



wwPDB EM Validation Summary Report ⓘ

Nov 4, 2024 – 05:54 AM JST

PDB ID : 7V5K
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.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

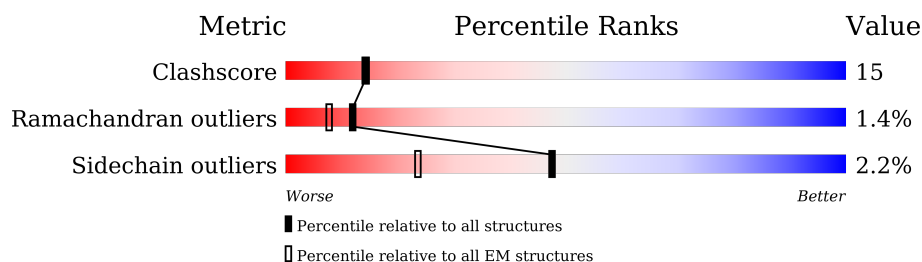
1 Overall quality at a glance

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.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1189	 69% 26% . .
1	B	1189	 66% 28% . .
1	C	1189	 67% 27% . .
2	D	212	 60% 38% .
2	F	212	 53% 45% .
2	H	212	 53% 44% .
3	E	222	 65% 34% .
3	G	222	 65% 35%

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Mol	Chain	Length	Quality of chain
3	I	222	<div><div></div><div>65%</div><div>33%</div><div></div></div>

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	Atoms					AltConf	Trace
2	D	212	Total	C	N	O	S	0	0
			1619	1015	266	332	6		
2	F	212	Total	C	N	O	S	0	0
			1619	1015	266	332	6		
2	H	212	Total	C	N	O	S	0	0
			1619	1015	266	332	6		

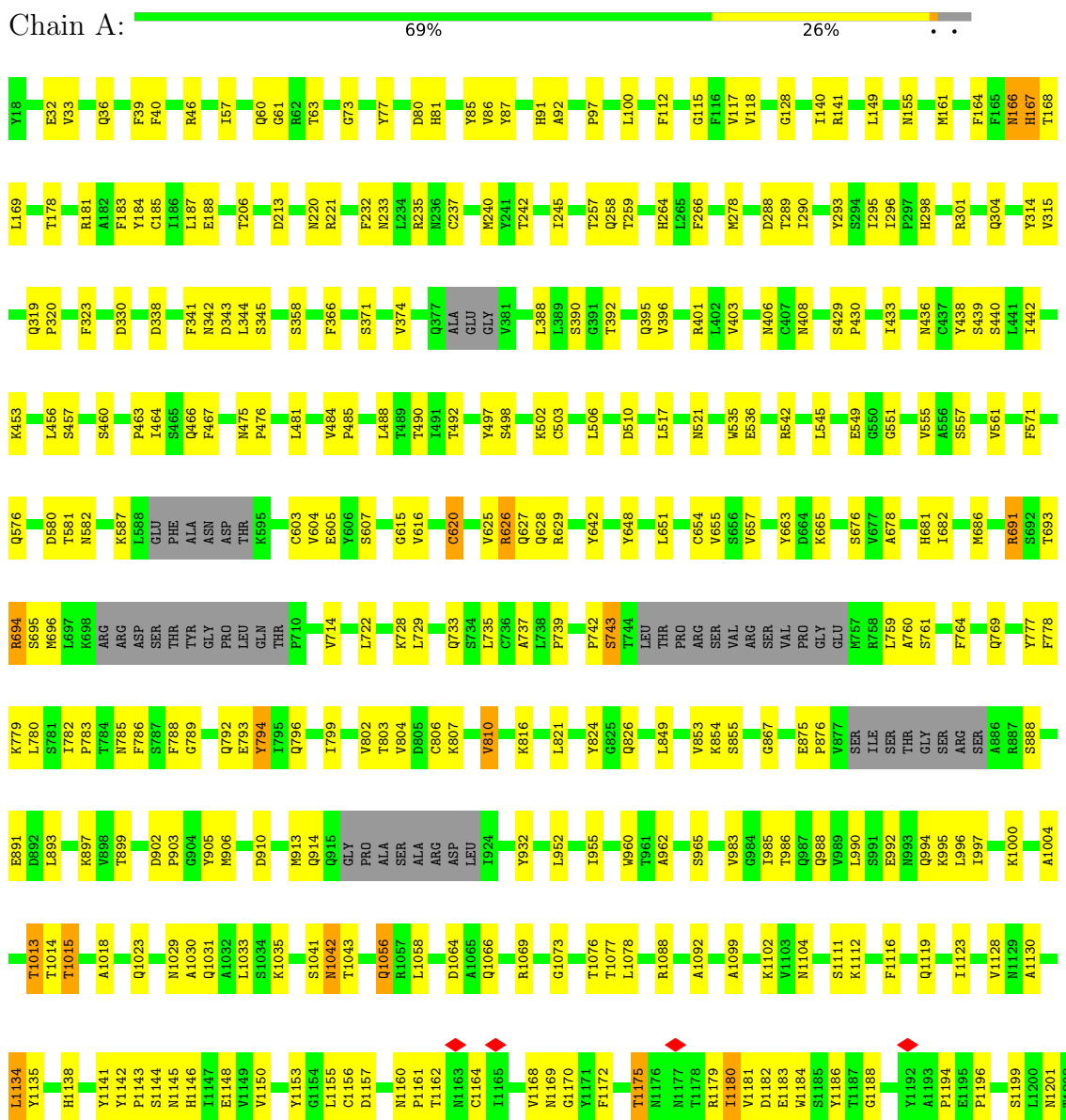
- Molecule 3 is a protein called 0722 H.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	222	Total	C	N	O	S	0	0
			1668	1057	275	329	7		
3	G	222	Total	C	N	O	S	0	0
			1668	1057	275	329	7		
3	I	222	Total	C	N	O	S	0	0
			1668	1057	275	329	7		

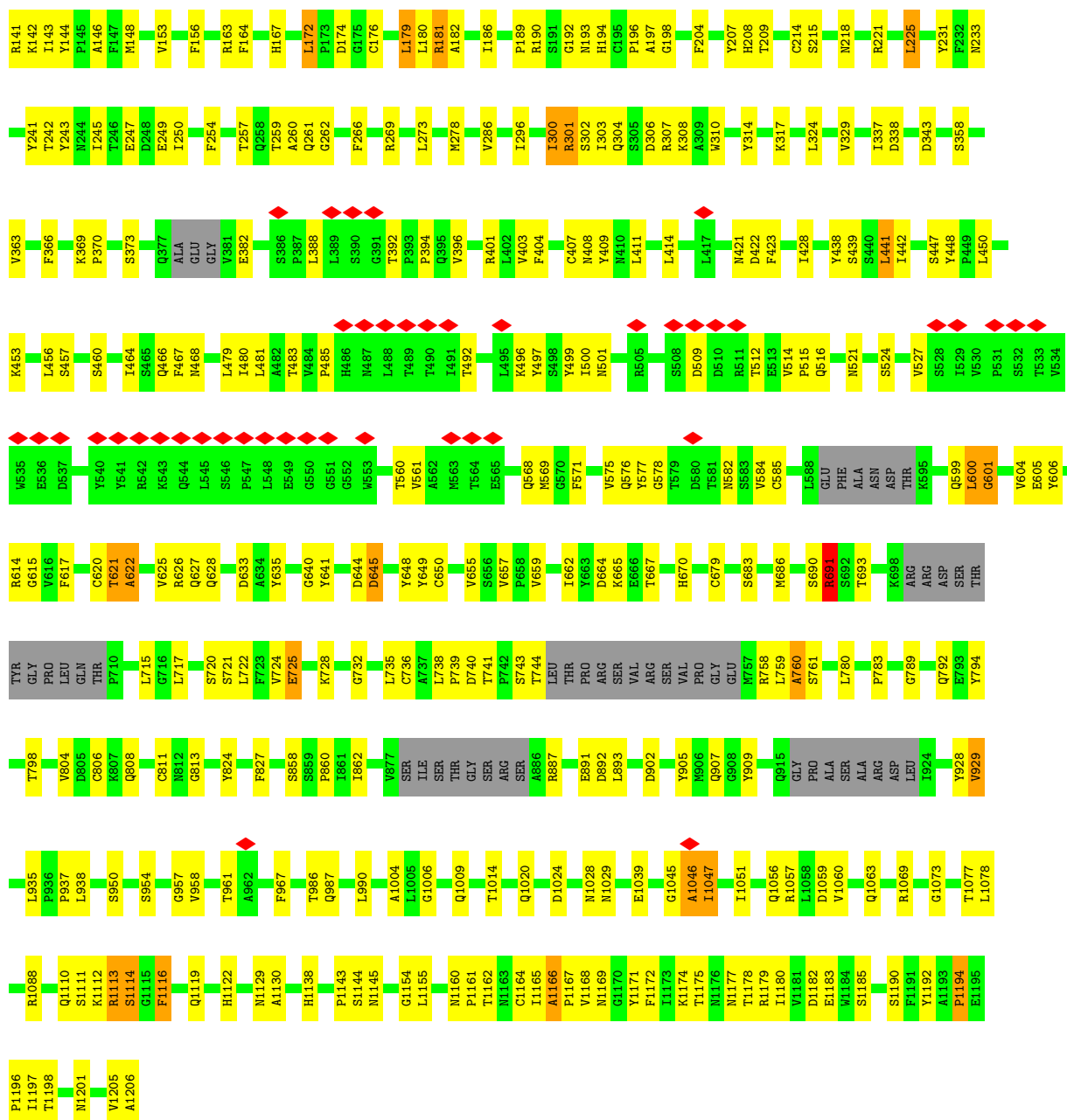
3 Residue-property plots

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.

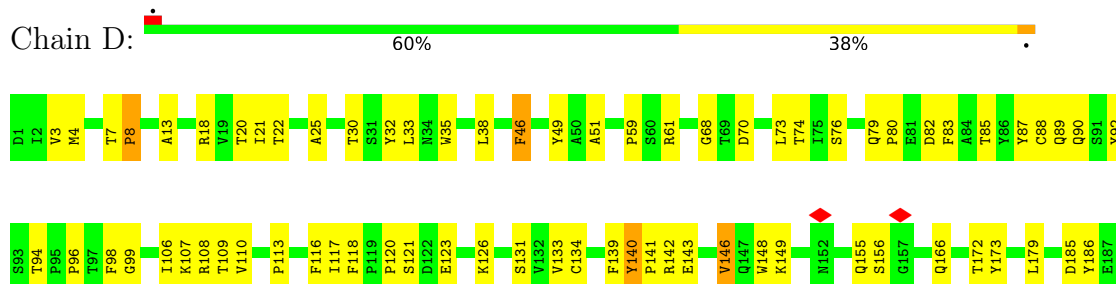
• Molecule 1: Spike glycoprotein



Y18	K27	S28	A29	C30	I31	E32	V33	D34	G55	Y58	P59	Q60	T63	N66	I69	Q78	D83	N84	Y85	V86	Y87	S88	A89	G90	H91	A92	T93	G94	T95	T96	P97	Q98	K99	L100	F101	A102	V103	N104	Y105	S106	I107	D108	V109	K110	V118	I130	V131	I132
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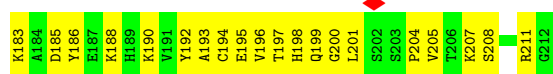
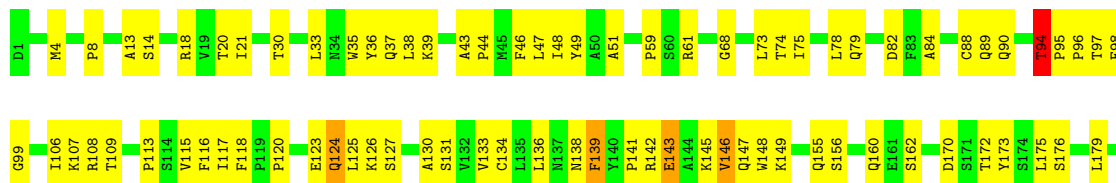
• Molecule 2: 0722 L





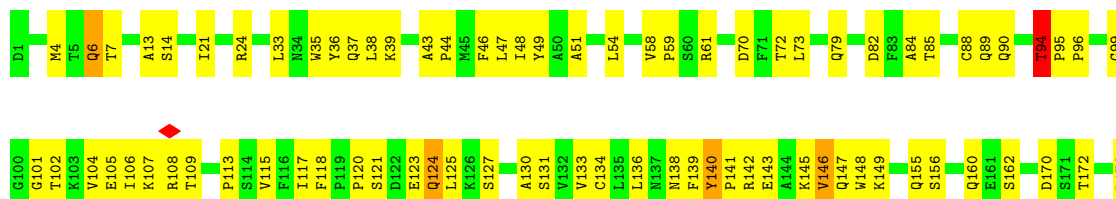
• Molecule 2: 0722 L

Chain F: 53% 45%



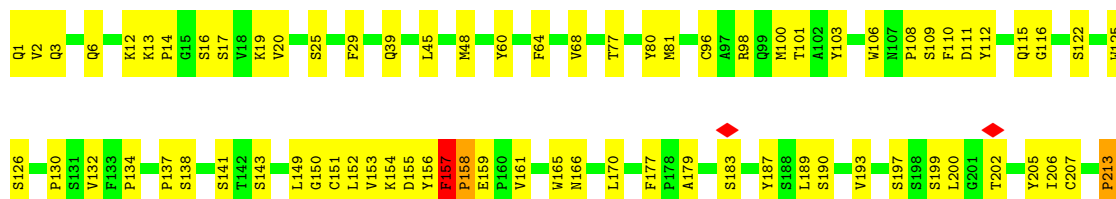
• Molecule 2: 0722 L

Chain H: 53% 44%



• Molecule 3: 0722 H

Chain E: 65% 34%

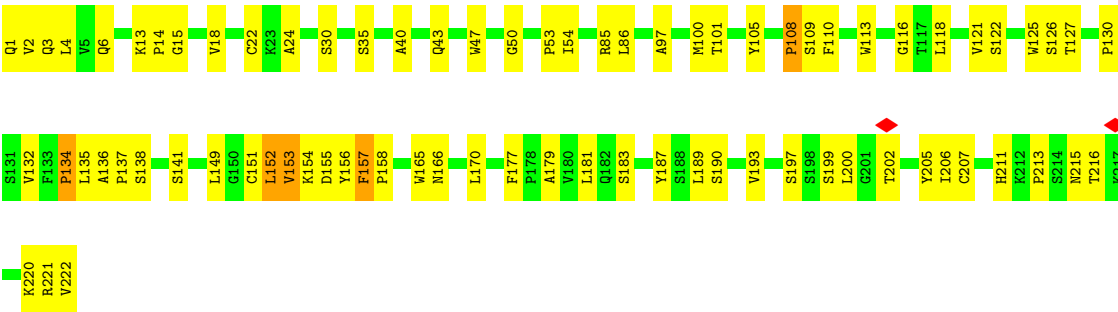


• Molecule 3: 0722 H

Chain G: 65% 35%



● 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 (\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 (\AA)	1.0825, 1.0825, 1.0825	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	0.54	5/9036 (0.1%)	0.62	4/12282 (0.0%)
1	B	0.55	1/9036 (0.0%)	0.66	4/12282 (0.0%)
1	C	0.53	1/9036 (0.0%)	0.62	0/12282
2	D	0.52	0/1655	0.62	0/2249
2	F	0.46	0/1655	0.63	1/2249 (0.0%)
2	H	0.51	1/1655 (0.1%)	0.67	0/2249
3	E	0.43	0/1711	0.65	1/2336 (0.0%)
3	G	0.41	0/1711	0.60	0/2336
3	I	0.55	0/1711	0.69	1/2336 (0.0%)
All	All	0.52	8/37206 (0.0%)	0.64	11/50601 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	C	0	2
All	All	0	4

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	696	MET	C-N	6.09	1.48	1.34
1	B	319	GLN	C-N	5.83	1.45	1.34
1	A	655	VAL	C-N	-5.82	1.20	1.34
1	A	654	CYS	C-N	-5.77	1.20	1.34
1	A	1175	THR	C-N	5.45	1.46	1.34

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1144	SER	O-C-N	-16.86	95.72	122.70
1	B	641	TYR	CB-CA-C	-16.44	77.52	110.40
3	E	157	PHE	CB-CA-C	7.68	125.76	110.40
1	B	641	TYR	N-CA-C	6.59	128.80	111.00
3	I	105	TYR	CB-CA-C	-6.16	98.09	110.40

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 ⓘ

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	8836	0	8558	214	0
1	B	8836	0	8564	260	0
1	C	8836	0	8558	262	0
2	D	1619	0	1571	60	0
2	F	1619	0	1571	79	0
2	H	1619	0	1571	82	0
3	E	1668	0	1624	62	0
3	G	1668	0	1624	65	0
3	I	1668	0	1624	64	0
All	All	36369	0	35265	1097	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 15.

The worst 5 of 1097 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:724:VAL:HG21	1:C:758:ARG:CG	1.76	1.14

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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%)	10	32
1	B	1127/1189 (95%)	1000 (89%)	104 (9%)	23 (2%)	6	21
1	C	1128/1189 (95%)	979 (87%)	131 (12%)	18 (2%)	8	27
2	D	210/212 (99%)	199 (95%)	9 (4%)	2 (1%)	13	39
2	F	210/212 (99%)	199 (95%)	9 (4%)	2 (1%)	13	39
2	H	210/212 (99%)	198 (94%)	11 (5%)	1 (0%)	25	56
3	E	220/222 (99%)	205 (93%)	12 (6%)	3 (1%)	9	30
3	G	220/222 (99%)	206 (94%)	14 (6%)	0	100	100
3	I	220/222 (99%)	208 (94%)	9 (4%)	3 (1%)	9	30
All	All	4672/4869 (96%)	4200 (90%)	405 (9%)	67 (1%)	12	30

5 of 67 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	166	ASN
1	A	737	ALA
1	A	759	LEU
1	A	1042	ASN
1	A	1184	TRP

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%)	961 (98%)	22 (2%)	47	79
1	B	983/1022 (96%)	969 (99%)	14 (1%)	62	87
1	C	982/1022 (96%)	961 (98%)	21 (2%)	48	80
2	D	186/186 (100%)	179 (96%)	7 (4%)	28	62
2	F	186/186 (100%)	178 (96%)	8 (4%)	25	57
2	H	186/186 (100%)	178 (96%)	8 (4%)	25	57
3	E	185/185 (100%)	183 (99%)	2 (1%)	70	90
3	G	185/185 (100%)	183 (99%)	2 (1%)	70	90
3	I	185/185 (100%)	181 (98%)	4 (2%)	47	79
All	All	4061/4179 (97%)	3973 (98%)	88 (2%)	47	79

5 of 88 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	3	VAL
2	F	146	VAL
2	D	70	ASP
3	E	183	SER
3	G	183	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	994	GLN
3	G	166	ASN
1	C	1020	GLN
1	C	1145	ASN
2	H	198	HIS

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.

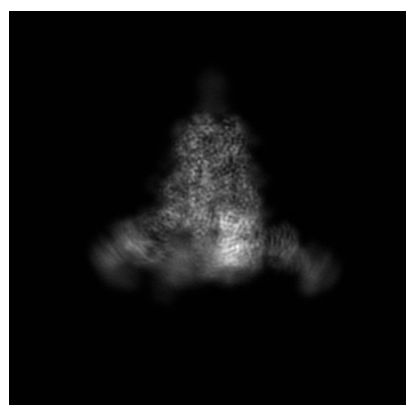
6 Map visualisation [i](#)

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.

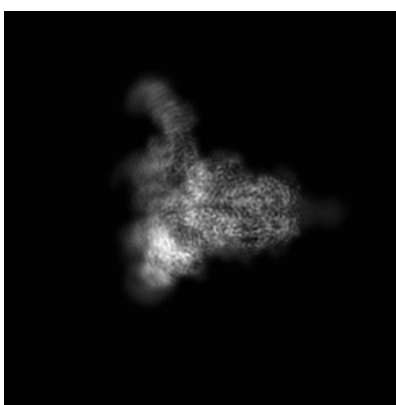
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

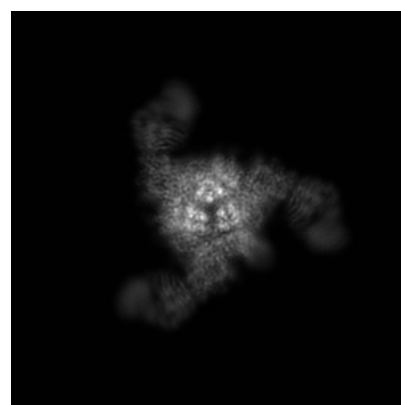
6.1.1 Primary map



X



Y

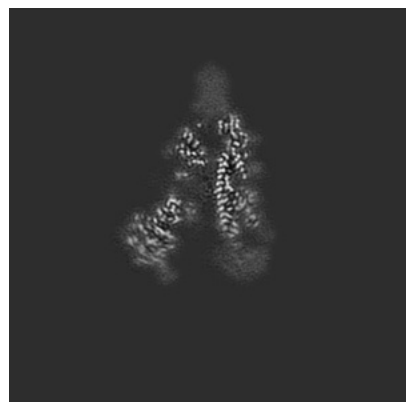


Z

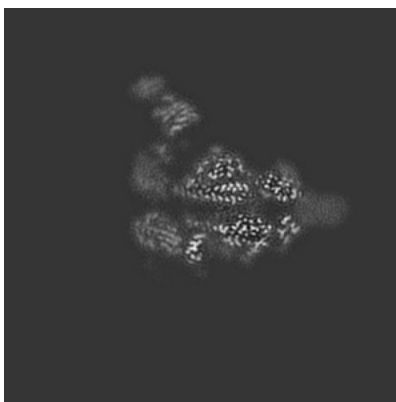
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

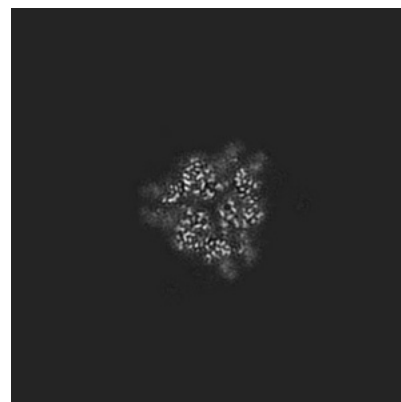
6.2.1 Primary map



X Index: 160



Y Index: 160

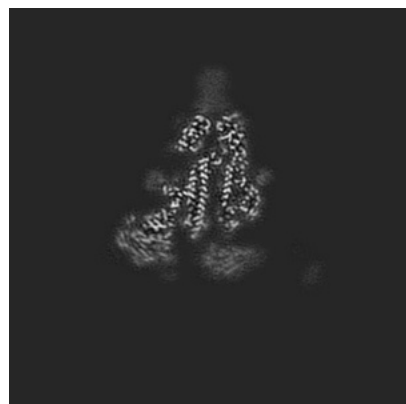


Z Index: 160

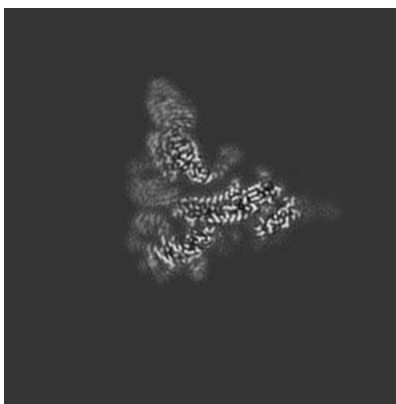
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

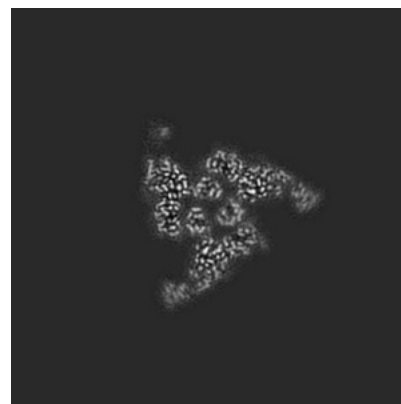
6.3.1 Primary map



X Index: 152



Y Index: 174

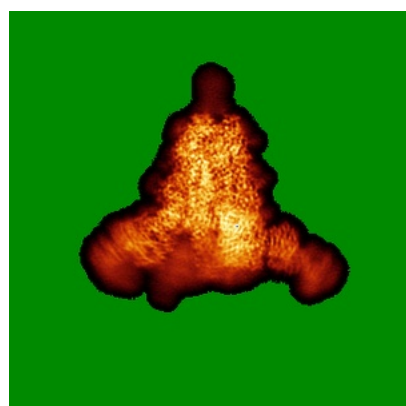


Z Index: 149

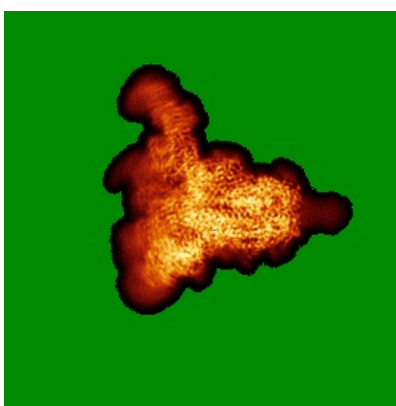
The images above show the largest variance slices of the map in three orthogonal directions.

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

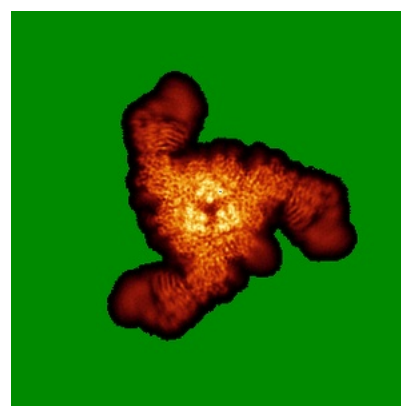
6.4.1 Primary map



X



Y

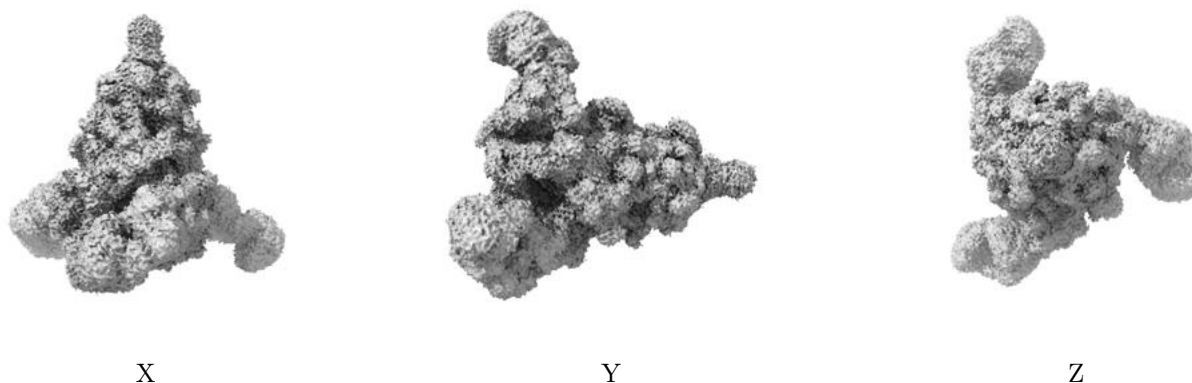


Z

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



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.

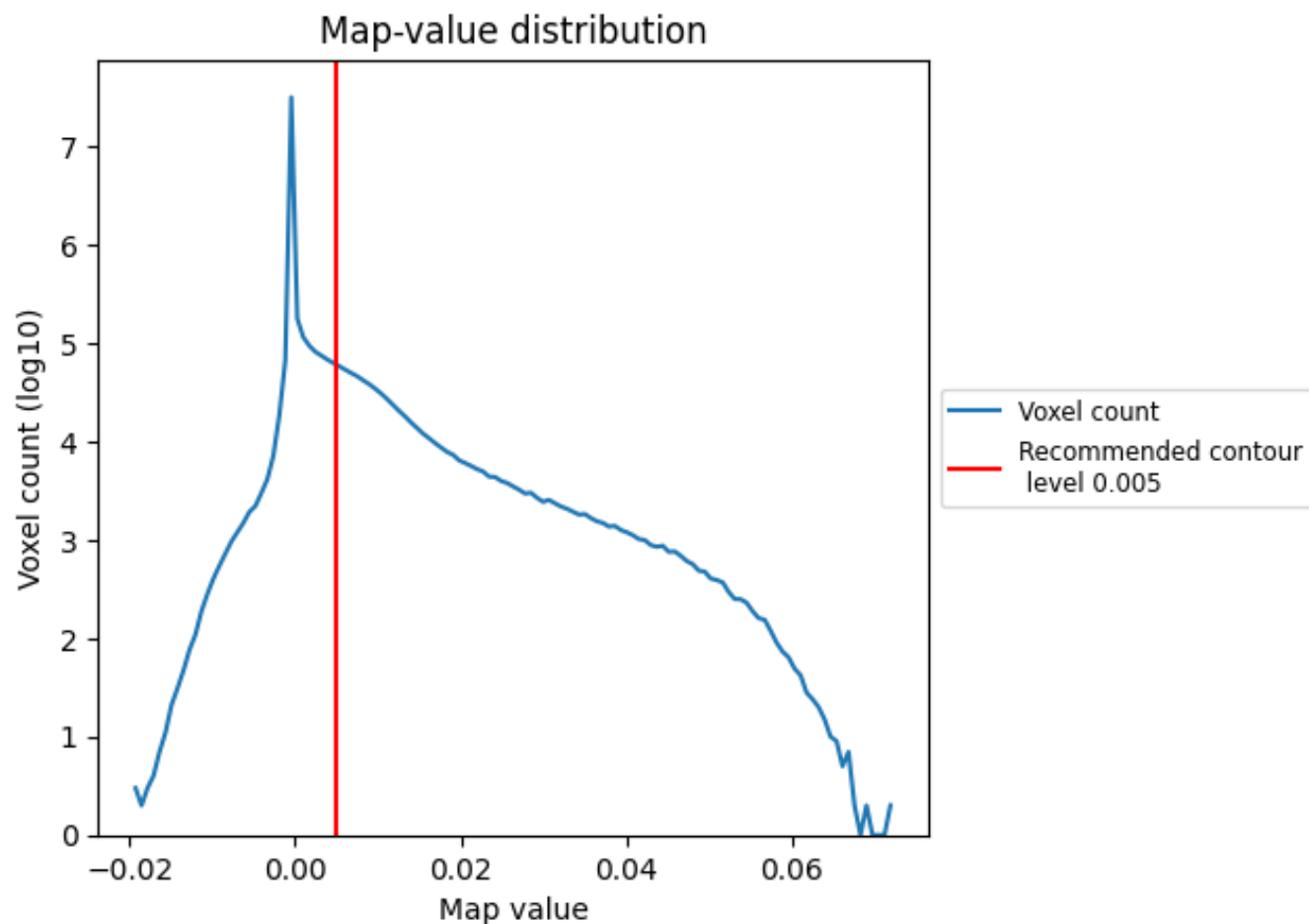
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

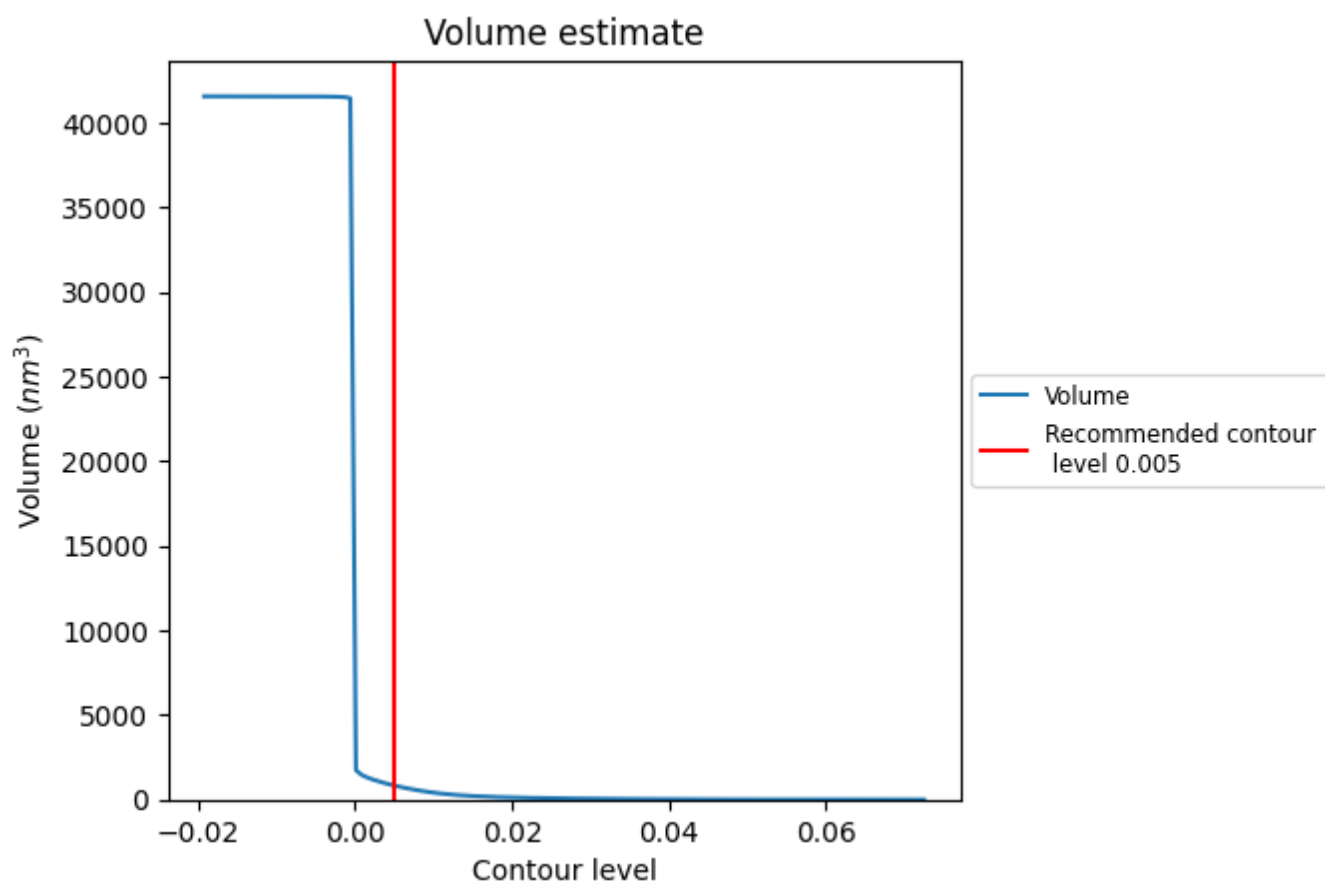
This section contains the results of statistical analysis of the map.

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.

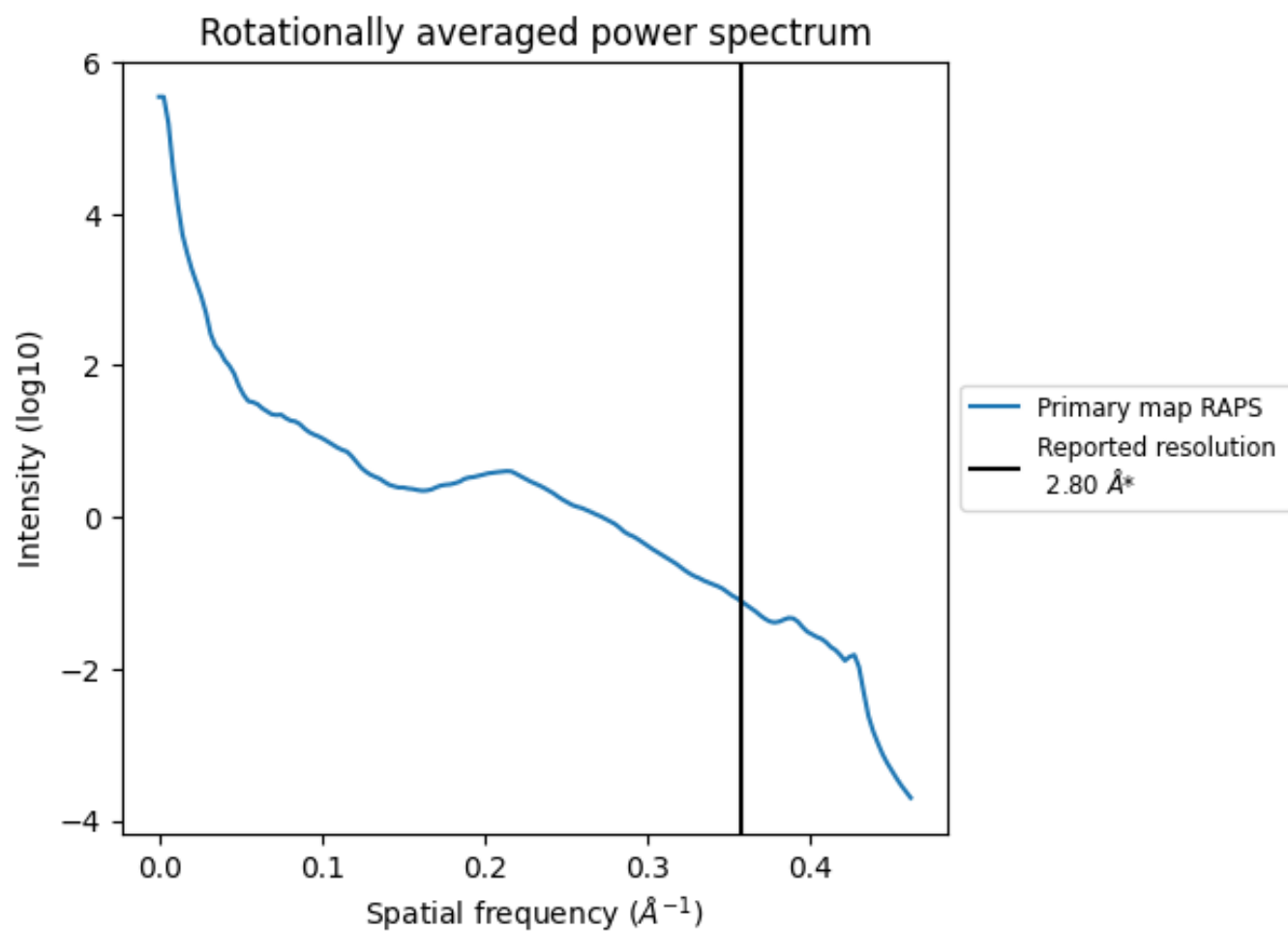
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 829 nm³; 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

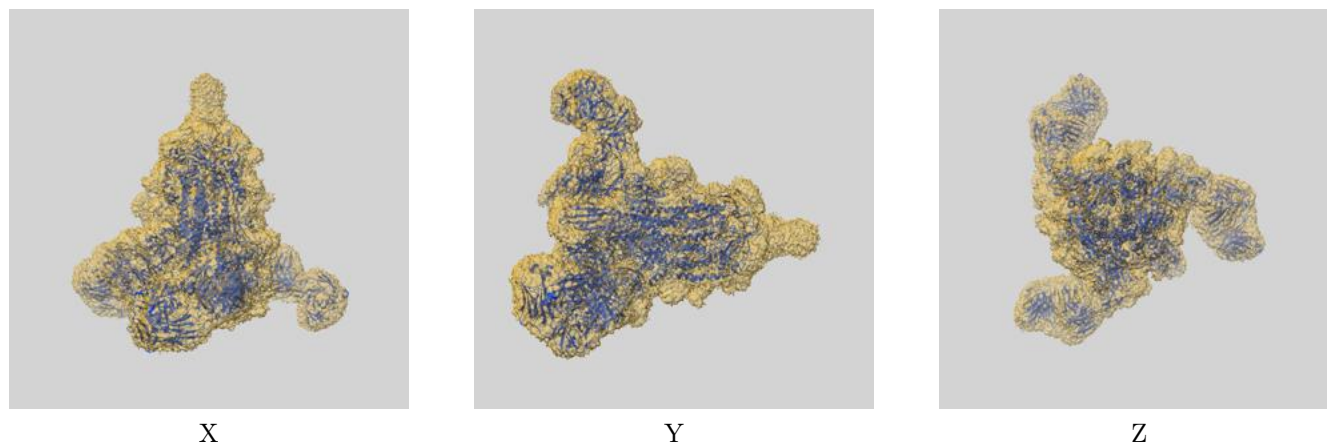
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

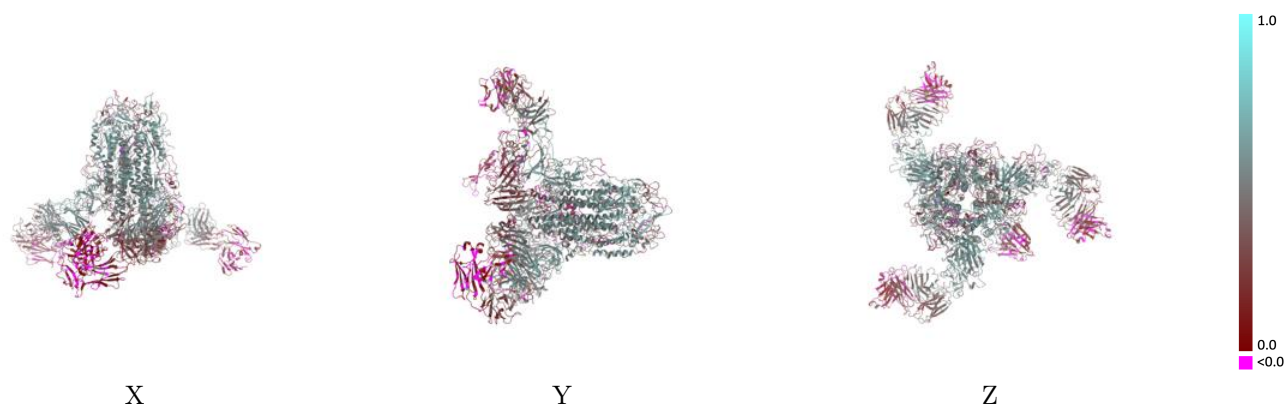
This section contains information regarding the fit between EMDB map EMD-31726 and PDB model 7V5K. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



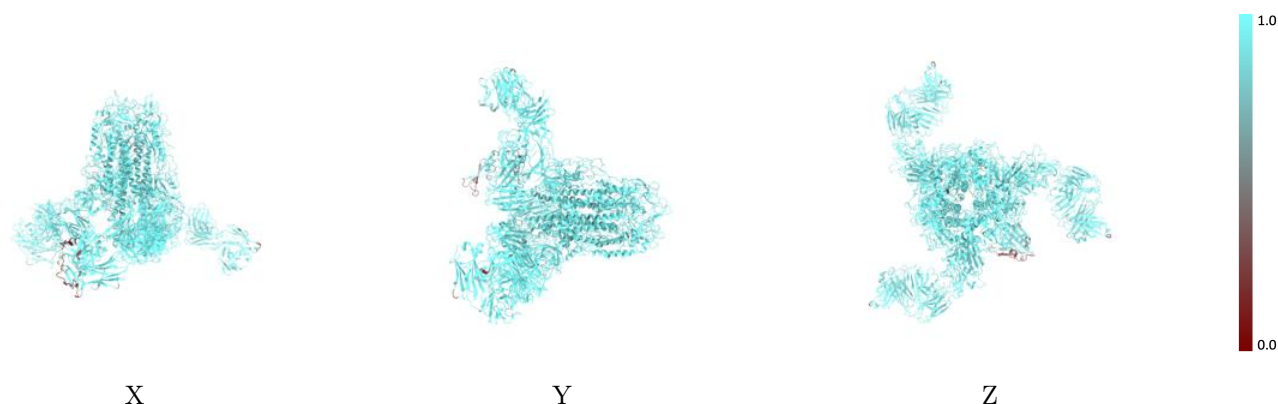
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



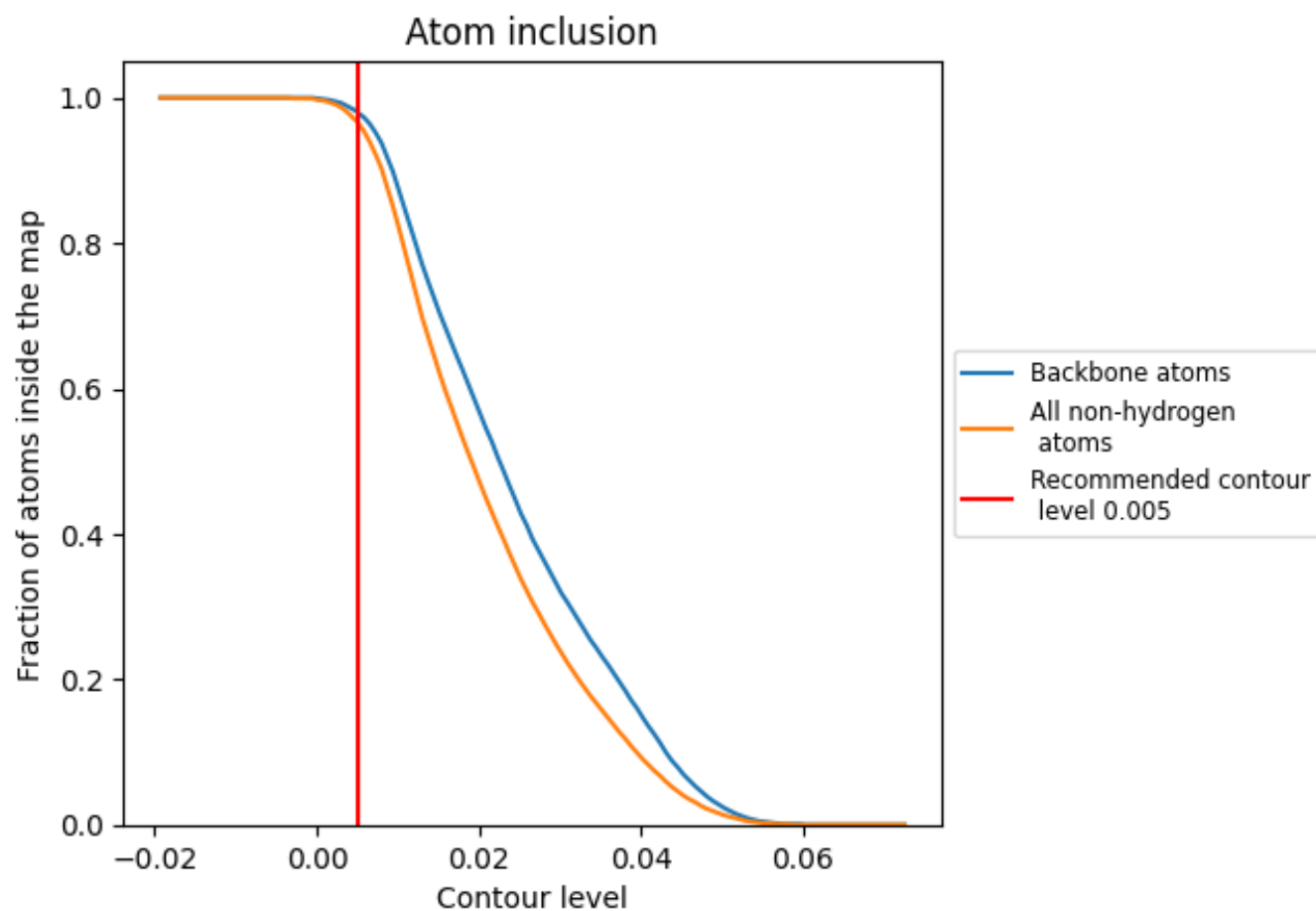
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	<div></div> 0.9670	<div></div> 0.3890
A	<div></div> 0.9770	<div></div> 0.4700
B	<div></div> 0.9780	<div></div> 0.4580
C	<div></div> 0.9350	<div></div> 0.3930
D	<div></div> 0.9620	<div></div> 0.1980
E	<div></div> 0.9840	<div></div> 0.2860
F	<div></div> 0.9750	<div></div> 0.2240
G	<div></div> 0.9840	<div></div> 0.3030
H	<div></div> 0.9730	<div></div> 0.1980
I	<div></div> 0.9750	<div></div> 0.3050

1.0

0.0

<0.0