



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 04:59 AM UTC

PDB ID : 8Z6T / pdb_00008z6t
EMDB ID : EMD-39804
Title : Structure of XBB.1.16 RBD in complex with antibody CYFN1006-1.
Authors : Wang, Y.J.; Sun, L.
Deposited on : 2024-04-19
Resolution : 2.92 Å(reported)

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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

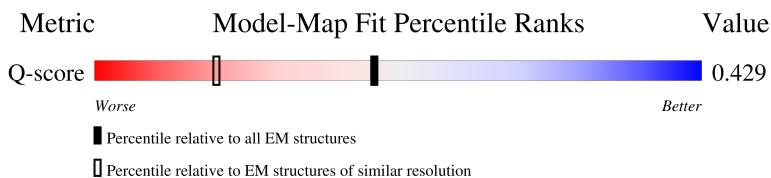
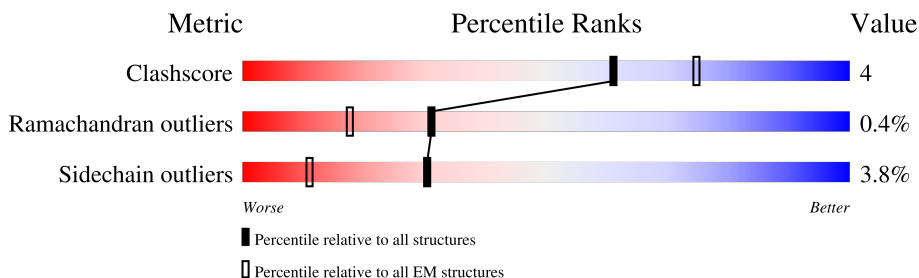
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.92 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	13007 (2.42 - 3.42)

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	1299	
2	C	215	
3	B	451	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4526 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,Fibritin,Expression Tag.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	196	Total	C	N	O	S	0	0
			1558	1004	263	283	8		

There are 81 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP P0DTC2
A	-5	PRO	-	expression tag	UNP P0DTC2
A	-4	MET	-	expression tag	UNP P0DTC2
A	-3	GLY	-	expression tag	UNP P0DTC2
A	-2	SER	-	expression tag	UNP P0DTC2
A	-1	LEU	-	expression tag	UNP P0DTC2
A	0	GLN	-	expression tag	UNP P0DTC2
A	1	PRO	-	expression tag	UNP P0DTC2
A	2	LEU	-	expression tag	UNP P0DTC2
A	3	ALA	-	expression tag	UNP P0DTC2
A	4	THR	-	expression tag	UNP P0DTC2
A	5	LEU	-	expression tag	UNP P0DTC2
A	6	TYR	-	expression tag	UNP P0DTC2
A	7	LEU	-	expression tag	UNP P0DTC2
A	8	LEU	-	expression tag	UNP P0DTC2
A	9	GLY	-	expression tag	UNP P0DTC2
A	10	MET	-	expression tag	UNP P0DTC2
A	11	LEU	-	expression tag	UNP P0DTC2
A	12	VAL	-	expression tag	UNP P0DTC2
A	13	ALA	-	expression tag	UNP P0DTC2
A	14	SER	-	expression tag	UNP P0DTC2
A	15	VAL	-	expression tag	UNP P0DTC2
A	16	LEU	-	expression tag	UNP P0DTC2
A	17	ALA	-	expression tag	UNP P0DTC2
A	23	ILE	THR	variant	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	28	SER	ALA	variant	UNP P0DTC2
A	84	ALA	VAL	variant	UNP P0DTC2
A	143	ASP	GLY	variant	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	146	GLN	HIS	variant	UNP P0DTC2
A	180	VAL	GLU	variant	UNP P0DTC2
A	183	GLU	GLN	variant	UNP P0DTC2
A	213	GLU	VAL	variant	UNP P0DTC2
A	252	VAL	GLY	variant	UNP P0DTC2
A	339	HIS	GLY	variant	UNP P0DTC2
A	346	THR	ARG	variant	UNP P0DTC2
A	368	ILE	LEU	variant	UNP P0DTC2
A	371	PHE	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	376	ALA	THR	variant	UNP P0DTC2
A	405	ASN	ASP	variant	UNP P0DTC2
A	408	SER	ARG	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	445	PRO	VAL	variant	UNP P0DTC2
A	446	SER	GLY	variant	UNP P0DTC2
A	460	LYS	ASN	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	ARG	THR	conflict	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2
A	486	PRO	PHE	variant	UNP P0DTC2
A	490	SER	PHE	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	679	LYS	ASN	variant	UNP P0DTC2
A	681	HIS	PRO	variant	UNP P0DTC2
A	682	GLY	ARG	conflict	UNP P0DTC2
A	683	SER	ARG	conflict	UNP P0DTC2
A	685	SER	-	insertion	UNP P0DTC2
A	686	SER	-	insertion	UNP P0DTC2
A	687	LYS	-	insertion	UNP P0DTC2
A	689	SER	-	insertion	UNP P0DTC2
A	768	LYS	ASN	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	800	TYR	ASP	conflict	UNP P0DTC2
A	821	PRO	PHE	conflict	UNP P0DTC2
A	896	PRO	ALA	conflict	UNP P0DTC2
A	903	PRO	ALA	conflict	UNP P0DTC2
A	946	PRO	ALA	conflict	UNP P0DTC2
A	958	HIS	GLN	variant	UNP P0DTC2
A	973	LYS	ASN	variant	UNP P0DTC2
A	990	PRO	LYS	conflict	UNP P0DTC2
A	991	PRO	VAL	conflict	UNP P0DTC2
A	1213	GLY	-	linker	UNP P0DTC2
A	1214	SER	-	linker	UNP P0DTC2

- Molecule 2 is a protein called CYFN1006-1 lighth chain.

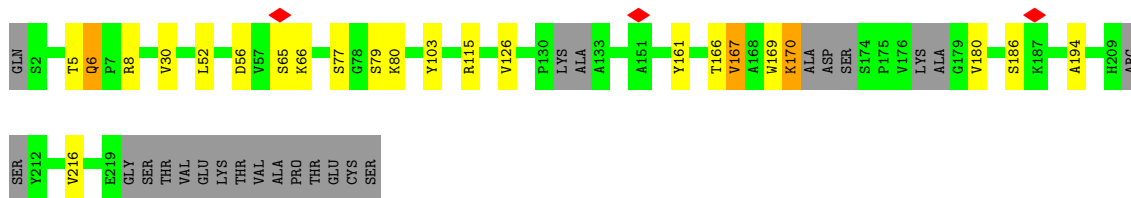
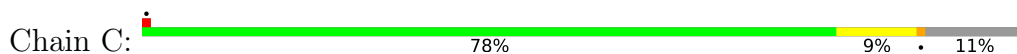
Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	191	Total	C	N	O	S	0	0
			1424	892	236	289	7		

- Molecule 3 is a protein called CYFN1006-1 heavy chain.

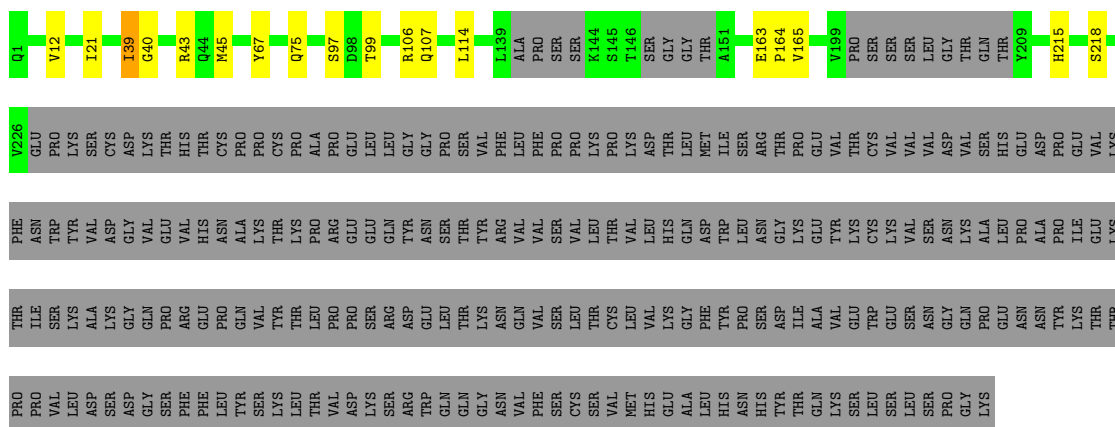
Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	202	Total	C	N	O	S	0	0
			1544	992	251	293	8		

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

- Molecule 2: CYFN1006-1 ligh chain



- Molecule 3: CYFN1006-1 heavy chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	936842	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.968	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	298.24, 298.24, 298.24	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.932, 0.932, 0.932	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	0.42	1/1607 (0.1%)	0.43	1/2190 (0.0%)
2	C	0.20	0/1455	0.37	0/1979
3	B	0.29	0/1584	0.31	0/2151
All	All	0.32	1/4646 (0.0%)	0.38	1/6320 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	443	SER	CA-C	-5.75	1.47	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	443	SER	CB-CA-C	-5.37	104.78	111.43

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	1558	0	1486	16	0
2	C	1424	0	1370	12	0
3	B	1544	0	1519	15	0
All	All	4526	0	4375	39	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (39) 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)
2:C:186:SER:OG	2:C:194:ALA:N	2.20	0.73
3:B:43:ARG:NH1	3:B:45:MET:SD	2.64	0.71
2:C:56:ASP:O	2:C:66:LYS:N	2.23	0.70
2:C:115:ARG:NH2	3:B:67:TYR:O	2.26	0.68
2:C:126:VAL:O	2:C:161:TYR:OH	2.20	0.59
3:B:75:GLN:N	3:B:75:GLN:OE1	2.35	0.59
1:A:401:VAL:HG22	1:A:509:ARG:HG2	1.85	0.59
3:B:215:HIS:ND1	3:B:218:SER:OG	2.22	0.58
1:A:369:TYR:OH	1:A:384:PRO:O	2.23	0.56
3:B:39:ILE:HD13	3:B:40:GLY:N	2.20	0.56
2:C:6:GLN:HE22	2:C:103:TYR:HA	1.71	0.55
1:A:405:ASN:N	1:A:504:GLY:O	2.40	0.54
1:A:417:ASN:OD1	1:A:418:ILE:N	2.42	0.53
1:A:363:ALA:N	1:A:525:CYS:O	2.39	0.53
1:A:358:ILE:HB	1:A:395:VAL:HG13	1.92	0.52
2:C:167:VAL:HG13	2:C:216:VAL:HG22	1.91	0.52
2:C:56:ASP:O	2:C:65:SER:N	2.43	0.51
2:C:52:LEU:HD22	3:B:114:LEU:HD11	1.95	0.48
2:C:169:TRP:NE1	2:C:180:VAL:HG21	2.29	0.48
3:B:99:THR:O	3:B:99:THR:HG23	2.14	0.47
1:A:493:GLN:OE1	1:A:493:GLN:N	2.48	0.46
1:A:457:ARG:NH2	1:A:459:SER:OG	2.50	0.45
2:C:52:LEU:CD2	3:B:114:LEU:HD11	2.47	0.45
3:B:163:GLU:N	3:B:164:PRO:CD	2.80	0.45
3:B:43:ARG:NH1	3:B:97:SER:O	2.50	0.45
3:B:114:LEU:C	3:B:114:LEU:HD13	2.43	0.43
1:A:378:LYS:O	1:A:433:VAL:HG22	2.19	0.43
1:A:445:PRO:HG3	1:A:499:PRO:HG3	2.01	0.43
1:A:393:THR:O	1:A:523:THR:OG1	2.28	0.43
1:A:341:VAL:HG12	2:C:30:VAL:HG21	2.00	0.42
1:A:354:ASN:OD1	1:A:355:ARG:N	2.53	0.42
1:A:358:ILE:HG22	1:A:524:VAL:HG11	2.00	0.42
3:B:215:HIS:CE1	3:B:218:SER:HG	2.25	0.42
2:C:170:LYS:HA	2:C:170:LYS:HD2	1.62	0.42
3:B:12:VAL:O	3:B:12:VAL:HG13	2.20	0.41
1:A:517:LEU:HD12	1:A:517:LEU:O	2.20	0.41
3:B:163:GLU:N	3:B:164:PRO:HD2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:LEU:HD23	1:A:518:LEU:N	2.36	0.41
3:B:163:GLU:O	3:B:165:VAL:N	2.53	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	194/1299 (15%)	184 (95%)	9 (5%)	1 (0%)	24	53
2	C	181/215 (84%)	172 (95%)	9 (5%)	0	100	100
3	B	194/451 (43%)	181 (93%)	12 (6%)	1 (0%)	24	53
All	All	569/1965 (29%)	537 (94%)	30 (5%)	2 (0%)	31	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	107	GLN
1	A	446	SER

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	169/1122 (15%)	162 (96%)	7 (4%)	27	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	162/181 (90%)	153 (94%)	9 (6%)	19	48
3	B	171/399 (43%)	168 (98%)	3 (2%)	51	79
All	All	502/1702 (30%)	483 (96%)	19 (4%)	30	62

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	336	CYS
1	A	346	THR
1	A	406	GLU
1	A	424	LYS
1	A	443	SER
1	A	468	ILE
1	A	517	LEU
2	C	5	THR
2	C	6	GLN
2	C	8	ARG
2	C	77	SER
2	C	79	SER
2	C	80	LYS
2	C	166	THR
2	C	167	VAL
2	C	170	LYS
3	B	21	ILE
3	B	39	ILE
3	B	106	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	394	ASN
1	A	474	GLN
2	C	6	GLN
3	B	107	GLN

5.3.3 RNA ⓘ

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-39804. These allow visual inspection of the internal detail of the map and identification of artifacts.

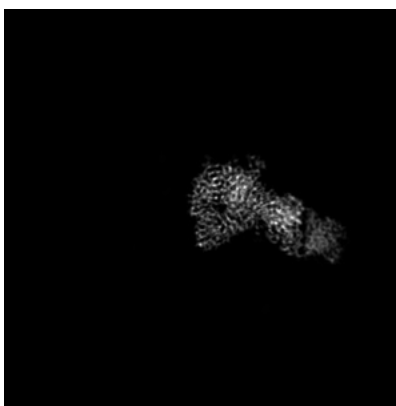
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

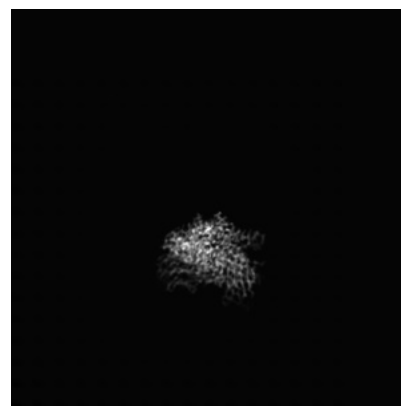
6.1.1 Primary map



X

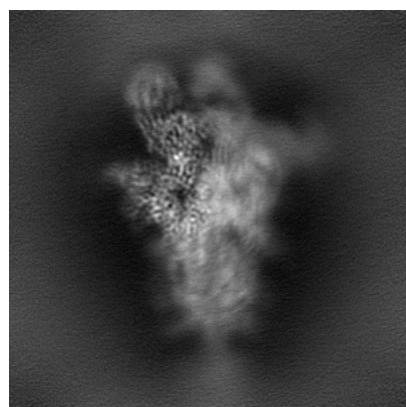


Y

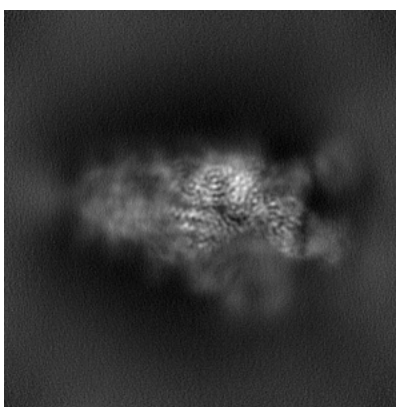


Z

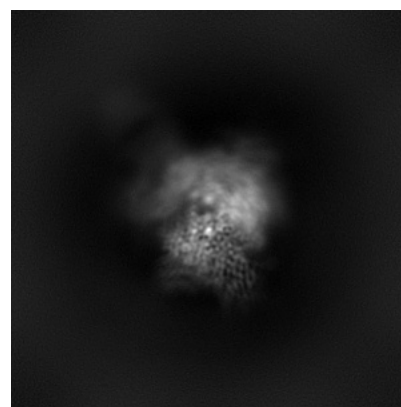
6.1.2 Raw map



X



Y



Z

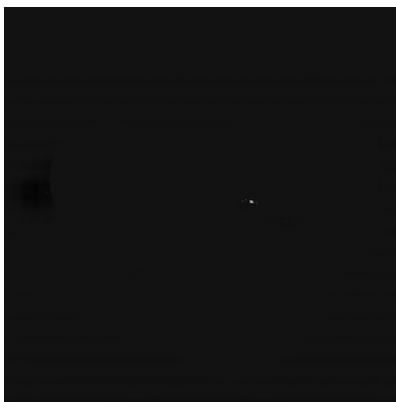
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

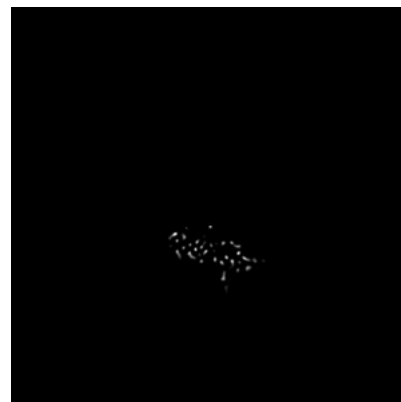
6.2.1 Primary map



X Index: 160

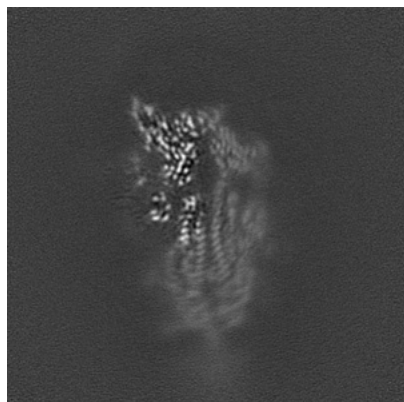


Y Index: 160

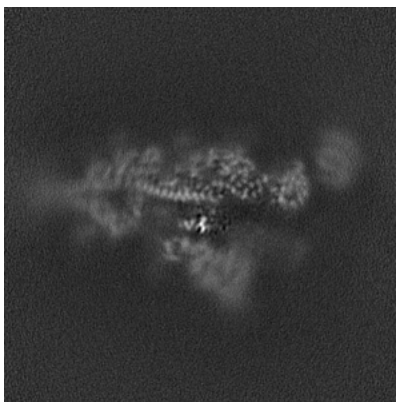


Z Index: 160

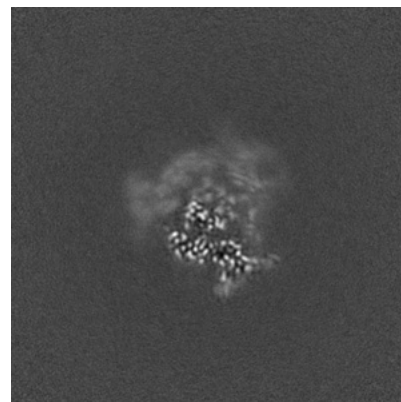
6.2.2 Raw map



X Index: 160



Y Index: 160

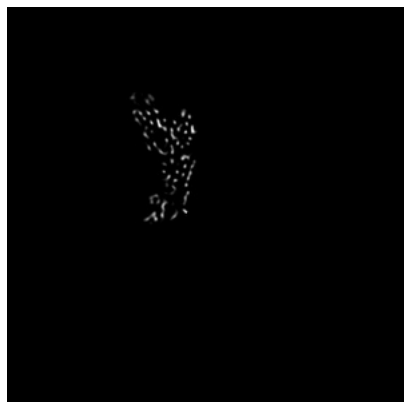


Z Index: 160

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: 156

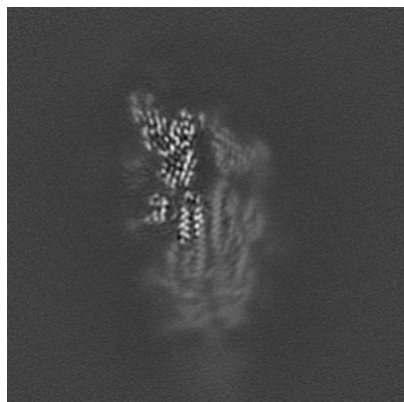


Y Index: 132

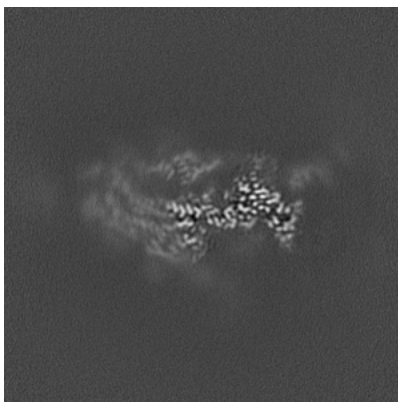


Z Index: 186

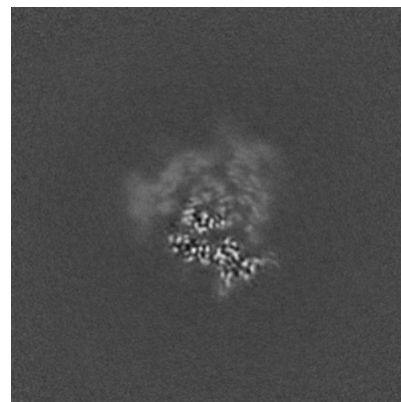
6.3.2 Raw map



X Index: 157



Y Index: 143

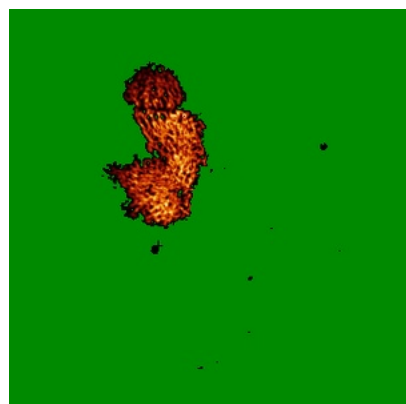


Z Index: 163

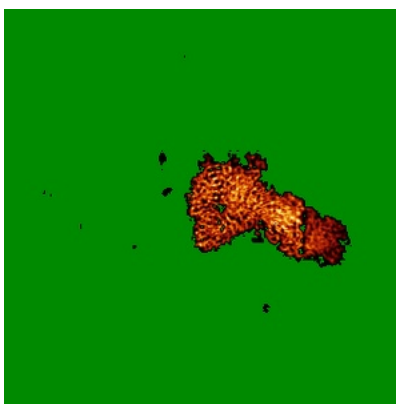
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

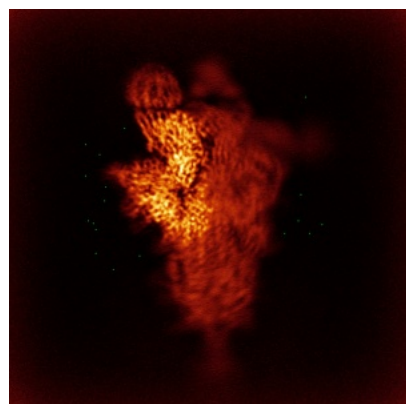


Y

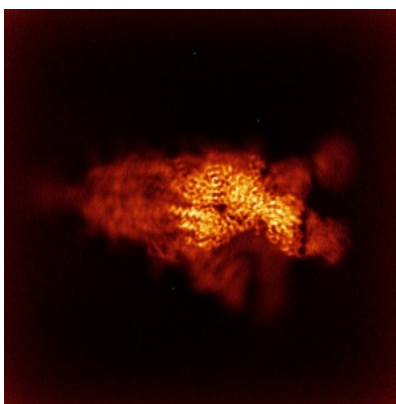


Z

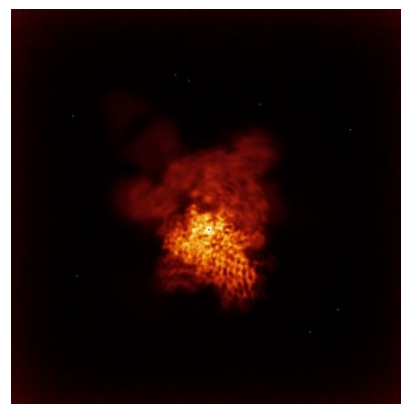
6.4.2 Raw map



X



Y

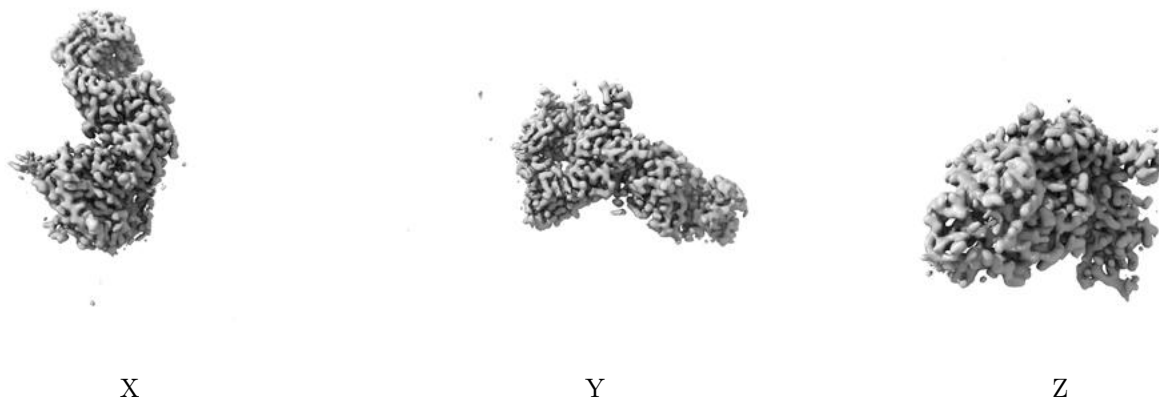


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.03. 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



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.

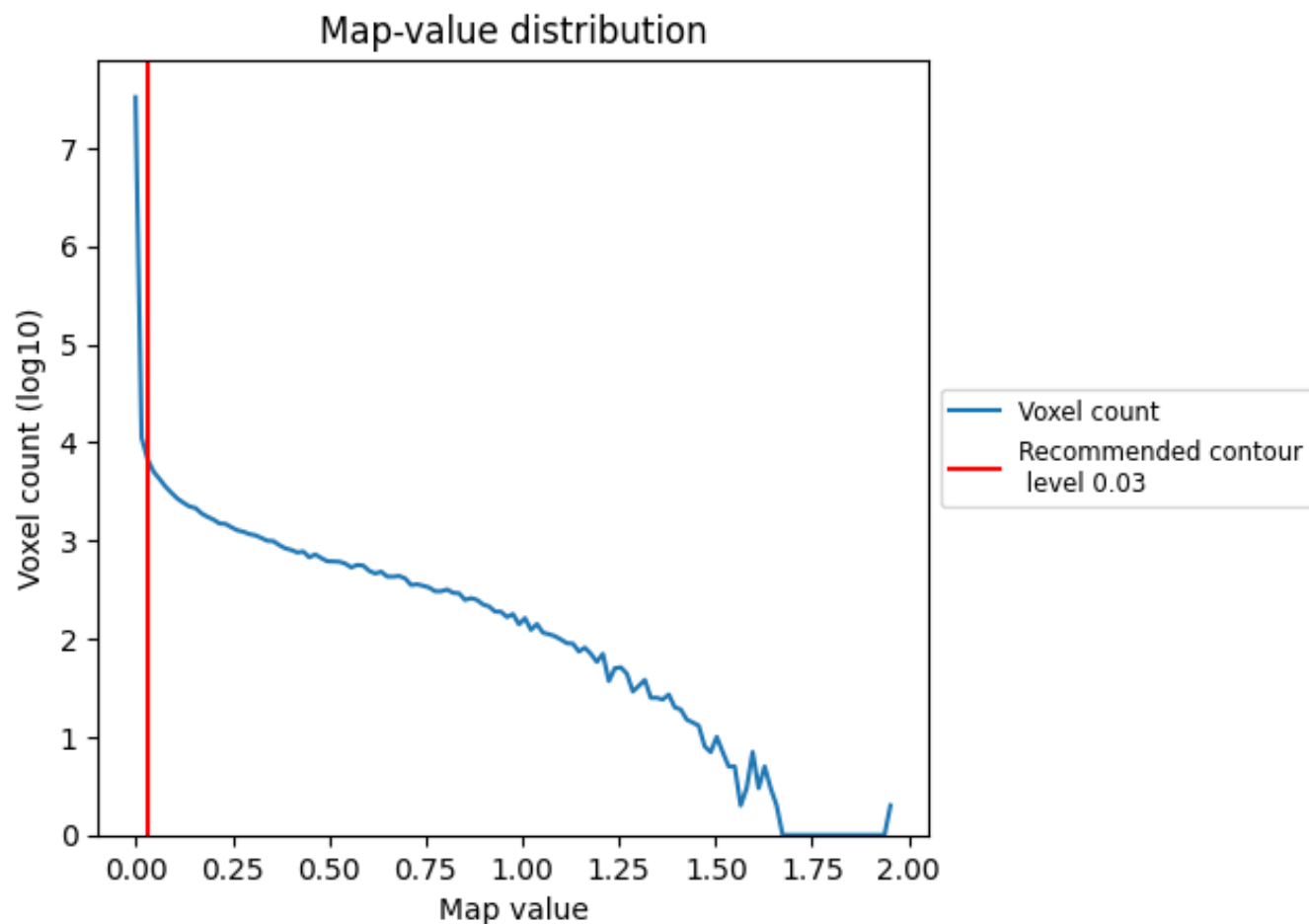
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

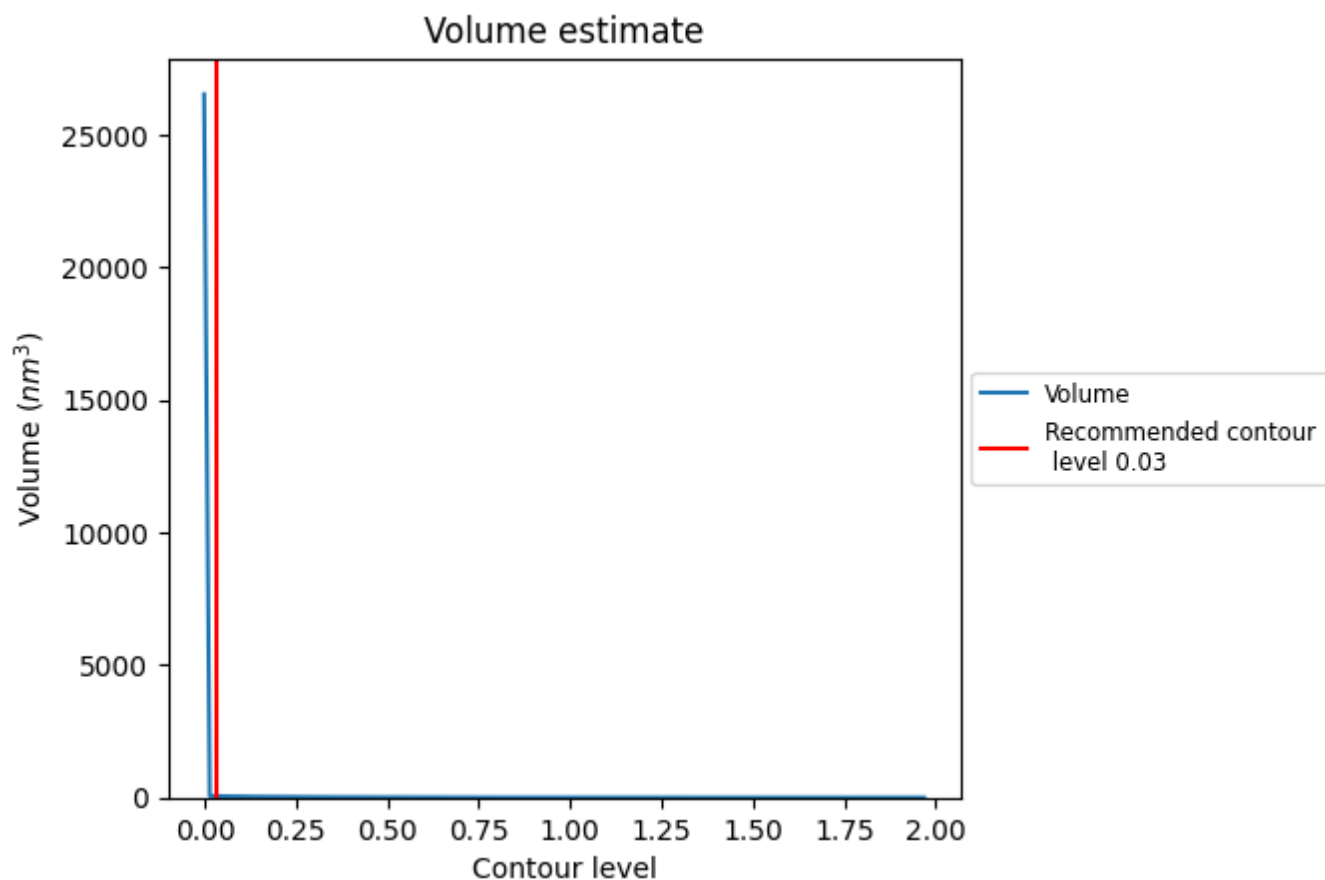
This section contains the results of statistical analysis of the map.

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.

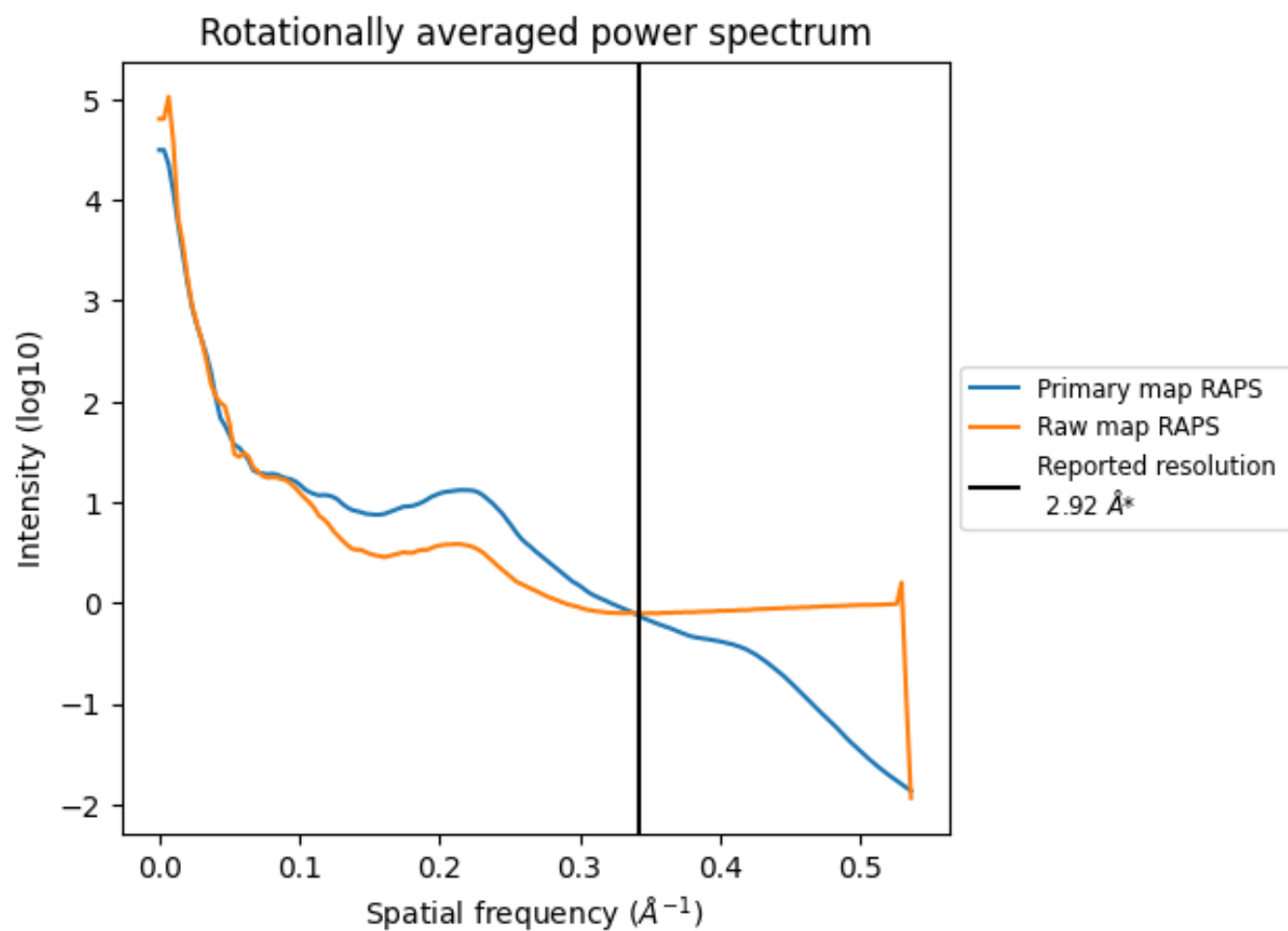
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 56 nm^3 ; this corresponds to an approximate mass of 51 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 ⓘ

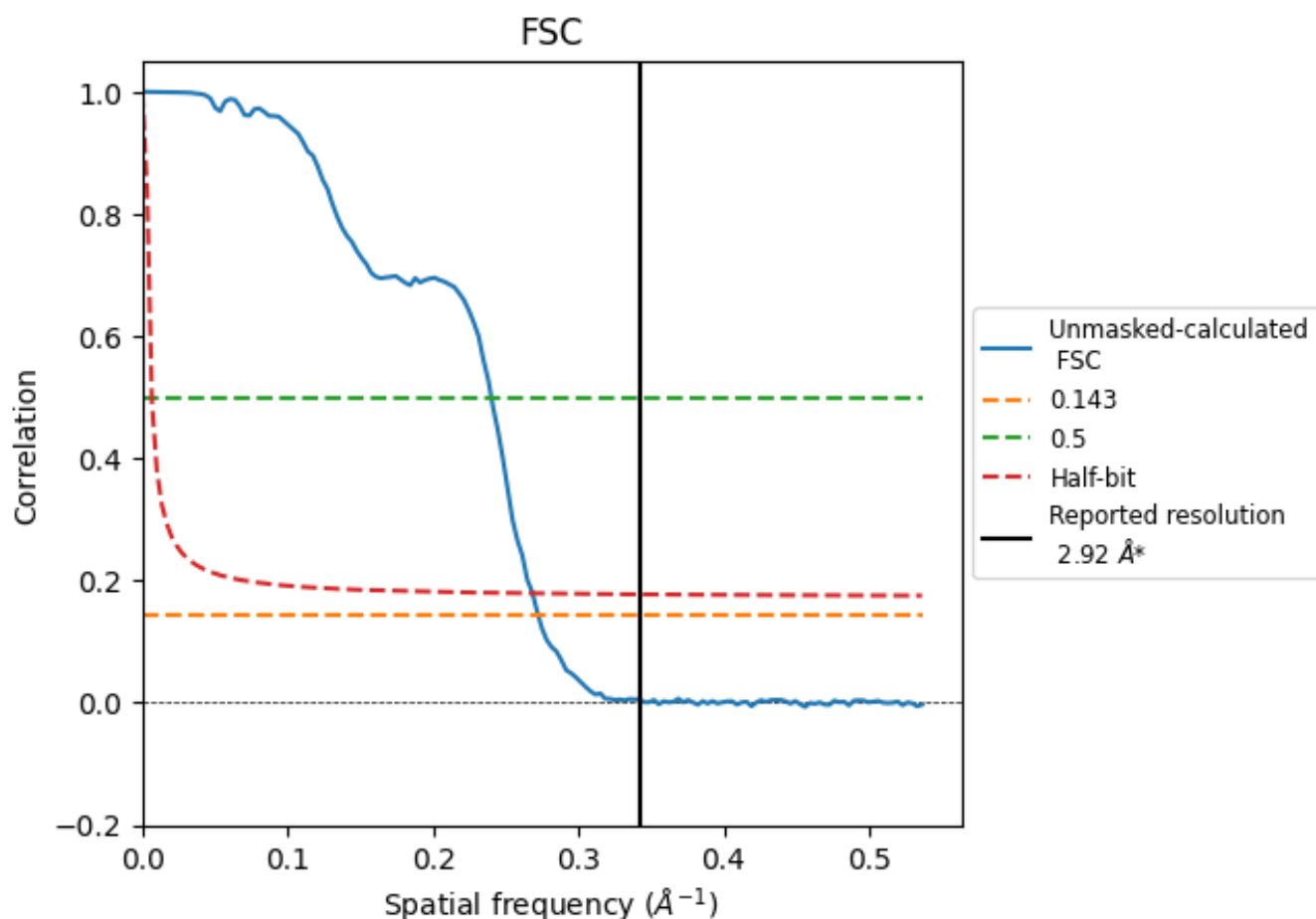


*Reported resolution corresponds to spatial frequency of $0.342 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.342 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

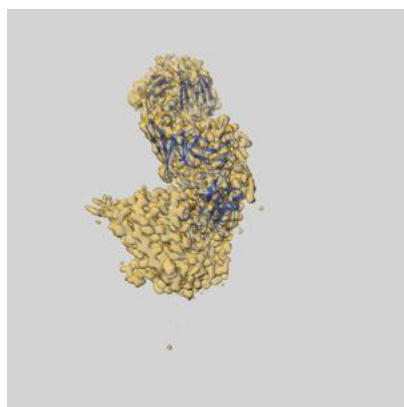
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.92	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.67	4.16	3.72

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.67 differs from the reported value 2.92 by more than 10 %

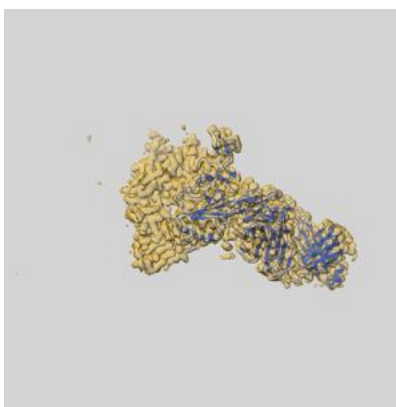
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-39804 and PDB model 8Z6T. Per-residue inclusion information can be found in section [3](#) on page [6](#).

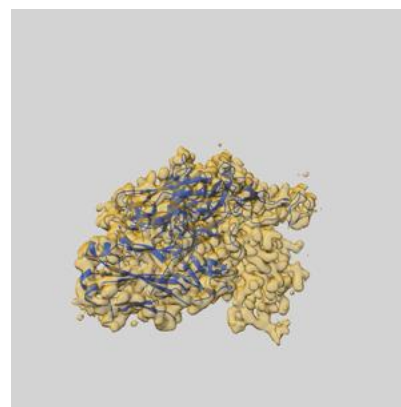
9.1 Map-model overlay [i](#)



X



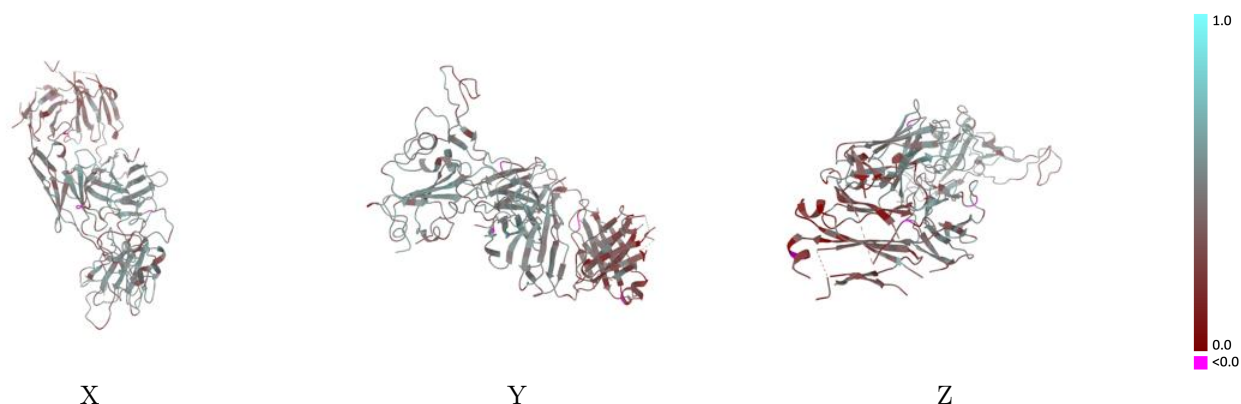
Y



Z

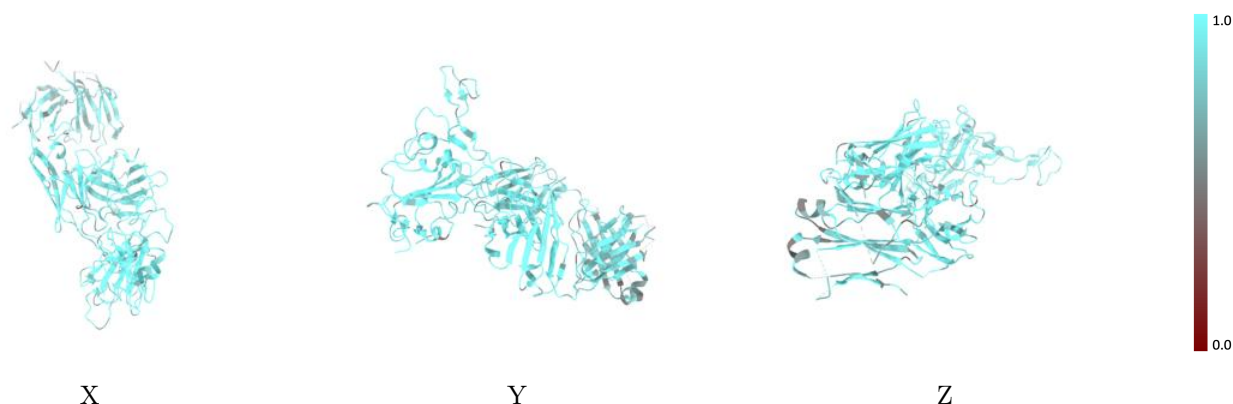
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



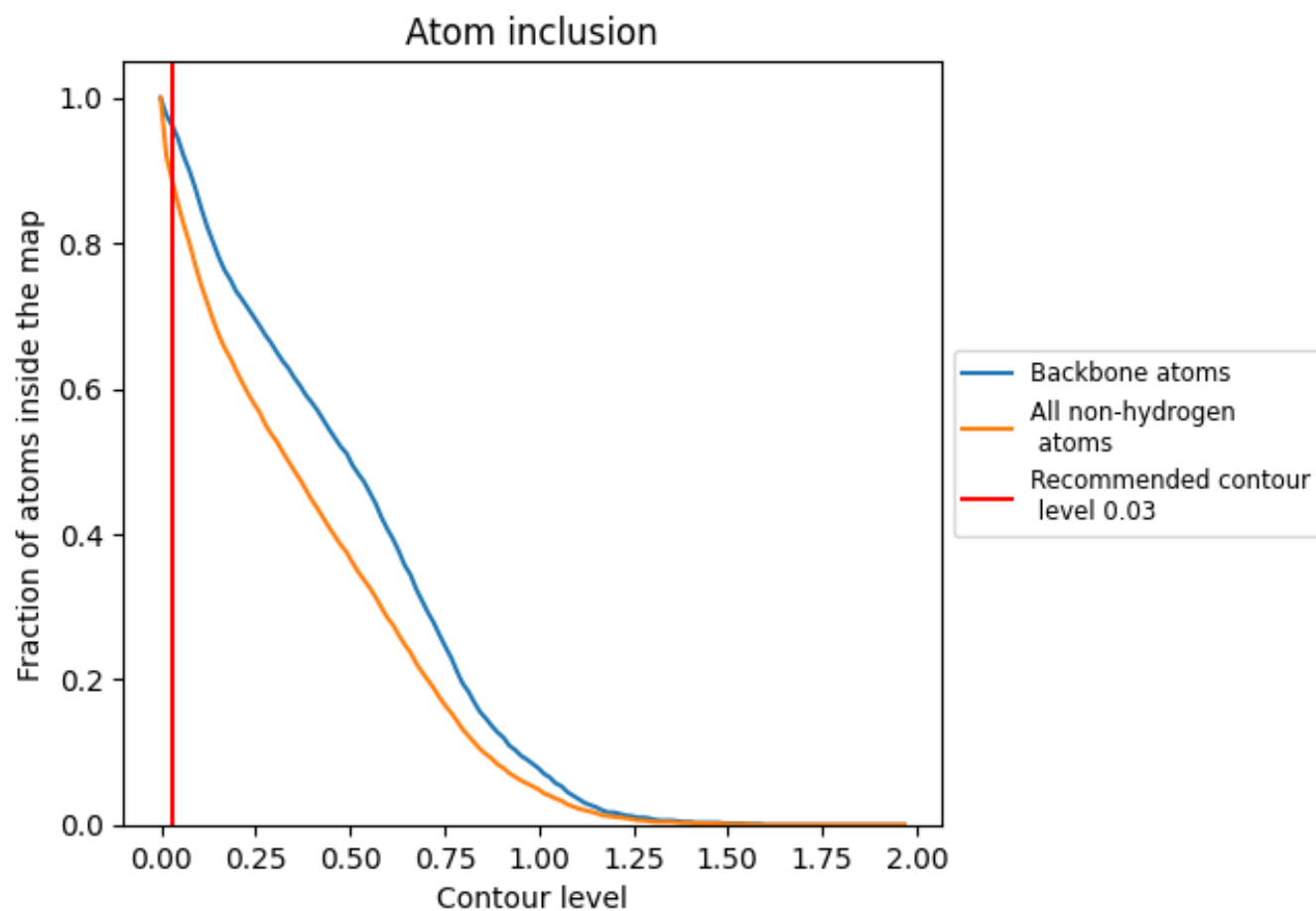
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 88% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8840	0.4290
A	0.9110	0.4770
B	0.8910	0.4250
C	0.8470	0.3790

