



Full wwPDB EM Validation Report ⓘ

Sep 27, 2026 – 12:44 AM JST

PDB ID : 9XW5 / pdb_00009xw5
EMDB ID : EMD-67325
Title : Cryo-EM structure of PI3Kalpha H1047R mutation in complex with STX-478
Authors : Liu, X.; Chen, Y.; Li, G.; Chen, A.; Zhou, Q.; Wang, M.-W.
Deposited on : 2025-11-27
Resolution : 3.31 Å(reported)

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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
Mogul : 1.8.5 (274361), CSD as541be (2020)
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 EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

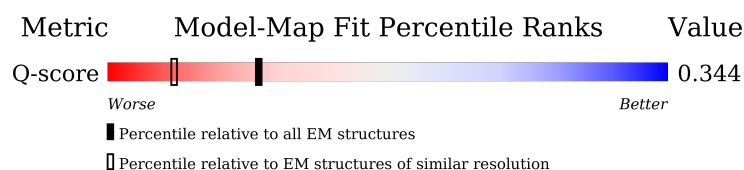
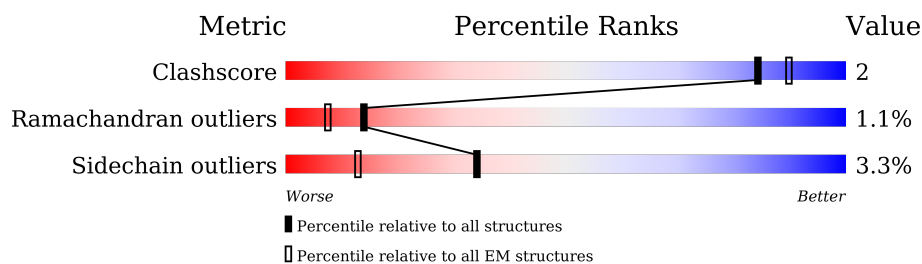
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.31 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	14550 (2.81 - 3.81)

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	9% 75% 13% • 12%
2	B	723	14% 36% • 61%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10333 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	966	7906	5055	1354	1433	64	1	0

There are 29 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
A	1047	ARG	HIS	engineered mutation	UNP P42336

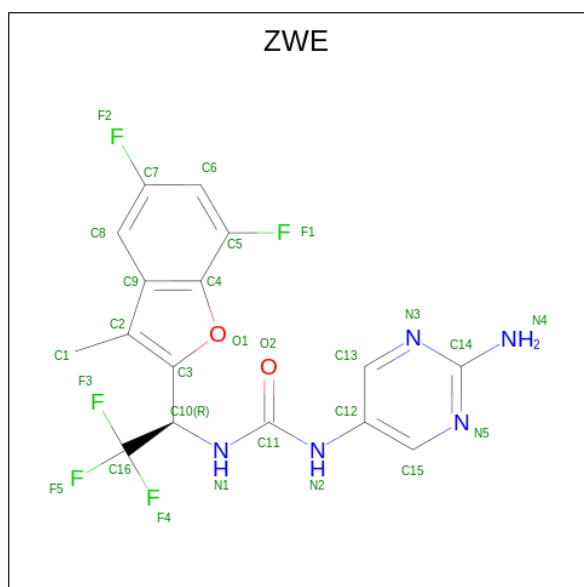
- Molecule 2 is a protein called Phosphatidylinositol 3-kinase regulatory subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	283	Total	C	N	O	S	0	0
			2399	1497	428	467	7		

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-(2-aminopyrimidin-5-yl)-N'-[(1R)-1-(5,7-difluoro-3-methyl-1-benzofuran-2-yl)-2,2,2-trifluoroethyl]urea (CCD ID: ZWE) (formula: C₁₆H₁₂F₅N₅O₂).

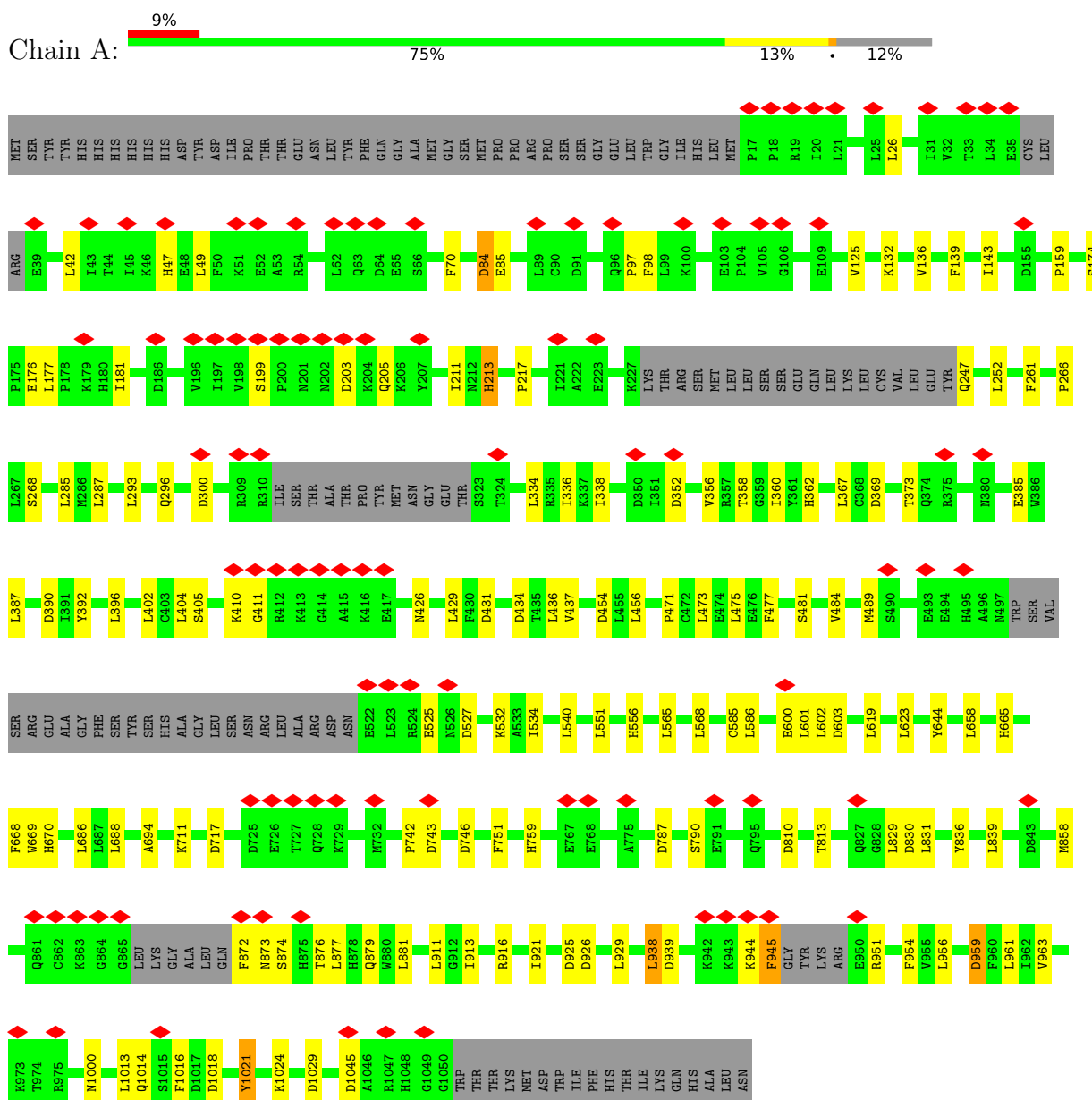


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	F	N	O	0
			28	16	5	5	2	

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



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E341
E342
V343
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V357
R358
D359
A360
S361
T362
K363
M364
H365
G366
D367
R366
D367
D394
I405

S412
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P418
K419
L420
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Y431
D434
Q435
V436
V437
K438
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D440
N441
I442
E443
A444
V445
G446
Y452
S460
D464
T471
Q475
T482
A486
I493
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Y504
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K513
R514
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G516
N517
E518

K519
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I539
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S541
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I559
D560
M563
K567
Q572
L573
R574
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Q579
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L581
L584
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ALA
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ARG

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	5684108	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.394	Depositor
Minimum map value	-1.059	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.077	Depositor
Map size (Å)	210.944, 210.944, 210.944	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.824, 0.824, 0.824	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.93	2/8078 (0.0%)	1.60	53/10906 (0.5%)
2	B	0.92	0/2439	1.65	12/3269 (0.4%)
All	All	0.93	2/10517 (0.0%)	1.61	65/14175 (0.5%)

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	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	810	ASP	CG-OD1	6.03	1.36	1.25
1	A	600	GLU	CD-OE2	6.01	1.36	1.25

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	434	ASP	CA-CB-CG	8.92	121.52	112.60
1	A	717	ASP	CA-CB-CG	8.15	120.75	112.60
1	A	392	TYR	CA-C-N	7.87	126.62	120.33
1	A	392	TYR	C-N-CA	7.87	126.62	120.33
1	A	746	ASP	CA-CB-CG	7.46	120.06	112.60
1	A	743	ASP	CA-CB-CG	7.39	120.00	112.60
1	A	369	ASP	CA-CB-CG	7.32	119.92	112.60
1	A	84	ASP	CA-CB-CG	7.10	119.70	112.60
1	A	959	ASP	CA-CB-CG	6.88	119.48	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	926	ASP	CA-CB-CG	6.84	119.44	112.60
1	A	527	ASP	CA-CB-CG	6.76	119.36	112.60
1	A	390	ASP	CA-CB-CG	6.71	119.31	112.60
2	B	605	ASP	CA-CB-CG	6.69	119.29	112.60
1	A	352	ASP	CA-CB-CG	6.64	119.24	112.60
1	A	431	ASP	CA-CB-CG	6.44	119.04	112.60
2	B	578	ASP	CA-C-N	6.40	129.69	120.79
2	B	578	ASP	C-N-CA	6.40	129.69	120.79
2	B	421	ASP	CA-CB-CG	6.37	118.97	112.60
2	B	579	GLN	CA-CB-CG	6.18	126.45	114.10
2	B	394	ASP	CA-CB-CG	6.07	118.67	112.60
1	A	213	HIS	CA-CB-CG	6.00	119.80	113.80
1	A	426	ASN	CA-CB-CG	5.95	118.55	112.60
1	A	787	ASP	CA-C-N	5.92	128.88	120.53
1	A	787	ASP	C-N-CA	5.92	128.88	120.53
1	A	830	ASP	CA-CB-CG	5.92	118.52	112.60
1	A	203	ASP	CA-CB-CG	5.91	118.51	112.60
1	A	1000	ASN	CA-CB-CG	5.91	118.51	112.60
2	B	540	ASP	CA-CB-CG	5.79	118.39	112.60
2	B	417	ASN	CA-CB-CG	5.76	118.36	112.60
1	A	300	ASP	CA-CB-CG	5.73	118.33	112.60
1	A	939	ASP	CA-CB-CG	5.68	118.28	112.60
1	A	836	TYR	CA-C-N	5.66	125.72	120.34
1	A	836	TYR	C-N-CA	5.66	125.72	120.34
1	A	603	ASP	CA-C-N	5.62	128.37	120.28
1	A	603	ASP	C-N-CA	5.62	128.37	120.28
1	A	787	ASP	CA-CB-CG	5.53	118.13	112.60
2	B	529	ASP	CA-CB-CG	5.47	118.07	112.60
1	A	925	ASP	CA-CB-CG	5.47	118.07	112.60
2	B	527	ASN	CA-CB-CG	5.43	118.03	112.60
1	A	1018	ASP	CA-CB-CG	5.42	118.02	112.60
1	A	945	PHE	CA-CB-CG	5.41	119.21	113.80
1	A	1045	ASP	CA-CB-CG	5.36	117.96	112.60
1	A	603	ASP	CA-CB-CG	5.36	117.96	112.60
1	A	954	PHE	CA-CB-CG	5.33	119.13	113.80
1	A	362	HIS	CE1-NE2-CD2	-5.22	103.78	109.00
1	A	665	HIS	ND1-CE1-NE2	5.22	113.62	108.40
1	A	266	PRO	CA-C-N	5.21	127.52	120.38
1	A	266	PRO	C-N-CA	5.21	127.52	120.38
1	A	454	ASP	CA-CB-CG	5.16	117.75	112.60
1	A	1029	ASP	CA-CB-CG	5.14	117.74	112.60
1	A	790	SER	CA-C-N	5.13	127.41	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	790	SER	C-N-CA	5.13	127.41	120.38
1	A	751	PHE	CA-CB-CG	5.12	118.92	113.80
1	A	261	PHE	CA-CB-CG	5.10	118.90	113.80
1	A	742	PRO	CA-C-N	5.08	127.04	120.44
1	A	742	PRO	C-N-CA	5.08	127.04	120.44
1	A	98	PHE	CA-CB-CG	5.07	118.87	113.80
1	A	670	HIS	CE1-NE2-CD2	-5.07	103.93	109.00
2	B	512	PHE	CA-CB-CG	5.03	118.83	113.80
1	A	47	HIS	ND1-CE1-NE2	5.03	113.43	108.40
1	A	362	HIS	ND1-CE1-NE2	5.02	113.42	108.40
2	B	560	ASP	CA-CB-CG	5.02	117.62	112.60
1	A	759	HIS	CE1-NE2-CD2	-5.01	103.99	109.00
1	A	47	HIS	CE1-NE2-CD2	-5.01	103.99	109.00
1	A	556	HIS	CE1-NE2-CD2	-5.01	103.99	109.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1021	TYR	Sidechain
1	A	644	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7906	0	7919	42	0
2	B	2399	0	2359	5	0
3	A	28	0	0	4	0
All	All	10333	0	10278	48	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 2.

All (48) 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:338:ILE:HD11	1:A:473:LEU:HD11	1.55	0.89
1:A:1021:TYR:CD2	3:A:1101:ZWE:F3	2.16	0.88
1:A:336:ILE:HD11	1:A:402:LEU:HD11	1.62	0.80
1:A:921:ILE:HD11	1:A:929:LEU:HD21	1.68	0.74
1:A:402:LEU:HD13	1:A:429:LEU:HD13	1.71	0.72
2:B:581:LEU:HD23	2:B:594:LEU:HD11	1.72	0.70
2:B:357:VAL:HG21	2:B:405:ILE:HD11	1.76	0.67
1:A:373:THR:HB	1:A:387:LEU:HD21	1.80	0.64
1:A:252:LEU:H	1:A:252:LEU:HD23	1.66	0.60
3:A:1101:ZWE:F5	3:A:1101:ZWE:C11	2.42	0.57
1:A:136:VAL:HG13	1:A:686:LEU:HD21	1.89	0.55
2:B:581:LEU:CD2	2:B:594:LEU:HD11	2.37	0.54
1:A:139:PHE:CE1	1:A:143:ILE:HD12	2.42	0.53
1:A:938:LEU:HD13	1:A:1013:LEU:HD11	1.90	0.53
1:A:436:LEU:HD12	1:A:484:VAL:HB	1.91	0.51
1:A:404:LEU:HD12	1:A:475:LEU:HD21	1.92	0.51
1:A:602:LEU:HD11	1:A:619:LEU:HD11	1.92	0.51
1:A:336:ILE:HD13	1:A:404:LEU:HD11	1.93	0.51
1:A:405:SER:HB3	1:A:456:LEU:HD23	1.93	0.51
1:A:911:LEU:O	3:A:1101:ZWE:F1	2.19	0.51
1:A:26:LEU:HD11	1:A:49:LEU:HD22	1.93	0.50
1:A:217:PRO:HB3	1:A:252:LEU:HD21	1.93	0.50
1:A:858:MET:HE2	1:A:858:MET:H	1.77	0.49
1:A:360:ILE:CD1	1:A:402:LEU:HD12	2.44	0.48
1:A:358:THR:HB	1:A:404:LEU:HD22	1.97	0.47
1:A:668:PHE:CD2	1:A:688:LEU:HD11	2.49	0.47
1:A:945:PHE:O	3:A:1101:ZWE:F4	2.23	0.46
1:A:829:LEU:HB3	1:A:831:LEU:HD23	1.98	0.46
1:A:334:LEU:HD21	1:A:396:LEU:HD11	1.98	0.45
1:A:540:LEU:HD12	1:A:1016:PHE:CZ	2.51	0.45
1:A:360:ILE:HG22	1:A:367:LEU:HD12	1.99	0.44
1:A:338:ILE:HD13	1:A:356:VAL:HG21	2.00	0.44
1:A:658:LEU:HD22	1:A:694:ALA:O	2.17	0.44
1:A:534:ILE:HG21	1:A:551:LEU:HD21	1.99	0.44
1:A:252:LEU:HD12	1:A:285:LEU:HD13	1.99	0.44
1:A:177:LEU:HD21	1:A:268:SER:HB2	2.00	0.43
1:A:956:LEU:HB3	1:A:961:LEU:HD21	2.00	0.43
1:A:913:ILE:HG22	1:A:916:ARG:HD3	2.00	0.43
1:A:49:LEU:HD11	1:A:70:PHE:CE1	2.53	0.43
1:A:565:LEU:HD23	1:A:601:LEU:HD21	2.02	0.42
2:B:452:TYR:CE1	2:B:573:LEU:HD22	2.54	0.42
1:A:872:PHE:O	1:A:876:THR:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:LEU:HD22	1:A:85:GLU:HA	2.01	0.42
1:A:669:TRP:HB3	1:A:839:LEU:HD21	2.01	0.41
1:A:410:LYS:HG2	1:A:411:GLY:H	1.86	0.41
1:A:619:LEU:HD22	1:A:623:LEU:HD22	2.03	0.41
1:A:877:LEU:HD22	1:A:963:VAL:HG21	2.02	0.41
2:B:584:LEU:HD23	2:B:594:LEU:HD13	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	953/1096 (87%)	878 (92%)	65 (7%)	10 (1%)	12	41
2	B	281/723 (39%)	257 (92%)	21 (8%)	3 (1%)	11	40
All	All	1234/1819 (68%)	1135 (92%)	86 (7%)	13 (1%)	14	40

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1014	GLN
1	A	176	GLU
1	A	477	PHE
2	B	602	ASN
1	A	159	PRO
1	A	481	SER
2	B	603	THR
1	A	97	PRO
1	A	489	MET
1	A	525	GLU
2	B	591	GLN
1	A	471	PRO

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Mol	Chain	Res	Type
1	A	199	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	885/999 (89%)	856 (97%)	29 (3%)	33	60
2	B	263/653 (40%)	254 (97%)	9 (3%)	32	59
All	All	1148/1652 (70%)	1110 (97%)	38 (3%)	34	60

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	ASP
1	A	125	VAL
1	A	132	LYS
1	A	174	SER
1	A	181	ILE
1	A	205	GLN
1	A	211	ILE
1	A	213	HIS
1	A	247	GLN
1	A	287	LEU
1	A	293	LEU
1	A	296	GLN
1	A	385	GLU
1	A	437	VAL
1	A	532	LYS
1	A	568	LEU
1	A	585	CYS
1	A	586	LEU
1	A	711	LYS
1	A	813	THR
1	A	873	ASN
1	A	874	SER

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Mol	Chain	Res	Type
1	A	879	GLN
1	A	881	LEU
1	A	938	LEU
1	A	944	LYS
1	A	951	ARG
1	A	959	ASP
1	A	1024	LYS
2	B	324	ASN
2	B	343	VAL
2	B	439	GLU
2	B	452	TYR
2	B	527	ASN
2	B	563	MET
2	B	567	LYS
2	B	579	GLN
2	B	605	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	ASN
1	A	180	HIS
1	A	189	GLN
1	A	212	ASN
1	A	219	GLN
1	A	388	ASN
1	A	495	HIS
1	A	661	GLN
1	A	676	HIS
1	A	703	ASN
1	A	714	ASN
1	A	728	GLN
1	A	825	GLN
1	A	855	HIS
1	A	861	GLN
1	A	875	HIS
1	A	920	ASN
1	A	996	ASN
1	A	1000	ASN
2	B	407	HIS
2	B	435	GLN
2	B	564	ASN

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	ZWE	A	1101	-	28,30,30	2.33	8 (28%)	37,45,45	2.35	13 (35%)

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	ZWE	A	1101	-	-	9/15/18/18	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1101	ZWE	O1-C3	-6.18	1.32	1.38
3	A	1101	ZWE	C14-N4	5.69	1.45	1.33
3	A	1101	ZWE	C11-N1	4.54	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1101	ZWE	C11-N2	3.81	1.45	1.37
3	A	1101	ZWE	C14-N5	-2.93	1.31	1.35
3	A	1101	ZWE	C14-N3	-2.42	1.32	1.35
3	A	1101	ZWE	O2-C11	-2.02	1.19	1.23
3	A	1101	ZWE	C9-C4	-2.01	1.36	1.39

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1101	ZWE	C12-C13-N3	-6.77	118.04	124.13
3	A	1101	ZWE	C12-C15-N5	-6.23	118.53	124.13
3	A	1101	ZWE	N2-C11-N1	3.84	119.12	113.76
3	A	1101	ZWE	C12-N2-C11	-3.25	119.97	126.61
3	A	1101	ZWE	O1-C4-C5	3.21	130.96	126.33
3	A	1101	ZWE	C8-C7-C6	-3.15	119.54	123.52
3	A	1101	ZWE	N5-C14-N3	-3.02	121.32	124.53
3	A	1101	ZWE	C13-N3-C14	2.72	121.49	116.44
3	A	1101	ZWE	C15-N5-C14	2.68	121.40	116.44
3	A	1101	ZWE	N4-C14-N3	2.55	120.02	117.44
3	A	1101	ZWE	F5-C16-C10	-2.26	107.92	112.02
3	A	1101	ZWE	F3-C16-C10	-2.20	108.02	112.02
3	A	1101	ZWE	C9-C8-C7	2.20	121.63	117.98

There are no chirality outliers.

All (9) torsion outliers are listed below:

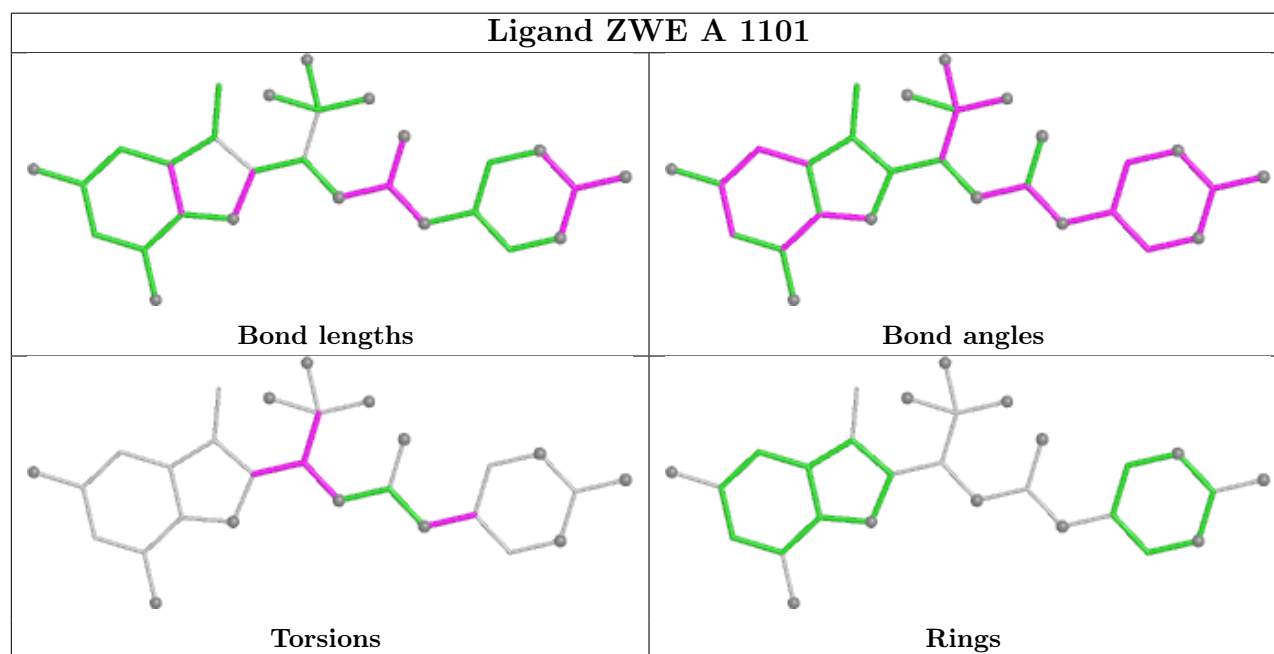
Mol	Chain	Res	Type	Atoms
3	A	1101	ZWE	C3-C10-N1-C11
3	A	1101	ZWE	C16-C10-N1-C11
3	A	1101	ZWE	C15-C12-N2-C11
3	A	1101	ZWE	C13-C12-N2-C11
3	A	1101	ZWE	C3-C10-C16-F3
3	A	1101	ZWE	C3-C10-C16-F4
3	A	1101	ZWE	C3-C10-C16-F5
3	A	1101	ZWE	N1-C10-C3-O1
3	A	1101	ZWE	N1-C10-C16-F5

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1101	ZWE	4	0

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.

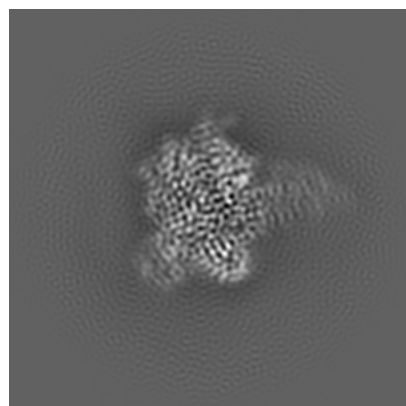
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-67325. These allow visual inspection of the internal detail of the map and identification of artifacts.

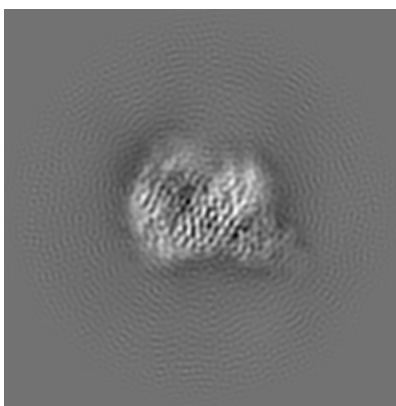
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

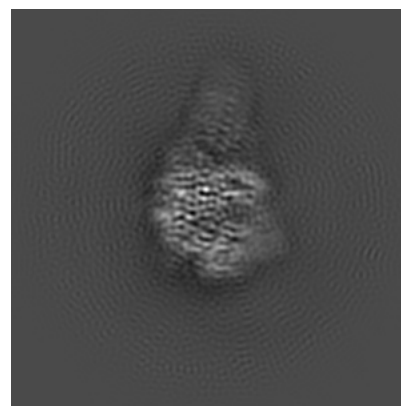
6.1.1 Primary map



X

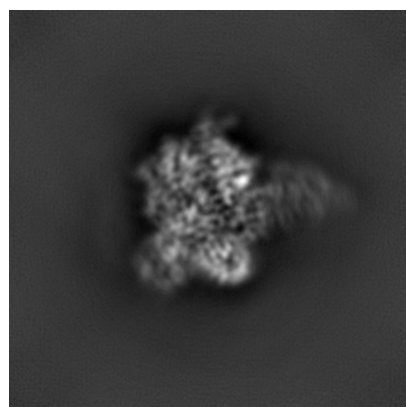


Y

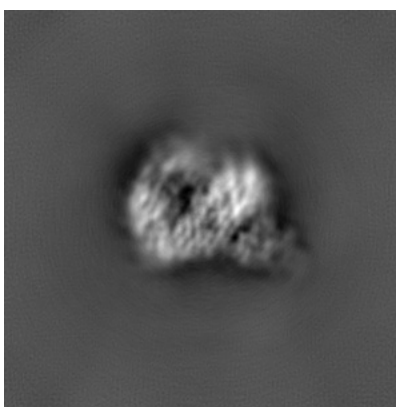


Z

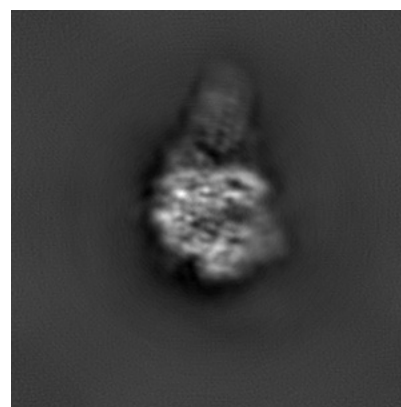
6.1.2 Raw map



X



Y

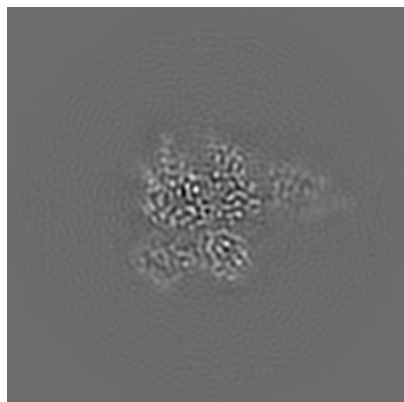


Z

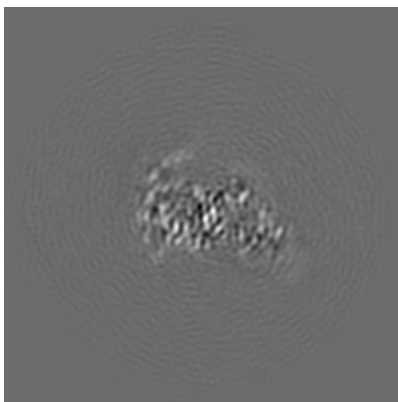
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

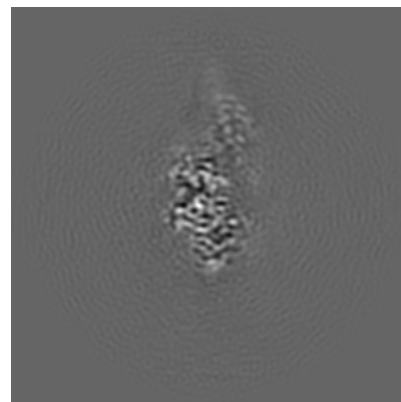
6.2.1 Primary map



X Index: 128

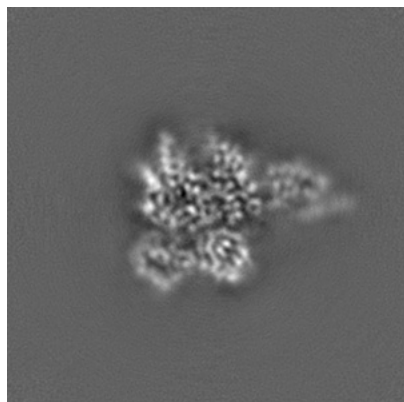


Y Index: 128

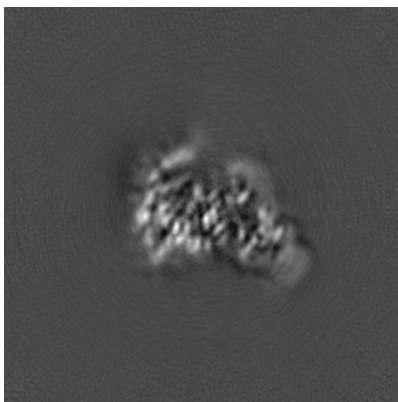


Z Index: 128

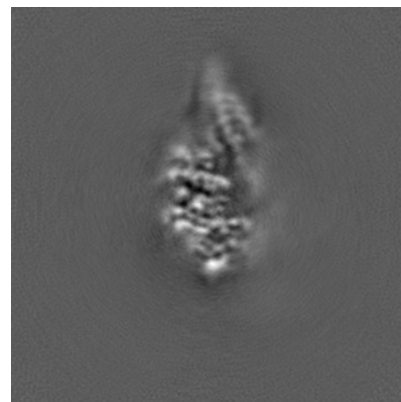
6.2.2 Raw map



X Index: 128



Y Index: 128

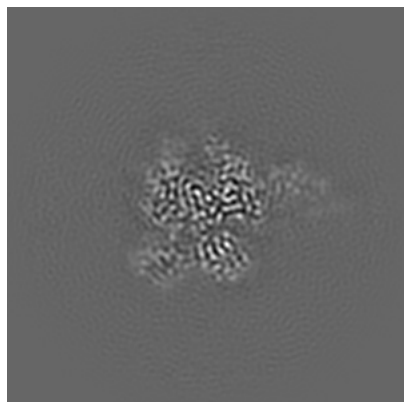


Z Index: 128

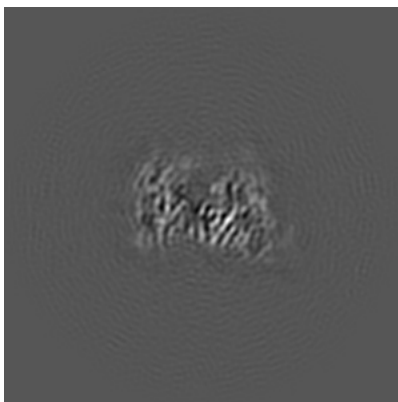
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

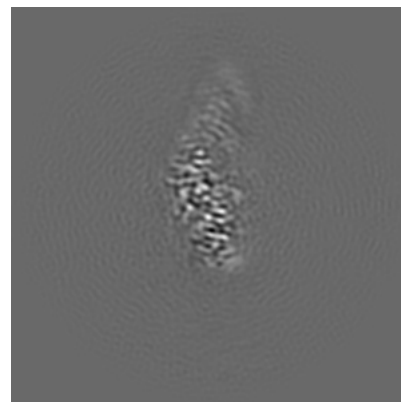
6.3.1 Primary map



X Index: 125

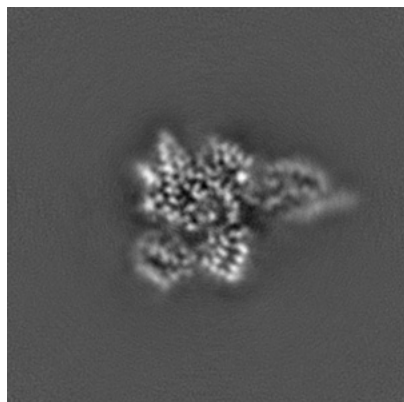


Y Index: 139

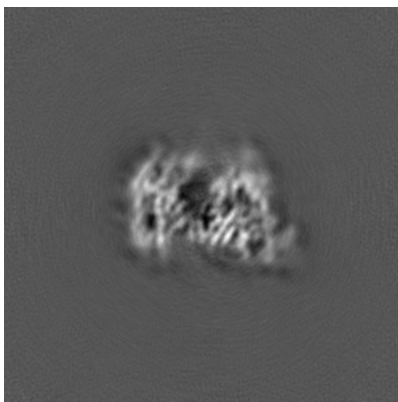


Z Index: 137

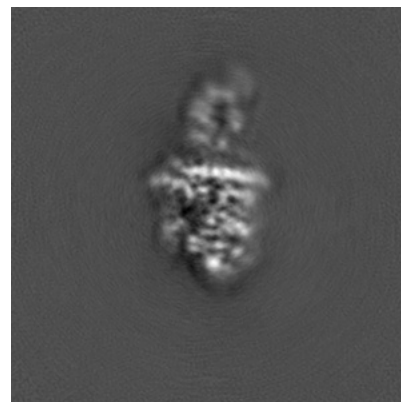
6.3.2 Raw map



X Index: 131



Y Index: 138

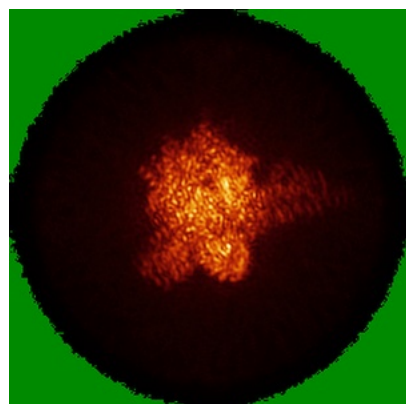


Z Index: 146

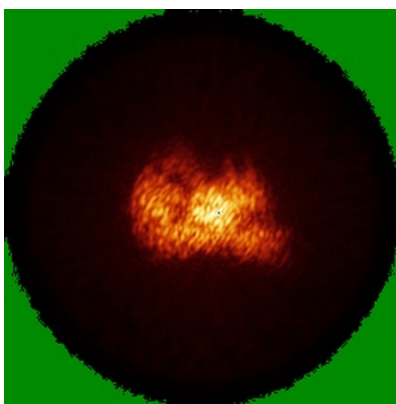
The images above show the largest variance slices of the map in three orthogonal directions.

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

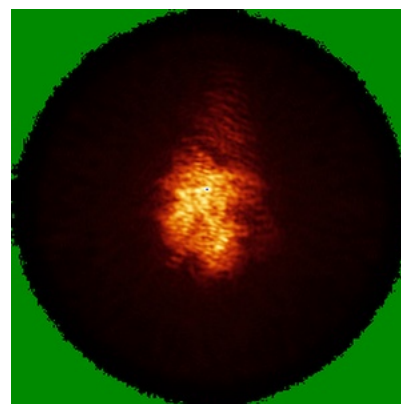
6.4.1 Primary map



X

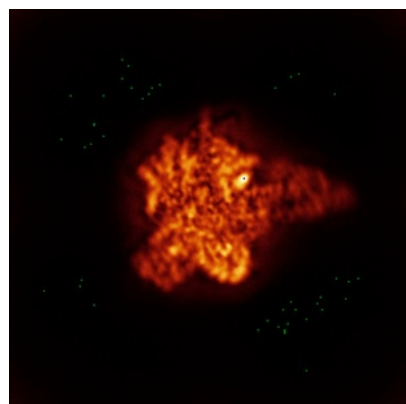


Y

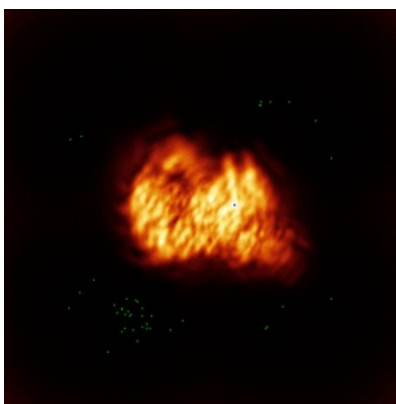


Z

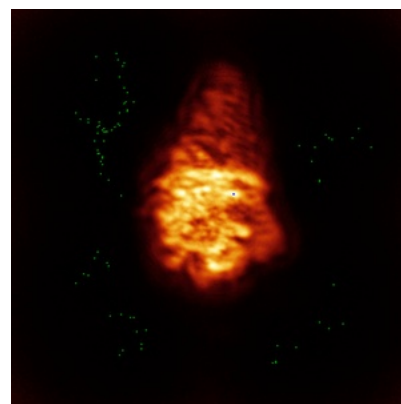
6.4.2 Raw map



X



Y

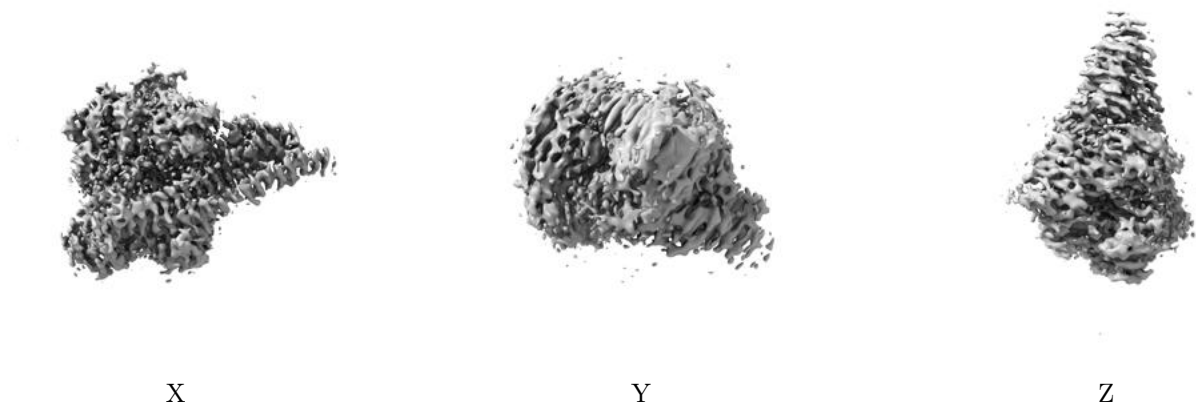


Z

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.

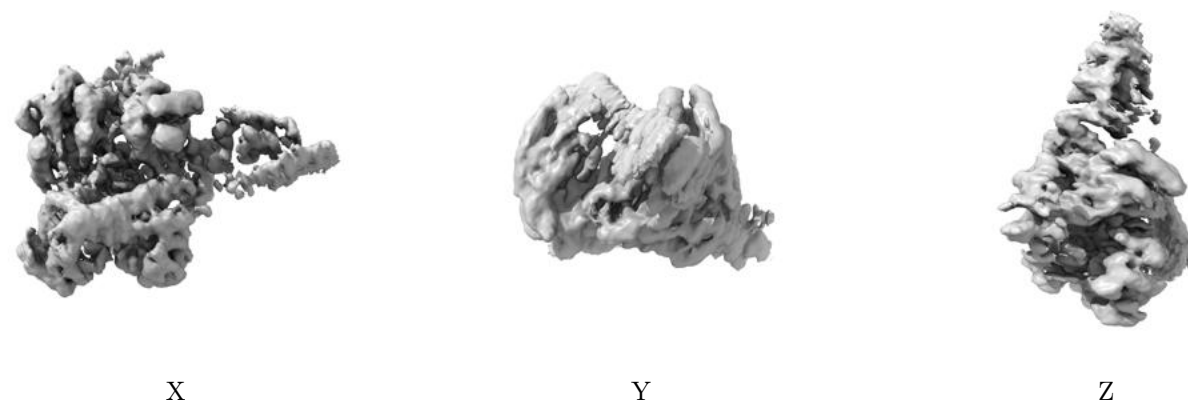
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.077. 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.

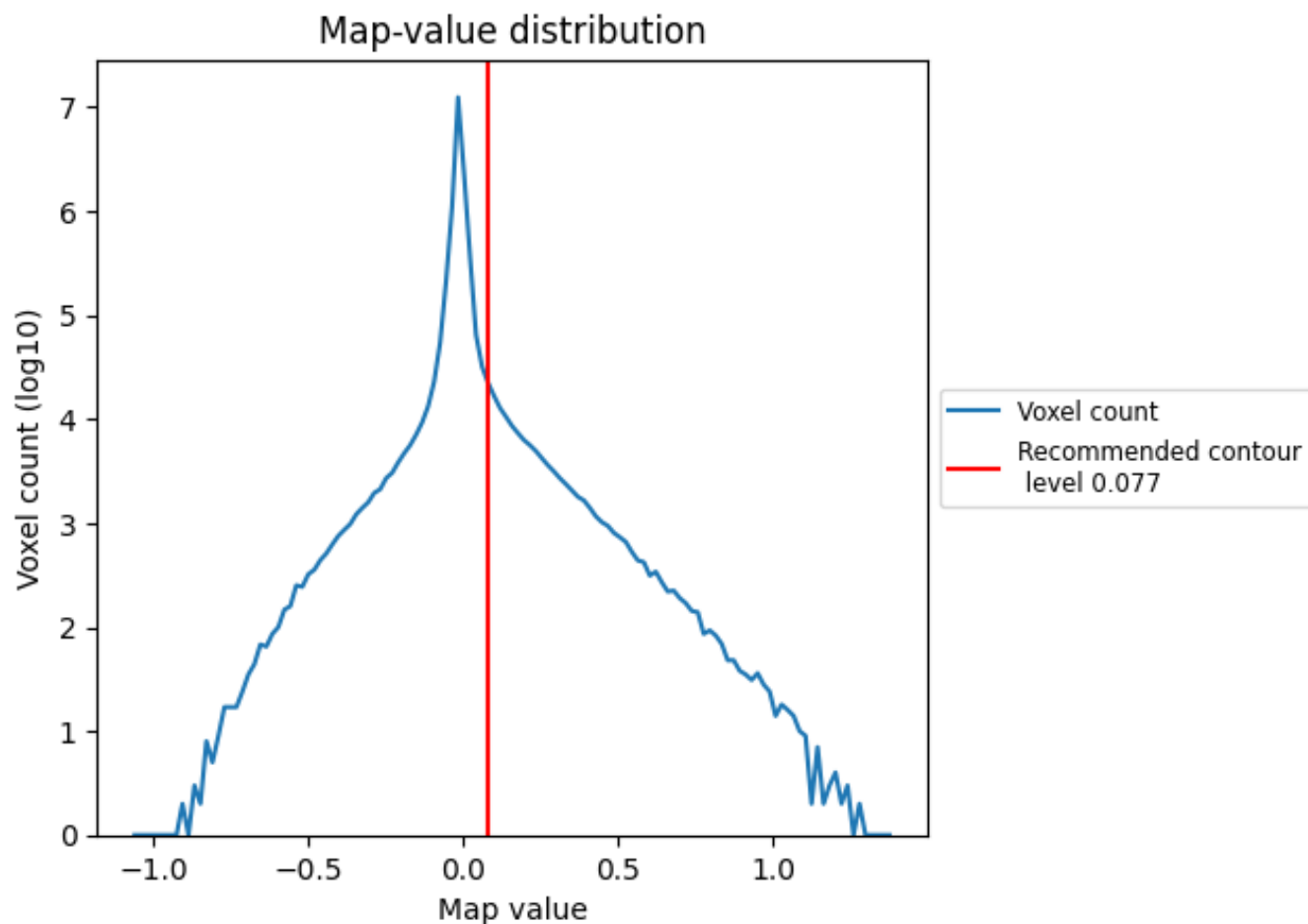
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

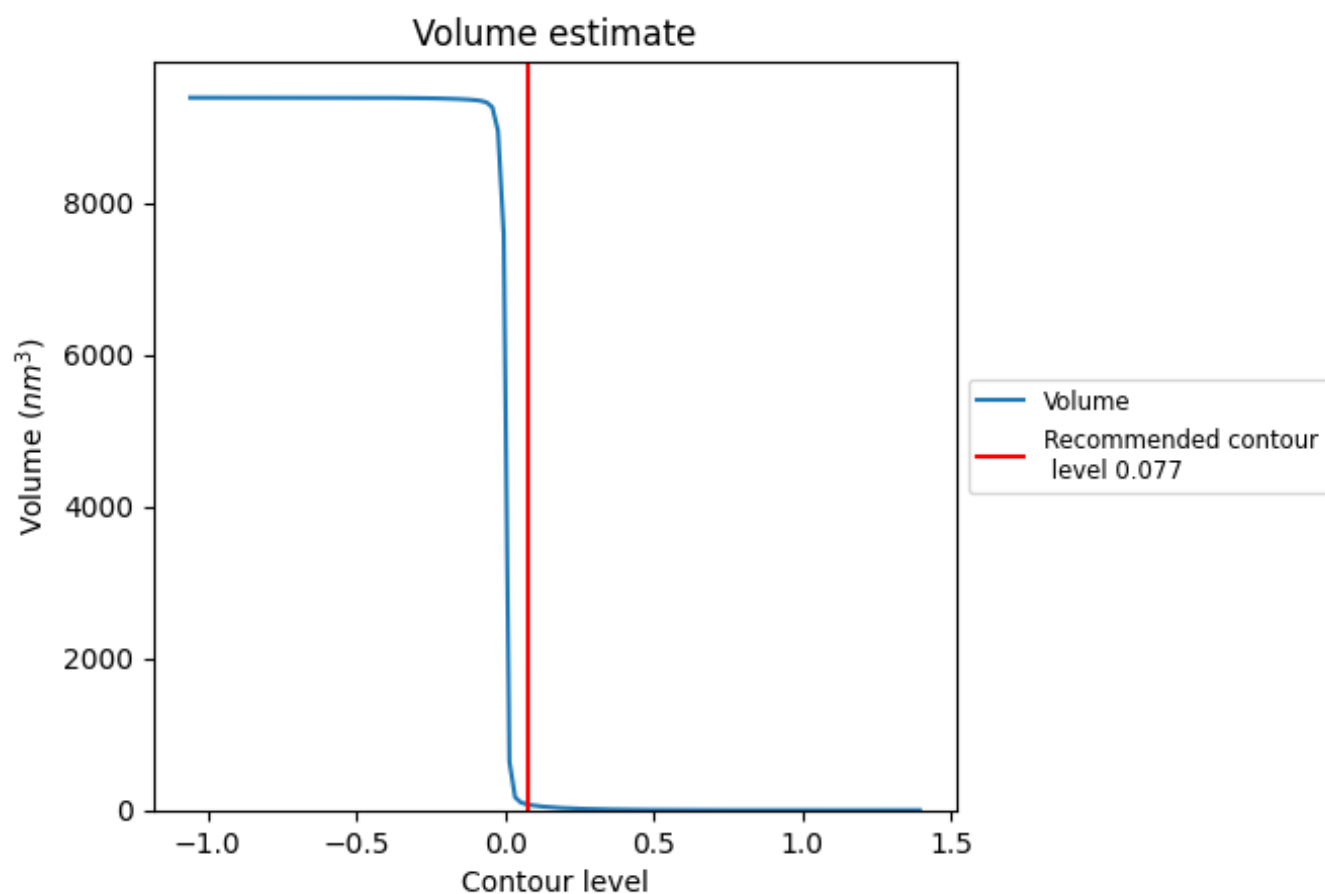
This section contains the results of statistical analysis of the map.

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.

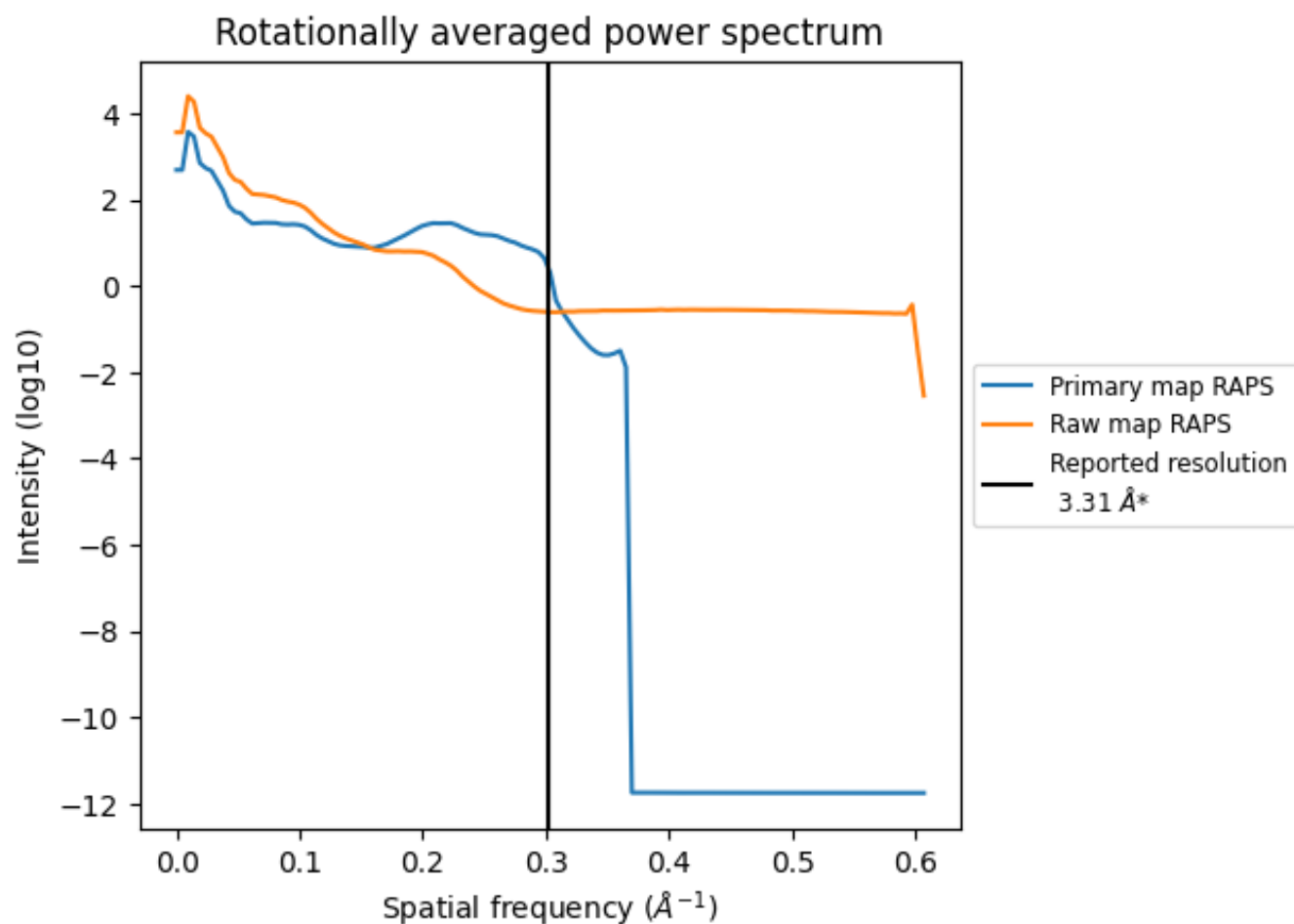
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 75 nm³; this corresponds to an approximate mass of 68 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 ⓘ

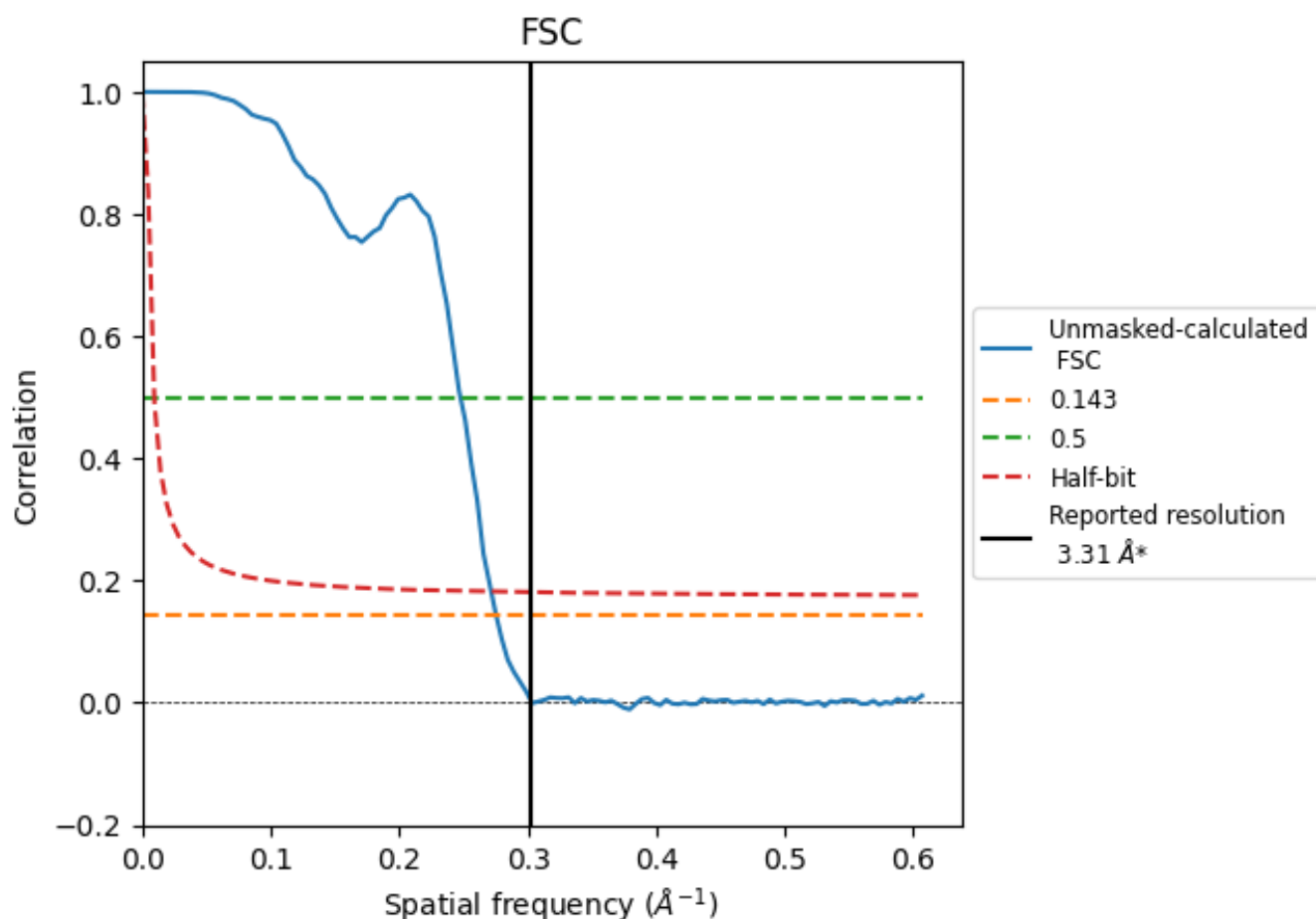


*Reported resolution corresponds to spatial frequency of 0.302 $\text{\AA}^{-1}$

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 0.302 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

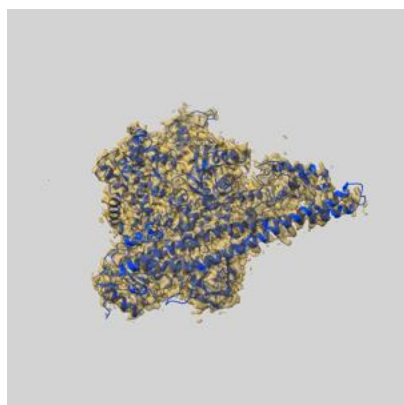
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.31	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.63	4.04	3.68

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

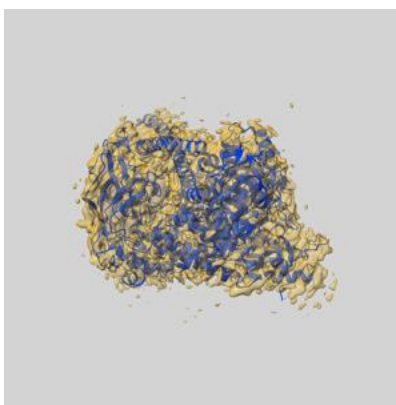
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-67325 and PDB model 9XW5. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

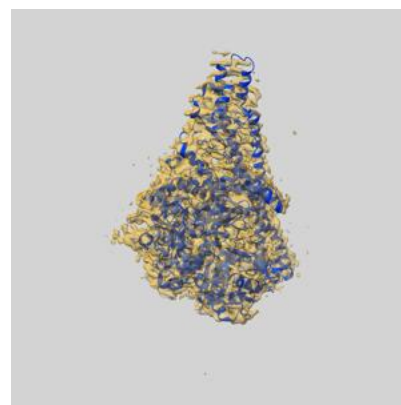
9.1 Map-model overlay [i](#)



X



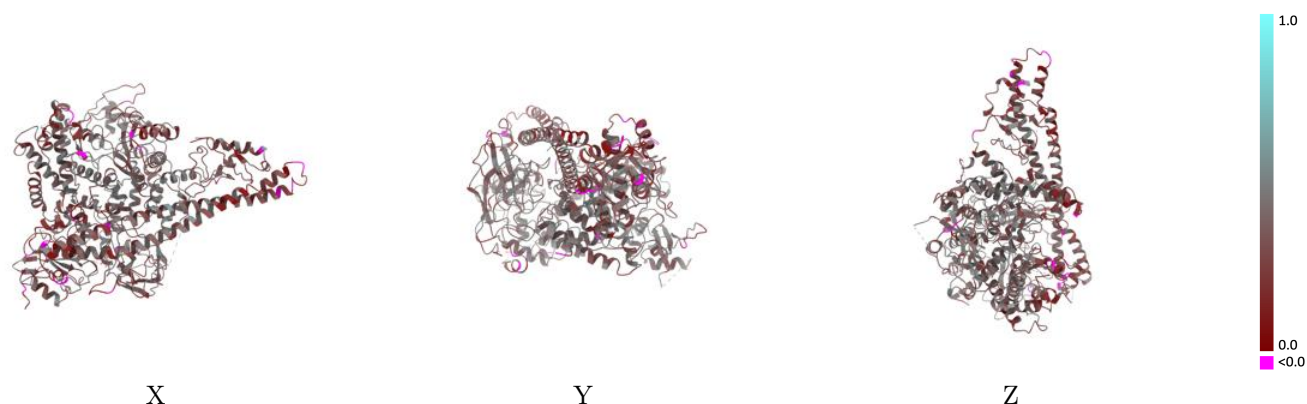
Y



Z

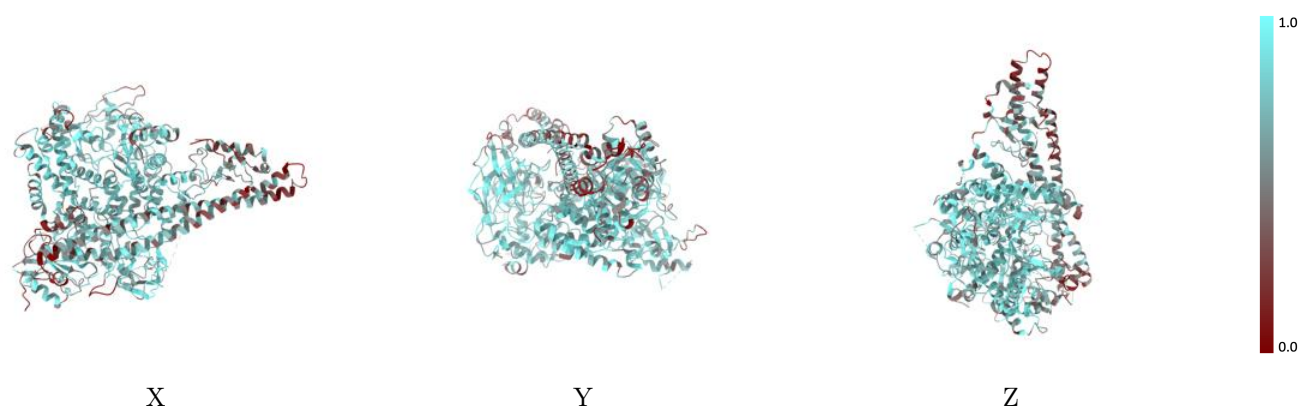
The images above show the 3D surface view of the map at the recommended contour level 0.077 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



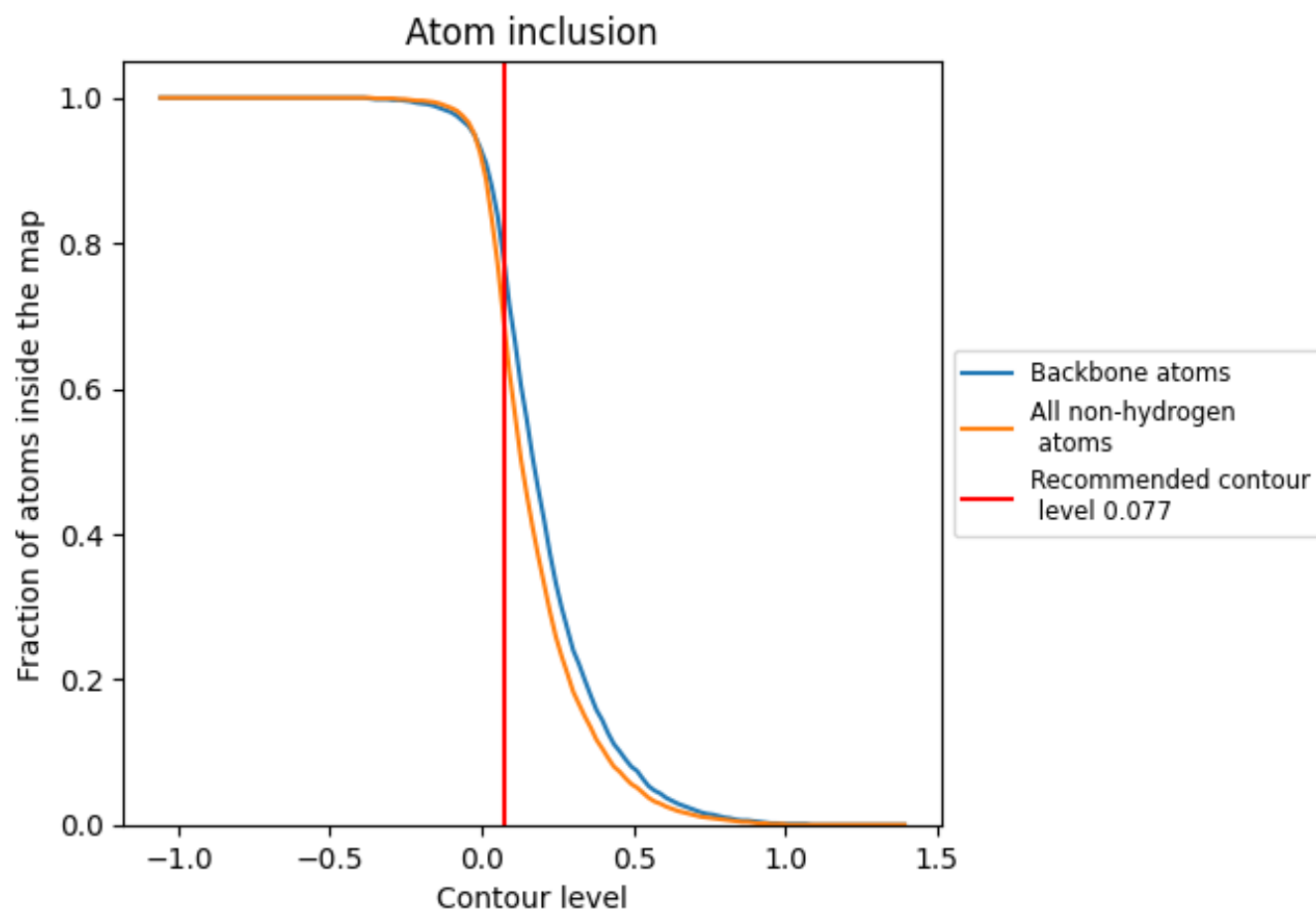
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.077).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 68% 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 (0.077) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6790	0.3440
A	0.7260	0.3580
B	0.5260	0.2970

