



## Full wwPDB EM Validation Report ⓘ

Apr 15, 2026 – 03:00 AM UTC

PDB ID : 9OFA / pdb\_00009ofa  
EMDB ID : EMD-70421  
Title : The structure of a Fungal Cyanide Hydratase from *Gloeocercospora sorghi*  
Authors : Justo Arevalo, S.; Valle-Riestra F, V.; Balan, A.; Farah, C.S.  
Deposited on : 2025-04-29  
Resolution : 2.04 Å (reported)  
Based on initial model : .

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

We welcome your comments at [validation@mail.wwpdb.org](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:

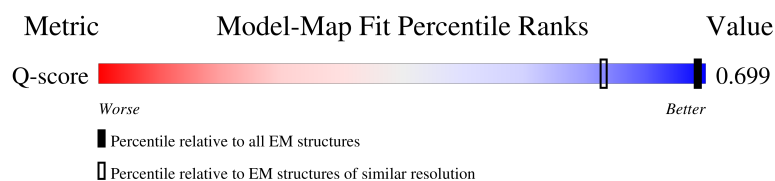
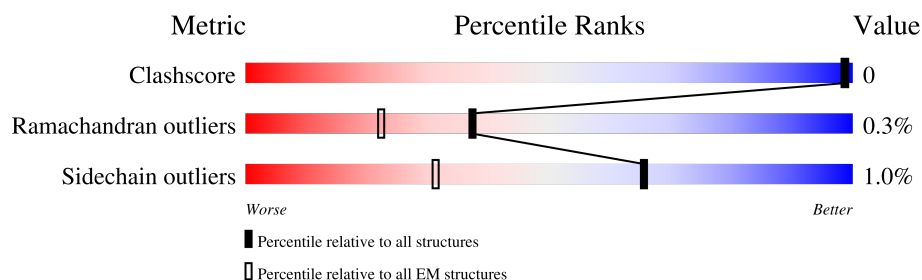
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : 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 2.04 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.



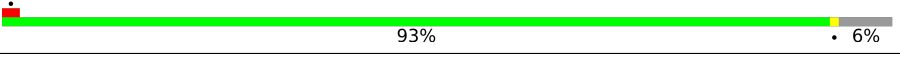
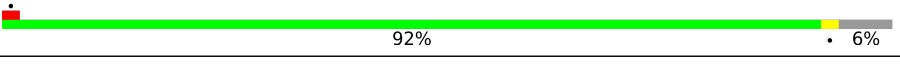
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1810 ( 1.55 - 2.54 )

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	368	<div> <div>19%</div> <div>93%</div> <div>...</div> </div>
1	B	368	<div> <div>8%</div> <div>91%</div> <div>6%</div> </div>
1	C	368	<div> <div>93%</div> <div>...</div> </div>
1	D	368	<div> <div>90%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
1	E	368	
1	F	368	
1	G	368	
1	H	368	
1	I	368	
1	J	368	
1	K	368	
1	L	368	
1	M	368	
1	N	368	
1	O	368	
1	P	368	
1	Q	368	
1	R	368	
1	S	368	
1	T	368	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 55218 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 Cyanide hydratase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	O	346	Total	C	N	O	S	0	0
			2720	1734	467	509	10		
1	N	355	Total	C	N	O	S	0	0
			2793	1776	480	527	10		
1	Q	346	Total	C	N	O	S	0	0
			2720	1734	467	509	10		
1	P	356	Total	C	N	O	S	0	0
			2797	1778	481	528	10		
1	S	346	Total	C	N	O	S	0	0
			2720	1734	467	509	10		
1	R	356	Total	C	N	O	S	0	0
			2797	1778	481	528	10		
1	T	353	Total	C	N	O	S	0	0
			2780	1769	478	523	10		
1	M	347	Total	C	N	O	S	0	0
			2729	1739	468	512	10		
1	L	354	Total	C	N	O	S	0	0
			2788	1773	479	526	10		
1	E	356	Total	C	N	O	S	0	0
			2797	1778	481	528	10		
1	D	345	Total	C	N	O	S	0	0
			2711	1729	466	506	10		
1	G	355	Total	C	N	O	S	0	0
			2793	1776	480	527	10		
1	F	346	Total	C	N	O	S	0	0
			2720	1734	467	509	10		
1	I	356	Total	C	N	O	S	0	0
			2797	1778	481	528	10		
1	H	346	Total	C	N	O	S	0	0
			2720	1734	467	509	10		
1	K	353	Total	C	N	O	S	0	0
			2780	1769	478	523	10		
1	J	350	Total	C	N	O	S	0	0
			2760	1758	474	518	10		

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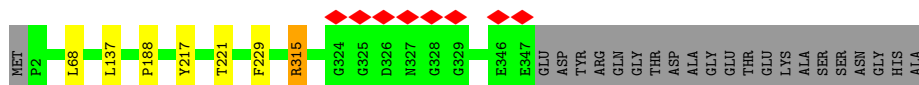
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	356	Total	C	N	O	S	0	0
			2797	1778	481	528	10		
1	C	354	Total	C	N	O	S	0	0
			2788	1773	479	526	10		
1	B	345	Total	C	N	O	S	0	0
			2711	1729	466	506	10		

### 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.

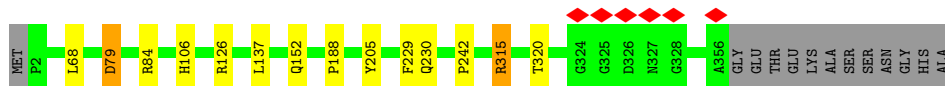
- Molecule 1: Cyanide hydratase

Chain O:  92% 6%

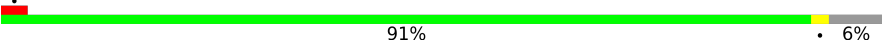


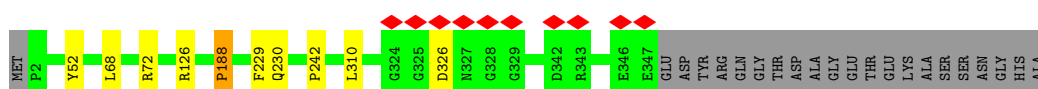
- Molecule 1: Cyanide hydratase

Chain N:  93% 6%



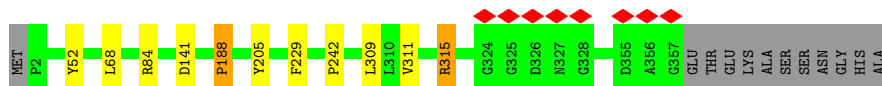
- Molecule 1: Cyanide hydratase

Chain Q:  91% 6%




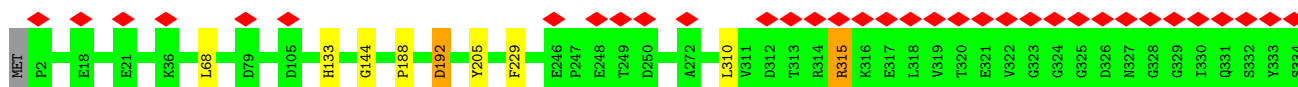
- Molecule 1: Cyanide hydratase

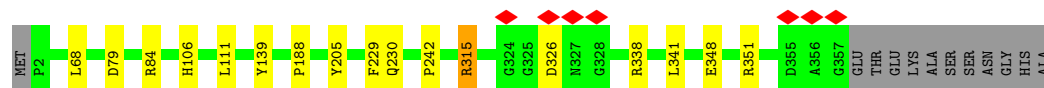
Chain P:  94% 6%




- Molecule 1: Cyanide hydratase

Chain S:  13% 91% 6%

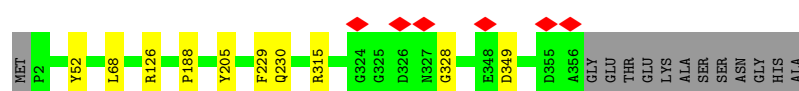




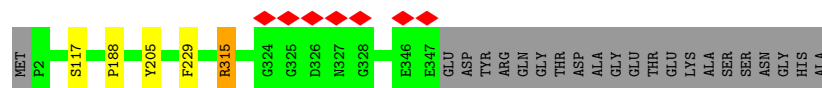
## ● Molecule 1: Cyanide hydratase

Chain D:  90% 6%

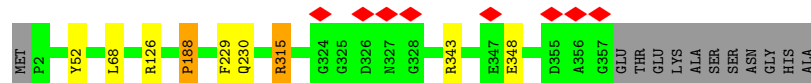
## ● Molecule 1: Cyanide hydratase

Chain G:  94% 6%

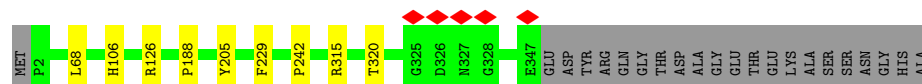
## ● Molecule 1: Cyanide hydratase

Chain F:  93% 6%

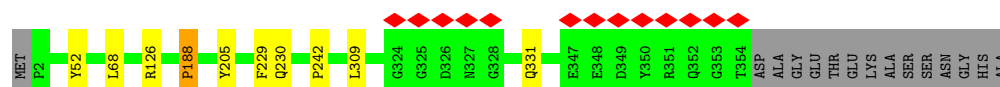
## ● Molecule 1: Cyanide hydratase

Chain I:  94% 6%

## ● Molecule 1: Cyanide hydratase

Chain H:  92% 6%

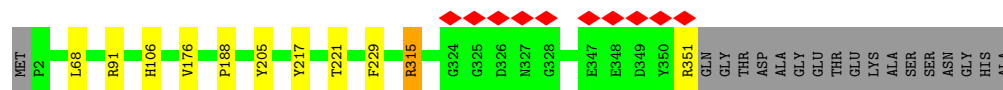
## ● Molecule 1: Cyanide hydratase

Chain K:  93% 6%

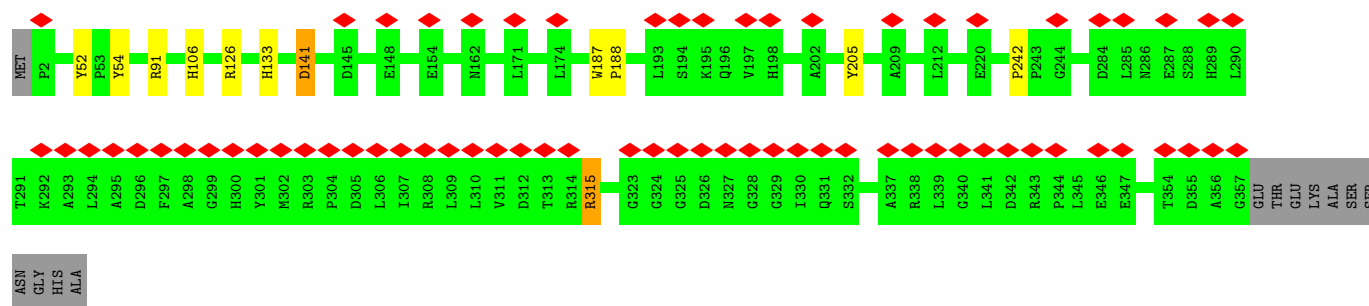
## ● Molecule 1: Cyanide hydratase

Chain J:  92% 5%

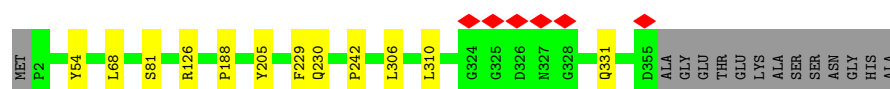




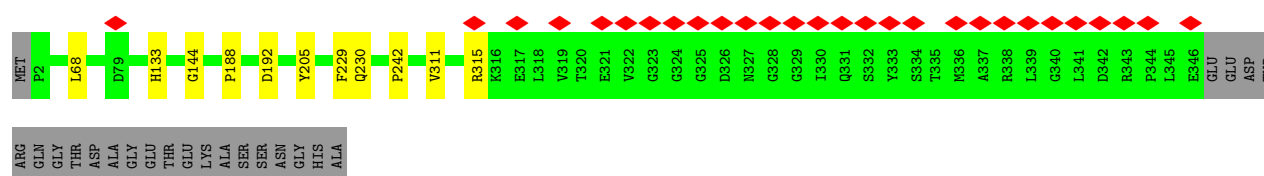
- Molecule 1: Cyanide hydratase



- Molecule 1: Cyanide hydratase



- Molecule 1: Cyanide hydratase



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	209895	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 ( $e^-/\text{\AA}^2$ )	55.59	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	165000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	3.968	Depositor
Minimum map value	-1.714	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.128	Depositor
Recommended contour level	0.5	Depositor
Map size ( $\text{\AA}$ )	393.66, 393.66, 393.66	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.8748, 0.8748, 0.8748	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	0.79	0/2869	1.33	7/3908 (0.2%)
1	B	0.77	0/2782	1.31	3/3791 (0.1%)
1	C	0.77	0/2860	1.31	3/3896 (0.1%)
1	D	0.77	0/2782	1.31	3/3791 (0.1%)
1	E	0.79	0/2869	1.32	8/3908 (0.2%)
1	F	0.78	0/2791	1.32	3/3803 (0.1%)
1	G	0.78	0/2865	1.33	5/3903 (0.1%)
1	H	0.78	0/2791	1.32	2/3803 (0.1%)
1	I	0.78	0/2869	1.32	4/3908 (0.1%)
1	J	0.78	0/2832	1.33	2/3858 (0.1%)
1	K	0.78	0/2852	1.31	4/3885 (0.1%)
1	L	0.78	0/2860	1.31	2/3896 (0.1%)
1	M	0.78	0/2800	1.31	3/3815 (0.1%)
1	N	0.79	0/2865	1.33	7/3903 (0.2%)
1	O	0.77	0/2791	1.31	1/3803 (0.0%)
1	P	0.78	1/2869 (0.0%)	1.31	4/3908 (0.1%)
1	Q	0.77	0/2791	1.31	4/3803 (0.1%)
1	R	0.76	0/2869	1.31	5/3908 (0.1%)
1	S	0.78	0/2791	1.32	4/3803 (0.1%)
1	T	0.80	0/2852	1.32	4/3885 (0.1%)
All	All	0.78	1/56650 (0.0%)	1.32	78/77178 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	2
1	C	0	3
1	D	0	4
1	E	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	2
1	G	0	3
1	H	0	3
1	I	0	1
1	J	0	3
1	K	0	2
1	L	0	2
1	M	0	2
1	N	0	3
1	O	0	1
1	P	0	2
1	Q	0	1
1	R	0	5
1	S	0	2
1	T	0	2
All	All	0	48

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	242	PRO	CA-C	5.17	1.54	1.51

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	349	ASP	N-CA-C	6.73	120.82	112.47
1	N	79	ASP	CA-CB-CG	6.57	119.17	112.60
1	T	326	ASP	CA-CB-CG	6.50	119.10	112.60
1	R	343	ARG	NE-CZ-NH2	6.43	124.99	119.20
1	I	343	ARG	NE-CZ-NH2	6.41	124.96	119.20
1	G	349	ASP	CA-CB-CG	6.38	118.98	112.60
1	R	326	ASP	CA-CB-CG	6.36	118.96	112.60
1	D	315	ARG	NE-CZ-NH2	6.26	124.84	119.20
1	K	309	LEU	CB-CA-C	6.12	120.40	109.38
1	O	315	ARG	NE-CZ-NH2	6.08	124.67	119.20
1	A	141	ASP	CA-CB-CG	6.03	118.63	112.60
1	K	242	PRO	N-CA-CB	6.00	106.55	103.19
1	S	315	ARG	NE-CZ-NH2	5.90	124.51	119.20
1	S	343	ARG	NE-CZ-NH2	5.90	124.51	119.20
1	E	315	ARG	NE-CZ-NH2	5.87	124.49	119.20
1	R	315	ARG	NE-CZ-NH2	5.80	124.42	119.20
1	S	192	ASP	CA-CB-CG	5.79	118.39	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	242	PRO	N-CA-CB	5.75	106.41	103.19
1	C	331	GLN	OE1-CD-NE2	-5.69	116.91	122.60
1	Q	242	PRO	N-CA-CB	5.66	106.36	103.19
1	I	315	ARG	NE-CZ-NH2	5.64	124.28	119.20
1	N	242	PRO	N-CA-CB	5.62	106.34	103.19
1	N	84	ARG	NE-CZ-NH2	5.59	124.23	119.20
1	R	72	ARG	NE-CZ-NH2	5.58	124.22	119.20
1	P	315	ARG	NE-CZ-NH2	5.56	124.20	119.20
1	L	152	GLN	OE1-CD-NE2	-5.56	117.04	122.60
1	L	315	ARG	NE-CZ-NH2	5.55	124.19	119.20
1	J	315	ARG	NE-CZ-NH2	5.54	124.18	119.20
1	C	242	PRO	N-CA-CB	5.49	106.26	103.19
1	A	242	PRO	N-CA-CB	5.49	106.26	103.19
1	E	242	PRO	N-CA-CB	5.45	106.24	103.19
1	A	126	ARG	NE-CZ-NH2	5.43	124.09	119.20
1	E	79	ASP	CA-CB-CG	5.41	118.01	112.60
1	F	315	ARG	NE-CZ-NH2	5.38	124.04	119.20
1	N	315	ARG	NE-CZ-NH2	5.37	124.03	119.20
1	B	242	PRO	N-CA-CB	5.36	106.19	103.19
1	G	315	ARG	NE-CZ-NH2	5.35	124.01	119.20
1	N	106	HIS	CB-CG-CD2	-5.34	124.26	131.20
1	E	84	ARG	NE-CZ-NH2	5.32	123.99	119.20
1	C	230	GLN	OE1-CD-NE2	-5.32	117.28	122.60
1	J	106	HIS	CB-CG-CD2	-5.28	124.33	131.20
1	B	230	GLN	OE1-CD-NE2	-5.28	117.32	122.60
1	I	230	GLN	OE1-CD-NE2	-5.27	117.33	122.60
1	D	343	ARG	NE-CZ-NH2	5.25	123.92	119.20
1	G	328	GLY	N-CA-C	5.25	117.67	110.69
1	N	152	GLN	OE1-CD-NE2	-5.24	117.36	122.60
1	M	141	ASP	CA-CB-CG	5.24	117.84	112.60
1	M	230	GLN	OE1-CD-NE2	-5.23	117.37	122.60
1	A	187	TRP	CA-C-N	5.22	126.37	119.84
1	A	187	TRP	C-N-CA	5.22	126.37	119.84
1	D	230	GLN	OE1-CD-NE2	-5.22	117.38	122.60
1	G	230	GLN	OE1-CD-NE2	-5.21	117.39	122.60
1	N	230	GLN	OE1-CD-NE2	-5.19	117.41	122.60
1	E	326	ASP	CA-CB-CG	5.17	117.77	112.60
1	K	331	GLN	OE1-CD-NE2	-5.17	117.43	122.60
1	K	230	GLN	OE1-CD-NE2	-5.16	117.44	122.60
1	E	351	ARG	NE-CZ-NH2	5.16	123.84	119.20
1	Q	230	GLN	OE1-CD-NE2	-5.14	117.46	122.60
1	I	126	ARG	NE-CZ-NH2	5.14	123.83	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	326	ASP	CA-CB-CG	5.10	117.70	112.60
1	M	106	HIS	CB-CG-CD2	-5.10	124.57	131.20
1	T	106	HIS	CB-CG-CD2	-5.10	124.57	131.20
1	P	84	ARG	NE-CZ-NH2	5.08	123.78	119.20
1	A	91	ARG	NE-CZ-NH2	5.07	123.77	119.20
1	R	230	GLN	OE1-CD-NE2	-5.07	117.53	122.60
1	E	338	ARG	NE-CZ-NH2	5.06	123.76	119.20
1	E	230	GLN	OE1-CD-NE2	-5.06	117.54	122.60
1	A	315	ARG	NE-CZ-NH2	5.06	123.75	119.20
1	P	242	PRO	N-CA-CB	5.06	106.02	103.19
1	T	315	ARG	NE-CZ-NH2	5.05	123.74	119.20
1	Q	72	ARG	NE-CZ-NH2	5.04	123.74	119.20
1	B	192	ASP	CA-CB-CG	5.04	117.64	112.60
1	P	141	ASP	CA-CB-CG	5.02	117.62	112.60
1	S	342	ASP	CA-CB-CG	5.02	117.62	112.60
1	H	106	HIS	CB-CG-CD2	-5.02	124.67	131.20
1	F	117	SER	CA-C-N	5.01	124.73	119.82
1	F	117	SER	C-N-CA	5.01	124.73	119.82
1	T	126	ARG	NE-CZ-NH2	5.00	123.70	119.20

There are no chirality outliers.

All (48) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	205	TYR	Sidechain
1	A	315	ARG	Sidechain
1	A	54	TYR	Sidechain
1	B	205	TYR	Sidechain
1	B	315	ARG	Sidechain
1	C	126	ARG	Sidechain
1	C	205	TYR	Sidechain
1	C	54	TYR	Sidechain
1	D	126	ARG	Sidechain
1	D	205	TYR	Sidechain
1	D	315	ARG	Sidechain
1	D	52	TYR	Sidechain
1	E	205	TYR	Sidechain
1	E	315	ARG	Sidechain
1	F	205	TYR	Sidechain
1	F	315	ARG	Sidechain
1	G	126	ARG	Sidechain
1	G	205	TYR	Sidechain

*Continued on next page...*

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Mol	Chain	Res	Type	Group
1	G	52	TYR	Sidechain
1	H	126	ARG	Sidechain
1	H	205	TYR	Sidechain
1	H	315	ARG	Sidechain
1	I	315	ARG	Sidechain
1	J	205	TYR	Sidechain
1	J	315	ARG	Sidechain
1	J	91	ARG	Sidechain
1	K	126	ARG	Sidechain
1	K	205	TYR	Sidechain
1	L	205	TYR	Sidechain
1	L	315	ARG	Sidechain
1	M	126	ARG	Sidechain
1	M	205	TYR	Sidechain
1	N	126	ARG	Sidechain
1	N	205	TYR	Sidechain
1	N	315	ARG	Sidechain
1	O	315	ARG	Sidechain
1	P	205	TYR	Sidechain
1	P	315	ARG	Sidechain
1	Q	126	ARG	Sidechain
1	R	126	ARG	Sidechain
1	R	205	TYR	Sidechain
1	R	301	TYR	Sidechain
1	R	315	ARG	Sidechain
1	R	71	TYR	Sidechain
1	S	205	TYR	Sidechain
1	S	315	ARG	Sidechain
1	T	205	TYR	Sidechain
1	T	315	ARG	Sidechain

## 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	A	2797	0	2744	1	0
1	B	2711	0	2676	1	0
1	C	2788	0	2736	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2711	0	2676	1	0
1	E	2797	0	2744	1	0
1	F	2720	0	2682	0	0
1	G	2793	0	2741	0	0
1	H	2720	0	2682	0	0
1	I	2797	0	2744	1	0
1	J	2760	0	2714	2	0
1	K	2780	0	2732	1	0
1	L	2788	0	2736	0	0
1	M	2729	0	2688	0	0
1	N	2793	0	2741	0	0
1	O	2720	0	2682	1	0
1	P	2797	0	2744	1	0
1	Q	2720	0	2682	1	0
1	R	2797	0	2744	1	0
1	S	2720	0	2682	1	0
1	T	2780	0	2732	0	0
All	All	55218	0	54302	12	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 0.

All (12) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:TYR:CD1	1:A:188:PRO:HB3	2.49	0.46
1:J:217:TYR:CE1	1:J:221:THR:HG21	2.52	0.45
1:C:306:LEU:HD22	1:B:144:GLY:HA2	1.98	0.45
1:S:144:GLY:HA2	1:R:306:LEU:HD22	1.99	0.44
1:J:176:VAL:HG12	1:J:221:THR:HA	2.02	0.41
1:O:217:TYR:CE1	1:O:221:THR:HG21	2.56	0.41
1:K:52:TYR:CG	1:K:188:PRO:HB2	2.55	0.41
1:I:52:TYR:CG	1:I:188:PRO:HB2	2.56	0.41
1:E:111:LEU:HD11	1:E:139:TYR:CD2	2.56	0.40
1:P:52:TYR:CG	1:P:188:PRO:HB2	2.57	0.40
1:D:78:MET:HE1	1:D:101:VAL:HG21	2.04	0.40
1:Q:52:TYR:CG	1:Q:188:PRO:HB2	2.57	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	354/368 (96%)	340 (96%)	12 (3%)	2 (1%)	21	13
1	B	343/368 (93%)	330 (96%)	11 (3%)	2 (1%)	21	13
1	C	352/368 (96%)	339 (96%)	12 (3%)	1 (0%)	36	30
1	D	343/368 (93%)	334 (97%)	8 (2%)	1 (0%)	36	30
1	E	354/368 (96%)	341 (96%)	11 (3%)	2 (1%)	21	13
1	F	344/368 (94%)	332 (96%)	11 (3%)	1 (0%)	36	30
1	G	353/368 (96%)	338 (96%)	14 (4%)	1 (0%)	36	30
1	H	344/368 (94%)	332 (96%)	11 (3%)	1 (0%)	36	30
1	I	354/368 (96%)	341 (96%)	12 (3%)	1 (0%)	36	30
1	J	348/368 (95%)	335 (96%)	12 (3%)	1 (0%)	36	30
1	K	351/368 (95%)	339 (97%)	11 (3%)	1 (0%)	36	30
1	L	352/368 (96%)	339 (96%)	12 (3%)	1 (0%)	36	30
1	M	345/368 (94%)	333 (96%)	11 (3%)	1 (0%)	36	30
1	N	353/368 (96%)	340 (96%)	12 (3%)	1 (0%)	36	30
1	O	344/368 (94%)	334 (97%)	9 (3%)	1 (0%)	36	30
1	P	354/368 (96%)	342 (97%)	11 (3%)	1 (0%)	36	30
1	Q	344/368 (94%)	331 (96%)	12 (4%)	1 (0%)	36	30
1	R	354/368 (96%)	343 (97%)	10 (3%)	1 (0%)	36	30
1	S	344/368 (94%)	332 (96%)	10 (3%)	2 (1%)	21	13
1	T	351/368 (95%)	337 (96%)	13 (4%)	1 (0%)	36	30
All	All	6981/7360 (95%)	6732 (96%)	225 (3%)	24 (0%)	37	30

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	188	PRO

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Mol	Chain	Res	Type
1	O	188	PRO
1	Q	188	PRO
1	P	188	PRO
1	M	188	PRO
1	L	188	PRO
1	E	188	PRO
1	D	188	PRO
1	G	188	PRO
1	F	188	PRO
1	I	188	PRO
1	H	188	PRO
1	K	188	PRO
1	B	188	PRO
1	N	188	PRO
1	S	188	PRO
1	R	188	PRO
1	A	106	HIS
1	A	133	HIS
1	B	133	HIS
1	S	133	HIS
1	T	106	HIS
1	E	106	HIS
1	C	188	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	298/307 (97%)	297 (100%)	1 (0%)	86	90
1	B	290/307 (94%)	287 (99%)	3 (1%)	68	72
1	C	298/307 (97%)	294 (99%)	4 (1%)	61	63
1	D	290/307 (94%)	286 (99%)	4 (1%)	59	60
1	E	298/307 (97%)	294 (99%)	4 (1%)	61	63
1	F	291/307 (95%)	290 (100%)	1 (0%)	86	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	298/307 (97%)	296 (99%)	2 (1%)	76	80
1	H	291/307 (95%)	288 (99%)	3 (1%)	68	72
1	I	298/307 (97%)	295 (99%)	3 (1%)	68	72
1	J	295/307 (96%)	292 (99%)	3 (1%)	68	72
1	K	297/307 (97%)	295 (99%)	2 (1%)	76	80
1	L	298/307 (97%)	295 (99%)	3 (1%)	68	72
1	M	292/307 (95%)	290 (99%)	2 (1%)	76	80
1	N	298/307 (97%)	293 (98%)	5 (2%)	53	53
1	O	291/307 (95%)	288 (99%)	3 (1%)	68	72
1	P	298/307 (97%)	294 (99%)	4 (1%)	61	63
1	Q	291/307 (95%)	288 (99%)	3 (1%)	68	72
1	R	298/307 (97%)	294 (99%)	4 (1%)	61	63
1	S	291/307 (95%)	287 (99%)	4 (1%)	59	60
1	T	297/307 (97%)	296 (100%)	1 (0%)	86	90
All	All	5898/6140 (96%)	5839 (99%)	59 (1%)	65	72

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	68	LEU
1	O	137	LEU
1	O	229	PHE
1	N	68	LEU
1	N	79	ASP
1	N	137	LEU
1	N	229	PHE
1	N	320	THR
1	Q	68	LEU
1	Q	229	PHE
1	Q	310	LEU
1	P	68	LEU
1	P	229	PHE
1	P	309	LEU
1	P	311	VAL
1	S	68	LEU
1	S	192	ASP
1	S	229	PHE

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Mol	Chain	Res	Type
1	S	310	LEU
1	R	68	LEU
1	R	229	PHE
1	R	310	LEU
1	R	326	ASP
1	T	68	LEU
1	M	68	LEU
1	M	229	PHE
1	L	68	LEU
1	L	229	PHE
1	L	311	VAL
1	E	68	LEU
1	E	229	PHE
1	E	341	LEU
1	E	348	GLU
1	D	68	LEU
1	D	137	LEU
1	D	229	PHE
1	D	320	THR
1	G	68	LEU
1	G	229	PHE
1	F	229	PHE
1	I	68	LEU
1	I	229	PHE
1	I	348	GLU
1	H	68	LEU
1	H	229	PHE
1	H	320	THR
1	K	68	LEU
1	K	229	PHE
1	J	68	LEU
1	J	229	PHE
1	J	351	ARG
1	A	141	ASP
1	C	68	LEU
1	C	81	SER
1	C	229	PHE
1	C	310	LEU
1	B	68	LEU
1	B	229	PHE
1	B	311	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52)

such sidechains are listed below:

Mol	Chain	Res	Type
1	O	93	ASN
1	N	93	ASN
1	N	152	GLN
1	N	352	GLN
1	Q	4	ASN
1	Q	93	ASN
1	Q	152	GLN
1	Q	300	HIS
1	P	93	ASN
1	R	93	ASN
1	R	106	HIS
1	R	300	HIS
1	T	93	ASN
1	T	106	HIS
1	T	204	ASN
1	M	93	ASN
1	L	93	ASN
1	L	300	HIS
1	E	93	ASN
1	E	327	ASN
1	E	352	GLN
1	D	4	ASN
1	D	93	ASN
1	D	152	GLN
1	D	162	ASN
1	D	286	ASN
1	D	300	HIS
1	G	93	ASN
1	G	352	GLN
1	F	4	ASN
1	F	19	ASN
1	F	93	ASN
1	F	113	GLN
1	F	300	HIS
1	I	93	ASN
1	I	352	GLN
1	H	4	ASN
1	H	93	ASN
1	K	93	ASN
1	K	152	GLN
1	K	162	ASN
1	J	93	ASN

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Mol	Chain	Res	Type
1	A	93	ASN
1	A	286	ASN
1	A	352	GLN
1	C	19	ASN
1	C	196	GLN
1	C	352	GLN
1	B	4	ASN
1	B	93	ASN
1	B	133	HIS
1	B	162	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

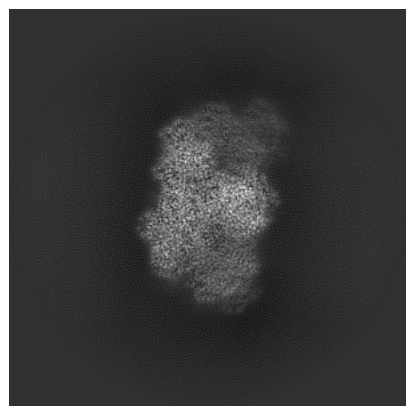
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70421. These allow visual inspection of the internal detail of the map and identification of artifacts.

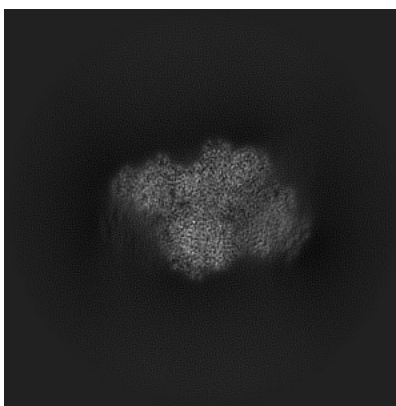
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

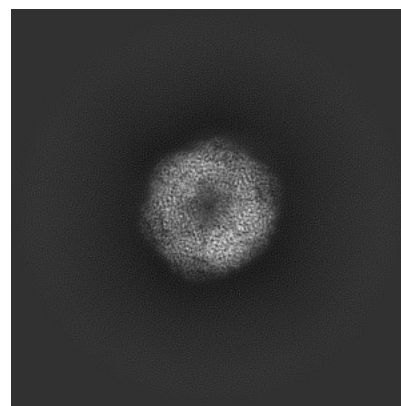
#### 6.1.1 Primary map



X

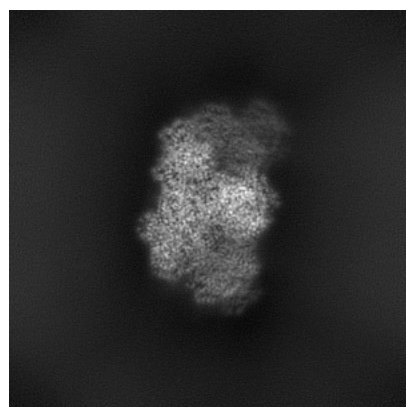


Y

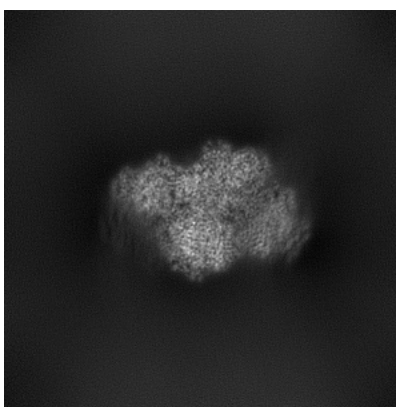


Z

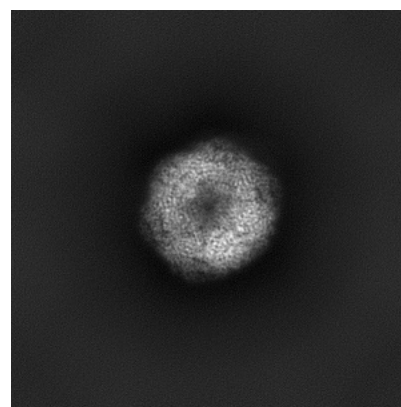
#### 6.1.2 Raw map



X



Y

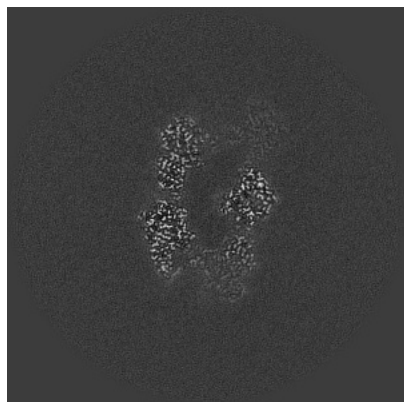


Z

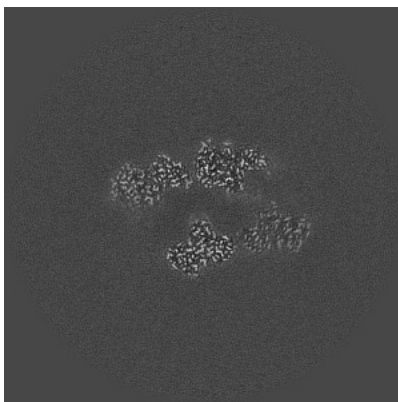
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

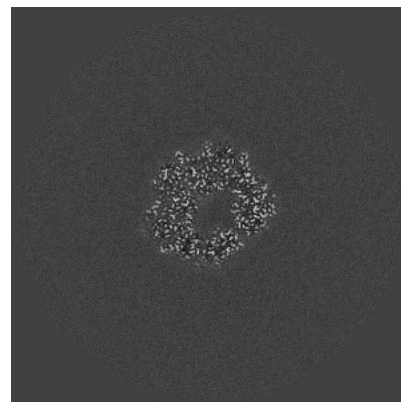
### 6.2.1 Primary map



X Index: 225

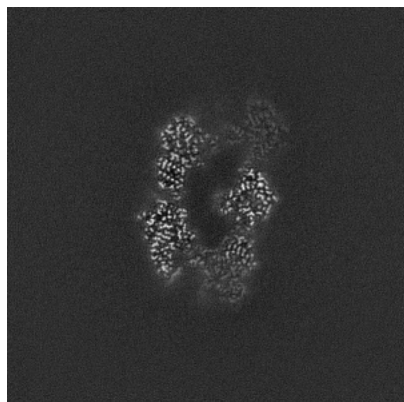


Y Index: 225

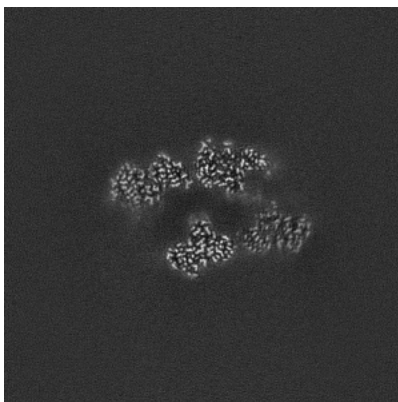


Z Index: 225

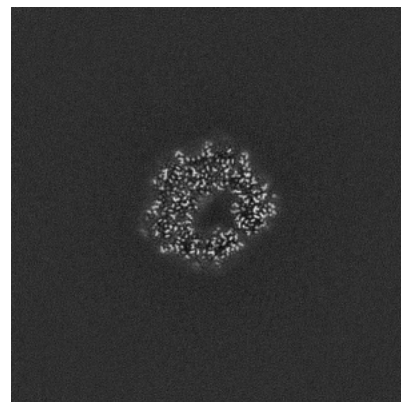
### 6.2.2 Raw map



X Index: 225



Y Index: 225



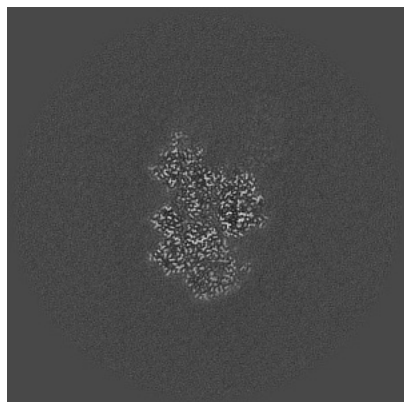
Z Index: 225

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

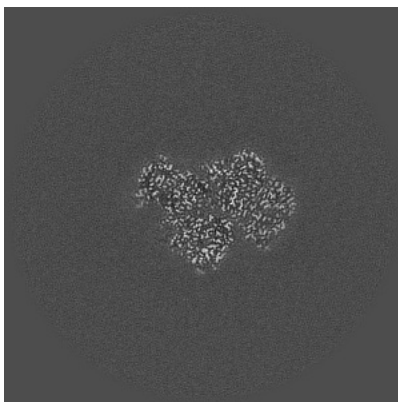


## 6.3 Largest variance slices [i](#)

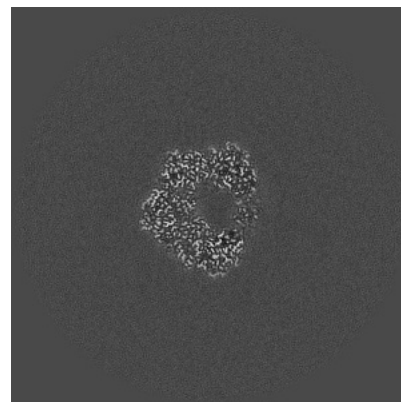
### 6.3.1 Primary map



X Index: 255

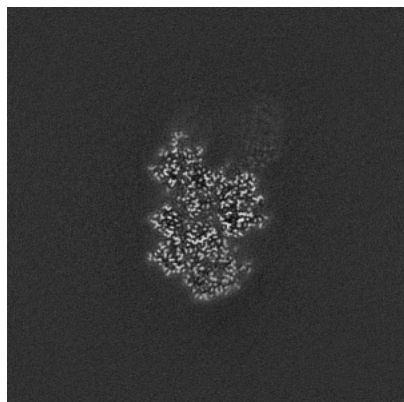


Y Index: 192

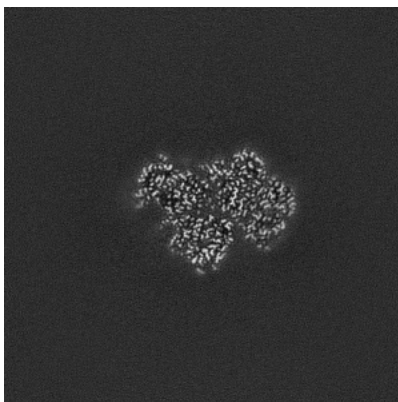


Z Index: 213

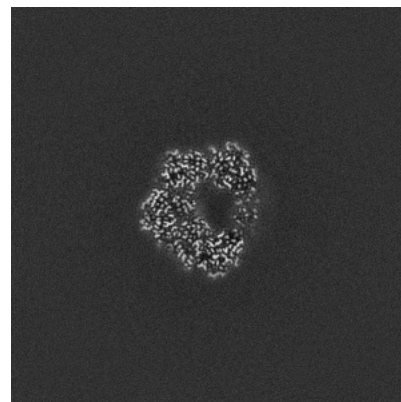
### 6.3.2 Raw map



X Index: 255



Y Index: 192

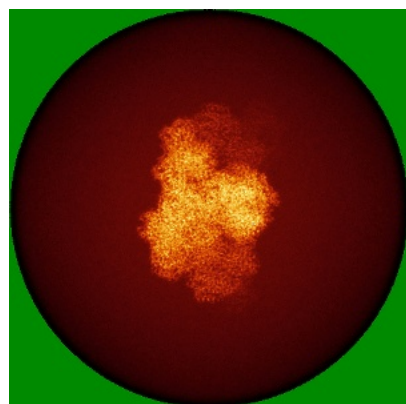


Z Index: 213

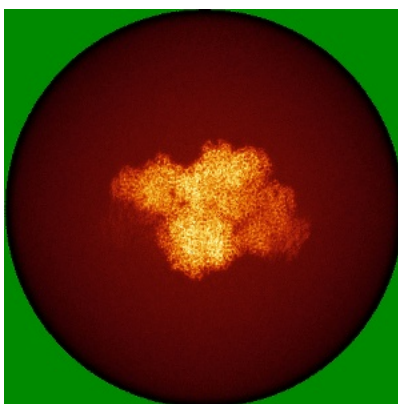
The images above show the largest variance slices of the map in three orthogonal directions.

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

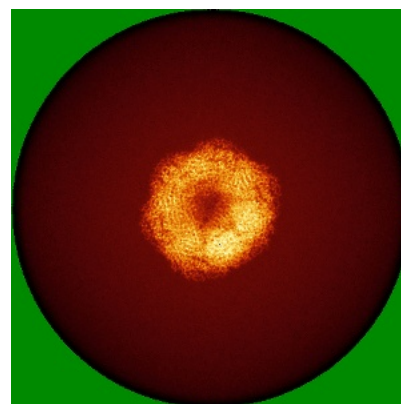
### 6.4.1 Primary map



X

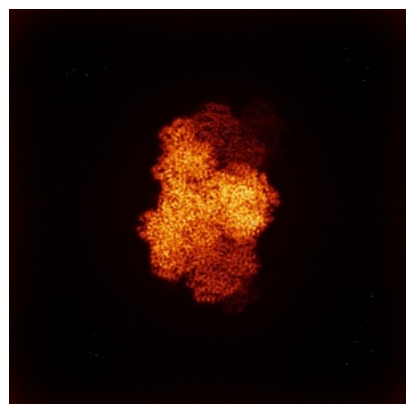


Y

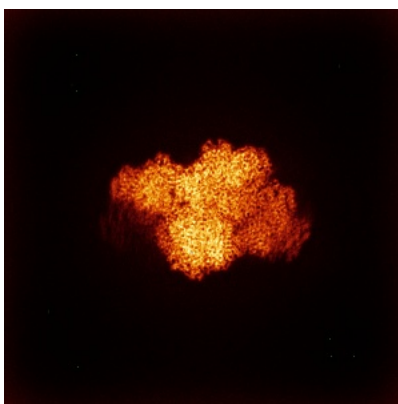


Z

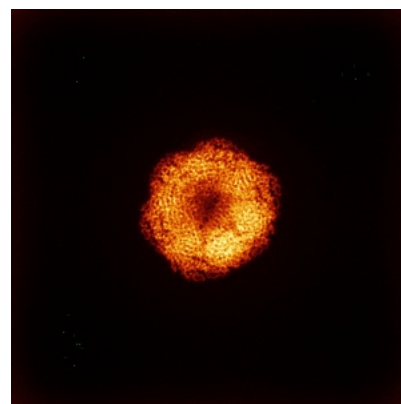
### 6.4.2 Raw map



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



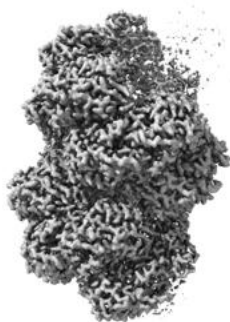
Y



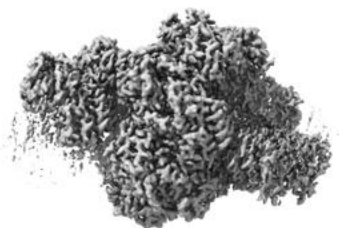
Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. 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.

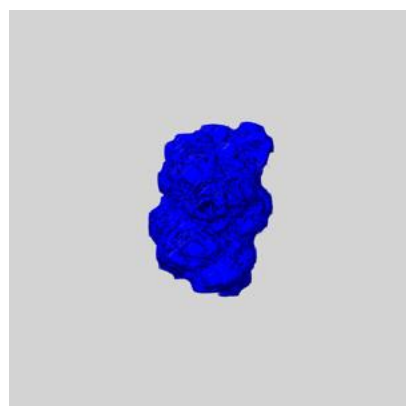
## 6.6 Mask visualisation [i](#)

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

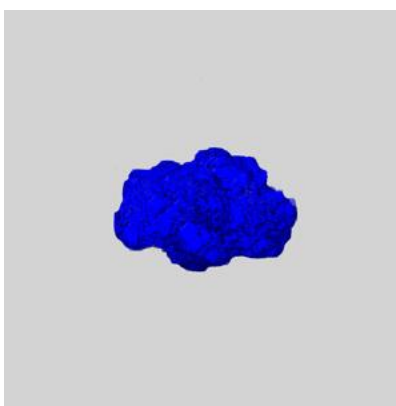
A mask typically either:

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

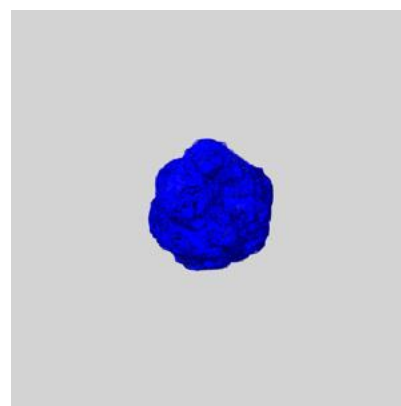
### 6.6.1 emd\_70421\_msk\_1.map [i](#)



X



Y

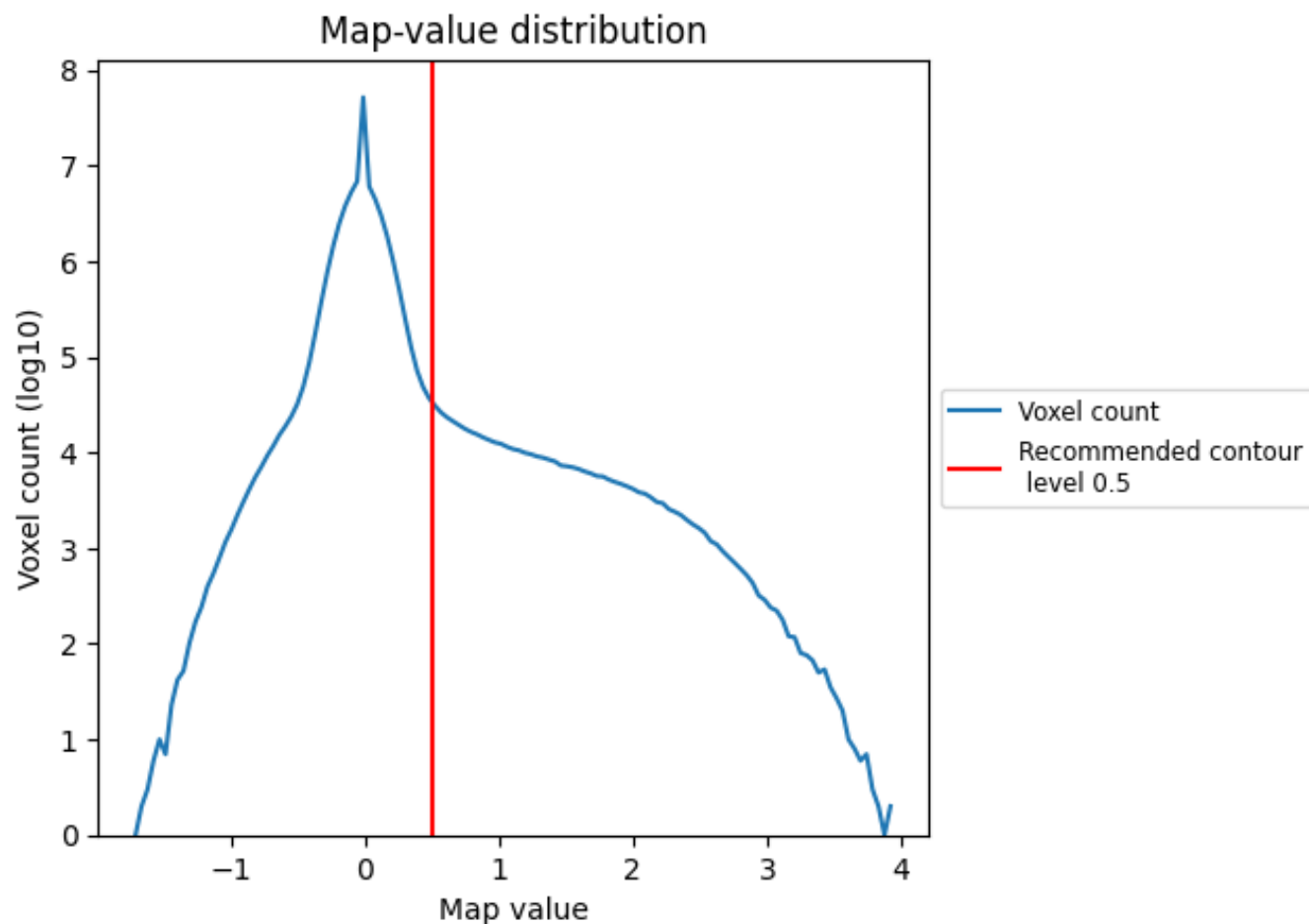


Z

## 7 Map analysis [i](#)

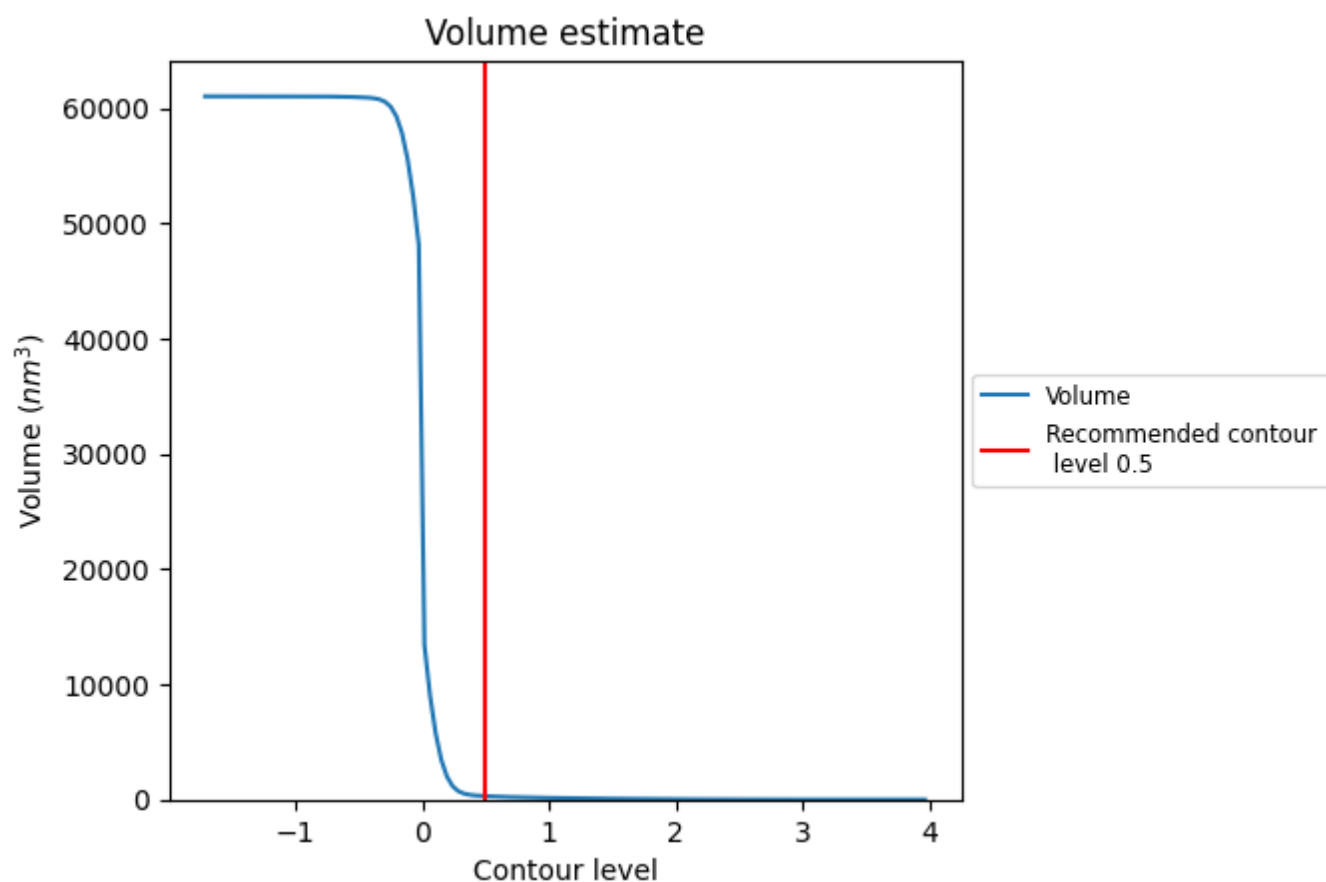
This section contains the results of statistical analysis of the map.

### 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.

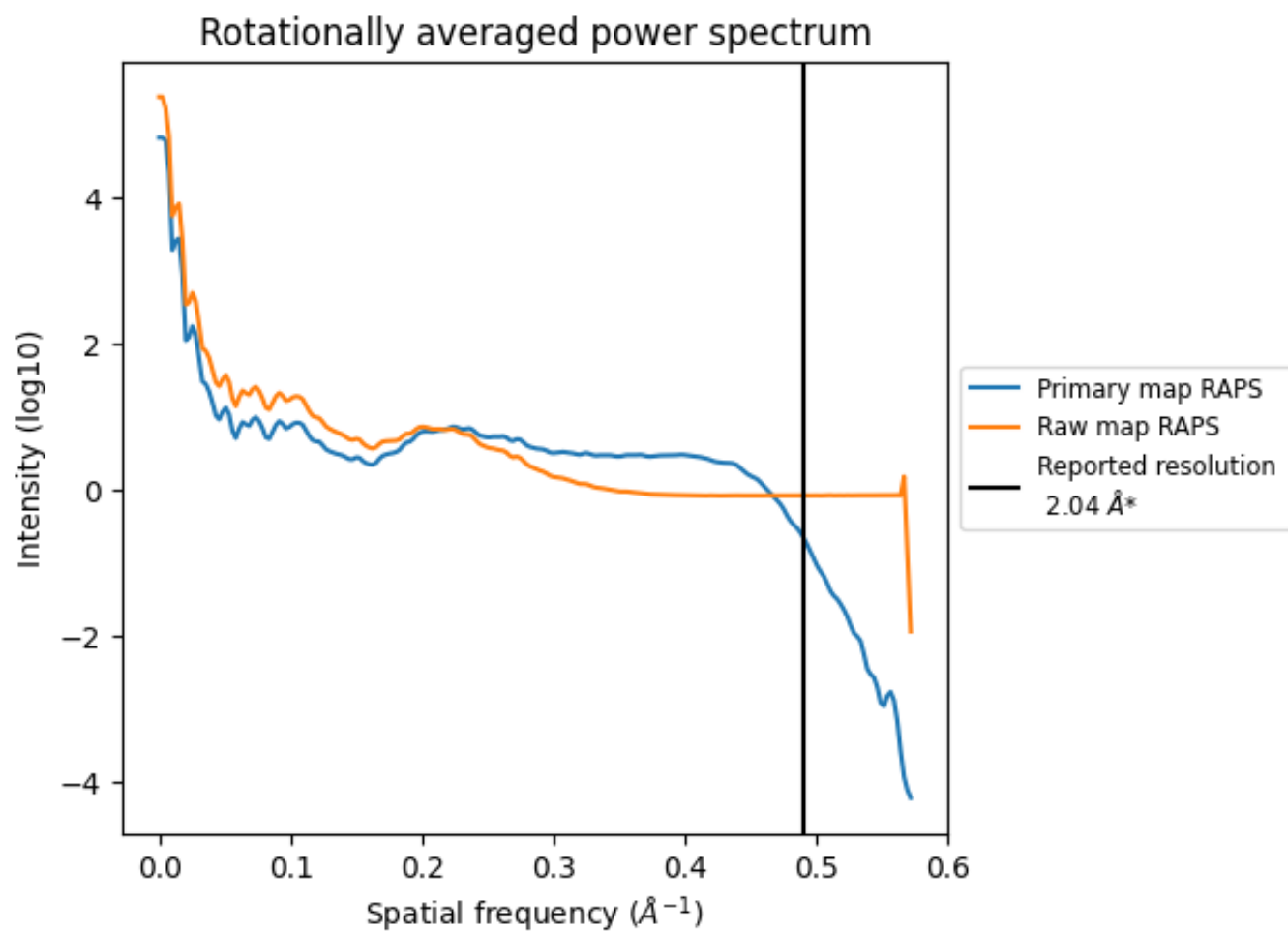
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 297 nm<sup>3</sup>; this corresponds to an approximate mass of 268 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 ⓘ

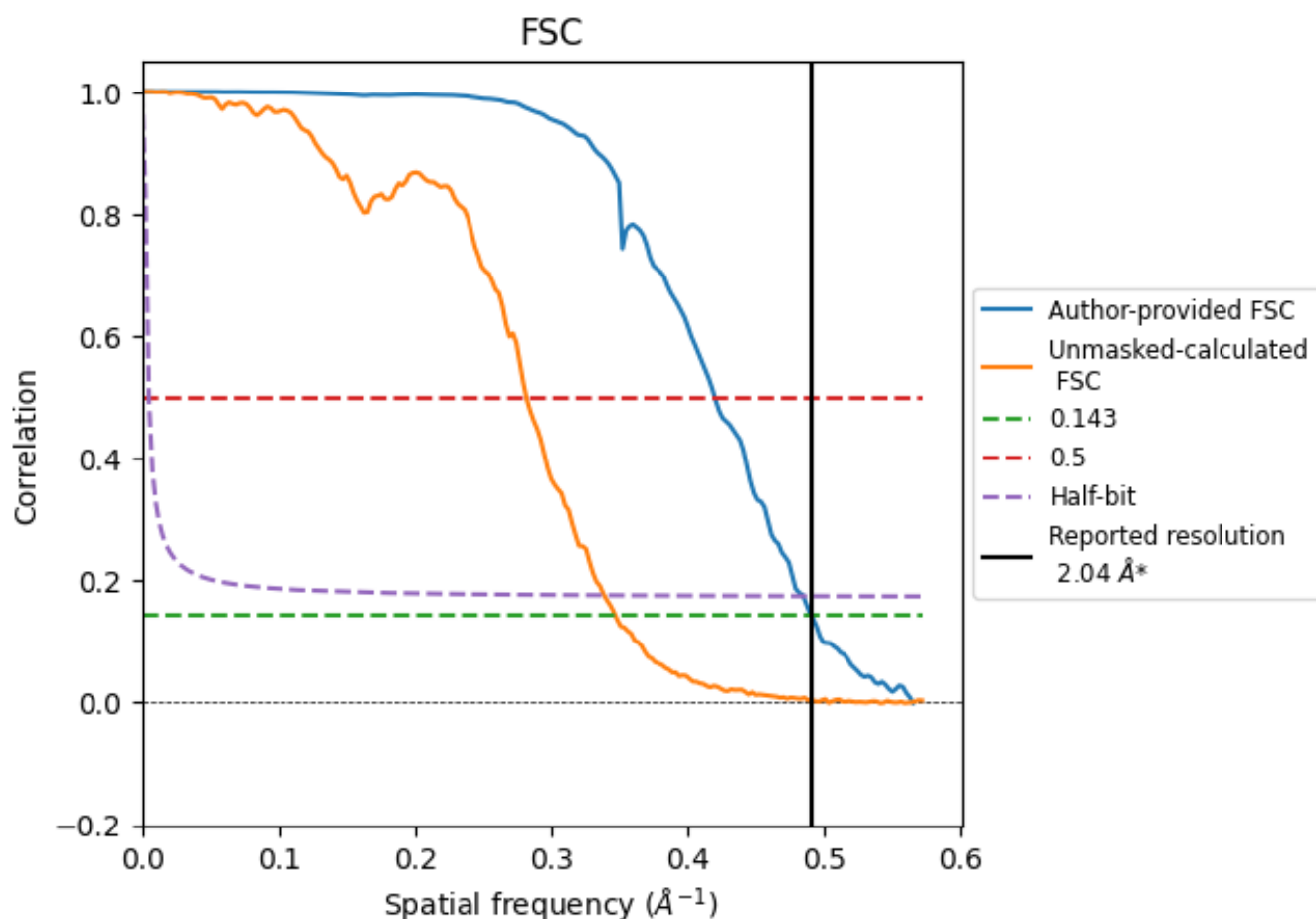


\*Reported resolution corresponds to spatial frequency of 0.490 Å<sup>-1</sup>

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



## 8.2 Resolution estimates [i](#)

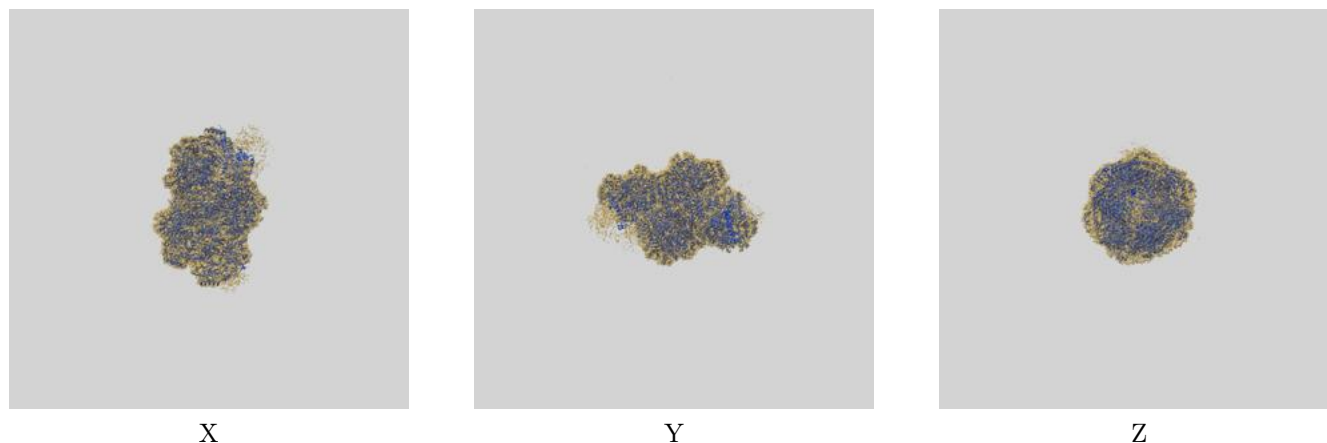
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.04	-	-
Author-provided FSC curve	2.04	2.38	2.06
Unmasked-calculated*	2.89	3.55	2.96

\*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 2.89 differs from the reported value 2.04 by more than 10 %

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

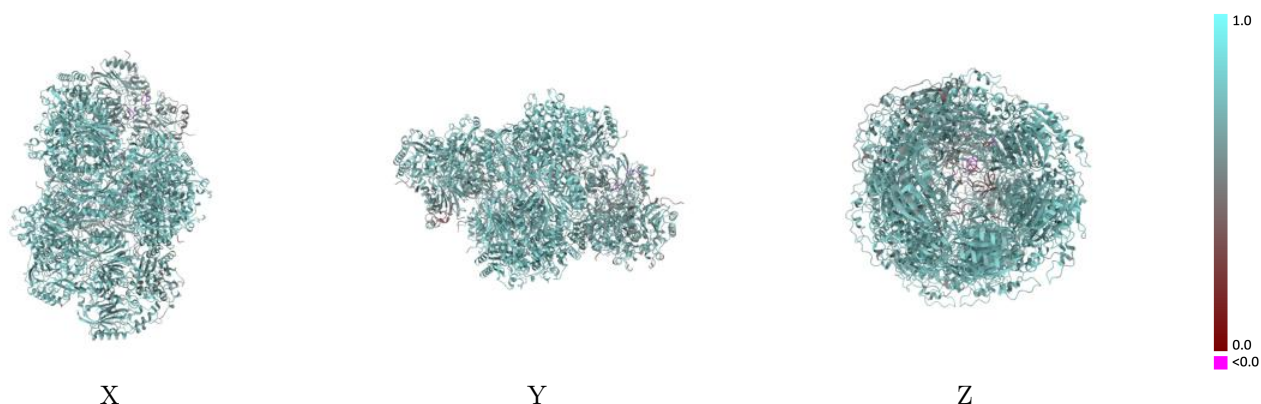
This section contains information regarding the fit between EMDB map EMD-70421 and PDB model 9OFA. Per-residue inclusion information can be found in section [3](#) on page [6](#).

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



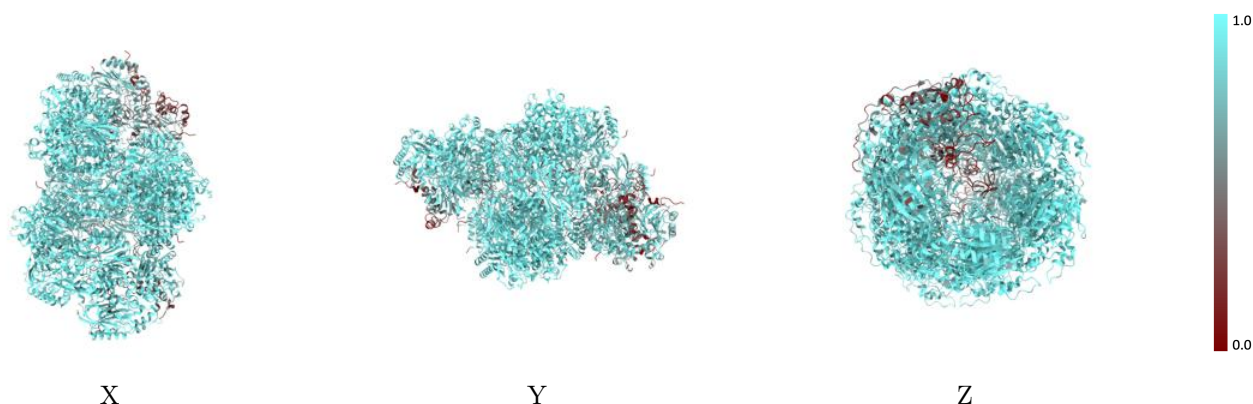
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



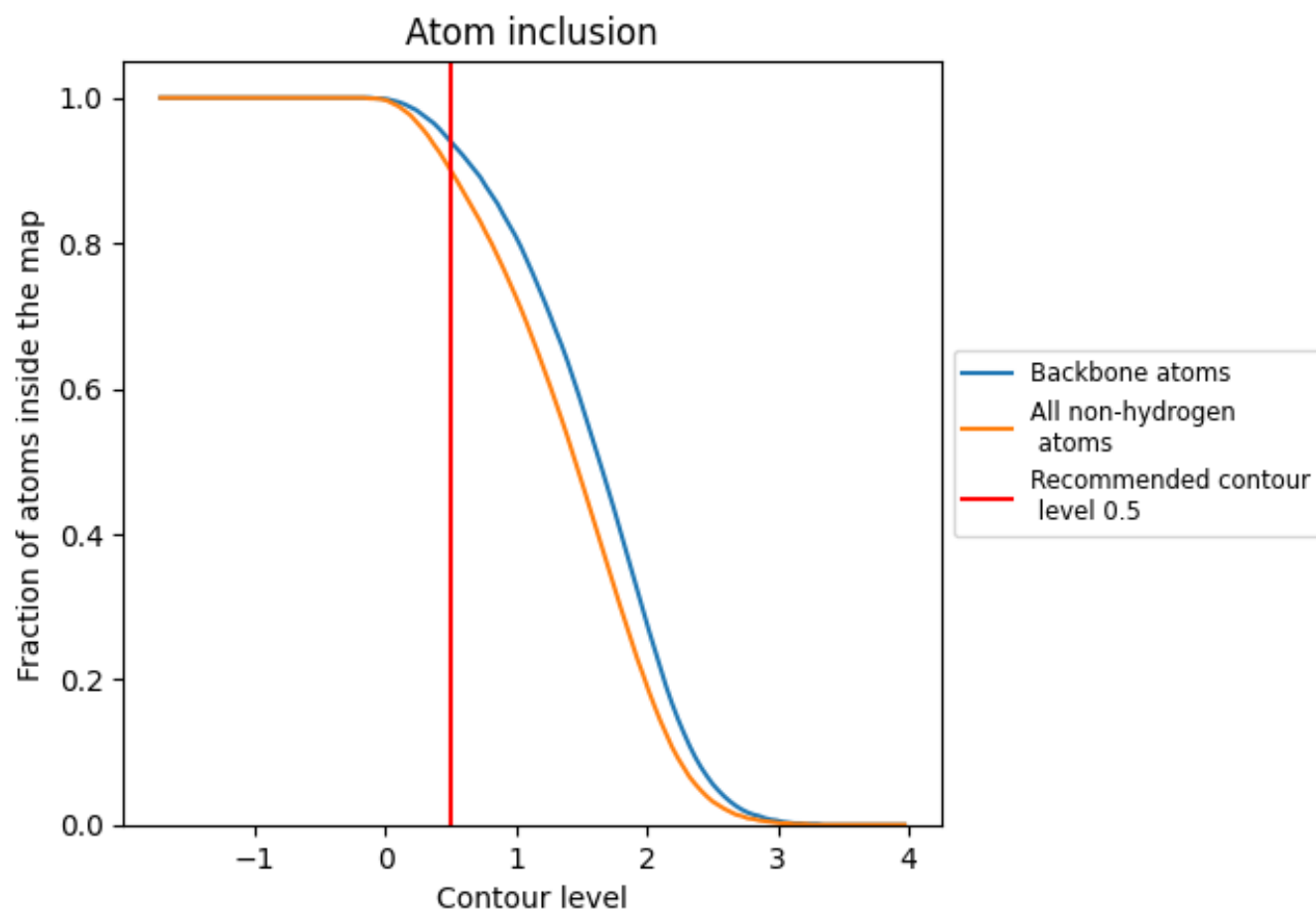
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).











































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 90% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9010	 0.6990
A	 0.7160	 0.6180
B	 0.8660	 0.6620
C	 0.9450	 0.7140
D	 0.9430	 0.7090
E	 0.9550	 0.7250
F	 0.9500	 0.7200
G	 0.9550	 0.7290
H	 0.9530	 0.7200
I	 0.9510	 0.7190
J	 0.9420	 0.7190
K	 0.9360	 0.7160
L	 0.9540	 0.7240
M	 0.9500	 0.7210
N	 0.9520	 0.7250
O	 0.9460	 0.7140
P	 0.9480	 0.7200
Q	 0.9280	 0.6920
R	 0.9100	 0.6910
S	 0.7540	 0.6340
T	 0.5620	 0.6070

