



Full wwPDB EM Validation Report ⓘ

Mar 30, 2026 – 01:05 AM UTC

PDB ID : 8YB4 / pdb_00008yb4
EMDB ID : EMD-39108
Title : Pfr conformer of Arabidopsis thaliana phytochrome B in complex with phytochrome-interacting factor 6
Authors : Wang, Z.; Wang, W.; Zhao, D.; Song, Y.; Xu, B.; Zhao, J.; Wang, J.
Deposited on : 2024-02-11
Resolution : 3.10 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:

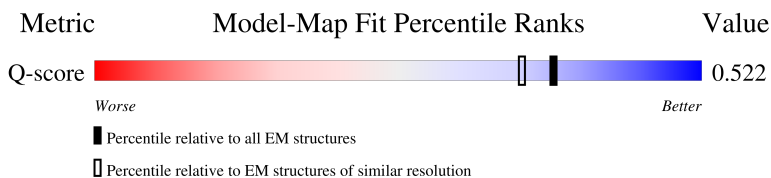
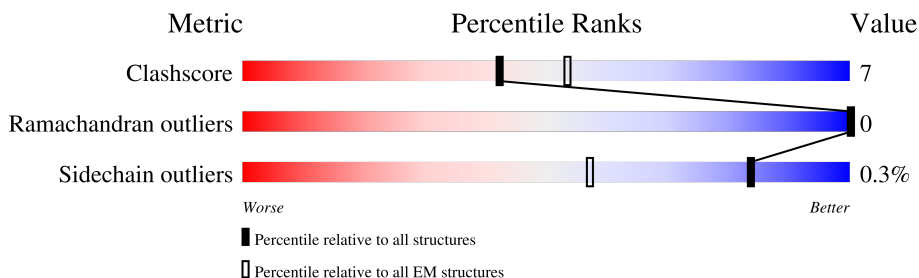
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the 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) : 2.49

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 3.10 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	14724 (2.60 - 3.60)

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	1177	
1	B	1177	
2	C	105	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8400 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 phytochrome B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	542	Total	C	N	O	S	0	0
			4211	2661	728	791	31		
1	A	477	Total	C	N	O	S	0	0
			3701	2347	641	683	30		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLY	-	expression tag	UNP P14713
B	-3	PRO	-	expression tag	UNP P14713
B	-2	LEU	-	expression tag	UNP P14713
B	-1	GLY	-	expression tag	UNP P14713
B	0	SER	-	expression tag	UNP P14713
A	-4	GLY	-	expression tag	UNP P14713
A	-3	PRO	-	expression tag	UNP P14713
A	-2	LEU	-	expression tag	UNP P14713
A	-1	GLY	-	expression tag	UNP P14713
A	0	SER	-	expression tag	UNP P14713

- Molecule 2 is a protein called phytochrome-interacting factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	48	Total	C	N	O	S	0	0
			402	247	70	81	4		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	GLY	-	expression tag	UNP Q8L5W7
C	-3	PRO	-	expression tag	UNP Q8L5W7
C	-2	LEU	-	expression tag	UNP Q8L5W7
C	-1	GLY	-	expression tag	UNP Q8L5W7
C	0	SER	-	expression tag	UNP Q8L5W7

- [illegible]

Mol	Chain	Residues	Atoms				AltConf
3	B	1	Total 43	C 33	N 4	O 6	0
3	A	1	Total 43	C 33	N 4	O 6	0

ILE
LEU
GLU
LEU
PRO
VAL
PRO
ARG
LYS
ARG
PRO
LEU
SER
THR
ALA
SER
GLY
SER
GLY
ASP
MET
MET
LEU
MET
MET
PRO
TYR

- Molecule 1: phytochrome B



GLY	PRO	LEU	GLY	SER	MET	VAL	SER	GLY	VAL	GLY	GLY	SER	GLY	GLY	ARG	GLY	GLY	GLY	GLY	GLU	GLU	GLU	PRO	SER	SER	SER	HIS	THR	PRO	ASN	ASN	ARG	ARG	GLY	GLY	GLU	GLN	ALA	GLN	SER	SER	SER	LEU	ARG	PRO	PRO	ARG	SER	SER	THR	GLU	SER	SER	MET	SER
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LYS	ILE	GLN	THR	THR	VAL	ASP	ALA	ARG	LEU	HIS	ALA	VAL	PHE	GLU	GLN	SER	GLY	GLU	SER	GLY	LYS	SER	PHE	ASP	TYR	SER	SER	GLN	LEU	LYS	THR	THR	THR	GLY	SER	SER	SER	VAL	PRO	GLU	GLN	GLN	ILE	THR	ALA	TYR	LEU	SER	ARG	ILE	GLN	ARG	G111	G115
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G119	M120	R129	S134	E135	N136	M144	PRO	GLN	SER	SER	VAL	PRO	THR	LEU	LEU	LYS	PRO	PRO	GLU	I156	G160	V163	L166	L175	A178	R182	T185	L186	L187	L205	H206	R207	T208	D209	V210	I214	I228	V232	Q233	D252	V260	V264
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G269
Y270
Z271
M274
V275
D281
E282
H283
G284
E289
S290
K291
R292
D293
P297
Y303
K317
R320
R321
R322
M323
I324
V325
D326
A329
Q336
S343
S349
T350
L351
I376
I377
N380
GLU
ASP
ASP
GLY
SER
ASN
VAL
ALA
GLY
SER
GLY
ARG
S392
S393
S264

Category	Count	Color	Marker
R395	10	Yellow	
V400	10	Yellow	
H404	10	Yellow	
R408	10	Yellow	
C409	10	Yellow	
I410	10	Yellow	
R415	10	Yellow	
F425	10	Yellow	
M431	10	Yellow	
M439	10	Yellow	
D453	10	Green	Red Diamond
M454	10	Green	Red Diamond
L455	10	Green	Red Diamond
L456	10	Green	Red Diamond
R457	10	Green	Red Diamond
D458	10	Green	Red Diamond
I463	10	Yellow	
S467	10	Green	Red Diamond
P468	10	Yellow	
S469	10	Green	
I470	10	Yellow	
V474	10	Yellow	
K475	10	Yellow	
H484	10	Green	Red Diamond
S495	10	Yellow	
E496	10	Yellow	
V497	10	Yellow	
K500	10	Yellow	
A511	10	Green	Red Diamond
D512	10	Green	Red Diamond
S513	10	Green	Red Diamond
T514	10	Green	
G515	10	Green	
L516	10	Yellow	
G522	10	Yellow	
D523	10	Green	
A524	10	Yellow	
A530	10	Green	Red Diamond
V541	10	Yellow	

K546	R547	F549	W552	W563	G564	G565	ALA	LYS	HIS	HIS	PRO	GLU	ASP	LYS	ASP	ASP	GLY	GLN	R578	M579	H580	P581	R582	F585	Q586	A587	F588	L589	E590	Q597	E603	M604	D605	H608	S609	Q611	L612	L613	L614	R615	K619	E620	S621	GLU	ALA	ALA	ALA	MET	ASN
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VAL	VAL	ASP	GLY	VAL	VAL	GLN	PRO	CYS	ARG	ASP	MET	ALA	GLY	GLU	GLN	GLY	ILE	ASP	GLU	LEU	GLY	ALA	VAL	ALA	ARG	GLU	MET	VAL	ARG	LEU	ILE	GLU	THR	THR	VAL	VAL	ILE	PRO	ILE	PHE	VAL	VAL	ASP	ALA	ALA	GLY	CYS	ILE	ASN	TRP	LYS	ILE	ALA	LEU	GLU	THR	TYR
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LEU SER VAL GLU MET LYS LEU ASP SER ASP ILE TYR LYS ASN ASN ARG ALA LEU ARG GLY ASP GLU LEU LEU SER ARG ALA LEU ARG GLY ASP GLU LEU LEU THR THR VAL ASN LYS LYS ASN LYS VAL VAL LYS LEU LEU LYS THR THR PHE SER PRO GLU GLU GLN GLY LYS ALA VAL PHE VAL VAL

ASN	ALA	CYS	SER	SER	LYS	ASP	TYR	LEU	ASN	ASN	VAL	VAL	GLY	VAL	CYS	PHE	VAL	GLY	GLN	ASP	THR	SER	GLN	LYS	ILE	ILE	VAL	VAL	MET	ASP	LYS	PHE	ILE	ILE	ASN	ILE	ILE	GLN	GLY	ASP	TRP	TRP	LYS	ALA	ILE	VAL	HTS	SER	PRO	PRO	ASN	PRO	LEU	ILE	PRO	PRO	ILE	ILE	PHE	ALA	ALA	ASP	GLU	ASN	THR
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[illegible]

PHE PRO PHE PRO PHE ASP ARG ASN GLY LYS PHE VAL GLN ALA LEU LEU THR ALA ASN LYS ARG VAL SER LEU GLY GLU GLY VAL LYS VAL ILE ILE GLY PHE PHE PHE LEU GLN ILE PRO PRO SER SER SER GLU LEU GLN GLN GLN ALA LEU ALA VAL GLN ARG ARG ARG ASP THR THR THR THR THR

[illegible]

	GLU	ASP	GLY	GLY	SER	PHE	VAL	LEU	LYS	ARG	GLU	GLU	PHE	PHE	GLN	ASN	ALA	ILE	ILE	SER	GLN	MET	PHE	LEU	LEU	ARG	ASP	GLY	GLY	LEU	LEU	GLN	LEU	LEU	ILE	ARG	ASP	ASP	ILE	PRO	GLU	GLU	GLI	GLI	LYS	SER	SER	PHE	PHX	GLY	GLN	GLN	GLN	GLN	LEU	LEU	FEN
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ALA	GLU	PHE	LEU	SER	ILE	ARG	TYP	PRO	SER	GLN	GLU	TRP	VAL	GLY	ILE	HIS	LEU	SER	SER	GLN	LEU	SER	LYS	GLN	MET	ASP	GLY	PHE	ALA	ALA	ALA	ILE	ARG	THR	GLU	PHE	GLY	GLY	GLU	GLY	GLY	PRO	ALA	CYS	MET	ASP	PHE	HIS	SER	ALA
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	325483	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.942	Depositor
Minimum map value	-0.629	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.105	Depositor
Map size (Å)	204.0, 204.0, 204.0	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	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: O6E

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.16	0/3775	0.37	0/5110
1	B	0.12	0/4295	0.29	0/5812
2	C	0.11	0/406	0.29	0/539
All	All	0.14	0/8476	0.33	0/11461

There are no bond length outliers.

There are no bond angle outliers.

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	3701	0	3699	65	0
1	B	4211	0	4185	48	0
2	C	402	0	377	2	0
3	A	43	0	0	0	0
3	B	43	0	0	0	0
All	All	8400	0	8261	112	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (112) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:VAL:HA	1:A:500:LYS:HE2	1.59	0.82
1:B:275:VAL:HG22	1:B:400:VAL:HG22	1.62	0.81
1:A:205:LEU:HG	1:A:214:ILE:HG22	1.72	0.71
1:A:455:LEU:HD12	1:A:463:ILE:HD11	1.73	0.69
1:B:448:GLN:NE2	1:B:452:CYS:SG	2.65	0.68
1:A:580:HIS:CE1	1:A:582:ARG:HG3	2.30	0.66
1:B:177:ARG:NH1	2:C:53:GLU:O	2.29	0.65
1:A:611:GLN:O	1:A:615:ARG:HG2	1.98	0.63
1:B:129:ARG:NH1	1:B:160:GLY:O	2.31	0.63
1:A:475:LYS:NZ	1:A:597:GLN:OE1	2.35	0.59
1:B:454:MET:HE1	1:B:466:GLN:HB2	1.83	0.59
1:B:480:ALA:HB3	1:B:551:PHE:HB2	1.84	0.59
1:A:474:VAL:HG13	1:A:603:GLU:HG2	1.83	0.59
1:B:379:GLY:O	1:B:393:SER:OG	2.21	0.58
1:A:586:GLN:O	1:A:590:GLU:HG3	2.03	0.58
1:B:544:ILE:HG22	1:B:545:THR:HG23	1.86	0.58
1:A:163:VAL:HA	1:A:166:LEU:HD12	1.86	0.57
1:B:60:GLN:CD	1:B:310:GLN:HE21	2.13	0.57
1:B:189:PRO:HB3	1:B:204:ILE:HG13	1.85	0.57
1:A:134:SER:OG	1:A:136:ASN:OD1	2.21	0.57
1:A:323:MET:SD	1:A:415:ARG:NH1	2.78	0.56
1:A:320:ARG:HD3	1:A:376:ILE:HD12	1.87	0.56
1:A:336:GLN:HE22	1:A:343:SER:HA	1.71	0.56
1:A:185:THR:HG22	1:A:186:LEU:H	1.71	0.55
1:A:392:SER:OG	1:A:393:SER:N	2.39	0.55
1:A:563:TRP:HD1	1:A:585:PHE:CD2	2.25	0.54
1:A:182:ARG:O	1:A:207:ARG:NH1	2.37	0.54
1:B:431:MET:SD	1:A:431:MET:HA	2.48	0.53
1:A:208:ILE:C	1:A:210:VAL:H	2.17	0.53
1:A:580:HIS:HE1	1:A:582:ARG:HG3	1.73	0.53
1:A:284:GLY:HA3	1:A:303:TYR:CZ	2.45	0.52
1:A:377:ILE:HD11	1:A:395:ARG:HH21	1.72	0.52
1:B:136:ASN:OD1	1:B:136:ASN:N	2.43	0.52
1:A:543:TYR:HA	1:A:549:PHE:HD1	1.75	0.52
1:A:546:LYS:HB2	1:A:547:ARG:NH1	2.24	0.52
1:B:428:GLN:O	1:B:431:MET:HB3	2.10	0.51
1:B:229:ALA:HA	1:B:232:VAL:HG22	1.92	0.51
1:B:125:GLU:HG2	1:B:212:VAL:HG23	1.92	0.51
1:A:118:GLY:HA3	1:A:351:LEU:HD21	1.92	0.51
1:A:271:ASP:HB2	1:A:404:HIS:HA	1.92	0.50
1:A:317:LYS:O	1:A:320:ARG:NH1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:604:MET:O	1:A:608:HIS:ND1	2.45	0.50
1:A:293:ASP:OD1	1:A:293:ASP:N	2.39	0.50
1:A:497:VAL:HA	1:A:500:LYS:CE	2.37	0.50
1:A:129:ARG:HH22	1:A:160:GLY:CA	2.24	0.50
1:A:409:CYS:O	1:A:410:ILE:HG22	2.12	0.49
1:B:54:MET:SD	1:B:54:MET:N	2.80	0.49
1:B:500:LYS:O	1:B:504:GLU:HG2	2.14	0.48
1:B:519:ASP:OD1	1:B:598:PRO:HA	2.13	0.48
1:A:320:ARG:O	1:A:321:VAL:HG23	2.13	0.48
1:A:611:GLN:HA	1:A:614:LEU:HD23	1.96	0.47
1:B:79:LYS:HB3	1:B:79:LYS:HE3	1.71	0.47
1:A:467:SER:HB2	1:A:468:PRO:HD3	1.96	0.47
1:A:610:LEU:O	1:A:614:LEU:HD22	2.15	0.47
1:B:186:LEU:C	1:A:233:GLN:HE21	2.23	0.46
1:A:274:MET:HG2	1:A:289:GLU:HG3	1.98	0.46
1:B:442:LYS:HB2	1:B:442:LYS:HE3	1.65	0.46
1:A:586:GLN:HA	1:A:589:LEU:HB2	1.96	0.46
1:B:224:PRO:O	1:B:228:ILE:HG13	2.16	0.46
1:B:542:ALA:HB3	1:B:550:LEU:HB2	1.96	0.46
1:A:291:LYS:HE3	1:A:297:PRO:HB3	1.97	0.45
1:A:495:SER:OG	1:A:496:GLU:N	2.49	0.45
1:B:526:TYR:HD1	1:B:527:PRO:HD2	1.81	0.45
1:A:115:GLN:HE22	1:A:324:ILE:HA	1.82	0.45
1:B:252:ASP:OD1	1:B:252:ASP:N	2.48	0.45
1:A:275:VAL:HG22	1:A:400:VAL:HG22	1.98	0.45
1:B:83:TYR:OH	1:B:307:ASP:OD1	2.34	0.45
1:A:268:THR:HB	1:A:270:TYR:HD1	1.82	0.45
1:A:281:ASP:OD1	1:A:283:HIS:ND1	2.39	0.45
1:A:522:GLY:C	1:A:524:ALA:H	2.25	0.45
1:A:260:VAL:HG21	1:A:425:PHE:CD1	2.52	0.45
1:A:516:LEU:HB3	1:A:541:VAL:HG12	1.99	0.45
1:B:580:HIS:CD2	1:B:581:PRO:HD2	2.52	0.45
1:A:585:PHE:O	1:A:586:GLN:HG2	2.17	0.44
1:A:120:MET:HE2	1:A:120:MET:HB2	1.79	0.44
1:A:129:ARG:HH22	1:A:160:GLY:HA2	1.82	0.44
1:A:326:ASP:HB3	1:A:329:ALA:HB2	1.98	0.44
1:B:373:MET:SD	1:B:418:CYS:HB3	2.58	0.43
1:B:272:ARG:HD3	1:B:274:MET:HE3	1.99	0.43
1:B:561:ILE:HG21	1:B:589:LEU:HD21	2.00	0.43
1:B:133:TYR:HE1	1:B:159:MET:HG2	1.82	0.43
1:A:470:ILE:HG22	1:A:552:TRP:HE1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:GLN:HE22	1:B:343:SER:HA	1.83	0.43
1:B:161:THR:OG1	1:B:162:ASP:N	2.51	0.43
1:A:252:ASP:OD1	1:A:252:ASP:N	2.52	0.43
1:B:556:HIS:CE1	1:B:558:ALA:HB3	2.53	0.43
1:A:264:VAL:O	1:A:268:THR:OG1	2.32	0.42
1:B:289:GLU:CD	1:B:298:TYR:H	2.28	0.42
1:B:452:CYS:SG	1:B:613:ILE:HG21	2.59	0.42
1:A:120:MET:HE1	1:A:349:SER:OG	2.19	0.42
1:A:439:MET:HE3	1:A:439:MET:HB3	1.81	0.42
1:B:120:MET:HE1	1:B:344:MET:HE2	2.01	0.42
1:A:175:LEU:HD23	1:A:175:LEU:HA	1.93	0.42
1:A:585:PHE:C	1:A:587:ALA:H	2.28	0.41
1:A:470:ILE:H	1:A:470:ILE:HG13	1.73	0.41
1:B:197:THR:OG1	1:B:198:GLY:N	2.53	0.41
1:B:344:MET:HE3	1:B:344:MET:HB3	1.90	0.41
1:B:323:MET:HE2	1:B:323:MET:HB3	1.86	0.41
1:A:178:ALA:HA	1:A:187:LEU:HD13	2.02	0.41
1:A:268:THR:O	1:A:408:ARG:NH1	2.53	0.41
1:B:138:ARG:HG3	1:B:157:LEU:HD23	2.02	0.41
1:B:321:VAL:HG11	1:B:415:ARG:HG2	2.01	0.41
1:B:453:ASP:OD1	1:B:453:ASP:C	2.64	0.41
1:B:539:MET:HE2	1:B:539:MET:HB3	1.86	0.41
1:B:122:ALA:HB2	1:B:344:MET:HE1	2.02	0.41
1:A:609:SER:O	1:A:613:ILE:HG12	2.20	0.41
2:C:49:LEU:HD23	2:C:49:LEU:HA	1.83	0.41
1:B:451:LEU:HD12	1:B:463:ILE:HB	2.03	0.40
1:B:461:ALA:O	1:B:464:VAL:HG22	2.21	0.40
1:B:521:LEU:HD13	1:B:526:TYR:HD2	1.85	0.40
1:A:208:ILE:HG13	1:A:210:VAL:H	1.87	0.40
1:A:228:ILE:O	1:A:232:VAL:HG23	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	469/1177 (40%)	442 (94%)	27 (6%)	0	100	100
1	B	534/1177 (45%)	515 (96%)	19 (4%)	0	100	100
2	C	44/105 (42%)	42 (96%)	2 (4%)	0	100	100
All	All	1047/2459 (43%)	999 (95%)	48 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	403/997 (40%)	401 (100%)	2 (0%)	81	85
1	B	460/997 (46%)	459 (100%)	1 (0%)	87	89
2	C	44/90 (49%)	44 (100%)	0	100	100
All	All	907/2084 (44%)	904 (100%)	3 (0%)	84	87

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

Mol	Chain	Res	Type
1	B	109	GLN
1	A	209	ASP
1	A	458	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	68	HIS
1	B	246	GLN
1	B	310	GLN
1	B	358	HIS

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Mol	Chain	Res	Type
1	B	448	GLN
1	B	580	HIS
1	A	115	GLN
1	A	235	GLN
1	A	319	ASN
1	A	336	GLN
1	A	378	ASN
1	A	404	HIS
1	A	484	HIS
2	C	41	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 ⓘ

2 ligands are 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	O6E	B	1201	1	46,46,46	0.85	2 (4%)	62,67,67	0.95	3 (4%)
3	O6E	A	1201	1	46,46,46	0.85	2 (4%)	62,67,67	0.95	3 (4%)

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	O6E	B	1201	1	-	10/26/74/74	0/4/4/4
3	O6E	A	1201	1	-	10/26/74/74	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1201	O6E	CAB-CBI	-3.06	1.39	1.47
3	A	1201	O6E	CAB-CBI	-3.02	1.39	1.47
3	A	1201	O6E	CBI-CBC	2.23	1.41	1.37
3	B	1201	O6E	CBI-CBC	2.20	1.41	1.37

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1201	O6E	CAW-CAP-CBL	3.18	135.86	128.06
3	A	1201	O6E	CAW-CAP-CBL	2.68	134.63	128.06
3	B	1201	O6E	CAP-CAW-CBC	2.64	132.24	126.97
3	A	1201	O6E	CAP-CAW-CBC	2.44	131.83	126.97
3	B	1201	O6E	CBD-CBJ-CBN	2.25	104.71	101.34
3	A	1201	O6E	CBD-CBJ-CBN	2.19	104.61	101.34

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1201	O6E	CAH-CAC-CBJ-CBN
3	A	1201	O6E	CAH-CAC-CBJ-CBN
3	B	1201	O6E	CBL-CAP-CAW-CBC
3	A	1201	O6E	CBL-CAP-CAW-CBC
3	B	1201	O6E	CBL-CAP-CAW-NAJ
3	A	1201	O6E	CBL-CAP-CAW-NAJ
3	B	1201	O6E	CAW-CAP-CBL-NAE
3	A	1201	O6E	CAW-CAP-CBL-NAE
3	B	1201	O6E	CAW-CAP-CBL-CBH
3	A	1201	O6E	CAW-CAP-CBL-CBH
3	B	1201	O6E	CAH-CAC-CBJ-CBD
3	A	1201	O6E	CAH-CAC-CBJ-CBD

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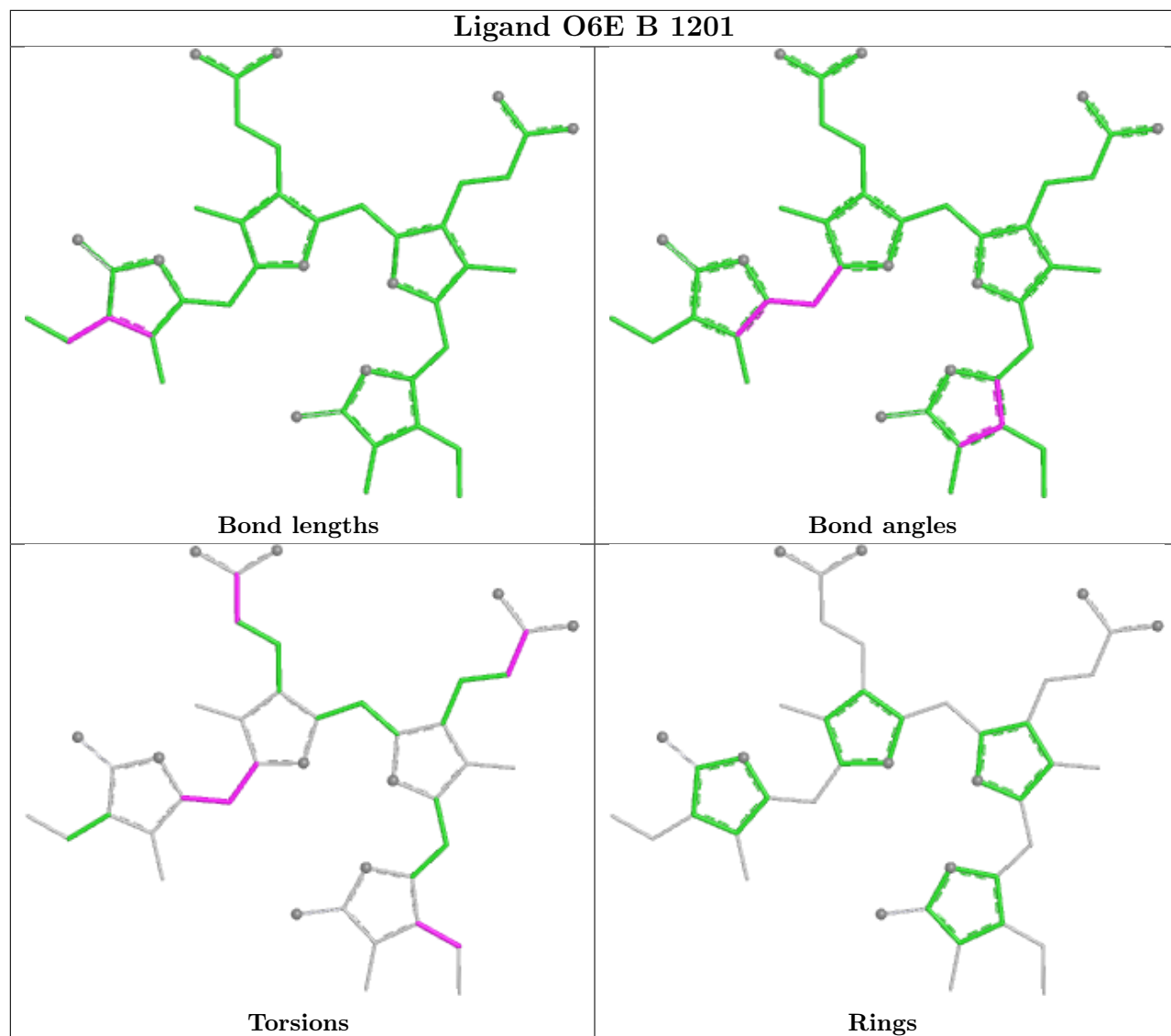
Continued from previous page...

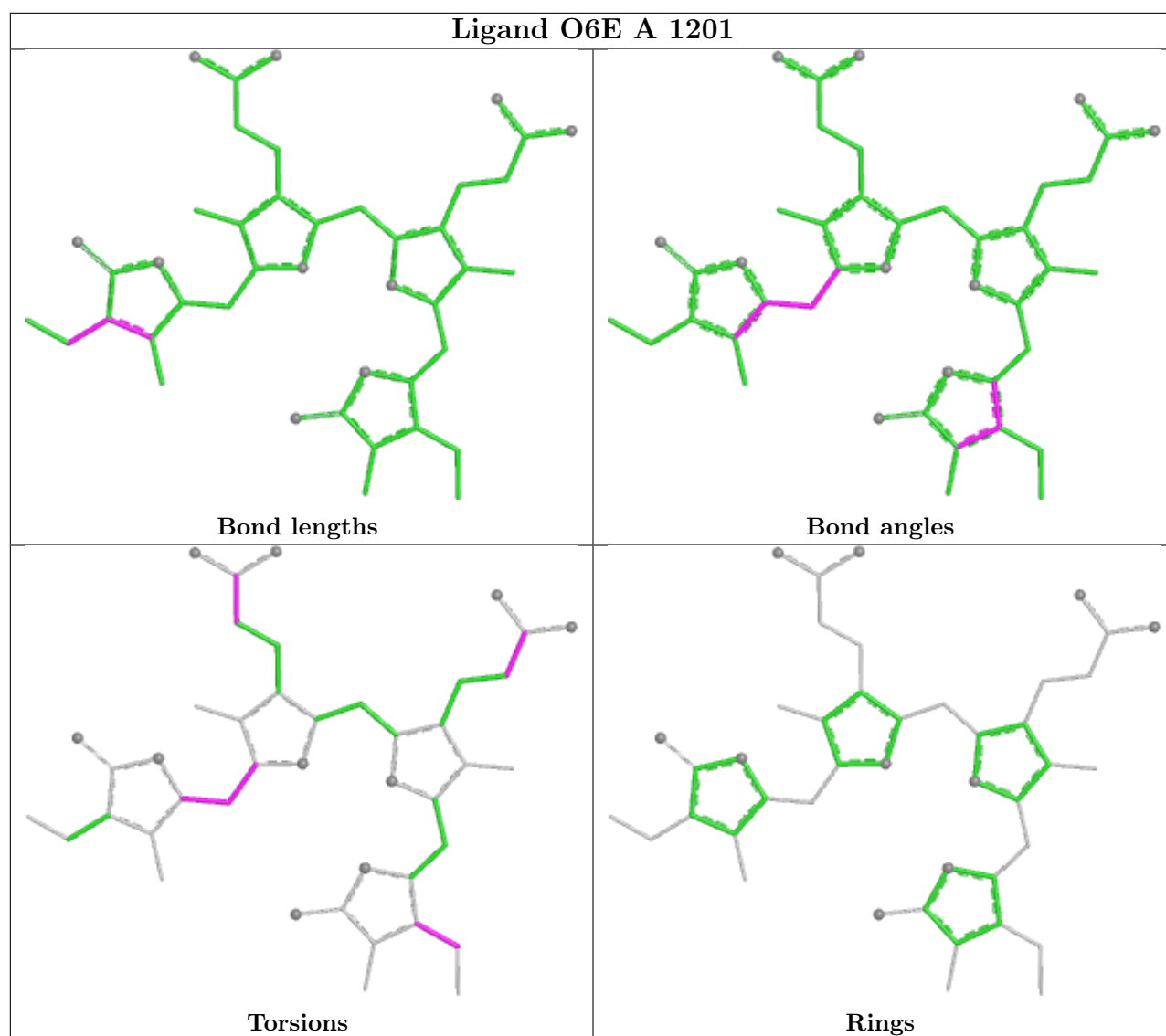
Mol	Chain	Res	Type	Atoms
3	A	1201	O6E	CAD-CAI-CAM-OBA
3	A	1201	O6E	CAA-CAF-CAL-OBF
3	B	1201	O6E	CAA-CAF-CAL-OAZ
3	A	1201	O6E	CAA-CAF-CAL-OAZ
3	A	1201	O6E	CAD-CAI-CAM-OBG
3	B	1201	O6E	CAD-CAI-CAM-OBG
3	B	1201	O6E	CAD-CAI-CAM-OBA
3	B	1201	O6E	CAA-CAF-CAL-OBF

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.

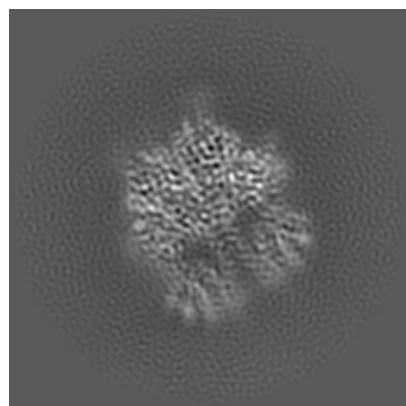
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39108. These allow visual inspection of the internal detail of the map and identification of artifacts.

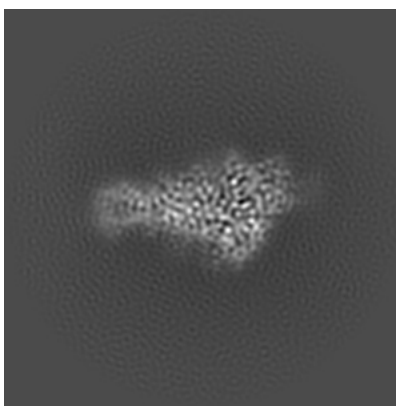
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

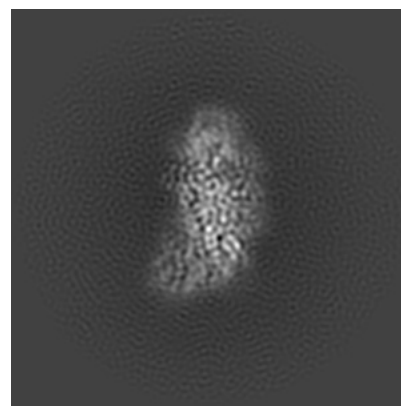
6.1.1 Primary map



X

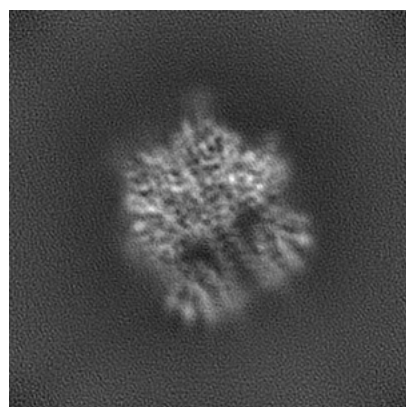


Y

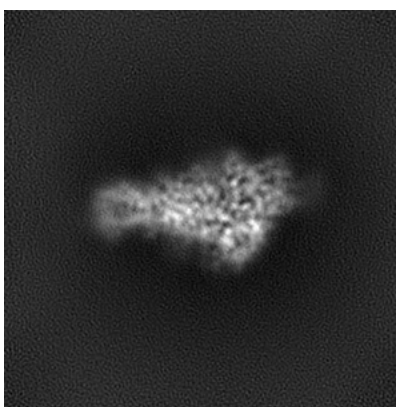


Z

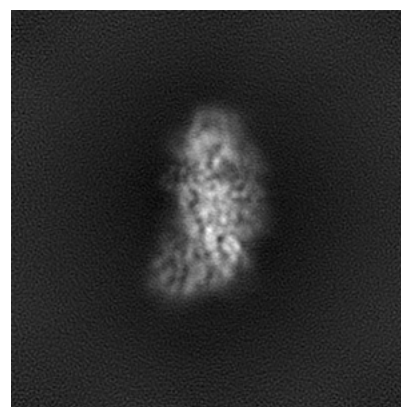
6.1.2 Raw map



X



Y

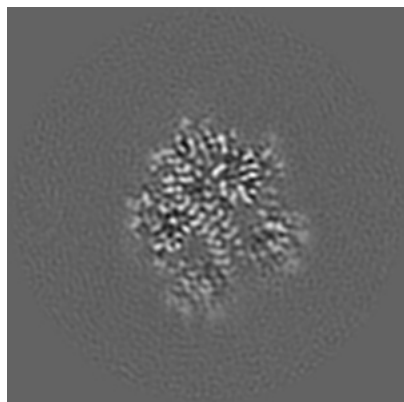


Z

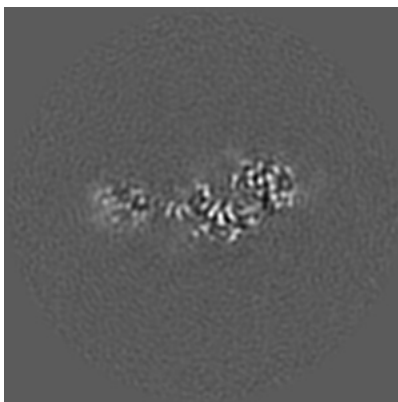
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

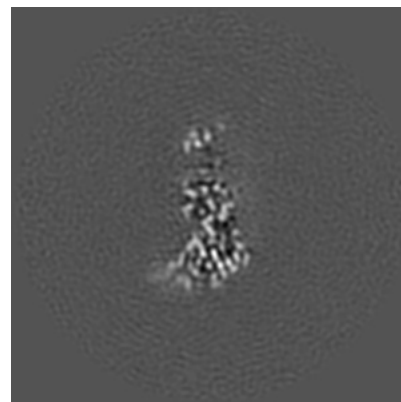
6.2.1 Primary map



X Index: 120

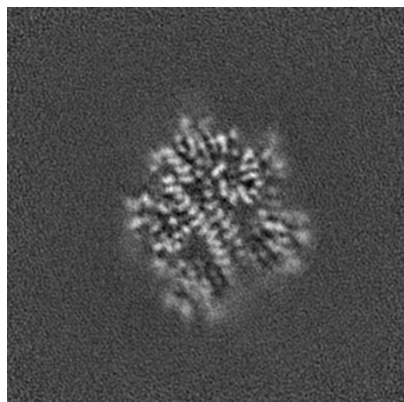


Y Index: 120

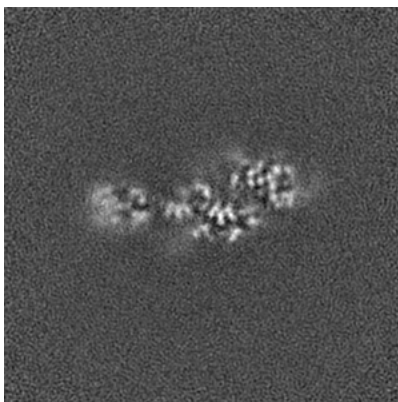


Z Index: 120

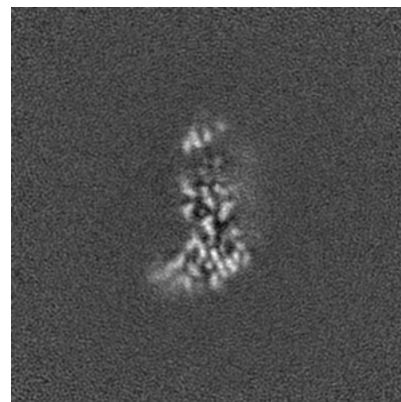
6.2.2 Raw map



X Index: 120



Y Index: 120

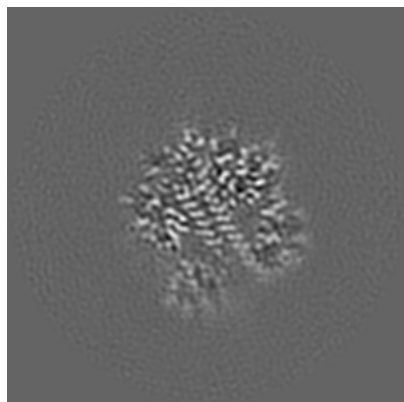


Z Index: 120

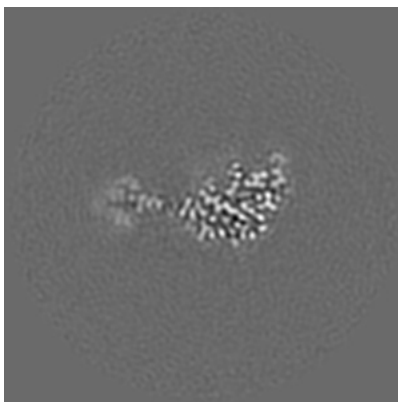
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

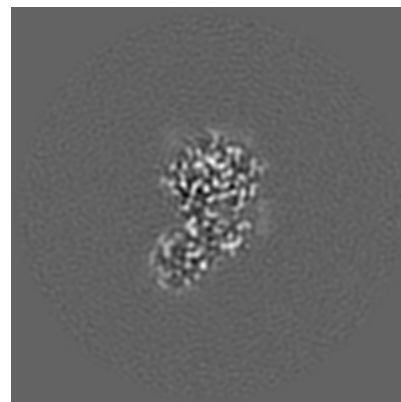
6.3.1 Primary map



X Index: 117

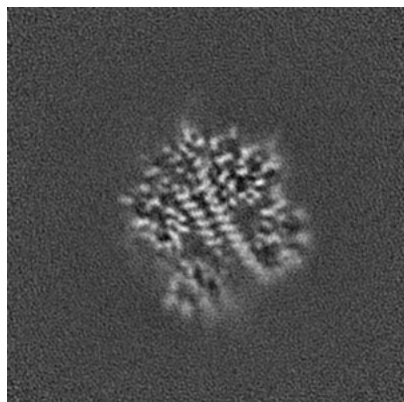


Y Index: 129

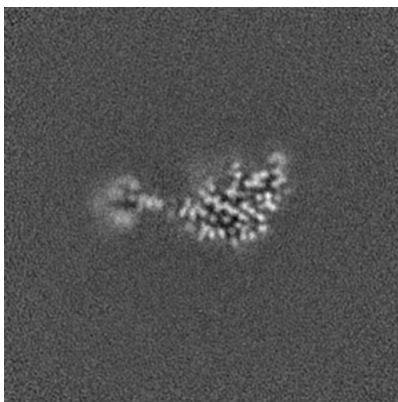


Z Index: 139

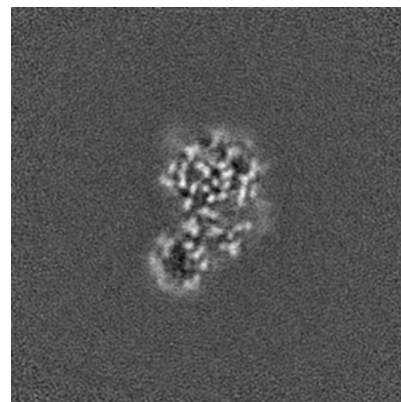
6.3.2 Raw map



X Index: 117



Y Index: 129

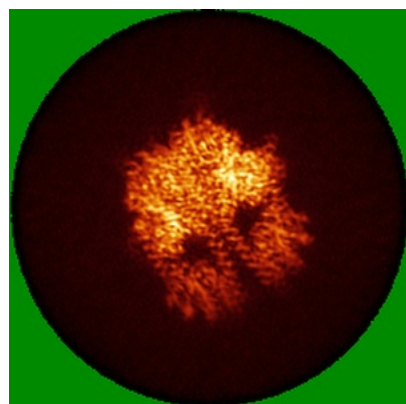


Z Index: 140

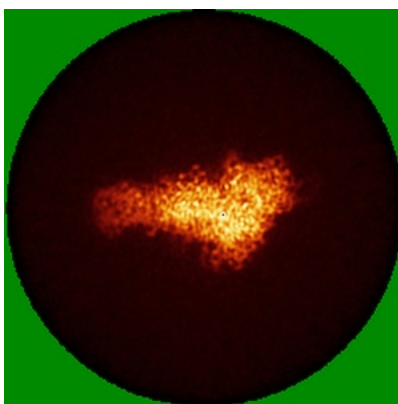
The images above show the largest variance slices of the map in three orthogonal directions.

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

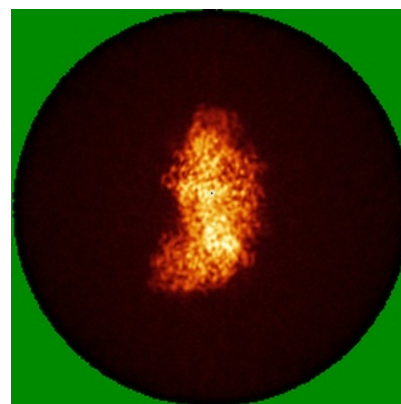
6.4.1 Primary map



X

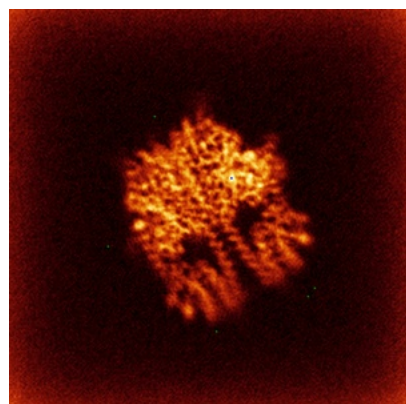


Y

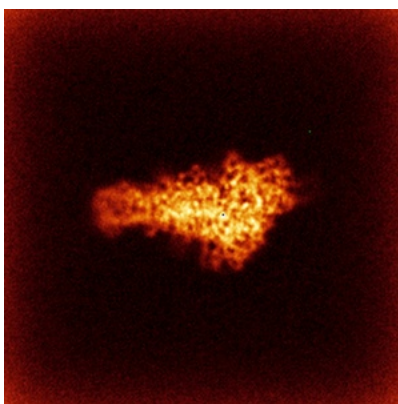


Z

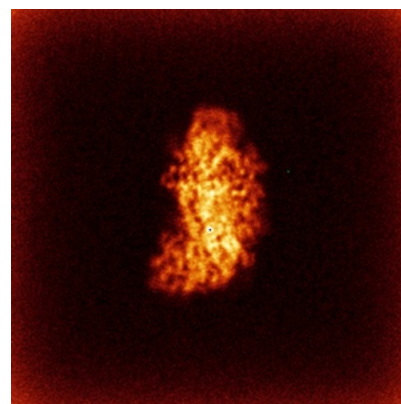
6.4.2 Raw map



X



Y

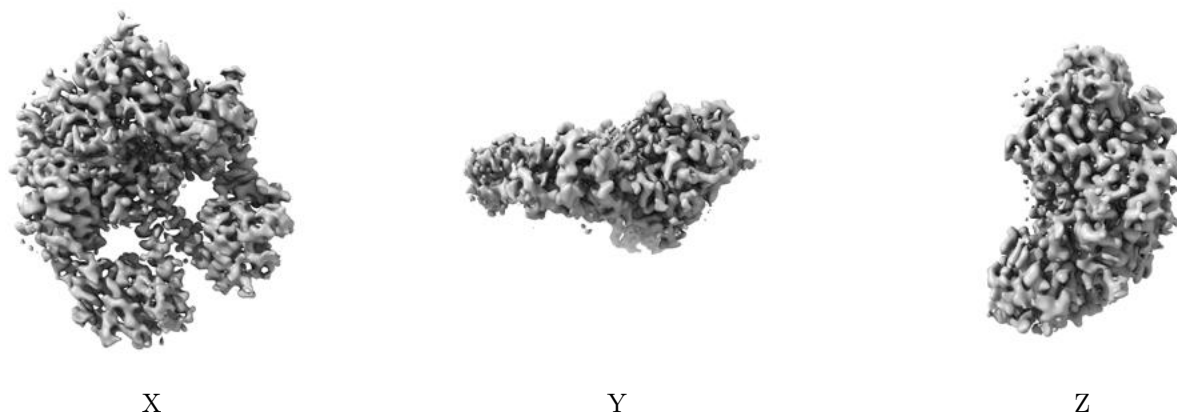


Z

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.

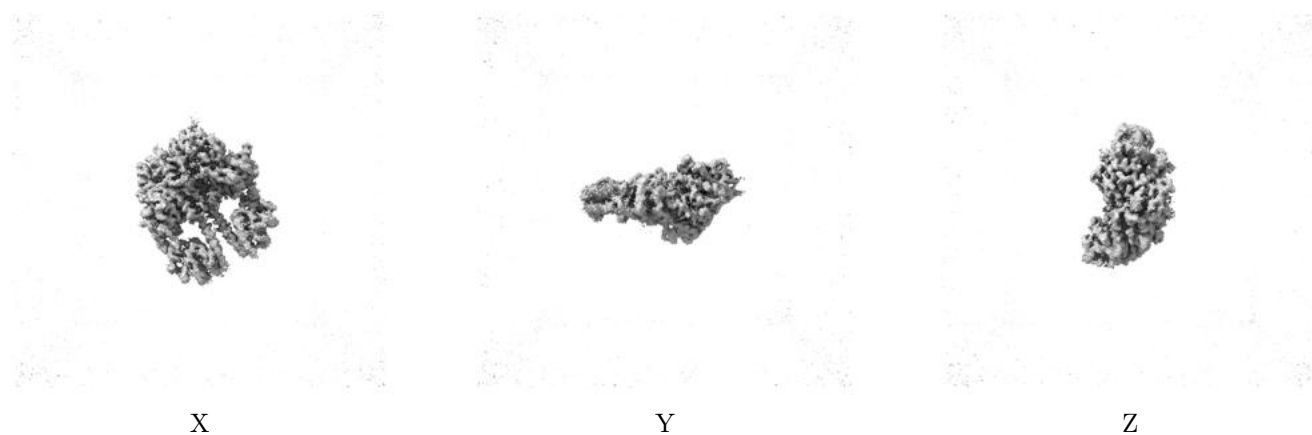
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.105. 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.

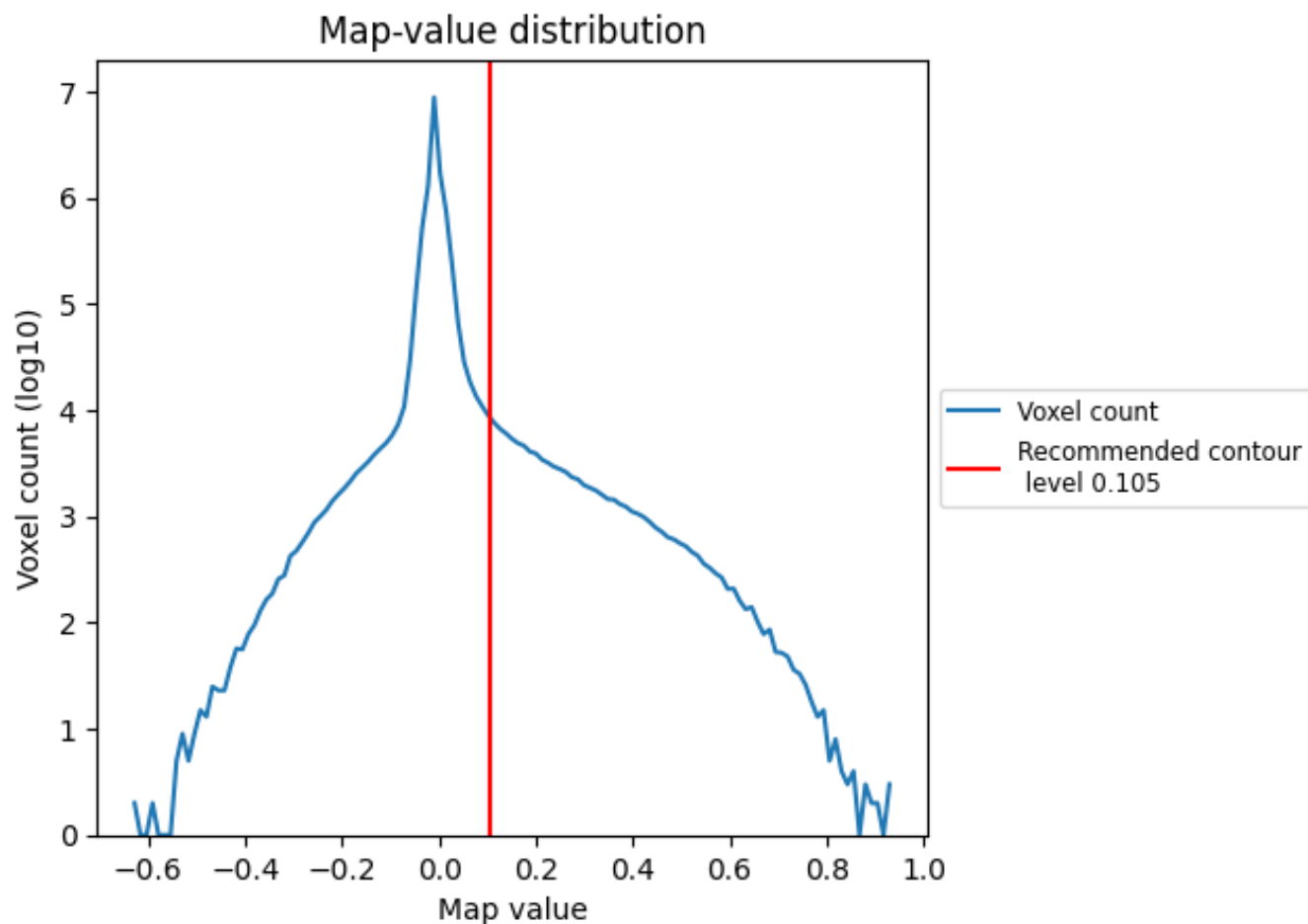
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

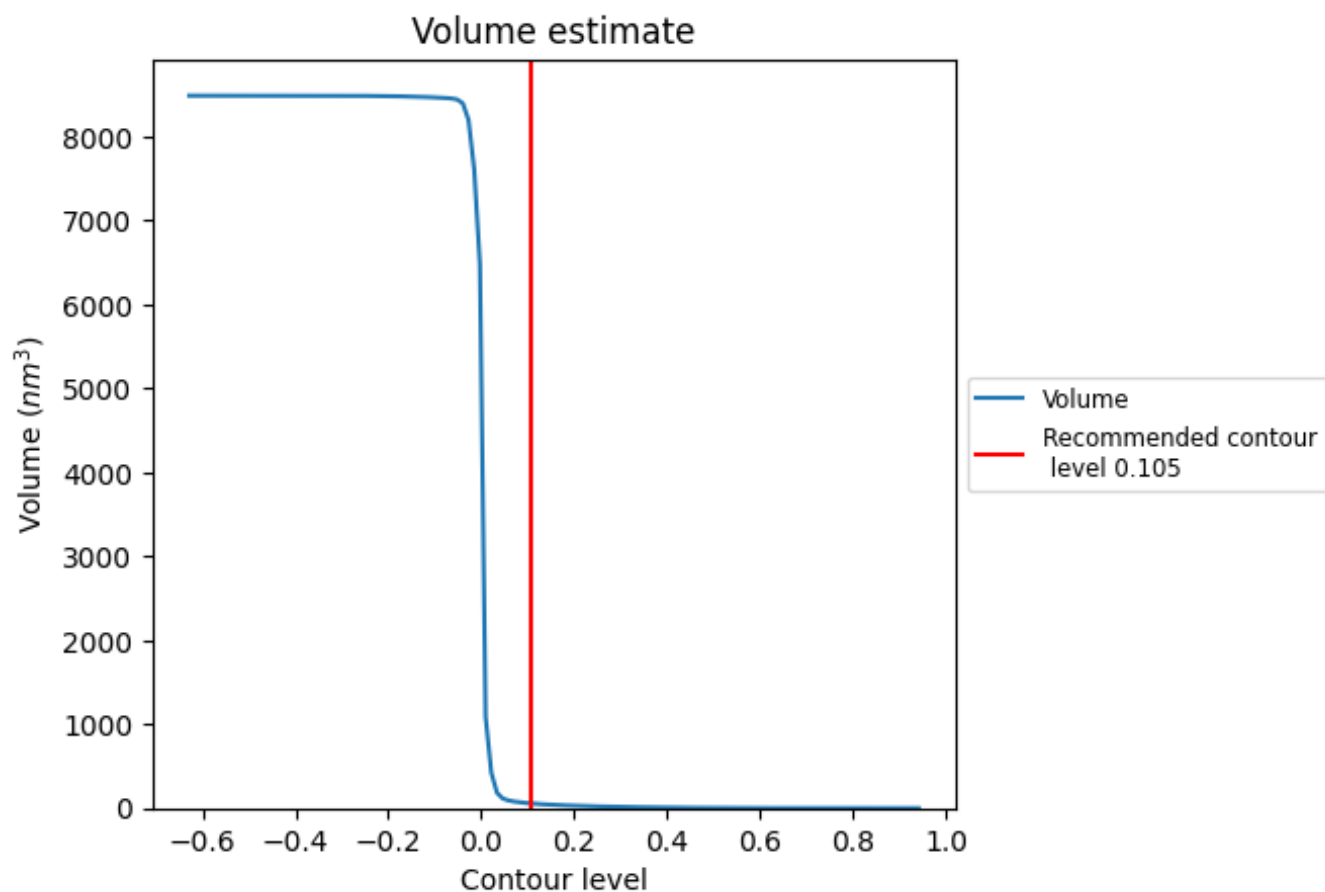
This section contains the results of statistical analysis of the map.

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.

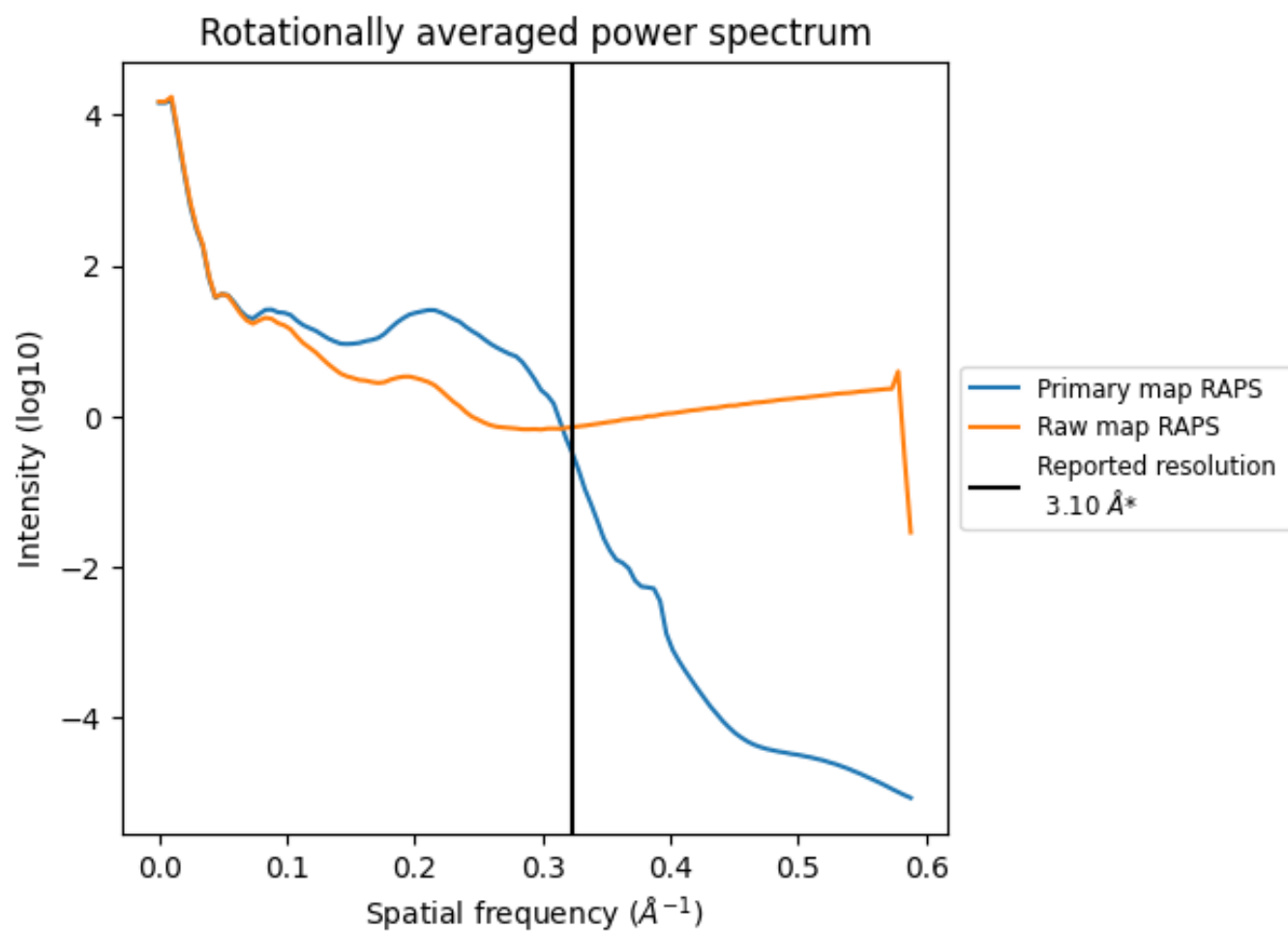
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 57 nm^3 ; this corresponds to an approximate mass of 52 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 ⓘ

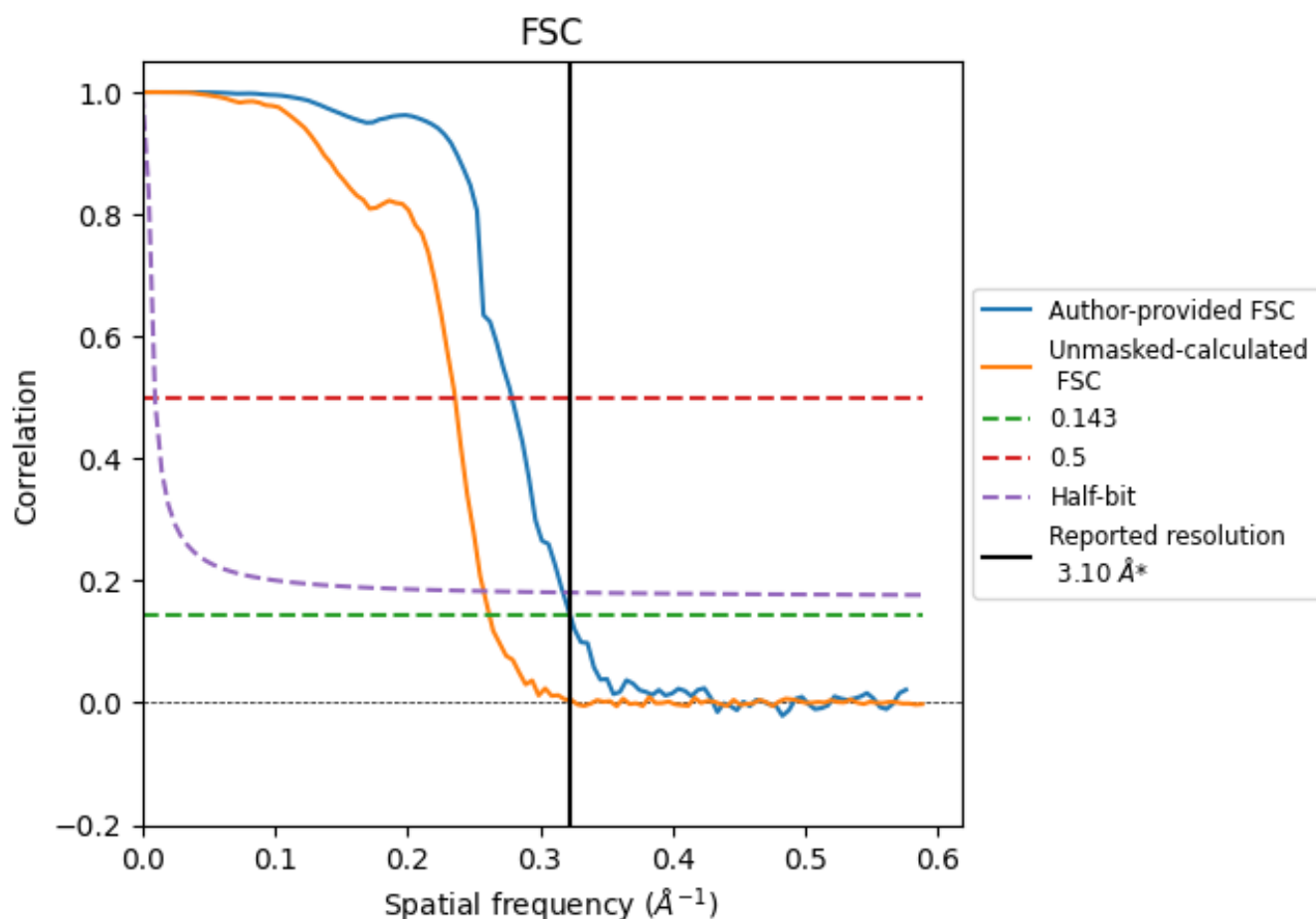


*Reported resolution corresponds to spatial frequency of 0.323 $\text{\AA}^{-1}$

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 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

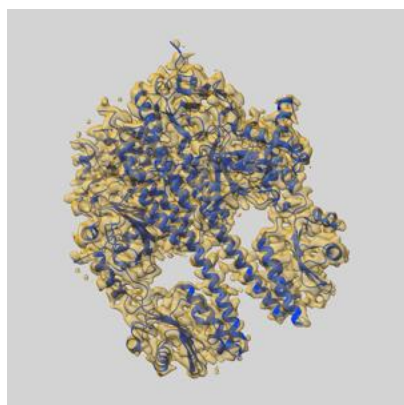
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.10	3.59	3.15
Unmasked-calculated*	3.82	4.24	3.88

*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 3.82 differs from the reported value 3.1 by more than 10 %

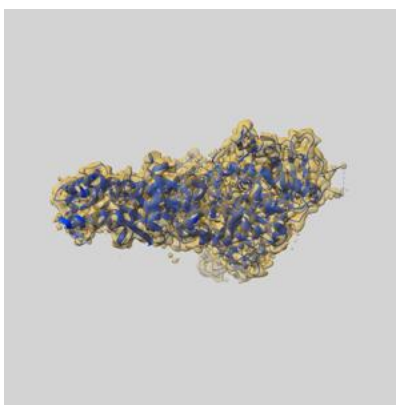
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-39108 and PDB model 8YB4. Per-residue inclusion information can be found in section [3](#) on page [5](#).

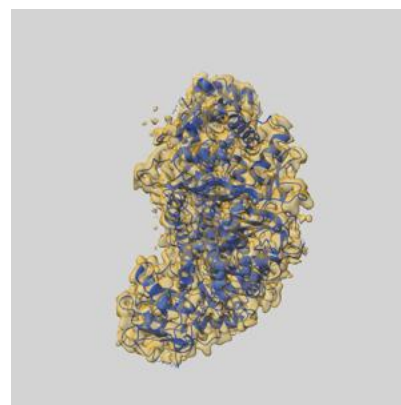
9.1 Map-model overlay [i](#)



X



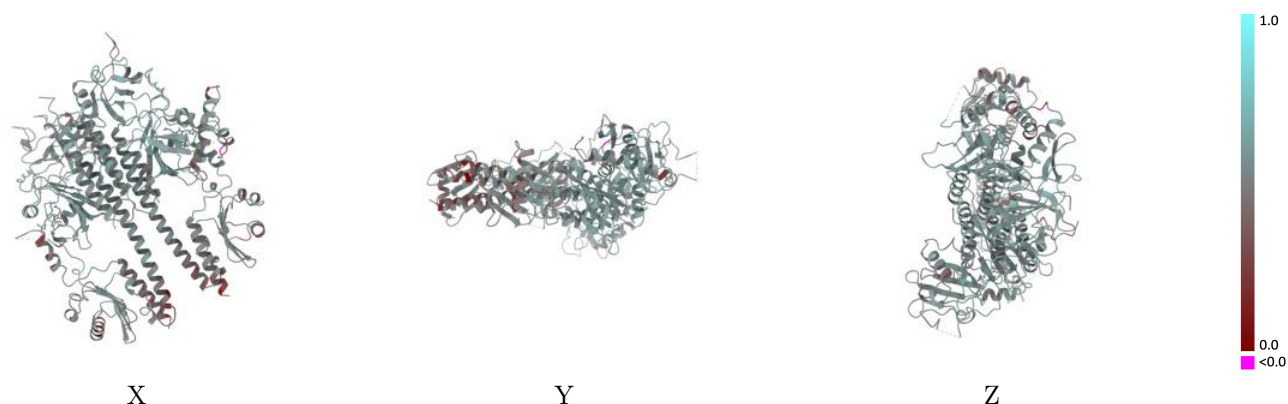
Y



Z

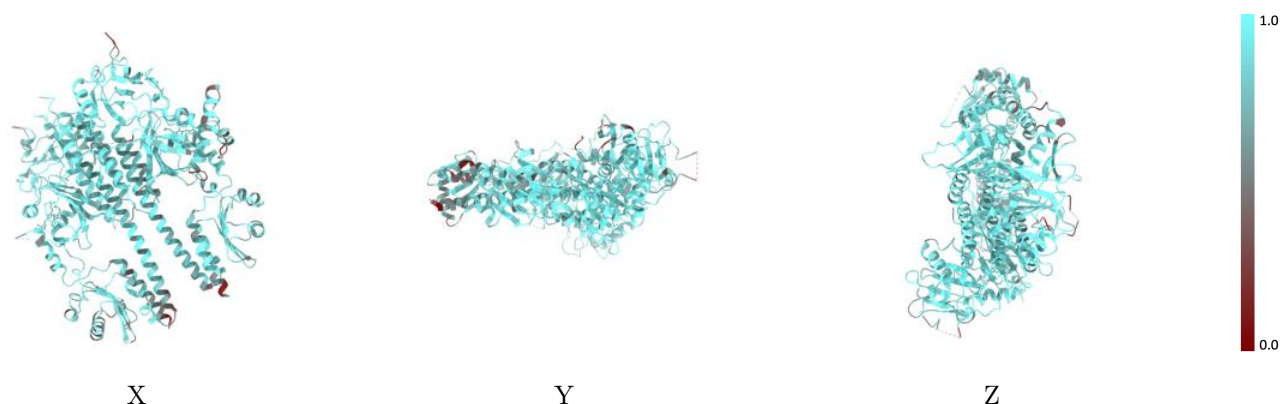
The images above show the 3D surface view of the map at the recommended contour level 0.105 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



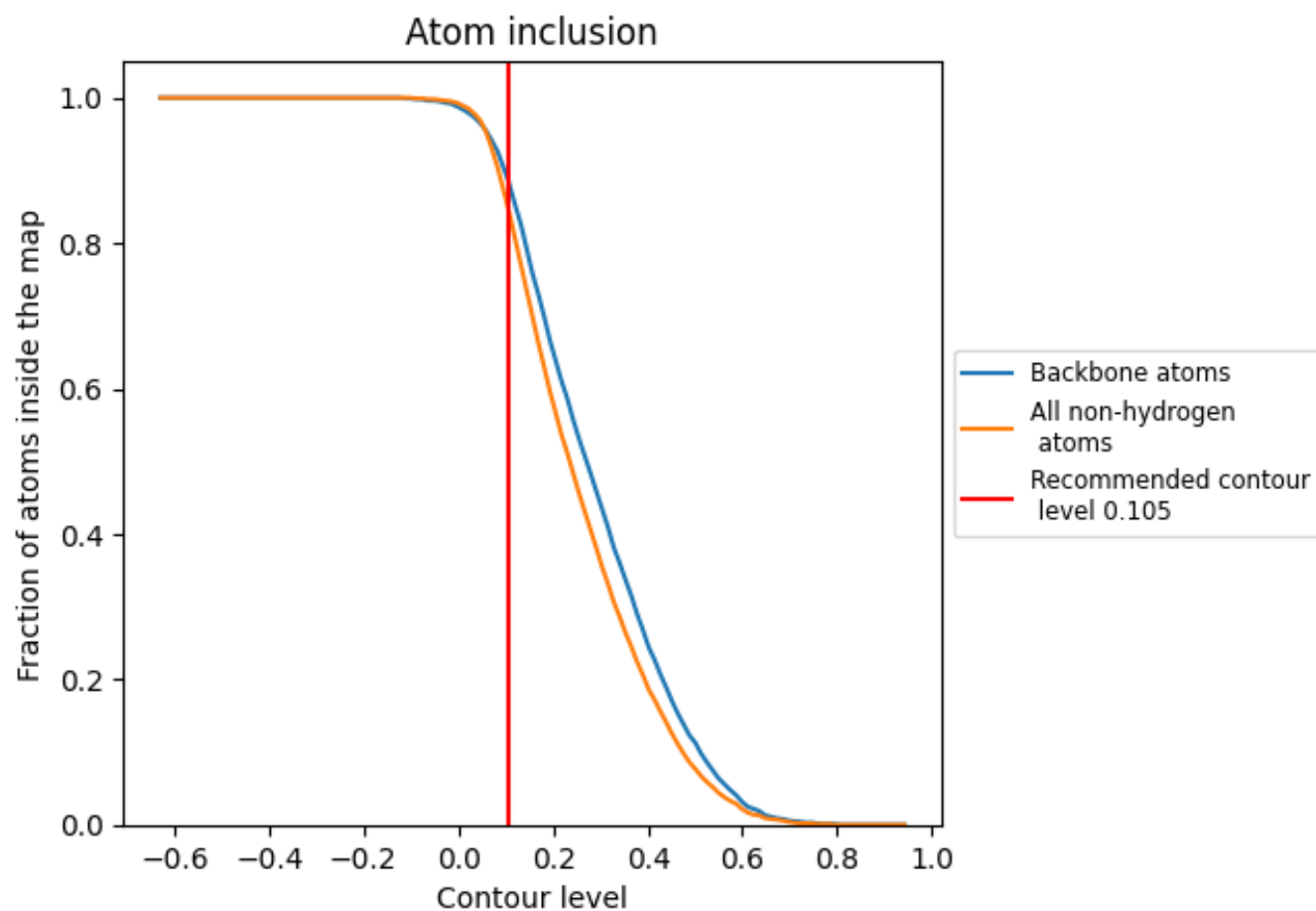
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.105).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 85% 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 (0.105) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8490	0.5220
A	0.8370	0.5110
B	0.8600	0.5290
C	0.8370	0.5510

