



Full wwPDB EM Validation Report ⓘ

Aug 29, 2026 – 12:54 PM EDT

PDB ID : 11YB / pdb_000011yb
EMDB ID : EMD-76179
Title : Structure of AlphaIbBeta3-R21C11 Fab in the near-bent conformation
Authors : Wang, J.L.; Collier, B.; Wang, L.; Li, J.H.
Deposited on : 2026-03-17
Resolution : 3.40 Å (reported)
Based on initial models : 8T2V, 7LA4

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:

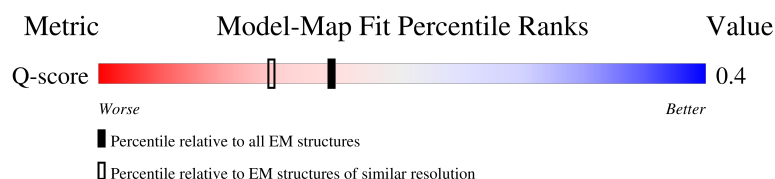
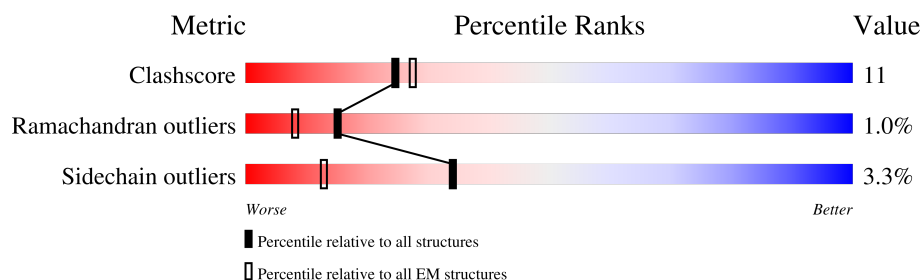
EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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	1039	7% 78% 10% 12%
2	B	788	74% 12% 12%
3	H	221	22% 29% 48%
4	L	211	19% 24% 6% 50%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 25517 atoms, of which 11628 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 Integrin alpha-IIb.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	912	Total	C	H	N	O	S	0	0
			13783	4409	6808	1214	1323	29		

- Molecule 2 is a protein called Integrin beta-3.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	690	Total	C	H	N	O	S	0	0
			10011	3185	4820	886	1055	65		

- Molecule 3 is a protein called R21C11 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	116	Total	C	N	O	S	0	0
			915	586	145	179	5		

- Molecule 4 is a protein called R21C11 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	105	Total	C	N	O	S	0	0
			800	506	131	161	2		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
5	A	5	Total	Ca	0
			5	5	
5	B	2	Total	Ca	0
			2	2	

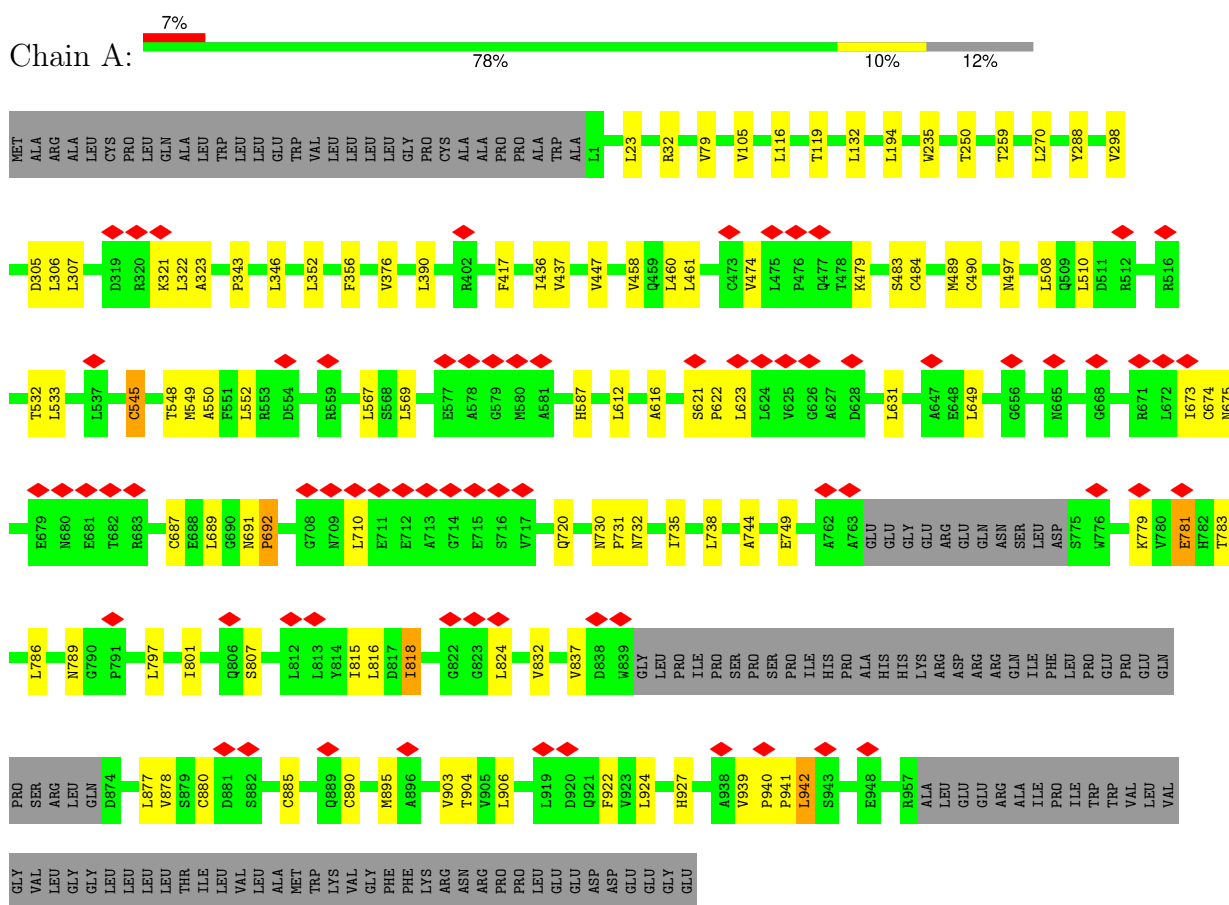
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
6	B	1	Total	Mg	0
			1	1	

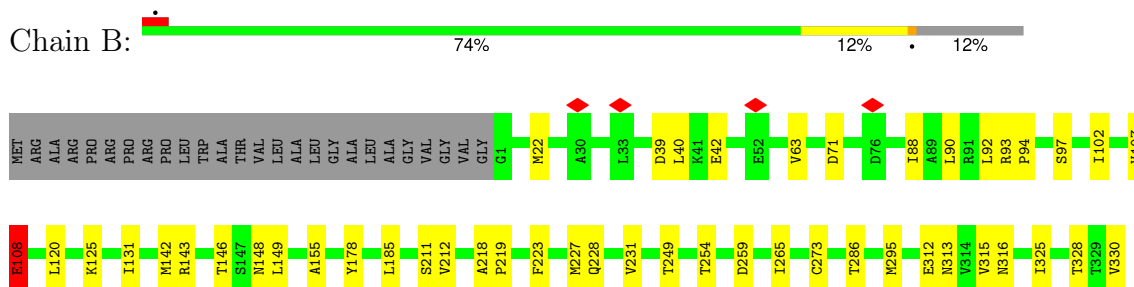
3 Residue-property plots [i](#)

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: Integrin alpha-IIb



• Molecule 2: Integrin beta-3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	49648	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 ($e^-/\text{\AA}^2$)	54	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.082	Depositor
Minimum map value	-1.921	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.048	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	344.0, 344.0, 344.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.16	0/7141	0.32	1/9735 (0.0%)
2	B	0.51	4/5283 (0.1%)	0.60	4/7158 (0.1%)
3	H	0.19	0/941	0.44	1/1276 (0.1%)
4	L	0.63	0/818	0.91	3/1109 (0.3%)
All	All	0.37	4/14183 (0.0%)	0.50	9/19278 (0.0%)

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
2	B	0	1
4	L	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	617	CYS	C-O	22.19	1.51	1.24
2	B	617	CYS	N-CA	10.35	1.59	1.46
2	B	617	CYS	CA-CB	9.00	1.68	1.53
2	B	626	HIS	C-O	6.56	1.32	1.24

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	617	CYS	N-CA-CB	16.44	138.28	110.49
2	B	471	CYS	CA-C-N	13.85	148.60	121.18
2	B	471	CYS	C-N-CA	13.85	148.60	121.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	617	CYS	N-CA-C	-7.56	94.69	110.80
4	L	60	ARG	N-CA-C	-6.48	106.58	114.75
3	H	1	GLU	N-CA-CB	-6.00	100.30	110.50
4	L	86	TYR	N-CA-CB	-5.52	102.47	110.70
1	A	545	CYS	CA-CB-SG	5.36	126.72	114.40
4	L	95	PHE	CB-CA-C	-5.27	102.60	112.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	143	ARG	Sidechain
4	L	60	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6975	6808	6815	78	0
2	B	5191	4820	4846	71	0
3	H	915	0	869	84	0
4	L	800	0	788	73	0
5	A	5	0	0	1	0
5	B	2	0	0	0	0
6	B	1	0	0	0	0
All	All	13889	11628	13318	289	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 11.

All (289) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:38:LYS:HB2	3:H:48:ILE:HD11	1.33	1.06
3:H:51:ILE:HD12	3:H:70:LEU:HB3	1.46	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:13:LYS:HG3	3:H:14:PRO:HD2	1.44	0.96
3:H:105:TRP:HB2	4:L:45:LEU:HD11	1.48	0.95
3:H:104:SER:HB3	4:L:88:LEU:HD13	1.54	0.89
3:H:23:LYS:HA	3:H:78:THR:HG22	1.56	0.87
1:A:783:THR:HG22	1:A:904:THR:HG22	1.58	0.85
4:L:3:LEU:HD11	4:L:32:LEU:HD21	1.58	0.84
2:B:616:GLU:O	2:B:617:CYS:C	2.25	0.80
1:A:490:CYS:HA	1:A:545:CYS:HB2	1.64	0.79
1:A:458:VAL:HG11	1:A:569:LEU:HD22	1.66	0.77
4:L:11:SER:HB3	4:L:106:LYS:HE3	1.67	0.77
4:L:3:LEU:CD1	4:L:32:LEU:HD21	2.14	0.77
1:A:895:MET:HE2	1:A:895:MET:HA	1.67	0.77
1:A:818:ILE:HD11	1:A:832:VAL:HG21	1.66	0.77
1:A:781:GLU:OE2	1:A:783:THR:HG23	1.84	0.77
3:H:50:TYR:HB3	3:H:59:GLU:HB2	1.65	0.77
3:H:68:THR:HG22	3:H:83:LEU:HD23	1.67	0.76
3:H:38:LYS:CB	3:H:48:ILE:HD11	2.14	0.75
3:H:58:SER:HB3	3:H:60:TYR:CE1	2.22	0.75
3:H:50:TYR:CB	3:H:59:GLU:HB2	2.18	0.73
4:L:90:GLY:HA2	4:L:95:PHE:CE1	2.24	0.72
2:B:231:VAL:HG23	2:B:273:CYS:HB3	1.72	0.72
3:H:95:TYR:HB2	3:H:109:TRP:HZ3	1.55	0.72
3:H:39:GLN:O	3:H:92:ALA:HB1	1.88	0.72
1:A:105:VAL:HG22	1:A:132:LEU:HG	1.71	0.71
1:A:490:CYS:HA	1:A:545:CYS:CB	2.20	0.71
4:L:16:GLU:O	4:L:77:VAL:HG12	1.91	0.71
4:L:29:TYR:HA	4:L:91:TYR:CZ	2.27	0.70
1:A:781:GLU:HB2	1:A:906:LEU:HD13	1.73	0.70
3:H:34:MET:HE1	3:H:98:ARG:HG3	1.72	0.70
3:H:59:GLU:OE2	4:L:93:ILE:HG12	1.91	0.70
3:H:105:TRP:HB2	4:L:45:LEU:CD1	2.22	0.69
3:H:39:GLN:HB2	3:H:45:LEU:HD23	1.74	0.69
4:L:34:TRP:HD1	4:L:47:ILE:HG22	1.58	0.68
3:H:114:LEU:HD23	3:H:115:VAL:N	2.08	0.68
1:A:479:LYS:HE2	1:A:479:LYS:HA	1.76	0.68
4:L:12:VAL:HG21	4:L:18:VAL:CG2	2.24	0.67
2:B:680:TYR:OH	3:H:102:SER:HB3	1.96	0.66
3:H:69:THR:C	3:H:70:LEU:HD12	2.21	0.66
4:L:27:SER:HB2	4:L:29:TYR:CE2	2.31	0.66
3:H:105:TRP:CG	4:L:48:LYS:HD2	2.32	0.65
4:L:28:ILE:O	4:L:28:ILE:HG22	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:13:THR:HG23	4:L:14:PRO:HD2	1.79	0.65
3:H:35:HIS:HD1	3:H:106:PHE:HE1	1.46	0.63
3:H:68:THR:HG22	3:H:83:LEU:CD2	2.28	0.63
2:B:375:LEU:HD12	2:B:375:LEU:O	1.97	0.63
4:L:45:LEU:HD23	4:L:46:LEU:H	1.62	0.63
1:A:259:THR:O	1:A:259:THR:HG22	2.00	0.62
3:H:13:LYS:CG	3:H:14:PRO:HD2	2.25	0.62
3:H:50:TYR:O	3:H:70:LEU:HD22	2.00	0.62
3:H:51:ILE:HD12	3:H:70:LEU:CB	2.25	0.62
3:H:5:GLN:HE21	3:H:23:LYS:HE3	1.64	0.62
3:H:27:TYR:HD2	3:H:29:PHE:H	1.48	0.62
4:L:45:LEU:HD22	4:L:54:ILE:HG13	1.82	0.62
2:B:390:LYS:HD2	4:L:55:SER:HB3	1.83	0.61
2:B:265:ILE:HD12	2:B:265:ILE:H	1.65	0.61
2:B:644:GLU:OE2	4:L:92:SER:HA	1.99	0.61
3:H:60:TYR:CE2	3:H:69:THR:HA	2.35	0.61
1:A:321:LYS:C	1:A:322:LEU:HD22	2.25	0.61
2:B:333:LEU:HD23	2:B:334:SER:O	2.01	0.61
4:L:18:VAL:HG21	4:L:103:LEU:HD11	1.82	0.61
1:A:250:THR:O	5:A:1103:CA:CA	1.78	0.60
4:L:18:VAL:O	4:L:73:SER:HA	2.02	0.60
3:H:2:VAL:O	3:H:3:GLN:HG2	2.02	0.59
3:H:69:THR:HB	3:H:82:GLN:OE1	2.02	0.59
4:L:4:THR:H	4:L:24:ALA:CB	2.14	0.59
4:L:45:LEU:HD22	4:L:54:ILE:CG1	2.32	0.59
1:A:720:GLN:HE21	1:A:735:ILE:HG23	1.67	0.59
3:H:104:SER:CB	4:L:88:LEU:HD13	2.30	0.59
1:A:786:LEU:HD13	1:A:797:LEU:HD21	1.84	0.58
1:A:569:LEU:C	1:A:569:LEU:HD23	2.28	0.58
1:A:674:CYS:HA	1:A:687:CYS:CB	2.34	0.58
4:L:13:THR:CG2	4:L:14:PRO:HD2	2.34	0.58
3:H:30:ILE:HG23	3:H:54:THR:HG22	1.86	0.58
4:L:22:CYS:HB2	4:L:34:TRP:CZ2	2.39	0.58
4:L:45:LEU:HD23	4:L:46:LEU:N	2.18	0.58
3:H:16:ALA:O	3:H:86:LEU:HG	2.04	0.58
1:A:235:TRP:CZ2	1:A:270:LEU:HD11	2.40	0.57
2:B:668:GLN:HG2	2:B:669:TYR:H	1.69	0.57
4:L:88:LEU:HD23	4:L:89:GLN:N	2.19	0.57
1:A:549:MET:HE3	1:A:550:ALA:N	2.20	0.57
2:B:535:MET:HE1	2:B:542:CYS:SG	2.44	0.57
3:H:105:TRP:CD2	4:L:48:LYS:HD2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:652:ALA:HB2	2:B:670:TYR:HA	1.84	0.57
1:A:674:CYS:HA	1:A:687:CYS:HB2	1.86	0.57
3:H:1:GLU:CD	3:H:1:GLU:H3	2.13	0.57
4:L:48:LYS:HD3	4:L:54:ILE:HD11	1.87	0.57
3:H:23:LYS:CA	3:H:78:THR:HG22	2.31	0.57
2:B:673:SER:HB3	3:H:31:SER:HB2	1.87	0.56
4:L:90:GLY:HA2	4:L:95:PHE:HE1	1.65	0.56
4:L:11:SER:HA	4:L:104:GLU:O	2.04	0.56
1:A:306:LEU:HD23	1:A:307:LEU:N	2.20	0.56
2:B:223:PHE:CZ	2:B:254:THR:HG21	2.40	0.55
3:H:60:TYR:OH	3:H:69:THR:HA	2.06	0.55
1:A:532:THR:C	1:A:533:LEU:HD22	2.32	0.55
3:H:5:GLN:NE2	3:H:23:LYS:HE3	2.21	0.55
1:A:436:ILE:HG22	1:A:447:VAL:HG22	1.88	0.55
3:H:4:LEU:HD23	3:H:22:CYS:SG	2.46	0.55
4:L:48:LYS:HB2	4:L:54:ILE:HD11	1.89	0.54
3:H:95:TYR:HB2	3:H:109:TRP:CZ3	2.41	0.54
1:A:484:CYS:HB2	1:A:549:MET:HE1	1.90	0.54
3:H:33:TRP:CD1	3:H:33:TRP:H	2.25	0.54
1:A:489:MET:O	1:A:545:CYS:HB2	2.08	0.54
4:L:48:LYS:HD3	4:L:54:ILE:CD1	2.38	0.54
1:A:744:ALA:N	1:A:939:VAL:HG21	2.23	0.54
3:H:37:VAL:HG21	3:H:109:TRP:HH2	1.73	0.53
2:B:102:ILE:CG2	2:B:425:LEU:HD22	2.38	0.53
4:L:5:GLN:HG3	4:L:100:GLY:H	1.73	0.53
1:A:649:LEU:HB2	1:A:689:LEU:HD21	1.91	0.53
1:A:616:ALA:HB1	1:A:738:LEU:HD11	1.90	0.53
3:H:35:HIS:ND1	3:H:106:PHE:HE1	2.06	0.53
4:L:23:ARG:HG2	4:L:24:ALA:H	1.74	0.53
1:A:484:CYS:HB2	1:A:549:MET:CE	2.39	0.53
3:H:62:GLN:O	3:H:63:LYS:HG3	2.09	0.53
1:A:460:LEU:HD12	1:A:461:LEU:N	2.24	0.52
1:A:789:ASN:OD1	1:A:789:ASN:C	2.51	0.52
2:B:679:LEU:HD12	2:B:679:LEU:N	2.24	0.52
2:B:120:LEU:HD12	2:B:155:ALA:HB1	1.92	0.52
1:A:691:ASN:O	1:A:692:PRO:C	2.51	0.52
1:A:824:LEU:HD11	1:A:903:VAL:CG2	2.39	0.52
1:A:924:LEU:C	1:A:924:LEU:HD23	2.35	0.52
2:B:218:ALA:HB3	2:B:219:PRO:HD3	1.92	0.51
1:A:390:LEU:N	1:A:390:LEU:HD12	2.25	0.51
3:H:2:VAL:HG21	3:H:108:TYR:CD2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:801:ILE:HD12	1:A:927:HIS:O	2.10	0.51
2:B:227:MET:O	2:B:231:VAL:HG22	2.11	0.51
4:L:12:VAL:HG12	4:L:16:GLU:HG2	1.93	0.51
1:A:490:CYS:CA	1:A:545:CYS:HB2	2.38	0.51
2:B:680:TYR:CZ	3:H:102:SER:HB3	2.45	0.51
2:B:627:ASP:O	2:B:628:GLU:C	2.54	0.50
2:B:40:LEU:HD12	2:B:42:GLU:OE2	2.11	0.50
2:B:107:VAL:O	2:B:108:GLU:C	2.54	0.50
3:H:81:MET:CE	3:H:83:LEU:HD21	2.42	0.50
1:A:194:LEU:HD12	1:A:194:LEU:C	2.37	0.50
3:H:39:GLN:CB	3:H:45:LEU:HD23	2.42	0.50
1:A:23:LEU:HD23	1:A:23:LEU:N	2.27	0.50
2:B:672:ASP:HB3	3:H:101:GLY:HA3	1.94	0.50
2:B:675:GLY:O	2:B:676:LYS:CB	2.59	0.50
2:B:22:MET:HE1	2:B:40:LEU:HD22	1.94	0.49
2:B:228:GLN:OE1	2:B:273:CYS:HB2	2.12	0.49
4:L:6:SER:HB3	4:L:21:SER:HB3	1.93	0.49
1:A:623:LEU:HD21	1:A:631:LEU:HD21	1.93	0.49
2:B:618:LYS:O	2:B:619:LYS:C	2.55	0.49
1:A:323:ALA:HB1	1:A:352:LEU:HD21	1.92	0.49
2:B:92:LEU:N	2:B:92:LEU:HD12	2.28	0.49
3:H:62:GLN:C	3:H:63:LYS:HG3	2.37	0.49
4:L:28:ILE:HA	4:L:67:GLY:O	2.13	0.49
2:B:501:CYS:C	2:B:502:LEU:HD22	2.37	0.49
1:A:552:LEU:HD12	1:A:552:LEU:O	2.13	0.49
2:B:63:VAL:HG12	2:B:88:ILE:HG22	1.94	0.49
4:L:22:CYS:HB2	4:L:34:TRP:CH2	2.48	0.49
2:B:312:GLU:O	2:B:315:VAL:HG12	2.13	0.48
1:A:877:LEU:HD12	1:A:878:VAL:N	2.28	0.48
2:B:644:GLU:CD	4:L:92:SER:HA	2.39	0.48
2:B:22:MET:SD	2:B:22:MET:C	2.97	0.48
1:A:321:LYS:O	1:A:322:LEU:HD22	2.14	0.48
1:A:549:MET:HE3	1:A:549:MET:C	2.38	0.48
3:H:20:MET:CE	3:H:113:THR:HB	2.43	0.48
4:L:48:LYS:O	4:L:49:SER:C	2.55	0.48
3:H:19:LYS:NZ	3:H:82:GLN:HE21	2.11	0.48
4:L:4:THR:H	4:L:24:ALA:HB3	1.77	0.48
2:B:142:MET:HG2	2:B:149:LEU:HD13	1.94	0.48
2:B:535:MET:SD	2:B:535:MET:C	2.97	0.48
2:B:672:ASP:CB	3:H:101:GLY:HA3	2.42	0.48
1:A:483:SER:HB3	1:A:552:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:TRP:HZ2	1:A:270:LEU:HD11	1.78	0.48
2:B:389:LEU:HD21	2:B:395:VAL:HG21	1.96	0.48
3:H:29:PHE:CD2	3:H:77:SER:HA	2.48	0.48
2:B:102:ILE:HG21	2:B:425:LEU:HD22	1.96	0.47
3:H:59:GLU:HA	3:H:59:GLU:OE1	2.14	0.47
1:A:105:VAL:HG13	1:A:132:LEU:HD12	1.96	0.47
1:A:807:SER:OG	1:A:815:ILE:HD13	2.13	0.47
3:H:35:HIS:HB2	3:H:97:SER:OG	2.14	0.47
4:L:25:SER:CB	4:L:68:THR:HA	2.45	0.47
3:H:23:LYS:CB	3:H:78:THR:HG22	2.45	0.47
1:A:474:VAL:HG21	1:A:479:LYS:HE2	1.97	0.47
1:A:880:CYS:HB2	1:A:885:CYS:HA	1.96	0.47
2:B:22:MET:O	2:B:22:MET:HE3	2.16	0.46
2:B:643:LYS:HE3	4:L:91:TYR:HD2	1.79	0.46
3:H:60:TYR:CZ	3:H:69:THR:HA	2.50	0.46
4:L:16:GLU:HG3	4:L:17:THR:N	2.29	0.46
2:B:131:ILE:HG22	2:B:131:ILE:O	2.15	0.46
1:A:941:PRO:HA	1:A:942:LEU:HA	1.80	0.46
2:B:313:ASN:C	2:B:313:ASN:OD1	2.59	0.46
1:A:710:LEU:HD23	1:A:710:LEU:H	1.81	0.45
2:B:90:LEU:HD23	2:B:92:LEU:HD11	1.98	0.45
4:L:29:TYR:HA	4:L:91:TYR:CE2	2.51	0.45
2:B:286:THR:HG22	2:B:286:THR:O	2.16	0.45
2:B:330:VAL:HG12	2:B:331:GLY:N	2.30	0.45
2:B:642:VAL:HG22	2:B:644:GLU:HG2	1.98	0.45
2:B:380:ILE:HG21	2:B:383:LEU:HD22	1.97	0.45
3:H:28:THR:O	3:H:29:PHE:HB3	2.17	0.45
2:B:364:GLU:H	2:B:364:GLU:CD	2.25	0.45
1:A:490:CYS:HA	1:A:545:CYS:HB3	1.98	0.45
1:A:824:LEU:HD12	1:A:890:CYS:HB3	1.99	0.45
2:B:668:GLN:HG2	2:B:669:TYR:N	2.31	0.45
1:A:510:LEU:HG	1:A:567:LEU:HD22	1.98	0.45
1:A:940:PRO:N	1:A:941:PRO:CD	2.80	0.45
3:H:20:MET:HE3	3:H:113:THR:HB	1.99	0.45
3:H:37:VAL:HG21	3:H:109:TRP:CH2	2.52	0.45
2:B:259:ASP:OD1	2:B:259:ASP:O	2.35	0.44
4:L:46:LEU:HD22	4:L:61:PHE:CD2	2.52	0.44
3:H:60:TYR:HE2	3:H:69:THR:HA	1.81	0.44
1:A:497:ASN:CG	1:A:497:ASN:O	2.60	0.44
3:H:32:TYR:CB	3:H:98:ARG:HD3	2.46	0.44
4:L:29:TYR:OH	4:L:89:GLN:NE2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:34:TRP:CD1	4:L:47:ILE:HG22	2.45	0.44
1:A:673:ILE:O	1:A:687:CYS:HB2	2.18	0.44
4:L:75:ASN:O	4:L:76:SER:C	2.61	0.44
2:B:223:PHE:CE1	2:B:295:MET:HE1	2.53	0.44
2:B:372:ALA:HB2	2:B:383:LEU:O	2.18	0.44
3:H:33:TRP:CD1	3:H:33:TRP:N	2.86	0.44
3:H:62:GLN:H	3:H:62:GLN:CD	2.24	0.44
4:L:93:ILE:HG22	4:L:94:PRO:HD3	1.99	0.44
1:A:674:CYS:HA	1:A:687:CYS:HB3	2.00	0.44
2:B:212:VAL:O	2:B:212:VAL:HG23	2.17	0.44
4:L:10:LEU:HD23	4:L:10:LEU:HA	1.74	0.43
4:L:23:ARG:CG	4:L:24:ALA:H	2.30	0.43
4:L:89:GLN:H	4:L:89:GLN:HG3	1.65	0.43
2:B:332:VAL:H	3:H:1:GLU:HG2	1.84	0.43
3:H:8:GLY:O	3:H:113:THR:HG23	2.18	0.43
3:H:60:TYR:CE2	3:H:70:LEU:HD13	2.53	0.43
1:A:489:MET:HE1	1:A:548:THR:OG1	2.19	0.43
2:B:315:VAL:HG13	2:B:316:ASN:N	2.33	0.43
2:B:653:VAL:O	2:B:653:VAL:HG23	2.18	0.43
3:H:2:VAL:HG21	3:H:108:TYR:CE2	2.54	0.43
3:H:16:ALA:HB3	3:H:86:LEU:HD12	1.99	0.43
4:L:29:TYR:CE1	4:L:89:GLN:HB3	2.53	0.43
1:A:298:VAL:HG22	1:A:305:ASP:OD2	2.19	0.43
1:A:343:PRO:CB	1:A:346:LEU:HD21	2.49	0.43
4:L:25:SER:HB2	4:L:68:THR:HA	2.00	0.43
4:L:35:TYR:HB2	4:L:86:TYR:HB2	2.01	0.43
2:B:407:PRO:HB2	2:B:409:GLU:OE1	2.19	0.42
3:H:43:GLN:HG3	3:H:44:GLY:N	2.34	0.42
1:A:730:ASN:N	1:A:731:PRO:HD3	2.34	0.42
3:H:5:GLN:HE21	3:H:23:LYS:CE	2.32	0.42
3:H:64:PHE:HA	3:H:67:LYS:HD2	2.01	0.42
1:A:356:PHE:CE1	1:A:376:VAL:HG11	2.54	0.42
1:A:417:PHE:CZ	1:A:437:VAL:HG21	2.55	0.42
1:A:815:ILE:HD12	1:A:815:ILE:H	1.85	0.42
1:A:878:VAL:HG21	1:A:922:PHE:CE1	2.53	0.42
3:H:20:MET:SD	3:H:94:TYR:HB2	2.59	0.42
3:H:107:VAL:HG12	3:H:108:TYR:CD1	2.53	0.42
1:A:691:ASN:HB2	1:A:692:PRO:HD2	2.01	0.42
1:A:32:ARG:HA	1:A:32:ARG:CZ	2.50	0.42
2:B:380:ILE:N	2:B:380:ILE:HD12	2.34	0.42
3:H:84:ILE:HD13	3:H:84:ILE:HA	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:20:LEU:O	4:L:71:ILE:HA	2.19	0.42
4:L:58:PRO:HG2	4:L:61:PHE:CD1	2.55	0.42
2:B:125:LYS:HA	2:B:212:VAL:HG11	2.02	0.42
2:B:178:TYR:CD2	2:B:178:TYR:C	2.98	0.42
4:L:23:ARG:HA	4:L:69:ASP:OD1	2.19	0.42
1:A:779:LYS:NZ	1:A:816:LEU:HD12	2.35	0.41
2:B:325:ILE:HB	2:B:328:THR:HG21	2.02	0.41
4:L:46:LEU:HA	4:L:46:LEU:HD23	1.80	0.41
1:A:105:VAL:HG13	1:A:132:LEU:CD1	2.50	0.41
2:B:608:CYS:CB	2:B:655:CYS:SG	3.08	0.41
4:L:32:LEU:HD22	4:L:88:LEU:O	2.20	0.41
2:B:93:ARG:HB2	2:B:94:PRO:HD2	2.00	0.41
4:L:3:LEU:HD23	4:L:24:ALA:HB3	2.02	0.41
2:B:185:LEU:HD22	2:B:211:SER:OG	2.20	0.41
2:B:626:HIS:O	2:B:627:ASP:C	2.64	0.41
3:H:74:LYS:H	3:H:74:LYS:HG2	1.62	0.41
4:L:29:TYR:HB3	4:L:91:TYR:CE1	2.56	0.41
4:L:58:PRO:HG2	4:L:61:PHE:CE1	2.56	0.41
2:B:629:ASN:O	2:B:630:THR:C	2.64	0.41
2:B:668:GLN:CG	2:B:669:TYR:H	2.33	0.41
1:A:489:MET:HE2	1:A:508:LEU:CD1	2.51	0.41
3:H:102:SER:O	3:H:103:SER:OG	2.33	0.41
3:H:114:LEU:HD23	3:H:114:LEU:C	2.44	0.41
4:L:32:LEU:HD13	4:L:33:HIS:N	2.36	0.41
1:A:79:VAL:O	1:A:79:VAL:HG23	2.21	0.41
1:A:612:LEU:HD22	1:A:612:LEU:N	2.36	0.41
1:A:880:CYS:HB2	1:A:885:CYS:CA	2.51	0.41
4:L:12:VAL:HG21	4:L:18:VAL:HG23	2.01	0.41
1:A:306:LEU:HD23	1:A:307:LEU:H	1.84	0.41
2:B:71:ASP:O	2:B:108:GLU:OE1	2.37	0.41
3:H:23:LYS:HB2	3:H:23:LYS:HE2	1.87	0.41
3:H:58:SER:HB3	3:H:60:TYR:HE1	1.77	0.41
4:L:6:SER:HB3	4:L:7:PRO:HD3	2.02	0.41
4:L:31:ASN:O	4:L:31:ASN:OD1	2.39	0.41
2:B:497:GLN:HG2	2:B:497:GLN:O	2.20	0.40
1:A:621:SER:N	1:A:622:PRO:HD2	2.36	0.40
2:B:389:LEU:HD21	2:B:395:VAL:CG2	2.51	0.40
4:L:3:LEU:HD21	4:L:23:ARG:O	2.20	0.40
2:B:639:ILE:N	2:B:639:ILE:HD12	2.37	0.40
3:H:27:TYR:HE2	3:H:29:PHE:HA	1.86	0.40
4:L:3:LEU:O	4:L:98:GLY:HA2	2.20	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	906/1039 (87%)	872 (96%)	32 (4%)	2 (0%)	43	71
2	B	688/788 (87%)	602 (88%)	74 (11%)	12 (2%)	7	28
3	H	114/221 (52%)	101 (89%)	12 (10%)	1 (1%)	14	42
4	L	103/211 (49%)	77 (75%)	23 (22%)	3 (3%)	3	19
All	All	1811/2259 (80%)	1652 (91%)	141 (8%)	18 (1%)	15	40

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	692	PRO
2	B	617	CYS
2	B	676	LYS
4	L	73	SER
2	B	108	GLU
2	B	616	GLU
2	B	618	LYS
2	B	672	ASP
3	H	107	VAL
4	L	39	SER
4	L	51	SER
2	B	619	LYS
2	B	645	LEU
2	B	673	SER
2	B	625	LEU
1	A	837	VAL
2	B	628	GLU
2	B	650	LYS

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	756/864 (88%)	746 (99%)	10 (1%)	61	71
2	B	583/690 (84%)	563 (97%)	20 (3%)	32	57
3	H	98/191 (51%)	93 (95%)	5 (5%)	21	48
4	L	92/189 (49%)	77 (84%)	15 (16%)	2	10
All	All	1529/1934 (79%)	1479 (97%)	50 (3%)	34	57

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	LEU
1	A	119	THR
1	A	288	TYR
1	A	587	HIS
1	A	675	ASN
1	A	732	ASN
1	A	749	GLU
1	A	781	GLU
1	A	818	ILE
1	A	942	LEU
2	B	39	ASP
2	B	97	SER
2	B	108	GLU
2	B	146	THR
2	B	148	ASN
2	B	249	THR
2	B	365	GLU
2	B	419	VAL
2	B	497	GLN
2	B	509	HIS
2	B	583	CYS
2	B	604	CYS
2	B	637	ASP
2	B	643	LYS

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Mol	Chain	Res	Type
2	B	644	GLU
2	B	656	THR
2	B	657	TYR
2	B	659	ASN
2	B	671	GLU
2	B	678	ILE
3	H	1	GLU
3	H	2	VAL
3	H	33	TRP
3	H	81	MET
3	H	100	TYR
4	L	4	THR
4	L	6	SER
4	L	32	LEU
4	L	47	ILE
4	L	48	LYS
4	L	51	SER
4	L	60	ARG
4	L	66	SER
4	L	68	THR
4	L	71	ILE
4	L	72	LEU
4	L	84	ILE
4	L	89	GLN
4	L	93	ILE
4	L	95	PHE

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	215	HIS
1	A	534	ASN
1	A	639	ASN
1	A	655	GLN
1	A	720	GLN
1	A	722	GLN
1	A	893	GLN
2	B	133	ASN
2	B	274	HIS
2	B	654	ASN
2	B	668	GLN
3	H	5	GLN

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Mol	Chain	Res	Type
4	L	5	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

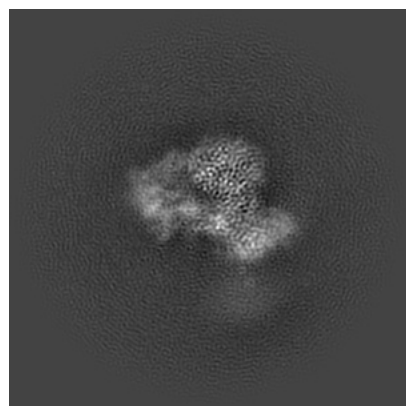
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-76179. These allow visual inspection of the internal detail of the map and identification of artifacts.

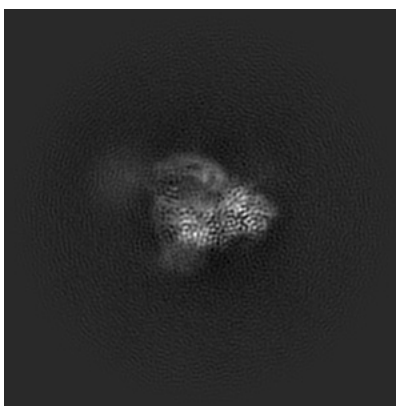
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

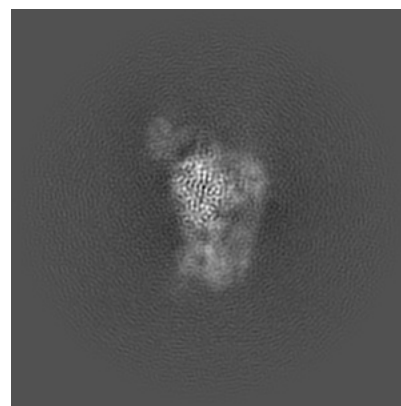
6.1.1 Primary map



X

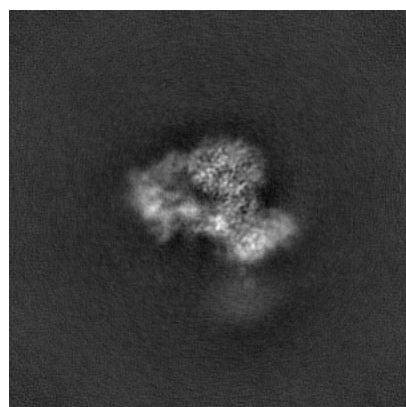


Y

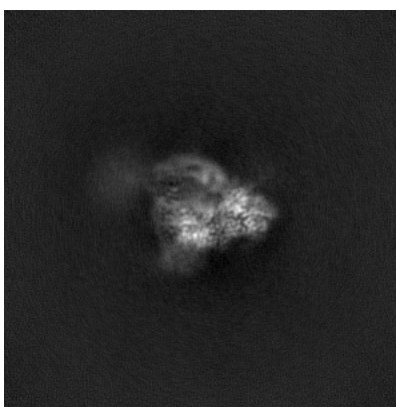


Z

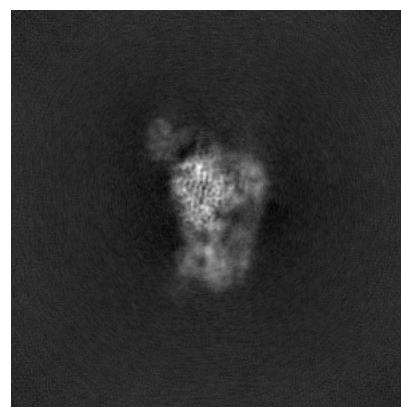
6.1.2 Raw map



X



Y

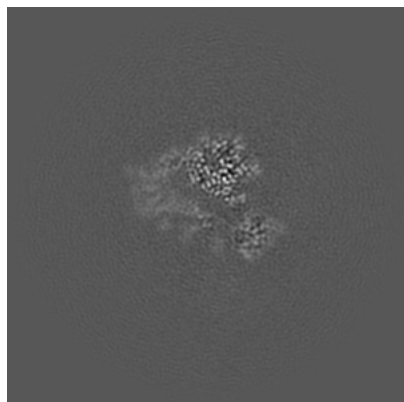


Z

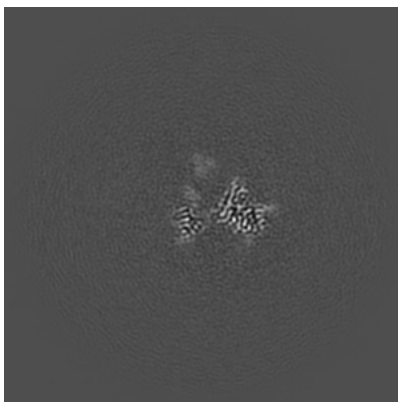
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

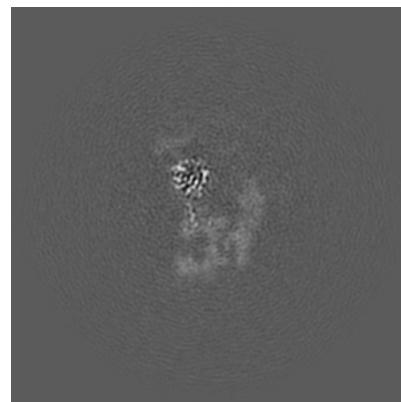
6.2.1 Primary map



X Index: 200

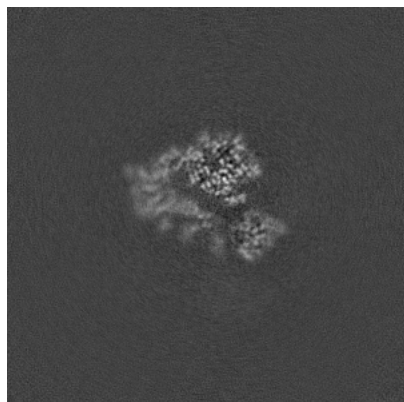


Y Index: 200

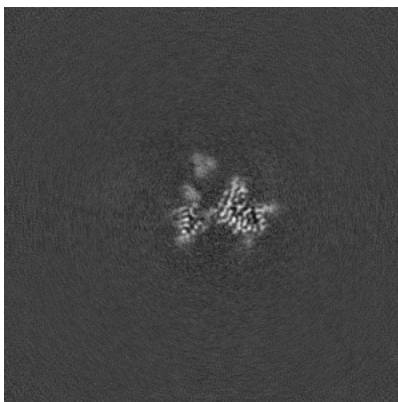


Z Index: 200

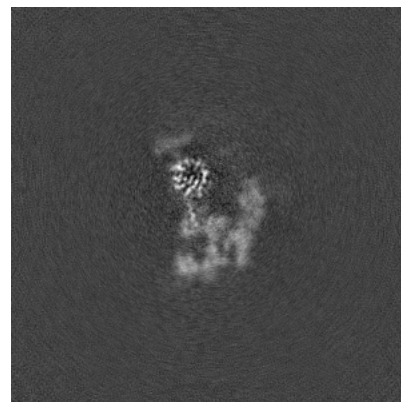
6.2.2 Raw map



X Index: 200



Y Index: 200

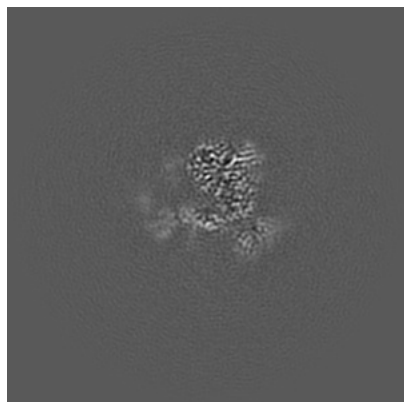


Z Index: 200

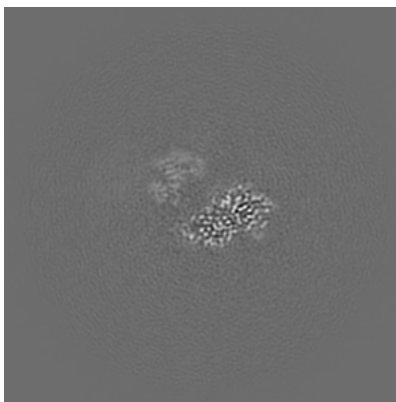
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

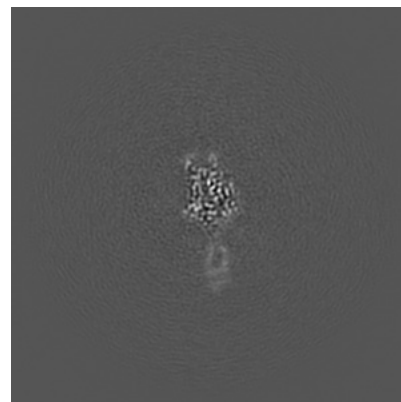
6.3.1 Primary map



X Index: 187

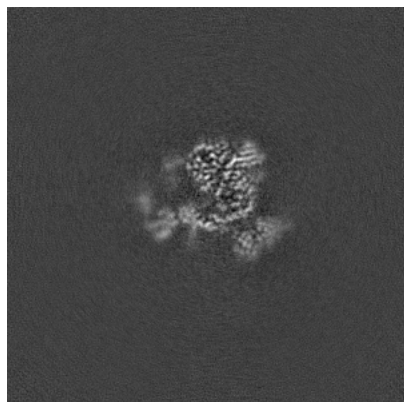


Y Index: 222

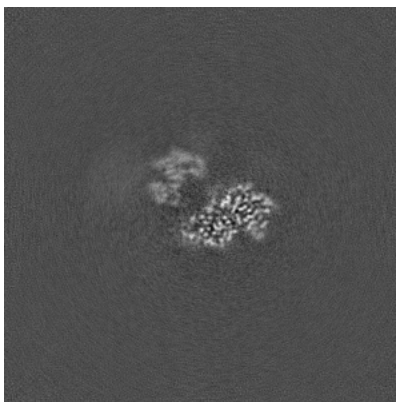


Z Index: 235

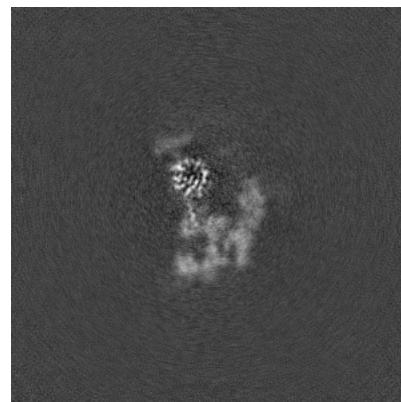
6.3.2 Raw map



X Index: 187



Y Index: 222

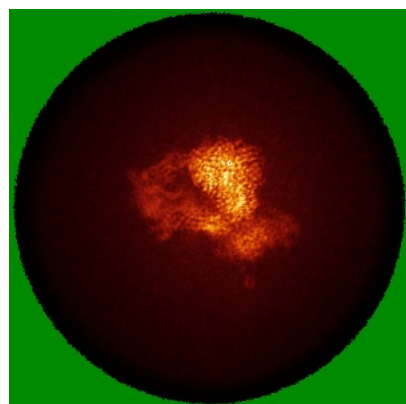


Z Index: 200

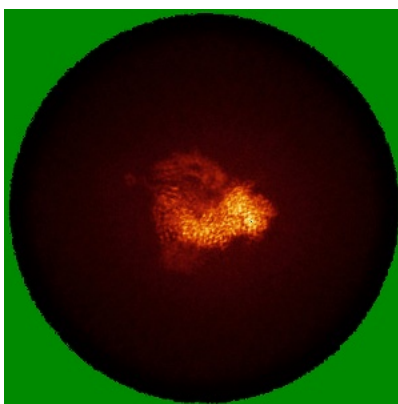
The images above show the largest variance slices of the map in three orthogonal directions.

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

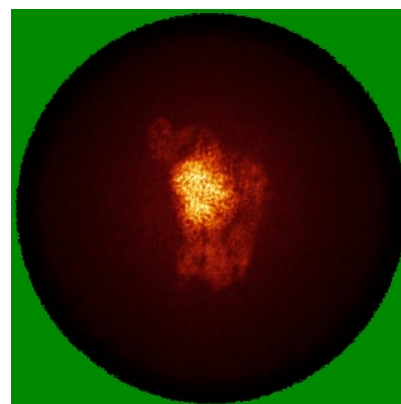
6.4.1 Primary map



X

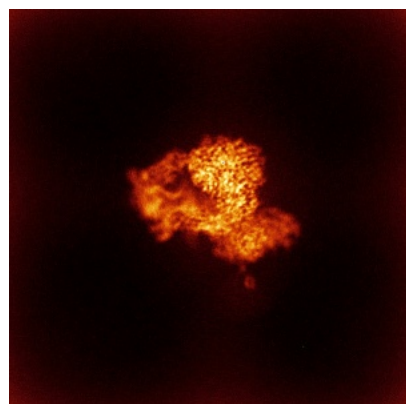


Y

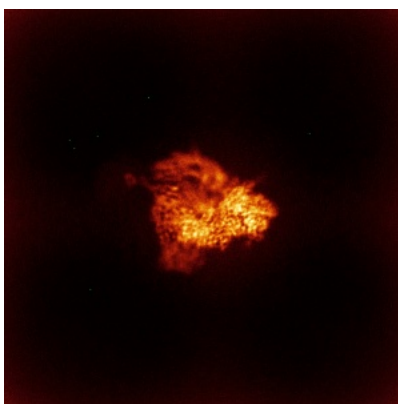


Z

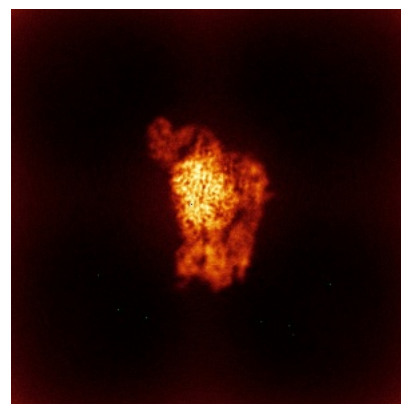
6.4.2 Raw map



X



Y

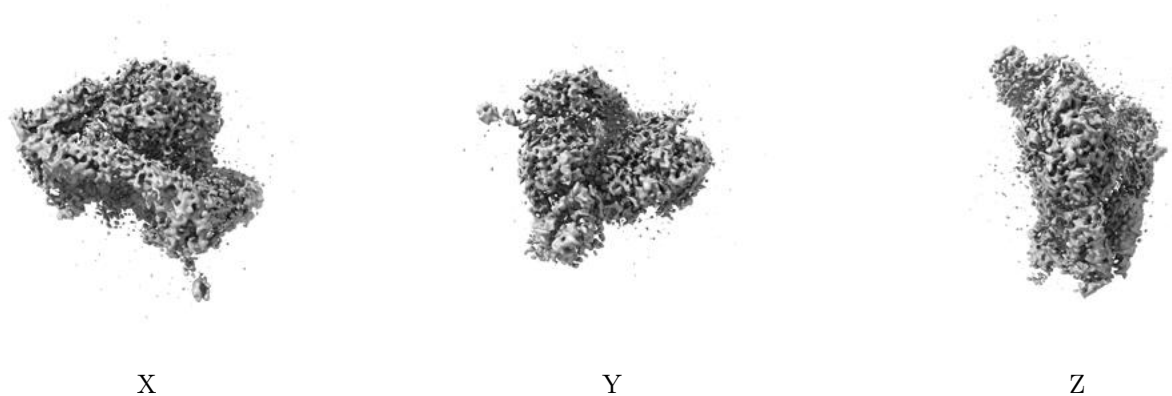


Z

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.

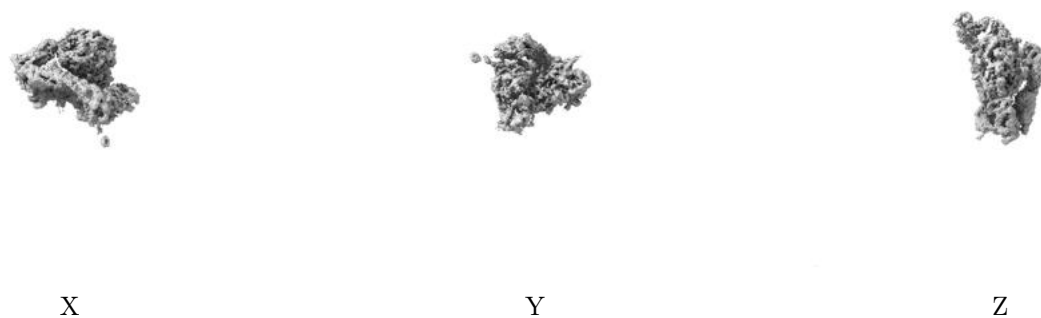
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. 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.

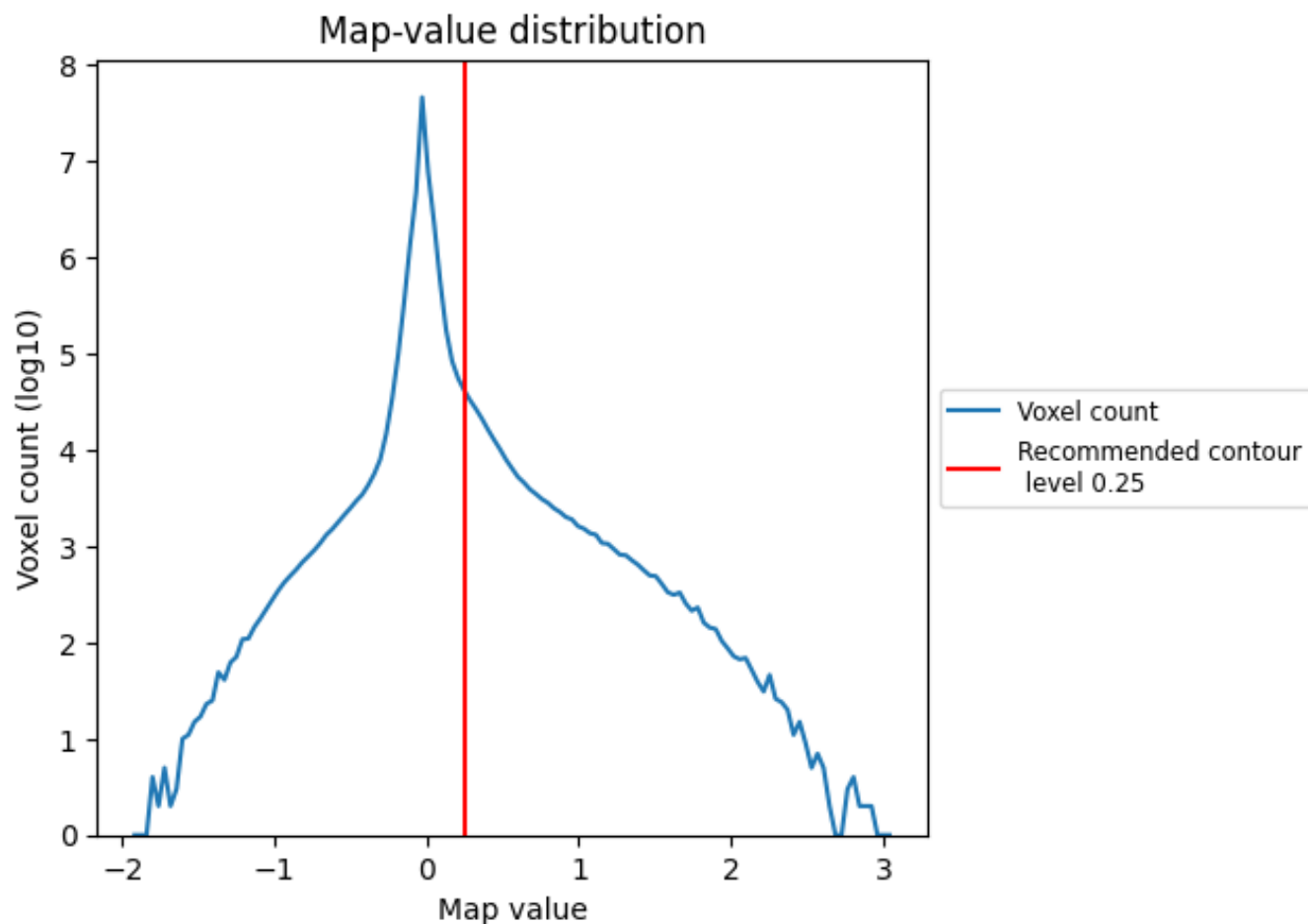
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

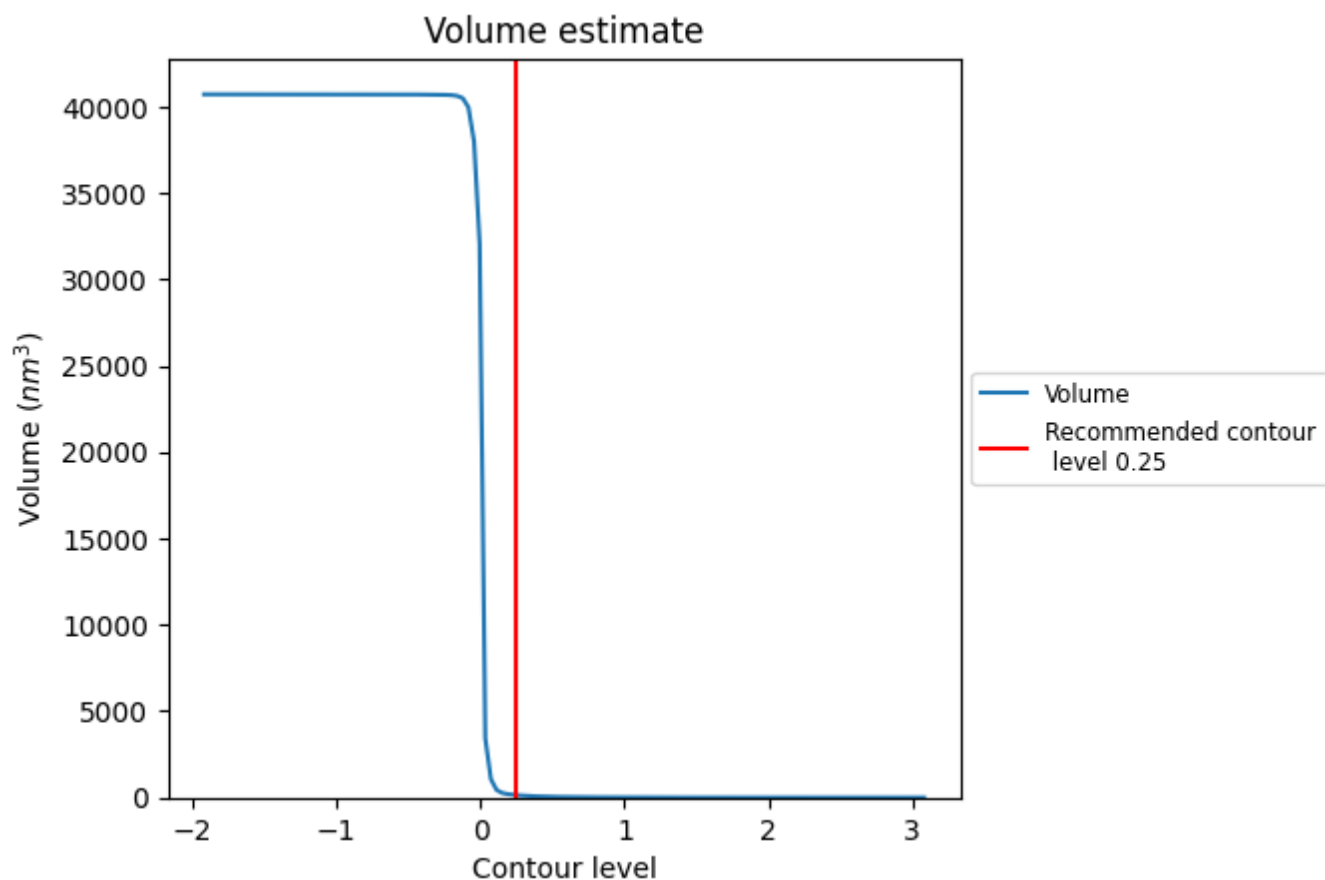
This section contains the results of statistical analysis of the map.

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.

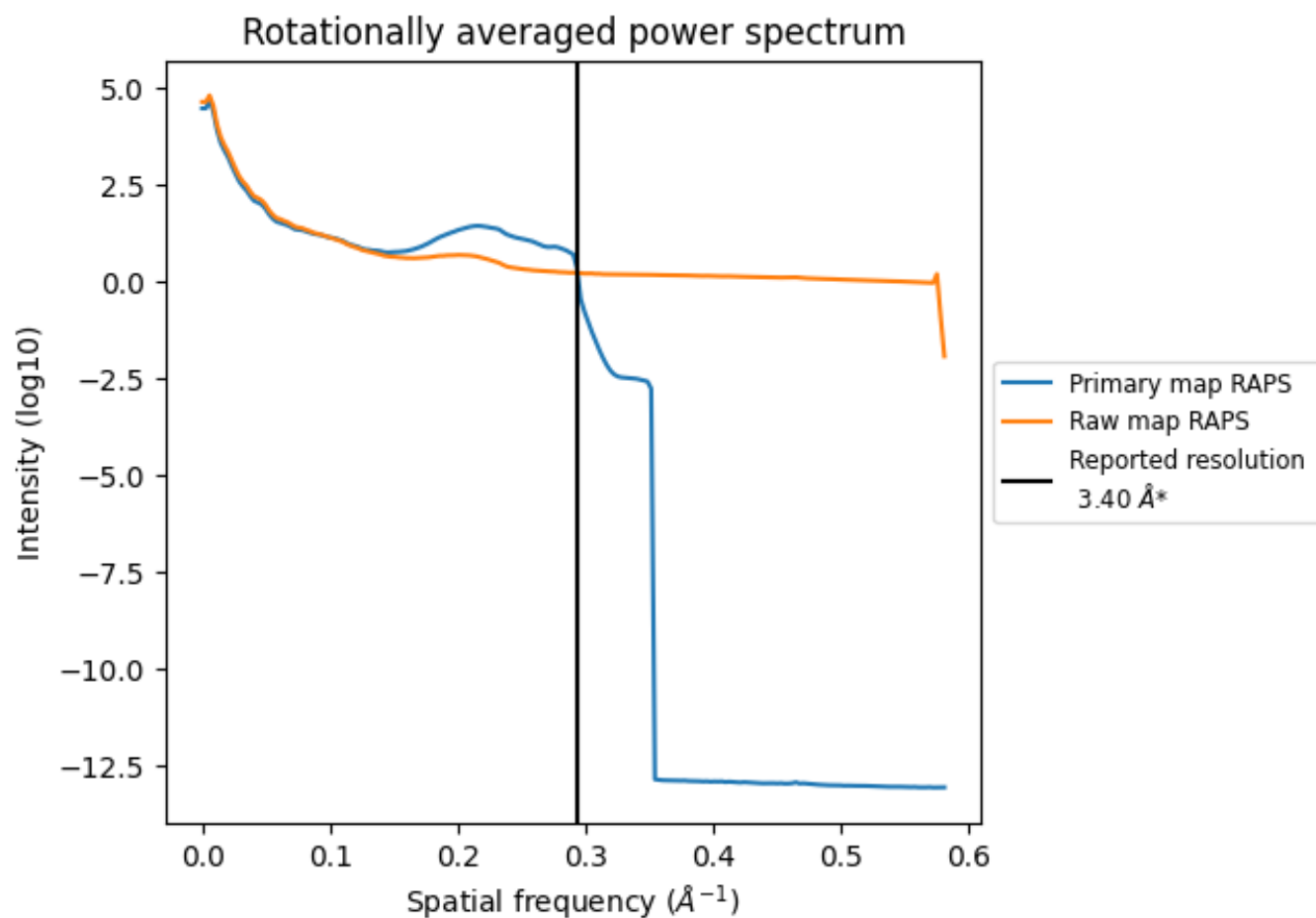
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 140 nm³; this corresponds to an approximate mass of 127 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 ⓘ

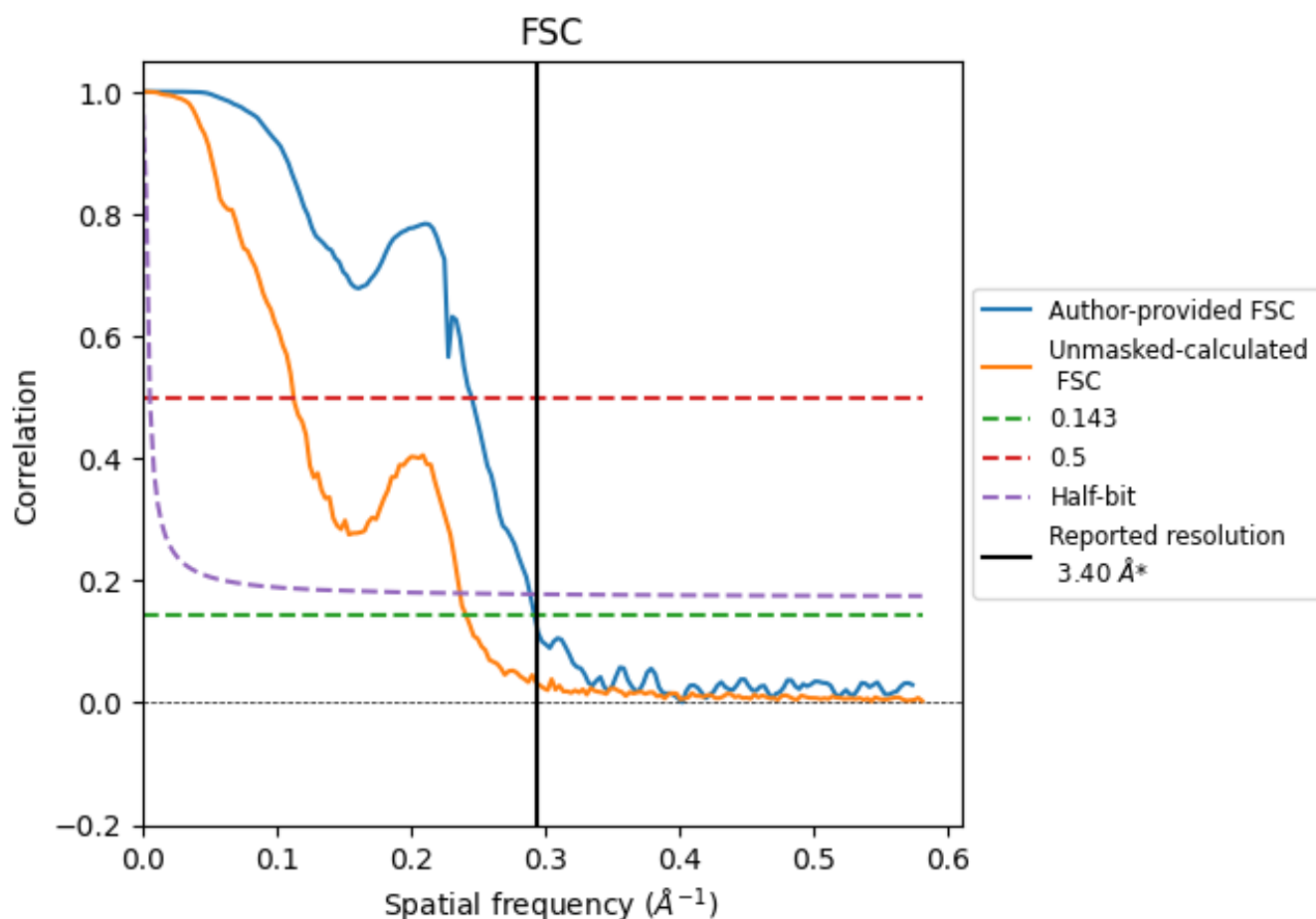


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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

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	3.42	4.07	3.46
Unmasked-calculated*	4.14	8.86	4.22

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

9 Map-model fit [i](#)

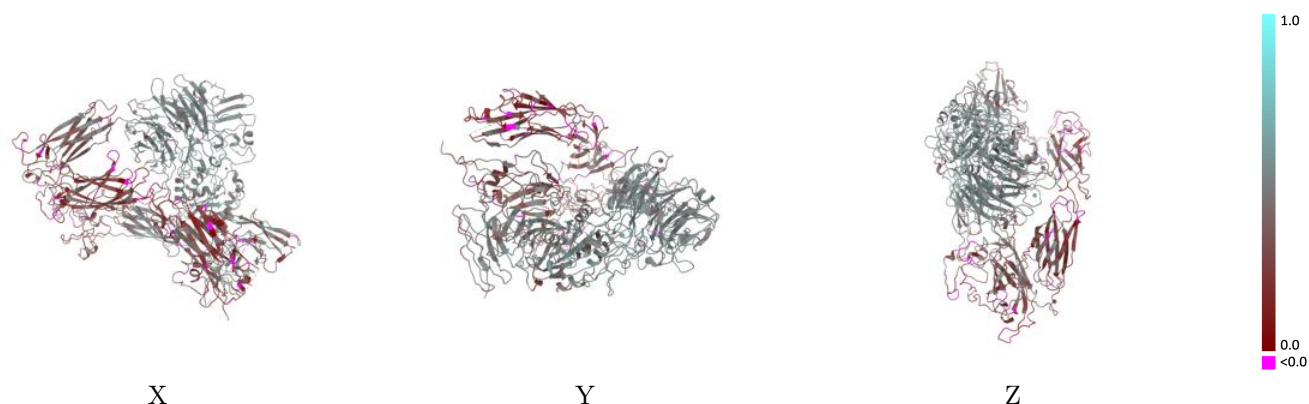
This section contains information regarding the fit between EMDB map EMD-76179 and PDB model 11YB. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



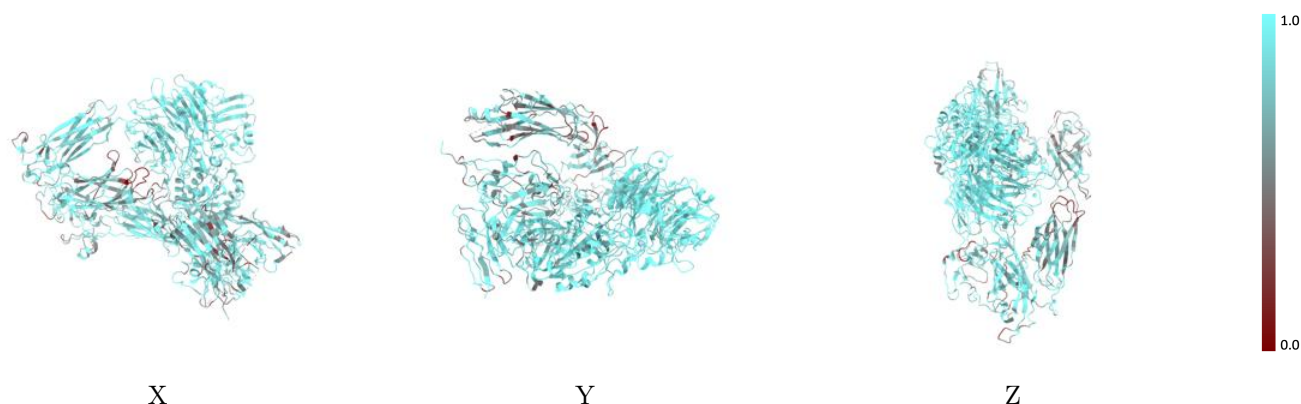
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



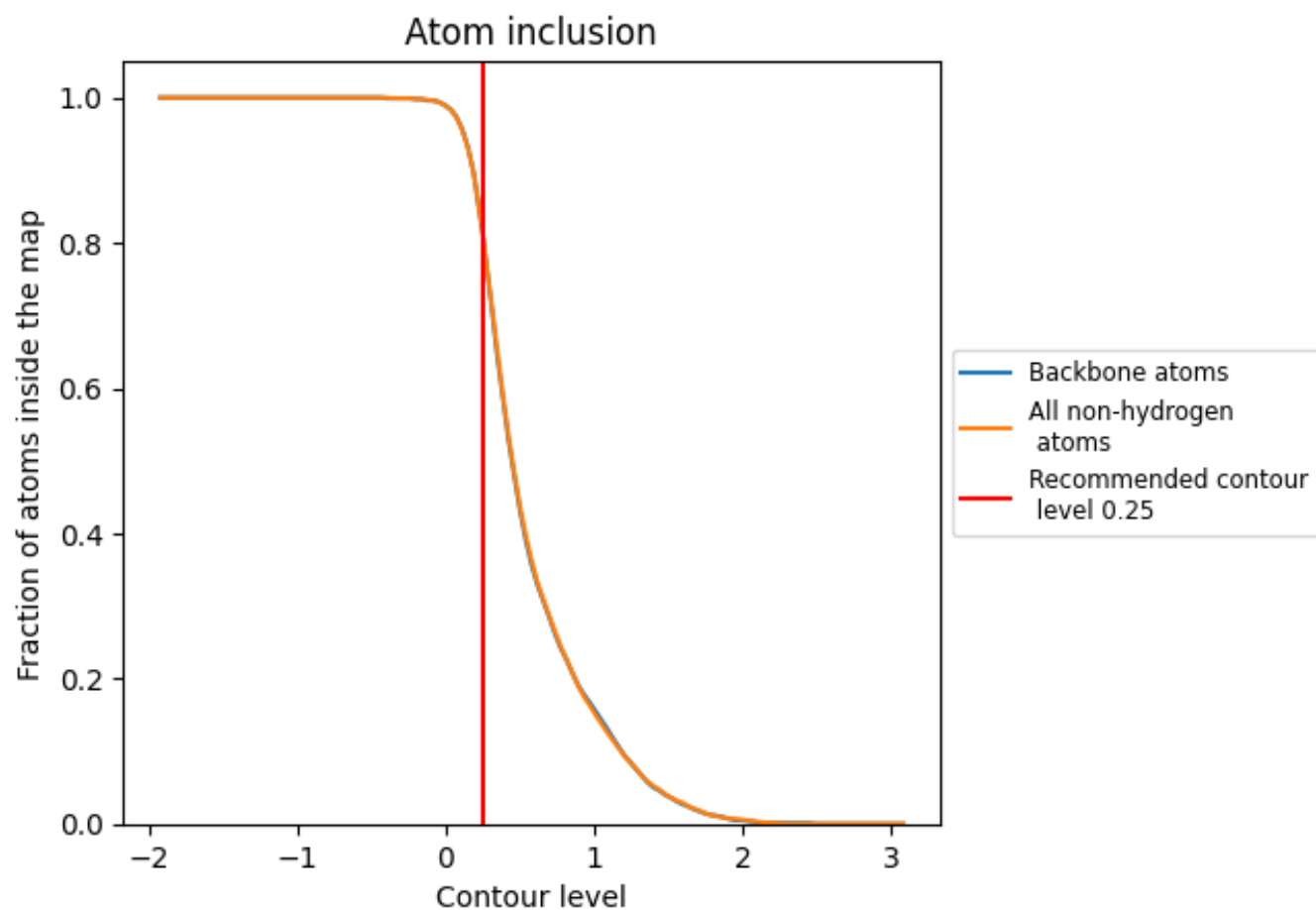
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.25).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 81% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8130	0.4000
A	0.8010	0.3830
B	0.8430	0.4050
H	0.8110	0.4320
L	0.8160	0.4800

