



Full wwPDB EM Validation Report ⓘ

Sep 27, 2026 – 02:33 AM JST

PDB ID : 9XD5 / pdb_00009xd5
EMDB ID : EMD-66755
Title : Crimean-Congo hemorrhagic fever virus RNA polymerase in complex with the 5' vRNA
Authors : Xue, L.; Gui, J.; Pan, H.; Chang, T.; Xiong, X.
Deposited on : 2025-10-27
Resolution : 2.72 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

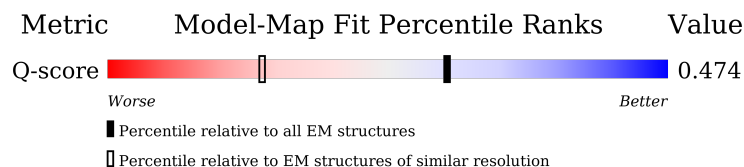
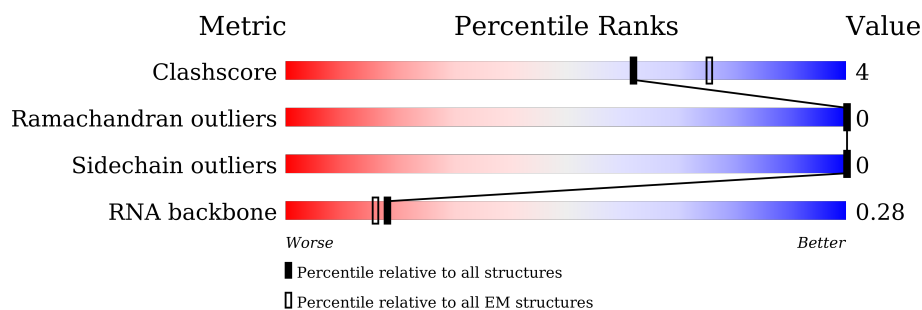
EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 2.72 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	10355 (2.22 - 3.22)

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	3945	
2	C	19	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12810 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	1571	Total	C	N	O	S	0	0
			12577	7953	2176	2357	91		

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

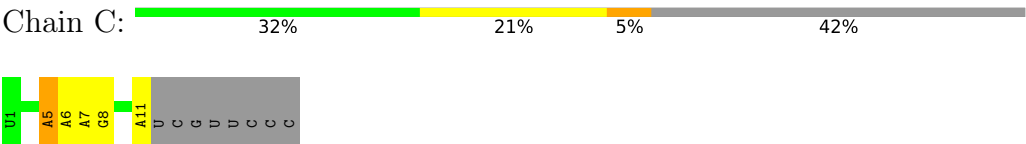
Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	11	Total	C	N	O	P	0	0
			232	106	45	71	10		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	

F2349	T2349	ASP	SER	LYS	LYS	SER	SER	ASN	K1808	LYS	ASP	T1417	G1201	GLY	GLY	GLU	LYS	THR	LYS
C2354	LYS	GLY	VAL	THR	THR	VAL	VAL	TRP	G1627	ARG	GLU	T1418	S1204	PHE	GLU	THR	LYS	TRP	LYS
G2357	LYS	LEU	LEU	LEU	LYS	GLY	GLY	SER	L1632	ARG	L1632	Y1419	LYS	SER	ASP	ASP	LYS	ASP	LYS
M2375	GLN	HIS	VAL	VAL	LYS	LEU	LEU	ILE	D1645	SER	D1645	Q1424	K1208	ASN	GLU	VAL	LEU	LEU	LEU
V2378	GLY	THR	CYS	ASP	ASP	THR	THR	GLU	L1646	PHE	L1646	L1440	R1212	C1102	GLY	VAL	GLY	LYS	LYS
V2382	GLU	LEU	THR	PHE	ALA	GLN	GLN	VAL	M1647	GLY	M1647	E1457	Q1213	T1103	ALA	ALA	LEU	LEU	LEU
V2382	VAL	ILE	GLN	THR	ALA	GLY	GLY	THR	D1653	ARG	D1653	E1457	Q1213	T1104	ILE	ILE	SER	GLU	GLU
M2394	MET	PHE	LYS	GLU	ILE	ASN	ASN	THR	E1654	TYR	E1654	L1462	K1217	D1105	THR	THR	LEU	LEU	LEU
L2394	ALA	ALA	ASP	ASP	ASN	ASN	ASN	THR	K1655	SER	K1655	L1462	K1217	V1110	GLN	GLN	LYS	GLY	GLY
R2399	ILE	THR	ASP	THR	THR	ILE	ILE	SER	K1656	GLN	K1656	S1469	R1222	R1111	LYS	LYS	LEU	LEU	LEU
R2399	VAL	VAL	VAL	VAL	ASN	ASN	ASN	VAL	S1223	LYS	S1223	L1499	W1224	G1116	ARG	VAL	VAL	ILE	ILE
P2404	GLN	LEU	GLU	GLU	GLN	GLY	GLY	ALA	R1659	PRO	R1659	L1262	W1224	G1116	ARG	VAL	VAL	LYS	LYS
P2404	LEU	LEU	GLU	GLU	GLN	ILE	ILE	SER	T1660	PHE	T1660	L1263	L1225	K1117	TYR	TYR	SER	SER	CYS
L2415	ALA	PHE	ASN	PHE	PHE	GLU	GLU	PRO	A1661	GLU	A1661	F1527	V1234	R1123	LEU	LEU	PHE	PHE	PHE
S2421	ALA	SER	SER	ALA	ALA	THR	THR	THR	L1664	ARG	L1664	L1512	V1241	R1124	ALA	ALA	ALA	ALA	ALA
S2432	GLN	TYR	SER	ALA	HIS	HIS	SER	HIS	V1670	GLY	V1670	Q1517	N1259	L1131	THR	THR	ALA	ALA	ASP
S2432	ALA	ASP	LEU	LEU	LEU	LEU	LEU	MET	M1524	GLY	M1524	M1524	N1259	L1131	THR	THR	ALA	ALA	ASP
R2435	ASN	LEU	LEU	ALA	ALA	GLU	GLU	LEU	LYS	VAL	LYS	L1525	L1262	M1135	THR	THR	LYS	LYS	LYS
L2436	THR	TRP	GLY	PRO	PRO	LEU	PHE	LYS	ALA	VAL	ALA	R1526	L1263	M1135	THR	THR	LYS	LYS	LYS
L2437	GLU	THR	PHE	THR	ASP	LEU	THR	ASP	F1527	PHE	F1527	F1527	L1263	M1135	THR	THR	LYS	LYS	LYS
M2466	ARG	THR	VAL	CYS	CYS	GLU	THR	CYS	L1536	ASN	L1536	L1536	V1292	C1143	SER	SER	SER	SER	SER
M2466	THR	THR	VAL	LEU	LEU	GLU	THR	PHE	K1837	ASP	K1837	L1536	V1292	C1143	SER	SER	SER	SER	SER
L2475	ALA	ALA	VAL	VAL	LYS	GLU	GLU	LEU	K1846	ASN	LYS	F1546	A1302	VAL	VAL	VAL	VAL	VAL	VAL
L2486	VAL	ASN	VAL	THR	LEU	LEU	LEU	LYS	M1850	TYR	M1850	K1306	K1306	SER	SER	SER	SER	SER	SER
E2492	ALA	ASN	LEU	LEU	GLY	GLU	GLU	LEU	L1851	GLN	L1851	C1550	K1306	ALA	ALA	ALA	ALA	ALA	ALA
V2510	ALA	GLY	THR	THR	LEU	LEU	LEU	ILE	R1852	GLN	R1852	I1316	K1306	LYS	LYS	LYS	THR	THR	THR
E2511	ALA	VAL	SER	SER	THR	THR	THR	LYS	GLY	ALA	GLY	I1553	V1321	HIS	HIS	ASP	ASP	GLU	GLU
H2512	GLN	ASN	ASN	ASN	VAL	VAL	VAL	ASN	LYS	ILE	ASN	I1553	V1321	ASP	ASP	ASP	ASP	VAL	VAL
K2521	GLY	LYS	GLY	GLY	ARG	GLY	GLY	LEU	LYS	THR	ASP	M1556	V1326	GLY	GLY	GLY	ARG	ARG	ARG
V2526	GLY	LEU	LEU	THR	THR	PHE	PHE	GLU	LYS	ILE	THR	L1560	V1326	ASN	ASN	ASN	ARG	ARG	ARG
V2526	ARG	GLY	GLY	GLY	HIS	GLN	GLN	GLU	THR	GLN	THR	Y1567	V1351	LEU	LEU	LEU	VAL	VAL	VAL
L2529	ASP	ARG	LEU	LEU	PRO	ILE	ILE	GLN	GLY	PHE	THR	E1352	T1351	ASP	ASP	ASP	LYS	LYS	LYS
L2533	VAL	THR	THR	THR	VAL	GLU	GLU	ASN	S1371	THR	S1371	W1572	K1373	R1169	GLY	GLY	ASN	ASN	ASN
V2542	GLN	GLY	ASP	ASP	PHE	GLY	GLY	ASN	F1754	ILE	F1754	V1372	K1373	D1173	SER	SER	SER	SER	SER
V2542	GLU	ARG	GLY	GLY	THR	GLY	GLY	ILE	Y1755	ALA	Y1755	Q1174	K1378	Q1174	ALA	ALA	PHE	PHE	PHE
R2557	THR	PRO	GLY	GLY	LYS	LEU	LEU	ILE	T1756	SER	T1756	L1176	K1378	R1175	LEU	LEU	PHE	PHE	PHE
R2557	GLY	GLY	GLY	GLY	LYS	LYS	LYS	GLY	P1774	VAL	P1774	C1384	K1384	L1176	GLY	GLY	ASN	ASN	ASN
K2566	THR	ARG	ASP	ASP	GLU	GLN	GLN	GLY	L1783	SER	L1783	I1608	L1386	D1181	LYS	LYS	LYS	LYS	LYS
T2567	VAL	SER	LEU	LEU	VAL	LEU	LEU	LYS	GLY	ASP	GLY	I1608	L1386	D1181	LEU	LEU	LEU	LEU	LEU
L2568	VAL	VAL	LEU	LEU	ILE	ILE	ILE	ASP	T1811	ARG	T1811	I1608	L1386	D1181	LEU	LEU	LEU	LEU	LEU
V2569	MET	ARG	HIS	HIS	LYS	THR	THR	CYS	M1621	ARG	M1621	I1608	L1386	D1181	LEU	LEU	LEU	LEU	LEU
V2569	LYS	SER	LYS	LYS	THR	THR	THR	ASP	ASP	ARG	ASP	I1608	L1386	D1181	LEU	LEU	LEU	LEU	LEU
F2573	VAL	VAL	THR	THR	ASP	THR	THR	ASP	R1804	LYS	R1804	I1608	L1386	D1181	LEU	LEU	LEU	LEU	LEU
L2574	ILE	ILE	THR	THR	LEU	LEU	LEU	LEU	K2318	GLY	K2318	I1608	L1386	D1181	LEU	LEU	LEU	LEU	LEU

- Molecule 2: RNA (5'-R(*UP*CP*UP*CP*AP*AP*AP*GP*AP*AP*AP*UP*CP*GP*UP*UP*CP*CP*C)-3')



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	155957	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)	600	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	1.779	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	262.8, 262.8, 262.8	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.876, 0.876, 0.876	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: ZN

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	0.16	0/12779	0.32	0/17213
2	C	0.17	0/260	0.31	0/403
All	All	0.16	0/13039	0.32	0/17616

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	12577	0	12754	110	0
2	C	232	0	121	2	0
3	A	1	0	0	0	0
All	All	12810	0	12875	110	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 (110) 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:2958:PHE:HB3	1:A:2992:THR:O	1.80	0.81
1:A:2399:ARG:HH12	1:A:2475:ILE:HG21	1.53	0.72
1:A:1536:LEU:HB2	1:A:2569:VAL:HB	1.73	0.71
1:A:1028:CYS:HB3	1:A:1065:CYS:HA	1.74	0.70
1:A:1632:LEU:HD22	1:A:2404:PRO:HD2	1.77	0.65
1:A:2590:VAL:HG13	1:A:2625:VAL:HG22	1.78	0.65
1:A:1608:ILE:HA	1:A:1611:ILE:HG12	1.81	0.63
1:A:2903:VAL:HG21	1:A:3152:LEU:HD21	1.81	0.62
1:A:3027:VAL:HA	1:A:3040:SER:O	2.02	0.59
1:A:2760:ILE:HD11	1:A:3058:LEU:HD11	1.84	0.58
1:A:2585:ARG:HH12	1:A:3086:VAL:HG13	1.69	0.57
1:A:2694:LEU:HD12	1:A:2830:ILE:HG13	1.87	0.57
1:A:2657:LEU:HD22	1:A:2666:LEU:HB2	1.87	0.57
1:A:1004:LEU:HD21	1:A:2542:TRP:HB3	1.87	0.56
1:A:1414:ILE:HD11	1:A:2599:ILE:HD11	1.87	0.55
1:A:1418:LEU:HB3	1:A:2595:PHE:HZ	1.70	0.55
1:A:1105:ASP:HB2	1:A:1213:GLN:HG3	1.89	0.55
1:A:1173:ASP:HA	1:A:1176:LEU:HD13	1.89	0.55
1:A:1241:VAL:HG21	1:A:1850:MET:HB3	1.89	0.55
1:A:1774:PRO:HD2	1:A:2557:ARG:HH21	1.72	0.54
1:A:1605:ARG:HH21	1:A:2590:VAL:HG21	1.72	0.54
1:A:1351:THR:HG23	1:A:1352:GLU:HG3	1.89	0.54
1:A:1083:PRO:HD3	1:A:1386:LEU:HD13	1.91	0.53
1:A:1306:LYS:HD2	1:A:2818:LEU:HD21	1.91	0.53
1:A:1111:ARG:HG2	1:A:1147:PRO:HG3	1.90	0.52
1:A:1417:THR:HB	1:A:2595:PHE:HE1	1.75	0.52
1:A:1262:LEU:HD23	1:A:1550:CYS:HB3	1.91	0.52
1:A:1259:ASN:HA	2:C:5:A:H62	1.74	0.51
1:A:1526:ARG:HD2	1:A:2580:PHE:HZ	1.75	0.51
1:A:1580:TRP:HE1	1:A:2582:MET:HG3	1.76	0.51
1:A:3173:ARG:HG3	1:A:3177:HIS:CE1	2.46	0.51
1:A:1292:VAL:HG11	1:A:1321:VAL:HG13	1.93	0.51
1:A:1411:TYR:HB2	1:A:1512:LEU:HD21	1.93	0.51
1:A:1457:GLU:HG3	1:A:1469:SER:HB3	1.92	0.51
1:A:2591:ILE:HA	1:A:2594:MET:HE2	1.93	0.50
1:A:1234:VAL:HG22	1:A:1373:LYS:HE2	1.93	0.50
1:A:2529:LEU:HD22	1:A:2533:LEU:HD23	1.93	0.50
1:A:1503:TYR:HE2	1:A:1595:THR:HG23	1.76	0.50
1:A:1035:ILE:HG12	1:A:1055:ASN:HD22	1.77	0.50
1:A:1143:CYS:HB2	1:A:1225:LEU:HD22	1.94	0.50
1:A:2837:ARG:HG2	1:A:2839:PHE:H	1.76	0.50
1:A:2375:MET:HA	1:A:2378:VAL:HG22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1103:LEU:HB2	1:A:1217:LYS:HE3	1.94	0.49
1:A:2349:PHE:O	1:A:2526:THR:HA	2.13	0.48
1:A:2630:ASN:HA	1:A:2633:PHE:CE2	2.48	0.48
1:A:2628:VAL:HG21	1:A:3218:LYS:HE2	1.96	0.48
1:A:1058:LEU:HD21	1:A:1263:LEU:HD22	1.96	0.47
1:A:2790:PRO:HG2	1:A:2793:ARG:HA	1.95	0.47
1:A:966:LEU:HB3	1:A:2394:ILE:HD11	1.97	0.47
1:A:1207:LEU:HG	1:A:1208:LYS:HD2	1.95	0.47
1:A:2354:CYS:HB3	1:A:2574:LEU:HD13	1.96	0.47
1:A:2655:LEU:HB2	1:A:2797:ILE:HD11	1.97	0.47
1:A:1124:VAL:HG13	1:A:1187:LEU:HD21	1.96	0.46
1:A:3152:LEU:HD13	1:A:3174:TYR:HD2	1.79	0.46
1:A:2837:ARG:HD2	1:A:2839:PHE:HB2	1.98	0.46
1:A:2680:ALA:HB1	1:A:2859:ILE:HG13	1.97	0.46
1:A:1110:VAL:HG12	1:A:1147:PRO:HD3	1.98	0.46
1:A:2655:LEU:HD12	1:A:2825:GLN:HG3	1.98	0.45
1:A:1462:LEU:HD13	1:A:1560:LEU:HD11	1.99	0.45
1:A:1580:TRP:HE3	1:A:1589:VAL:HG11	1.81	0.45
1:A:2415:LEU:HD22	1:A:2437:LEU:HG	1.98	0.45
1:A:1424:GLN:HB3	1:A:3219:GLU:HB3	1.99	0.45
1:A:1804:ARG:HD2	1:A:2382:VAL:HG11	1.99	0.45
1:A:2357:GLY:HA2	1:A:2567:THR:HG23	1.99	0.45
1:A:1526:ARG:HH21	1:A:1527:PHE:HZ	1.66	0.44
1:A:3197:MET:HE1	1:A:3207:PRO:HB3	2.00	0.44
1:A:2492:GLU:HG3	1:A:2510:VAL:HB	1.99	0.44
1:A:2638:GLN:HE22	1:A:2667:PHE:H	1.66	0.44
1:A:1645:ASP:HB3	1:A:1664:LEU:HD11	2.00	0.44
1:A:934:VAL:HG12	1:A:967:VAL:HG13	2.00	0.44
1:A:2573:PHE:HA	1:A:2581:MET:O	2.18	0.44
1:A:954:LEU:HD21	1:A:1646:LEU:HD21	1.98	0.43
1:A:2581:MET:HE3	1:A:2581:MET:HB3	1.83	0.43
1:A:949:PRO:HG3	1:A:2466:ASN:HB3	2.00	0.43
1:A:1783:LEU:O	1:A:1787:ILE:HG23	2.18	0.43
1:A:2318:LYS:HD2	1:A:2579:GLU:HB2	2.00	0.43
1:A:1524:MET:HE1	1:A:2566:LYS:HD3	2.01	0.43
1:A:1316:ILE:HG12	1:A:2628:VAL:HG22	2.00	0.42
1:A:1407:LEU:HG	1:A:1512:LEU:HD23	2.00	0.42
1:A:1378:LYS:HD3	1:A:1378:LYS:HA	1.82	0.42
1:A:1524:MET:HB3	1:A:1546:PHE:CE1	2.55	0.42
1:A:2660:LEU:HD13	1:A:2860:ILE:HG13	2.01	0.42
1:A:3026:CYS:O	1:A:3041:VAL:HA	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1298:LYS:HE3	1:A:1298:LYS:HB2	1.82	0.42
1:A:1517:GLN:HE22	2:C:5:A:P	2.42	0.42
1:A:1846:LYS:HG2	1:A:1850:MET:HE3	2.02	0.42
1:A:981:ILE:HD11	1:A:1790:PHE:HB2	2.01	0.42
1:A:1131:LEU:O	1:A:1135:MET:HG3	2.20	0.42
1:A:1645:ASP:C	1:A:1647:MET:H	2.27	0.42
1:A:2378:VAL:HG11	1:A:2486:LEU:HD11	2.02	0.42
1:A:3101:LEU:HD21	1:A:3108:VAL:HG21	2.02	0.42
1:A:1302:ALA:HB1	1:A:2818:LEU:HD11	2.02	0.41
1:A:1371:SER:O	1:A:1384:CYS:HA	2.21	0.41
1:A:1424:GLN:HE22	1:A:2628:VAL:HB	1.86	0.41
1:A:1755:TYR:CE2	1:A:1757:PRO:HG3	2.55	0.41
1:A:2621:MET:HE2	1:A:2621:MET:HB3	1.98	0.41
1:A:1184:ARG:HD2	1:A:1208:LYS:NZ	2.35	0.41
1:A:1553:ILE:HA	1:A:1556:ASN:HD22	1.86	0.41
1:A:2791:LEU:HD21	1:A:2818:LEU:HD12	2.03	0.41
1:A:1015:LEU:HD11	1:A:1567:TYR:HB2	2.02	0.41
1:A:962:MET:HE2	1:A:962:MET:HB3	1.81	0.41
1:A:1326:VAL:HG13	1:A:1440:LEU:HD21	2.02	0.40
1:A:1659:ARG:C	1:A:1661:ALA:H	2.29	0.40
1:A:1526:ARG:HG3	1:A:1611:ILE:HD12	2.02	0.40
1:A:2797:ILE:HG23	1:A:2824:ILE:HD12	2.03	0.40
1:A:1419:TYR:CZ	1:A:1499:LEU:HB3	2.56	0.40
1:A:2512:HIS:HA	1:A:2521:LYS:HG2	2.03	0.40
1:A:1014:MET:HG3	1:A:1539:PRO:HB3	2.02	0.40
1:A:1224:TRP:CD2	1:A:1391:MET:HG3	2.57	0.40
1:A:2819:GLU:O	1:A:2823:ARG:HG3	2.20	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	1541/3945 (39%)	1469 (95%)	72 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1447/3601 (40%)	1447 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1002	HIS
1	A	1055	ASN
1	A	1433	ASN
1	A	1517	GLN
1	A	1758	ASN
1	A	1776	HIS
1	A	2302	ASN
1	A	2428	HIS
1	A	2476	HIS
1	A	2695	GLN
1	A	2857	ASN
1	A	3098	GLN
1	A	3186	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	10/19 (52%)	5 (50%)	0

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	5	A
2	C	6	A
2	C	7	A
2	C	8	G
2	C	11	A

There are no RNA pucker outliers to report.

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](#)

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

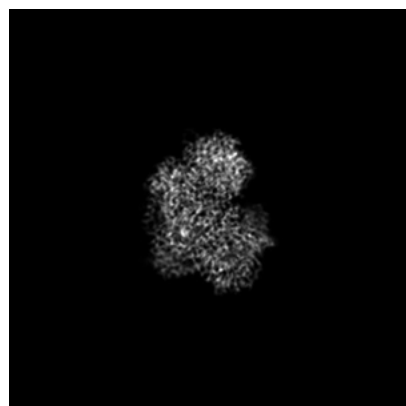
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66755. These allow visual inspection of the internal detail of the map and identification of artifacts.

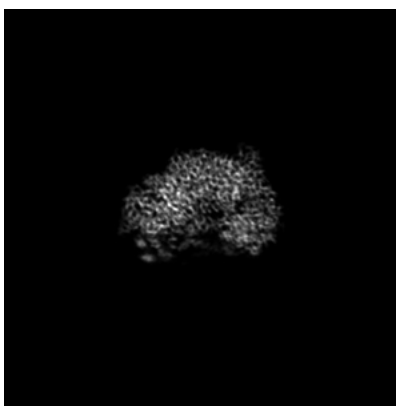
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

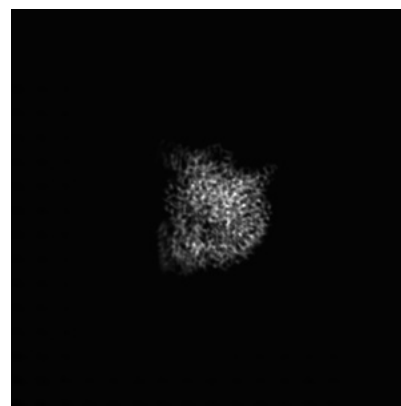
6.1.1 Primary map



X

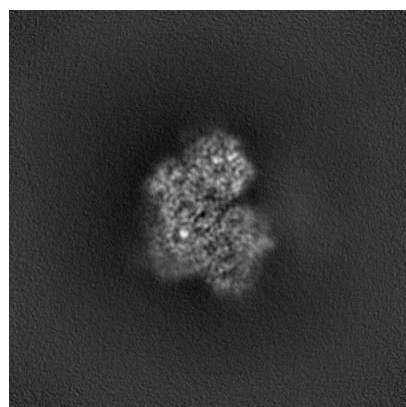


Y

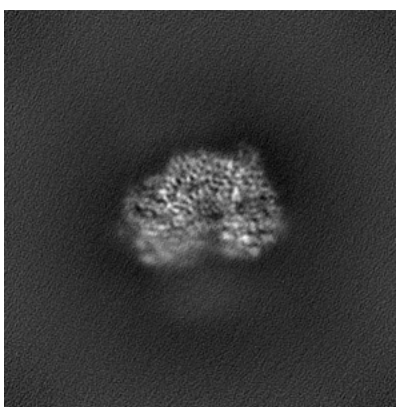


Z

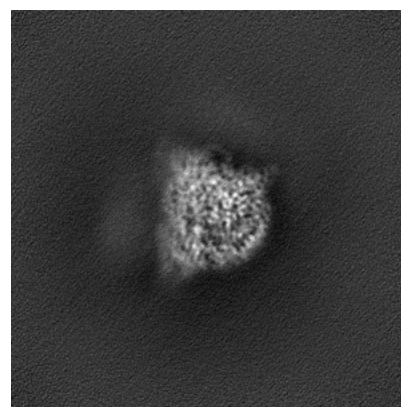
6.1.2 Raw map



X



Y

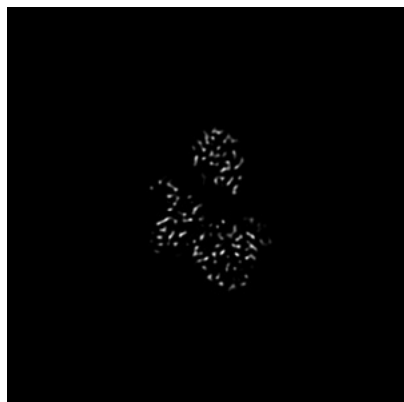


Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 150

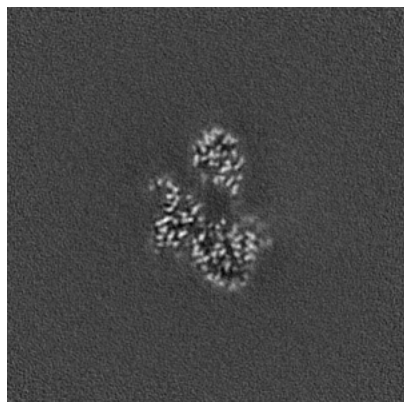


Y Index: 150

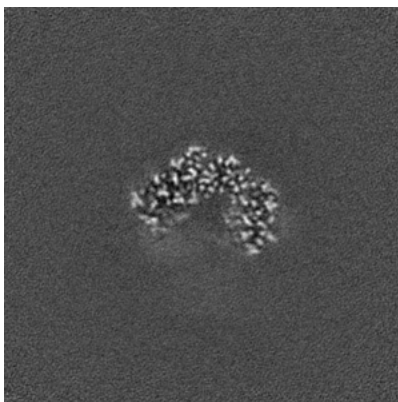


Z Index: 150

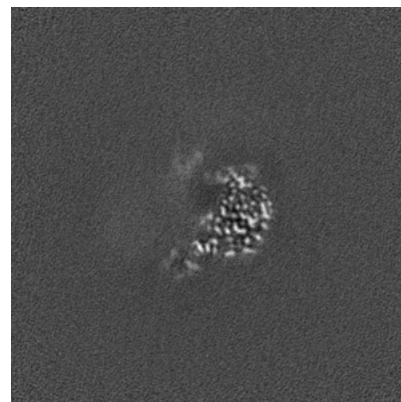
6.2.2 Raw map



X Index: 150



Y Index: 150



Z Index: 150

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: 162

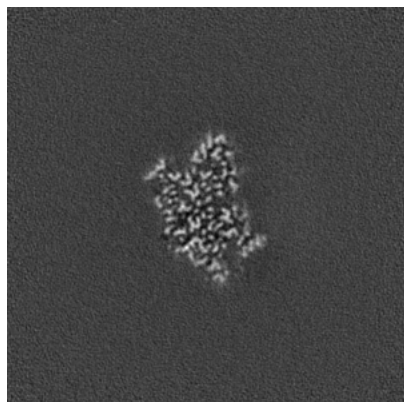


Y Index: 162

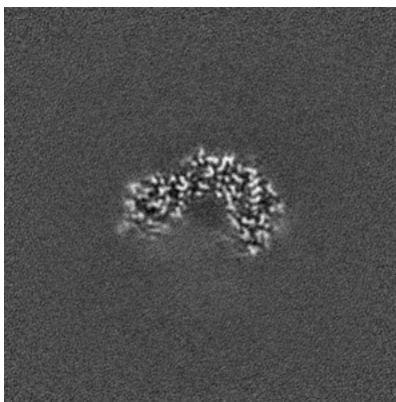


Z Index: 130

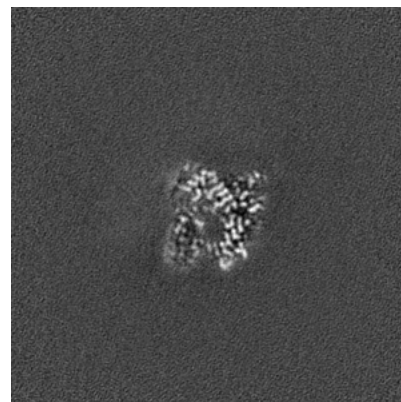
6.3.2 Raw map



X Index: 162



Y Index: 156

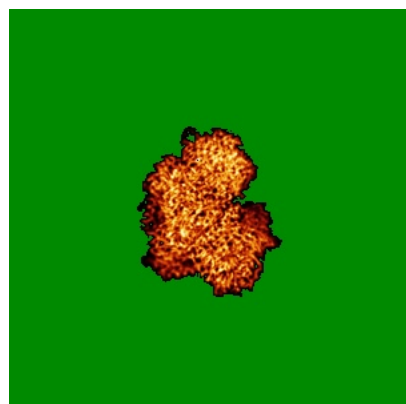


Z Index: 172

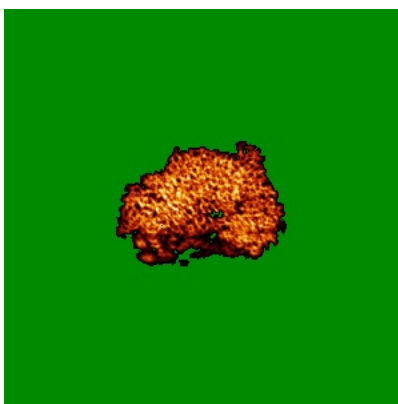
The images above show the largest variance slices of the map in three orthogonal directions.

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

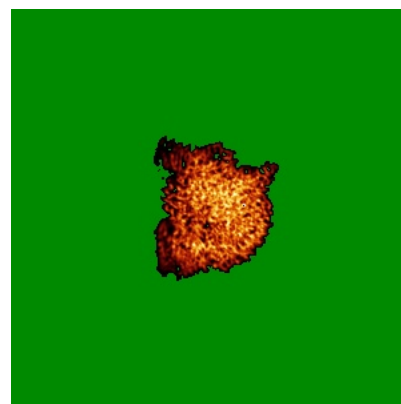
6.4.1 Primary map



X

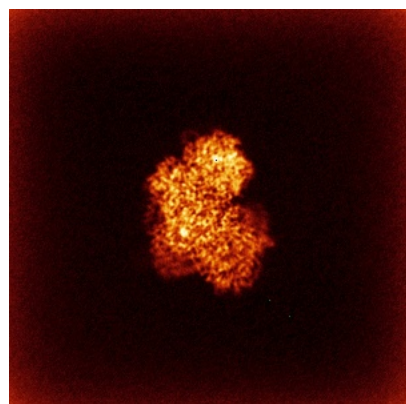


Y

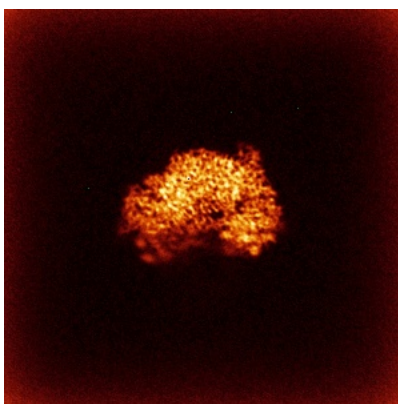


Z

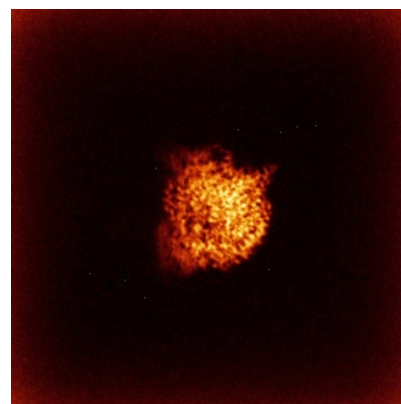
6.4.2 Raw map



X



Y

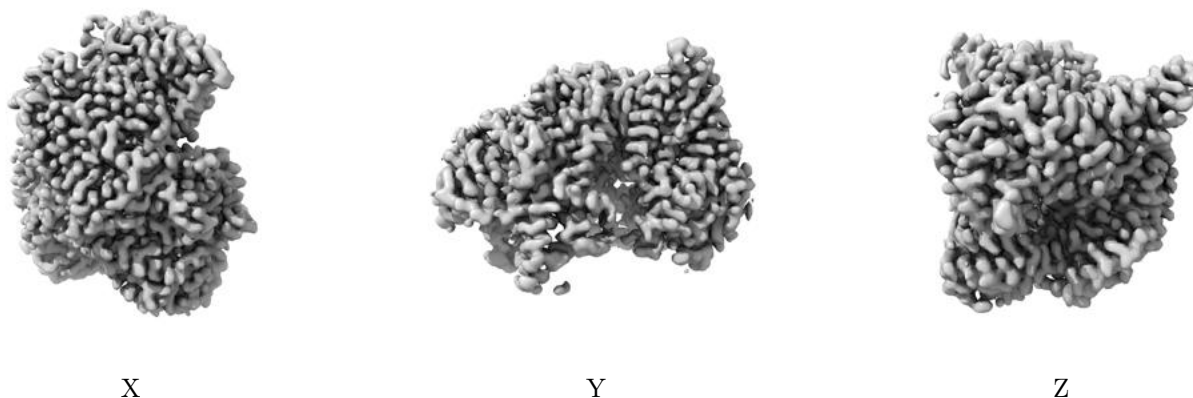


Z

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.

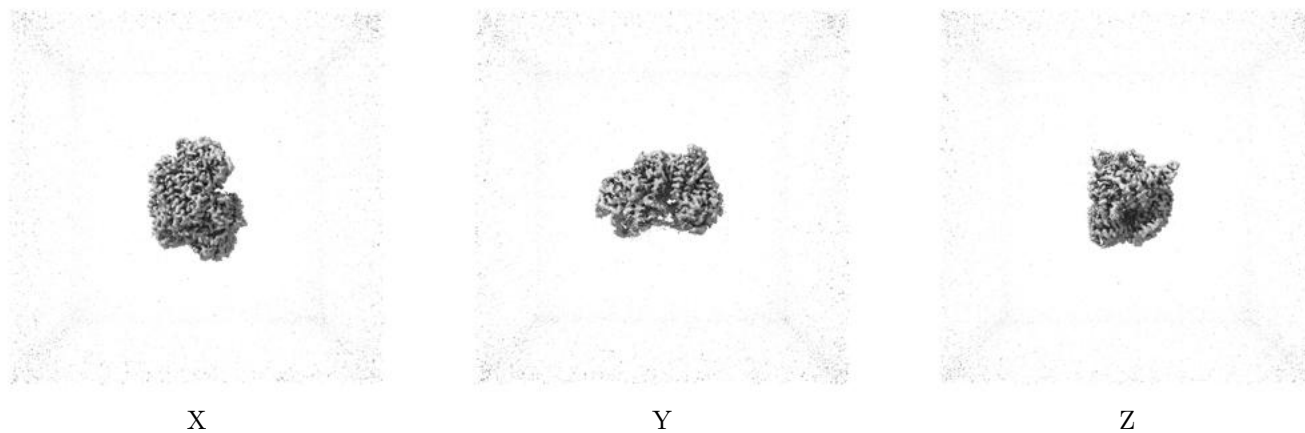
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

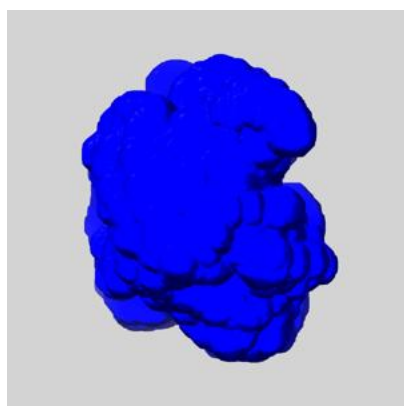
6.6 Mask visualisation [i](#)

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

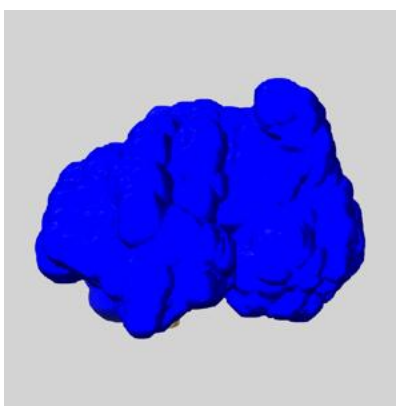
A mask typically either:

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

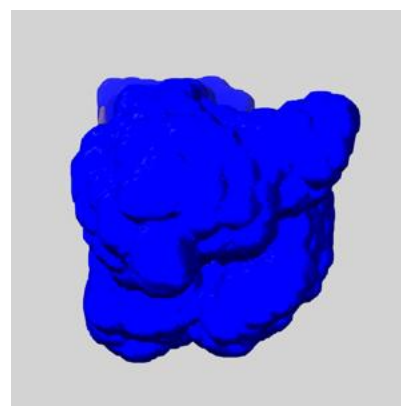
6.6.1 emd_66755_msk_1.map [i](#)



X



Y

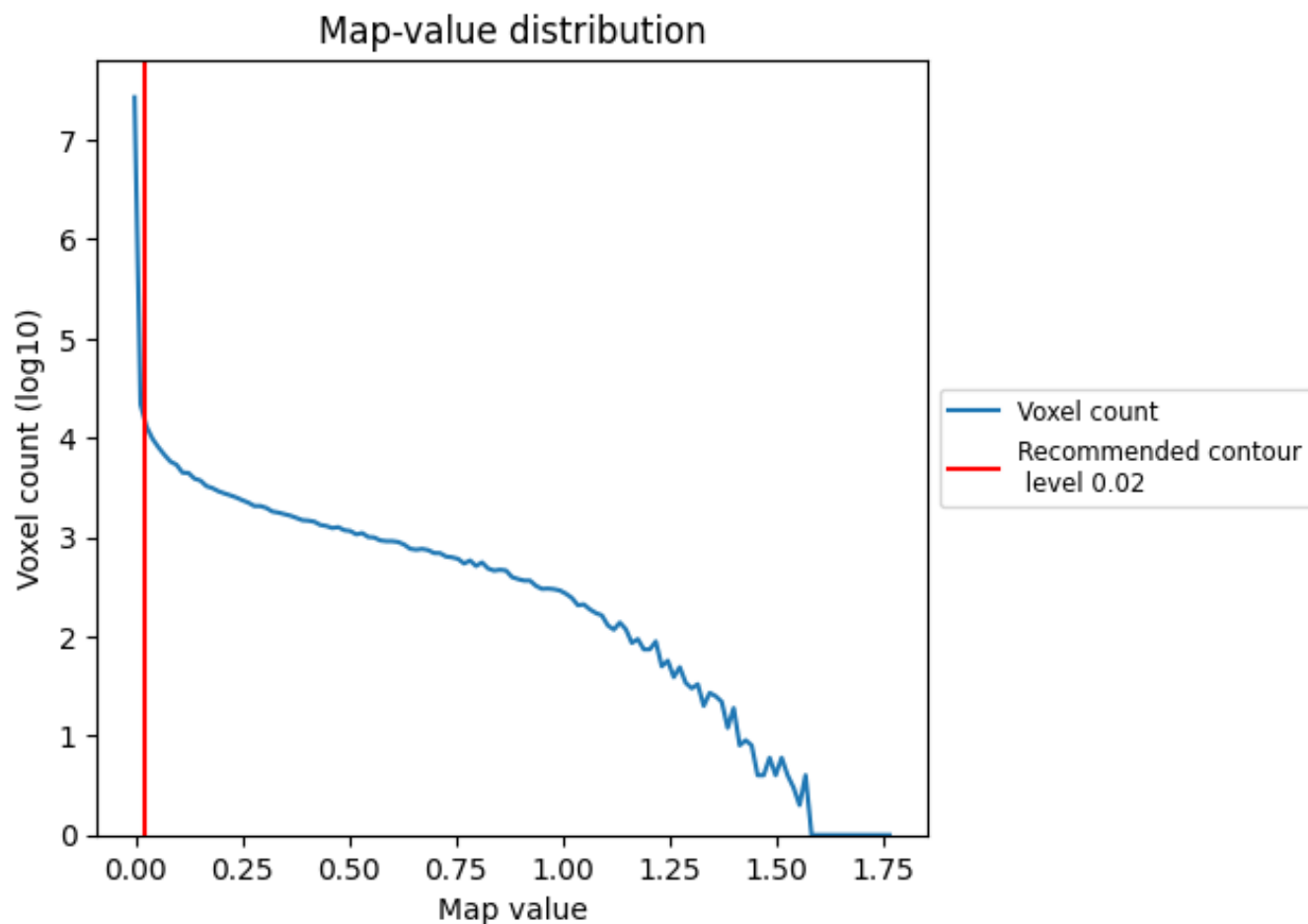


Z

7 Map analysis [i](#)

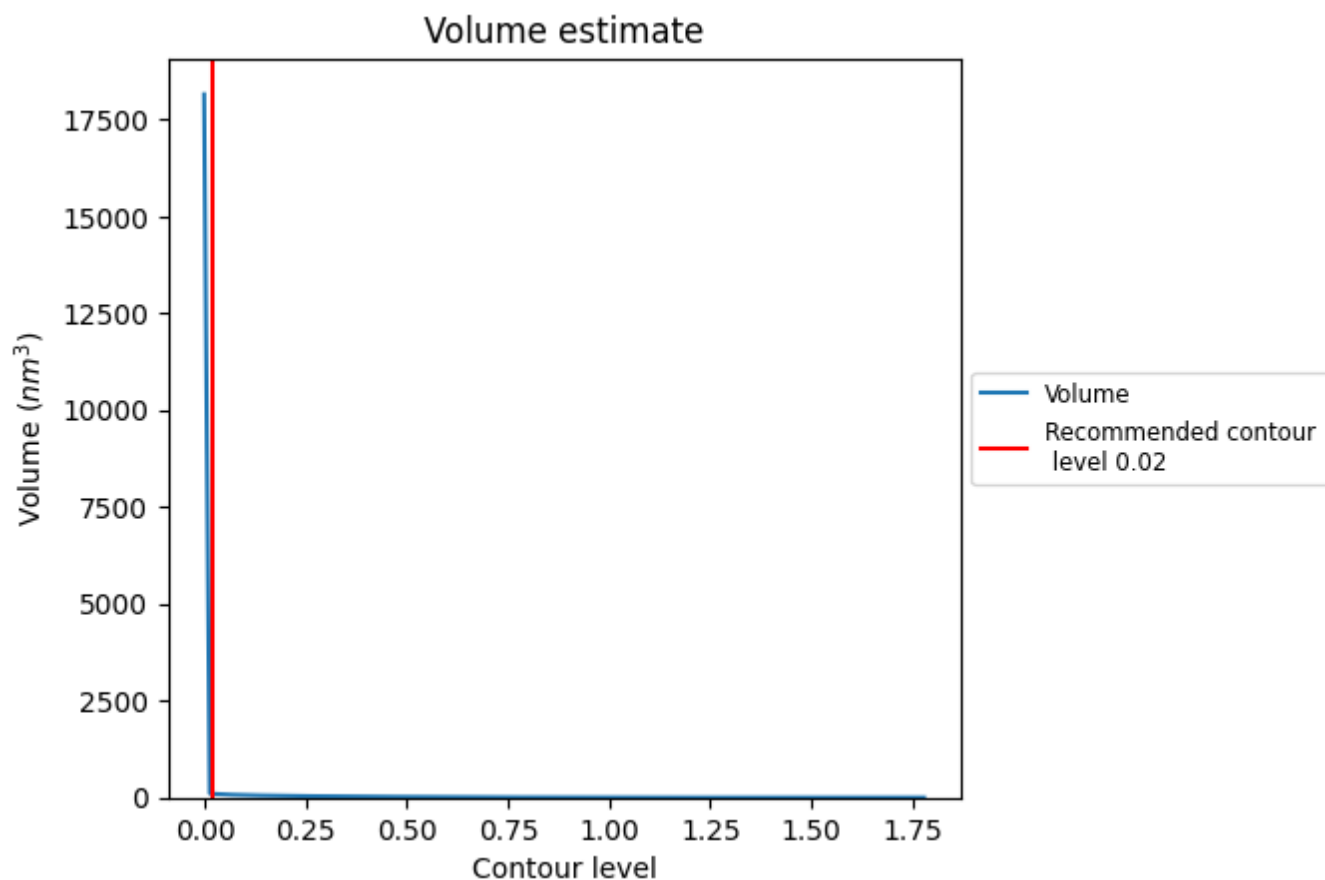
This section contains the results of statistical analysis of the map.

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.

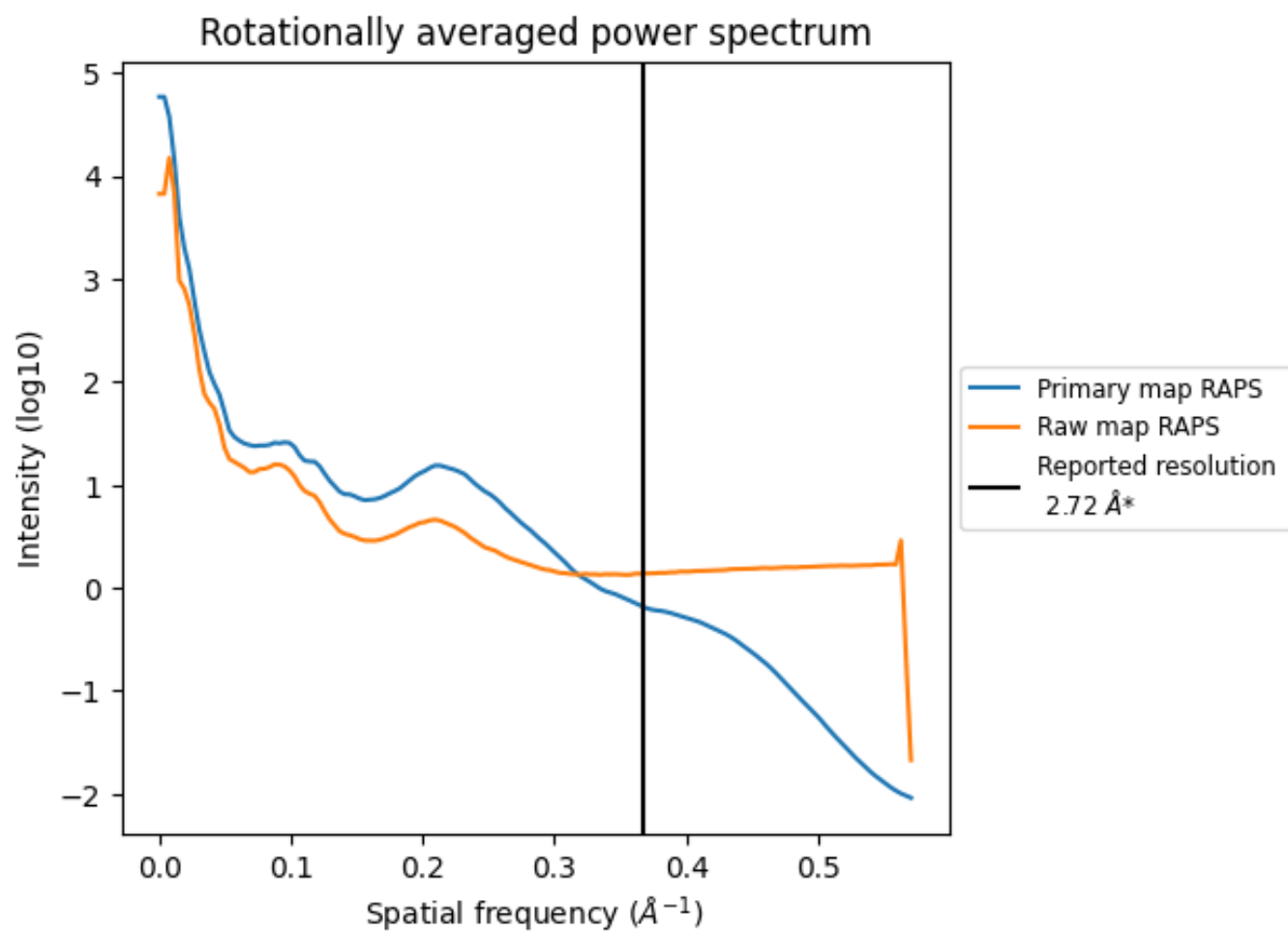
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 99 nm³; this corresponds to an approximate mass of 90 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 ⓘ

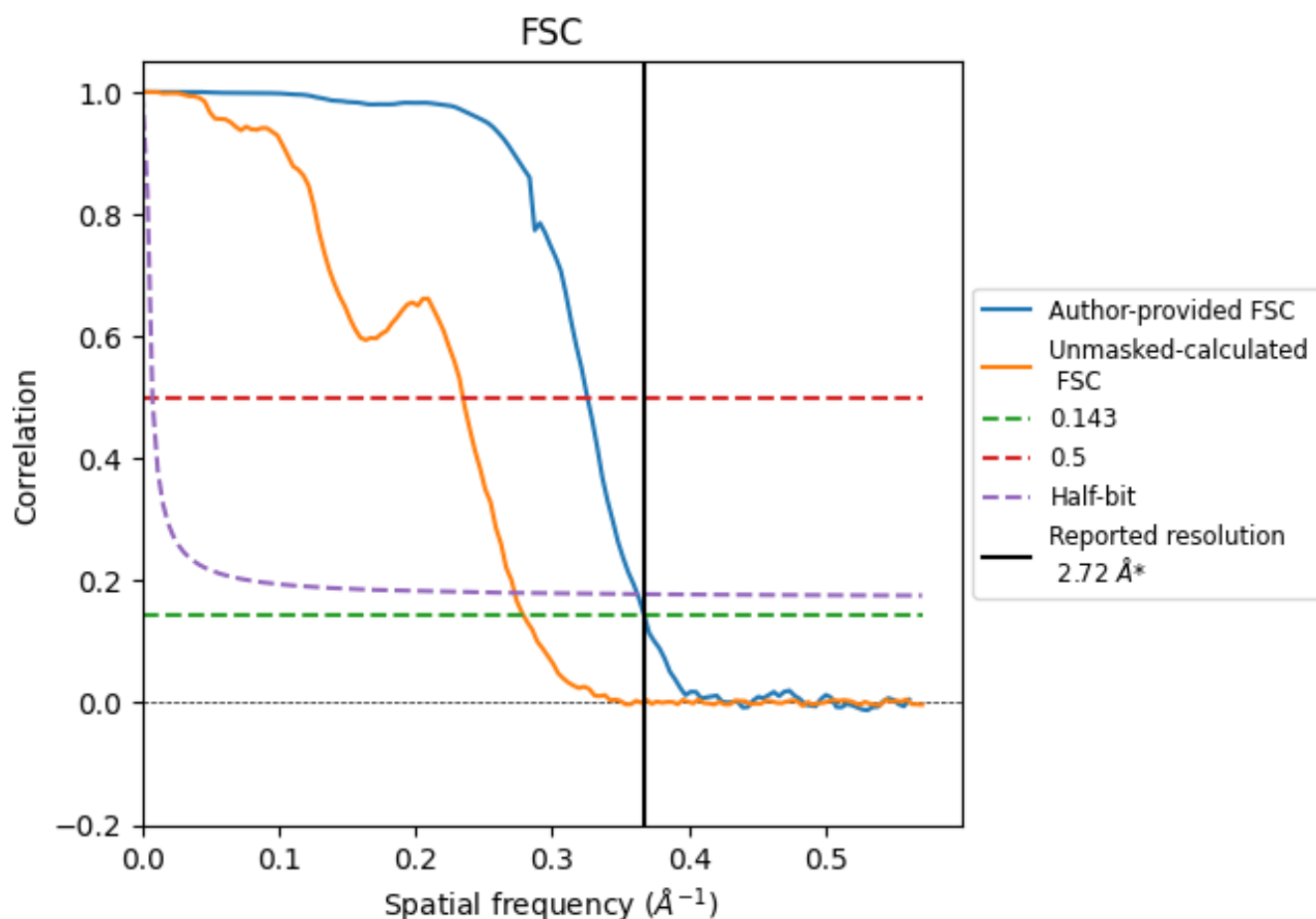


*Reported resolution corresponds to spatial frequency of 0.368 Å⁻¹

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 0.368 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

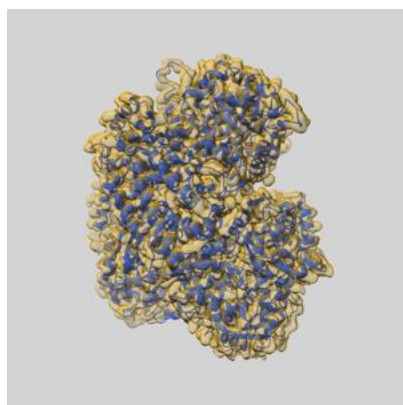
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.72	-	-
Author-provided FSC curve	2.72	3.07	2.76
Unmasked-calculated*	3.58	4.26	3.67

*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 3.58 differs from the reported value 2.72 by more than 10 %

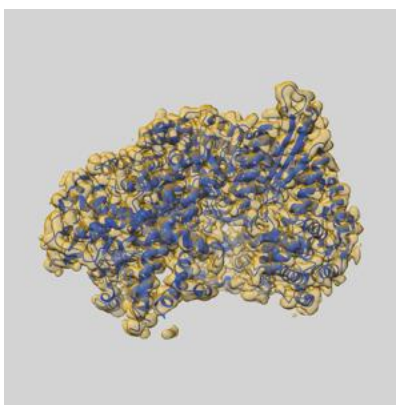
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-66755 and PDB model 9XD5. Per-residue inclusion information can be found in section [3](#) on page [4](#).

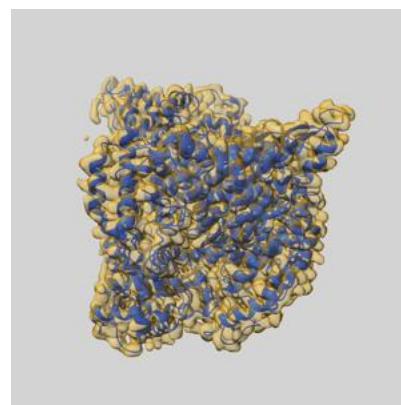
9.1 Map-model overlay [i](#)



X



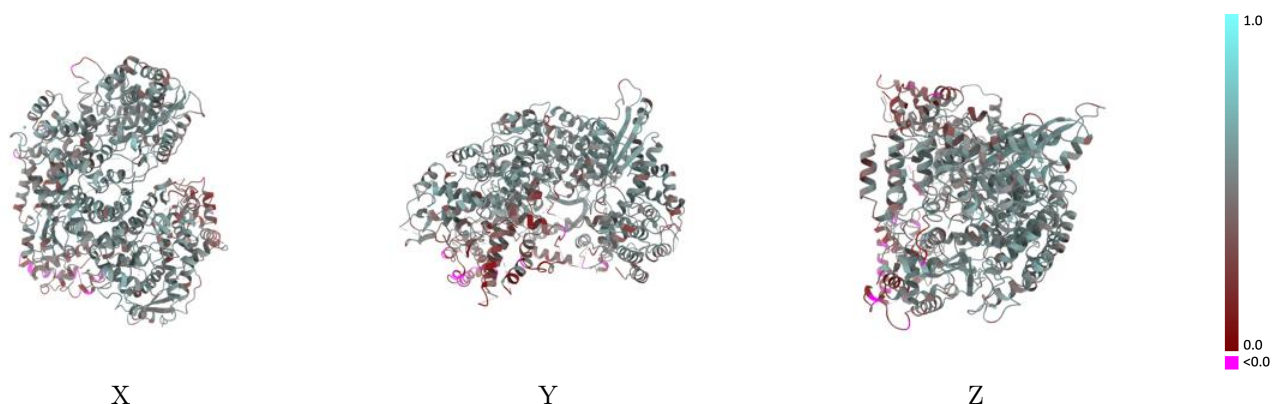
Y



Z

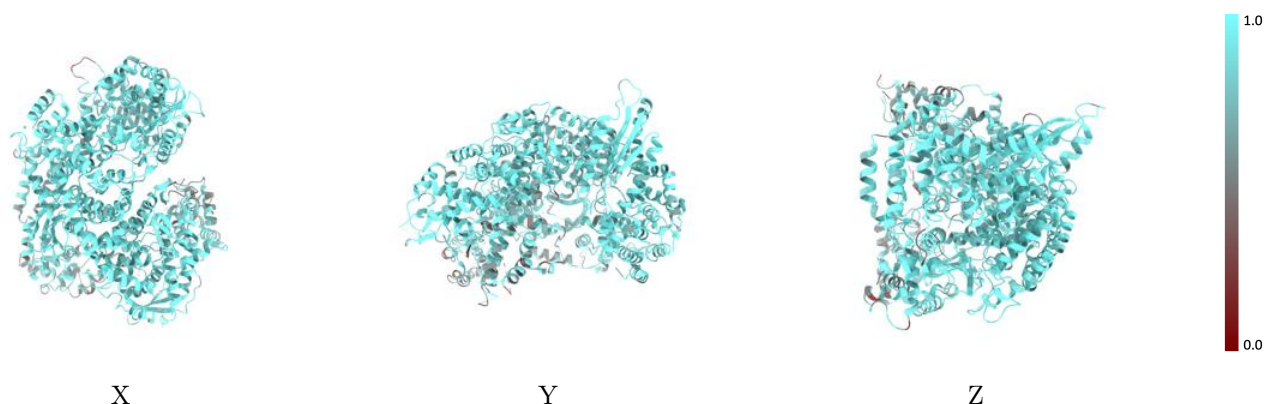
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



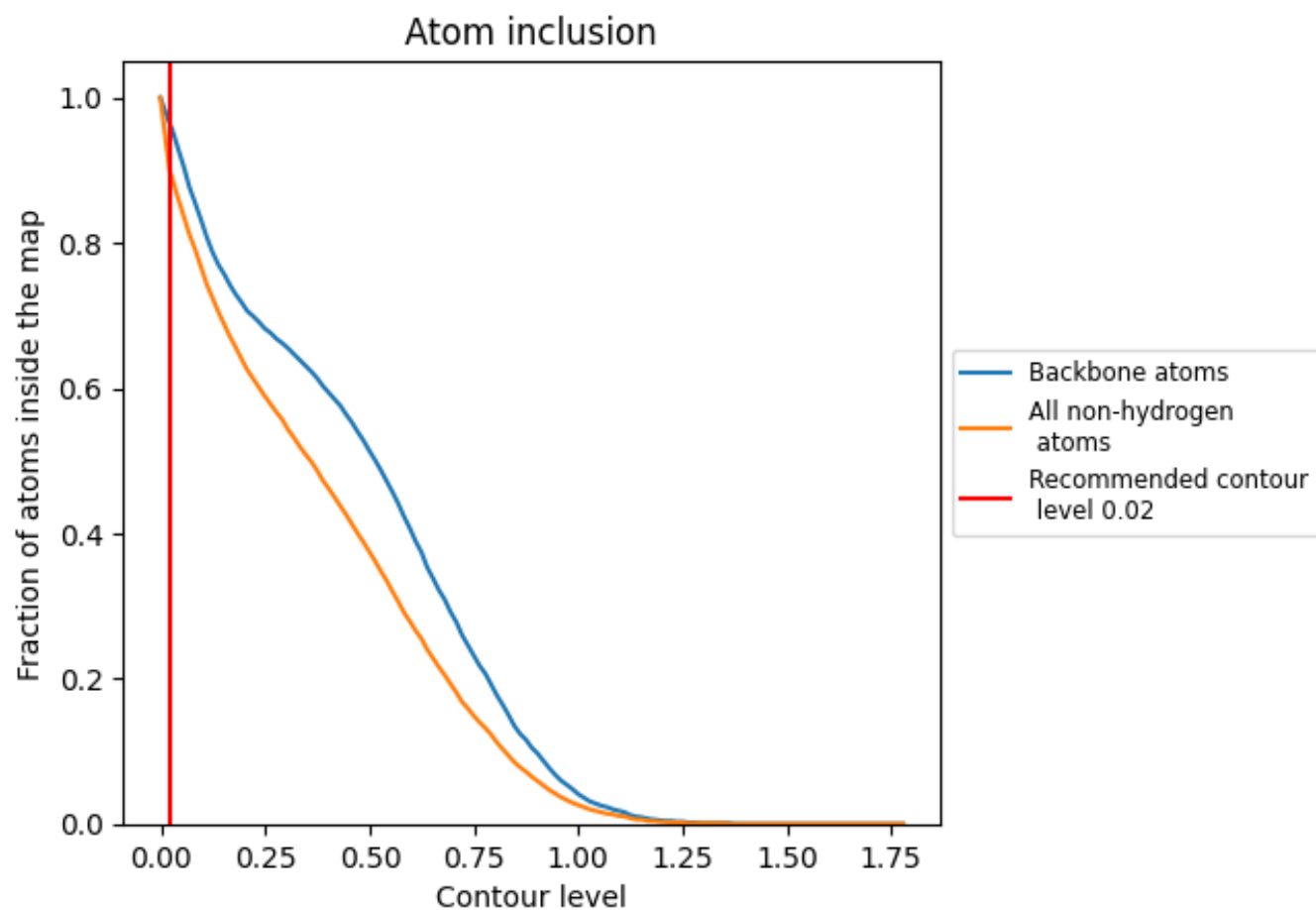
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 90% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9000	0.4740
A	0.8990	0.4730
C	0.9780	0.5510

