wwPDB EM Validation Summary Report (i)

Aug 7, 2026 – 12:04 AM JST

PDB ID	:	9L9P / pdb_00009l9p
EMDB ID	:	EMD-62912
Title	:	Cryo-EM structure of bacteriophage T1 tail tip complex
Authors	:	Chen, Y.; Liu, H.R.
Deposited on	:	2024-12-30
Resolution	:	4.30 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

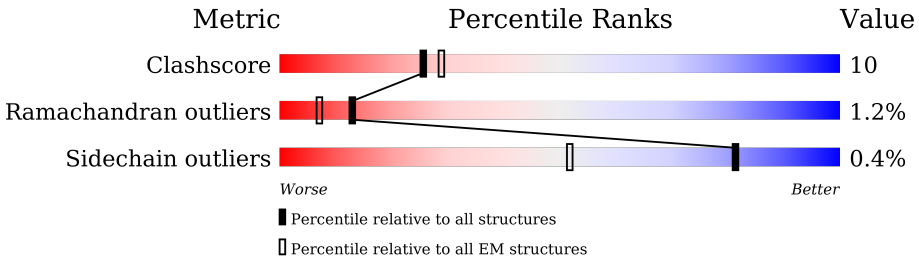
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

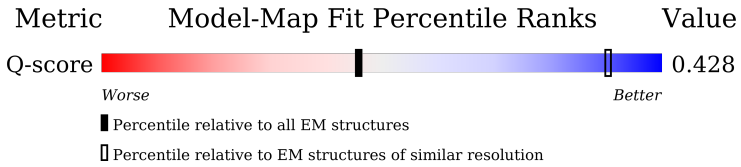
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4585 (3.80 - 4.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	S	1172	5% 50% 18% • 31%
2	A	199	• 34% •• 64%
3	J	260	• 70% 23% 7%
4	H	117	19% 81% 16% ••

Continued on next page...

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Mol	Chain	Length	Quality of chain
5	B	957	96%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 9999 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 Putative tail fiber protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	S	808	Total	C	N	O	S	0	0
			6408	4033	1095	1256	24		

- Molecule 2 is a protein called Putative tail assembly protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	72	Total	C	N	O	S	0	0
			504	324	80	92	8		

- Molecule 3 is a protein called Putative minor tail protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	242	Total	C	N	O	S	0	0
			1894	1196	326	361	11		

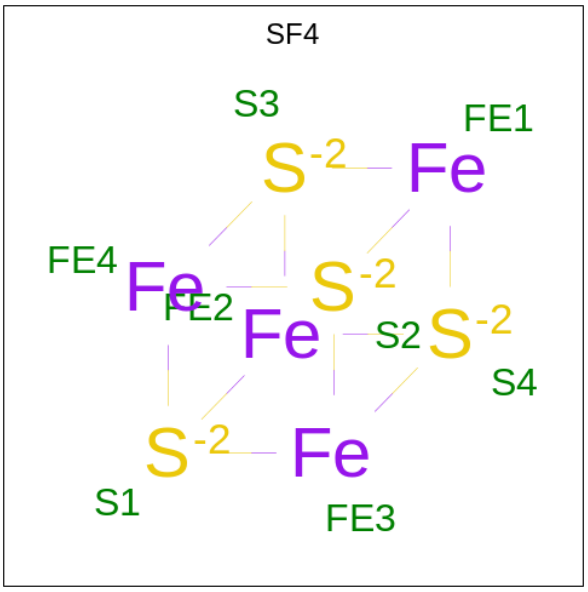
- Molecule 4 is a protein called Putative minor tail protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	116	Total	C	N	O	S	0	0
			902	570	151	174	7		

- Molecule 5 is a protein called Tape measure protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	36	Total	C	N	O	S	0	0
			283	174	49	56	4		

- Molecule 6 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



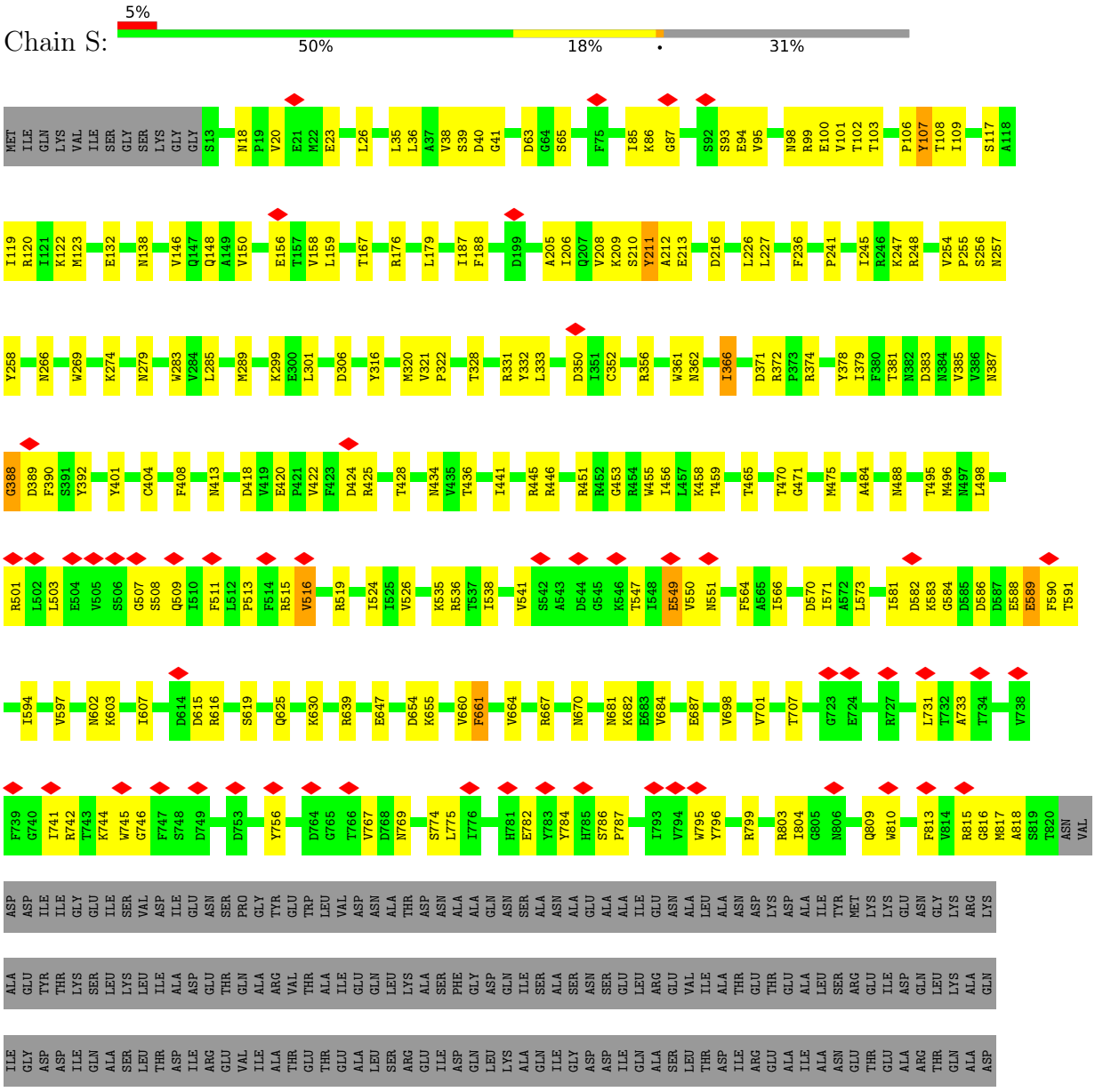
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
6	J	1	8	4	4	0

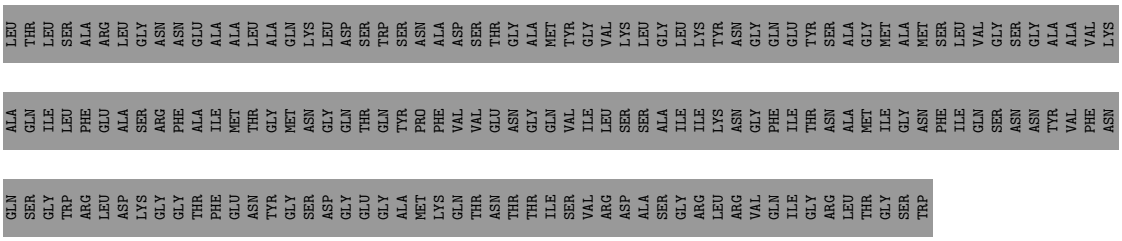
3 Residue-property plots (i)

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: Putative tail fiber protein

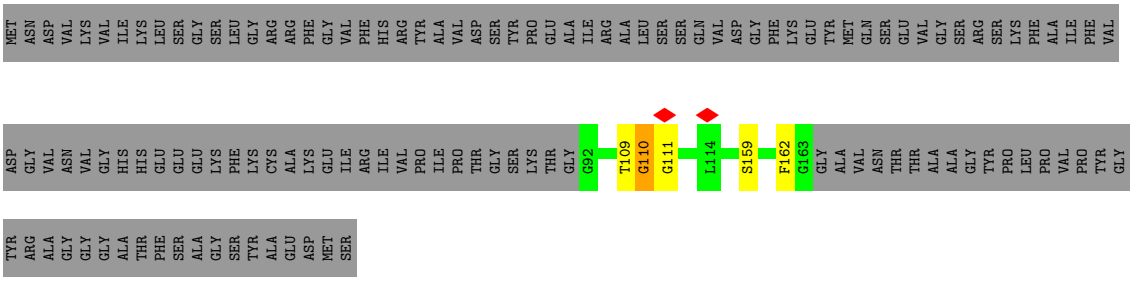
Chain S:





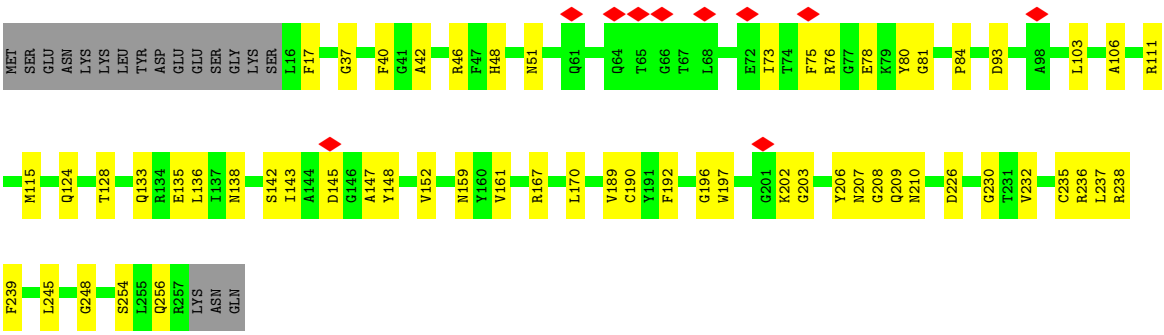
• Molecule 2: Putative tail assembly protein

Chain A:



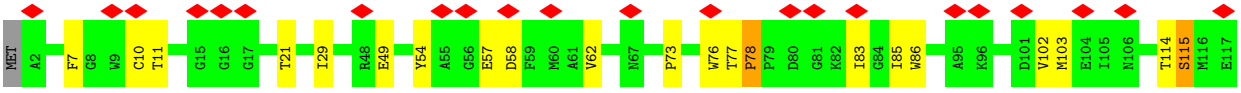
• Molecule 3: Putative minor tail protein

Chain J:



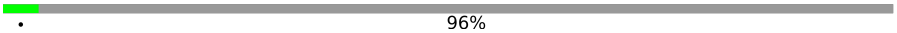
• Molecule 4: Putative minor tail protein

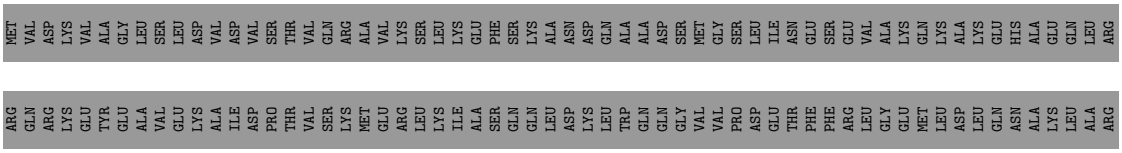
Chain H:

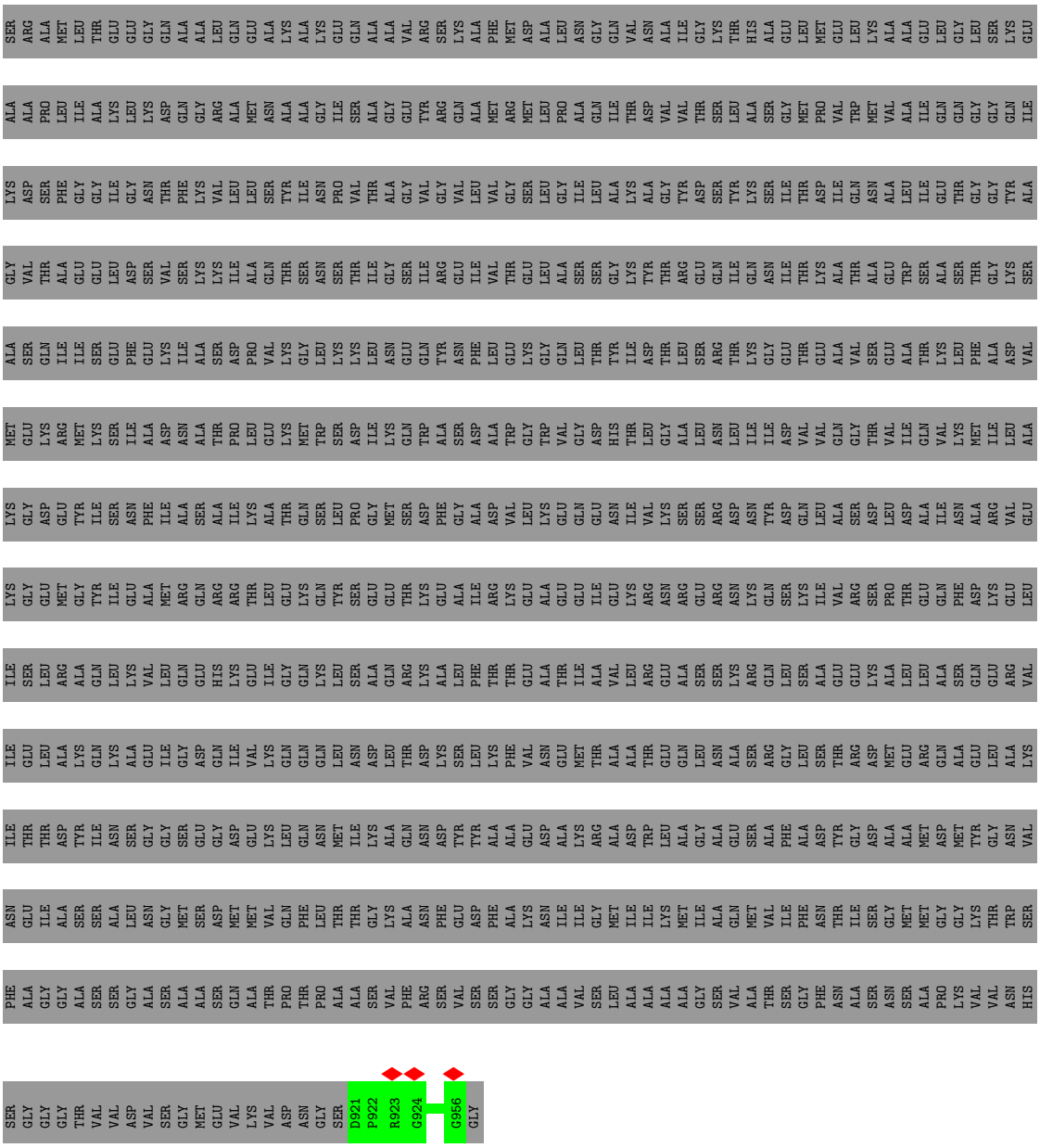


• Molecule 5: Tape measure protein

Chain B:






SER ARG ALA MET LEU THR GLU GLU GLY GLN ALA ALA LEU GLN GLU ALA LYS ALA LYS GLU GLN ALA ALA VAL ARG SER LYS ALA PHE MET ASP ALA LEU ASN GLY GLN VAL ASN ALA ILE GLY LYS THR HIS ALA GLU LEU MET GLU LEU LYS ALA ALA GLU LEU GLY LEU SER LYS GLU
ALA ALA PRO LEU ILE ALA LYS LEU LYS ASP GLN GLY ARG ALA MET ASN ALA ALA GLY ILE SER ALA GLY GLU TYR ARG GLN ALA MET ARG MET LEU PRO ALA GLN ILE THR ASP VAL VAL THR SER LEU ALA SER GLY MET PRO VAL TRP MET VAL ALA ALA ILE GLN GLN GLY GLY GLY ILE
LYS ASP SER PHE GLY GLY ILE GLY ASN THR PHE LYS VAL LEU LEU SER TYR ILE ASN PRO VAL THR ALA GLY VAL GLY VAL LEU VAL GLY SER LEU GLY ILE LEU ALA LYS ALA GLY TYR ASP SER TYR LYS SER ILE THR ASP ILE GLN ASN ALA ALA LEU ILE GLU THR GLY GLY LYS ALA
GLY VAL THR ALA GLU GLU LEU ASP SER VAL THR ILE LYS LYS ILE ALA GLN THR SER ASN SER THR ILE GLY SER ILE ARG GLU ILE VAL THR GLU LEU ALA SER SER GLY LYS TYR THR ARG GLU GLN ILE GLN ASN ILE THR LYS ALA ALA THR ALA GLU TRP SER ALA SER THR GLY LYS SER
ALA SER GLN ILE ILE SER GLU PHE GLU LYS ILE ALA SER ASP PRO VAL LYS GLY LEU LYS LYS LEU ASN GLU GLN LEU THR TYR ILE ASP THR LEU SER ARG THR LYS GLY GLU THR LEU ASN LEU ILE LYS ALA THR LYS LEU PHE ALA ASP VAL
MET GLU LYS ARG MET LYS SER ILE ALA ASP ASN ALA THR PRO LEU GLU LYS MET TRP SER ASP ILE LYS GLN TRP ALA SER ASP ALA TRP GLY TRP VAL GLY ASP HIS THR LEU GLY ALA LEU ASN LEU ILE ILE ASP VAL VAL GLN GLY THR VAL ILE GLN VAL LYS MET LEU ILE ALA
LYS GLY ASP GLU TYR ILE SER ASN PHE ILE ALA SER ALA ILE LYS ALA THR GLN SER LEU PRO GLY MET SER ASP PHE GLY ALA ASP VAL LEU LYS GLU GLN GLU ASN ILE VAL LYS SER SER ARG ASP ASN TYR ASP GLN LEU ALA SER ASP LEU ASP ALA ILE ASN ALA ARG VAL GLU
LYS GLY GLU MET GLY TYR ILE GLU ALA MET ARG GLN ARG ARG THR LEU GLU LYS GLN TYR SER GLU GLU THR LYS GLU ALA ILE ARG LYS GLU ALA GLU GLU ILE GLU LYS ARG ASN ARG GLU ARG ASN LYS GLN SER LYS ILE VAL ARG SER PRO THR GLU GLN PHE ASP LYS GLU LEU
ILE SER LEU ARG ALA GLN LEU LYS VAL LEU GLN GLU HIS LYS GLU ILE GLY GLN LYS LEU SER ALA GLN ARG LYS ALA LEU PHE THR THR GLU ALA THR ILE ALA VAL LEU ARG GLU ALA SER SER LYS ARG GLN LEU SER ALA GLU GLU LYS ALA LEU LEU LEU ALA SER GLN GLU ARG VAL
ILE GLU LEU ALA LYS GLN LYS ALA GLU ILE GLY ASP GLN ILE VAL LYS GLN GLN LEU GLN LEU ASN ASP LEU THR ASP LYS SER LEU LYS PHE VAL ASN GLU MET THR ALA ALA THR GLU GLN LEU ASN ALA SER ARG GLY LEU SER THR ARG ASP MET GLU ARG GLN ALA GLU LEU ALA LYS
ILE THR THR ASP TYR ILE ASN SER GLY GLY SER GLU GLY ASP GLU GLY GLN ASN ASP TYR TYR ALA ALA GLU ASP ALA LYS ALA ARG ALA ASP TRP LEU ALA GLY ALA GLU SER ALA PHE ALA ASP TYR GLY ASP ALA ALA MET ASP MET TYR GLY ASN VAL
ASN GLU ILE ALA SER SER GLY MET MET SER ASP MET MET VAL GLN PHE LEU THR THR GLY LYS ALA ASN PHE GLU ASP PHE ALA LYS ASN ILE ILE GLY MET ILE ILE ILE LYS MET ILE ALA GLN MET VAL ALA GLY MET ILE GLY LYS THR TRP SER
PHE ALA GLY GLY ALA SER SER GLY ALA SER ALA ALA SER VAL PHE ARG SER VAL SER SER GLY GLY ALA ALA ALA VAL SER LEU ALA ALA ALA ALA GLY SER VAL ALA THR SER GLY PHE ASN ALA SER ASN SER ALA PRO LYS VAL VAL ASN HIS
SER GLY GLY GLY THR VAL VAL ASP VAL SER GLY MET GLU VAL LYS VAL ASP ASN GLY SER D921 P922 R923 G924 G956 GLY

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	4467	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	32	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	25.300	Depositor
Minimum map value	-8.842	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.819	Depositor
Recommended contour level	4	Depositor
Map size (Å)	326.4, 326.4, 326.4	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4

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	S	0.17	0/6547	0.44	0/8898
2	A	0.13	0/513	0.36	0/688
3	J	0.14	0/1937	0.40	0/2621
4	H	0.15	0/925	0.41	0/1254
5	B	0.12	0/286	0.32	0/378
All	All	0.16	0/10208	0.43	0/13839

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

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	S	6408	0	6224	149	0
2	A	504	0	508	3	0
3	J	1894	0	1836	41	0
4	H	902	0	854	14	0
5	B	283	0	276	0	0
6	J	8	0	0	1	0
All	All	9999	0	9698	203	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 10.

The worst 5 of 203 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:S:392:TYR:HB2	3:J:161:VAL:HB	1.49	0.92
1:S:381:THR:HG23	1:S:383:ASP:H	1.44	0.83
1:S:741:ILE:HG12	1:S:787:PRO:HB3	1.64	0.80
3:J:196:GLY:HA3	3:J:202:LYS:HD3	1.66	0.77
1:S:498:LEU:HD11	1:S:516:VAL:HB	1.68	0.74

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	S	806/1172 (69%)	708 (88%)	88 (11%)	10 (1%)	10 42
2	A	70/199 (35%)	66 (94%)	3 (4%)	1 (1%)	9 39
3	J	240/260 (92%)	214 (89%)	24 (10%)	2 (1%)	16 52
4	H	114/117 (97%)	101 (89%)	11 (10%)	2 (2%)	6 33
5	B	34/957 (4%)	32 (94%)	2 (6%)	0	100 100
All	All	1264/2705 (47%)	1121 (89%)	128 (10%)	15 (1%)	13 42

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	S	150	VAL
1	S	589	GLU
1	S	388	GLY
3	J	51	ASN
1	S	516	VAL

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	S	713/1001 (71%)	710 (100%)	3 (0%)	84 82
2	A	51/150 (34%)	51 (100%)	0	100 100
3	J	202/219 (92%)	201 (100%)	1 (0%)	81 81
4	H	98/99 (99%)	98 (100%)	0	100 100
5	B	31/766 (4%)	31 (100%)	0	100 100
All	All	1095/2235 (49%)	1091 (100%)	4 (0%)	81 82

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

Mol	Chain	Res	Type
1	S	107	TYR
1	S	211	TYR
1	S	321	VAL
3	J	93	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	S	760	GLN
3	J	120	ASN
4	H	14	GLN
3	J	138	ASN
3	J	256	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	SF4	J	301	3	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	SF4	J	301	3	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

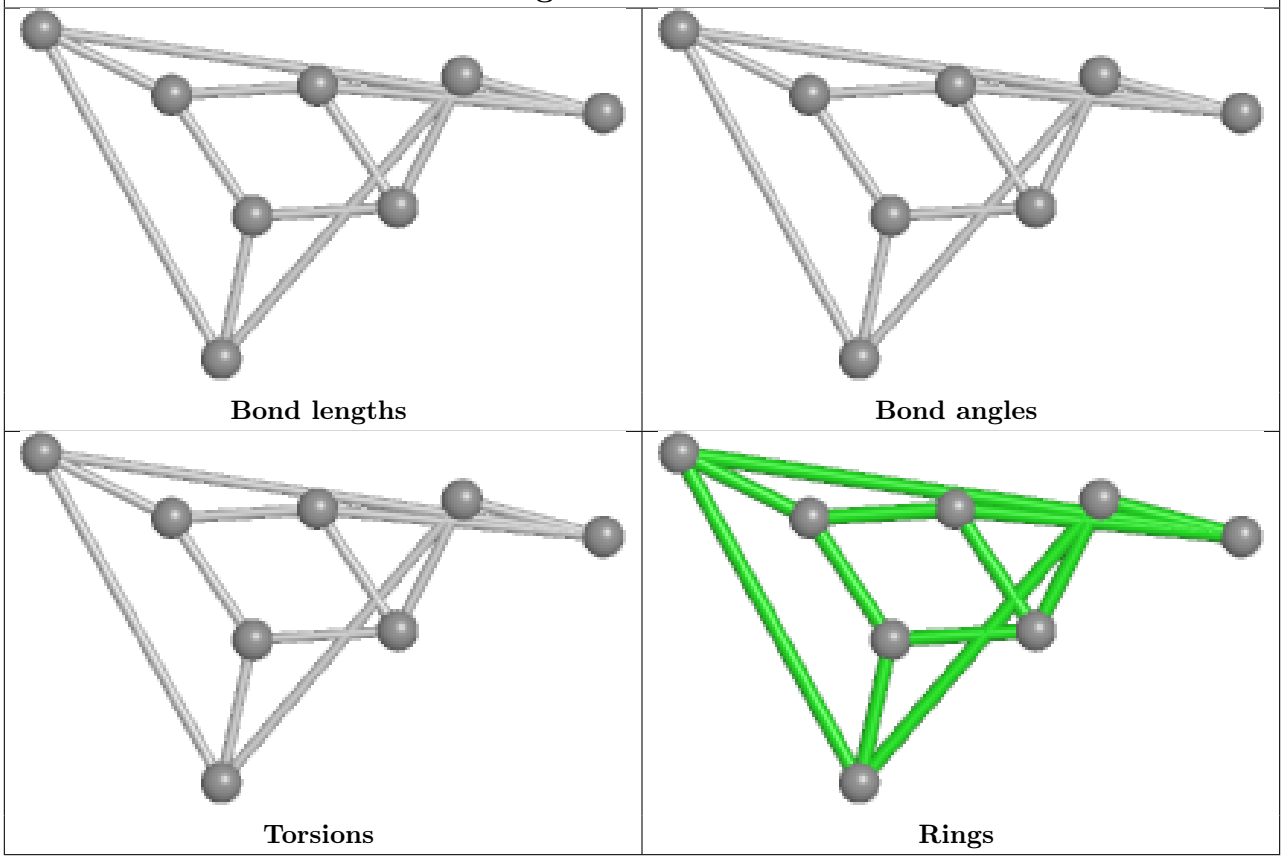
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	J	301	SF4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand SF4 J 301



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

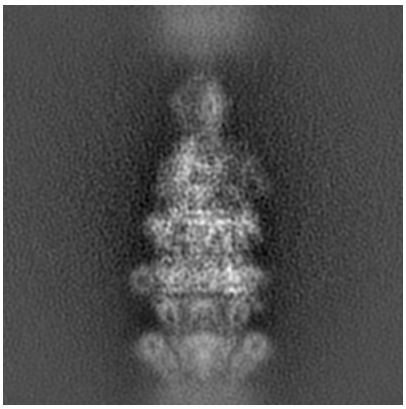
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-62912. These allow visual inspection of the internal detail of the map and identification of artifacts.

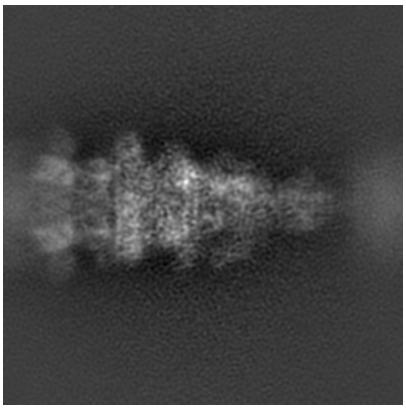
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

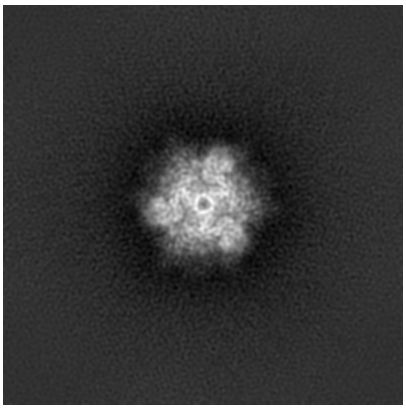
6.1.1 Primary map



X

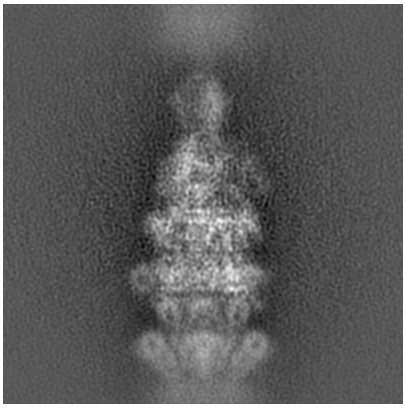


Y

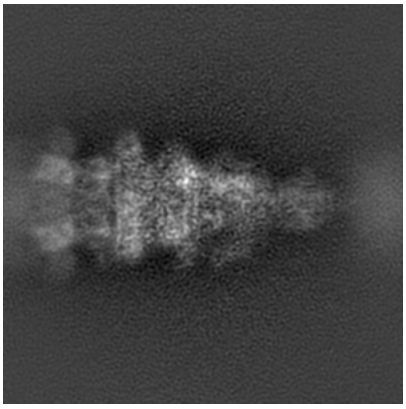


Z

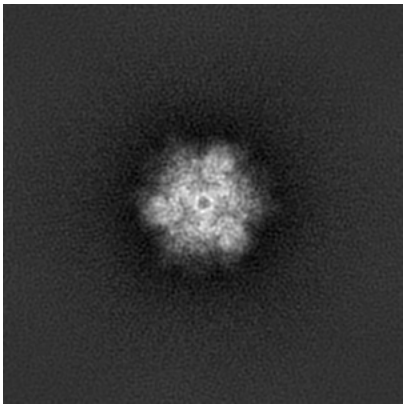
6.1.2 Raw map



X



Y

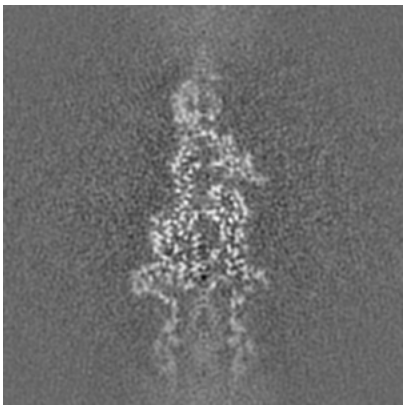


Z

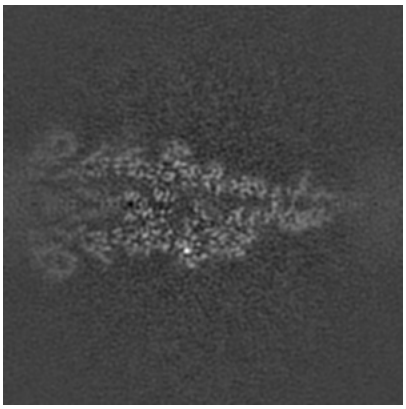
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

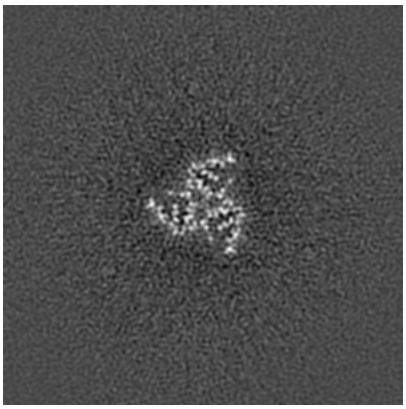
6.2.1 Primary map



X Index: 120

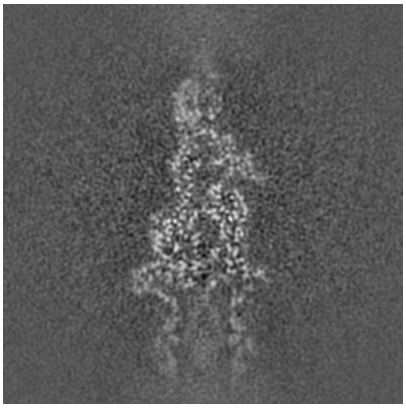


Y Index: 120

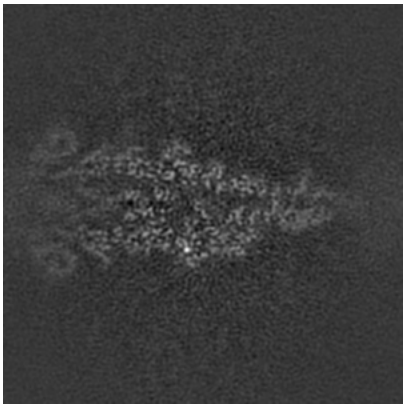


Z Index: 120

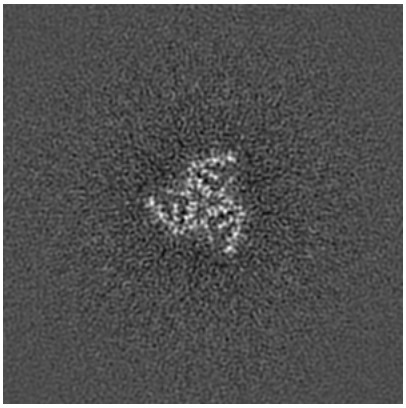
6.2.2 Raw map



X Index: 120



Y Index: 120

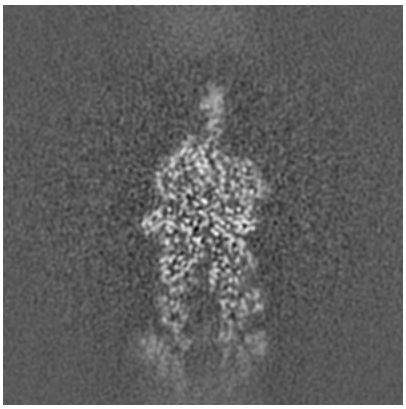


Z Index: 120

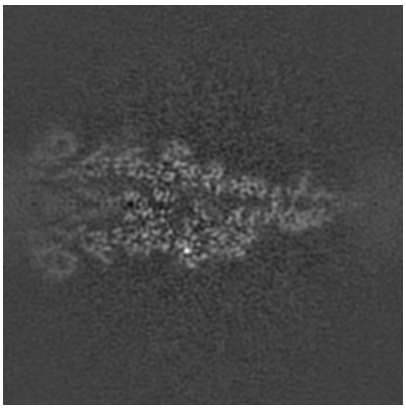
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

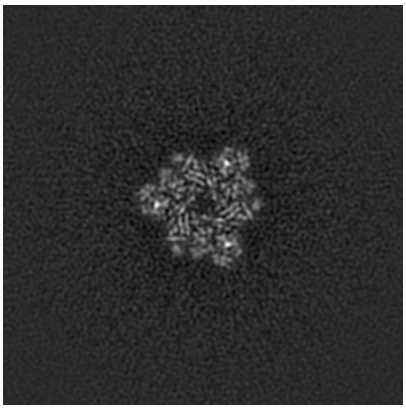
6.3.1 Primary map



X Index: 132

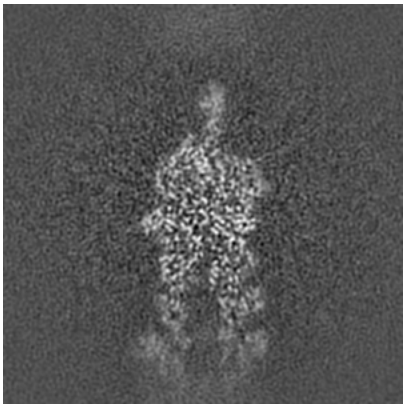


Y Index: 120

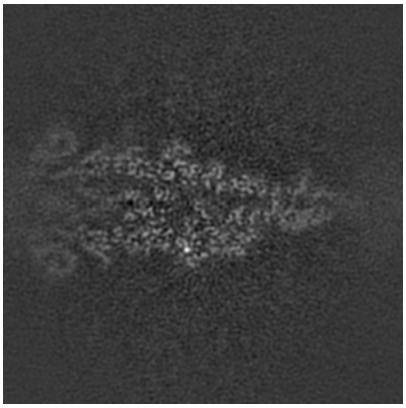


Z Index: 109

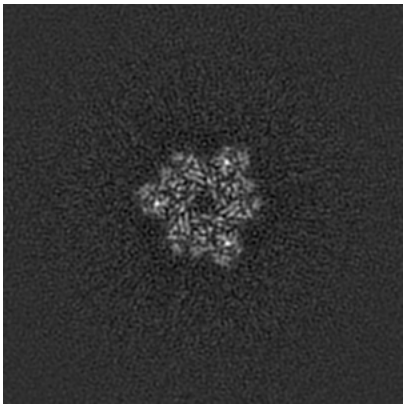
6.3.2 Raw map



X Index: 132



Y Index: 120

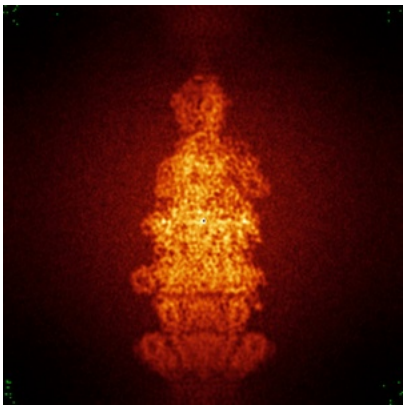


Z Index: 109

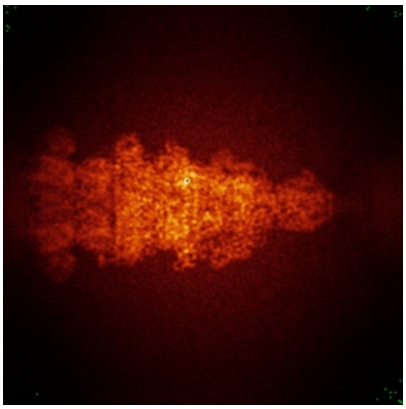
The images above show the largest variance slices of the map in three orthogonal directions.

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

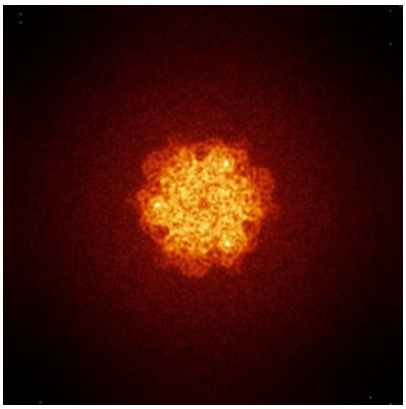
6.4.1 Primary map



X

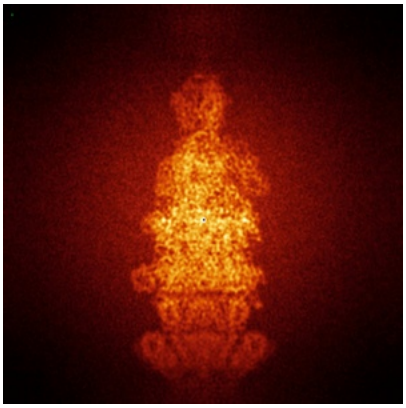


Y

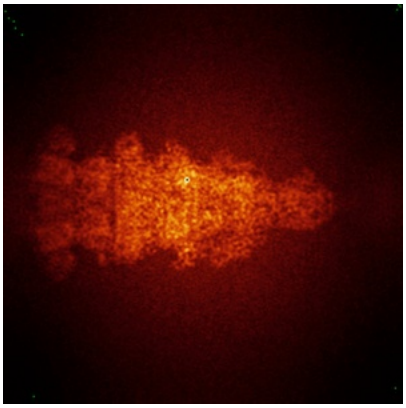


Z

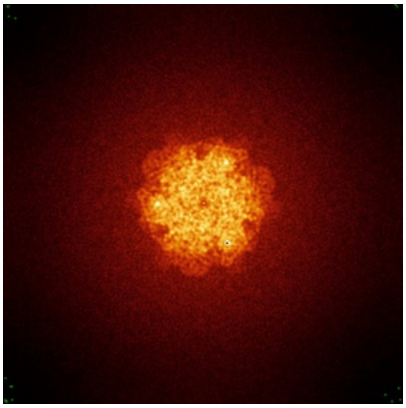
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

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

6.5.2 Raw map

X Y Z

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

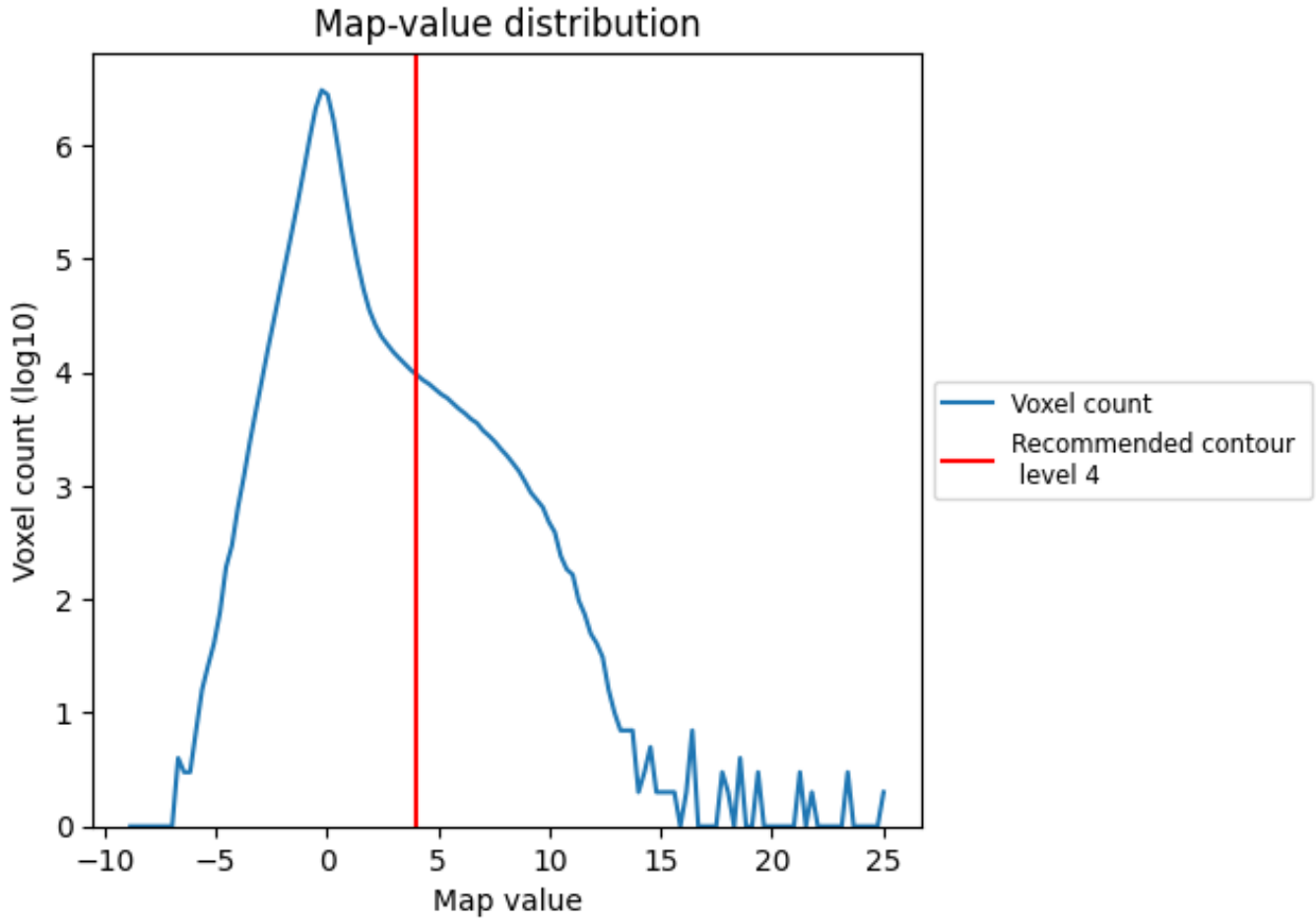
6.6 Mask visualisation (i)

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

7 Map analysis

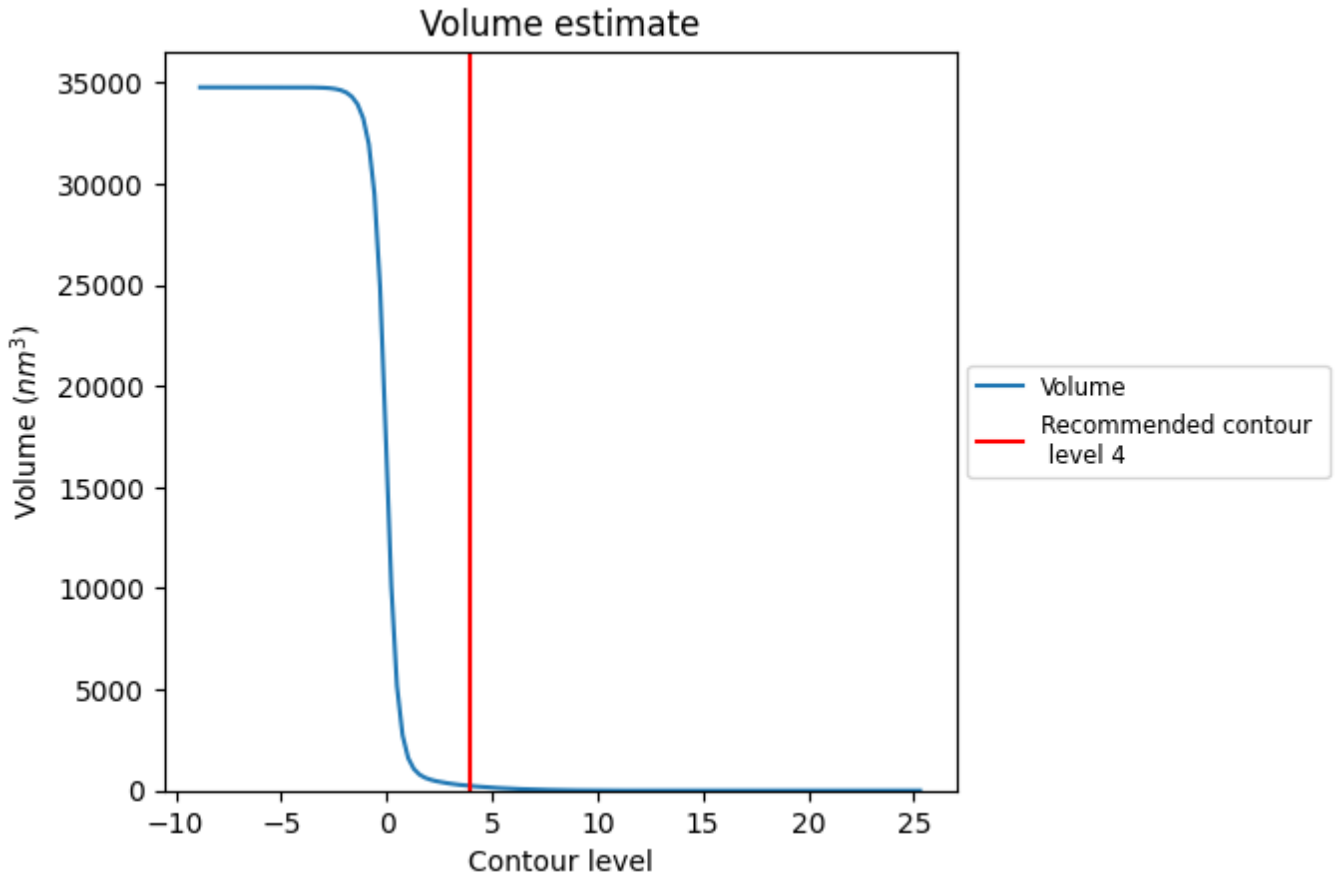
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

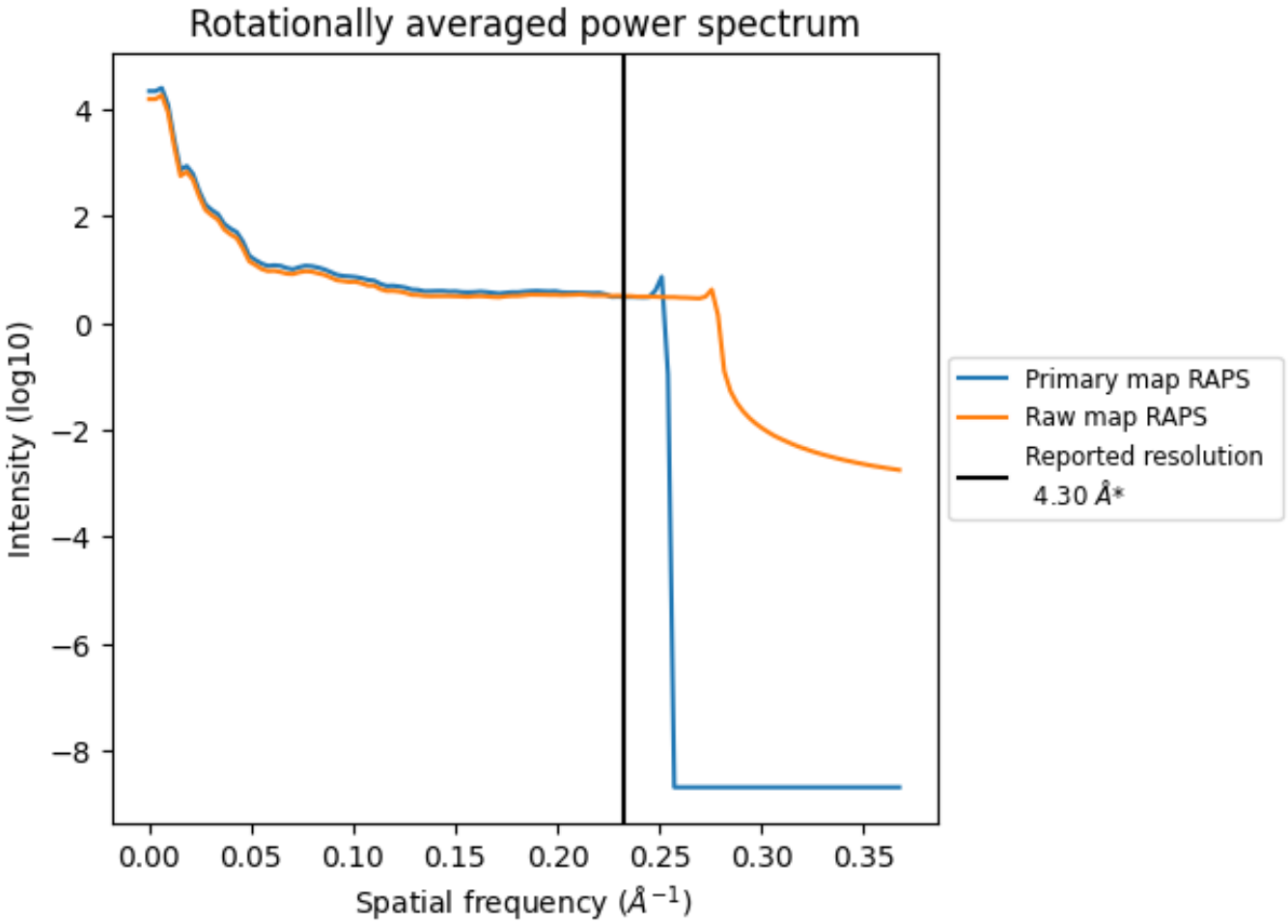
7.2 Volume estimate (i)



The volume at the recommended contour level is 226 nm^3; this corresponds to an approximate mass of 204 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)

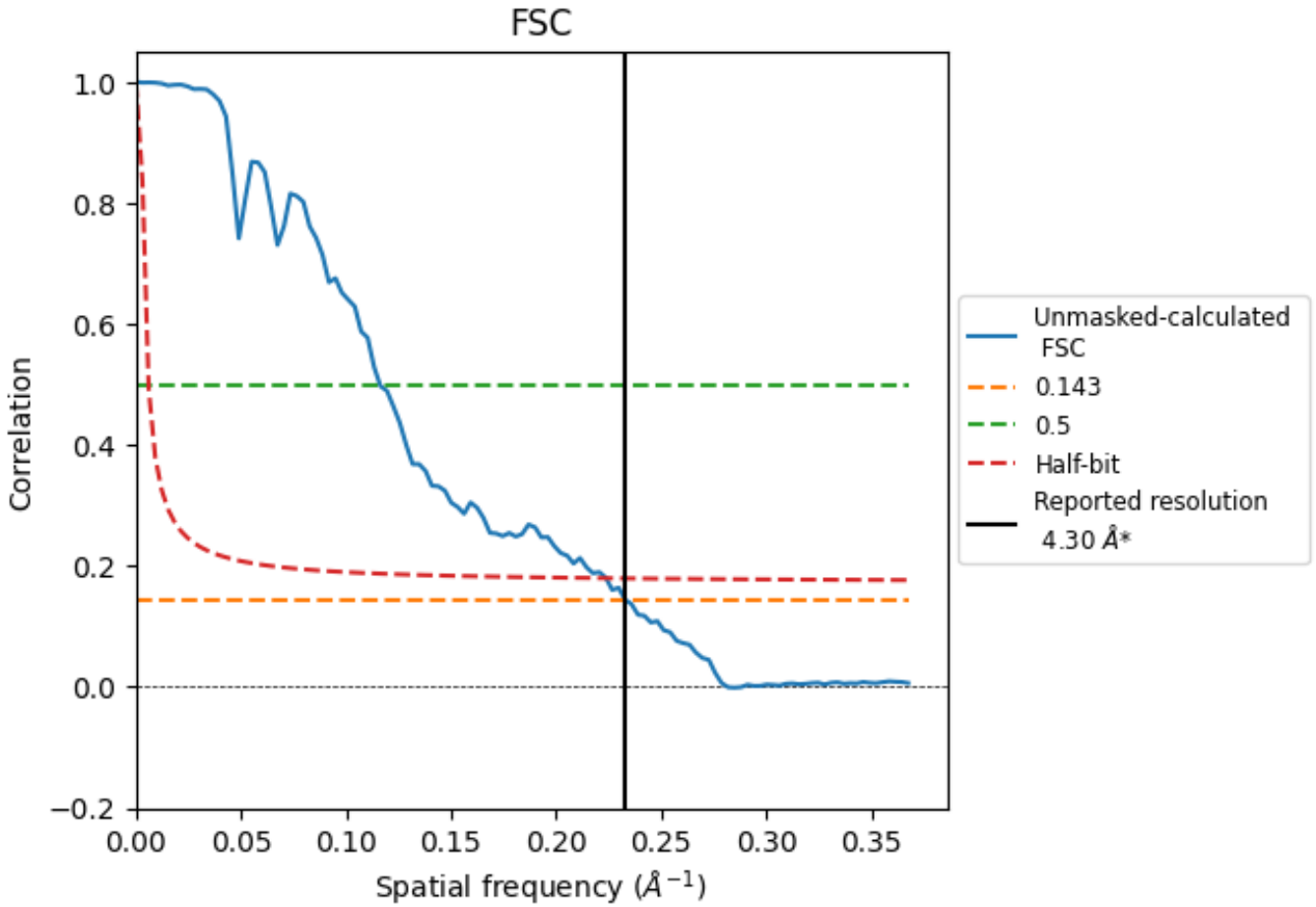


*Reported resolution corresponds to spatial frequency of 0.233 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.233 Å^{-1}

8.2 Resolution estimates (i)

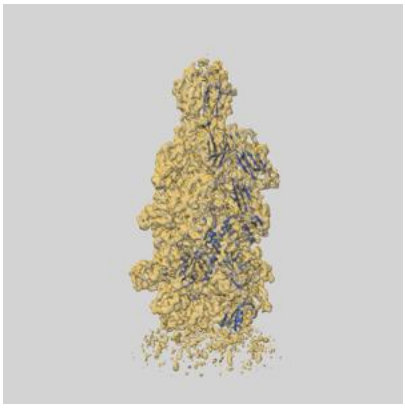
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.29	8.61	4.47

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

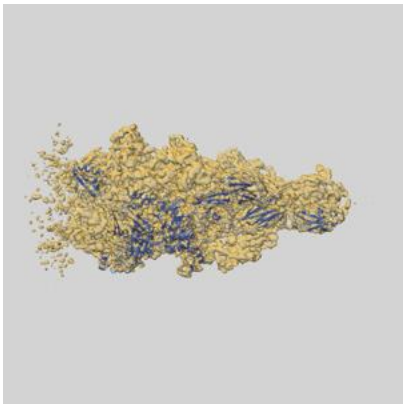
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-62912 and PDB model 9L9P. Per-residue inclusion information can be found in section 3 on page 6.

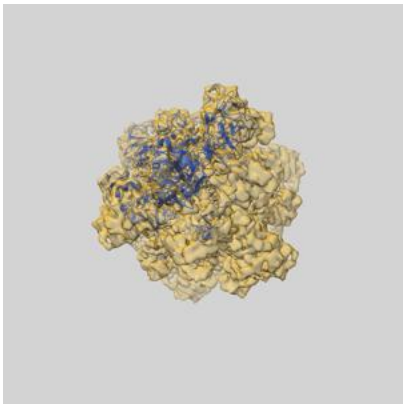
9.1 Map-model overlay



X



Y



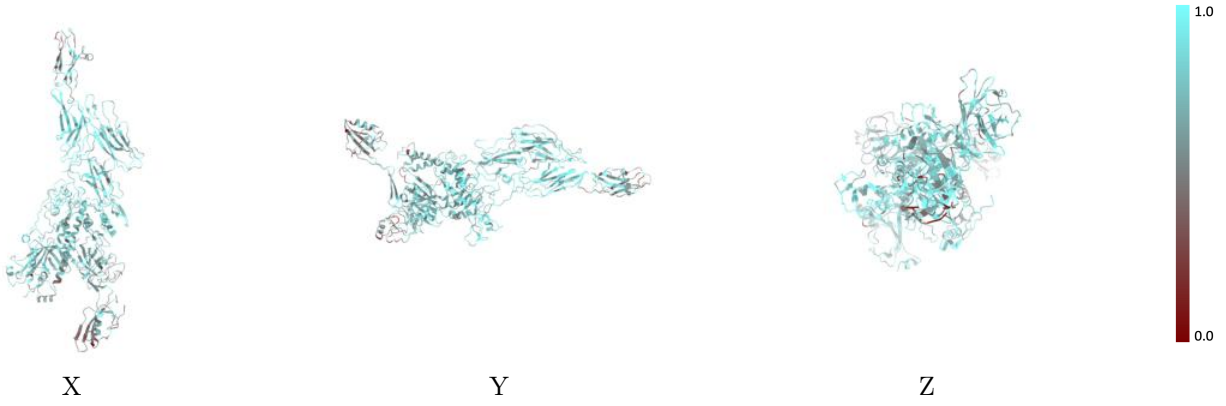
Z

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 Q-score mapped to coordinate model (i)

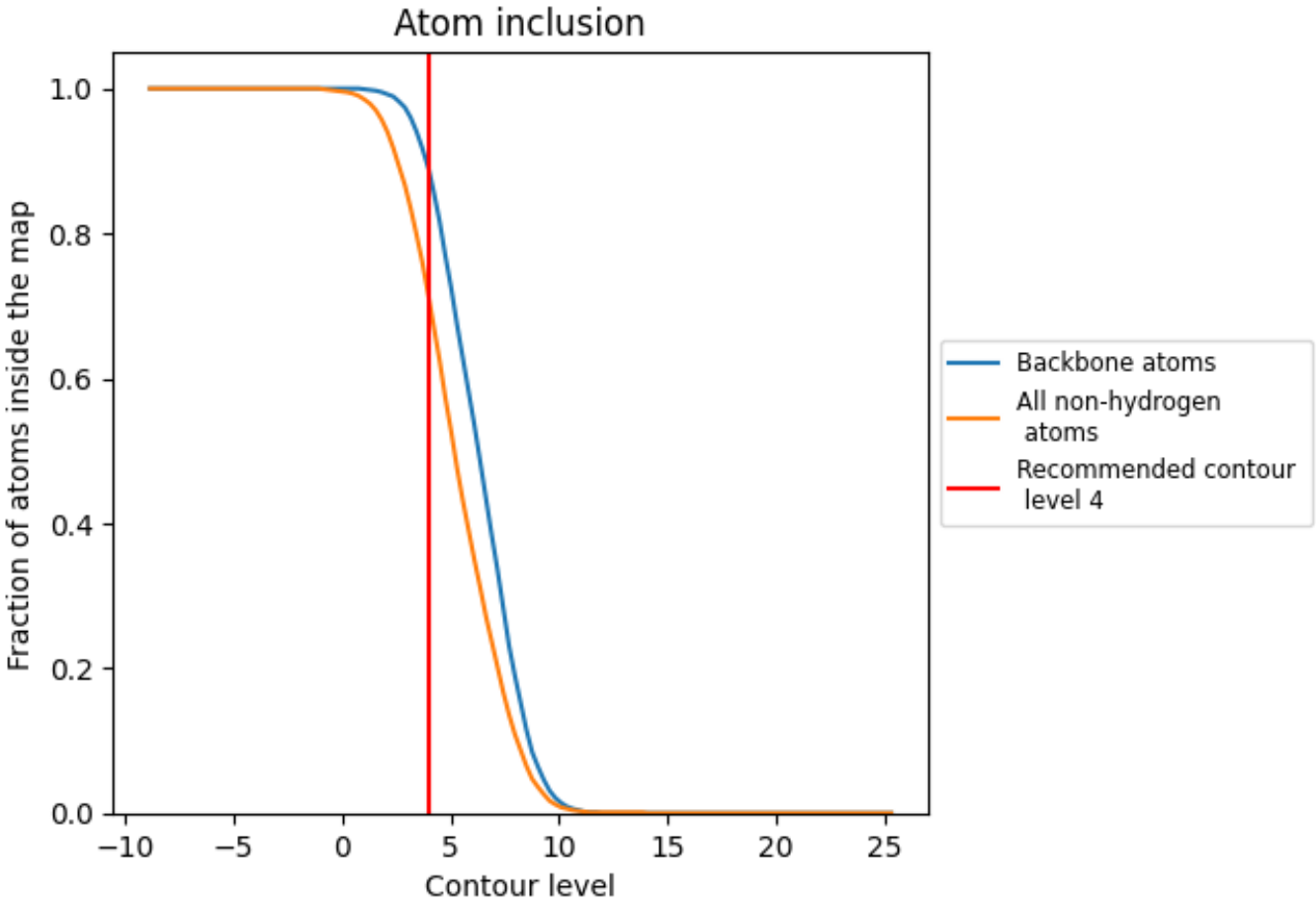
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7110	0.4280
A	0.7150	0.4840
B	0.6790	0.4610
H	0.5660	0.4340
J	0.7290	0.4320
S	0.7270	0.4210