



wwPDB EM Validation Summary Report ⓘ

Mar 29, 2026 – 11:16 AM UTC

PDB ID : 7V5K / pdb_00007v5k
EMDB ID : EMD-31726
Title : MERS S ectodomain trimer in complex with neutralizing antibody 0722 (state 1)
Authors : Wang, X.; Zhao, J.; Wang, Z.; Zeng, J.; Zhang, S.; Wang, Y.
Deposited on : 2021-08-17
Resolution : 2.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

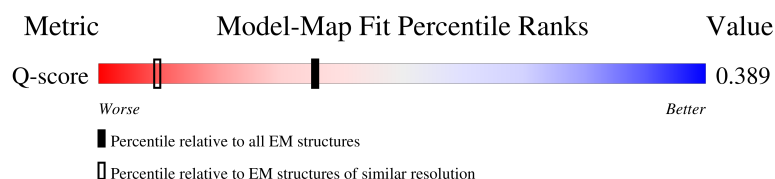
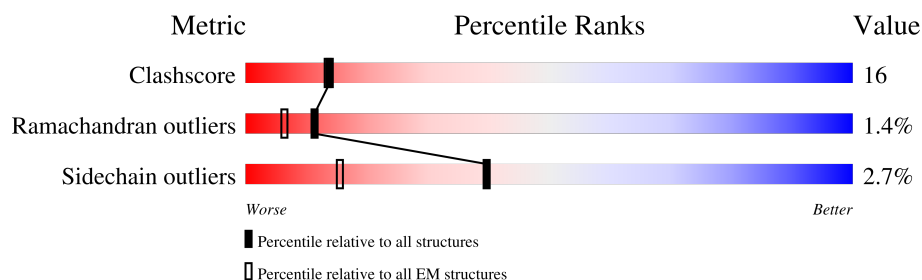
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.80 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.



Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	212	 50% 46% .
2	H	212	 51% 44% .
3	E	222	 64% 35% .
3	G	222	 65% 34%
3	I	222	 64% 33% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 36369 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1141	Total	C	N	O	S	0	0
			8836	5616	1462	1707	51		
1	B	1141	Total	C	N	O	S	0	0
			8836	5616	1462	1707	51		
1	C	1141	Total	C	N	O	S	1	0
			8836	5615	1463	1707	51		

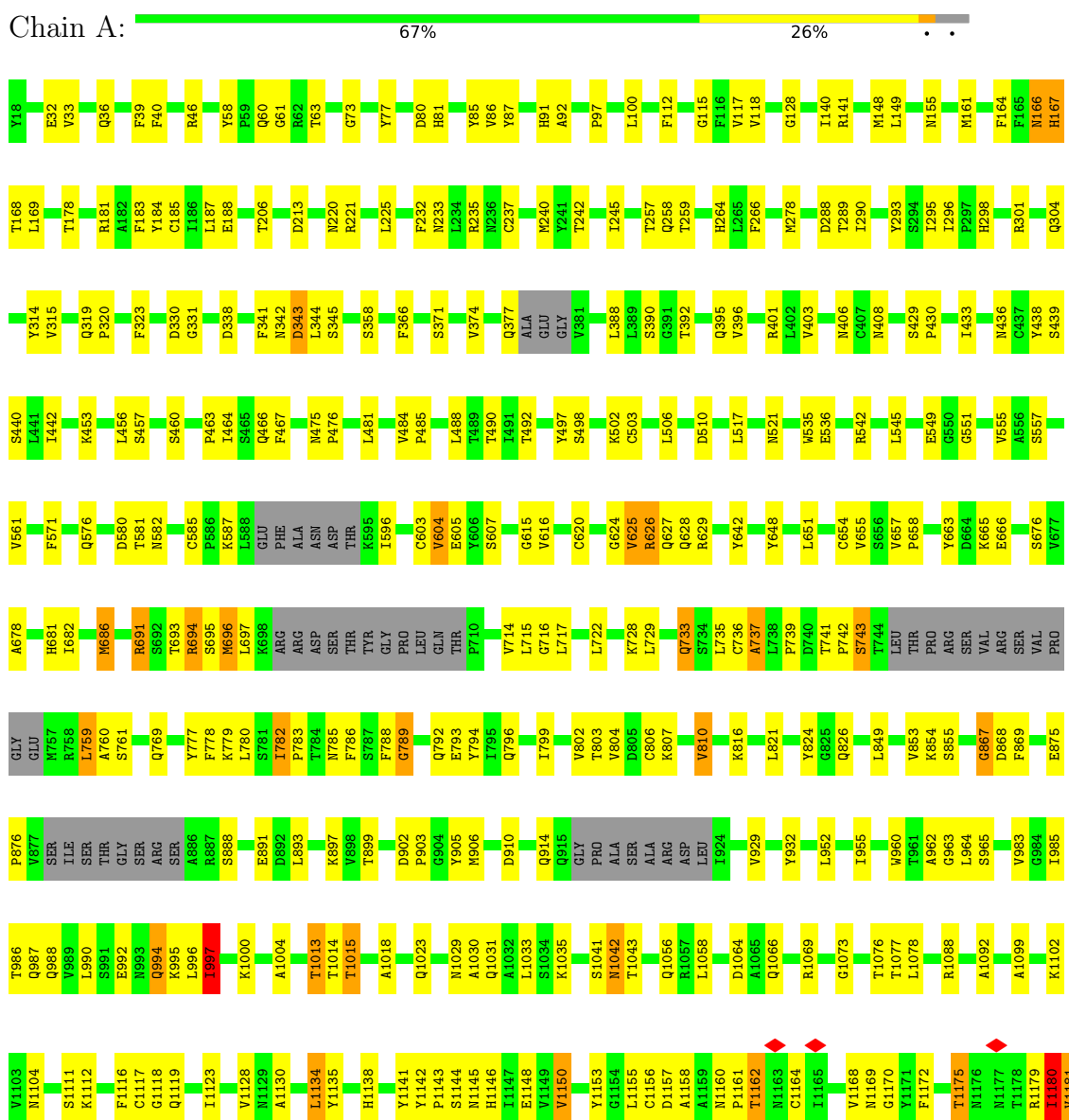
- Molecule 2 is a protein called 0722 L.

Mol	Chain	Residues
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3 Residue-property plots

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.

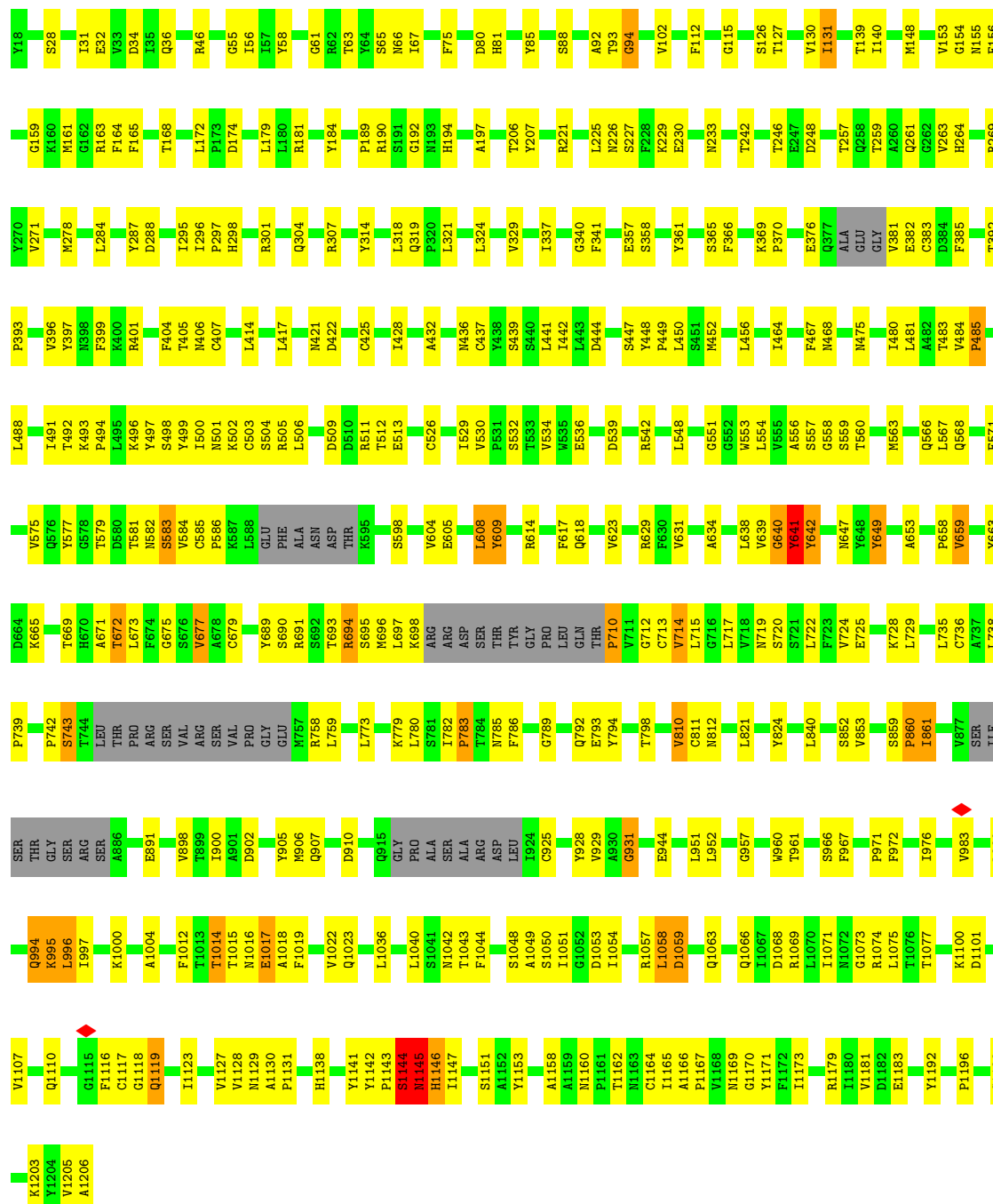
• Molecule 1: Spike glycoprotein

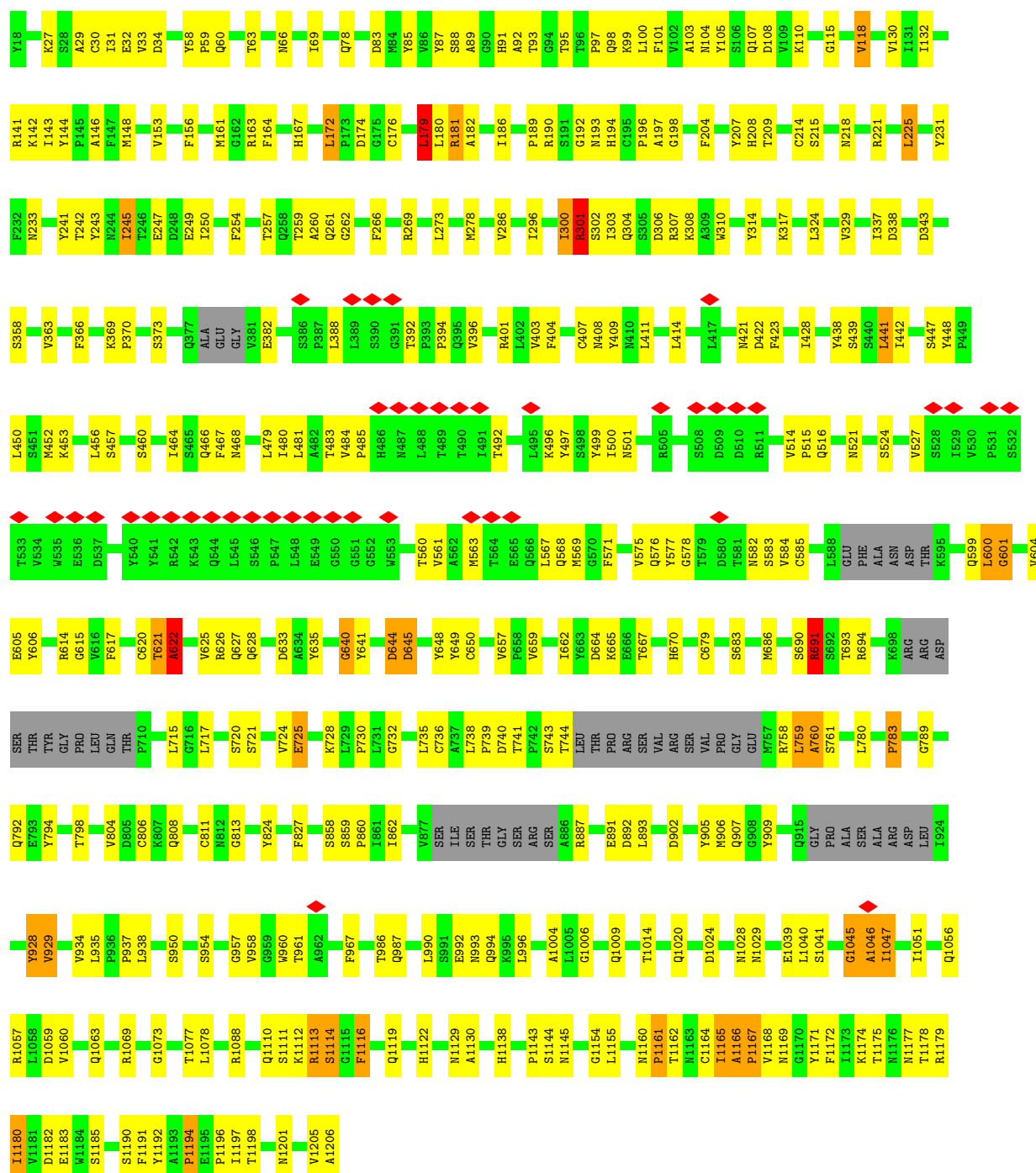




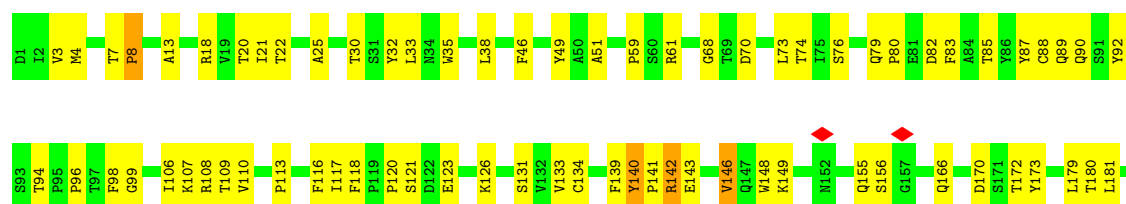
• Molecule 1: Spike glycoprotein

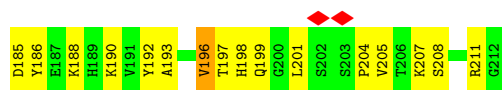
Chain B: 64% 29%





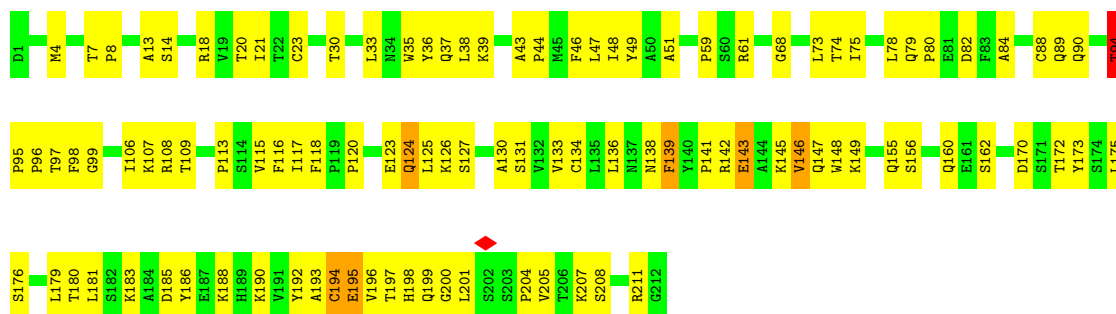
• Molecule 2: 0722 L





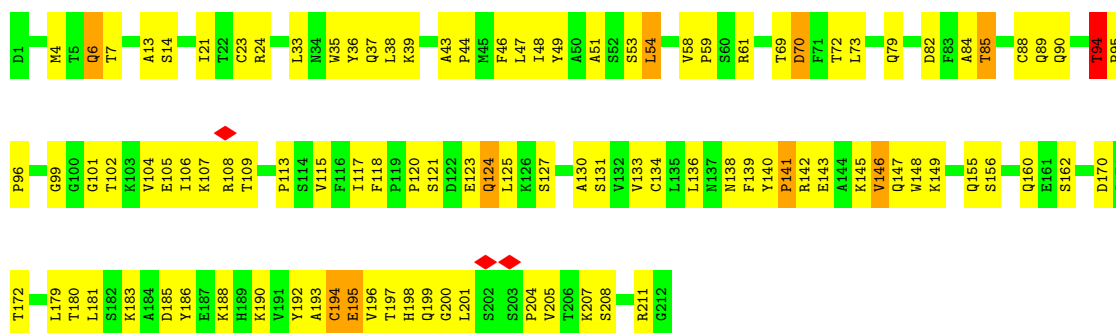
• Molecule 2: 0722 L

Chain F: 50% 46%



• Molecule 2: 0722 L

Chain H: 51% 44%



• Molecule 3: 0722 H



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1463548	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.073	Depositor
Minimum map value	-0.019	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.005	Depositor
Map size ($\text{\AA}$)	346.4, 346.4, 346.4	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0825, 1.0825, 1.0825	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.69	14/9036 (0.2%)	0.84	23/12282 (0.2%)
1	B	0.69	5/9036 (0.1%)	0.94	13/12282 (0.1%)
1	C	0.65	5/9036 (0.1%)	0.82	19/12282 (0.2%)
2	D	0.76	0/1655	0.92	0/2249
2	F	0.62	3/1655 (0.2%)	0.85	2/2249 (0.1%)
2	H	0.74	7/1655 (0.4%)	0.89	4/2249 (0.2%)
3	E	0.50	1/1711 (0.1%)	0.74	2/2336 (0.1%)
3					

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1144	SER	O-C-N	-36.05	95.72	122.03
1	B	641	TYR	CB-CA-C	-16.53	77.52	110.42
2	F	142	ARG	N-CA-C	-9.31	102.11	113.19
1	B	641	TYR	N-CA-C	8.45	128.80	110.80
3	E	157	PHE	CB-CA-C	7.92	125.76	110.17

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1144	SER	Mainchain
1	B	640	GLY	Mainchain
1	C	1190	SER	Mainchain
1	C	300	ILE	Mainchain

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

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:724:VAL:CG2	1:C:758:ARG:HG3	1.83	1.08
1:B:406:ASN:H	1:B:583:SER:HB3	1.24	1.02
1:C:724:VAL:HG21	1:C:758:ARG:HG3	1.00	0.99
1:A:580:ASP:HB2	1:B:61:GLY:HA2	1.46	0.96

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	1127/1189 (95%)	1006 (89%)	106 (9%)	15 (1%)	9	31
1	B	1127/1189 (95%)	1000 (89%)				

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	983/1022 (96%)	957 (97%)	26 (3%)	40	75
1	B	983/1022 (96%)	954 (97%)	29 (3%)	36	72
1	C	982/1022 (96%)	957 (98%)	25 (2%)	42	76
2	D	186/186 (100%)	179 (96%)	7 (4%)	29	64
2	F	186/186 (100%)	178 (96%)	8 (4%)	26	60
2	H	186/186 (100%)	179 (96%)	7 (4%)	29	64
3	E	185/185 (100%)	183 (99%)	2 (1%)	65	87
3	G	185/185 (100%)	183 (99%)	2 (1%)	65	87
3	I	185/185 (100%)	180 (97%)	5 (3%)	39	74
All	All	4061/4179 (97				

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](#)

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.

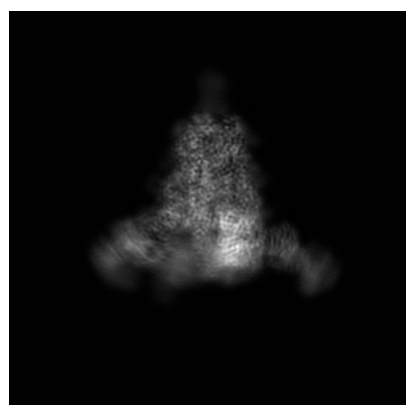
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31726. These allow visual inspection of the internal detail of the map and identification of artifacts.

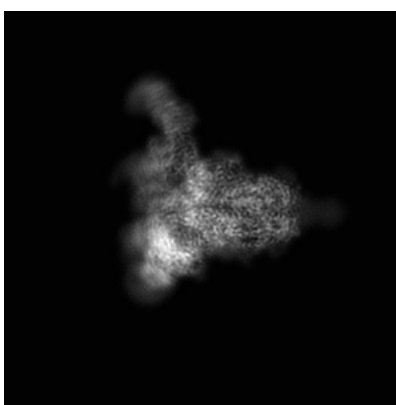
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

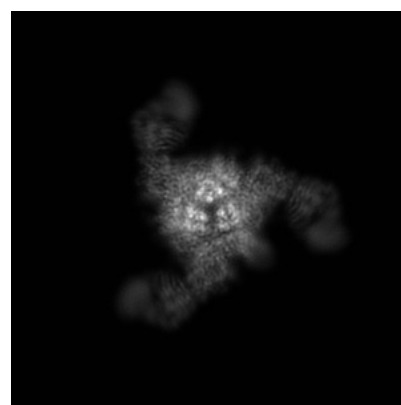
6.1.1 Primary map



X



Y

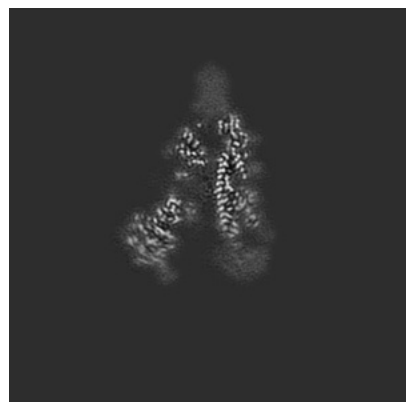


Z

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

6.2 Central slices [i](#)

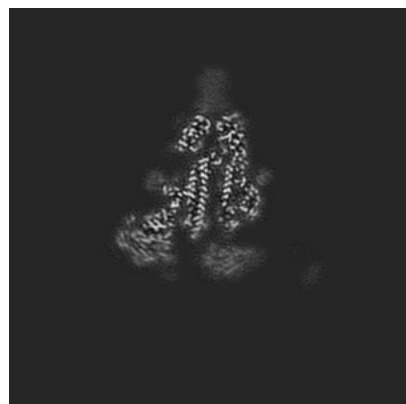
6.2.1 Primary map



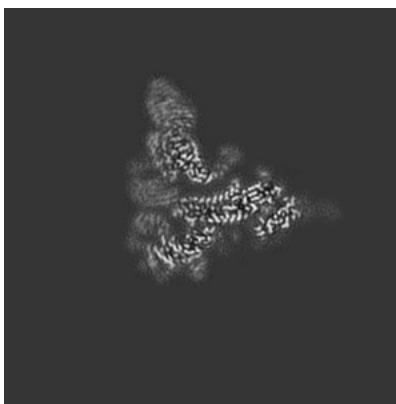
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

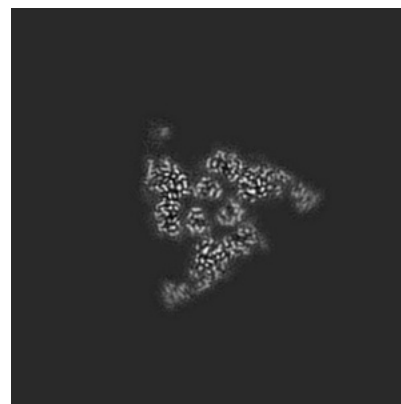
6.3.1 Primary map



X Index: 152



Y Index: 174

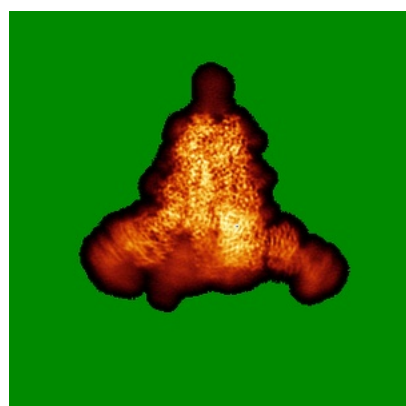


Z Index: 149

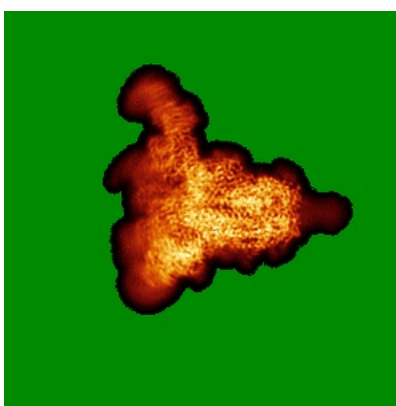
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map

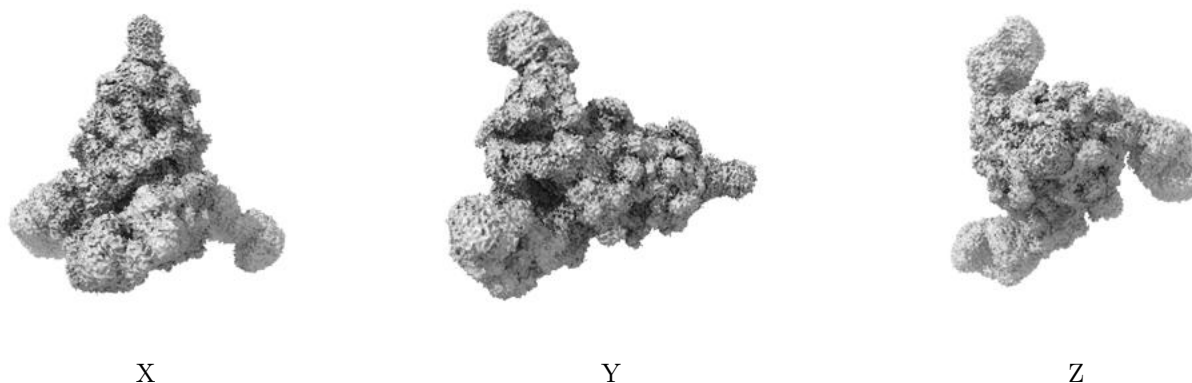


X



6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

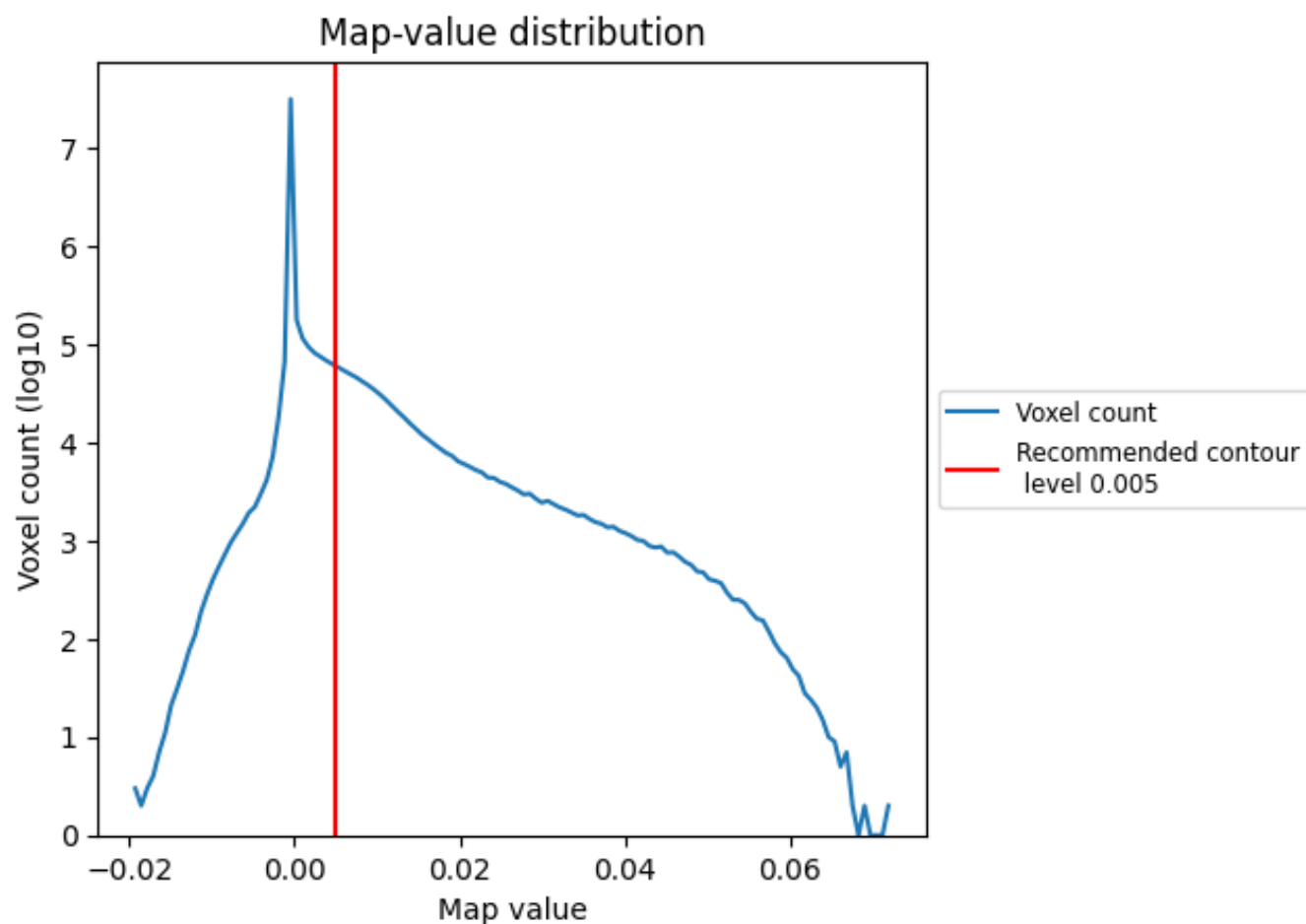
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

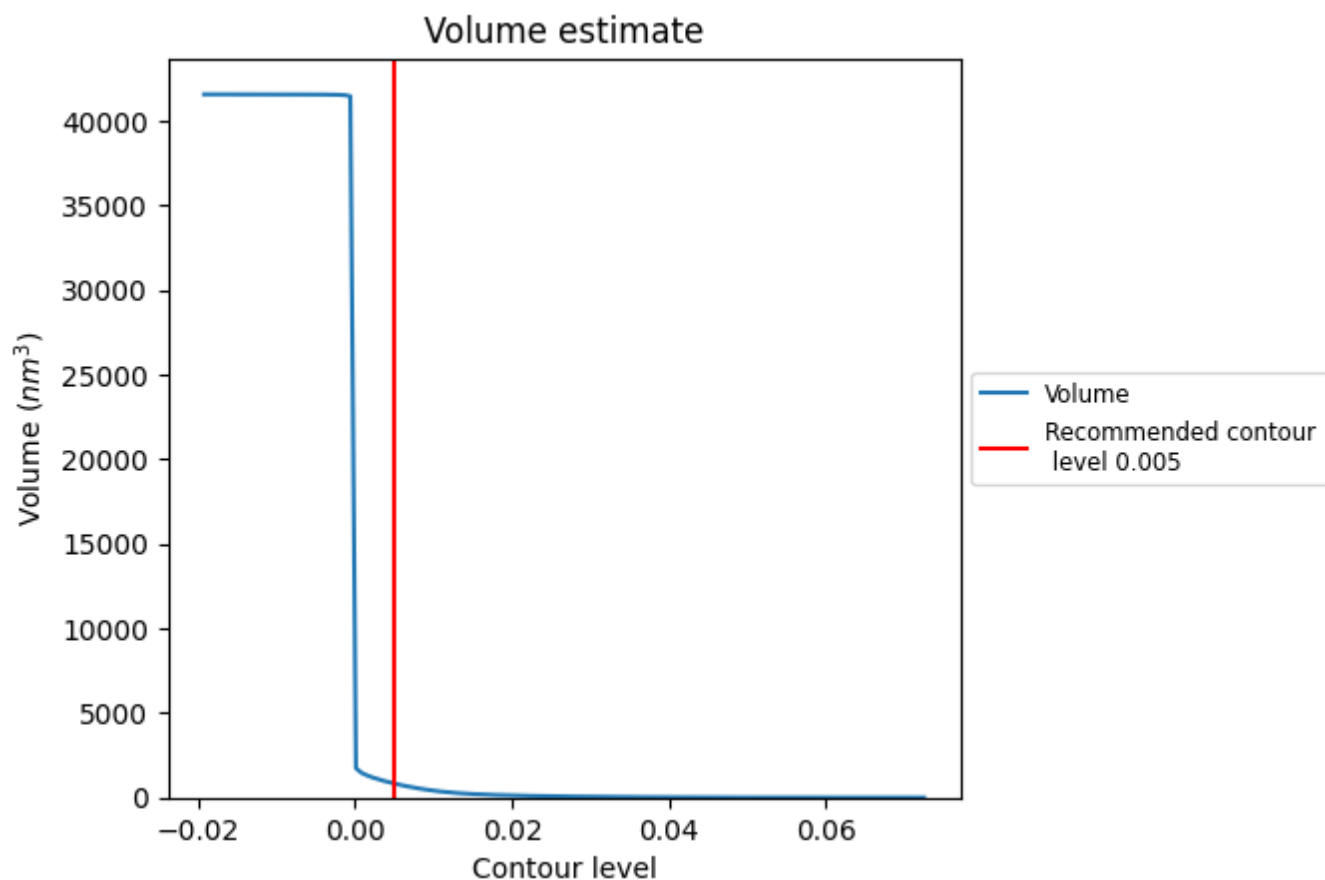
This section contains the results of statistical analysis of the map.

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.

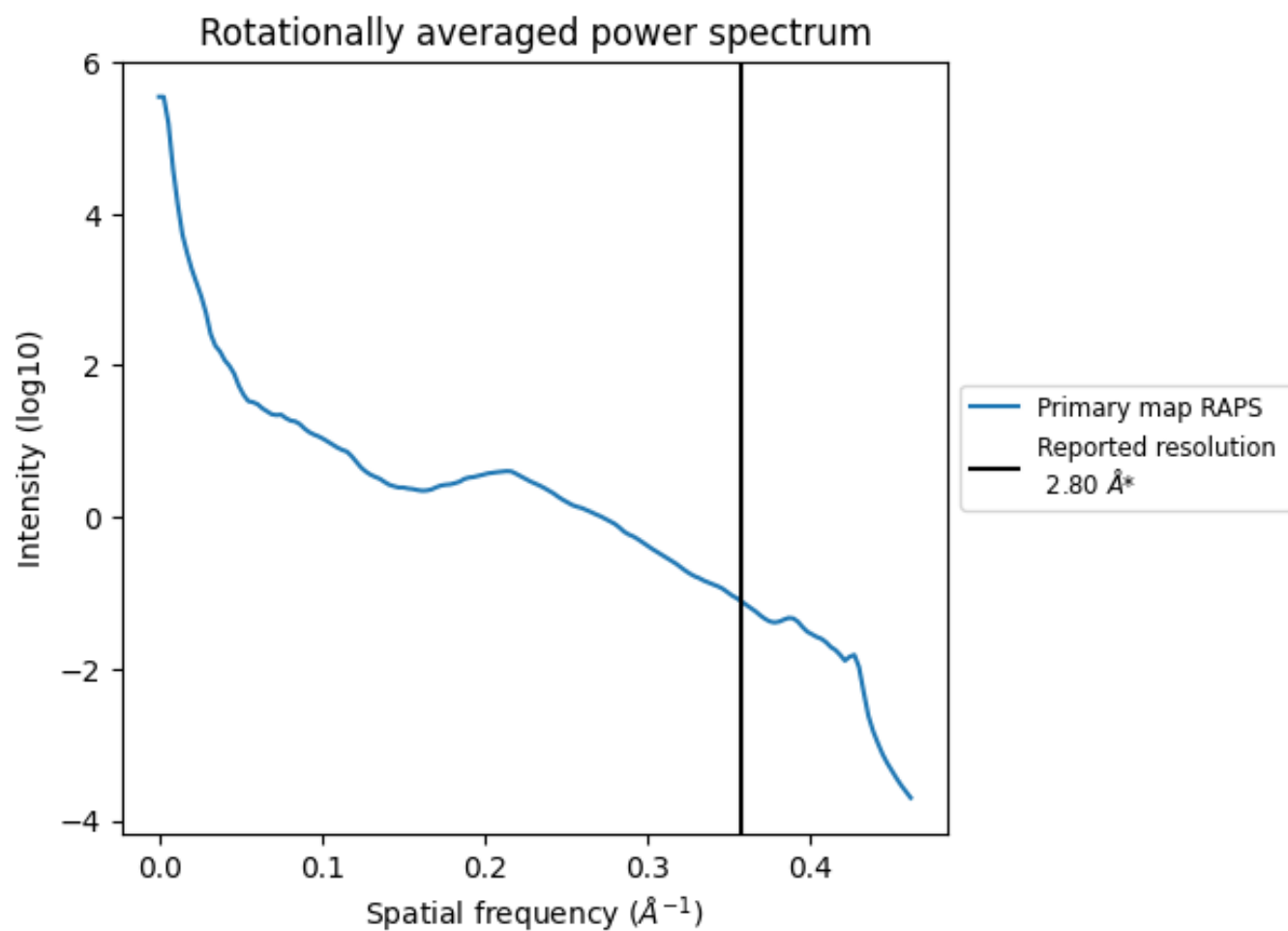
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 829 nm^3 ; this corresponds to an approximate mass of 749 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 0.357 Å⁻¹

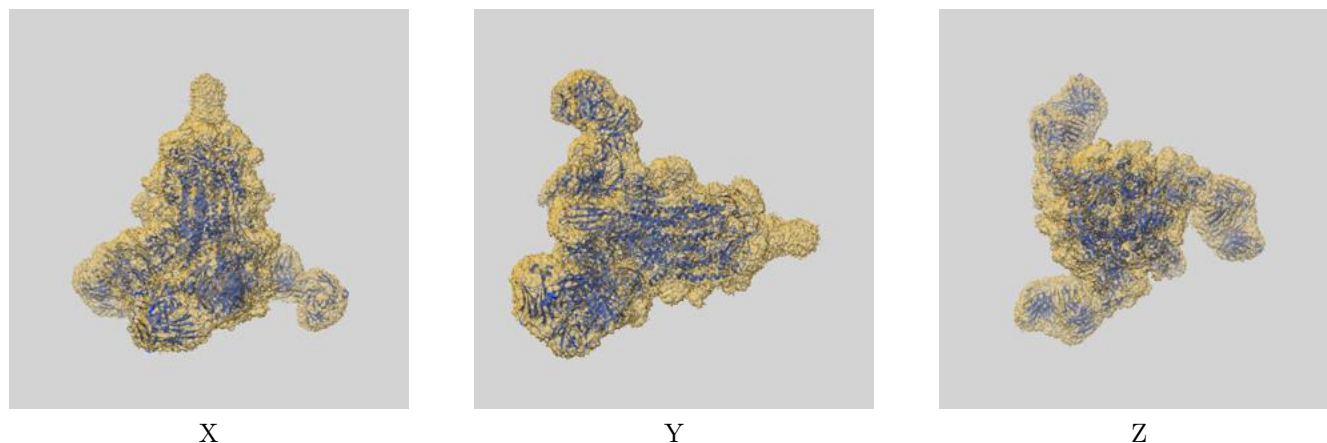
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

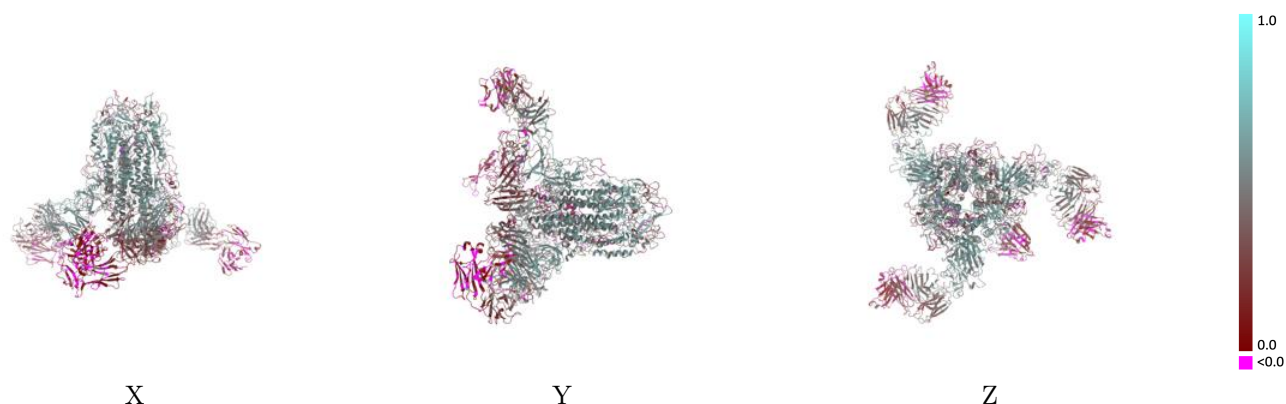
This section contains information regarding the fit between EMDB map EMD-31726 and PDB model 7V5K. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



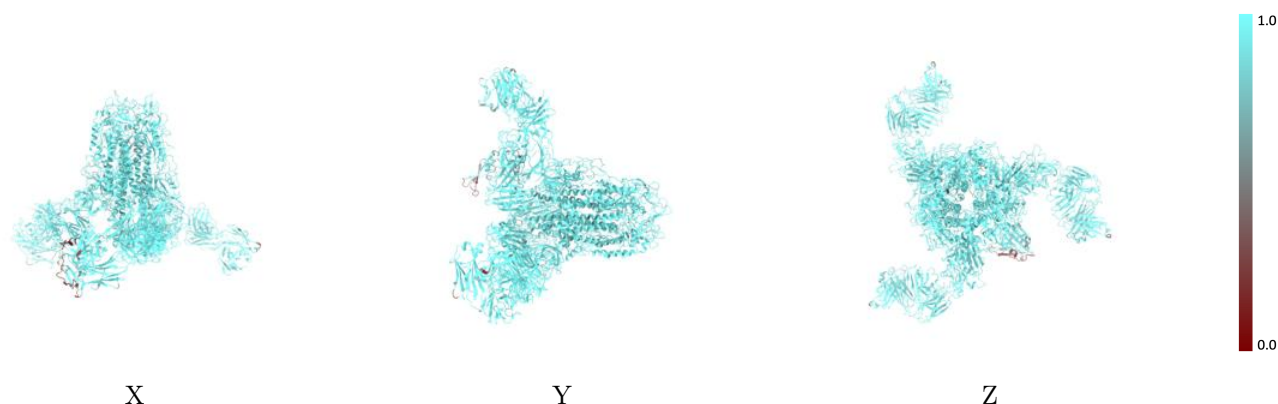
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



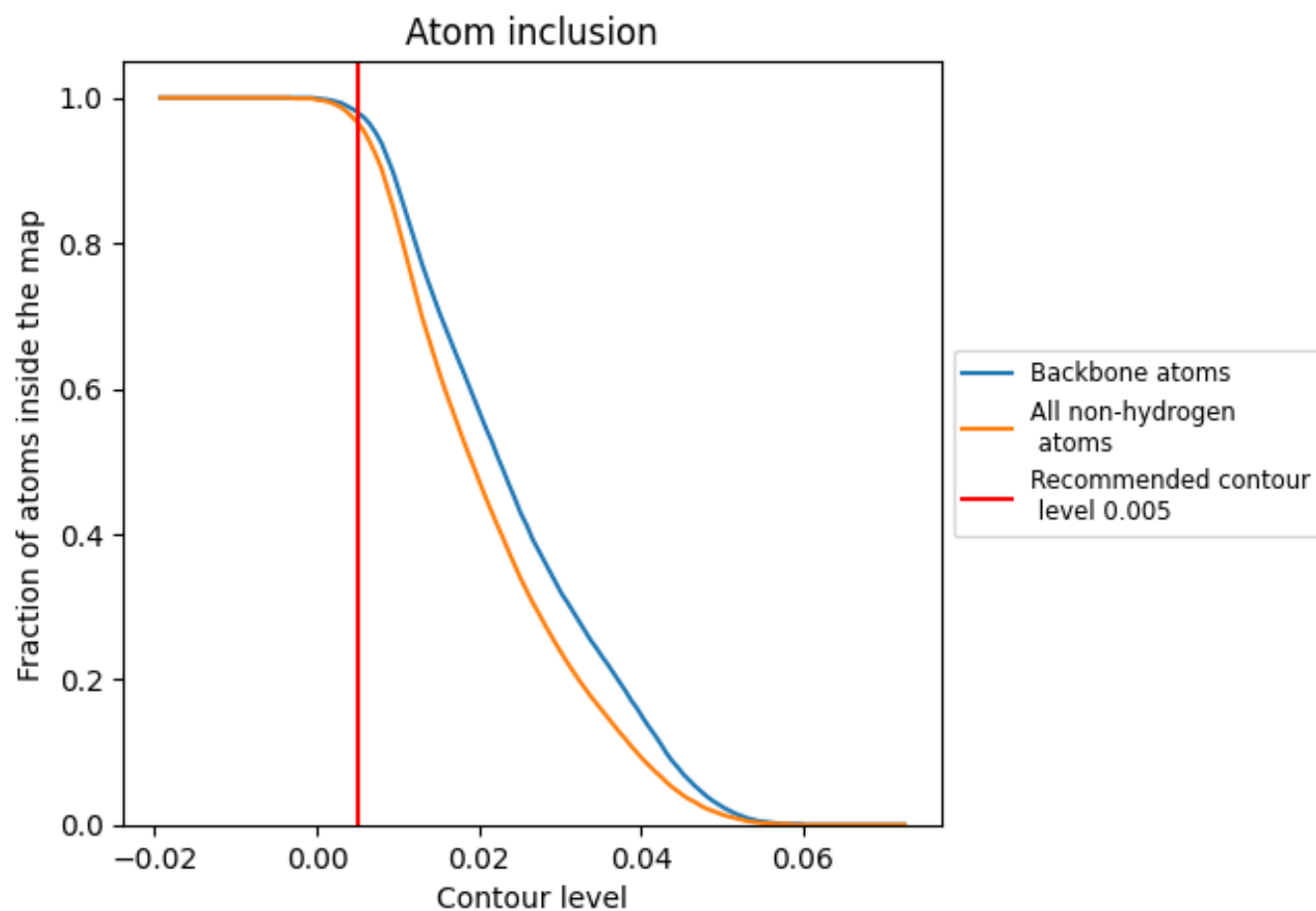
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.005).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 97% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9670	0.3890
A	0.9770	0.4700
B	0.9780	0.4580
C	0.9350	0.3930
D	0.9620	0.1980
E	0.9840	0.2860
F	0.9750	0.2240
G	0.9840	0.3030
H	0.9730	0.1980
I	0.9750	0.3050

