



Full wwPDB EM Validation Report ⓘ

Oct 6, 2024 – 03:12 AM JST

PDB ID : 7E39
EMDB ID : EMD-30977
Title : SARS-CoV-2 spike in complex with the Ab4 neutralizing antibody (State 3)
Authors : Liu, C.
Deposited on : 2021-02-08
Resolution : 3.70 Å(reported)

This is a Full wwPDB EM Validation 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
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

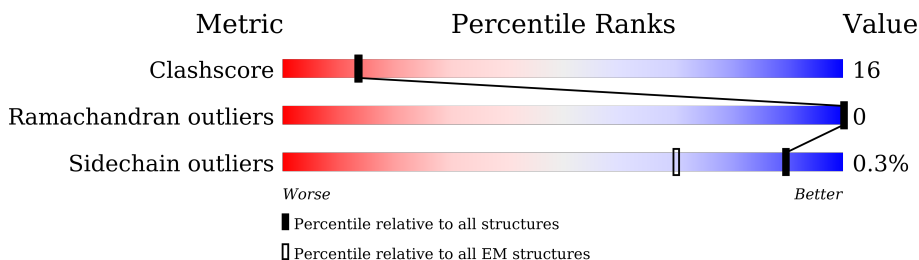
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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	194	 70% 30%
2	B	214	 26% 23% 50%
3	C	448	 19% 6% 75%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3074 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 protein S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	194	Total	C	N	O	S	0	0
			1536	984	256	288	8		

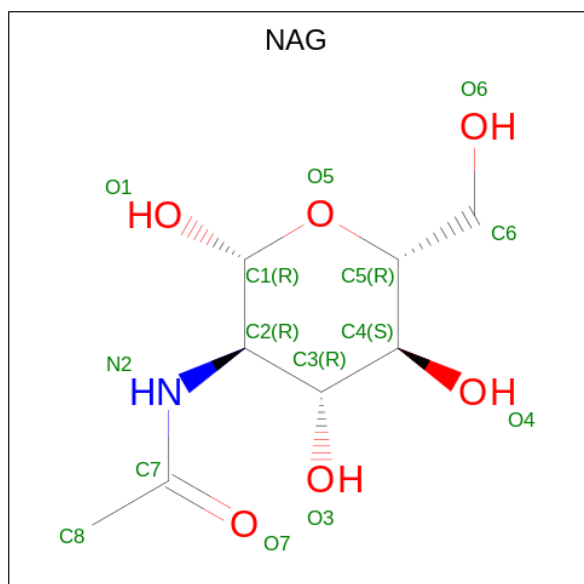
- Molecule 2 is a protein called Light Chain of Ab4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	106	Total	C	N	O	S	0	0
			819	518	138	159	4		

- Molecule 3 is a protein called Heavy Chain of Ab4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	114	Total	C	N	O	S	0	0
			705	436	130	136	3		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	

GLY	GLN	VAL	LYS	ALA
SER	PRO	GLU	THR	LEU
PHE	ARG	VAL	HIS	THR
PHE	GLU	HIS	THR	SER
LEU	PRO	ASN	CYS	GLY
TYR	GLN	ALA	PRO	VAL
SER	VAL	LYS	PRO	HIS
LYS	TYR	THR	CYS	THR
LYS	THR	LYS	PRO	PHE
THR	LEU	PRO	ALA	PRO
VAL	PRO	ARG	PRO	ALA
ASP	PRO	GLU	GLU	VAL
LYS	SER	GLU	ALA	LEU
SER	ARG	GLN	ALA	GLN
ARG	GLU	TYR	GLY	SER
TRP	GLU	ASN	GLY	SER
GLN	MET	SER	PRO	GLY
GLN	THR	THR	SER	LEU
GLY	LYS	TYR	VAL	TYR
ASN	ASN	ARG	PHE	SER
VAL	GLN	VAL	PHE	LEU
PHE	VAL	VAL	PHE	SER
SER	SER	SER	PRO	VAL
CYS	LEU	VAL	PRO	VAL
SER	THR	LEU	LYS	VAL
VAL	CYS	THR	PRO	VAL
VAL	LEU	VAL	LYS	VAL
MET	LEU	VAL	ASP	PRO
HIS	VAL	HIS	THR	SER
GLU	LYS	HIS	THR	SER
ALA	GLY	GLN	LEU	SER
LEU	PHE	ASP	MET	SER
HIS	TYR	TRP	ILE	LEU
ASN	PRO	LEU	SER	GLY
HIS	SER	ASN	ARG	THR
TYR	ASP	GLY	THR	GLN
THR	ILE	LYS	PRO	THR
GLN	ALA	GLU	GLU	TYR
LYS	VAL	TYR	VAL	ILE
SER	GLU	LYS	THR	CYS
LEU	TRP	CYS	CYS	ASN
SER	GLU	LYS	VAL	VAL
LEU	SER	VAL	VAL	ASN
SER	ASN	SER	VAL	HIS
PRO	GLY	ASN	ASP	LYS
GLY	GLN	LYS	VAL	PRO
LYS	GLU	ALA	SER	SER
	GLU	LEU	HIS	ASN
	ASN	PRO	GLU	THR
	ASN	ALA	ASP	LYS
	TYR	PRO	PRO	VAL
	LYS	ILE	GLU	ASP
	THR	GLU	VAL	LYS
	PRO	THR	PHE	VAL
	PRO	ILE	ASN	GLU
	VAL	SER	TRP	PRO
	LEU	LYS	TYR	LYS
	ASP	ALA	VAL	SER
	SER	LYS	ASP	CYS
	ASN	GLY	GLY	ASN

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	108702	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	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 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.082	Depositor
Minimum map value	-0.035	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.016	Depositor
Map size (\AA)	345.6, 345.6, 345.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.08, 1.08, 1.08	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.34	0/1579	0.49	0/2149
2	B	0.31	0/839	0.57	0/1138
3	C	0.28	0/718	0.49	0/986
All	All	0.32	0/3136	0.51	0/4273

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	1536	0	1452	38	0
2	B	819	0	798	37	0
3	C	705	0	482	22	0
4	A	14	0	13	0	0
All	All	3074	0	2745	92	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 16.

All (92) 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)
3:C:2:VAL:HA	3:C:25:SER:O	1.75	0.86
2:B:39:LYS:NZ	2:B:81:GLU:O	2.13	0.79
2:B:89:LEU:HD11	2:B:96:TYR:HB3	1.63	0.79
2:B:39:LYS:NZ	2:B:81:GLU:OE2	2.17	0.74
1:A:454:ARG:NH2	1:A:469:SER:O	2.22	0.73
2:B:22:THR:HG22	2:B:72:THR:HG22	1.74	0.70
1:A:518:LEU:HG	1:A:519:HIS:H	1.58	0.68
1:A:405:ASP:O	1:A:408:ARG:NH1	2.28	0.67
2:B:33:LEU:HB3	2:B:51:ALA:HB2	1.77	0.66
1:A:496:GLY:O	1:A:501:ASN:ND2	2.27	0.66
1:A:486:PHE:N	3:C:101:VAL:O	2.27	0.65
3:C:100:THR:OG1	3:C:104:GLY:N	2.27	0.65
2:B:79:GLN:HE22	2:B:81:GLU:HB3	1.62	0.65
2:B:63:SER:OG	2:B:74:THR:OG1	2.16	0.63
1:A:334:ASN:OD1	1:A:335:LEU:N	2.31	0.63
1:A:336:CYS:H	1:A:363:ALA:HB2	1.63	0.63
2:B:79:GLN:NE2	2:B:81:GLU:HB3	2.16	0.61
1:A:418:ILE:HA	1:A:422:ASN:HD22	1.65	0.60
1:A:411:ALA:HB3	1:A:414:GLN:HG3	1.84	0.59
3:C:98:ARG:NH1	3:C:99:GLU:O	2.34	0.59
1:A:384:PRO:HA	1:A:387:LEU:HD23	1.84	0.59
1:A:440:ASN:OD1	1:A:441:LEU:N	2.37	0.58
1:A:494:SER:OG	1:A:495:TYR:N	2.37	0.58
1:A:380:TYR:CE2	1:A:412:PRO:HD2	2.40	0.57
3:C:37:VAL:O	3:C:95:TYR:N	2.30	0.57
3:C:98:ARG:HH12	3:C:100:THR:HG23	1.70	0.56
1:A:478:THR:HG22	3:C:33:GLY:H	1.71	0.55
2:B:55:LEU:HD12	2:B:56:SER:H	1.71	0.55
1:A:498:GLN:H	1:A:501:ASN:ND2	2.04	0.55
3:C:59:TYR:OH	3:C:69:THR:N	2.40	0.55
2:B:39:LYS:HB2	2:B:42:LYS:HG2	1.88	0.54
3:C:89:GLU:N	3:C:89:GLU:OE1	2.41	0.53
1:A:438:SER:OG	1:A:442:ASP:OD2	2.23	0.53
1:A:365:TYR:HB2	1:A:387:LEU:HD11	1.91	0.52
2:B:6:GLN:HG2	2:B:23:CYS:SG	2.50	0.52
2:B:20:THR:HG22	2:B:74:THR:HG22	1.92	0.52
2:B:6:GLN:HB2	2:B:100:GLN:O	2.11	0.51
1:A:447:GLY:HA2	1:A:497:PHE:O	2.10	0.51
2:B:29:ILE:O	2:B:68:GLU:HA	2.10	0.51
2:B:24:ARG:NH1	2:B:26:ARG:HD3	2.25	0.50
3:C:98:ARG:HH12	3:C:100:THR:CG2	2.24	0.50
2:B:38:GLN:OE1	3:C:45:LEU:HD11	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:ASN:O	1:A:443:SER:OG	2.30	0.50
2:B:27:GLN:HG3	2:B:28:GLY:H	1.75	0.50
1:A:474:GLN:NE2	1:A:478:THR:O	2.44	0.49
2:B:17:ASP:OD1	2:B:18:ARG:N	2.43	0.49
3:C:97:ALA:HA	3:C:108:TRP:HA	1.93	0.49
1:A:417:LYS:NZ	1:A:455:LEU:HG	2.27	0.49
3:C:38:ARG:HA	3:C:94:TYR:HA	1.94	0.49
1:A:421:TYR:CD1	1:A:457:ARG:HB3	2.47	0.49
1:A:342:PHE:HE2	1:A:434:ILE:HG21	1.78	0.48
3:C:72:ARG:O	3:C:76:LYS:N	2.46	0.48
3:C:40:ALA:HA	3:C:92:ALA:HA	1.96	0.48
2:B:39:LYS:HE2	2:B:84:ALA:HB2	1.96	0.48
2:B:3:GLN:OE1	2:B:4:MET:N	2.47	0.48
3:C:5:VAL:O	3:C:22:CYS:HA	2.13	0.48
2:B:32:TYR:HB3	2:B:91:HIS:NE2	2.29	0.47
2:B:35:TRP:CE2	2:B:73:LEU:HB2	2.50	0.47
3:C:91:THR:HG22	3:C:115:THR:HA	1.96	0.47
1:A:431:GLY:HA2	1:A:515:PHE:CD2	2.50	0.47
1:A:412:PRO:HB3	1:A:426:PRO:O	2.15	0.46
2:B:18:ARG:HD2	2:B:76:SER:HA	1.98	0.45
2:B:33:LEU:HD12	2:B:89:LEU:O	2.16	0.45
2:B:62:PHE:CD1	2:B:75:ILE:HD12	2.51	0.45
3:C:59:TYR:HH	3:C:69:THR:H	1.64	0.45
2:B:30:SER:OG	2:B:31:ASN:N	2.50	0.45
2:B:14:SER:HB3	2:B:106:ILE:HD12	1.99	0.45
2:B:33:LEU:O	2:B:51:ALA:N	2.51	0.44
2:B:49:TYR:O	2:B:53:SER:OG	2.23	0.44
2:B:32:TYR:HA	2:B:50:ALA:HA	1.99	0.44
1:A:388:ASN:O	1:A:388:ASN:ND2	2.49	0.44
1:A:403:ARG:O	1:A:406:GLU:HG2	2.18	0.43
3:C:92:ALA:HB3	3:C:94:TYR:CE2	2.53	0.43
1:A:497:PHE:CE2	1:A:507:PRO:HB3	2.54	0.43
1:A:377:PHE:HE2	1:A:384:PRO:HB3	1.84	0.43
1:A:456:PHE:HD2	1:A:491:PRO:HA	1.83	0.43
1:A:490:PHE:CE2	1:A:492:LEU:HB2	2.53	0.43
1:A:416:GLY:O	1:A:420:ASP:N	2.50	0.43
2:B:24:ARG:HH12	2:B:26:ARG:HD3	1.84	0.42
2:B:94:TYR:N	2:B:95:PRO:HD2	2.34	0.42
1:A:392:PHE:CD1	1:A:515:PHE:HB3	2.55	0.42
1:A:418:ILE:HA	1:A:422:ASN:ND2	2.31	0.42
2:B:61:ARG:NH2	2:B:79:GLN:HE21	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:PHE:HA	2:B:49:TYR:CE1	2.54	0.42
2:B:32:TYR:HB2	2:B:92:ASN:OD1	2.20	0.42
1:A:479:PRO:HG3	3:C:53:PHE:CZ	2.55	0.41
1:A:365:TYR:CB	1:A:387:LEU:HD11	2.50	0.41
1:A:355:ARG:NH2	1:A:398:ASP:OD2	2.48	0.41
2:B:83:PHE:CE2	2:B:105:GLU:HB3	2.56	0.41
3:C:38:ARG:HD3	3:C:94:TYR:CZ	2.56	0.40
2:B:18:ARG:HA	2:B:75:ILE:O	2.20	0.40
3:C:102:SER:OG	3:C:103:TYR:N	2.55	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	192/194 (99%)	178 (93%)	14 (7%)	0	100	100
2	B	104/214 (49%)	87 (84%)	17 (16%)	0	100	100
3	C	110/448 (25%)	100 (91%)	10 (9%)	0	100	100
All	All	406/856 (47%)	365 (90%)	41 (10%)	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	167/167 (100%)	166 (99%)	1 (1%)	84	90
2	B	91/188 (48%)	91 (100%)	0	100	100
3	C	36/394 (9%)	36 (100%)	0	100	100
All	All	294/749 (39%)	293 (100%)	1 (0%)	90	94

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

Mol	Chain	Res	Type
1	A	388	ASN

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 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	$\# Z > 2$
4	NAG	A	601	1	14,14,15	0.21	0	17,19,21	0.45	0

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
4	NAG	A	601	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	NAG	C4-C5-C6-O6
4	A	601	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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.

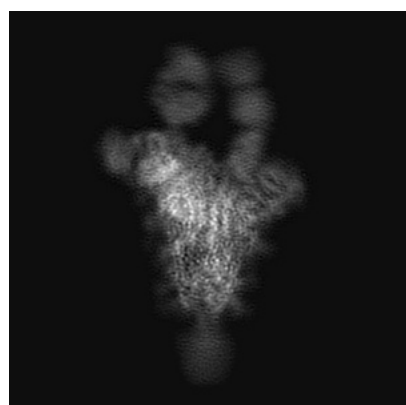
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30977. These allow visual inspection of the internal detail of the map and identification of artifacts.

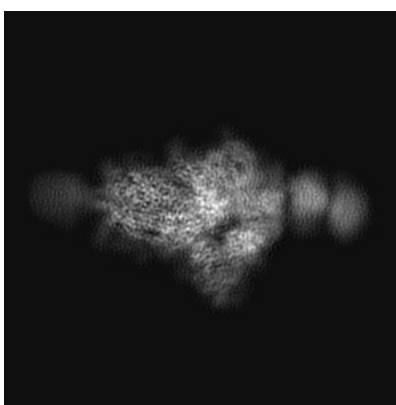
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

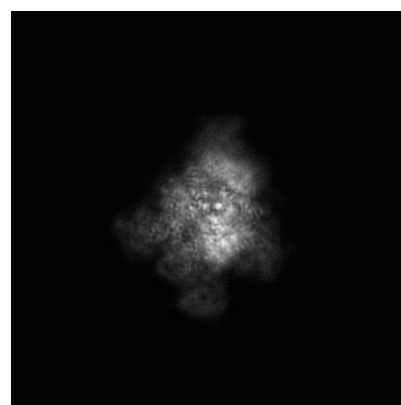
6.1.1 Primary map



X



Y

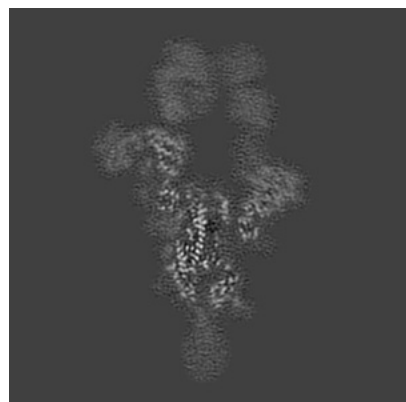


Z

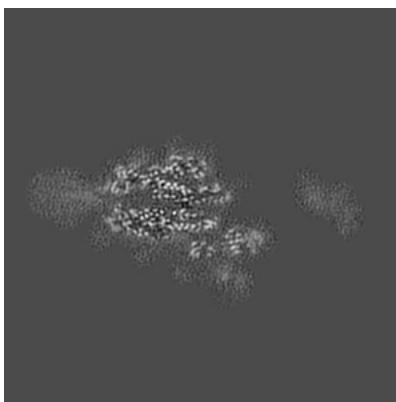
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 160



Y Index: 160

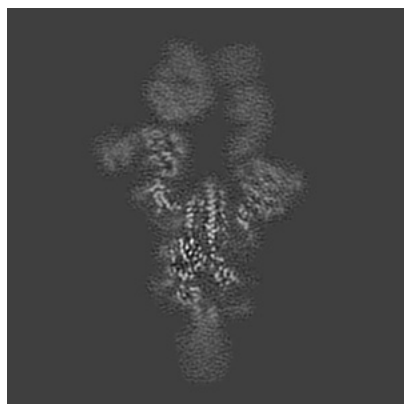


Z Index: 160

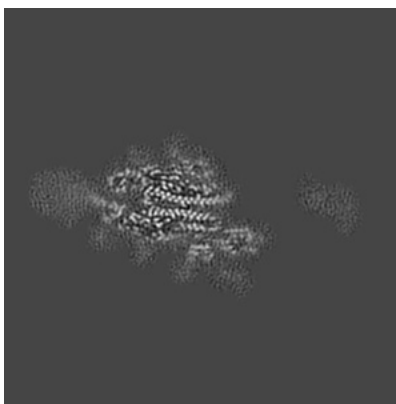
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

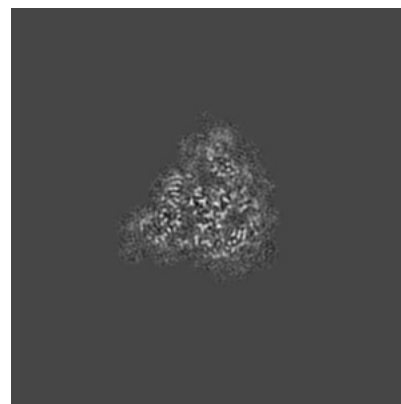
6.3.1 Primary map



X Index: 166



Y Index: 163

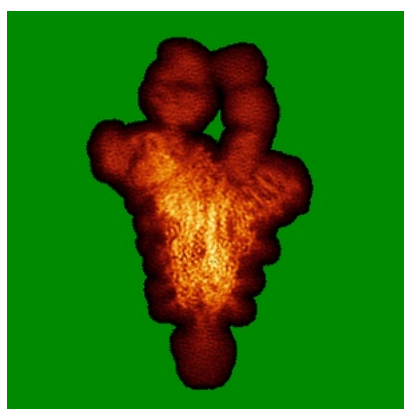


Z Index: 158

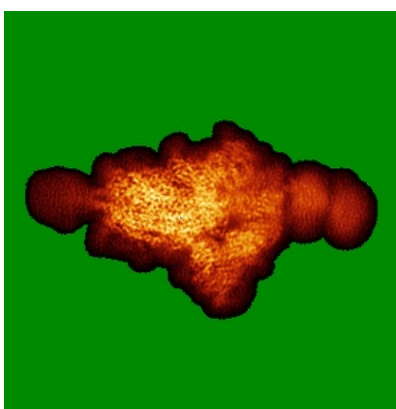
The images above show the largest variance slices of the map in three orthogonal directions.

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

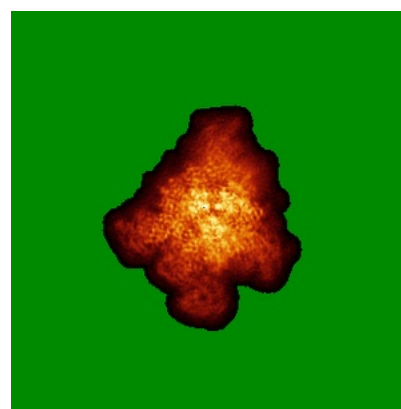
6.4.1 Primary map



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

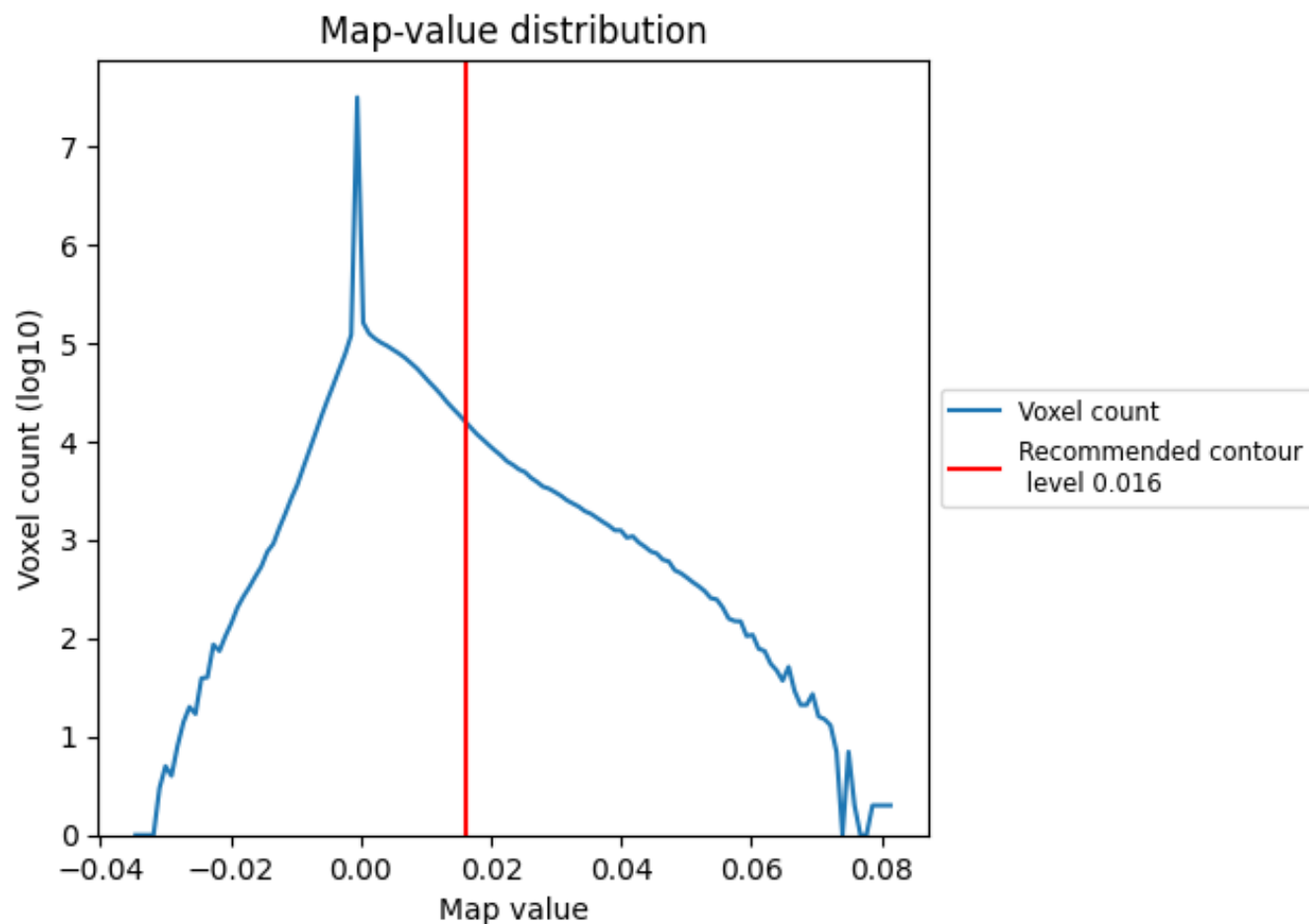
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

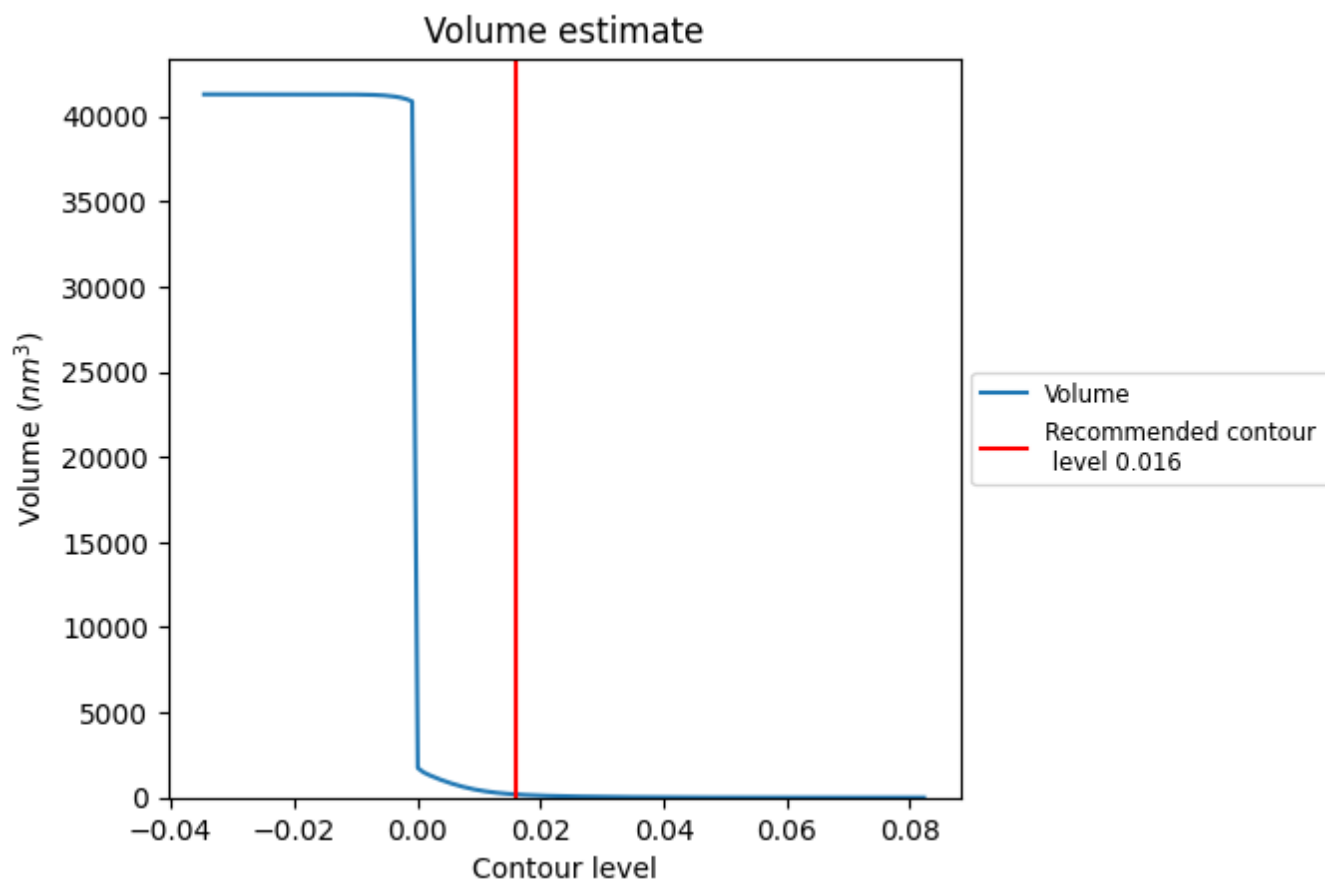
This section contains the results of statistical analysis of the map.

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.

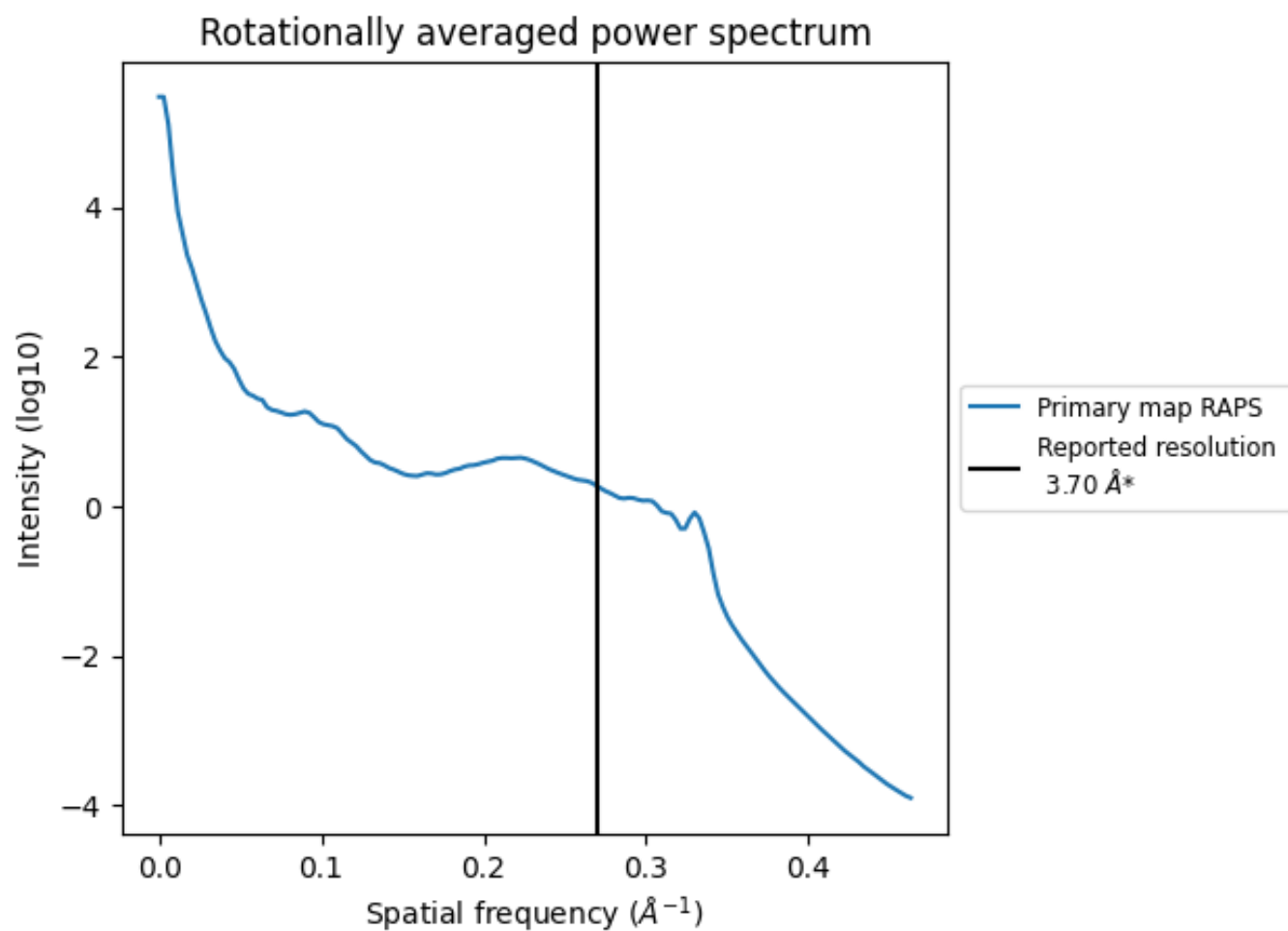
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 186 nm^3 ; this corresponds to an approximate mass of 168 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 ⓘ

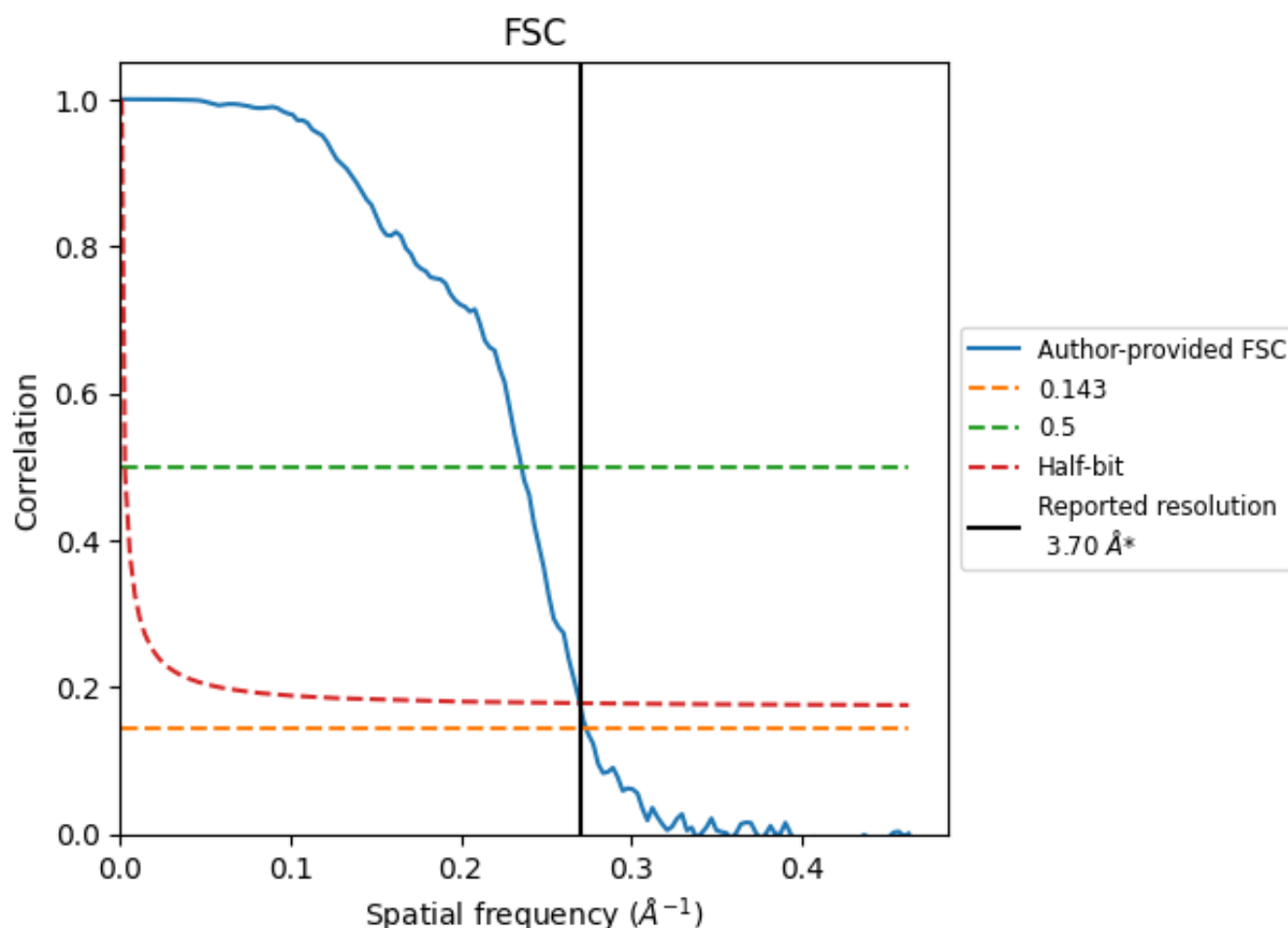


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 0.270 Å⁻¹

8.2 Resolution estimates [i](#)

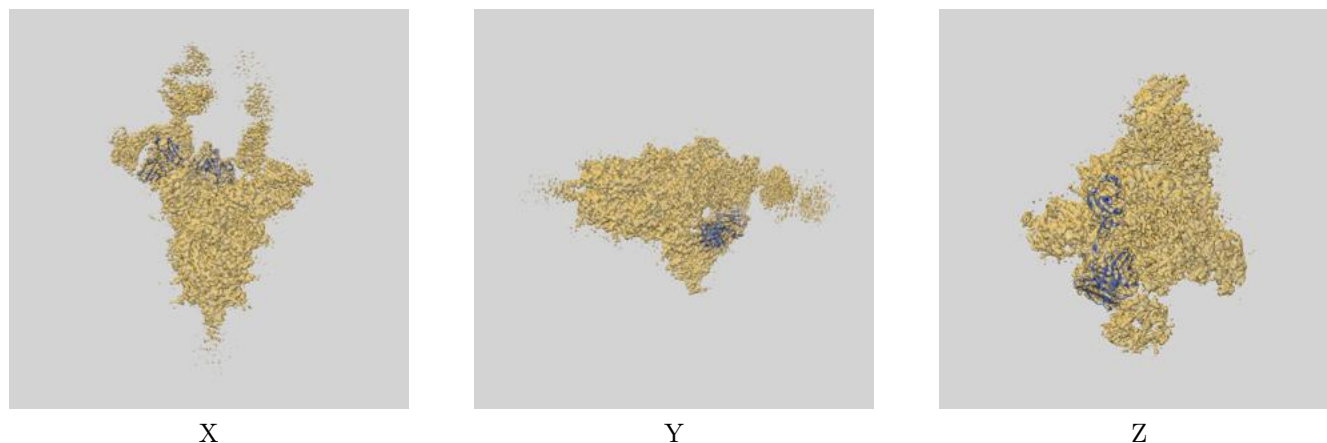
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.65	4.24	3.71
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

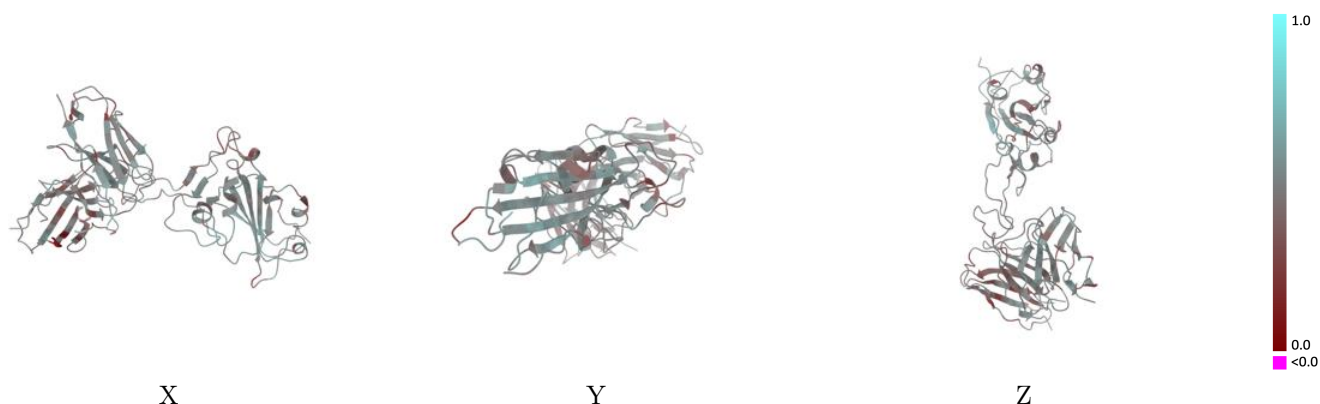
This section contains information regarding the fit between EMDB map EMD-30977 and PDB model 7E39. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



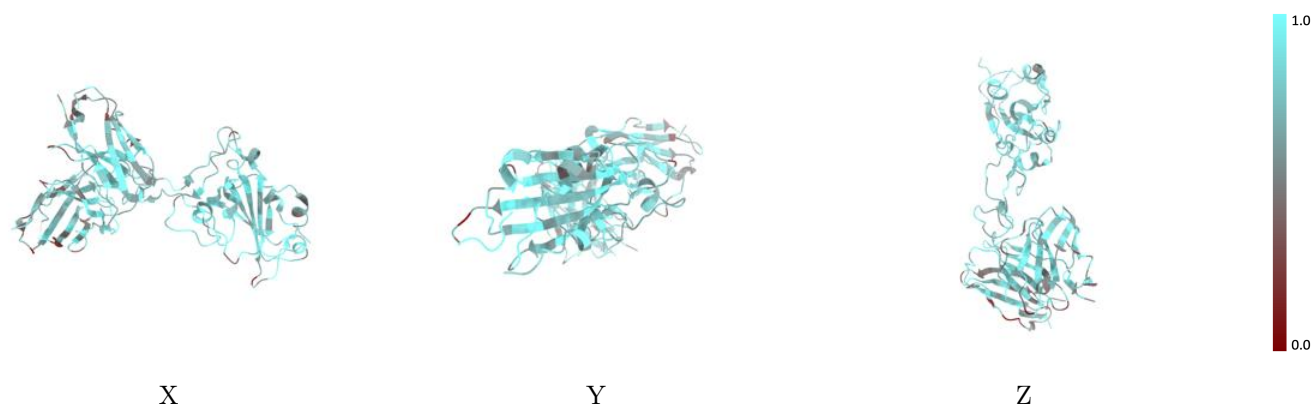
The images above show the 3D surface view of the map at the recommended contour level 0.016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



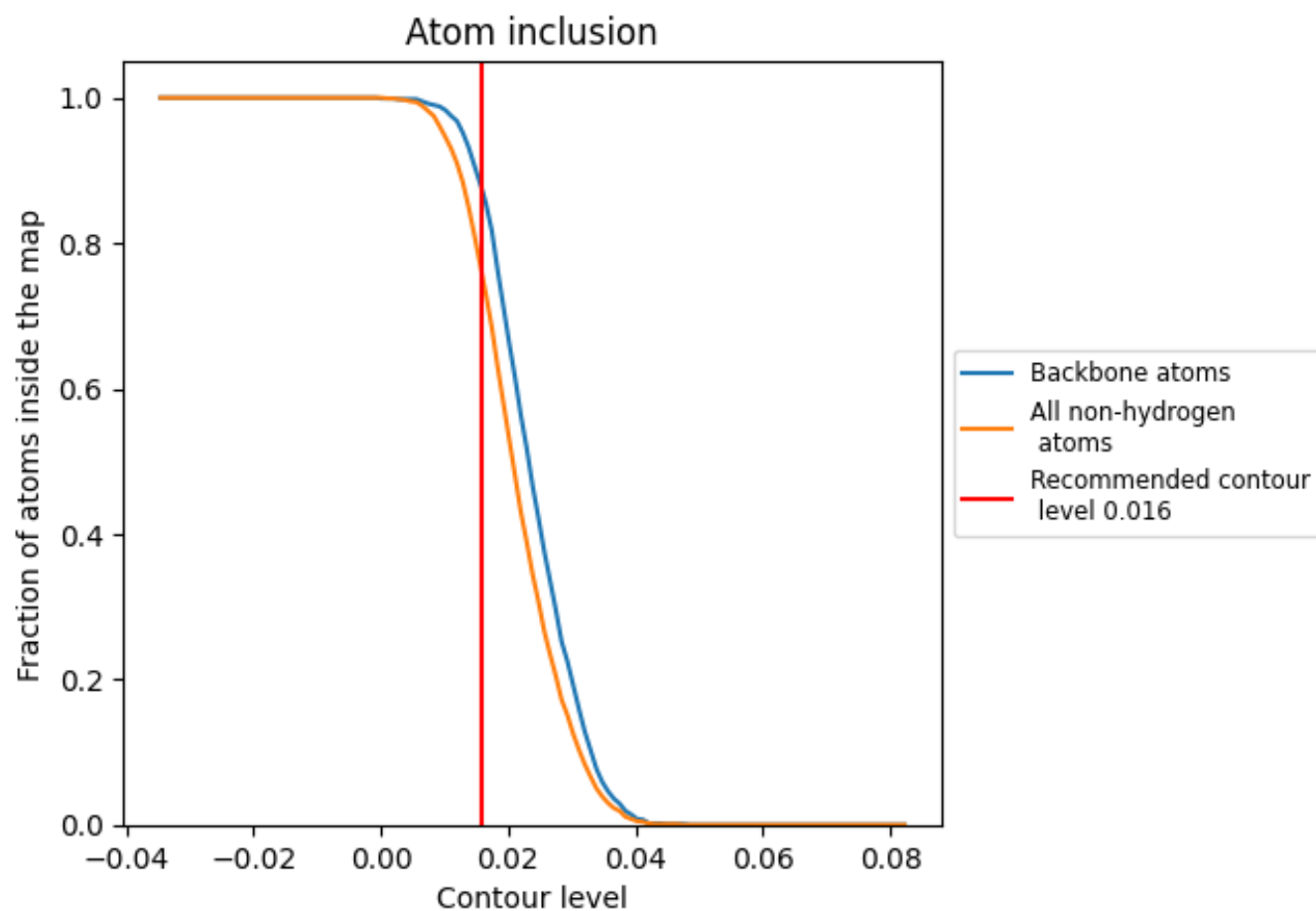
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.016).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 75% 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 (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7530	<div></div> 0.4760
A	<div></div> 0.7740	<div></div> 0.4890
B	<div></div> 0.7340	<div></div> 0.4820
C	<div></div> 0.7290	<div></div> 0.4420

