Full wwPDB EM Validation Report ⓘ

May 14, 2025 – 12:14 PM JST

PDB ID	:	8XJZ / pdb_00008xjz
EMDB ID	:	EMD-38411
Title	:	Cryo-EM structure of colibactin assembly line polyketide synthase ClbI KS-AT didomain crosslinked with its precursor module, ClbH
Authors	:	Kim, M.; Kim, J.; Kang, J.Y.
Deposited on	:	2023-12-22
Resolution	:	3.67 Å(reported)
Based on initial model	:	.

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:

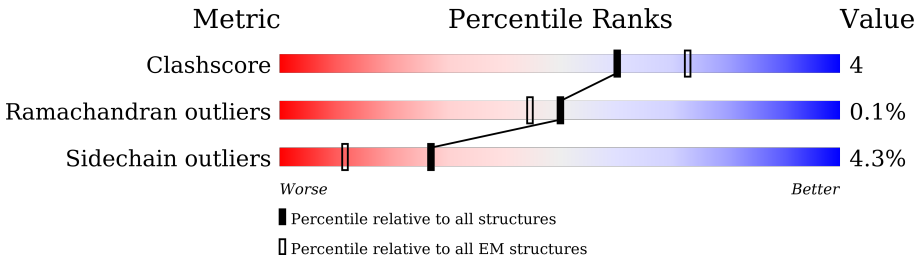
EMDB validation analysis	:	0.0.1.dev118
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 3.67 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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	921	10% 80% 12% • 7%
1	B	921	15% 83% 11% • 6%
2	C	1634	• • 97%
3	D	26	8% 100%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 13651 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 Polyketide synthase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	859	Total	C	N	O	S	0	0
			6508	4116	1130	1236	26		
1	B	867	Total	C	N	O	S	0	0
			6576	4159	1145	1246	26		

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	896	LYS	-	expression tag	UNP Q0P7J9
A	897	LEU	-	expression tag	UNP Q0P7J9
A	898	SER	-	expression tag	UNP Q0P7J9
A	899	SER	-	expression tag	UNP Q0P7J9
A	900	GLY	-	expression tag	UNP Q0P7J9
A	901	LEU	-	expression tag	UNP Q0P7J9
A	902	GLU	-	expression tag	UNP Q0P7J9
A	903	VAL	-	expression tag	UNP Q0P7J9
A	904	LEU	-	expression tag	UNP Q0P7J9
A	905	PHE	-	expression tag	UNP Q0P7J9
A	906	GLN	-	expression tag	UNP Q0P7J9
A	907	GLY	-	expression tag	UNP Q0P7J9
A	908	PRO	-	expression tag	UNP Q0P7J9
A	909	SER	-	expression tag	UNP Q0P7J9
A	910	SER	-	expression tag	UNP Q0P7J9
A	911	GLY	-	expression tag	UNP Q0P7J9
A	912	HIS	-	expression tag	UNP Q0P7J9
A	913	HIS	-	expression tag	UNP Q0P7J9
A	914	HIS	-	expression tag	UNP Q0P7J9
A	915	HIS	-	expression tag	UNP Q0P7J9
A	916	HIS	-	expression tag	UNP Q0P7J9
A	917	HIS	-	expression tag	UNP Q0P7J9
A	918	HIS	-	expression tag	UNP Q0P7J9
A	919	HIS	-	expression tag	UNP Q0P7J9
A	920	HIS	-	expression tag	UNP Q0P7J9
A	921	HIS	-	expression tag	UNP Q0P7J9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	896	LYS	-	expression tag	UNP Q0P7J9
B	897	LEU	-	expression tag	UNP Q0P7J9
B	898	SER	-	expression tag	UNP Q0P7J9
B	899	SER	-	expression tag	UNP Q0P7J9
B	900	GLY	-	expression tag	UNP Q0P7J9
B	901	LEU	-	expression tag	UNP Q0P7J9
B	902	GLU	-	expression tag	UNP Q0P7J9
B	903	VAL	-	expression tag	UNP Q0P7J9
B	904	LEU	-	expression tag	UNP Q0P7J9
B	905	PHE	-	expression tag	UNP Q0P7J9
B	906	GLN	-	expression tag	UNP Q0P7J9
B	907	GLY	-	expression tag	UNP Q0P7J9
B	908	PRO	-	expression tag	UNP Q0P7J9
B	909	SER	-	expression tag	UNP Q0P7J9
B	910	SER	-	expression tag	UNP Q0P7J9
B	911	GLY	-	expression tag	UNP Q0P7J9
B	912	HIS	-	expression tag	UNP Q0P7J9
B	913	HIS	-	expression tag	UNP Q0P7J9
B	914	HIS	-	expression tag	UNP Q0P7J9
B	915	HIS	-	expression tag	UNP Q0P7J9
B	916	HIS	-	expression tag	UNP Q0P7J9
B	917	HIS	-	expression tag	UNP Q0P7J9
B	918	HIS	-	expression tag	UNP Q0P7J9
B	919	HIS	-	expression tag	UNP Q0P7J9
B	920	HIS	-	expression tag	UNP Q0P7J9
B	921	HIS	-	expression tag	UNP Q0P7J9

- Molecule 2 is a protein called Peptide synthetase.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	54	Total	C	N	O	S	0	0
			437	282	78	75	2		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-35	MET	-	initiating methionine	UNP Q0P7J8
C	-34	GLY	-	expression tag	UNP Q0P7J8
C	-33	SER	-	expression tag	UNP Q0P7J8
C	-32	SER	-	expression tag	UNP Q0P7J8
C	-31	HIS	-	expression tag	UNP Q0P7J8
C	-30	HIS	-	expression tag	UNP Q0P7J8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-29	HIS	-	expression tag	UNP Q0P7J8
C	-28	HIS	-	expression tag	UNP Q0P7J8
C	-27	HIS	-	expression tag	UNP Q0P7J8
C	-26	HIS	-	expression tag	UNP Q0P7J8
C	-25	SER	-	expression tag	UNP Q0P7J8
C	-24	SER	-	expression tag	UNP Q0P7J8
C	-23	GLY	-	expression tag	UNP Q0P7J8
C	-22	LEU	-	expression tag	UNP Q0P7J8
C	-21	VAL	-	expression tag	UNP Q0P7J8
C	-20	PRO	-	expression tag	UNP Q0P7J8
C	-19	ARG	-	expression tag	UNP Q0P7J8
C	-18	GLY	-	expression tag	UNP Q0P7J8
C	-17	SER	-	expression tag	UNP Q0P7J8
C	-16	HIS	-	expression tag	UNP Q0P7J8
C	-15	MET	-	expression tag	UNP Q0P7J8
C	-14	ALA	-	expression tag	UNP Q0P7J8
C	-13	SER	-	expression tag	UNP Q0P7J8
C	-12	MET	-	expression tag	UNP Q0P7J8
C	-11	THR	-	expression tag	UNP Q0P7J8
C	-10	GLY	-	expression tag	UNP Q0P7J8
C	-9	GLY	-	expression tag	UNP Q0P7J8
C	-8	GLN	-	expression tag	UNP Q0P7J8
C	-7	GLN	-	expression tag	UNP Q0P7J8
C	-6	MET	-	expression tag	UNP Q0P7J8
C	-5	GLY	-	expression tag	UNP Q0P7J8
C	-4	ARG	-	expression tag	UNP Q0P7J8
C	-3	GLY	-	expression tag	UNP Q0P7J8
C	-2	SER	-	expression tag	UNP Q0P7J8
C	-1	GLU	-	expression tag	UNP Q0P7J8
C	0	PHE	-	expression tag	UNP Q0P7J8

- Molecule 3 is a protein called polypeptide from ClbH.

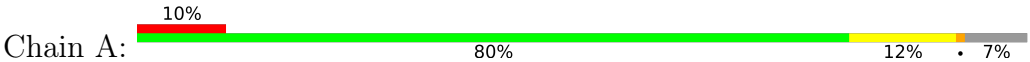
Mol	Chain	Residues	Atoms				AltConf	Trace
3	D	26	Total	C	N	O	0	0
			130	78	26	26		

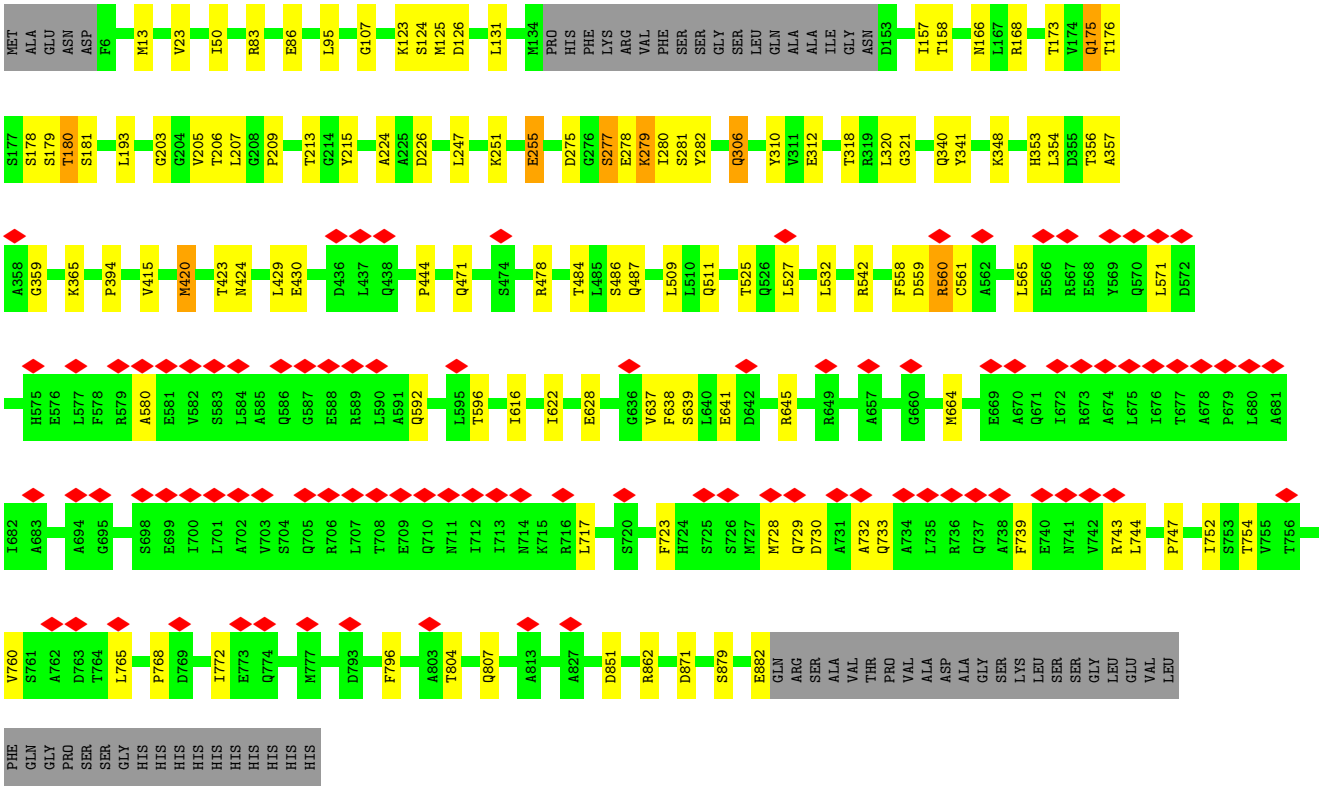
3 Residue-property plots (i)

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: Polyketide synthase

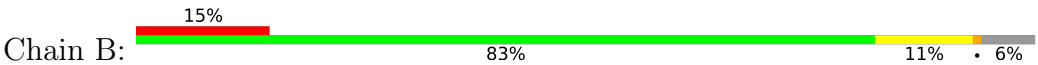
Chain A:

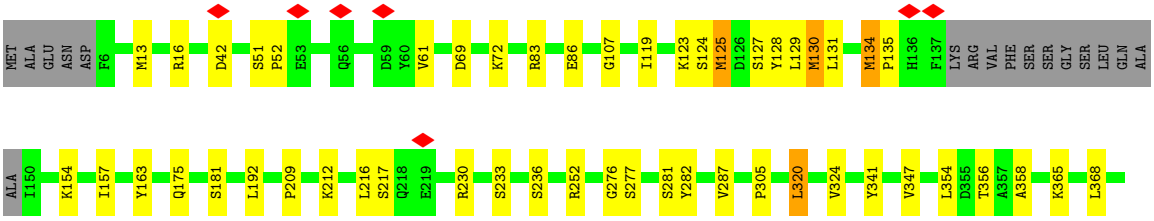


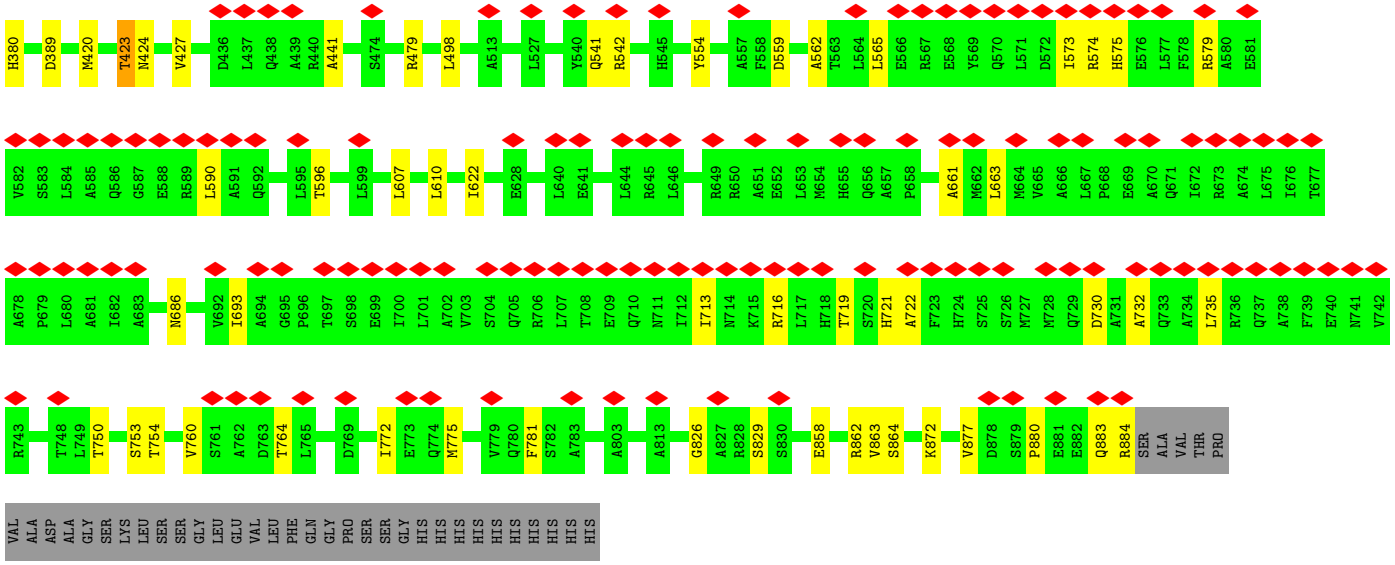


• Molecule 1: Polyketide synthase

Chain B:

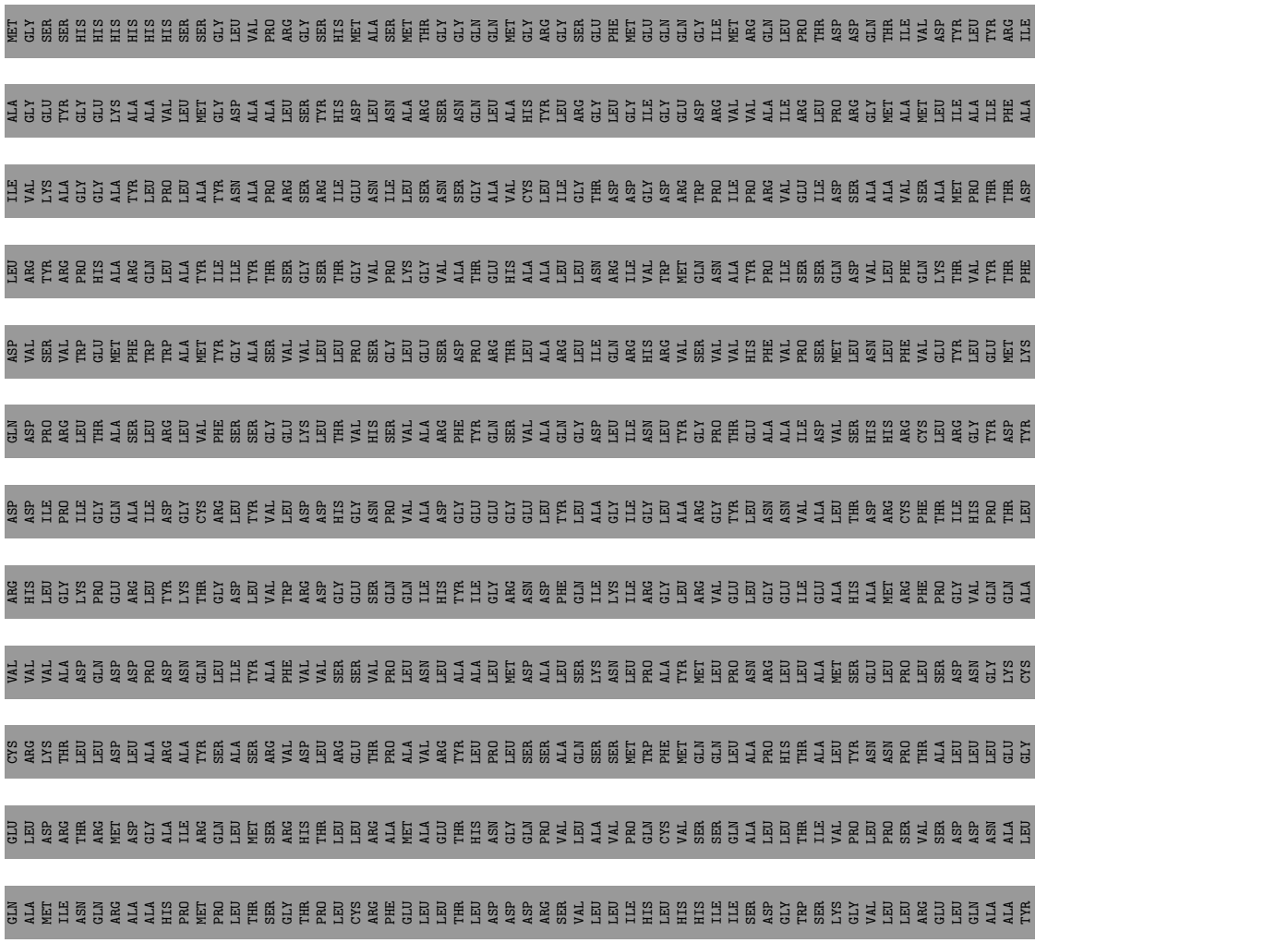


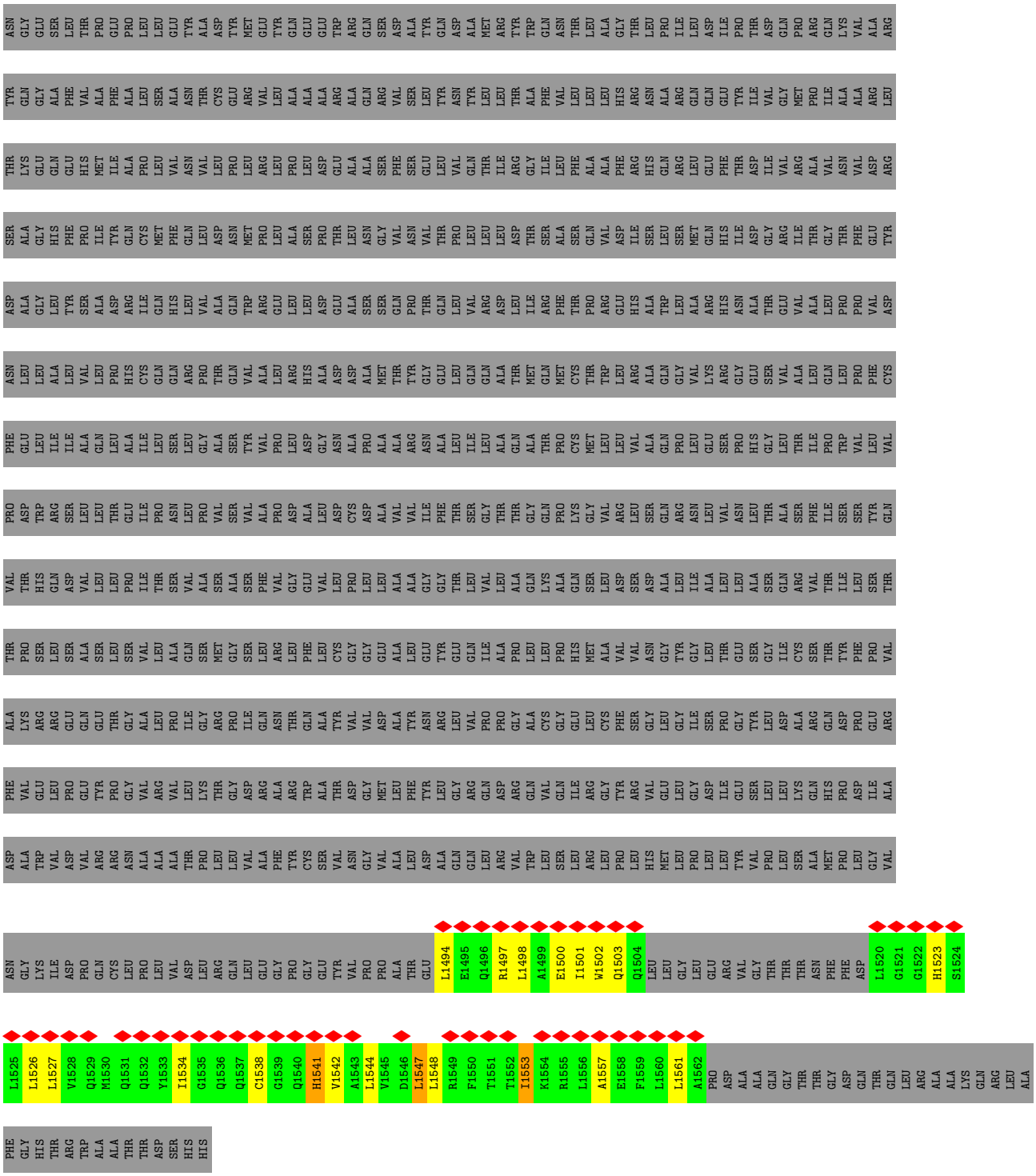




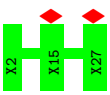
• Molecule 2: Peptide synthetase

Chain C: 97%





• Molecule 3: polypeptide from ClbH



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	246050	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.278	Depositor
Minimum map value	-0.163	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.026	Depositor
Map size (Å)	279.0912, 279.0912, 279.0912	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0902, 1.0902, 1.0902	Depositor

5 Model quality

5.1 Standard geometry

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	0.52	0/6651	0.72	5/9063 (0.1%)
1	B	0.51	0/6722	0.72	3/9159 (0.0%)
2	C	0.51	0/442	0.89	2/594 (0.3%)
All	All	0.51	0/13815	0.72	10/18816 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	209	PRO	N-CA-C	7.41	119.74	110.70
1	A	484	THR	N-CA-C	-6.61	106.16	114.56
1	A	558	PHE	N-CA-C	-5.94	104.93	111.82
1	A	486	SER	N-CA-C	-5.92	106.09	113.38
2	C	1553	ILE	N-CA-C	-5.45	107.54	112.12
1	B	423	THR	N-CA-C	-5.40	108.47	114.62
1	B	130	MET	N-CA-C	-5.28	105.90	114.09
2	C	1547	LEU	N-CA-C	-5.27	106.85	113.28
1	B	209	PRO	N-CA-C	5.03	116.84	110.70
1	A	768	PRO	CA-N-CD	-5.02	104.97	112.00

There are no chirality outliers.

There are no planarity outliers.

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	6508	0	6399	61	0
1	B	6576	0	6463	51	0
2	C	437	0	452	9	0
3	D	130	0	29	0	0
All	All	13651	0	13343	116	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (116) 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:175:GLN:HA	1:A:180:THR:HG23	1.65	0.79
2:C:1527:LEU:HB3	2:C:1544:LEU:HD11	1.73	0.70
1:A:310:TYR:OH	1:A:365:LYS:NZ	2.30	0.65
1:A:348:LYS:HD3	1:A:353:HIS:HB2	1.79	0.64
1:A:340:GLN:H	1:A:394:PRO:HA	1.62	0.63
1:A:180:THR:HB	1:A:356:THR:HG23	1.83	0.60
2:C:1523:HIS:HB3	2:C:1526:LEU:HG	1.83	0.59
1:A:641:GLU:OE2	1:A:645:ARG:NH1	2.36	0.59
1:B:123:LYS:HG3	1:B:157:ILE:HD12	1.85	0.59
1:A:124:SER:OG	1:A:125:MET:N	2.33	0.58
1:A:879:SER:HB3	1:A:882:GLU:H	1.68	0.58
1:B:16:ARG:NH1	1:B:69:ASP:O	2.37	0.58
1:A:471:GLN:NE2	1:A:511:GLN:OE1	2.35	0.57
1:B:83:ARG:NH1	1:B:86:GLU:OE2	2.38	0.57
1:B:661:ALA:H	1:B:722:ALA:HB2	1.70	0.56
1:B:192:LEU:O	1:B:252:ARG:NH1	2.38	0.56
1:A:123:LYS:NZ	1:A:126:ASP:OD1	2.38	0.56
1:A:729:GLN:O	1:A:733:GLN:NE2	2.36	0.56
1:B:305:PRO:O	1:B:341:TYR:OH	2.24	0.56
1:A:444:PRO:O	1:A:478:ARG:NH1	2.39	0.55
1:B:661:ALA:HB1	1:B:716:ARG:HH22	1.70	0.55
1:A:166:ASN:ND2	1:B:276:GLY:O	2.39	0.55
1:A:565:LEU:HD23	1:A:571:LEU:HD11	1.89	0.54
1:B:107:GLY:O	1:B:862:ARG:NH2	2.39	0.54
1:A:166:ASN:HD22	1:B:277:SER:HG	1.54	0.54
1:B:441:ALA:O	1:B:479:ARG:NH1	2.41	0.54
1:A:83:ARG:NH1	1:A:86:GLU:OE1	2.40	0.53
1:B:441:ALA:HB3	1:B:858:GLU:HG3	1.89	0.53
1:A:203:GLY:HA3	1:A:247:LEU:HD23	1.89	0.53
2:C:1494:LEU:HA	2:C:1497:ARG:HD2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:ASN:OD1	1:A:168:ARG:NH2	2.43	0.52
1:A:542:ARG:NH1	1:A:580:ALA:O	2.42	0.52
1:B:732:ALA:HB1	1:B:772:ILE:HG23	1.91	0.52
1:B:559:ASP:OD1	1:B:574:ARG:NH2	2.42	0.52
1:A:622:ILE:HG22	1:A:752:ILE:HB	1.92	0.51
1:B:181:SER:OG	1:B:356:THR:O	2.23	0.51
1:B:233:SER:O	1:B:236:SER:OG	2.26	0.50
1:A:50:ILE:HD11	1:A:213:THR:HG22	1.93	0.50
1:B:354:LEU:HB2	1:B:358:ALA:HB2	1.94	0.49
2:C:1498:LEU:HA	2:C:1501:ILE:HB	1.96	0.48
1:A:871:ASP:OD1	1:A:871:ASP:N	2.42	0.48
1:A:318:THR:HG23	1:A:321:GLY:H	1.79	0.48
1:A:107:GLY:HA3	1:A:862:ARG:HD3	1.96	0.48
1:B:565:LEU:HD22	1:B:573:ILE:HD11	1.96	0.48
1:B:72:LYS:HD2	1:B:872:LYS:HB3	1.97	0.47
1:A:723:PHE:HD1	1:A:728:MET:HE1	1.79	0.47
1:A:157:ILE:HG23	1:A:158:THR:HG23	1.97	0.47
1:B:134:MET:H	1:B:134:MET:HG2	1.42	0.47
1:A:747:PRO:HG3	1:A:765:LEU:HD23	1.96	0.47
1:B:760:VAL:HG13	1:B:764:THR:HB	1.97	0.47
1:B:686:ASN:HA	1:B:781:PHE:HB3	1.97	0.46
1:B:575:HIS:HA	1:B:579:ARG:HG2	1.97	0.46
1:A:730:ASP:OD1	1:A:730:ASP:N	2.40	0.46
1:B:281:SER:OG	1:B:282:TYR:N	2.48	0.46
1:A:628:GLU:OE2	1:A:754:THR:OG1	2.30	0.46
1:A:851:ASP:OD1	1:A:851:ASP:N	2.45	0.46
1:A:13:MET:HE3	1:A:23:VAL:HG11	1.98	0.46
1:A:226:ASP:OD1	1:A:226:ASP:N	2.42	0.46
1:A:312:GLU:HB3	1:A:415:VAL:HA	1.97	0.46
1:B:13:MET:HE1	1:B:368:LEU:HG	1.98	0.46
1:B:347:VAL:HG22	1:B:365:LYS:HD3	1.98	0.46
1:B:554:TYR:HB2	1:B:610:LEU:HD13	1.98	0.45
1:B:389:ASP:OD1	1:B:389:ASP:N	2.46	0.45
1:B:590:LEU:O	1:B:596:THR:OG1	2.33	0.45
1:B:753:SER:OG	1:B:754:THR:N	2.50	0.45
1:A:592:GLN:O	1:A:596:THR:OG1	2.30	0.45
1:A:616:ILE:HD13	1:A:616:ILE:HA	1.87	0.45
1:A:306:GLN:HE21	1:A:306:GLN:HB2	1.45	0.45
1:A:173:THR:HB	1:B:175:GLN:HB3	1.99	0.44
1:A:420:MET:HE3	1:A:420:MET:HB3	1.74	0.44
1:B:125:MET:HB3	1:B:125:MET:HE3	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:LEU:HD13	1:B:320:LEU:HA	1.79	0.44
1:A:743:ARG:NH2	1:A:744:LEU:O	2.51	0.44
1:B:230:ARG:HG2	1:B:380:HIS:HB3	1.99	0.44
1:B:562:ALA:HA	1:B:573:ILE:HD13	1.99	0.44
1:A:251:LYS:HE2	1:A:255:GLU:HB2	2.00	0.44
1:A:281:SER:OG	1:A:282:TYR:N	2.51	0.44
1:B:212:LYS:HB3	1:B:212:LYS:HE2	1.66	0.44
1:B:287:VAL:HG22	1:B:324:VAL:HG13	1.99	0.44
1:A:664:MET:HB2	1:A:717:LEU:HD11	1.99	0.44
1:A:760:VAL:HG21	1:A:765:LEU:HD22	1.99	0.44
1:A:277:SER:H	1:B:163:TYR:HD1	1.66	0.44
1:A:83:ARG:HA	1:A:83:ARG:HD2	1.91	0.43
1:A:166:ASN:ND2	1:B:277:SER:OG	2.33	0.43
1:A:560:ARG:HE	1:A:560:ARG:HB2	1.20	0.43
1:B:826:GLY:O	1:B:829:SER:OG	2.35	0.43
2:C:1534:ILE:HG22	2:C:1541:HIS:H	1.84	0.43
2:C:1502:TRP:HB3	2:C:1553:ILE:HG21	2.01	0.42
1:A:357:ALA:C	1:A:359:GLY:H	2.27	0.42
1:A:95:LEU:HD13	1:A:205:VAL:HB	2.00	0.42
1:B:735:LEU:HD21	1:B:775:MET:HE1	2.00	0.42
1:A:131:LEU:HD22	1:A:879:SER:HB2	2.02	0.42
1:A:804:THR:HA	1:A:807:GLN:HE22	1.83	0.42
2:C:1500:GLU:HA	2:C:1503:GLN:HB2	2.01	0.42
1:A:279:LYS:HE2	1:A:279:LYS:HB3	1.71	0.42
1:B:42:ASP:OD1	1:B:42:ASP:N	2.53	0.42
1:B:730:ASP:N	1:B:730:ASP:OD1	2.52	0.42
1:A:215:TYR:OH	1:A:224:ALA:O	2.30	0.42
1:B:123:LYS:HE3	1:B:154:LYS:HG2	2.00	0.42
1:A:306:GLN:HA	1:A:341:TYR:OH	2.20	0.42
1:A:320:LEU:HD12	1:A:320:LEU:HA	1.90	0.41
1:B:622:ILE:HD13	1:B:622:ILE:HG21	1.91	0.41
1:B:663:LEU:HD23	1:B:693:ILE:HD11	2.02	0.41
1:B:880:PRO:HA	1:B:883:GLN:HE21	1.84	0.41
1:A:739:PHE:HD1	1:A:739:PHE:HA	1.81	0.41
1:B:51:SER:HA	1:B:52:PRO:HD3	1.90	0.41
2:C:1494:LEU:HB3	2:C:1561:LEU:HD11	2.02	0.41
1:A:532:LEU:HD13	1:A:796:PHE:HB3	2.02	0.41
1:A:125:MET:HE2	1:A:125:MET:HB3	1.87	0.40
1:A:732:ALA:HB1	1:A:772:ILE:HD12	2.02	0.40
2:C:1553:ILE:O	2:C:1557:ALA:HB2	2.21	0.40
1:A:193:LEU:HA	1:A:193:LEU:HD23	1.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:LEU:HD12	1:A:509:LEU:HA	1.87	0.40
1:B:713:ILE:H	1:B:713:ILE:HG13	1.76	0.40
1:B:719:THR:HG22	1:B:721:HIS:H	1.87	0.40
1:B:750:THR:O	1:B:750:THR:OG1	2.40	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	855/921 (93%)	765 (90%)	90 (10%)	0	100 100
1	B	863/921 (94%)	768 (89%)	94 (11%)	1 (0%)	48 78
2	C	50/1634 (3%)	46 (92%)	4 (8%)	0	100 100
All	All	1768/3476 (51%)	1579 (89%)	188 (11%)	1 (0%)	50 78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	135	PRO

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	671/721 (93%)	641 (96%)	30 (4%)	23 49
1	B	678/721 (94%)	653 (96%)	25 (4%)	29 54
2	C	46/1362 (3%)	41 (89%)	5 (11%)	5 24
All	All	1395/2804 (50%)	1335 (96%)	60 (4%)	27 50

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	175	GLN
1	A	176	THR
1	A	178	SER
1	A	179	SER
1	A	180	THR
1	A	181	SER
1	A	206	THR
1	A	207	LEU
1	A	255	GLU
1	A	275	ASP
1	A	277	SER
1	A	278	GLU
1	A	279	LYS
1	A	280	ILE
1	A	306	GLN
1	A	354	LEU
1	A	420	MET
1	A	423	THR
1	A	424	ASN
1	A	429	LEU
1	A	430	GLU
1	A	487	GLN
1	A	525	THR
1	A	527	LEU
1	A	559	ASP
1	A	560	ARG
1	A	561	CYS
1	A	637	VAL
1	A	638	PHE
1	A	639	SER
1	B	61	VAL
1	B	119	ILE
1	B	124	SER
1	B	125	MET

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Mol	Chain	Res	Type
1	B	127	SER
1	B	128	TYR
1	B	129	LEU
1	B	130	MET
1	B	131	LEU
1	B	134	MET
1	B	216	LEU
1	B	217	SER
1	B	320	LEU
1	B	420	MET
1	B	423	THR
1	B	424	ASN
1	B	427	VAL
1	B	498	LEU
1	B	541	GLN
1	B	542	ARG
1	B	607	LEU
1	B	863	VAL
1	B	864	SER
1	B	877	VAL
1	B	884	ARG
2	C	1538	CYS
2	C	1541	HIS
2	C	1542	VAL
2	C	1547	LEU
2	C	1548	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	190	GLN
1	A	274	ASN
1	A	306	GLN
1	A	314	HIS
1	A	487	GLN
1	A	504	HIS
1	A	524	GLN
1	A	671	GLN
1	A	759	HIS
1	B	24	GLN
1	B	91	GLN
1	B	228	HIS

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Mol	Chain	Res	Type
1	B	597	GLN
1	B	686	ASN
1	B	710	GLN
1	B	729	GLN
1	B	789	GLN
1	B	810	ASN
1	B	812	HIS
1	B	835	HIS
1	B	883	GLN
2	C	1532	GLN
2	C	1536	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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

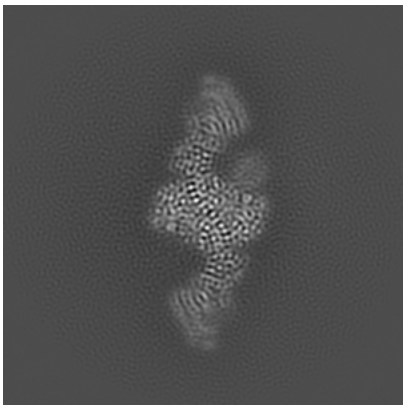
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-38411. These allow visual inspection of the internal detail of the map and identification of artifacts.

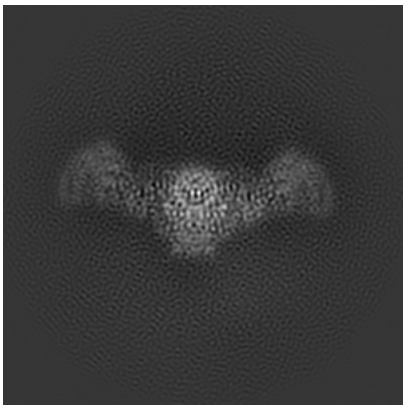
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

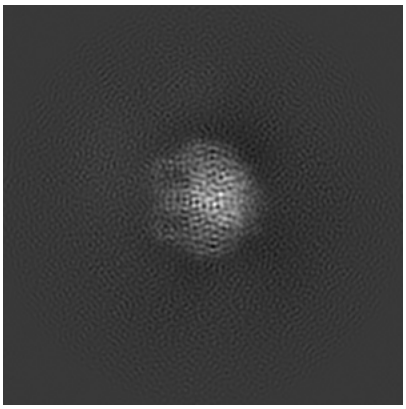
6.1.1 Primary map



X

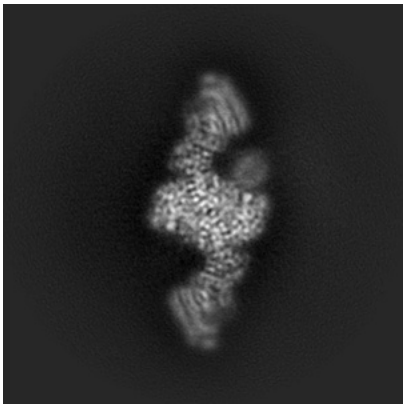


Y

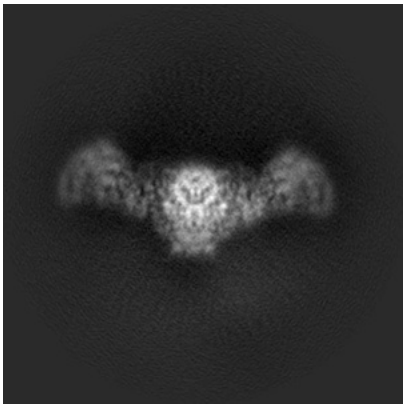


Z

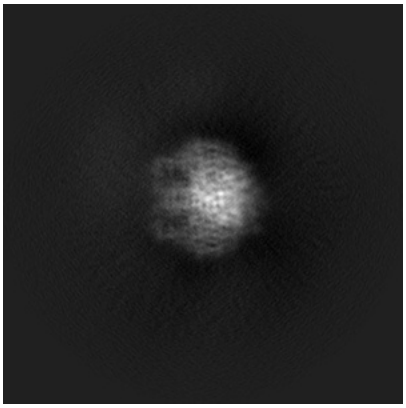
6.1.2 Raw map



X



Y

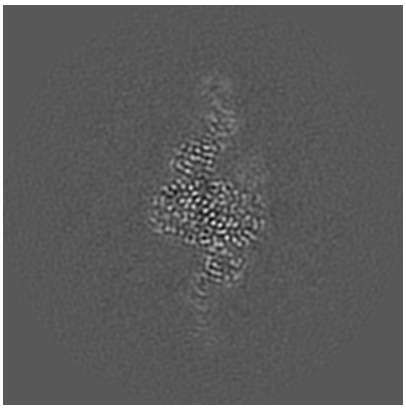


Z

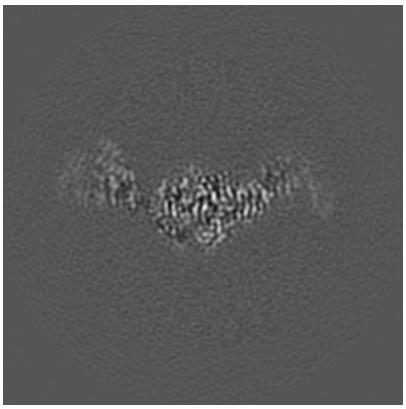
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

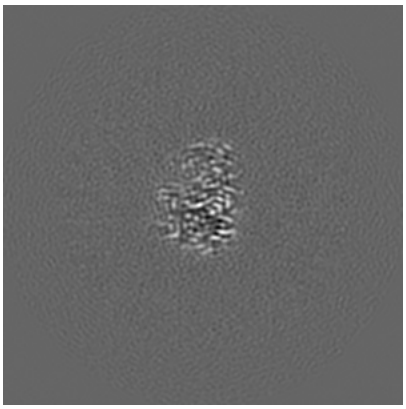
6.2.1 Primary map



X Index: 128

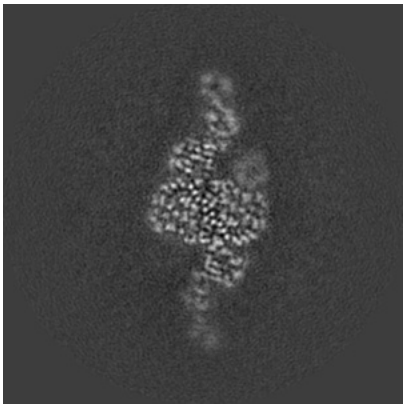


Y Index: 128

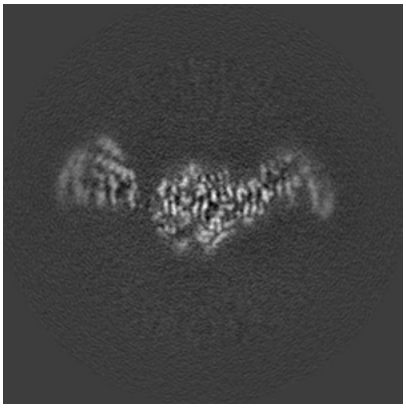


Z Index: 128

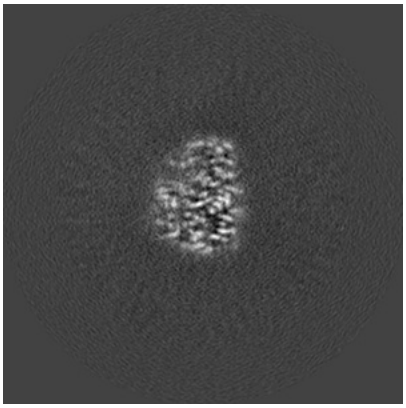
6.2.2 Raw map



X Index: 128



Y Index: 128

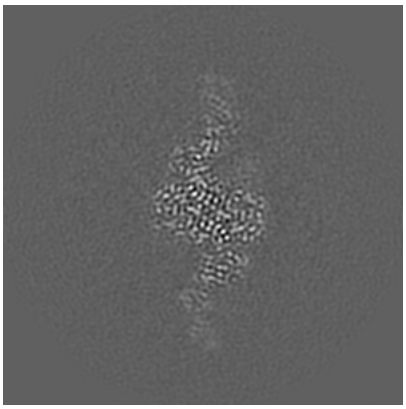


Z Index: 128

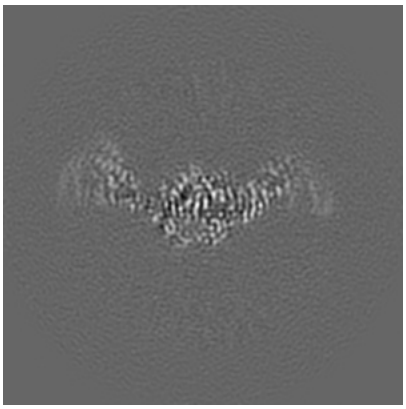
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

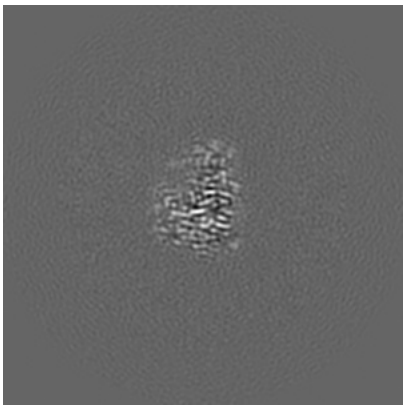
6.3.1 Primary map



X Index: 131

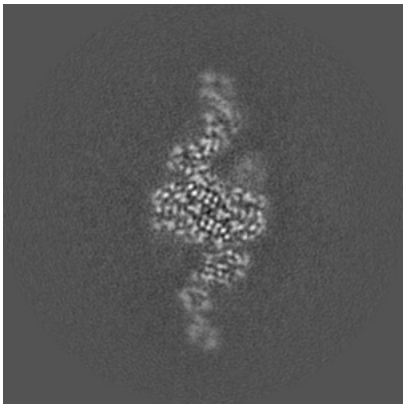


Y Index: 129

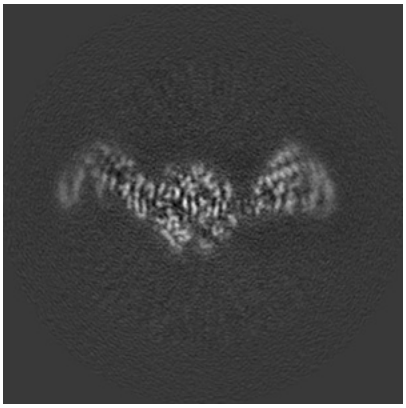


Z Index: 130

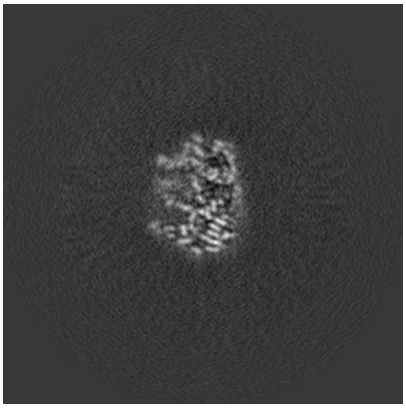
6.3.2 Raw map



X Index: 131



Y Index: 134

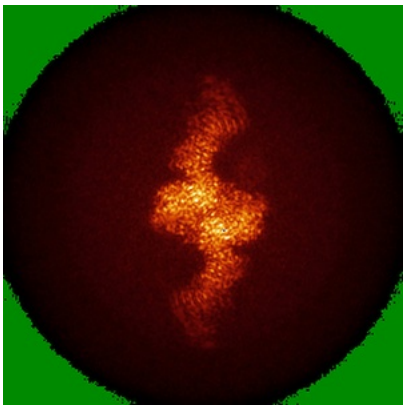


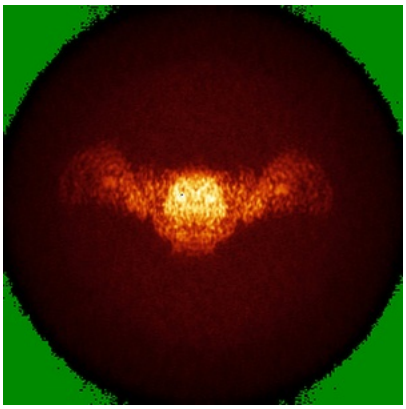
Z Index: 125

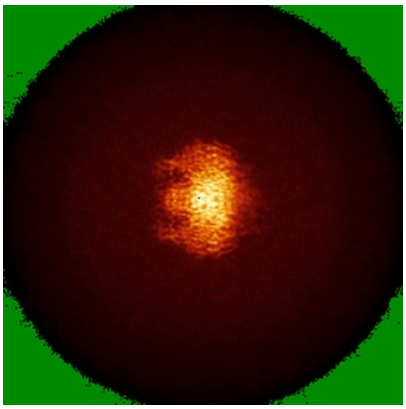
The images above show the largest variance slices of the map in three orthogonal directions.

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

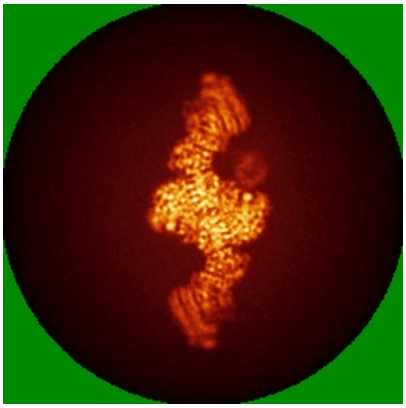
6.4.1 Primary map

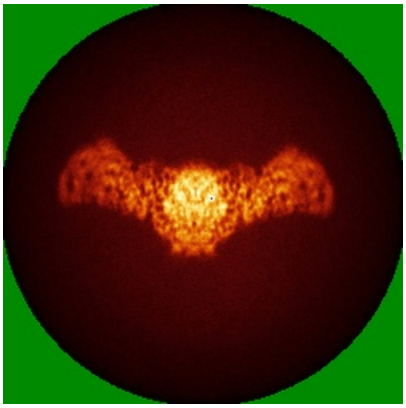

X

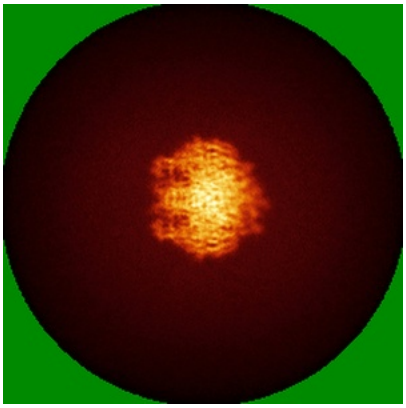

Y


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 0.026. 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.

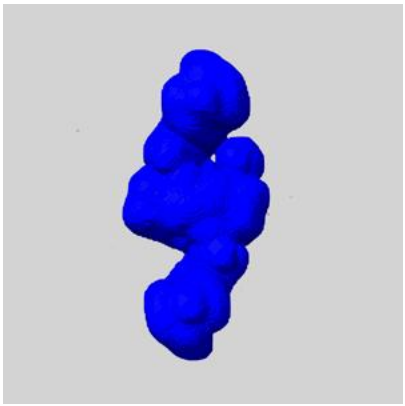
6.6 Mask visualisation

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

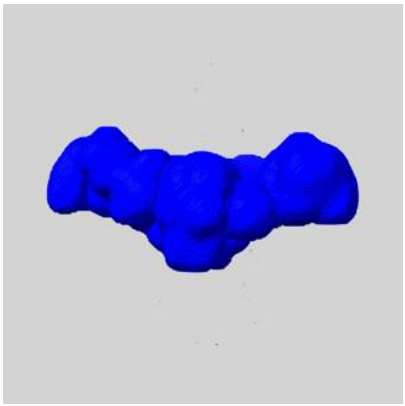
A mask typically either:

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

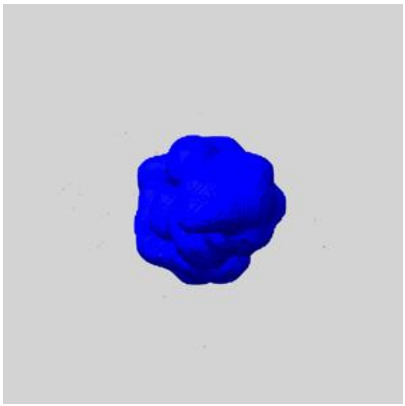
6.6.1 emd_38411_msk_1.map



X



Y

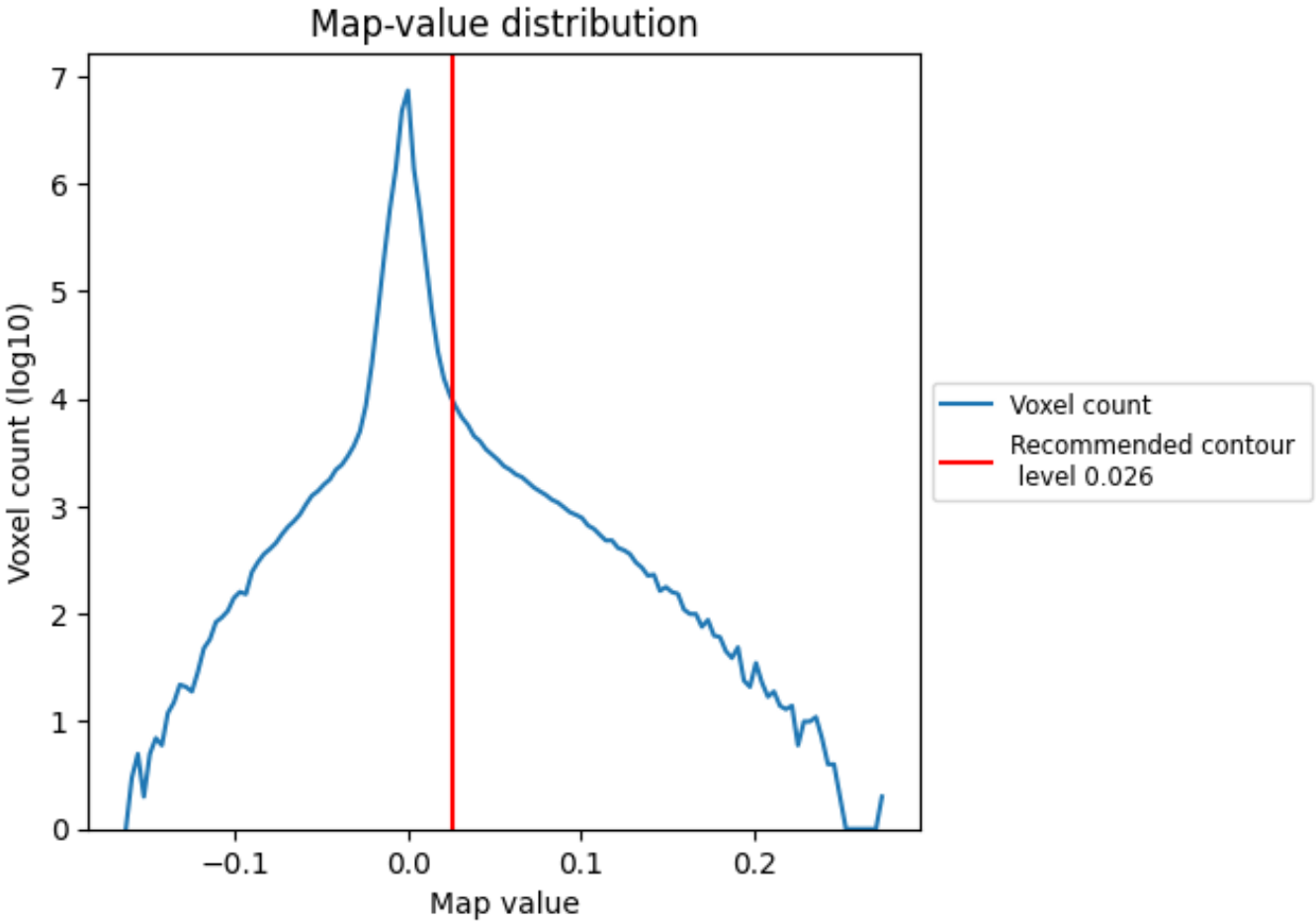


Z

7 Map analysis

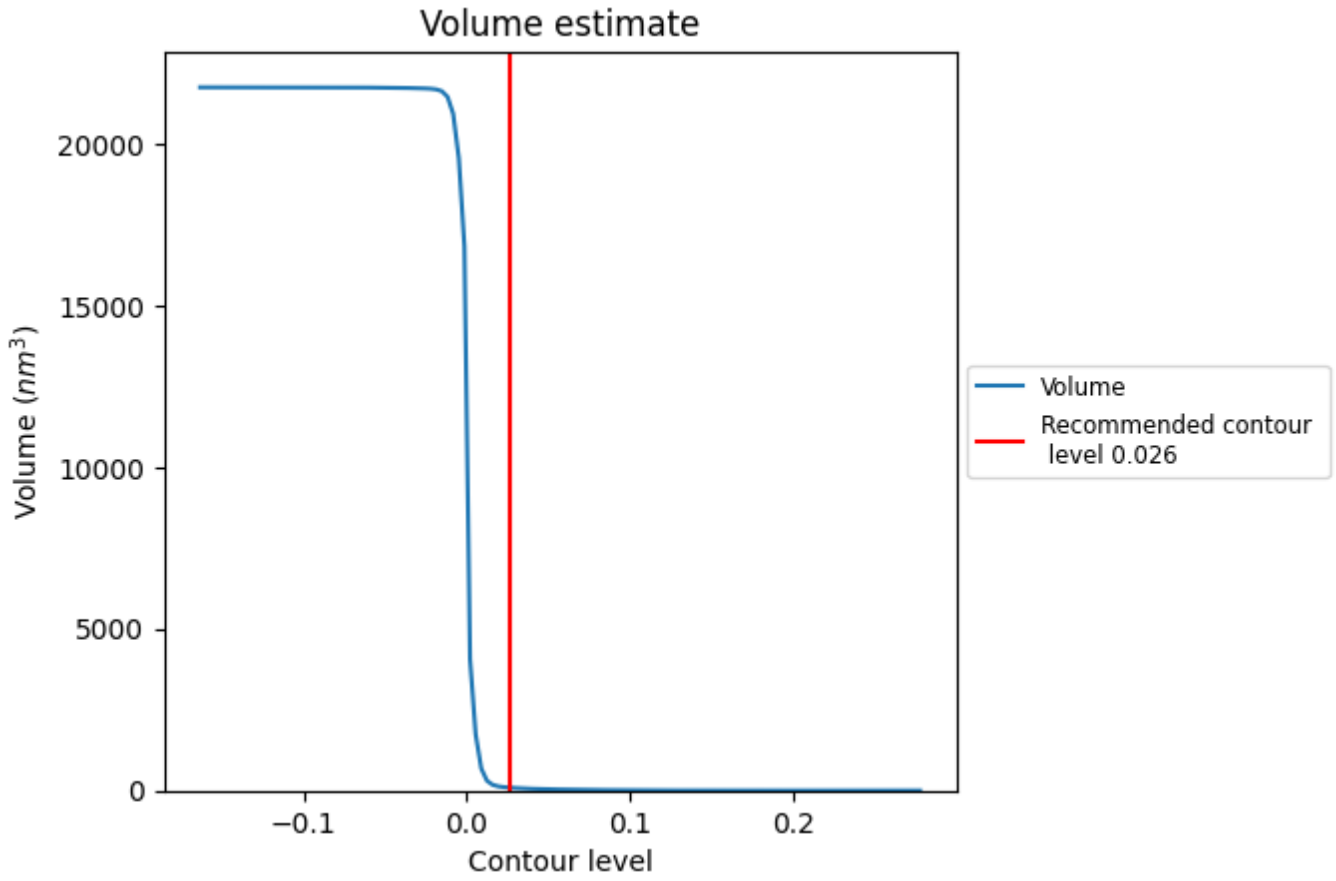
This section contains the results of statistical analysis of the map.

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.

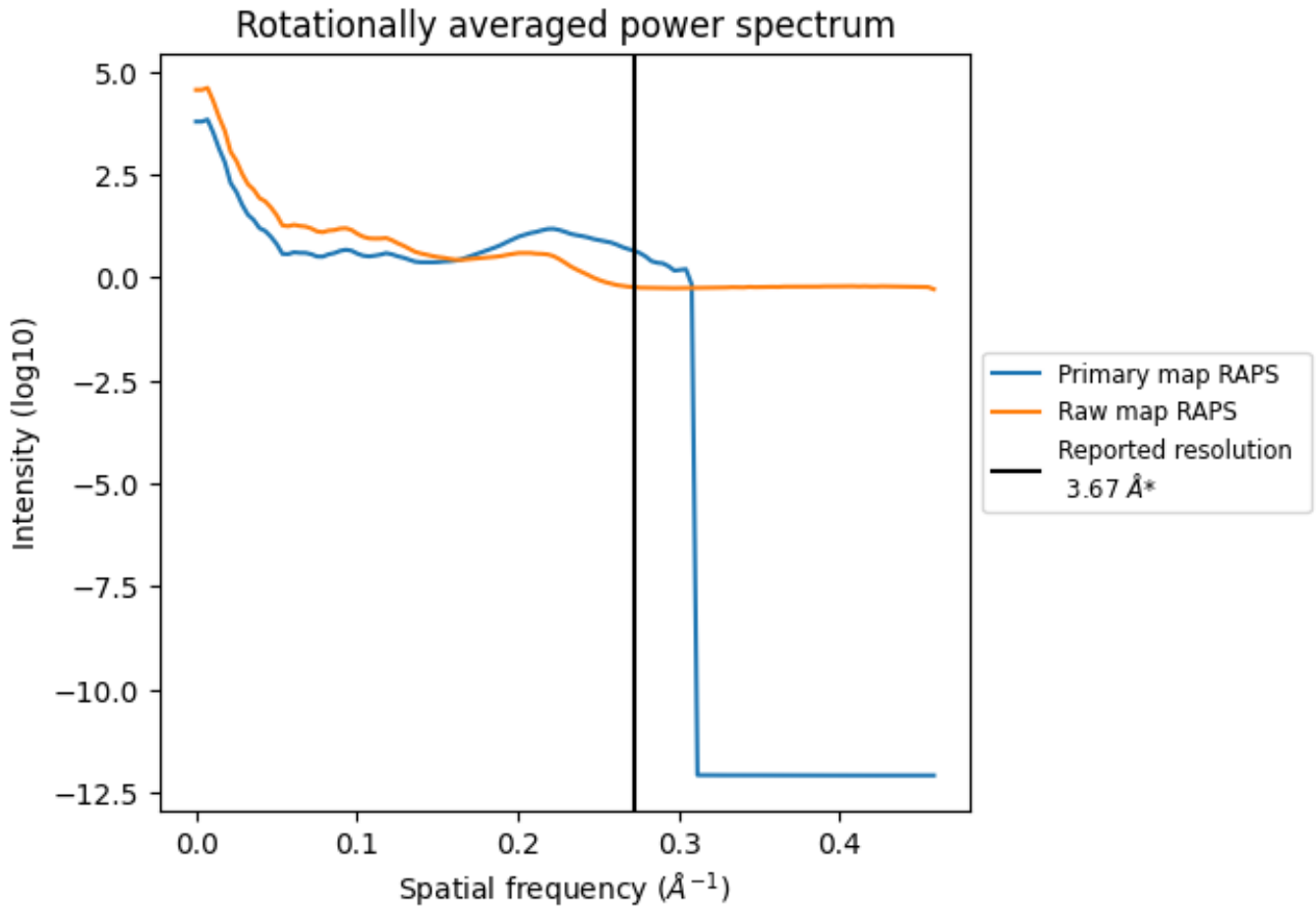
7.2 Volume estimate



The volume at the recommended contour level is 91 nm^3; this corresponds to an approximate mass of 82 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)

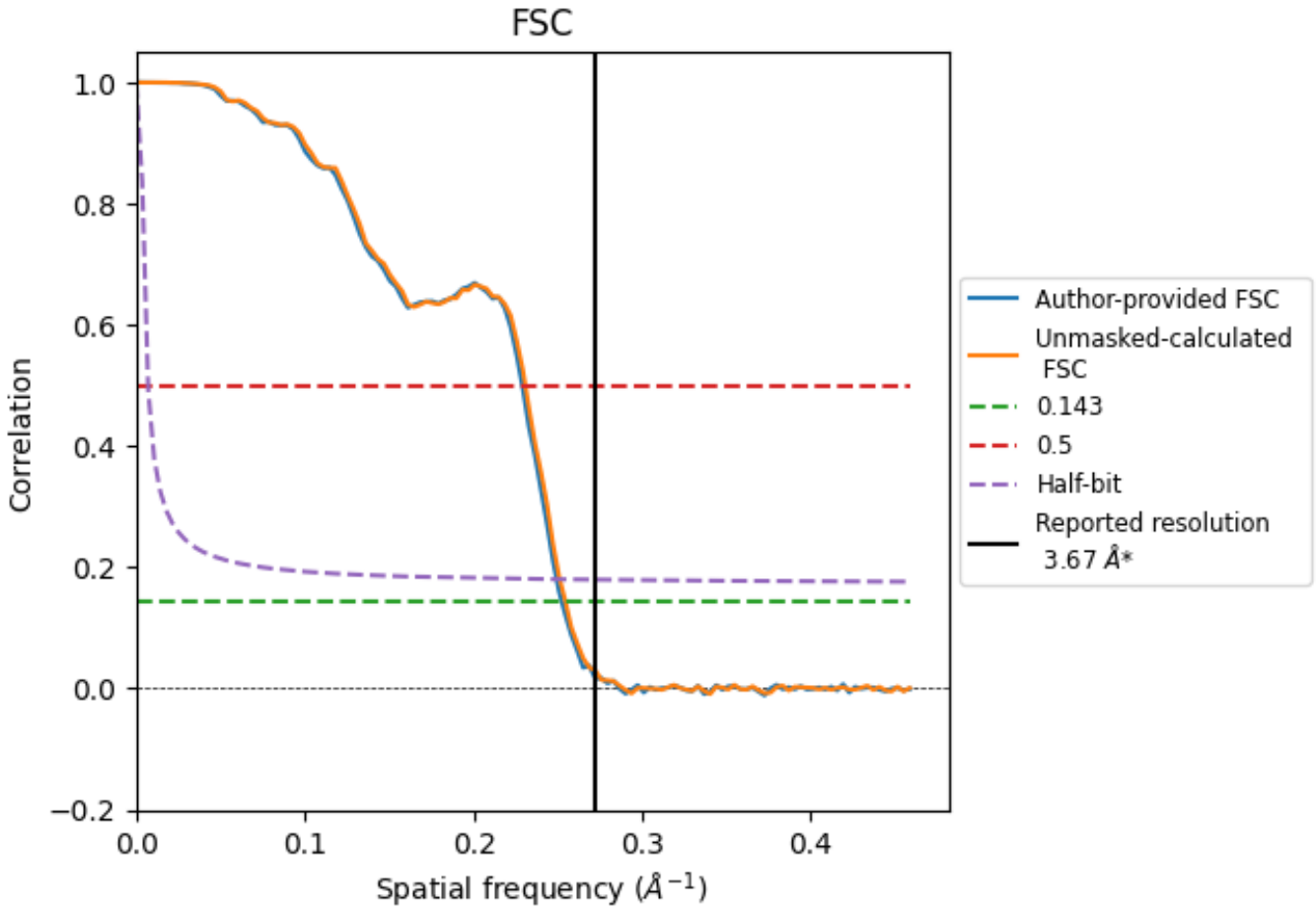


*Reported resolution corresponds to spatial frequency of 0.272 $Å^{-1}$

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 0.272 Å^{-1}

8.2 Resolution estimates (i)

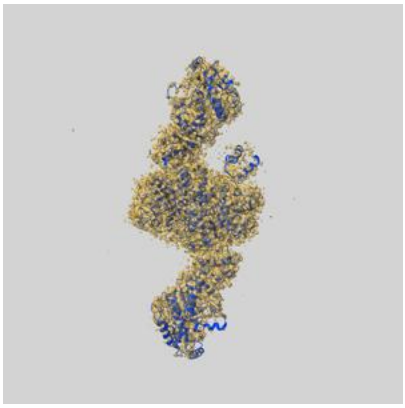
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.67	-	-
Author-provided FSC curve	3.96	4.37	4.01
Unmasked-calculated*	3.93	4.33	3.98

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

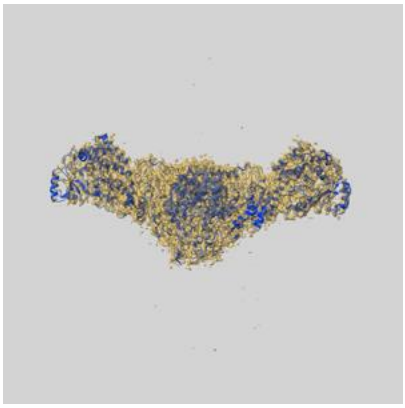
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-38411 and PDB model 8XJZ. Per-residue inclusion information can be found in section 3 on page 6.

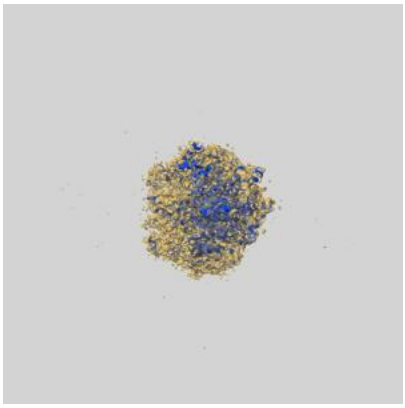
9.1 Map-model overlay



X



Y



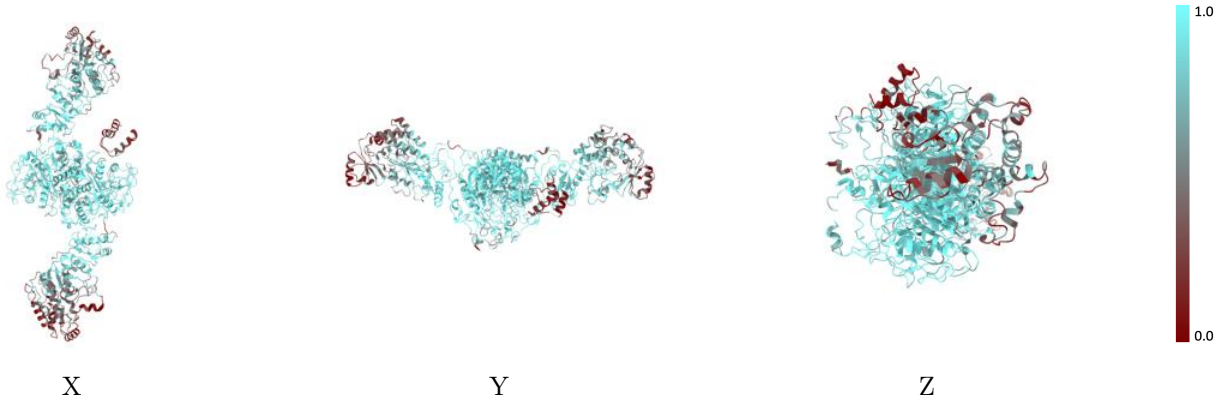
Z

The images above show the 3D surface view of the map at the recommended contour level 0.026 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)

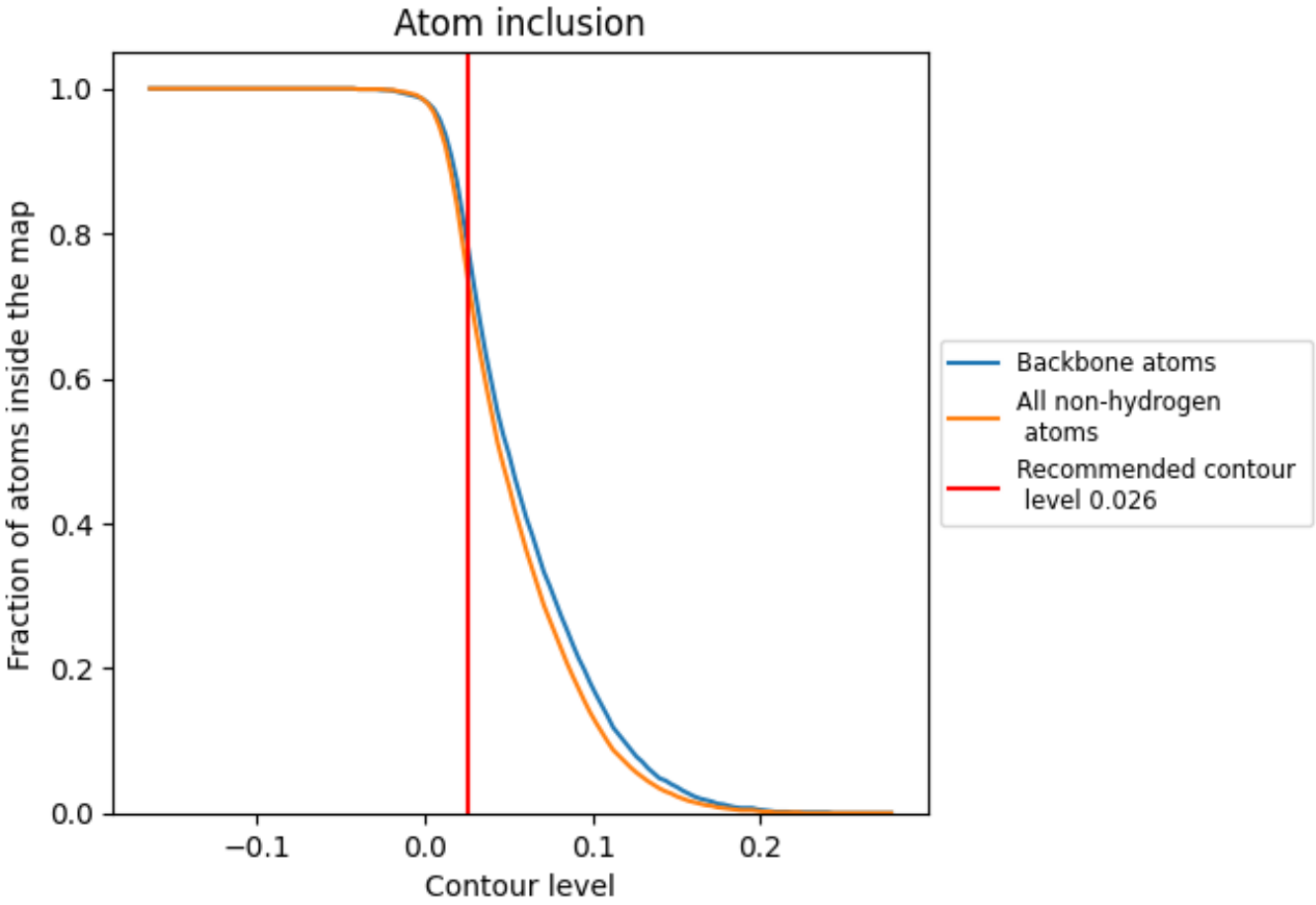
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.026).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 73% 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 (0.026) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7330	0.4720
A	0.7780	0.4870
B	0.7240	0.4780
C	0.1750	0.1940
D	0.7610	0.4100