



## Full wwPDB EM Validation Report ⓘ

Apr 8, 2026 – 10:59 PM UTC

PDB ID : 9QPO / pdb\_00009qpo  
EMDB ID : EMD-53276  
Title : CryoEM structure of human MATa2 in complex with MATBv2 at 2.6 Å resolution  
Authors : Khaja, F.; Antonyuk, S.V.; Muench, S.P.; Hasnain, S.S.  
Deposited on : 2025-03-27  
Resolution : 2.60 Å (reported)  
Based on initial model : 4ndn

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:

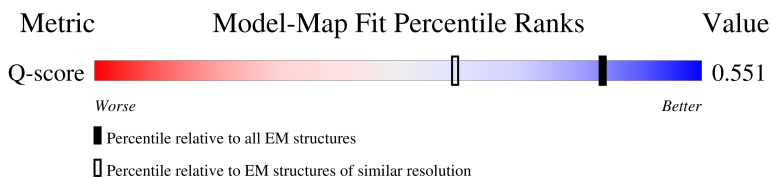
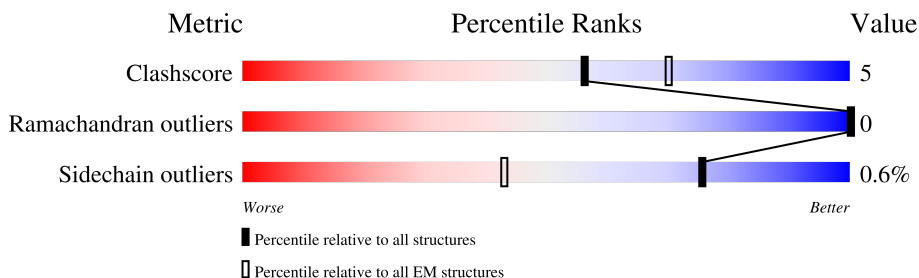
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : 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 2.60 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.



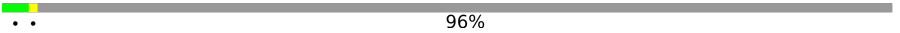
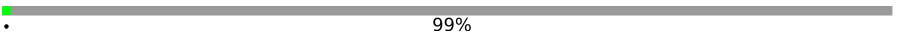
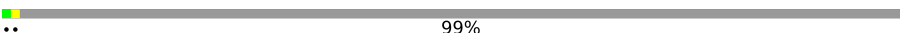
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8728 ( 2.10 - 3.10 )

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	395	86% 8% 6%
1	B	395	83% 11% 6%
1	C	395	80% 14% 6%
1	D	395	84% 12% .

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Mol	Chain	Length	Quality of chain
2	E	334	 96%
2	F	334	 99%
2	G	334	 99%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11801 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 S-adenosylmethionine synthase isoform type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	371	Total	C	N	O	S	0	0
			2881	1822	505	543	11		
1	B	371	Total	C	N	O	S	0	0
			2877	1821	502	543	11		
1	C	372	Total	C	N	O	S	0	0
			2889	1828	504	546	11		
1	D	380	Total	C	N	O	S	0	0
			2950	1865	516	558	11		

- Molecule 2 is a protein called Isoform 2 of Methionine adenosyltransferase 2 subunit beta.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	E	13	Total	C	N	O	0	0
			125	83	24	18		
2	G	4	Total	C	N	O	4	0
			35	24	6	5		
2	F	4	Total	C	N	O	4	0
			36	24	6	6		

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-10	MET	-	initiating methionine	UNP Q9NZL9
E	-9	VAL	-	expression tag	UNP Q9NZL9
E	-8	GLY	-	expression tag	UNP Q9NZL9
E	-7	ARG	-	expression tag	UNP Q9NZL9
E	-6	GLU	-	expression tag	UNP Q9NZL9
E	-5	LYS	-	expression tag	UNP Q9NZL9
E	-4	GLU	-	expression tag	UNP Q9NZL9
E	-3	LEU	-	expression tag	UNP Q9NZL9
E	-2	SER	-	expression tag	UNP Q9NZL9
E	-1	ILE	MET	conflict	UNP Q9NZL9
E	0	HIS	PRO	conflict	UNP Q9NZL9

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1	PHE	GLU	conflict	UNP Q9NZL9
E	2	VAL	MET	conflict	UNP Q9NZL9
E	4	GLY	-	insertion	UNP Q9NZL9
E	5	SER	-	insertion	UNP Q9NZL9
E	6	CYS	GLU	conflict	UNP Q9NZL9
E	7	ARG	ASP	conflict	UNP Q9NZL9
E	8	LEU	MET	conflict	UNP Q9NZL9
E	9	VAL	GLU	conflict	UNP Q9NZL9
E	10	GLU	GLN	conflict	UNP Q9NZL9
G	-10	MET	-	initiating methionine	UNP Q9NZL9
G	-9	VAL	-	expression tag	UNP Q9NZL9
G	-8	GLY	-	expression tag	UNP Q9NZL9
G	-7	ARG	-	expression tag	UNP Q9NZL9
G	-6	GLU	-	expression tag	UNP Q9NZL9
G	-5	LYS	-	expression tag	UNP Q9NZL9
G	-4	GLU	-	expression tag	UNP Q9NZL9
G	-3	LEU	-	expression tag	UNP Q9NZL9
G	-2	SER	-	expression tag	UNP Q9NZL9
G	-1	ILE	MET	conflict	UNP Q9NZL9
G	0	HIS	PRO	conflict	UNP Q9NZL9
G	1	PHE	GLU	conflict	UNP Q9NZL9
G	2	VAL	MET	conflict	UNP Q9NZL9
G	4	GLY	-	insertion	UNP Q9NZL9
G	5	SER	-	insertion	UNP Q9NZL9
G	6	CYS	GLU	conflict	UNP Q9NZL9
G	7	ARG	ASP	conflict	UNP Q9NZL9
G	8	LEU	MET	conflict	UNP Q9NZL9
G	9	VAL	GLU	conflict	UNP Q9NZL9
G	10	GLU	GLN	conflict	UNP Q9NZL9
F	-10	MET	-	initiating methionine	UNP Q9NZL9
F	-9	VAL	-	expression tag	UNP Q9NZL9
F	-8	GLY	-	expression tag	UNP Q9NZL9
F	-7	ARG	-	expression tag	UNP Q9NZL9
F	-6	GLU	-	expression tag	UNP Q9NZL9
F	-5	LYS	-	expression tag	UNP Q9NZL9
F	-4	GLU	-	expression tag	UNP Q9NZL9
F	-3	LEU	-	expression tag	UNP Q9NZL9
F	-2	SER	-	expression tag	UNP Q9NZL9
F	-1	ILE	MET	conflict	UNP Q9NZL9
F	0	HIS	PRO	conflict	UNP Q9NZL9
F	1	PHE	GLU	conflict	UNP Q9NZL9
F	2	VAL	MET	conflict	UNP Q9NZL9

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Chain	Residue	Modelled	Actual	Comment	Reference
F	4	GLY	-	insertion	UNP Q9NZL9
F	5	SER	-	insertion	UNP Q9NZL9
F	6	CYS	GLU	conflict	UNP Q9NZL9
F	7	ARG	ASP	conflict	UNP Q9NZL9
F	8	LEU	MET	conflict	UNP Q9NZL9
F	9	VAL	GLU	conflict	UNP Q9NZL9
F	10	GLU	GLN	conflict	UNP Q9NZL9

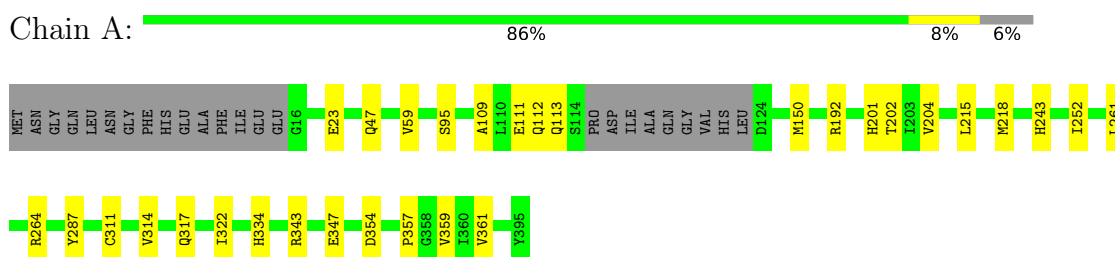
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	AltConf
3	B	2	Total O 2 2	0
3	C	3	Total O 3 3	0
3	D	3	Total O 3 3	0

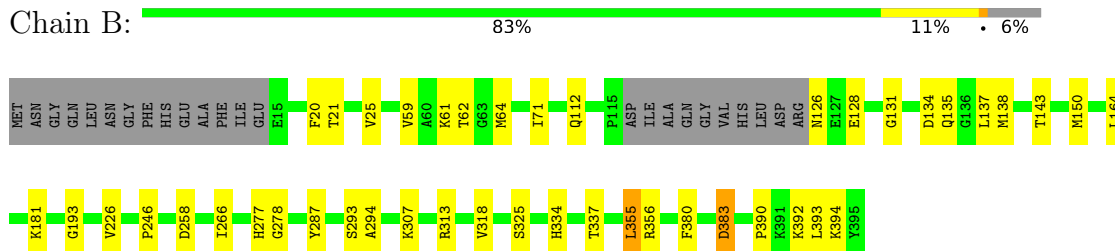
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

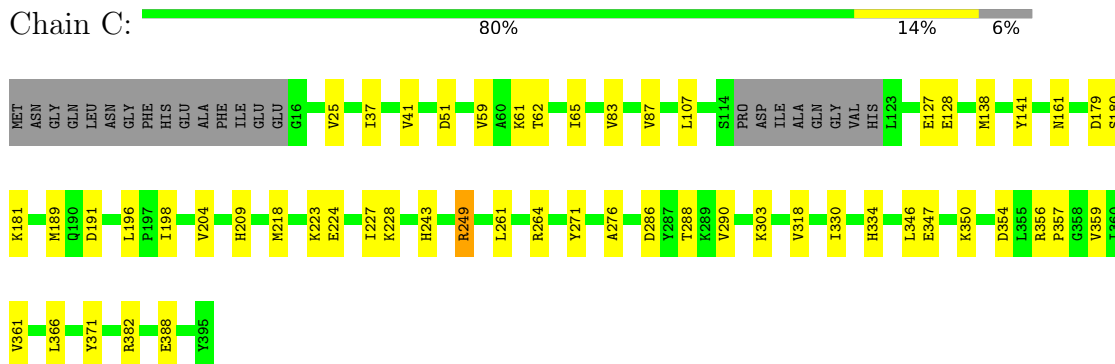
- Molecule 1: S-adenosylmethionine synthase isoform type-2



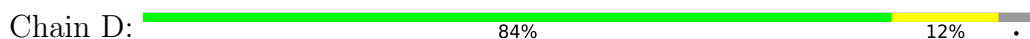
- Molecule 1: S-adenosylmethionine synthase isoform type-2

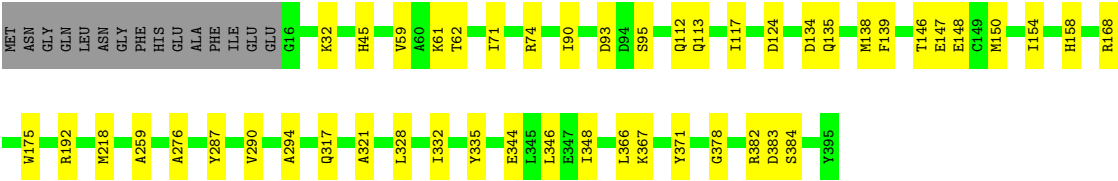


- Molecule 1: S-adenosylmethionine synthase isoform type-2

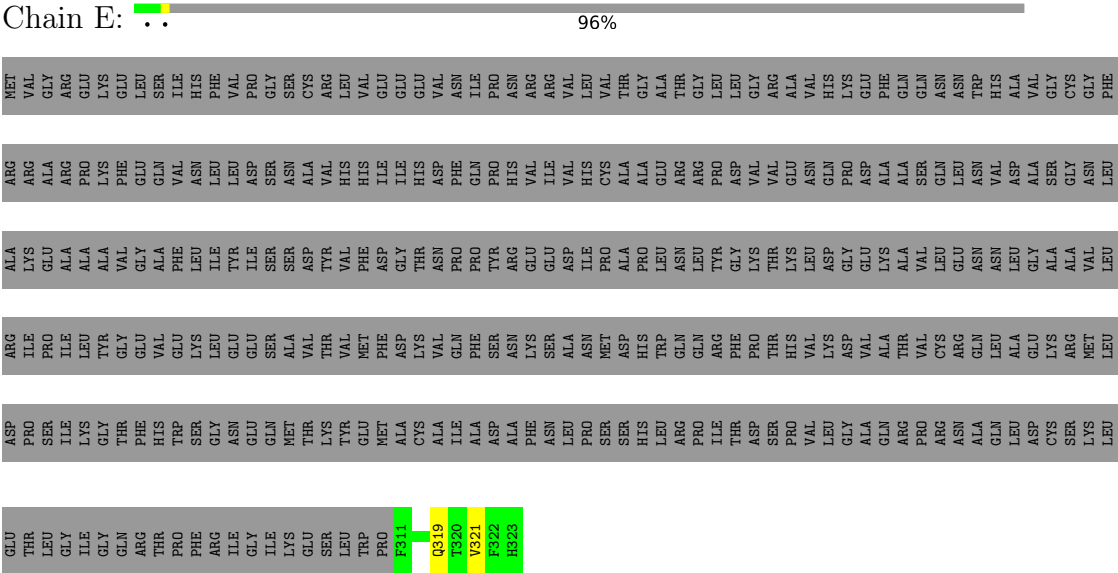


- Molecule 1: S-adenosylmethionine synthase isoform type-2

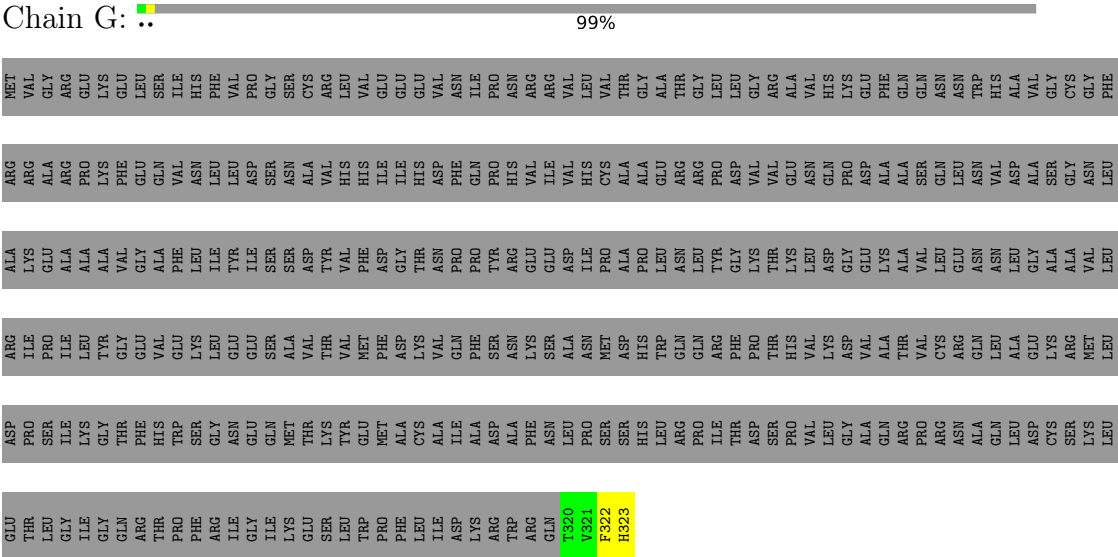




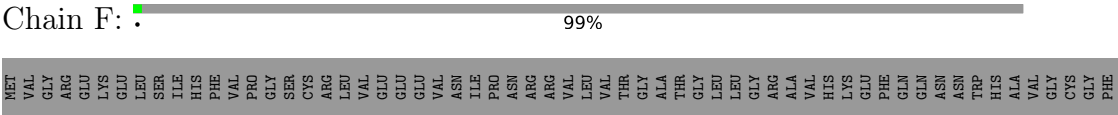
● Molecule 2: Isoform 2 of Methionine adenosyltransferase 2 subunit beta



● Molecule 2: Isoform 2 of Methionine adenosyltransferase 2 subunit beta



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GLU	THR	ASP	ARG	ALA	ARG
THR	LEU	SER	ILE	LYS	ARG
ILE	GLY	ILE	ILE	ALA	ARG
GLY	GLY	LYS	LEU	ALA	PRO
GLN	THR	THR	TYR	ALA	LYS
ARG	PHE	PHE	GLY	VAL	PHE
THR	HIS	THR	GLU	ALA	GLN
PRO	PRO	TRP	VAL	PHE	VAL
PHE	PHE	SER	LYS	LEU	ASN
ARG	ARG	GLY	LEU	ILE	LEU
ILE	ASN	ASN	GLU	TYR	LEU
GLY	GLU	GLU	GLU	ILE	ASP
ILE	GLN	SER	SER	SER	ASN
LYS	LYS	MET	ALA	ASP	ASN
GLU	THR	THR	VAL	ASP	ALA
SER	LYS	THR	THR	TYR	VAL
THR	TYR	VAL	VAL	VAL	HIS
LEU	LEU	GLU	MET	PHE	HIS
TRP	TRP	MET	PHE	ASP	ILE
PRO	PHE	ALA	ASP	GLY	ILE
PHE	LEU	CYS	LYS	THR	ILE
LEU	ILE	ALA	VAL	ASN	ASP
ASP	ASP	ILE	GLN	PRO	PHE
LYS	LYS	ALA	PHE	PRO	GLN
ARG	ARG	ASP	SER	TYR	PRO
TRP	TRP	ALA	ASN	ARG	HIS
ARG	ARG	PHE	LYS	GLU	VAL
GLN	GLN	ASN	SER	GLU	ILE
T320	V321	LEU	ASN	ASP	VAL
F322	F323	PRO	ASN	ILE	HIS
H323		SER	MET	PRO	CYS
		SER	ASP	ALA	ALA
		HIS	HIS	PRO	ALA
		LEU	TRP	LEU	GLU
		ARG	GLN	ASN	ARG
		PRO	GLN	LEU	PRO
		ILE	ARG	TYR	ARG
		THR	PHE	LYS	ASP
		ASP	PRO	GLY	VAL
		SER	THR	THR	VAL
		PRO	HIS	LYS	GLN
		VAL	VAL	LEU	ASN
		LEU	LYS	ASP	GLN
		GLY	ASP	GLY	PRO
		ALA	VAL	GLU	ASP
		GLN	ALA	LYS	ALA
		ARG	THR	VAL	ALA
		PRO	VAL	VAL	SER
		ARG	CYS	LEU	GLN
		ASN	ARG	GLU	LEU
		ALA	GLN	ASN	ASN
		GLN	LEU	ASN	VAL
		LEU	ALA	GLY	ASP
		ASP	GLU	LEU	ALA
		CYS	LYS	ALA	GLY
		SER	ARG	ALA	SER
		LYS	MET	ALA	ASN
		LEU	THR	VAL	ILE

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	135219	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 ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.141	Depositor
Minimum map value	-0.522	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.0573	Depositor
Map size (Å)	281.2, 281.2, 281.2	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.74, 0.74, 0.74	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	0/2937	0.34	0/3970
1	B	0.12	0/2934	0.34	0/3968
1	C	0.14	0/2945	0.36	0/3981
1	D	0.14	0/3009	0.33	0/4071
2	E	0.12	0/129	0.27	0/171
2	F	0.47	0/37	0.85	0/48
2	G	0.50	0/36	0.91	0/48
All	All	0.14	0/12027	0.35	0/16257

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2881	0	2878	24	0
1	B	2877	0	2872	30	0
1	C	2889	0	2885	37	0
1	D	2950	0	2944	34	0
2	E	125	0	123	1	0
2	F	36	0	27	1	0
2	G	35	0	27	2	0
3	B	2	0	0	0	0
3	C	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	3	0	0	0	0
All	All	11801	0	11756	115	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 5.

All (115) 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:C:223:LYS:HA	1:C:227:ILE:HD12	1.67	0.75
1:B:394:LYS:HE3	1:B:394:LYS:HA	1.71	0.71
1:D:147:GLU:OE2	1:D:147:GLU:N	2.22	0.71
1:C:127:GLU:OE2	1:C:127:GLU:N	2.25	0.70
1:D:134:ASP:OD1	1:D:135:GLN:N	2.27	0.68
1:D:61:LYS:HD3	1:D:259:ALA:HB2	1.74	0.67
1:D:74:ARG:HD2	1:D:117:ILE:HD11	1.76	0.67
1:A:354:ASP:HB3	1:A:359:VAL:HG11	1.77	0.67
1:B:193:GLY:O	1:B:313:ARG:NH1	2.28	0.66
1:C:61:LYS:HG3	1:C:62:THR:HG22	1.78	0.66
1:B:150:MET:HE2	1:B:380:PHE:HB2	1.77	0.65
1:D:192:ARG:HH11	1:D:192:ARG:HA	1.62	0.65
1:D:321:ALA:HB2	1:D:328:LEU:HD11	1.78	0.65
1:C:318:VAL:HG22	1:C:330:ILE:HG12	1.79	0.64
1:C:209:HIS:CD2	1:C:218:MET:HE1	2.33	0.63
1:B:134:ASP:OD1	1:B:135:GLN:N	2.33	0.62
1:C:204:VAL:HG22	1:C:243:HIS:HB2	1.81	0.62
1:A:95:SER:HB3	1:D:95:SER:HB3	1.81	0.62
1:C:354:ASP:HB3	1:C:359:VAL:HG11	1.81	0.62
1:A:47:GLN:O	1:A:47:GLN:NE2	2.33	0.61
1:D:383:ASP:OD1	1:D:384:SER:N	2.35	0.60
1:B:383:ASP:N	1:B:383:ASP:OD1	2.34	0.60
1:B:61:LYS:HG3	1:B:62:THR:H	1.66	0.60
1:C:347:GLU:HA	1:C:350:LYS:HZ2	1.67	0.59
1:D:192:ARG:HA	1:D:192:ARG:NH1	2.17	0.59
1:B:313:ARG:NH2	2:E:321:VAL:O	2.34	0.59
1:B:334:HIS:O	1:B:337:THR:OG1	2.21	0.58
1:B:318:VAL:HG11	1:B:355:LEU:HD23	1.86	0.58
1:C:249:ARG:HH11	1:C:249:ARG:HB2	1.68	0.57
1:D:148:GLU:OE1	1:D:148:GLU:N	2.34	0.57
1:C:161:ASN:ND2	1:C:180:SER:OG	2.38	0.57
1:C:83:VAL:O	1:C:87:VAL:HG12	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:ASP:N	1:B:258:ASP:OD1	2.40	0.55
1:A:215:LEU:HA	1:A:218:MET:HE2	1.88	0.55
1:C:286:ASP:OD1	1:C:288:THR:OG1	2.24	0.55
1:A:343:ARG:HH12	1:A:347:GLU:HB2	1.71	0.54
1:C:179:ASP:OD1	1:C:180:SER:N	2.40	0.54
1:B:287:TYR:O	1:B:293:SER:OG	2.24	0.54
1:D:124:ASP:OD1	1:D:124:ASP:N	2.42	0.53
1:A:59:VAL:HG21	1:B:59:VAL:HG21	1.90	0.53
1:C:59:VAL:HG22	1:C:261:LEU:HD22	1.91	0.52
1:A:322:ILE:HG22	1:B:246:PRO:HG2	1.92	0.51
1:C:191:ASP:HB3	1:C:196:LEU:HD23	1.92	0.51
1:B:61:LYS:HG3	1:B:62:THR:N	2.25	0.51
1:D:90:ILE:O	1:D:168:ARG:NH2	2.44	0.50
1:B:307:LYS:HD2	1:B:390:PRO:HG3	1.94	0.49
1:C:25:VAL:HG12	1:C:181:LYS:HG2	1.93	0.49
1:C:59:VAL:HG21	1:D:59:VAL:HG21	1.93	0.49
1:B:138:MET:HG2	1:B:294:ALA:HB3	1.95	0.48
1:C:128:GLU:O	1:C:356:ARG:NH1	2.46	0.48
1:D:45:HIS:CE1	1:D:71:ILE:HG21	2.48	0.48
1:B:128:GLU:O	1:B:356:ARG:NH1	2.47	0.48
1:D:344:GLU:O	1:D:348:ILE:HG13	2.14	0.48
1:A:192:ARG:H	1:A:192:ARG:CZ	2.27	0.48
1:A:23:GLU:OE1	1:B:135:GLN:NE2	2.44	0.47
1:D:378:GLY:O	1:D:382:ARG:NH1	2.48	0.47
1:C:189:MET:SD	1:C:198:ILE:HD11	2.56	0.46
1:C:366:LEU:O	1:C:371:TYR:OH	2.31	0.46
1:A:201:HIS:ND1	1:A:202:THR:OG1	2.48	0.45
1:A:204:VAL:HG22	1:A:243:HIS:HB2	1.99	0.45
1:C:303:LYS:NZ	1:C:388:GLU:OE1	2.39	0.45
1:A:317:GLN:HE22	1:B:21:THR:H	1.64	0.45
1:B:25:VAL:HG12	1:B:181:LYS:HG3	1.99	0.45
1:A:357:PRO:O	1:A:361:VAL:HG13	2.17	0.44
1:D:290:VAL:O	1:D:294:ALA:HB3	2.17	0.44
1:D:135:GLN:HB3	1:D:321:ALA:HA	1.99	0.44
1:D:138:MET:N	1:D:138:MET:SD	2.91	0.44
1:D:146:THR:OG1	1:D:150:MET:O	2.29	0.44
1:C:276:ALA:HB2	2:G:322[B]:PHE:CE2	2.52	0.44
1:C:330:ILE:HG22	1:C:346:LEU:HD21	2.00	0.44
1:C:181:LYS:HB3	1:D:135:GLN:HE21	1.83	0.43
1:D:32:LYS:HA	1:D:32:LYS:HD3	1.53	0.43
1:A:311:CYS:SG	1:A:314:VAL:HB	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:GLU:OE2	1:C:224:GLU:HA	2.19	0.43
1:C:357:PRO:O	1:C:361:VAL:HG12	2.18	0.43
1:D:175:TRP:CZ3	1:D:218:MET:HG2	2.53	0.43
1:C:141:TYR:HB3	1:C:271:TYR:CE1	2.54	0.43
1:A:287:TYR:HD1	1:A:361:VAL:HG11	1.84	0.43
1:A:252:ILE:HD12	1:A:252:ILE:HA	1.87	0.42
1:D:366:LEU:O	1:D:371:TYR:OH	2.33	0.42
1:A:261:LEU:HD12	1:A:264:ARG:HH11	1.84	0.42
1:B:131:GLY:HA2	1:B:325:SER:HA	2.01	0.42
1:C:51:ASP:OD1	1:C:51:ASP:N	2.52	0.42
1:D:332:ILE:HG12	1:D:346:LEU:HD13	2.02	0.42
1:A:109:ALA:HB2	1:C:107:LEU:HD23	2.02	0.42
1:B:392:LYS:HD3	1:B:393:LEU:N	2.34	0.42
1:D:61:LYS:HD2	1:D:62:THR:H	1.84	0.42
1:D:287:TYR:CE2	1:D:367:LYS:HG2	2.55	0.42
1:B:164:LEU:HG	1:B:226:VAL:HG11	2.01	0.42
1:C:223:LYS:HG2	1:C:228:LYS:HZ2	1.84	0.42
1:D:154:ILE:HG13	1:D:158:HIS:CD2	2.55	0.42
1:B:137:LEU:O	1:B:278:GLY:HA3	2.20	0.42
1:C:347:GLU:HA	1:C:350:LYS:NZ	2.35	0.42
1:C:382:ARG:O	1:C:388:GLU:HG3	2.20	0.42
1:A:317:GLN:NE2	1:B:20:PHE:HA	2.34	0.42
1:B:64:MET:HE2	1:B:64:MET:HB3	1.83	0.42
1:C:65:ILE:HG21	1:C:83:VAL:HG11	2.02	0.42
1:D:335:TYR:HE1	2:G:323[B]:HIS:N	2.18	0.42
1:A:111:GLU:OE2	1:A:112:GLN:N	2.53	0.41
1:D:139:PHE:CZ	1:D:317:GLN:HG3	2.55	0.41
1:A:111:GLU:HG3	1:A:113:GLN:H	1.85	0.41
1:B:266:ILE:HD12	1:B:277:HIS:CE1	2.54	0.41
1:C:249:ARG:HB2	1:C:249:ARG:NH1	2.34	0.41
1:D:112:GLN:NE2	1:D:113:GLN:O	2.54	0.41
1:D:138:MET:HG2	1:D:294:ALA:HB3	2.02	0.41
1:A:192:ARG:H	1:A:192:ARG:NH1	2.17	0.41
1:C:37:ILE:O	1:C:41:VAL:HG23	2.21	0.41
1:D:93:ASP:OD1	1:D:93:ASP:N	2.51	0.41
1:A:317:GLN:HE22	1:B:20:PHE:HA	1.86	0.41
1:A:150:MET:HE3	1:A:150:MET:HB3	1.77	0.41
1:C:138:MET:HE2	1:C:290:VAL:C	2.46	0.41
1:D:276:ALA:HB2	2:F:322[A]:PHE:CE2	2.56	0.41
1:B:138:MET:SD	1:B:138:MET:N	2.94	0.40
1:C:261:LEU:HD12	1:C:264:ARG:HH11	1.86	0.40

*Continued on next page...*

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:ILE:O	1:B:112:GLN:HA	2.20	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	367/395 (93%)	362 (99%)	5 (1%)	0	100	100
1	B	367/395 (93%)	360 (98%)	7 (2%)	0	100	100
1	C	368/395 (93%)	360 (98%)	8 (2%)	0	100	100
1	D	378/395 (96%)	372 (98%)	6 (2%)	0	100	100
2	E	11/334 (3%)	11 (100%)	0	0	100	100
2	F	2/334 (1%)	2 (100%)	0	0	100	100
2	G	2/334 (1%)	2 (100%)	0	0	100	100
All	All	1495/2582 (58%)	1469 (98%)	26 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	306/327 (94%)	305 (100%)	1 (0%)	86	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	306/327 (94%)	302 (99%)	4 (1%)	61	82
1	C	307/327 (94%)	305 (99%)	2 (1%)	76	89
1	D	314/327 (96%)	314 (100%)	0	100	100
2	E	13/285 (5%)	12 (92%)	1 (8%)	12	27
2	F	4/285 (1%)	4 (100%)	0	100	100
2	G	4/285 (1%)	4 (100%)	0	100	100
All	All	1254/2163 (58%)	1246 (99%)	8 (1%)	76	91

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	334	HIS
1	B	126	ASN
1	B	143	THR
1	B	355	LEU
1	B	383	ASP
1	C	249	ARG
1	C	334	HIS
2	E	319	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	135	GLN
1	A	183	GLN
1	A	317	GLN
1	B	183	GLN
1	B	256	GLN
1	B	372	GLN
1	C	36	GLN
1	C	161	ASN
1	C	190	GLN
1	D	183	GLN
1	D	187	GLN



### 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 [i](#)

There are no chain breaks in this entry.

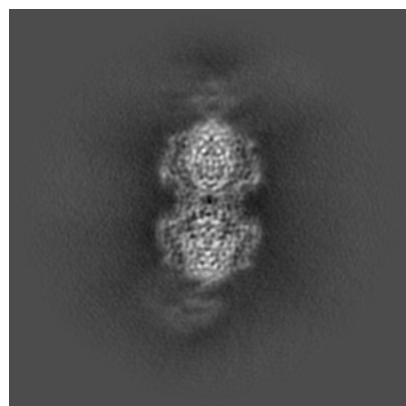
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53276. These allow visual inspection of the internal detail of the map and identification of artifacts.

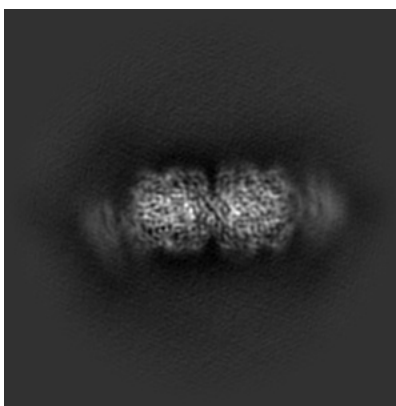
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

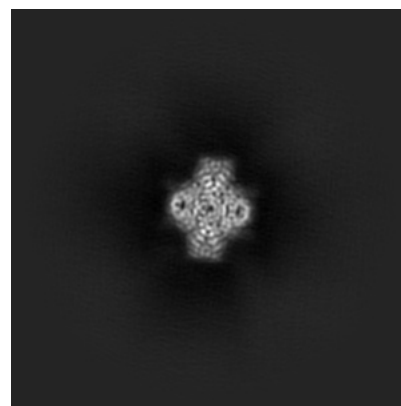
#### 6.1.1 Primary map



X

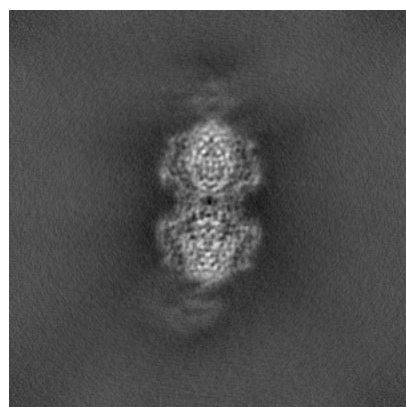


Y

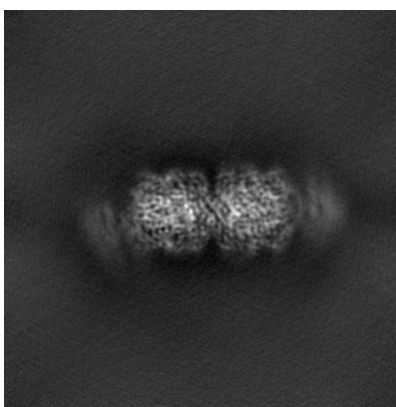


Z

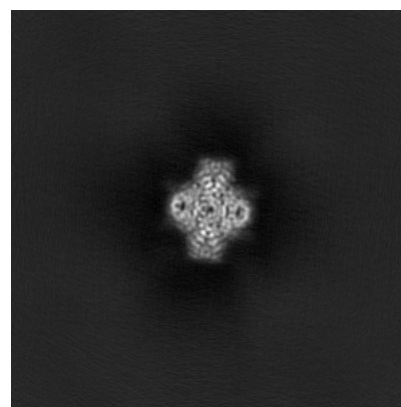
#### 6.1.2 Raw map



X



Y

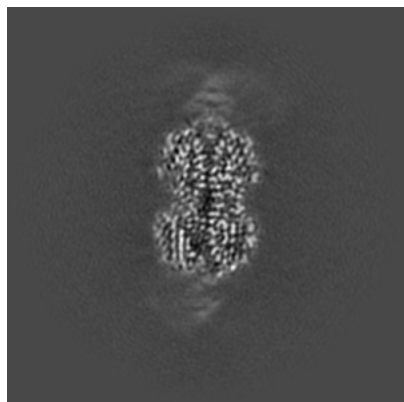


Z

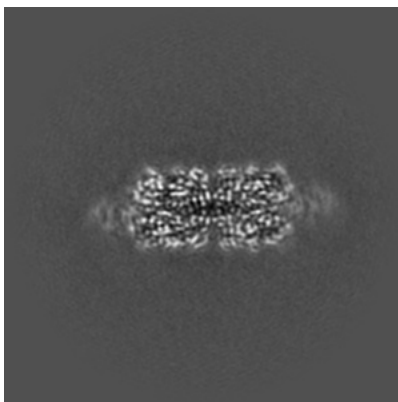
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

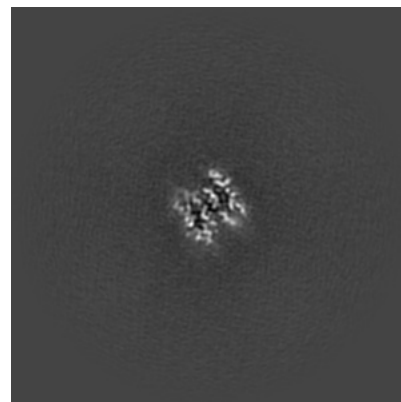
### 6.2.1 Primary map



X Index: 190

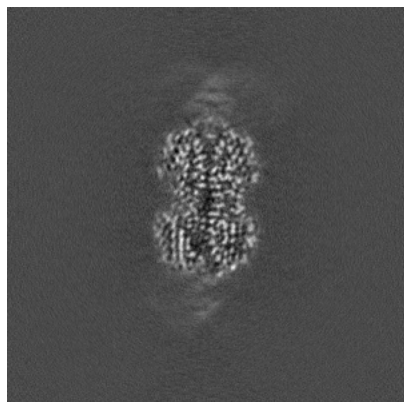


Y Index: 190

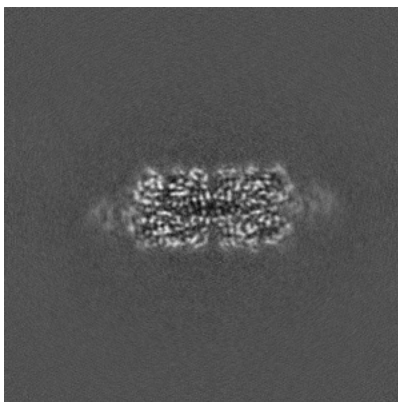


Z Index: 190

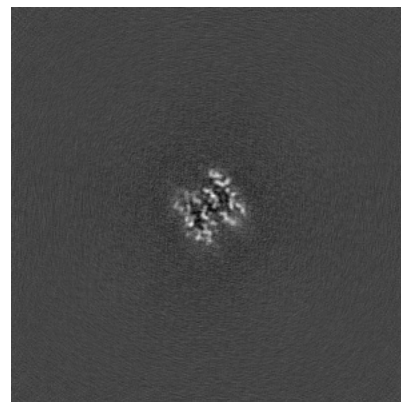
### 6.2.2 Raw map



X Index: 190



Y Index: 190

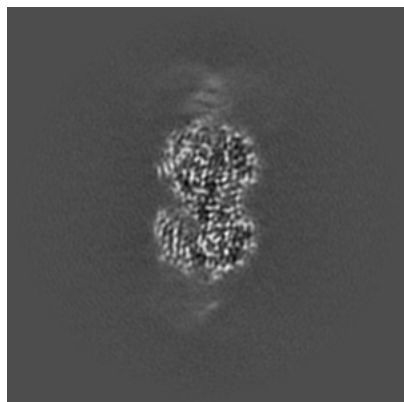


Z Index: 190

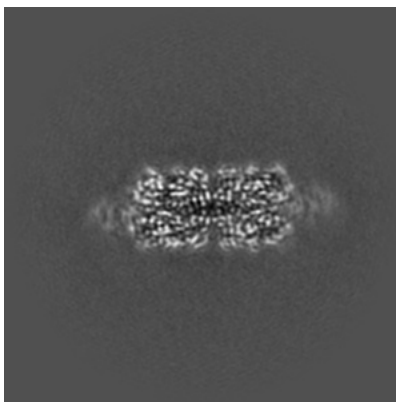
The images above show central slices of the map in three orthogonal directions.

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

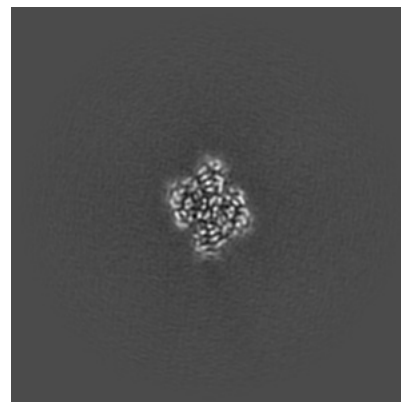
### 6.3.1 Primary map



X Index: 193

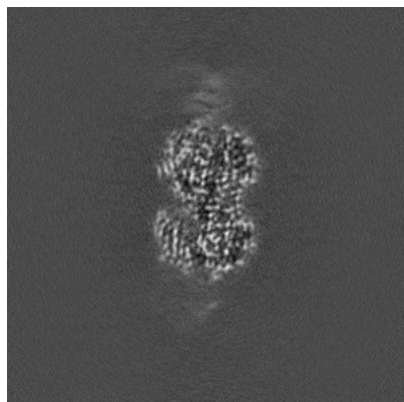


Y Index: 190

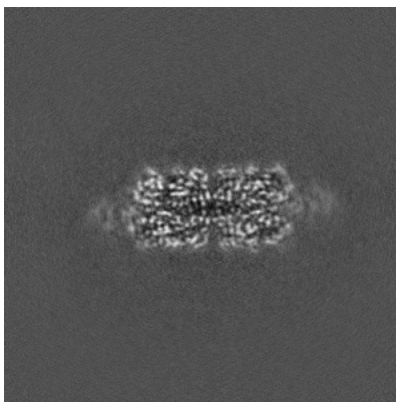


Z Index: 156

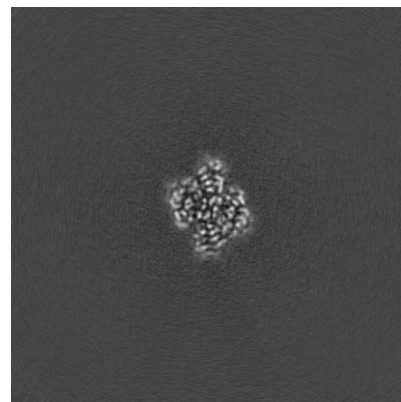
### 6.3.2 Raw map



X Index: 193



Y Index: 190

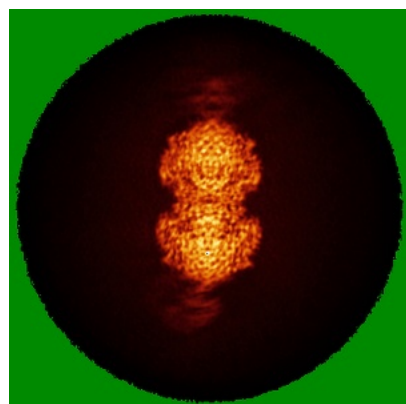


Z Index: 156

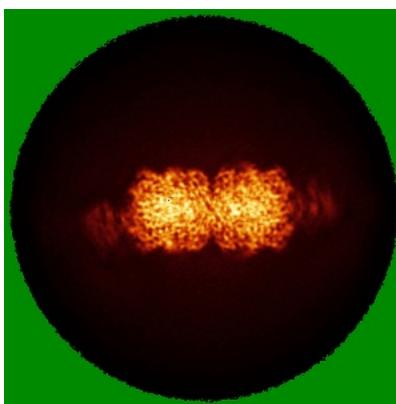
The images above show the largest variance slices of the map in three orthogonal directions.

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

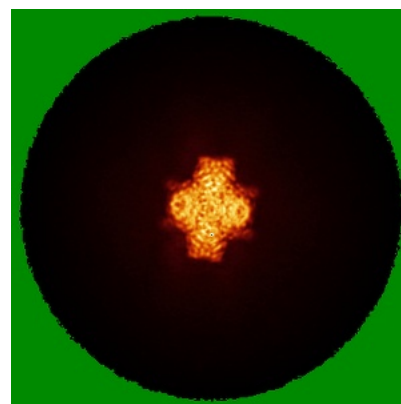
### 6.4.1 Primary map



X

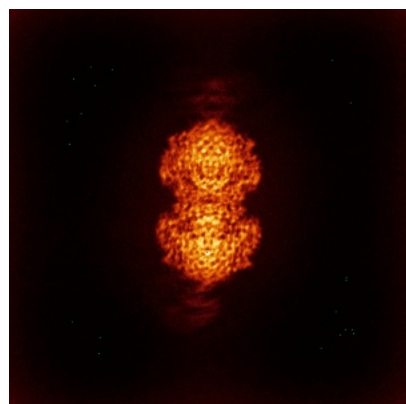


Y

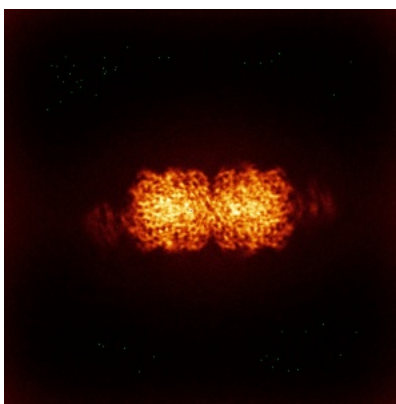


Z

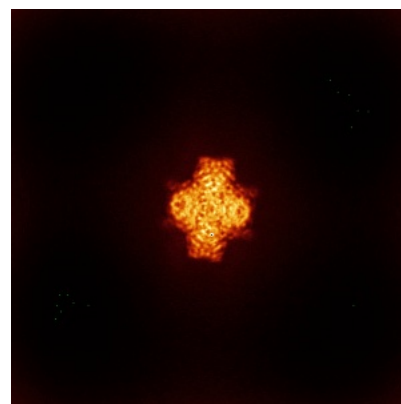
### 6.4.2 Raw map



X



Y

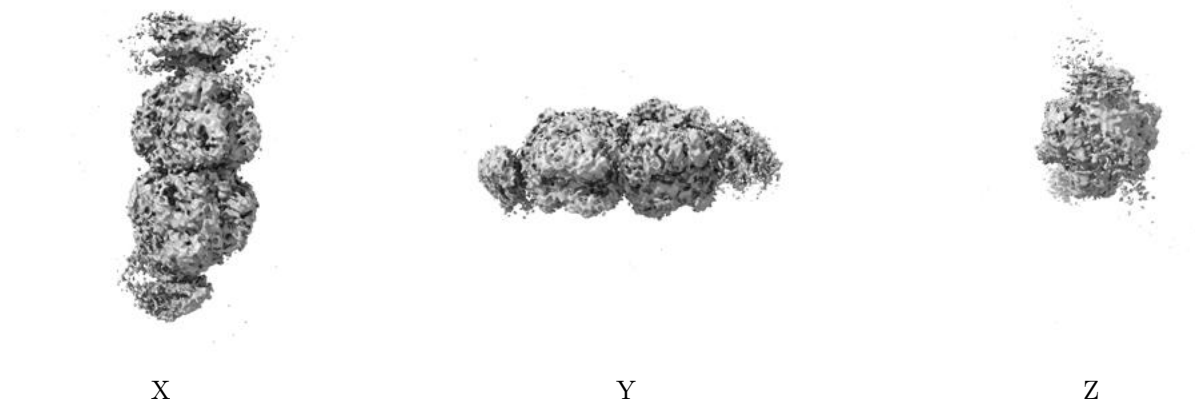


Z

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.

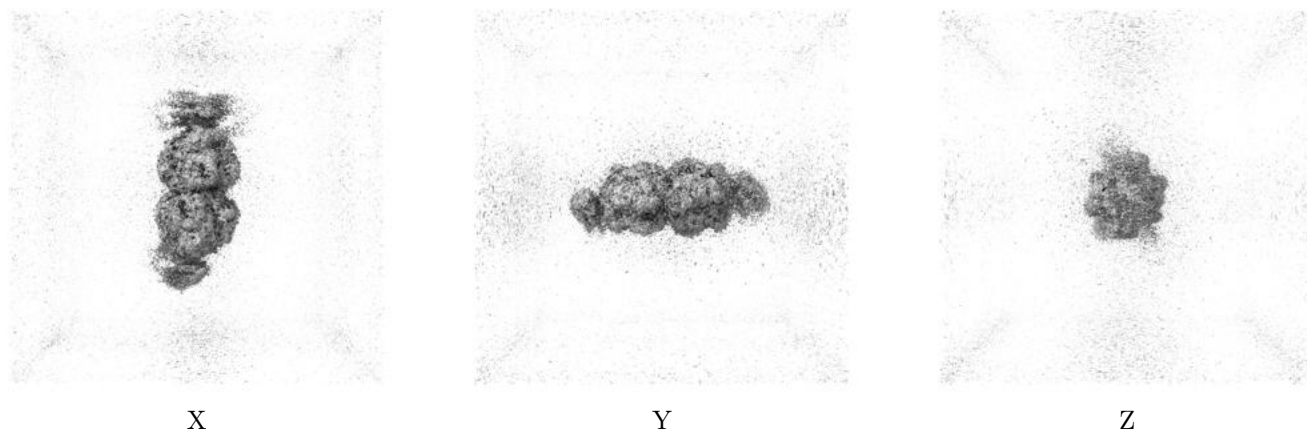
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0573. 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.



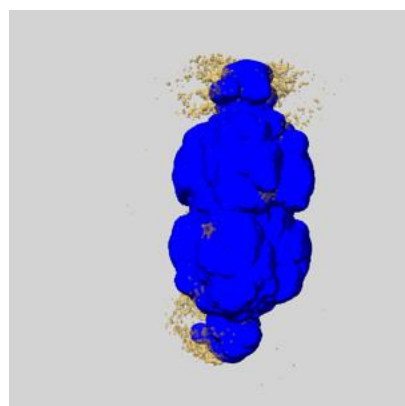
## 6.6 Mask visualisation [i](#)

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

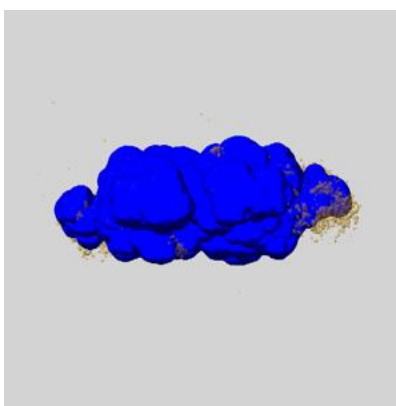
A mask typically either:

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

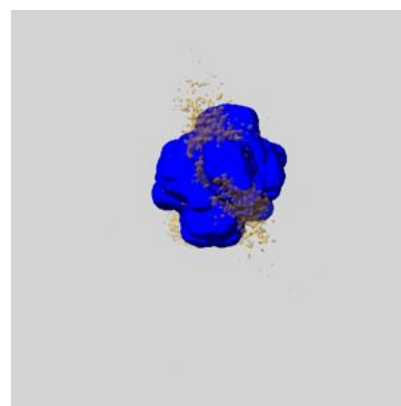
### 6.6.1 emd\_53276\_msk\_1.map [i](#)



X



Y

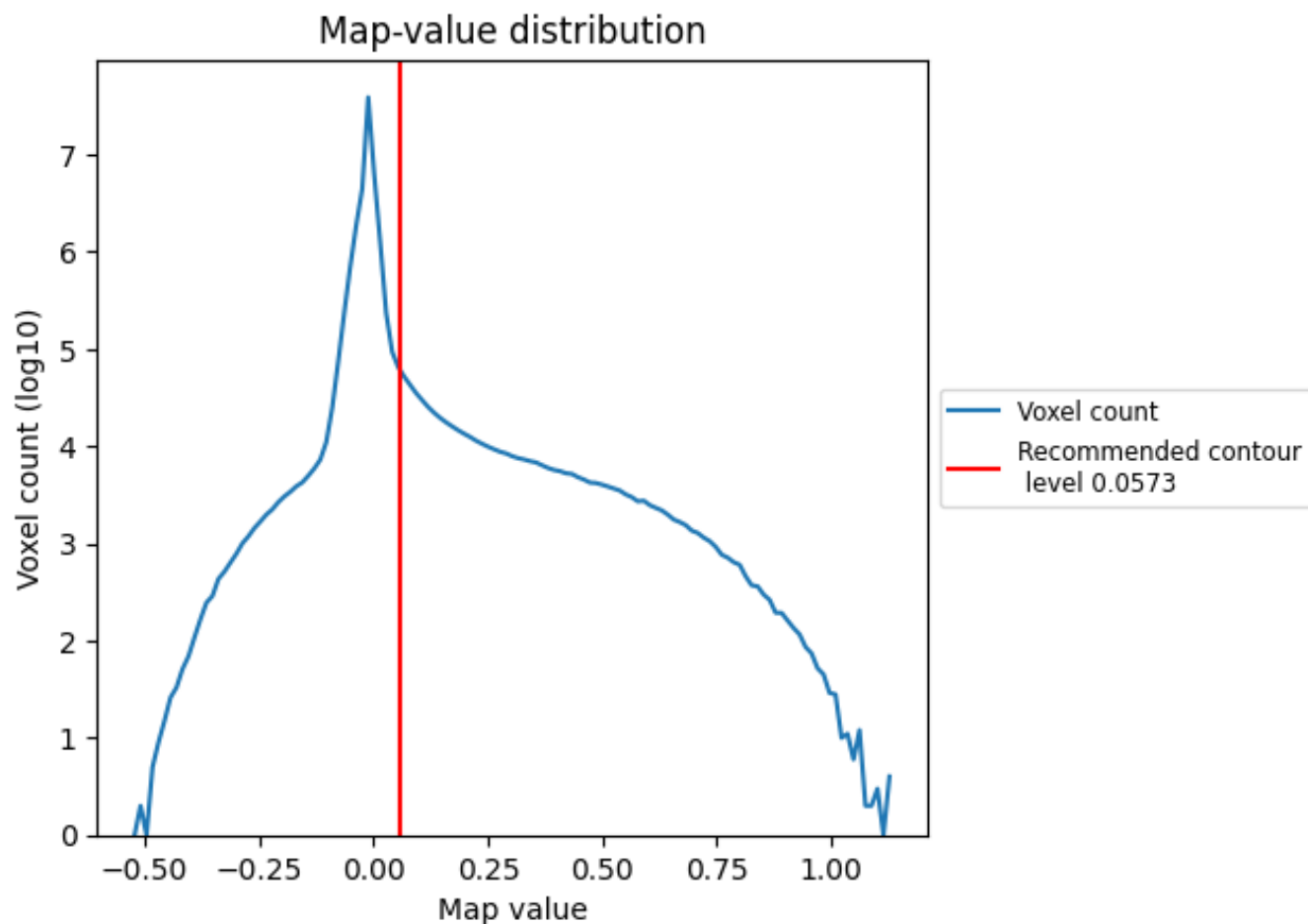


Z

## 7 Map analysis [i](#)

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

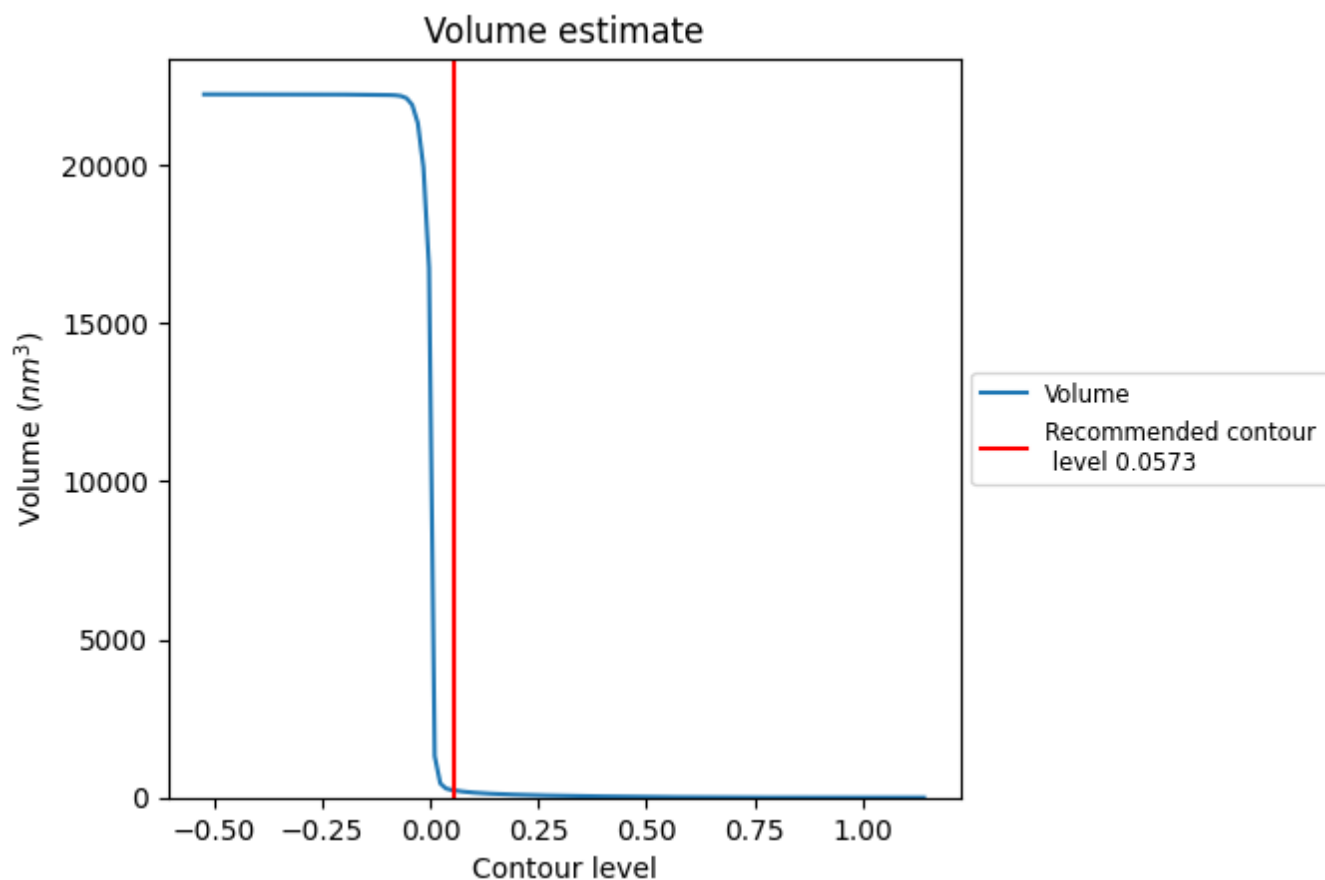
### 7.1 Map-value distribution [i](#)



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.



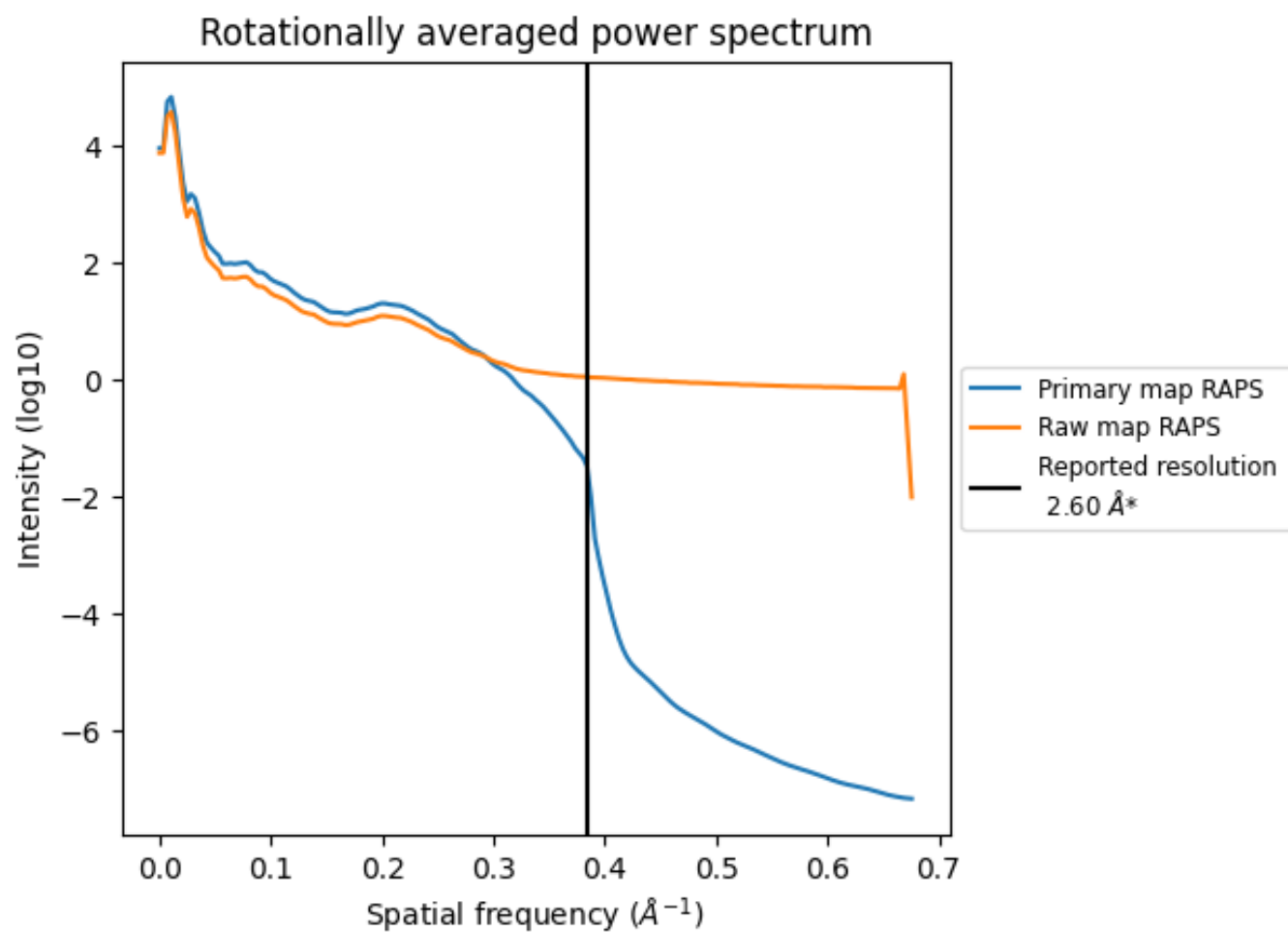
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 223 nm<sup>3</sup>; this corresponds to an approximate mass of 202 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 [i](#)

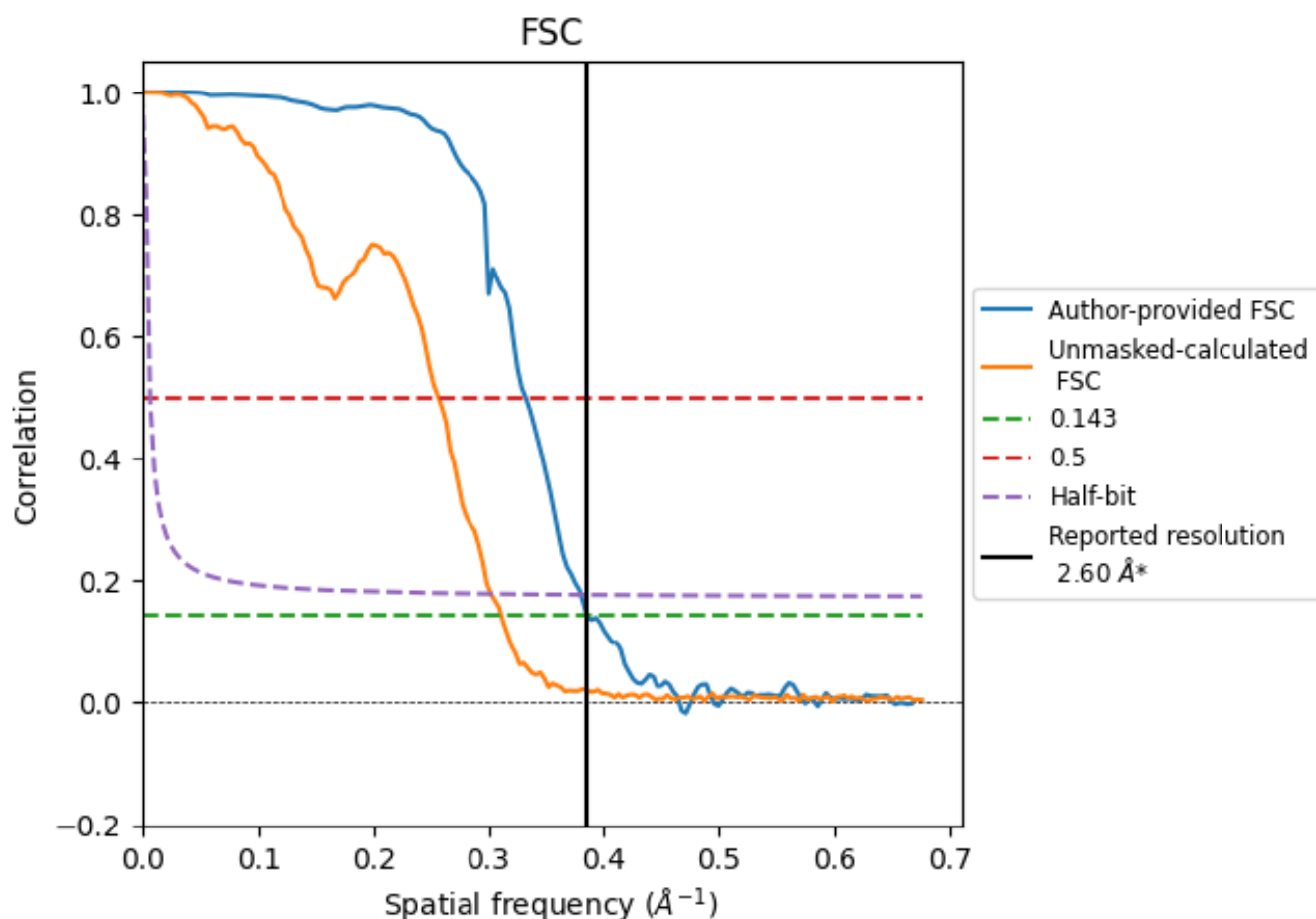


\*Reported resolution corresponds to spatial frequency of 0.385 Å<sup>-1</sup>

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

## 8.2 Resolution estimates [i](#)

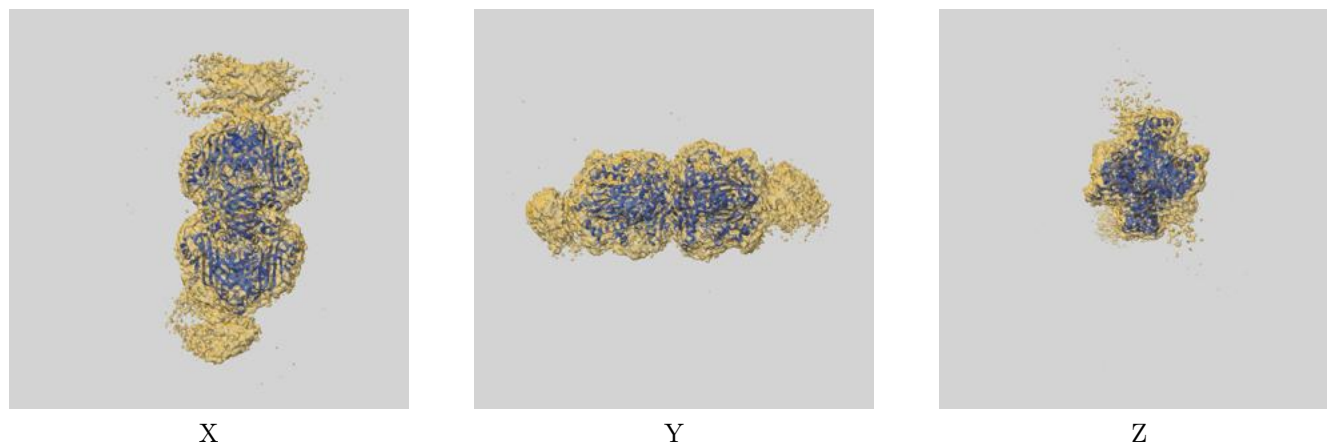
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.60	3.01	2.63
Unmasked-calculated*	3.21	3.90	3.31

\*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 3.21 differs from the reported value 2.6 by more than 10 %

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

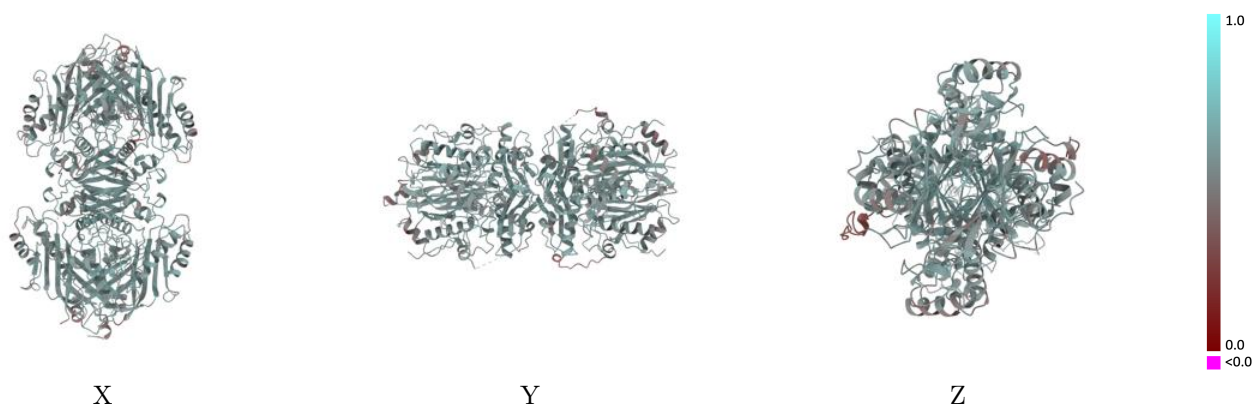
This section contains information regarding the fit between EMDB map EMD-53276 and PDB model 9QPO. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

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



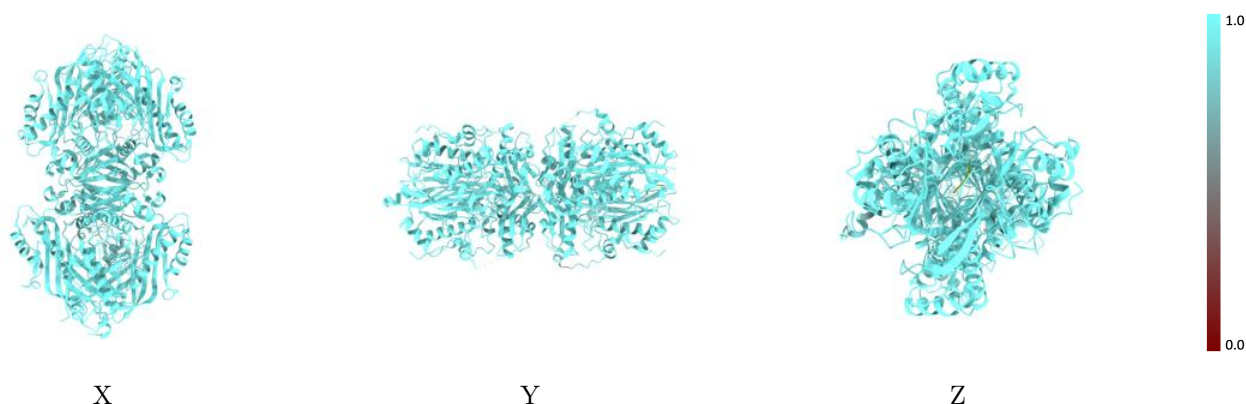
The images above show the 3D surface view of the map at the recommended contour level 0.0573 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



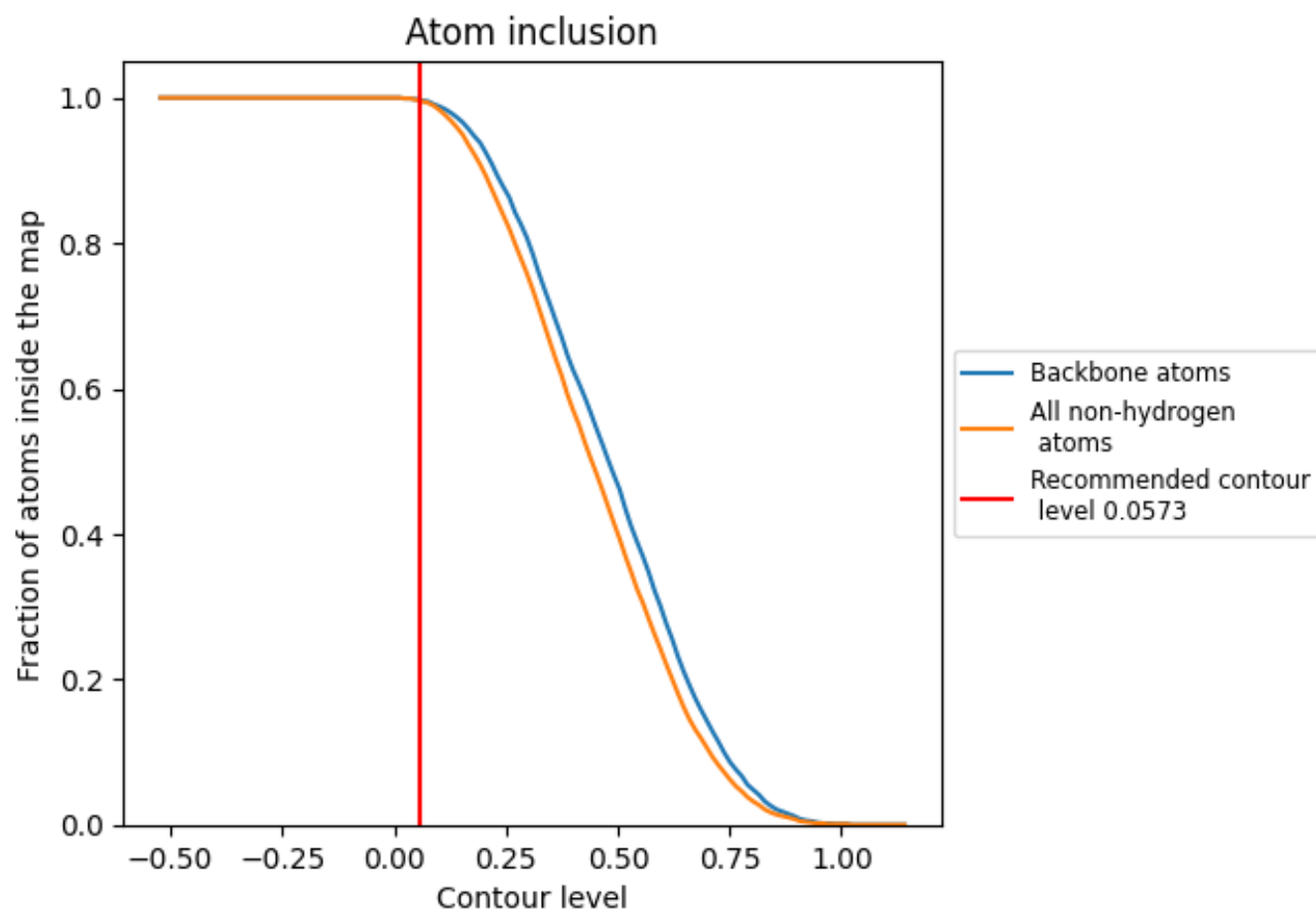
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0573).

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 100% of all backbone atoms, 100% 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 (0.0573) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9960	<div><div></div></div> 0.5510
A	<div><div></div></div> 0.9990	<div><div></div></div> 0.5610
B	<div><div></div></div> 0.9990	<div><div></div></div> 0.5550
C	<div><div></div></div> 0.9970	<div><div></div></div> 0.5410
D	<div><div></div></div> 0.9930	<div><div></div></div> 0.5490
E	<div><div></div></div> 0.9670	<div><div></div></div> 0.4900
F	<div><div></div></div> 0.9440	<div><div></div></div> 0.5730

1.0

0.0

<0.0