



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 04:35 AM UTC

PDB ID : 9HVY / pdb_00009hvy
EMDB ID : EMD-52445
Title : Cryo-EM structure of human separase-SCC1 (1-631) fusion protein
Authors : Yu, J.; Schmidt, S.; Botto, M.; Boland, A.
Deposited on : 2025-01-02
Resolution : 3.50 Å(reported)
Based on initial model : 7NJ1

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

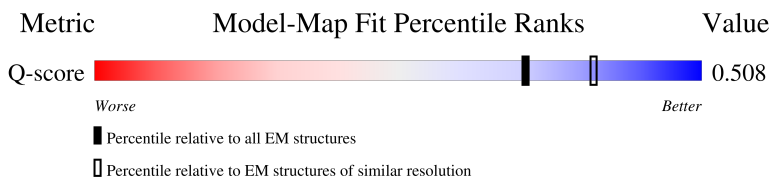
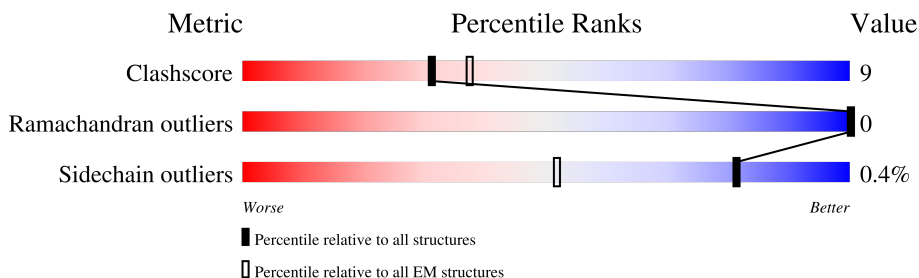
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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	2819	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10456 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 Double-strand-break repair protein rad21 homolog,Separin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1396	Total	C	N	O	S	0	0
			10455	6632	1835	1939	49		

There are 74 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	GLY	-	linker	UNP O60216
A	-26	GLY	-	linker	UNP O60216
A	-25	SER	-	linker	UNP O60216
A	-24	GLY	-	linker	UNP O60216
A	-23	GLY	-	linker	UNP O60216
A	-22	GLY	-	linker	UNP O60216
A	-21	GLY	-	linker	UNP O60216
A	-20	SER	-	linker	UNP O60216
A	-19	GLY	-	linker	UNP O60216
A	-18	GLY	-	linker	UNP O60216
A	-17	GLY	-	linker	UNP O60216
A	-16	GLY	-	linker	UNP O60216
A	-15	SER	-	linker	UNP O60216
A	-14	GLY	-	linker	UNP O60216
A	-13	GLY	-	linker	UNP O60216
A	-12	SER	-	linker	UNP O60216
A	-11	GLY	-	linker	UNP O60216
A	-10	GLY	-	linker	UNP O60216
A	-9	SER	-	linker	UNP O60216
A	-8	GLY	-	linker	UNP O60216
A	-7	GLY	-	linker	UNP O60216
A	-6	GLY	-	linker	UNP O60216
A	-5	SER	-	linker	UNP O60216
A	-4	GLY	-	linker	UNP O60216
A	-3	GLY	-	linker	UNP O60216
A	-2	GLY	-	linker	UNP O60216
A	-1	SER	-	linker	UNP O60216
A	0	GLY	-	linker	UNP O60216

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Chain	Residue	Modelled	Actual	Comment	Reference
A	25	ASP	ALA	conflict	UNP Q14674
A	116	VAL	ALA	conflict	UNP Q14674
A	1329	SER	ARG	conflict	UNP Q14674
A	1561	GLN	ARG	conflict	UNP Q14674
A	2029	SER	CYS	conflict	UNP Q14674
A	2037	HIS	ARG	conflict	UNP Q14674
A	2121	SER	-	expression tag	UNP Q14674
A	2122	SER	-	expression tag	UNP Q14674
A	2123	LEU	-	expression tag	UNP Q14674
A	2124	ALA	-	expression tag	UNP Q14674
A	2125	GLU	-	expression tag	UNP Q14674
A	2126	GLU	-	expression tag	UNP Q14674
A	2127	ASN	-	expression tag	UNP Q14674
A	2128	LEU	-	expression tag	UNP Q14674
A	2129	TYR	-	expression tag	UNP Q14674
A	2130	PHE	-	expression tag	UNP Q14674
A	2131	GLN	-	expression tag	UNP Q14674
A	2132	SER	-	expression tag	UNP Q14674
A	2133	TRP	-	expression tag	UNP Q14674
A	2134	SER	-	expression tag	UNP Q14674
A	2135	HIS	-	expression tag	UNP Q14674
A	2136	PRO	-	expression tag	UNP Q14674
A	2137	GLN	-	expression tag	UNP Q14674
A	2138	PHE	-	expression tag	UNP Q14674
A	2139	GLU	-	expression tag	UNP Q14674
A	2140	LYS	-	expression tag	UNP Q14674
A	2141	GLY	-	expression tag	UNP Q14674
A	2142	GLY	-	expression tag	UNP Q14674
A	2143	GLY	-	expression tag	UNP Q14674
A	2144	SER	-	expression tag	UNP Q14674
A	2145	GLY	-	expression tag	UNP Q14674
A	2146	GLY	-	expression tag	UNP Q14674
A	2147	GLY	-	expression tag	UNP Q14674
A	2148	SER	-	expression tag	UNP Q14674
A	2149	GLY	-	expression tag	UNP Q14674
A	2150	GLY	-	expression tag	UNP Q14674
A	2151	GLY	-	expression tag	UNP Q14674
A	2152	SER	-	expression tag	UNP Q14674
A	2153	TRP	-	expression tag	UNP Q14674
A	2154	SER	-	expression tag	UNP Q14674
A	2155	HIS	-	expression tag	UNP Q14674
A	2156	PRO	-	expression tag	UNP Q14674

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Chain	Residue	Modelled	Actual	Comment	Reference
A	2157	GLN	-	expression tag	UNP Q14674
A	2158	PHE	-	expression tag	UNP Q14674
A	2159	GLU	-	expression tag	UNP Q14674
A	2160	LYS	-	expression tag	UNP Q14674

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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



GLN	V2023	L2056	D2063	V2064	L2040	D2065	D2066	L2067	D2068	L2081	V2104	L2105	L2106	P2116	L2119	R2120	SER	SER	LEU	ALA	GLU	GLU	ASN	LEU	TYR	PHE	GLN	SER	TRP	SER	HIS	PRO	GLN	PHE	GLU	LYS	GLY	GLY	GLY	SER	GLY	GLY	SER	GLY	GLY	SER	TRP	SER	PRO
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	131299	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	150000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	14.583	Depositor
Minimum map value	-0.092	Depositor
Average map value	-0.017	Depositor
Map value standard deviation	0.319	Depositor
Recommended contour level	2.7	Depositor
Map size (Å)	351.324, 351.324, 351.324	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9759, 0.9759, 0.9759	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	0.25	0/10649	0.43	2/14497 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	331	PRO	N-CA-CB	6.74	110.42	103.00
1	A	332	PRO	N-CA-CB	6.20	110.14	103.33

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	10455	0	10254	182	0
2	A	1	0	0	0	0
All	All	10456	0	10254	182	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 9.

All (182) 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:1748:LEU:HD23	1:A:1797:SER:CB	1.79	1.13
1:A:1748:LEU:HD23	1:A:1797:SER:HB2	1.47	0.93
1:A:1879:ARG:O	1:A:1879:ARG:NH1	2.07	0.86
1:A:1748:LEU:CD2	1:A:1797:SER:HB2	2.15	0.77
1:A:490:VAL:HG13	1:A:494:THR:HB	1.68	0.73
1:A:699:ARG:HB2	1:A:702:ARG:HH21	1.52	0.73
1:A:1953:ASN:ND2	1:A:1962:GLU:OE1	2.24	0.71
1:A:1941:GLN:HE21	1:A:2120:ARG:HH12	1.38	0.70
1:A:573:LEU:HD11	1:A:576:TRP:CD2	2.27	0.70
1:A:697:ILE:HD11	1:A:957:ASP:HB3	1.72	0.70
1:A:1150:LEU:HD23	1:A:1156:LEU:HD13	1.73	0.69
1:A:894:SER:HB3	1:A:897:TRP:HD1	1.57	0.69
1:A:347:LEU:O	1:A:351:THR:N	2.24	0.69
1:A:1748:LEU:HD23	1:A:1797:SER:OG	1.94	0.67
1:A:1930:ILE:HG23	1:A:1935:ALA:HB3	1.75	0.66
1:A:573:LEU:HD23	1:A:581:LEU:HD13	1.78	0.66
1:A:1258:ILE:HG23	1:A:1259:PRO:HD3	1.78	0.66
1:A:515:LYS:HZ1	1:A:552:VAL:HA	1.61	0.66
1:A:1818:GLU:HA	1:A:1821:ARG:HH21	1.61	0.65
1:A:722:LYS:HE3	1:A:722:LYS:HA	1.79	0.64
1:A:735:PHE:HE1	1:A:1022:GLN:HA	1.62	0.64
1:A:741:ALA:O	1:A:745:LYS:HG2	1.98	0.63
1:A:1843:LEU:HA	1:A:1846:ALA:HB2	1.81	0.62
1:A:1723:ASN:OD1	1:A:1751:ARG:NH1	2.32	0.62
1:A:513:SER:HA	1:A:516:LYS:HD2	1.82	0.61
1:A:1748:LEU:HD21	1:A:1793:SER:OG	2.00	0.61
1:A:1828:ASP:OD1	1:A:1828:ASP:N	2.32	0.61
1:A:1962:GLU:HG2	1:A:1966:ARG:HH12	1.65	0.61
1:A:475:GLU:O	1:A:479:ILE:HG12	2.01	0.60
1:A:492:PRO:HG3	1:A:535:GLN:HE22	1.66	0.59
1:A:675:ASP:HA	1:A:678:ALA:HB3	1.82	0.59
1:A:1729:ARG:NH1	1:A:1805:LEU:O	2.31	0.59
1:A:563:GLU:OE1	1:A:563:GLU:N	2.23	0.59
1:A:356:ARG:O	1:A:360:ILE:N	2.36	0.58
1:A:1214:LEU:HD12	1:A:1214:LEU:N	2.18	0.57
1:A:333:LEU:O	1:A:337:TYR:N	2.35	0.57
1:A:654:ARG:O	1:A:658:GLN:HG3	2.04	0.57
1:A:1242:SER:HA	1:A:1245:LYS:NZ	2.20	0.56
1:A:697:ILE:CD1	1:A:957:ASP:HB3	2.35	0.56
1:A:1727:LEU:HD22	1:A:1805:LEU:HD23	1.87	0.55
1:A:1234:GLY:HA2	1:A:1243:LEU:HD13	1.88	0.54
1:A:2064:VAL:HG12	1:A:2106:ILE:HD12	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1852:GLN:OE1	1:A:1852:GLN:N	2.21	0.54
1:A:872:GLN:HE22	1:A:1259:PRO:HG3	1.71	0.54
1:A:1714:ALA:HB3	1:A:1724:THR:HB	1.90	0.54
1:A:495:TYR:HB3	1:A:498:VAL:CG2	2.37	0.53
1:A:535:GLN:HG2	1:A:576:TRP:CH2	2.42	0.53
1:A:1669:PRO:HG3	1:A:1933:TYR:CG	2.43	0.53
1:A:1748:LEU:CD2	1:A:1797:SER:CB	2.68	0.53
1:A:1952:LEU:HD21	1:A:1962:GLU:HA	1.90	0.53
1:A:2105:LEU:C	1:A:2106:ILE:HD13	2.35	0.52
1:A:446:GLY:O	1:A:448:GLU:N	2.43	0.52
1:A:492:PRO:HG3	1:A:535:GLN:NE2	2.24	0.52
1:A:486:HIS:O	1:A:490:VAL:HG23	2.10	0.51
1:A:1193:GLU:O	1:A:1196:GLU:HG3	2.11	0.51
1:A:655:GLU:HA	1:A:658:GLN:OE1	2.09	0.51
1:A:1774:ARG:O	1:A:1778:THR:HG23	2.10	0.51
1:A:1199:THR:HG23	1:A:1212:PRO:HG2	1.92	0.51
1:A:563:GLU:H	1:A:563:GLU:CD	2.16	0.51
1:A:1214:LEU:N	1:A:1214:LEU:CD1	2.73	0.51
1:A:789:PRO:HB2	1:A:822:LEU:HD11	1.93	0.51
1:A:1291:SER:HB2	1:A:1609:GLY:HA3	1.92	0.51
1:A:1879:ARG:HH11	1:A:1879:ARG:C	2.11	0.50
1:A:535:GLN:HG2	1:A:576:TRP:CZ2	2.47	0.50
1:A:755:LYS:HG2	1:A:798:LEU:HD11	1.92	0.50
1:A:950:ILE:HG21	1:A:959:LEU:HD21	1.93	0.50
1:A:880:LEU:O	1:A:884:VAL:HG23	2.12	0.49
1:A:735:PHE:CE1	1:A:1022:GLN:HA	2.46	0.49
1:A:570:ARG:HD2	1:A:613:LEU:HD11	1.94	0.49
1:A:897:TRP:O	1:A:901:ARG:HG3	2.13	0.49
1:A:511:VAL:HG11	1:A:530:TRP:HZ3	1.77	0.49
1:A:798:LEU:O	1:A:802:VAL:HG23	2.13	0.49
1:A:1140:LEU:H	1:A:1140:LEU:HD23	1.78	0.49
1:A:1890:HIS:CE1	1:A:2116:PRO:HD3	2.48	0.49
1:A:1859:TYR:CE1	1:A:1866:PRO:HB2	2.48	0.48
1:A:514:LEU:HD22	1:A:526:MET:HE2	1.96	0.48
1:A:627:THR:O	1:A:630:VAL:HG22	2.13	0.48
1:A:1004:VAL:HG21	1:A:2040:LEU:HD21	1.96	0.48
1:A:1762:LYS:O	1:A:1766:GLU:HG2	2.14	0.47
1:A:1144:PRO:O	1:A:1197:ARG:NH2	2.44	0.47
1:A:1791:ILE:HD12	1:A:2104:TYR:HD1	1.79	0.47
1:A:1242:SER:HA	1:A:1245:LYS:HZ2	1.78	0.47
1:A:550:VAL:HG21	1:A:591:ALA:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:603:ARG:O	1:A:607:ILE:HG13	2.14	0.47
1:A:1826:LEU:HD12	1:A:1829:CYS:HB3	1.97	0.47
1:A:527:VAL:O	1:A:531:LEU:HG	2.15	0.46
1:A:514:LEU:HD22	1:A:526:MET:CE	2.45	0.46
1:A:563:GLU:HA	1:A:566:LEU:HD12	1.98	0.46
1:A:898:TYR:HD2	1:A:949:ILE:HD11	1.79	0.46
1:A:1943:VAL:HG23	1:A:1996:ASP:HB3	1.95	0.46
1:A:511:VAL:HG11	1:A:530:TRP:CZ3	2.51	0.46
1:A:1943:VAL:HG13	1:A:2119:LEU:HD23	1.97	0.46
1:A:1748:LEU:HD11	1:A:1793:SER:OG	2.16	0.46
1:A:447:GLN:O	1:A:451:ASP:N	2.44	0.45
1:A:522:GLN:HA	1:A:525:LYS:HG2	1.97	0.45
1:A:992:GLU:HG3	1:A:1029:LEU:HD21	1.97	0.45
1:A:562:LYS:HE3	1:A:562:LYS:HA	1.97	0.45
1:A:1823:GLN:HE21	1:A:1834:PRO:HB2	1.81	0.45
1:A:495:TYR:HB3	1:A:498:VAL:HG23	1.97	0.45
1:A:1250:GLY:O	1:A:1254:VAL:HG23	2.17	0.45
1:A:961:THR:CG2	1:A:1020:LYS:HE2	2.47	0.45
1:A:515:LYS:HZ1	1:A:552:VAL:HG22	1.82	0.45
1:A:1251:LEU:HD12	1:A:1251:LEU:HA	1.83	0.45
1:A:495:TYR:HB3	1:A:498:VAL:HG21	1.98	0.44
1:A:511:VAL:HA	1:A:526:MET:HE1	1.99	0.44
1:A:1890:HIS:NE2	1:A:1916:THR:OG1	2.40	0.44
1:A:696:GLY:O	1:A:699:ARG:HG3	2.16	0.44
1:A:961:THR:HG22	1:A:1020:LYS:HE2	1.99	0.44
1:A:982:GLN:O	1:A:986:GLU:HG2	2.16	0.44
1:A:1221:GLU:OE1	1:A:1221:GLU:N	2.40	0.44
1:A:1991:ALA:HA	1:A:1995:HIS:HD1	1.83	0.44
1:A:507:PHE:O	1:A:508:ARG:C	2.61	0.43
1:A:626:ALA:O	1:A:630:VAL:HG13	2.17	0.43
1:A:830:SER:HB2	1:A:1213:SER:HB2	1.99	0.43
1:A:861:ASP:OD1	1:A:861:ASP:N	2.42	0.43
1:A:1818:GLU:CA	1:A:1821:ARG:HH21	2.30	0.43
1:A:1820:SER:HA	1:A:1836:ARG:HH11	1.83	0.43
1:A:548:PHE:O	1:A:552:VAL:HG23	2.18	0.43
1:A:663:VAL:C	1:A:664:ARG:HD2	2.44	0.43
1:A:774:ALA:O	1:A:778:ILE:HG13	2.18	0.43
1:A:891:GLN:OE1	1:A:891:GLN:N	2.42	0.43
1:A:1748:LEU:O	1:A:1748:LEU:HG	2.18	0.43
1:A:544:GLU:H	1:A:544:GLU:CD	2.22	0.43
1:A:970:PHE:HZ	1:A:977:LEU:HA	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1573:THR:O	1:A:1577:ILE:HG12	2.19	0.43
1:A:1888:ASN:OD1	1:A:1888:ASN:C	2.61	0.43
1:A:591:ALA:O	1:A:595:VAL:HG23	2.19	0.43
1:A:979:GLN:O	1:A:983:VAL:HG23	2.19	0.43
1:A:682:LEU:O	1:A:686:ILE:HG13	2.18	0.43
1:A:674:LEU:O	1:A:675:ASP:HB3	2.20	0.42
1:A:971:LEU:O	1:A:973:TYR:HD1	2.03	0.42
1:A:2016:LEU:HD12	1:A:2016:LEU:HA	1.84	0.42
1:A:610:LEU:HD22	1:A:628:HIS:CE1	2.54	0.42
1:A:1687:PHE:HA	1:A:1688:PRO:HA	1.90	0.42
1:A:971:LEU:HD23	1:A:971:LEU:HA	1.94	0.42
1:A:551:ARG:CZ	1:A:551:ARG:HB3	2.50	0.42
1:A:778:ILE:HG12	1:A:978:VAL:HG22	2.02	0.42
1:A:2063:ASP:O	1:A:2063:ASP:OD1	2.38	0.42
1:A:481:GLU:HA	1:A:510:GLN:HE22	1.83	0.42
1:A:2023:VAL:HG13	1:A:2056:LEU:HB3	2.01	0.42
1:A:610:LEU:HD22	1:A:628:HIS:NE2	2.35	0.42
1:A:1622:GLU:CD	1:A:1922:ARG:HH12	2.28	0.42
1:A:1711:LEU:HB2	1:A:1895:LEU:HD23	2.01	0.42
1:A:1992:LEU:HD12	1:A:1992:LEU:HA	1.87	0.42
1:A:791:GLN:H	1:A:791:GLN:HG2	1.65	0.42
1:A:527:VAL:HG21	1:A:549:TRP:HE3	1.84	0.41
1:A:755:LYS:HE2	1:A:755:LYS:HB3	1.87	0.41
1:A:797:LEU:HD11	1:A:1206:LEU:HD23	2.03	0.41
1:A:959:LEU:O	1:A:961:THR:HG23	2.20	0.41
1:A:650:LEU:O	1:A:654:ARG:HG3	2.21	0.41
1:A:1962:GLU:HG2	1:A:1966:ARG:NH1	2.31	0.41
1:A:697:ILE:HD11	1:A:957:ASP:C	2.46	0.41
1:A:2066:ASP:OD2	1:A:2068:ASP:HB2	2.20	0.41
1:A:553:LYS:HD3	1:A:553:LYS:HA	1.82	0.41
1:A:556:ALA:HB1	1:A:564:LEU:HD12	2.01	0.41
1:A:569:LEU:O	1:A:573:LEU:HB2	2.21	0.41
1:A:726:ASP:CG	1:A:727:ARG:H	2.28	0.41
1:A:640:ASP:OD1	1:A:640:ASP:C	2.63	0.41
1:A:1850:THR:O	1:A:1854:ILE:HG13	2.20	0.41
1:A:1954:PRO:HB3	1:A:2009:PHE:HZ	1.84	0.41
1:A:2081:LEU:HD13	1:A:2081:LEU:HA	1.95	0.41
1:A:573:LEU:HD12	1:A:573:LEU:O	2.21	0.41
1:A:801:ILE:O	1:A:805:ARG:HG3	2.21	0.41
1:A:1667:ASP:HB2	1:A:1669:PRO:HD2	2.03	0.41
1:A:1787:MET:HG2	1:A:2104:TYR:O	2.20	0.41

Continued on next page...

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1818:GLU:HA	1:A:1821:ARG:HE	1.85	0.41
1:A:1972:GLU:HG3	1:A:1975:TRP:CE3	2.56	0.41
1:A:2106:ILE:HG22	1:A:2106:ILE:O	2.21	0.41
1:A:732:ASN:HA	1:A:735:PHE:HB3	2.03	0.41
1:A:499:PRO:HA	1:A:500:PRO:HD3	1.85	0.40
1:A:1199:THR:HG23	1:A:1212:PRO:CG	2.52	0.40
1:A:586:ARG:HE	1:A:586:ARG:HB2	1.67	0.40
1:A:1050:ASP:O	1:A:1054:VAL:HG23	2.21	0.40
1:A:1146:CYS:SG	1:A:1147:ASP:N	2.95	0.40
1:A:715:ASN:OD1	1:A:715:ASN:N	2.49	0.40
1:A:857:SER:O	1:A:861:ASP:OD1	2.39	0.40
1:A:1137:PRO:HG2	1:A:1140:LEU:HD22	2.04	0.40
1:A:655:GLU:O	1:A:659:LEU:HG	2.22	0.40
1:A:898:TYR:CD2	1:A:949:ILE:HD11	2.56	0.40
1:A:1258:ILE:CG2	1:A:1259:PRO:HD3	2.49	0.40
1:A:1823:GLN:NE2	1:A:1834:PRO:HB2	2.36	0.40
1:A:1949:PHE:HA	1:A:1976:ARG:O	2.21	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	1380/2819 (49%)	1326 (96%)	54 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	1068/2388 (45%)	1064 (100%)	4 (0%)	84 81

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	504	HIS
1	A	959	LEU
1	A	1215	VAL
1	A	1258	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	535	GLN
1	A	541	HIS
1	A	601	GLN
1	A	605	ASN
1	A	679	GLN
1	A	809	HIS
1	A	835	HIS
1	A	926	GLN
1	A	943	HIS
1	A	1048	GLN
1	A	1599	HIS
1	A	1911	GLN
1	A	1941	GLN
1	A	2037	HIS
1	A	2060	ASN
1	A	2095	GLN
1	A	2098	GLN

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 [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.

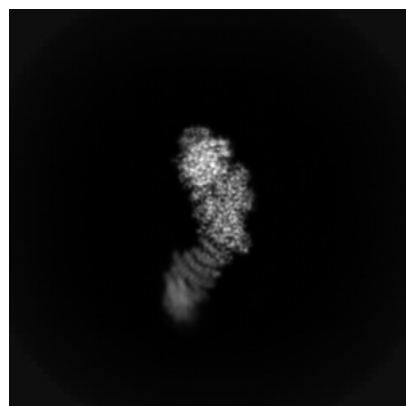
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52445. These allow visual inspection of the internal detail of the map and identification of artifacts.

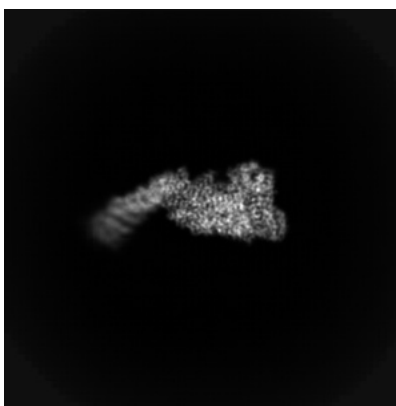
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

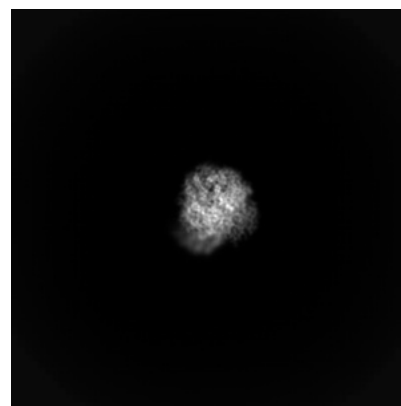
6.1.1 Primary map



X

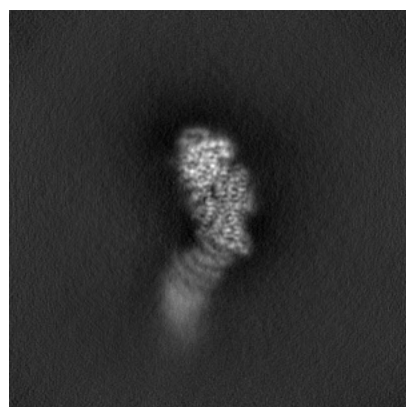


Y

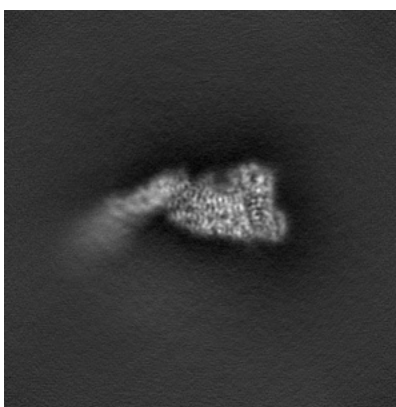


Z

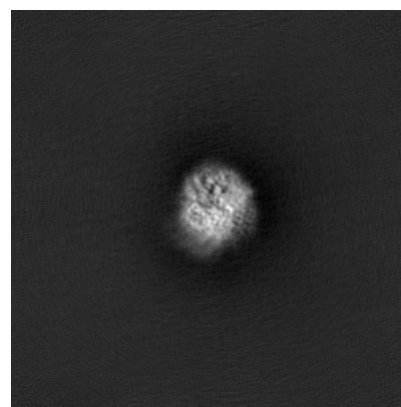
6.1.2 Raw map



X



Y

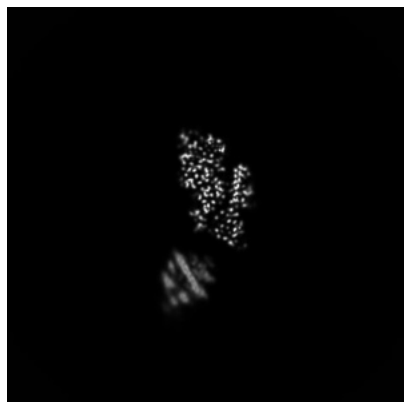


Z

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

6.2 Central slices [i](#)

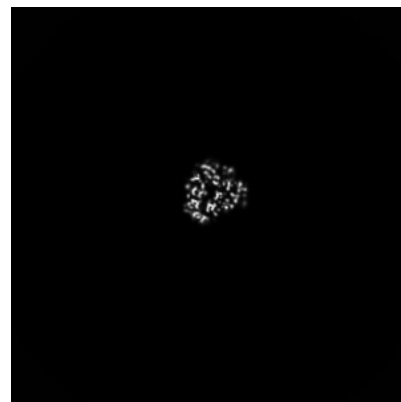
6.2.1 Primary map



X Index: 180

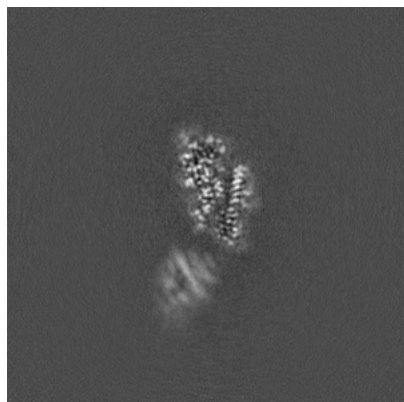


Y Index: 180

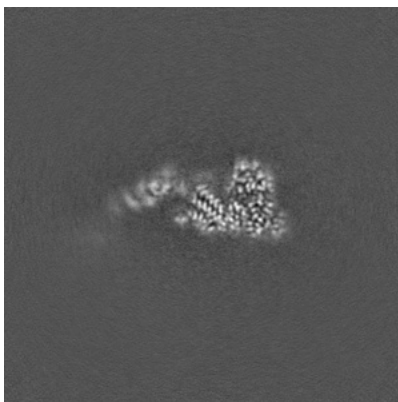


Z Index: 180

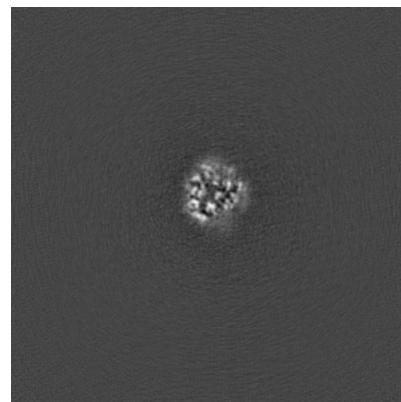
6.2.2 Raw map



X Index: 180



Y Index: 180

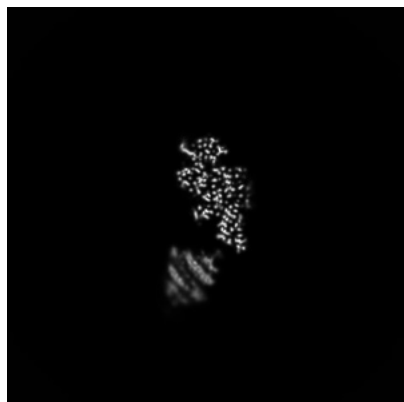


Z Index: 180

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

6.3 Largest variance slices [i](#)

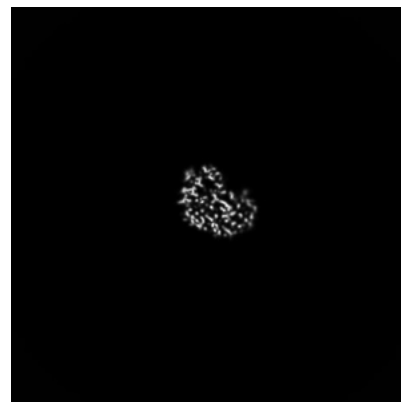
6.3.1 Primary map



X Index: 184

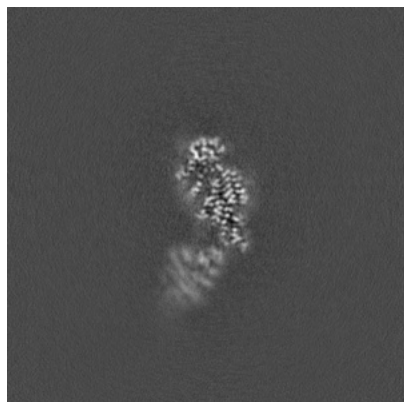


Y Index: 179

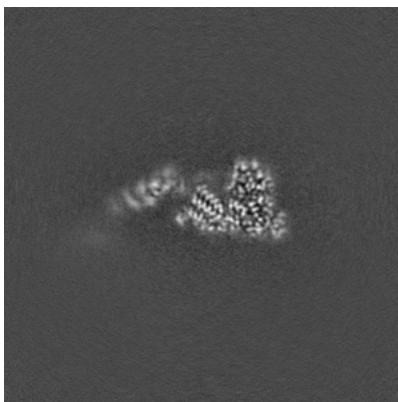


Z Index: 212

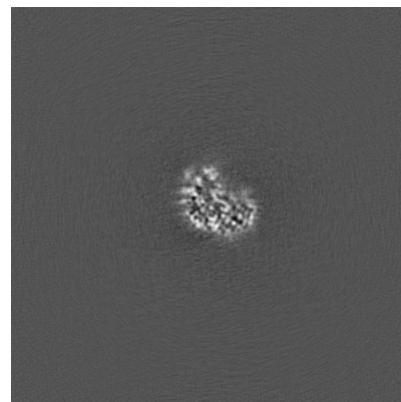
6.3.2 Raw map



X Index: 188



Y Index: 179



Z Index: 213

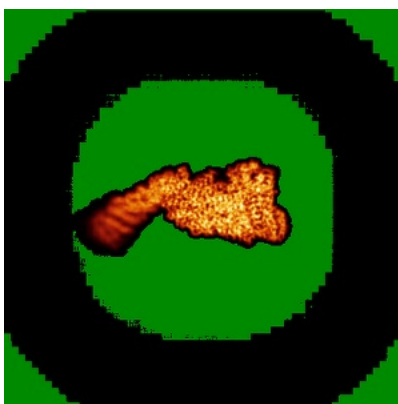
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

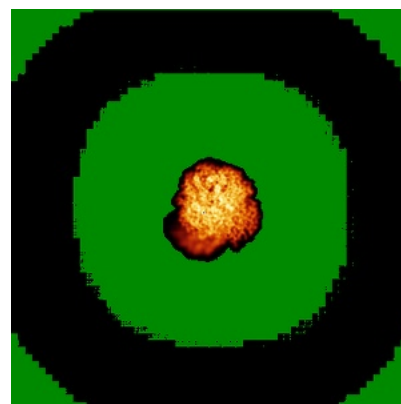
6.4.1 Primary map



X



Y

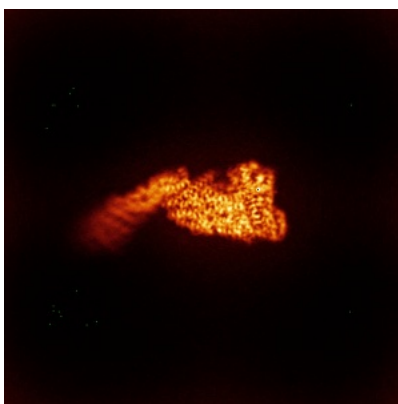


Z

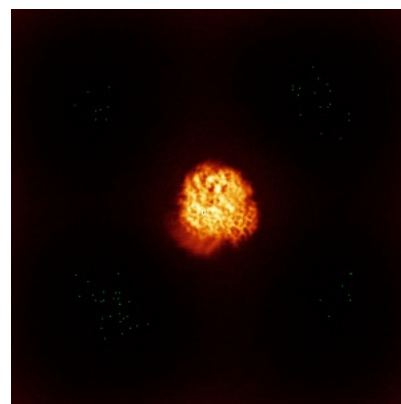
6.4.2 Raw map



X



Y

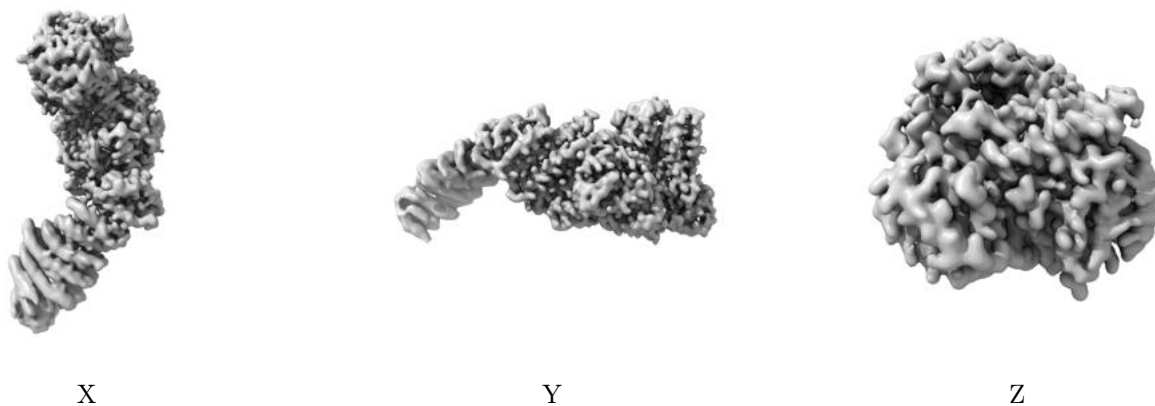


Z

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.

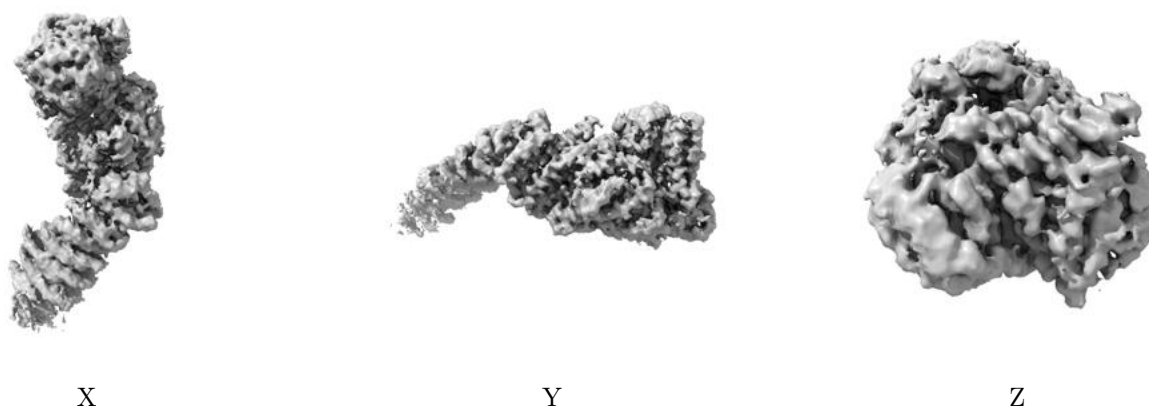
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

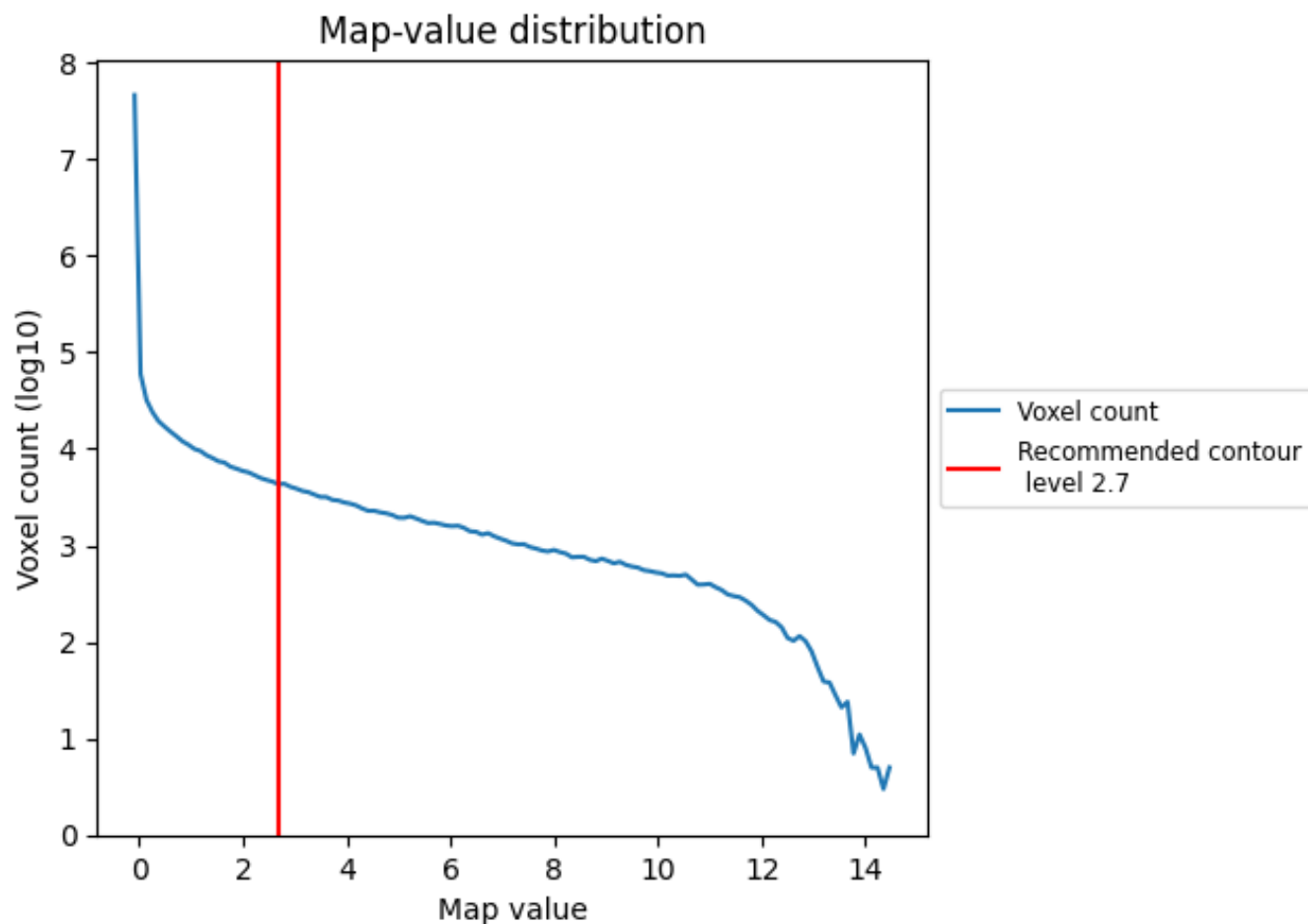
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

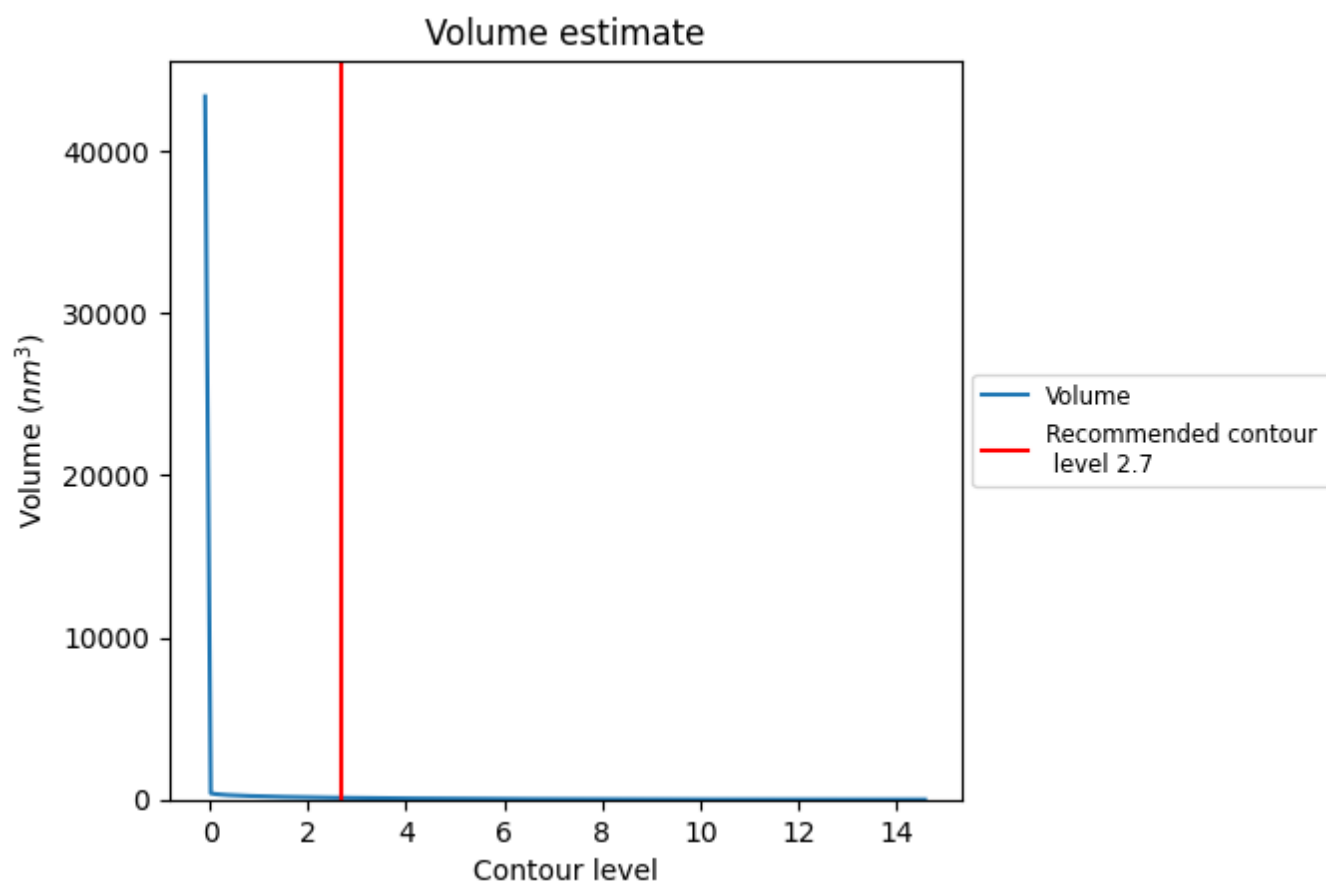
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

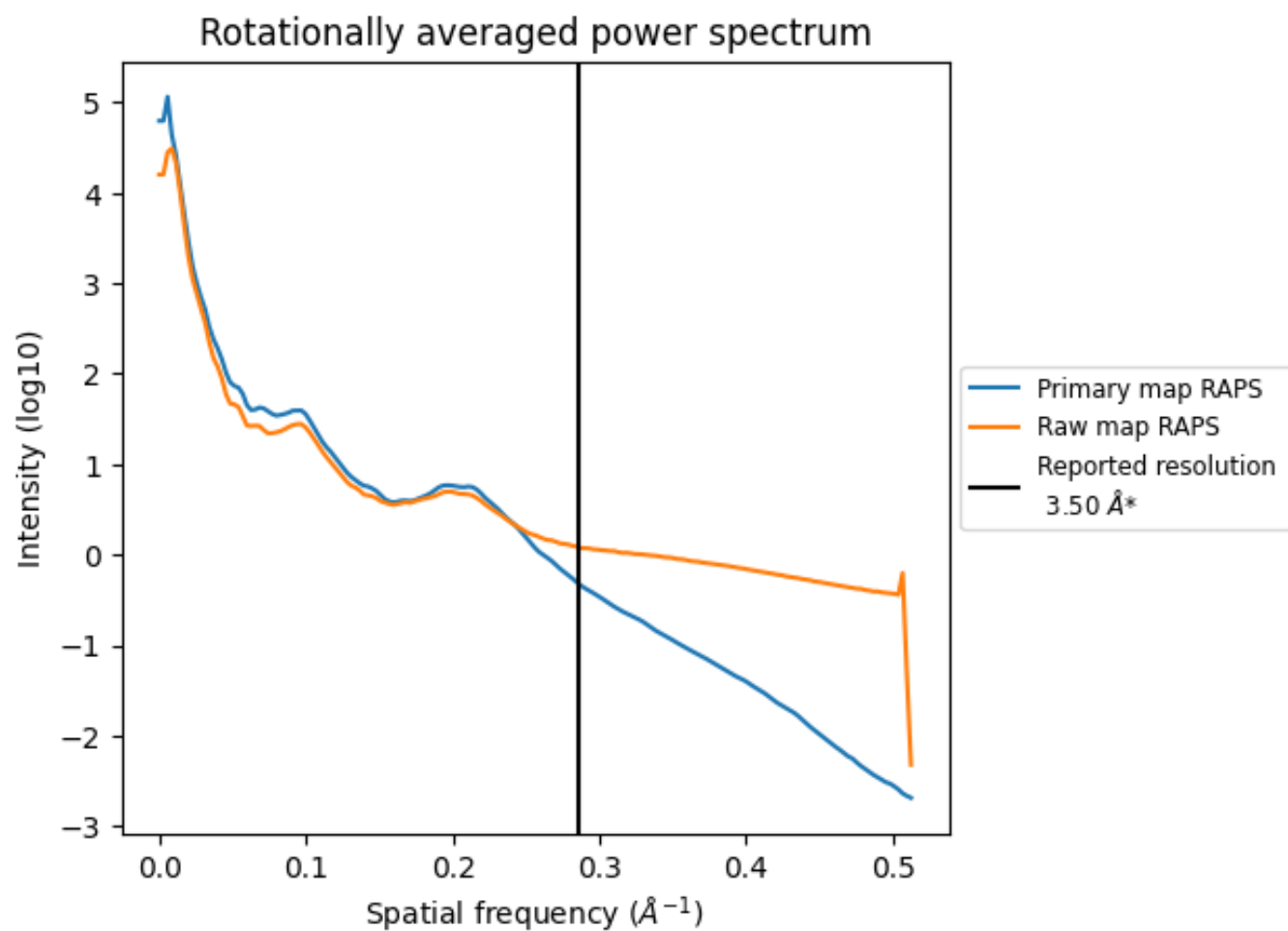
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 109 nm³; this corresponds to an approximate mass of 98 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 ⓘ

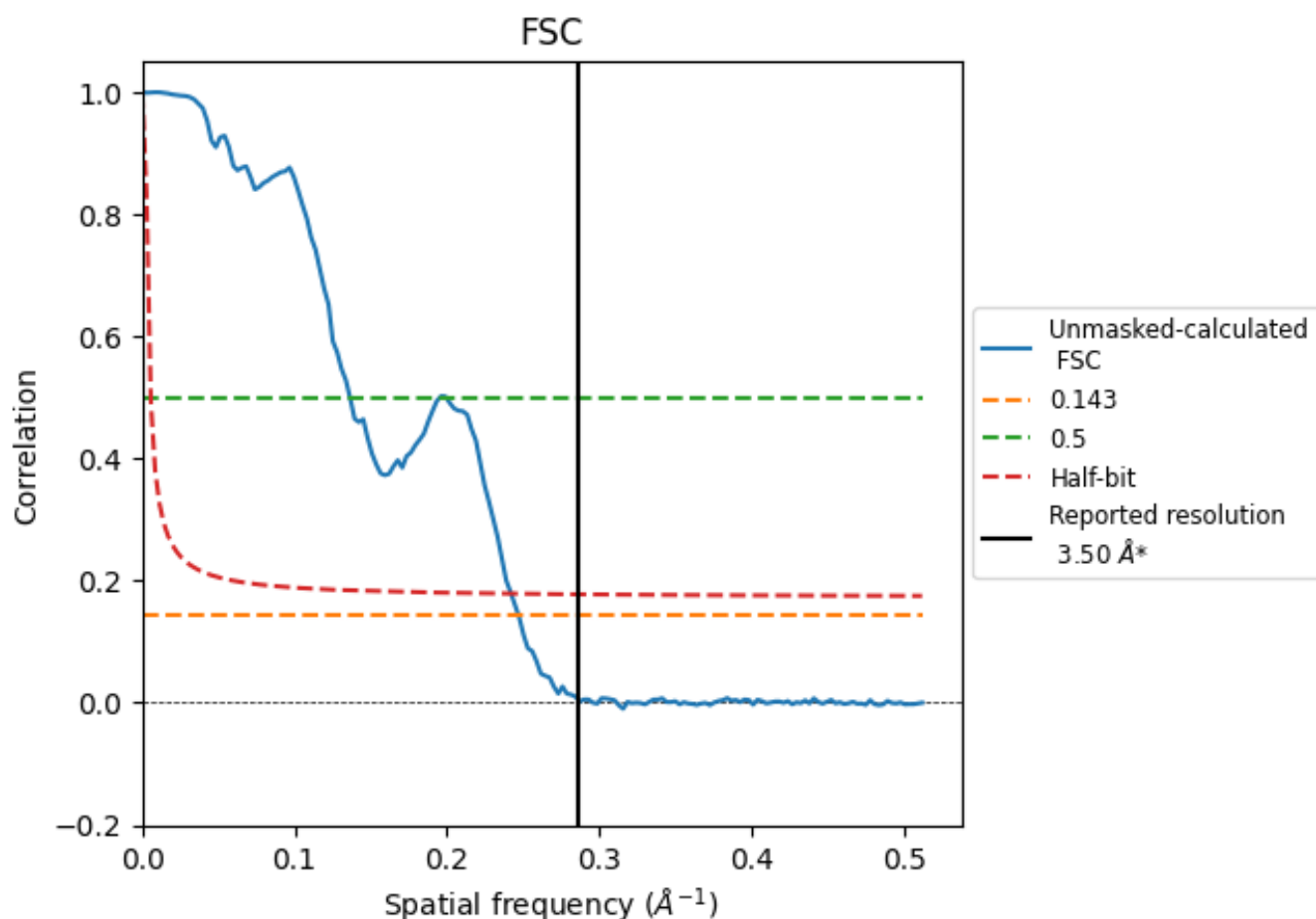


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

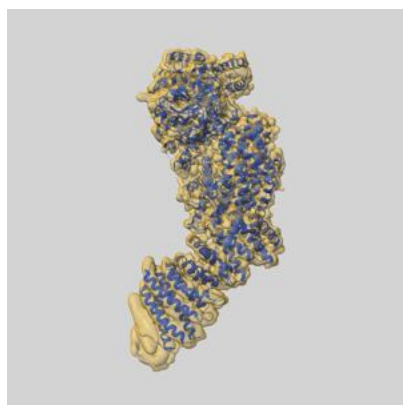
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.05	7.33	4.13

*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 4.05 differs from the reported value 3.5 by more than 10 %

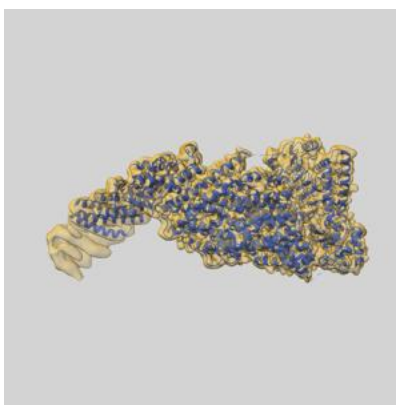
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52445 and PDB model 9HVY. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

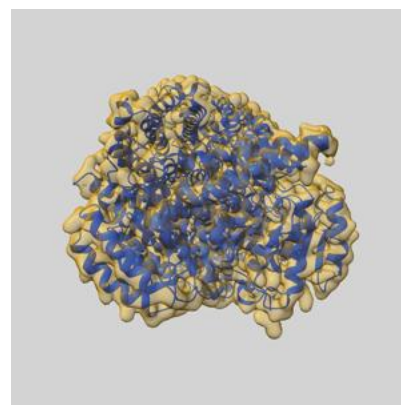
9.1 Map-model overlay [i](#)



X



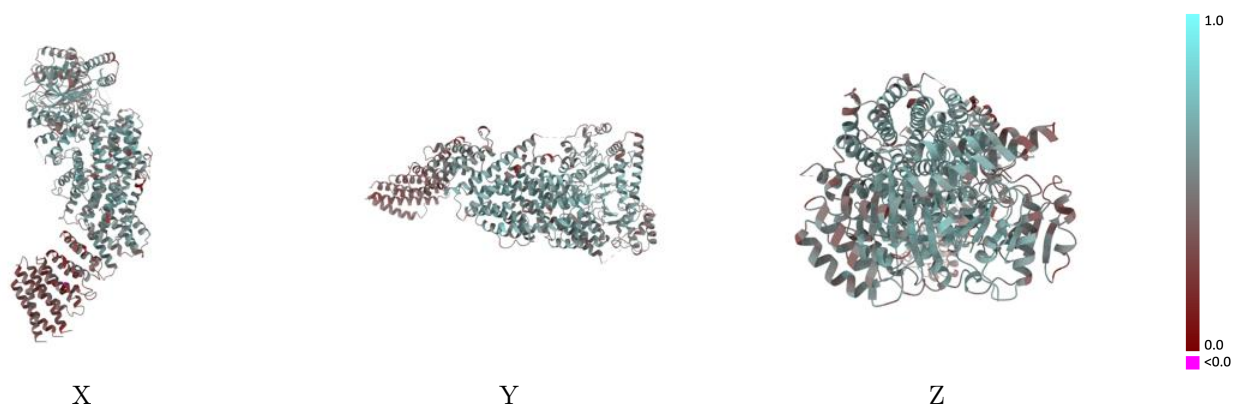
Y



Z

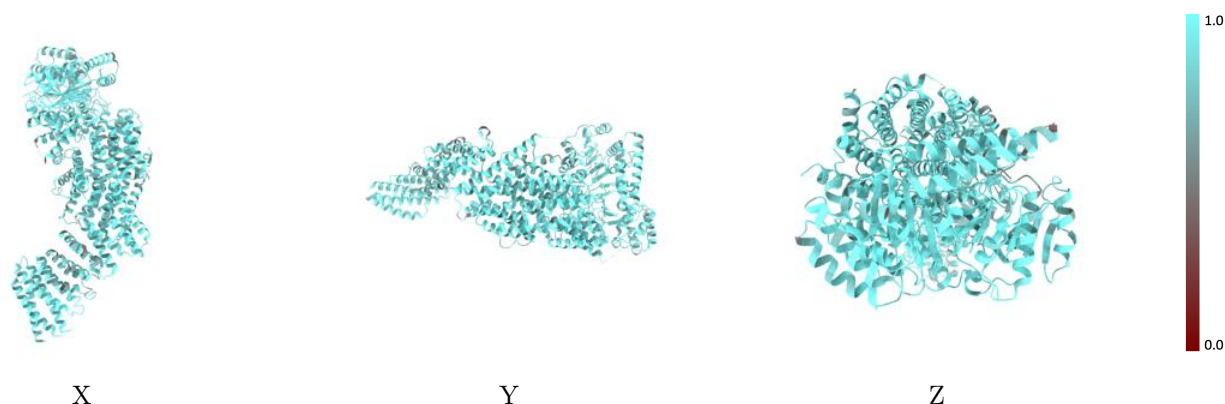
The images above show the 3D surface view of the map at the recommended contour level 2.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



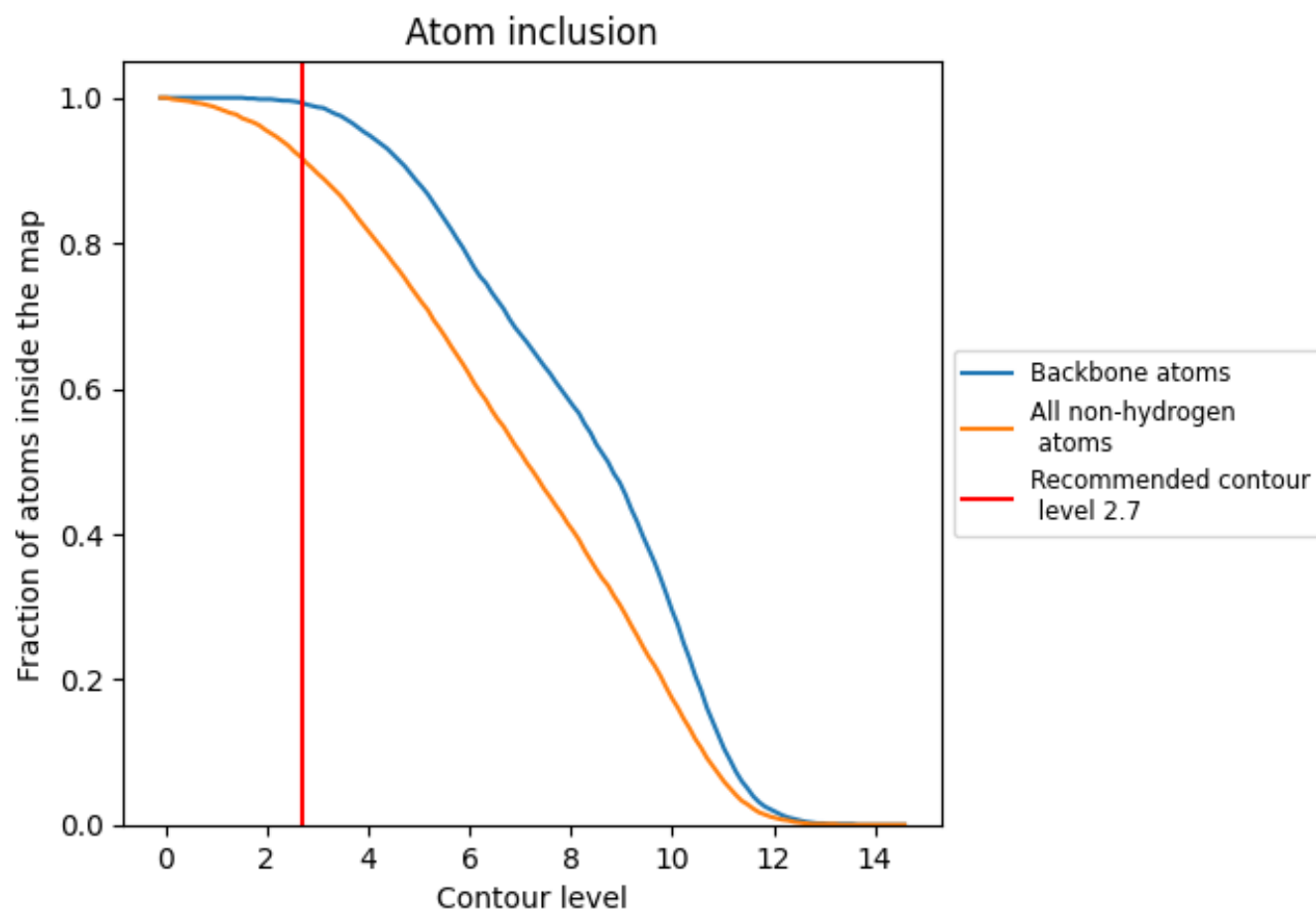
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.7).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 92% 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 (2.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9170	<div><div></div></div> 0.5080
A	<div><div></div></div> 0.9170	<div><div></div></div> 0.5080

