



Full wwPDB EM Validation Report ⓘ

Sep 19, 2021 – 06:42 PM JST

PDB ID : 7VFF
EMDB ID : EMD-31951
Title : Cryo-EM structure of Vaccinia virus scaffolding protein D13 with N-terminal 17 residue truncation
Deposited on : 2021-09-13
Resolution : 4.10 Å (reported)
Based on initial model : 6BEI

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

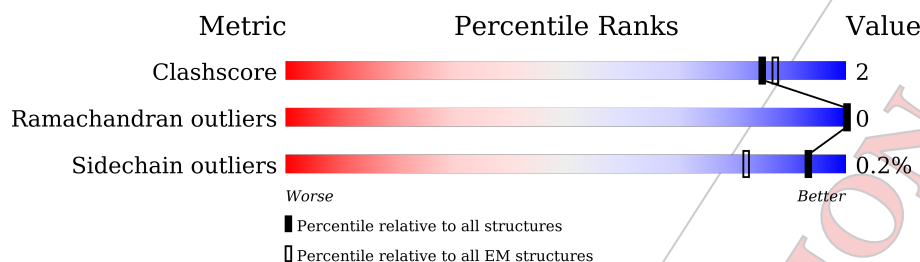
EMDB validation analysis : 0.0.0.dev97
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.1

1 Overall quality at a glance

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

The reported resolution of this entry is 4.10 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	531	 94% 5%
1	B	531	 94% 6%
1	C	531	 93% 6%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 12579 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

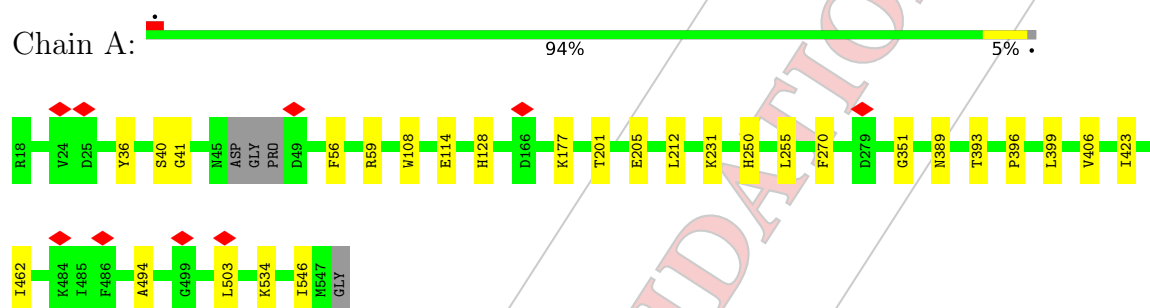
- Molecule 1 is a protein called Scaffold protein D13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	527	Total 4193	2681	681	819	12	0	0
1	B	527	Total 4193	2681	681	819	12	0	0
1	C	527	Total 4193	2681	681	819	12	0	0

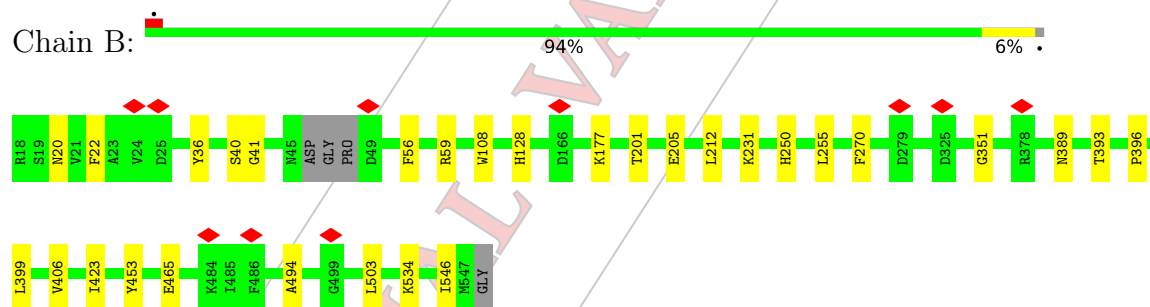
3 Residue-property plots [i](#)

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.

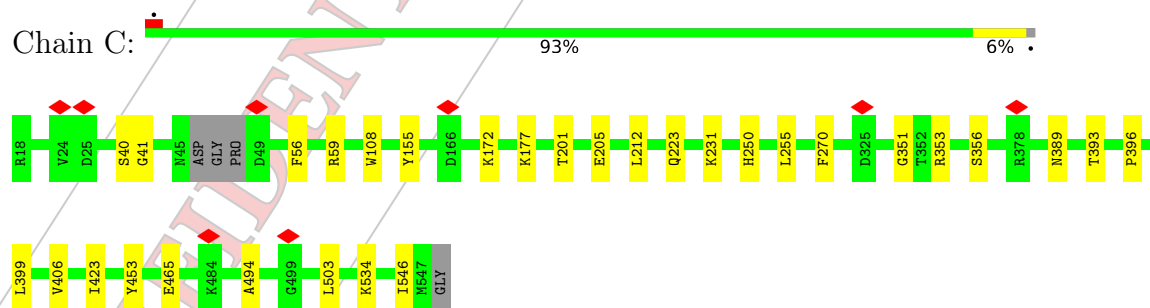
- Molecule 1: Scaffold protein D13



- Molecule 1: Scaffold protein D13



- Molecule 1: Scaffold protein D13



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	156813	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	92000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	38.371	Depositor
Minimum map value	-24.914	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	6.0	Depositor
Map size (Å)	286.72, 286.72, 286.72	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.12, 1.12, 1.12	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	0.41	0/4285	0.51	0/5830
1	B	0.41	0/4285	0.51	0/5830
1	C	0.41	0/4285	0.51	0/5830
All	All	0.41	0/12855	0.51	0/17490

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4193	0	4143	20	0
1	B	4193	0	4143	23	0
1	C	4193	0	4143	22	0
All	All	12579	0	12429	56	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (56) 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:36:TYR:HB2	1:B:453:TYR:CE1	2.27	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:396:PRO:HD2	1:C:399:LEU:HD12	1.77	0.67
1:A:396:PRO:HD2	1:A:399:LEU:HD12	1.77	0.66
1:B:396:PRO:HD2	1:B:399:LEU:HD12	1.77	0.66
1:A:36:TYR:HB2	1:B:453:TYR:HE1	1.63	0.63
1:A:59:ARG:HB2	1:A:177:LYS:HZ3	1.69	0.57
1:B:59:ARG:HB2	1:B:177:LYS:HZ3	1.69	0.57
1:C:59:ARG:HB2	1:C:177:LYS:HZ3	1.71	0.55
1:B:255:LEU:HD13	1:B:503:LEU:HD13	1.89	0.55
1:C:255:LEU:HD13	1:C:503:LEU:HD13	1.89	0.54
1:A:255:LEU:HD13	1:A:503:LEU:HD13	1.89	0.54
1:A:128:HIS:NE2	1:B:465:GLU:OE1	2.39	0.54
1:B:108:TRP:HA	1:B:231:LYS:NZ	2.24	0.53
1:C:108:TRP:HA	1:C:231:LYS:NZ	2.24	0.52
1:A:108:TRP:HA	1:A:231:LYS:NZ	2.24	0.52
1:B:36:TYR:HB2	1:C:453:TYR:CE1	2.45	0.52
1:A:201:THR:O	1:A:205:GLU:HG3	2.11	0.51
1:C:201:THR:O	1:C:205:GLU:HG3	2.11	0.51
1:B:201:THR:O	1:B:205:GLU:HG3	2.11	0.51
1:B:250:HIS:HA	1:B:494:ALA:HB2	1.94	0.50
1:C:250:HIS:HA	1:C:494:ALA:HB2	1.94	0.48
1:B:128:HIS:NE2	1:C:465:GLU:OE1	2.40	0.48
1:A:250:HIS:HA	1:A:494:ALA:HB2	1.94	0.48
1:B:36:TYR:HB2	1:C:453:TYR:HE1	1.78	0.48
1:A:56:PHE:CE2	1:A:212:LEU:HB2	2.50	0.47
1:C:56:PHE:CE2	1:C:212:LEU:HB2	2.50	0.46
1:B:56:PHE:CE2	1:B:212:LEU:HB2	2.50	0.46
1:A:41:GLY:HA3	1:A:56:PHE:CE1	2.51	0.45
1:B:41:GLY:HA3	1:B:56:PHE:CE1	2.51	0.44
1:C:41:GLY:HA3	1:C:56:PHE:CE1	2.51	0.44
1:C:351:GLY:O	1:C:406:VAL:HG22	2.19	0.43
1:B:20:ASN:ND2	1:C:223:GLN:HB2	2.33	0.43
1:A:59:ARG:HB2	1:A:177:LYS:NZ	2.34	0.43
1:A:351:GLY:O	1:A:406:VAL:HG22	2.19	0.43
1:A:534:LYS:HB2	1:A:546:ILE:HD11	2.01	0.43
1:B:270:PHE:CD2	1:B:423:ILE:HD12	2.54	0.43
1:B:59:ARG:HB2	1:B:177:LYS:NZ	2.34	0.43
1:A:462:ILE:HG13	1:C:155:TYR:CE2	2.53	0.43
1:B:351:GLY:O	1:B:406:VAL:HG22	2.19	0.43
1:A:389:ASN:O	1:A:393:THR:HG23	2.19	0.42
1:C:389:ASN:O	1:C:393:THR:HG23	2.19	0.42
1:B:534:LYS:HB2	1:B:546:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:534:LYS:HB2	1:C:546:ILE:HD11	2.01	0.42
1:A:270:PHE:CD2	1:A:423:ILE:HD12	2.54	0.42
1:C:270:PHE:CD2	1:C:423:ILE:HD12	2.54	0.42
1:B:22:PHE:O	1:C:172:LYS:NZ	2.35	0.41
1:B:389:ASN:O	1:B:393:THR:HG23	2.19	0.41
1:C:108:TRP:HA	1:C:231:LYS:HZ3	1.83	0.41
1:A:56:PHE:CD2	1:A:212:LEU:HB2	2.55	0.41
1:A:108:TRP:HA	1:A:231:LYS:HZ3	1.85	0.41
1:B:56:PHE:CD2	1:B:212:LEU:HB2	2.55	0.41
1:C:59:ARG:HB2	1:C:177:LYS:NZ	2.34	0.41
1:B:108:TRP:HA	1:B:231:LYS:HZ3	1.85	0.41
1:A:114:GLU:OE1	1:A:114:GLU:HA	2.22	0.40
1:C:56:PHE:CD2	1:C:212:LEU:HB2	2.55	0.40
1:C:353:ARG:HB2	1:C:356:SER:HB2	2.04	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	523/531 (98%)	504 (96%)	19 (4%)	0	100	100
1	B	523/531 (98%)	504 (96%)	19 (4%)	0	100	100
1	C	523/531 (98%)	504 (96%)	19 (4%)	0	100	100
All	All	1569/1593 (98%)	1512 (96%)	57 (4%)	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	485/487 (100%)	484 (100%)	1 (0%)	93	96
1	B	485/487 (100%)	484 (100%)	1 (0%)	93	96
1	C	485/487 (100%)	484 (100%)	1 (0%)	93	96
All	All	1455/1461 (100%)	1452 (100%)	3 (0%)	93	96

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

Mol	Chain	Res	Type
1	A	40	SER
1	B	40	SER
1	C	40	SER

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 [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.

CONFIDENTIAL VALIDATION REPORT

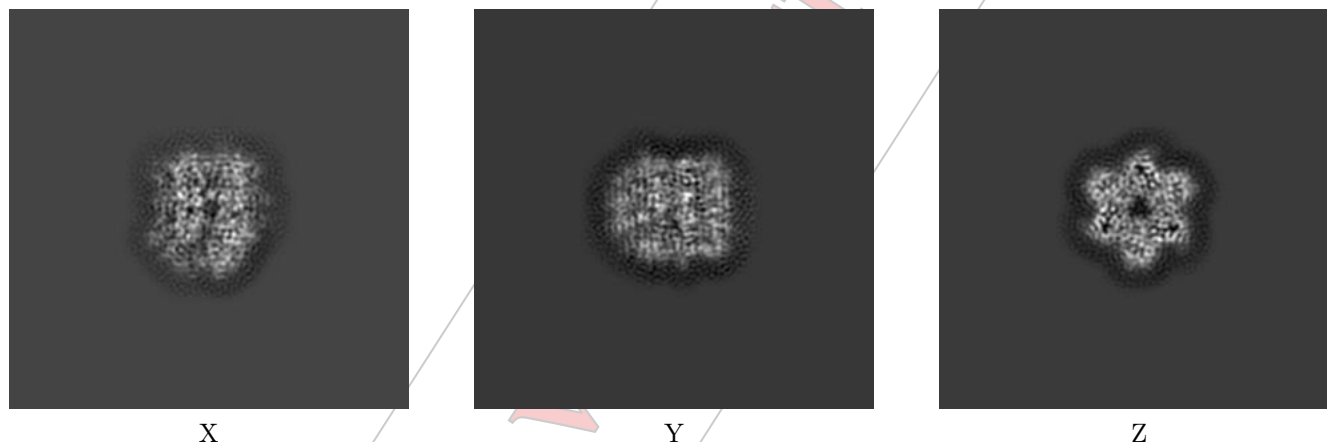
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31951. These allow visual inspection of the internal detail of the map and identification of artifacts.

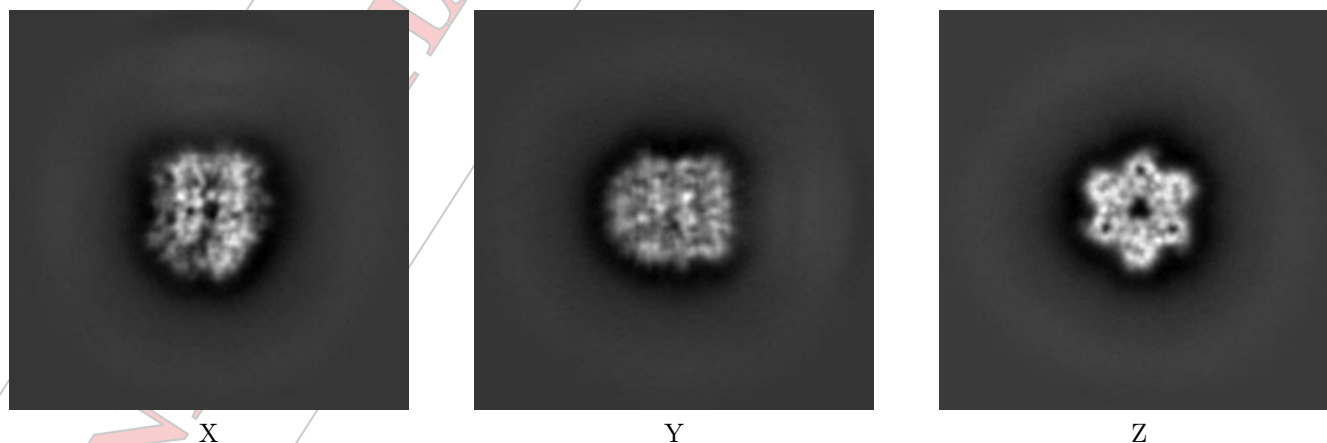
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



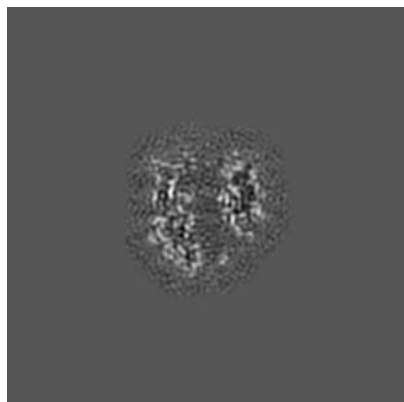
6.1.2 Raw map



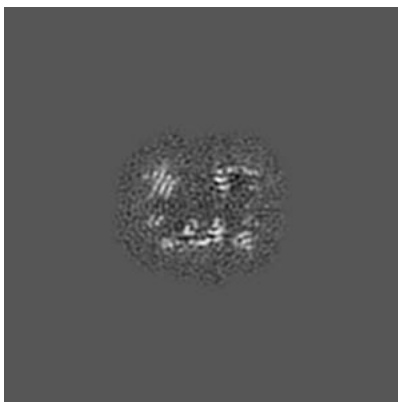
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 128

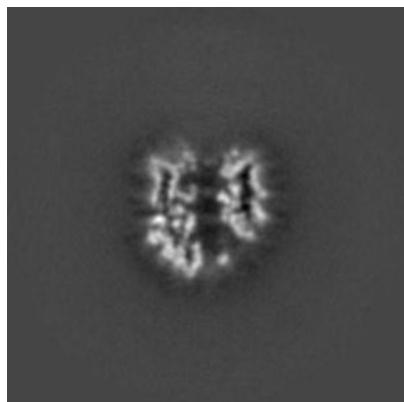


Y Index: 128

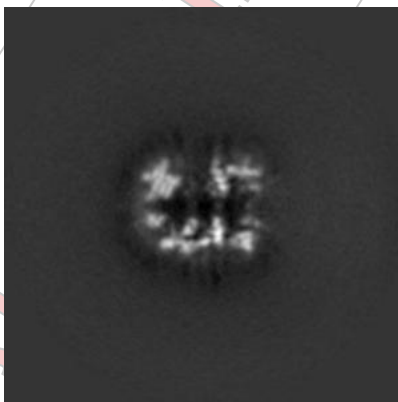


Z Index: 128

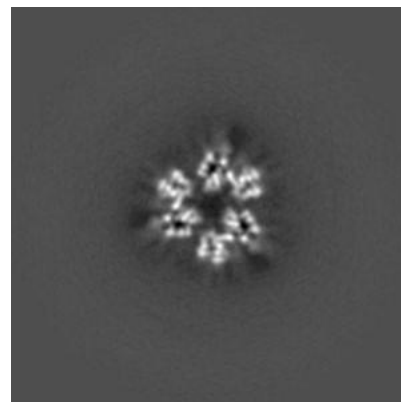
6.2.2 Raw map



X Index: 128



Y Index: 128

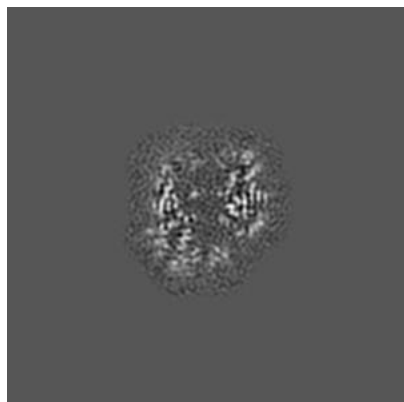


Z Index: 128

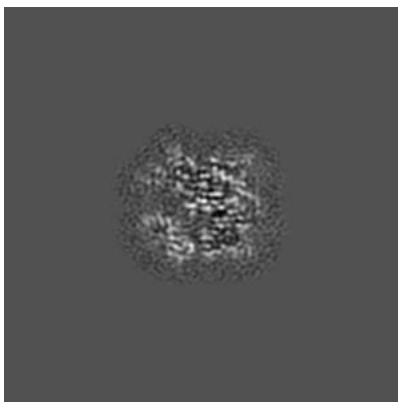
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

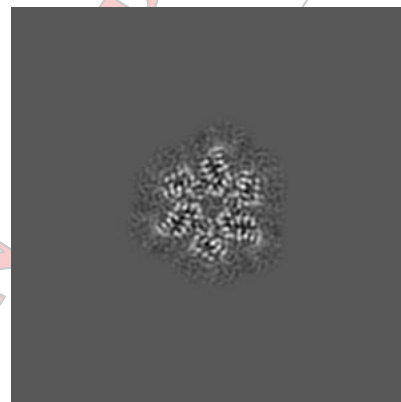
6.3.1 Primary map



X Index: 132

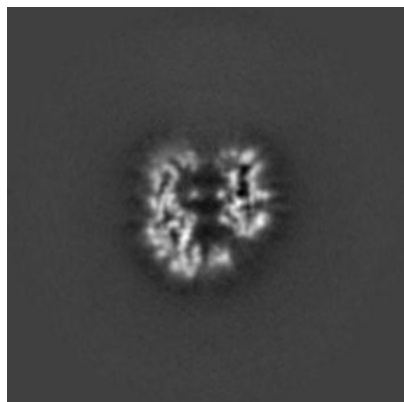


Y Index: 144

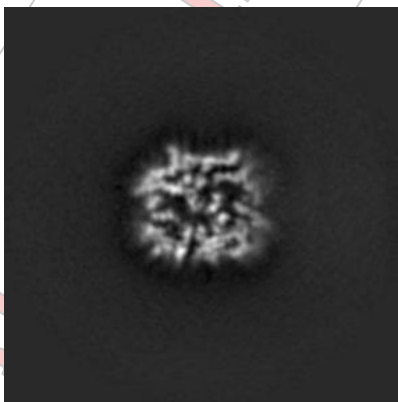


Z Index: 135

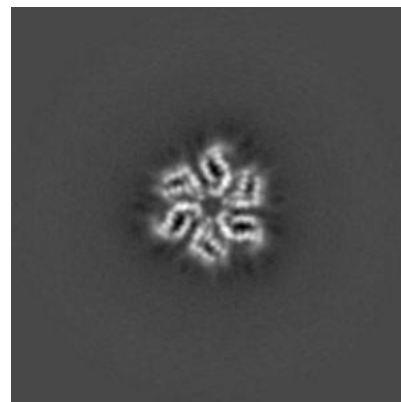
6.3.2 Raw map



X Index: 131



Y Index: 138

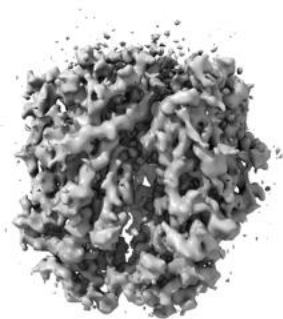


Z Index: 136

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



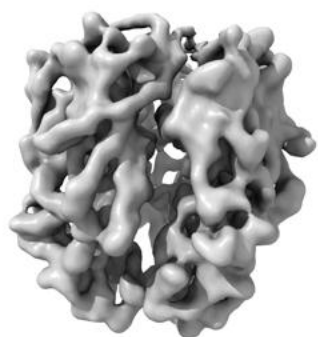
Y



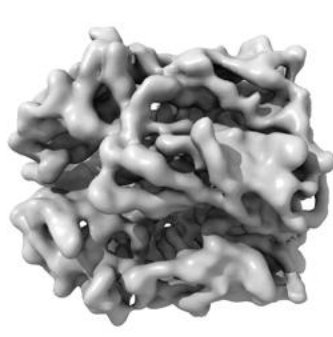
Z

The images above show the 3D surface view of the map at the recommended contour level 6.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

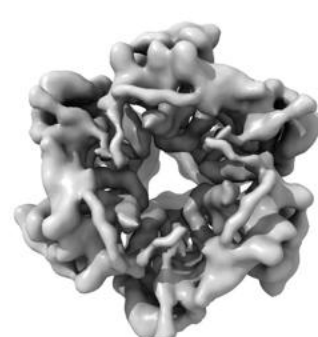
6.4.2 Raw map



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.

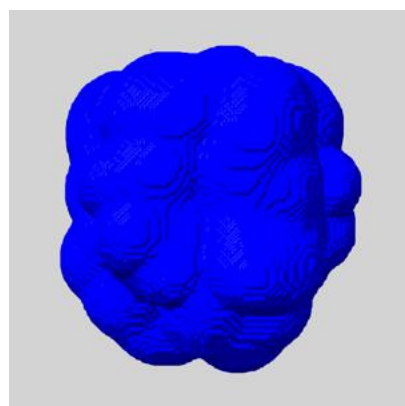
6.5 Mask visualisation [i](#)

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

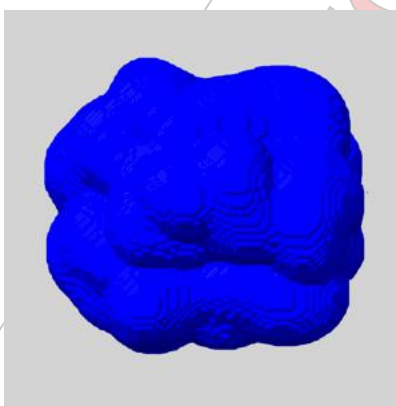
A mask typically either:

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

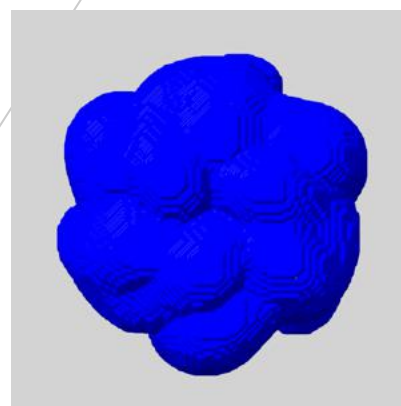
6.5.1 D_1300024106_em-mask-volume_P1.map.V2 [i](#)



X



Y

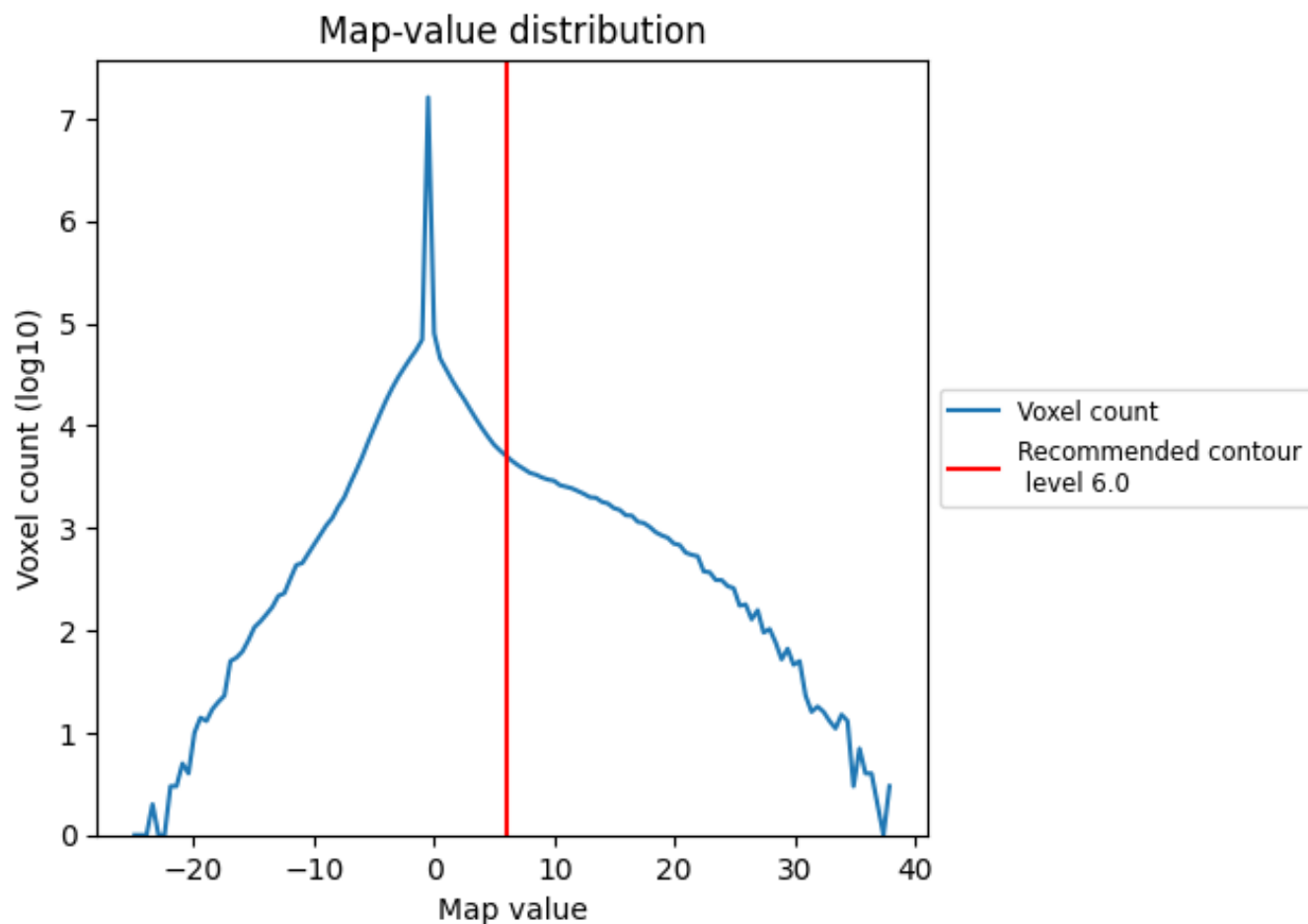


Z

7 Map analysis [i](#)

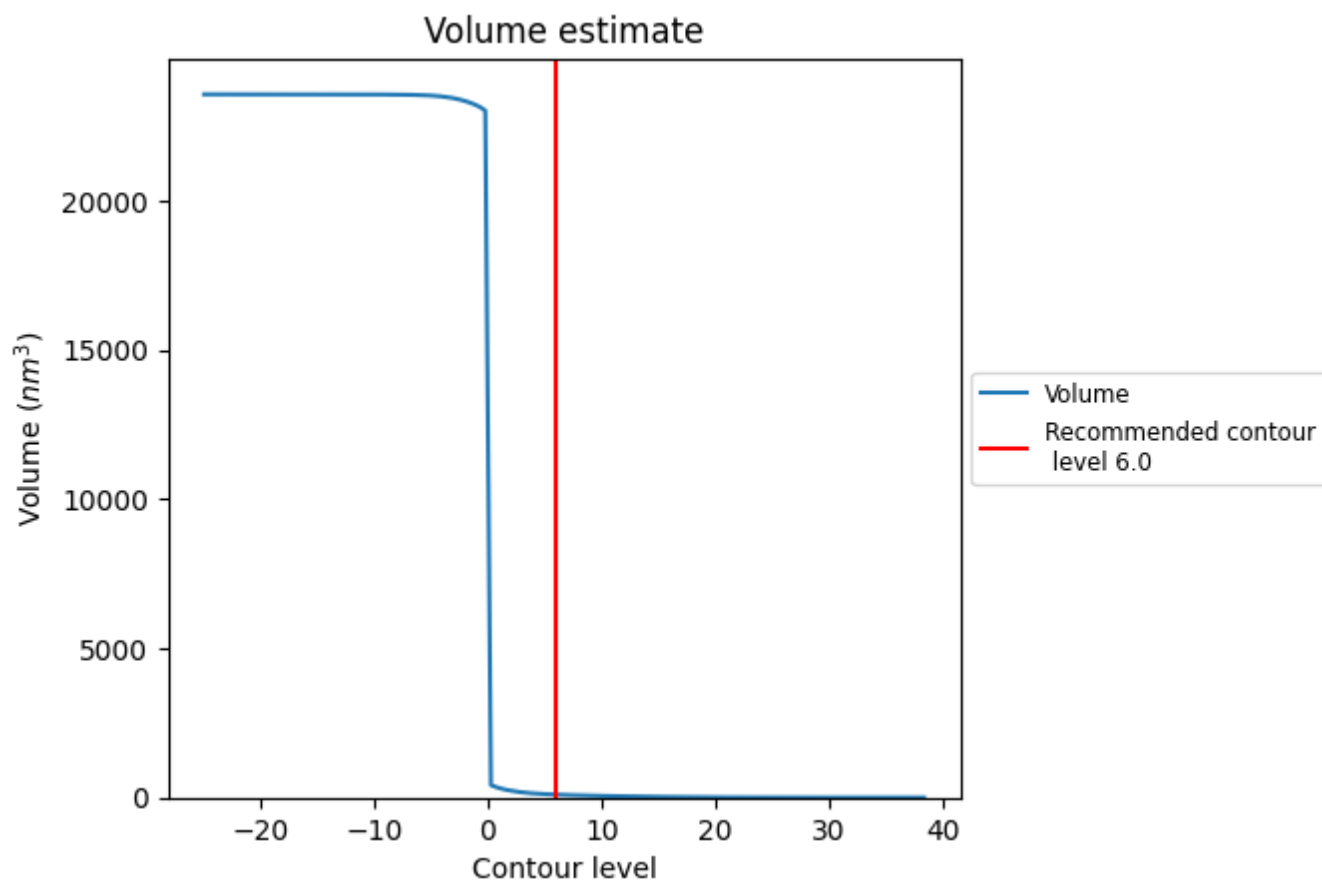
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

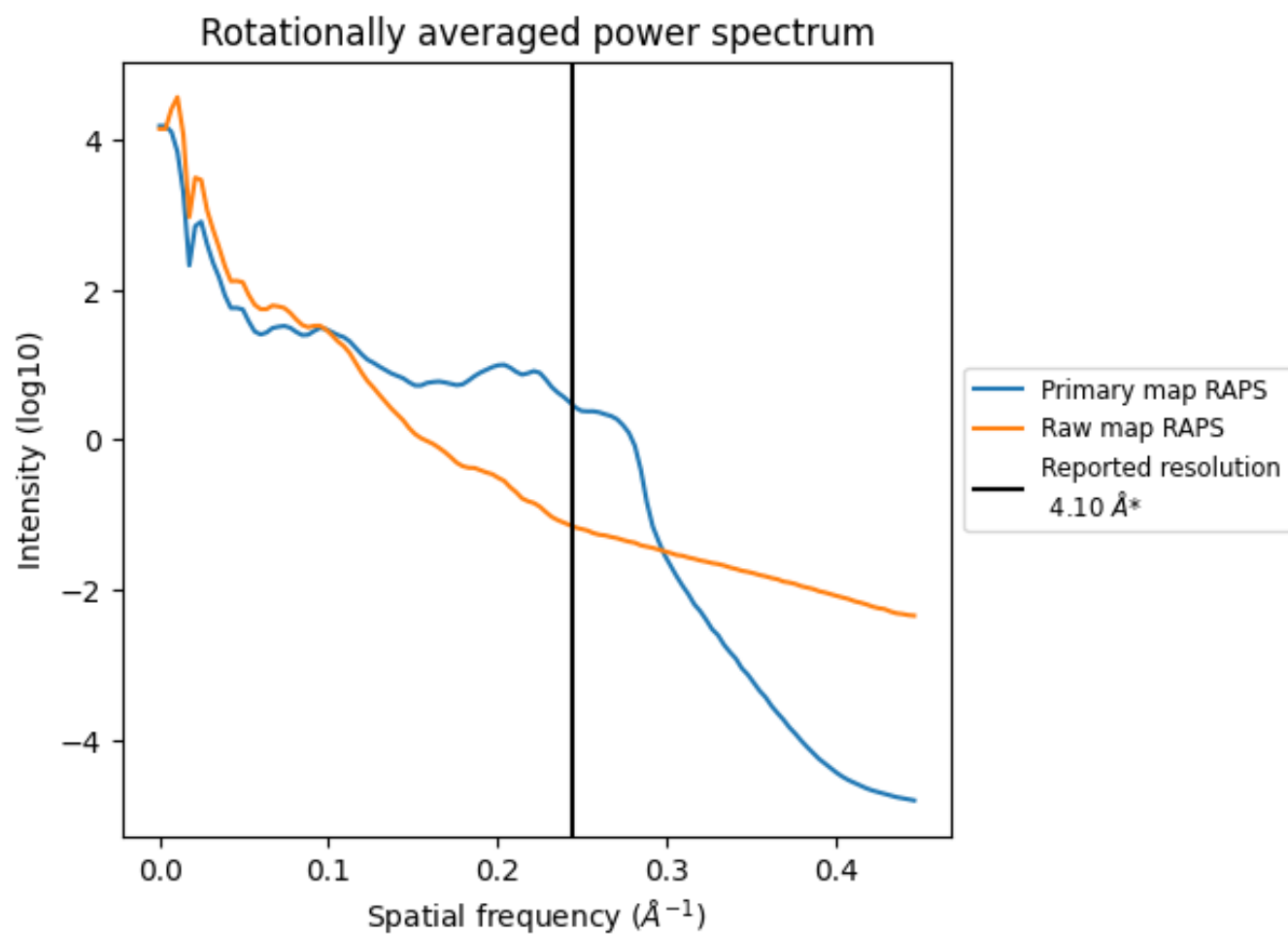
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 99 nm^3 ; this corresponds to an approximate mass of 89 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

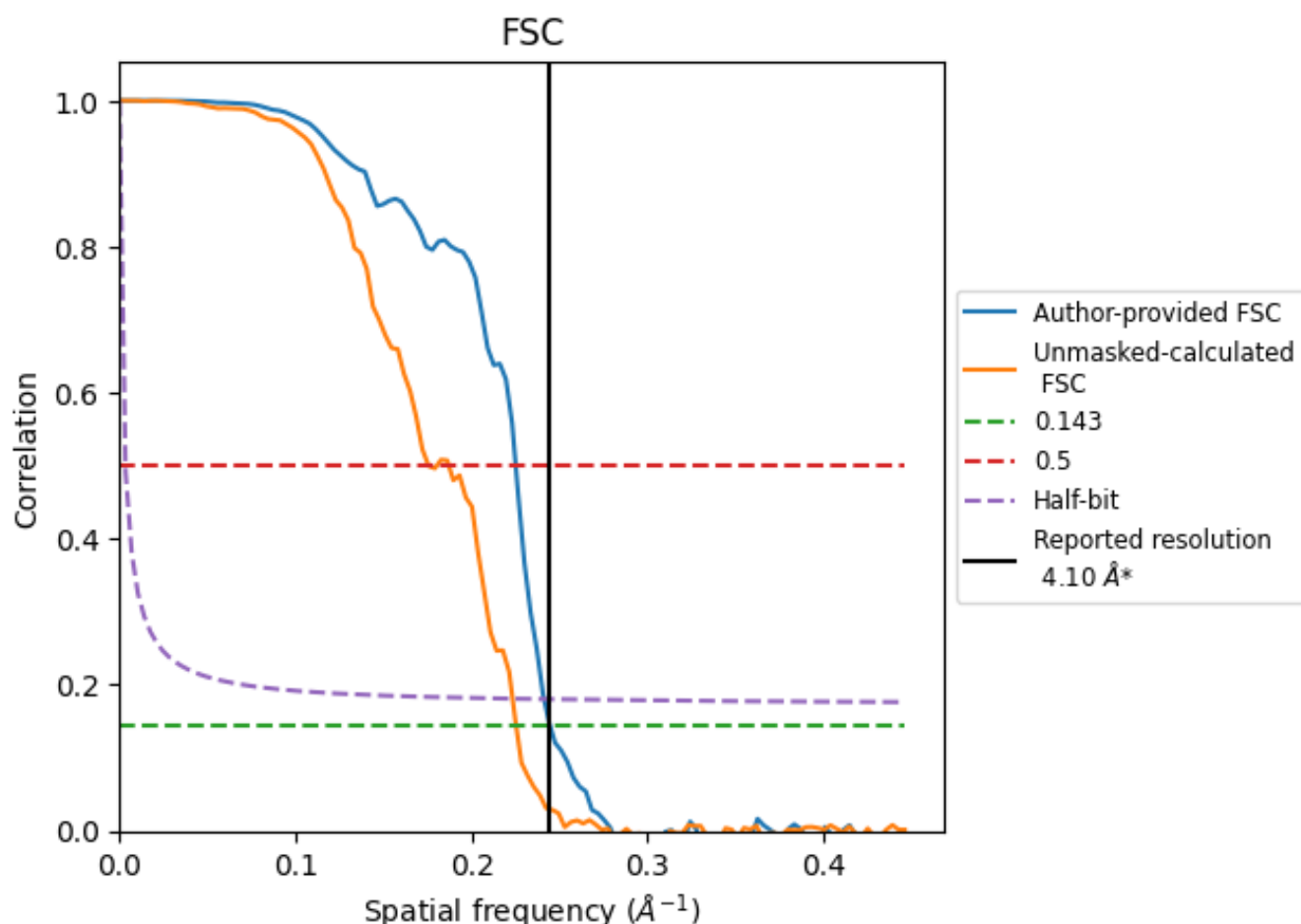


*Reported resolution corresponds to spatial frequency of $0.244 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.244 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

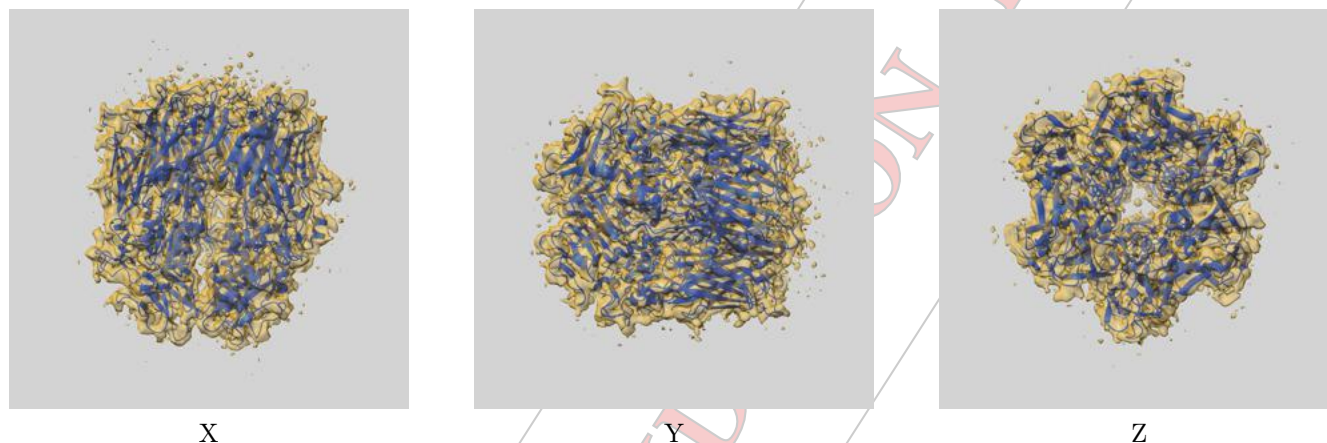
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.08	4.44	4.14
Unmasked-calculated*	4.43	5.69	4.48

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

9 Map-model fit [i](#)

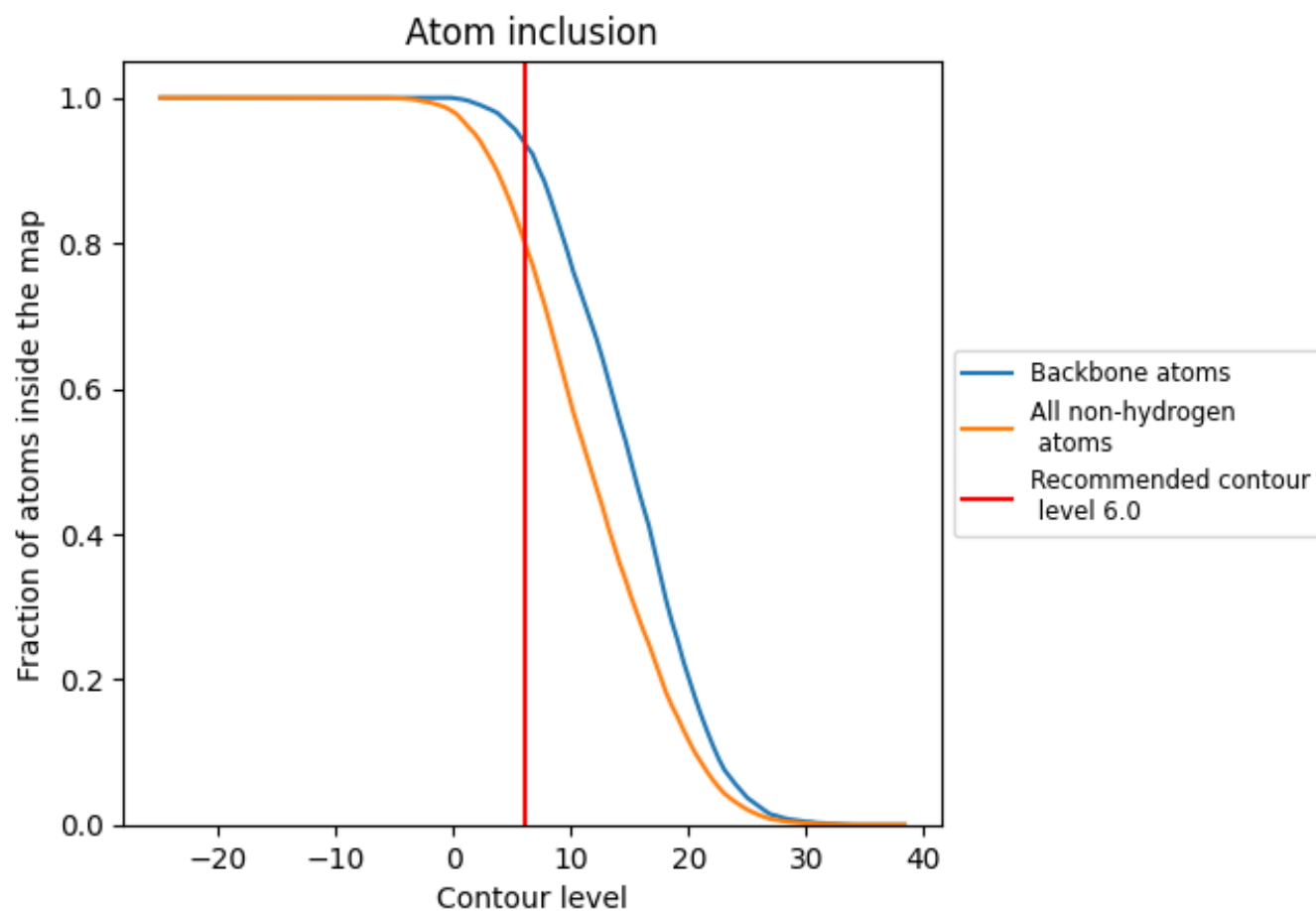
This section contains information regarding the fit between EMDB map EMD-31951 and PDB model 7VFF. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 6.0 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 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.



Full wwPDB EM Validation Report ⓘ

Sep 19, 2021 – 06:43 PM JST

PDB ID : 7VFG
EMDB ID : EMD-31952
Title : Cryo-EM structure of Vaccinia virus scaffolding protein D13 trimer doublet
Deposited on : 2021-09-13
Resolution : 3.87 Å(reported)
Based on initial model : 6BEI

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

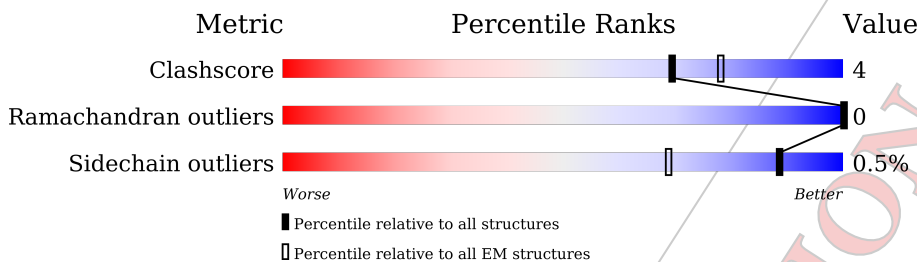
EMDB validation analysis : 0.0.0.dev97
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.1

1 Overall quality at a glance

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

The reported resolution of this entry is 3.87 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	549	 11% 88% 8% .
1	B	549	 9% 88% 8% .
1	C	549	 7% 86% 10% .
1	D	549	 9% 88% 8% .
1	E	549	 8% 87% 9% .
1	F	549	 11% 88% 8% .

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 25044 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Scaffold protein D13.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	527	Total	C	N	O	S	2	0
			4174	2672	679	810	13		
1	F	527	Total	C	N	O	S	2	0
			4174	2672	679	810	13		
1	D	527	Total	C	N	O	S	2	0
			4174	2672	679	810	13		
1	C	527	Total	C	N	O	S	2	0
			4174	2672	679	810	13		
1	A	527	Total	C	N	O	S	2	0
			4174	2672	679	810	13		
1	B	527	Total	C	N	O	S	2	0
			4174	2672	679	810	13		

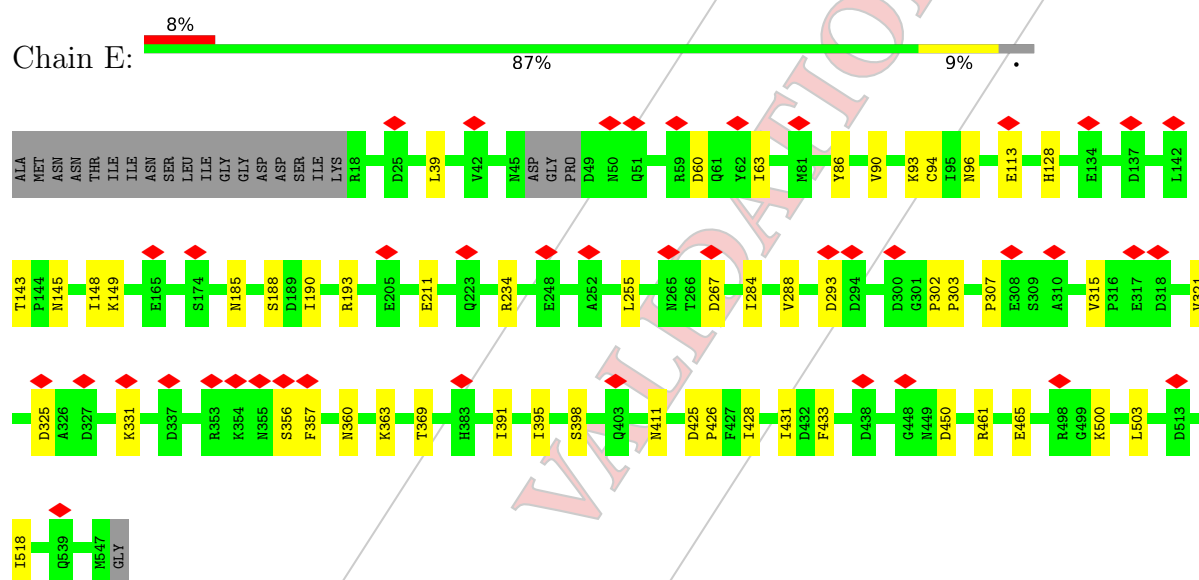
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	0	ALA	-	expression tag	UNP P68440
F	0	ALA	-	expression tag	UNP P68440
D	0	ALA	-	expression tag	UNP P68440
C	0	ALA	-	expression tag	UNP P68440
A	0	ALA	-	expression tag	UNP P68440
B	0	ALA	-	expression tag	UNP P68440

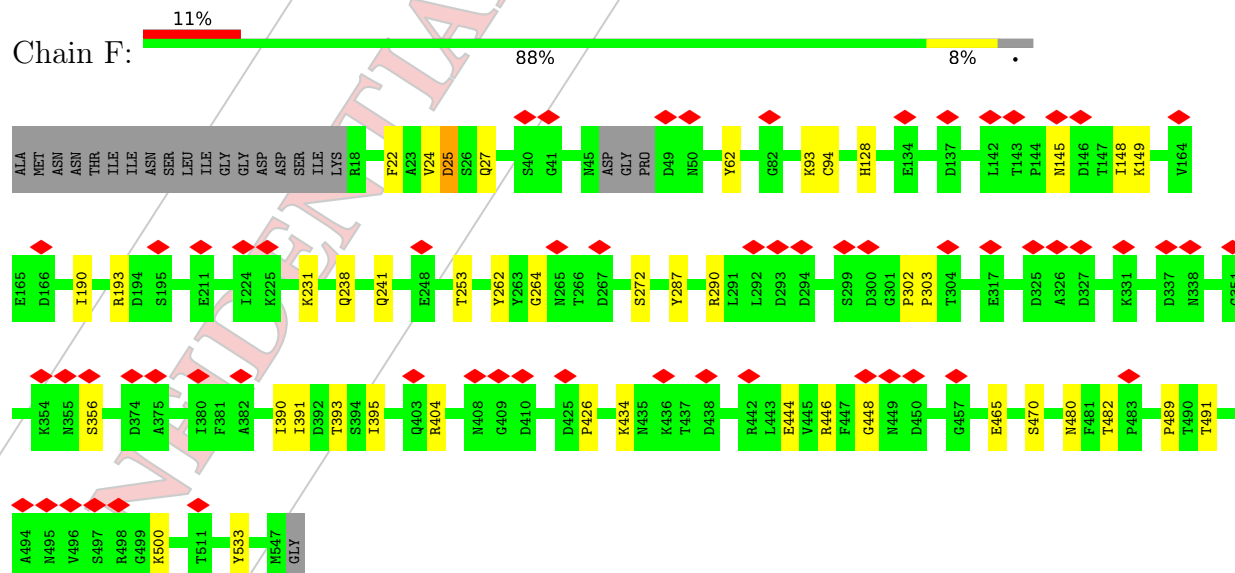
3 Residue-property plots [i](#)

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.

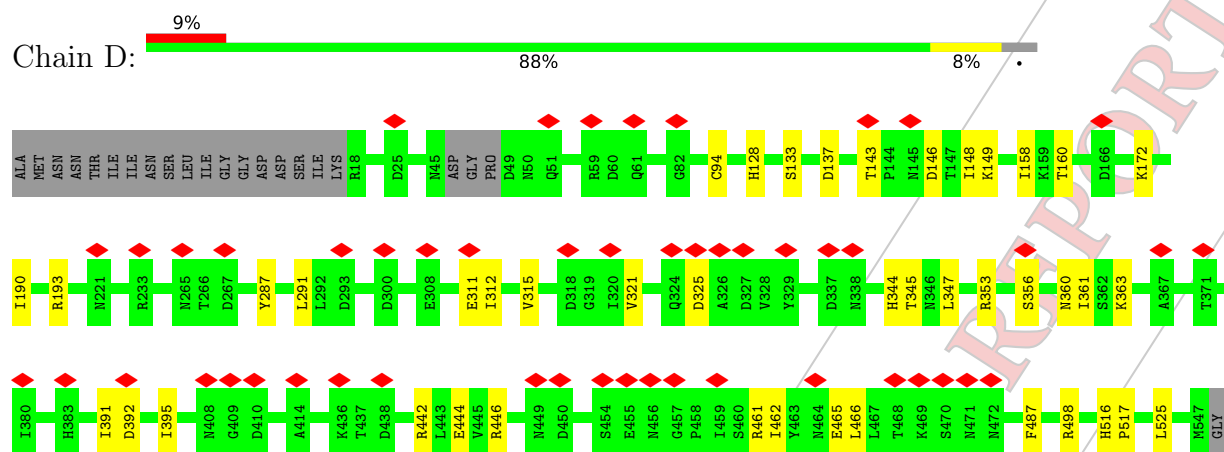
• Molecule 1: Scaffold protein D13



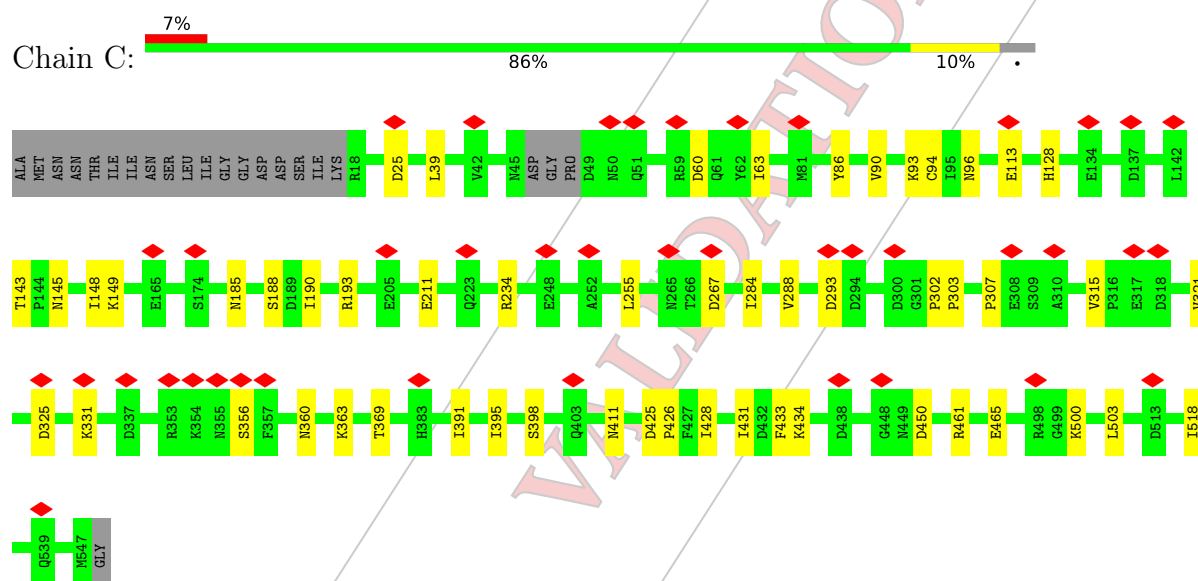
• Molecule 1: Scaffold protein D13



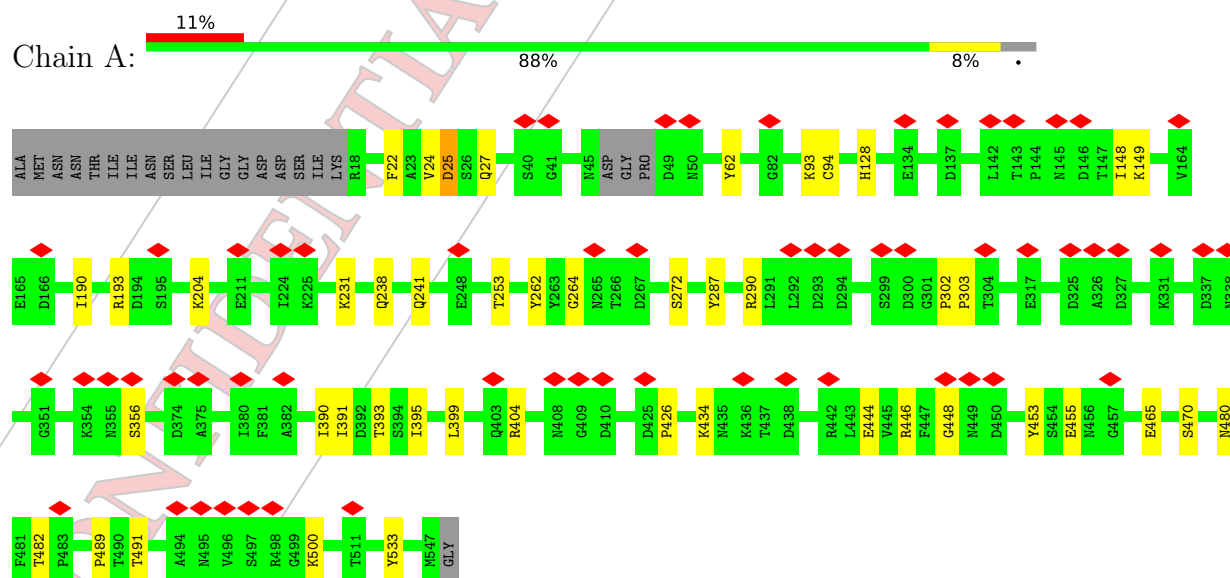
• Molecule 1: Scaffold protein D13



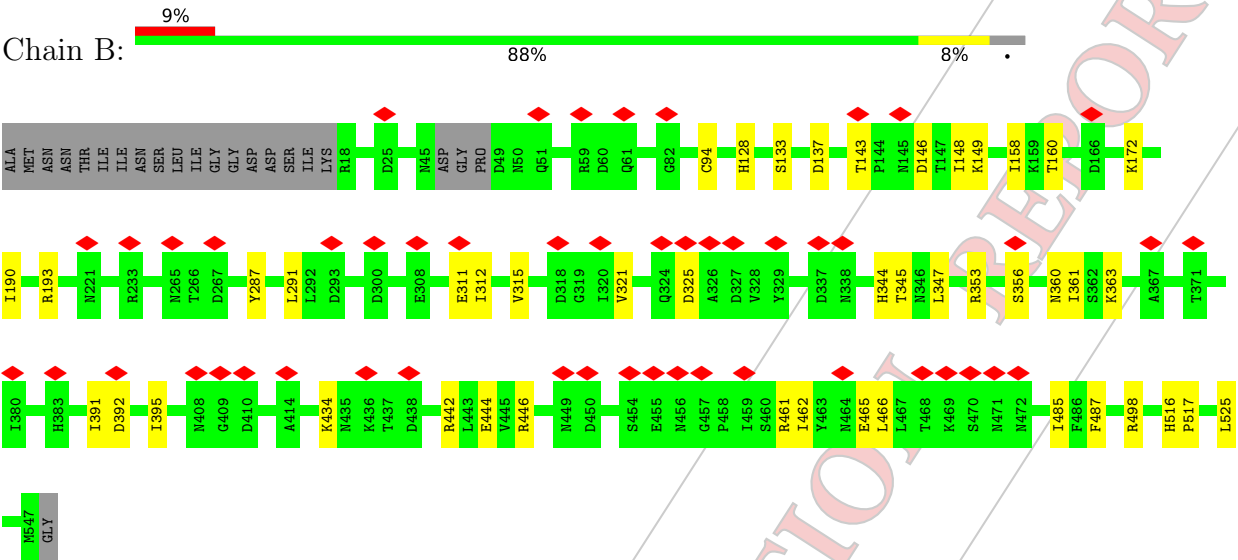
• Molecule 1: Scaffold protein D13



• Molecule 1: Scaffold protein D13



● Molecule 1: Scaffold protein D13



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	42854	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	92000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	29.742	Depositor
Minimum map value	-18.701	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	6.0	Depositor
Map size (Å)	286.72, 286.72, 286.72	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.12, 1.12, 1.12	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	0.38	0/4266	0.52	0/5807
1	B	0.40	0/4266	0.52	0/5807
1	C	0.38	0/4266	0.52	0/5807
1	D	0.40	0/4266	0.52	0/5807
1	E	0.38	0/4266	0.52	0/5807
1	F	0.38	0/4266	0.52	0/5807
All	All	0.39	0/25596	0.52	0/34842

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4174	0	4114	29	0
1	B	4174	0	4114	40	0
1	C	4174	0	4114	32	0
1	D	4174	0	4114	38	0
1	E	4174	0	4114	32	0
1	F	4174	0	4114	27	0
All	All	25044	0	24684	182	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 4.

All (182) 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:D:442:ARG:HH21	1:B:442:ARG:HH21	1.17	0.88
1:B:444:GLU:OE2	1:B:446:ARG:NH1	2.25	0.70
1:B:287:TYR:CE2	1:B:392:ASP:OD2	2.45	0.70
1:D:444:GLU:OE2	1:D:446:ARG:NH1	2.25	0.69
1:D:287:TYR:CE2	1:D:392:ASP:OD2	2.46	0.68
1:A:448:GLY:HA3	1:A:500:LYS:HG2	1.75	0.68
1:D:312:ILE:HG12	1:D:344:HIS:HA	1.77	0.67
1:E:148:ILE:HG22	1:E:149:LYS:HG2	1.78	0.66
1:E:465:GLU:OE2	1:D:128:HIS:NE2	2.26	0.66
1:B:312:ILE:HG12	1:B:344:HIS:HA	1.77	0.66
1:F:448:GLY:HA3	1:F:500:LYS:HG2	1.75	0.66
1:C:465:GLU:OE2	1:B:128:HIS:NE2	2.27	0.66
1:C:148:ILE:HG22	1:C:149:LYS:HG2	1.77	0.65
1:C:60:ASP:HB3	1:C:63:ILE:HD12	1.81	0.63
1:B:361:ILE:HD11	1:B:392:ASP:CG	2.19	0.63
1:E:60:ASP:HB3	1:E:63:ILE:HD12	1.81	0.63
1:A:93:LYS:HD2	1:A:426:PRO:HD2	1.81	0.63
1:D:361:ILE:HD11	1:D:392:ASP:CG	2.19	0.63
1:F:93:LYS:HD2	1:F:426:PRO:HD2	1.81	0.62
1:C:325:ASP:OD1	1:C:363:LYS:NZ	2.33	0.61
1:D:360:ASN:HB3	1:D:363:LYS:HD3	1.83	0.61
1:E:325:ASP:OD1	1:E:363:LYS:NZ	2.34	0.60
1:F:25:ASP:N	1:F:25:ASP:OD1	2.35	0.60
1:A:287:TYR:CG	1:A:393:THR:HG22	2.38	0.59
1:E:356:SER:HG	1:E:357[B]:PHE:H	1.49	0.59
1:F:287:TYR:CG	1:F:393:THR:HG22	2.38	0.59
1:D:148:ILE:HG22	1:D:149:LYS:HG2	1.84	0.59
1:A:272:SER:HB3	1:A:290:ARG:HG3	1.84	0.59
1:B:360:ASN:HB3	1:B:363:LYS:HD3	1.83	0.59
1:F:272:SER:HB3	1:F:290:ARG:HG3	1.85	0.58
1:E:39:LEU:O	1:E:211:GLU:HG3	2.04	0.58
1:C:39:LEU:O	1:C:211:GLU:HG3	2.04	0.58
1:B:148:ILE:HG22	1:B:149:LYS:HG2	1.84	0.58
1:E:128:HIS:NE2	1:F:465:GLU:OE2	2.32	0.57
1:D:353:ARG:HE	1:D:356:SER:HB2	1.69	0.57
1:C:128:HIS:NE2	1:A:465:GLU:OE2	2.31	0.56
1:B:353:ARG:HE	1:B:356:SER:HB2	1.69	0.56
1:F:94[A]:CYS:SG	1:F:190:ILE:HG21	2.45	0.56
1:D:361:ILE:CD1	1:D:392:ASP:OD1	2.54	0.56
1:F:148:ILE:HG22	1:F:149:LYS:HG2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94[A]:CYS:SG	1:C:190:ILE:HG21	2.47	0.55
1:A:94[A]:CYS:SG	1:A:190:ILE:HG21	2.45	0.55
1:E:94[A]:CYS:SG	1:E:190:ILE:HG21	2.47	0.55
1:B:361:ILE:CD1	1:B:392:ASP:OD1	2.55	0.55
1:C:391:ILE:O	1:C:395:ILE:HG13	2.07	0.55
1:A:148:ILE:HG22	1:A:149:LYS:HG2	1.88	0.55
1:A:25:ASP:N	1:A:25:ASP:OD1	2.35	0.54
1:E:391:ILE:O	1:E:395:ILE:HG13	2.07	0.54
1:A:390:ILE:O	1:A:393:THR:OG1	2.22	0.54
1:D:498:ARG:HD2	1:A:62:TYR:HE2	1.73	0.54
1:F:62:TYR:HE2	1:B:498:ARG:HD2	1.73	0.53
1:F:390:ILE:O	1:F:393:THR:OG1	2.22	0.53
1:C:113:GLU:OE1	1:C:234:ARG:NH2	2.42	0.53
1:B:287:TYR:CE2	1:B:291:LEU:HD11	2.44	0.53
1:D:287:TYR:CE2	1:D:291:LEU:HD11	2.44	0.52
1:E:113:GLU:OE1	1:E:234:ARG:NH2	2.42	0.52
1:E:293:ASP:N	1:E:293:ASP:OD1	2.42	0.52
1:C:93:LYS:HD2	1:C:426:PRO:HD2	1.92	0.51
1:D:311:GLU:O	1:D:345:THR:OG1	2.28	0.51
1:C:360:ASN:HB3	1:C:363:LYS:HD3	1.92	0.51
1:E:93:LYS:HD2	1:E:426:PRO:HD2	1.93	0.51
1:C:293:ASP:OD1	1:C:293:ASP:N	2.43	0.51
1:D:291:LEU:HD22	1:D:347:LEU:HD21	1.93	0.49
1:E:360:ASN:HB3	1:E:363:LYS:HD3	1.93	0.49
1:F:262:TYR:CZ	1:F:264:GLY:HA3	2.48	0.48
1:A:262:TYR:CZ	1:A:264:GLY:HA3	2.47	0.48
1:B:361:ILE:HD13	1:B:392:ASP:OD1	2.13	0.48
1:C:93:LYS:NZ	1:C:425:ASP:OD2	2.44	0.48
1:D:353:ARG:NH1	1:B:325:ASP:OD2	2.47	0.48
1:D:361:ILE:HD13	1:D:392:ASP:OD1	2.13	0.48
1:D:325:ASP:OD2	1:B:353:ARG:NH1	2.47	0.48
1:D:361:ILE:HD11	1:D:392:ASP:OD1	2.14	0.48
1:B:94[A]:CYS:SG	1:B:190:ILE:HD13	2.54	0.48
1:D:94[A]:CYS:SG	1:D:190:ILE:HD13	2.54	0.47
1:A:434:LYS:HB3	1:A:434:LYS:HE3	1.73	0.47
1:B:361:ILE:HD11	1:B:392:ASP:OD1	2.14	0.47
1:D:143:THR:N	1:D:146:ASP:OD2	2.48	0.47
1:D:94[A]:CYS:SG	1:D:190:ILE:HG21	2.55	0.47
1:B:291:LEU:HD22	1:B:347:LEU:HD21	1.95	0.47
1:B:143:THR:N	1:B:146:ASP:OD2	2.48	0.47
1:C:255:LEU:HD13	1:C:503:LEU:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:HIS:NE2	1:B:465:GLU:OE2	2.45	0.46
1:B:311:GLU:O	1:B:345:THR:OG1	2.29	0.46
1:B:353:ARG:NE	1:B:356:SER:HB2	2.30	0.46
1:D:315:VAL:HG22	1:D:321:VAL:HG21	1.98	0.46
1:C:96:ASN:HB2	1:C:185:ASN:OD1	2.16	0.46
1:F:128:HIS:NE2	1:D:465:GLU:OE2	2.45	0.46
1:C:143:THR:HG23	1:C:145:ASN:H	1.81	0.46
1:E:143:THR:HG23	1:E:145:ASN:H	1.81	0.46
1:C:431:ILE:HD12	1:C:518:ILE:HG12	1.98	0.45
1:B:94[A]:CYS:SG	1:B:190:ILE:HG21	2.55	0.45
1:F:404:ARG:HH11	1:F:404:ARG:HG2	1.82	0.45
1:D:353:ARG:NE	1:D:356:SER:HB2	2.30	0.45
1:A:253:THR:HG22	1:A:491:THR:HG22	1.99	0.45
1:B:315:VAL:HG22	1:B:321:VAL:HG21	1.97	0.45
1:E:255:LEU:HD13	1:E:503:LEU:HD13	1.97	0.45
1:E:331:LYS:O	1:E:369:THR:HA	2.17	0.45
1:B:133:SER:O	1:B:137:ASP:HB2	2.17	0.45
1:D:442:ARG:NE	1:B:442:ARG:NE	2.64	0.45
1:E:96:ASN:HB2	1:E:185:ASN:OD1	2.16	0.45
1:E:431:ILE:HD12	1:E:518:ILE:HG12	1.98	0.45
1:D:133:SER:O	1:D:137:ASP:HB2	2.16	0.45
1:A:404:ARG:NH1	1:A:404:ARG:HG2	2.32	0.45
1:F:231:LYS:HE2	1:F:533:TYR:CE1	2.52	0.44
1:F:253:THR:HG22	1:F:491:THR:HG22	1.99	0.44
1:C:94[A]:CYS:SG	1:C:190:ILE:HD13	2.58	0.44
1:A:404:ARG:HG2	1:A:404:ARG:HH11	1.82	0.44
1:C:302:PRO:HA	1:C:303:PRO:HD3	1.90	0.44
1:C:331:LYS:O	1:C:369:THR:HA	2.17	0.44
1:A:444:GLU:OE1	1:A:446:ARG:NE	2.50	0.44
1:E:94[A]:CYS:SG	1:E:190:ILE:HD13	2.58	0.44
1:C:284:ILE:O	1:C:288:VAL:HG23	2.17	0.44
1:F:404:ARG:HG2	1:F:404:ARG:NH1	2.33	0.44
1:F:434:LYS:HB3	1:F:434:LYS:HE3	1.73	0.44
1:A:231:LYS:HE2	1:A:533:TYR:CE1	2.52	0.44
1:E:450:ASP:OD2	1:E:500:LYS:HE3	2.18	0.44
1:B:391:ILE:O	1:B:395:ILE:HG13	2.18	0.44
1:E:284:ILE:O	1:E:288:VAL:HG23	2.17	0.44
1:E:93:LYS:NZ	1:E:425:ASP:OD2	2.44	0.43
1:A:302:PRO:HA	1:A:303:PRO:HD3	1.92	0.43
1:D:466:LEU:HD23	1:D:466:LEU:HA	1.82	0.43
1:E:428:ILE:HD12	1:E:433:PHE:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:353:ARG:HG2	1:D:356:SER:HB3	2.00	0.43
1:B:434:LYS:HA	1:B:434:LYS:HD2	1.85	0.43
1:D:391:ILE:O	1:D:395:ILE:HG13	2.18	0.43
1:B:516:HIS:ND1	1:B:517:PRO:HD2	2.33	0.43
1:D:516:HIS:ND1	1:D:517:PRO:HD2	2.34	0.43
1:C:428:ILE:HD12	1:C:433:PHE:CD1	2.53	0.43
1:E:302:PRO:HA	1:E:303:PRO:HD3	1.90	0.43
1:C:315:VAL:HG22	1:C:321:VAL:HG21	2.01	0.43
1:F:145:ASN:OD1	1:F:145:ASN:N	2.51	0.43
1:D:525:LEU:HD12	1:D:525:LEU:HA	1.86	0.43
1:C:450:ASP:OD2	1:C:500:LYS:HE3	2.18	0.43
1:E:315:VAL:HG22	1:E:321:VAL:HG21	2.01	0.43
1:B:462:ILE:HD13	1:B:462:ILE:HA	1.85	0.42
1:F:22:PHE:HD1	1:D:172:LYS:HE3	1.83	0.42
1:A:204:LYS:HB3	1:A:204:LYS:HE3	1.76	0.42
1:B:461:ARG:HH11	1:B:461:ARG:HG2	1.84	0.42
1:C:461:ARG:HH11	1:C:461:ARG:HG2	1.83	0.42
1:C:86:TYR:HB3	1:C:90:VAL:HG11	2.02	0.42
1:F:27:GLN:HB2	1:D:487:PHE:CD2	2.55	0.42
1:C:86:TYR:HB3	1:C:90:VAL:CG1	2.49	0.42
1:E:86:TYR:HB3	1:E:90:VAL:CG1	2.49	0.42
1:C:267:ASP:OD1	1:C:398:SER:OG	2.37	0.42
1:A:238:GLN:HB2	1:A:241:GLN:HG2	2.00	0.42
1:F:444:GLU:OE1	1:F:446:ARG:NE	2.51	0.42
1:A:391:ILE:O	1:A:395:ILE:HG13	2.20	0.42
1:B:353:ARG:HG2	1:B:356:SER:HB3	2.01	0.42
1:E:267:ASP:OD1	1:E:398:SER:OG	2.38	0.42
1:E:461:ARG:HG2	1:E:461:ARG:HH11	1.83	0.42
1:E:307:PRO:HG2	1:E:411:ASN:HA	2.02	0.42
1:D:461:ARG:HG2	1:D:461:ARG:HH11	1.84	0.42
1:A:399:LEU:HD23	1:A:399:LEU:HA	1.85	0.42
1:E:86:TYR:HB3	1:E:90:VAL:HG11	2.02	0.41
1:F:302:PRO:HA	1:F:303:PRO:HD3	1.92	0.41
1:B:461:ARG:HG2	1:B:461:ARG:NH1	2.35	0.41
1:B:525:LEU:HD12	1:B:525:LEU:HA	1.86	0.41
1:F:238:GLN:HB2	1:F:241:GLN:HG2	2.00	0.41
1:C:307:PRO:HG2	1:C:411:ASN:HA	2.01	0.41
1:A:22:PHE:HD1	1:B:172:LYS:HE3	1.84	0.41
1:C:434:LYS:HA	1:C:434:LYS:HD2	1.92	0.41
1:F:391:ILE:O	1:F:395:ILE:HG13	2.20	0.41
1:C:428:ILE:HD12	1:C:433:PHE:HD1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:461:ARG:HG2	1:D:461:ARG:NH1	2.35	0.41
1:A:453:TYR:OH	1:A:455:GLU:OE1	2.38	0.41
1:A:465:GLU:HG2	1:A:470:SER:O	2.21	0.41
1:F:465:GLU:HG2	1:F:470:SER:O	2.21	0.41
1:A:27:GLN:HB2	1:B:487:PHE:CD2	2.55	0.41
1:A:480:ASN:ND2	1:A:489:PRO:HB3	2.36	0.40
1:D:158:ILE:O	1:D:160:THR:HG23	2.21	0.40
1:B:466:LEU:HD23	1:B:466:LEU:HA	1.81	0.40
1:B:485:ILE:HD13	1:B:485:ILE:HA	1.86	0.40
1:E:428:ILE:HD12	1:E:433:PHE:HD1	1.85	0.40
1:F:480:ASN:ND2	1:F:489:PRO:HB3	2.36	0.40
1:D:462:ILE:HD13	1:D:462:ILE:HA	1.85	0.40
1:B:158:ILE:O	1:B:160:THR:HG23	2.21	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	524/549 (95%)	506 (97%)	18 (3%)	0	100	100
1	B	524/549 (95%)	506 (97%)	18 (3%)	0	100	100
1	C	524/549 (95%)	504 (96%)	20 (4%)	0	100	100
1	D	524/549 (95%)	506 (97%)	18 (3%)	0	100	100
1	E	524/549 (95%)	504 (96%)	20 (4%)	0	100	100
1	F	524/549 (95%)	506 (97%)	18 (3%)	0	100	100
All	All	3144/3294 (95%)	3032 (96%)	112 (4%)	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	479/502 (95%)	475 (99%)	4 (1%)	81	89
1	B	479/502 (95%)	478 (100%)	1 (0%)	93	96
1	C	479/502 (95%)	476 (99%)	3 (1%)	86	91
1	D	479/502 (95%)	478 (100%)	1 (0%)	93	96
1	E	479/502 (95%)	477 (100%)	2 (0%)	91	94
1	F	479/502 (95%)	475 (99%)	4 (1%)	81	89
All	All	2874/3012 (95%)	2859 (100%)	15 (0%)	89	93

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	188	SER
1	E	193	ARG
1	F	24	VAL
1	F	25	ASP
1	F	193	ARG
1	F	482	THR
1	D	193	ARG
1	C	25	ASP
1	C	188	SER
1	C	193	ARG
1	A	24	VAL
1	A	25	ASP
1	A	193	ARG
1	A	482	THR
1	B	193	ARG

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 [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.

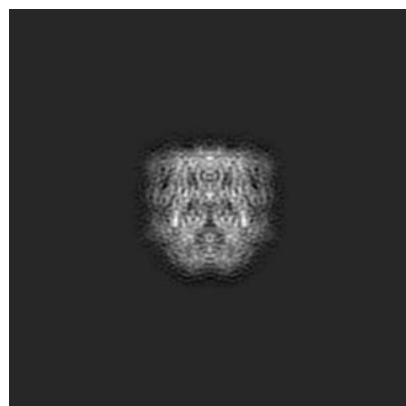
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31952. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

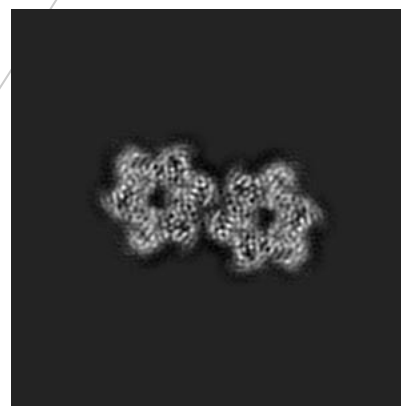
6.1.1 Primary map



X

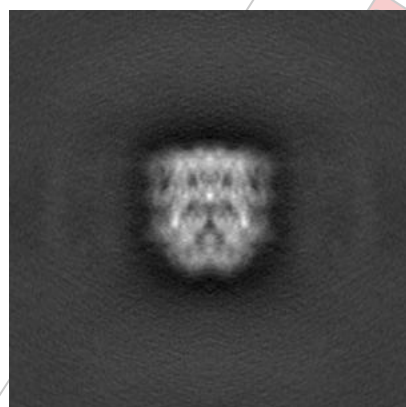


Y

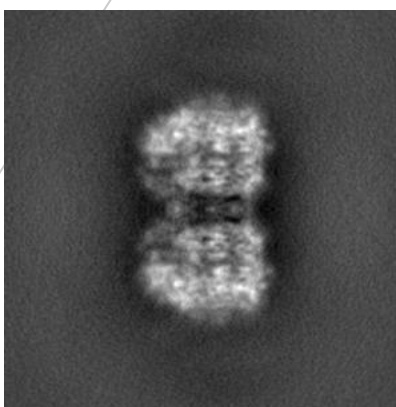


Z

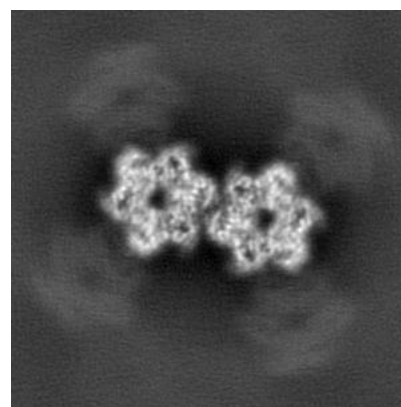
6.1.2 Raw map



X



Y

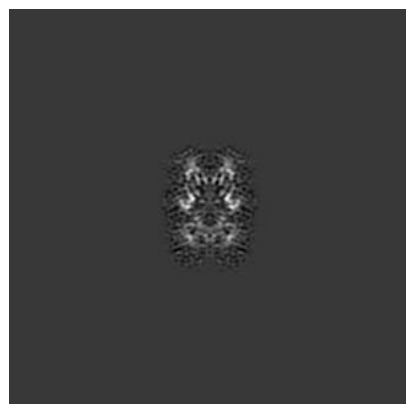


Z

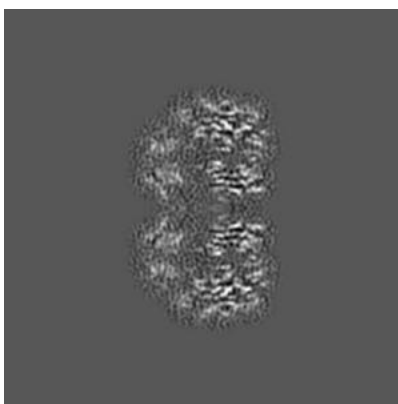
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

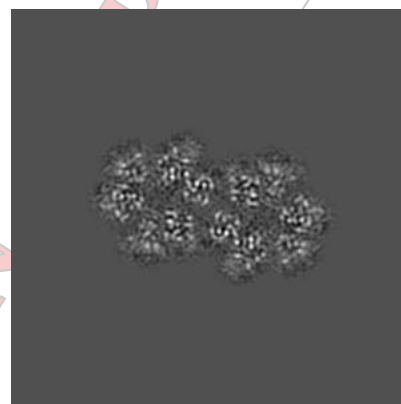
6.2.1 Primary map



X Index: 128

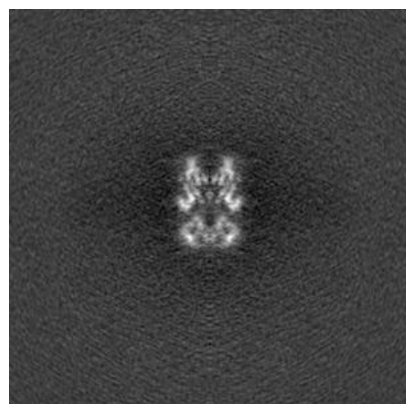


Y Index: 128

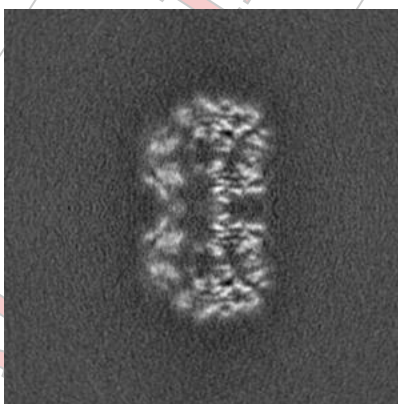


Z Index: 128

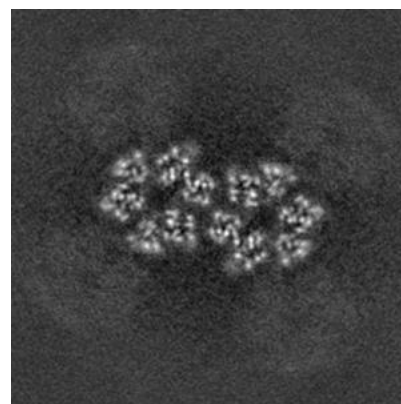
6.2.2 Raw map



X Index: 128



Y Index: 128

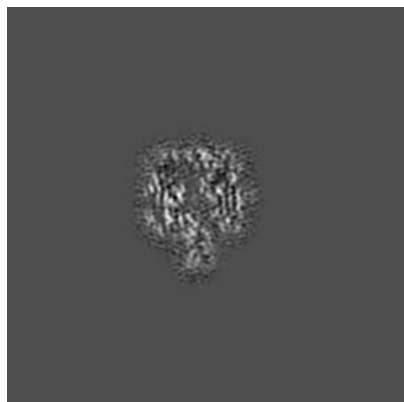


Z Index: 128

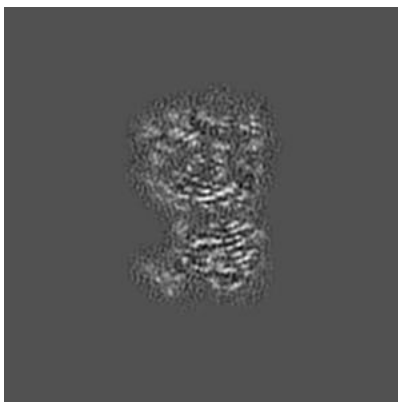
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

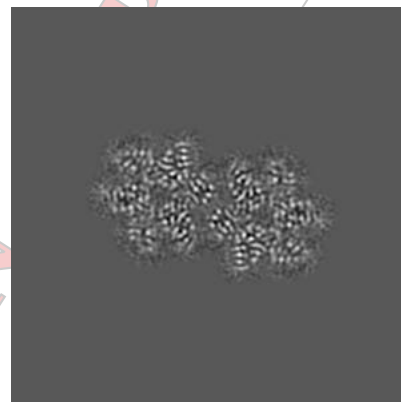
6.3.1 Primary map



X Index: 149

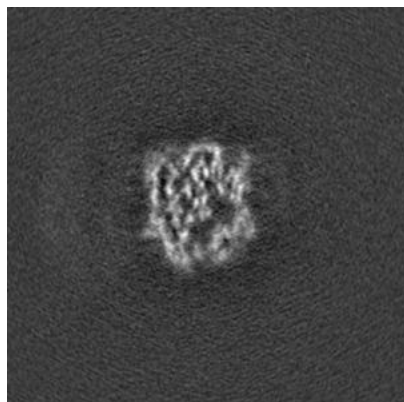


Y Index: 113

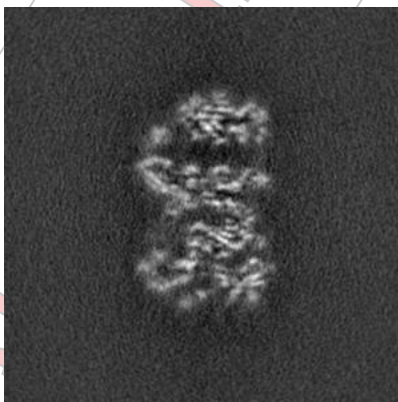


Z Index: 136

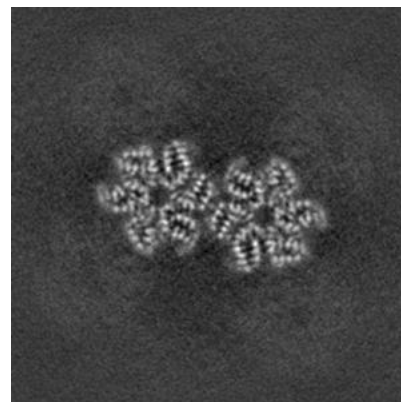
6.3.2 Raw map



X Index: 177



Y Index: 121

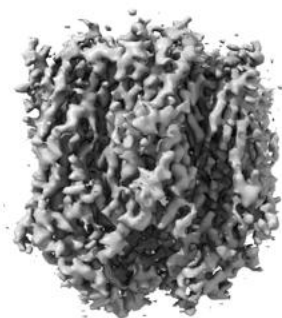


Z Index: 138

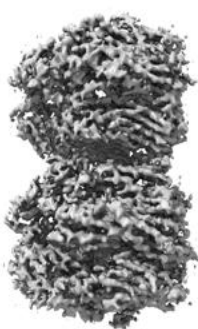
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

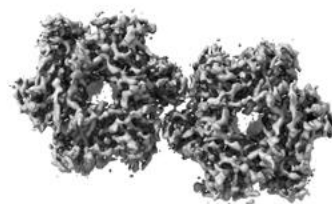
6.4.1 Primary map



X



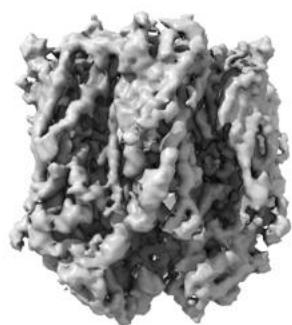
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 6.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

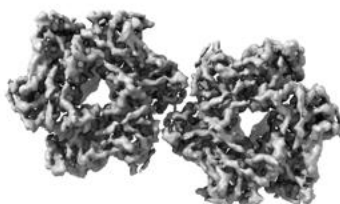
6.4.2 Raw map



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.

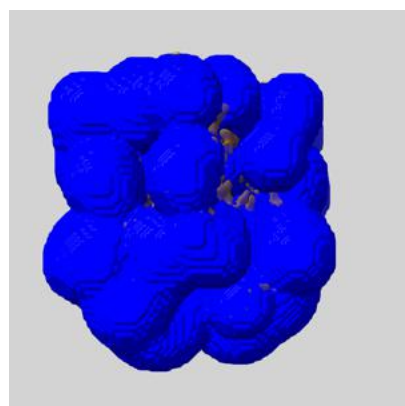
6.5 Mask visualisation [i](#)

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

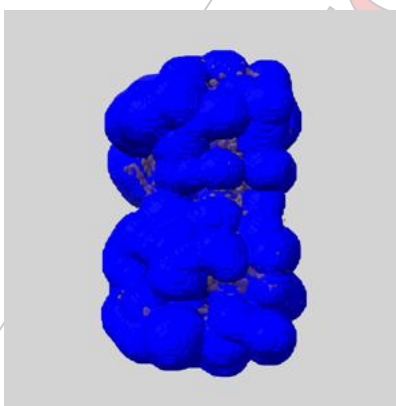
A mask typically either:

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

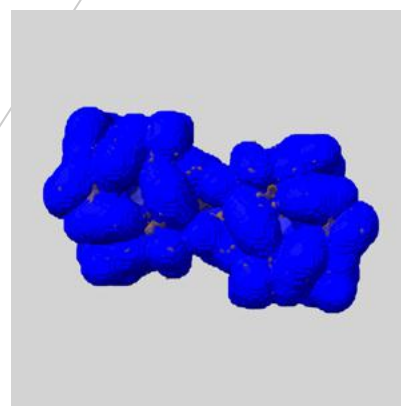
6.5.1 D_1300024107_em-mask-volume_P1.map.V2 [i](#)



X



Y

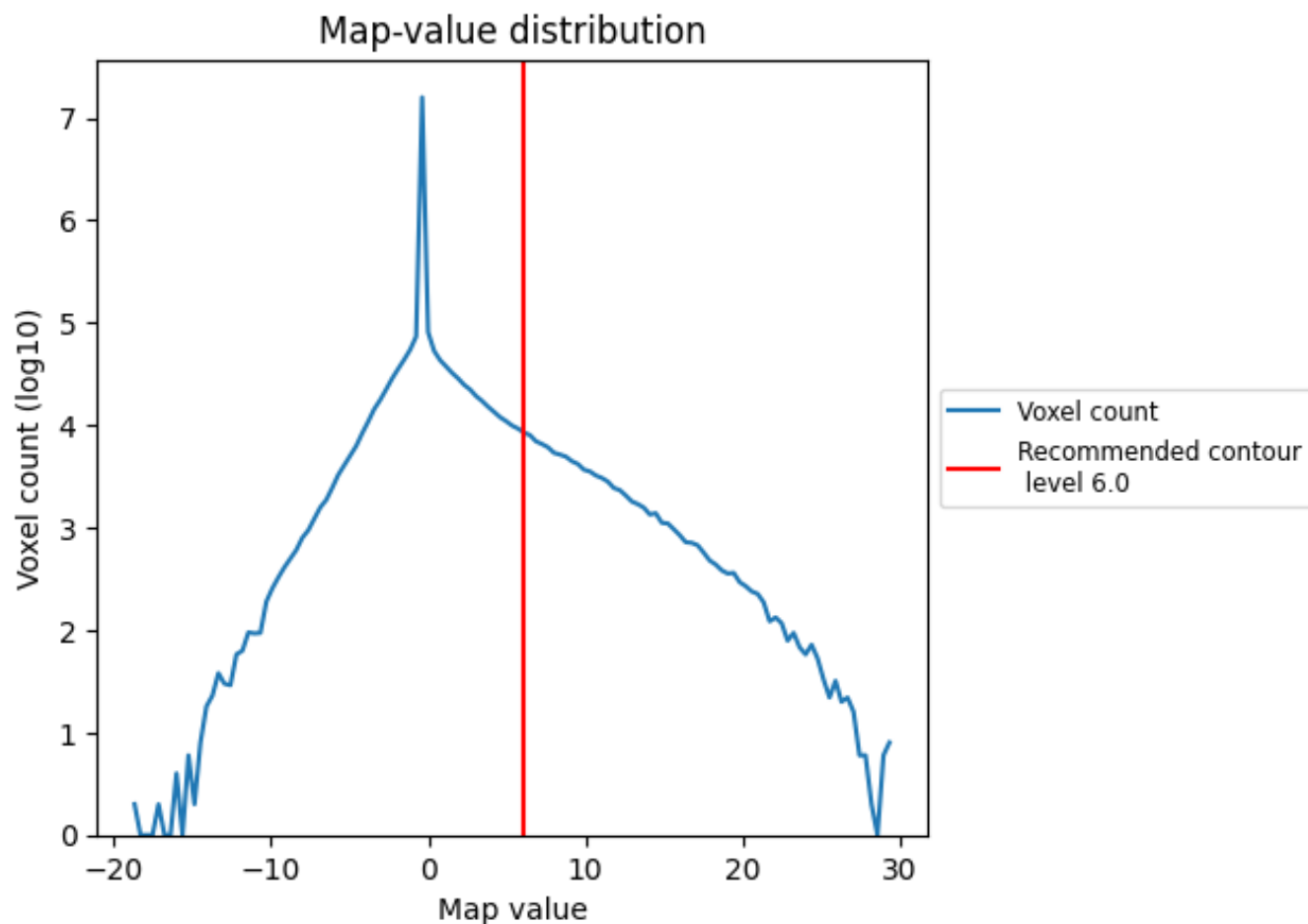


Z

7 Map analysis [i](#)

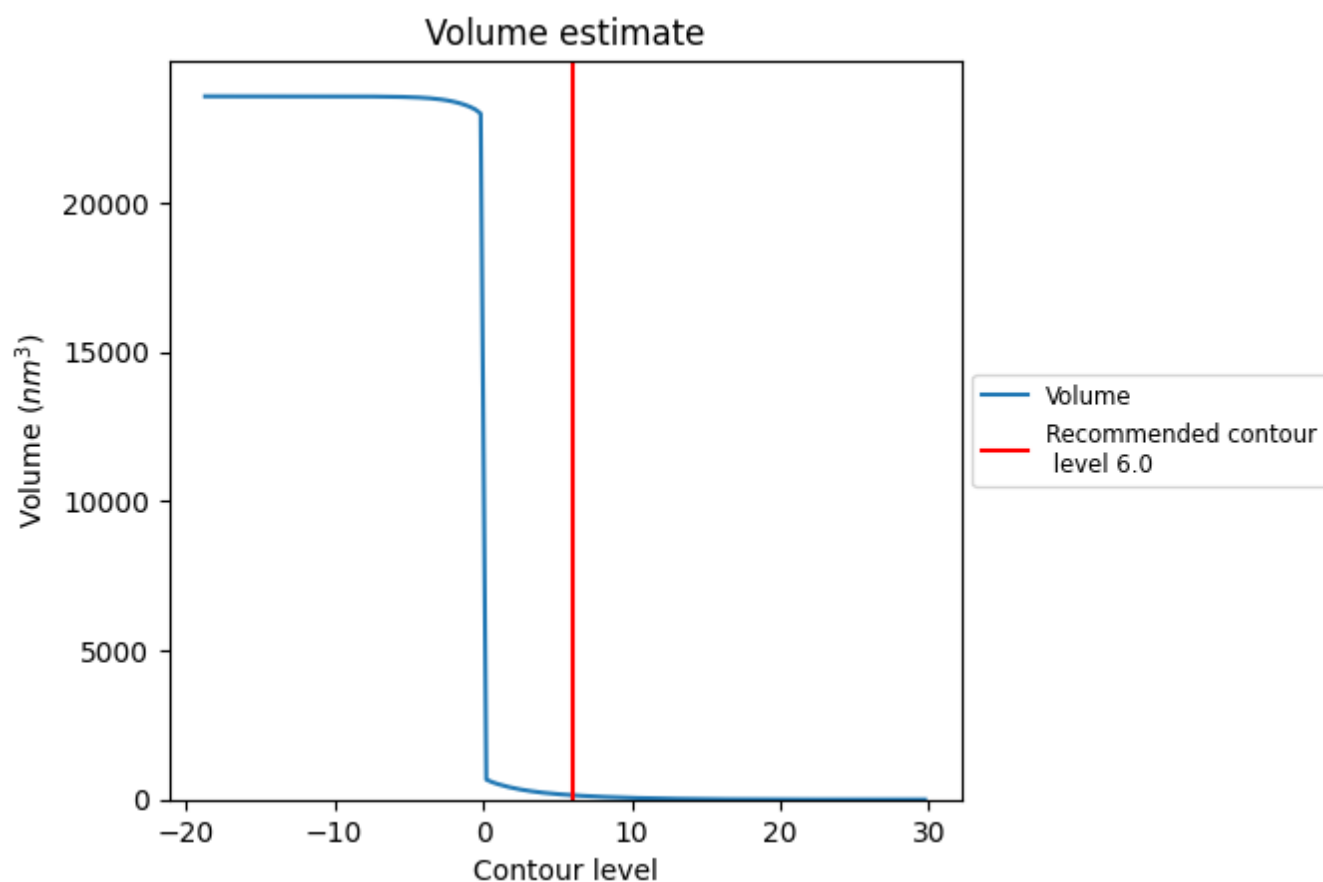
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

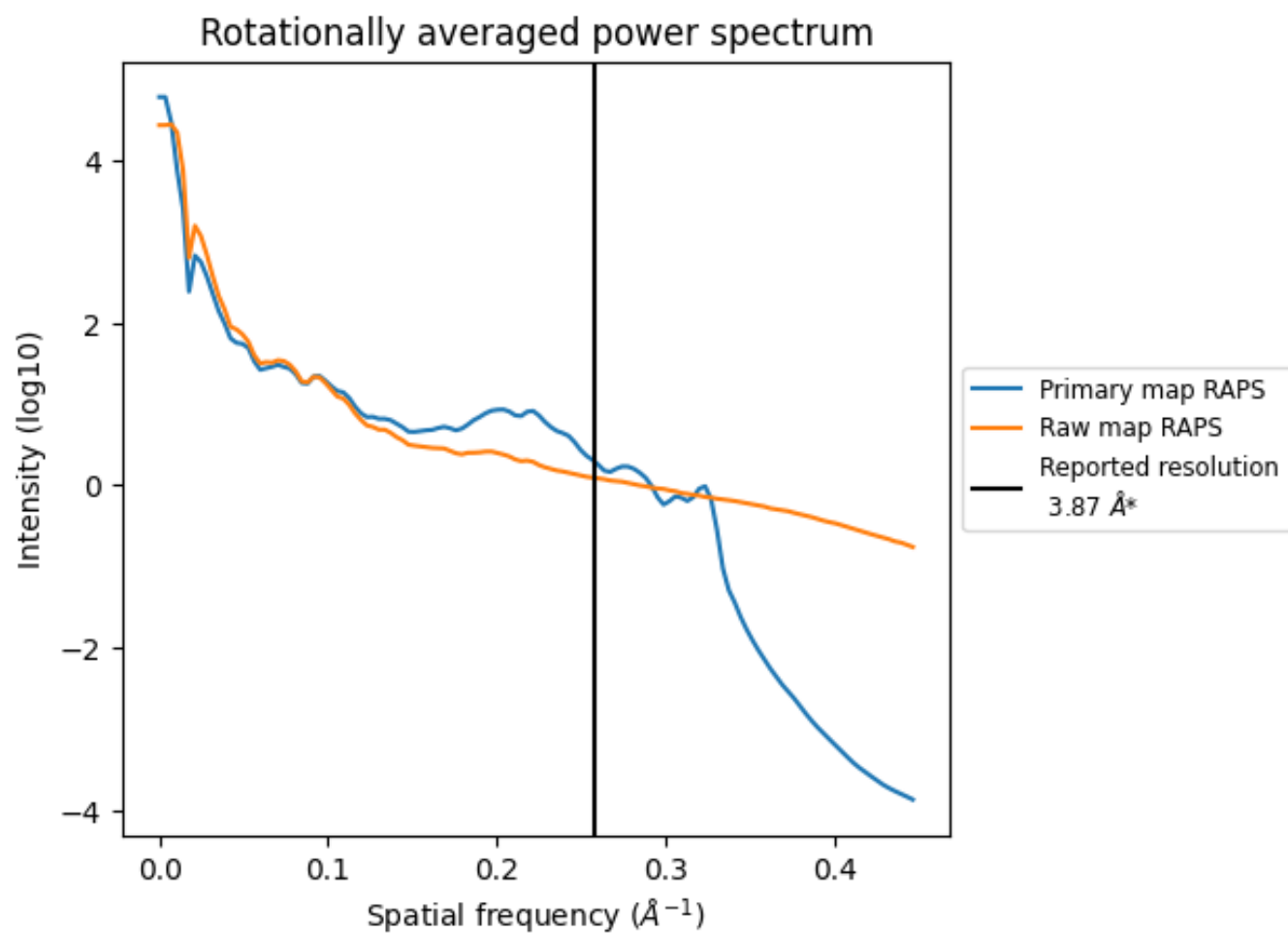
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 147 nm^3 ; this corresponds to an approximate mass of 133 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

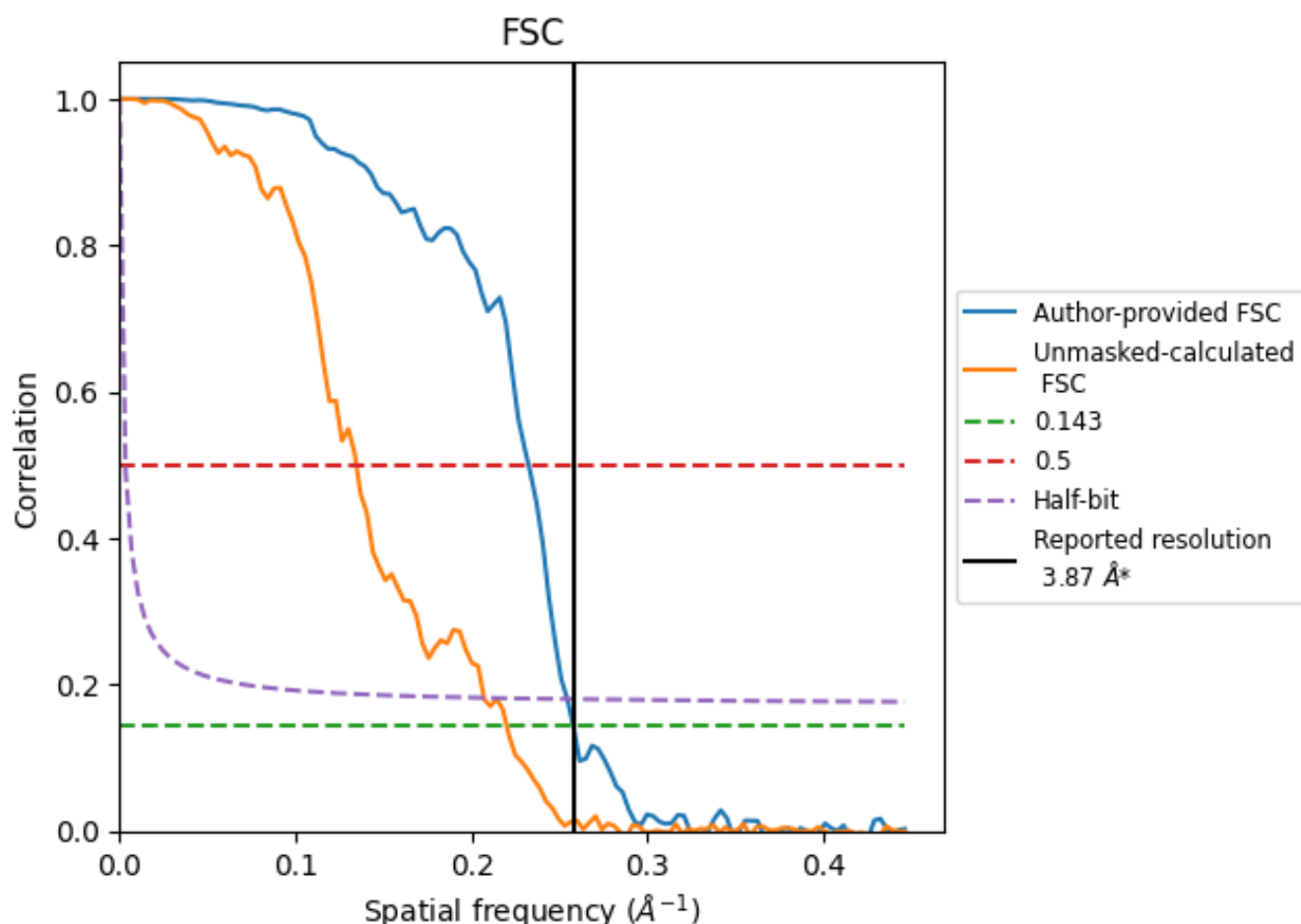


*Reported resolution corresponds to spatial frequency of 0.258 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.258 Å⁻¹

8.2 Resolution estimates [i](#)

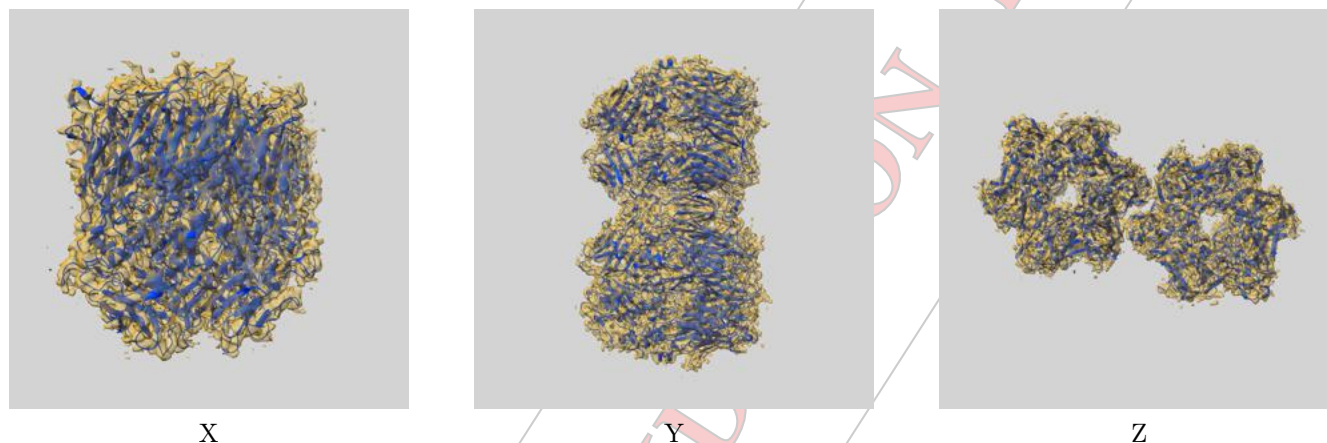
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.87	-	-
Author-provided FSC curve	3.88	4.30	3.93
Unmasked-calculated*	4.54	7.43	4.83

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.54 differs from the reported value 3.87 by more than 10 %

9 Map-model fit [i](#)

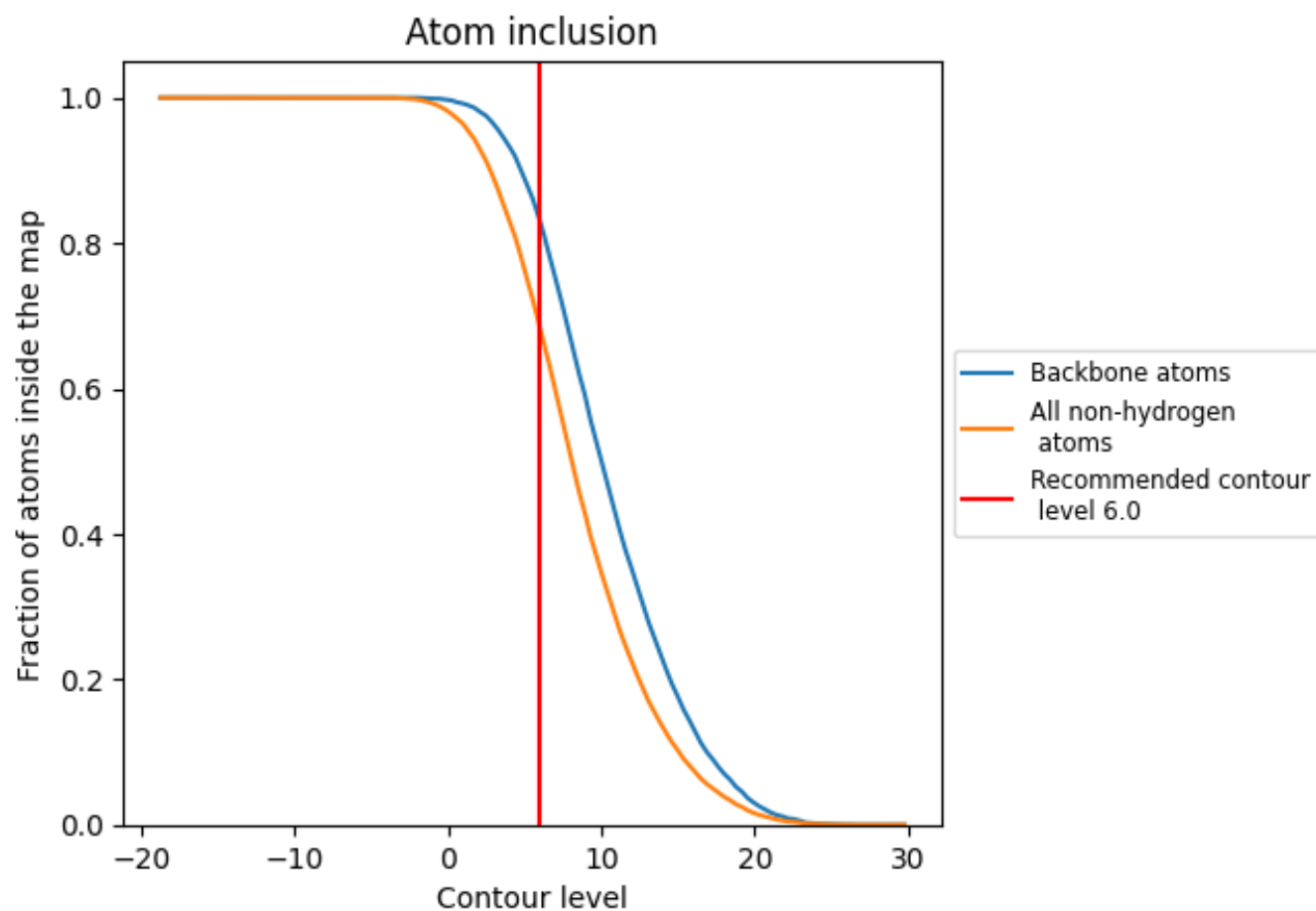
This section contains information regarding the fit between EMDB map EMD-31952 and PDB model 7VFG. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 6.0 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 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.



Full wwPDB EM Validation Report ⓘ

Oct 14, 2021 – 05:51 PM JST

PDB ID : 7VFH
EMDB ID : EMD-31954
Title : Cryo-EM structure of Vaccinia virus scaffolding protein D13 trimer sextet
Deposited on : 2021-09-13
Resolution : 3.90 Å (reported)
Based on initial model : 6BEI

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

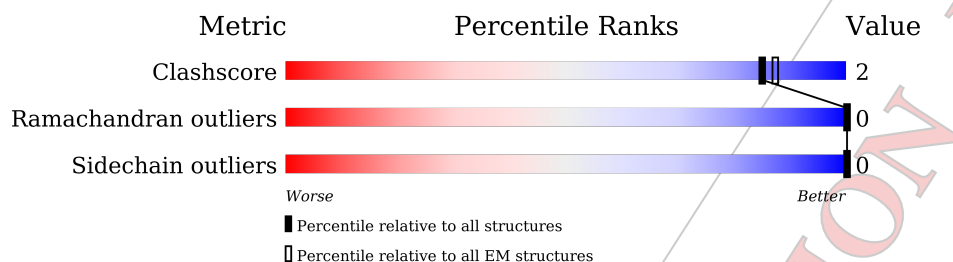
EMDB validation analysis : 0.0.0.dev97
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

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 3.90 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	531	10% 93% 6%
1	B	531	12% 93% 6%
1	C	531	7% 94% 5%
1	D	531	13% 94% 5%
1	E	531	25% 93% 6%
1	F	531	11% 93% 6%
1	G	531	11% 93% 6%
1	H	531	14% 94% 6%

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Mol	Chain	Length	Quality of chain	
1	I	531	5%	93% 6%
1	J	531	7%	93% 6%
1	K	531	9%	94% 5%
1	L	531	5%	94% 5%
1	M	531	11%	94% 5%
1	N	531	19%	92% 7%
1	O	531	5%	93% 7%
1	P	531	12%	93% 6%
1	Q	531	15%	93% 6%
1	R	531	5%	93% 6%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 75474 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Scaffold protein D13.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	527	Total	C	N	O	S	0	0
			4193	2681	681	819	12		
1	B	527	Total	C	N	O	S	0	0
			4193	2681	681	819	12		
1	C	527	Total	C	N	O	S	0	0
			4193	2681	681	819	12		
1	D	527	Total	C	N	O	S	0	0
			4193	2681	681	819	12		
1	E	527	Total	C	N	O	S	0	0
			4193	2681	681	819	12		
1	F	527	Total	C	N	O	S	0	0
			4193	2681	681	819	12		
1	G	527	Total	C	N	O	S	0	0
			4193	2681	681	819	12		
1	H	527	Total	C	N	O	S	0	0
			4193	2681	681	819	12		
1	I	527	Total	C	N	O	S	0	0
			4193	2681	681	819	12		
1	L	527	Total	C	N	O	S	0	0
			4193	2681	681	819	12		
1	J	527	Total	C	N	O	S	0	0
			4193	2681	681	819	12		
1	K	527	Total	C	N	O	S	0	0
			4193	2681	681	819	12		
1	N	527	Total	C	N	O	S	0	0
			4193	2681	681	819	12		
1	O	527	Total	C	N	O	S	0	0
			4193	2681	681	819	12		
1	M	527	Total	C	N	O	S	0	0
			4193	2681	681	819	12		
1	Q	527	Total	C	N	O	S	0	0
			4193	2681	681	819	12		
1	R	527	Total	C	N	O	S	0	0
			4193	2681	681	819	12		

Continued on next page...

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	P	527	4193	2681	681	819	12	0	0

CONFIDENTIAL

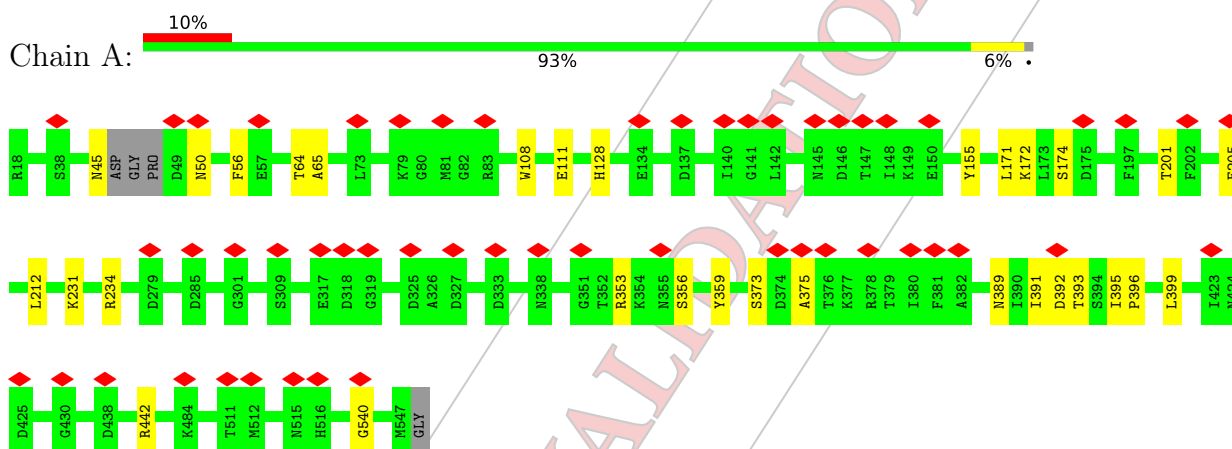
VALIDATION

REPORT

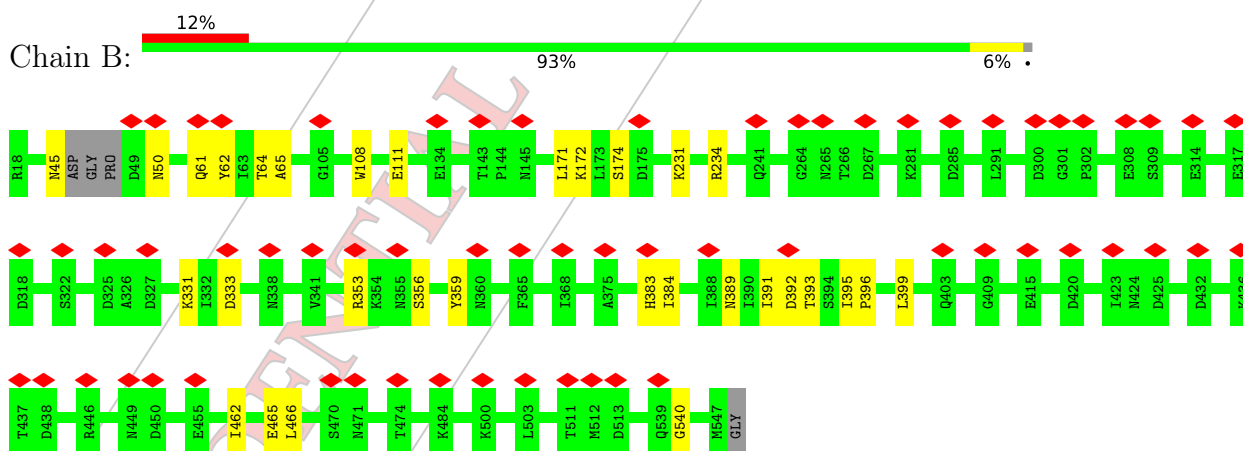
3 Residue-property plots [i](#)

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.

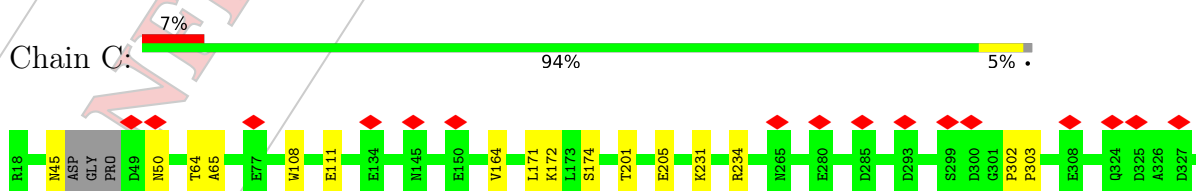
- Molecule 1: Scaffold protein D13

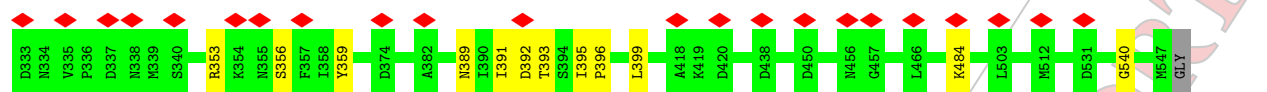


- Molecule 1: Scaffold protein D13

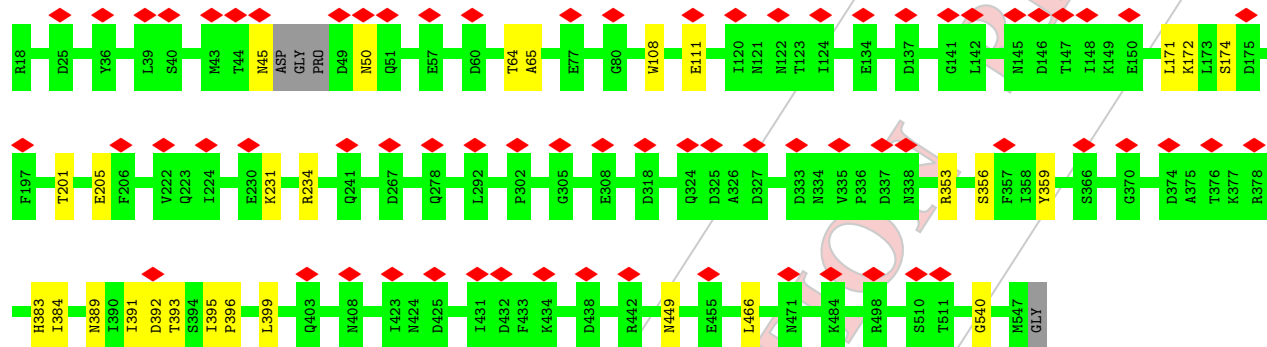


- Molecule 1: Scaffold protein D13

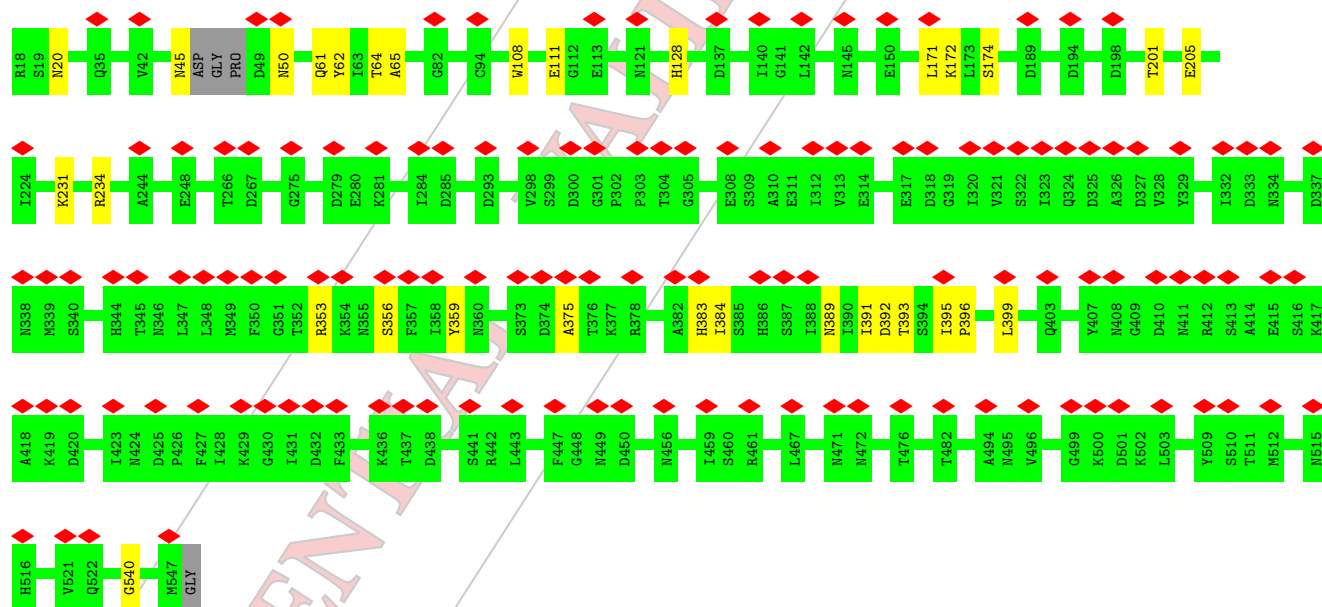




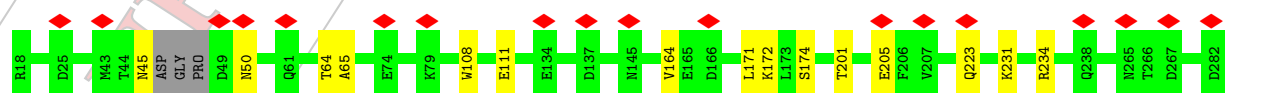
- Molecule 1: Scaffold protein D13

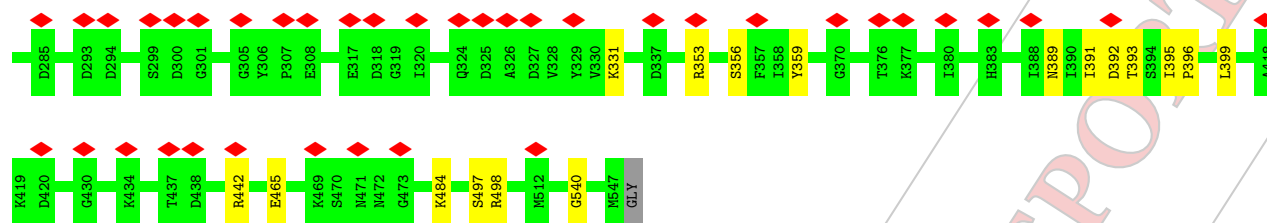


- Molecule 1: Scaffold protein D13

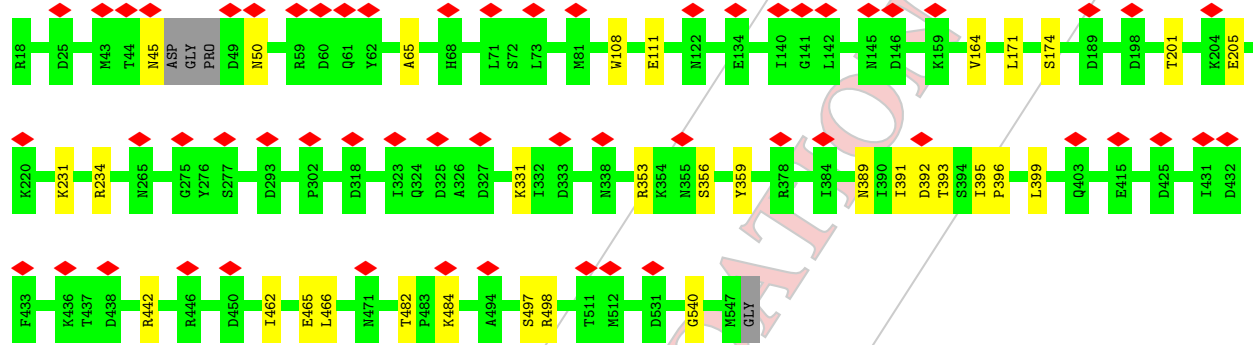
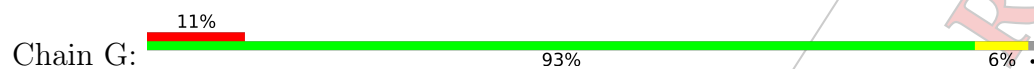


- Molecule 1: Scaffold protein D13

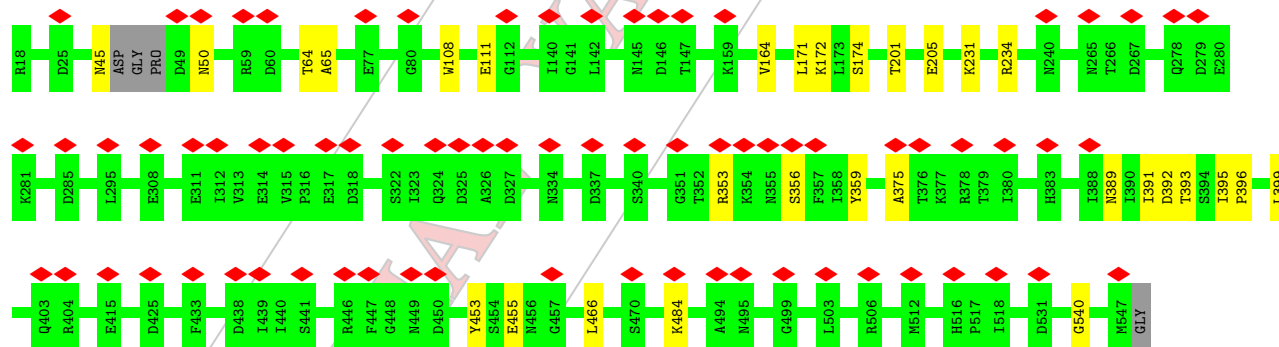
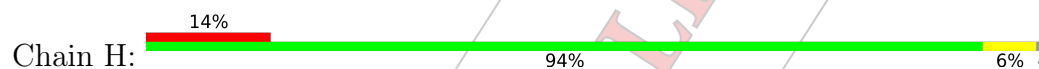




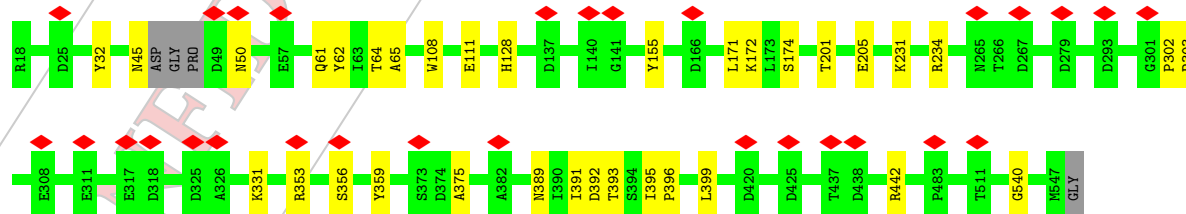
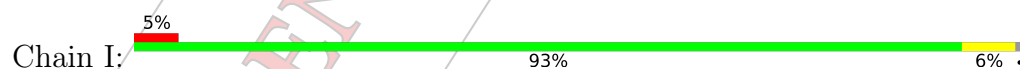
• Molecule 1: Scaffold protein D13



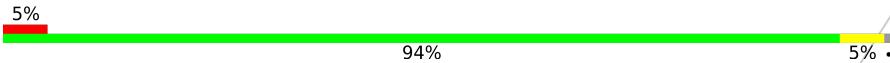
• Molecule 1: Scaffold protein D13

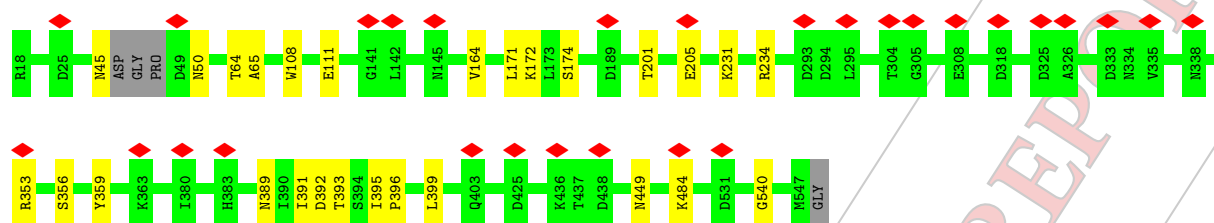


• Molecule 1: Scaffold protein D13

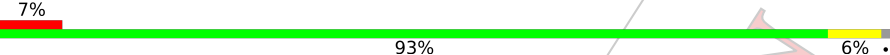


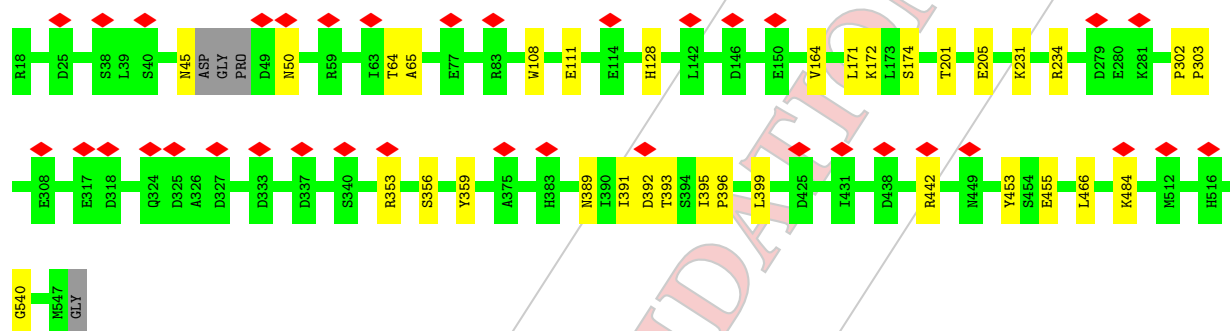
• Molecule 1: Scaffold protein D13

Chain L: 

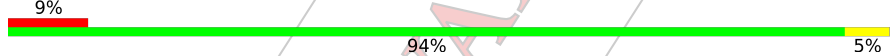


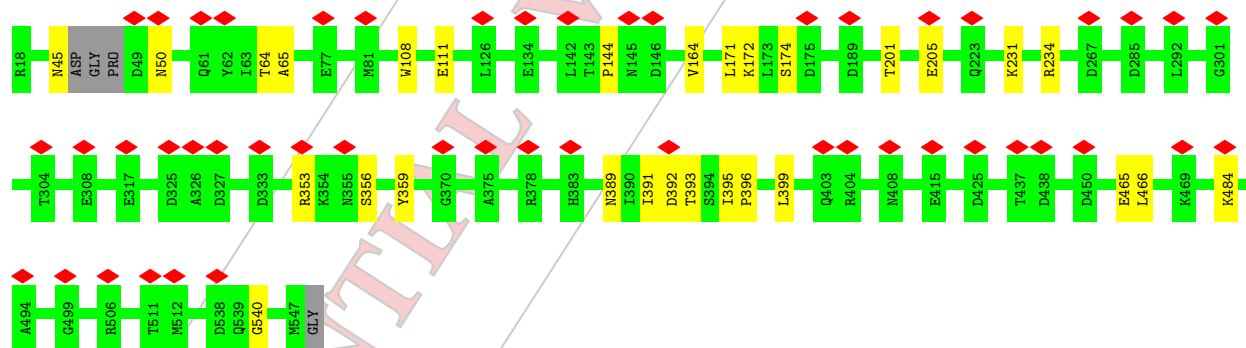
• Molecule 1: Scaffold protein D13

Chain J: 

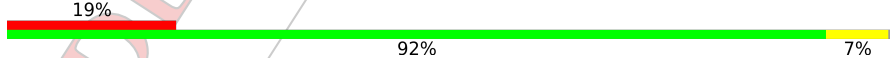


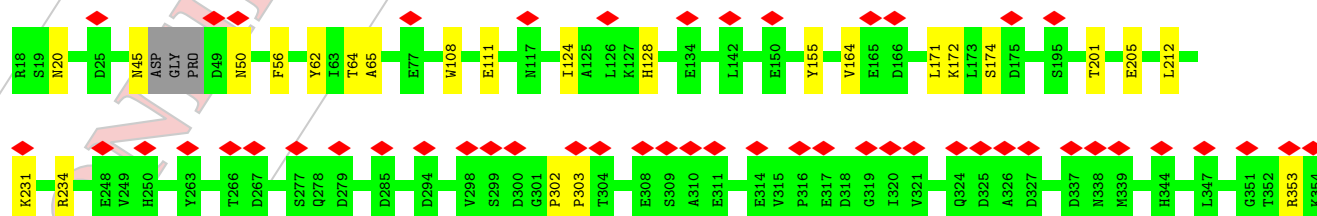
• Molecule 1: Scaffold protein D13

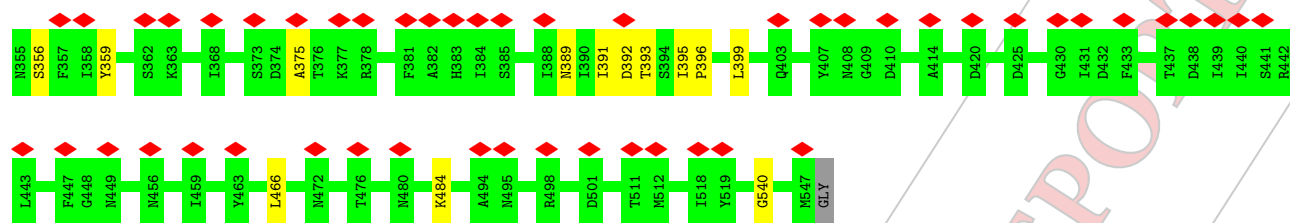
Chain K: 



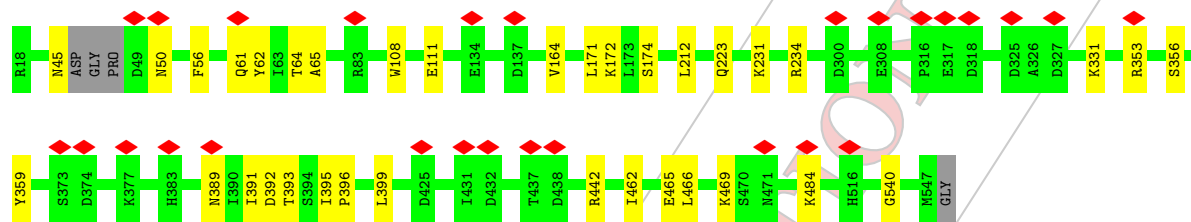
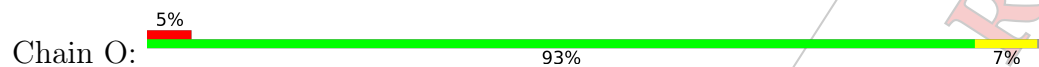
• Molecule 1: Scaffold protein D13

Chain N: 

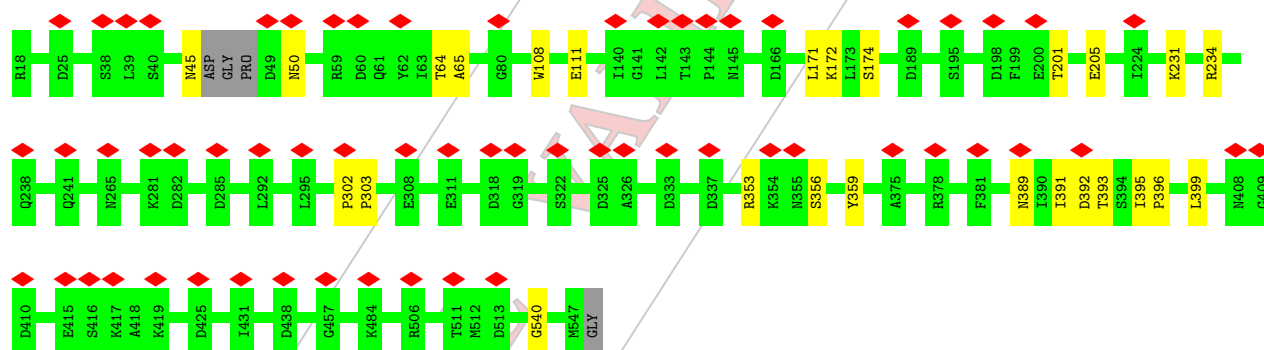
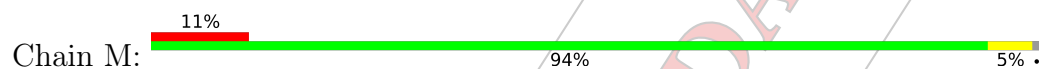




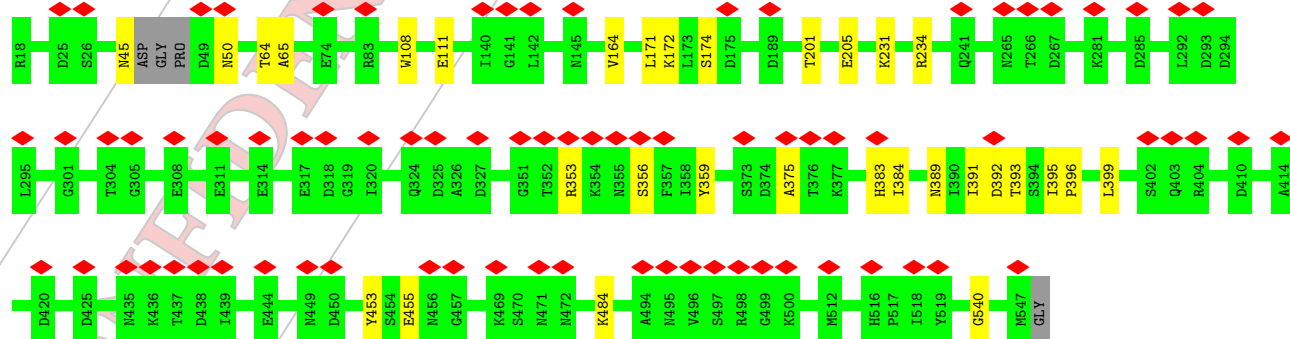
• Molecule 1: Scaffold protein D13



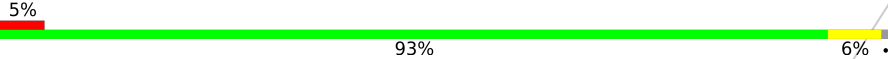
• Molecule 1: Scaffold protein D13

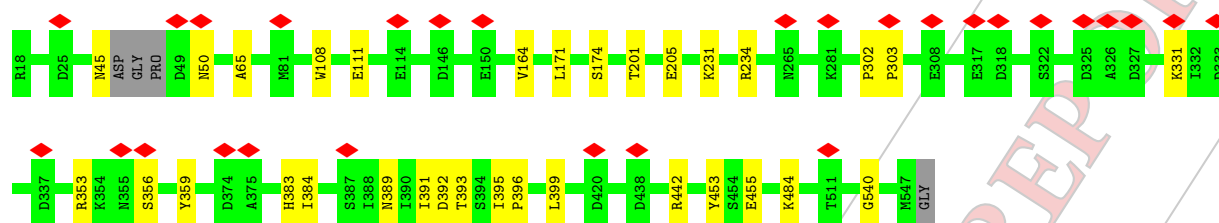


• Molecule 1: Scaffold protein D13

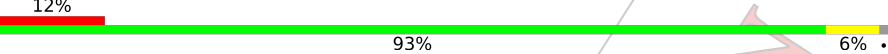


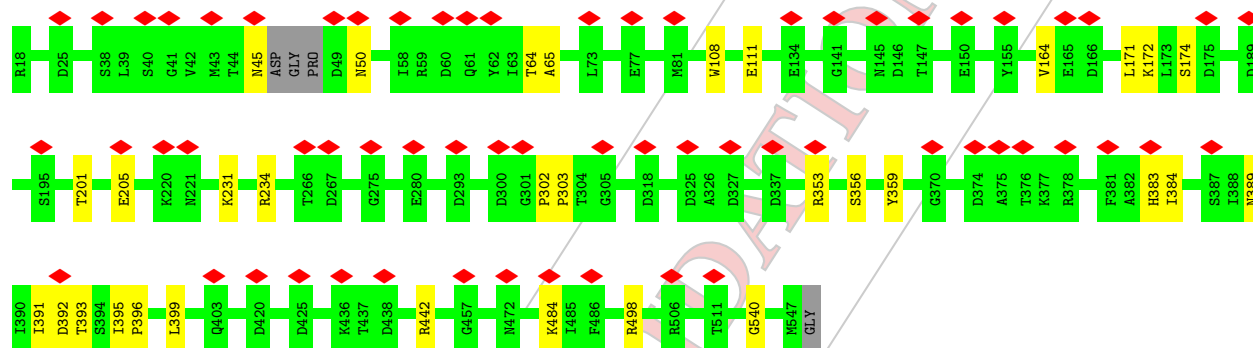
• Molecule 1: Scaffold protein D13

Chain R:  5% 93% 6%



• Molecule 1: Scaffold protein D13

Chain P:  12% 93% 6%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	247311	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	23.476	Depositor
Minimum map value	-9.367	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4.5	Depositor
Map size (Å)	355.84, 355.84, 355.84	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.39	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	0.26	0/4285	0.46	0/5830
1	B	0.26	0/4285	0.46	0/5830
1	C	0.26	0/4285	0.46	0/5830
1	D	0.26	0/4285	0.46	0/5830
1	E	0.26	0/4285	0.46	0/5830
1	F	0.26	0/4285	0.46	0/5830
1	G	0.26	0/4285	0.46	0/5830
1	H	0.26	0/4285	0.46	0/5830
1	I	0.26	0/4285	0.46	0/5830
1	J	0.26	0/4285	0.46	0/5830
1	K	0.26	0/4285	0.46	0/5830
1	L	0.26	0/4285	0.46	0/5830
1	M	0.26	0/4285	0.46	0/5830
1	N	0.26	0/4285	0.46	0/5830
1	O	0.26	0/4285	0.46	0/5830
1	P	0.26	0/4285	0.46	0/5830
1	Q	0.26	0/4285	0.46	0/5830
1	R	0.26	0/4285	0.46	0/5830
All	All	0.26	0/77130	0.46	0/104940

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4193	0	4143	22	0
1	B	4193	0	4143	33	0
1	C	4193	0	4143	14	0
1	D	4193	0	4143	30	0
1	E	4193	0	4143	18	0
1	F	4193	0	4143	19	0
1	G	4193	0	4143	20	0
1	H	4193	0	4143	17	0
1	I	4193	0	4143	24	0
1	J	4193	0	4143	20	0
1	K	4193	0	4143	17	0
1	L	4193	0	4143	31	0
1	M	4193	0	4143	15	0
1	N	4193	0	4143	25	0
1	O	4193	0	4143	39	0
1	P	4193	0	4143	17	0
1	Q	4193	0	4143	16	0
1	R	4193	0	4143	20	0
All	All	75474	0	74574	327	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (327) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:TYR:CE2	1:D:449:ASN:HB3	1.76	1.21
1:L:449:ASN:HB3	1:O:62:TYR:CE2	1.97	1.00
1:L:449:ASN:HD21	1:O:61:GLN:NE2	1.63	0.96
1:B:62:TYR:CZ	1:D:449:ASN:CB	2.49	0.95
1:B:62:TYR:CE2	1:D:449:ASN:CB	2.51	0.93
1:B:62:TYR:CZ	1:D:449:ASN:HB3	2.03	0.93
1:A:442:ARG:HH21	1:R:442:ARG:HH21	1.01	0.92
1:I:442:ARG:HH21	1:J:442:ARG:HH21	1.08	0.92
1:B:61:GLN:NE2	1:D:449:ASN:HD21	1.73	0.86
1:B:62:TYR:CZ	1:D:449:ASN:HB2	2.11	0.85
1:A:442:ARG:HH21	1:R:442:ARG:NH2	1.79	0.81
1:A:442:ARG:NH2	1:R:442:ARG:HH21	1.79	0.79
1:O:442:ARG:HH21	1:P:442:ARG:HH21	1.30	0.77
1:F:442:ARG:HH21	1:G:442:ARG:HH21	1.34	0.75
1:L:449:ASN:CB	1:O:62:TYR:CE2	2.70	0.75
1:B:62:TYR:CD2	1:D:449:ASN:HB3	2.22	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:GLN:HE21	1:D:449:ASN:HD21	1.38	0.71
1:F:174:SER:HB2	1:F:540:GLY:HA2	1.74	0.70
1:K:174:SER:HB2	1:K:540:GLY:HA2	1.74	0.70
1:A:174:SER:HB2	1:A:540:GLY:HA2	1.74	0.70
1:M:174:SER:HB2	1:M:540:GLY:HA2	1.74	0.70
1:J:174:SER:HB2	1:J:540:GLY:HA2	1.74	0.70
1:Q:174:SER:HB2	1:Q:540:GLY:HA2	1.74	0.70
1:L:174:SER:HB2	1:L:540:GLY:HA2	1.74	0.69
1:I:174:SER:HB2	1:I:540:GLY:HA2	1.74	0.69
1:G:174:SER:HB2	1:G:540:GLY:HA2	1.74	0.69
1:R:174:SER:HB2	1:R:540:GLY:HA2	1.74	0.69
1:P:174:SER:HB2	1:P:540:GLY:HA2	1.74	0.69
1:B:174:SER:HB2	1:B:540:GLY:HA2	1.74	0.69
1:E:174:SER:HB2	1:E:540:GLY:HA2	1.74	0.69
1:C:174:SER:HB2	1:C:540:GLY:HA2	1.74	0.69
1:N:174:SER:HB2	1:N:540:GLY:HA2	1.74	0.69
1:H:174:SER:HB2	1:H:540:GLY:HA2	1.74	0.69
1:O:174:SER:HB2	1:O:540:GLY:HA2	1.74	0.69
1:D:174:SER:HB2	1:D:540:GLY:HA2	1.74	0.68
1:I:442:ARG:HH21	1:J:442:ARG:NH2	1.88	0.67
1:N:128:HIS:NE2	1:O:465:GLU:OE1	2.28	0.66
1:L:449:ASN:HD21	1:O:61:GLN:CD	2.00	0.65
1:L:449:ASN:HD21	1:O:61:GLN:HE21	1.43	0.64
1:L:449:ASN:CB	1:O:62:TYR:CZ	2.81	0.64
1:N:20:ASN:ND2	1:O:223:GLN:HB2	2.13	0.64
1:L:449:ASN:HB3	1:O:62:TYR:CD2	2.33	0.64
1:K:144:PRO:HG2	1:M:353:ARG:NH2	2.13	0.63
1:I:442:ARG:NH2	1:J:442:ARG:HH21	1.89	0.62
1:L:449:ASN:HB2	1:O:62:TYR:CZ	2.37	0.60
1:L:449:ASN:HB3	1:O:62:TYR:CZ	2.37	0.59
1:G:465:GLU:OE1	1:I:128:HIS:NE2	2.36	0.58
1:B:62:TYR:OH	1:D:449:ASN:HB2	2.03	0.58
1:L:449:ASN:ND2	1:O:61:GLN:CG	2.67	0.58
1:E:201:THR:O	1:E:205:GLU:HG3	2.04	0.58
1:L:201:THR:O	1:L:205:GLU:HG3	2.04	0.58
1:H:45:ASN:HB3	1:H:50:ASN:HB3	1.86	0.57
1:O:45:ASN:HB3	1:O:50:ASN:HB3	1.87	0.57
1:Q:45:ASN:HB3	1:Q:50:ASN:HB3	1.86	0.57
1:R:201:THR:O	1:R:205:GLU:HG3	2.04	0.57
1:P:45:ASN:HB3	1:P:50:ASN:HB3	1.86	0.57
1:J:45:ASN:HB3	1:J:50:ASN:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:THR:O	1:C:205:GLU:HG3	2.04	0.57
1:D:201:THR:O	1:D:205:GLU:HG3	2.04	0.57
1:A:201:THR:O	1:A:205:GLU:HG3	2.05	0.57
1:J:201:THR:O	1:J:205:GLU:HG3	2.04	0.57
1:F:201:THR:O	1:F:205:GLU:HG3	2.04	0.57
1:I:201:THR:O	1:I:205:GLU:HG3	2.04	0.57
1:L:45:ASN:HB3	1:L:50:ASN:HB3	1.86	0.57
1:C:45:ASN:HB3	1:C:50:ASN:HB3	1.86	0.57
1:F:45:ASN:HB3	1:F:50:ASN:HB3	1.86	0.57
1:G:201:THR:O	1:G:205:GLU:HG3	2.04	0.57
1:G:331:LYS:HB3	1:I:375:ALA:HB1	1.87	0.57
1:M:201:THR:O	1:M:205:GLU:HG3	2.04	0.57
1:I:45:ASN:HB3	1:I:50:ASN:HB3	1.86	0.57
1:N:201:THR:O	1:N:205:GLU:HG3	2.04	0.57
1:P:201:THR:O	1:P:205:GLU:HG3	2.04	0.57
1:N:155:TYR:CD2	1:O:462:ILE:HG13	2.39	0.57
1:N:359:TYR:OH	1:N:392:ASP:OD1	2.21	0.57
1:G:45:ASN:HB3	1:G:50:ASN:HB3	1.86	0.56
1:Q:201:THR:O	1:Q:205:GLU:HG3	2.04	0.56
1:F:359:TYR:OH	1:F:392:ASP:OD1	2.21	0.56
1:K:201:THR:O	1:K:205:GLU:HG3	2.04	0.56
1:A:373:SER:OG	1:B:333:ASP:OD2	2.21	0.56
1:K:45:ASN:HB3	1:K:50:ASN:HB3	1.86	0.56
1:N:375:ALA:HB1	1:O:331:LYS:HB3	1.86	0.56
1:H:201:THR:O	1:H:205:GLU:HG3	2.04	0.56
1:N:45:ASN:HB3	1:N:50:ASN:HB3	1.86	0.56
1:R:45:ASN:HB3	1:R:50:ASN:HB3	1.86	0.56
1:E:45:ASN:HB3	1:E:50:ASN:HB3	1.86	0.56
1:M:45:ASN:HB3	1:M:50:ASN:HB3	1.86	0.56
1:B:45:ASN:HB3	1:B:50:ASN:HB3	1.86	0.55
1:E:375:ALA:HB1	1:F:331:LYS:HB3	1.89	0.55
1:A:45:ASN:HB3	1:A:50:ASN:HB3	1.86	0.55
1:D:45:ASN:HB3	1:D:50:ASN:HB3	1.86	0.55
1:E:359:TYR:OH	1:E:392:ASP:OD1	2.21	0.55
1:G:359:TYR:OH	1:G:392:ASP:OD1	2.21	0.55
1:E:128:HIS:NE2	1:F:465:GLU:OE1	2.37	0.55
1:B:359:TYR:OH	1:B:392:ASP:OD1	2.21	0.54
1:B:62:TYR:CE2	1:D:449:ASN:O	2.60	0.54
1:M:359:TYR:OH	1:M:392:ASP:OD1	2.21	0.54
1:J:359:TYR:OH	1:J:392:ASP:OD1	2.21	0.54
1:N:124:ILE:HD13	1:O:469:LYS:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:359:TYR:OH	1:R:392:ASP:OD1	2.21	0.53
1:L:449:ASN:ND2	1:O:61:GLN:HG3	2.24	0.53
1:I:359:TYR:OH	1:I:392:ASP:OD1	2.21	0.53
1:K:359:TYR:OH	1:K:392:ASP:OD1	2.21	0.53
1:C:353:ARG:HB2	1:C:356:SER:HB2	1.92	0.52
1:O:359:TYR:OH	1:O:392:ASP:OD1	2.21	0.52
1:Q:359:TYR:OH	1:Q:392:ASP:OD1	2.21	0.52
1:C:359:TYR:OH	1:C:392:ASP:OD1	2.21	0.52
1:D:359:TYR:OH	1:D:392:ASP:OD1	2.21	0.52
1:M:353:ARG:HB2	1:M:356:SER:HB2	1.92	0.52
1:I:353:ARG:HB2	1:I:356:SER:HB2	1.92	0.52
1:Q:353:ARG:HB2	1:Q:356:SER:HB2	1.92	0.52
1:A:353:ARG:HB2	1:A:356:SER:HB2	1.92	0.52
1:F:353:ARG:HB2	1:F:356:SER:HB2	1.92	0.52
1:K:353:ARG:HB2	1:K:356:SER:HB2	1.92	0.52
1:O:353:ARG:HB2	1:O:356:SER:HB2	1.92	0.52
1:D:353:ARG:HB2	1:D:356:SER:HB2	1.92	0.51
1:E:353:ARG:HB2	1:E:356:SER:HB2	1.92	0.51
1:H:353:ARG:HB2	1:H:356:SER:HB2	1.92	0.51
1:H:375:ALA:HB1	1:I:331:LYS:HB3	1.92	0.51
1:B:353:ARG:HB2	1:B:356:SER:HB2	1.92	0.51
1:B:62:TYR:CE2	1:D:449:ASN:C	2.83	0.51
1:G:353:ARG:HB2	1:G:356:SER:HB2	1.92	0.51
1:J:353:ARG:HB2	1:J:356:SER:HB2	1.92	0.51
1:G:391:ILE:O	1:G:395:ILE:HG13	2.11	0.51
1:J:391:ILE:O	1:J:395:ILE:HG13	2.11	0.51
1:R:353:ARG:HB2	1:R:356:SER:HB2	1.92	0.51
1:L:353:ARG:HB2	1:L:356:SER:HB2	1.92	0.51
1:L:359:TYR:OH	1:L:392:ASP:OD1	2.21	0.51
1:Q:391:ILE:O	1:Q:395:ILE:HG13	2.11	0.51
1:I:391:ILE:O	1:I:395:ILE:HG13	2.11	0.50
1:O:391:ILE:O	1:O:395:ILE:HG13	2.11	0.50
1:P:353:ARG:HB2	1:P:356:SER:HB2	1.92	0.50
1:A:128:HIS:NE2	1:B:465:GLU:OE1	2.40	0.50
1:A:391:ILE:O	1:A:395:ILE:HG13	2.11	0.50
1:B:62:TYR:HE2	1:D:449:ASN:O	1.94	0.50
1:L:391:ILE:O	1:L:395:ILE:HG13	2.11	0.50
1:A:359:TYR:OH	1:A:392:ASP:OD1	2.21	0.50
1:B:391:ILE:O	1:B:395:ILE:HG13	2.11	0.50
1:P:391:ILE:O	1:P:395:ILE:HG13	2.11	0.50
1:D:391:ILE:O	1:D:395:ILE:HG13	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:391:ILE:O	1:K:395:ILE:HG13	2.11	0.50
1:N:353:ARG:HB2	1:N:356:SER:HB2	1.92	0.50
1:R:391:ILE:O	1:R:395:ILE:HG13	2.11	0.50
1:H:391:ILE:O	1:H:395:ILE:HG13	2.11	0.50
1:C:391:ILE:O	1:C:395:ILE:HG13	2.11	0.50
1:M:391:ILE:O	1:M:395:ILE:HG13	2.11	0.50
1:P:359:TYR:OH	1:P:392:ASP:OD1	2.21	0.50
1:F:391:ILE:O	1:F:395:ILE:HG13	2.11	0.50
1:G:111:GLU:OE1	1:G:234:ARG:HD3	2.13	0.49
1:D:111:GLU:OE1	1:D:234:ARG:HD3	2.13	0.49
1:H:111:GLU:OE1	1:H:234:ARG:HD3	2.13	0.49
1:K:111:GLU:OE1	1:K:234:ARG:HD3	2.13	0.49
1:O:111:GLU:OE1	1:O:234:ARG:HD3	2.13	0.49
1:F:111:GLU:OE1	1:F:234:ARG:HD3	2.13	0.49
1:N:391:ILE:O	1:N:395:ILE:HG13	2.11	0.49
1:Q:453:TYR:OH	1:Q:455:GLU:OE1	2.26	0.49
1:P:111:GLU:OE1	1:P:234:ARG:HD3	2.13	0.49
1:E:111:GLU:OE1	1:E:234:ARG:HD3	2.13	0.49
1:B:111:GLU:OE1	1:B:234:ARG:HD3	2.13	0.49
1:B:61:GLN:CD	1:D:449:ASN:OD1	2.51	0.49
1:G:396:PRO:HD2	1:G:399:LEU:HD12	1.95	0.49
1:J:111:GLU:OE1	1:J:234:ARG:HD3	2.13	0.49
1:N:111:GLU:OE1	1:N:234:ARG:HD3	2.13	0.49
1:Q:111:GLU:OE1	1:Q:234:ARG:HD3	2.13	0.49
1:I:111:GLU:OE1	1:I:234:ARG:HD3	2.13	0.49
1:I:396:PRO:HD2	1:I:399:LEU:HD12	1.95	0.49
1:M:111:GLU:OE1	1:M:234:ARG:HD3	2.13	0.49
1:R:396:PRO:HD2	1:R:399:LEU:HD12	1.95	0.49
1:L:396:PRO:HD2	1:L:399:LEU:HD12	1.95	0.48
1:D:396:PRO:HD2	1:D:399:LEU:HD12	1.95	0.48
1:E:391:ILE:O	1:E:395:ILE:HG13	2.11	0.48
1:C:111:GLU:OE1	1:C:234:ARG:HD3	2.13	0.48
1:Q:396:PRO:HD2	1:Q:399:LEU:HD12	1.95	0.48
1:A:111:GLU:OE1	1:A:234:ARG:HD3	2.13	0.48
1:H:359:TYR:OH	1:H:392:ASP:OD1	2.21	0.48
1:H:396:PRO:HD2	1:H:399:LEU:HD12	1.95	0.48
1:B:396:PRO:HD2	1:B:399:LEU:HD12	1.95	0.48
1:C:396:PRO:HD2	1:C:399:LEU:HD12	1.95	0.48
1:H:65:ALA:HA	1:H:171:LEU:O	2.14	0.48
1:L:111:GLU:OE1	1:L:234:ARG:HD3	2.13	0.48
1:L:449:ASN:OD1	1:O:61:GLN:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:396:PRO:HD2	1:K:399:LEU:HD12	1.95	0.48
1:O:396:PRO:HD2	1:O:399:LEU:HD12	1.95	0.48
1:Q:65:ALA:HA	1:Q:171:LEU:O	2.14	0.48
1:R:111:GLU:OE1	1:R:234:ARG:HD3	2.13	0.48
1:P:65:ALA:HA	1:P:171:LEU:O	2.14	0.48
1:P:396:PRO:HD2	1:P:399:LEU:HD12	1.95	0.48
1:R:65:ALA:HA	1:R:171:LEU:O	2.14	0.48
1:A:396:PRO:HD2	1:A:399:LEU:HD12	1.95	0.48
1:E:65:ALA:HA	1:E:171:LEU:O	2.14	0.48
1:K:65:ALA:HA	1:K:171:LEU:O	2.14	0.48
1:N:396:PRO:HD2	1:N:399:LEU:HD12	1.95	0.48
1:E:396:PRO:HD2	1:E:399:LEU:HD12	1.95	0.47
1:J:396:PRO:HD2	1:J:399:LEU:HD12	1.95	0.47
1:L:65:ALA:HA	1:L:171:LEU:O	2.14	0.47
1:L:449:ASN:ND2	1:O:61:GLN:CD	2.67	0.47
1:F:396:PRO:HD2	1:F:399:LEU:HD12	1.95	0.47
1:O:65:ALA:HA	1:O:171:LEU:O	2.14	0.47
1:F:65:ALA:HA	1:F:171:LEU:O	2.14	0.47
1:B:65:ALA:HA	1:B:171:LEU:O	2.14	0.47
1:C:65:ALA:HA	1:C:171:LEU:O	2.14	0.47
1:E:61:GLN:OE1	1:G:497:SER:HB2	2.15	0.47
1:G:65:ALA:HA	1:G:171:LEU:O	2.14	0.47
1:M:65:ALA:HA	1:M:171:LEU:O	2.14	0.47
1:M:396:PRO:HD2	1:M:399:LEU:HD12	1.95	0.47
1:I:65:ALA:HA	1:I:171:LEU:O	2.14	0.47
1:J:128:HIS:NE2	1:K:465:GLU:OE1	2.46	0.47
1:B:62:TYR:HE2	1:D:449:ASN:C	2.18	0.47
1:J:65:ALA:HA	1:J:171:LEU:O	2.14	0.47
1:N:20:ASN:HD21	1:O:223:GLN:HB2	1.80	0.46
1:N:65:ALA:HA	1:N:171:LEU:O	2.14	0.46
1:A:375:ALA:HB1	1:B:331:LYS:HB3	1.97	0.46
1:D:65:ALA:HA	1:D:171:LEU:O	2.14	0.46
1:A:65:ALA:HA	1:A:171:LEU:O	2.14	0.46
1:J:453:TYR:OH	1:J:455:GLU:OE1	2.26	0.46
1:F:497:SER:HB2	1:I:61:GLN:OE1	2.16	0.45
1:N:108:TRP:HA	1:N:231:LYS:HZ3	1.81	0.45
1:D:108:TRP:HA	1:D:231:LYS:NZ	2.32	0.45
1:Q:375:ALA:HB1	1:R:331:LYS:HB3	1.98	0.45
1:B:108:TRP:HA	1:B:231:LYS:NZ	2.32	0.45
1:C:108:TRP:HA	1:C:231:LYS:NZ	2.32	0.45
1:E:108:TRP:HA	1:E:231:LYS:NZ	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:108:TRP:HA	1:G:231:LYS:NZ	2.32	0.45
1:H:389:ASN:O	1:H:393:THR:HG23	2.17	0.45
1:H:108:TRP:HA	1:H:231:LYS:NZ	2.32	0.45
1:N:389:ASN:O	1:N:393:THR:HG23	2.17	0.45
1:Q:108:TRP:HA	1:Q:231:LYS:NZ	2.32	0.45
1:P:389:ASN:O	1:P:393:THR:HG23	2.17	0.45
1:F:108:TRP:HA	1:F:231:LYS:NZ	2.32	0.45
1:G:389:ASN:O	1:G:393:THR:HG23	2.17	0.45
1:I:389:ASN:O	1:I:393:THR:HG23	2.17	0.45
1:L:108:TRP:HA	1:L:231:LYS:NZ	2.32	0.45
1:J:108:TRP:HA	1:J:231:LYS:NZ	2.32	0.45
1:J:389:ASN:O	1:J:393:THR:HG23	2.17	0.45
1:Q:389:ASN:O	1:Q:393:THR:HG23	2.17	0.45
1:D:389:ASN:O	1:D:393:THR:HG23	2.17	0.45
1:E:389:ASN:O	1:E:393:THR:HG23	2.17	0.45
1:G:482:THR:HG23	1:I:32:TYR:OH	2.17	0.45
1:L:449:ASN:CG	1:O:61:GLN:CG	2.86	0.45
1:F:389:ASN:O	1:F:393:THR:HG23	2.17	0.45
1:O:389:ASN:O	1:O:393:THR:HG23	2.17	0.45
1:C:389:ASN:O	1:C:393:THR:HG23	2.17	0.45
1:I:108:TRP:HA	1:I:231:LYS:NZ	2.32	0.45
1:L:449:ASN:HD21	1:O:61:GLN:CG	2.29	0.45
1:K:389:ASN:O	1:K:393:THR:HG23	2.17	0.45
1:M:108:TRP:HA	1:M:231:LYS:NZ	2.32	0.45
1:R:108:TRP:HA	1:R:231:LYS:NZ	2.32	0.45
1:A:108:TRP:HA	1:A:231:LYS:NZ	2.32	0.44
1:B:389:ASN:O	1:B:393:THR:HG23	2.17	0.44
1:K:108:TRP:HA	1:K:231:LYS:NZ	2.32	0.44
1:R:453:TYR:OH	1:R:455:GLU:OE1	2.26	0.44
1:N:155:TYR:CE2	1:O:462:ILE:HG13	2.53	0.44
1:P:108:TRP:HA	1:P:231:LYS:NZ	2.32	0.44
1:R:389:ASN:O	1:R:393:THR:HG23	2.17	0.44
1:B:61:GLN:CG	1:D:449:ASN:OD1	2.66	0.44
1:L:449:ASN:OD1	1:O:61:GLN:CD	2.56	0.44
1:O:108:TRP:HA	1:O:231:LYS:NZ	2.32	0.44
1:L:389:ASN:O	1:L:393:THR:HG23	2.17	0.43
1:A:389:ASN:O	1:A:393:THR:HG23	2.17	0.43
1:F:498:ARG:NH1	1:I:62:TYR:HE2	2.16	0.43
1:N:108:TRP:HA	1:N:231:LYS:NZ	2.32	0.43
1:M:389:ASN:O	1:M:393:THR:HG23	2.17	0.43
1:E:62:TYR:HE2	1:G:498:ARG:NH1	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:466:LEU:HD23	1:D:466:LEU:HA	1.91	0.43
1:G:462:ILE:HG13	1:I:155:TYR:CD2	2.54	0.43
1:N:466:LEU:HD23	1:N:466:LEU:HA	1.91	0.43
1:K:144:PRO:HG2	1:M:353:ARG:CZ	2.49	0.42
1:L:449:ASN:OD1	1:O:61:GLN:CG	2.67	0.42
1:J:302:PRO:HA	1:J:303:PRO:HD3	1.94	0.42
1:C:302:PRO:HA	1:C:303:PRO:HD3	1.94	0.42
1:B:466:LEU:HD23	1:B:466:LEU:HA	1.91	0.42
1:A:108:TRP:HA	1:A:231:LYS:HZ3	1.85	0.42
1:H:108:TRP:HA	1:H:231:LYS:HZ3	1.85	0.42
1:C:64:THR:O	1:C:172:LYS:HA	2.20	0.41
1:L:64:THR:O	1:L:172:LYS:HA	2.21	0.41
1:I:302:PRO:HA	1:I:303:PRO:HD3	1.94	0.41
1:J:466:LEU:HD23	1:J:466:LEU:HA	1.91	0.41
1:N:64:THR:O	1:N:172:LYS:HA	2.20	0.41
1:E:64:THR:O	1:E:172:LYS:HA	2.20	0.41
1:A:155:TYR:CD2	1:B:462:ILE:HG13	2.56	0.41
1:E:20:ASN:ND2	1:F:223:GLN:HB2	2.35	0.41
1:B:61:GLN:HG2	1:D:449:ASN:OD1	2.21	0.41
1:G:466:LEU:HD23	1:G:466:LEU:HA	1.91	0.41
1:H:453:TYR:OH	1:H:455:GLU:OE1	2.26	0.41
1:N:302:PRO:HA	1:N:303:PRO:HD3	1.94	0.41
1:D:64:THR:O	1:D:172:LYS:HA	2.21	0.41
1:I:64:THR:O	1:I:172:LYS:HA	2.20	0.41
1:J:64:THR:O	1:J:172:LYS:HA	2.20	0.41
1:O:64:THR:O	1:O:172:LYS:HA	2.21	0.41
1:F:164:VAL:HG21	1:F:484:LYS:HD2	2.03	0.41
1:H:164:VAL:HG21	1:H:484:LYS:HD2	2.03	0.41
1:I:108:TRP:HA	1:I:231:LYS:HZ3	1.86	0.41
1:L:108:TRP:HA	1:L:231:LYS:HZ3	1.85	0.41
1:Q:64:THR:O	1:Q:172:LYS:HA	2.21	0.41
1:Q:164:VAL:HG21	1:Q:484:LYS:HD2	2.03	0.41
1:A:64:THR:O	1:A:172:LYS:HA	2.21	0.41
1:A:442:ARG:NE	1:R:442:ARG:NE	2.68	0.41
1:C:164:VAL:HG21	1:C:484:LYS:HD2	2.03	0.41
1:H:64:THR:O	1:H:172:LYS:HA	2.20	0.41
1:J:164:VAL:HG21	1:J:484:LYS:HD2	2.03	0.41
1:K:466:LEU:HD23	1:K:466:LEU:HA	1.91	0.41
1:O:466:LEU:HD23	1:O:466:LEU:HA	1.91	0.41
1:M:64:THR:O	1:M:172:LYS:HA	2.20	0.41
1:P:164:VAL:HG21	1:P:484:LYS:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:164:VAL:HG21	1:N:484:LYS:HD2	2.03	0.41
1:Q:383:HIS:O	1:Q:384:ILE:HD13	2.21	0.40
1:R:164:VAL:HG21	1:R:484:LYS:HD2	2.03	0.40
1:P:64:THR:O	1:P:172:LYS:HA	2.21	0.40
1:P:302:PRO:HA	1:P:303:PRO:HD3	1.94	0.40
1:E:383:HIS:O	1:E:384:ILE:HD13	2.22	0.40
1:K:64:THR:O	1:K:172:LYS:HA	2.21	0.40
1:O:164:VAL:HG21	1:O:484:LYS:HD2	2.03	0.40
1:R:302:PRO:HA	1:R:303:PRO:HD3	1.94	0.40
1:A:56:PHE:HD2	1:A:212:LEU:HD22	1.87	0.40
1:D:383:HIS:O	1:D:384:ILE:HD13	2.22	0.40
1:G:164:VAL:HG21	1:G:484:LYS:HD2	2.03	0.40
1:N:56:PHE:HD2	1:N:212:LEU:HD22	1.86	0.40
1:M:302:PRO:HA	1:M:303:PRO:HD3	1.94	0.40
1:B:64:THR:O	1:B:172:LYS:HA	2.20	0.40
1:L:164:VAL:HG21	1:L:484:LYS:HD2	2.03	0.40
1:O:56:PHE:HD2	1:O:212:LEU:HD22	1.87	0.40
1:B:383:HIS:O	1:B:384:ILE:HD13	2.22	0.40
1:F:64:THR:O	1:F:172:LYS:HA	2.20	0.40
1:H:466:LEU:HD23	1:H:466:LEU:HA	1.91	0.40
1:K:164:VAL:HG21	1:K:484:LYS:HD2	2.03	0.40
1:N:62:TYR:HE2	1:P:498:ARG:NH1	2.20	0.40
1:R:383:HIS:O	1:R:384:ILE:HD13	2.22	0.40
1:P:383:HIS:O	1:P:384:ILE:HD13	2.21	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	523/531 (98%)	503 (96%)	20 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	523/531 (98%)	503 (96%)	20 (4%)	0	100	100
1	C	523/531 (98%)	503 (96%)	20 (4%)	0	100	100
1	D	523/531 (98%)	503 (96%)	20 (4%)	0	100	100
1	E	523/531 (98%)	503 (96%)	20 (4%)	0	100	100
1	F	523/531 (98%)	503 (96%)	20 (4%)	0	100	100
1	G	523/531 (98%)	503 (96%)	20 (4%)	0	100	100
1	H	523/531 (98%)	503 (96%)	20 (4%)	0	100	100
1	I	523/531 (98%)	503 (96%)	20 (4%)	0	100	100
1	J	523/531 (98%)	503 (96%)	20 (4%)	0	100	100
1	K	523/531 (98%)	503 (96%)	20 (4%)	0	100	100
1	L	523/531 (98%)	503 (96%)	20 (4%)	0	100	100
1	M	523/531 (98%)	503 (96%)	20 (4%)	0	100	100
1	N	523/531 (98%)	503 (96%)	20 (4%)	0	100	100
1	O	523/531 (98%)	503 (96%)	20 (4%)	0	100	100
1	P	523/531 (98%)	503 (96%)	20 (4%)	0	100	100
1	Q	523/531 (98%)	503 (96%)	20 (4%)	0	100	100
1	R	523/531 (98%)	503 (96%)	20 (4%)	0	100	100
All	All	9414/9558 (98%)	9054 (96%)	360 (4%)	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	485/487 (100%)	485 (100%)	0	100	100
1	B	485/487 (100%)	485 (100%)	0	100	100
1	C	485/487 (100%)	485 (100%)	0	100	100
1	D	485/487 (100%)	485 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	485/487 (100%)	485 (100%)	0	100	100
1	F	485/487 (100%)	485 (100%)	0	100	100
1	G	485/487 (100%)	485 (100%)	0	100	100
1	H	485/487 (100%)	485 (100%)	0	100	100
1	I	485/487 (100%)	485 (100%)	0	100	100
1	J	485/487 (100%)	485 (100%)	0	100	100
1	K	485/487 (100%)	485 (100%)	0	100	100
1	L	485/487 (100%)	485 (100%)	0	100	100
1	M	485/487 (100%)	485 (100%)	0	100	100
1	N	485/487 (100%)	485 (100%)	0	100	100
1	O	485/487 (100%)	485 (100%)	0	100	100
1	P	485/487 (100%)	485 (100%)	0	100	100
1	Q	485/487 (100%)	485 (100%)	0	100	100
1	R	485/487 (100%)	485 (100%)	0	100	100
All	All	8730/8766 (100%)	8730 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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	61	GLN
1	O	61	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 [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.

CONFIDENTIAL VALIDATION REPORT

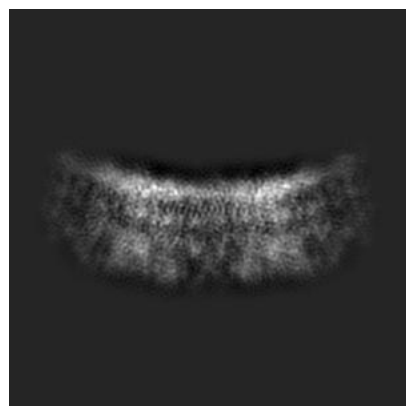
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31954. These allow visual inspection of the internal detail of the map and identification of artifacts.

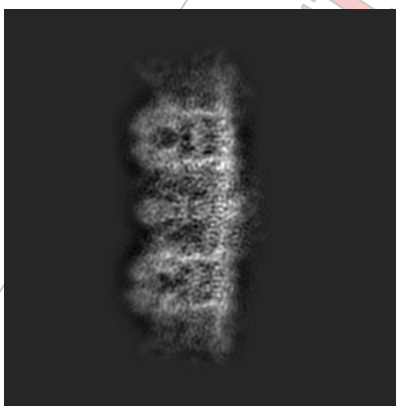
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

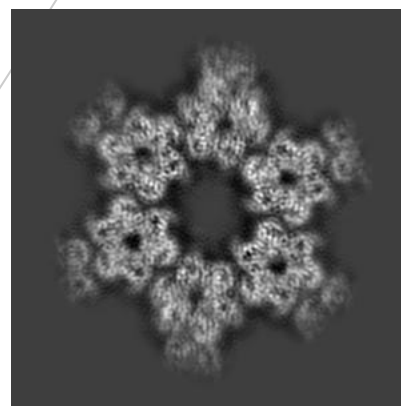
6.1.1 Primary map



X

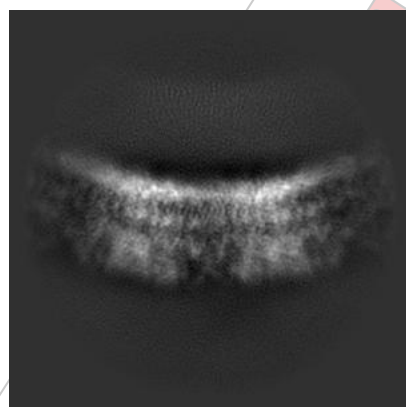


Y

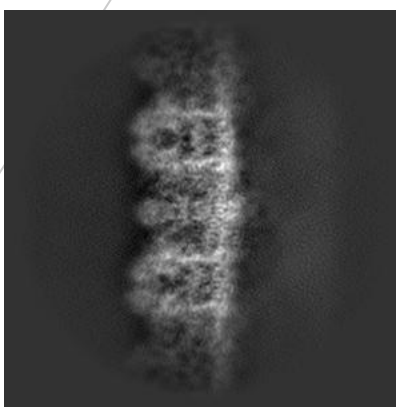


Z

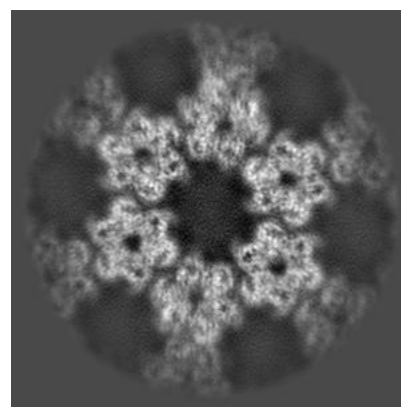
6.1.2 Raw map



X



Y

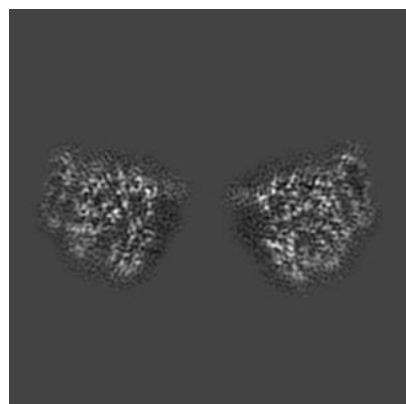


Z

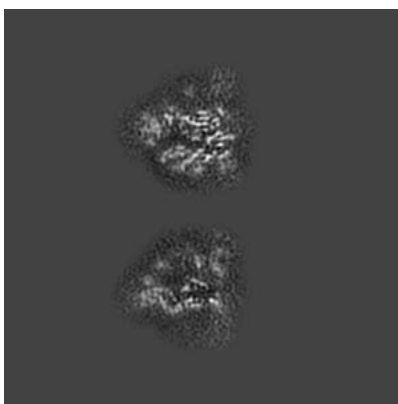
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

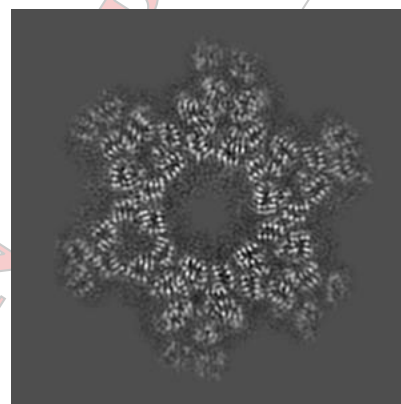
6.2.1 Primary map



X Index: 128

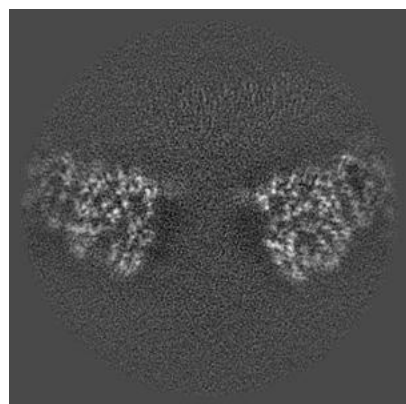


Y Index: 128

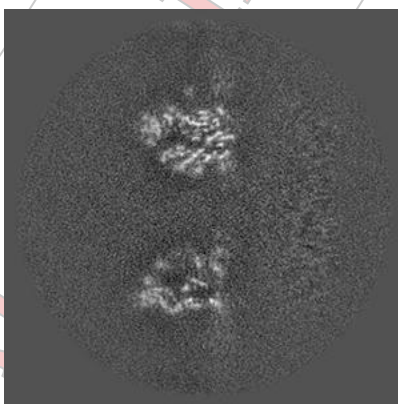


Z Index: 128

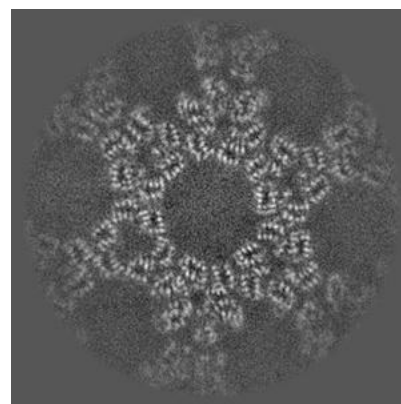
6.2.2 Raw map



X Index: 128



Y Index: 128

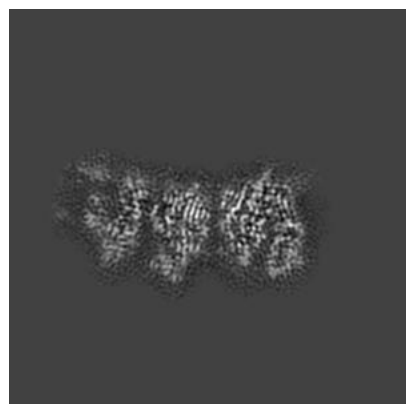


Z Index: 128

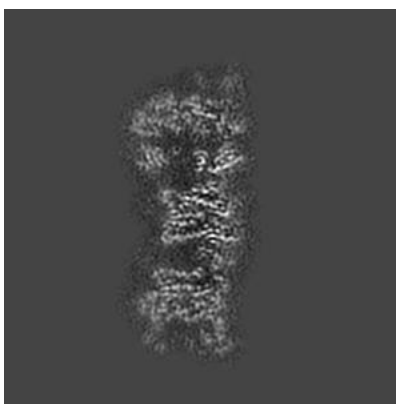
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

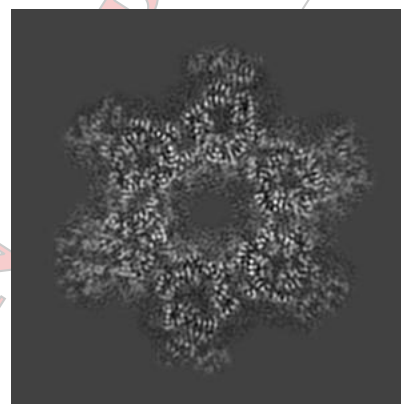
6.3.1 Primary map



X Index: 96

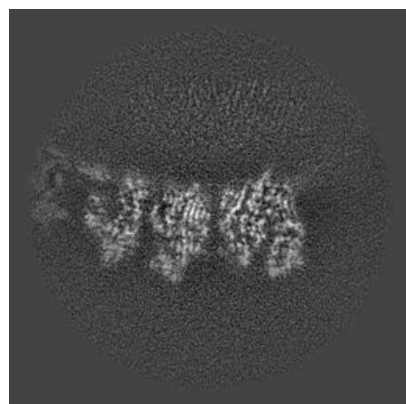


Y Index: 87

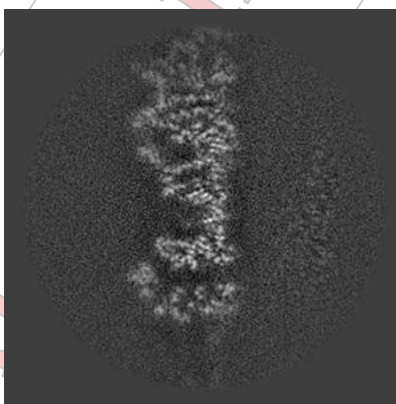


Z Index: 137

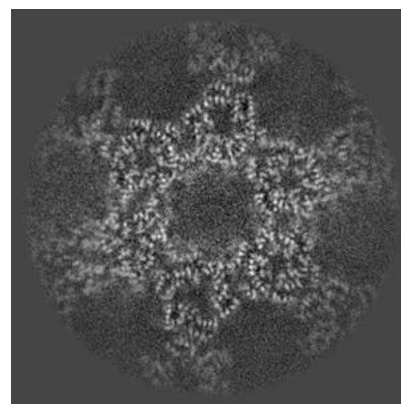
6.3.2 Raw map



X Index: 96



Y Index: 160



Z Index: 137

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 4.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



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

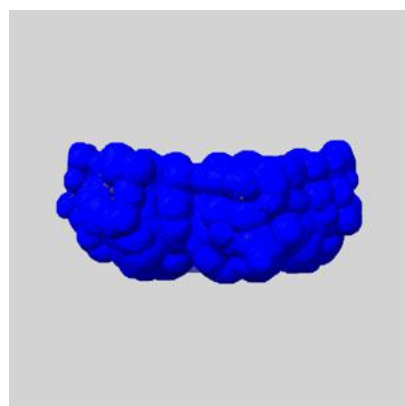
6.5 Mask visualisation [i](#)

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

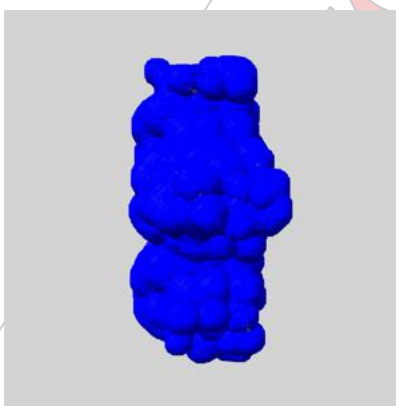
A mask typically either:

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

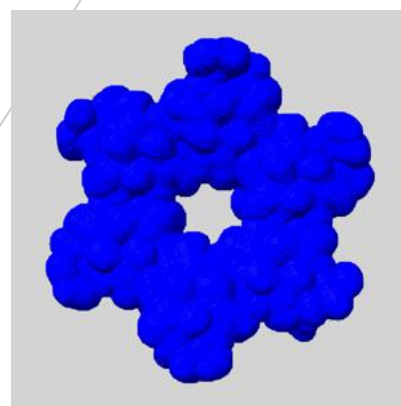
6.5.1 D_1300024109_em-mask-volume_P1.map.V3 [i](#)



X



Y

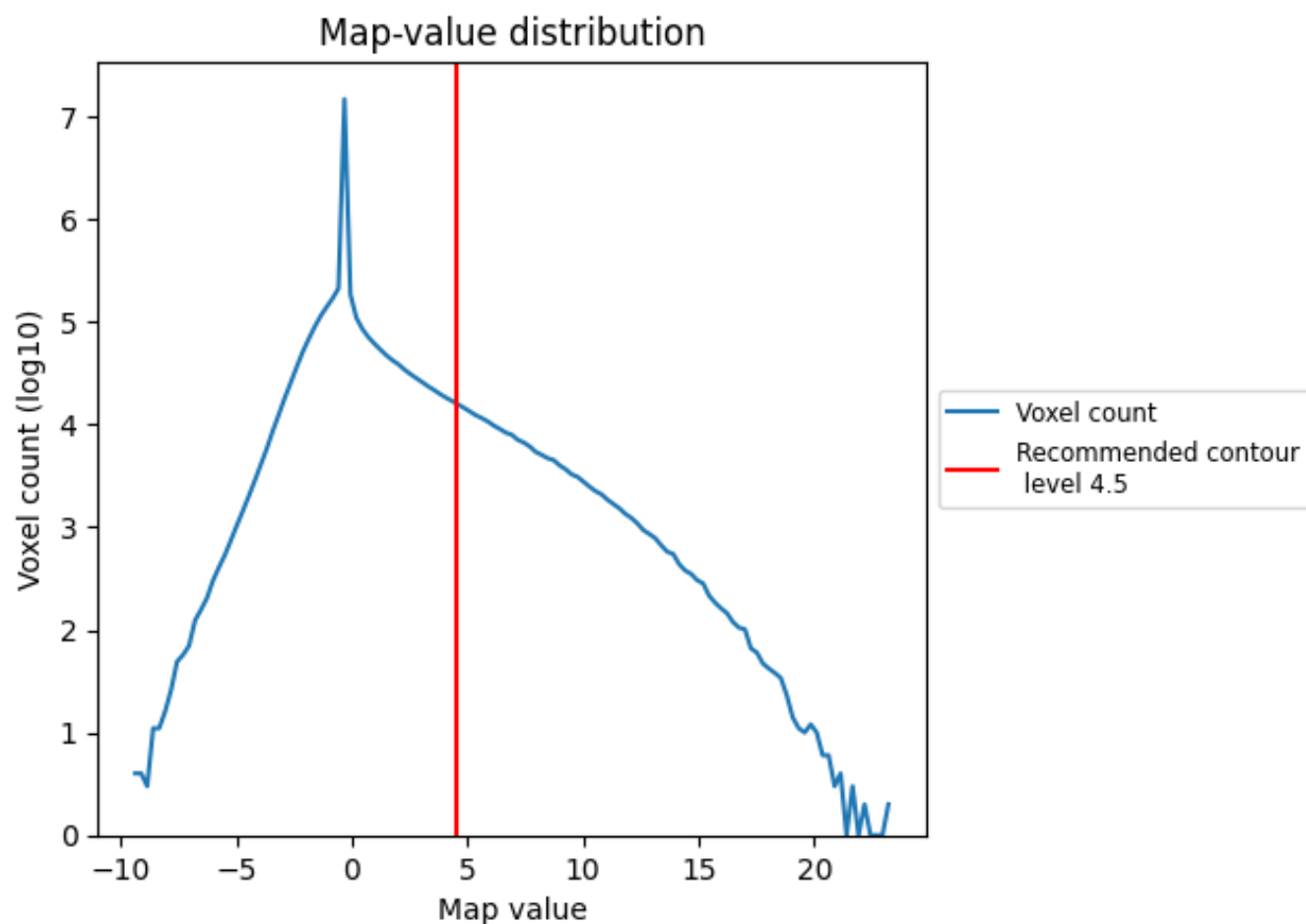


Z

7 Map analysis [i](#)

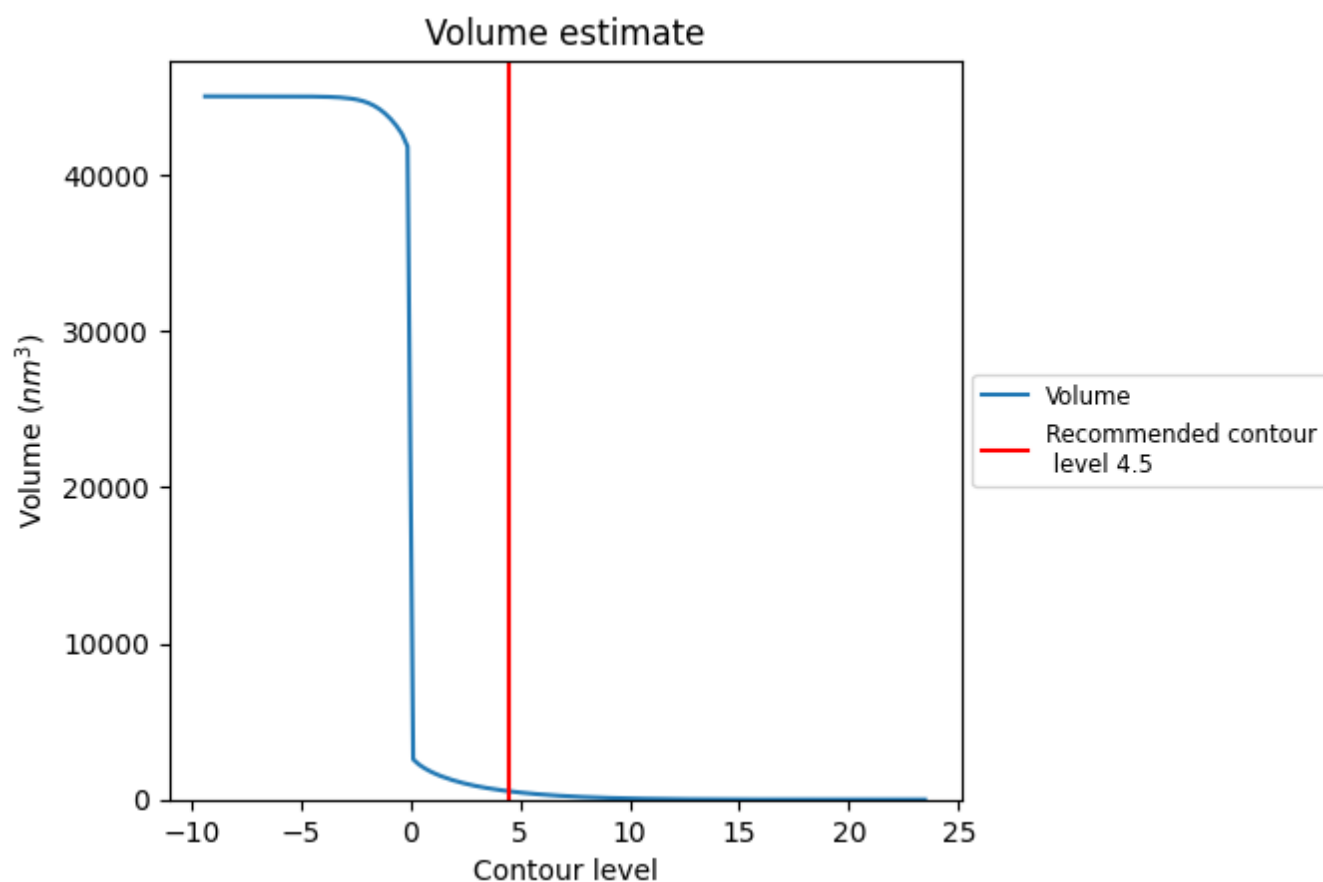
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

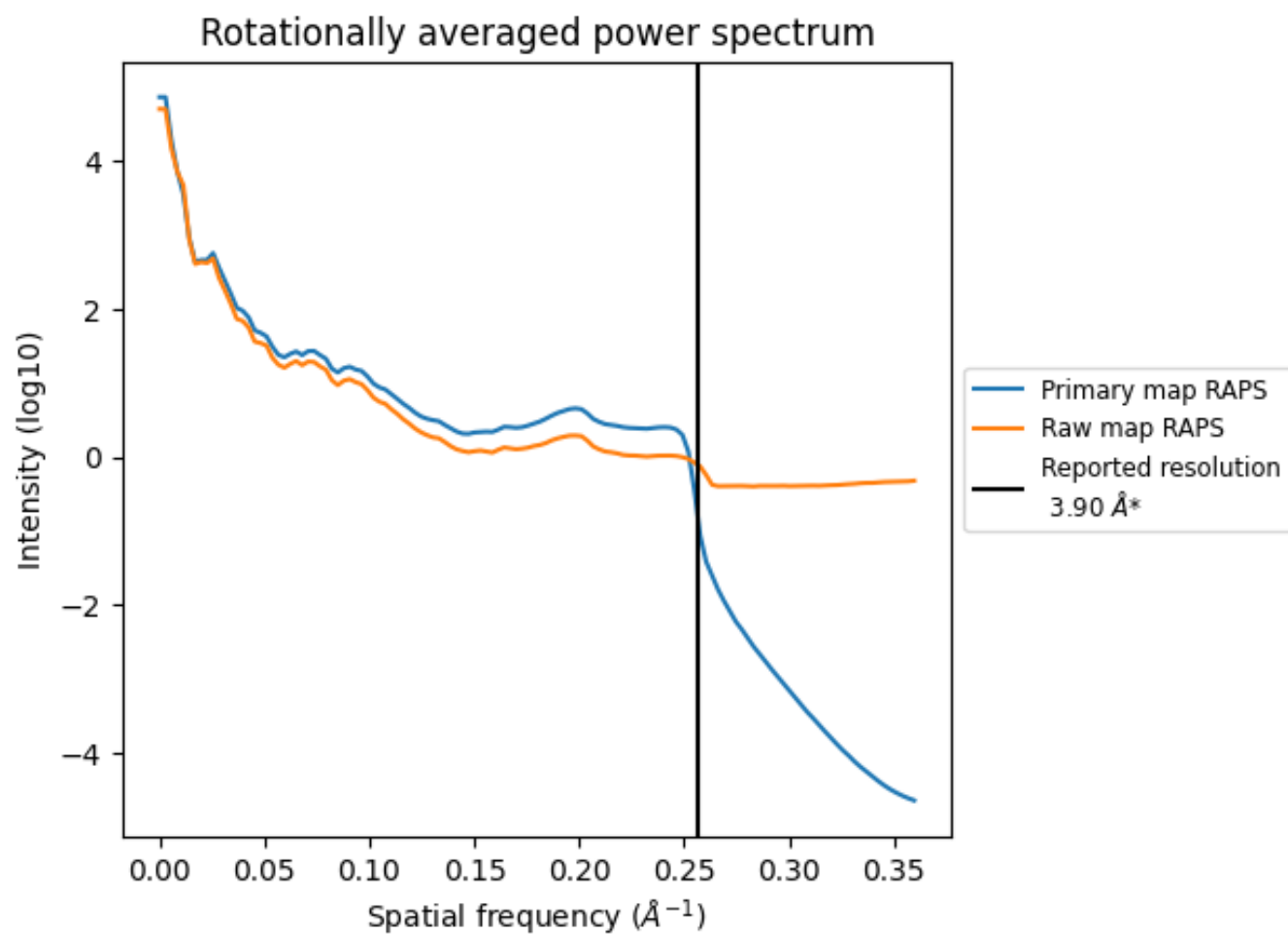
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 533 nm³; this corresponds to an approximate mass of 481 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

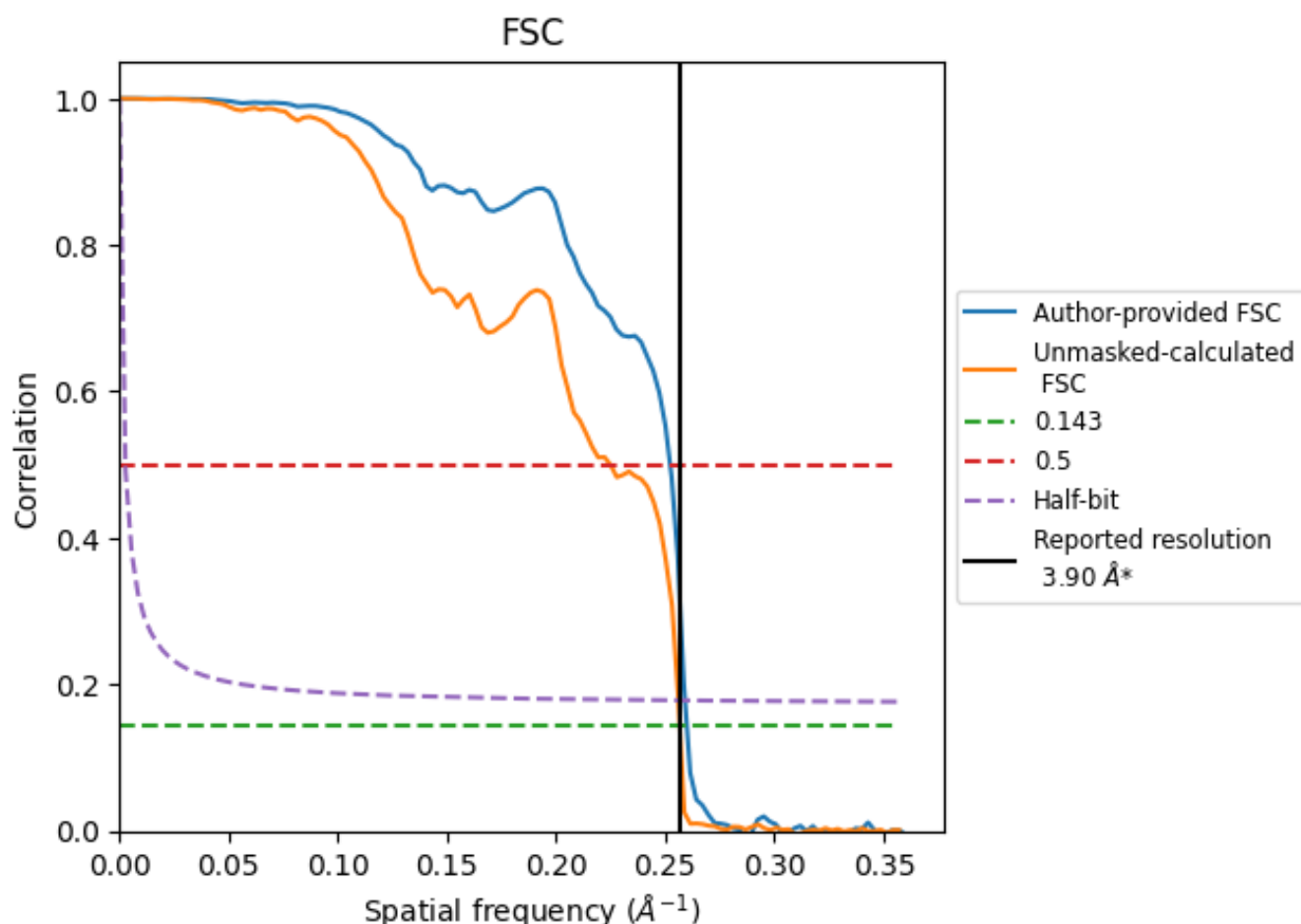


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

8.2 Resolution estimates [i](#)

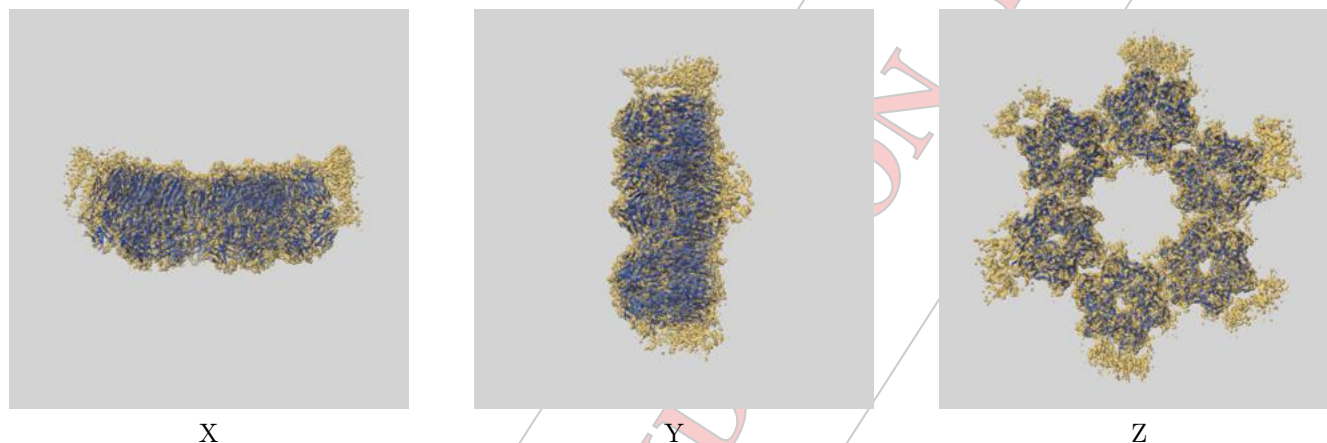
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.85	3.97	3.86
Unmasked-calculated*	3.90	4.45	3.91

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

9 Map-model fit [i](#)

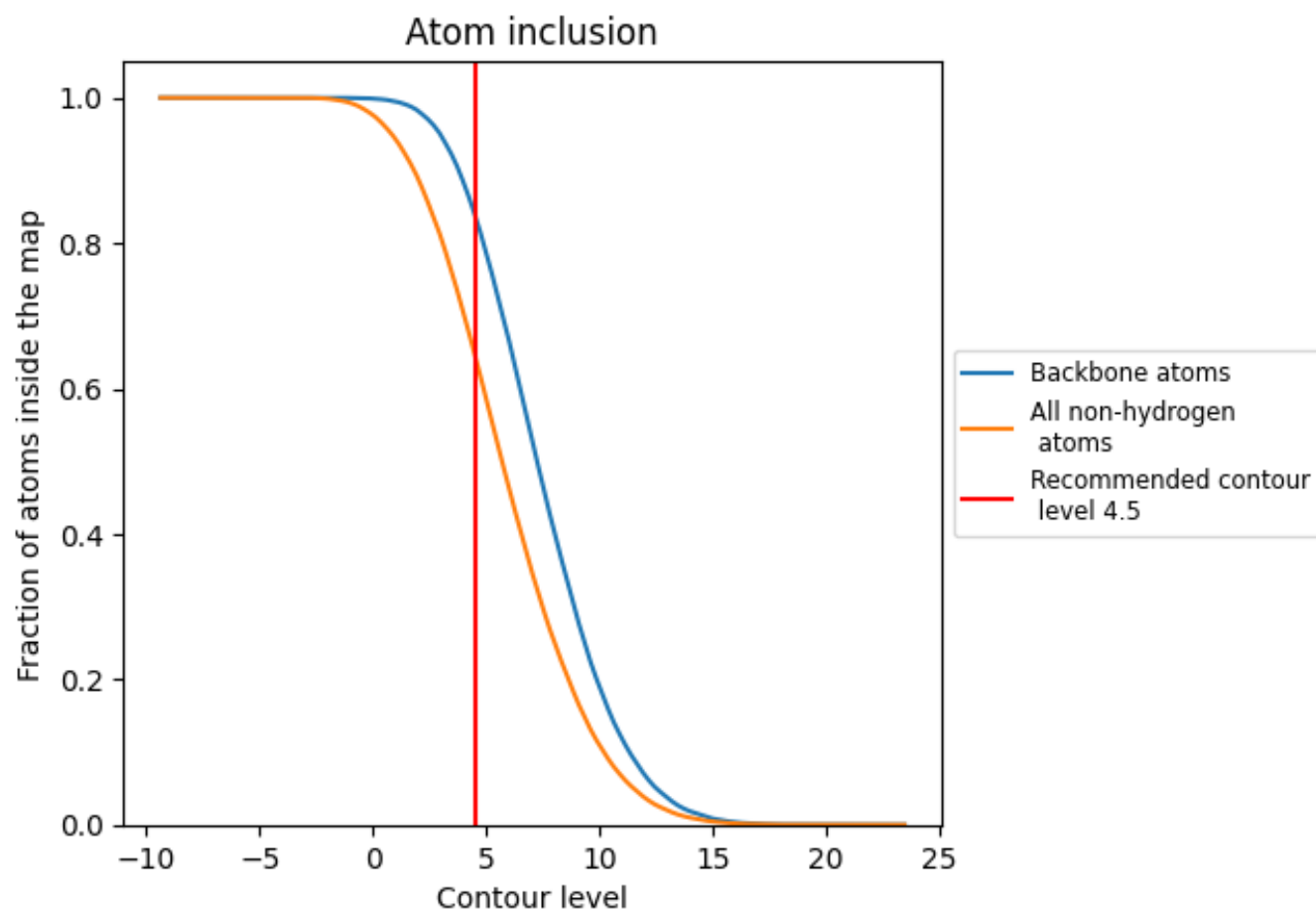
This section contains information regarding the fit between EMDB map EMD-31954 and PDB model 7VFH. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 4.5 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 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 65% of all non-hydrogen atoms, are inside the map.



Full wwPDB EM Validation Report ⓘ

Sep 24, 2021 – 08:26 PM JST

PDB ID : 7VFD
EMDB ID : EMD-31949
Title : Cryo-EM structure of Vaccinia virus scaffolding protein D13
Deposited on : 2021-09-13
Resolution : 2.25 Å (reported)
Based on initial model : 6BEI

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

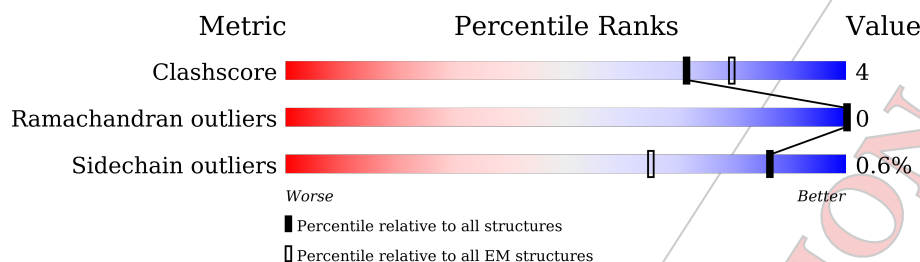
EMDB validation analysis : 0.0.0.dev97
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

1 Overall quality at a glance

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

The reported resolution of this entry is 2.25 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	549	90% 9%
1	B	549	88% 11%
1	C	549	88% 10%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13262 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Scaffold protein D13.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	541	Total	C	N	O	S	2	0
			4304	2750	700	840	14		
1	B	541	Total	C	N	O	S	2	0
			4304	2750	700	840	14		
1	C	541	Total	C	N	O	S	2	0
			4304	2750	700	840	14		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ALA	-	expression tag	UNP P68440
B	0	ALA	-	expression tag	UNP P68440
C	0	ALA	-	expression tag	UNP P68440

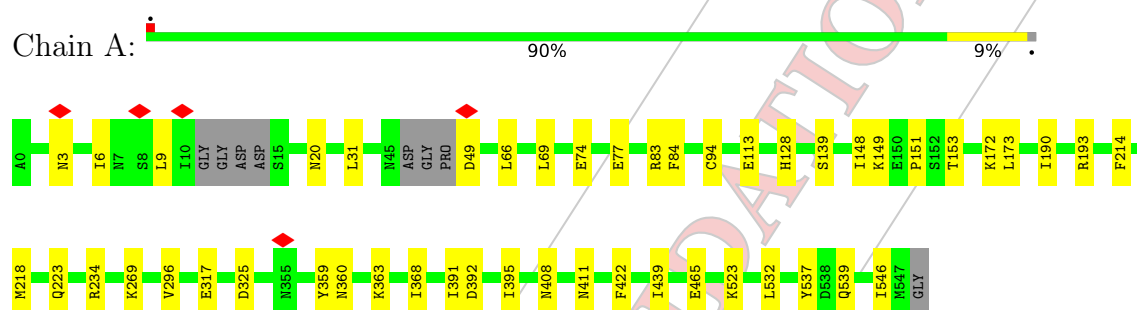
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		AltConf
2	A	111	Total	O	0
			111	111	
2	B	117	Total	O	0
			117	117	
2	C	122	Total	O	0
			122	122	

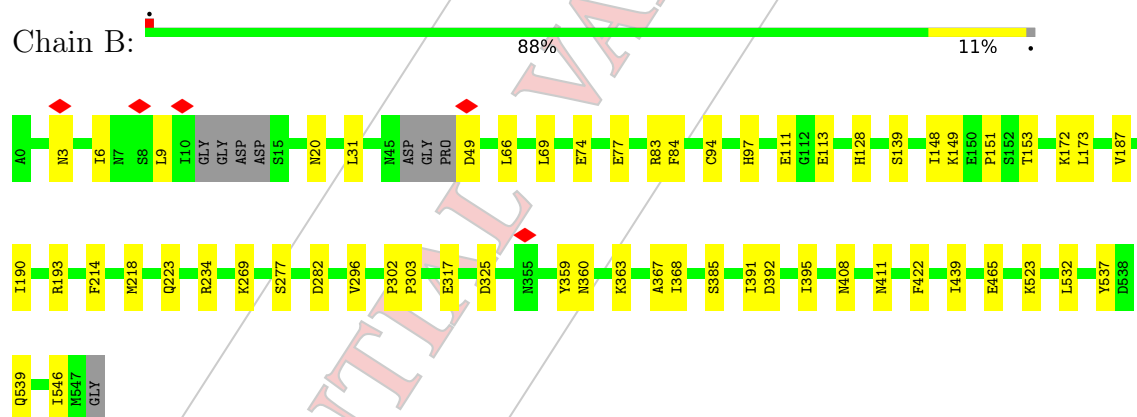
3 Residue-property plots [i](#)

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.

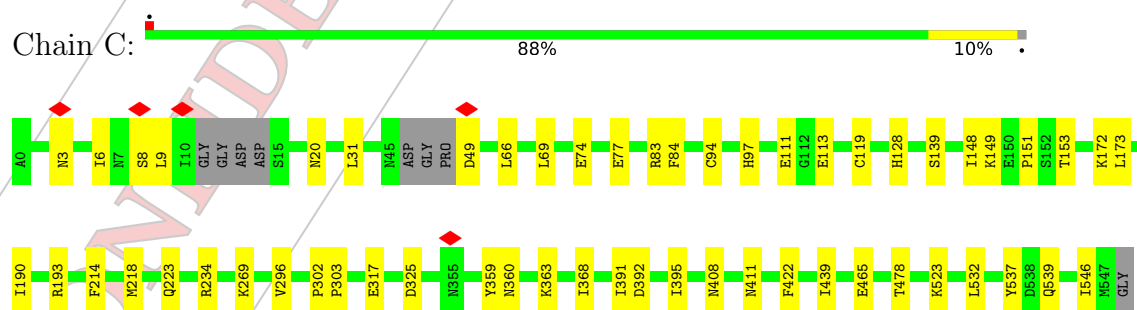
- Molecule 1: Scaffold protein D13



- Molecule 1: Scaffold protein D13



- Molecule 1: Scaffold protein D13



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	130384	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	155000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	42.581	Depositor
Minimum map value	-22.933	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4.0	Depositor
Map size (Å)	265.216, 265.216, 265.216	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.036, 1.036, 1.036	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	0.28	0/4395	0.45	0/5977
1	B	0.28	0/4395	0.45	0/5977
1	C	0.28	0/4395	0.45	0/5977
All	All	0.28	0/13185	0.45	0/17931

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4304	0	4266	31	0
1	B	4304	0	4266	36	0
1	C	4304	0	4266	36	0
2	A	111	0	0	0	0
2	B	117	0	0	2	0
2	C	122	0	0	2	0
All	All	13262	0	12798	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 4.

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:128:HIS:NE2	1:B:465:GLU:OE2	2.30	0.64
1:A:465:GLU:OE2	1:C:128:HIS:NE2	2.31	0.62
1:B:128:HIS:NE2	1:C:465:GLU:OE2	2.31	0.62
1:A:84:PHE:HB3	1:A:148:ILE:HG21	1.84	0.59
1:C:84:PHE:HB3	1:C:148:ILE:HG21	1.84	0.59
1:C:74:GLU:OE1	1:C:153:THR:OG1	2.20	0.59
1:B:74:GLU:OE1	1:B:153:THR:OG1	2.20	0.58
1:B:84:PHE:HB3	1:B:148:ILE:HG21	1.84	0.58
1:A:74:GLU:OE1	1:A:153:THR:OG1	2.21	0.58
1:B:359:TYR:OH	1:B:392:ASP:OD1	2.25	0.55
1:A:3:ASN:HA	1:A:6:ILE:HG12	1.90	0.54
1:A:532:LEU:HG	1:A:546:ILE:HD12	1.89	0.54
1:C:3:ASN:HA	1:C:6:ILE:HG12	1.89	0.54
1:B:532:LEU:HG	1:B:546:ILE:HD12	1.89	0.54
1:A:408:ASN:ND2	1:A:411:ASN:OD1	2.39	0.53
1:C:478:THR:HG23	2:C:664:HOH:O	2.08	0.53
1:C:532:LEU:HG	1:C:546:ILE:HD12	1.89	0.53
1:B:3:ASN:HA	1:B:6:ILE:HG12	1.89	0.53
1:C:359:TYR:OH	1:C:392:ASP:OD1	2.25	0.53
1:B:139:SER:HB2	1:B:148:ILE:HG23	1.91	0.53
1:A:139:SER:HB2	1:A:148:ILE:HG23	1.91	0.52
1:C:139:SER:HB2	1:C:148:ILE:HG23	1.91	0.52
1:A:359:TYR:OH	1:A:392:ASP:OD1	2.25	0.51
1:B:408:ASN:ND2	1:B:411:ASN:OD1	2.39	0.50
1:C:69:LEU:HD23	1:C:214:PHE:HB3	1.94	0.50
1:C:94[A]:CYS:SG	1:C:190:ILE:HG21	2.52	0.50
1:B:69:LEU:HD23	1:B:214:PHE:HB3	1.94	0.49
1:A:218:MET:SD	1:C:6:ILE:HA	2.52	0.48
1:B:113:GLU:OE2	1:B:234:ARG:NH1	2.32	0.48
1:C:408:ASN:ND2	1:C:411:ASN:OD1	2.39	0.48
1:A:69:LEU:HD23	1:A:214:PHE:HB3	1.94	0.48
1:B:6:ILE:HA	1:C:218:MET:SD	2.54	0.48
1:A:94[A]:CYS:SG	1:A:190:ILE:HG21	2.52	0.48
1:B:94[A]:CYS:SG	1:B:190:ILE:HG21	2.52	0.48
1:A:6:ILE:HA	1:B:218:MET:SD	2.53	0.47
1:A:269:LYS:HE3	1:A:422:PHE:CZ	2.50	0.47
1:C:269:LYS:HE3	1:C:422:PHE:CZ	2.50	0.47
1:C:325:ASP:OD1	1:C:363:LYS:NZ	2.48	0.47
1:B:269:LYS:HE3	1:B:422:PHE:CZ	2.50	0.47
1:A:31:LEU:HG	1:C:9:LEU:HD22	1.96	0.46
1:A:9:LEU:HD22	1:B:31:LEU:HG	1.97	0.46
1:A:439:ILE:HD13	1:A:523:LYS:HD2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:ASP:N	1:C:49:ASP:OD1	2.49	0.46
1:B:9:LEU:HD22	1:C:31:LEU:HG	1.97	0.46
1:B:325:ASP:OD1	1:B:363:LYS:NZ	2.48	0.46
1:B:20:ASN:ND2	1:C:223:GLN:HB2	2.31	0.46
1:B:49:ASP:N	1:B:49:ASP:OD1	2.49	0.45
1:A:49:ASP:OD1	1:A:49:ASP:N	2.49	0.45
1:C:439:ILE:HD13	1:C:523:LYS:HD2	1.98	0.45
1:C:391:ILE:O	1:C:395:ILE:HG13	2.17	0.45
1:A:113:GLU:OE2	1:A:234:ARG:NH1	2.32	0.45
1:A:172:LYS:HB2	1:A:537:TYR:CE1	2.51	0.45
1:A:223:GLN:HB2	1:C:20:ASN:ND2	2.31	0.45
1:B:172:LYS:HB2	1:B:537:TYR:CE1	2.51	0.45
1:B:439:ILE:HD13	1:B:523:LYS:HD2	1.98	0.45
1:B:391:ILE:O	1:B:395:ILE:HG13	2.17	0.45
1:C:172:LYS:HB2	1:C:537:TYR:CE1	2.51	0.45
1:A:391:ILE:O	1:A:395:ILE:HG13	2.17	0.45
1:A:20:ASN:ND2	1:B:223:GLN:HB2	2.31	0.44
1:C:113:GLU:OE2	1:C:234:ARG:NH1	2.32	0.44
1:A:325:ASP:OD1	1:A:363:LYS:NZ	2.48	0.44
1:C:119:CYS:HB2	2:C:715:HOH:O	2.18	0.43
1:B:296:VAL:HG21	1:B:368:ILE:HG21	2.00	0.43
2:B:654:HOH:O	1:C:8:SER:HB2	2.18	0.43
1:A:296:VAL:HG21	1:A:368:ILE:HG21	2.00	0.43
1:B:77:GLU:HB2	1:B:151:PRO:HG3	2.01	0.43
1:C:296:VAL:HG21	1:C:368:ILE:HG21	2.00	0.43
1:B:302:PRO:HA	1:B:303:PRO:HD3	1.93	0.42
1:A:77:GLU:HB2	1:A:151:PRO:HG3	2.01	0.42
1:B:148:ILE:HG22	1:B:149:LYS:HG2	2.02	0.42
1:C:302:PRO:HA	1:C:303:PRO:HD3	1.93	0.42
1:A:148:ILE:HG22	1:A:149:LYS:HG2	2.02	0.42
1:C:97:HIS:HD2	1:C:111:GLU:OE2	2.03	0.42
1:C:83:ARG:HA	1:C:139:SER:O	2.20	0.42
1:C:94[A]:CYS:SG	1:C:190:ILE:HD13	2.60	0.42
1:C:360:ASN:HB3	1:C:363:LYS:HD2	2.02	0.42
1:B:94[A]:CYS:SG	1:B:190:ILE:HD13	2.60	0.42
1:B:83:ARG:HA	1:B:139:SER:O	2.20	0.41
1:C:148:ILE:HG22	1:C:149:LYS:HG2	2.02	0.41
1:C:66:LEU:HD23	1:C:173:LEU:HD11	2.01	0.41
1:C:77:GLU:HB2	1:C:151:PRO:HG3	2.01	0.41
1:A:83:ARG:HA	1:A:139:SER:O	2.20	0.41
1:B:360:ASN:HB3	1:B:363:LYS:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:ASN:HB3	1:A:363:LYS:HD2	2.02	0.41
1:A:94[A]:CYS:SG	1:A:190:ILE:HD13	2.60	0.41
1:B:66:LEU:HD23	1:B:173:LEU:HD11	2.01	0.41
1:B:97:HIS:HD2	1:B:111:GLU:OE2	2.03	0.41
1:A:66:LEU:HD23	1:A:173:LEU:HD11	2.01	0.40
1:B:187:VAL:HG12	2:B:628:HOH:O	2.22	0.40
1:B:367:ALA:HB3	1:B:385:SER:HB2	2.03	0.40
1:B:277:SER:HB3	1:B:282:ASP:OD2	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	536/549 (98%)	516 (96%)	20 (4%)	0	100	100
1	B	536/549 (98%)	516 (96%)	20 (4%)	0	100	100
1	C	536/549 (98%)	516 (96%)	20 (4%)	0	100	100
All	All	1608/1647 (98%)	1548 (96%)	60 (4%)	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	499/502 (99%)	496 (99%)	3 (1%)	86	91
1	B	499/502 (99%)	496 (99%)	3 (1%)	86	91
1	C	499/502 (99%)	496 (99%)	3 (1%)	86	91
All	All	1497/1506 (99%)	1488 (99%)	9 (1%)	86	91

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	193	ARG
1	A	317	GLU
1	A	539	GLN
1	B	193	ARG
1	B	317	GLU
1	B	539	GLN
1	C	193	ARG
1	C	317	GLU
1	C	539	GLN

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

CONFIDENTIAL VALIDATION REPORT

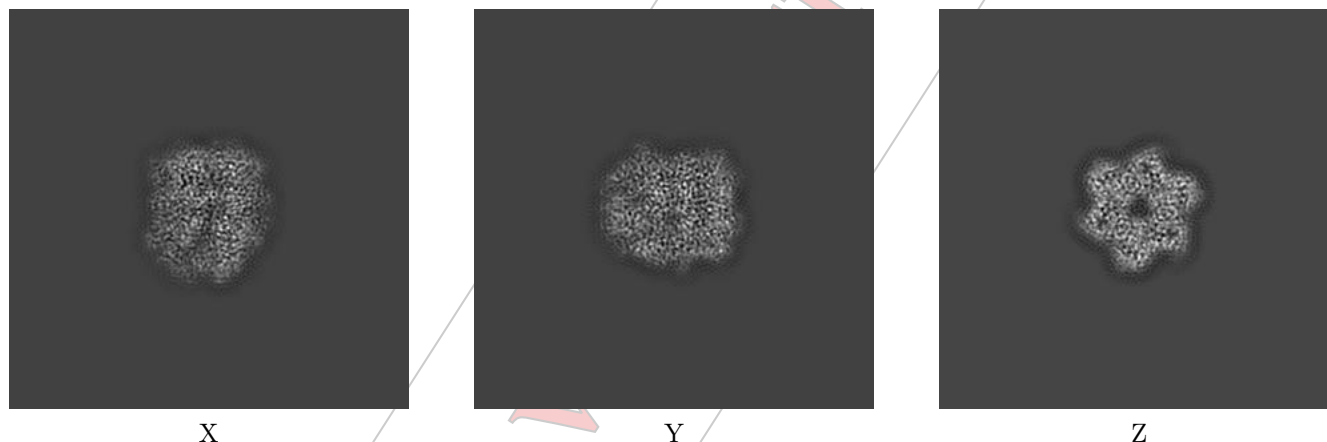
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31949. These allow visual inspection of the internal detail of the map and identification of artifacts.

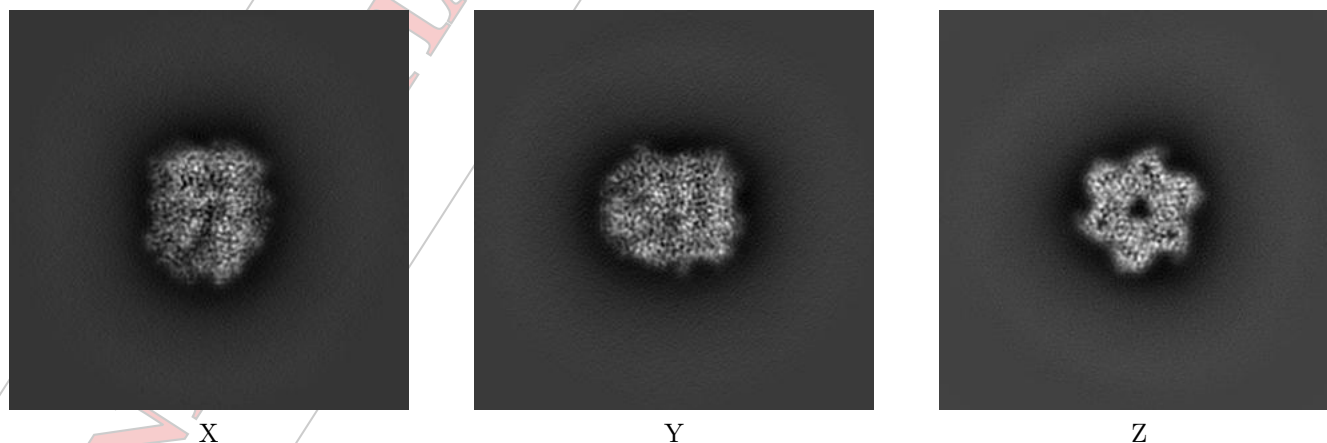
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



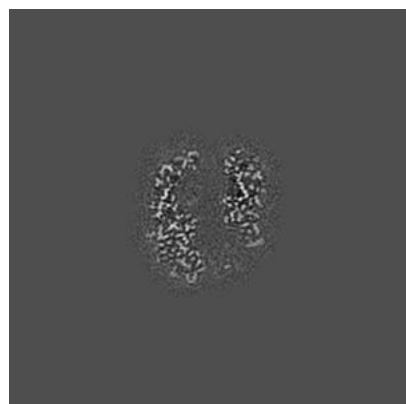
6.1.2 Raw map



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

6.2 Central slices [i](#)

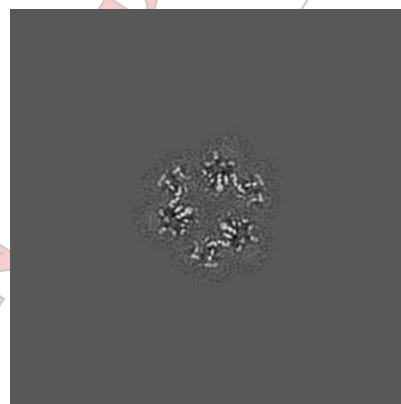
6.2.1 Primary map



X Index: 128

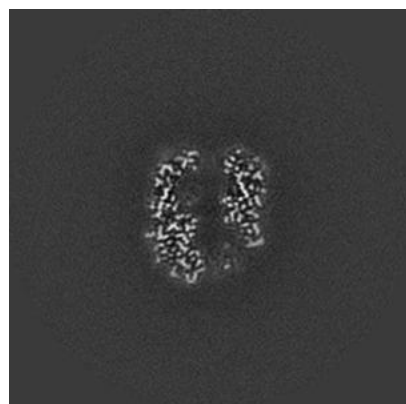


Y Index: 128

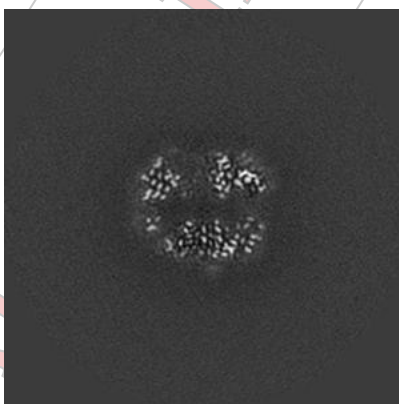


Z Index: 128

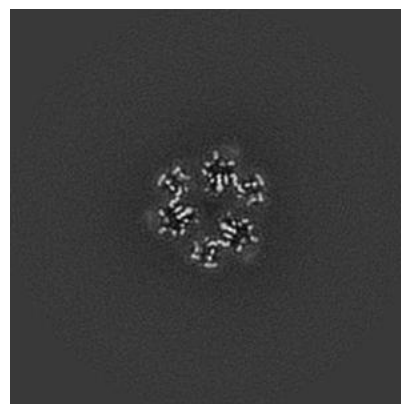
6.2.2 Raw map



X Index: 128



Y Index: 128

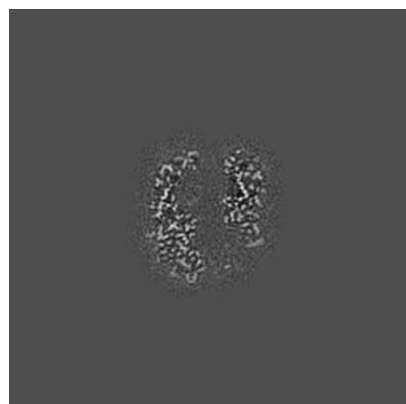


Z Index: 128

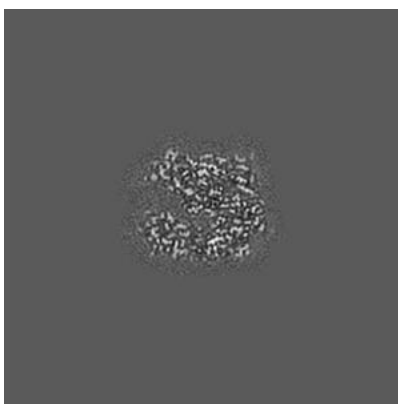
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

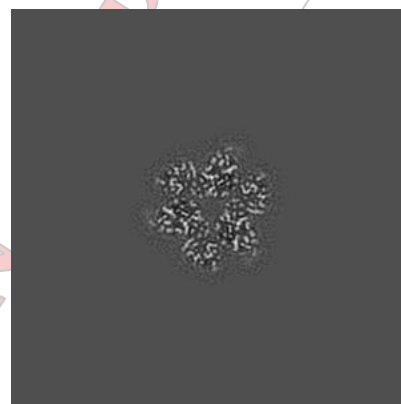
6.3.1 Primary map



X Index: 128

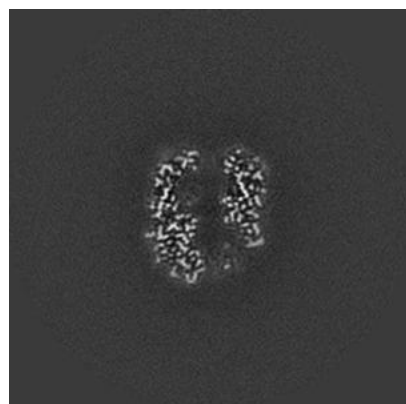


Y Index: 143

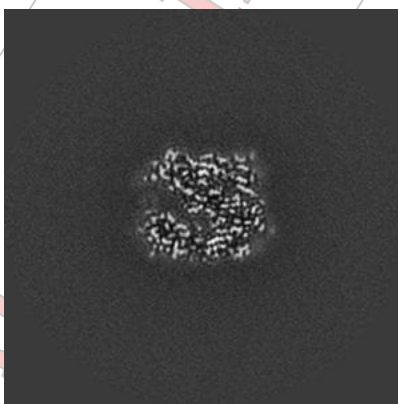


Z Index: 134

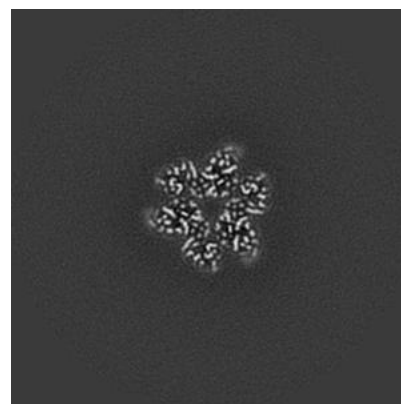
6.3.2 Raw map



X Index: 128



Y Index: 143

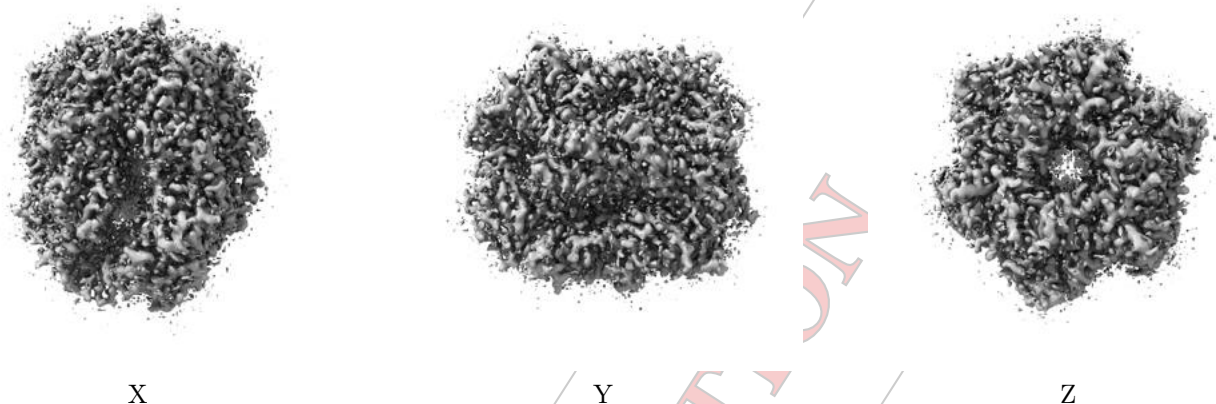


Z Index: 134

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

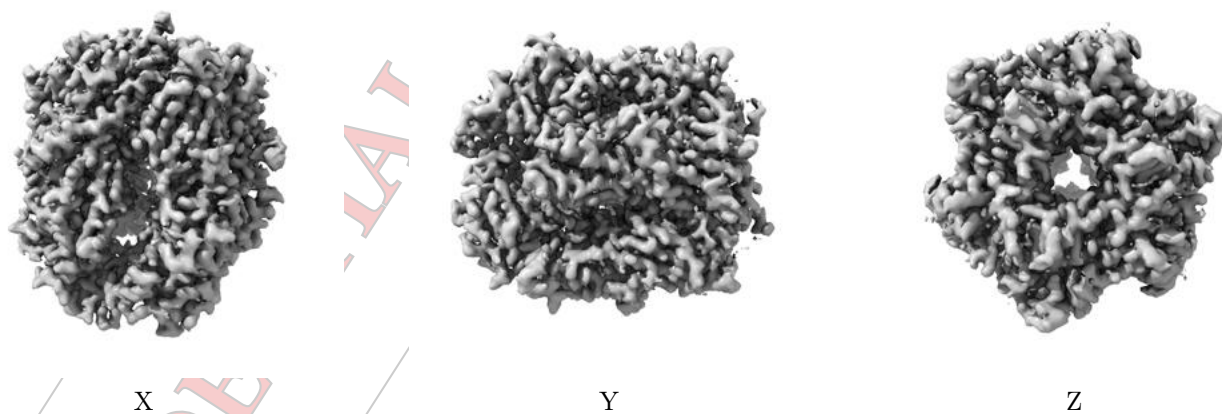
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 4.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



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

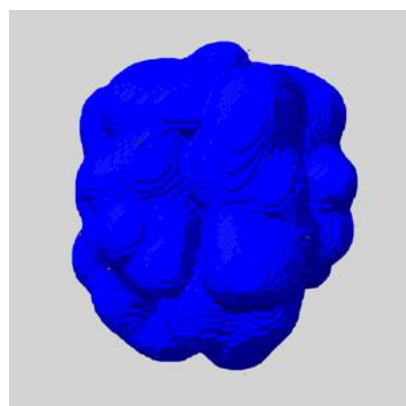
6.5 Mask visualisation [i](#)

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

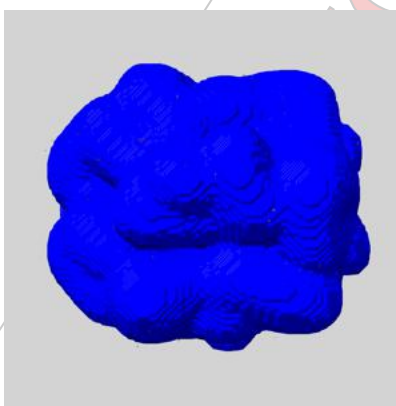
A mask typically either:

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

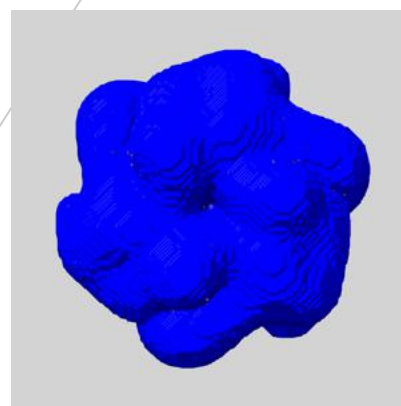
6.5.1 D_1300024103_em-mask-volume_P1.map.V2 [i](#)



X



Y

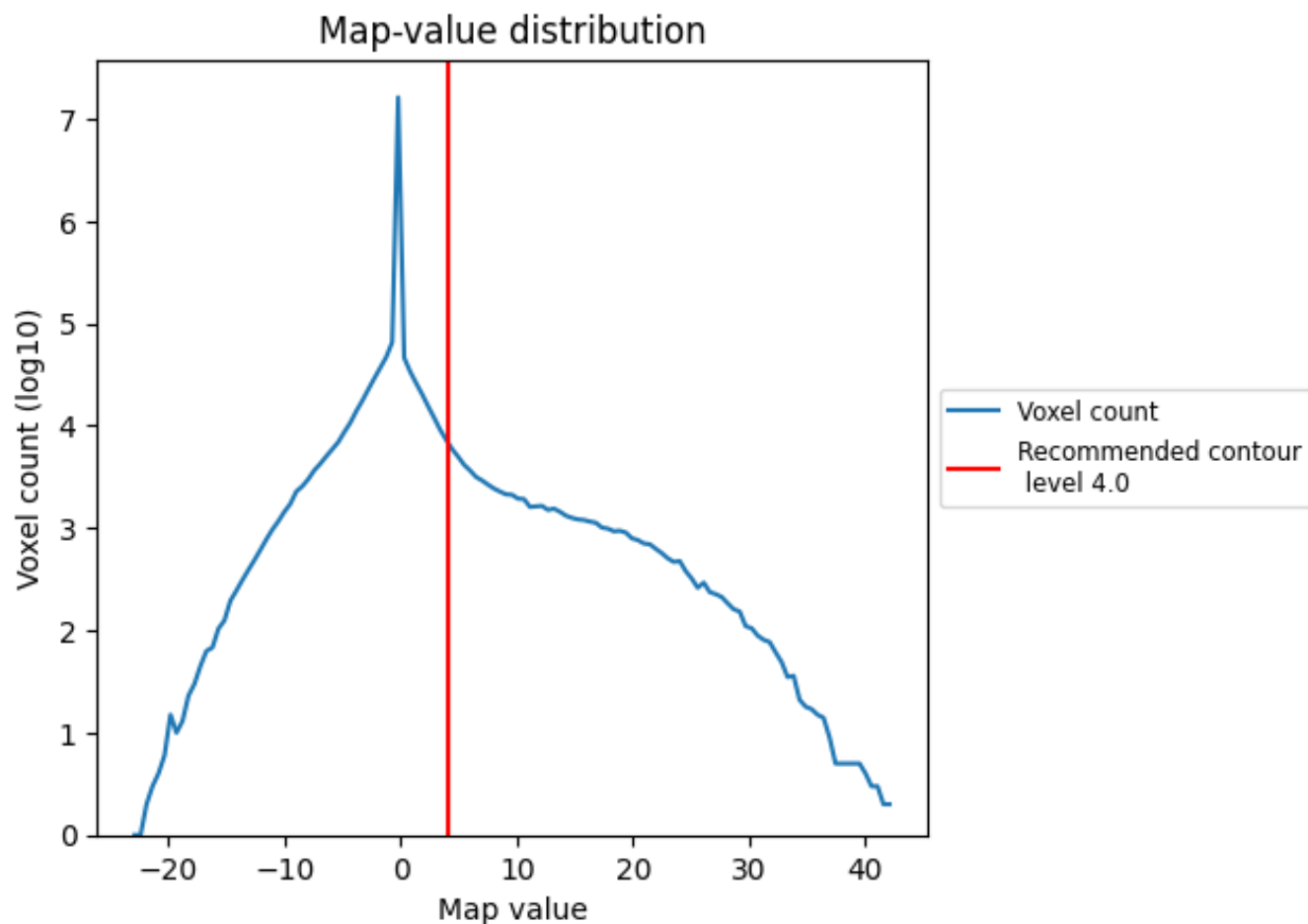


Z

7 Map analysis [i](#)

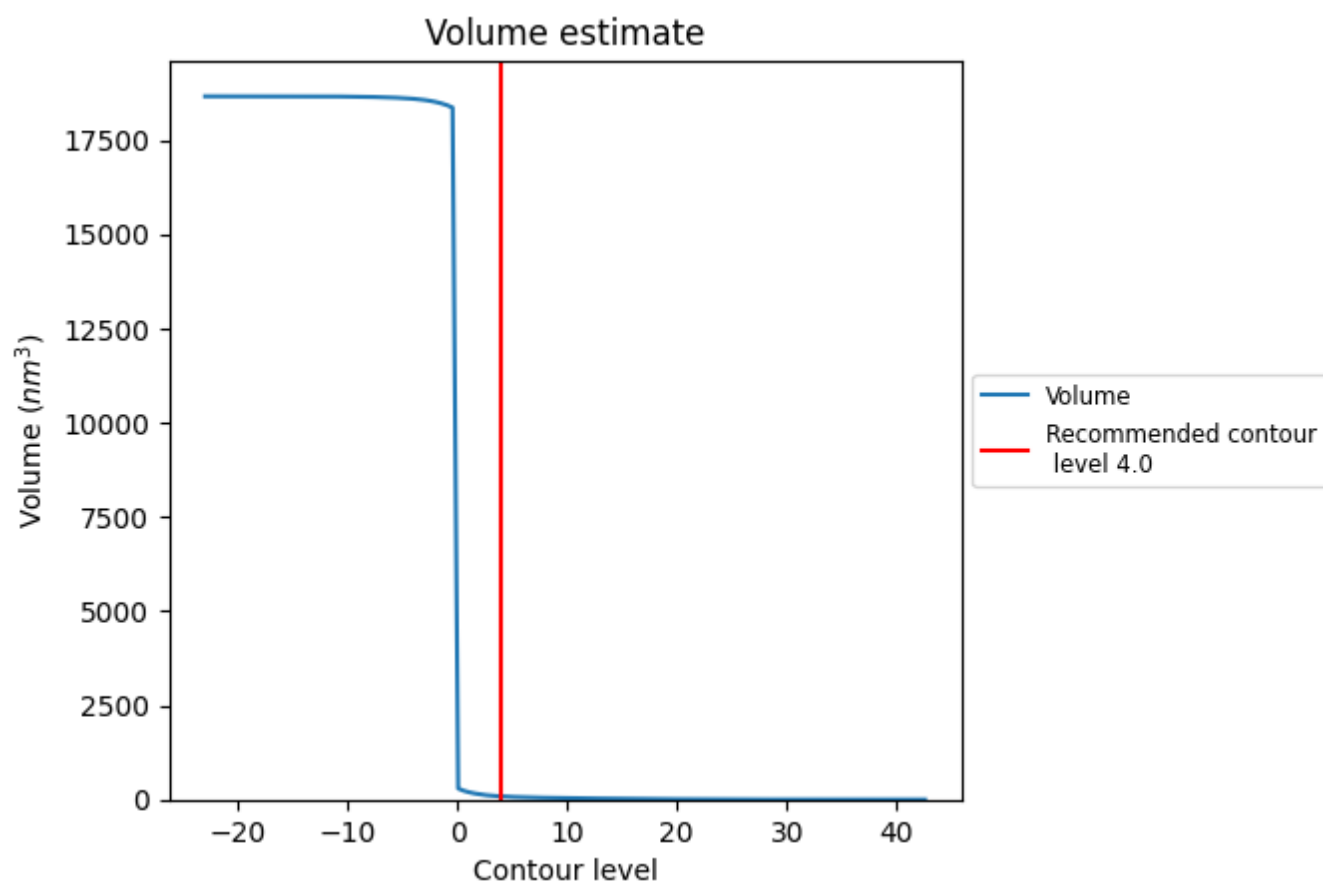
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

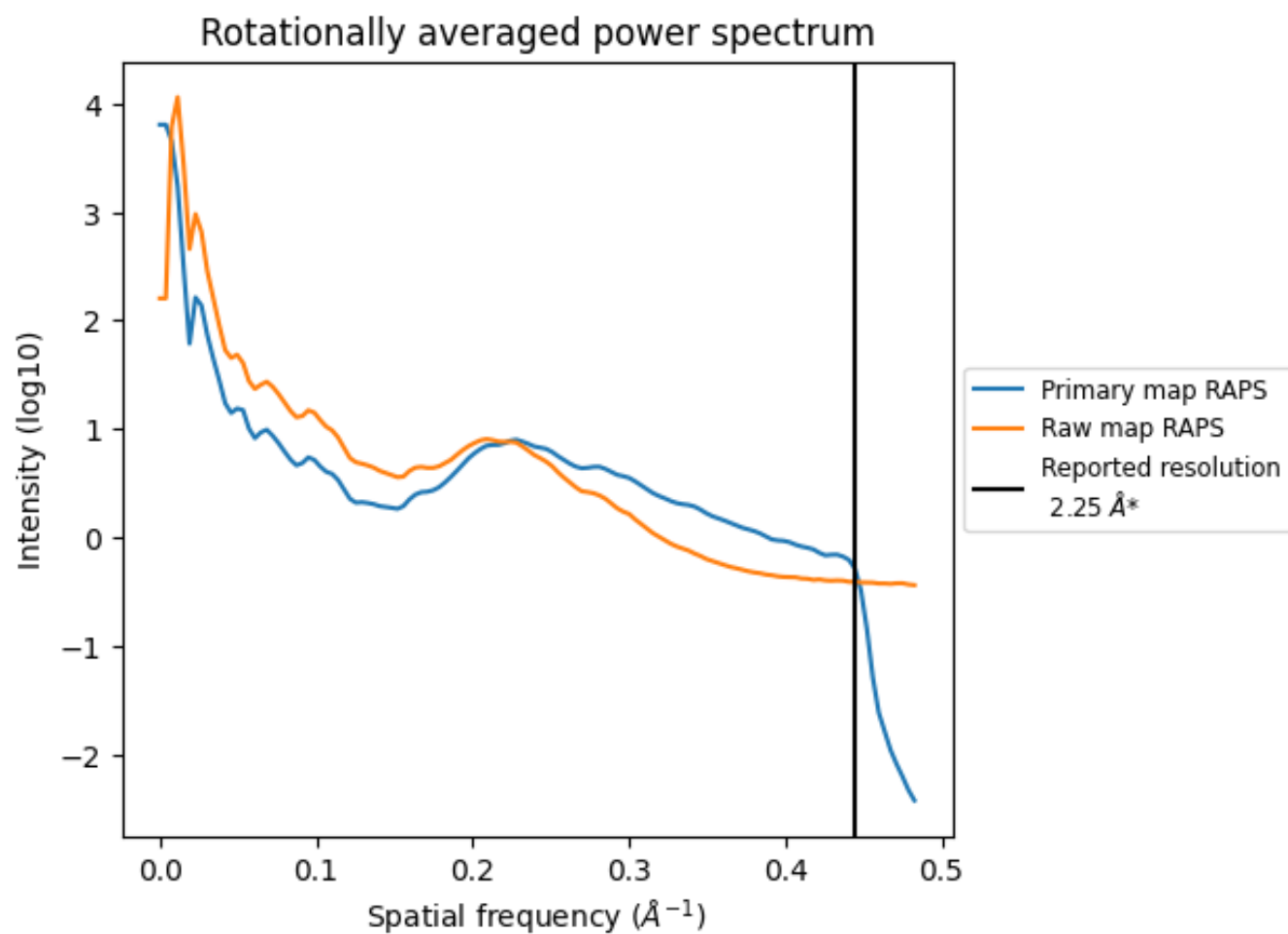
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 85 nm^3 ; this corresponds to an approximate mass of 77 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

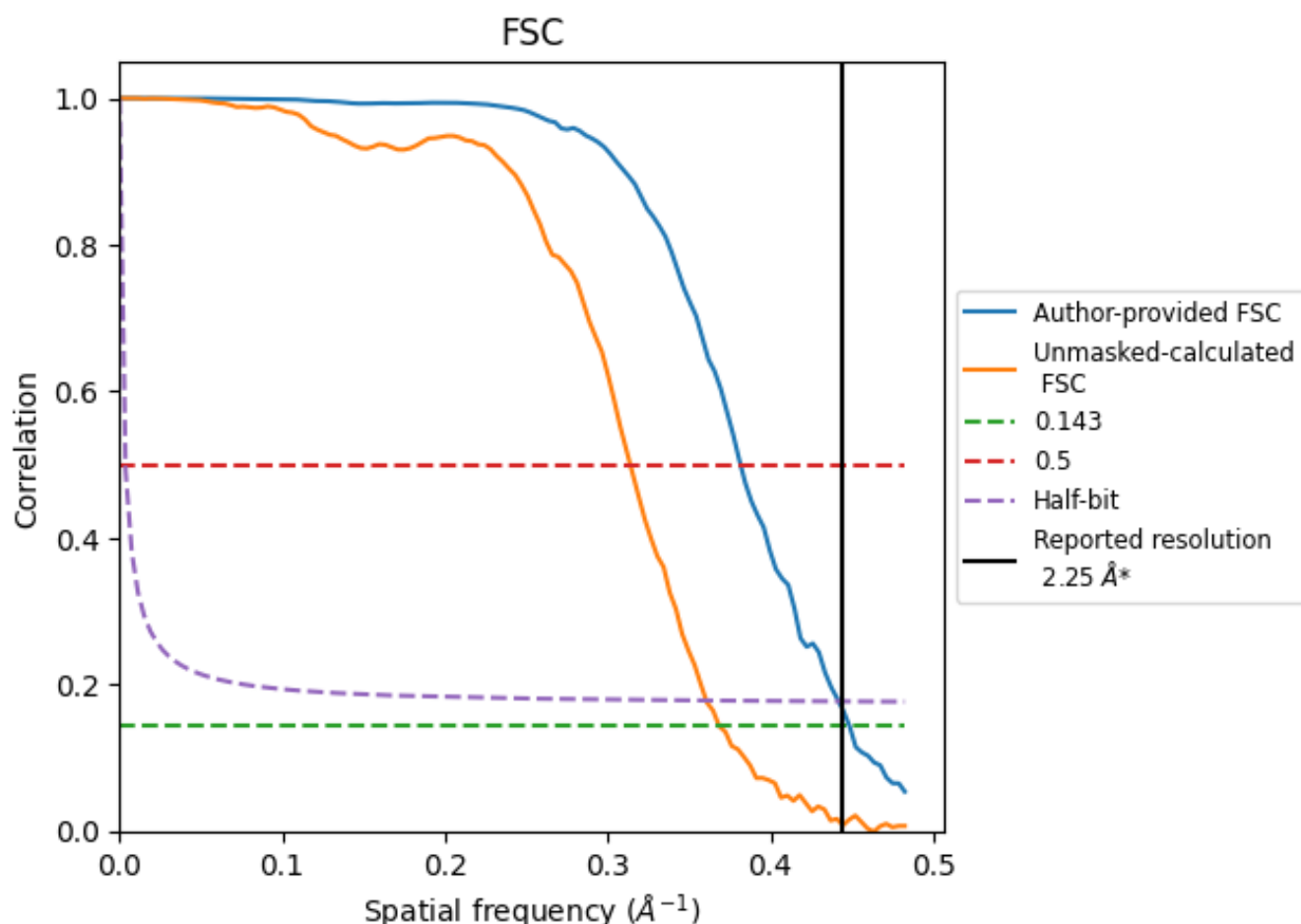


*Reported resolution corresponds to spatial frequency of 0.444 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.444 Å⁻¹

8.2 Resolution estimates [i](#)

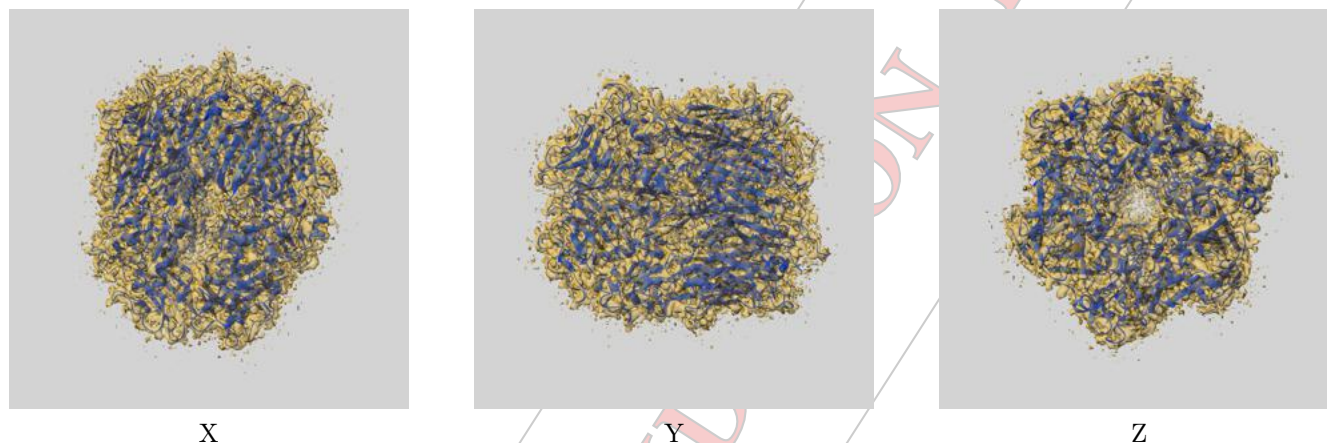
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.25	-	-
Author-provided FSC curve	2.23	2.62	2.26
Unmasked-calculated*	2.71	3.19	2.77

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.71 differs from the reported value 2.25 by more than 10 %

9 Map-model fit [i](#)

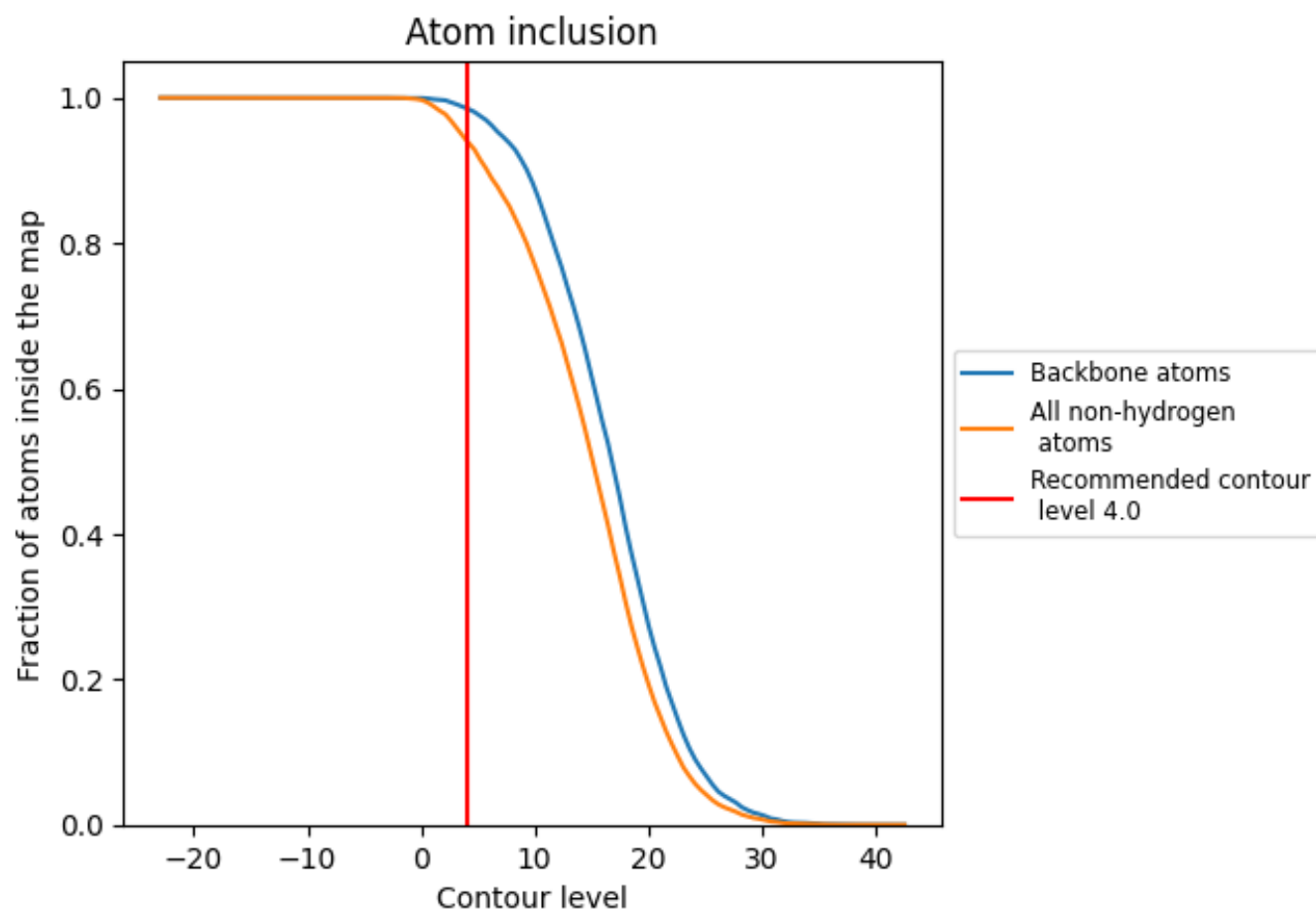
This section contains information regarding the fit between EMDB map EMD-31949 and PDB model 7VFD. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 4.0 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 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.



Full wwPDB EM Validation Report ⓘ

Sep 19, 2021 – 06:29 PM JST

PDB ID : 7VFE
EMDB ID : EMD-31950
Title : Cryo-EM structure of Vaccinia virus scaffolding protein D13 with N-terminal polyhistidine tag
Deposited on : 2021-09-13
Resolution : 2.63 Å (reported)
Based on initial model : 6BEI

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

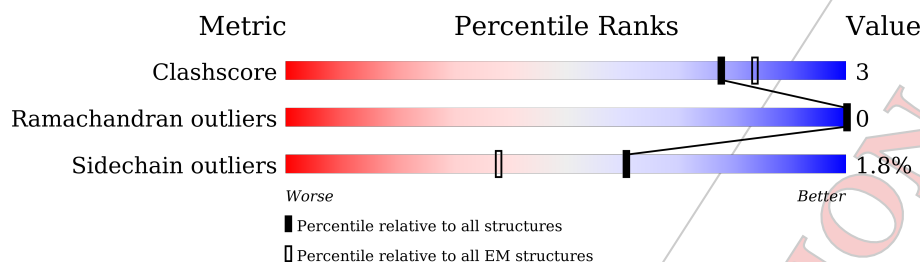
EMDB validation analysis : 0.0.0.dev97
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.1

1 Overall quality at a glance

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

The reported resolution of this entry is 2.63 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	569	 83% 10% 7%
1	B	569	 83% 9% 7%
1	C	569	 84% 9% 7%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 12630 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Scaffold protein D13.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	529	Total	C	N	O	S	0	0
			4210	2693	684	821	12		
1	B	529	Total	C	N	O	S	0	0
			4210	2693	684	821	12		
1	C	529	Total	C	N	O	S	0	0
			4210	2693	684	821	12		

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	HIS	-	expression tag	UNP P68440
A	-19	HIS	-	expression tag	UNP P68440
A	-18	HIS	-	expression tag	UNP P68440
A	-17	HIS	-	expression tag	UNP P68440
A	-16	HIS	-	expression tag	UNP P68440
A	-15	HIS	-	expression tag	UNP P68440
A	-14	ASP	-	expression tag	UNP P68440
A	-13	TYR	-	expression tag	UNP P68440
A	-12	ASP	-	expression tag	UNP P68440
A	-11	ILE	-	expression tag	UNP P68440
A	-10	PRO	-	expression tag	UNP P68440
A	-9	THR	-	expression tag	UNP P68440
A	-8	THR	-	expression tag	UNP P68440
A	-7	GLU	-	expression tag	UNP P68440
A	-6	ASN	-	expression tag	UNP P68440
A	-5	LEU	-	expression tag	UNP P68440
A	-4	TYR	-	expression tag	UNP P68440
A	-3	PHE	-	expression tag	UNP P68440
A	-2	GLN	-	expression tag	UNP P68440
A	-1	GLY	-	expression tag	UNP P68440
A	0	ALA	-	expression tag	UNP P68440
B	-20	HIS	-	expression tag	UNP P68440
B	-19	HIS	-	expression tag	UNP P68440
B	-18	HIS	-	expression tag	UNP P68440

Continued on next page...

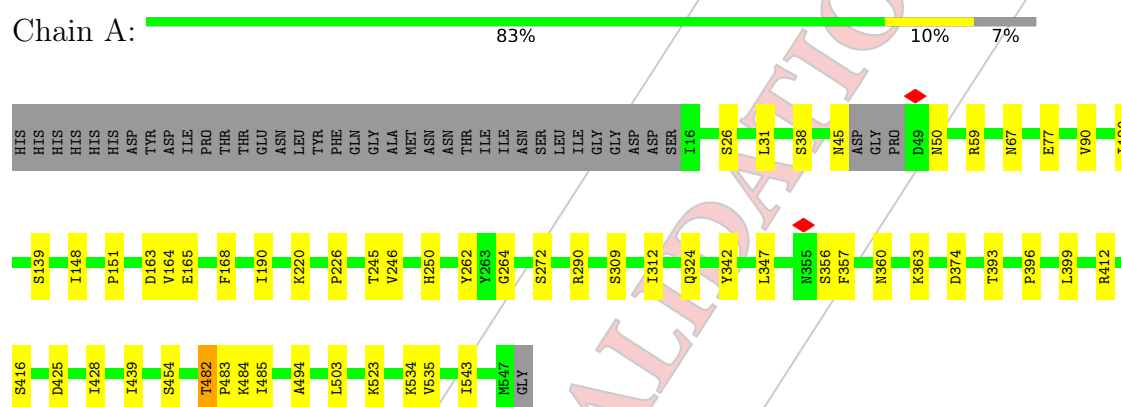
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	HIS	-	expression tag	UNP P68440
B	-16	HIS	-	expression tag	UNP P68440
B	-15	HIS	-	expression tag	UNP P68440
B	-14	ASP	-	expression tag	UNP P68440
B	-13	TYR	-	expression tag	UNP P68440
B	-12	ASP	-	expression tag	UNP P68440
B	-11	ILE	-	expression tag	UNP P68440
B	-10	PRO	-	expression tag	UNP P68440
B	-9	THR	-	expression tag	UNP P68440
B	-8	THR	-	expression tag	UNP P68440
B	-7	GLU	-	expression tag	UNP P68440
B	-6	ASN	-	expression tag	UNP P68440
B	-5	LEU	-	expression tag	UNP P68440
B	-4	TYR	-	expression tag	UNP P68440
B	-3	PHE	-	expression tag	UNP P68440
B	-2	GLN	-	expression tag	UNP P68440
B	-1	GLY	-	expression tag	UNP P68440
B	0	ALA	-	expression tag	UNP P68440
C	-20	HIS	-	expression tag	UNP P68440
C	-19	HIS	-	expression tag	UNP P68440
C	-18	HIS	-	expression tag	UNP P68440
C	-17	HIS	-	expression tag	UNP P68440
C	-16	HIS	-	expression tag	UNP P68440
C	-15	HIS	-	expression tag	UNP P68440
C	-14	ASP	-	expression tag	UNP P68440
C	-13	TYR	-	expression tag	UNP P68440
C	-12	ASP	-	expression tag	UNP P68440
C	-11	ILE	-	expression tag	UNP P68440
C	-10	PRO	-	expression tag	UNP P68440
C	-9	THR	-	expression tag	UNP P68440
C	-8	THR	-	expression tag	UNP P68440
C	-7	GLU	-	expression tag	UNP P68440
C	-6	ASN	-	expression tag	UNP P68440
C	-5	LEU	-	expression tag	UNP P68440
C	-4	TYR	-	expression tag	UNP P68440
C	-3	PHE	-	expression tag	UNP P68440
C	-2	GLN	-	expression tag	UNP P68440
C	-1	GLY	-	expression tag	UNP P68440
C	0	ALA	-	expression tag	UNP P68440

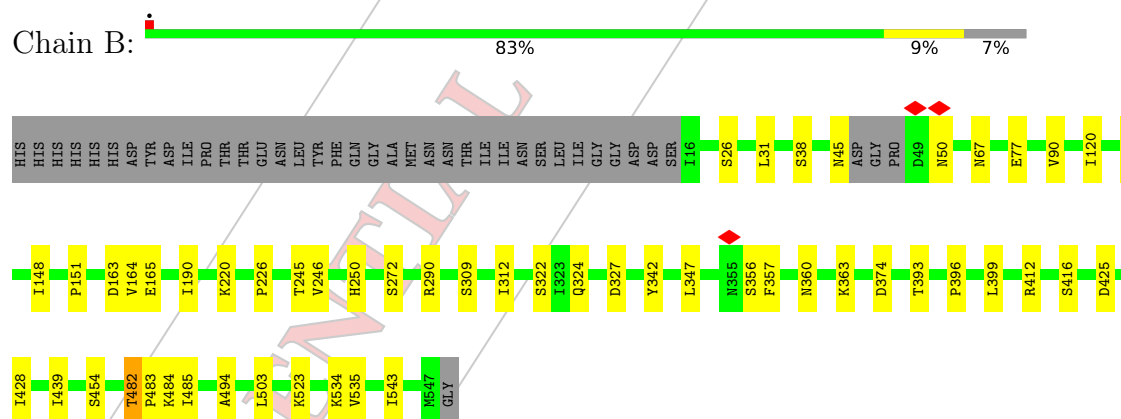
3 Residue-property plots [i](#)

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.

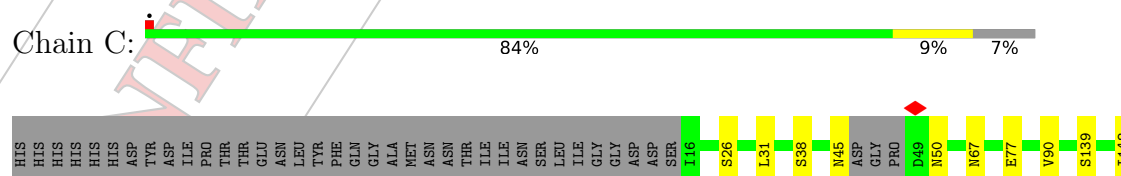
• Molecule 1: Scaffold protein D13

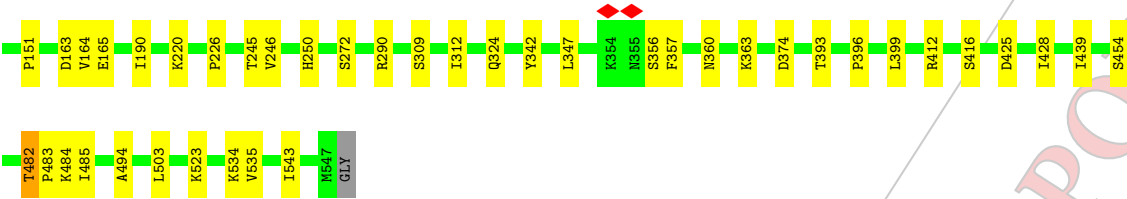


• Molecule 1: Scaffold protein D13



• Molecule 1: Scaffold protein D13





CONFIDENTIAL VALIDATION REPORT

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	173354	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	155000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	37.893	Depositor
Minimum map value	-21.522	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	5.0	Depositor
Map size (Å)	265.216, 265.216, 265.216	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.036, 1.036, 1.036	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	0.43	0/4302	0.47	0/5852
1	B	0.43	0/4302	0.47	0/5852
1	C	0.43	0/4302	0.47	0/5852
All	All	0.43	0/12906	0.47	0/17556

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4210	0	4167	26	0
1	B	4210	0	4167	24	0
1	C	4210	0	4167	22	0
All	All	12630	0	12501	72	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 3.

All (72) 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:C:165:GLU:HG3	1:C:485:ILE:HG12	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:GLU:HG3	1:B:485:ILE:HG12	1.75	0.67
1:A:165:GLU:HG3	1:A:485:ILE:HG12	1.76	0.66
1:C:164:VAL:HG21	1:C:484:LYS:HG2	1.77	0.65
1:A:164:VAL:HG21	1:A:484:LYS:HG2	1.77	0.65
1:B:164:VAL:HG21	1:B:484:LYS:HG2	1.77	0.65
1:A:250:HIS:HA	1:A:494:ALA:HB2	1.82	0.61
1:C:45:ASN:HB3	1:C:50:ASN:HB3	1.82	0.61
1:B:45:ASN:HB3	1:B:50:ASN:HB3	1.82	0.61
1:C:250:HIS:HA	1:C:494:ALA:HB2	1.82	0.61
1:B:250:HIS:HA	1:B:494:ALA:HB2	1.82	0.61
1:A:45:ASN:HB3	1:A:50:ASN:HB3	1.82	0.60
1:C:226:PRO:HB2	1:C:534:LYS:HE3	1.84	0.59
1:A:226:PRO:HB2	1:A:534:LYS:HE3	1.84	0.58
1:B:226:PRO:HB2	1:B:534:LYS:HE3	1.84	0.58
1:B:396:PRO:HD2	1:B:399:LEU:HD12	1.87	0.57
1:C:396:PRO:HD2	1:C:399:LEU:HD12	1.87	0.56
1:B:90:VAL:HG23	1:B:190:ILE:HB	1.88	0.56
1:A:396:PRO:HD2	1:A:399:LEU:HD12	1.87	0.55
1:A:90:VAL:HG23	1:A:190:ILE:HB	1.88	0.55
1:C:90:VAL:HG23	1:C:190:ILE:HB	1.88	0.54
1:A:139:SER:HB2	1:A:148:ILE:HG22	1.90	0.53
1:B:139:SER:HB2	1:B:148:ILE:HG22	1.90	0.53
1:A:360:ASN:HB3	1:A:363:LYS:HD3	1.91	0.53
1:C:139:SER:HB2	1:C:148:ILE:HG22	1.90	0.53
1:B:272:SER:HB3	1:B:290:ARG:HG3	1.91	0.53
1:A:324:GLN:O	1:A:363:LYS:NZ	2.42	0.52
1:C:324:GLN:O	1:C:363:LYS:NZ	2.42	0.52
1:B:31:LEU:HD23	1:B:220:LYS:HD2	1.92	0.52
1:B:324:GLN:O	1:B:363:LYS:NZ	2.42	0.52
1:C:272:SER:HB3	1:C:290:ARG:HG3	1.91	0.52
1:A:272:SER:HB3	1:A:290:ARG:HG3	1.91	0.52
1:B:360:ASN:HB3	1:B:363:LYS:HD3	1.91	0.52
1:C:360:ASN:HB3	1:C:363:LYS:HD3	1.91	0.52
1:A:356:SER:OG	1:A:357:PHE:N	2.44	0.51
1:B:439:ILE:HD12	1:B:523:LYS:HD2	1.93	0.51
1:A:31:LEU:HD23	1:A:220:LYS:HD2	1.92	0.51
1:C:31:LEU:HD23	1:C:220:LYS:HD2	1.92	0.51
1:C:356:SER:OG	1:C:357:PHE:N	2.44	0.51
1:A:439:ILE:HD12	1:A:523:LYS:HD2	1.93	0.51
1:C:439:ILE:HD12	1:C:523:LYS:HD2	1.93	0.50
1:A:77:GLU:HB2	1:A:151:PRO:HD3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:GLU:HB2	1:C:151:PRO:HD3	1.94	0.49
1:B:77:GLU:HB2	1:B:151:PRO:HD3	1.94	0.49
1:B:482:THR:HG22	1:B:483:PRO:HD2	1.96	0.47
1:A:347:LEU:HD11	1:A:412:ARG:HG2	1.98	0.46
1:A:482:THR:HG22	1:A:483:PRO:HD2	1.96	0.46
1:C:482:THR:HG22	1:C:483:PRO:HD2	1.96	0.46
1:B:356:SER:OG	1:B:357:PHE:N	2.44	0.46
1:C:535:VAL:HG22	1:C:543:ILE:HG22	1.98	0.46
1:A:535:VAL:HG22	1:A:543:ILE:HG22	1.98	0.45
1:B:322:SER:OG	1:B:327:ASP:OD1	2.29	0.45
1:B:535:VAL:HG22	1:B:543:ILE:HG22	1.98	0.45
1:B:347:LEU:HD11	1:B:412:ARG:HG2	1.98	0.45
1:C:347:LEU:HD11	1:C:412:ARG:HG2	1.98	0.45
1:A:67:ASN:HB2	1:A:163:ASP:OD1	2.17	0.44
1:C:67:ASN:HB2	1:C:163:ASP:OD1	2.17	0.44
1:C:246:VAL:HG13	1:C:503:LEU:HB2	2.00	0.44
1:A:120:ILE:HD12	1:A:120:ILE:HA	1.84	0.44
1:A:246:VAL:HG13	1:A:503:LEU:HB2	2.00	0.44
1:B:67:ASN:HB2	1:B:163:ASP:OD1	2.17	0.43
1:B:246:VAL:HG13	1:B:503:LEU:HB2	2.00	0.43
1:A:425:ASP:HB3	1:A:428:ILE:HD11	2.00	0.43
1:B:425:ASP:HB3	1:B:428:ILE:HD11	2.00	0.42
1:C:425:ASP:HB3	1:C:428:ILE:HD11	2.00	0.42
1:A:59:ARG:HA	1:A:59:ARG:HD2	1.84	0.42
1:B:120:ILE:HD12	1:B:120:ILE:HA	1.84	0.42
1:B:312:ILE:HG22	1:B:342:TYR:HB3	2.02	0.41
1:A:312:ILE:HG22	1:A:342:TYR:HB3	2.02	0.41
1:C:312:ILE:HG22	1:C:342:TYR:HB3	2.02	0.41
1:A:262:TYR:CZ	1:A:264:GLY:HA3	2.56	0.41
1:A:168:PHE:HB3	1:A:485:ILE:HD11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	525/569 (92%)	505 (96%)	20 (4%)	0	100	100
1	B	525/569 (92%)	505 (96%)	20 (4%)	0	100	100
1	C	525/569 (92%)	505 (96%)	20 (4%)	0	100	100
All	All	1575/1707 (92%)	1515 (96%)	60 (4%)	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	487/521 (94%)	478 (98%)	9 (2%)	59	75
1	B	487/521 (94%)	478 (98%)	9 (2%)	59	75
1	C	487/521 (94%)	478 (98%)	9 (2%)	59	75
All	All	1461/1563 (94%)	1434 (98%)	27 (2%)	61	75

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	SER
1	A	38	SER
1	A	245	THR
1	A	309	SER
1	A	374	ASP
1	A	393	THR
1	A	416	SER
1	A	454	SER
1	A	482	THR
1	B	26	SER
1	B	38	SER
1	B	245	THR
1	B	309	SER

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Mol	Chain	Res	Type
1	B	374	ASP
1	B	393	THR
1	B	416	SER
1	B	454	SER
1	B	482	THR
1	C	26	SER
1	C	38	SER
1	C	245	THR
1	C	309	SER
1	C	374	ASP
1	C	393	THR
1	C	416	SER
1	C	454	SER
1	C	482	THR

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 [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 ⓘ

There are no chain breaks in this entry.

CONFIDENTIAL VALIDATION REPORT

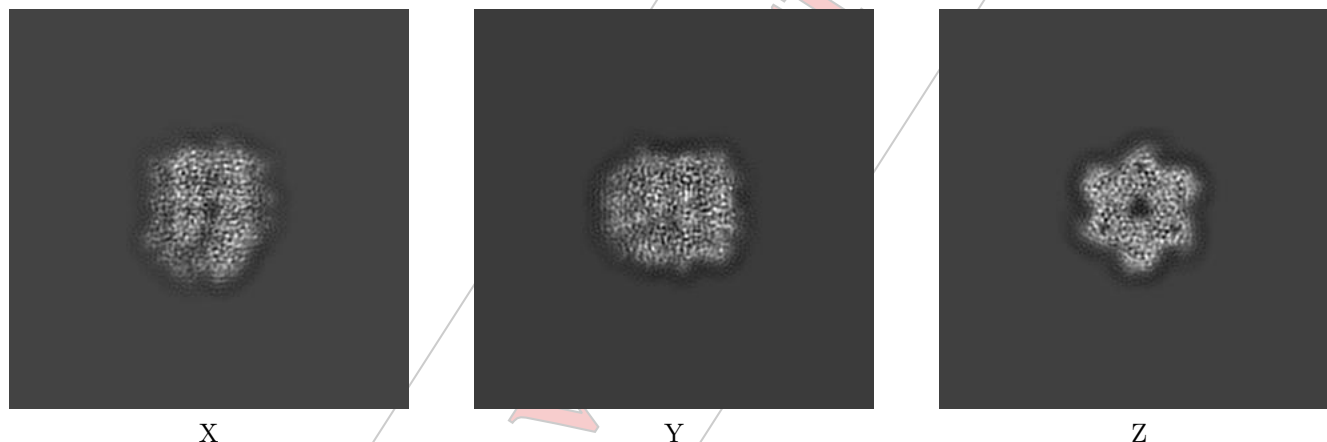
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31950. These allow visual inspection of the internal detail of the map and identification of artifacts.

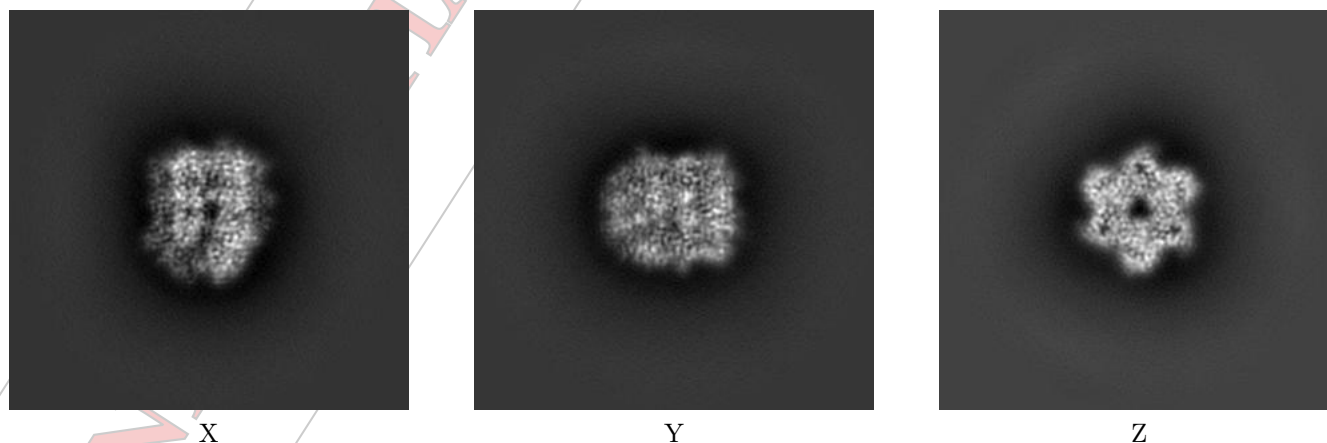
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



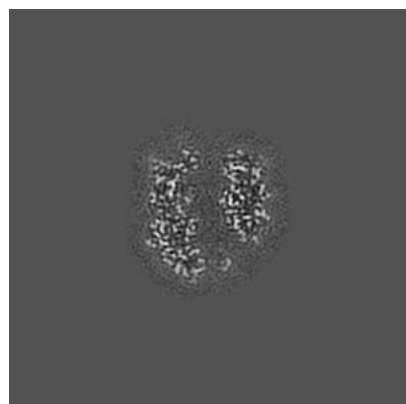
6.1.2 Raw map



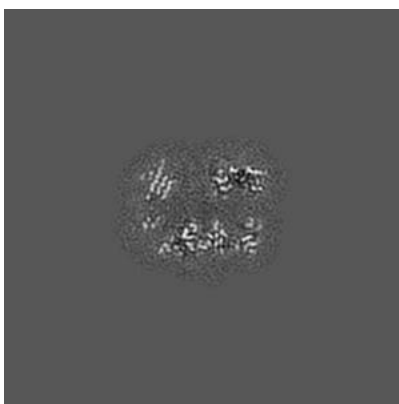
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

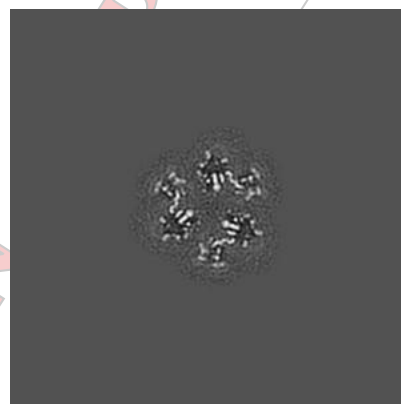
6.2.1 Primary map



X Index: 128

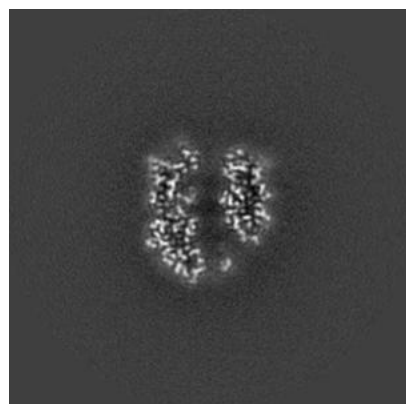


Y Index: 128

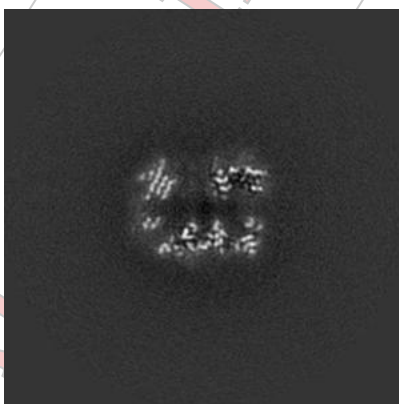


Z Index: 128

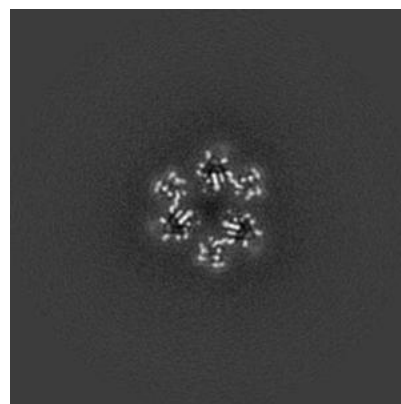
6.2.2 Raw map



X Index: 128



Y Index: 128

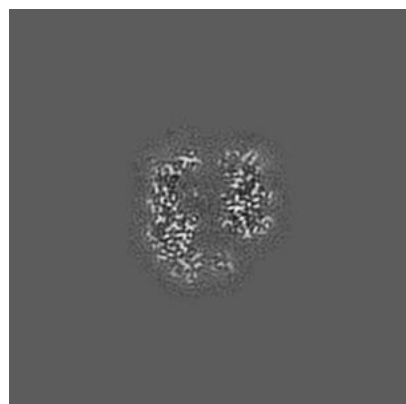


Z Index: 128

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

6.3 Largest variance slices [i](#)

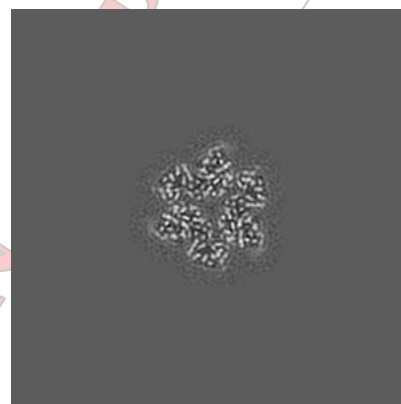
6.3.1 Primary map



X Index: 131

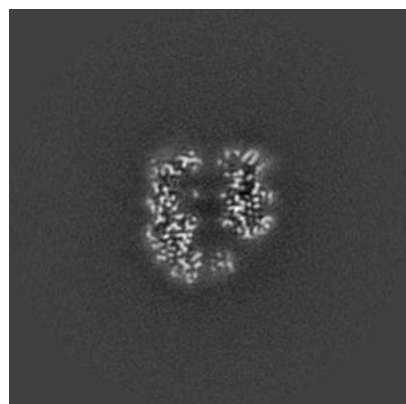


Y Index: 145

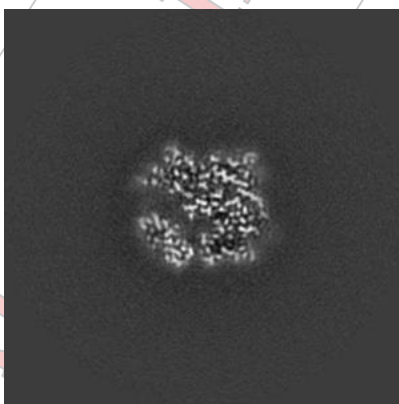


Z Index: 135

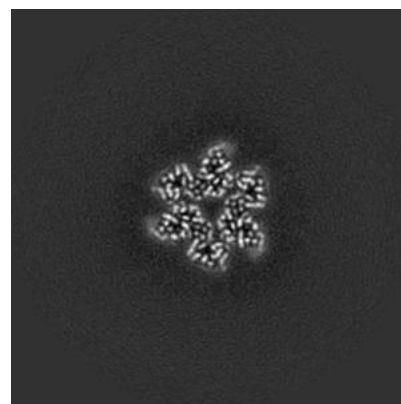
6.3.2 Raw map



X Index: 131



Y Index: 145

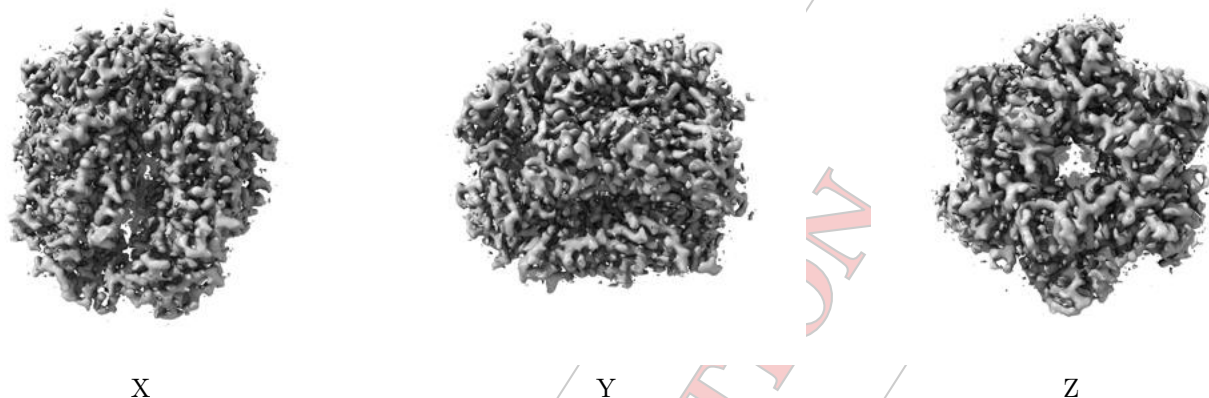


Z Index: 135

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

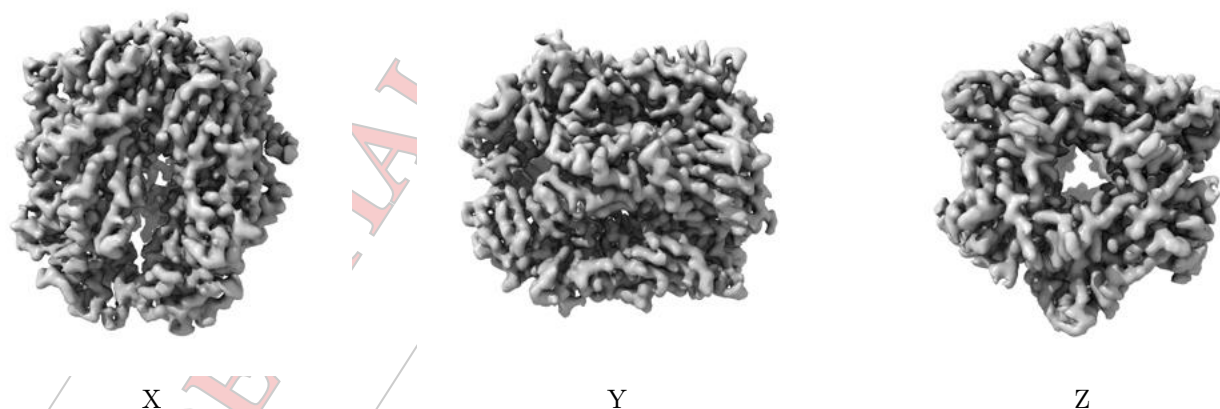
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 5.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



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

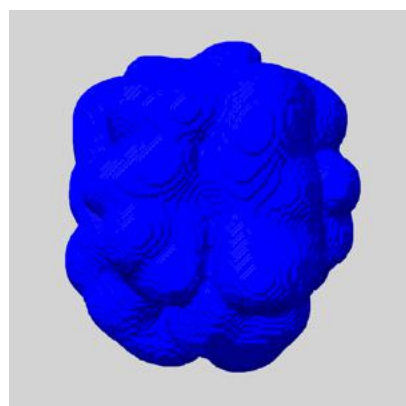
6.5 Mask visualisation [i](#)

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

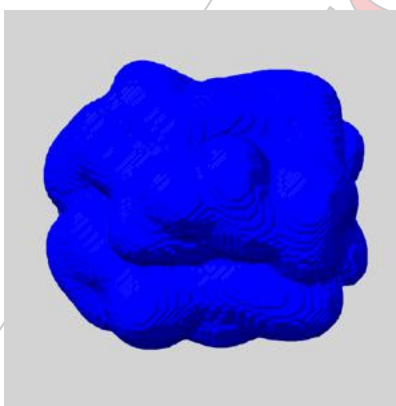
A mask typically either:

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

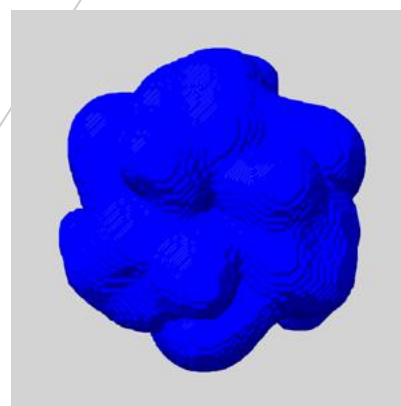
6.5.1 D_1300024105_em-mask-volume_P1.map.V2 [i](#)



X



Y

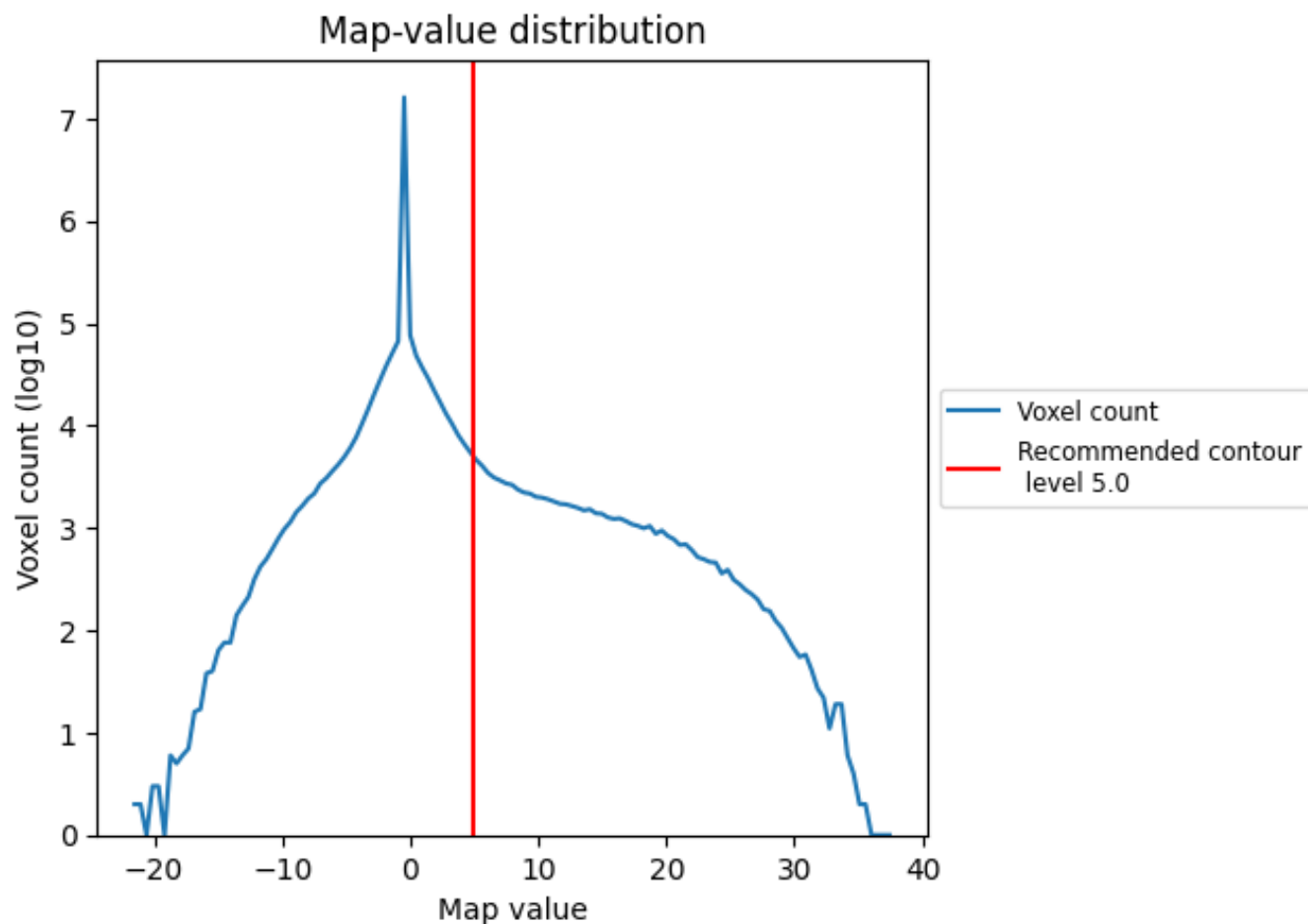


Z

7 Map analysis [i](#)

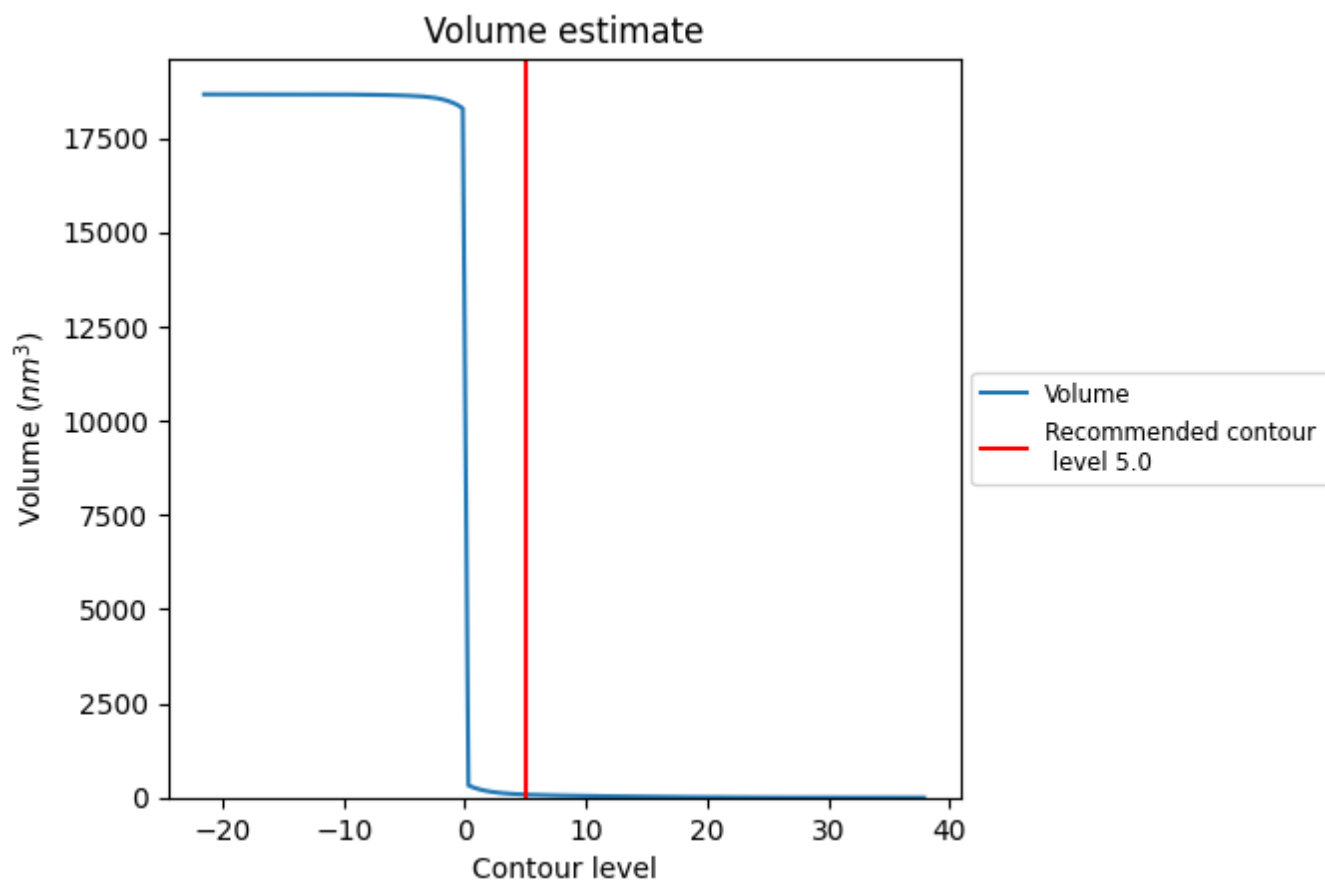
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

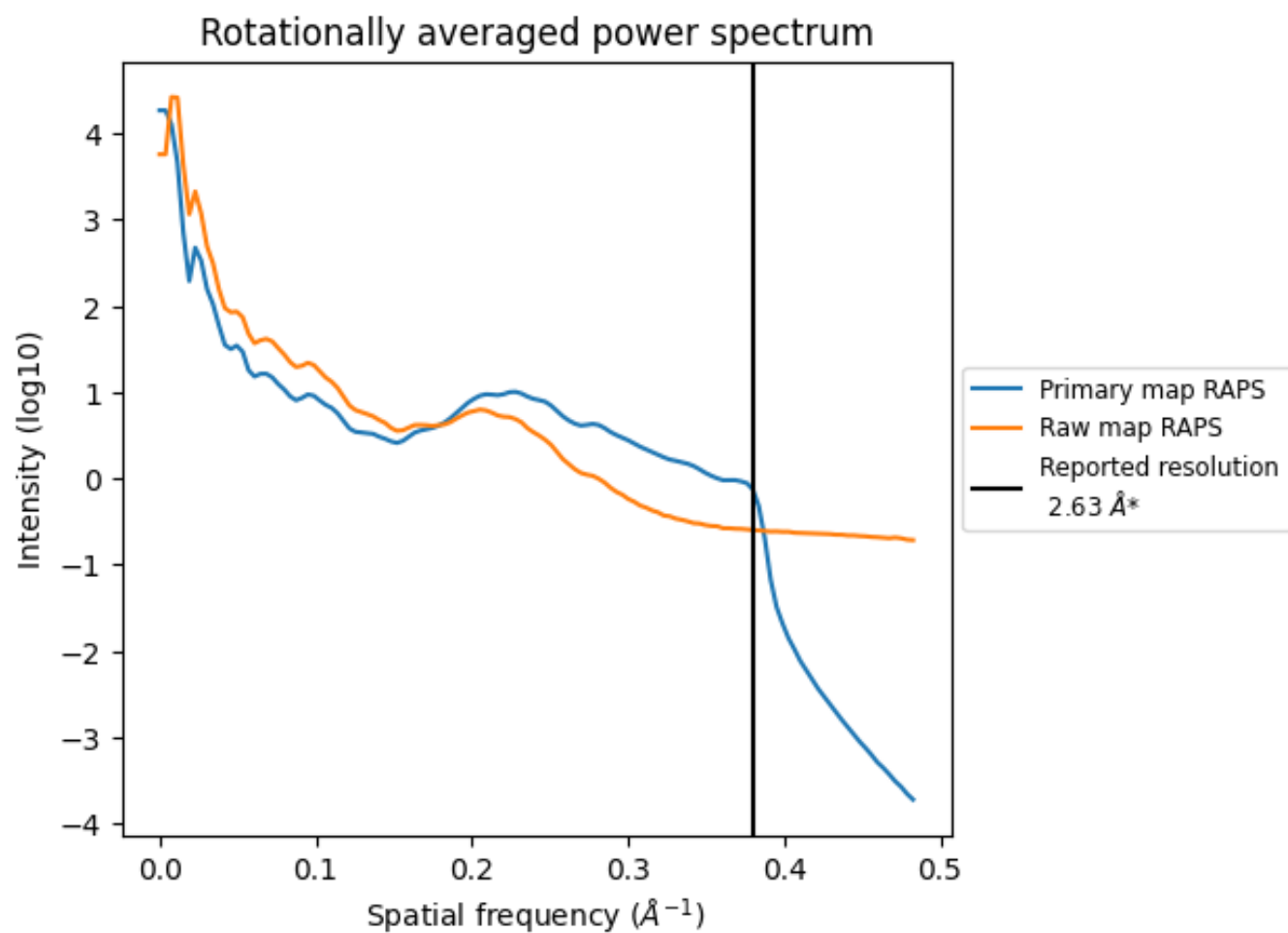
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 80 nm^3 ; this corresponds to an approximate mass of 72 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

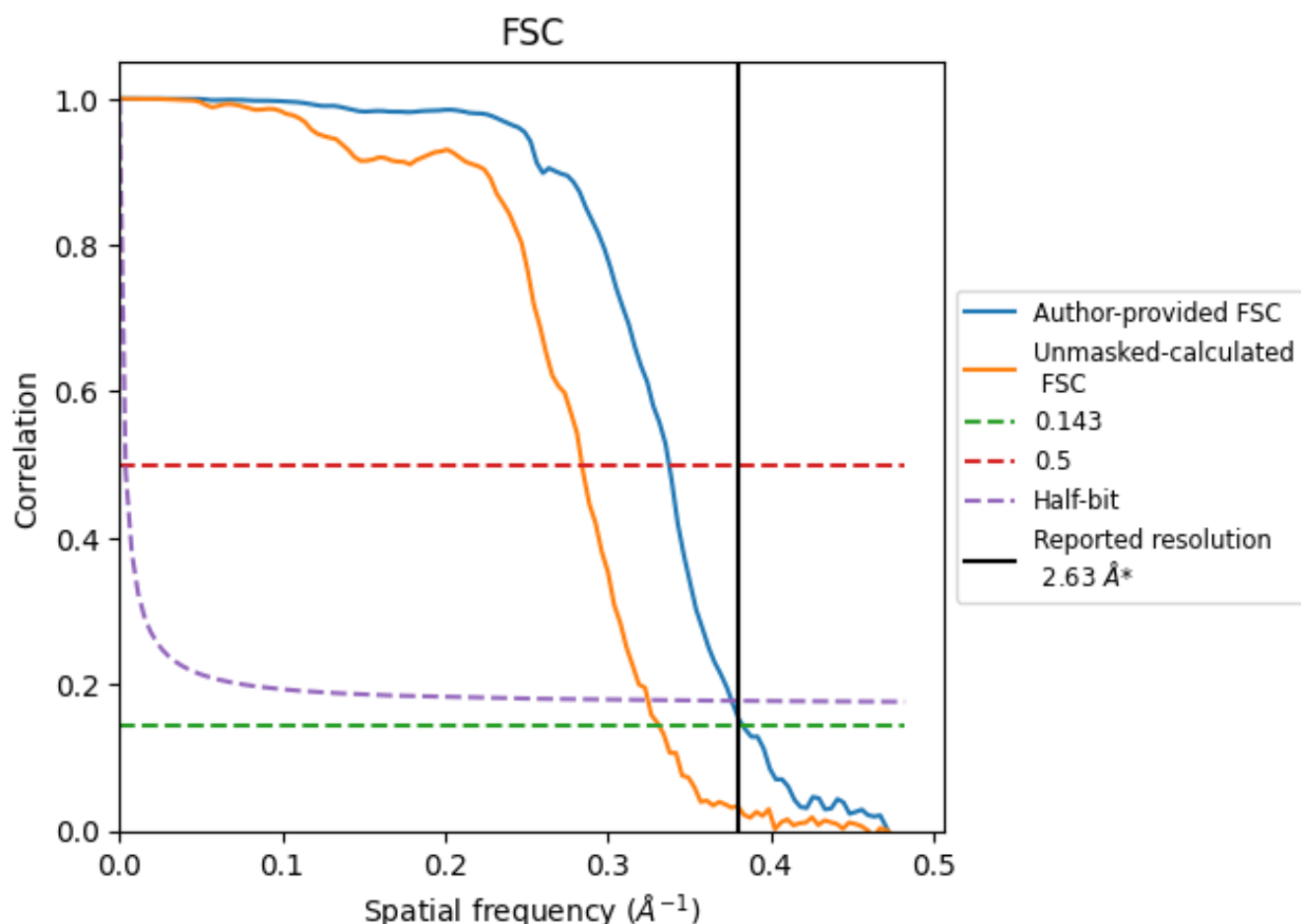


*Reported resolution corresponds to spatial frequency of 0.380 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.380 Å⁻¹

8.2 Resolution estimates [i](#)

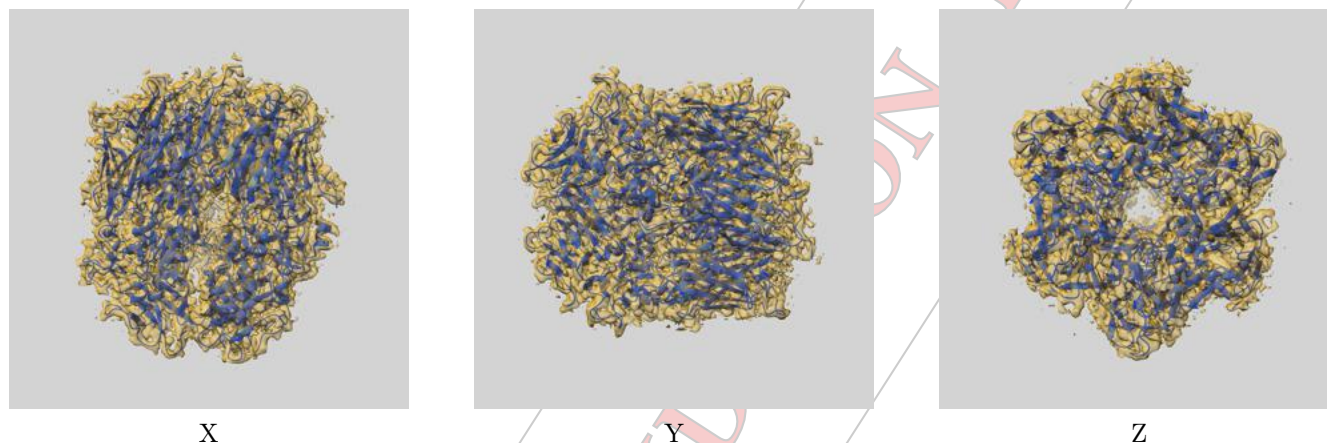
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.63	-	-
Author-provided FSC curve	2.61	2.96	2.66
Unmasked-calculated*	3.01	3.52	3.08

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.01 differs from the reported value 2.63 by more than 10 %

9 Map-model fit [i](#)

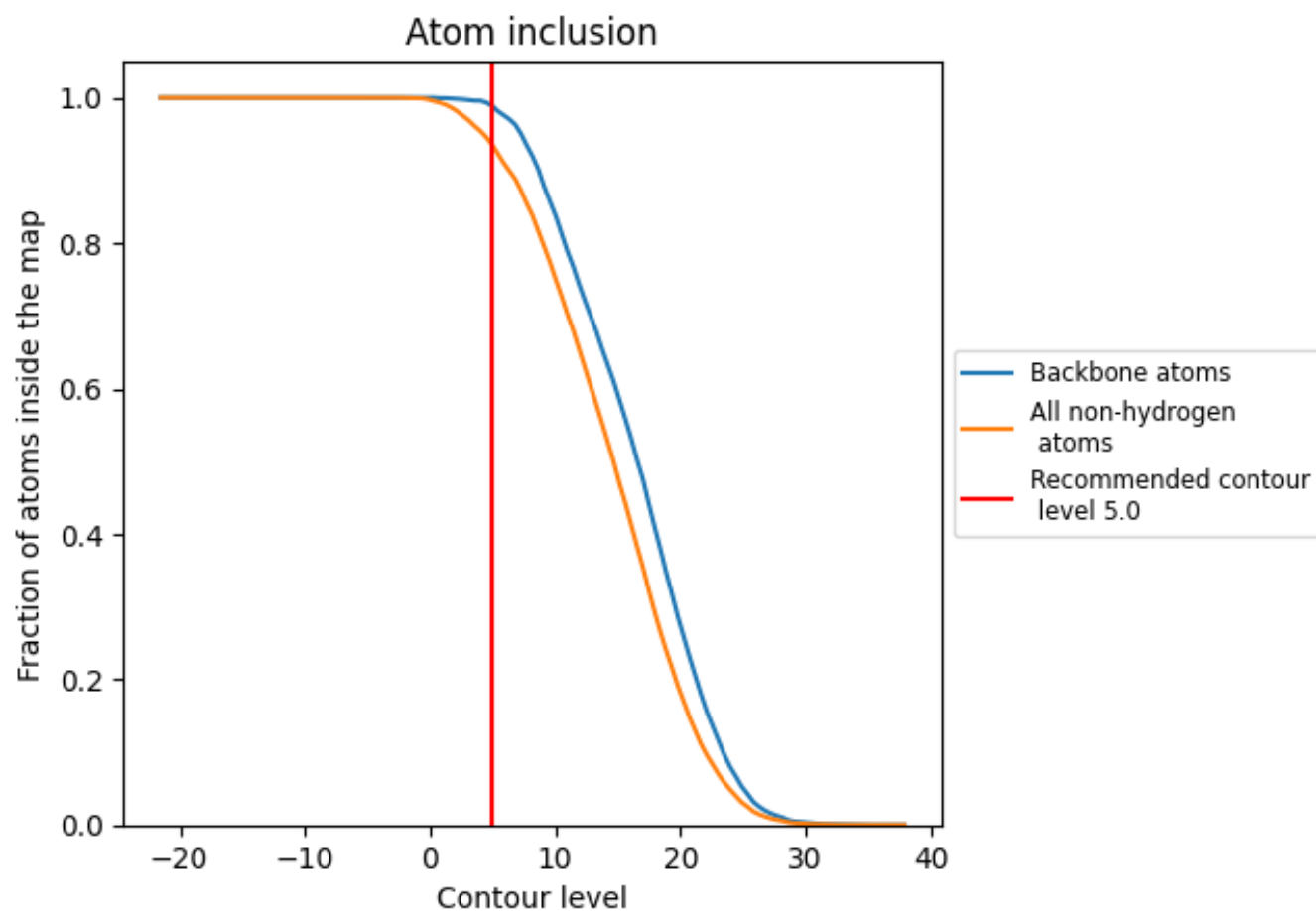
This section contains information regarding the fit between EMDB map EMD-31950 and PDB model 7VFE. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 5.0 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 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.