



## Full wwPDB EM Validation Report ⓘ

Oct 15, 2025 – 01:37 am BST

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](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>.

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

EMDB validation analysis : 0.0.1.dev129  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.46

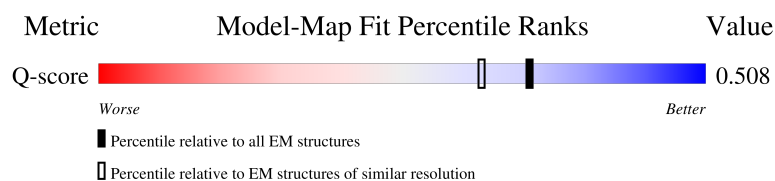
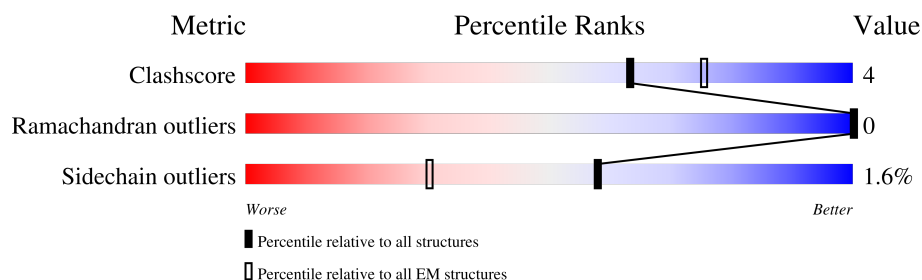
# 1 Overall quality at a glance

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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
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  $\geq 3$ , 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	E	158	<div> <div>17%</div> <div>78%</div> <div>5%</div> <div>17%</div> </div>
1	F	158	<div> <div>17%</div> <div>79%</div> <div>•</div> <div>17%</div> </div>
2	A	5193	<div> <div>18%</div> <div>80%</div> </div>
2	B	5193	<div> <div>18%</div> <div>80%</div> </div>

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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











- Molecule 2: E3 ubiquitin-protein ligase UBR4

SER	ALA	SER	MET
PRO	CYS	GLU	THR
GLU	ALA	ILE	SER
LEU	VAL	LEU	GLY
ARG	SER	HIS	GLY
GLN	GLN	HIS	GLU
	LYS	GLU	GLU
GLU	HIS	LYS	ALA
VAL	LEU	LEU	ALA
GLN	ILE	TYR	ALA
MET	LEU	GLU	ALA
ASN	LEU	PRO	ALA
PHE	ILE	PHE	ALA
LEU	LYS	TYR	ALA
LEU	GLY	SER	PRO
ASN	GLY	SER	ALA
GLN	LEU	SER	PRO
LEU	CYS	PHE	GLY
THR	THR	VAL	THR
SER	GLY	ALA	PRO
VAL	CYS	LEU	ALA
PHE	SER	SER	THR
ASN	ARG	THR	GLY
PRO	LEU	HIS	ALA
ARG	ASP	TYR	ASP
THR	ARG	ILE	THR
VAL	THR	THR	THR
ALA	GLU	THR	PRO
SER	ILE	VAL	GLY
GLN	ILE	CYS	TRP
PRO	THR	SER	GLU
ILE	PHE	LEU	VAL
SER	THR	ILE	ALA
THR	ALA	PRO	VAL
GLN	MET	ARG	ARG
THR	MET	ASN	PRO
LEU	LYS	GLN	LEU
VAL	SER	LEU	LEU
GLU	ALA	GLN	SER
GLY	LYS	SER	ALA
GLU	LEU	VAL	SER
ASN	PRO	ALA	TYR
ASP	GLN	ALA	SER
GLU	THR	ALA	ALA
GLN	VAL	CYS	PHE
SER	LYS	LYS	GLU
SER	THR	VAL	MET
THR	LEU	LYS	LYS
ASP	SER	ILE	GLU
GLN	ASP	GLU	LEU
ALA	VAL	PHE	PRO
SER	GLU	SER	GLN
LEU	ASP	LEU	LEU
ILE	GLN	LEU	VAL
LYS	LYS	ARG	ALA
THR	GLU	LEU	SER
THR	LEU	GLU	VAL
ASN	ALA	ASN	ILE
VAL	SER	PRO	GLU
PHE	THR	ASP	THR
THR	VAL	THR	CTR









- 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	GLY	VAL	TYR	TYR
	ASP	ILE	SER	ARG	THR	ASP
	ILE	GLN	VAL	HIS	GLU	TYR
	MET	SER	ARG	VAL	THR	ASP
	PRO	THR	ARG	VAL	THR	LEU
	LEU	ALA	SER	ARG	SER	CYS
	ASP	ALA	ALA	MET	LEU	ALA
	VAL	THR	GLY	PHE	GLU	SER
	ALA	ASN	GLY	HIS	HIS	CYS
	LEU	ILE	GLN	PRO	VAL	TYR
	GLU	ALA	ASN	GLY	THR	GLU
	ASN	ASN	SER	ARG	SER	SER
	LEU	THR	SER	GLY	GLY	ALA
	LEU	SER	GLY	LEU	HIS	ALA
	LYS	SER	PRO	GLY	ALA	THR
	GLU	GLN	SER	GLY	GLU	THR
	ASN	GLN	LEU	ARG	VAL	THR
	GLU	ASN	GLN	SER	ILE	ASP
	PRO	\$299	LEU	SER	CYS	HIS
	PRO	L296	GLN	ASN	PRO	PRO
	PRO	ASN	MET	HIS	GLY	GLN
	PRO	ASP	GLN	PHE	CYS	CYS
	PRO	PRO	LEU	THR	ALA	ALA
	LEU	F300	GLN	SER	ALA	ILE
	SER	M301	LEU	SER	LEU	LEU
	ALA		GLU	SER	PRO	THR
	TRP	E305	ARG	THR	GLY	ARG
	SER	B306	GLN	GLY	GLY	THR
	HIS		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%)	17	46
2	A	904/4531 (20%)	890 (98%)	14 (2%)	60	80
2	B	904/4531 (20%)	890 (98%)	14 (2%)	60	80
3	C	38/339 (11%)	38 (100%)	0	100	100
3	D	38/339 (11%)	37 (97%)	1 (3%)	41	68
All	All	1956/10012 (20%)	1924 (98%)	32 (2%)	58	79

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.

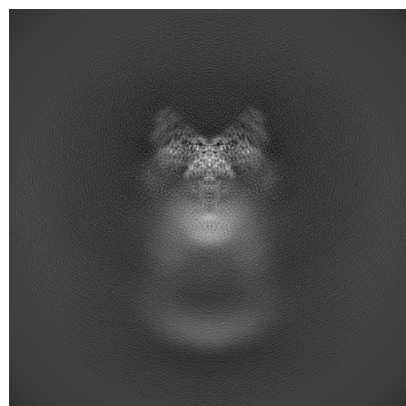
## 6 Map visualisation [i](#)

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.

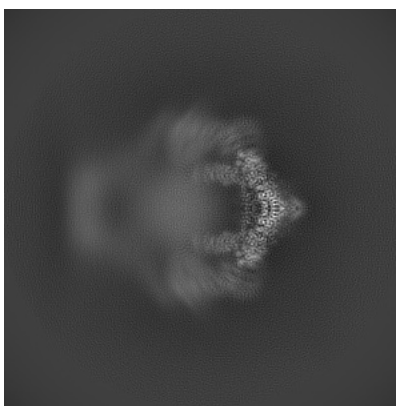
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

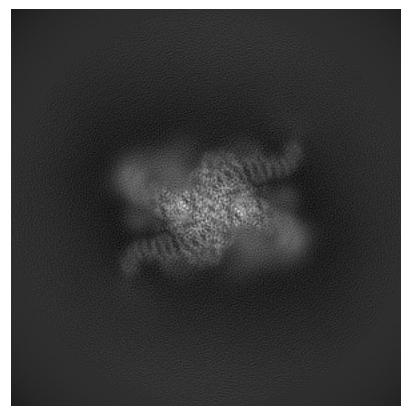
#### 6.1.1 Primary map



X

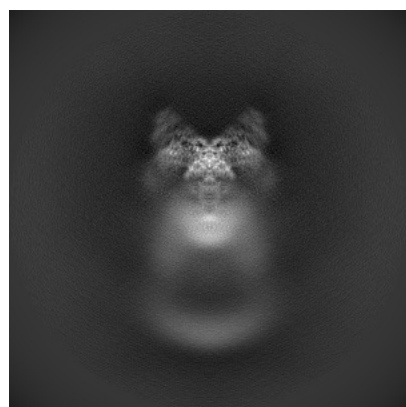


Y

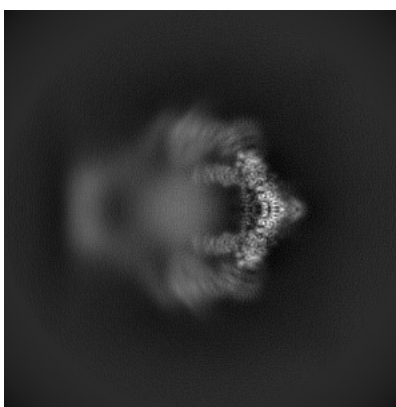


Z

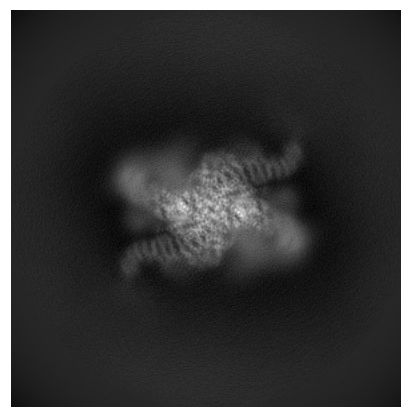
#### 6.1.2 Raw map



X



Y

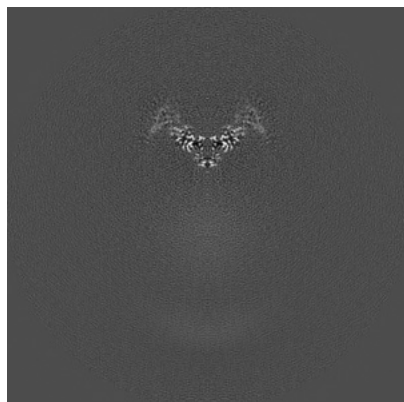


Z

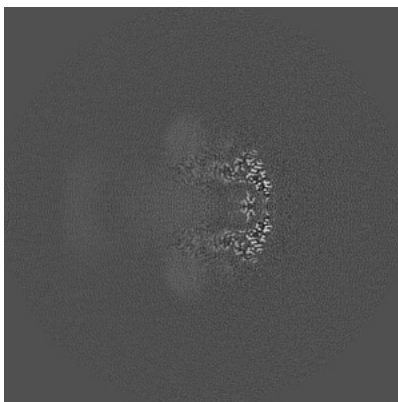
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

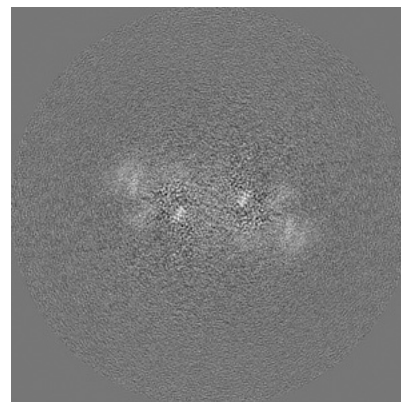
### 6.2.1 Primary map



X Index: 192

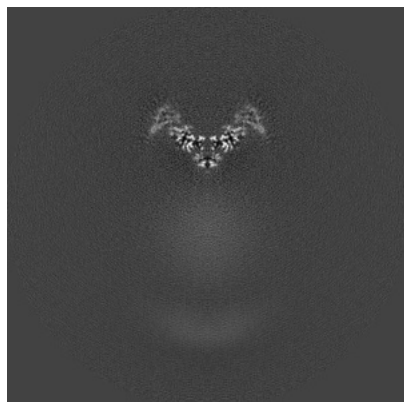


Y Index: 192

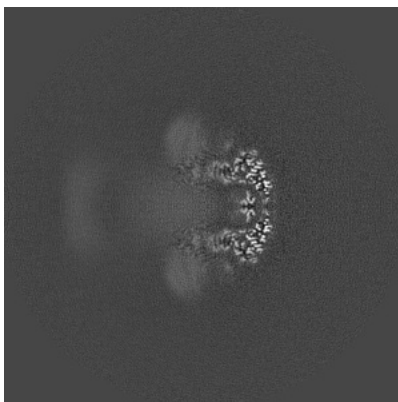


Z Index: 192

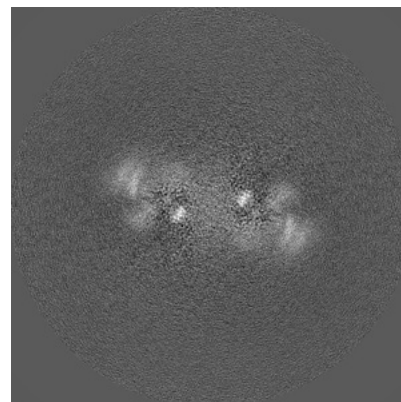
### 6.2.2 Raw map



X Index: 192



Y Index: 192

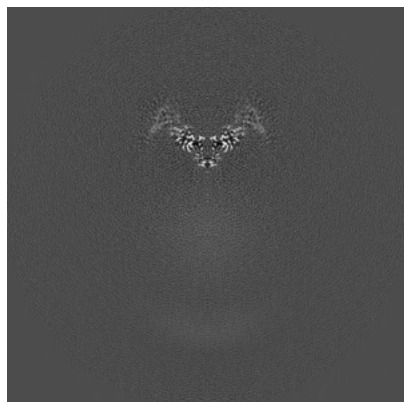


Z Index: 192

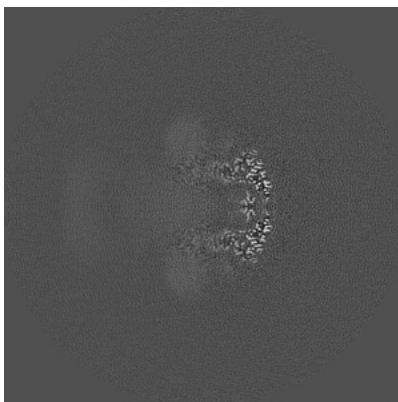
The images above show central slices of the map in three orthogonal directions.

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

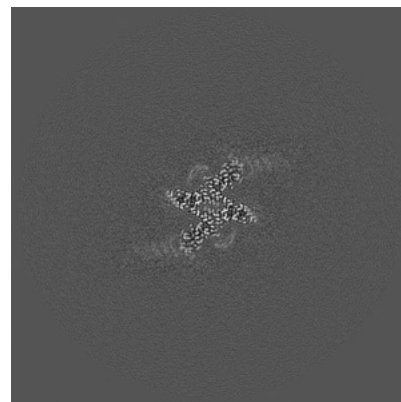
### 6.3.1 Primary map



X Index: 192

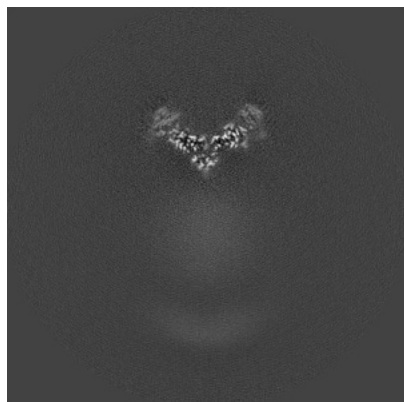


Y Index: 192

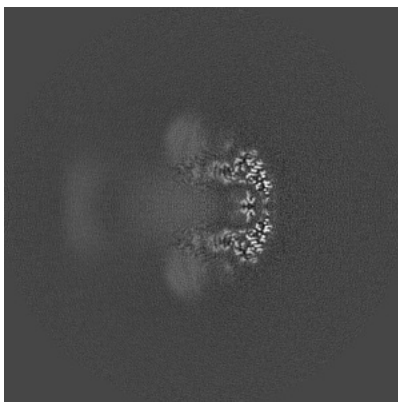


Z Index: 249

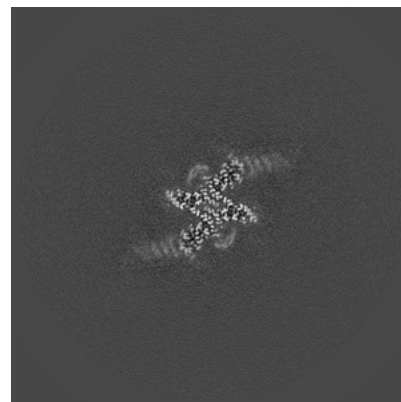
### 6.3.2 Raw map



X Index: 188



Y Index: 192



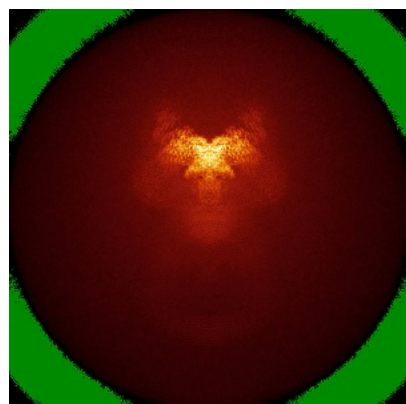
Z Index: 249

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

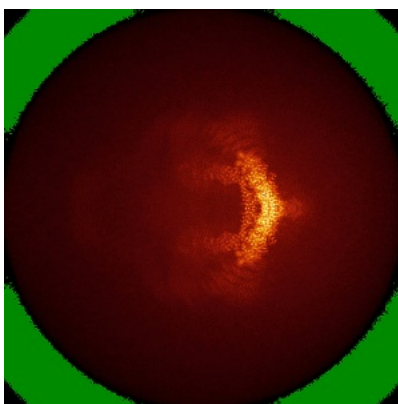


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

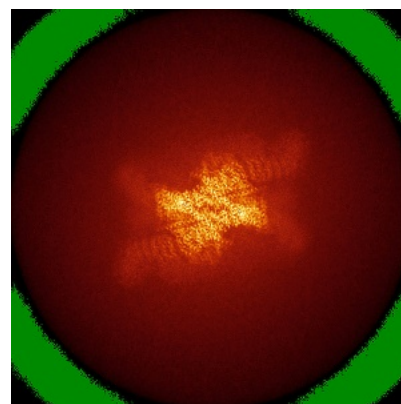
### 6.4.1 Primary map



X

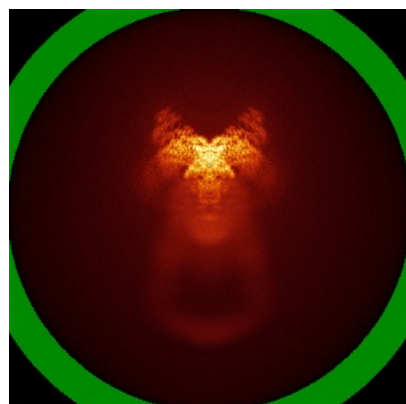


Y

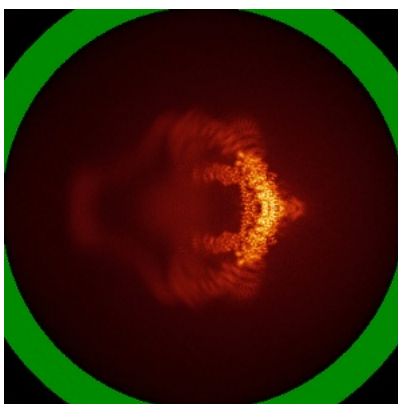


Z

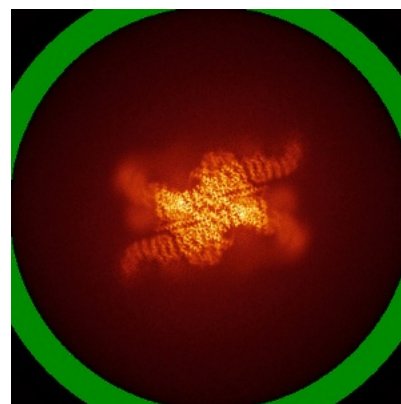
### 6.4.2 Raw map



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



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.

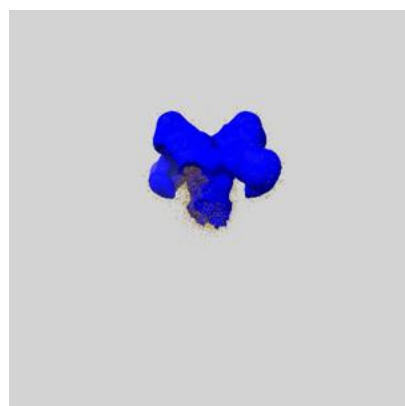
## 6.6 Mask visualisation [i](#)

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

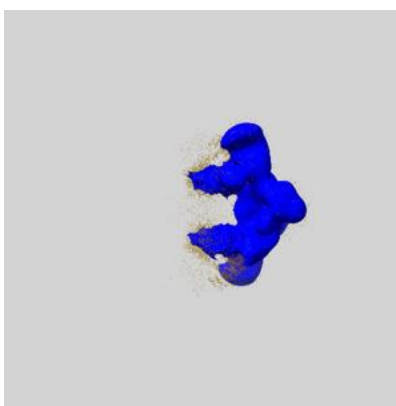
A mask typically either:

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

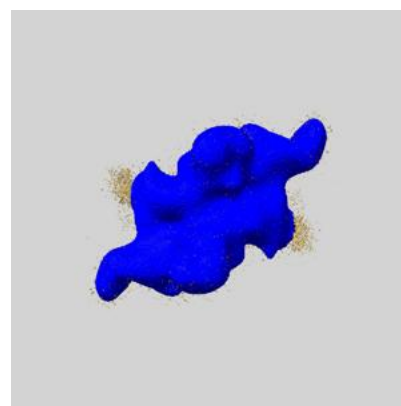
### 6.6.1 emd\_53426\_msk\_1.map [i](#)



X



Y



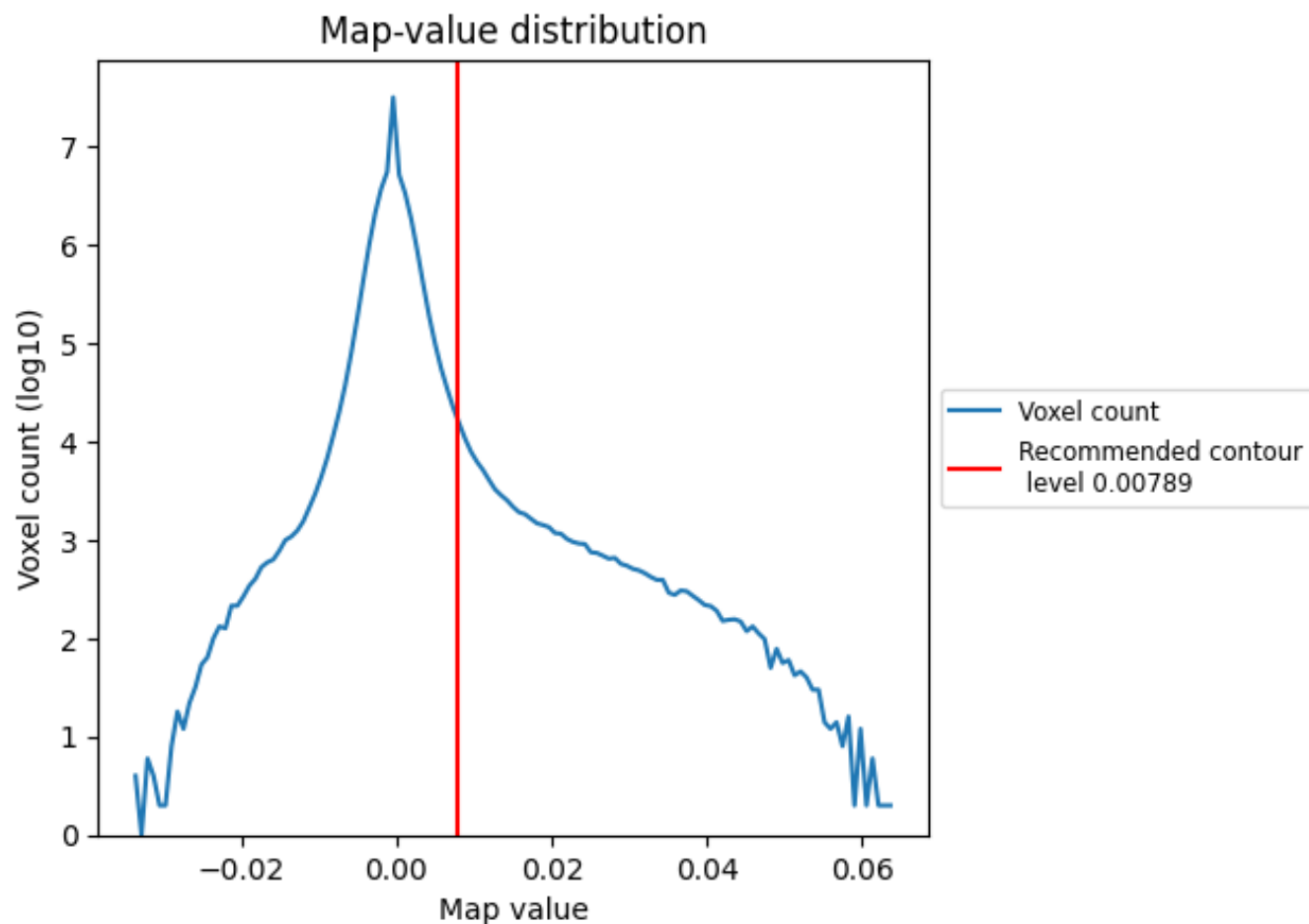
Z



## 7 Map analysis [i](#)

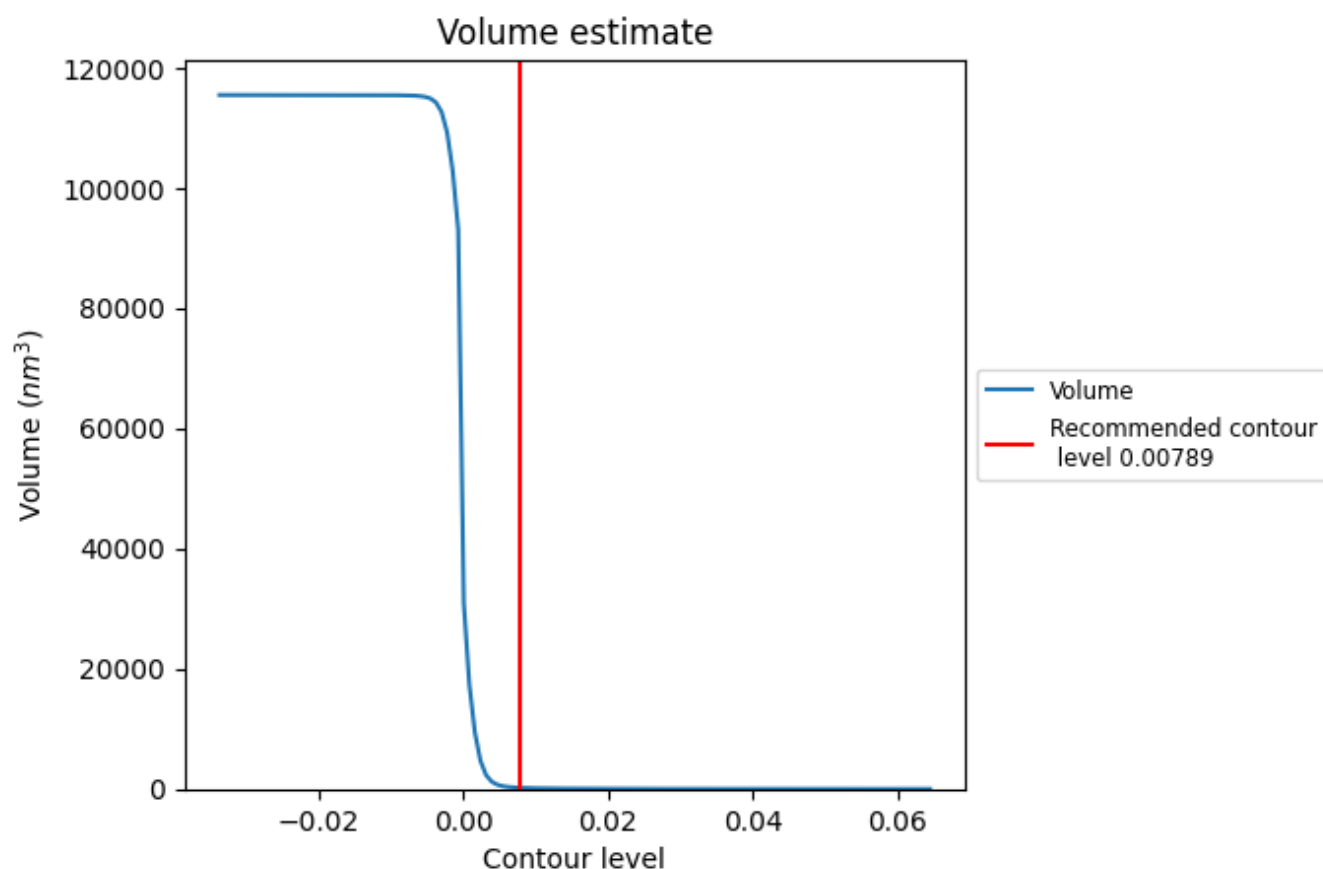
This section contains the results of statistical analysis of the map.

### 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.

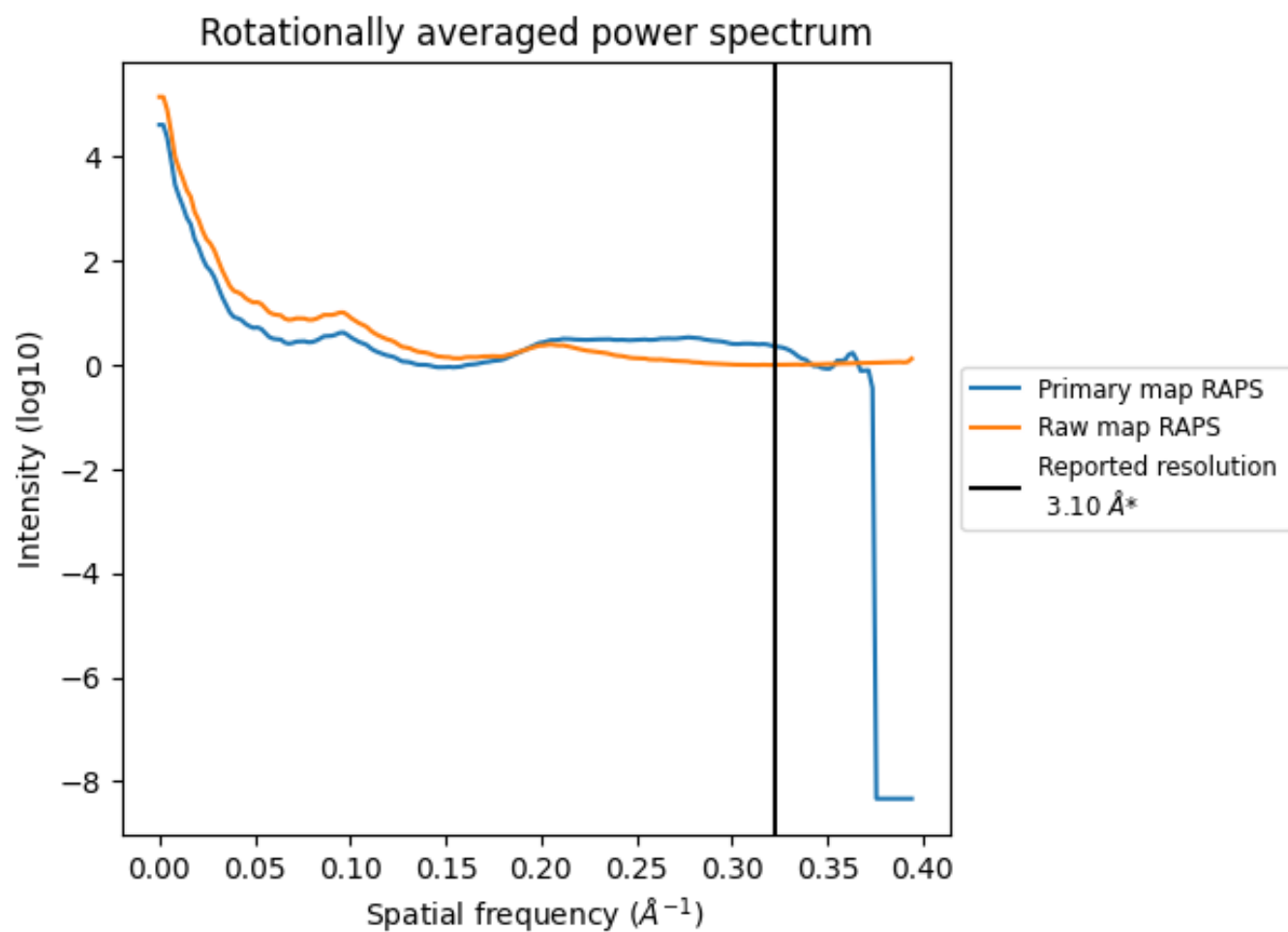
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 188 nm<sup>3</sup>; 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 ⓘ

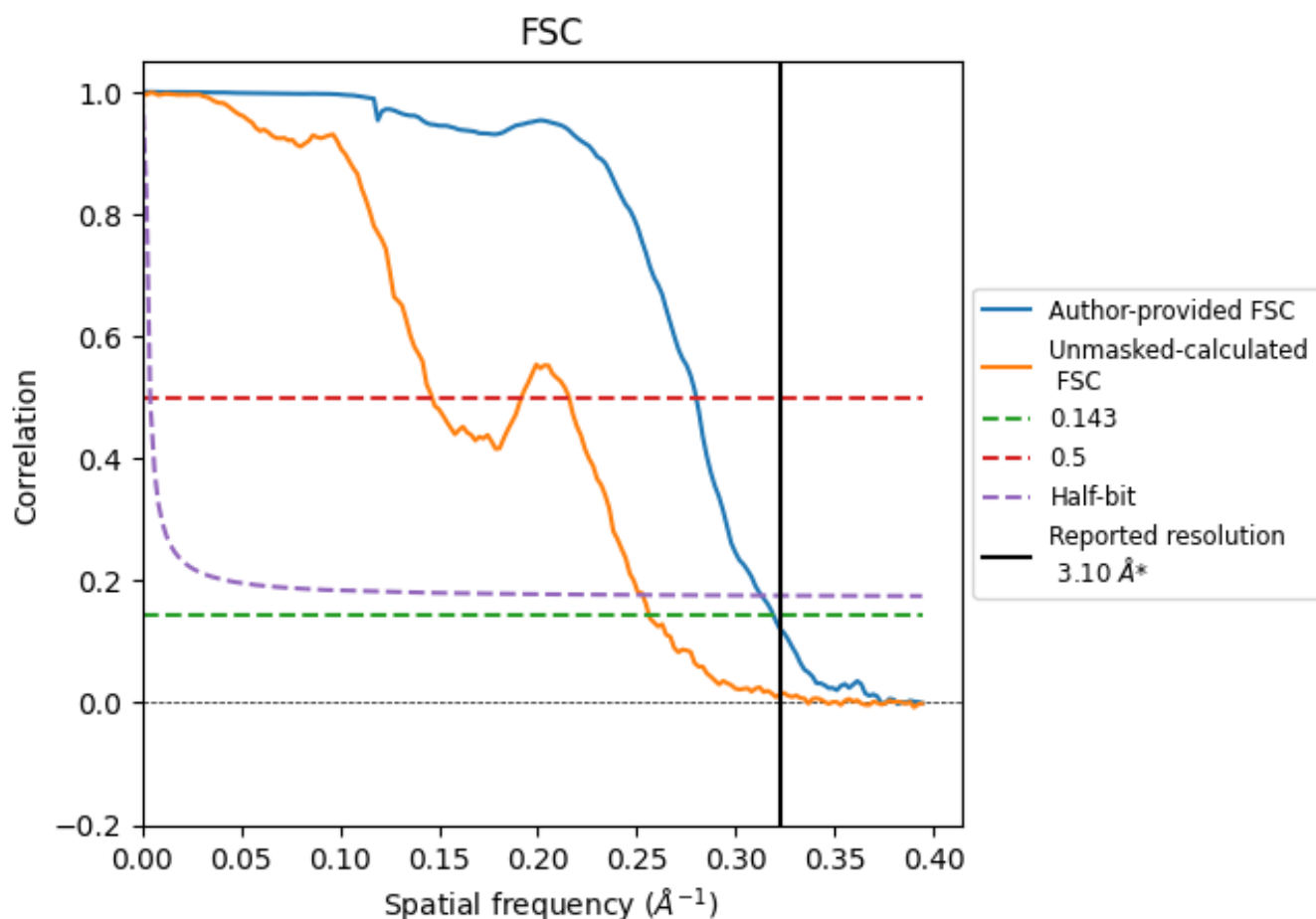


\*Reported resolution corresponds to spatial frequency of 0.323 Å<sup>-1</sup>

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

## 8.2 Resolution estimates [i](#)

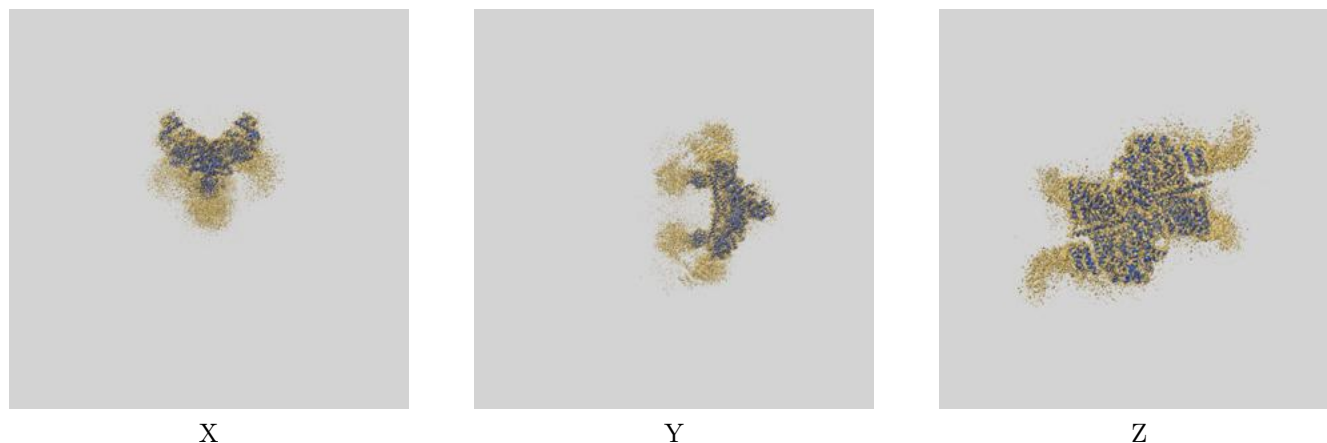
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.13	3.57	3.19
Unmasked-calculated*	3.90	6.83	3.95

\*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](#)

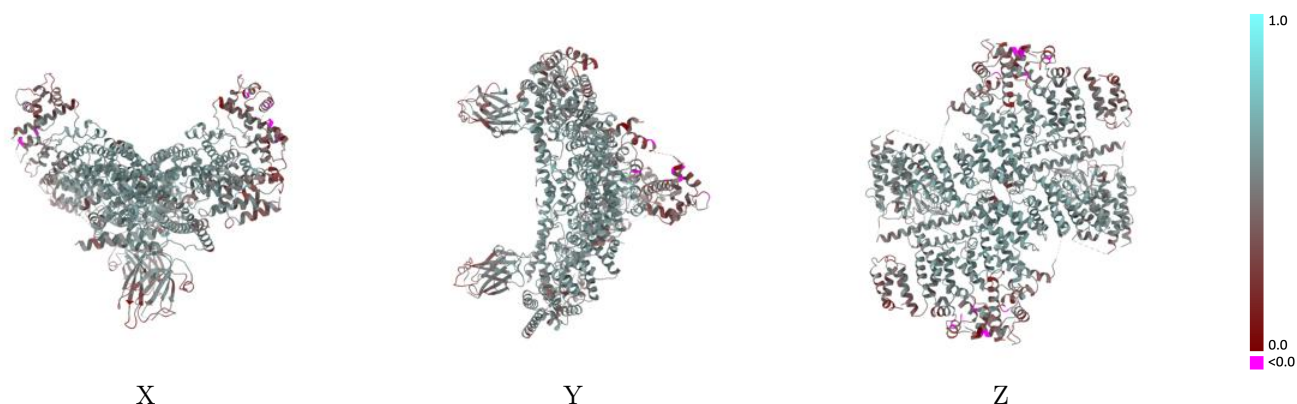
This section contains information regarding the fit between EMDB map EMD-53426 and PDB model 9QWS. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

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



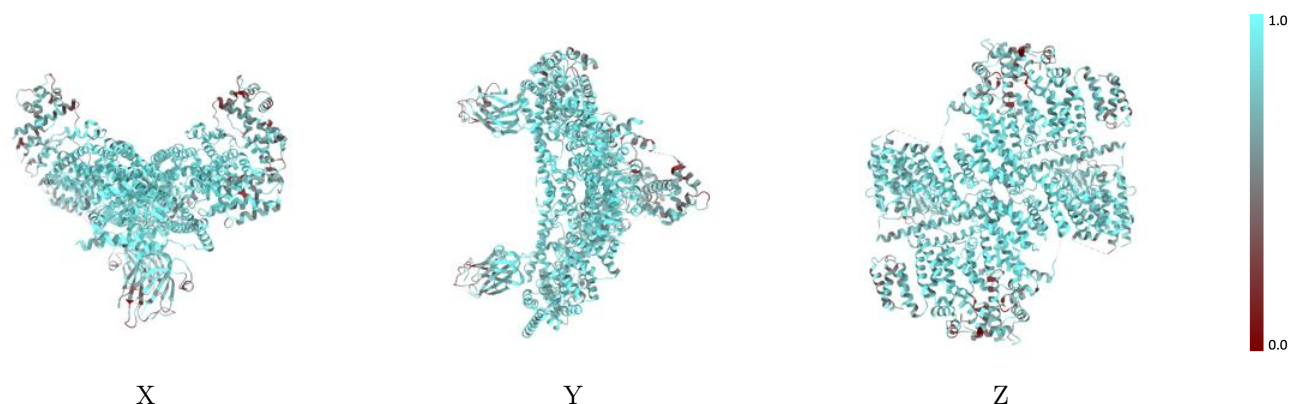
The images above show the 3D surface view of the map at the recommended contour level 0.00789 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



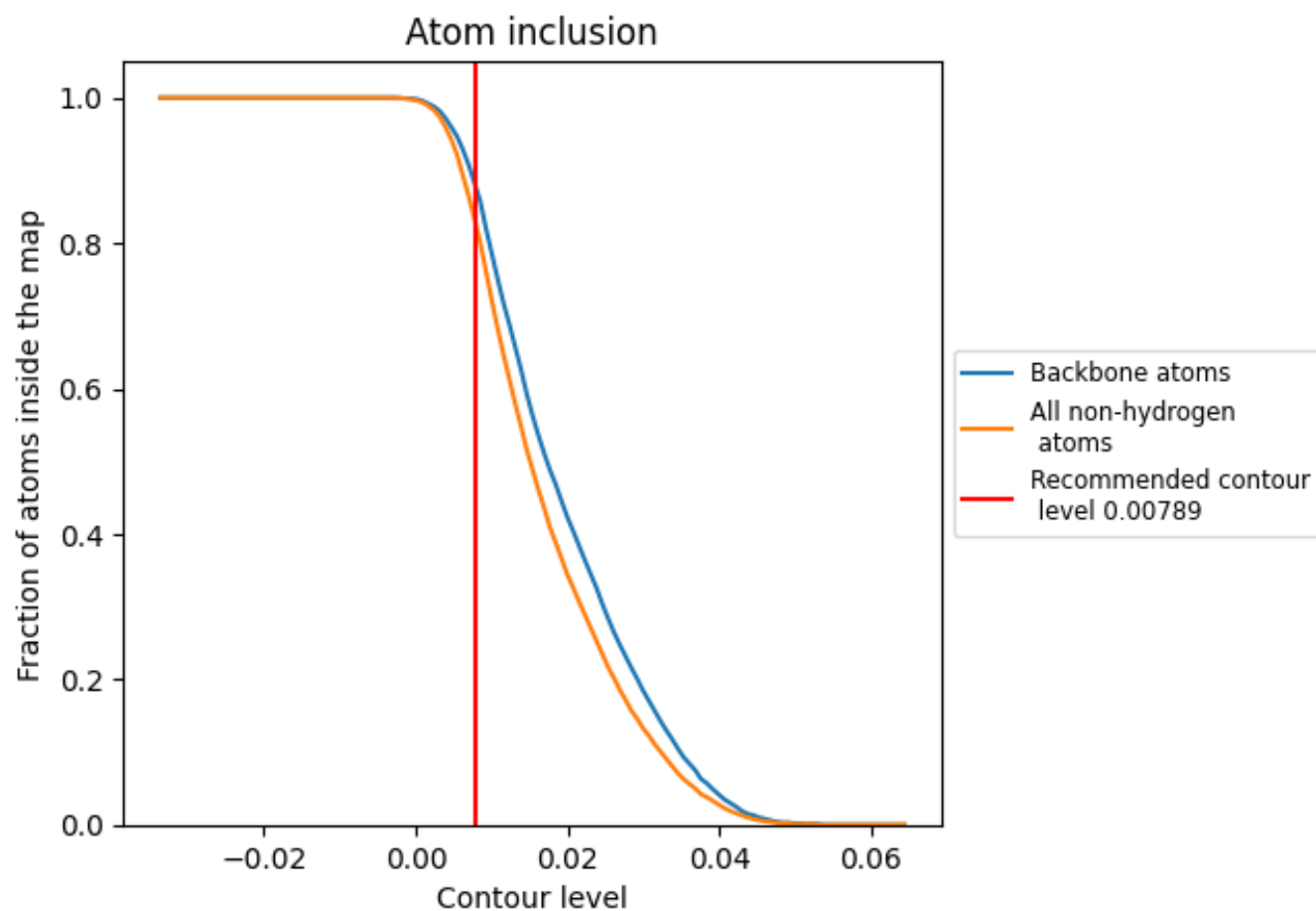
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	<div><div></div>0.8280</div>	<div><div></div>0.5080</div>
A	<div><div></div>0.8430</div>	<div><div></div>0.5180</div>
B	<div><div></div>0.8450</div>	<div><div></div>0.5190</div>
C	<div><div></div>0.8800</div>	<div><div></div>0.5370</div>
D	<div><div></div>0.8770</div>	<div><div></div>0.5350</div>
E	<div><div></div>0.6350</div>	<div><div></div>0.3760</div>
F	<div><div></div>0.6350</div>	<div><div></div>0.3820</div>

1.0

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