1	A	403	PHE	CG-CD2	28.62	1.81	1.38
1	A	403	PHE	CG-CD1	28.35	1.81	1.38
1	A	407	LEU	CB-CG	23.86	2.21	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	407	LEU	CA-CB-CG	21.06	163.74	115.30
1	A	407	LEU	CB-CG-CD2	13.63	134.17	111.00
1	A	407	LEU	CB-CG-CD1	11.36	130.31	111.00
1	B	262	ARG	NE-CZ-NH2	6.63	123.61	120.30
1	A	407	LEU	CD1-CG-CD2	-6.59	90.74	110.50
1	A	403	PHE	CD1-CG-CD2	5.59	125.57	118.30
1	A	403	PHE	CB-CG-CD1	-5.52	116.93	120.80
1	A	395	LEU	CA-CB-CG	5.19	127.25	115.30

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	3029	2978	2977	101	0
1	B	2832	2768	2763	64	0
All	All	5861	5746	5740	165	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 14.

All (165) 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:403:PHE:CD2	1:A:403:PHE:CG	1.81	1.67
1:A:403:PHE:CG	1:A:403:PHE:CD1	1.81	1.65
1:A:403:PHE:CD2	1:A:407:LEU:HB2	1.40	1.53
1:A:403:PHE:CD1	1:A:407:LEU:HB3	1.42	1.52
1:A:403:PHE:CE2	1:A:407:LEU:HG	1.64	1.31
1:A:403:PHE:CZ	1:A:407:LEU:HG	1.70	1.26
1:A:403:PHE:CD1	1:A:403:PHE:CE1	2.24	1.25
1:A:403:PHE:CE2	1:A:403:PHE:CZ	2.24	1.25
1:A:403:PHE:CD2	1:A:403:PHE:CE2	2.27	1.23
1:A:403:PHE:CZ	1:A:403:PHE:CE1	2.26	1.22
1:A:403:PHE:CE2	1:A:407:LEU:CB	2.21	1.22
1:A:403:PHE:CD2	1:A:407:LEU:CB	2.23	1.21
1:A:403:PHE:CE1	1:A:407:LEU:CB	2.23	1.20
1:A:403:PHE:CD1	1:A:407:LEU:CB	2.25	1.20
1:A:403:PHE:CZ	1:A:407:LEU:CB	2.25	1.18
1:A:407:LEU:CB	1:A:407:LEU:CG	2.21	1.17
1:A:407:LEU:HG	1:A:407:LEU:CB	1.76	1.16
1:A:403:PHE:CG	1:A:407:LEU:CB	2.31	1.12
1:A:403:PHE:CG	1:A:407:LEU:HB3	1.90	1.05
1:A:403:PHE:CE2	1:A:407:LEU:HB2	1.94	1.00
1:A:403:PHE:CZ	1:A:407:LEU:CG	2.46	0.99
1:A:403:PHE:CE2	1:A:407:LEU:CG	2.49	0.94
1:A:403:PHE:CE1	1:A:407:LEU:CG	2.51	0.93
1:A:403:PHE:CG	1:A:407:LEU:HB2	2.04	0.92
1:A:403:PHE:CD1	1:A:407:LEU:CG	2.58	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:PHE:CE1	1:A:407:LEU:HB3	2.08	0.86
1:A:287:GLY:HA3	1:A:396:PRO:HD2	1.60	0.83
1:A:403:PHE:CD2	1:A:407:LEU:CG	2.63	0.81
1:A:403:PHE:CG	1:A:407:LEU:CG	2.70	0.74
1:B:6:PRO:HD2	1:B:41:ARG:HD2	1.68	0.74
1:B:60:GLY:HA3	1:B:212:GLY:H	1.54	0.72
1:A:403:PHE:CE1	1:A:407:LEU:CD2	2.73	0.72
1:A:13:PRO:HG2	1:A:15:ILE:HG12	1.73	0.71
1:A:10:ARG:HH22	1:A:113:LEU:H	1.36	0.70
1:B:209:ARG:HH11	1:B:221:LEU:HD13	1.57	0.69
1:B:412:SER:O	1:B:416:SER:N	2.19	0.68
1:A:121:LEU:HD23	1:A:123:TYR:H	1.59	0.68
1:B:9:GLN:OE1	1:B:43:GLN:NE2	2.27	0.67
1:A:293:ARG:HB2	1:A:384:GLN:HE21	1.61	0.66
1:A:41:ARG:NH2	1:A:47:ASN:HA	2.10	0.66
1:A:292:ILE:HG22	1:A:293:ARG:HG3	1.78	0.64
1:B:346:PHE:HA	1:B:349:GLN:HG3	1.80	0.64
1:A:11:ASN:ND2	1:A:181:GLN:HE22	1.95	0.64
1:B:60:GLY:O	1:B:214:GLY:N	2.31	0.64
1:A:403:PHE:CD2	1:A:407:LEU:CD1	2.81	0.64
1:A:376:ALA:HA	1:A:404:SER:HB2	1.79	0.63
1:B:277:ARG:HD2	1:B:330:TRP:CD1	2.33	0.63
1:B:7:GLN:HG2	1:B:40:ARG:H	1.64	0.63
1:B:15:ILE:HG12	1:B:26:SER:H	1.62	0.63
1:A:265:THR:HA	1:A:335:GLY:H	1.64	0.63
1:B:293:ARG:NH2	1:B:368:PRO:O	2.29	0.62
1:A:375:LYS:O	1:A:408:GLN:NE2	2.26	0.61
1:B:89:ARG:HH12	1:B:127:LYS:HD2	1.65	0.61
1:B:43:GLN:HG3	1:B:114:GLY:H	1.66	0.61
1:A:66:PHE:HD2	1:A:135:THR:HG23	1.66	0.60
1:A:157:ILE:H	1:A:178:GLY:HA3	1.65	0.60
1:B:177:ARG:HB3	1:B:180:SER:HB3	1.83	0.60
1:A:294:GLN:HG2	1:A:388:LYS:HB3	1.82	0.60
1:B:277:ARG:HB2	1:B:331:LEU:HD23	1.82	0.60
1:B:125:ALA:N	1:B:128:ASP:OD2	2.36	0.59
1:B:123:TYR:HB2	1:B:128:ASP:HB2	1.86	0.58
1:B:189:ARG:NH2	1:B:241:GLN:OE1	2.32	0.57
1:A:289:GLN:HE22	1:A:383:PRO:HG2	1.69	0.57
1:B:277:ARG:HD2	1:B:330:TRP:HD1	1.69	0.57
1:B:147:GLY:O	1:B:149:ARG:NH2	2.38	0.57
1:A:408:GLN:HA	1:A:411:MET:HG2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:ARG:HH21	1:B:178:GLY:N	2.03	0.56
1:B:191:ARG:NH2	1:B:241:GLN:OE1	2.38	0.56
1:A:384:GLN:O	1:A:385:ARG:NH2	2.38	0.56
1:B:49:THR:HG22	1:B:92:ARG:HG2	1.88	0.56
1:A:144:ASP:OD1	1:A:185:ARG:NH2	2.39	0.56
1:A:40:ARG:C	1:A:41:ARG:HD2	2.27	0.55
1:A:160:GLN:HE21	1:A:229:GLN:HB3	1.71	0.55
1:B:146:ILE:O	1:B:149:ARG:NH1	2.24	0.54
1:A:68:ARG:HG2	1:A:139:LEU:H	1.73	0.54
1:A:11:ASN:HD22	1:A:181:GLN:HE22	1.54	0.54
1:A:205:THR:H	1:A:220:ALA:HB1	1.73	0.54
1:A:332:THR:HG22	1:A:338:LYS:HE3	1.88	0.54
1:B:73:PRO:HD2	1:B:137:GLY:H	1.72	0.54
1:A:6:PRO:HG3	1:A:46:PRO:HD3	1.88	0.54
1:B:109:TYR:OH	1:B:181:GLN:OE1	2.26	0.54
1:A:325:THR:OG1	1:A:328:GLY:O	2.25	0.54
1:B:60:GLY:CA	1:B:212:GLY:H	2.21	0.54
1:B:163:GLN:HB3	1:B:194:SER:HA	1.89	0.53
1:A:286:PHE:HB3	1:A:400:LEU:HB3	1.90	0.53
1:A:111:TYR:HE2	1:A:113:LEU:HD23	1.74	0.53
1:B:260:GLN:HE22	1:B:311:ALA:H	1.57	0.53
1:B:226:ARG:HD2	1:B:229:GLN:HE21	1.74	0.53
1:A:403:PHE:CG	1:A:407:LEU:CD1	2.92	0.52
1:B:177:ARG:O	1:B:181:GLN:N	2.33	0.52
1:A:403:PHE:CZ	1:A:407:LEU:CA	2.93	0.51
1:A:51:SER:OG	1:A:52:TRP:N	2.42	0.51
1:B:177:ARG:HD3	1:B:179:GLY:N	2.26	0.51
1:B:174:GLU:N	1:B:174:GLU:OE1	2.44	0.51
1:B:372:LYS:NZ	1:B:374:LYS:H	2.08	0.51
1:A:227:LEU:HA	1:A:230:LEU:HG	1.93	0.51
1:B:177:ARG:HH21	1:B:178:GLY:H	1.59	0.50
1:A:97:GLY:HA3	1:A:217:ALA:H	1.76	0.50
1:A:98:ASP:HB2	1:A:212:GLY:HA2	1.93	0.50
1:A:131:ILE:HG22	1:A:133:VAL:HG23	1.94	0.50
1:A:163:GLN:HE22	1:A:233:LYS:HB2	1.76	0.50
1:A:8:ASN:HB2	1:A:11:ASN:OD1	2.12	0.49
1:B:107:ARG:HH22	1:B:176:SER:HB2	1.77	0.49
1:A:40:ARG:O	1:A:41:ARG:HD2	2.12	0.49
1:B:349:GLN:HA	1:B:352:LEU:HB2	1.94	0.49
1:A:224:LEU:HD23	1:A:227:LEU:HD21	1.95	0.49
1:B:4:ASN:ND2	1:B:149:ARG:H	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ARG:HH22	1:A:47:ASN:HA	1.76	0.48
1:A:374:LYS:HB3	1:A:405:LYS:NZ	2.28	0.48
1:B:14:ARG:HG3	1:B:20:PRO:HB3	1.94	0.48
1:B:219:LEU:HA	1:B:223:LEU:HD22	1.94	0.48
1:B:177:ARG:HD3	1:B:179:GLY:H	1.77	0.48
1:A:403:PHE:CD2	1:A:407:LEU:HD12	2.49	0.48
1:A:403:PHE:CD1	1:A:403:PHE:CB	2.85	0.47
1:B:290:GLU:OE1	1:B:360:TYR:OH	2.31	0.47
1:A:294:GLN:NE2	1:A:385:ARG:O	2.40	0.47
1:B:8:ASN:N	1:B:11:ASN:OD1	2.42	0.47
1:B:160:GLN:OE1	1:B:226:ARG:NH1	2.46	0.47
1:A:404:SER:OG	1:A:405:LYS:N	2.48	0.47
1:A:297:ASP:OD1	1:A:298:TYR:N	2.49	0.46
1:B:42:PRO:HG2	1:B:118:GLU:HA	1.96	0.46
1:B:277:ARG:HB3	1:B:330:TRP:NE1	2.31	0.46
1:B:219:LEU:HA	1:B:223:LEU:HD13	1.97	0.46
1:A:254:ALA:HB1	1:A:259:ARG:HB2	1.97	0.46
1:A:58:GLN:HB2	1:A:108:TRP:HZ3	1.81	0.45
1:A:403:PHE:CG	1:A:407:LEU:HD13	2.51	0.45
1:B:7:GLN:HG2	1:B:39:GLN:HA	1.99	0.45
1:A:97:GLY:HA3	1:A:217:ALA:HB3	1.99	0.45
1:B:276:ARG:HD3	1:B:276:ARG:H	1.82	0.44
1:A:15:ILE:HD11	1:A:40:ARG:HH11	1.82	0.44
1:B:9:GLN:H	1:B:43:GLN:HE22	1.65	0.44
1:A:59:HIS:HA	1:A:105:SER:HB2	1.99	0.44
1:A:226:ARG:NH2	1:A:229:GLN:OE1	2.50	0.44
1:A:88:ARG:HH12	1:A:127:LYS:HB3	1.83	0.44
1:A:403:PHE:CD2	1:A:407:LEU:HG	2.47	0.44
1:A:403:PHE:CE1	1:A:407:LEU:C	2.91	0.44
1:A:387:LYS:HA	1:A:387:LYS:HD2	1.85	0.43
1:B:9:GLN:OE1	1:B:9:GLN:N	2.44	0.43
1:B:61:LYS:HD2	1:B:216:ASP:HA	1.99	0.43
1:A:87:TYR:HA	1:A:108:TRP:CD1	2.54	0.43
1:A:22:ASP:OD2	1:A:133:VAL:HG13	2.19	0.43
1:B:181:GLN:O	1:B:185:ARG:NH2	2.52	0.43
1:A:14:ARG:HH12	1:A:32:ARG:H	1.67	0.43
1:A:16:THR:HG21	1:A:40:ARG:HD2	2.01	0.42
1:A:160:GLN:HG2	1:A:229:GLN:HB3	2.01	0.42
1:B:61:LYS:HB3	1:B:215:GLY:O	2.20	0.42
1:B:415:ASP:OD1	1:B:416:SER:N	2.53	0.42
1:B:280:GLU:HG3	1:B:330:TRP:CE3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:LYS:HB3	1:A:405:LYS:HZ1	1.85	0.42
1:B:244:GLN:HB3	1:B:246:VAL:HG23	2.01	0.42
1:B:348:ASP:OD1	1:B:349:GLN:N	2.53	0.41
1:A:167:LEU:HD23	1:A:171:PHE:HB3	2.03	0.41
1:A:403:PHE:CD1	1:A:403:PHE:O	2.73	0.41
1:B:74:ILE:HD12	1:B:138:ALA:HA	2.03	0.41
1:B:226:ARG:O	1:B:229:GLN:HG3	2.20	0.41
1:B:374:LYS:NZ	1:B:402:ASP:OD2	2.47	0.41
1:A:340:ASP:OD1	1:A:340:ASP:N	2.53	0.41
1:B:74:ILE:HD13	1:B:137:GLY:O	2.20	0.41
1:A:10:ARG:NH2	1:A:113:LEU:H	2.11	0.41
1:A:242:GLN:HA	1:A:393:THR:HG21	2.04	0.40
1:A:258:PRO:HB3	1:A:260:GLN:NE2	2.37	0.40
1:A:374:LYS:HD2	1:A:374:LYS:HA	1.85	0.40
1:B:121:LEU:HD12	1:B:121:LEU:O	2.22	0.40
1:A:280:GLU:HG3	1:A:283:GLN:HE22	1.86	0.40
1:B:15:ILE:HG23	1:B:26:SER:OG	2.22	0.40

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	392/419 (94%)	328 (84%)	64 (16%)	0	100	100
1	B	356/419 (85%)	306 (86%)	50 (14%)	0	100	100
All	All	748/838 (89%)	634 (85%)	114 (15%)	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	317/339 (94%)	314 (99%)	3 (1%)	78	88
1	B	300/339 (88%)	296 (99%)	4 (1%)	69	82
All	All	617/678 (91%)	610 (99%)	7 (1%)	74	85

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	189	ARG
1	A	237	LYS
1	B	177	ARG
1	B	237	LYS
1	B	265	THR
1	B	276	ARG

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	181	GLN
1	A	289	GLN
1	B	229	GLN
1	B	260	GLN

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 monosaccharides 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 (i)

There are no chain breaks in this entry.

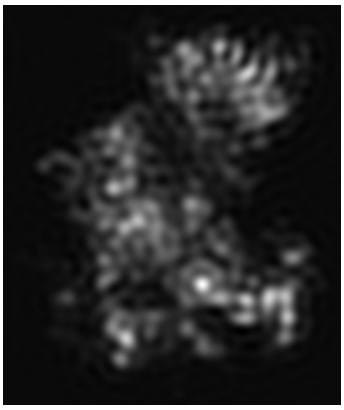
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-40657. These allow visual inspection of the internal detail of the map and identification of artifacts.

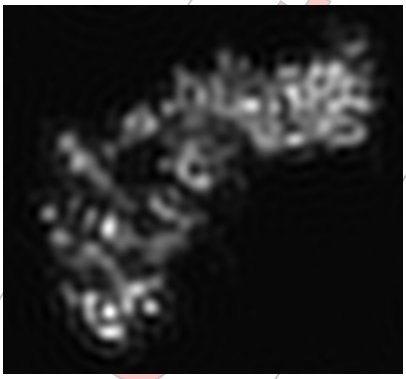
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

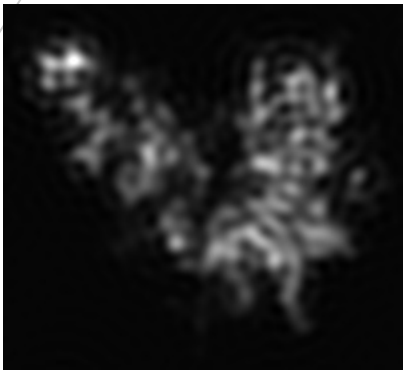
6.1.1 Primary map



X

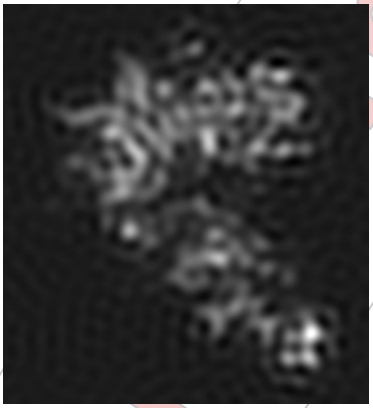


Y

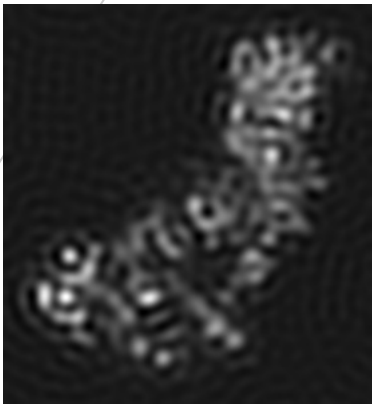


Z

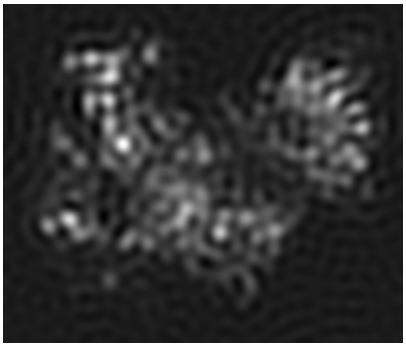
6.1.2 Raw map



X



Y

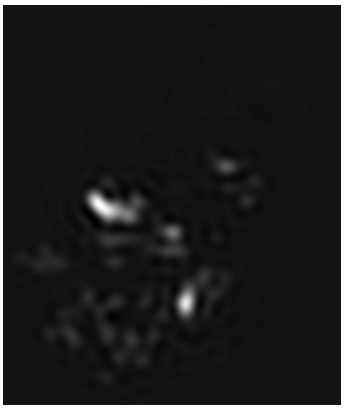


Z

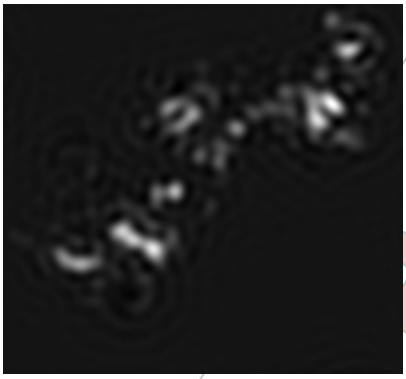
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

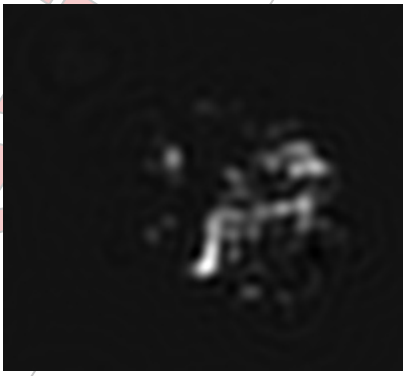
6.2.1 Primary map



X Index: 42

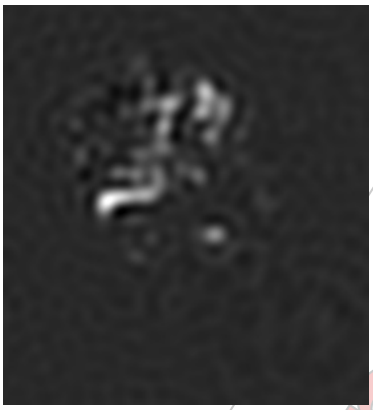


Y Index: 38

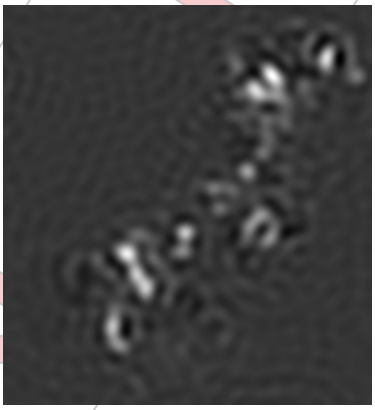


Z Index: 45

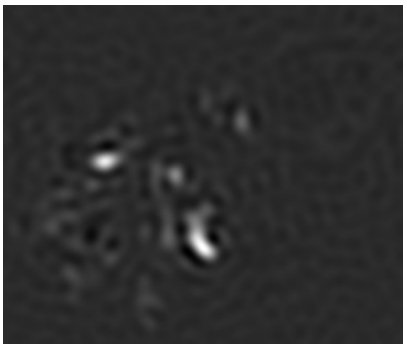
6.2.2 Raw map



X Index: 45



Y Index: 38

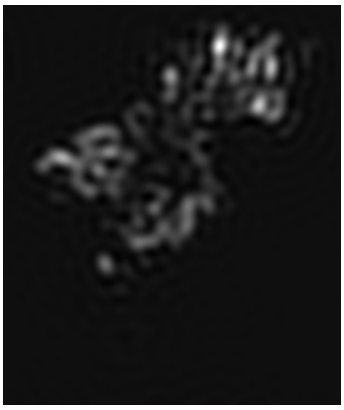


Z Index: 42

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

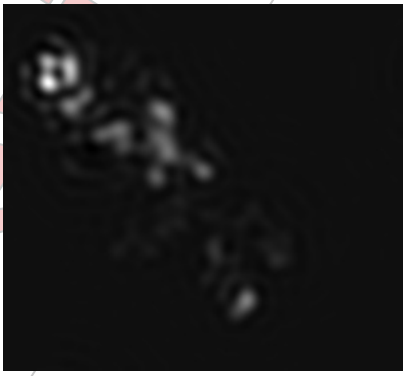
6.3 Largest variance slices (i)

6.3.1 Primary map



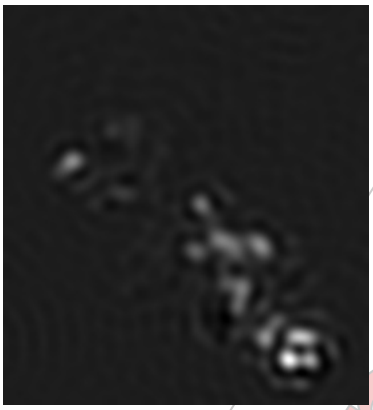
X Index: 61

Y Index: 64

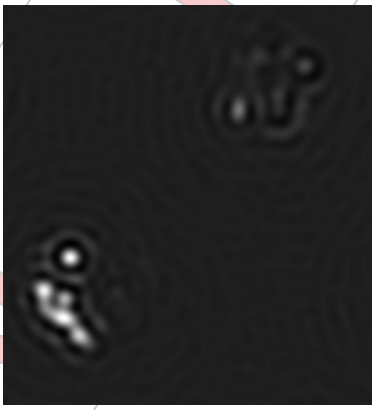


Z Index: 24

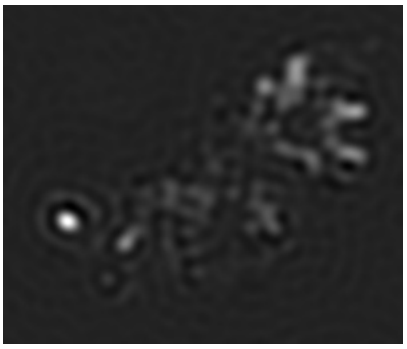
6.3.2 Raw map



X Index: 24



Y Index: 64

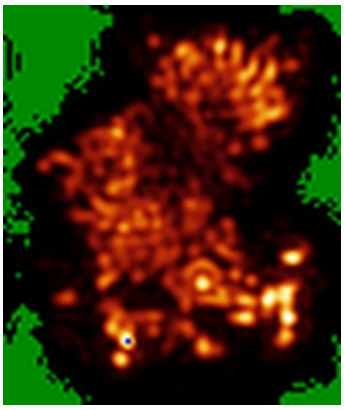


Z Index: 53

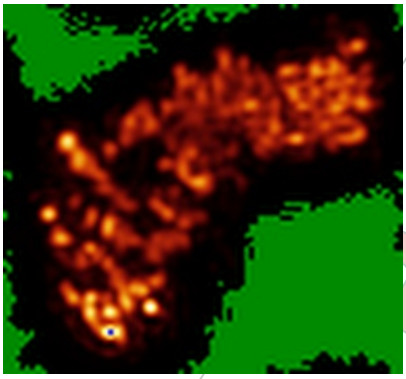
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color)

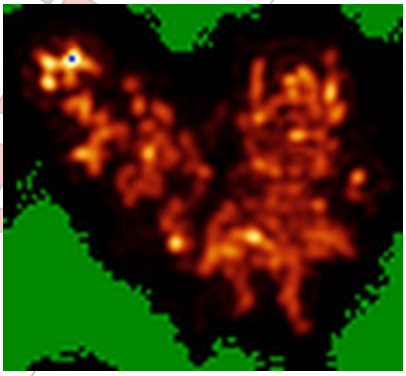
6.4.1 Primary map



X

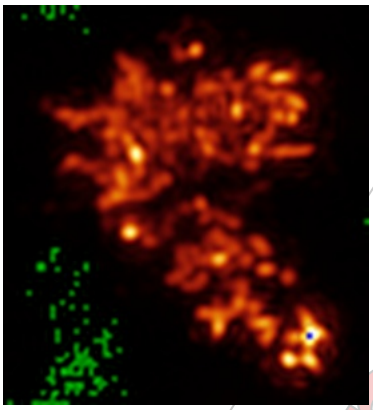


Y

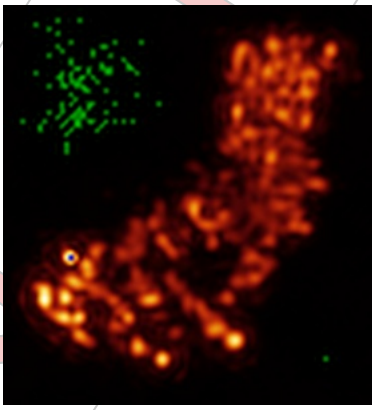


Z

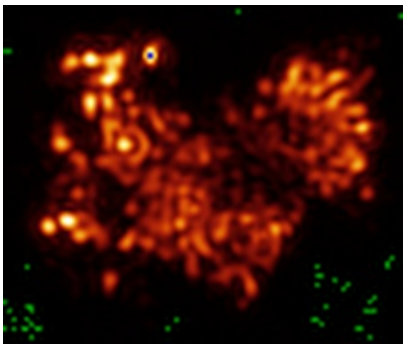
6.4.2 Raw map



X



Y

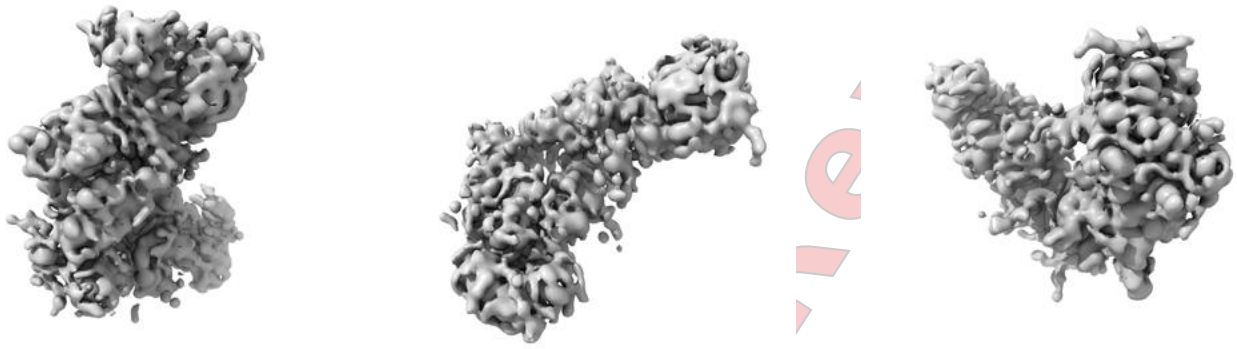


Z

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)

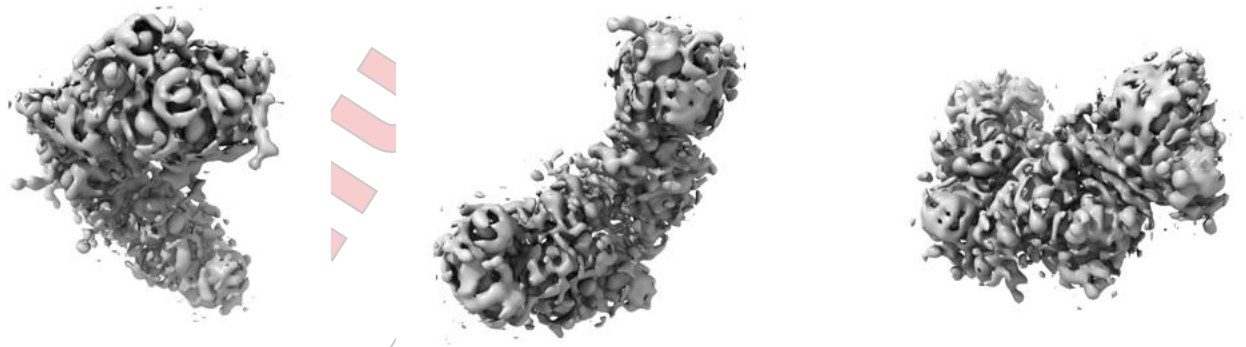
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.4. 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.

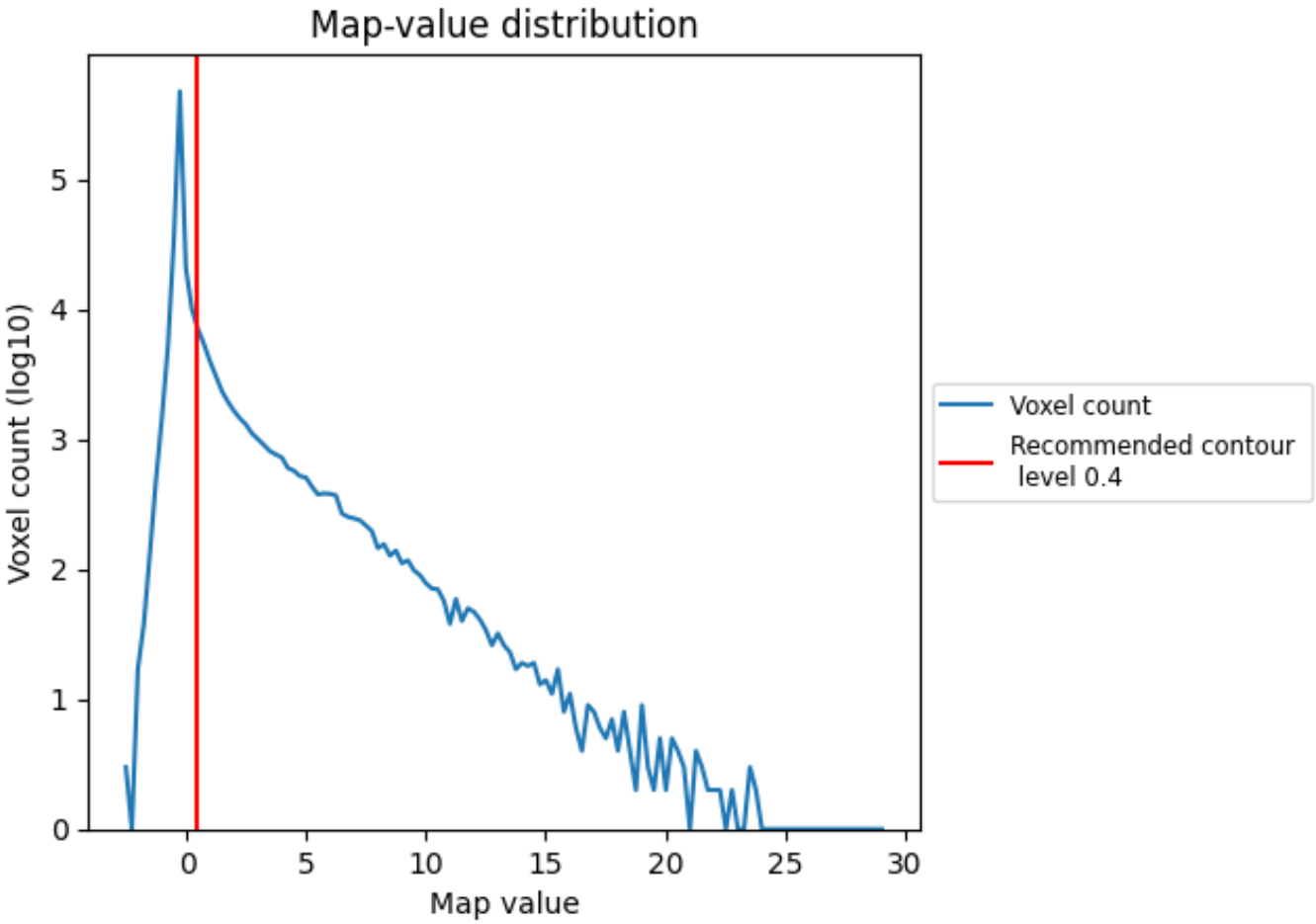
6.6 Mask visualisation (i)

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

7 Map analysis

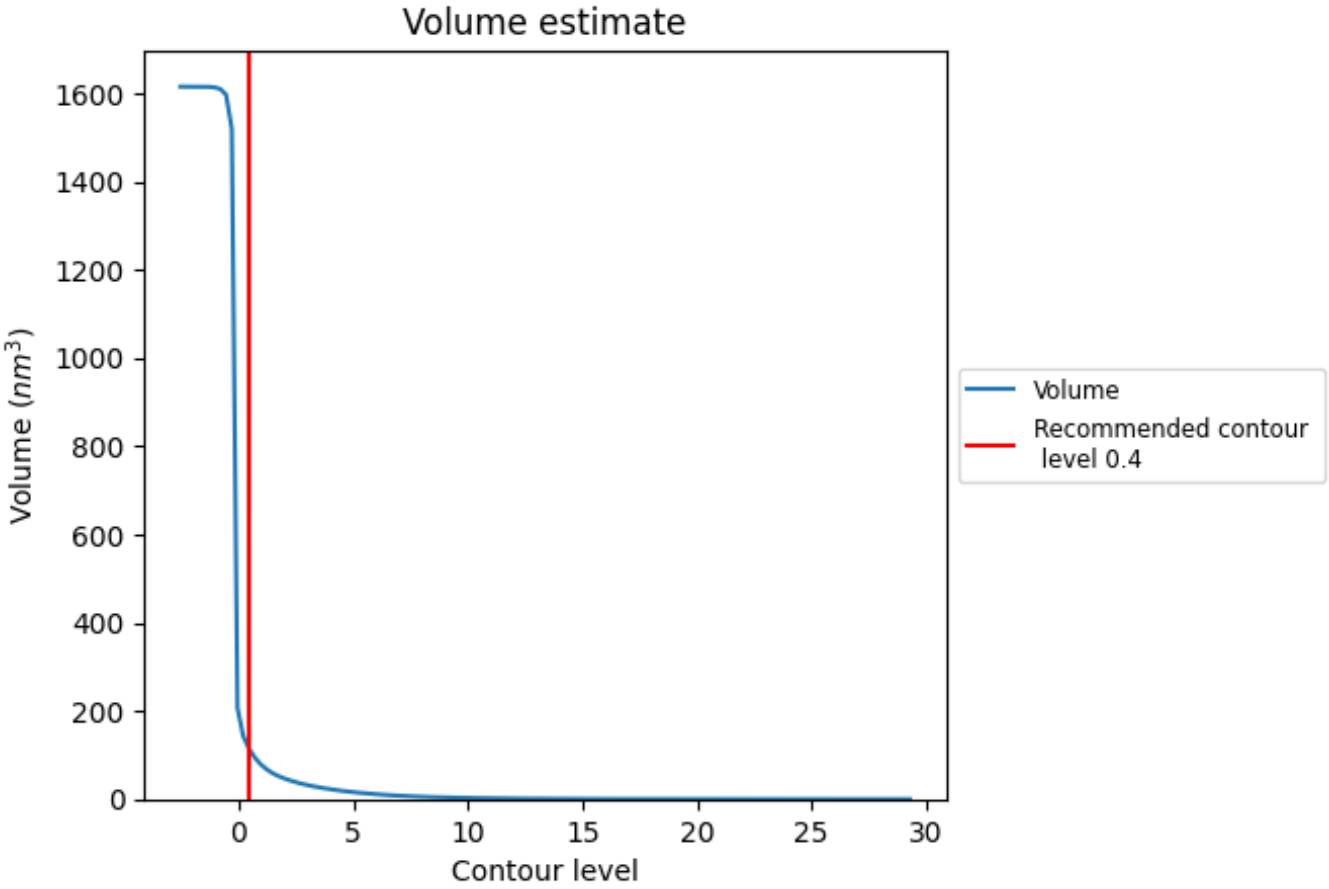
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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 119 nm^3; this corresponds to an approximate mass of 108 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.

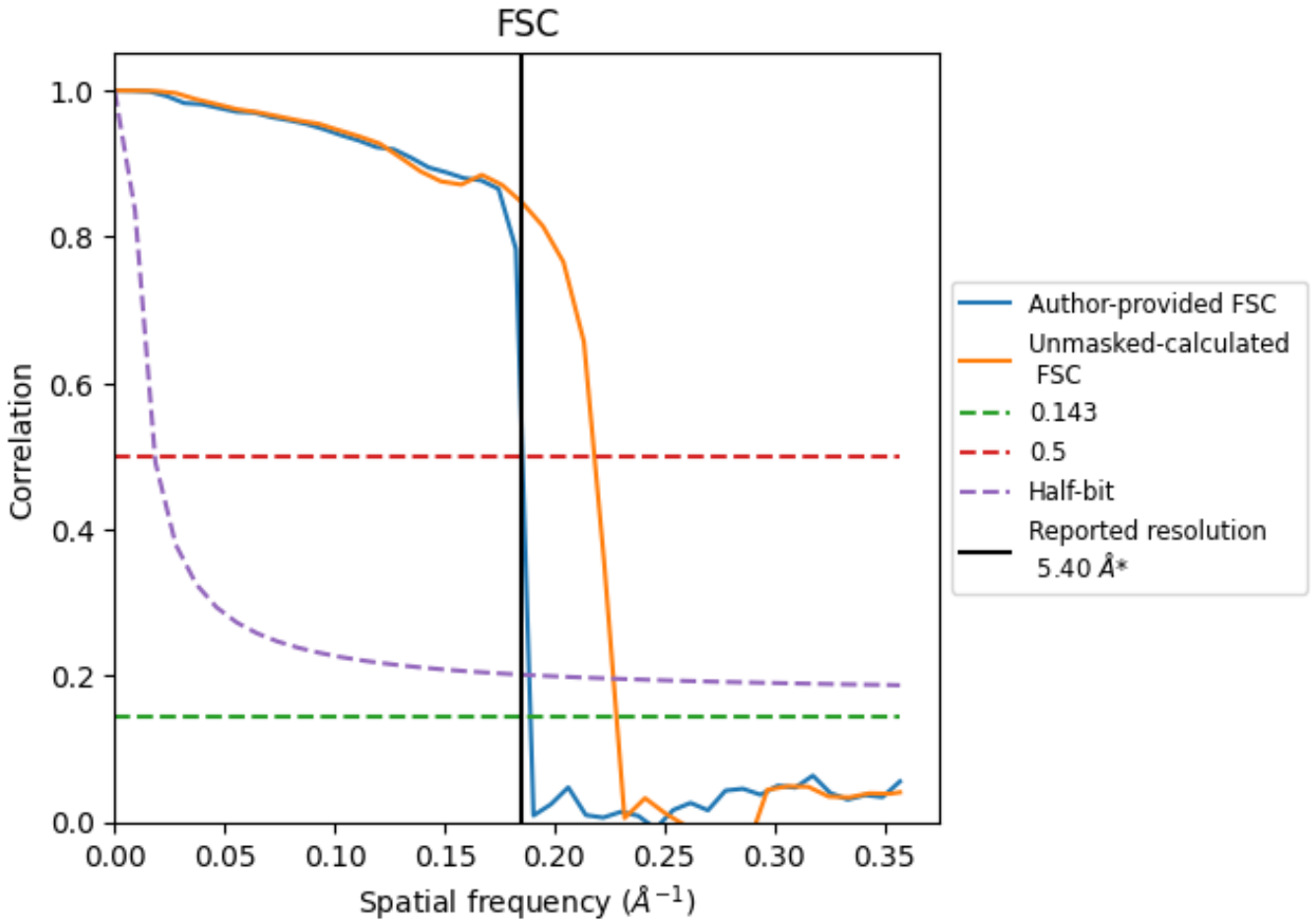
7.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.185 Å^{-1}

8.2 Resolution estimates (i)

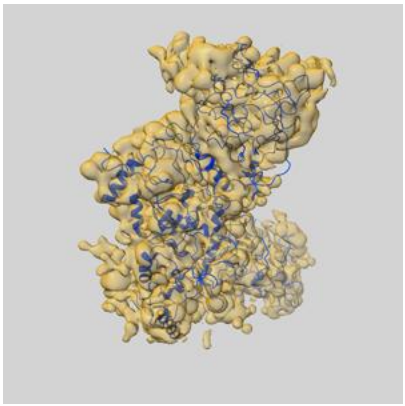
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	5.40	-
Author-provided FSC curve	5.29	5.39	5.30
Unmasked-calculated*	4.38	4.58	4.41

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.5 CUT-OFF 4.58 differs from the reported value 5.4 by more than 10 %

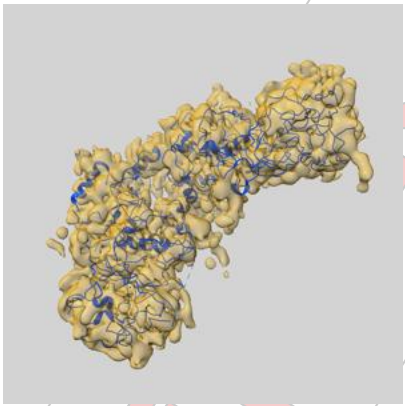
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-40657 and PDB model 8SOH. Per-residue inclusion information can be found in section 3 on page 4.

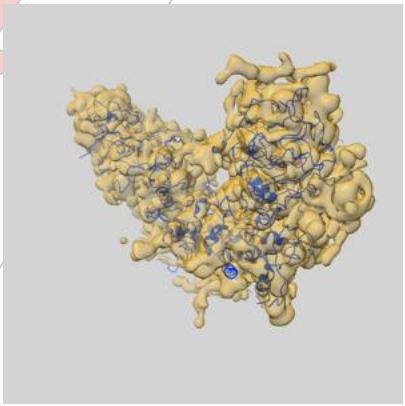
9.1 Map-model overlay



X



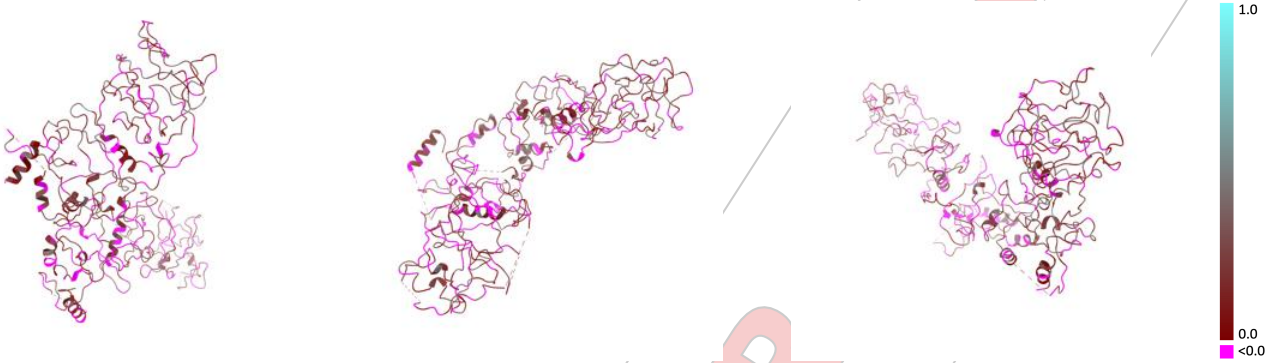
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.4 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



X Y Z

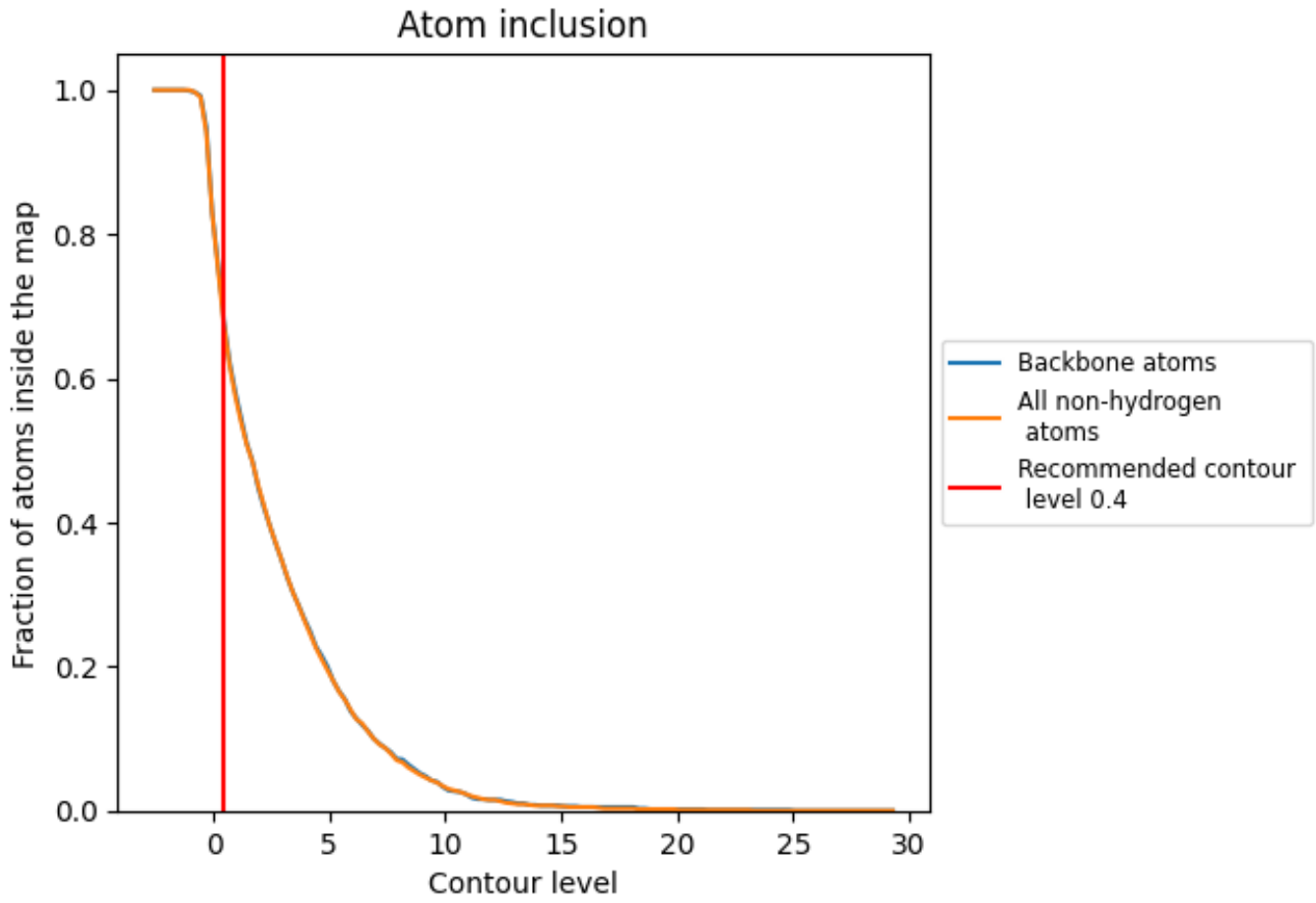
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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 (0.4).

9.4 Atom inclusion (i)



At the recommended contour level, 70% of all backbone atoms, 69% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6920	0.1210
A	0.7720	0.1480
B	0.6230	0.0920