



Full wwPDB EM Validation Report ⓘ

Jun 8, 2026 – 10:19 am BST

PDB ID : 9T0E / pdb_00009t0e
EMDB ID : EMD-55399
Title : Structure of Crimean Congo hemorrhagic fever virus (CCHFV) L protein bound to 5' vRNA and nanobody 20096.
Authors : Keown, J.R.; Carrique, L.; Grimes, J.M.
Deposited on : 2025-10-17
Resolution : 2.30 Å(reported)
Based on initial model : .

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.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

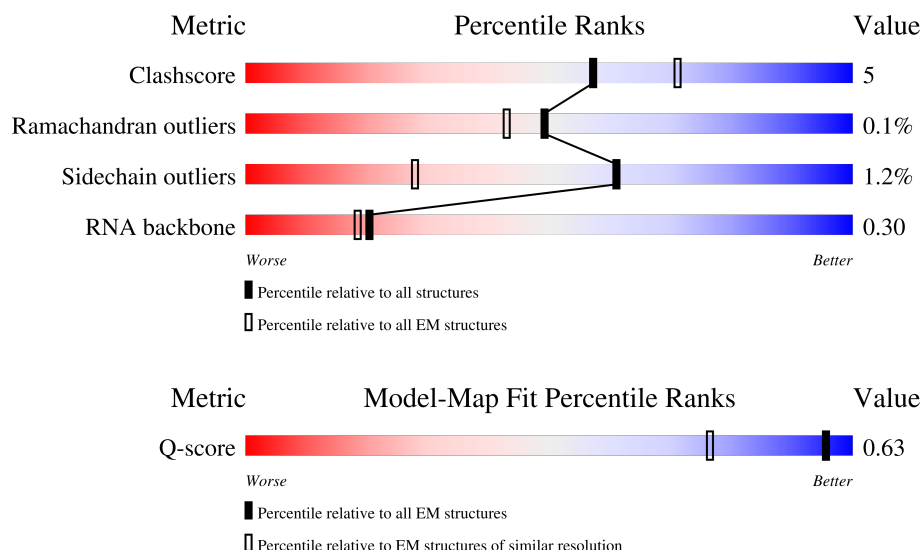
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.30 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	-
RNA backbone	8273	3508	-
Q-score	-	25397	4254 (1.80 - 2.80)

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 $\leq 5\%$. 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	C	130	<div> <div>19%</div> <div> <div></div> <div>71%</div> <div>19%</div> <div>• 9%</div> </div> </div>
2	R	16	<div> <div>6%</div> <div> <div></div> <div>44%</div> <div>31%</div> <div>6%</div> <div>19%</div> </div> </div>
3	A	3990	<div> <div>•</div> <div> <div></div> <div>37%</div> <div>5%</div> <div>58%</div> </div> </div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 29390 atoms, of which 14560 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 Nanobody 20096.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	C	118	Total	C	H	N	O	S	0	0
			1776	561	880	162	169	4		

- Molecule 2 is a RNA chain called RNA (5'-R(P*UP*CP*UP*CP*AP*AP*AP*GP*AP*UP*AP*UP*A)-3').

Mol	Chain	Residues	Atoms						AltConf	Trace
2	R	13	Total	C	H	N	O	P	0	0
			414	124	139	49	89	13		

- Molecule 3 is a protein called RNA-directed RNA polymerase L.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	A	1671	Total	C	H	N	O	S	0	0
			26903	8459	13541	2301	2507	95		

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-44	MET	-	initiating methionine	UNP Q6TQR6
A	-43	TRP	-	expression tag	UNP Q6TQR6
A	-42	SER	-	expression tag	UNP Q6TQR6
A	-41	HIS	-	expression tag	UNP Q6TQR6
A	-40	PRO	-	expression tag	UNP Q6TQR6
A	-39	GLN	-	expression tag	UNP Q6TQR6
A	-38	PHE	-	expression tag	UNP Q6TQR6
A	-37	GLU	-	expression tag	UNP Q6TQR6
A	-36	LYS	-	expression tag	UNP Q6TQR6
A	-35	GLY	-	expression tag	UNP Q6TQR6
A	-34	GLY	-	expression tag	UNP Q6TQR6
A	-33	GLY	-	expression tag	UNP Q6TQR6
A	-32	SER	-	expression tag	UNP Q6TQR6
A	-31	GLY	-	expression tag	UNP Q6TQR6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-30	GLY	-	expression tag	UNP Q6TQR6
A	-29	GLY	-	expression tag	UNP Q6TQR6
A	-28	SER	-	expression tag	UNP Q6TQR6
A	-27	GLY	-	expression tag	UNP Q6TQR6
A	-26	GLY	-	expression tag	UNP Q6TQR6
A	-25	SER	-	expression tag	UNP Q6TQR6
A	-24	SER	-	expression tag	UNP Q6TQR6
A	-23	ALA	-	expression tag	UNP Q6TQR6
A	-22	TRP	-	expression tag	UNP Q6TQR6
A	-21	SER	-	expression tag	UNP Q6TQR6
A	-20	HIS	-	expression tag	UNP Q6TQR6
A	-19	PRO	-	expression tag	UNP Q6TQR6
A	-18	GLN	-	expression tag	UNP Q6TQR6
A	-17	PHE	-	expression tag	UNP Q6TQR6
A	-16	GLU	-	expression tag	UNP Q6TQR6
A	-15	LYS	-	expression tag	UNP Q6TQR6
A	-14	HIS	-	expression tag	UNP Q6TQR6
A	-13	HIS	-	expression tag	UNP Q6TQR6
A	-12	HIS	-	expression tag	UNP Q6TQR6
A	-11	HIS	-	expression tag	UNP Q6TQR6
A	-10	HIS	-	expression tag	UNP Q6TQR6
A	-9	HIS	-	expression tag	UNP Q6TQR6
A	-8	HIS	-	expression tag	UNP Q6TQR6
A	-7	HIS	-	expression tag	UNP Q6TQR6
A	-6	GLU	-	expression tag	UNP Q6TQR6
A	-5	ASN	-	expression tag	UNP Q6TQR6
A	-4	LEU	-	expression tag	UNP Q6TQR6
A	-3	TYR	-	expression tag	UNP Q6TQR6
A	-2	PHE	-	expression tag	UNP Q6TQR6
A	-1	GLN	-	expression tag	UNP Q6TQR6
A	0	GLY	-	expression tag	UNP Q6TQR6
A	1047	GLY	GLU	conflict	UNP Q6TQR6
A	1660	PRO	THR	conflict	UNP Q6TQR6
A	1675	THR	ASN	conflict	UNP Q6TQR6

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
4	A	2	Total Zn 2 2	0

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	A	2	Total 2	Mg 2	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		AltConf
6	C	2	Total 2	O 2	0
6	R	4	Total 4	O 4	0
6	A	287	Total 287	O 287	0





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

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	52000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.489	Depositor
Minimum map value	-0.279	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	277.4, 277.4, 277.4	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.72999996, 0.72999996, 0.72999996	Depositor

5 Model quality

5.1 Standard geometry

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

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	C	0.19	0/913	0.34	0/1236
2	R	0.25	0/307	0.28	0/475
3	A	0.23	0/13583	0.33	0/18310
All	All	0.23	0/14803	0.33	0/20021

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	C	896	880	880	22	0
2	R	275	139	140	1	0
3	A	13362	13541	13538	118	0
4	A	2	0	0	0	0
5	A	2	0	0	0	0
6	A	287	0	0	16	0
6	C	2	0	0	0	0
6	R	4	0	0	0	0
All	All	14830	14560	14558	139	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 5.

All (139) 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:A:1520:LYS:NZ	6:A:4101:HOH:O	1.92	1.03
3:A:1344:GLU:OE2	6:A:4102:HOH:O	1.93	0.86
3:A:2966:LEU:O	3:A:2969:ARG:NE	2.11	0.82
3:A:2897:ASP:O	3:A:2898:THR:OG1	1.96	0.82
3:A:1007:ASN:O	6:A:4103:HOH:O	2.02	0.77
3:A:1104:THR:OG1	3:A:1216:SER:OG	2.01	0.76
3:A:3199:LYS:NZ	3:A:3200:GLY:O	2.19	0.76
3:A:1006:GLN:OE1	6:A:4106:HOH:O	2.06	0.73
3:A:1409:SER:O	6:A:4102:HOH:O	2.05	0.73
3:A:2769:THR:O	6:A:4104:HOH:O	2.04	0.73
3:A:1604:ASP:OD2	6:A:4105:HOH:O	2.06	0.71
3:A:1427:ARG:O	6:A:4107:HOH:O	2.10	0.70
3:A:1104:THR:HG1	3:A:1216:SER:HG	1.36	0.69
3:A:2587:THR:O	6:A:4108:HOH:O	2.10	0.68
3:A:2268:ALA:HB2	3:A:2399:ARG:HH21	1.60	0.66
3:A:1184:ARG:HD2	3:A:1207:LEU:HD13	1.78	0.65
3:A:2521:LYS:NZ	6:A:4112:HOH:O	2.29	0.65
3:A:2903:VAL:HG21	3:A:3152:LEU:HD21	1.79	0.65
3:A:1851:LEU:O	3:A:1854:LYS:NZ	2.30	0.64
3:A:3033:GLU:OE1	3:A:3033:GLU:N	2.31	0.63
3:A:3109:MET:HG2	3:A:3149:ILE:HD11	1.82	0.62
3:A:1075:THR:O	3:A:1080:LYS:NZ	2.33	0.62
1:C:63:VAL:HG13	1:C:67:PHE:CD2	2.35	0.61
3:A:1117:LYS:O	3:A:1118:THR:OG1	2.13	0.61
3:A:2661:SER:O	6:A:4109:HOH:O	2.16	0.61
3:A:1583:ARG:NH1	3:A:1588:GLU:OE2	2.34	0.60
3:A:1130:TYR:O	3:A:1134:LEU:HD13	2.02	0.60
3:A:3168:LEU:O	3:A:3171:VAL:HG12	2.02	0.59
3:A:1620:GLU:OE2	3:A:1620:GLU:HA	2.01	0.59
3:A:1245:ILE:HD11	3:A:1850:MET:HE1	1.83	0.58
1:C:102:PRO:O	3:A:2350:TYR:OH	2.19	0.57
3:A:2837:ARG:NH1	3:A:3019:LEU:O	2.35	0.57
1:C:41:PRO:O	1:C:43:ARG:NH2	2.38	0.57
3:A:1789:GLU:OE1	3:A:2377:GLN:NE2	2.37	0.57
1:C:93:TYR:CD1	1:C:116:VAL:HG11	2.41	0.56
3:A:1787:ILE:CD1	3:A:2490:LEU:HD22	2.36	0.55
3:A:1810:TRP:CD2	3:A:2250:ILE:HG21	2.43	0.54
3:A:1896:GLU:N	3:A:1896:GLU:OE1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1806:ASP:OD1	3:A:1808:LYS:N	2.39	0.54
3:A:2694:LEU:HD12	3:A:2830:ILE:HG13	1.91	0.53
3:A:2837:ARG:NH2	3:A:3024:ILE:O	2.40	0.53
3:A:1201:GLY:O	3:A:1205:ASN:ND2	2.42	0.52
3:A:2435:ARG:O	3:A:2439:ASP:OD2	2.27	0.52
3:A:1882:LEU:O	3:A:1887:LYS:NZ	2.42	0.52
3:A:1171:ASP:N	3:A:1171:ASP:OD1	2.43	0.52
1:C:93:TYR:CE1	1:C:116:VAL:HG11	2.45	0.52
3:A:2966:LEU:HD12	3:A:2992:THR:HG21	1.91	0.52
3:A:1798:GLU:CD	3:A:1798:GLU:H	2.18	0.52
3:A:1179:LYS:O	3:A:1183:VAL:HG23	2.10	0.51
1:C:71:ARG:HB3	1:C:78:VAL:HG12	1.92	0.51
3:A:1792:MET:HE1	3:A:1800:ILE:HD11	1.91	0.51
3:A:1787:ILE:HD12	3:A:2490:LEU:HD22	1.93	0.50
3:A:3028:ASN:OD1	3:A:3042:ILE:HD11	2.10	0.50
1:C:90:THR:HG22	1:C:118:VAL:H	1.76	0.50
3:A:1570:VAL:HG12	3:A:1570:VAL:O	2.12	0.49
3:A:1347:LEU:O	3:A:1351:THR:HG23	2.11	0.49
3:A:2802:MET:O	3:A:2805:SER:OG	2.29	0.49
3:A:2748:LEU:HD12	3:A:2752:LEU:CD2	2.43	0.49
3:A:2384:ASP:OD1	3:A:2384:ASP:N	2.40	0.49
3:A:1121:GLU:N	3:A:1121:GLU:OE1	2.46	0.49
3:A:2953:MET:HA	3:A:2953:MET:HE2	1.94	0.49
1:C:87:PRO:O	1:C:90:THR:HG23	2.13	0.48
3:A:2563:ASP:OD1	3:A:2563:ASP:N	2.44	0.48
1:C:11:LEU:HD13	1:C:117:THR:OG1	2.13	0.48
1:C:90:THR:HG22	1:C:118:VAL:N	2.29	0.48
3:A:1671:ARG:NE	6:A:4122:HOH:O	2.45	0.48
3:A:1559:ARG:NH2	6:A:4119:HOH:O	2.36	0.47
3:A:1118:THR:OG1	3:A:1121:GLU:OE1	2.31	0.47
2:R:7:A:C4	3:A:2414:VAL:HG22	2.50	0.47
3:A:3116:SER:O	3:A:3119:SER:OG	2.22	0.47
3:A:1848:VAL:HG22	3:A:1894:ILE:HG23	1.97	0.47
1:C:34:MET:HE2	1:C:78:VAL:HG13	1.97	0.46
1:C:67:PHE:CD1	1:C:82:MET:HB3	2.50	0.46
3:A:2477:HIS:ND1	3:A:2516:SER:OG	2.49	0.46
3:A:2678:ALA:O	3:A:2682:GLU:HG3	2.16	0.46
3:A:2329:LEU:HD12	3:A:2581:MET:HE1	1.97	0.45
3:A:2429:SER:OG	3:A:2432:ASP:OD1	2.34	0.45
3:A:1341:LYS:NZ	6:A:4125:HOH:O	2.48	0.45
3:A:1537:VAL:HG13	3:A:1539:PRO:HD3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:CYS:O	1:C:77:THR:HB	2.17	0.45
1:C:6:GLU:OE2	1:C:6:GLU:N	2.48	0.44
3:A:1103:LEU:HD13	3:A:1107:ASP:HB2	1.98	0.44
3:A:2819:GLU:OE1	6:A:4104:HOH:O	2.21	0.44
3:A:2645:VAL:HG12	3:A:2954:LYS:HE2	1.99	0.44
3:A:1073:SER:O	3:A:1074:ASN:HB2	2.18	0.44
3:A:2748:LEU:HD12	3:A:2752:LEU:HD21	1.98	0.44
3:A:2897:ASP:O	3:A:2898:THR:CB	2.66	0.44
3:A:1204:SER:O	3:A:1208:LYS:HG2	2.18	0.44
3:A:1130:TYR:CE2	3:A:1134:LEU:HD11	2.52	0.43
3:A:2792:ASP:OD1	6:A:4110:HOH:O	2.21	0.43
3:A:1462:LEU:HD13	3:A:1560:LEU:HD11	1.99	0.43
3:A:2963:PHE:O	3:A:2965:SER:N	2.50	0.43
3:A:1171:ASP:N	3:A:1173:ASP:OD1	2.51	0.43
3:A:1133:LYS:HG2	3:A:1154:HIS:NE2	2.33	0.43
3:A:2657:LEU:HD22	3:A:2666:LEU:HB2	2.01	0.43
3:A:2991:ILE:HD13	3:A:2991:ILE:N	2.34	0.43
1:C:59:TYR:HB3	1:C:63:VAL:HG21	2.01	0.43
3:A:1427:ARG:NH1	3:A:3083:ASN:O	2.49	0.43
3:A:1125:LYS:O	3:A:1128:VAL:HG12	2.19	0.43
3:A:1135:MET:CE	3:A:1206:SER:HB2	2.49	0.43
3:A:1245:ILE:HD11	3:A:1850:MET:CE	2.48	0.43
3:A:1461:ALA:HB2	3:A:1564:THR:CG2	2.49	0.43
3:A:1375:PRO:HD3	3:A:1382:MET:HG2	2.01	0.43
3:A:1638:ARG:CD	3:A:2364:PRO:HB2	2.49	0.43
3:A:2415:LEU:HD22	3:A:2437:LEU:HD13	2.00	0.43
1:C:63:VAL:HG13	1:C:67:PHE:HB2	2.01	0.42
3:A:1403:ARG:NH2	3:A:1617:TYR:OH	2.51	0.42
3:A:1854:LYS:O	3:A:1855:LEU:HB2	2.18	0.42
3:A:2444:TRP:CD2	3:A:2450:VAL:HG11	2.55	0.42
3:A:3012:THR:HG22	3:A:3013:THR:N	2.34	0.42
3:A:1429:LEU:O	3:A:1432:ILE:HG22	2.20	0.42
3:A:3081:GLU:OE1	3:A:3221:ARG:NH1	2.53	0.42
3:A:3112:LEU:HD21	3:A:3135:ARG:HB2	2.02	0.41
3:A:1135:MET:HE2	3:A:1206:SER:HB2	2.01	0.41
3:A:1810:TRP:CE2	3:A:2250:ILE:HG21	2.55	0.41
3:A:3174:TYR:O	3:A:3178:LEU:HD23	2.20	0.41
1:C:85:LEU:O	1:C:118:VAL:HG21	2.20	0.41
3:A:1104:THR:O	3:A:1105:ASP:HB3	2.19	0.41
3:A:2990:ILE:C	3:A:2991:ILE:HD13	2.45	0.41
3:A:1134:LEU:O	3:A:1138:MET:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:3099:VAL:HG22	3:A:3099:VAL:O	2.20	0.41
3:A:1069:GLY:O	3:A:1258:ASN:ND2	2.46	0.41
3:A:1173:ASP:OD1	3:A:1173:ASP:N	2.51	0.41
3:A:1772:LYS:HD2	3:A:1778:MET:HE1	2.03	0.41
3:A:1117:LYS:O	3:A:1121:GLU:HB2	2.20	0.41
3:A:1841:GLY:O	3:A:1845:LYS:HG2	2.20	0.41
3:A:1153:THR:HG21	3:A:1225:LEU:HD21	2.03	0.41
3:A:2319:GLU:OE1	3:A:2319:GLU:N	2.49	0.41
3:A:2332:MET:HE1	3:A:2571:ASP:HB2	2.03	0.41
3:A:3026:CYS:SG	3:A:3046:LEU:HD23	2.61	0.41
1:C:13:GLN:OE1	1:C:13:GLN:N	2.47	0.41
1:C:63:VAL:HG13	1:C:67:PHE:HD2	1.80	0.41
3:A:927:THR:HA	3:A:2384:ASP:HB2	2.02	0.40
3:A:1457:GLU:HG2	3:A:1469:SER:HB2	2.03	0.40
1:C:4:LEU:HD13	1:C:95:CYS:SG	2.62	0.40
1:C:92:VAL:O	1:C:92:VAL:HG13	2.20	0.40
3:A:1186:GLU:O	3:A:1191:LYS:NZ	2.45	0.40
3:A:3205:THR:HG22	3:A:3206:GLU:N	2.36	0.40
1:C:90:THR:HG22	1:C:117:THR:HA	2.03	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	C	116/130 (89%)	112 (97%)	3 (3%)	1 (1%)	14	17
3	A	1645/3990 (41%)	1598 (97%)	46 (3%)	1 (0%)	48	60
All	All	1761/4120 (43%)	1710 (97%)	49 (3%)	2 (0%)	49	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	67	PHE
3	A	2423	GLY

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	C	91/102 (89%)	90 (99%)	1 (1%)	65	81
3	A	1534/3635 (42%)	1516 (99%)	18 (1%)	63	79
All	All	1625/3737 (44%)	1606 (99%)	19 (1%)	61	79

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

Mol	Chain	Res	Type
1	C	21	SER
3	A	1139	SER
3	A	1248	SER
3	A	1356	SER
3	A	1434	SER
3	A	1458	ILE
3	A	1630	SER
3	A	1787	ILE
3	A	2291	VAL
3	A	2296	THR
3	A	2564	SER
3	A	2596	THR
3	A	2610	MET
3	A	2764	SER
3	A	2805	SER
3	A	2912	VAL
3	A	3094	SER
3	A	3112	LEU
3	A	3151	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	76	ASN
1	C	96	ASN
1	C	104	GLN
3	A	1034	ASN
3	A	1247	ASN
3	A	1390	ASN
3	A	1433	ASN
3	A	1521	GLN
3	A	1606	GLN
3	A	1758	ASN
3	A	2331	ASN
3	A	2476	HIS
3	A	2607	GLN
3	A	2777	ASN
3	A	2785	ASN
3	A	2795	ASN
3	A	2857	ASN
3	A	3140	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	R	12/16 (75%)	6 (50%)	0

All (6) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	R	2	C
2	R	5	A
2	R	7	A
2	R	8	G
2	R	10	U
2	R	12	U

There are no RNA pucker outliers to report.

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

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](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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.

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.

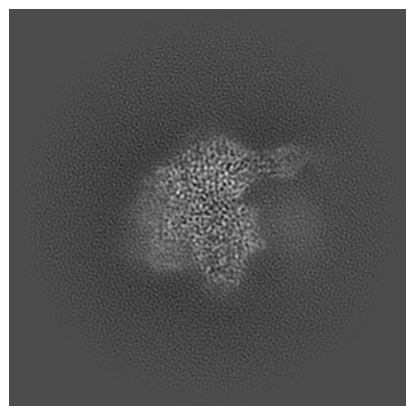
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55399. These allow visual inspection of the internal detail of the map and identification of artifacts.

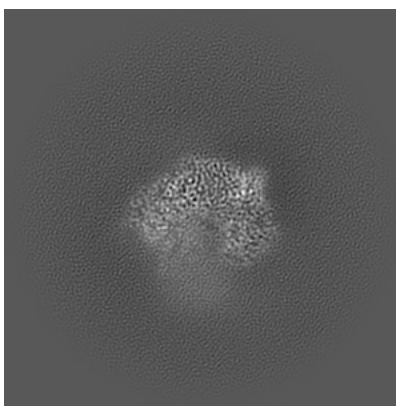
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

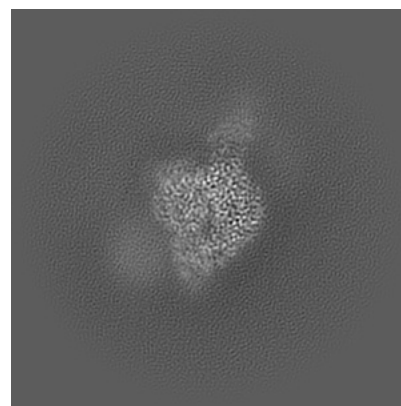
6.1.1 Primary map



X

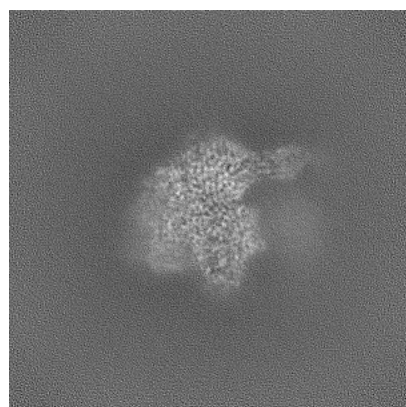


Y

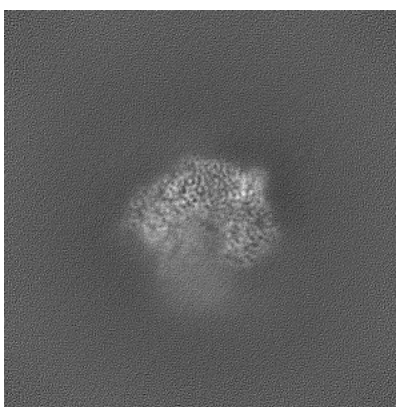


Z

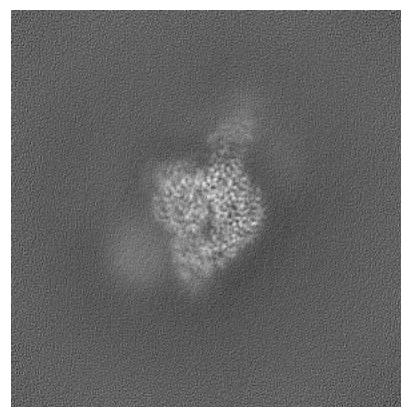
6.1.2 Raw map



X



Y

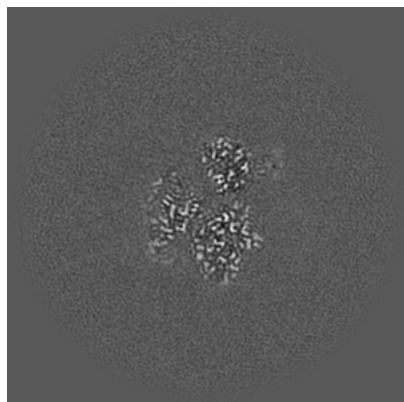


Z

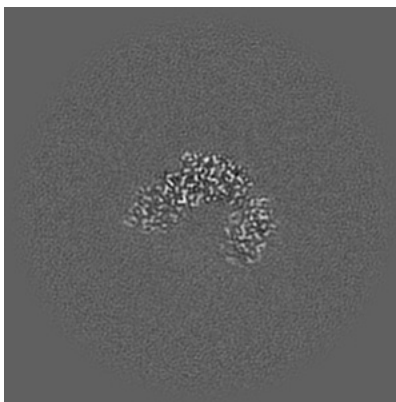
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

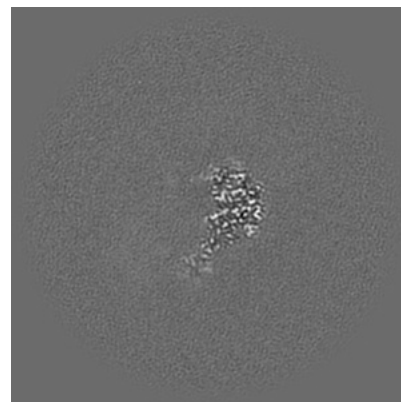
6.2.1 Primary map



X Index: 190

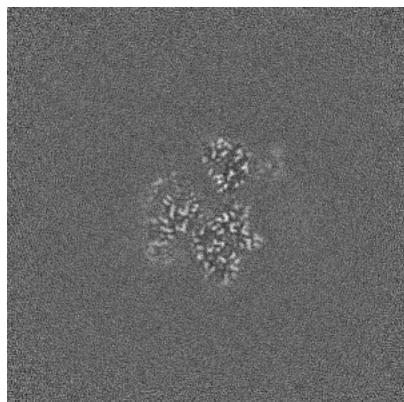


Y Index: 190

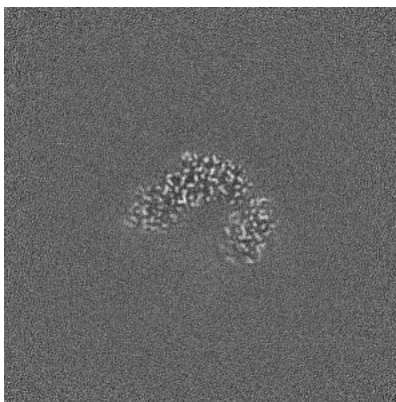


Z Index: 190

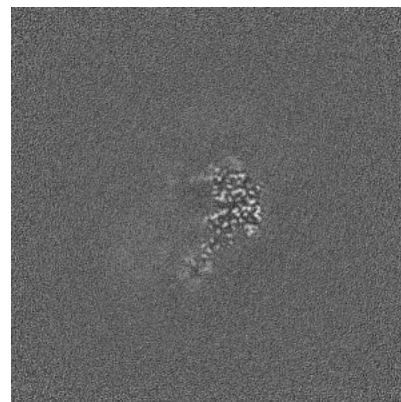
6.2.2 Raw map



X Index: 190



Y Index: 190

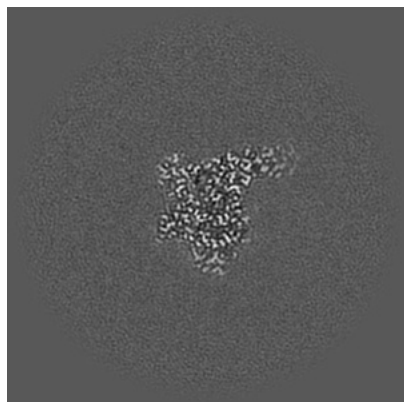


Z Index: 190

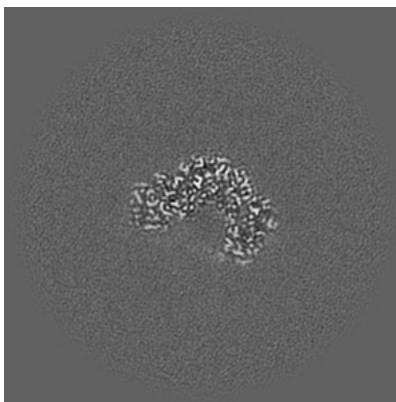
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

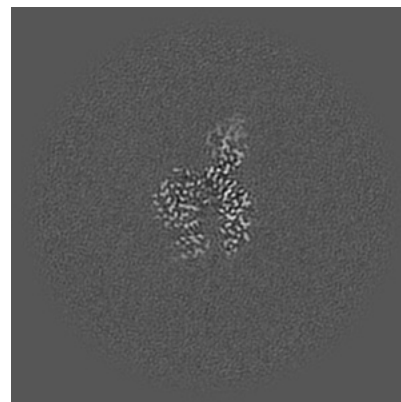
6.3.1 Primary map



X Index: 206

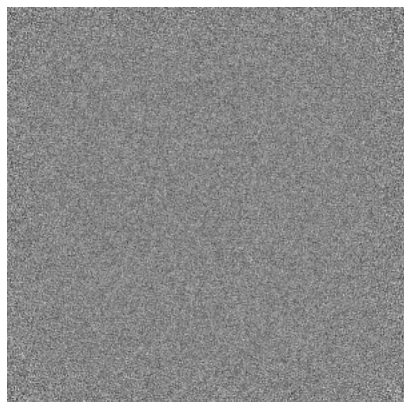


Y Index: 200

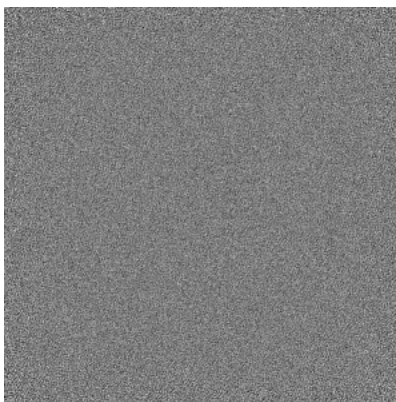


Z Index: 227

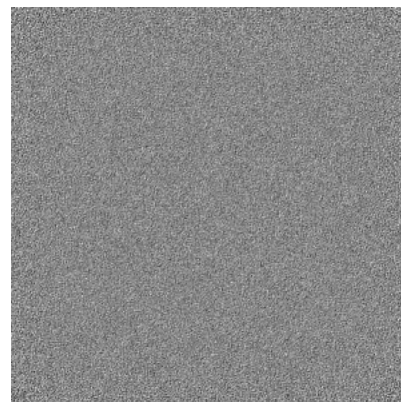
6.3.2 Raw map



X Index: 0



Y Index: 0

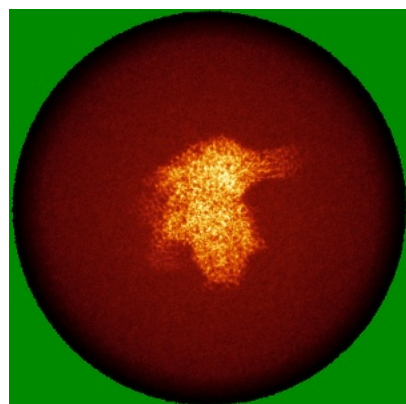


Z Index: 0

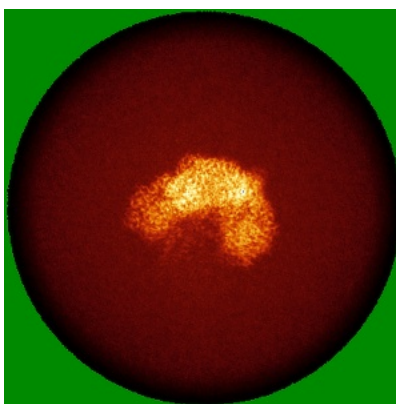
The images above show the largest variance slices of the map in three orthogonal directions.

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

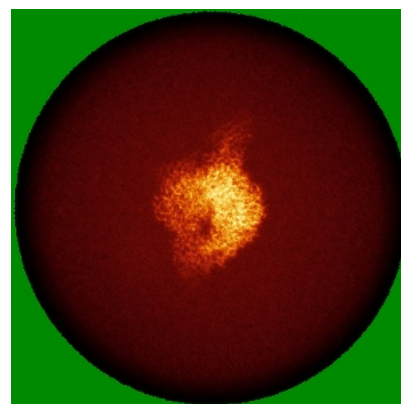
6.4.1 Primary map



X

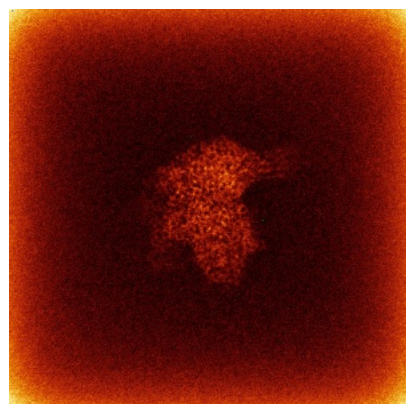


Y

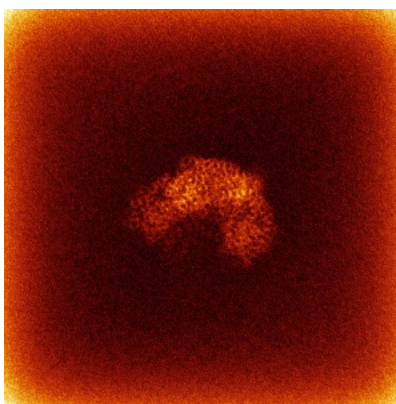


Z

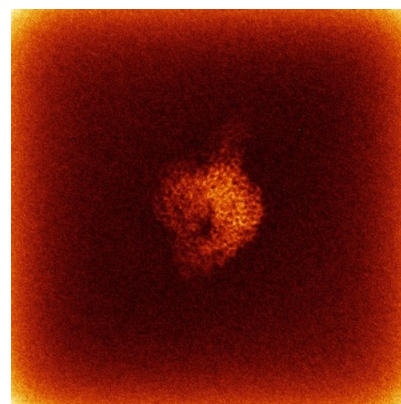
6.4.2 Raw map



X



Y

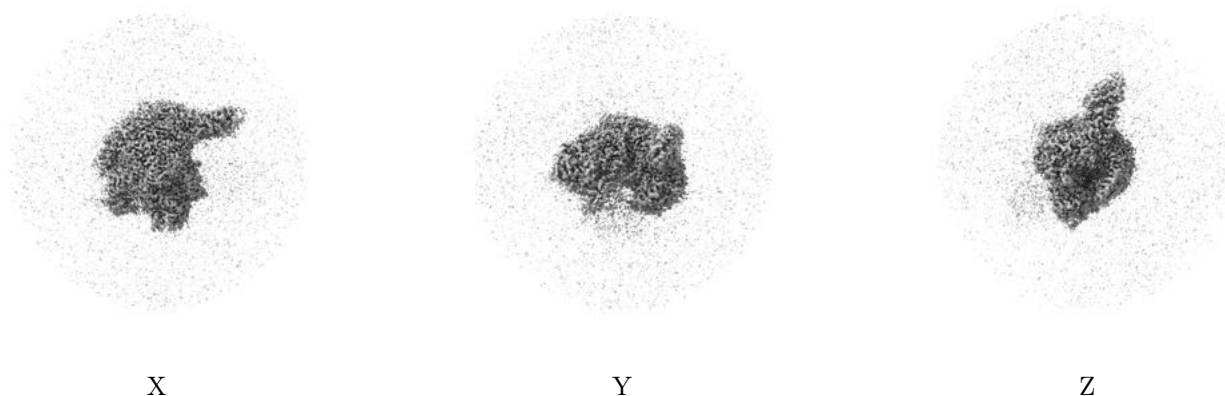


Z

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.

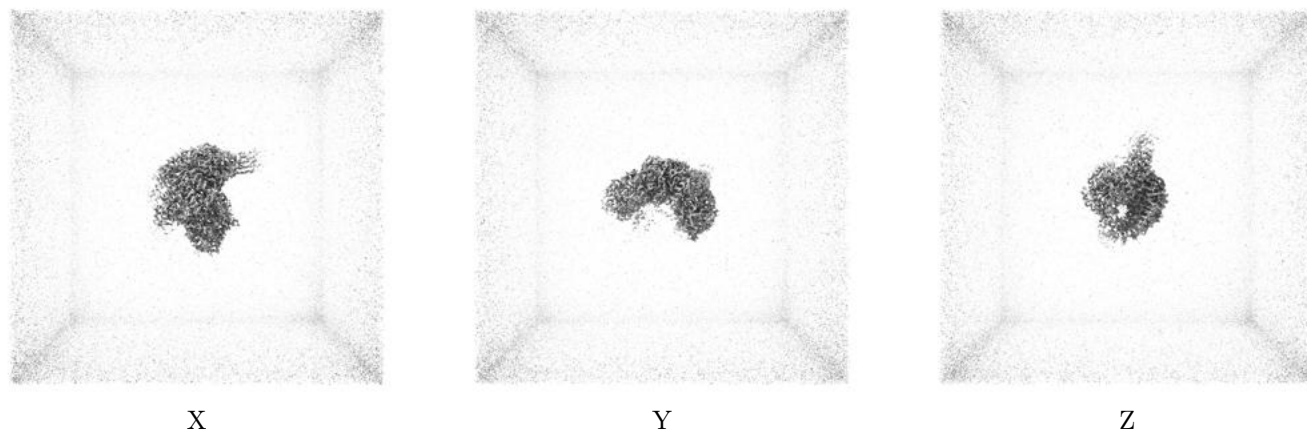
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. 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.

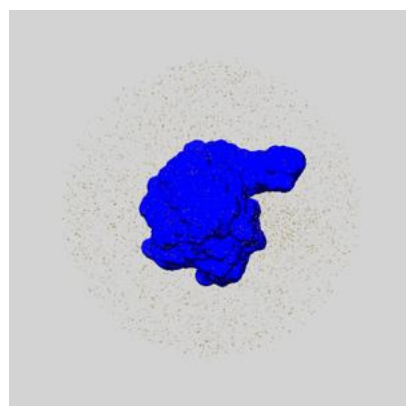
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

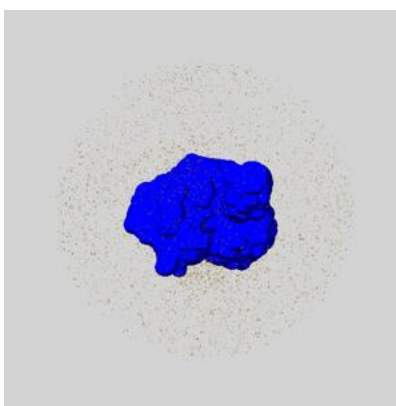
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

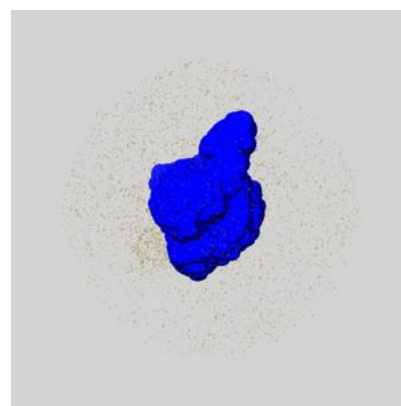
6.6.1 emd_55399_msk_1.map [i](#)



X



Y

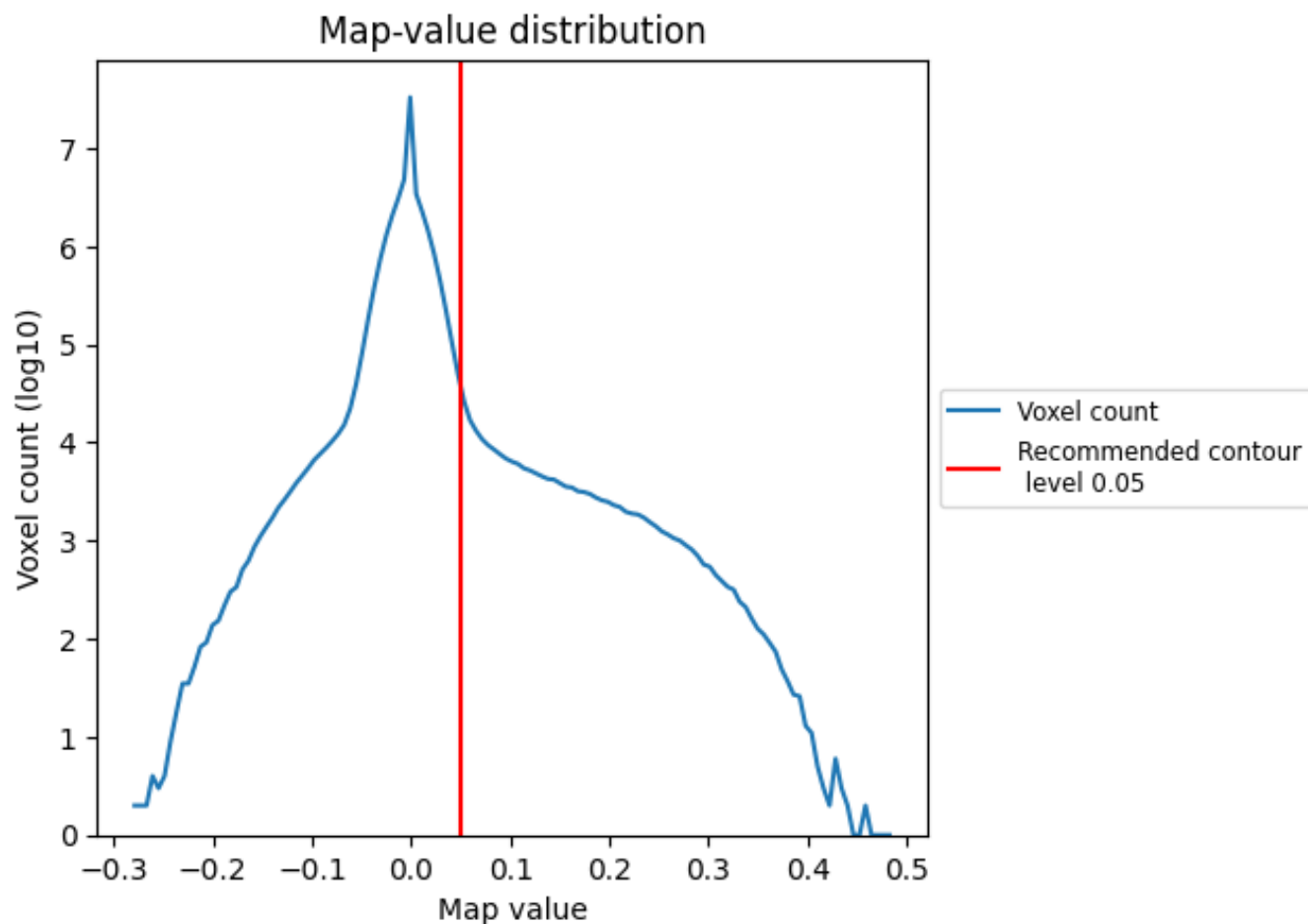


Z

7 Map analysis [i](#)

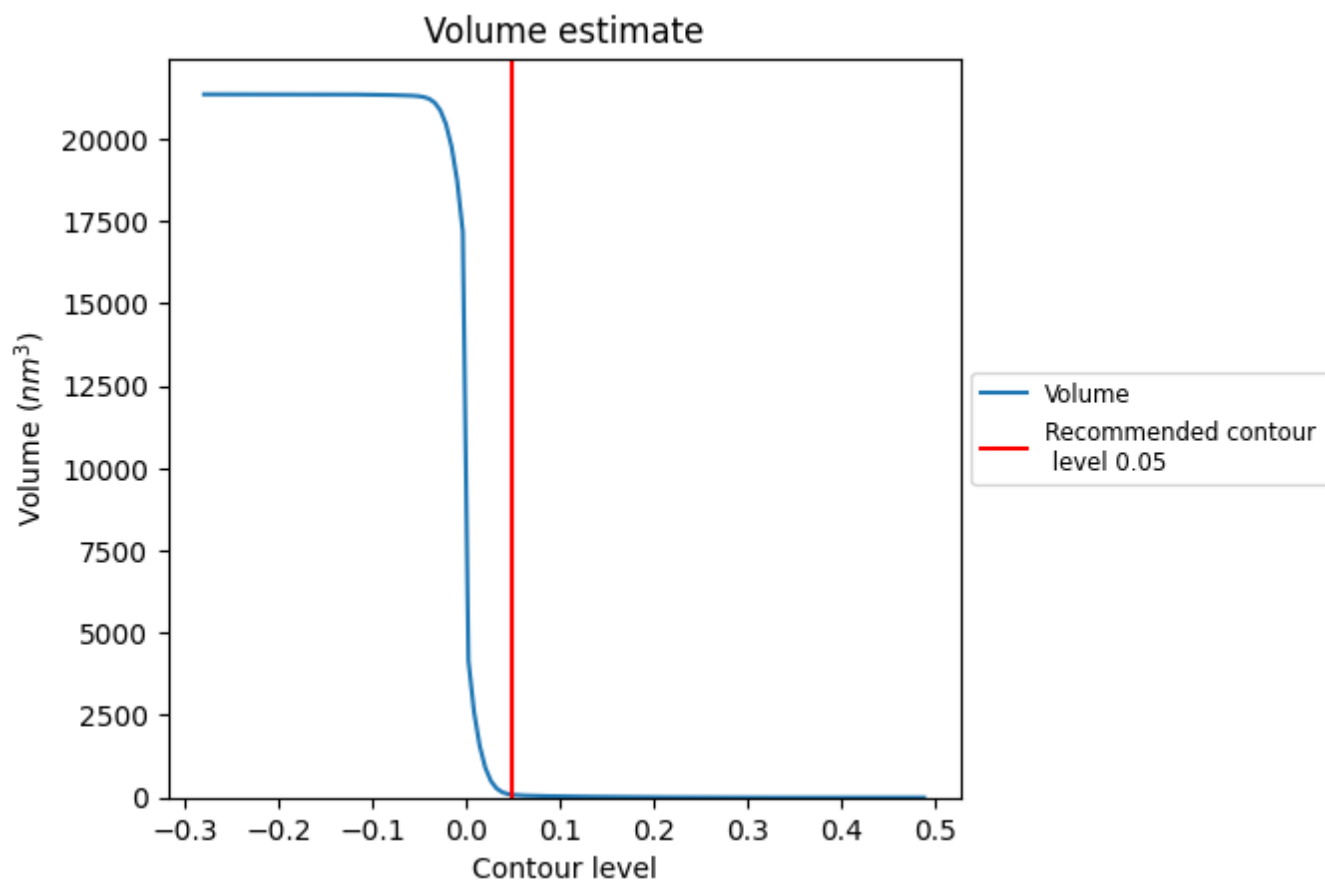
This section contains the results of statistical analysis of the map.

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.

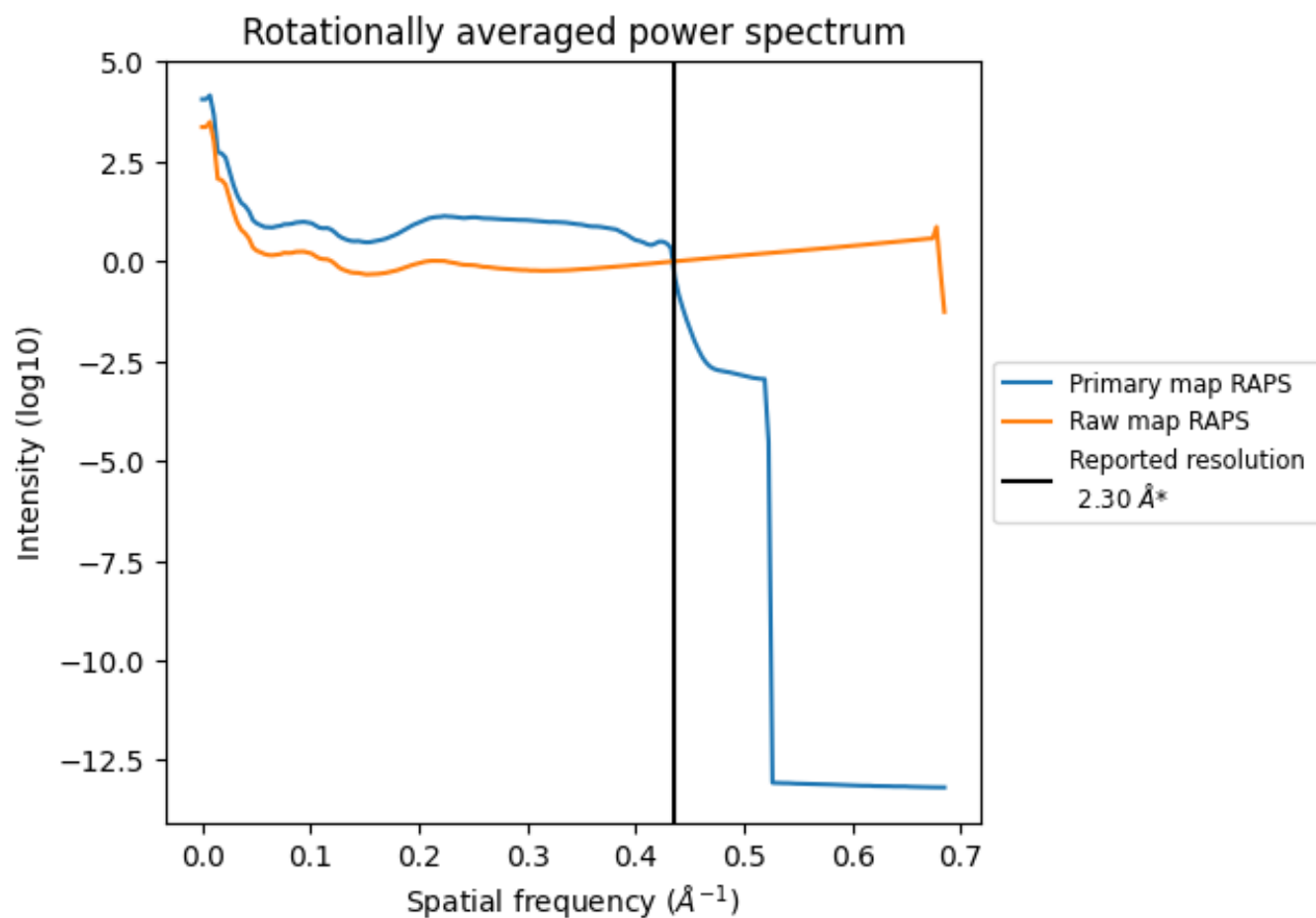
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 86 nm³; this corresponds to an approximate mass of 77 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 ⓘ

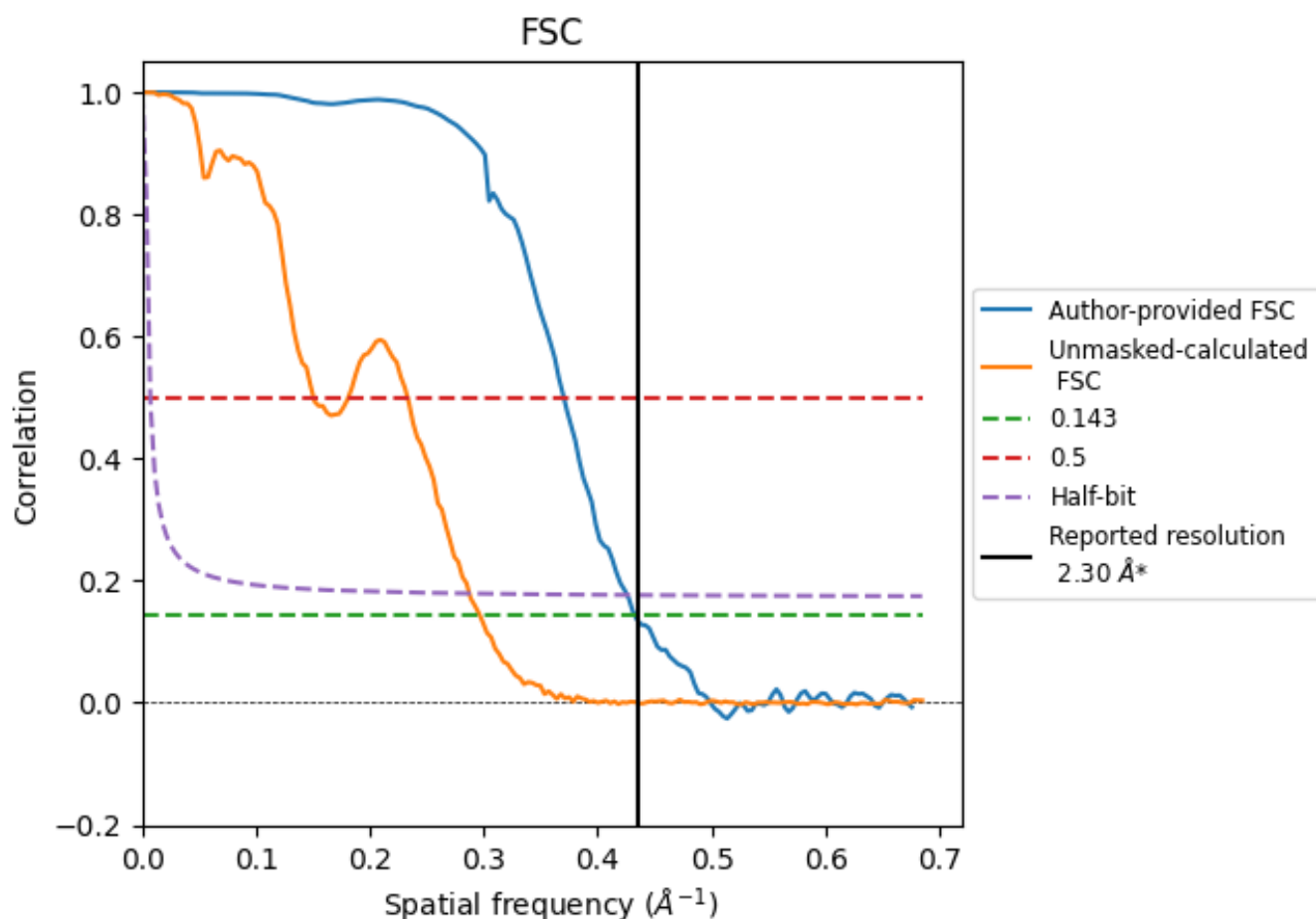


*Reported resolution corresponds to spatial frequency of 0.435 Å⁻¹

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 0.435 \AA^{-1}

8.2 Resolution estimates [i](#)

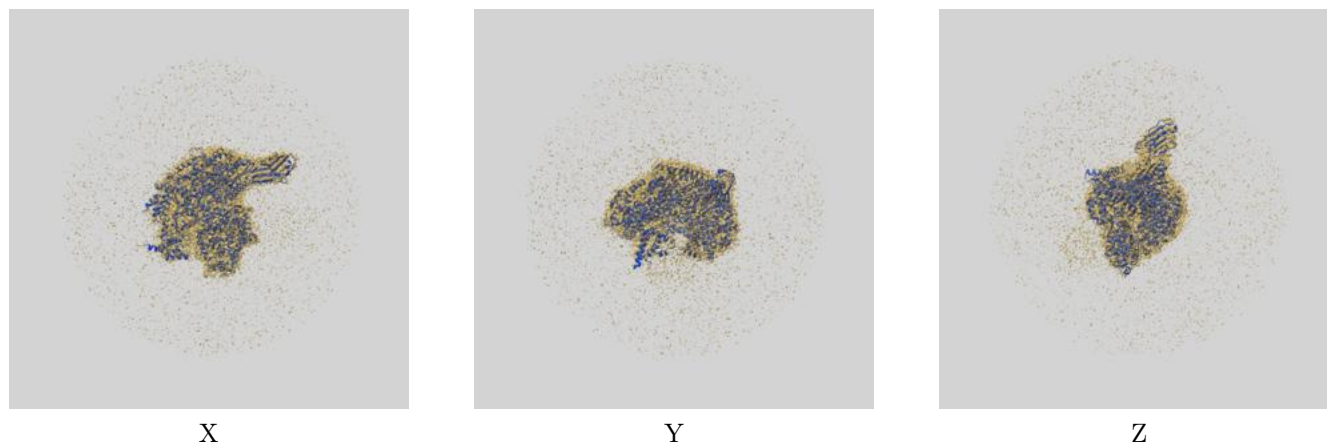
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.30	-	-
Author-provided FSC curve	2.31	2.70	2.35
Unmasked-calculated*	3.37	6.64	3.48

*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 3.37 differs from the reported value 2.3 by more than 10 %

9 Map-model fit [i](#)

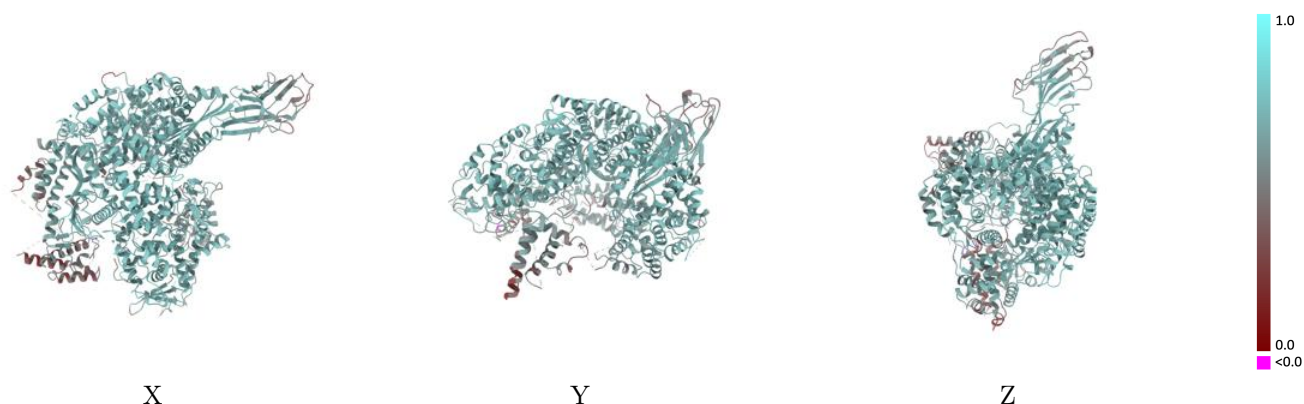
This section contains information regarding the fit between EMDB map EMD-55399 and PDB model 9T0E. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



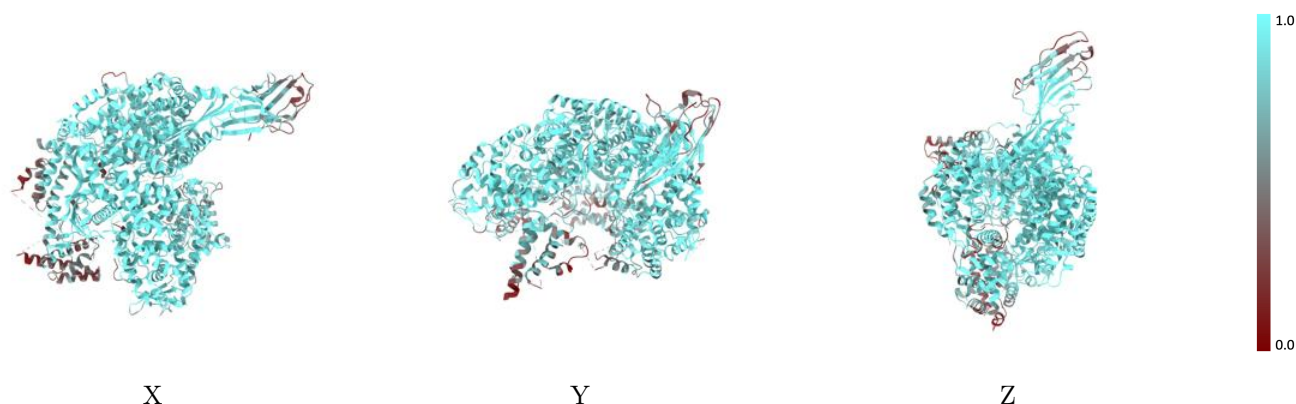
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



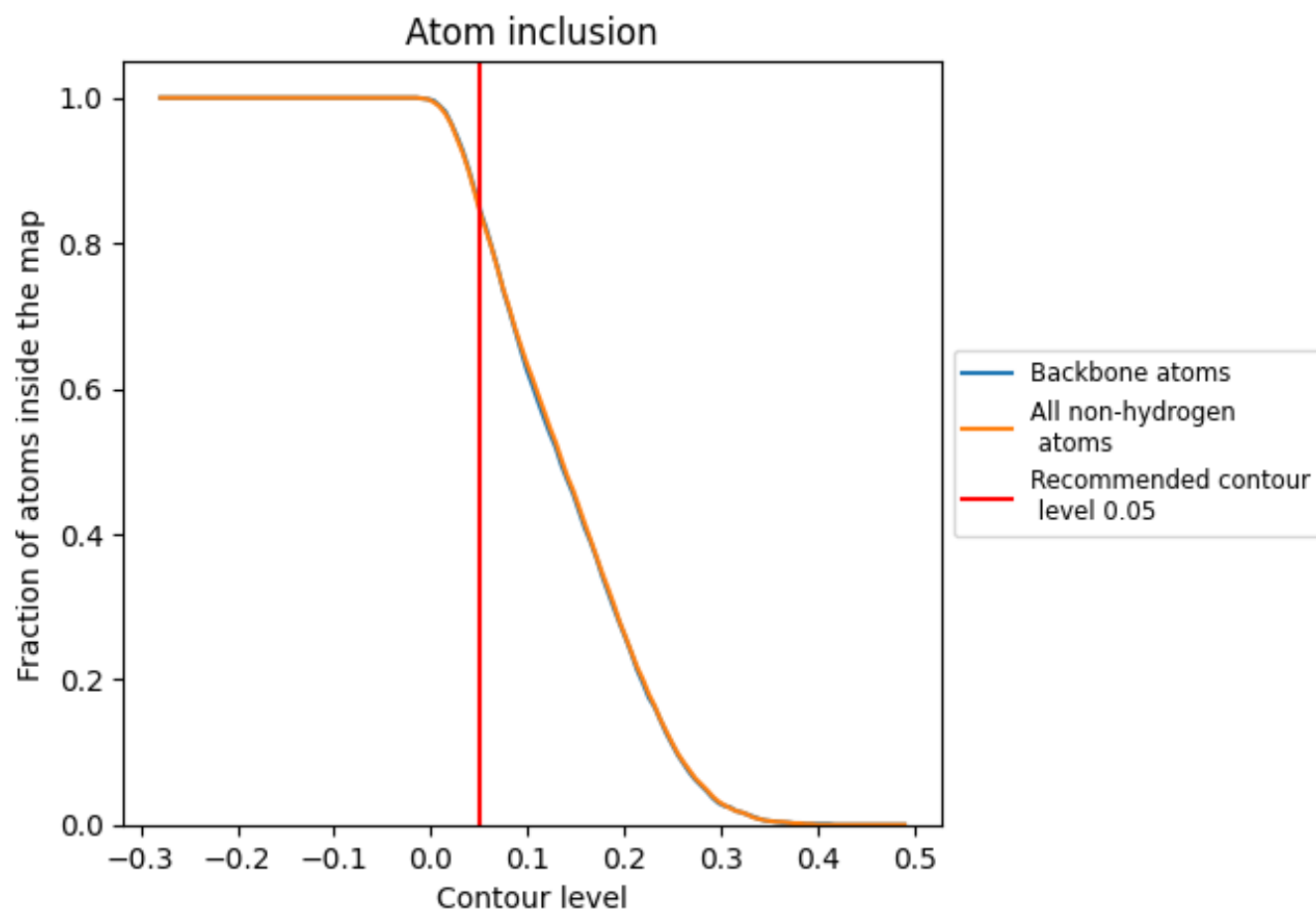
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 85% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8460	<div></div> 0.6300
A	<div></div> 0.8600	<div></div> 0.6340
C	<div></div> 0.6910	<div></div> 0.5610
R	<div></div> 0.9130	<div></div> 0.6490

