



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 01:19 PM UTC

PDB ID : 8ILV / pdb_00008ilv
EMDB ID : EMD-35547
Title : Cryo-EM structure of PI3Kalpha in complex with compound 18
Authors : Zhou, Q.; Liu, X.; Neri, D.; Li, W.; Favalli, N.; Bassi, G.; Yang, S.; Yang, D.;
Vogt, P.K.; Wang, M.-W.
Deposited on : 2023-03-04
Resolution : 3.19 Å(reported)
Based on initial model : 7MYN

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMD archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

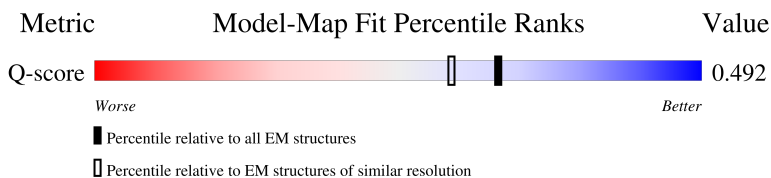
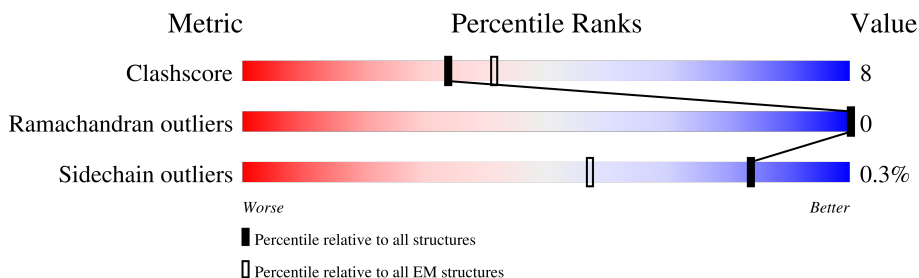
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.19 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	14455 (2.69 - 3.69)

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	1096	
2	B	723	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10218 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 Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic sub-unit alpha isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	971	7933	5071	1359	1440	63	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	MET	-	initiating methionine	UNP P42336
A	-26	SER	-	expression tag	UNP P42336
A	-25	TYR	-	expression tag	UNP P42336
A	-24	TYR	-	expression tag	UNP P42336
A	-23	HIS	-	expression tag	UNP P42336
A	-22	HIS	-	expression tag	UNP P42336
A	-21	HIS	-	expression tag	UNP P42336
A	-20	HIS	-	expression tag	UNP P42336
A	-19	HIS	-	expression tag	UNP P42336
A	-18	HIS	-	expression tag	UNP P42336
A	-17	ASP	-	expression tag	UNP P42336
A	-16	TYR	-	expression tag	UNP P42336
A	-15	ASP	-	expression tag	UNP P42336
A	-14	ILE	-	expression tag	UNP P42336
A	-13	PRO	-	expression tag	UNP P42336
A	-12	THR	-	expression tag	UNP P42336
A	-11	THR	-	expression tag	UNP P42336
A	-10	GLU	-	expression tag	UNP P42336
A	-9	ASN	-	expression tag	UNP P42336
A	-8	LEU	-	expression tag	UNP P42336
A	-7	TYR	-	expression tag	UNP P42336
A	-6	PHE	-	expression tag	UNP P42336
A	-5	GLN	-	expression tag	UNP P42336
A	-4	GLY	-	expression tag	UNP P42336
A	-3	ALA	-	expression tag	UNP P42336
A	-2	MET	-	expression tag	UNP P42336
A	-1	GLY	-	expression tag	UNP P42336

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Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP P42336

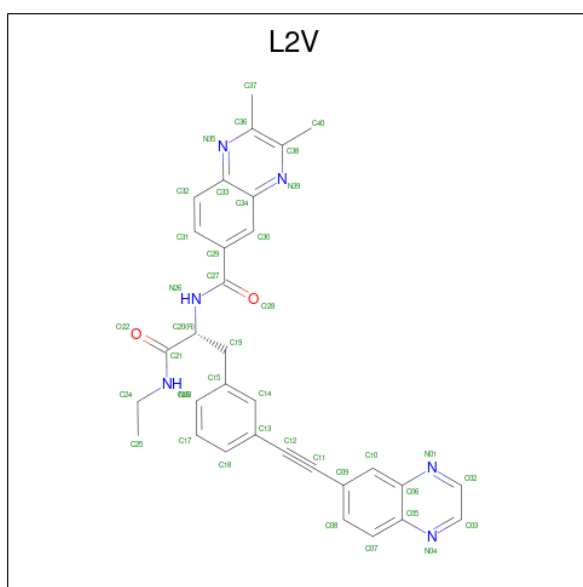
- Molecule 2 is a protein called Phosphatidylinositol 3-kinase regulatory subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	265	Total	C	N	O	S	0	0
			2241	1405	398	432	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	2	MET	-	initiating methionine	UNP P27986

- Molecule 3 is N-[(2R)-1-(ethylamino)-1-oxidanylidene-3-[3-(2-quinoxalin-6-ylethynyl)phenyl]propan-2-yl]-2,3-dimethyl-quinoxaline-6-carboxamide (CCD ID: L2V) (formula: C₃₂H₂₈N₆O₂).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			40	32	6	2	

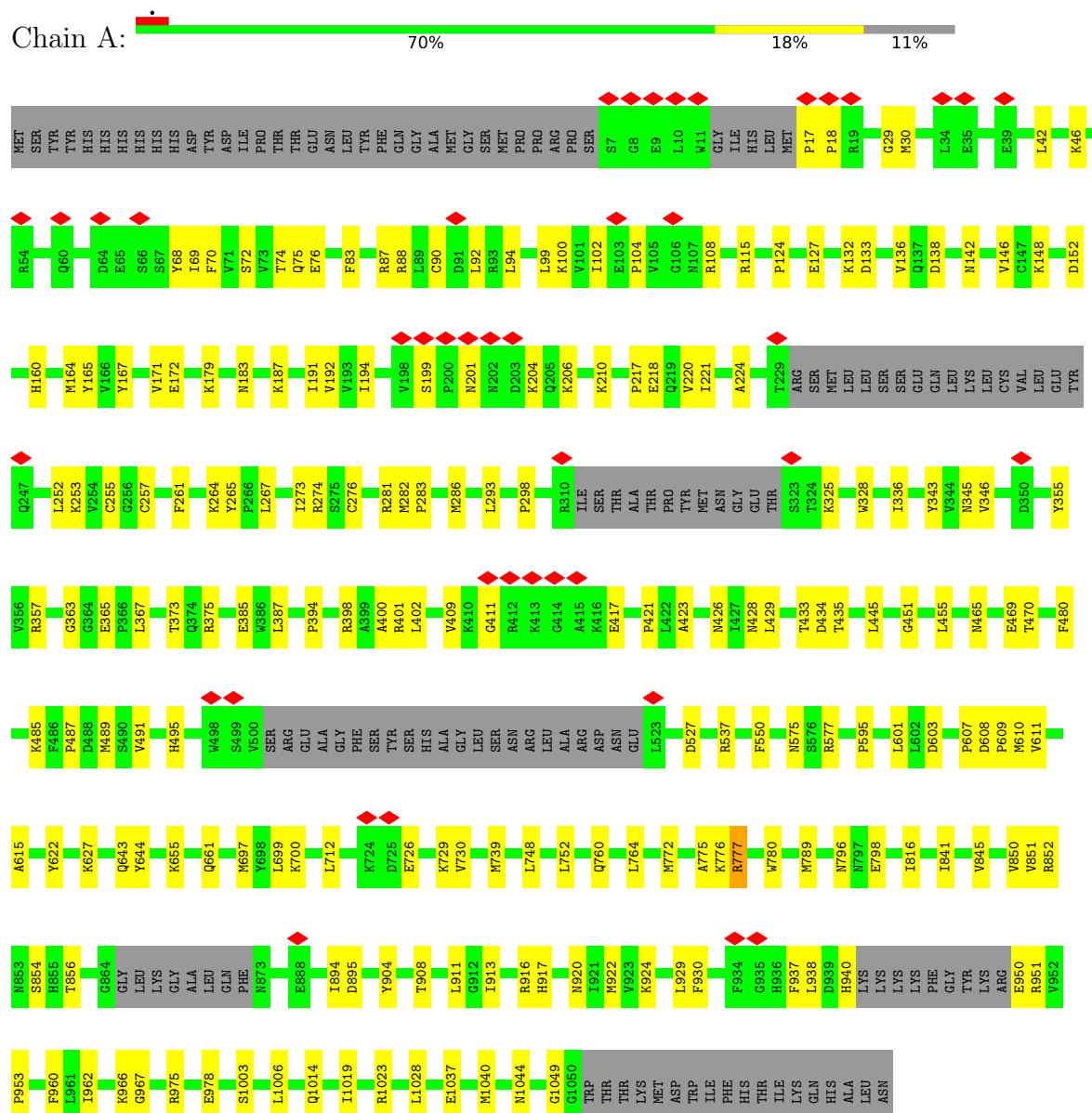
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		AltConf
4	A	4	Total	O	0
			4	4	

3 Residue-property plots

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: Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit alpha isoform



- Molecule 2: Phosphatidylinositol 3-kinase regulatory subunit alpha



MET	THR	PHE	LEU	TYR	GLN	PRO	GLN	Q115	R523	LEU	ALA
ALA	THR	ALA	ALA	LEU	PRO	ALA	PRO	D421	I524	PRO	THR
GLY	GLY	PRO	ASP	LEU	PRO	PRO	ALA	V422	N527	HIS	GLY
TYR	ARG	ASP	PHE	HIS	LEU	ALA	LEU	K423	Y528	ASP	GLY
GLN	GLY	ILE	LYS	PHE	PRO	PRO	LEU	S429	D529	GLU	PHE
TYR	ASP	ALA	ARG	PHE	PRO	PRO	PRO	K430	K532	LYS	ALA
ARG	PHE	PRO	TYR	LYS	PRO	PRO	PRO	D434	I538	THR	GLU
LEU	GLY	PRO	LEU	SER	PRO	PRO	PRO	Q435	I539	ASN	TYR
TYR	GLY	PRO	LEU	THR	LYS	LYS	LYS	V436	D540	VAL	LEU
ASP	TYR	LYS	LEU	THR	PRO	PRO	PRO	V437	R543	GLY	TYR
LYS	GLY	VAL	ASN	SER	THR	THR	THR	K438	R543	SER	SER
LYS	TYR	VAL	VAL	LYS	VAL	VAL	VAL	E439	K551	ASN	SER
GLU	ILE	ALA	ILE	LEU	ALA	ALA	ALA	D440	R557	ARG	LYS
ARG	GLY	ILE	PRO	LEU	ASN	ASN	ASN	N441	K561	LYS	GLU
GLU	ARG	GLY	ILE	ASN	ALA	ALA	ALA	I442	K561	ALA	LEU
LYS	LYS	ALA	ALA	ALA	GLY	GLY	GLY	E443	N664	GLU	VAL
ASP	LYS	VAL	VAL	ARG	MET	MET	MET	A444	P568	ASN	VAL
ILE	ILE	LYS	VAL	VAL	N323	N324	N325	K448	I571	LEU	HIS
ASP	GLY	GLY	TYR	SER	D330	A331	E332	L449	Q572	LEU	GLN
LEU	PRO	GLY	GLY	GLU	ILE	ILE	ILE	R472	L573	ARG	THR
HIS	PRO	THR	THR	GLU	PHE	PHE	PHE	E476	Y580	GLY	HIS
LEU	PRO	THR	THR	GLU	ILE	ILE	ILE	R481	K587	LYS	ASN
GLY	PRO	THR	THR	GLU	ILE	ILE	ILE	I493	G588	THR	ASP
ASP	LYS	THR	THR	GLY	THR	THR	THR	F494	V589	VAL	ASP
ILE	ILE	ILE	ILE	SER	PRO	PRO	PRO	E495	R590	ARG	LEU
LEU	LEU	LEU	LEU	ALA	ALA	ALA	ALA	E496	Q591	GLY	LEU
VAL	VAL	VAL	VAL	GLY	GLY	GLY	GLY	C498	K592	SER	VAL
ALA	PRO	ALA	ALA	SER	TYR	TYR	TYR	Q499	K593	LYS	THR
LEU	GLY	GLY	GLY	ASP	ASP	ASP	ASP	T500	L594	GLN	LEU
GLY	LEU	LEU	LEU	GLN	GLN	GLN	GLN	Q501	N595	ALA	ALA
THR	LYS	LEU	LEU	ASN	ASN	ASN	ASN	E502	E596	VAL	TYR
ASP	GLY	GLY	GLY	GLY	GLY	GLY	GLY	R503	W597	CYS	VAL
GLN	ALA	ALA	ALA	VAL	VAL	VAL	VAL	Y504	L598	SER	GLN
ARG	ARG	ARG	ARG	THR	THR	THR	THR	S505	GLY	VAL	ARG
				ILE	ILE	ILE	ILE	K506	ASN	VAL	ARG
				GLY	GLY	GLY	GLY	E507	GLU	ASP	
				ILE	ILE	ILE	ILE	Y508	ASN	GLY	
				ILE	ILE	ILE	ILE	I509	THR	GLY	
				LEU	LEU	LEU	LEU	E510	GLU	VAL	
				SER	SER	SER	SER	K511	ASP	VAL	
				THR	THR	THR	THR	PHE	TYR	GLY	
				GLY	GLY	GLY	GLY	LYS	SER	THR	
				TRP	TRP	TRP	TRP	ARG	LEU	LEU	
				LEU	LEU	LEU	LEU	GLY	VAL	VAL	
				ASN	ASN	ASN	ASN	GLY	GLY	LYS	
				THR	THR	THR	THR	ASN	ASP	THR	
				GLY	GLY	GLY	GLY	GLY	ASP	ASP	
				ILE	ILE	ILE	ILE	ILE	ASP	ASP	
				GLN	GLN	GLN	GLN	GLN	ASP	ASP	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	232150	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 ($e^-/\text{\AA}^2$)	70	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.655	Depositor
Minimum map value	-3.678	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.098	Depositor
Recommended contour level	0.42	Depositor
Map size ($\text{\AA}$)	274.176, 274.176, 274.176	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.071, 1.071, 1.071	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: L2V

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	0.13	0/8108	0.30	2/10957 (0.0%)
2	B	0.10	0/2279	0.26	1/3057 (0.0%)
All	All	0.12	0/10387	0.29	3/14014 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	775	ALA	N-CA-C	10.90	124.69	111.40
1	A	775	ALA	CB-CA-C	-5.79	101.06	110.79
2	B	324	ASN	N-CA-C	-5.28	106.89	113.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7933	0	7928	135	0
2	B	2241	0	2208	42	0
3	A	40	0	0	0	0
4	A	4	0	0	0	0
All	All	10218	0	10136	167	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 8.

All (167) 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)
2:B:436:VAL:O	2:B:438:LYS:NZ	2.07	0.86
1:A:595:PRO:HG3	1:A:622:TYR:HB3	1.60	0.83
1:A:367:LEU:O	1:A:575:ASN:ND2	2.20	0.74
1:A:76:GLU:N	1:A:76:GLU:OE1	2.24	0.70
1:A:950:GLU:HG2	1:A:951:ARG:HH21	1.56	0.69
2:B:387:ASP:OD1	2:B:389:LYS:NZ	2.24	0.69
1:A:282:MET:HE3	1:A:283:PRO:HD2	1.74	0.69
1:A:253:LYS:NZ	1:A:257:CYS:O	2.26	0.69
2:B:498:CYS:SG	2:B:532:LYS:NZ	2.65	0.69
1:A:780:TRP:NE1	1:A:798:GLU:OE1	2.24	0.69
1:A:398:ARG:NH2	1:A:434:ASP:OD1	2.26	0.68
1:A:124:PRO:HG2	1:A:127:GLU:HG2	1.77	0.66
1:A:218:GLU:OE1	1:A:264:LYS:NZ	2.28	0.66
1:A:328:TRP:HA	1:A:394:PRO:HB3	1.75	0.66
1:A:298:PRO:HG2	1:A:697:MET:HG3	1.78	0.65
2:B:331:ALA:O	2:B:430:LYS:NZ	2.31	0.64
1:A:1037:GLU:N	1:A:1037:GLU:OE1	2.31	0.64
1:A:30:MET:HA	2:B:527:ASN:HD21	1.62	0.63
1:A:69:ILE:HB	1:A:104:PRO:HG3	1.82	0.62
1:A:42:LEU:HD21	1:A:92:LEU:HD11	1.82	0.61
1:A:75:GLN:NE2	1:A:94:LEU:O	2.34	0.61
1:A:375:ARG:HH21	1:A:409:VAL:HG21	1.67	0.60
1:A:357:ARG:NH2	2:B:349:ASP:OD2	2.35	0.59
1:A:401:ARG:NH1	1:A:426:ASN:OD1	2.35	0.59
1:A:252:LEU:HB2	1:A:261:PHE:HB2	1.84	0.59
1:A:451:GLY:O	1:A:1014:GLN:NE2	2.34	0.58
1:A:411:GLY:HA2	1:A:417:GLU:HG2	1.84	0.58
1:A:220:VAL:HG21	1:A:267:LEU:HD13	1.86	0.58
2:B:333:TRP:CD1	2:B:333:TRP:H	2.21	0.58
1:A:363:GLY:HA3	1:A:607:PRO:HG3	1.86	0.58
1:A:343:TYR:OH	2:B:557:ARG:NH1	2.32	0.58
1:A:76:GLU:HG3	1:A:124:PRO:HD3	1.87	0.57
1:A:72:SER:HB2	1:A:94:LEU:HD21	1.86	0.57
2:B:540:ASP:OD1	2:B:543:ARG:NH1	2.38	0.57
1:A:217:PRO:HB3	1:A:252:LEU:HD23	1.85	0.56
1:A:841:ILE:HG13	1:A:845:VAL:HG12	1.85	0.56
1:A:88:ARG:NH1	1:A:90:CYS:SG	2.77	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:GLU:HG2	1:A:387:LEU:HD12	1.85	0.56
1:A:191:ILE:HG22	1:A:210:LYS:HG2	1.87	0.56
1:A:854:SER:HB3	1:A:922:MET:HE3	1.86	0.56
1:A:87:ARG:HD3	1:A:115:ARG:HH21	1.71	0.56
2:B:506:LYS:HD3	2:B:509:ILE:HD11	1.88	0.56
2:B:524:ILE:HD12	2:B:524:ILE:H	1.71	0.56
1:A:171:VAL:HG11	1:A:265:TYR:HD2	1.71	0.55
1:A:100:LYS:HD3	1:A:102:ILE:HD11	1.87	0.55
1:A:435:THR:OG1	1:A:485:LYS:NZ	2.39	0.55
1:A:160:HIS:NE2	1:A:164:MET:SD	2.78	0.55
1:A:255:CYS:HB3	1:A:789:MET:HG2	1.88	0.55
1:A:1023:ARG:HA	1:A:1028:LEU:HD12	1.89	0.55
1:A:253:LYS:HB3	1:A:286:MET:HG2	1.89	0.55
2:B:347:LEU:HB2	2:B:378:ASN:HD21	1.72	0.54
1:A:373:THR:HG22	1:A:387:LEU:HD11	1.90	0.54
2:B:386:ARG:HG2	2:B:396:LEU:HD12	1.90	0.54
2:B:568:PRO:HA	2:B:571:ILE:HD12	1.90	0.54
1:A:83:PHE:O	1:A:108:ARG:NH1	2.40	0.54
2:B:332:GLU:OE1	2:B:429:SER:OG	2.24	0.53
1:A:917:HIS:ND1	1:A:920:ASN:OD1	2.41	0.53
1:A:138:ASP:O	1:A:142:ASN:ND2	2.31	0.53
1:A:428:ASN:ND2	1:A:643:GLN:OE1	2.40	0.53
1:A:798:GLU:HB2	1:A:850:VAL:HB	1.90	0.53
1:A:76:GLU:H	1:A:76:GLU:CD	2.17	0.52
1:A:975:ARG:NE	1:A:978:GLU:OE1	2.42	0.52
2:B:412:SER:HA	2:B:423:LYS:HB3	1.92	0.52
1:A:400:ALA:HB3	1:A:429:LEU:HB2	1.91	0.51
1:A:199:SER:OG	1:A:201:ASN:OD1	2.20	0.51
1:A:148:LYS:O	1:A:148:LYS:HD3	2.10	0.51
1:A:908:THR:HA	1:A:913:ILE:HD12	1.93	0.50
1:A:726:GLU:HG3	1:A:730:VAL:HB	1.94	0.50
1:A:74:THR:HG22	1:A:75:GLN:H	1.76	0.50
1:A:100:LYS:HD2	2:B:493:ILE:HG23	1.93	0.50
1:A:423:ALA:HB1	1:A:445:LEU:HB3	1.92	0.50
1:A:133:ASP:HB2	1:A:136:VAL:HG12	1.93	0.49
1:A:171:VAL:HG11	1:A:265:TYR:CD2	2.47	0.49
1:A:192:VAL:HG23	1:A:283:PRO:HB2	1.95	0.48
1:A:398:ARG:HG2	1:A:609:PRO:HG2	1.96	0.48
2:B:337:ASP:OD1	2:B:337:ASP:N	2.42	0.48
1:A:421:PRO:HG3	1:A:455:LEU:HA	1.94	0.48
1:A:894:ILE:HG21	1:A:966:LYS:HD2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:ARG:NH1	1:A:644:TYR:OH	2.45	0.48
1:A:469:GLU:OE1	2:B:481:ARG:NH2	2.45	0.47
2:B:386:ARG:HG3	2:B:387:ASP:OD2	2.15	0.47
1:A:46:LYS:NZ	1:A:68:TYR:O	2.33	0.46
1:A:916:ARG:HH21	1:A:920:ASN:HB3	1.80	0.46
2:B:441:ASN:N	2:B:441:ASN:OD1	2.49	0.46
1:A:69:ILE:HD12	1:A:69:ILE:HA	1.87	0.46
1:A:777:ARG:HD3	1:A:777:ARG:HA	1.47	0.46
1:A:1006:LEU:HD21	1:A:1019:ILE:HD11	1.98	0.46
2:B:347:LEU:HD22	2:B:354:THR:HG23	1.96	0.46
2:B:442:ILE:HD11	2:B:587:LYS:HE3	1.96	0.46
1:A:132:LYS:HE2	1:A:132:LYS:HB2	1.70	0.46
1:A:487:PRO:HB3	1:A:491:VAL:HB	1.97	0.45
1:A:851:VAL:HG21	1:A:930:PHE:CE2	2.51	0.45
1:A:167:TYR:CE2	1:A:293:LEU:HD11	2.52	0.45
1:A:489:MET:HE1	1:A:610:MET:HE2	1.99	0.45
1:A:29:GLY:HA3	2:B:501:GLN:CD	2.41	0.45
1:A:485:LYS:HB2	1:A:485:LYS:HE2	1.65	0.45
1:A:187:LYS:HA	1:A:187:LYS:HD2	1.76	0.45
2:B:363:LYS:HA	2:B:363:LYS:HD2	1.75	0.45
2:B:439:GLU:HB3	2:B:444:ALA:HB3	1.98	0.45
1:A:83:PHE:HE1	1:A:104:PRO:HB3	1.82	0.45
1:A:495:HIS:HE2	1:A:577:ARG:HG3	1.82	0.45
1:A:627:LYS:HD3	1:A:627:LYS:HA	1.72	0.45
1:A:789:MET:HE2	1:A:789:MET:HB2	1.76	0.45
2:B:412:SER:OG	2:B:421:ASP:O	2.29	0.44
1:A:194:ILE:HD12	1:A:224:ALA:HB2	2.00	0.44
1:A:365:GLU:O	1:A:365:GLU:HG3	2.18	0.44
1:A:904:TYR:CE2	1:A:930:PHE:HA	2.52	0.44
2:B:372:LEU:HD21	2:B:374:LYS:HE3	2.00	0.44
1:A:281:ARG:HG2	1:A:282:MET:H	1.83	0.44
1:A:355:TYR:HE2	1:A:357:ARG:HB2	1.83	0.44
1:A:655:LYS:HE3	1:A:655:LYS:HB3	1.89	0.44
1:A:29:GLY:HA2	2:B:497:GLN:HE22	1.82	0.43
1:A:739:MET:SD	1:A:764:LEU:HD21	2.58	0.43
1:A:179:LYS:HA	1:A:179:LYS:HD2	1.81	0.43
1:A:165:TYR:O	1:A:661:GLN:HB2	2.18	0.43
1:A:856:THR:HG22	1:A:922:MET:SD	2.58	0.43
2:B:448:LYS:HD3	2:B:448:LYS:HA	1.83	0.43
1:A:179:LYS:HE3	1:A:183:ASN:HD21	1.84	0.43
1:A:796:ASN:O	1:A:852:ARG:NH2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:PHE:CE1	1:A:99:LEU:HD21	2.54	0.43
1:A:194:ILE:O	1:A:206:LYS:HA	2.19	0.43
1:A:700:LYS:HA	1:A:700:LYS:HD2	1.87	0.43
1:A:276:CYS:HB3	1:A:283:PRO:HG3	1.99	0.42
1:A:895:ASP:OD1	1:A:895:ASP:C	2.62	0.42
1:A:924:LYS:HB3	1:A:924:LYS:HE3	1.90	0.42
1:A:204:LYS:HE2	1:A:204:LYS:HB2	1.65	0.42
1:A:851:VAL:HG21	1:A:930:PHE:CZ	2.54	0.42
1:A:937:PHE:HD2	1:A:938:LEU:HG	1.83	0.42
1:A:527:ASP:HB2	1:A:550:PHE:HZ	1.85	0.42
2:B:551:LYS:HA	2:B:551:LYS:HD3	1.75	0.42
1:A:537:ARG:HE	1:A:537:ARG:HB2	1.58	0.42
1:A:752:LEU:HD23	1:A:760:GLN:HG2	2.02	0.42
1:A:146:VAL:HG23	1:A:655:LYS:HG2	2.02	0.42
1:A:608:ASP:HB3	1:A:611:VAL:HG23	2.02	0.42
1:A:962:ILE:HG23	1:A:967:GLY:HA2	2.01	0.42
1:A:850:VAL:HG12	1:A:852:ARG:H	1.83	0.42
1:A:325:LYS:NZ	1:A:480:PHE:O	2.46	0.41
1:A:940:HIS:HB3	1:A:951:ARG:HD3	2.00	0.41
1:A:699:LEU:HD23	1:A:699:LEU:HA	1.85	0.41
1:A:221:ILE:HD13	1:A:221:ILE:HA	1.81	0.41
1:A:816:ILE:HG21	1:A:911:LEU:HD21	2.02	0.41
2:B:449:LEU:HD12	2:B:580:TYR:HB3	2.03	0.41
1:A:346:VAL:HG23	2:B:564:ASN:HB3	2.01	0.41
1:A:1044:ASN:OD1	1:A:1049:GLY:N	2.54	0.41
2:B:372:LEU:O	2:B:379:LYS:N	2.49	0.41
1:A:172:GLU:OE1	1:A:274:ARG:NH1	2.53	0.41
1:A:1040:MET:O	1:A:1044:ASN:HB2	2.20	0.41
2:B:591:GLN:HA	2:B:594:LEU:HD12	2.02	0.41
1:A:729:LYS:HB3	1:A:729:LYS:HE3	1.66	0.41
2:B:472:ARG:O	2:B:476:GLU:HG2	2.21	0.41
1:A:152:ASP:OD1	1:A:152:ASP:C	2.64	0.41
1:A:17:PRO:HA	1:A:18:PRO:HD3	1.98	0.41
1:A:29:GLY:HA3	2:B:501:GLN:OE1	2.21	0.41
1:A:465:ASN:ND2	1:A:470:THR:HG21	2.35	0.41
1:A:929:LEU:HD11	1:A:960:PHE:HE2	1.85	0.41
2:B:394:ASP:OD1	2:B:394:ASP:N	2.54	0.41
2:B:538:ILE:HD13	2:B:538:ILE:HA	1.86	0.41
2:B:573:LEU:HD23	2:B:573:LEU:HA	1.84	0.41
1:A:345:ASN:C	2:B:561:LYS:HD3	2.45	0.41
1:A:336:ILE:HD13	1:A:402:LEU:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:LEU:HG	1:A:273:ILE:HD13	2.02	0.40
1:A:601:LEU:HB2	1:A:615:ALA:HB2	2.02	0.40
1:A:433:THR:O	1:A:433:THR:OG1	2.35	0.40
1:A:908:THR:HB	1:A:953:PRO:HG2	2.03	0.40
2:B:389:LYS:HE2	2:B:396:LEU:HB2	2.04	0.40
1:A:603:ASP:OD2	1:A:1003:SER:OG	2.23	0.40
1:A:712:LEU:HG	1:A:748:LEU:HD21	2.03	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	957/1096 (87%)	917 (96%)	40 (4%)	0	100	100
2	B	261/723 (36%)	254 (97%)	7 (3%)	0	100	100
All	All	1218/1819 (67%)	1171 (96%)	47 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	888/999 (89%)	885 (100%)	3 (0%)	86	88

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	245/653 (38%)	245 (100%)	0	100	100
All	All	1133/1652 (69%)	1130 (100%)	3 (0%)	84	88

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	772	MET
1	A	776	LYS
1	A	777	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	ASN
1	A	157	ASN
1	A	731	GLN
1	A	940	HIS
2	B	407	HIS
2	B	497	GLN
2	B	579	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 ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	L2V	A	1101	-	44,44,44	1.09	2 (4%)	60,61,61	0.67	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	L2V	A	1101	-	-	7/24/24/24	0/5/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1101	L2V	C38-N39	3.55	1.36	1.32
3	A	1101	L2V	C36-N35	3.18	1.36	1.32

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

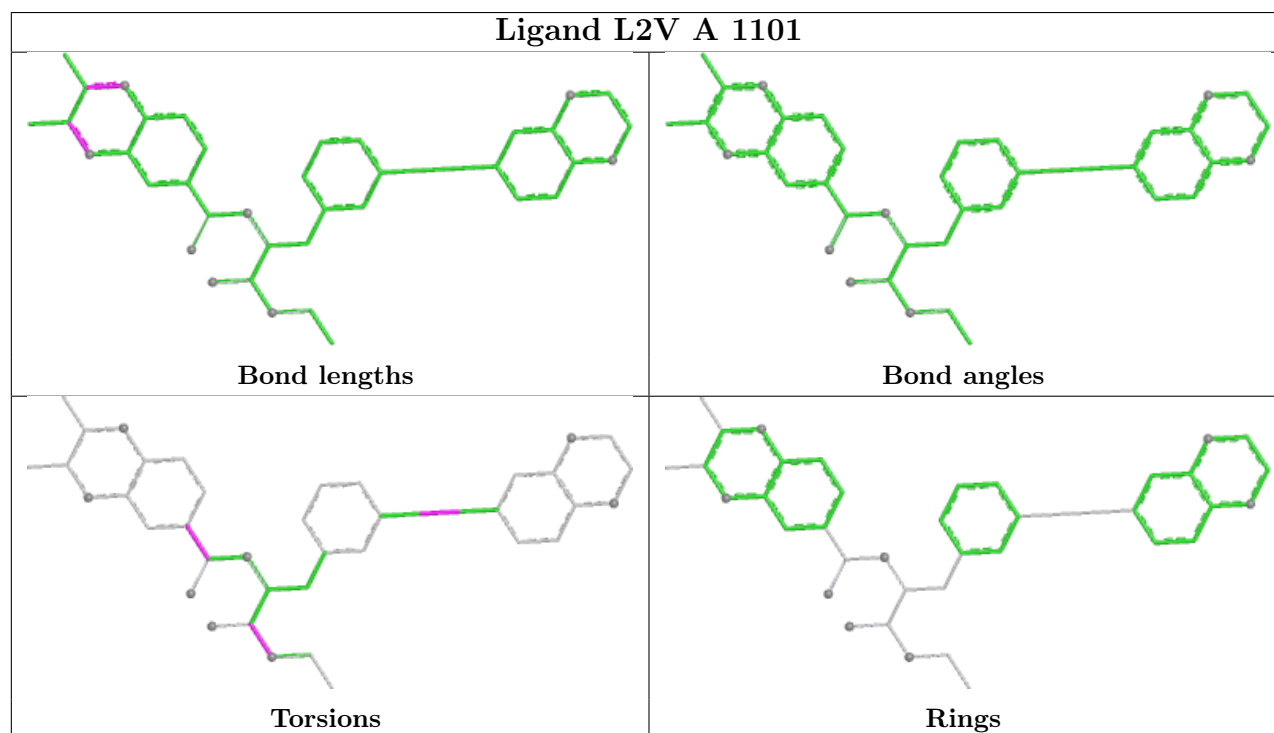
Mol	Chain	Res	Type	Atoms
3	A	1101	L2V	O22-C21-N23-C24
3	A	1101	L2V	C20-C21-N23-C24
3	A	1101	L2V	O28-C27-C29-C31
3	A	1101	L2V	N26-C27-C29-C31
3	A	1101	L2V	O28-C27-C29-C30
3	A	1101	L2V	N26-C27-C29-C30
3	A	1101	L2V	C09-C11-C12-C13

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

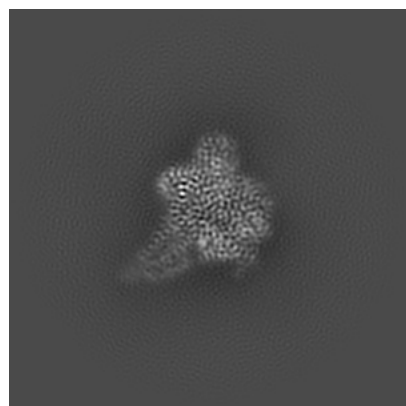
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35547. These allow visual inspection of the internal detail of the map and identification of artifacts.

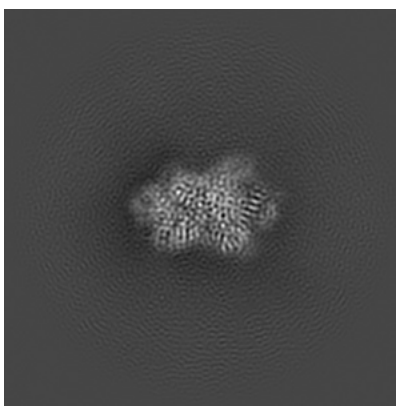
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

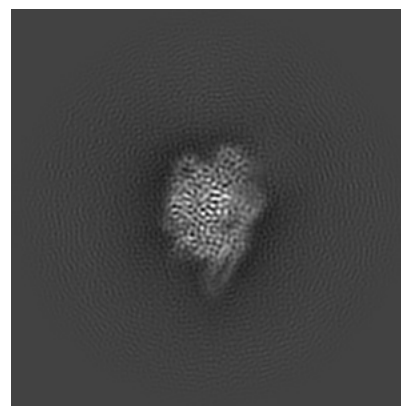
6.1.1 Primary map



X

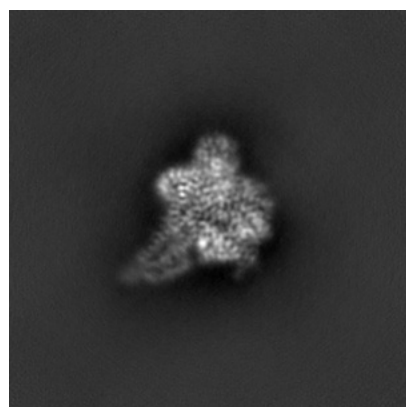


Y

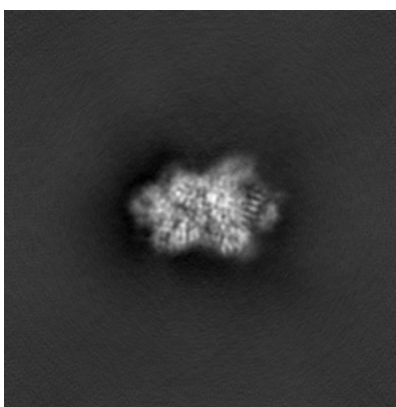


Z

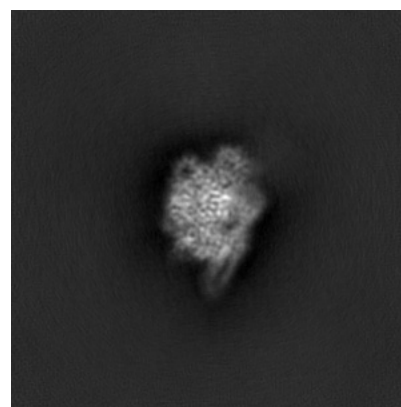
6.1.2 Raw map



X



Y

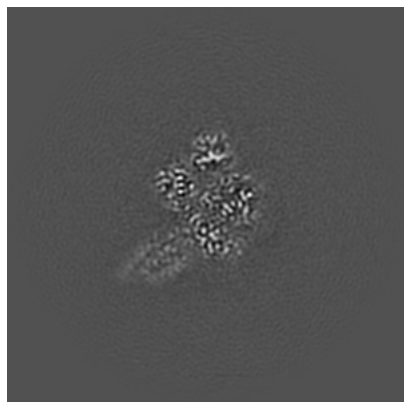


Z

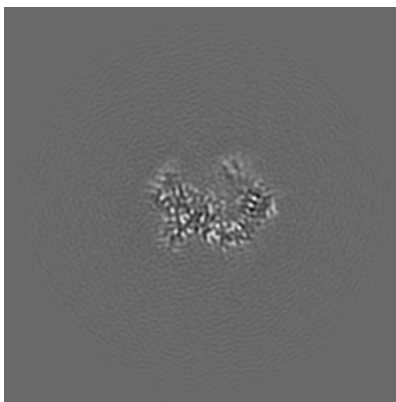
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

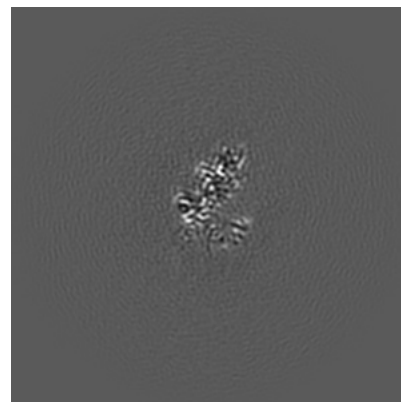
6.2.1 Primary map



X Index: 128

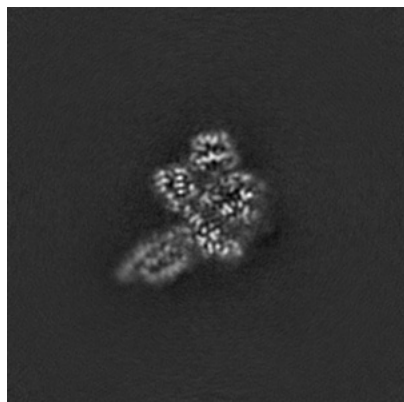


Y Index: 128

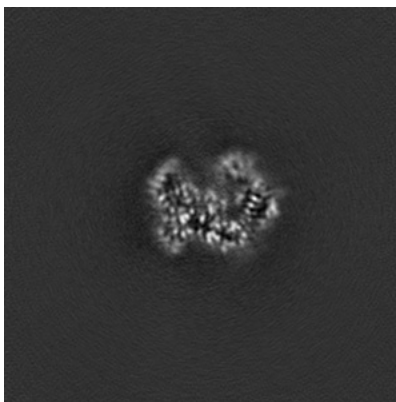


Z Index: 128

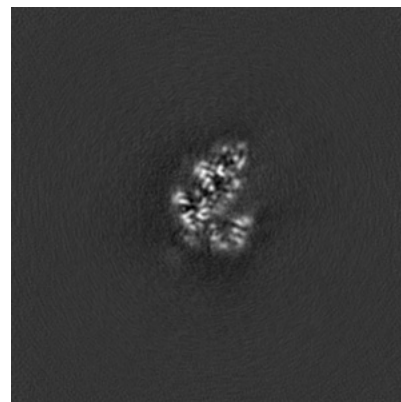
6.2.2 Raw map



X Index: 128



Y Index: 128

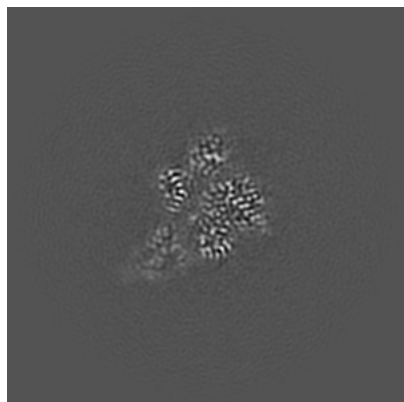


Z Index: 128

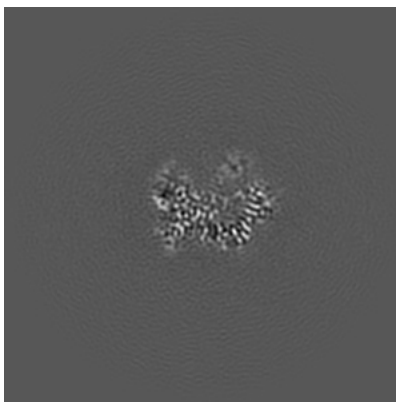
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

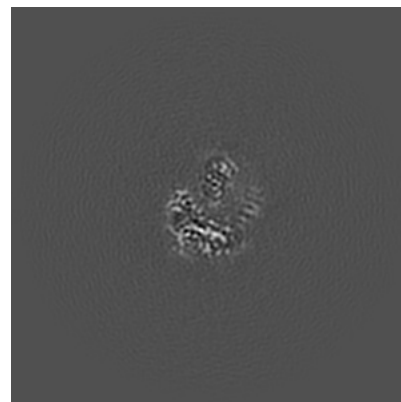
6.3.1 Primary map



X Index: 133

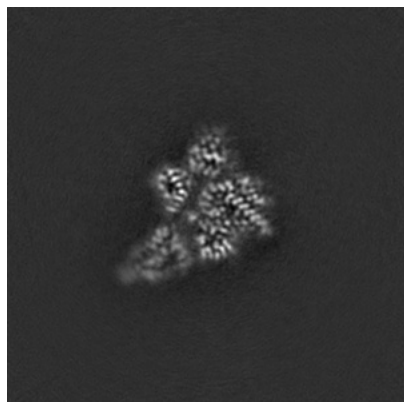


Y Index: 130

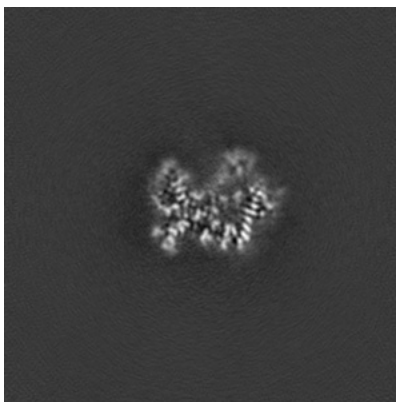


Z Index: 141

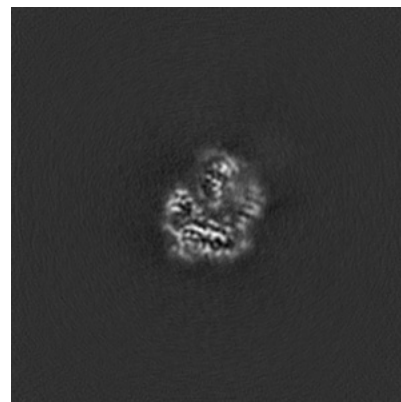
6.3.2 Raw map



X Index: 133



Y Index: 131

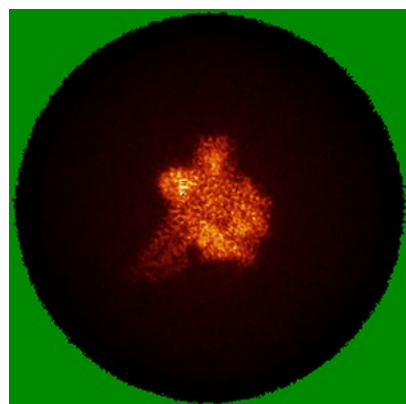


Z Index: 141

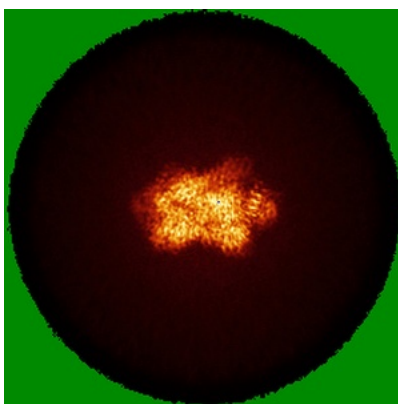
The images above show the largest variance slices of the map in three orthogonal directions.

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

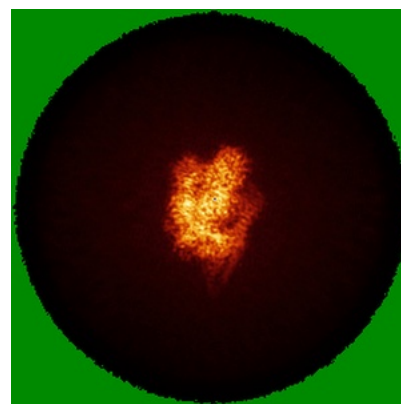
6.4.1 Primary map



X

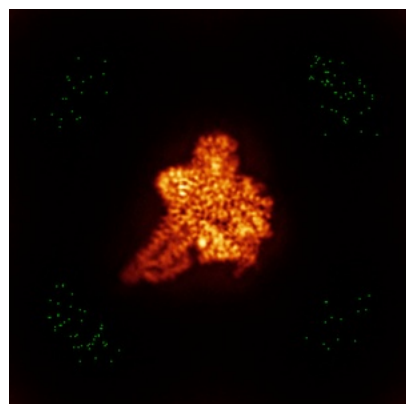


Y

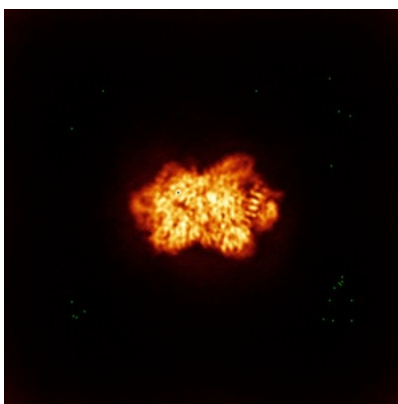


Z

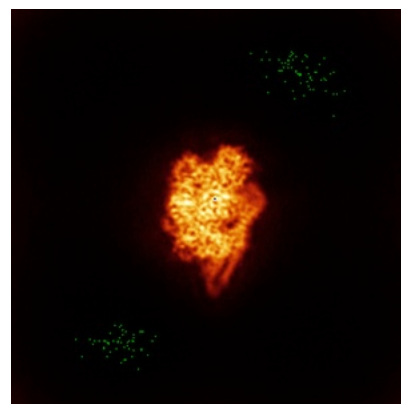
6.4.2 Raw map



X



Y

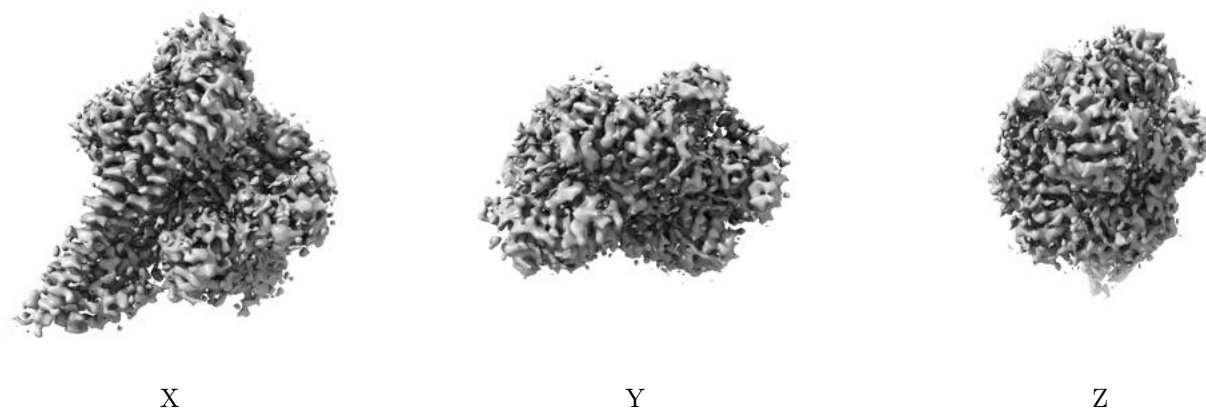


Z

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

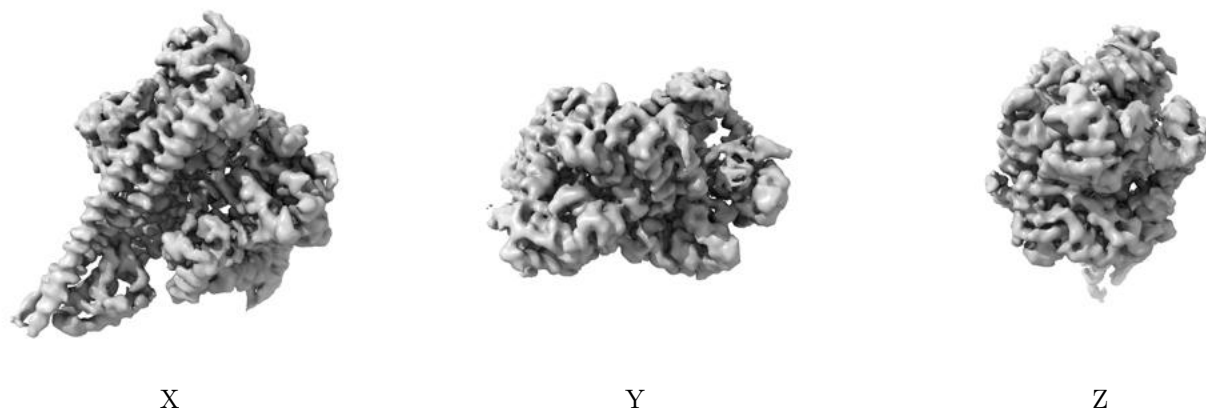
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.42. 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.

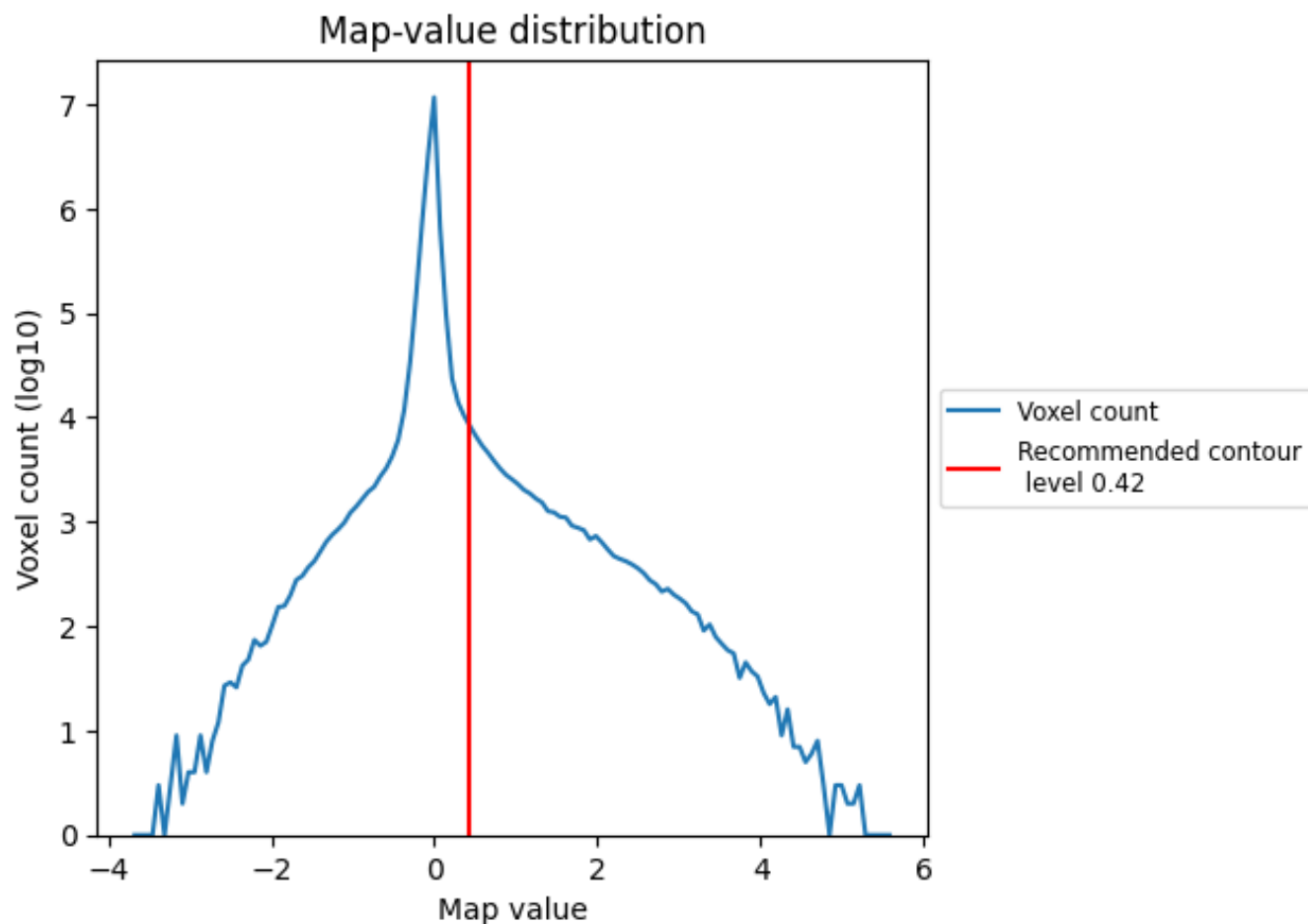
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

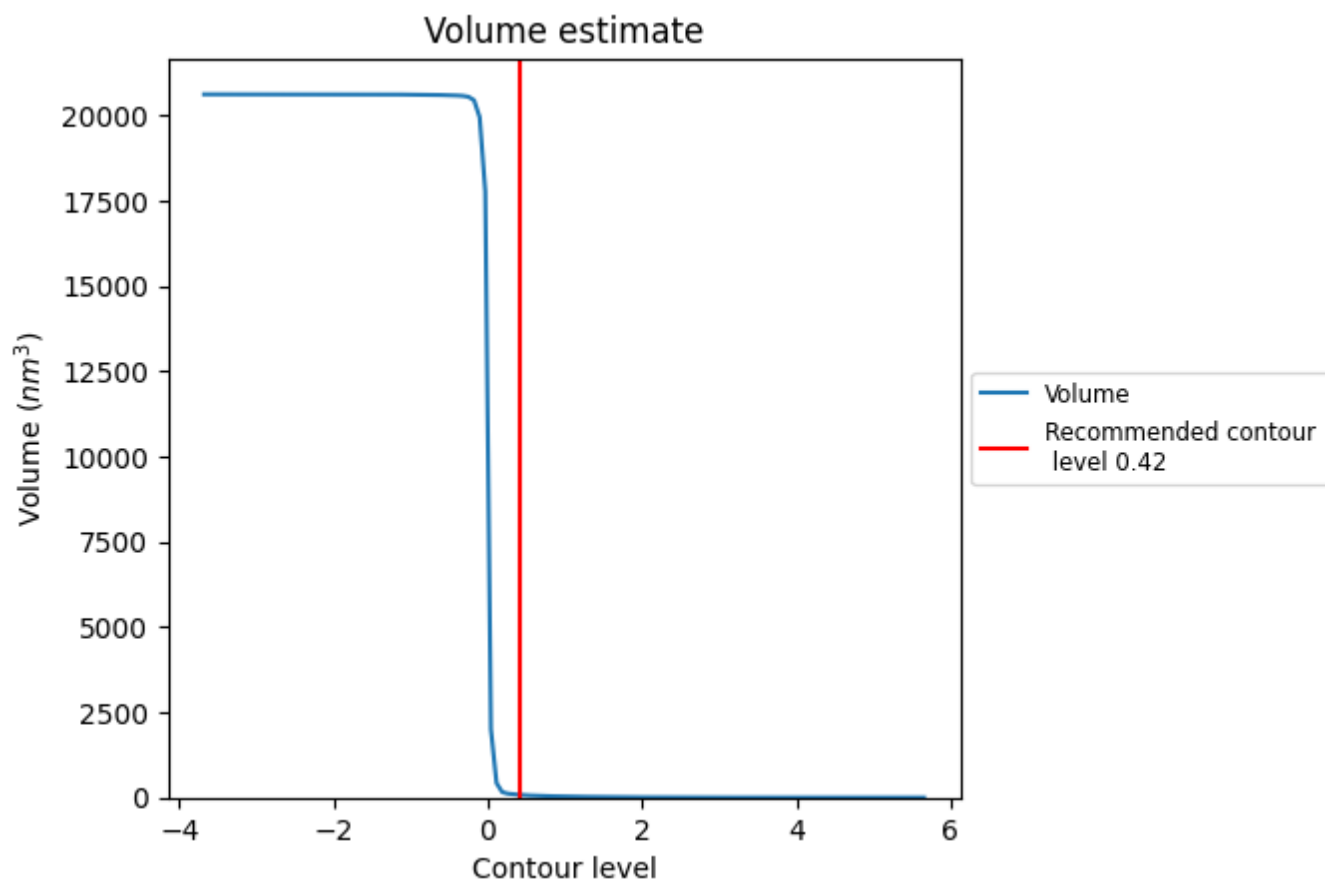
This section contains the results of statistical analysis of the map.

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.

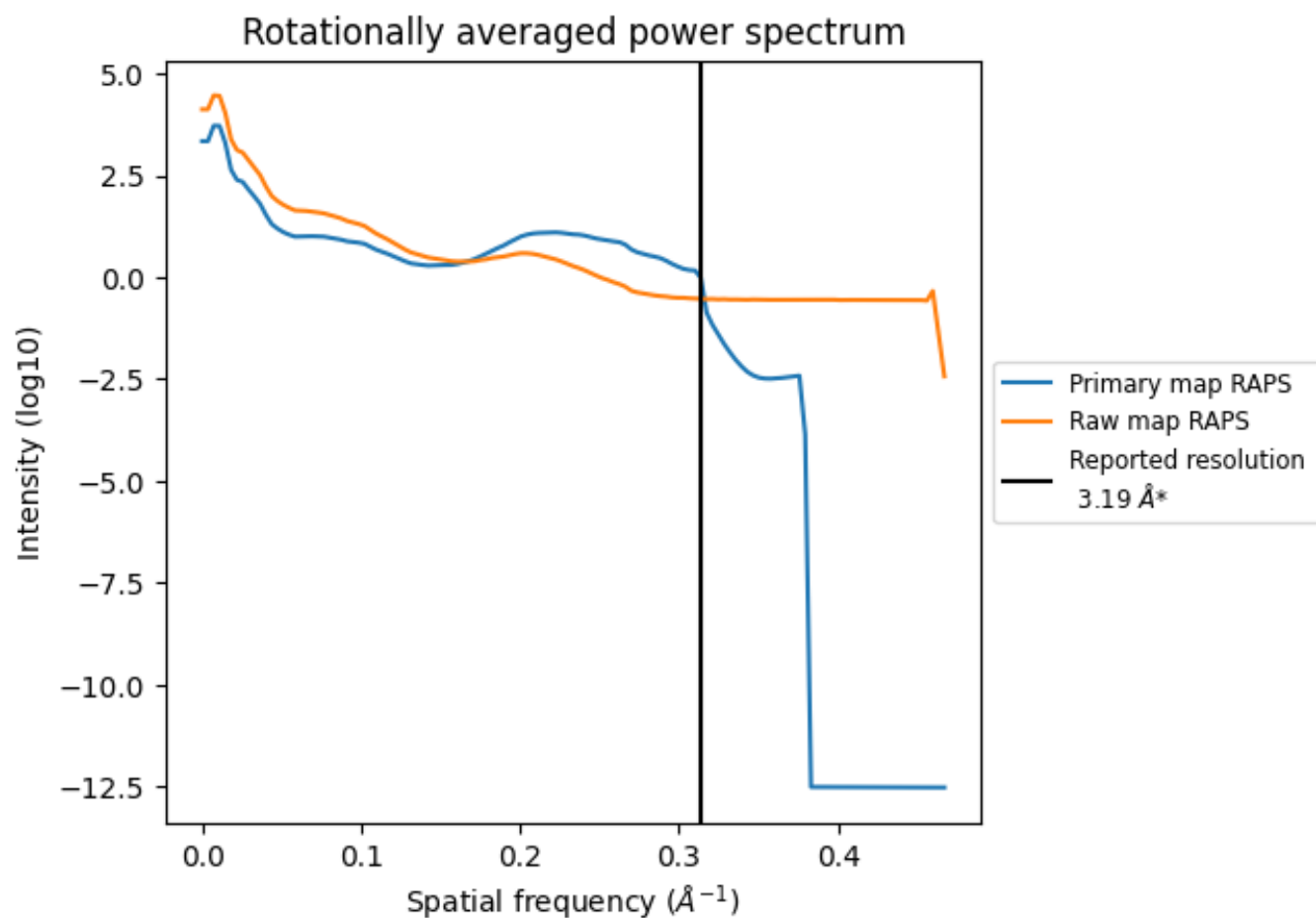
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 79 nm³; this corresponds to an approximate mass of 71 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 ⓘ

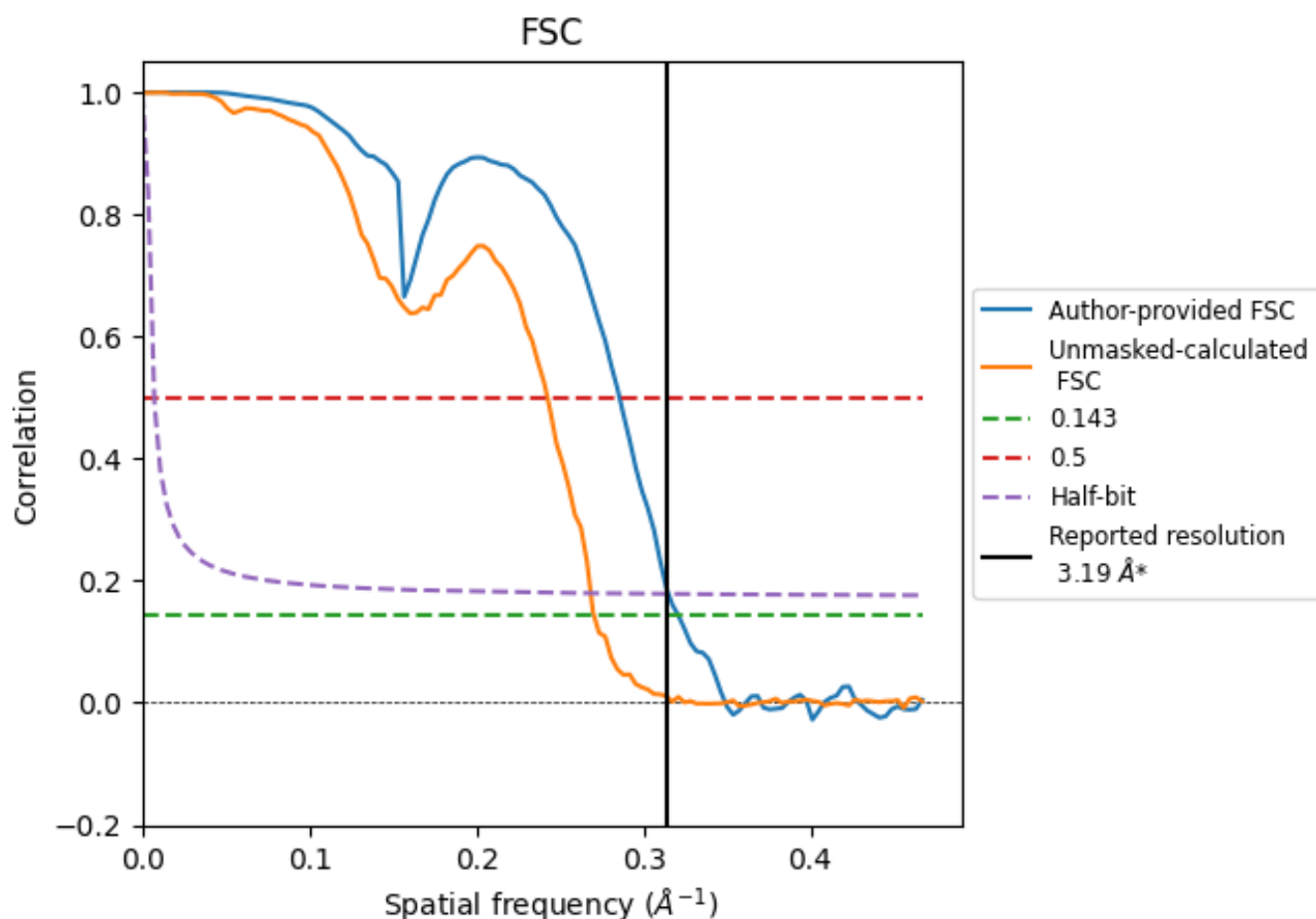


*Reported resolution corresponds to spatial frequency of 0.313 $\text{\AA}^{-1}$

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 0.313 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

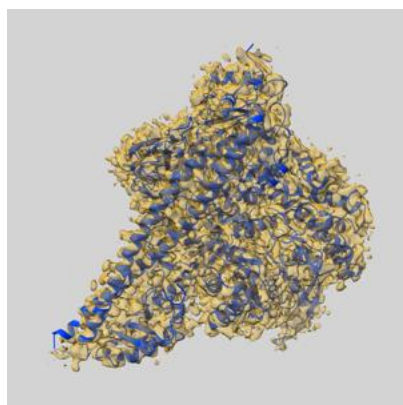
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.19	-	-
Author-provided FSC curve	3.12	3.50	3.17
Unmasked-calculated*	3.70	4.12	3.72

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.70 differs from the reported value 3.19 by more than 10 %

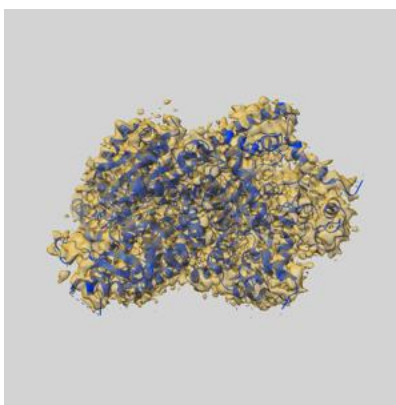
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-35547 and PDB model 8ILV. Per-residue inclusion information can be found in section 3 on page 5.

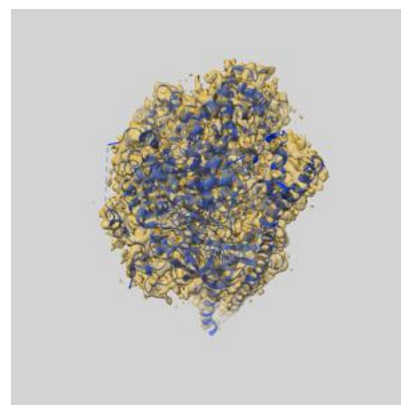
9.1 Map-model overlay [i](#)



X



Y



Z

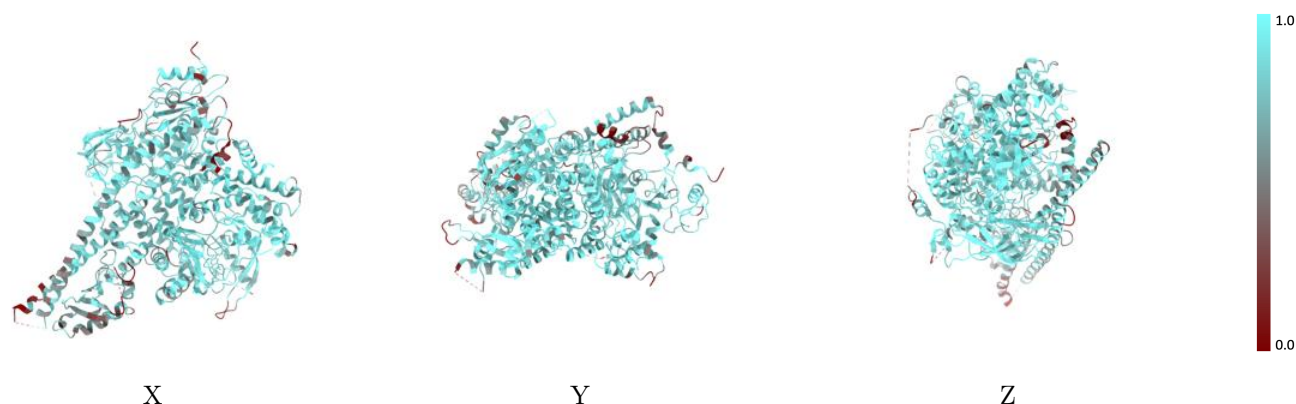
The images above show the 3D surface view of the map at the recommended contour level 0.42 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



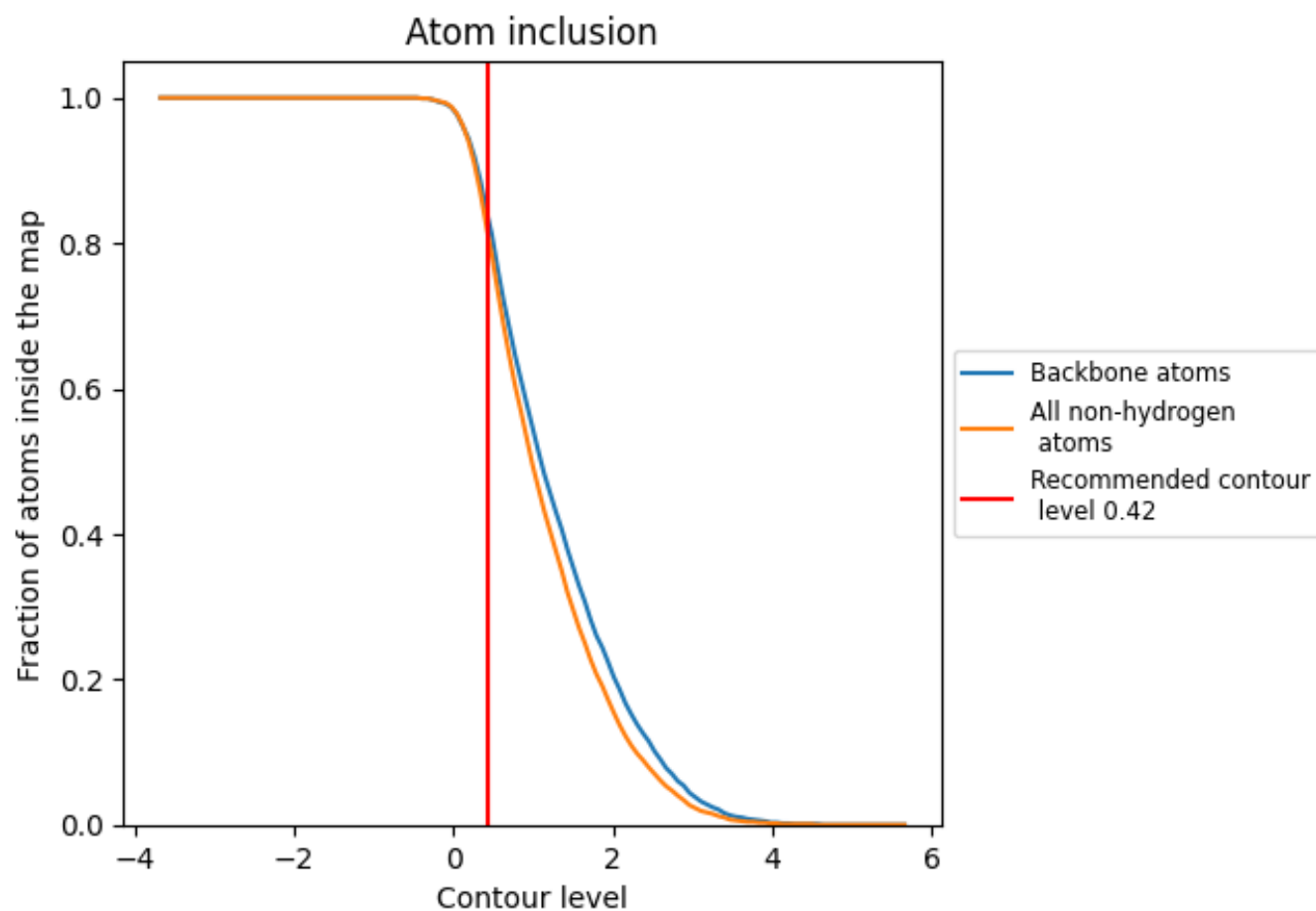
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.42).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 82% 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 (0.42) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8170	0.4920
A	0.8430	0.5050
B	0.7320	0.4450

