Full wwPDB EM Validation Report ⓘ

Oct 17, 2026 – 10:14 am BST

PDB ID	:	9TE2 / pdb_00009te2
EMDB ID	:	EMD-55817
Title	:	Cryo-EM structure of C5*-CVFBb (state 2.3)
Authors	:	Joergensen, M.H.; Andersen, G.R.; Almeida, A.V.d.
Deposited on	:	2025-11-25
Resolution	:	3.89 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:

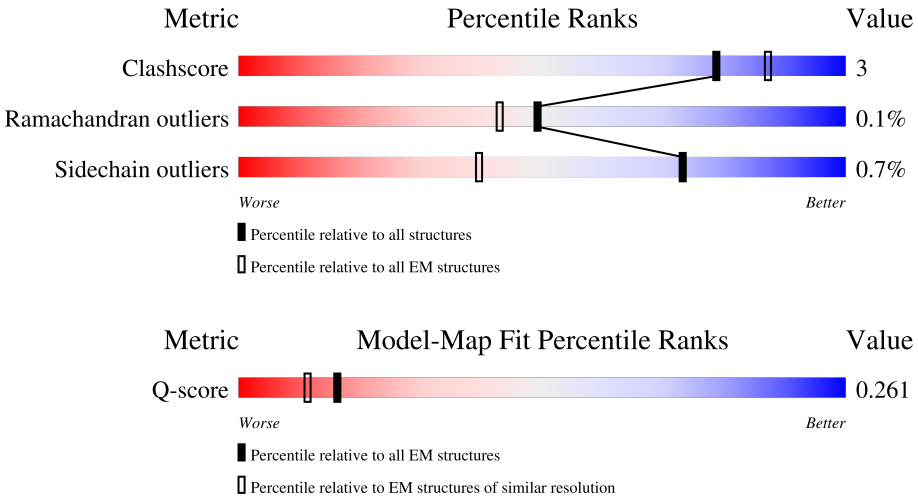
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 3.89 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	8712 (3.39 - 4.39)

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 <=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	659	93% 7%
2	C	999	16% 83%
3	B	627	91% 8%
4	D	252	81% 12% 7%

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Mol	Chain	Length	Quality of chain
5	E	379	
6	J	764	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 20334 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 Complement C5 beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	657	5195	3330	838	1014	13	0	0

- Molecule 2 is a protein called Complement C5 alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	172	1364	877	230	250	7	0	0

- Molecule 3 is a protein called Cobra venom factor alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	626	4893	3125	824	928	16	0	0

- Molecule 4 is a protein called Cobra venom factor gamma chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	234	1865	1199	312	349	5	0	0

- Molecule 5 is a protein called Cobra venom factor beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	373	3007	1895	507	585	20	0	0

- Molecule 6 is a protein called Complement factor B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	J	505	4007	2546	689	752	20	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	279	GLY	ASP	engineered mutation	UNP P00751
J	699	ALA	SER	engineered mutation	UNP P00751

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
7	J	1	Total	Mg	0
			1	1	

- Molecule 8 is water.

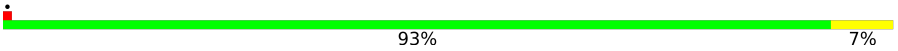
Mol	Chain	Residues	Atoms		AltConf
8	J	2	Total	O	0
			2	2	

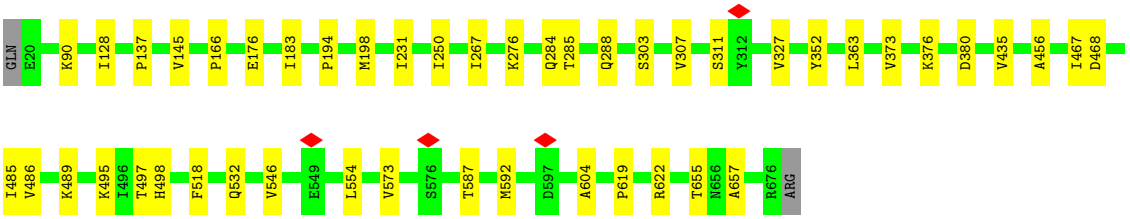
3 Residue-property plots (i)

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: Complement C5 beta chain

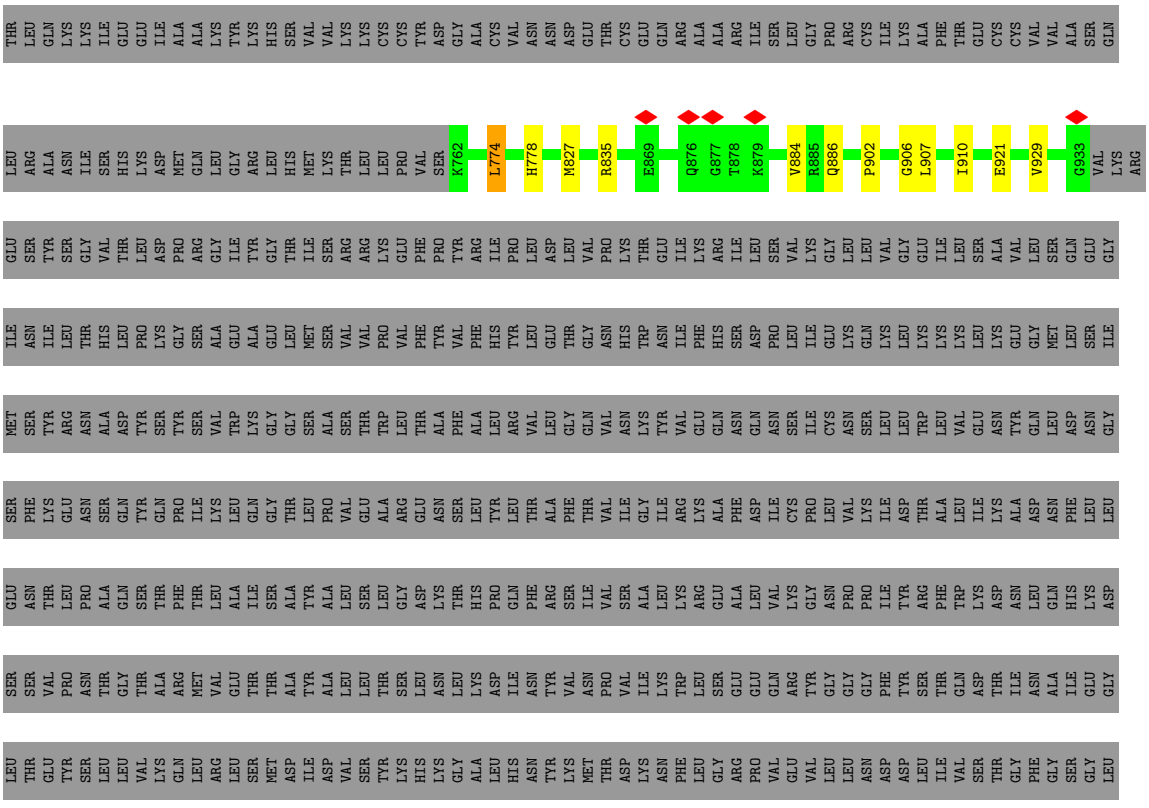
Chain A:

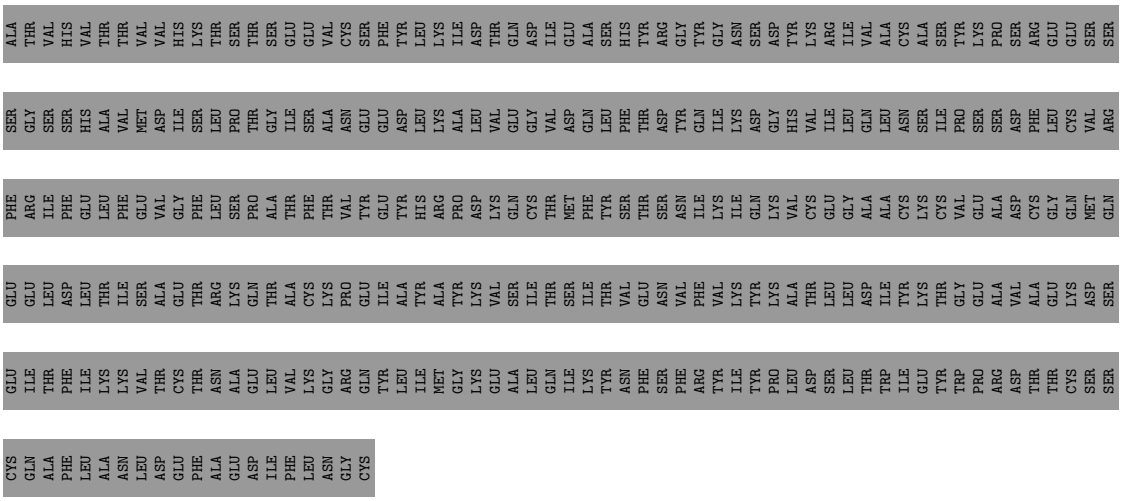




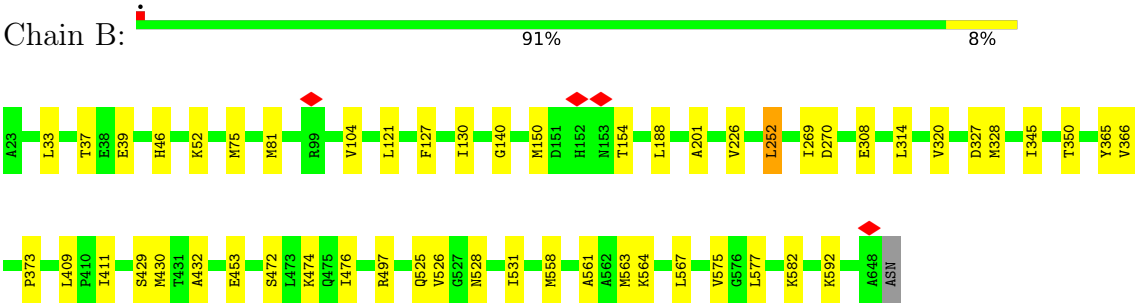
• Molecule 2: Complement C5 alpha chain

Chain C:

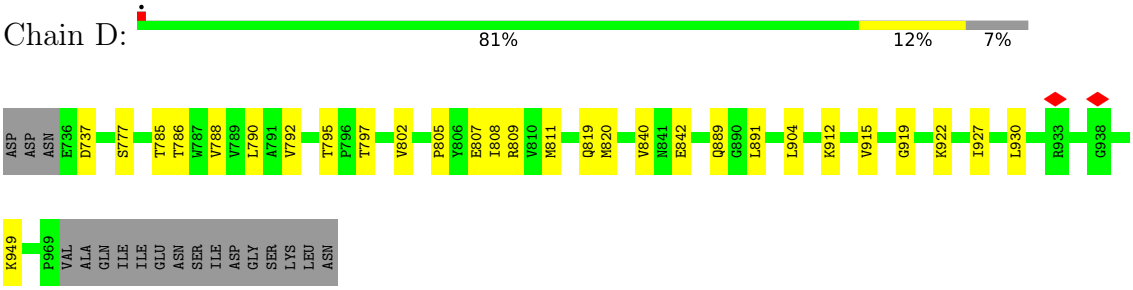




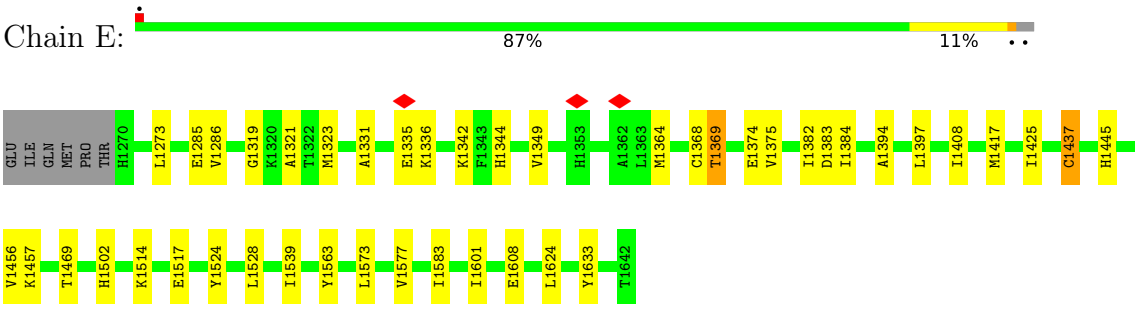
• Molecule 3: Cobra venom factor alpha chain



• Molecule 4: Cobra venom factor gamma chain

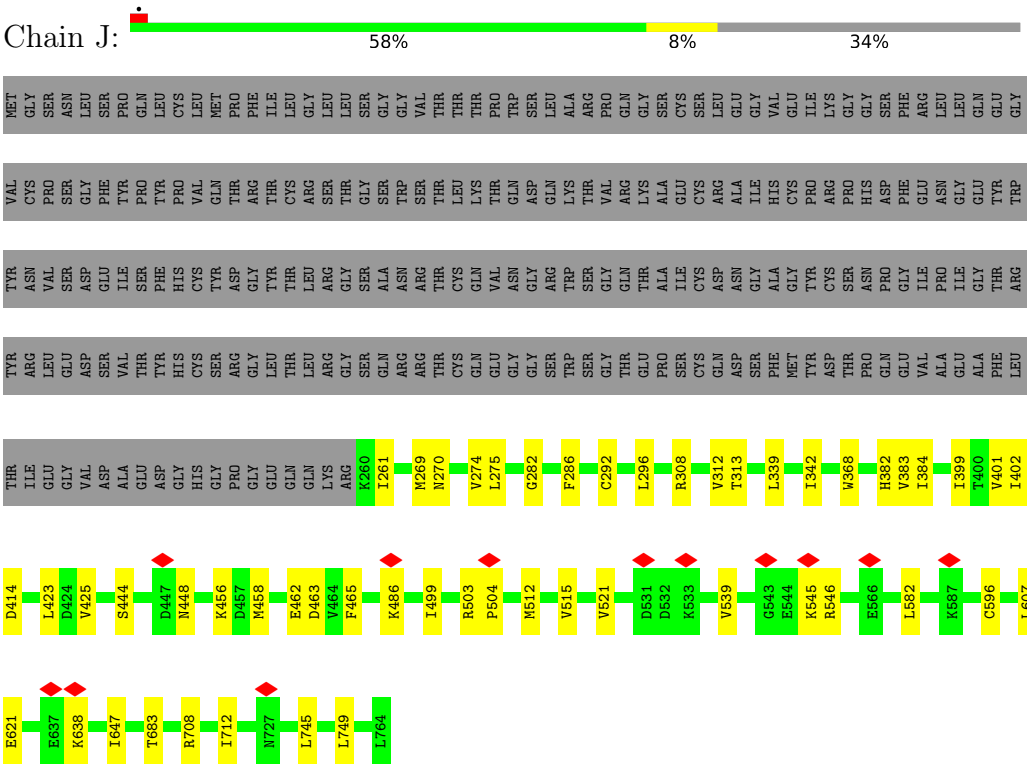


• Molecule 5: Cobra venom factor beta chain



• Molecule 6: Complement factor B

Chain J:


58%
8%
34%
MET GLY SER ASN LEU SER PRO GLN LEU CYS LEU MET PRO PHE ILE LEU GLY LEU LEU SER GLY GLY VAL THR THR THR PRO TRP SER LEU ALA ARG PRO GLN GLY SER CYS SER LEU GLU GLY VAL GLU ILE LYS GLY GLY SER PHE ARG LEU LEU GLN GLU GLY GLN ALA LEU GLU TYR
VAL CYS PRO SER GLY PHE TYR PRO TYR PRO VAL GLN THR ARG THR CYS ARG SER THR GLY SER TRP SER THR LEU LYS THR GLN ASP GLN LYS THR VAL ARG LYS ALA GLU CYS ARG ALA ILE HIS CYS PRO ARG PRO HIS ASP PHE GLU ASN GLY GLU TYR TRP PRO ARG SER PRO TYR
TYR ASN VAL SER ASP GLU ILE SER PHE HIS CYS TYR ASP GLY TYR THR LEU ARG GLY SER ALA ASN ARG ARG THR CYS GLN VAL ASN GLY GLY ARG TRP SER GLY GLN THR ALA ILE CYS ASP ASN GLY ALA GLY TYR CYS SER ASN PRO GLY ILE PRO ILE GLY THR ARG LYS VAL GLY SER GLN
TYR ARG LEU GLU ASP SER VAL THR TYR HIS CYS SER ARG GLY LEU THR LEU ARG GLY SER GLN ARG ARG THR CYS GLN GLU GLY GLY SER TRP SER GLY THR GLU PRO SER CYS GLN ASP SER PHE MET TYR ASP THR PRO GLN GLU VAL ALA GLU ALA PHE LEU SER SER LEU THR GLU
THR ILE GLU GLY VAL ASP ALA GLU ASP GLY HIS GLY PRO GLY GLU GLN GLN LYS ARG K260 I261 M269 N270 V274 L275 G282 F286 C292 L296 R308 V312 T313 L339 I342 W368 H382 V383 I384 I399 T400 V401 I402 D403 E404 I405 R406
D414 L423 D424 V425 S444 D447 N448 K456 D457 M458 E462 D463 V464 F465 K486 I499 R503 P504 M512 V515 V521 D531 D532 K533 V539 G543 E544 K545 R546 E566 L582 K587 C596 L607 R608 L609 T613 Q618
E621 E637 K638 I647 T683 R708 I712 N727 L745 L749 L764

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	23989	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 ($e^-/Å^2$)	59.9	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.784	Depositor
Minimum map value	-0.384	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	387.0, 387.0, 387.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.29, 1.29, 1.29	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.32	0/5316	0.77	6/7230 (0.1%)
2	C	0.31	0/1395	0.80	2/1891 (0.1%)
3	B	0.31	0/5004	0.75	4/6809 (0.1%)
4	D	0.37	0/1903	0.82	2/2582 (0.1%)
5	E	0.34	0/3061	0.86	9/4140 (0.2%)
6	J	0.32	0/4095	0.80	5/5542 (0.1%)
All	All	0.32	0/20774	0.79	28/28194 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	C	0	1
4	D	0	1
All	All	0	3

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	284	GLN	CA-C-N	8.02	136.86	121.54
1	A	284	GLN	C-N-CA	8.02	136.86	121.54
2	C	774	LEU	CA-CB-CG	6.96	140.66	116.30
5	E	1335	GLU	CA-CB-CG	6.16	126.42	114.10
6	J	296	LEU	CA-CB-CG	6.01	137.33	116.30
5	E	1514	LYS	CA-CB-CG	5.87	125.84	114.10
1	A	532	GLN	CA-CB-CG	5.82	125.75	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	949	LYS	CA-CB-CG	5.75	125.60	114.10
6	J	269	MET	CB-CG-SD	5.72	129.85	112.70
5	E	1517	GLU	CA-CB-CG	5.66	125.43	114.10
2	C	827	MET	CB-CG-SD	5.66	129.66	112.70
3	B	81	MET	CA-CB-CG	5.65	125.39	114.10
6	J	638	LYS	CA-CB-CG	5.50	125.10	114.10
6	J	448	ASN	CA-CB-CG	5.44	118.04	112.60
5	E	1437	CYS	CA-CB-SG	5.36	126.73	114.40
5	E	1608	GLU	CA-CB-CG	5.29	124.69	114.10
5	E	1323	MET	CB-CG-SD	5.27	128.50	112.70
3	B	308	GLU	CB-CG-CD	5.25	121.53	112.60
3	B	528	ASN	CA-CB-CG	5.22	117.82	112.60
5	E	1573	LEU	CA-C-N	5.22	129.83	122.46
5	E	1573	LEU	C-N-CA	5.22	129.83	122.46
3	B	453	GLU	CA-CB-CG	5.18	124.46	114.10
1	A	380	ASP	N-CA-CB	-5.13	108.32	114.17
4	D	922	LYS	CA-CB-CG	5.07	124.25	114.10
1	A	532	GLN	CB-CG-CD	5.06	121.20	112.60
5	E	1342	LYS	CA-CB-CG	5.06	124.21	114.10
1	A	90	LYS	CB-CG-CD	5.05	122.93	111.30
6	J	368	TRP	CA-CB-CG	5.02	123.14	113.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	518	PHE	Peptide
2	C	778	HIS	Peptide
4	D	904	LEU	Peptide

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	5195	0	5114	21	0
2	C	1364	0	1380	5	0
3	B	4893	0	4896	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1865	0	1907	15	0
5	E	3007	0	2959	20	0
6	J	4007	0	3999	30	0
7	J	1	0	0	0	0
8	J	2	0	0	0	0
All	All	20334	0	20255	112	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 3.

All (112) 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)
6:J:545:LYS:HG3	6:J:546:ARG:HG2	1.74	0.68
4:D:786:THR:HA	4:D:808:ILE:O	1.97	0.64
3:B:127:PHE:HB2	3:B:150:MET:HB3	1.83	0.60
6:J:282:GLY:O	6:J:286:PHE:HB2	2.01	0.60
4:D:840:VAL:HG13	4:D:842:GLU:H	1.66	0.59
2:C:835:ARG:HA	2:C:902:PRO:HG2	1.84	0.59
6:J:274:VAL:HA	6:J:312:VAL:O	2.02	0.59
5:E:1382:ILE:HB	5:E:1425:ILE:HB	1.85	0.58
3:B:567:LEU:HD11	3:B:577:LEU:HD11	1.85	0.57
6:J:499:ILE:HG12	6:J:539:VAL:HG12	1.87	0.56
3:B:140:GLY:HA2	3:B:188:LEU:O	2.06	0.55
3:B:327:ASP:HB2	4:D:819:GLN:HG2	1.87	0.55
6:J:618:GLN:HA	6:J:621:GLU:HG2	1.89	0.54
6:J:647:ILE:HG22	6:J:683:THR:HG22	1.89	0.54
6:J:463:ASP:HB2	6:J:486:LYS:HZ3	1.72	0.53
6:J:292:CYS:HB2	6:J:458:MET:HE1	1.90	0.53
4:D:795:THR:HG22	4:D:797:THR:H	1.74	0.52
1:A:176:GLU:HB2	1:A:183:ILE:HD11	1.91	0.52
3:B:472:SER:HB2	3:B:526:VAL:HG11	1.90	0.52
1:A:619:PRO:HA	1:A:622:ARG:HH12	1.74	0.51
6:J:261:ILE:HG22	6:J:383:VAL:HG21	1.91	0.51
5:E:1528:LEU:HD12	5:E:1577:VAL:HA	1.93	0.51
1:A:573:VAL:HG12	1:A:592:MET:HG2	1.92	0.50
2:C:884:VAL:HG13	2:C:886:GLN:HG2	1.93	0.50
3:B:269:ILE:HG13	3:B:270:ASP:H	1.77	0.50
5:E:1397:LEU:HD11	5:E:1408:ILE:HG21	1.93	0.50
6:J:399:ILE:HD13	6:J:402:ILE:HD11	1.93	0.49
5:E:1368:CYS:HA	5:E:1437:CYS:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:1349:VAL:HA	5:E:1364:MET:O	2.13	0.48
6:J:521:VAL:HG23	6:J:582:LEU:HD11	1.96	0.48
3:B:575:VAL:HA	4:D:792:VAL:O	2.14	0.48
6:J:596:CYS:HB2	6:J:712:ILE:HG23	1.94	0.48
1:A:267:ILE:HG12	1:A:327:VAL:HG22	1.94	0.48
6:J:275:LEU:HB3	6:J:313:THR:HG22	1.96	0.48
1:A:373:VAL:HG11	1:A:435:VAL:HG11	1.96	0.48
4:D:891:LEU:HB3	4:D:912:LYS:HD2	1.96	0.48
5:E:1383:ASP:O	5:E:1456:VAL:HA	2.14	0.48
6:J:607:LEU:HA	6:J:708:ARG:HG3	1.96	0.47
4:D:889:GLN:HA	4:D:915:VAL:HG12	1.96	0.47
2:C:906:GLY:H	2:C:929:VAL:HB	1.79	0.47
3:B:409:LEU:HB3	3:B:432:ALA:HB3	1.97	0.47
5:E:1374:GLU:HG2	5:E:1375:VAL:HG13	1.96	0.47
5:E:1457:LYS:HG2	5:E:1469:THR:HG22	1.96	0.47
4:D:786:THR:HG22	4:D:809:ARG:HA	1.97	0.46
3:B:411:ILE:O	3:B:429:SER:HA	2.15	0.46
4:D:811:MET:HE2	4:D:811:MET:HB2	1.80	0.46
5:E:1344:HIS:O	5:E:1369:THR:HA	2.15	0.46
6:J:402:ILE:HA	6:J:405:ILE:HD12	1.98	0.46
3:B:558:MET:HB2	3:B:561:ALA:HB2	1.97	0.46
1:A:468:ASP:HB3	1:A:485:ILE:HB	1.98	0.46
3:B:345:ILE:HG22	3:B:366:VAL:HG22	1.98	0.46
3:B:563:MET:O	4:D:777:SER:HA	2.16	0.46
1:A:489:LYS:HE2	1:A:489:LYS:HB2	1.73	0.45
3:B:252:LEU:HD12	3:B:582:LYS:HB3	1.98	0.45
3:B:476:ILE:HG13	3:B:497:ARG:HD3	1.98	0.45
3:B:52:LYS:O	3:B:75:MET:HB3	2.16	0.45
6:J:274:VAL:HG22	6:J:312:VAL:HB	1.97	0.45
3:B:592:LYS:HE2	3:B:592:LYS:HB3	1.82	0.45
3:B:130:ILE:HD11	3:B:201:ALA:HB2	1.97	0.45
6:J:401:VAL:O	6:J:404:GLU:HB3	2.17	0.45
4:D:919:GLY:HA3	5:E:1331:ALA:O	2.17	0.45
5:E:1563:TYR:HB3	5:E:1601:ILE:HD11	1.99	0.45
1:A:128:ILE:HG22	1:A:145:VAL:HG13	1.99	0.44
1:A:363:LEU:HG	1:A:456:ALA:HA	1.99	0.44
5:E:1502:HIS:HE1	5:E:1624:LEU:HD21	1.83	0.44
4:D:820:MET:HB3	4:D:820:MET:HE2	1.81	0.44
1:A:352:TYR:HA	1:A:376:LYS:O	2.18	0.44
4:D:788:VAL:HG22	4:D:807:GLU:HG2	1.99	0.44
5:E:1384:ILE:HG12	5:E:1456:VAL:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:604:ALA:HB2	2:C:774:LEU:HD23	2.00	0.44
6:J:339:LEU:HA	6:J:342:ILE:HD12	1.99	0.44
6:J:425:VAL:HB	6:J:444:SER:HB2	2.00	0.44
3:B:37:THR:HG23	3:B:154:THR:HG22	2.00	0.43
4:D:790:LEU:HD23	4:D:805:PRO:HB3	2.01	0.43
6:J:515:VAL:HG22	6:J:521:VAL:HG22	2.00	0.43
1:A:267:ILE:HB	1:A:288:GLN:HG3	2.00	0.43
1:A:554:LEU:HD11	1:A:655:THR:HG21	1.99	0.43
4:D:930:LEU:HB2	5:E:1321:ALA:HB3	2.00	0.43
1:A:495:LYS:HZ2	1:A:546:VAL:HB	1.83	0.43
1:A:137:PRO:HB3	1:A:194:PRO:HG3	2.01	0.43
5:E:1285:GLU:HG2	5:E:1286:VAL:HG23	2.00	0.43
6:J:382:HIS:HB2	6:J:423:LEU:HG	2.00	0.43
3:B:350:THR:HG21	3:B:430:MET:HE1	2.01	0.42
6:J:270:ASN:HA	6:J:308:ARG:O	2.19	0.42
6:J:503:ARG:HD3	6:J:504:PRO:HD2	2.00	0.42
1:A:231:ILE:HG22	1:A:250:ILE:HG23	2.01	0.42
1:A:467:ILE:HG22	1:A:486:VAL:HG22	2.01	0.42
1:A:497:THR:HG23	1:A:498:HIS:CD2	2.55	0.42
3:B:33:LEU:HD12	3:B:39:GLU:HG2	2.01	0.42
6:J:403:ASP:O	6:J:406:ARG:HB2	2.20	0.42
2:C:907:LEU:HG	2:C:910:ILE:HD11	2.02	0.41
3:B:365:TYR:HE1	3:B:373:PRO:HB3	1.85	0.41
5:E:1273:LEU:HA	5:E:1319:GLY:HA3	2.02	0.41
1:A:166:PRO:HB3	1:A:198:MET:H	1.84	0.41
1:A:655:THR:HB	1:A:657:ALA:H	1.85	0.41
3:B:104:VAL:HB	3:B:121:LEU:HD21	2.03	0.41
6:J:462:GLU:HA	6:J:465:PHE:CD1	2.55	0.41
6:J:609:LEU:HD13	6:J:613:THR:HG21	2.02	0.41
6:J:745:LEU:O	6:J:749:LEU:HB2	2.20	0.41
6:J:402:ILE:O	6:J:405:ILE:HB	2.20	0.41
3:B:411:ILE:HD12	3:B:430:MET:HG2	2.02	0.41
6:J:456:LYS:HD2	6:J:456:LYS:HA	1.91	0.41
5:E:1336:LYS:HD3	5:E:1336:LYS:H	1.86	0.41
1:A:303:SER:O	1:A:307:VAL:HB	2.21	0.41
3:B:531:ILE:HD13	3:B:531:ILE:HA	1.91	0.41
5:E:1417:MET:HE1	5:E:1445:HIS:CG	2.56	0.41
5:E:1394:ALA:H	5:E:1417:MET:HA	1.86	0.41
5:E:1524:TYR:HD2	5:E:1583:ILE:HD11	1.86	0.41
3:B:46:HIS:CG	3:B:525:GLN:HG2	2.55	0.40
3:B:226:VAL:HG21	3:B:320:VAL:HG11	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:474:LYS:HA	3:B:474:LYS:HD3	1.93	0.40
6:J:282:GLY:O	6:J:286:PHE:CB	2.66	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	655/659 (99%)	621 (95%)	32 (5%)	2 (0%)	36 69
2	C	170/999 (17%)	162 (95%)	8 (5%)	0	100 100
3	B	624/627 (100%)	597 (96%)	27 (4%)	0	100 100
4	D	232/252 (92%)	223 (96%)	8 (3%)	1 (0%)	30 64
5	E	371/379 (98%)	356 (96%)	15 (4%)	0	100 100
6	J	503/764 (66%)	484 (96%)	19 (4%)	0	100 100
All	All	2555/3680 (69%)	2443 (96%)	109 (4%)	3 (0%)	49 80

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	311	SER
4	D	737	ASP
1	A	285	THR

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	582/584 (100%)	580 (100%)	2 (0%)	86	85
2	C	156/886 (18%)	155 (99%)	1 (1%)	78	80
3	B	547/548 (100%)	543 (99%)	4 (1%)	76	78
4	D	211/227 (93%)	208 (99%)	3 (1%)	59	71
5	E	339/345 (98%)	336 (99%)	3 (1%)	70	75
6	J	444/663 (67%)	441 (99%)	3 (1%)	76	78
All	All	2279/3253 (70%)	2263 (99%)	16 (1%)	73	78

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	276	LYS
1	A	587	THR
2	C	921	GLU
3	B	252	LEU
3	B	314	LEU
3	B	328	MET
3	B	564	LYS
4	D	785	THR
4	D	802	VAL
4	D	927	ILE
5	E	1369	THR
5	E	1539	ILE
5	E	1633	TYR
6	J	384	ILE
6	J	414	ASP
6	J	512	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	462	GLN
1	A	498	HIS
1	A	500	ASN
1	A	570	GLN
1	A	613	GLN
1	A	647	HIS
3	B	59	HIS

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Mol	Chain	Res	Type
3	B	102	GLN
3	B	153	ASN
3	B	176	ASN
3	B	385	HIS
3	B	471	ASN
3	B	557	GLN
3	B	615	GLN
3	B	646	GLN
5	E	1274	ASN
5	E	1330	ASN
5	E	1502	HIS
6	J	285	ASN
6	J	417	ASN
6	J	435	ASN
6	J	438	ASN
6	J	617	GLN
6	J	661	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

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

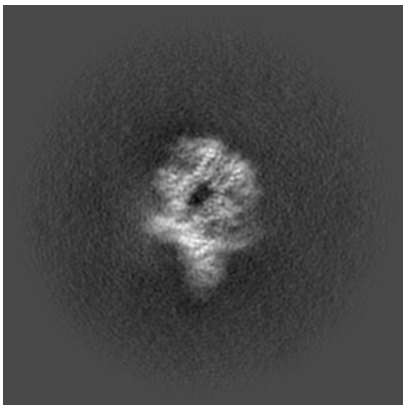
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-55817. These allow visual inspection of the internal detail of the map and identification of artifacts.

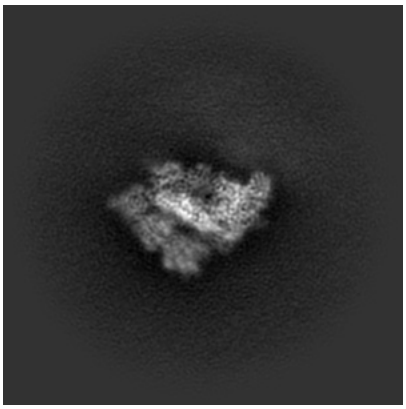
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

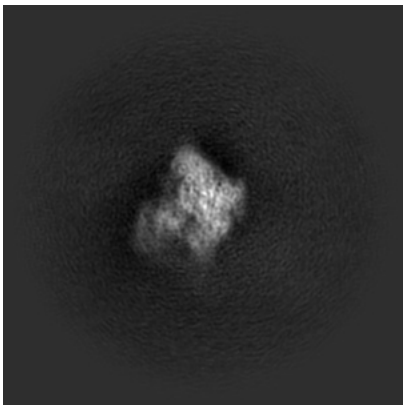
6.1.1 Primary map



X

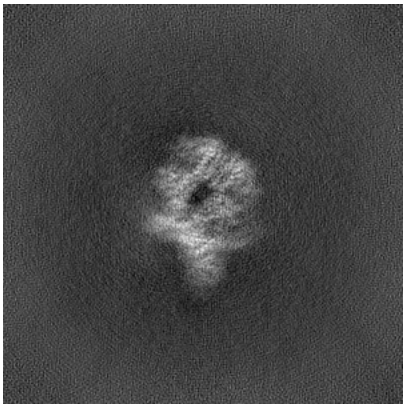


Y

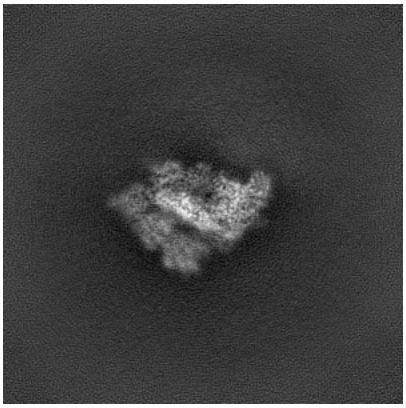


Z

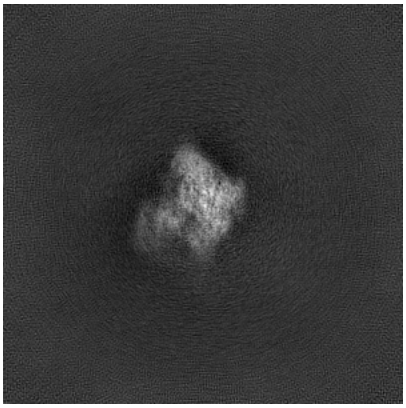
6.1.2 Raw map



X



Y

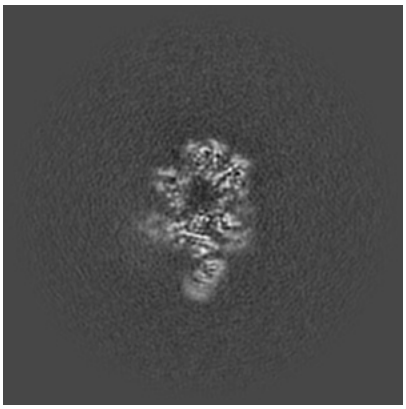


Z

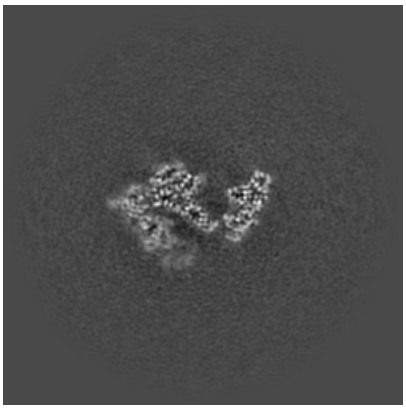
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

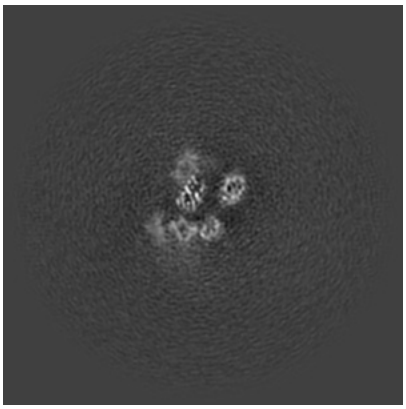
6.2.1 Primary map



X Index: 150

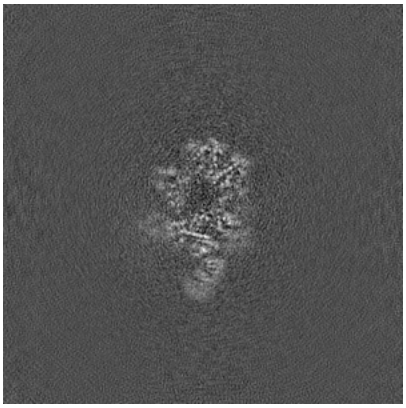


Y Index: 150

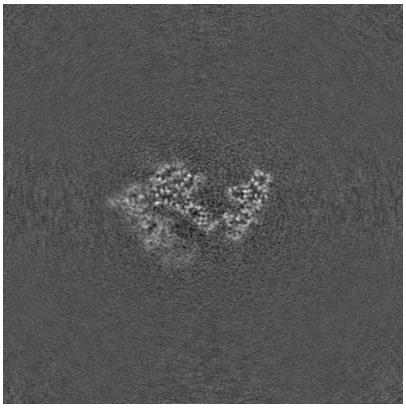


Z Index: 150

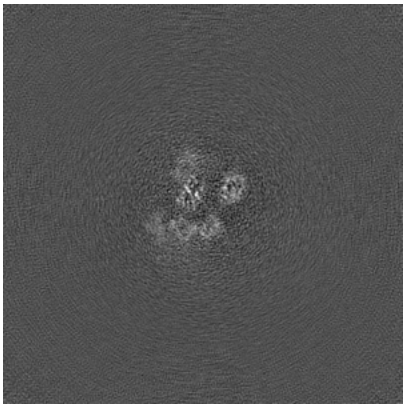
6.2.2 Raw map



X Index: 150



Y Index: 150



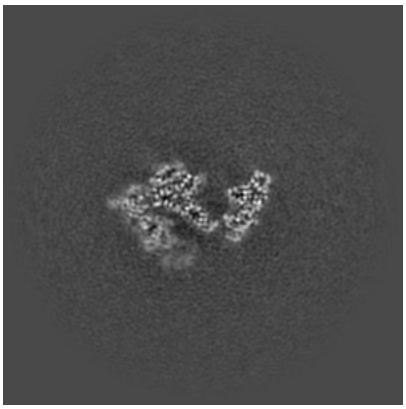
Z Index: 150

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

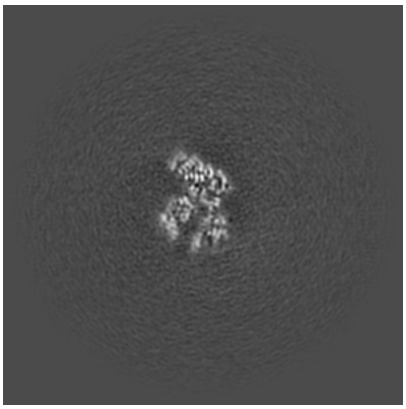
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 151

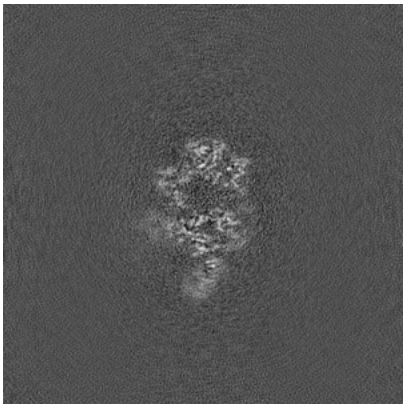


Y Index: 150

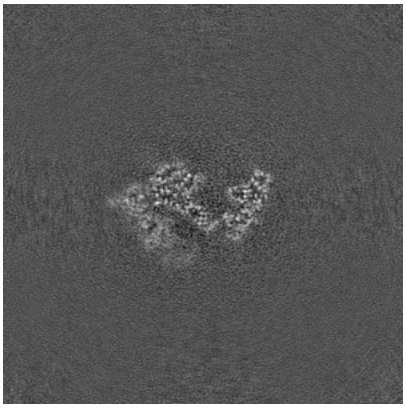


Z Index: 170

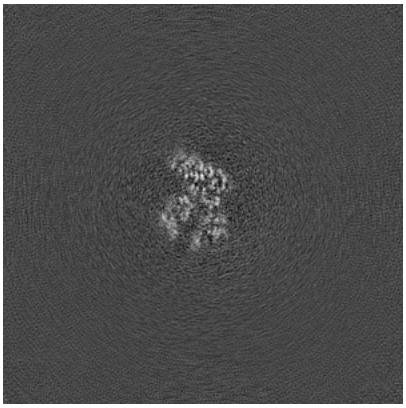
6.3.2 Raw map



X Index: 151



Y Index: 150

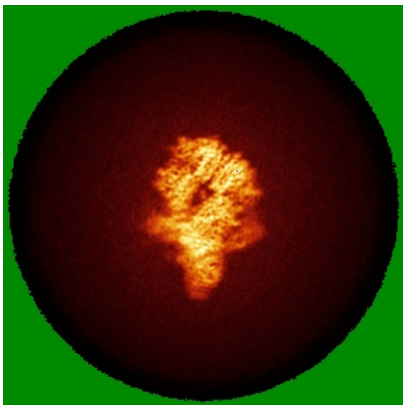


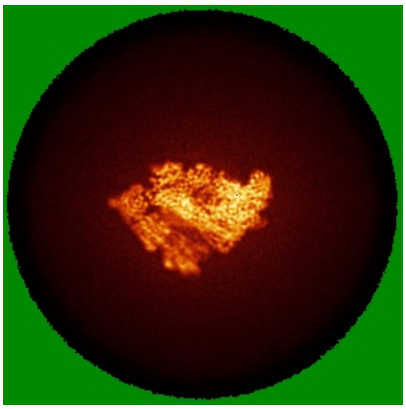
Z Index: 170

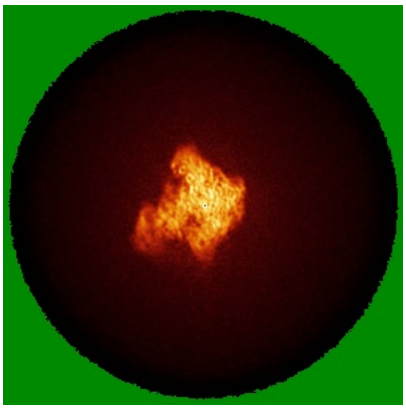
The images above show the largest variance slices of the map in three orthogonal directions.

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

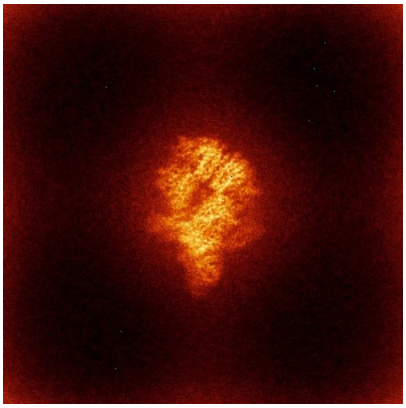
6.4.1 Primary map

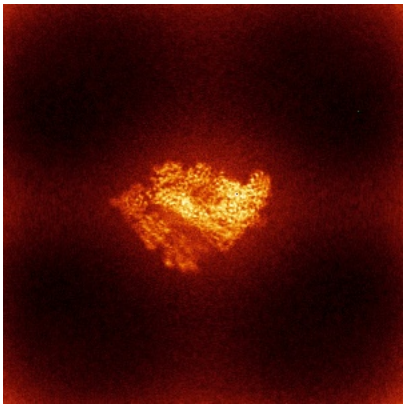

X

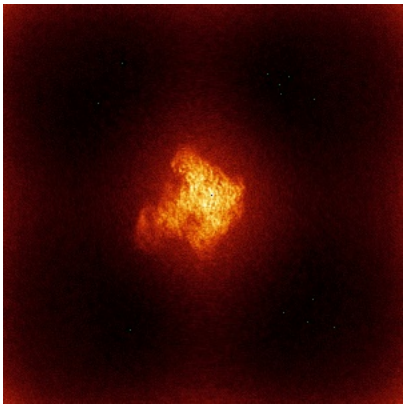

Y


Z

6.4.2 Raw map


X


Y


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

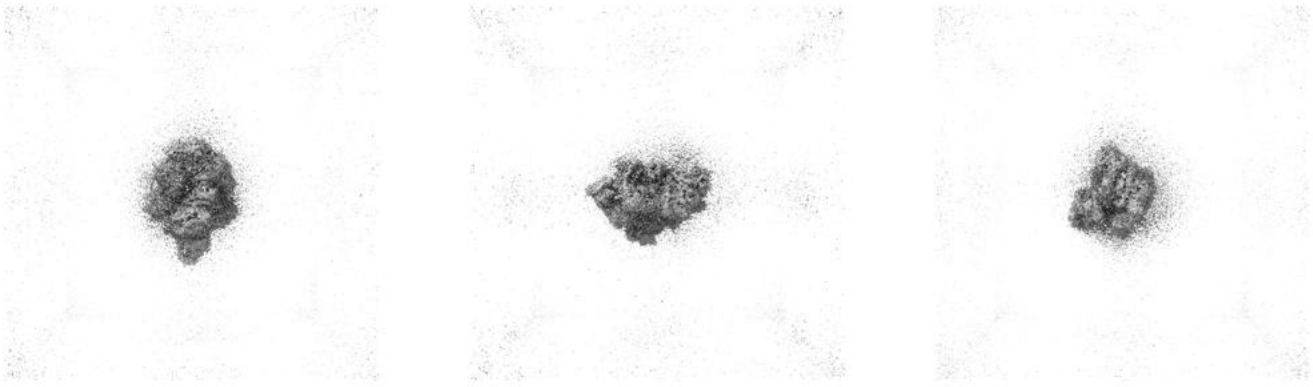
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

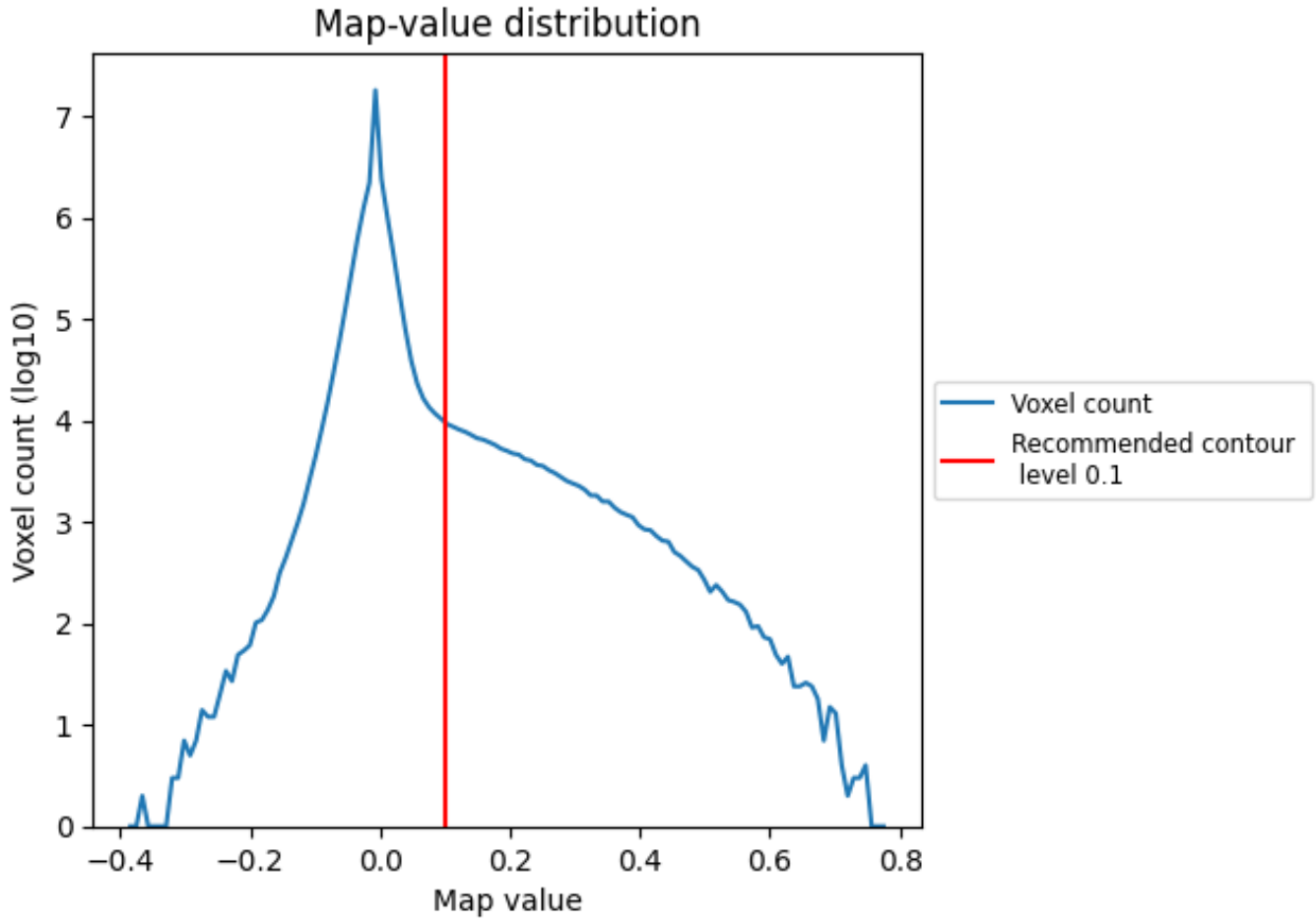
6.6 Mask visualisation (i)

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

7 Map analysis

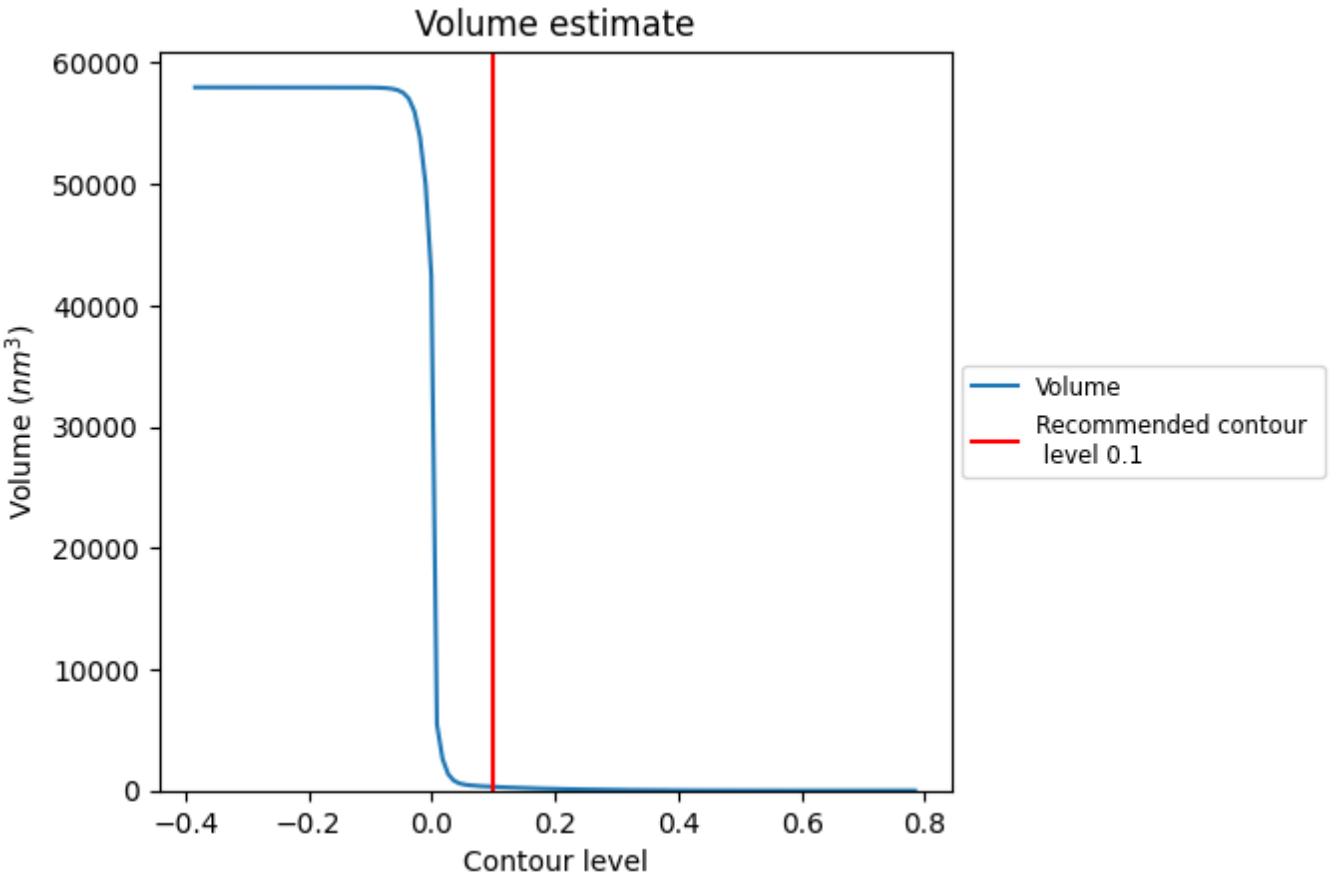
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

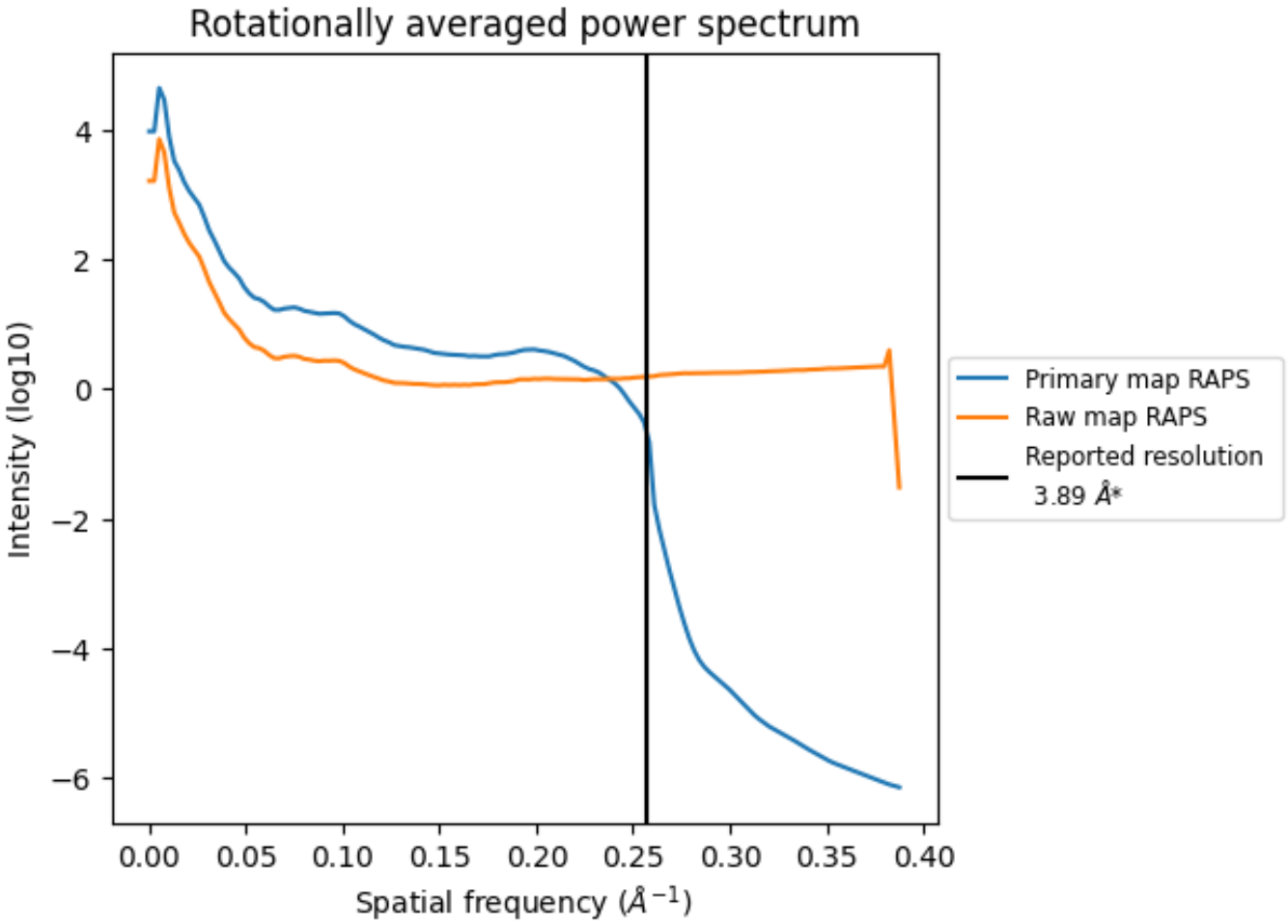
7.2 Volume estimate



The volume at the recommended contour level is 308 nm^3; this corresponds to an approximate mass of 279 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 (i)

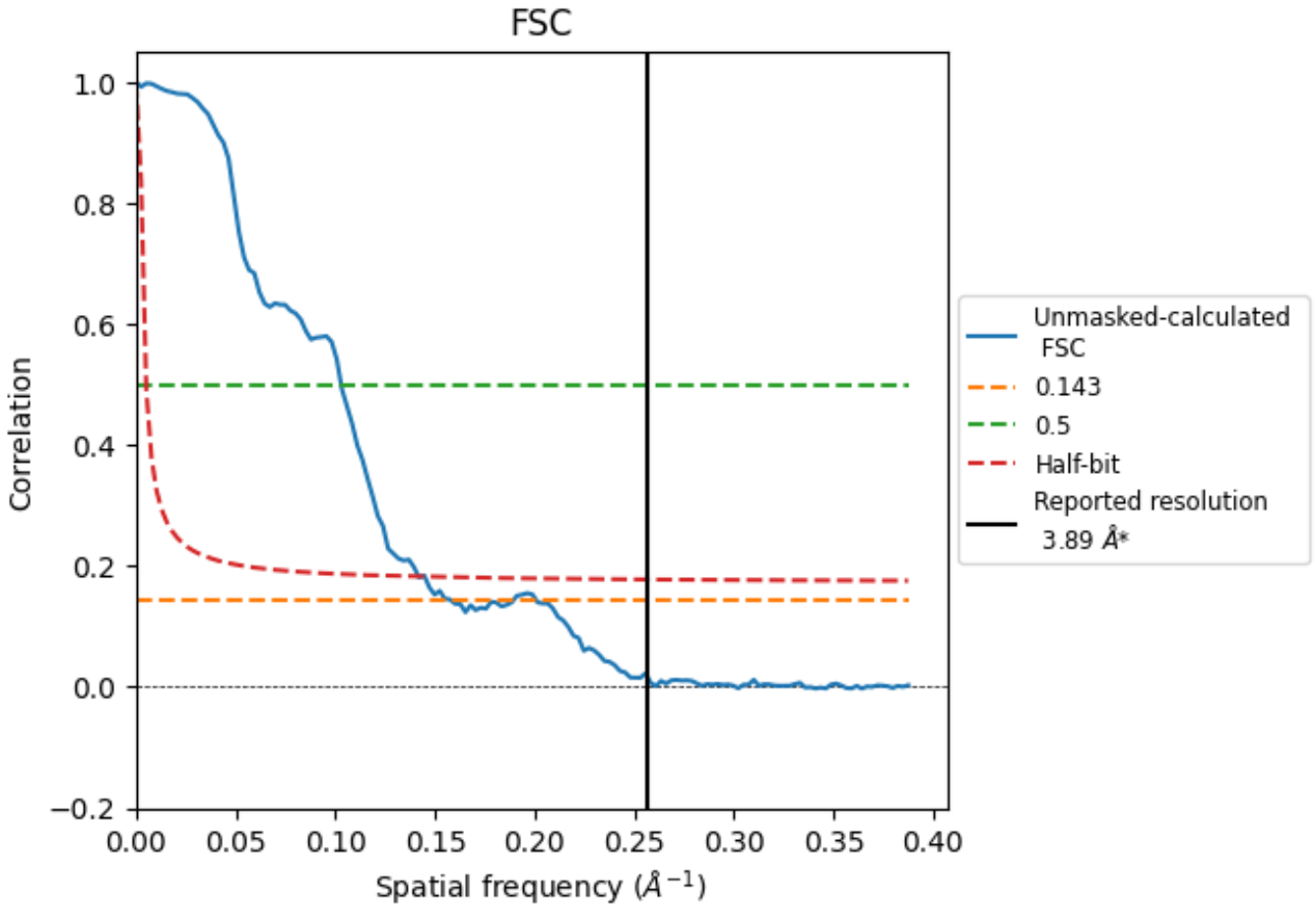


*Reported resolution corresponds to spatial frequency of 0.257 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.257 Å^{-1}

8.2 Resolution estimates (i)

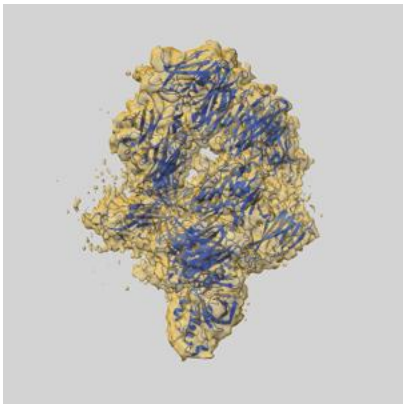
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.89	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.32	9.72	7.05

*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 6.32 differs from the reported value 3.89 by more than 10 %

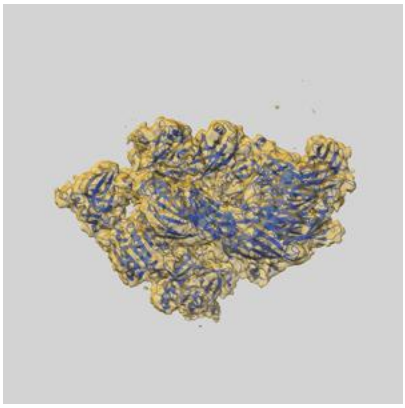
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-55817 and PDB model 9TE2. Per-residue inclusion information can be found in section 3 on page 6.

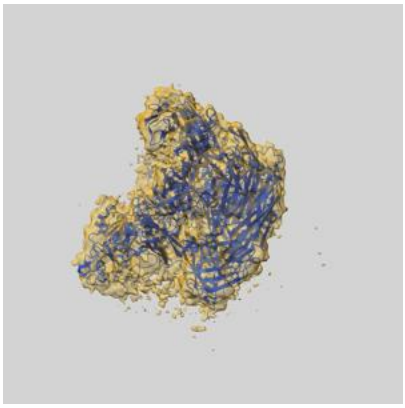
9.1 Map-model overlay



X



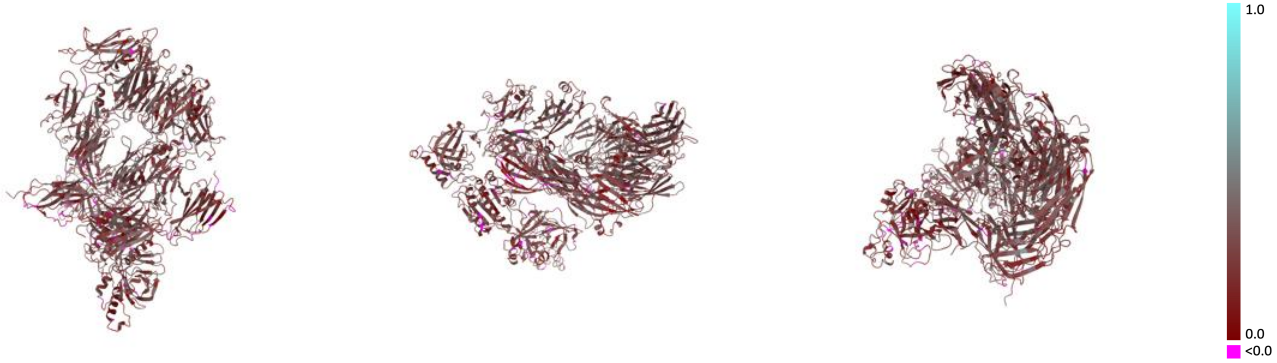
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 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.

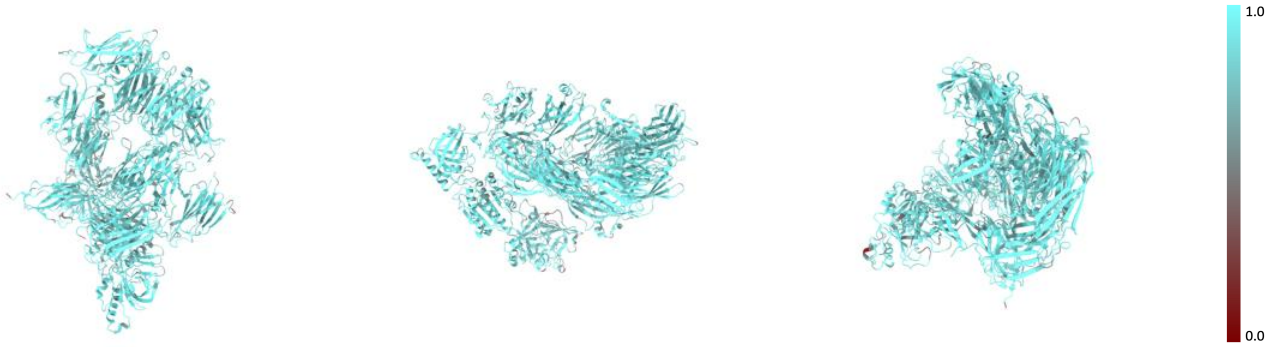
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

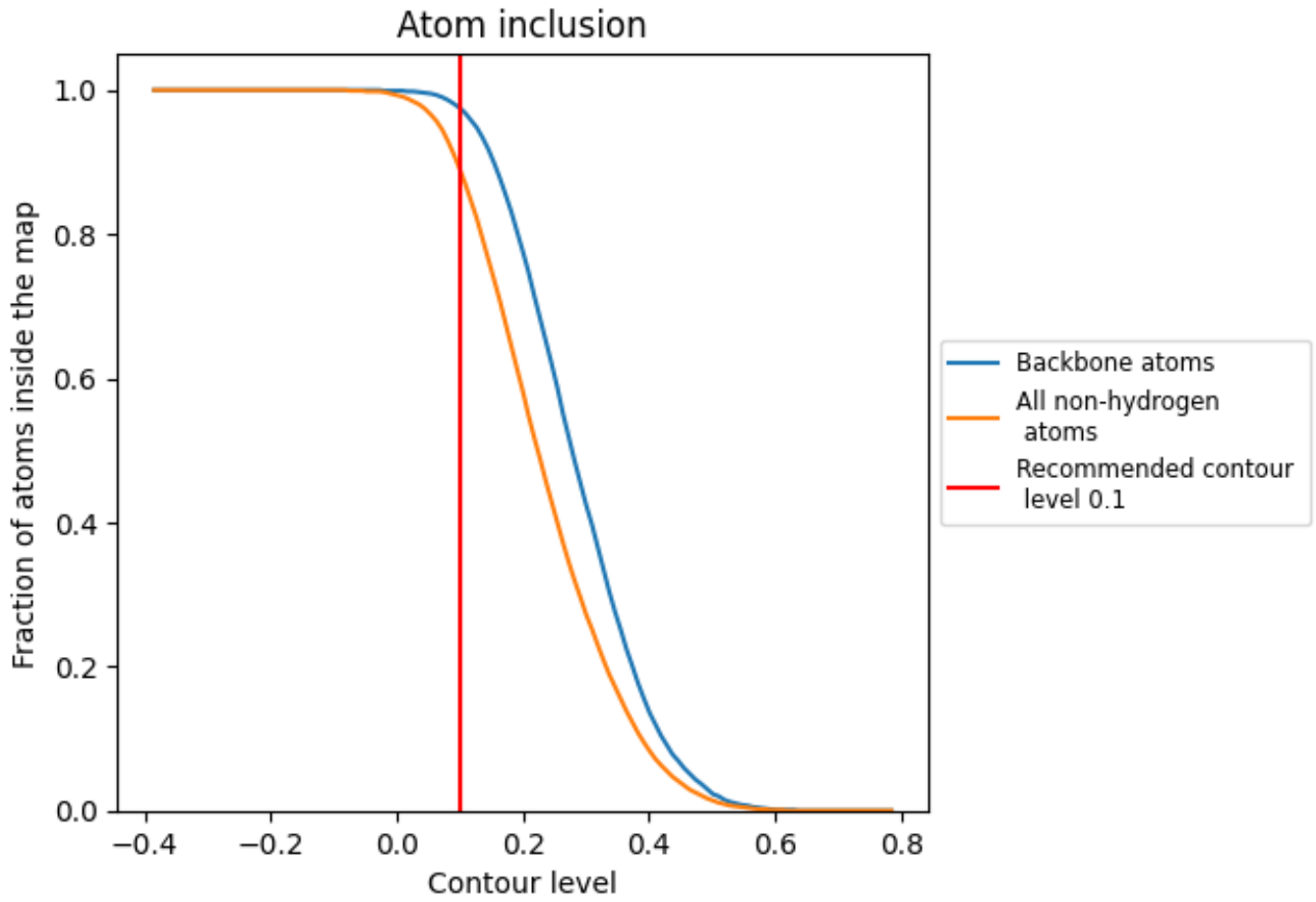
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 89% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8900	0.2610
A	0.8930	0.2760
B	0.9080	0.2870
C	0.8780	0.2630
D	0.8810	0.2780
E	0.8970	0.2480
J	0.8670	0.2090