



## Full wwPDB EM Validation Report ⓘ

Jun 1, 2026 – 10:20 AM EDT

PDB ID : 9PUW / pdb\_00009puw  
EMDB ID : EMD-71878  
Title : Insulin Receptor bound to Ins-AC-S2  
Authors : Vogel, A.; Hill, C.P.; Blakely, A.  
Deposited on : 2025-07-31  
Resolution : 3.64 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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  
MolProbity : 4-5-2 with Phenix2.0  
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

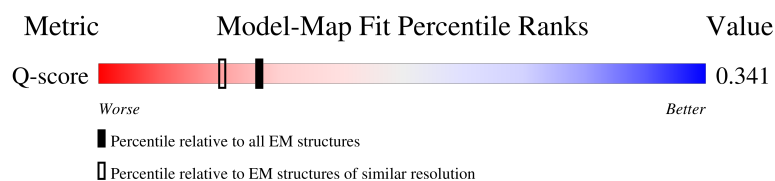
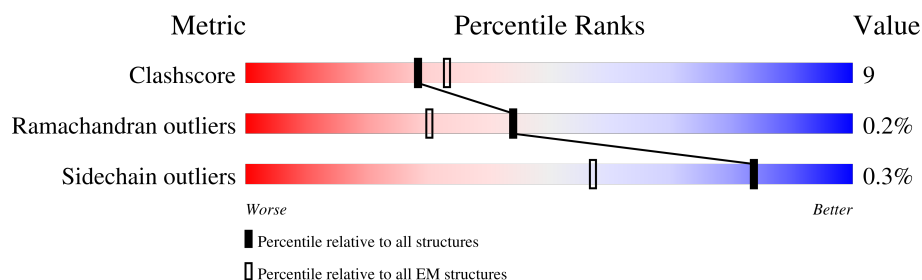
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.64 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	11633 ( 3.14 - 4.14 )

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  $\geq 3$ , 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	960	 61% 17% 22%
1	B	960	 64% 18% 19%
1	M	960	 99%
1	N	960	 99%

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	C	51	<div><div><div></div><div></div><div></div></div><div><div></div><div></div><div></div></div><div>80%12%8%</div></div>
2	Q	51	<div><div><div></div><div></div><div></div></div><div><div></div><div></div><div></div></div><div>76%16%8%</div></div>
3	P	29	<div><div><div></div><div></div><div></div></div><div><div></div><div></div><div></div></div><div>52%28%21%</div></div>
3	R	29	<div><div><div></div><div></div><div></div></div><div><div></div><div></div><div></div></div><div>69%21%7%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26929 atoms, of which 13249 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 Isoform Long of Insulin receptor.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	749	Total	C	H	N	O	S	0	0
			11964	3849	5910	1042	1120	43		
1	B	782	Total	C	H	N	O	S	0	0
			12474	4017	6149	1088	1173	47		
1	M	11	Total	C	H	N	O		0	0
			186	67	88	14	17			
1	N	11	Total	C	H	N	O		0	0
			186	67	88	14	17			

There are 124 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	918	SER	-	expression tag	UNP P06213
A	919	SER	-	expression tag	UNP P06213
A	920	GLY	-	expression tag	UNP P06213
A	921	PRO	-	expression tag	UNP P06213
A	922	SER	-	expression tag	UNP P06213
A	923	GLY	-	expression tag	UNP P06213
A	924	SER	-	expression tag	UNP P06213
A	925	HIS	-	expression tag	UNP P06213
A	926	HIS	-	expression tag	UNP P06213
A	927	HIS	-	expression tag	UNP P06213
A	928	HIS	-	expression tag	UNP P06213
A	929	HIS	-	expression tag	UNP P06213
A	930	HIS	-	expression tag	UNP P06213
A	931	GLY	-	expression tag	UNP P06213
A	932	SER	-	expression tag	UNP P06213
A	933	ASP	-	expression tag	UNP P06213
A	934	TYR	-	expression tag	UNP P06213
A	935	LYS	-	expression tag	UNP P06213
A	936	ASP	-	expression tag	UNP P06213
A	937	ASP	-	expression tag	UNP P06213
A	938	ASP	-	expression tag	UNP P06213
A	939	ASP	-	expression tag	UNP P06213

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	940	LYS	-	expression tag	UNP P06213
A	941	ASP	-	expression tag	UNP P06213
A	942	TYR	-	expression tag	UNP P06213
A	943	LYS	-	expression tag	UNP P06213
A	944	ASP	-	expression tag	UNP P06213
A	945	ASP	-	expression tag	UNP P06213
A	946	ASP	-	expression tag	UNP P06213
A	947	ASP	-	expression tag	UNP P06213
A	948	LYS	-	expression tag	UNP P06213
B	918	SER	-	expression tag	UNP P06213
B	919	SER	-	expression tag	UNP P06213
B	920	GLY	-	expression tag	UNP P06213
B	921	PRO	-	expression tag	UNP P06213
B	922	SER	-	expression tag	UNP P06213
B	923	GLY	-	expression tag	UNP P06213
B	924	SER	-	expression tag	UNP P06213
B	925	HIS	-	expression tag	UNP P06213
B	926	HIS	-	expression tag	UNP P06213
B	927	HIS	-	expression tag	UNP P06213
B	928	HIS	-	expression tag	UNP P06213
B	929	HIS	-	expression tag	UNP P06213
B	930	HIS	-	expression tag	UNP P06213
B	931	GLY	-	expression tag	UNP P06213
B	932	SER	-	expression tag	UNP P06213
B	933	ASP	-	expression tag	UNP P06213
B	934	TYR	-	expression tag	UNP P06213
B	935	LYS	-	expression tag	UNP P06213
B	936	ASP	-	expression tag	UNP P06213
B	937	ASP	-	expression tag	UNP P06213
B	938	ASP	-	expression tag	UNP P06213
B	939	ASP	-	expression tag	UNP P06213
B	940	LYS	-	expression tag	UNP P06213
B	941	ASP	-	expression tag	UNP P06213
B	942	TYR	-	expression tag	UNP P06213
B	943	LYS	-	expression tag	UNP P06213
B	944	ASP	-	expression tag	UNP P06213
B	945	ASP	-	expression tag	UNP P06213
B	946	ASP	-	expression tag	UNP P06213
B	947	ASP	-	expression tag	UNP P06213
B	948	LYS	-	expression tag	UNP P06213
M	930	SER	-	expression tag	UNP P06213
M	931	SER	-	expression tag	UNP P06213

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
M	932	GLY	-	expression tag	UNP P06213
M	933	PRO	-	expression tag	UNP P06213
M	934	SER	-	expression tag	UNP P06213
M	935	GLY	-	expression tag	UNP P06213
M	936	SER	-	expression tag	UNP P06213
M	937	HIS	-	expression tag	UNP P06213
M	938	HIS	-	expression tag	UNP P06213
M	939	HIS	-	expression tag	UNP P06213
M	940	HIS	-	expression tag	UNP P06213
M	941	HIS	-	expression tag	UNP P06213
M	942	HIS	-	expression tag	UNP P06213
M	943	GLY	-	expression tag	UNP P06213
M	944	SER	-	expression tag	UNP P06213
M	945	ASP	-	expression tag	UNP P06213
M	946	TYR	-	expression tag	UNP P06213
M	947	LYS	-	expression tag	UNP P06213
M	948	ASP	-	expression tag	UNP P06213
M	949	ASP	-	expression tag	UNP P06213
M	950	ASP	-	expression tag	UNP P06213
M	951	ASP	-	expression tag	UNP P06213
M	952	LYS	-	expression tag	UNP P06213
M	953	ASP	-	expression tag	UNP P06213
M	954	TYR	-	expression tag	UNP P06213
M	955	LYS	-	expression tag	UNP P06213
M	956	ASP	-	expression tag	UNP P06213
M	957	ASP	-	expression tag	UNP P06213
M	958	ASP	-	expression tag	UNP P06213
M	959	ASP	-	expression tag	UNP P06213
M	960	LYS	-	expression tag	UNP P06213
N	930	SER	-	expression tag	UNP P06213
N	931	SER	-	expression tag	UNP P06213
N	932	GLY	-	expression tag	UNP P06213
N	933	PRO	-	expression tag	UNP P06213
N	934	SER	-	expression tag	UNP P06213
N	935	GLY	-	expression tag	UNP P06213
N	936	SER	-	expression tag	UNP P06213
N	937	HIS	-	expression tag	UNP P06213
N	938	HIS	-	expression tag	UNP P06213
N	939	HIS	-	expression tag	UNP P06213
N	940	HIS	-	expression tag	UNP P06213
N	941	HIS	-	expression tag	UNP P06213
N	942	HIS	-	expression tag	UNP P06213

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
N	943	GLY	-	expression tag	UNP P06213
N	944	SER	-	expression tag	UNP P06213
N	945	ASP	-	expression tag	UNP P06213
N	946	TYR	-	expression tag	UNP P06213
N	947	LYS	-	expression tag	UNP P06213
N	948	ASP	-	expression tag	UNP P06213
N	949	ASP	-	expression tag	UNP P06213
N	950	ASP	-	expression tag	UNP P06213
N	951	ASP	-	expression tag	UNP P06213
N	952	LYS	-	expression tag	UNP P06213
N	953	ASP	-	expression tag	UNP P06213
N	954	TYR	-	expression tag	UNP P06213
N	955	LYS	-	expression tag	UNP P06213
N	956	ASP	-	expression tag	UNP P06213
N	957	ASP	-	expression tag	UNP P06213
N	958	ASP	-	expression tag	UNP P06213
N	959	ASP	-	expression tag	UNP P06213
N	960	LYS	-	expression tag	UNP P06213

- Molecule 2 is a protein called Ins-AC-S2 chain A.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	C	47	Total	C	H	N	O	S	0	0
			671	216	319	57	75	4		
2	Q	47	Total	C	H	N	O	S	0	0
			671	216	319	57	75	4		

- Molecule 3 is a protein called Insulin chain B.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	P	23	Total	C	H	N	O	S	0	0
			354	120	171	30	31	2		
3	R	27	Total	C	H	N	O	S	0	0
			423	143	205	36	37	2		





[illegible]

- Molecule 1: Isoform Long of Insulin receptor

Chain N:  99%

[illegible]



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	314550	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.696	Depositor
Minimum map value	-0.600	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.0311	Depositor
Map size ( $\text{\AA}$ )	339.19998, 339.19998, 339.19998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.06, 1.06, 1.06	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.14	0/6202	0.29	0/8408
1	B	0.14	0/6482	0.29	0/8791
1	M	0.07	0/101	0.18	0/137
1	N	0.10	0/101	0.21	0/137
2	C	0.11	0/358	0.32	0/484
2	Q	0.16	0/358	0.36	0/484
3	P	0.08	0/188	0.27	0/253
3	R	0.15	0/224	0.39	0/302
All	All	0.14	0/14014	0.29	0/18996

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	312	CYS	Peptide

### 5.2 Too-close contacts [i](#)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6054	5910	5905	114	0
1	B	6325	6149	6142	123	0
1	M	98	88	87	2	0
1	N	98	88	87	1	0
2	C	352	319	319	7	0
2	Q	352	319	319	6	0
3	P	183	171	170	6	0
3	R	218	205	205	8	0
All	All	13680	13249	13234	255	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 9.

All (255) 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:B:38:MET:HE3	1:B:66:VAL:HG22	1.55	0.89
3:R:4:GLN:N	3:R:4:GLN:OE1	2.07	0.87
1:A:613:LEU:HD21	1:A:781:ILE:HD13	1.65	0.79
1:A:374:TYR:OH	1:B:374:TYR:OH	2.01	0.78
1:A:452:GLN:N	1:A:452:GLN:OE1	2.18	0.76
1:B:378:SER:OG	1:B:410:GLN:O	2.03	0.75
1:A:387:LEU:HD12	1:A:420:THR:O	1.88	0.74
1:B:481:SER:O	1:B:590:THR:OG1	2.05	0.74
1:B:577:ARG:NH2	1:B:578:THR:O	2.21	0.73
1:A:38:MET:HB2	1:A:66:VAL:HG13	1.69	0.73
1:A:16:ASN:N	1:A:38:MET:SD	2.62	0.72
1:B:353:GLU:O	1:B:357:ASN:ND2	2.23	0.72
1:A:334:THR:HG22	1:A:335:VAL:HG23	1.71	0.71
1:A:556:LEU:HD23	1:A:562:TYR:CE2	2.25	0.71
1:A:775:HIS:NE2	1:A:837:GLU:O	2.21	0.70
1:B:556:LEU:HD23	1:B:562:TYR:CE2	2.26	0.69
1:A:249:GLN:OE1	1:A:277:TYR:OH	2.11	0.69
1:B:151:ASP:OD1	1:B:152:ASN:N	2.26	0.68
1:A:776:PHE:N	1:A:805:THR:OG1	2.27	0.68
1:A:38:MET:CB	1:A:66:VAL:HG13	2.24	0.68
1:A:368:LEU:HD23	1:A:369:LYS:N	2.10	0.67
1:B:11:MET:SD	1:B:11:MET:N	2.69	0.66
1:A:465:GLN:N	1:A:465:GLN:OE1	2.28	0.66
1:B:826:ASN:OD1	1:B:906:THR:OG1	2.12	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:34:GLU:N	2:C:34:GLU:OE1	2.28	0.66
1:A:653:LEU:HD22	1:A:843:VAL:HG11	1.76	0.66
1:A:258:PHE:O	1:A:262:LEU:HD22	1.97	0.65
3:R:21:GLU:OE2	3:R:21:GLU:N	2.28	0.65
1:B:517:GLU:OE1	1:B:582:LYS:NZ	2.30	0.64
1:A:17:LEU:HD21	1:A:46:PHE:CE2	2.33	0.64
1:B:629:LEU:HD11	1:B:631:PHE:CE2	2.33	0.64
1:B:24:GLU:OE2	1:B:53:LYS:NZ	2.32	0.62
1:A:379:LEU:O	1:A:412:TRP:NE1	2.33	0.62
1:A:339:SER:OG	1:A:340:LEU:N	2.29	0.61
1:B:605:SER:OG	1:B:806:MET:SD	2.50	0.61
1:A:630:VAL:HG22	1:A:783:LEU:HD12	1.83	0.60
1:A:342:ILE:HD11	1:A:382:PHE:CZ	2.35	0.60
1:A:13:ILE:HG21	1:A:20:LEU:HD22	1.82	0.60
1:A:342:ILE:HD11	1:A:382:PHE:HZ	1.67	0.60
1:B:584:ASP:OD1	1:B:584:ASP:N	2.34	0.60
1:B:638:ASP:OD2	1:B:656:ARG:NH1	2.35	0.60
1:B:556:LEU:HD23	1:B:562:TYR:CD2	2.38	0.59
1:B:55:ILE:HD12	1:B:78:ASN:O	2.02	0.59
1:B:806:MET:SD	1:B:806:MET:N	2.76	0.58
1:B:496:ASP:OD1	1:B:498:ARG:NE	2.35	0.58
1:B:633:GLU:O	1:B:780:ARG:N	2.36	0.58
1:A:125:LEU:HD21	1:A:128:LEU:HD21	1.84	0.57
1:B:829:HIS:NE2	1:B:869:GLU:O	2.37	0.57
1:A:18:THR:O	1:A:21:HIS:ND1	2.34	0.57
1:B:293:THR:OG1	1:B:304:CYS:SG	2.60	0.57
1:B:363:GLU:N	1:B:363:GLU:OE1	2.38	0.57
1:A:613:LEU:O	1:A:767:SER:OG	2.13	0.56
1:A:653:LEU:CD2	1:A:843:VAL:HG11	2.36	0.56
1:B:58:THR:O	1:B:84:GLY:N	2.39	0.56
1:A:526:SER:O	1:B:345:ARG:NH2	2.40	0.55
1:B:54:LEU:HD21	1:B:57:ILE:HD11	1.89	0.55
1:B:620:ASP:OD2	1:B:622:ASN:ND2	2.39	0.55
1:A:213:LEU:HD13	1:A:229:ARG:HD3	1.88	0.55
1:A:637:GLU:N	1:A:637:GLU:OE1	2.39	0.55
1:B:342:ILE:HD11	1:B:382:PHE:HZ	1.70	0.55
1:B:342:ILE:HD11	1:B:382:PHE:CZ	2.42	0.55
1:B:65:ARG:HD2	3:R:12:VAL:HG11	1.88	0.55
1:B:572:PHE:HD1	1:B:578:THR:HG22	1.72	0.55
3:P:14:ALA:O	3:P:18:VAL:HG23	2.07	0.54
1:A:283:LYS:HB2	1:A:285:ILE:HD11	1.88	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:464:ASP:OD1	1:B:465:GLN:N	2.41	0.54
1:B:13:ILE:HD13	1:B:20:LEU:CD1	2.37	0.54
1:B:85:SER:O	1:B:114:ARG:NH1	2.41	0.54
1:A:65:ARG:NH1	1:A:67:TYR:OH	2.40	0.54
1:B:531:VAL:O	1:B:531:VAL:HG12	2.09	0.53
1:B:760:GLU:OE1	1:B:761:LYS:N	2.37	0.53
1:A:36:LEU:HD23	1:A:36:LEU:N	2.24	0.53
1:A:819:THR:OG1	1:A:831:MET:HE2	2.08	0.53
1:B:888:ALA:O	1:B:895:GLY:N	2.39	0.53
1:M:708:TYR:O	1:M:712:VAL:HG13	2.08	0.53
1:B:35:ILE:HG22	1:B:38:MET:HE1	1.90	0.52
1:B:38:MET:CE	1:B:66:VAL:HG22	2.33	0.52
1:B:65:ARG:NH2	3:R:9:SER:OG	2.42	0.52
1:A:532:VAL:HG23	1:A:532:VAL:O	2.09	0.52
1:A:866:PHE:O	1:A:870:ARG:N	2.40	0.52
1:B:13:ILE:HD13	1:B:20:LEU:HD13	1.92	0.52
1:B:776:PHE:N	1:B:805:THR:OG1	2.42	0.52
2:Q:12:SER:N	2:Q:15:GLN:OE1	2.37	0.52
1:B:36:LEU:N	1:B:36:LEU:HD23	2.25	0.52
1:B:873:ARG:O	1:B:875:ARG:NH2	2.43	0.52
1:B:788:GLN:OE1	1:B:794:ARG:NH2	2.42	0.52
1:A:613:LEU:HD21	1:A:781:ILE:HG21	1.91	0.52
1:A:630:VAL:HG22	1:A:783:LEU:CD1	2.40	0.52
1:B:379:LEU:O	1:B:412:TRP:NE1	2.42	0.52
1:A:873:ARG:O	1:A:875:ARG:NH1	2.42	0.52
1:B:572:PHE:CD1	1:B:578:THR:HG22	2.44	0.52
1:A:368:LEU:HD23	1:A:369:LYS:H	1.75	0.51
1:A:489:TRP:CE3	1:A:566:VAL:HG21	2.45	0.51
1:B:842:ILE:HG21	1:B:845:TYR:CZ	2.45	0.51
1:A:625:ILE:H	1:A:625:ILE:HD12	1.75	0.51
1:B:530:THR:O	1:B:530:THR:HG22	2.09	0.51
2:C:36:TRP:HA	2:C:39:ILE:HG22	1.92	0.51
1:A:65:ARG:NE	1:A:97:GLU:OE1	2.40	0.51
1:A:13:ILE:HG21	1:A:20:LEU:CD2	2.41	0.51
1:B:65:ARG:NH1	1:B:97:GLU:OE1	2.41	0.51
1:B:81:VAL:HG13	1:B:111:ASN:O	2.11	0.51
1:B:629:LEU:O	1:B:784:GLN:N	2.44	0.51
1:A:111:ASN:OD1	1:A:112:ILE:N	2.44	0.50
1:B:477:TYR:HE1	1:B:486:LEU:HD23	1.76	0.50
1:B:488:ARG:NH2	2:C:39:ILE:HD13	2.26	0.50
1:B:824:GLU:N	1:B:824:GLU:OE1	2.43	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:540:SER:OG	1:B:541:ASN:N	2.43	0.50
1:A:453:GLU:N	1:A:453:GLU:OE1	2.45	0.50
1:A:463:GLY:O	1:A:466:ALA:HB2	2.12	0.49
1:B:387:LEU:HD12	1:B:420:THR:O	2.12	0.49
1:B:788:GLN:NE2	1:B:792:GLU:O	2.38	0.49
1:B:869:GLU:OE1	1:B:873:ARG:N	2.45	0.49
1:A:556:LEU:HD23	1:A:562:TYR:CZ	2.46	0.49
1:A:59:ASP:OD1	1:A:85:SER:OG	2.30	0.49
1:B:213:LEU:N	1:B:227:ALA:O	2.44	0.49
1:A:344:ILE:HG22	1:A:344:ILE:O	2.12	0.49
1:A:485:ILE:HG21	1:A:588:VAL:HG11	1.95	0.49
1:B:249:GLN:O	1:B:250:ASP:OD1	2.30	0.49
1:B:651:LEU:HD23	1:B:651:LEU:H	1.78	0.49
1:B:566:VAL:HG12	1:B:567:LYS:N	2.27	0.49
1:B:635:GLN:OE1	1:B:635:GLN:N	2.44	0.49
1:A:248:PHE:HB2	1:A:254:VAL:HG22	1.93	0.49
1:A:643:GLU:OE2	1:A:863:ARG:NH2	2.39	0.49
1:A:278:VAL:O	1:A:285:ILE:N	2.45	0.48
1:A:308:CYS:N	1:A:309:PRO:HD3	2.28	0.48
1:B:483:ASP:OD1	1:B:483:ASP:N	2.45	0.48
1:A:821:GLU:HG3	1:A:831:MET:HE1	1.94	0.48
3:P:21:GLU:N	3:P:21:GLU:OE1	2.46	0.48
3:P:7:CYS:O	3:P:11:LEU:N	2.30	0.48
1:A:246:TYR:N	1:A:254:VAL:O	2.42	0.48
1:A:417:HIS:ND1	1:A:418:ASN:O	2.45	0.48
1:B:488:ARG:CZ	2:C:39:ILE:HD13	2.43	0.48
1:A:409:ARG:NH2	1:A:520:GLY:O	2.46	0.48
3:P:6:LEU:HD22	3:P:11:LEU:HA	1.95	0.48
1:B:629:LEU:HD12	1:B:630:VAL:N	2.29	0.48
1:A:56:MET:SD	1:A:57:ILE:N	2.87	0.48
1:A:485:ILE:CG2	1:A:588:VAL:HG11	2.43	0.48
1:B:9:PRO:O	1:B:11:MET:HE3	2.14	0.48
1:A:869:GLU:OE1	1:A:873:ARG:NE	2.44	0.48
2:Q:24:LEU:HD22	2:Q:25:PRO:HD2	1.95	0.47
1:B:478:ILE:O	1:B:479:ARG:NH1	2.48	0.47
1:B:788:GLN:NE2	1:B:791:PRO:O	2.47	0.47
1:B:400:PHE:CD2	1:B:442:MET:HE1	2.50	0.47
1:A:496:ASP:O	1:A:497:PHE:CD1	2.68	0.47
1:B:278:VAL:HG11	1:B:288:CYS:SG	2.54	0.47
1:B:538:LEU:HD12	1:B:539:ARG:N	2.30	0.47
1:N:706:GLU:OE1	1:N:706:GLU:N	2.48	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:GLU:O	1:A:359:GLY:N	2.46	0.47
1:B:507:TYR:O	1:B:530:THR:HG23	2.14	0.47
1:B:52:PRO:O	1:B:78:ASN:ND2	2.41	0.47
1:A:324:VAL:HG22	1:A:353:GLU:HG3	1.96	0.47
1:A:574:ASP:OD1	1:A:574:ASP:N	2.48	0.47
3:R:1:PHE:O	3:R:2:VAL:HB	2.15	0.46
1:A:23:LEU:HD12	1:A:26:CYS:SG	2.56	0.46
1:A:429:HIS:HE1	1:B:571:THR:HG23	1.80	0.46
1:A:37:LEU:N	1:A:37:LEU:HD12	2.30	0.46
1:B:293:THR:OG1	1:B:308:CYS:SG	2.74	0.46
3:P:13:GLU:O	3:P:17:LEU:HG	2.16	0.46
1:B:28:VAL:HG22	1:B:55:ILE:CG2	2.45	0.46
1:A:796:SER:OG	1:A:797:VAL:N	2.49	0.45
1:B:611:ILE:HD12	1:B:773:LEU:CD1	2.46	0.45
1:A:13:ILE:HG23	1:A:19:ARG:HB2	1.98	0.45
1:A:830:LEU:N	1:A:872:CYS:O	2.42	0.45
1:A:622:ASN:O	1:A:787:ASN:ND2	2.50	0.45
1:B:34:GLN:HB3	1:B:36:LEU:HD22	1.99	0.45
3:R:1:PHE:CD1	3:R:1:PHE:C	2.93	0.45
1:A:475:PHE:HE2	1:A:583:SER:HG	1.65	0.45
1:B:11:MET:HE1	1:B:29:ILE:HG12	1.99	0.45
1:B:249:GLN:C	1:B:250:ASP:OD1	2.60	0.44
2:C:39:ILE:O	2:C:43:VAL:HG23	2.17	0.44
1:A:343:ASN:O	1:A:373:SER:HA	2.17	0.44
1:A:348:ASN:H	1:A:350:LEU:CD2	2.30	0.44
1:B:578:THR:O	1:B:578:THR:OG1	2.31	0.44
2:C:3:VAL:HG22	1:M:711:ASN:OD1	2.17	0.44
1:A:431:ASN:O	1:A:432:PRO:C	2.60	0.44
1:A:469:GLU:OE2	1:A:567:LYS:NZ	2.43	0.44
1:B:828:VAL:HG21	1:B:903:PHE:CE1	2.52	0.44
1:A:124:GLU:N	1:A:124:GLU:OE1	2.51	0.44
1:A:247:HIS:ND1	1:A:282:ASN:OD1	2.51	0.44
1:B:394:GLU:OE1	1:B:395:ILE:N	2.44	0.44
1:A:99:VAL:HG12	1:A:100:HIS:CD2	2.52	0.44
1:A:336:ILE:HG22	1:A:338:GLY:H	1.81	0.44
1:A:363:GLU:N	1:A:363:GLU:OE1	2.51	0.44
1:B:612:ILE:HG22	1:B:769:VAL:HG12	2.00	0.44
1:A:282:ASN:OD1	1:A:282:ASN:C	2.60	0.44
1:B:790:THR:HB	1:B:791:PRO:HD3	2.00	0.44
1:A:621:PRO:HB3	1:A:625:ILE:HD11	1.99	0.43
3:P:14:ALA:HA	3:P:17:LEU:HD12	2.00	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:ASP:O	1:A:498:ARG:N	2.52	0.43
1:B:776:PHE:O	1:B:804:ARG:NH1	2.47	0.43
1:A:615:TRP:HH2	1:A:762:VAL:HG21	1.81	0.43
1:A:790:THR:HB	1:A:791:PRO:HD3	2.01	0.43
1:A:781:ILE:N	1:A:801:VAL:O	2.47	0.43
1:B:65:ARG:NH2	1:B:97:GLU:OE1	2.51	0.43
1:A:343:ASN:O	1:A:344:ILE:C	2.62	0.43
1:A:549:PRO:HA	2:Q:43:VAL:HG11	2.01	0.43
1:B:532:VAL:HG21	1:B:551:TRP:NE1	2.33	0.43
1:A:487:LEU:O	1:A:550:GLY:HA2	2.19	0.42
1:A:566:VAL:HG12	1:A:567:LYS:N	2.33	0.42
1:B:370:ILE:HG22	1:B:405:ASN:OD1	2.19	0.42
1:A:370:ILE:HG22	1:A:405:ASN:OD1	2.19	0.42
1:B:847:VAL:HG22	1:B:886:ILE:HG12	1.99	0.42
1:A:390:GLY:O	1:A:393:LEU:HD21	2.20	0.42
2:Q:9:SER:OG	2:Q:10:ILE:N	2.50	0.42
1:A:38:MET:HE2	1:A:41:THR:HG23	2.01	0.42
1:B:574:ASP:OD1	1:B:575:GLU:N	2.52	0.42
1:A:350:LEU:CB	1:A:354:LEU:HD12	2.50	0.42
1:A:633:GLU:O	1:A:780:ARG:N	2.47	0.42
1:A:46:PHE:CE2	1:A:69:LEU:HD21	2.55	0.42
1:A:429:HIS:CE1	1:A:458:ALA:HB2	2.55	0.42
1:B:33:LEU:HD23	1:B:61:LEU:HD13	2.01	0.42
1:B:338:GLY:O	1:B:366:GLY:N	2.51	0.42
1:A:41:THR:OG1	1:A:67:TYR:O	2.24	0.42
1:B:80:THR:HG21	1:B:226:VAL:HG11	2.02	0.42
1:B:109:LEU:HD23	1:B:109:LEU:C	2.45	0.42
1:B:547:ASN:O	1:B:548:HIS:C	2.61	0.42
1:B:611:ILE:HD12	1:B:773:LEU:HD13	2.02	0.42
1:A:80:THR:O	1:A:110:MET:N	2.49	0.42
1:A:116:SER:OG	1:A:117:VAL:N	2.53	0.42
1:A:789:ASP:OD1	1:A:790:THR:N	2.52	0.42
1:B:79:LEU:O	1:B:109:LEU:N	2.52	0.41
1:B:869:GLU:OE2	1:B:875:ARG:NH2	2.53	0.41
1:A:483:ASP:O	1:A:556:LEU:HD13	2.20	0.41
1:B:87:LEU:HD21	1:B:115:GLY:HA2	2.02	0.41
1:B:504:MET:HE2	1:B:569:LEU:HD13	2.02	0.41
1:A:600:ASP:OD2	1:A:600:ASP:C	2.64	0.41
1:B:321:ILE:CD1	1:B:340:LEU:HD22	2.51	0.41
1:B:589:GLN:O	1:B:589:GLN:HG3	2.20	0.41
1:B:787:ASN:OD1	1:B:794:ARG:NH1	2.53	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:4:GLU:OE1	2:Q:4:GLU:N	2.50	0.41
1:B:14:ARG:HD2	3:R:26:TYR:CZ	2.55	0.41
1:B:513:GLN:OE1	1:B:561:GLN:NE2	2.53	0.41
2:Q:10:ILE:HD12	3:R:4:GLN:C	2.45	0.41
1:A:112:ILE:HD12	1:A:137:LEU:HD11	2.03	0.41
1:B:530:THR:O	1:B:530:THR:CG2	2.68	0.41
1:B:382:PHE:CD2	1:B:385:LEU:HD12	2.56	0.41
1:B:505:LEU:HD12	1:B:566:VAL:HG22	2.03	0.41
1:A:542:ASP:N	1:A:542:ASP:OD1	2.54	0.41
1:B:158:ILE:HD12	1:B:185:HIS:CE1	2.56	0.41
1:B:489:TRP:CE3	1:B:566:VAL:HG21	2.56	0.41
1:B:41:THR:OG1	1:B:67:TYR:O	2.36	0.41
1:B:279:ILE:HA	1:B:284:CYS:HA	2.02	0.41
1:B:646:TYR:CD1	1:B:651:LEU:HD13	2.55	0.41
1:A:566:VAL:CG1	1:A:567:LYS:N	2.84	0.40
1:A:370:ILE:CD1	1:A:379:LEU:HD11	2.51	0.40
1:B:139:SER:OG	1:B:141:GLU:OE2	2.39	0.40
1:A:222:PRO:HA	1:A:225:CYS:SG	2.62	0.40
1:A:350:LEU:HB2	1:A:354:LEU:HD12	2.03	0.40
1:B:355:GLU:OE2	1:B:383:ARG:NE	2.35	0.40
1:B:517:GLU:CD	1:B:582:LYS:HZ3	2.24	0.40
1:B:538:LEU:C	1:B:539:ARG:HG3	2.47	0.40
1:B:377:VAL:O	1:B:377:VAL:HG12	2.20	0.40
2:C:3:VAL:HG23	2:C:4:GLU:N	2.36	0.40
1:A:38:MET:HB3	1:A:66:VAL:HG13	2.01	0.40
1:A:429:HIS:CE1	1:B:571:THR:HG23	2.56	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	739/960 (77%)	653 (88%)	86 (12%)	0	100	100
1	B	772/960 (80%)	698 (90%)	72 (9%)	2 (0%)	36	64
1	M	9/960 (1%)	9 (100%)	0	0	100	100
1	N	9/960 (1%)	9 (100%)	0	0	100	100
2	C	45/51 (88%)	41 (91%)	4 (9%)	0	100	100
2	Q	45/51 (88%)	40 (89%)	5 (11%)	0	100	100
3	P	21/29 (72%)	20 (95%)	1 (5%)	0	100	100
3	R	25/29 (86%)	24 (96%)	0	1 (4%)	2	17
All	All	1665/4000 (42%)	1494 (90%)	168 (10%)	3 (0%)	44	71

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	792	GLU
3	R	2	VAL
1	B	539	ARG

### 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	680/868 (78%)	678 (100%)	2 (0%)	86	81
1	B	711/868 (82%)	709 (100%)	2 (0%)	86	81
1	M	11/868 (1%)	11 (100%)	0	100	100
1	N	11/868 (1%)	11 (100%)	0	100	100
2	C	38/42 (90%)	38 (100%)	0	100	100
2	Q	38/42 (90%)	38 (100%)	0	100	100
3	P	19/25 (76%)	19 (100%)	0	100	100
3	R	23/25 (92%)	23 (100%)	0	100	100
All	All	1531/3606 (42%)	1527 (100%)	4 (0%)	84	81

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	546	GLN
1	A	579	TYR
1	B	266	CYS
1	B	546	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	HIS
1	A	410	GLN
1	A	527	ASN
1	A	858	HIS
1	B	32	HIS
1	B	111	ASN
1	B	185	HIS
1	B	281	ASN
1	B	357	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

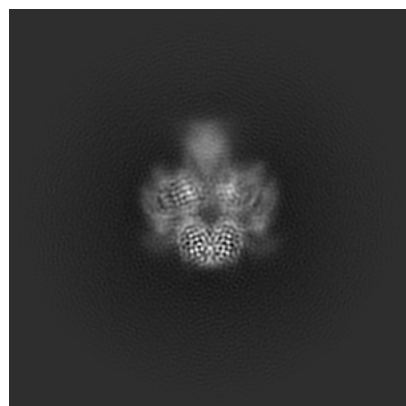
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71878. These allow visual inspection of the internal detail of the map and identification of artifacts.

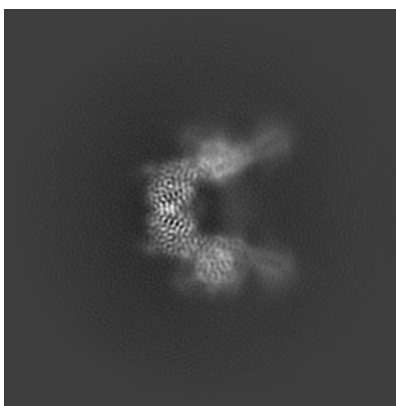
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

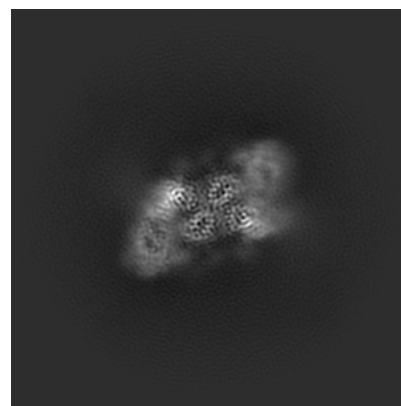
#### 6.1.1 Primary map



X

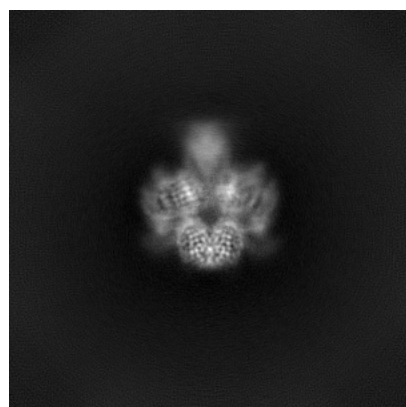


Y

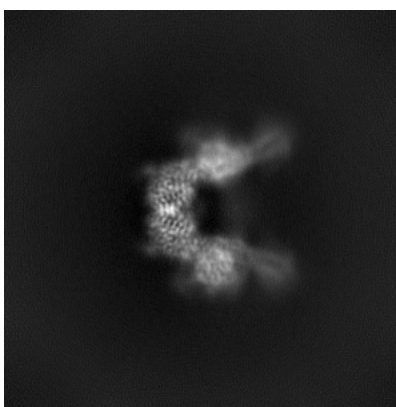


Z

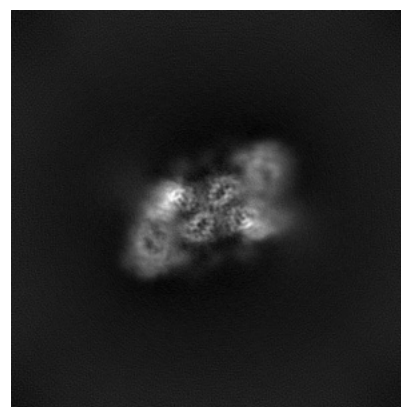
#### 6.1.2 Raw map



X



Y

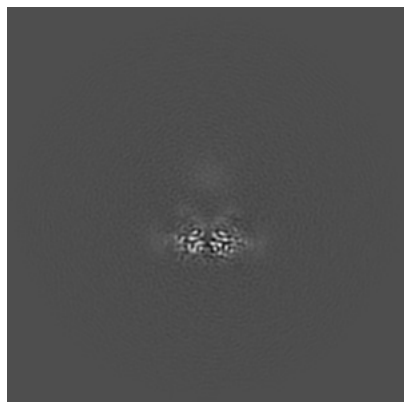


Z

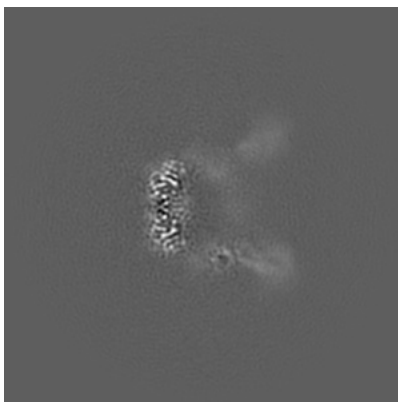
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

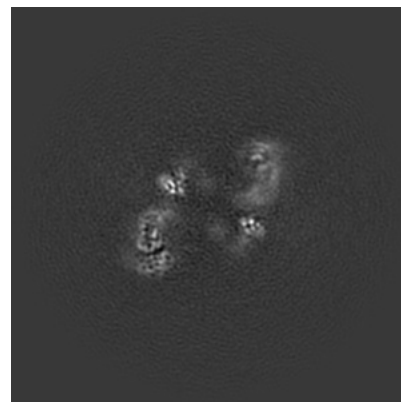
### 6.2.1 Primary map



X Index: 160

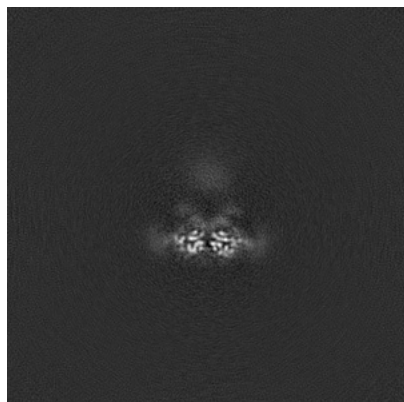


Y Index: 160

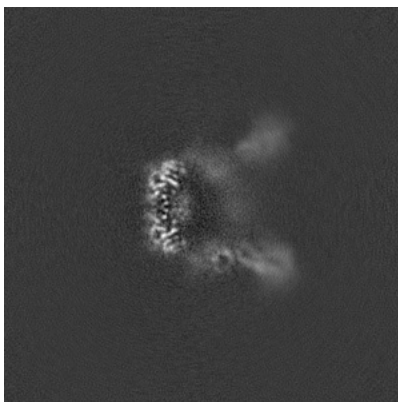


Z Index: 160

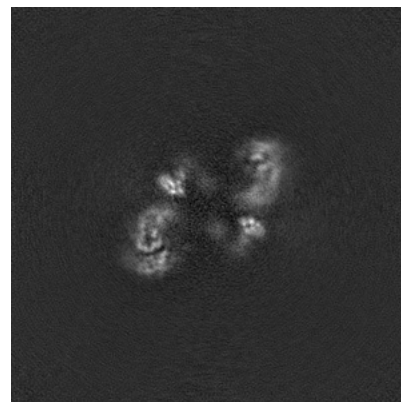
### 6.2.2 Raw map



X Index: 160



Y Index: 160

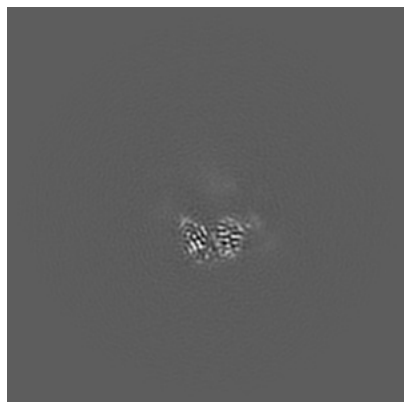


Z Index: 160

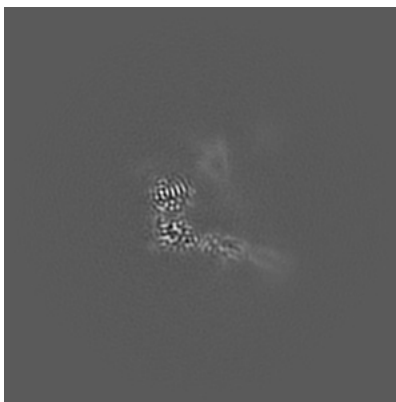
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

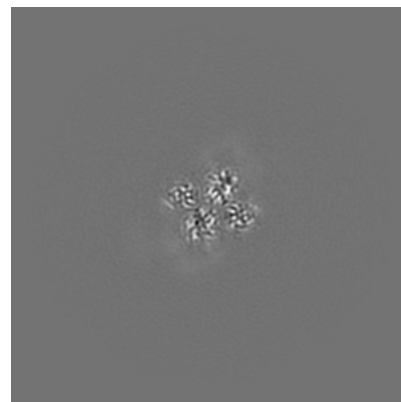
### 6.3.1 Primary map



X Index: 175

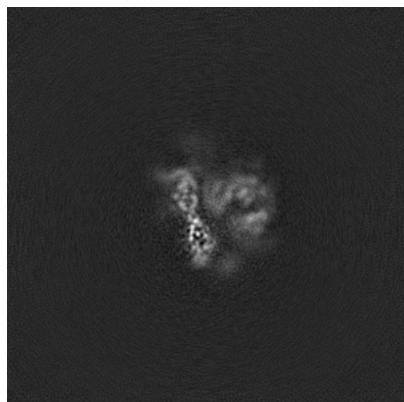


Y Index: 171

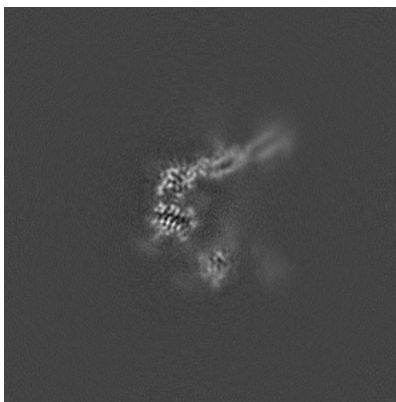


Z Index: 134

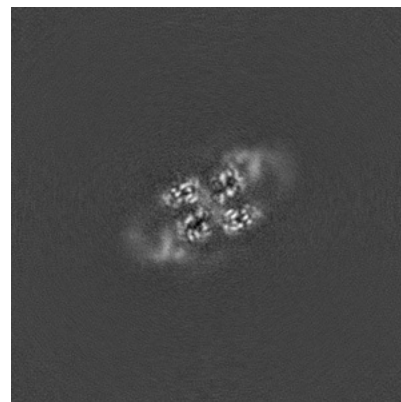
### 6.3.2 Raw map



X Index: 190



Y Index: 146



Z Index: 143

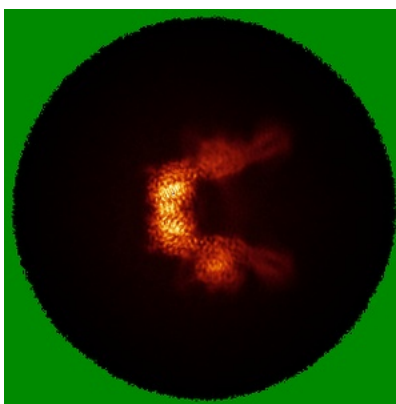
The images above show the largest variance slices of the map in three orthogonal directions.

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

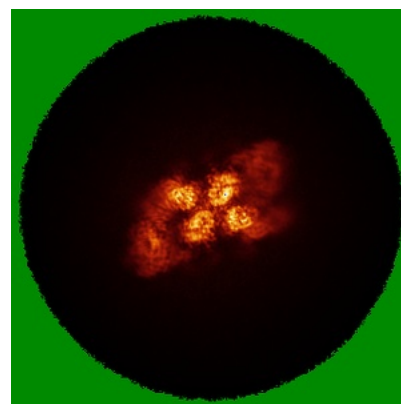
### 6.4.1 Primary map



X



Y

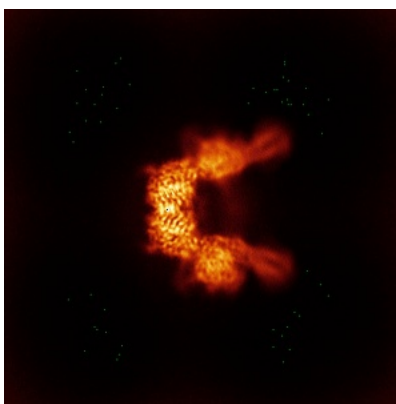


Z

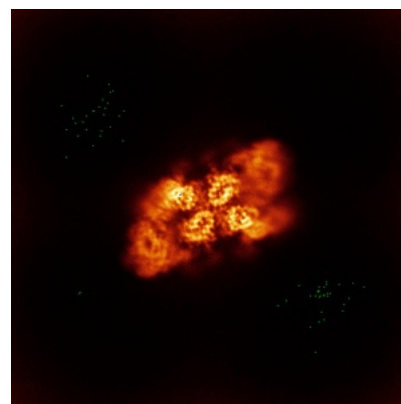
### 6.4.2 Raw map



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.

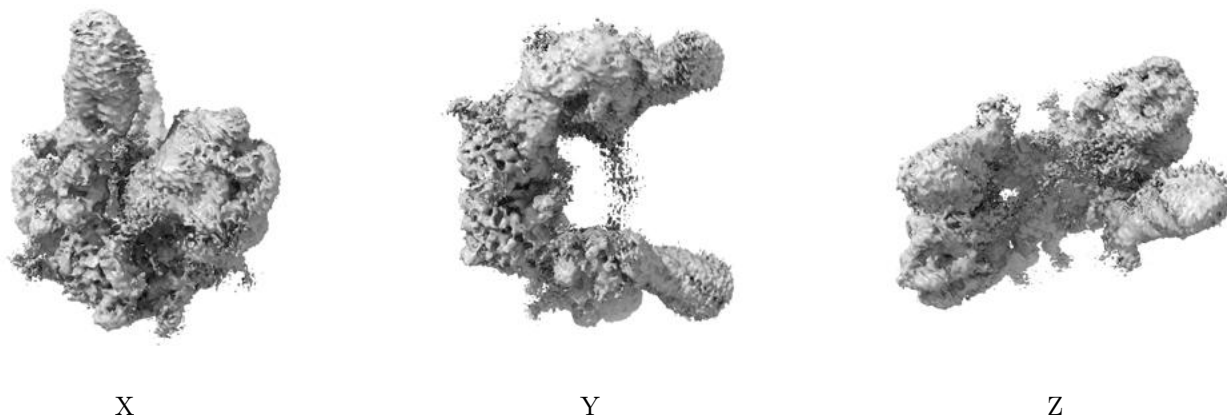
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0311. 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.

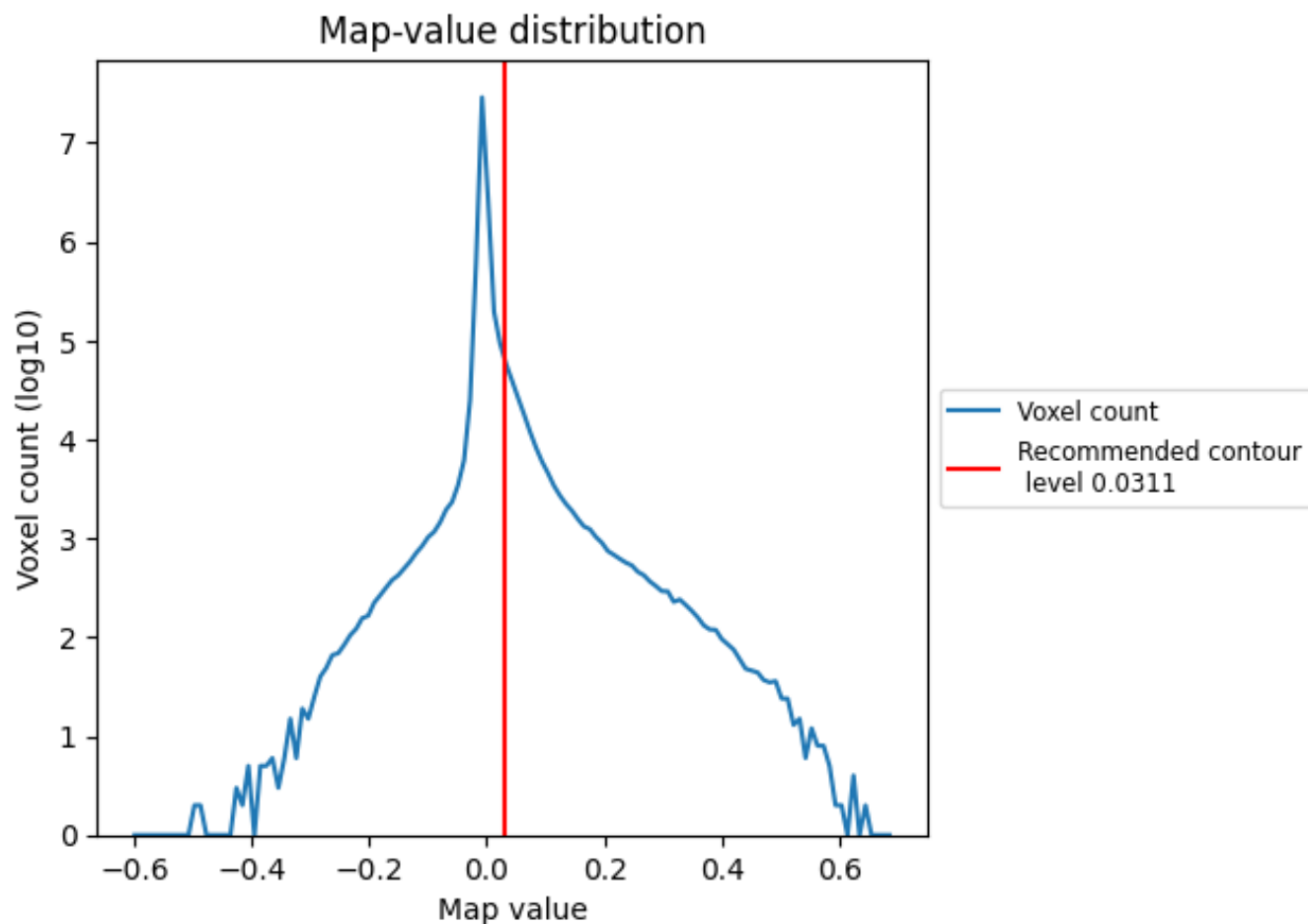
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

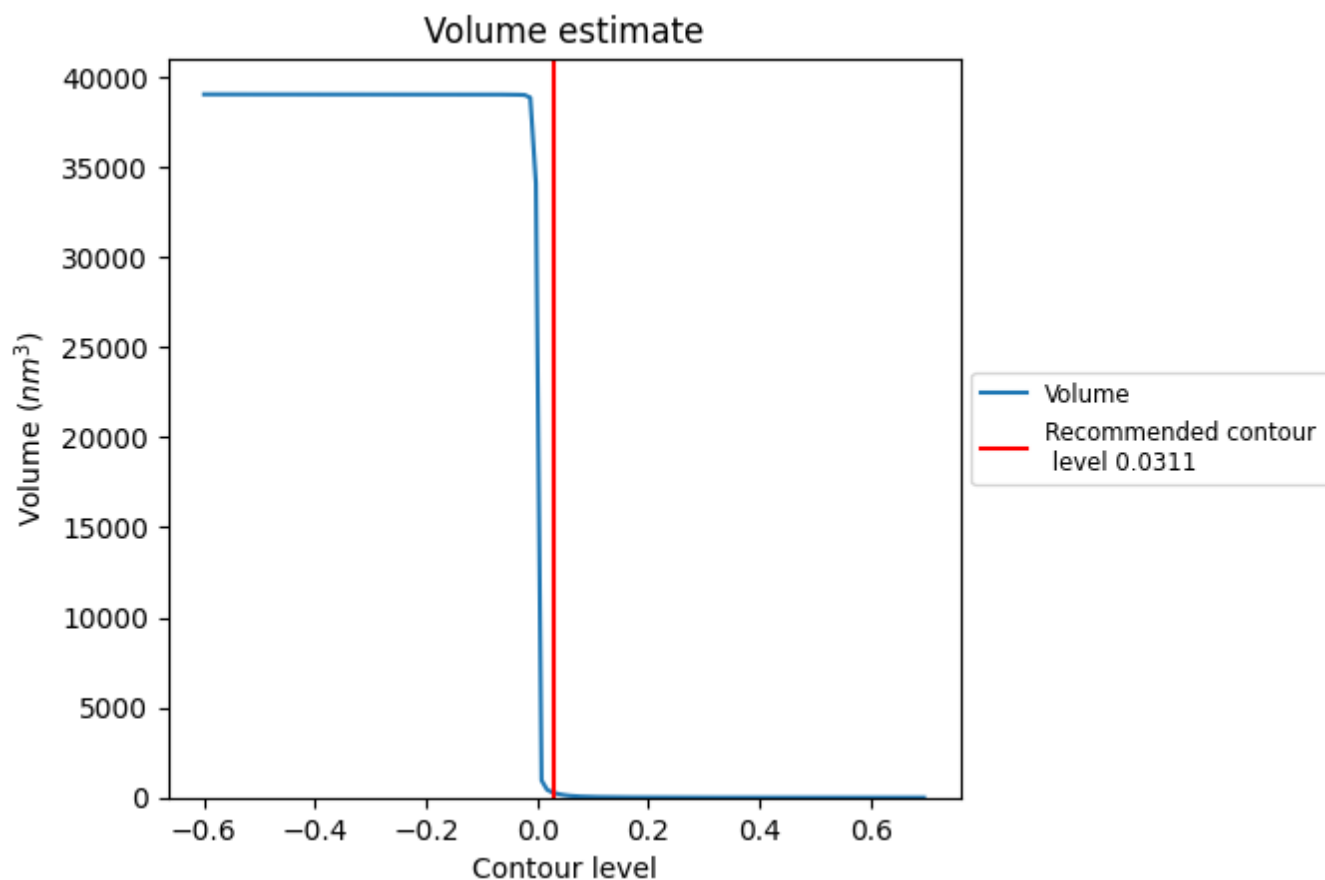
This section contains the results of statistical analysis of the map.

### 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.

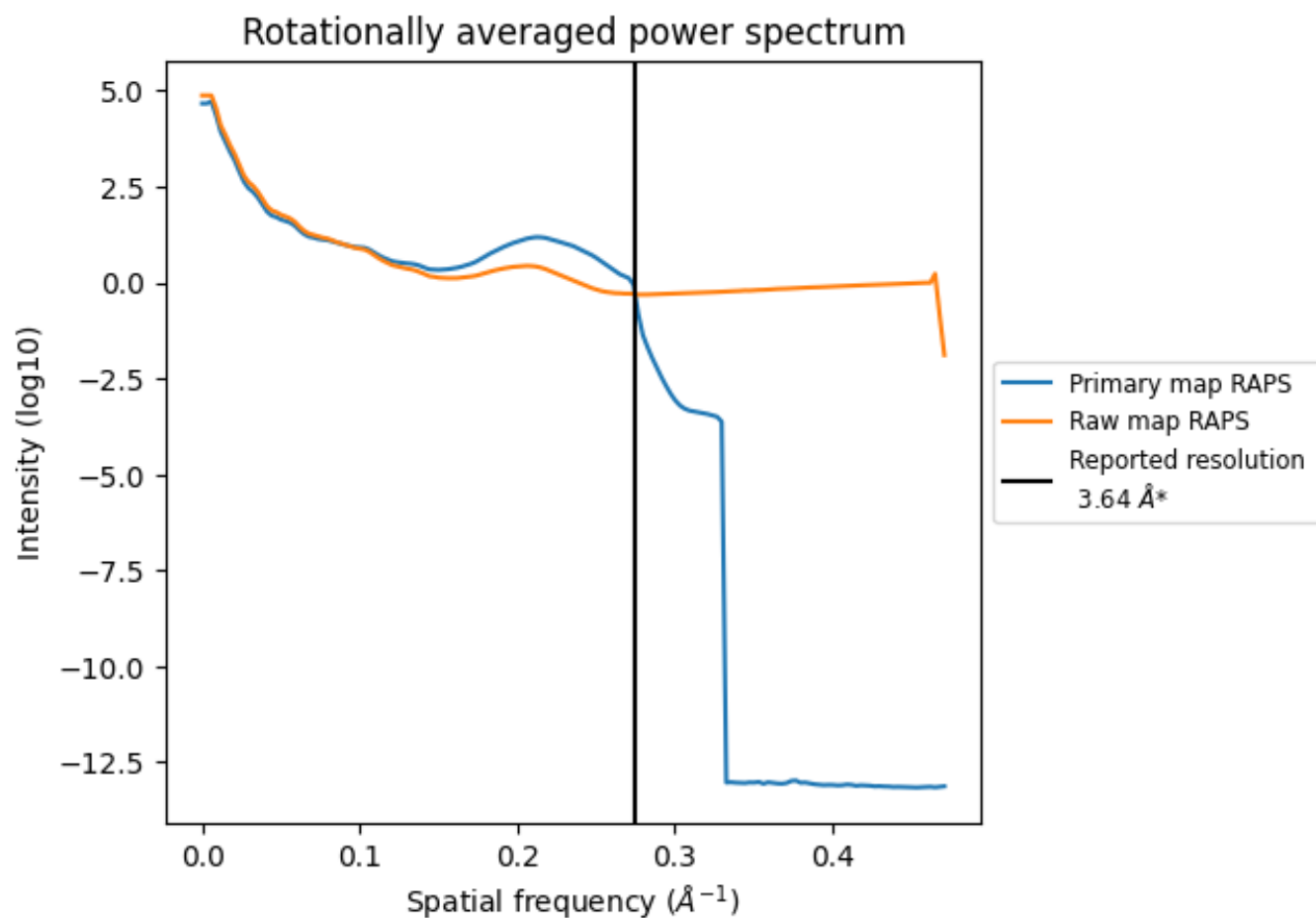
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 254 nm<sup>3</sup>; this corresponds to an approximate mass of 229 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 ⓘ

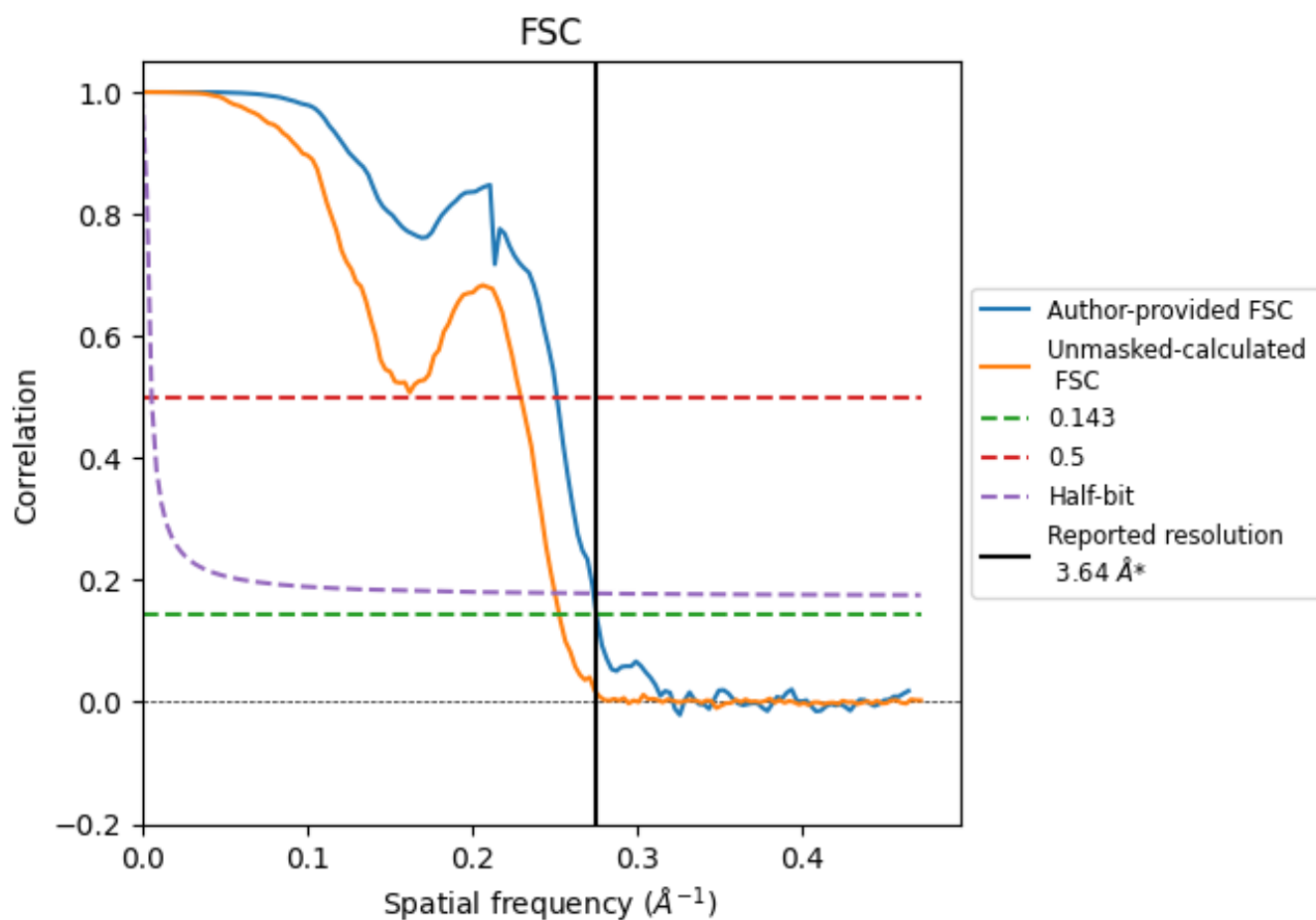


\*Reported resolution corresponds to spatial frequency of 0.275 Å<sup>-1</sup>

## 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  $0.275 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

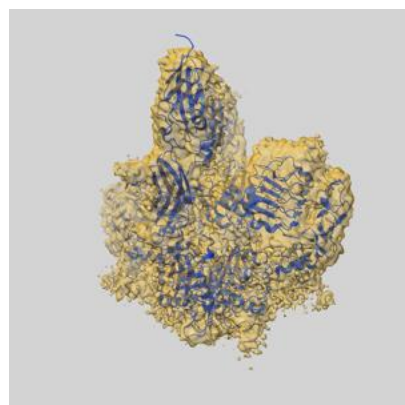
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.64	-	-
Author-provided FSC curve	3.63	3.98	3.66
Unmasked-calculated*	3.96	4.36	4.00

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

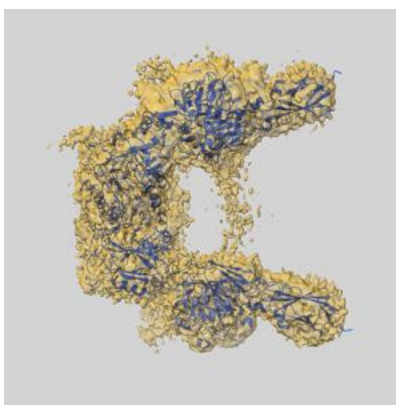
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-71878 and PDB model 9PUW. Per-residue inclusion information can be found in section [3](#) on page [8](#).

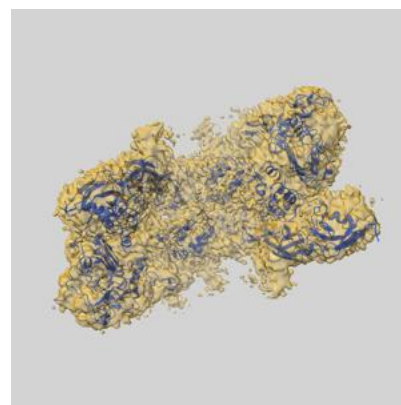
### 9.1 Map-model overlay [i](#)



X



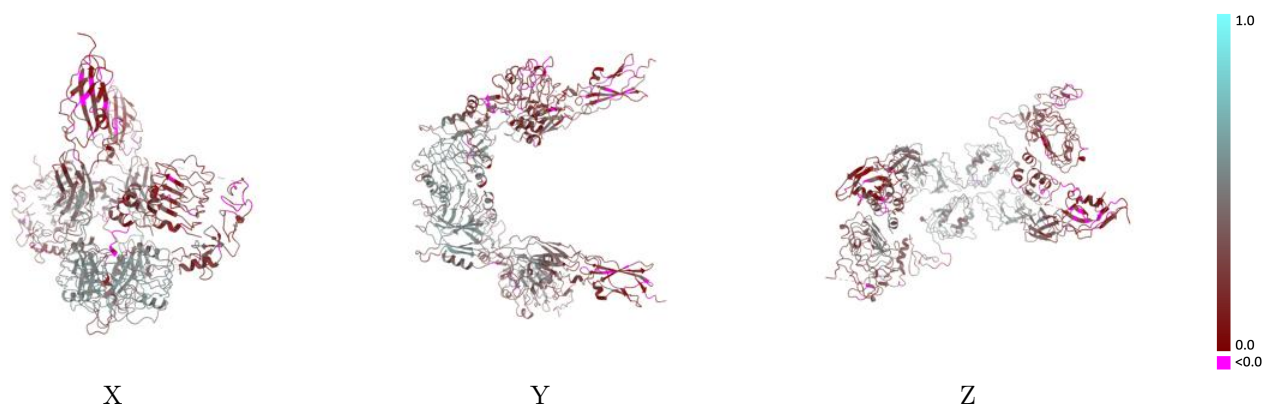
Y



Z

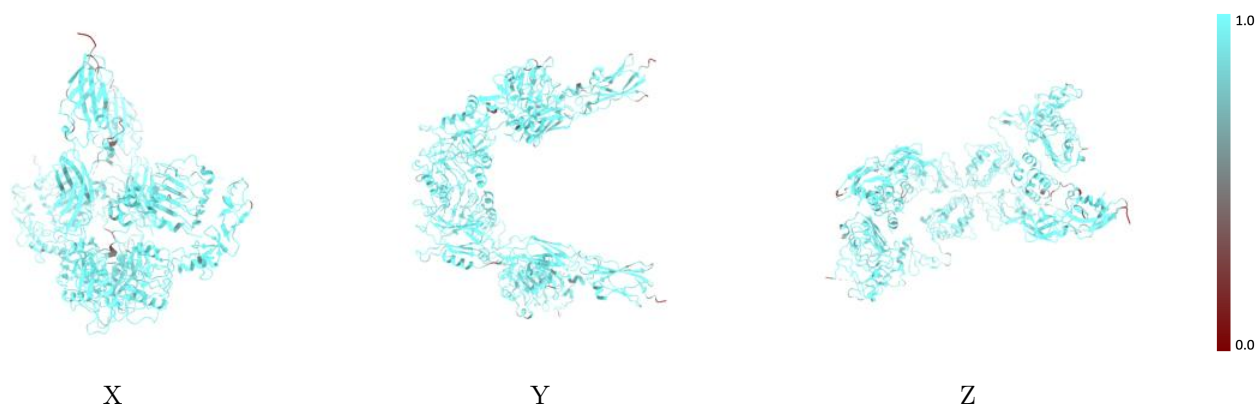
The images above show the 3D surface view of the map at the recommended contour level 0.0311 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



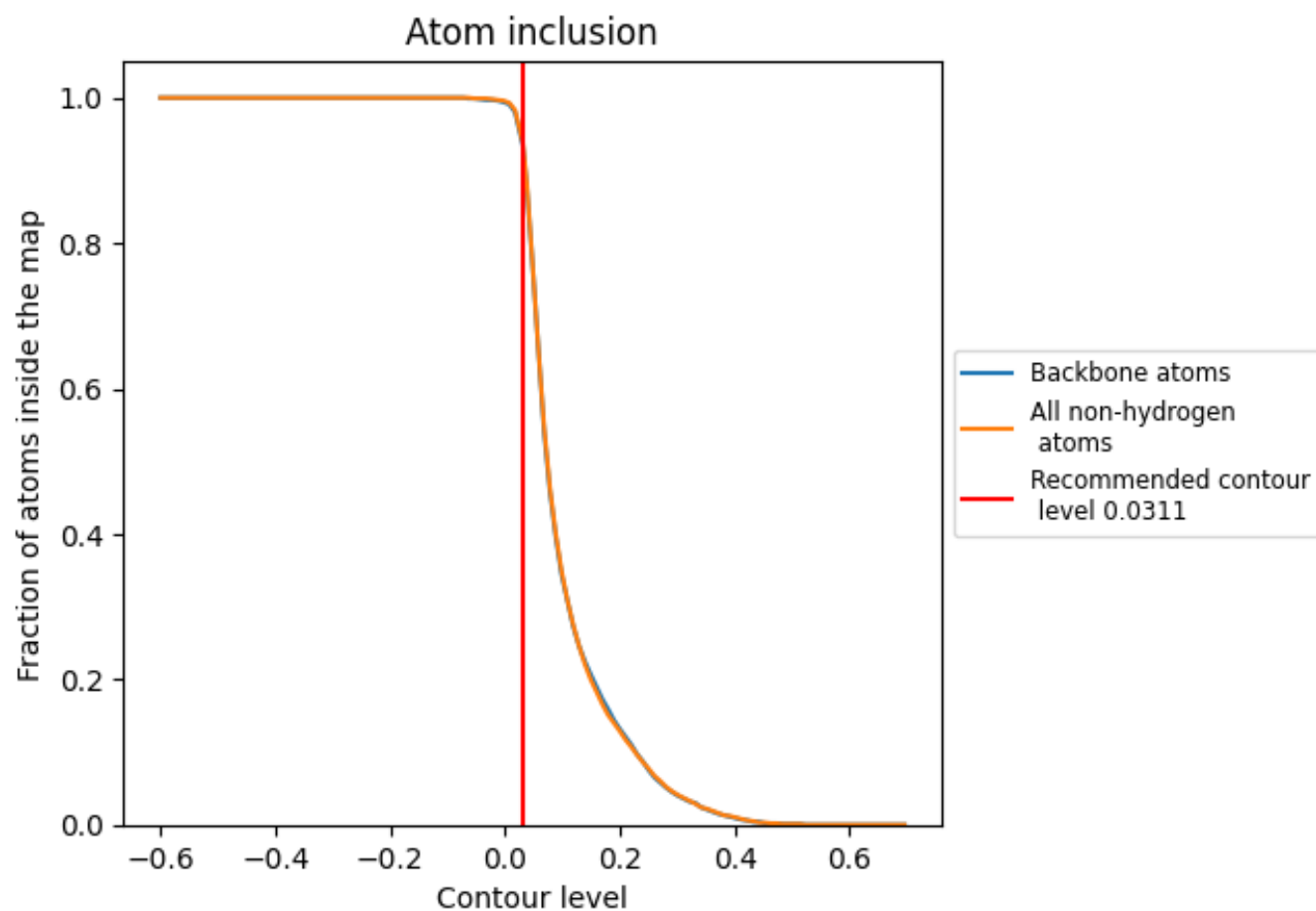
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0311).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 94% 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 (0.0311) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9390	<div><div></div></div> 0.3410
A	<div><div></div></div> 0.9420	<div><div></div></div> 0.3340
B	<div><div></div></div> 0.9350	<div><div></div></div> 0.3560
C	<div><div></div></div> 0.9220	<div><div></div></div> 0.2830
M	<div><div></div></div> 0.9690	<div><div></div></div> 0.1610
N	<div><div></div></div> 0.9590	<div><div></div></div> 0.4490
P	<div><div></div></div> 0.9720	<div><div></div></div> 0.2070
Q	<div><div></div></div> 0.9280	<div><div></div></div> 0.3490
R	<div><div></div></div> 0.9530	<div><div></div></div> 0.3290

1.0

0.0

<0.0