



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 10:39 AM UTC

PDB ID : 9QWS / pdb_00009qws
EMDB ID : EMD-53426
Title : Cryo-EM structure of the human UBR4/KCMF1/CALM1 complex (C-term dimer interface focused refinement)
Authors : Grabarczyk, D.B.; Clausen, T.
Deposited on : 2025-04-15
Resolution : 3.10 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

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:

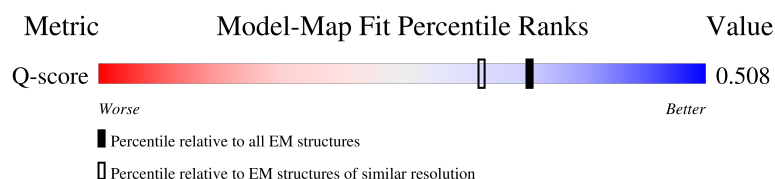
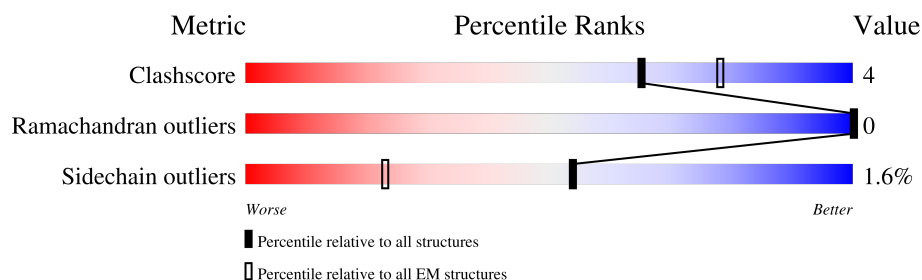
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.10 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	E	158	
1	F	158	
2	A	5193	
2	B	5193	

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Mol	Chain	Length	Quality of chain
3	C	391	9% 90%
3	D	391	9% 90%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18574 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 Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	131	Total	C	N	O	S	0	0
			762	465	136	159	2		
1	F	131	Total	C	N	O	S	0	0
			762	465	136	159	2		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-8	MET	-	initiating methionine	UNP P0DP23
E	-7	ASP	-	expression tag	UNP P0DP23
E	-6	TYR	-	expression tag	UNP P0DP23
E	-5	LYS	-	expression tag	UNP P0DP23
E	-4	ASP	-	expression tag	UNP P0DP23
E	-3	ASP	-	expression tag	UNP P0DP23
E	-2	ASP	-	expression tag	UNP P0DP23
E	-1	ASP	-	expression tag	UNP P0DP23
E	0	LYS	-	expression tag	UNP P0DP23
F	-8	MET	-	initiating methionine	UNP P0DP23
F	-7	ASP	-	expression tag	UNP P0DP23
F	-6	TYR	-	expression tag	UNP P0DP23
F	-5	LYS	-	expression tag	UNP P0DP23
F	-4	ASP	-	expression tag	UNP P0DP23
F	-3	ASP	-	expression tag	UNP P0DP23
F	-2	ASP	-	expression tag	UNP P0DP23
F	-1	ASP	-	expression tag	UNP P0DP23
F	0	LYS	-	expression tag	UNP P0DP23

- Molecule 2 is a protein called E3 ubiquitin-protein ligase UBR4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	1036	Total	C	N	O	S	0	0
			8197	5224	1415	1503	55		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1036	Total	C	N	O	S	0	0
			8197	5224	1415	1503	55		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5184	HIS	-	expression tag	UNP Q5T4S7
A	5185	HIS	-	expression tag	UNP Q5T4S7
A	5186	HIS	-	expression tag	UNP Q5T4S7
A	5187	HIS	-	expression tag	UNP Q5T4S7
A	5188	HIS	-	expression tag	UNP Q5T4S7
A	5189	HIS	-	expression tag	UNP Q5T4S7
A	5190	HIS	-	expression tag	UNP Q5T4S7
A	5191	HIS	-	expression tag	UNP Q5T4S7
A	5192	HIS	-	expression tag	UNP Q5T4S7
A	5193	HIS	-	expression tag	UNP Q5T4S7
B	5184	HIS	-	expression tag	UNP Q5T4S7
B	5185	HIS	-	expression tag	UNP Q5T4S7
B	5186	HIS	-	expression tag	UNP Q5T4S7
B	5187	HIS	-	expression tag	UNP Q5T4S7
B	5188	HIS	-	expression tag	UNP Q5T4S7
B	5189	HIS	-	expression tag	UNP Q5T4S7
B	5190	HIS	-	expression tag	UNP Q5T4S7
B	5191	HIS	-	expression tag	UNP Q5T4S7
B	5192	HIS	-	expression tag	UNP Q5T4S7
B	5193	HIS	-	expression tag	UNP Q5T4S7

- Molecule 3 is a protein called E3 ubiquitin-protein ligase KCMF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	40	Total	C	N	O	S	0	0
			327	201	58	66	2		
3	D	40	Total	C	N	O	S	0	0
			327	201	58	66	2		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	382	SER	-	expression tag	UNP Q9P0J7
C	383	ALA	-	expression tag	UNP Q9P0J7
C	384	TRP	-	expression tag	UNP Q9P0J7
C	385	SER	-	expression tag	UNP Q9P0J7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	386	HIS	-	expression tag	UNP Q9P0J7
C	387	PRO	-	expression tag	UNP Q9P0J7
C	388	GLN	-	expression tag	UNP Q9P0J7
C	389	PHE	-	expression tag	UNP Q9P0J7
C	390	GLU	-	expression tag	UNP Q9P0J7
C	391	LYS	-	expression tag	UNP Q9P0J7
D	382	SER	-	expression tag	UNP Q9P0J7
D	383	ALA	-	expression tag	UNP Q9P0J7
D	384	TRP	-	expression tag	UNP Q9P0J7
D	385	SER	-	expression tag	UNP Q9P0J7
D	386	HIS	-	expression tag	UNP Q9P0J7
D	387	PRO	-	expression tag	UNP Q9P0J7
D	388	GLN	-	expression tag	UNP Q9P0J7
D	389	PHE	-	expression tag	UNP Q9P0J7
D	390	GLU	-	expression tag	UNP Q9P0J7
D	391	LYS	-	expression tag	UNP Q9P0J7

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total 1	Zn 1	0
4	B	1	Total 1	Zn 1	0





V4312	C4313	I4314	E4315	T4316	A4317	K4318	R4319	Y4320	M4321	L4322	D4323	I4331	R4334	I4338	I4339	TYR	PRO	GLU	GLU	ASN	GLU	GLU	VAL	T4214	K4215	E4216	L4228	S4229	T4230	L4238	S4247	E4250	T4254	L4262	V4266	L4273	L4276	V4277	T4287	L4291	T4302	E4305	T4306	M4310	A4311	
R3857	A3858	L3859	L3862	C3875	V3879	R3888	N3893	L3896	L3905	R3916	L3928	L3932	I3979	L4019	L4020	S4031	K4032	K4033	D4036	A4041	L4042	T4043	T4044	V4045	Q4055	K4073	L4077	R4078	G4079	ILE	ASP	GLY	ASN	ASN	GLY	LYS	ALA	PRO	TYR	SER	ASN	PRO	GLY	M4310	A4311	
L4097	R4104	F4108	L4109	S4110	R4111	R4112	G4113	K4114	L4119	M4126	L4184	V4198	L4206	G4210	T4214	K4215	E4216	L4228	S4229	T4230	L4238	S4247	E4250	T4254	L4262	V4266	L4273	L4276	V4277	T4287	L4291	T4302	E4305	T4306	M4310	A4311										
ASN	VAL	TYR	GLN	CYS	HIS	LYS	CYS	ARG	ILE	ASN	TYR	ASP	GLU	LYS	ASP	PRO	F3698	F3705	C3706	K3707	R3710	M3714	I3739	F3775	GLN	ASP	ASP	SER	GLY	THR	ALA	GLY	ILE	SER	T3788	R3825	D3832	E3837	S3842	SER	ARG	THR	SER	VAL	GLN	P3849
R3857	A3858	L3859	L3862	C3875	V3879	R3888	N3893	L3896	L3905	R3916	L3928	L3932	I3979	L4019	L4020	S4031	K4032	K4033	D4036	A4041	L4042	T4043	T4044	V4045	Q4055	K4073	L4077	R4078	G4079	ILE	ASP	GLY	ASN	ASN	GLY	LYS	ALA	PRO	TYR	SER	ASN	PRO	GLY	M4310	A4311	
P3609	A3610	K3614	V3618	Q3619	L3620	G3623	T3624	T3625	E3626	V3627	K3628	I3629	P3630	L3631	P3632	L3633	N3639	I3640	H3641	A3645	P3646	F3647	TYR	GLU	ASN	GLN	ALA	ASP	GLY	THR	THR	LEU	GLN	CYS	PRO	ARG	ASN	SER	PRO	GLY	ASN	GLY	GLU			
L3412	L3416	L3431	R3463	T3479	Q3480	Q3481	L3504	T3505	Y3513	E3521	Y3525	Y3544	I3545	K3546	S3548	S3549	I3550	D3553	T3554	R3555	T3556	T3557	K3564	S3572	T3575	V3576	K3577	I3578	G3579	D3580	L3581	K3582	R3583	T3584	Y3593	Y3594	N3595	V3599	L3605	K3606	N3607	K3608				
ILE	PRO	PRO	VAL	PHE	ASP	HIS	SER	TRP	PHE	TYR	PHE	LEU	SER	GLY	SER	ALA	ILE	GLN	THR	PRO	PHE	VAL	VAL	LYS	ARG	GLY	SER	THR	GLN	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	
THR	SER	GLN	LEU	LEU	PRO	HIS	THR	THR	SER	SER	PRO	PRO	ASP	MET	TYR	PRO	PHE	PHE	LEU	ILE	SER	GLN	VAL	LYS	GLY	ARG	GLN	THR	GLN	LEU	THR	VAL	MET	LYS	ASN	SER	LEU	ARG	LEU	GLN	PRO	ASN	THR	ARG		
VAL	PHE	MET	SER	THR	ARG	LYS	SER	GLY	LYS	SER	ILE	CYS	TYR	SER	SER	SER	LEU	ILE	SER	SER	ALA	THR	LEU	ALA	SER	SER	GLY	VAL	ASP	ASP	VAL	TYR	CYS	LEU	HIS	THR	VAL	ALA	TYR	GLY	ASP	VAL	ALA			
GLN	VAL	ILE	MET	LEU	THR	LEU	THR	ASP	GLY	GLU	ASP	GLU	LYS	ASP	GLY	LYS	GLY	THR	GLU	GLN	LEU	ALA	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	
SER	THR	THR	THR	HIS	GLN	GLY	GLY	ASP	GLY	GLU	GLY	GLY	GLY	THR	HIS	THR	SER	ALA	GLN	GLY	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
LEU	ILE	ARG	VAL	GLY	ARG	PRO	ARG	ASN	ARG	GLY	VAL	THR	PRO	SER	ALA	SER	PRO	ASN	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY

- Molecule 2: E3 ubiquitin-protein ligase UBR4

[illegible]









- Molecule 3: E3 ubiquitin-protein ligase KCMF1



GLN	L324	ALA	LEU	PRO	PHE	MET
	PHE	GLN	SER	ASN	ASP	SER
GLU	L325	ALA	SER	HIS	LEU	ARG
LYS		ARG	GLN	VAL	TYR	HIS
	E331	GLN	SER	ASP	GLY	GLY
	GLU	GLN	SER	ASP	GLY	VAL
	SER	GLN	TYR	PHE	GLU	VAL
	SER	GLU	SER	ALA	ALA	CYS
	SER	GLU	PRO	ALA	PHE	ASP
	ASP	ALA	SER	HIS	SER	ALA
	GLU	ARG	ASN	LEU	VAL	CYS
	ASP	ASN	ARG	THR	GLU	LEU
	ASP	ALA	GLU	LEU	GLN	LYS
	ARG	THR	ALA	GLU	PRO	GLY
	GLY	ARG	MET	HIS	GLN	ASN
	GLU	ARG	ASP	ALA	SER	PHE
	MET	THR	PRO	ALA	PHE	ARG
	ALA	ASN	ILE	PRO	THR	GLY
	ASP	THR	ALA	ARG	CYS	ARG
	PHE	SER	GLU	ASP	PRO	ARG
	GLY	SER	LEU	LEU	TYR	TYR
	ALA	SER	LEU	ASP	CYS	LYS
	MET	VAL	LEU	GLU	GLY	CYS
	GLY	THR	GLN	SER	LYS	LEU
	CYS	THR	GLN	SER	MET	ILE
	VAL	ILE	SER	GLY	GLY	CYS
	ASP	ILE	SER	VAL	TYR	TYR
	ILE	GLN	VAL	ARG	THR	ASP
	MET	SER	ARG	HIS	GLU	TYR
	PRO	THR	ARG	VAL	THR	ASP
	LEU	ALA	SER	ARG	SER	LEU
	ASP	THR	ALA	MET	LEU	CYS
	VAL	THR	GLY	PHE	GLN	ALA
	ALA	ASN	GLY	HIS	HIS	SER
	LEU	ILE	GLN	PRO	TYR	CYS
	GLU	ALA	ASN	GLY	VAL	ALA
	ASN	ASN	SER	ARG	GLU	GLY
	LEU	THR	SER	GLY	GLU	ALA
	LYS	SER	PRO	GLY	HIS	THR
	GLU	GLN	SER	GLY	ALA	THR
	ASN	GLN	LEU	ARG	VAL	THR
	ASN	ASN	GLN	ARG	ILE	ASP
	PRO	GLU	LEU	SER	CYS	HIS
	PRO	ASN	GLN	MET	PRO	PRO
	PRO	ASN	MET	HIS	ILE	CYS
	PRO	ASP	GLN	PHE	ALA	GLN
	LEU	PRO	LEU	THR	ALA	CYS
	SER	ALA	GLN	SER	ALA	ILE
	TRP	ALA	GLU	SER	PRO	LEU
	SER	E305	ARG	THR	GLY	ARG
	HIS	B306	GLN	GLY	GLY	THR
			TYR	GLY	ASP	VAL

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	135406	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)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.064	Depositor
Minimum map value	-0.034	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00789	Depositor
Map size (Å)	486.912, 486.912, 486.912	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.268, 1.268, 1.268	Depositor

5 Model quality

5.1 Standard geometry

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

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	E	0.10	0/764	0.32	0/1046
1	F	0.11	0/764	0.31	0/1046
2	A	0.15	0/8340	0.30	0/11285
2	B	0.15	0/8340	0.31	0/11285
3	C	0.16	0/327	0.31	0/435
3	D	0.16	0/327	0.30	0/435
All	All	0.15	0/18862	0.30	0/25532

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

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	E	762	0	504	5	0
1	F	762	0	504	4	0
2	A	8197	0	8368	67	0
2	B	8197	0	8368	70	0
3	C	327	0	327	4	0
3	D	327	0	327	4	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
All	All	18574	0	18398	147	0

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

All (147) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3555:ARG:HH12	2:A:3557:THR:HB	1.48	0.78
2:B:3270:ILE:HD11	2:B:3632:PRO:HG2	1.67	0.76
2:B:3555:ARG:HH12	2:B:3557:THR:HB	1.51	0.76
2:A:3270:ILE:HD11	2:A:3632:PRO:HG2	1.67	0.75
2:B:4093:ARG:O	2:B:4097:LEU:HD12	1.91	0.71
2:A:4093:ARG:O	2:A:4097:LEU:HD12	1.91	0.70
2:B:3575:THR:HG22	2:B:3628:LYS:HD3	1.75	0.69
2:B:3909:LEU:HD12	2:B:3925:VAL:HG13	1.73	0.69
2:A:3575:THR:HG22	2:A:3628:LYS:HD3	1.76	0.68
2:A:3739:ILE:HD11	2:A:3825:ARG:HG2	1.76	0.67
2:B:3739:ILE:HD11	2:B:3825:ARG:HG2	1.77	0.65
1:F:52:MET:HE3	1:F:52:MET:HA	1.79	0.64
2:A:4492:LEU:HD22	2:A:4508:LEU:HD13	1.79	0.63
2:B:3888:ARG:HG3	2:B:3928:LEU:HB2	1.81	0.63
2:A:3888:ARG:HG3	2:A:3928:LEU:HB2	1.82	0.62
2:B:4492:LEU:HD22	2:B:4508:LEU:HD13	1.82	0.61
2:A:4479:MET:HE3	2:A:4479:MET:H	1.65	0.60
2:A:4339:ILE:HD13	2:A:4475:MET:HB3	1.83	0.59
2:B:4210:GLY:O	2:B:4214:THR:HG23	2.03	0.59
1:E:52:MET:HA	1:E:52:MET:HE3	1.86	0.58
2:B:4206:LEU:HD13	2:B:4262:LEU:HD11	1.84	0.58
2:B:3547:LEU:HD21	2:B:3563:VAL:HG11	1.86	0.57
2:A:3546:LYS:HZ3	2:A:3549:SER:N	2.03	0.57
2:B:3905:LEU:HD23	2:B:3932:LEU:HD11	1.87	0.56
2:B:4312:VAL:O	2:B:4316:THR:HG23	2.05	0.56
2:A:3618:VAL:HG21	2:A:3629:ILE:HG12	1.88	0.56
2:B:4216:GLU:HG2	2:B:4238:LEU:HB2	1.87	0.56
2:B:3618:VAL:HG21	2:B:3629:ILE:HG12	1.87	0.56
2:B:4339:ILE:HD13	2:B:4475:MET:HB3	1.89	0.55
2:A:4206:LEU:HD13	2:A:4262:LEU:HD11	1.89	0.54
2:A:4216:GLU:HG2	2:A:4238:LEU:HB2	1.90	0.54
2:B:3857:ARG:HH21	2:B:3862:LEU:HD13	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:46:GLU:O	1:F:50:GLN:HG2	2.07	0.53
2:A:4312:VAL:O	2:A:4316:THR:HG23	2.07	0.53
2:A:3575:THR:OG1	2:A:3714:MET:HB3	2.09	0.53
2:B:3278:ALA:O	2:B:3282:ILE:HG22	2.09	0.53
2:A:3905:LEU:HD23	2:A:3932:LEU:HD11	1.90	0.52
2:B:3576:VAL:HB	2:B:3627:VAL:HG23	1.91	0.52
2:A:3857:ARG:HH21	2:A:3862:LEU:HD13	1.74	0.52
2:B:3575:THR:OG1	2:B:3714:MET:HB3	2.09	0.52
2:A:3278:ALA:O	2:A:3282:ILE:HG22	2.10	0.51
2:A:3576:VAL:HB	2:A:3627:VAL:HG23	1.92	0.51
2:B:3252:ARG:HH11	2:B:3252:ARG:HG3	1.76	0.51
2:B:3546:LYS:NZ	2:B:3548:SER:HB2	2.25	0.51
2:A:3252:ARG:HG3	2:A:3252:ARG:HH11	1.76	0.51
2:B:3595:ASN:OD1	2:B:3639:ASN:HB2	2.11	0.50
1:E:46:GLU:O	1:E:50:GLN:HG2	2.11	0.50
2:A:3595:ASN:OD1	2:A:3639:ASN:HB2	2.12	0.50
2:B:4006:PRO:O	2:B:4010:GLU:HG3	2.12	0.50
2:B:4273:LEU:HA	2:B:4276:LEU:HD23	1.94	0.49
2:B:3332:VAL:HG11	2:B:3434:HIS:NE2	2.28	0.49
2:B:4306:THR:HG22	2:B:4475:MET:HE3	1.94	0.49
2:A:3593:TYR:HB2	2:A:3641:MET:HB3	1.94	0.48
2:A:4310:MET:HB2	2:A:4475:MET:HE2	1.93	0.48
2:B:4266:VAL:HG13	2:B:4291:LEU:HG	1.95	0.48
2:B:4041:ALA:HA	2:B:4078:ARG:HH12	1.79	0.48
2:A:3505:THR:HG22	2:A:3916:ARG:HH22	1.79	0.47
2:B:4327:THR:OG1	2:B:4328:PRO:HD3	2.14	0.47
2:B:3505:THR:HG22	2:B:3916:ARG:HH22	1.80	0.47
2:A:4210:GLY:O	2:A:4214:THR:HG23	2.14	0.47
2:A:4306:THR:HG22	2:A:4475:MET:HE3	1.96	0.46
2:A:4266:VAL:HG13	2:A:4291:LEU:HG	1.98	0.46
3:D:301:MET:HE3	3:D:306:ARG:HA	1.95	0.46
2:B:3599:VAL:HG21	2:B:3605:LEU:HB2	1.97	0.46
2:B:3513:TYR:CZ	2:B:3525:TYR:HB3	2.51	0.46
2:B:3614:LYS:HA	2:B:3614:LYS:HD2	1.75	0.46
2:B:3905:LEU:HG	2:B:3909:LEU:HD23	1.97	0.46
2:A:3513:TYR:CZ	2:A:3525:TYR:HB3	2.51	0.46
2:B:3546:LYS:HZ2	2:B:3548:SER:HB2	1.80	0.46
2:A:3270:ILE:O	2:A:3274:GLU:HG2	2.16	0.46
2:A:4273:LEU:HA	2:A:4276:LEU:HD23	1.97	0.46
2:A:3223:LYS:O	2:A:3227:LEU:HD22	2.16	0.45
2:B:3875:CYS:O	2:B:3879:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:4055:GLN:HG2	2:A:4119:LEU:HD23	1.98	0.45
2:B:3580:ASP:HB3	2:B:3710:ARG:HD3	1.99	0.45
2:B:4310:MET:HB2	2:B:4475:MET:HE2	1.98	0.45
2:A:4020:LEU:HD13	3:C:324:LEU:HD11	1.99	0.45
2:A:4198:VAL:HG22	2:A:4254:ILE:HD11	1.98	0.45
2:B:3593:TYR:HB2	2:B:3641:MET:HB3	1.98	0.45
1:F:43:ASN:O	1:F:43:ASN:ND2	2.45	0.45
2:A:4313:CYS:SG	2:A:4331:ILE:HG23	2.57	0.45
2:B:4238:LEU:HG	2:B:4287:THR:HG21	1.99	0.45
2:A:4247:SER:HA	2:A:4250:GLU:OE1	2.17	0.44
2:A:3875:CYS:O	2:A:3879:VAL:HG23	2.17	0.44
2:A:3546:LYS:NZ	2:A:3548:SER:HB2	2.31	0.44
2:A:4033:LYS:HE2	3:C:307:GLN:HE22	1.82	0.44
2:A:3599:VAL:HG21	2:A:3605:LEU:HB2	2.00	0.44
2:A:4031:SER:HB3	3:C:306:ARG:HG2	1.99	0.44
3:D:324:LEU:HD23	3:D:324:LEU:HA	1.89	0.44
2:A:3412:LEU:O	2:A:3416:LEU:HB2	2.17	0.44
2:A:3553:ASP:H	2:A:3564:LYS:HG2	1.82	0.44
2:B:3270:ILE:O	2:B:3274:GLU:HG2	2.18	0.44
2:B:4158:ARG:HD2	3:D:325:LEU:HD13	2.00	0.44
2:A:3544:TYR:C	2:A:3545:ILE:HD13	2.43	0.43
2:A:4334:ARG:O	2:A:4338:ILE:HG12	2.18	0.43
2:B:4313:CYS:SG	2:B:4331:ILE:HG23	2.58	0.43
2:B:3929:MET:HE2	2:B:3943:MET:HE2	2.01	0.43
2:B:4335:LEU:O	2:B:4339:ILE:HG12	2.19	0.43
2:B:4302:THR:O	2:B:4305:GLU:HG3	2.19	0.43
2:B:4163:LEU:HD23	2:B:4163:LEU:HA	1.86	0.43
2:B:3412:LEU:O	2:B:3416:LEU:HB2	2.19	0.43
2:A:3979:ILE:HD12	2:A:4019:ILE:HD13	2.00	0.42
2:B:4100:LYS:NZ	2:B:4104:ARG:HH22	2.17	0.42
2:A:4238:LEU:HG	2:A:4287:THR:HG21	2.00	0.42
2:B:3494:VAL:HG22	2:B:3905:LEU:HD13	2.01	0.42
2:A:3244:LEU:HD13	2:A:3244:LEU:HA	1.91	0.42
2:B:3267:ASP:O	2:B:3270:ILE:HG22	2.20	0.42
2:A:3267:ASP:O	2:A:3270:ILE:HG22	2.20	0.42
2:B:3244:LEU:HD13	2:B:3244:LEU:HA	1.89	0.42
2:B:4073:LYS:HB3	2:B:4073:LYS:HE3	1.71	0.42
2:A:4073:LYS:HB3	2:A:4073:LYS:HE3	1.71	0.42
1:F:49:LEU:HD23	1:F:49:LEU:HA	1.88	0.42
2:A:3479:THR:HG22	2:A:3481:GLN:HG2	2.02	0.42
2:A:4302:THR:O	2:A:4305:GLU:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3521:GLU:HG2	2:B:3773:GLU:HB2	2.01	0.41
2:B:3893:ASN:HB3	2:B:3896:LEU:HB2	2.02	0.41
1:E:49:LEU:HD23	1:E:49:LEU:HA	1.89	0.41
2:A:3614:LYS:HD2	2:A:3614:LYS:HA	1.75	0.41
2:A:3893:ASN:HB3	2:A:3896:LEU:HB2	2.02	0.41
2:A:4043:THR:HG22	2:A:4045:VAL:H	1.85	0.41
2:B:3479:THR:HG22	2:B:3481:GLN:HG2	2.02	0.41
2:B:3920:ALA:O	2:B:3924:GLU:HG3	2.20	0.41
2:B:3544:TYR:C	2:B:3545:ILE:HD13	2.45	0.41
2:B:4043:THR:HG22	2:B:4045:VAL:H	1.85	0.41
2:A:3572:SER:O	2:A:3631:LEU:HB2	2.20	0.41
1:E:34:GLY:HA3	1:E:49:LEU:HD11	2.01	0.41
2:A:4228:LEU:HD21	2:B:3825:ARG:HB3	2.03	0.41
2:B:3243:LEU:HD11	2:B:3271:SER:HB2	2.03	0.41
2:B:3633:LEU:HD23	2:B:3633:LEU:HA	1.82	0.41
2:B:3736:VAL:O	2:B:3739:ILE:HG22	2.21	0.41
1:E:21:ASP:HA	1:E:28:ILE:HG22	2.02	0.41
2:A:3633:LEU:HD23	2:A:3633:LEU:HA	1.82	0.41
2:B:4031:SER:HB3	3:D:306:ARG:HG2	2.03	0.41
2:B:4310:MET:O	2:B:4314:ILE:HG12	2.21	0.41
2:A:3328:CYS:SG	2:A:3431:LEU:HA	2.61	0.41
2:A:3580:ASP:HB3	2:A:3710:ARG:HD3	2.02	0.41
2:A:4314:ILE:O	2:A:4318:LYS:HG2	2.21	0.41
2:B:4273:LEU:HA	2:B:4273:LEU:HD23	1.95	0.41
2:B:4282:LYS:O	2:B:4286:GLU:HG2	2.20	0.41
2:A:4310:MET:O	2:A:4314:ILE:HG12	2.20	0.41
2:B:4314:ILE:O	2:B:4318:LYS:HG2	2.21	0.41
2:A:3307:VAL:O	2:A:3311:VAL:HG23	2.21	0.40
2:A:3595:ASN:HD21	2:A:3605:LEU:HD11	1.86	0.40
2:B:3914:LEU:HA	2:B:3914:LEU:HD23	1.88	0.40
2:A:4041:ALA:HA	2:A:4078:ARG:HH12	1.85	0.40
3:C:309:MET:HE2	3:C:309:MET:HB2	1.94	0.40
2:A:3463:ARG:H	2:A:3463:ARG:HG3	1.68	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	E	125/158 (79%)	125 (100%)	0	0	100	100
1	F	125/158 (79%)	125 (100%)	0	0	100	100
2	A	1022/5193 (20%)	999 (98%)	23 (2%)	0	100	100
2	B	1022/5193 (20%)	1002 (98%)	20 (2%)	0	100	100
3	C	36/391 (9%)	36 (100%)	0	0	100	100
3	D	36/391 (9%)	36 (100%)	0	0	100	100
All	All	2366/11484 (21%)	2323 (98%)	43 (2%)	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	E	36/136 (26%)	35 (97%)	1 (3%)	38	66
1	F	36/136 (26%)	34 (94%)	2 (6%)	19	49
2	A	904/4531 (20%)	890 (98%)	14 (2%)	57	75
2	B	904/4531 (20%)	890 (98%)	14 (2%)	57	75
3	C	38/339 (11%)	38 (100%)	0	100	100
3	D	38/339 (11%)	37 (97%)	1 (3%)	40	68
All	All	1956/10012 (20%)	1924 (98%)	32 (2%)	54	75

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	45	THR
2	A	3230	LEU
2	A	3244	LEU
2	A	3311	VAL
2	A	3315	VAL
2	A	3504	LEU
2	A	3550	ILE
2	A	3554	THR
2	A	3625	THR
2	A	3832	ASP
2	A	4077	ILE
2	A	4126	ASN
2	A	4184	LEU
2	A	4230	THR
2	A	4277	VAL
2	B	3230	LEU
2	B	3244	LEU
2	B	3311	VAL
2	B	3540	VAL
2	B	3550	ILE
2	B	3566	ILE
2	B	3627	VAL
2	B	3724	ASP
2	B	3832	ASP
2	B	3968	LEU
2	B	4077	ILE
2	B	4223	LEU
2	B	4229	SER
2	B	4277	VAL
3	D	305	GLU
1	F	19	LEU
1	F	43	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	3400	ASN
2	A	3410	GLN
2	A	3427	GLN
2	A	3506	ASN
2	A	3569	HIS

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Mol	Chain	Res	Type
2	A	3759	GLN
2	A	3762	ASN
2	A	4234	GLN
2	B	3400	ASN
2	B	3410	GLN
2	B	3506	ASN
2	B	3560	GLN
2	B	3569	HIS
2	B	3591	ASN
2	B	3759	GLN
2	B	3762	ASN
2	B	3941	GLN
2	B	4503	HIS

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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

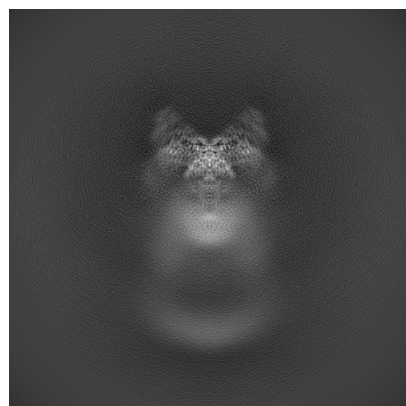
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53426. These allow visual inspection of the internal detail of the map and identification of artifacts.

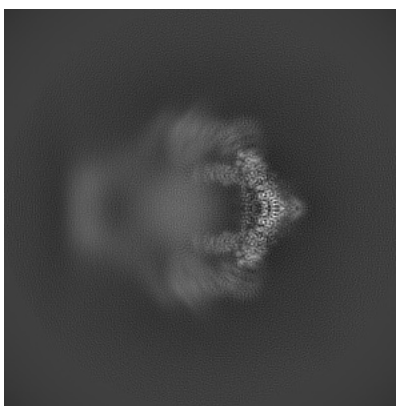
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

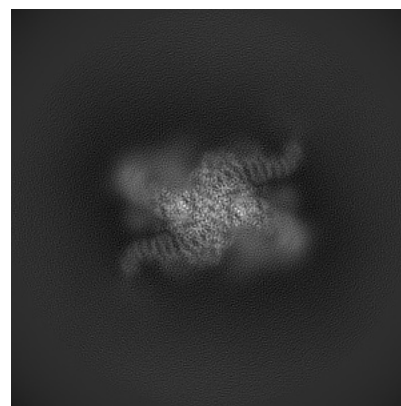
6.1.1 Primary map



X

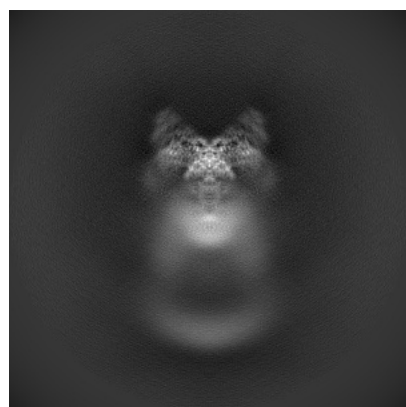


Y

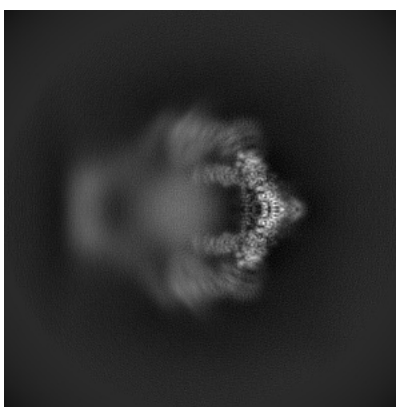


Z

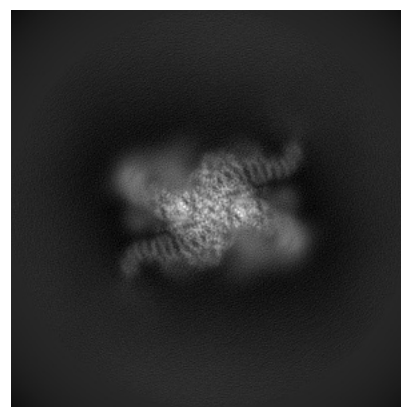
6.1.2 Raw map



X



Y

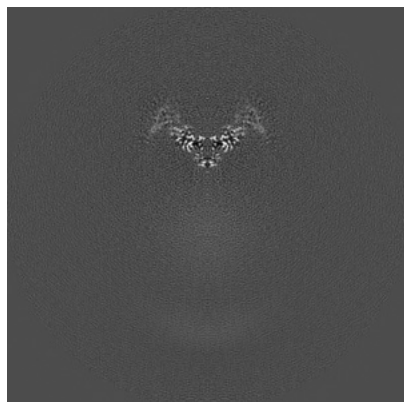


Z

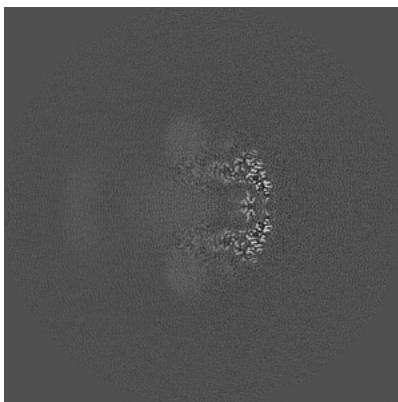
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

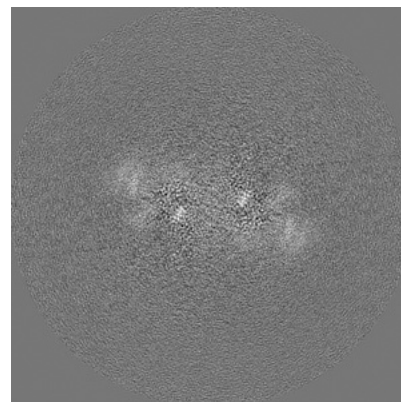
6.2.1 Primary map



X Index: 192

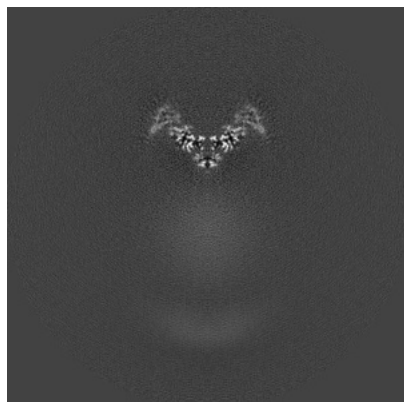


Y Index: 192

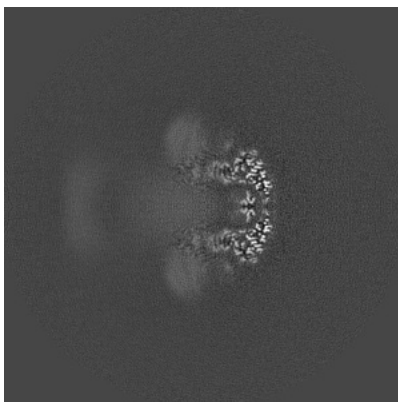


Z Index: 192

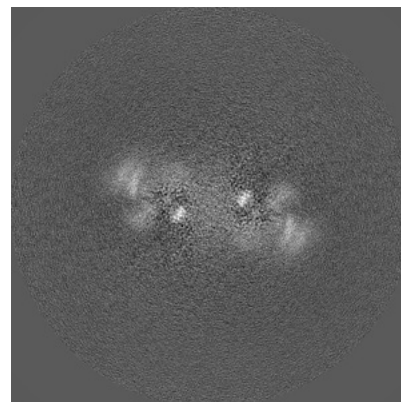
6.2.2 Raw map



X Index: 192



Y Index: 192

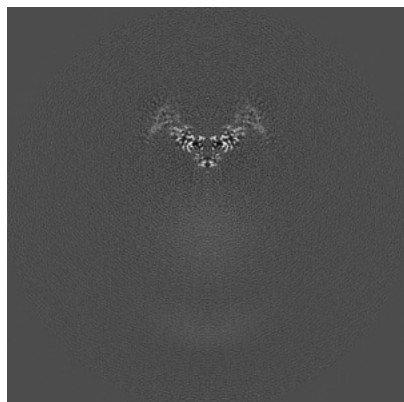


Z Index: 192

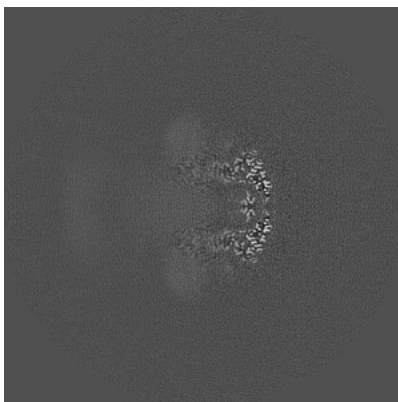
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

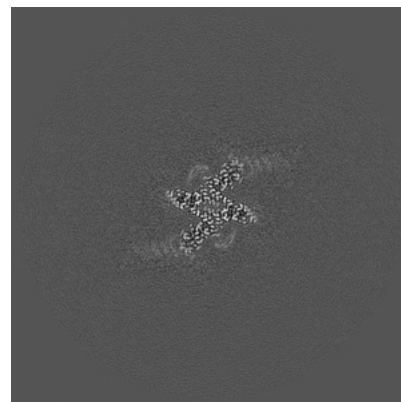
6.3.1 Primary map



X Index: 192

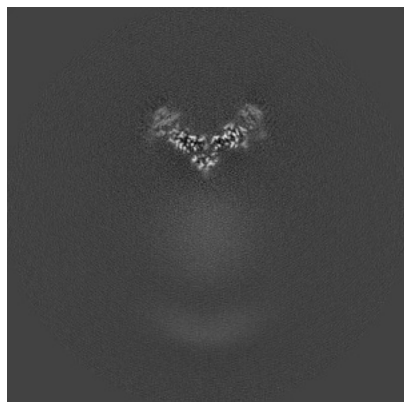


Y Index: 192

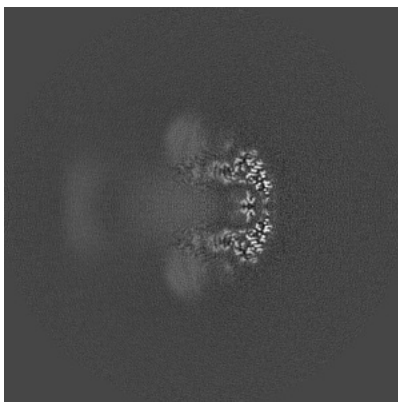


Z Index: 249

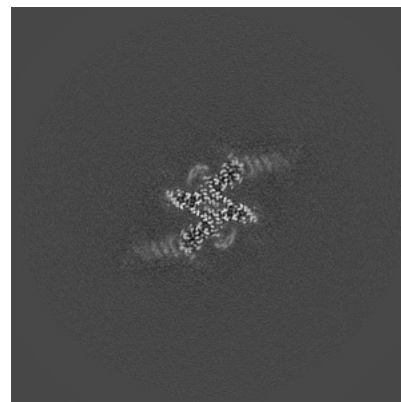
6.3.2 Raw map



X Index: 188



Y Index: 192

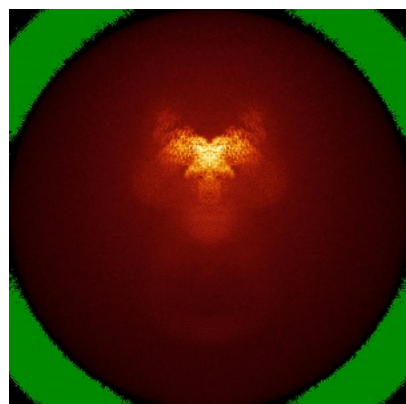


Z Index: 249

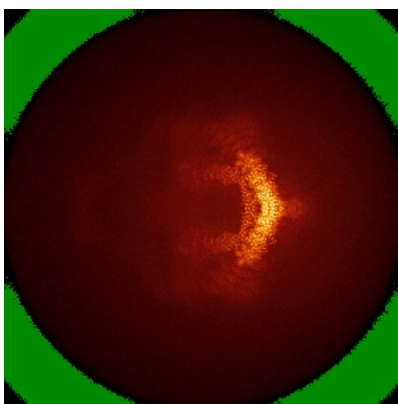
The images above show the largest variance slices of the map in three orthogonal directions.

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

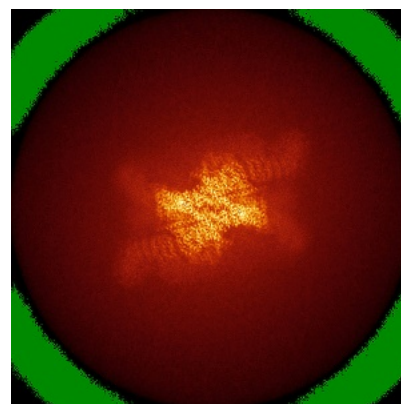
6.4.1 Primary map



X

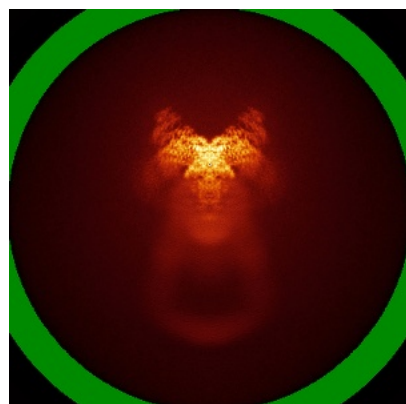


Y

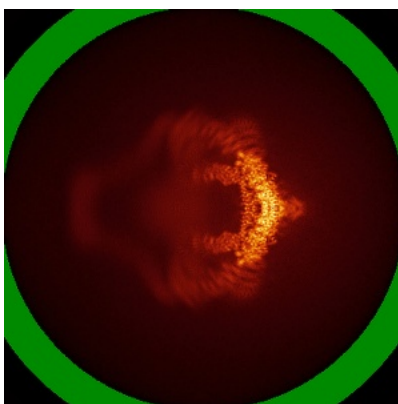


Z

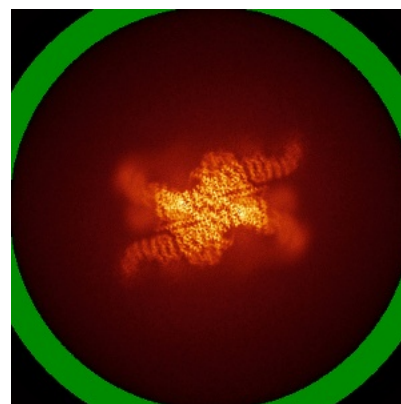
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00789. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

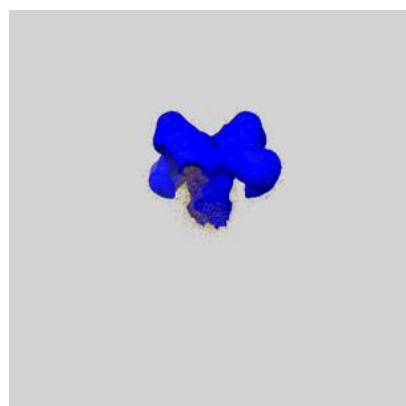
6.6 Mask visualisation [i](#)

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

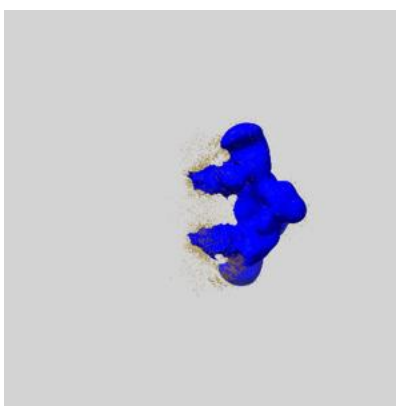
A mask typically either:

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

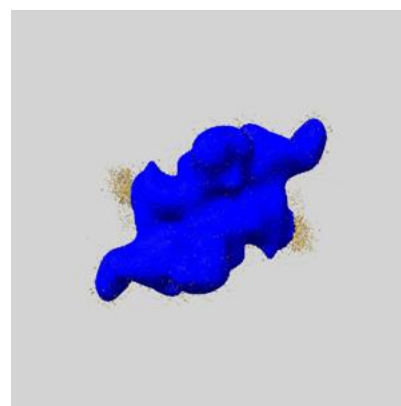
6.6.1 emd_53426_msk_1.map [i](#)



X



Y

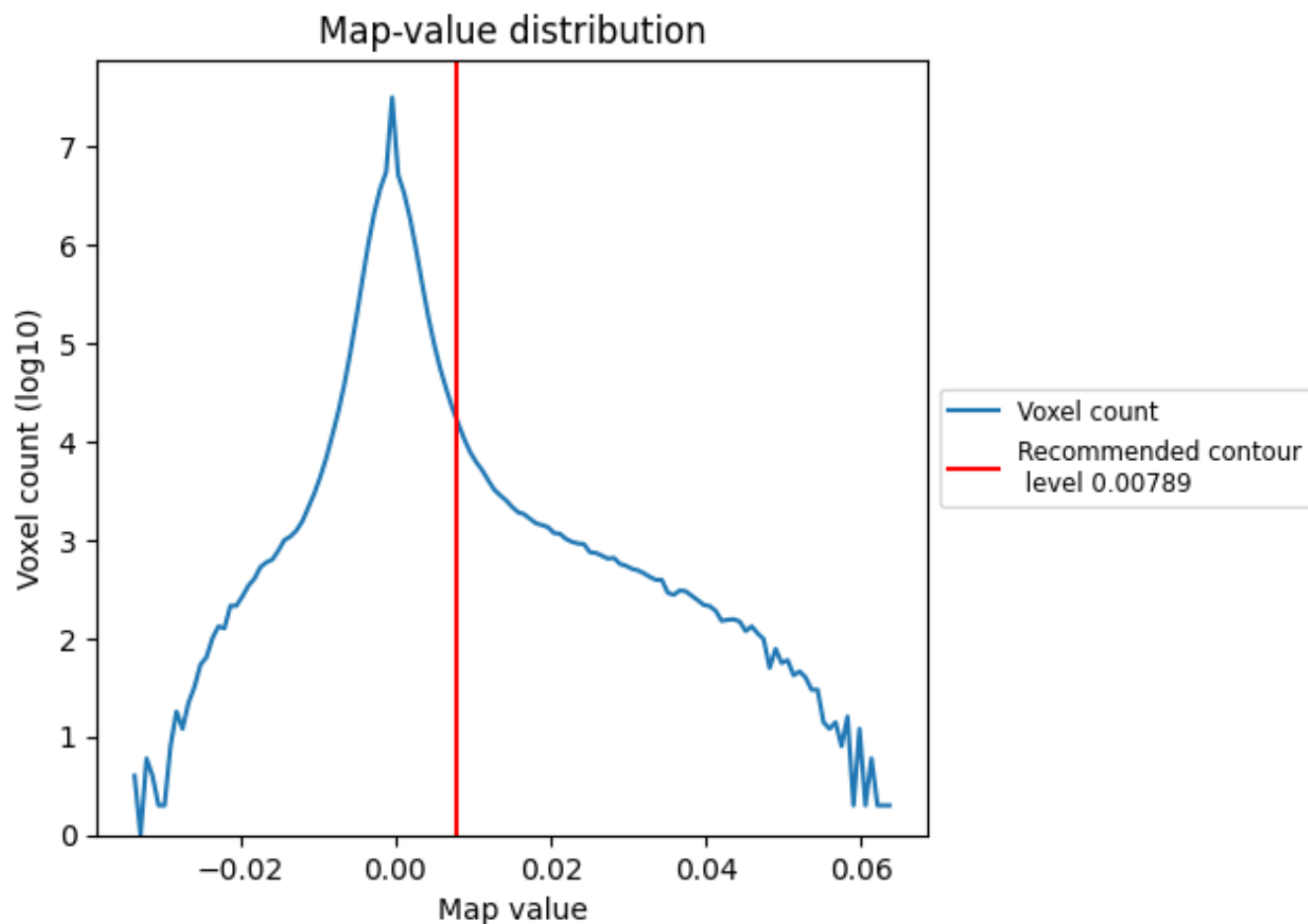


Z

7 Map analysis [i](#)

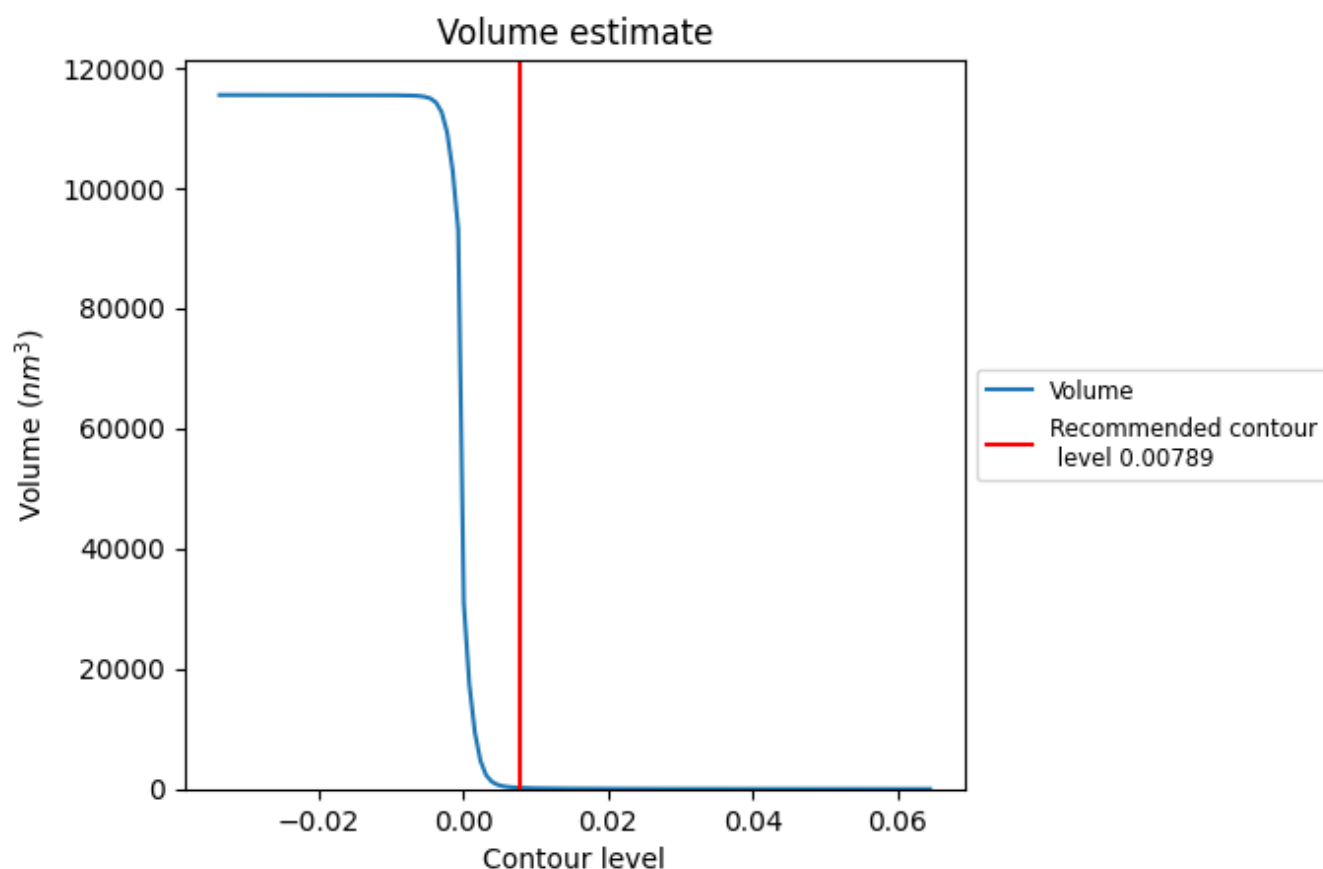
This section contains the results of statistical analysis of the map.

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.

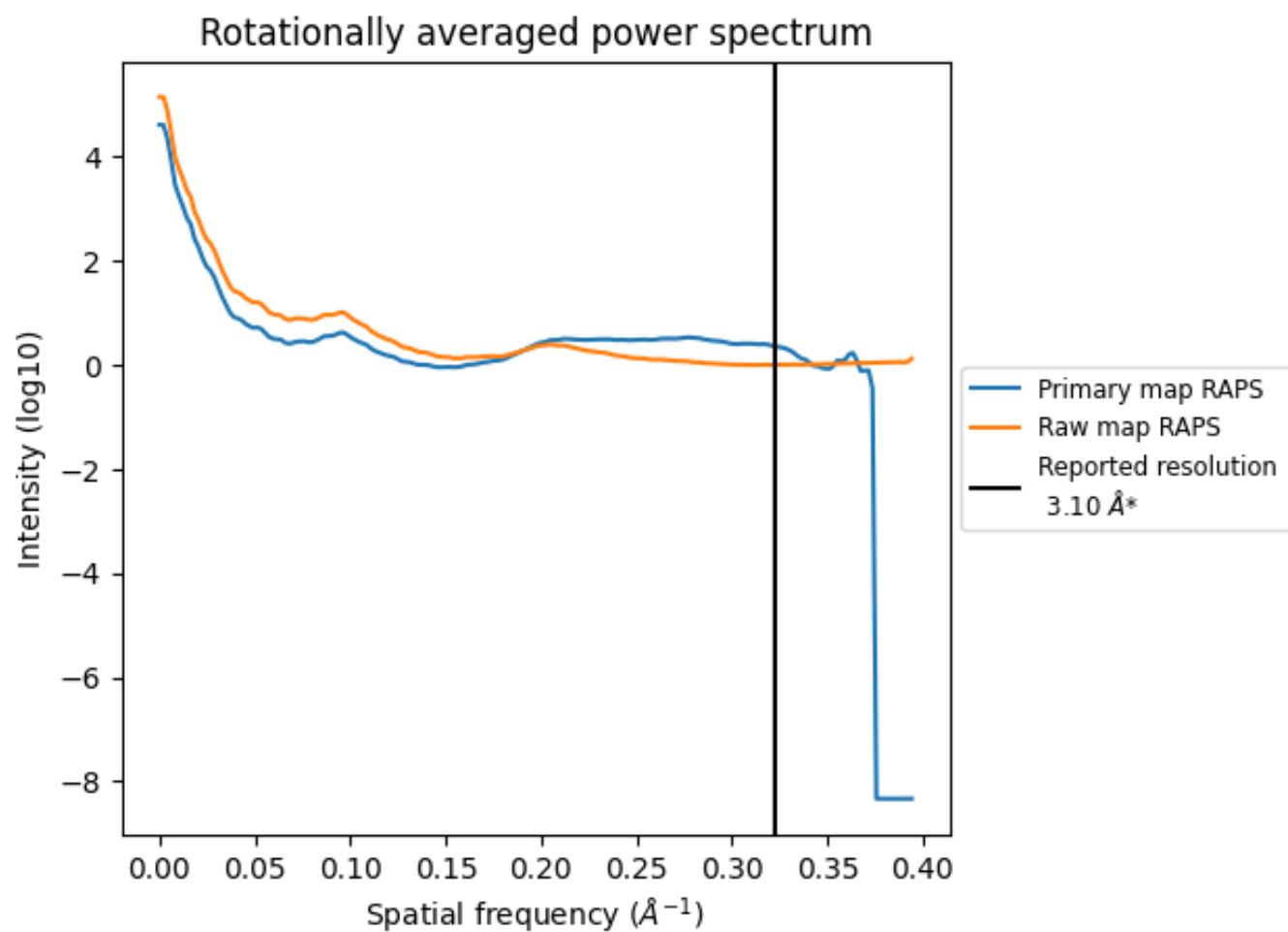
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 188 nm³; this corresponds to an approximate mass of 169 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 ⓘ

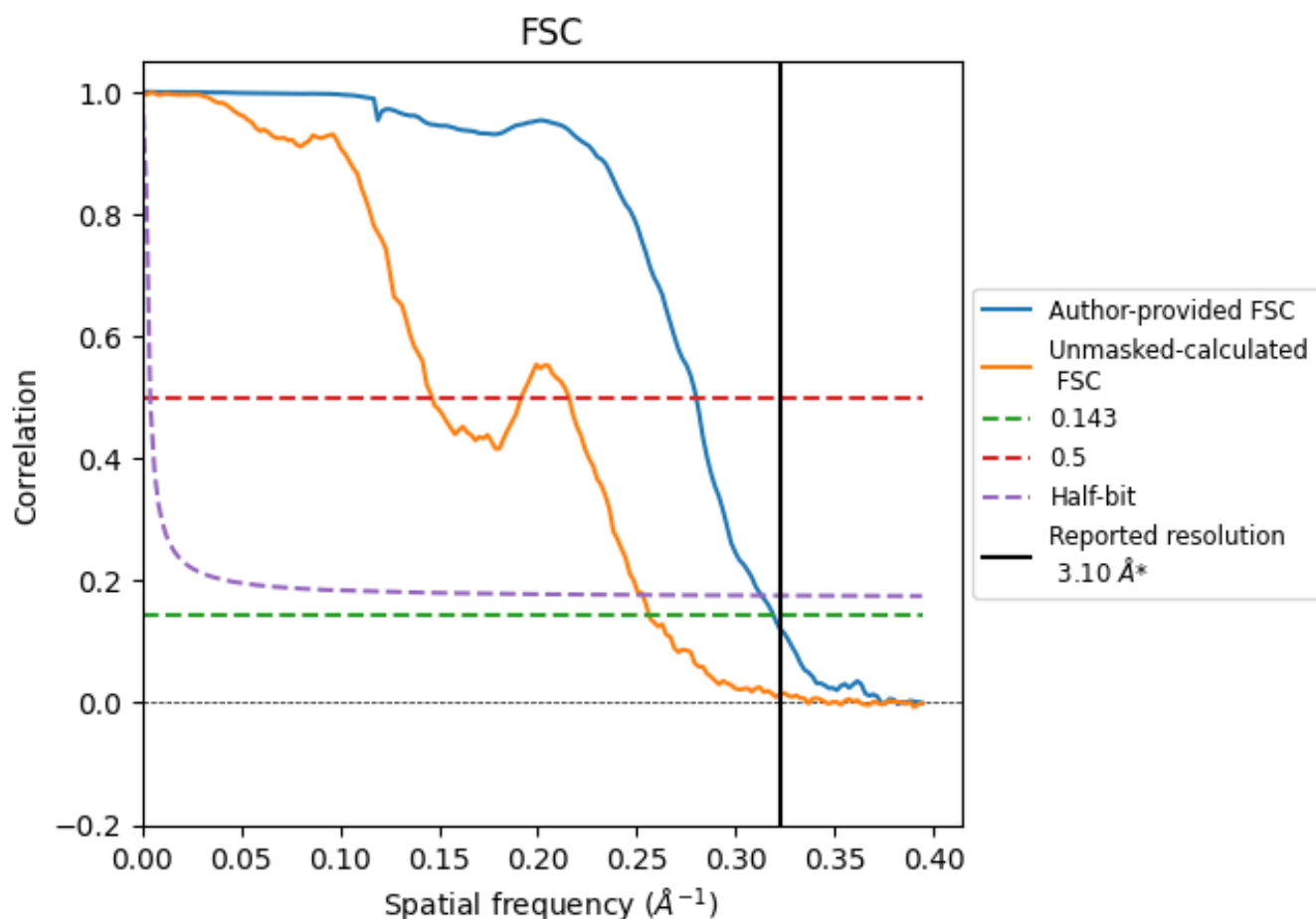


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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](#)

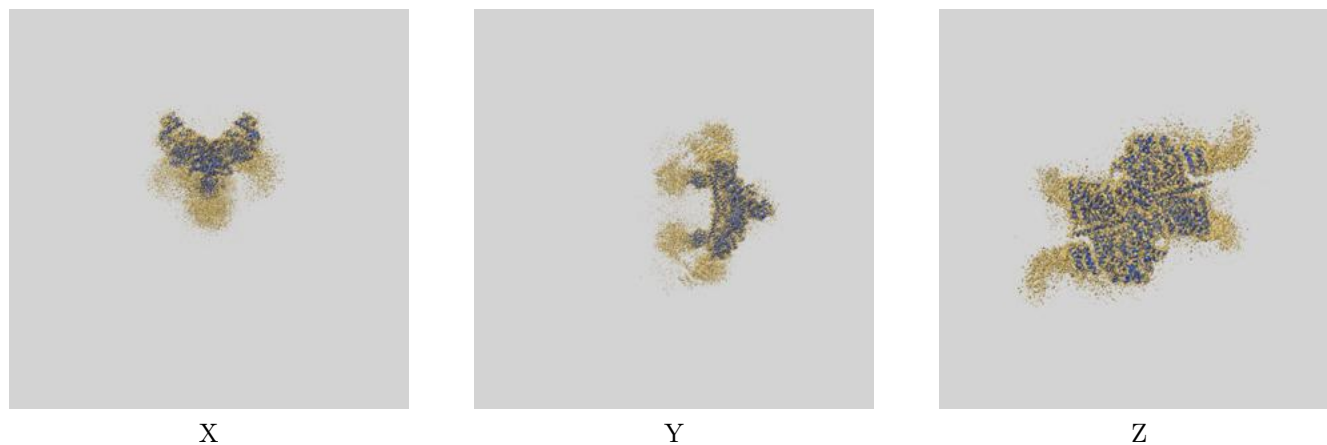
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.13	3.57	3.19
Unmasked-calculated*	3.90	6.83	3.95

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

9 Map-model fit [i](#)

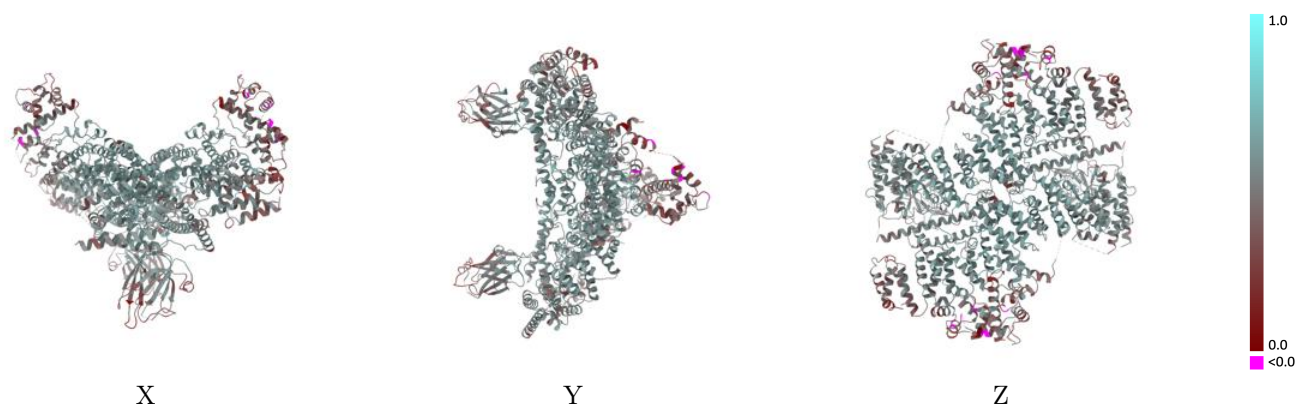
This section contains information regarding the fit between EMDB map EMD-53426 and PDB model 9QWS. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



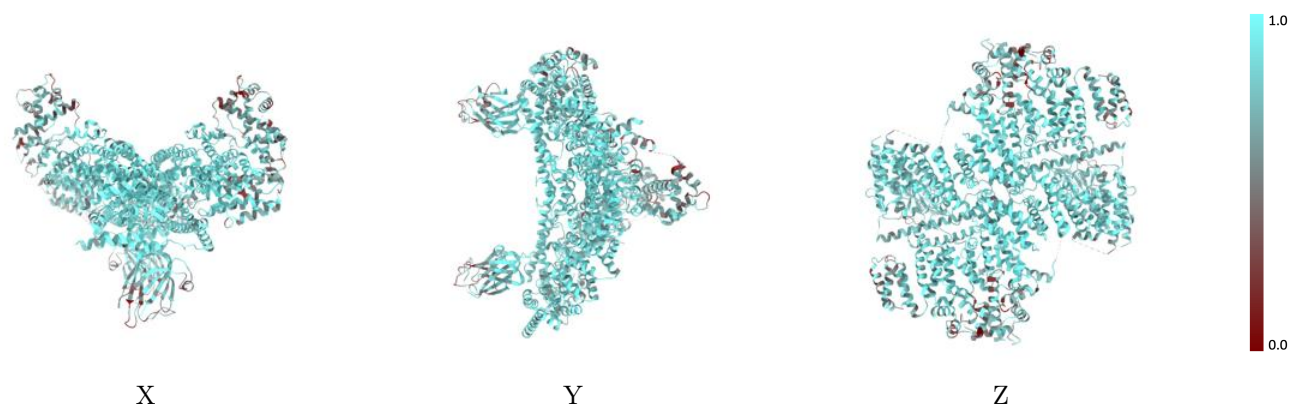
The images above show the 3D surface view of the map at the recommended contour level 0.00789 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



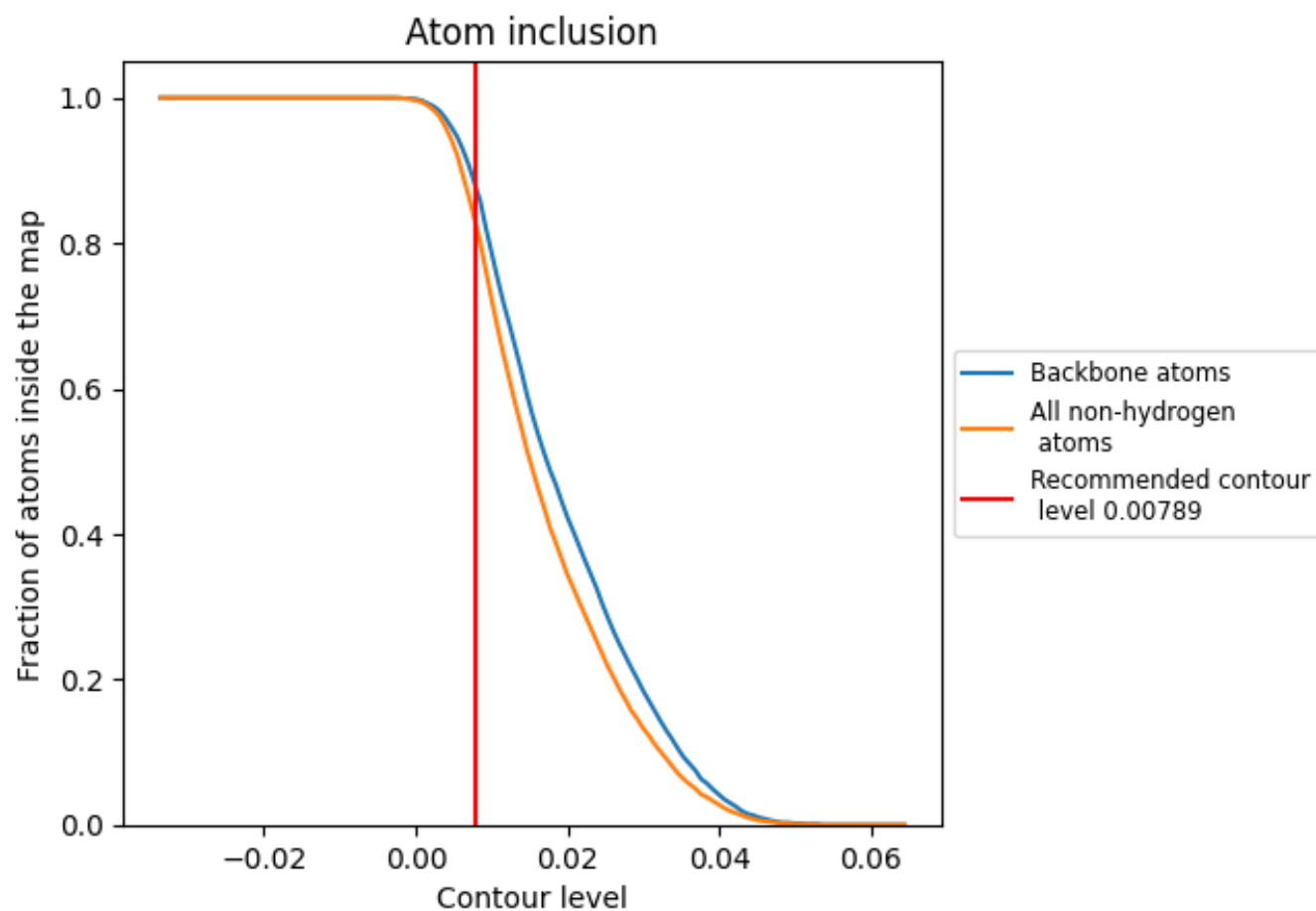
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00789).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 83% 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 (0.00789) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8280	0.5080
A	0.8430	0.5180
B	0.8450	0.5190
C	0.8800	0.5370
D	0.8770	0.5350
E	0.6350	0.3760
F	0.6350	0.3820

1.0

0.0

<0.0