



## Full wwPDB EM Validation Report ⓘ

Jun 25, 2025 – 09:06 AM JST

PDB ID : 7X6S / pdb\_00007x6s  
EMDB ID : EMD-33026  
Title : lymphocytic choriomeningitis virus RNA-dependent RNA polymerase (LCMV-L protein)  
Authors : Liu, L.; Lou, Z.  
Deposited on : 2022-03-08  
Resolution : 3.40 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev118  
MolProbity : 4-5-2 with Phenix2.0rc1  
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) : 2.44

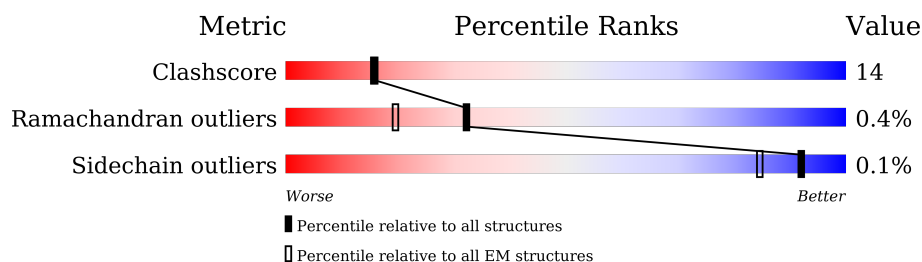
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.40 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  $\geq 3$ , 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	2210	 48% 16% 34%

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 10987 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 RNA-directed RNA polymerase L.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1453	Total	C	N	O	S	2	0
			10986	6987	1854	2079	66		

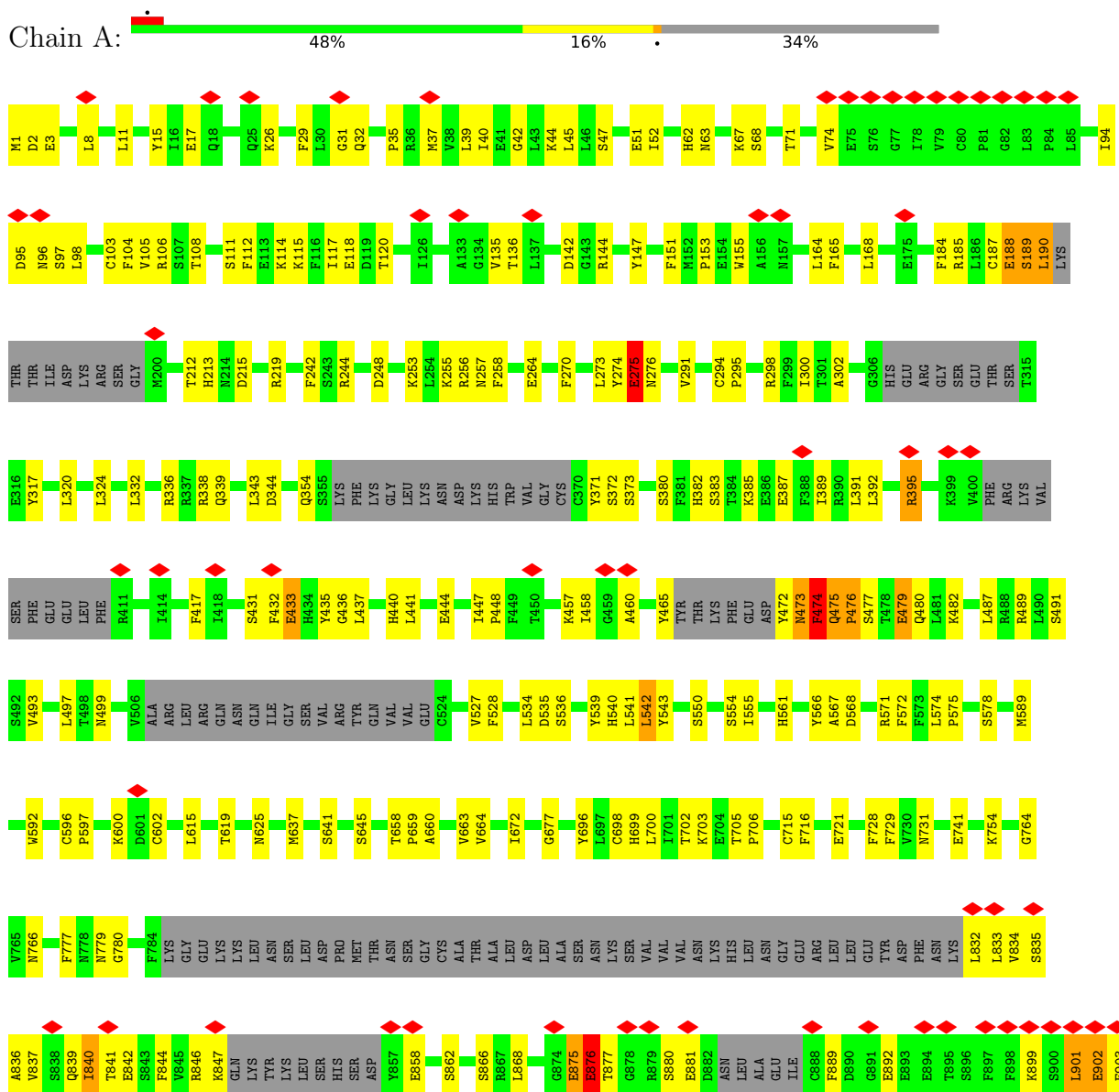
- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Mn	0
			1	1	

### 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: RNA-directed RNA polymerase L





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	112276	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 ( $e^-/\text{\AA}^2$ )	1.3	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.424	Depositor
Minimum map value	-1.483	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.075	Depositor
Recommended contour level	0.254	Depositor
Map size ( $\text{\AA}$ )	216.00002, 216.00002, 216.00002	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	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: MN

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	0.48	8/11199 (0.1%)	0.86	67/15156 (0.4%)

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	A	0	2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	474	PHE	C-O	-8.59	1.13	1.24
1	A	475	GLN	CA-CB	7.69	1.65	1.53
1	A	876	GLU	N-CA	-7.38	1.36	1.46
1	A	1603	ILE	C-O	-7.34	1.16	1.24
1	A	475	GLN	CA-C	5.82	1.60	1.52
1	A	476	PRO	CA-C	5.26	1.59	1.52
1	A	188	GLU	N-CA	-5.11	1.39	1.46
1	A	1459	TRP	C-O	-5.02	1.17	1.24

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	877	THR	N-CA-C	-19.53	81.56	107.73
1	A	1459	TRP	N-CA-C	-19.30	90.05	114.56
1	A	188	GLU	N-CA-C	-14.52	88.25	109.15
1	A	1154	CYS	N-CA-C	14.40	131.88	112.30
1	A	875	GLU	O-C-N	12.24	138.87	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1322	ASP	N-CA-C	-11.39	93.42	108.34
1	A	395	ARG	CB-CA-C	-9.75	93.29	109.27
1	A	473	ASN	CA-C-N	9.34	139.38	121.54
1	A	473	ASN	C-N-CA	9.34	139.38	121.54
1	A	1456	VAL	O-C-N	-9.22	113.04	122.54
1	A	1157	ASN	N-CA-C	-9.20	93.92	108.63
1	A	1788	LEU	CA-C-N	8.92	137.41	121.89
1	A	1788	LEU	C-N-CA	8.92	137.41	121.89
1	A	1321	ASP	CB-CA-C	-8.52	89.41	110.46
1	A	476	PRO	CB-CA-C	8.36	125.36	111.56
1	A	1209	TYR	CB-CA-C	-8.14	96.43	109.13
1	A	1178	ASN	N-CA-C	-8.06	93.59	107.61
1	A	875	GLU	CA-C-N	7.74	136.33	121.54
1	A	875	GLU	C-N-CA	7.74	136.33	121.54
1	A	476	PRO	N-CA-C	-7.54	96.94	112.47
1	A	840	ILE	N-CA-C	7.40	117.53	110.42
1	A	901	LEU	N-CA-C	7.36	120.97	107.73
1	A	275	GLU	CB-CA-C	7.29	124.92	110.42
1	A	1180	SER	N-CA-C	-7.12	95.64	110.80
1	A	1322	ASP	N-CA-CB	7.06	123.57	110.87
1	A	187	CYS	O-C-N	7.00	132.05	122.46
1	A	1457	LYS	N-CA-C	-6.97	95.96	110.80
1	A	1788	LEU	N-CA-C	-6.96	95.98	110.80
1	A	877	THR	CB-CA-C	-6.92	97.80	112.82
1	A	1338	ASP	CB-CA-C	6.92	123.80	110.17
1	A	371	TYR	N-CA-C	-6.92	96.23	108.13
1	A	1178	ASN	CB-CA-C	6.86	120.32	110.79
1	A	354	GLN	N-CA-C	-6.80	99.43	109.62
1	A	542	LEU	N-CA-C	-6.75	96.52	108.13
1	A	473	ASN	CB-CA-C	6.71	123.77	110.42
1	A	566	TYR	N-CA-C	-6.71	97.13	108.26
1	A	1338	ASP	N-CA-C	-6.70	95.00	109.81
1	A	1641	HIS	N-CA-C	-6.62	99.69	109.62
1	A	1319	SER	CB-CA-C	6.61	120.12	109.27
1	A	566	TYR	CB-CA-C	6.38	119.96	110.14
1	A	542	LEU	CB-CA-C	6.37	119.54	110.24
1	A	383	SER	CB-CA-C	6.29	119.15	110.34
1	A	1666	ARG	N-CA-C	-6.05	98.50	108.48
1	A	1541	ASN	N-CA-C	-6.03	97.33	108.24
1	A	389	ILE	N-CA-C	-5.96	103.47	110.21
1	A	1480	THR	N-CA-C	-5.93	98.20	108.52
1	A	371	TYR	CB-CA-C	5.89	118.84	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1182	ASP	N-CA-C	-5.70	98.98	108.32
1	A	1083	ALA	N-CA-C	-5.61	97.78	108.17
1	A	876	GLU	CB-CA-C	5.61	121.59	110.42
1	A	902	GLU	N-CA-C	5.53	120.01	112.88
1	A	1789	SER	N-CA-CB	5.48	119.81	110.71
1	A	1458	ASP	CA-C-O	5.45	128.30	120.51
1	A	1458	ASP	N-CA-C	-5.41	99.28	110.80
1	A	729	PHE	N-CA-C	5.36	118.52	111.28
1	A	677	GLY	N-CA-C	-5.26	103.62	112.77
1	A	479	GLU	N-CA-C	5.22	119.21	113.21
1	A	474	PHE	N-CA-C	5.21	121.89	110.80
1	A	1789	SER	N-CA-C	-5.18	99.16	108.48
1	A	1203	LYS	N-CA-C	-5.18	96.85	107.67
1	A	1454	THR	N-CA-C	-5.12	98.71	107.61
1	A	840	ILE	CB-CA-C	-5.08	105.46	111.97
1	A	433	GLU	N-CA-C	-5.07	103.14	110.64
1	A	1524	GLY	CA-C-N	5.06	132.63	123.27
1	A	1524	GLY	C-N-CA	5.06	132.63	123.27
1	A	383	SER	N-CA-C	-5.03	99.63	107.93
1	A	1671	LEU	N-CA-C	5.02	118.98	113.21

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1788	LEU	Mainchain
1	A	876	GLU	Mainchain

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10986	0	10137	301	0
2	A	1	0	0	0	0
All	All	10987	0	10137	301	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 14.

All (301) 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:A:1685:SER:CB	1:A:1790:LEU:HD23	1.80	1.11
1:A:147:TYR:OH	1:A:1090:PHE:CD1	2.11	1.02
1:A:899:LYS:HG2	1:A:902:GLU:OE2	1.60	1.01
1:A:184:PHE:O	1:A:188:GLU:CB	2.17	0.93
1:A:839:GLN:HE22	1:A:868:LEU:HA	1.35	0.90
1:A:899:LYS:CG	1:A:902:GLU:OE2	2.23	0.86
1:A:1334:LEU:O	1:A:1338:ASP:O	1.95	0.85
1:A:499:ASN:OD1	1:A:543:TYR:OH	1.97	0.82
1:A:1641:HIS:O	1:A:1641:HIS:ND1	2.12	0.81
1:A:876:GLU:HG3	1:A:1275:HIS:CE1	2.15	0.81
1:A:473:ASN:HD22	1:A:561:HIS:HE1	1.29	0.78
1:A:457:LYS:O	1:A:460:ALA:N	2.16	0.77
1:A:1083:ALA:O	1:A:1087:ASN:ND2	2.18	0.77
1:A:1789:SER:C	1:A:1790:LEU:HD12	2.10	0.76
1:A:165:PHE:CE2	1:A:190:LEU:HD12	2.21	0.76
1:A:475:GLN:N	1:A:476:PRO:HD3	2.04	0.72
1:A:17:GLU:O	1:A:26:LYS:NZ	2.24	0.71
1:A:190:LEU:N	1:A:190:LEU:HD13	2.05	0.71
1:A:1645:VAL:H	1:A:1654:TYR:HE2	1.37	0.70
1:A:658:THR:O	1:A:660:ALA:N	2.24	0.70
1:A:876:GLU:CG	1:A:1275:HIS:CE1	2.75	0.70
1:A:294:CYS:HB2	1:A:295:PRO:HD3	1.74	0.69
1:A:840:ILE:HA	1:A:946:HIS:ND1	2.07	0.69
1:A:1459:TRP:CZ3	1:A:1467:ARG:NH1	2.61	0.69
1:A:637:MET:HE3	1:A:1370:ALA:HB1	1.73	0.69
1:A:836:ALA:CB	1:A:949:LYS:HB3	2.24	0.68
1:A:96:ASN:O	1:A:135:VAL:HA	1.93	0.67
1:A:836:ALA:HB1	1:A:949:LYS:HB3	1.75	0.67
1:A:185:ARG:O	1:A:188:GLU:O	2.13	0.66
1:A:432:PHE:HA	1:A:436:GLY:H	1.61	0.66
1:A:385:LYS:HG2	1:A:387:GLU:H	1.59	0.66
1:A:833:LEU:HD12	1:A:834:VAL:HG23	1.77	0.65
1:A:147:TYR:OH	1:A:1090:PHE:HD1	1.77	0.65
1:A:1643:THR:OG1	1:A:1654:TYR:HB2	1.98	0.64
1:A:1790:LEU:HD12	1:A:1790:LEU:N	2.11	0.64
1:A:754:LYS:NZ	1:A:1354:GLY:O	2.26	0.64
1:A:1274:SER:HG	1:A:1275:HIS:HD1	1.42	0.64
1:A:63:ASN:ND2	1:A:67:LYS:O	2.24	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:LEU:O	1:A:440:HIS:ND1	2.29	0.63
1:A:1792:SER:O	1:A:1796:LYS:NZ	2.27	0.63
1:A:876:GLU:CG	1:A:1275:HIS:HE1	2.12	0.62
1:A:903:GLU:OE2	1:A:903:GLU:HA	1.99	0.62
1:A:880:SER:OG	1:A:881:GLU:N	2.33	0.62
1:A:1274:SER:OG	1:A:1275:HIS:ND1	2.31	0.61
1:A:108:THR:HG1	1:A:111:SER:HG	1.46	0.61
1:A:528:PHE:HB2	1:A:543:TYR:CE2	2.36	0.61
1:A:480:GLN:O	1:A:482:LYS:N	2.34	0.61
1:A:539:TYR:O	1:A:540:HIS:ND1	2.33	0.60
1:A:332:LEU:O	1:A:332:LEU:HD23	2.02	0.59
1:A:889:PHE:HA	1:A:892:GLU:HB2	1.85	0.59
1:A:833:LEU:HD12	1:A:833:LEU:C	2.27	0.59
1:A:862:SER:OG	1:A:1245:LYS:NZ	2.24	0.59
1:A:475:GLN:N	1:A:476:PRO:CD	2.66	0.58
1:A:1546:LEU:HD23	1:A:1546:LEU:H	1.68	0.58
1:A:899:LYS:HG2	1:A:902:GLU:CD	2.26	0.58
1:A:1621:ASN:OD1	1:A:1622:LYS:N	2.30	0.58
1:A:899:LYS:CG	1:A:902:GLU:CD	2.77	0.58
1:A:842:GLU:O	1:A:846:ARG:N	2.36	0.58
1:A:899:LYS:CD	1:A:902:GLU:OE2	2.52	0.57
1:A:473:ASN:O	1:A:474:PHE:CD2	2.57	0.57
1:A:1677:TRP:O	1:A:1680:ILE:N	2.37	0.57
1:A:1685:SER:CB	1:A:1790:LEU:CD2	2.69	0.57
1:A:1541:ASN:OD1	1:A:1541:ASN:O	2.22	0.57
1:A:637:MET:O	1:A:641:SER:HB3	2.04	0.57
1:A:432:PHE:HA	1:A:436:GLY:N	2.19	0.57
1:A:189:SER:O	1:A:189:SER:OG	2.18	0.56
1:A:343:LEU:HD13	1:A:447:ILE:HD12	1.87	0.56
1:A:68[A]:SER:HB3	1:A:71:THR:HG1	1.71	0.56
1:A:1455:ASP:OD2	1:A:1459:TRP:HZ2	1.89	0.56
1:A:493:VAL:O	1:A:497:LEU:N	2.31	0.56
1:A:615:LEU:O	1:A:619:THR:OG1	2.14	0.56
1:A:8:LEU:HB3	1:A:29:PHE:HZ	1.71	0.56
1:A:51:GLU:HB3	1:A:62:HIS:HE2	1.69	0.56
1:A:550:SER:OG	1:A:568:ASP:OD1	2.16	0.55
1:A:497:LEU:C	1:A:499:ASN:H	2.14	0.55
1:A:1282:MET:SD	1:A:1282:MET:O	2.65	0.55
1:A:1267:PHE:O	1:A:1271:ILE:N	2.40	0.54
1:A:637:MET:CE	1:A:1370:ALA:HB1	2.37	0.54
1:A:535:ASP:O	1:A:536:SER:C	2.51	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1179:TYR:CE2	1:A:1181:MET:HB3	2.43	0.54
1:A:295:PRO:HG2	1:A:298:ARG:H	1.73	0.53
1:A:1089:CYS:O	1:A:1091:TYR:N	2.41	0.53
1:A:1426:LEU:O	1:A:1430:ILE:HG13	2.08	0.53
1:A:876:GLU:OE2	1:A:876:GLU:HA	2.08	0.53
1:A:1437:LEU:HD22	1:A:1607:PHE:CE1	2.44	0.53
1:A:372:SER:O	1:A:373:SER:OG	2.17	0.52
1:A:1338:ASP:OD1	1:A:1338:ASP:N	2.39	0.52
1:A:190:LEU:N	1:A:190:LEU:CD1	2.73	0.52
1:A:947:LEU:O	1:A:951:ILE:HG12	2.09	0.52
1:A:1119:VAL:HG23	1:A:1120:GLY:H	1.74	0.52
1:A:94:ILE:HG12	1:A:95:ASP:H	1.74	0.52
1:A:274:TYR:C	1:A:276:ASN:H	2.17	0.52
1:A:833:LEU:CD1	1:A:834:VAL:HG23	2.40	0.52
1:A:527:VAL:HG21	1:A:542:LEU:HD22	1.91	0.52
1:A:574:LEU:HD21	1:A:700:LEU:HD22	1.92	0.51
1:A:1154:CYS:SG	1:A:1373:PHE:HZ	2.34	0.51
1:A:264:GLU:OE2	1:A:264:GLU:N	2.41	0.51
1:A:1179:TYR:O	1:A:1181:MET:N	2.43	0.51
1:A:52:ILE:HG13	1:A:62:HIS:CG	2.45	0.51
1:A:35:PRO:O	1:A:39:LEU:HD23	2.10	0.51
1:A:117:ILE:O	1:A:120:THR:OG1	2.26	0.51
1:A:600:LYS:O	1:A:602:CYS:N	2.39	0.51
1:A:1805:VAL:HG12	1:A:1806:LEU:H	1.76	0.51
1:A:703:LYS:HG3	1:A:703:LYS:O	2.10	0.51
1:A:473:ASN:OD1	1:A:474:PHE:N	2.43	0.51
1:A:721:GLU:OE2	1:A:1259:THR:OG1	2.27	0.51
1:A:844:PHE:HA	1:A:847:LYS:HE3	1.93	0.51
1:A:1499:PHE:CE1	1:A:1502:GLU:OE1	2.64	0.51
1:A:391:LEU:HD23	1:A:395:ARG:NH1	2.25	0.50
1:A:839:GLN:NE2	1:A:868:LEU:HA	2.14	0.50
1:A:1235:VAL:O	1:A:1239:MET:HG2	2.12	0.50
1:A:1800:ASP:OD1	1:A:1801:GLU:N	2.44	0.50
1:A:343:LEU:HD12	1:A:447:ILE:HG13	1.93	0.50
1:A:1123:ARG:HD2	1:A:1124:GLU:N	2.26	0.50
1:A:114:LYS:O	1:A:117:ILE:HG12	2.12	0.49
1:A:255:LYS:O	1:A:257:ASN:N	2.45	0.49
1:A:696:TYR:CE2	1:A:1386:LEU:HD22	2.46	0.49
1:A:841:THR:CG2	1:A:909:ILE:HG23	2.42	0.49
1:A:1445:LEU:O	1:A:1649:ASP:HB2	2.12	0.49
1:A:39:LEU:HD11	1:A:168:LEU:HD22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1790:LEU:N	1:A:1790:LEU:CD1	2.75	0.49
1:A:302:ALA:HA	1:A:479:GLU:OE1	2.13	0.49
1:A:1649:ASP:OD1	1:A:1649:ASP:N	2.45	0.49
1:A:165:PHE:CD2	1:A:190:LEU:HD12	2.48	0.49
1:A:917:ARG:NE	1:A:943:LYS:HZ3	2.11	0.49
1:A:190:LEU:HD13	1:A:190:LEU:H	1.76	0.48
1:A:106:ARG:HH12	1:A:115:LYS:NZ	2.11	0.48
1:A:106:ARG:HH12	1:A:115:LYS:HZ1	1.61	0.48
1:A:317:TYR:OH	1:A:344:ASP:OD1	2.20	0.48
1:A:914:ARG:HH21	1:A:917:ARG:HH22	1.61	0.48
1:A:1119:VAL:HG23	1:A:1120:GLY:N	2.28	0.48
1:A:392:LEU:HA	1:A:395:ARG:NH1	2.28	0.48
1:A:534:LEU:O	1:A:535:ASP:C	2.56	0.48
1:A:1455:ASP:OD2	1:A:1459:TRP:CZ2	2.66	0.48
1:A:1789:SER:CB	1:A:1793:HIS:HB2	2.43	0.48
1:A:1776:ASP:N	1:A:1776:ASP:OD1	2.44	0.48
1:A:63:ASN:OD1	1:A:67:LYS:N	2.30	0.48
1:A:71:THR:HA	1:A:74:VAL:HG12	1.96	0.48
1:A:258:PHE:O	1:A:1343:LEU:HD11	2.13	0.48
1:A:294:CYS:SG	1:A:663:VAL:HG21	2.54	0.48
1:A:1216:HIS:HA	1:A:1219:THR:HG22	1.94	0.48
1:A:380:SER:C	1:A:382:HIS:H	2.21	0.48
1:A:754:LYS:O	1:A:766:ASN:ND2	2.35	0.48
1:A:1515:ALA:HA	1:A:1518:GLN:HG2	1.96	0.48
1:A:554:SER:OG	1:A:555:ILE:N	2.47	0.47
1:A:837:VAL:HB	1:A:909:ILE:HG21	1.95	0.47
1:A:1334:LEU:O	1:A:1338:ASP:C	2.56	0.47
1:A:1545:PRO:O	1:A:1620:ARG:NH2	2.47	0.47
1:A:645:SER:OG	1:A:1362:PRO:O	2.28	0.47
1:A:1452:THR:HG22	1:A:1471:LEU:HB2	1.96	0.47
1:A:213:HIS:CD2	1:A:741:GLU:HG2	2.48	0.47
1:A:589:MET:HA	1:A:592:TRP:CE3	2.50	0.47
1:A:242:PHE:C	1:A:244:ARG:H	2.22	0.47
1:A:372:SER:O	1:A:373:SER:CB	2.62	0.47
1:A:1319:SER:O	1:A:1320:SER:CB	2.62	0.47
1:A:153:PRO:HB2	1:A:155:TRP:HD1	1.80	0.47
1:A:696:TYR:C	1:A:698:CYS:H	2.23	0.47
1:A:834:VAL:HA	1:A:837:VAL:HG22	1.96	0.47
1:A:876:GLU:HG2	1:A:1275:HIS:CE1	2.47	0.47
1:A:1282:MET:O	1:A:1283:GLY:C	2.56	0.47
1:A:104:PHE:HE2	1:A:112:PHE:HD1	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:PHE:O	1:A:435:TYR:N	2.36	0.47
1:A:37:MET:HA	1:A:40:ILE:HG12	1.97	0.46
1:A:699:HIS:CE1	1:A:1119:VAL:HG11	2.50	0.46
1:A:1452:THR:OG1	1:A:1455:ASP:OD1	2.32	0.46
1:A:1499:PHE:C	1:A:1501:GLU:H	2.21	0.46
1:A:8:LEU:HB3	1:A:29:PHE:CZ	2.48	0.46
1:A:832:LEU:C	1:A:834:VAL:N	2.71	0.46
1:A:1653:LEU:HD23	1:A:1672:LEU:HD21	1.96	0.46
1:A:147:TYR:OH	1:A:1090:PHE:CG	2.60	0.46
1:A:1353:SER:HB3	1:A:1358:LYS:O	2.15	0.46
1:A:1642:VAL:CB	1:A:1653:LEU:HD13	2.46	0.46
1:A:103[B]:CYS:HB2	1:A:142:ASP:HB3	1.98	0.46
1:A:431:SER:C	1:A:433:GLU:N	2.73	0.46
1:A:1438:LEU:HA	1:A:1438:LEU:HD23	1.75	0.46
1:A:1645:VAL:N	1:A:1654:TYR:HE2	2.08	0.46
1:A:1805:VAL:HG12	1:A:1806:LEU:N	2.30	0.46
1:A:291:VAL:HA	1:A:294:CYS:SG	2.56	0.46
1:A:417:PHE:HE2	1:A:448:PRO:HA	1.80	0.46
1:A:248:ASP:O	1:A:253:LYS:NZ	2.32	0.46
1:A:948:ARG:HG2	1:A:952:LEU:HD23	1.98	0.46
1:A:1407:CYS:HB3	1:A:1450:LEU:HD13	1.97	0.46
1:A:31:GLY:O	1:A:32:GLN:NE2	2.49	0.46
1:A:696:TYR:HH	1:A:1377:PHE:HE1	1.62	0.46
1:A:114:LYS:O	1:A:118:GLU:OE1	2.33	0.45
1:A:1438:LEU:HD13	1:A:1449:LEU:HD21	1.98	0.45
1:A:343:LEU:CD1	1:A:447:ILE:HG21	2.46	0.45
1:A:696:TYR:C	1:A:698:CYS:N	2.74	0.45
1:A:832:LEU:C	1:A:834:VAL:H	2.24	0.45
1:A:332:LEU:HD23	1:A:332:LEU:C	2.42	0.45
1:A:441:LEU:HA	1:A:444:GLU:HG3	1.97	0.45
1:A:1181:MET:HA	1:A:1364:SER:HB2	1.97	0.45
1:A:497:LEU:C	1:A:499:ASN:N	2.75	0.45
1:A:901:LEU:O	1:A:901:LEU:HD12	2.16	0.45
1:A:917:ARG:HH22	1:A:947:LEU:HD12	1.81	0.45
1:A:1154:CYS:SG	1:A:1373:PHE:CZ	3.09	0.45
1:A:1753:GLN:O	1:A:1756:PRO:HD2	2.16	0.45
1:A:1:MET:HB3	1:A:2:ASP:H	1.58	0.45
1:A:754:LYS:HD3	1:A:764:GLY:HA3	1.98	0.45
1:A:417:PHE:CE2	1:A:448:PRO:HA	2.52	0.45
1:A:487:LEU:O	1:A:487:LEU:HD23	2.17	0.45
1:A:1104:PRO:HB3	1:A:1223:TRP:CZ2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:625:ASN:OD1	1:A:664:VAL:HG21	2.17	0.44
1:A:731:ASN:O	1:A:731:ASN:ND2	2.50	0.44
1:A:1090:PHE:CD1	1:A:1090:PHE:O	2.69	0.44
1:A:1192:PRO:HA	1:A:1195:PHE:HD2	1.82	0.44
1:A:44:LYS:O	1:A:47:SER:OG	2.24	0.44
1:A:1379:VAL:O	1:A:1380:TRP:C	2.60	0.44
1:A:868:LEU:HD11	1:A:949:LYS:HE3	2.00	0.44
1:A:153:PRO:HB2	1:A:155:TRP:CD1	2.52	0.44
1:A:489:ARG:C	1:A:491:SER:H	2.25	0.44
1:A:876:GLU:HG2	1:A:1275:HIS:HE1	1.82	0.44
1:A:274:TYR:O	1:A:276:ASN:N	2.50	0.44
1:A:832:LEU:HA	1:A:835:SER:HB3	2.00	0.44
1:A:475:GLN:H	1:A:476:PRO:HD3	1.81	0.43
1:A:777:PHE:CZ	1:A:1297:LEU:HD22	2.53	0.43
1:A:1263:PHE:HA	1:A:1266:TYR:CD2	2.52	0.43
1:A:1334:LEU:O	1:A:1338:ASP:N	2.28	0.43
1:A:1447:PRO:O	1:A:1471:LEU:HD23	2.18	0.43
1:A:105:VAL:HA	1:A:144:ARG:O	2.18	0.43
1:A:477:SER:C	1:A:479:GLU:H	2.27	0.43
1:A:1099:TYR:HB2	1:A:1104:PRO:HA	1.99	0.43
1:A:1194:LEU:C	1:A:1194:LEU:HD23	2.44	0.43
1:A:527:VAL:CG2	1:A:542:LEU:HD22	2.49	0.43
1:A:51:GLU:HB3	1:A:62:HIS:NE2	2.33	0.43
1:A:1745:LEU:HD23	1:A:1745:LEU:H	1.83	0.43
1:A:212:THR:HA	1:A:215:ASP:OD2	2.19	0.43
1:A:300:ILE:C	1:A:302:ALA:N	2.77	0.43
1:A:1749:ILE:HD12	1:A:1749:ILE:H	1.84	0.43
1:A:1343:LEU:HD12	1:A:1343:LEU:HA	1.72	0.43
1:A:1435:LEU:HD23	1:A:1435:LEU:HA	1.64	0.43
1:A:98:LEU:N	1:A:136:THR:O	2.49	0.42
1:A:273:LEU:HB3	1:A:274:TYR:CD2	2.54	0.42
1:A:541:LEU:O	1:A:542:LEU:HD23	2.19	0.42
1:A:596:CYS:HB2	1:A:597:PRO:HD3	2.01	0.42
1:A:1280:ILE:HG13	1:A:1280:ILE:O	2.18	0.42
1:A:164:LEU:O	1:A:168:LEU:HD23	2.19	0.42
1:A:391:LEU:O	1:A:395:ARG:NH1	2.53	0.42
1:A:275:GLU:OE2	1:A:275:GLU:N	2.51	0.42
1:A:1534:ASP:HA	1:A:1655:ILE:O	2.19	0.42
1:A:320:LEU:HG	1:A:324:LEU:HD23	2.00	0.42
1:A:575:PRO:HA	1:A:578:SER:OG	2.20	0.42
1:A:339:GLN:O	1:A:343:LEU:HD23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:875:GLU:HG3	1:A:1274:SER:HB3	2.00	0.42
1:A:1355:LEU:HD23	1:A:1355:LEU:HA	1.85	0.42
1:A:3:GLU:OE1	1:A:3:GLU:N	2.44	0.42
1:A:858:GLU:N	1:A:858:GLU:OE2	2.52	0.42
1:A:911:ARG:HH21	1:A:915:GLY:N	2.18	0.42
1:A:385:LYS:HE2	1:A:465:TYR:HE1	1.83	0.42
1:A:473:ASN:OD1	1:A:474:PHE:O	2.38	0.42
1:A:589:MET:HG2	1:A:592:TRP:HZ3	1.84	0.42
1:A:1298:SER:HB2	1:A:1358:LYS:NZ	2.34	0.42
1:A:866:SER:OG	1:A:1241:LYS:HG2	2.20	0.42
1:A:904:LYS:NZ	1:A:905:VAL:O	2.53	0.42
1:A:215:ASP:O	1:A:219:ARG:HB2	2.19	0.41
1:A:270:PHE:HE2	1:A:672:ILE:HD12	1.84	0.41
1:A:589:MET:HA	1:A:592:TRP:CZ3	2.55	0.41
1:A:779:ASN:OD1	1:A:780:GLY:N	2.53	0.41
1:A:253:LYS:HE2	1:A:253:LYS:HB2	1.82	0.41
1:A:571:ARG:HE	1:A:702:THR:CG2	2.33	0.41
1:A:1456:VAL:HG11	1:A:1813:SER:HA	2.02	0.41
1:A:1748:LYS:HD2	1:A:1752:ASP:HB2	2.03	0.41
1:A:96:ASN:HA	1:A:135:VAL:HG12	2.02	0.41
1:A:567:ALA:HB1	1:A:572:PHE:HE2	1.85	0.41
1:A:1089:CYS:O	1:A:1090:PHE:C	2.62	0.41
1:A:1127:ILE:HG13	1:A:1127:ILE:O	2.20	0.41
1:A:1220:LEU:O	1:A:1223:TRP:HB2	2.20	0.41
1:A:1307:GLY:HA2	1:A:1312:GLU:O	2.21	0.41
1:A:256:ARG:C	1:A:258:PHE:N	2.78	0.41
1:A:441:LEU:HD12	1:A:444:GLU:HB2	2.02	0.41
1:A:472:TYR:N	1:A:472:TYR:HD2	2.19	0.41
1:A:1170:ILE:HD13	1:A:1170:ILE:HA	1.91	0.41
1:A:42:GLY:O	1:A:45:LEU:HG	2.21	0.41
1:A:184:PHE:HB3	1:A:1091:TYR:CE1	2.56	0.41
1:A:1126:TYR:CE1	1:A:1283:GLY:HA2	2.56	0.41
1:A:95:ASP:OD1	1:A:95:ASP:N	2.53	0.41
1:A:472:TYR:N	1:A:472:TYR:CD2	2.88	0.41
1:A:1693:TRP:C	1:A:1695:LEU:H	2.27	0.41
1:A:11:LEU:HD12	1:A:15:TYR:CE1	2.56	0.41
1:A:392:LEU:HA	1:A:395:ARG:CZ	2.51	0.41
1:A:899:LYS:HE3	1:A:899:LYS:HB2	1.79	0.41
1:A:52:ILE:HB	1:A:151:PHE:HE2	1.86	0.40
1:A:97:SER:HA	1:A:136:THR:H	1.86	0.40
1:A:1411:ASP:OD1	1:A:1467:ARG:NH1	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1450:LEU:HD12	1:A:1450:LEU:HA	1.88	0.40
1:A:1789:SER:O	1:A:1790:LEU:HD12	2.20	0.40
1:A:336:ARG:C	1:A:338:ARG:H	2.28	0.40
1:A:457:LYS:O	1:A:458:ILE:C	2.64	0.40
1:A:715:CYS:HB2	1:A:1124:GLU:OE2	2.21	0.40
1:A:1110:LYS:HE3	1:A:1110:LYS:HB2	1.68	0.40
1:A:1447:PRO:C	1:A:1448:PHE:HD1	2.29	0.40
1:A:1793:HIS:CD2	1:A:1797:TRP:HD1	2.39	0.40
1:A:300:ILE:C	1:A:302:ALA:H	2.28	0.40
1:A:114:LYS:O	1:A:115:LYS:C	2.64	0.40
1:A:705:THR:O	1:A:706:PRO:C	2.65	0.40
1:A:480:GLN:C	1:A:482:LYS:H	2.30	0.40
1:A:497:LEU:O	1:A:499:ASN:N	2.43	0.40
1:A:715:CYS:SG	1:A:716:PHE:N	2.94	0.40
1:A:728:PHE:CD2	1:A:728:PHE:N	2.88	0.40
1:A:1262:ILE:HG22	1:A:1266:TYR:CZ	2.56	0.40
1:A:1653:LEU:O	1:A:1655:ILE:N	2.55	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	1421/2210 (64%)	1191 (84%)	224 (16%)	6 (0%)	30	60

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	189	SER
1	A	474	PHE
1	A	1090	PHE
1	A	659	PRO

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Mol	Chain	Res	Type
1	A	1654	TYR
1	A	275	GLU

### 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	1112/2034 (55%)	1111 (100%)	1 (0%)	92 97

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

Mol	Chain	Res	Type
1	A	190	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	213	HIS
1	A	394	ASN
1	A	561	HIS
1	A	839	GLN
1	A	1087	ASN
1	A	1122	ASN
1	A	1224	HIS
1	A	1431	GLN
1	A	1530	ASN
1	A	1659	GLN
1	A	1784	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 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 ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is 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 ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

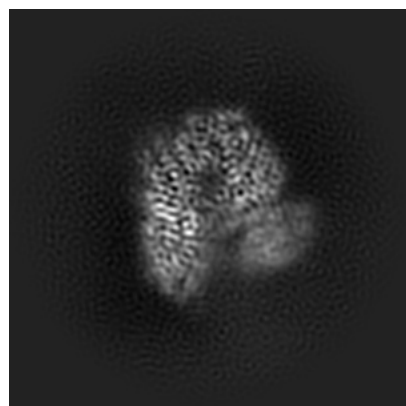
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33026. These allow visual inspection of the internal detail of the map and identification of artifacts.

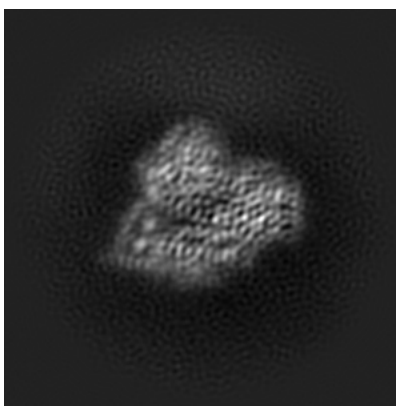
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

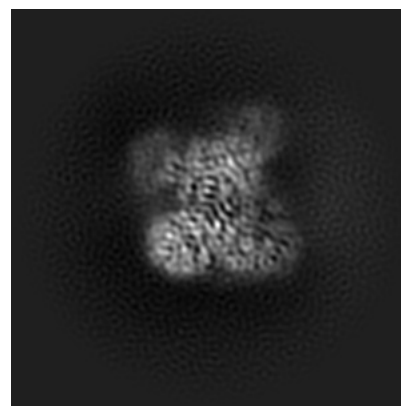
#### 6.1.1 Primary map



X

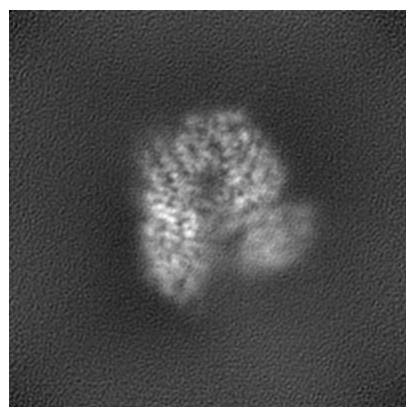


Y

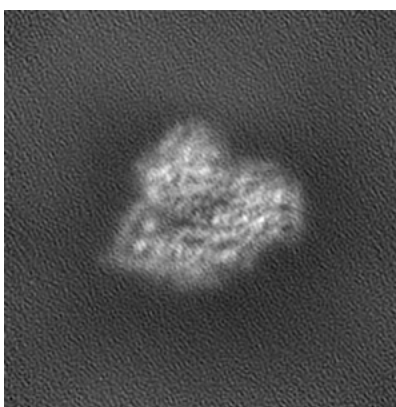


Z

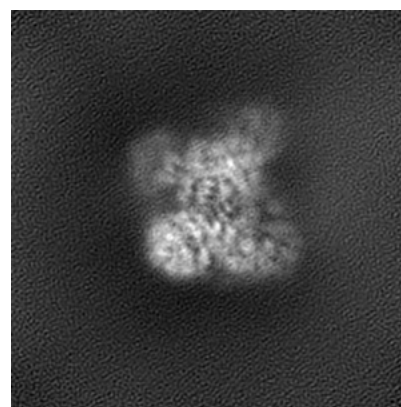
#### 6.1.2 Raw map



X



Y

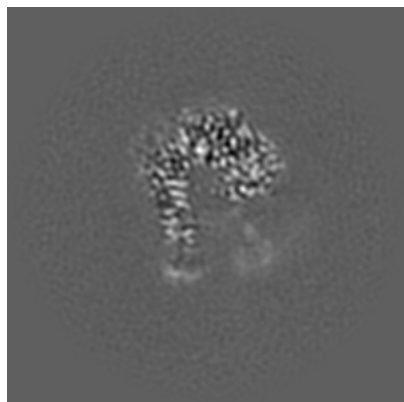


Z

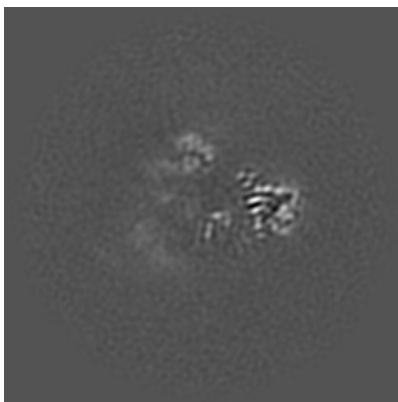
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

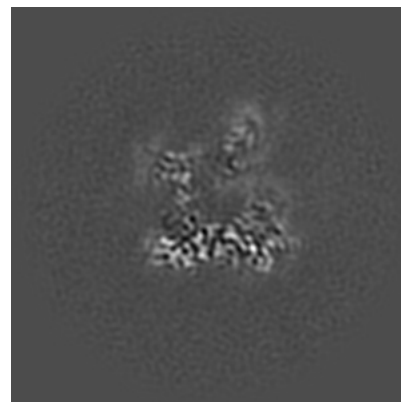
### 6.2.1 Primary map



X Index: 100

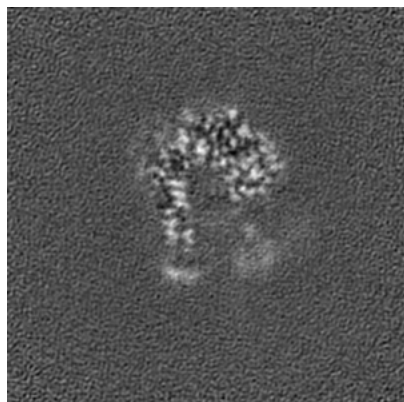


Y Index: 100

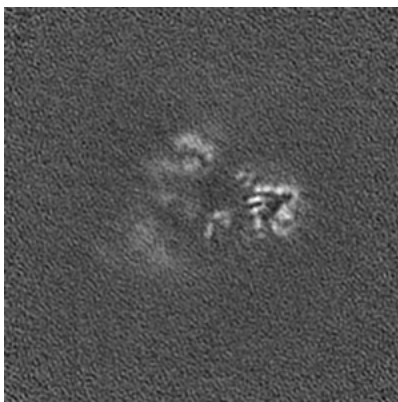


Z Index: 100

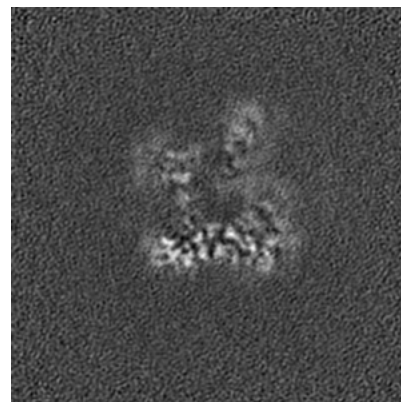
### 6.2.2 Raw map



X Index: 100



Y Index: 100

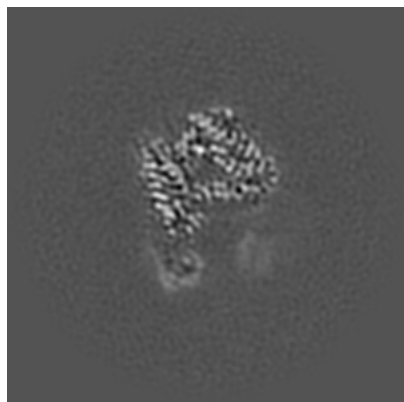


Z Index: 100

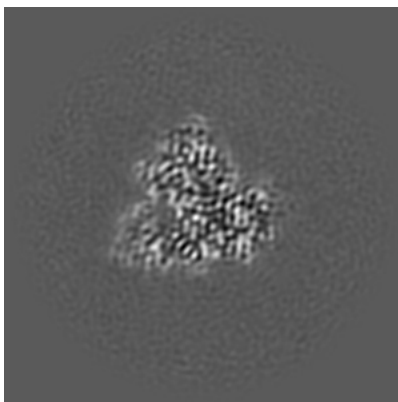
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

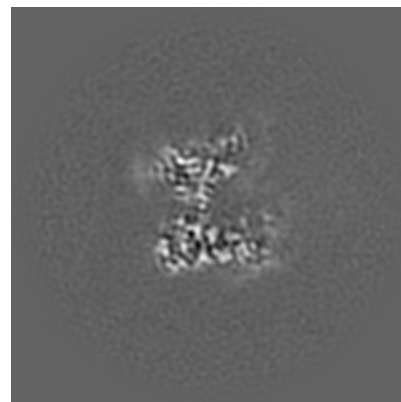
### 6.3.1 Primary map



X Index: 95

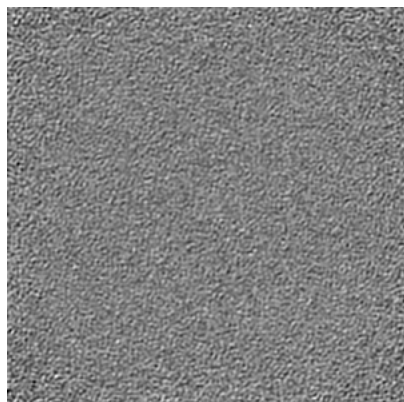


Y Index: 82

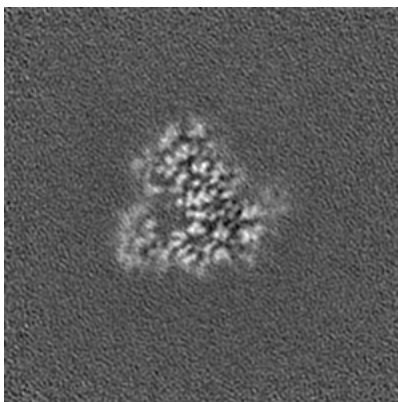


Z Index: 106

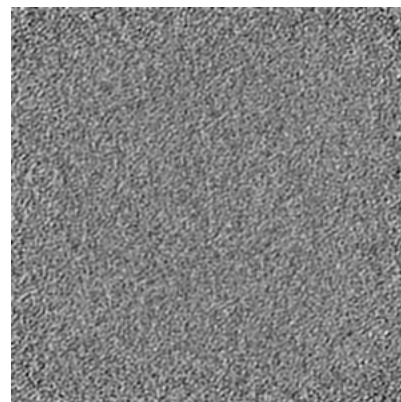
### 6.3.2 Raw map



X Index: 0



Y Index: 79



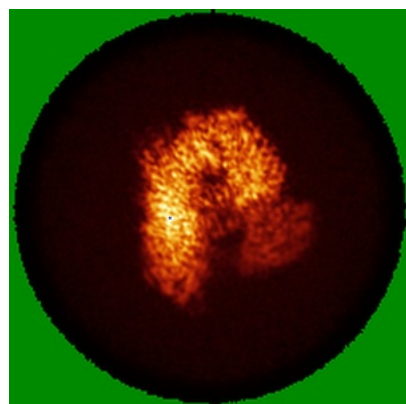
Z Index: 0

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

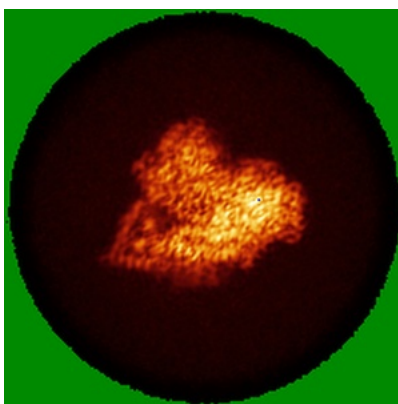


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

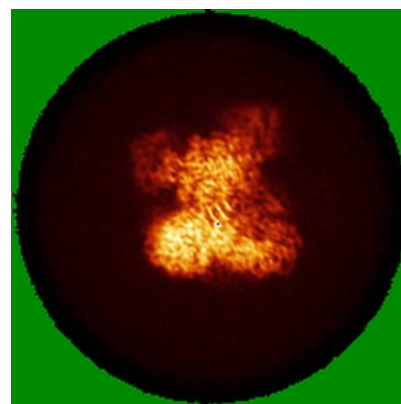
### 6.4.1 Primary map



X

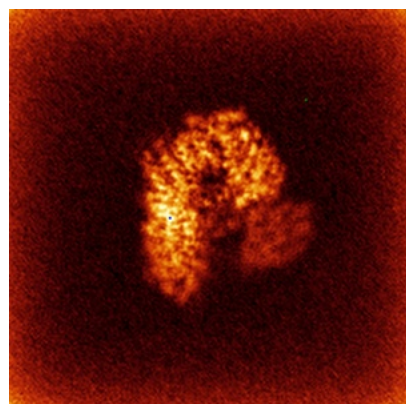


Y

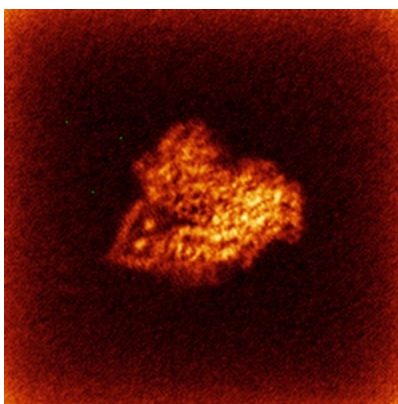


Z

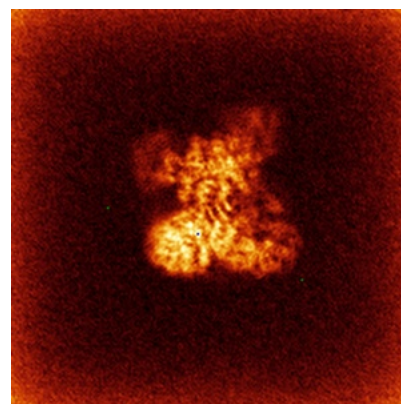
### 6.4.2 Raw map



X



Y

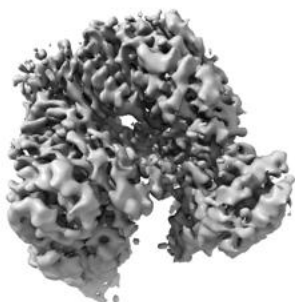


Z

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](#)

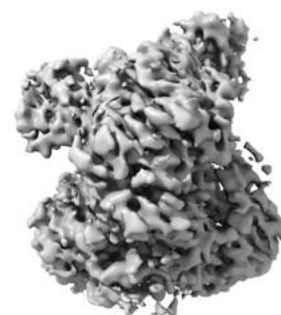
### 6.5.1 Primary map



X



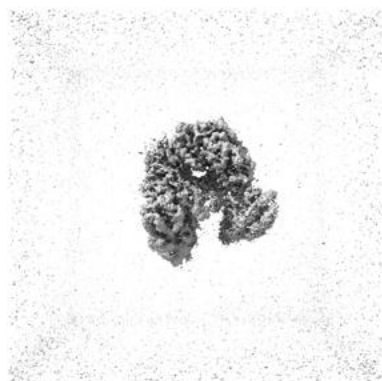
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.254. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

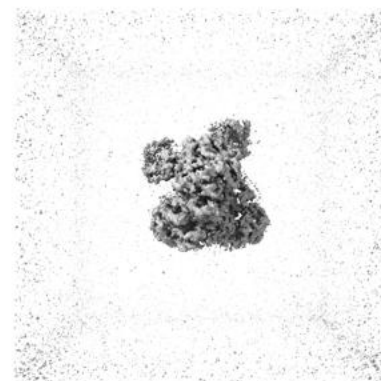
### 6.5.2 Raw map



X



Y



Z

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](#)

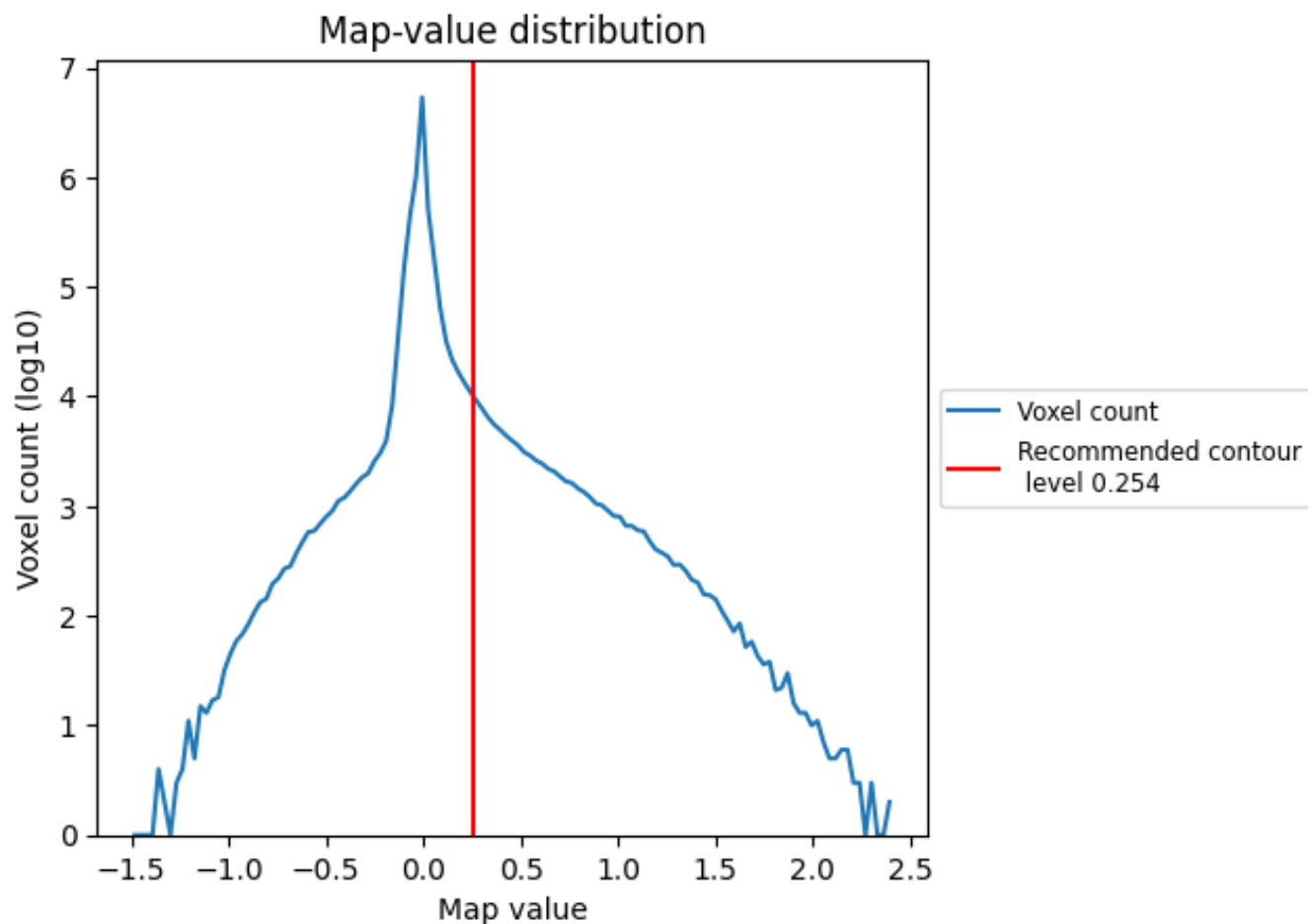
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

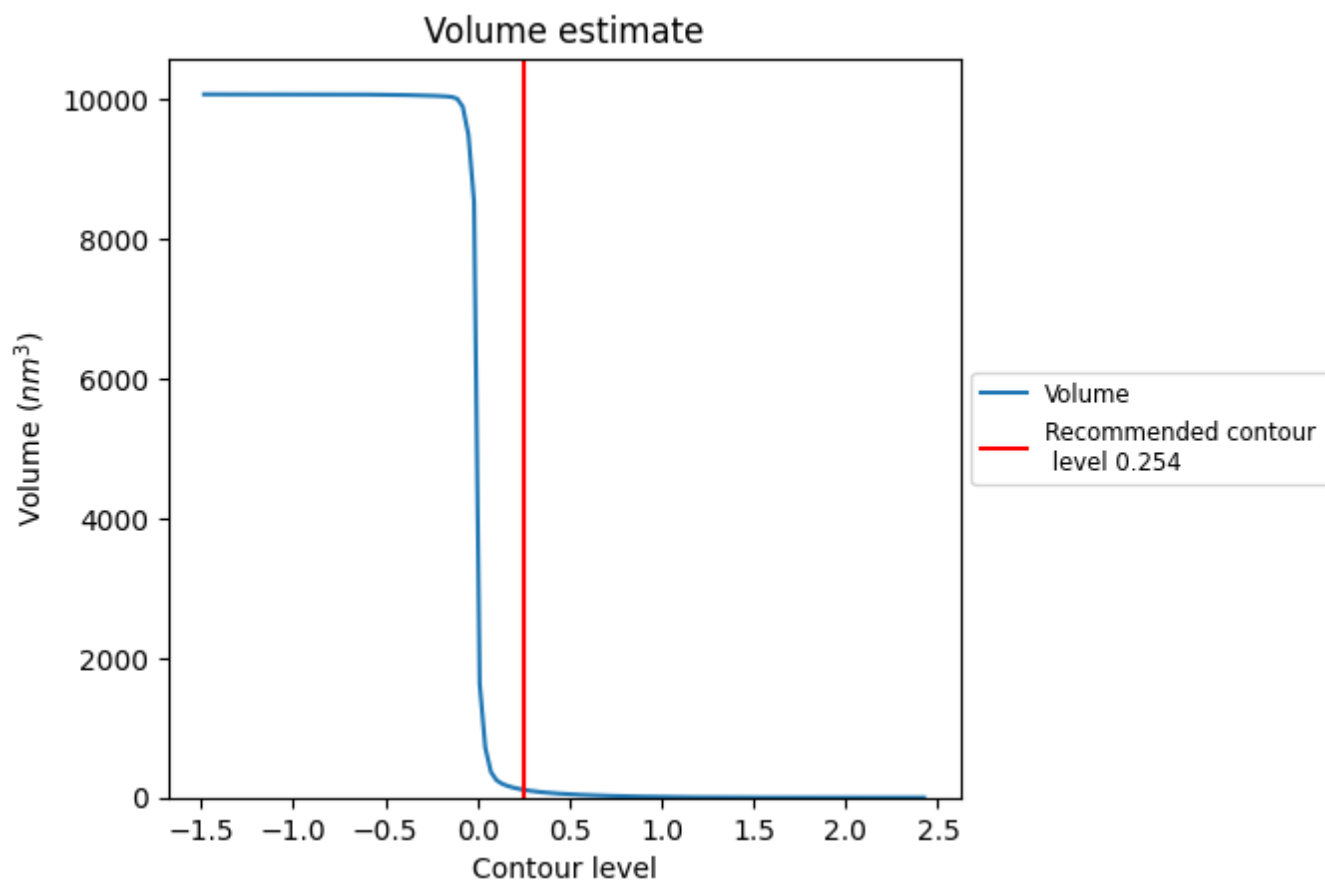
This section contains the results of statistical analysis of the map.

### 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.

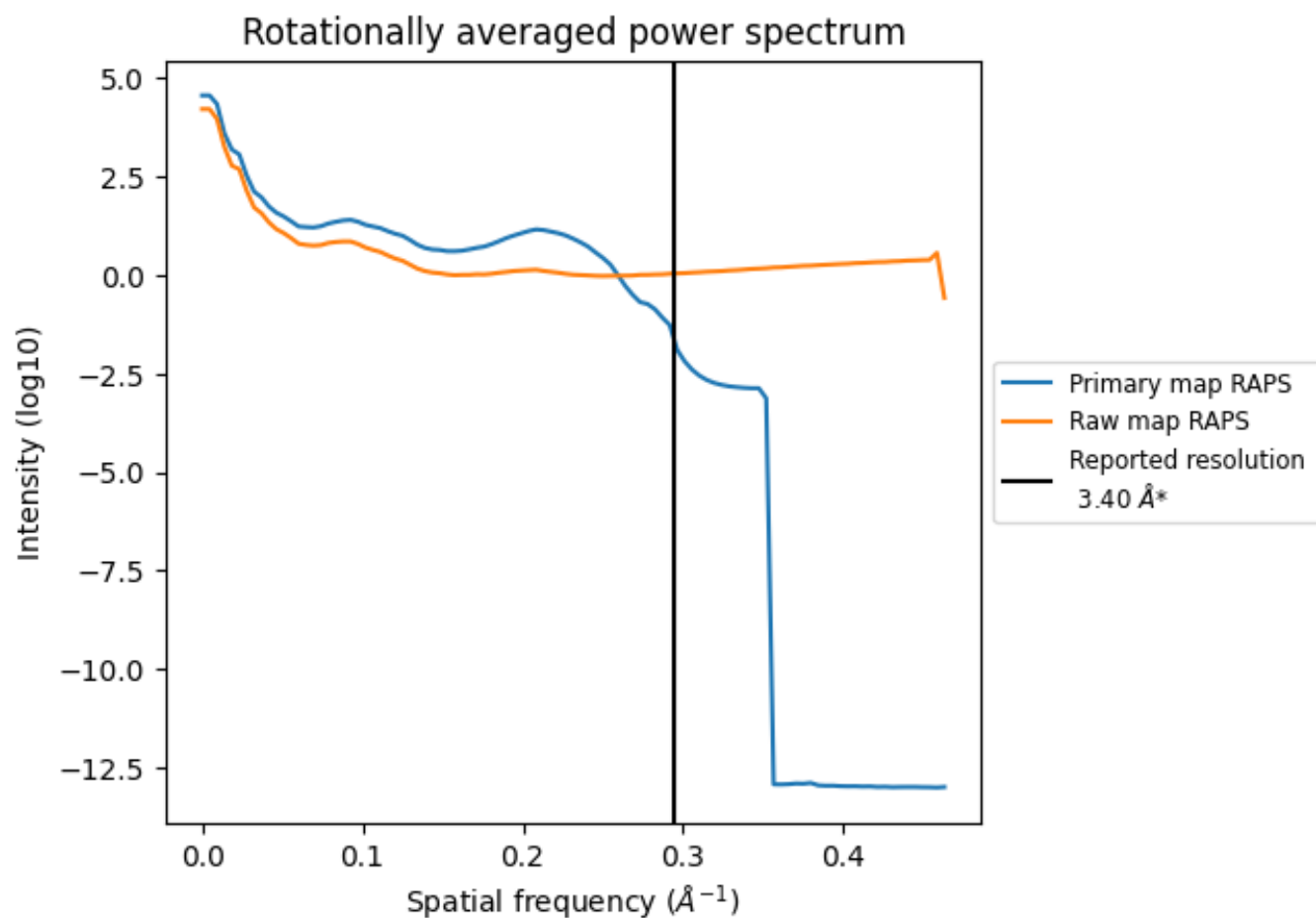
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 110 nm<sup>3</sup>; this corresponds to an approximate mass of 99 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 ⓘ

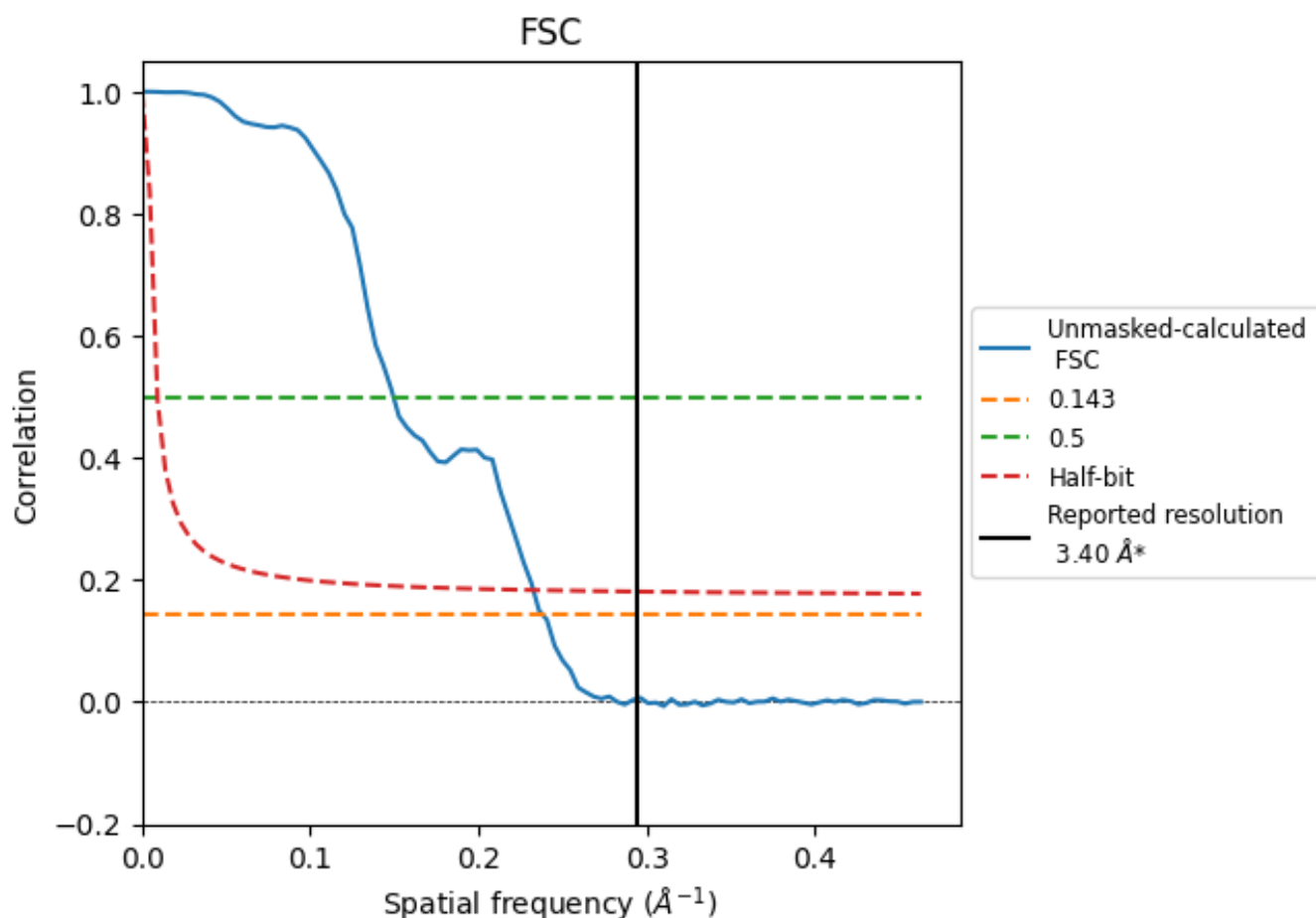


\*Reported resolution corresponds to spatial frequency of 0.294 Å<sup>-1</sup>

## 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 0.294  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

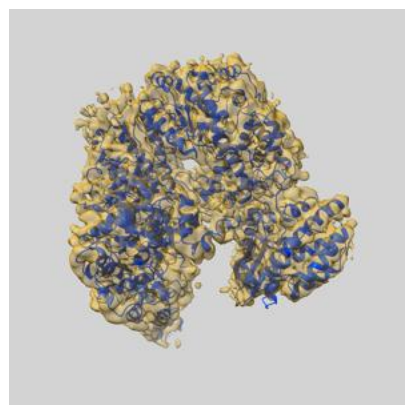
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.20	6.69	4.30

\*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 4.20 differs from the reported value 3.4 by more than 10 %

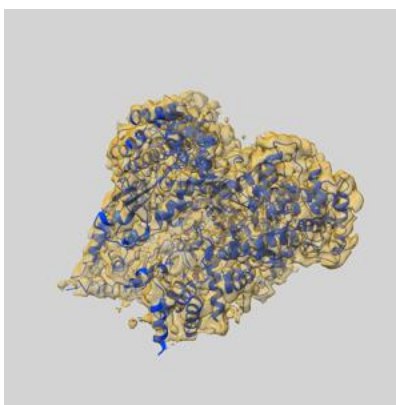
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-33026 and PDB model 7X6S. Per-residue inclusion information can be found in section [3](#) on page [4](#).

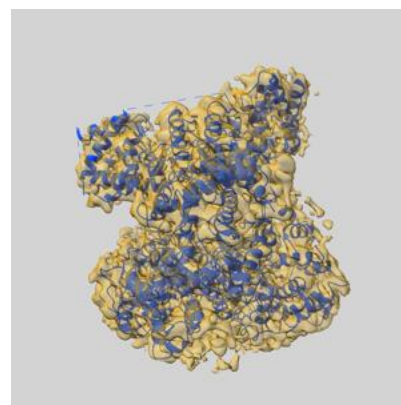
### 9.1 Map-model overlay [i](#)



X



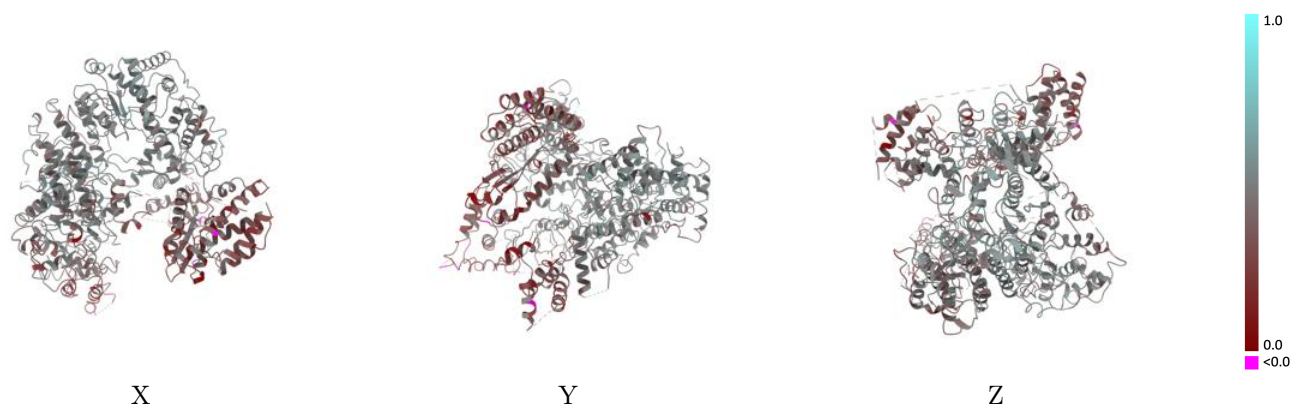
Y



Z

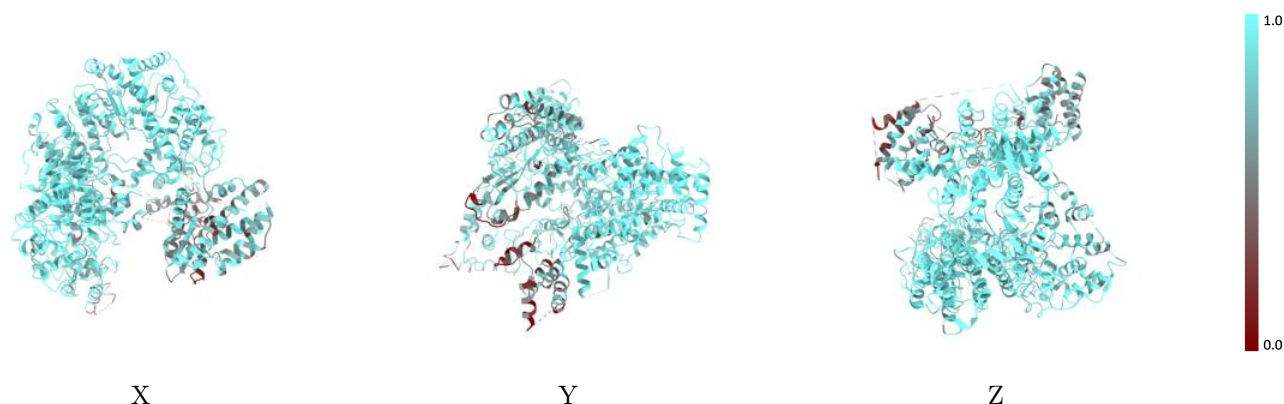
The images above show the 3D surface view of the map at the recommended contour level 0.254 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



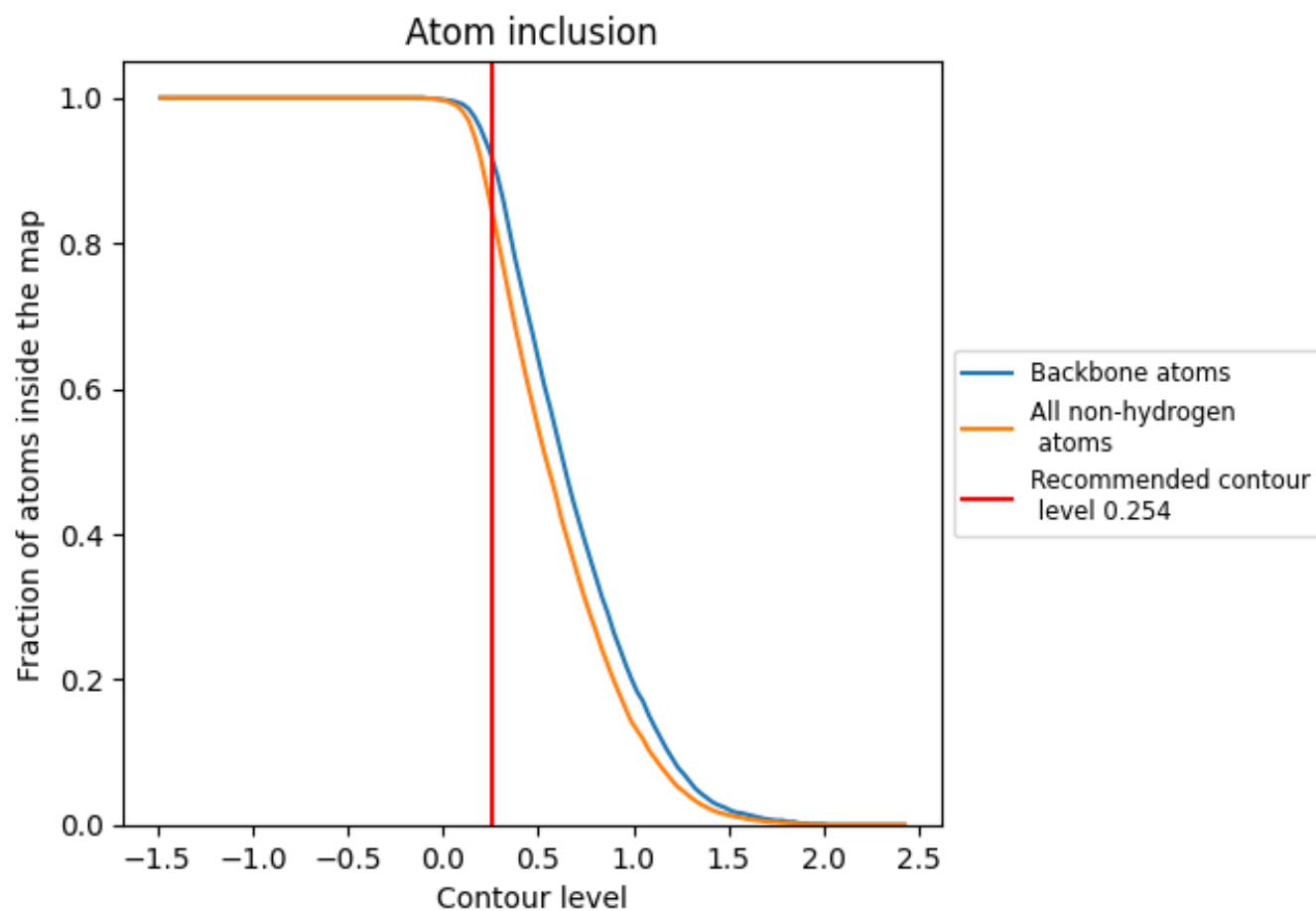
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.254).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 92% 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 (0.254) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8490	<div><div></div></div> 0.4270
A	<div><div></div></div> 0.8490	<div><div></div></div> 0.4270

