



## Full wwPDB EM Validation Report ⓘ

Jul 20, 2025 – 07:11 am BST

PDB ID : 9F5W / pdb\_00009f5w  
EMDB ID : EMD-50201  
Title : Human condensin II - M18BP1 complex  
Authors : Borsellini, A.; Vannini, A.  
Deposited on : 2024-04-30  
Resolution : 7.50 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.dev118  
MolProbity : 4-5-2 with Phenix2.0rc1  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.44

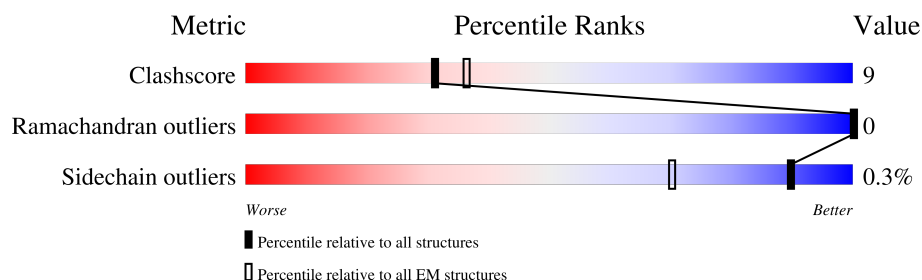
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 7.50 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1197	
2	B	1305	
3	D	1498	
4	H	640	
5	M	652	
6	G	1143	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 23030 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 Structural maintenance of chromosomes protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	513	Total	C	N	O	S	0	0
			4087	2587	709	773	18		

- Molecule 2 is a protein called Structural maintenance of chromosomes protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	533	Total	C	N	O	S	0	0
			4344	2767	742	815	20		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	HIS	-	expression tag	UNP Q9NTJ3
B	-15	HIS	-	expression tag	UNP Q9NTJ3
B	-14	HIS	-	expression tag	UNP Q9NTJ3
B	-13	HIS	-	expression tag	UNP Q9NTJ3
B	-12	HIS	-	expression tag	UNP Q9NTJ3
B	-11	HIS	-	expression tag	UNP Q9NTJ3
B	-10	HIS	-	expression tag	UNP Q9NTJ3
B	-9	HIS	-	expression tag	UNP Q9NTJ3
B	-8	HIS	-	expression tag	UNP Q9NTJ3
B	-7	HIS	-	expression tag	UNP Q9NTJ3
B	-6	LEU	-	expression tag	UNP Q9NTJ3
B	-5	GLU	-	expression tag	UNP Q9NTJ3
B	-4	VAL	-	expression tag	UNP Q9NTJ3
B	-3	LEU	-	expression tag	UNP Q9NTJ3
B	-2	PHE	-	expression tag	UNP Q9NTJ3
B	-1	GLN	-	expression tag	UNP Q9NTJ3
B	0	GLY	-	expression tag	UNP Q9NTJ3
B	1	PRO	-	expression tag	UNP Q9NTJ3

- Molecule 3 is a protein called Condensin-2 complex subunit D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1113	Total	C	N	O	S	0	0
			8964	5760	1531	1618	55		

- Molecule 4 is a protein called Condensin-2 complex subunit H2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	252	Total	C	N	O	S	0	0
			2034	1303	334	381	16		

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	606	GLU	-	expression tag	UNP Q6IBW4
H	607	ASN	-	expression tag	UNP Q6IBW4
H	608	LEU	-	expression tag	UNP Q6IBW4
H	609	TYR	-	expression tag	UNP Q6IBW4
H	610	PHE	-	expression tag	UNP Q6IBW4
H	611	GLN	-	expression tag	UNP Q6IBW4
H	612	SER	-	expression tag	UNP Q6IBW4
H	613	TRP	-	expression tag	UNP Q6IBW4
H	614	SER	-	expression tag	UNP Q6IBW4
H	615	HIS	-	expression tag	UNP Q6IBW4
H	616	PRO	-	expression tag	UNP Q6IBW4
H	617	GLN	-	expression tag	UNP Q6IBW4
H	618	PHE	-	expression tag	UNP Q6IBW4
H	619	GLU	-	expression tag	UNP Q6IBW4
H	620	LYS	-	expression tag	UNP Q6IBW4
H	621	GLY	-	expression tag	UNP Q6IBW4
H	622	GLY	-	expression tag	UNP Q6IBW4
H	623	GLY	-	expression tag	UNP Q6IBW4
H	624	SER	-	expression tag	UNP Q6IBW4
H	625	GLY	-	expression tag	UNP Q6IBW4
H	626	GLY	-	expression tag	UNP Q6IBW4
H	627	GLY	-	expression tag	UNP Q6IBW4
H	628	SER	-	expression tag	UNP Q6IBW4
H	629	GLY	-	expression tag	UNP Q6IBW4
H	630	GLY	-	expression tag	UNP Q6IBW4
H	631	GLY	-	expression tag	UNP Q6IBW4
H	632	SER	-	expression tag	UNP Q6IBW4
H	633	TRP	-	expression tag	UNP Q6IBW4
H	634	SER	-	expression tag	UNP Q6IBW4
H	635	HIS	-	expression tag	UNP Q6IBW4
H	636	PRO	-	expression tag	UNP Q6IBW4

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Chain	Residue	Modelled	Actual	Comment	Reference
H	637	GLN	-	expression tag	UNP Q6IBW4
H	638	PHE	-	expression tag	UNP Q6IBW4
H	639	GLU	-	expression tag	UNP Q6IBW4
H	640	LYS	-	expression tag	UNP Q6IBW4

- Molecule 5 is a protein called Maltose/maltodextrin-binding periplasmic protein,Mis18-binding protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	M	5	Total	C	N	O	0	0
			48	32	7	9		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	491	MET	-	initiating methionine	UNP P0AEX9
M	863	GLY	-	linker	UNP P0AEX9
M	864	SER	-	linker	UNP P0AEX9
M	865	GLU	-	linker	UNP P0AEX9
M	866	ASN	-	linker	UNP P0AEX9
M	867	LEU	-	linker	UNP P0AEX9
M	868	TYR	-	linker	UNP P0AEX9
M	869	PHE	-	linker	UNP P0AEX9
M	870	GLN	-	linker	UNP P0AEX9
M	871	GLY	-	linker	UNP P0AEX9
M	872	SER	-	linker	UNP P0AEX9
M	1133	LEU	-	expression tag	UNP Q6P0N0
M	1134	GLU	-	expression tag	UNP Q6P0N0
M	1135	HIS	-	expression tag	UNP Q6P0N0
M	1136	HIS	-	expression tag	UNP Q6P0N0
M	1137	HIS	-	expression tag	UNP Q6P0N0
M	1138	HIS	-	expression tag	UNP Q6P0N0
M	1139	HIS	-	expression tag	UNP Q6P0N0
M	1140	HIS	-	expression tag	UNP Q6P0N0
M	1141	HIS	-	expression tag	UNP Q6P0N0
M	1142	HIS	-	expression tag	UNP Q6P0N0

- Molecule 6 is a protein called Condensin-2 complex subunit G2.

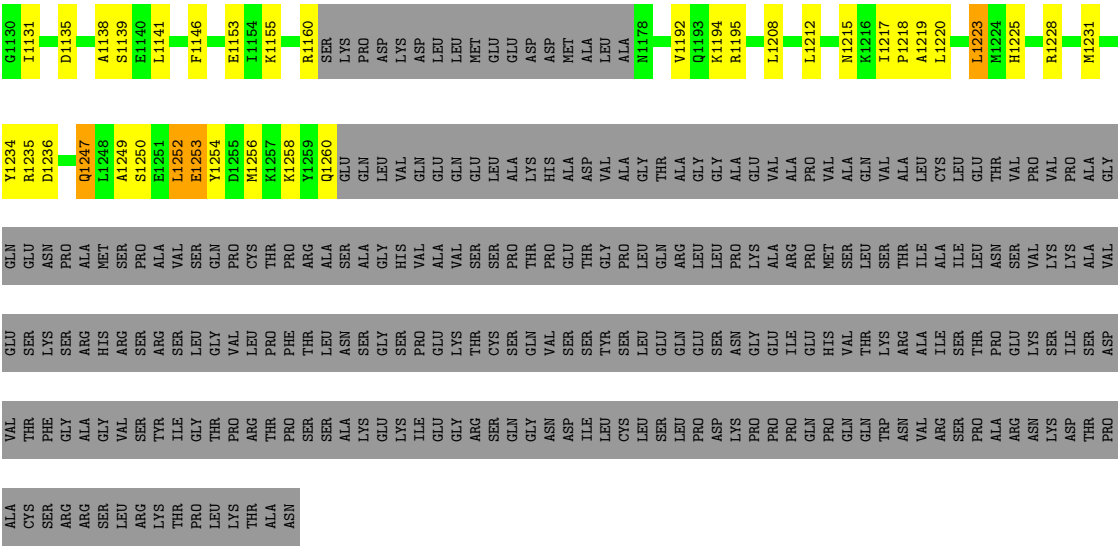
Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	433	Total	C	N	O	S	0	0
			3553	2289	622	614	28		



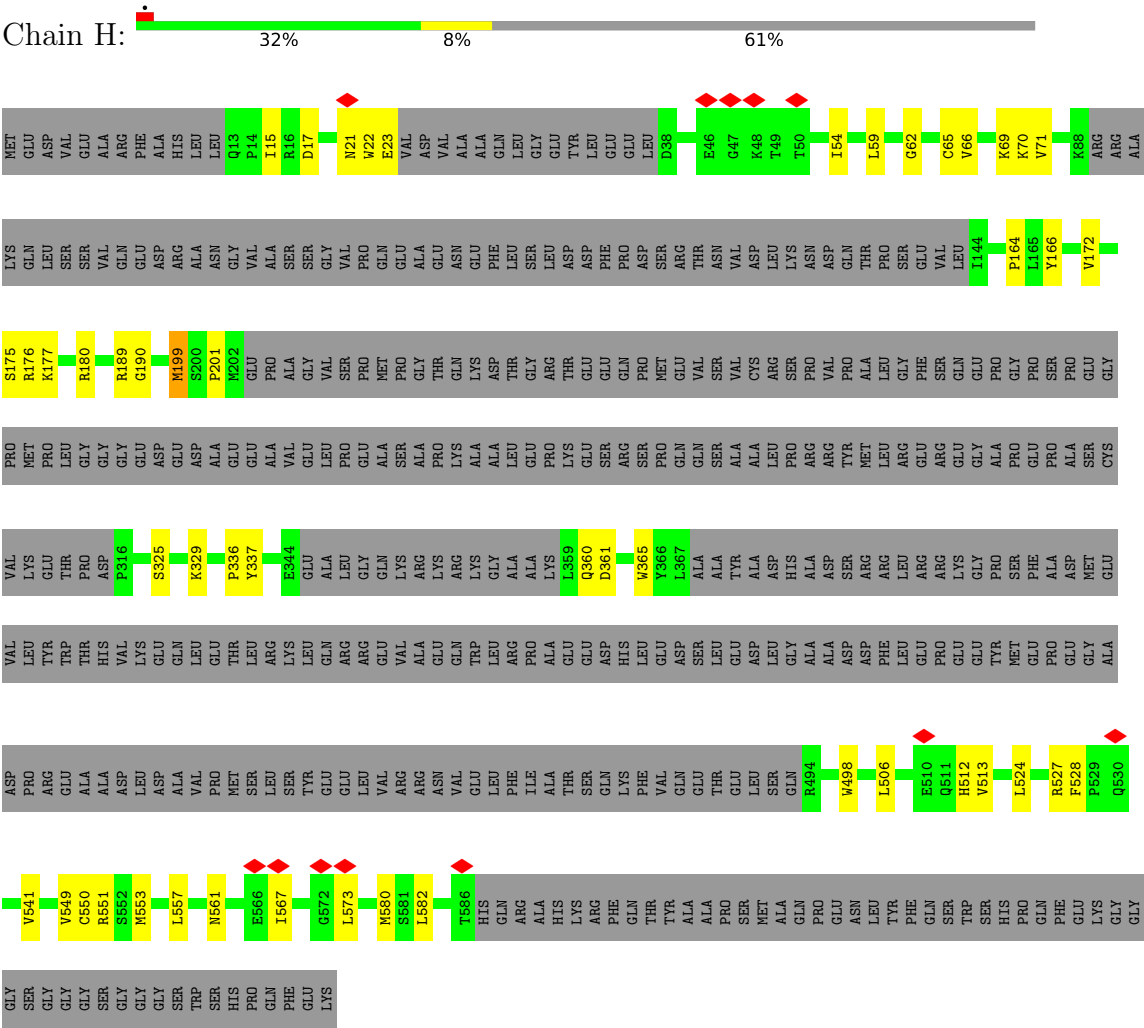








● Molecule 4: Condensin-2 complex subunit H2



● Molecule 5: Maltose/maltodextrin-binding periplasmic protein,Mis18-binding protein 1

99%

[illegible]

## Chain G:



I822	A341	D197	GLU	VAL	MET
S525	R342	L200	CYS	LEU	GLU
P528	R347		ILE	GLU	ARG
Q631	P388	K207	LEU	PRO	THR
		D208	ASN	VAL	PHI
V535	R393	M209	GLY	ASP	VAL
V536		L210	ILE	GLY	GLN
C637	I397	E211	LEU	TRP	ALA
E638		E212	TVR	GLN	VAL
R639	K402	L215	ALA	VAL	SER
		M216	LEU	LYS	
N647	L427	I217	PRO	GLU	GLU
H648			SER	GLN	LEU
A649	T431	I220	ARG	GLY	GLU
	S432	K221	ARG	GLU	PHI
R652	S433		LYS	ASP	
	A434	G225	LEU	ASN	LEU
Q656	D435	R226	GLN	ASP	GLN
Y657		F228	SER	GLU	PHI
	V440		SER	THR	VAL
H561			ILE	GLU	GLN
	C443	L232	GLN	HIS	LEU
H576	L444		ASP	GLY	ASP
	P445	Q255	LEU	SER	LYS
	M446		CYS	LEU	LYS
ASN	I447	L258	VAL	GLU	GLU
ALA	L448		VAL	MET	ALA
CYS	D449	T282	THR	ARG	SER
			TRP	LYS	ASP
GLN	P462	I265	TRP	LEU	PRO
ARG			GLU	ILE	PHI
ALA	R465	R268	LYS	GLU	SER
ARG			GLY	ILE	LEU
VAL	L468	A280	LEU	ILE	ASN
GLU	H469		PRO	TYR	GLU
PRO	D470	D284	ALA	ALA	LEU
			LYS	ILE	LEU
PRO			GLU	THR	LEU
GLU	R476	Q287	ASP	THR	ASP
ASP			THR	VAL	GLU
GLU	V480	M290	GLY	VAL	LEU
GLU	D481	F291	LYS	ILE	SER
GLU	M482	H292	THR	LEU	ARG
ASP	K487	L296	ALA	ALA	LYS
GLY			PHI	VAL	GLN
			VAL	SER	LYS
			VAL	THR	GLU
			VAL	VAL	GLU
			ASN	ILE	TRP
			L170	ASN	LEU
			L171	GLN	THR
			R172	SER	ARG
				SER	LEU
			L176	GLU	LYS
				TYR	ASN
			C184	ASN	LEU
			L330	GLU	LEU
			L185	ALA	LEU
			L186	ALA	LEU
			L187	LEU	THR
			L188	LEU	ASP
			L189	LYS	LYS

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

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	24490	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.125	Depositor
Minimum map value	-0.033	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0248	Depositor
Map size ( $\text{\AA}$ )	384.0, 384.0, 384.0	wwPDB
Map dimensions	160, 160, 160	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	2.4, 2.4, 2.4	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	0.27	0/4147	0.60	0/5574
2	B	0.30	0/4424	0.60	0/5945
3	D	0.31	0/9144	0.64	8/12363 (0.1%)
4	H	0.24	0/2084	0.52	0/2826
5	M	0.12	0/50	0.32	0/66
6	G	0.26	0/3632	0.58	0/4902
All	All	0.29	0/23481	0.61	8/31676 (0.0%)

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
2	B	0	1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	344	GLU	CA-C-O	-7.12	113.37	120.70
3	D	1247	GLN	CA-C-O	-6.68	112.44	120.32
3	D	1252	LEU	CA-C-O	-5.76	114.77	120.82
3	D	1253	GLU	N-CA-CB	5.73	118.64	110.16
3	D	342	VAL	CA-C-N	-5.68	113.05	120.44
3	D	342	VAL	C-N-CA	-5.68	113.05	120.44
3	D	1252	LEU	CA-C-N	-5.37	112.67	120.29
3	D	1252	LEU	C-N-CA	-5.37	112.67	120.29

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	272	ARG	Sidechain

## 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	4087	0	4187	69	0
2	B	4344	0	4363	106	0
3	D	8964	0	9157	154	0
4	H	2034	0	1982	35	0
5	M	48	0	32	0	0
6	G	3553	0	3634	56	0
All	All	23030	0	23355	397	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (397) 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:B:143:SER:HA	2:B:146:ILE:HD12	1.60	0.83
2:B:1094:ALA:O	2:B:1098:LYS:HB3	1.78	0.82
1:A:1096:SER:HA	1:A:1099:LEU:HD23	1.69	0.74
2:B:1232:ILE:HG23	4:H:498:TRP:HE1	1.53	0.73
1:A:963:LYS:HD3	2:B:1035:TRP:HZ3	1.55	0.72
3:D:345:LEU:HD12	3:D:349:ILE:HB	1.72	0.71
3:D:1247:GLN:HG3	6:G:336:TRP:CZ3	2.26	0.70
2:B:327:ILE:HG22	2:B:1036:HIS:ND1	2.07	0.69
2:B:219:ASP:H	2:B:224:ARG:HH12	1.39	0.69
3:D:7:LEU:HA	3:D:60:SER:HB2	1.76	0.68
3:D:488:ILE:HG13	3:D:542:VAL:HB	1.74	0.68
2:B:327:ILE:HG21	2:B:1037:LYS:HA	1.76	0.68
3:D:96:PHE:HB3	3:D:113:GLY:HA2	1.76	0.67
2:B:345:HIS:HB2	2:B:1020:GLN:HG3	1.76	0.66
1:A:167:GLU:HA	1:A:172:ARG:HD2	1.78	0.65
1:A:173:MET:HE1	4:H:59:LEU:HG	1.79	0.65
1:A:214:ARG:HB3	1:A:983:VAL:HG22	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1008:VAL:O	1:A:1012:LYS:HB2	1.97	0.64
3:D:593:VAL:O	3:D:597:LYS:HB2	1.97	0.64
2:B:164:PHE:HB2	2:B:183:PHE:HB2	1.82	0.62
2:B:1193:GLY:HA2	2:B:1196:LYS:HD2	1.80	0.62
2:B:278:ASN:HA	2:B:281:ARG:HD2	1.82	0.62
3:D:645:GLN:HA	3:D:649:GLN:HB2	1.82	0.62
3:D:967:ASP:HA	3:D:970:ILE:HD12	1.82	0.61
2:B:82:LEU:HD11	2:B:164:PHE:HB3	1.83	0.61
1:A:196:LYS:HB3	1:A:1004:LYS:HE2	1.82	0.61
2:B:87:ILE:HG12	2:B:162:VAL:HG23	1.83	0.61
2:B:1099:LYS:HA	2:B:1103:TYR:HB2	1.82	0.61
4:H:22:TRP:HD1	4:H:23:GLU:HG2	1.66	0.60
2:B:150:ASP:OD1	2:B:1270:ASN:ND2	2.35	0.60
2:B:251:LEU:HD21	2:B:1170:PHE:HA	1.84	0.60
3:D:828:LEU:HB2	3:D:863:ILE:HG21	1.82	0.60
6:G:443:CYS:O	6:G:447:ILE:HD12	2.02	0.59
1:A:1048:LEU:HD22	1:A:1127:ILE:HG22	1.83	0.59
2:B:248:GLU:HG3	2:B:252:GLU:HB2	1.84	0.59
2:B:1261:ARG:NH1	2:B:1276:ALA:O	2.36	0.59
1:A:968:ARG:NH2	2:B:1040:SER:O	2.35	0.59
6:G:292:HIS:O	6:G:296:LEU:N	2.36	0.58
2:B:127:LEU:HD21	2:B:226:LEU:HD22	1.85	0.58
2:B:295:LYS:HG2	2:B:1099:LYS:HD2	1.85	0.58
2:B:332:LYS:NZ	2:B:1064:GLU:OE1	2.38	0.57
1:A:978:LYS:HA	2:B:1088:PRO:HD2	1.86	0.57
1:A:177:LYS:HE3	4:H:54:ILE:HG13	1.87	0.57
3:D:769:LEU:O	3:D:774:ARG:NH2	2.38	0.57
4:H:164:PRO:O	4:H:176:ARG:NH1	2.38	0.57
1:A:1149:MET:SD	1:A:1149:MET:N	2.79	0.56
2:B:154:ASP:O	2:B:191:ARG:NH2	2.39	0.56
2:B:240:PRO:HB2	2:B:1173:GLY:HA3	1.87	0.56
2:B:1039:ILE:HB	2:B:1052:ILE:HD12	1.87	0.56
2:B:1118:ASP:O	2:B:1122:GLN:NE2	2.38	0.56
6:G:444:LEU:HD12	6:G:482:MET:HE3	1.88	0.56
2:B:146:ILE:HG22	2:B:147:HIS:H	1.69	0.56
3:D:717:PRO:HA	3:D:720:MET:HG2	1.86	0.56
1:A:1059:PRO:HG3	1:A:1069:GLU:HB2	1.87	0.56
6:G:341:ALA:O	6:G:347:ARG:NH1	2.39	0.56
3:D:706:VAL:HG11	3:D:722:LEU:HD21	1.88	0.56
6:G:287:GLN:HB3	6:G:330:LEU:HD11	1.87	0.56
1:A:137:ASN:ND2	4:H:62:GLY:O	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:175:LEU:HG	6:G:209:MET:HB3	1.88	0.56
3:D:221:LYS:HG2	3:D:267:LEU:HB3	1.86	0.56
3:D:924:ILE:HG21	3:D:961:VAL:HG22	1.88	0.56
1:A:7:ILE:HB	1:A:80:SER:H	1.70	0.56
1:A:1003:LYS:HG2	1:A:1006:ARG:HH21	1.69	0.56
3:D:257:HIS:O	3:D:333:GLN:NE2	2.38	0.56
1:A:963:LYS:HD3	2:B:1035:TRP:CZ3	2.39	0.56
2:B:93:LYS:HA	2:B:147:HIS:HA	1.88	0.56
6:G:487:LYS:NZ	6:G:521:LEU:O	2.39	0.56
4:H:557:LEU:O	4:H:561:ASN:ND2	2.39	0.55
3:D:550:ILE:HG21	3:D:587:GLN:HE21	1.72	0.55
3:D:311:GLU:O	3:D:318:ARG:NH1	2.38	0.55
3:D:1135:ASP:H	3:D:1138:ALA:HB3	1.72	0.55
1:A:8:LEU:HA	1:A:79:VAL:HG12	1.87	0.55
3:D:1256:MET:SD	3:D:1260:GLN:NE2	2.78	0.55
1:A:4:LYS:NZ	1:A:100:GLU:OE1	2.39	0.55
2:B:1042:ILE:HG22	2:B:1052:ILE:HD11	1.88	0.55
3:D:542:VAL:HA	3:D:545:MET:HG3	1.88	0.55
3:D:550:ILE:HA	3:D:558:ARG:HG2	1.88	0.55
3:D:926:THR:HA	3:D:929:LYS:HD3	1.89	0.54
3:D:379:VAL:HG13	3:D:422:LEU:HD11	1.90	0.54
6:G:433:SER:OG	6:G:435:ASP:OD1	2.25	0.54
3:D:824:CYS:HB3	3:D:863:ILE:HG23	1.88	0.54
3:D:722:LEU:HD22	3:D:726:ALA:HB2	1.90	0.54
3:D:668:TRP:HE3	3:D:671:LEU:HD11	1.73	0.54
2:B:92:PHE:HB3	2:B:95:TYR:HB2	1.89	0.54
3:D:146:THR:HA	3:D:149:LYS:HB2	1.89	0.54
3:D:956:ALA:O	3:D:960:ASN:ND2	2.41	0.54
1:A:145:ILE:HB	1:A:1113:ASP:HB3	1.90	0.53
1:A:182:GLN:HA	1:A:185:ILE:HG12	1.90	0.53
3:D:955:VAL:HB	3:D:994:ILE:HD11	1.90	0.53
3:D:1112:ARG:NH1	3:D:1155:LYS:O	2.42	0.53
1:A:157:LYS:HB2	1:A:160:GLU:HB2	1.90	0.53
3:D:110:ARG:HH22	3:D:152:PRO:HA	1.73	0.53
3:D:772:SER:O	3:D:776:LYS:NZ	2.40	0.53
3:D:1231:MET:HE1	3:D:1256:MET:HB2	1.91	0.53
6:G:462:PRO:O	6:G:465:ARG:NH1	2.41	0.53
3:D:646:LEU:O	3:D:650:ASN:ND2	2.42	0.53
3:D:1112:ARG:HH12	3:D:1160:ARG:HH22	1.56	0.53
3:D:16:PRO:HG3	3:D:42:ILE:HG12	1.91	0.53
2:B:1145:LYS:HD3	2:B:1209:HIS:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:709:HIS:O	3:D:715:SER:OG	2.24	0.53
3:D:781:VAL:HG11	3:D:802:LEU:HD21	1.90	0.53
3:D:110:ARG:NH1	3:D:150:SER:O	2.42	0.53
2:B:278:ASN:HB3	2:B:1117:ARG:HD3	1.91	0.53
6:G:402:LYS:HA	6:G:446:MET:HE1	1.90	0.53
2:B:1086:MET:HB3	2:B:1088:PRO:HD3	1.91	0.52
1:A:185:ILE:HA	1:A:188:LYS:HG2	1.92	0.52
2:B:213:LEU:HD22	2:B:218:ILE:HD12	1.91	0.52
2:B:338:GLU:HA	2:B:341:LYS:HE2	1.90	0.52
3:D:1013:TRP:HB3	3:D:1018:PHE:HE1	1.74	0.52
3:D:693:SER:HA	3:D:698:PHE:HE2	1.74	0.52
4:H:512:HIS:HB3	4:H:551:ARG:HH12	1.73	0.52
6:G:184:CYS:SG	6:G:188:ARG:NH1	2.81	0.52
2:B:278:ASN:HB3	2:B:1117:ARG:CD	2.39	0.52
3:D:284:LEU:HD23	3:D:289:HIS:HB3	1.91	0.52
3:D:628:VAL:HA	3:D:636:GLN:HG2	1.91	0.52
6:G:225:GLY:HA2	6:G:228:PHE:CE1	2.45	0.52
2:B:81:ARG:NH1	2:B:82:LEU:O	2.42	0.52
2:B:269:VAL:HG12	2:B:273:ARG:HE	1.75	0.52
6:G:504:LEU:HD22	6:G:547:ASN:HD22	1.75	0.52
2:B:1055:ILE:HB	2:B:1063:LEU:HD21	1.91	0.52
4:H:65:CYS:HB2	4:H:70:LYS:HG3	1.91	0.52
2:B:214:ARG:NH2	2:B:221:ASP:OD1	2.43	0.51
2:B:1082:ARG:O	2:B:1086:MET:HG2	2.10	0.51
3:D:57:LEU:HD23	3:D:119:LEU:HD13	1.91	0.51
3:D:233:LYS:HE3	3:D:288:ILE:HG13	1.91	0.51
1:A:158:PRO:HA	1:A:161:ILE:HG22	1.91	0.51
6:G:522:ILE:HG22	6:G:525:SER:HB2	1.91	0.51
1:A:170:GLY:HA2	1:A:172:ARG:HH11	1.76	0.51
6:G:220:ILE:HG23	6:G:265:ILE:HD11	1.92	0.51
6:G:262:ILE:HD13	6:G:265:ILE:HD12	1.92	0.51
2:B:108:PHE:HB2	2:B:1260:ASP:H	1.76	0.50
3:D:977:ASP:N	3:D:977:ASP:OD1	2.43	0.50
1:A:954:ALA:O	1:A:958:LYS:NZ	2.44	0.50
4:H:360:GLN:HG2	6:G:549:ALA:HB2	1.93	0.50
1:A:1095:LEU:HD12	1:A:1096:SER:N	2.26	0.50
2:B:68:PRO:HB3	2:B:1131:ARG:HH22	1.77	0.50
2:B:87:ILE:HD12	2:B:101:LEU:HD22	1.94	0.50
2:B:1256:PHE:HB2	2:B:1262:LEU:HD22	1.93	0.50
2:B:89:ASN:HB3	2:B:92:PHE:HB2	1.94	0.50
6:G:227:ARG:HH21	6:G:268:ARG:HG2	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ILE:HA	1:A:48:LEU:HG	1.94	0.49
2:B:1101:GLU:O	2:B:1105:GLN:N	2.44	0.49
2:B:1250:SER:OG	2:B:1251:LEU:N	2.45	0.49
3:D:224:LEU:HD23	3:D:227:LEU:HD12	1.94	0.49
2:B:106:LYS:HE3	2:B:107:ARG:HH11	1.76	0.49
3:D:1155:LYS:O	3:D:1160:ARG:NH1	2.46	0.49
1:A:7:ILE:HG13	1:A:80:SER:HB3	1.93	0.49
2:B:1091:GLY:HA2	2:B:1094:ALA:HB3	1.95	0.49
2:B:1094:ALA:O	2:B:1098:LYS:CB	2.58	0.49
3:D:695:LYS:HB3	3:D:697:LYS:HG2	1.93	0.49
3:D:1138:ALA:HA	3:D:1141:LEU:HD12	1.95	0.49
6:G:557:TYR:O	6:G:561:HIS:ND1	2.46	0.49
1:A:240:LEU:HD22	1:A:947:LEU:HB3	1.94	0.49
3:D:243:ILE:HG21	3:D:299:VAL:HG23	1.95	0.49
3:D:1250:SER:HA	3:D:1253:GLU:OE1	2.13	0.49
4:H:177:LYS:O	4:H:180:ARG:NH2	2.41	0.49
2:B:329:GLU:HB2	2:B:1064:GLU:HA	1.95	0.49
1:A:200:GLU:O	1:A:204:THR:OG1	2.31	0.49
1:A:1108:PRO:HG2	1:A:1109:ILE:HD12	1.95	0.49
2:B:265:GLU:HA	2:B:268:LYS:HD2	1.94	0.49
4:H:164:PRO:HA	4:H:175:SER:HA	1.95	0.49
3:D:832:GLU:OE2	3:D:874:ARG:NH1	2.46	0.49
6:G:280:ALA:O	6:G:284:ASP:HB2	2.13	0.48
3:D:32:PHE:HB3	3:D:139:MET:HB3	1.94	0.48
1:A:211:LYS:HA	1:A:214:ARG:HG2	1.95	0.48
2:B:236:ALA:HB1	2:B:1196:LYS:HD3	1.95	0.48
2:B:278:ASN:OD1	2:B:281:ARG:NH1	2.46	0.48
3:D:342:VAL:O	3:D:343:ASP:C	2.55	0.48
3:D:838:ILE:O	3:D:843:ASN:ND2	2.41	0.48
3:D:1235:ARG:CZ	3:D:1256:MET:HE2	2.44	0.48
3:D:567:SER:O	3:D:570:LYS:NZ	2.36	0.48
3:D:603:LEU:HD13	3:D:620:TRP:CD1	2.49	0.48
2:B:1090:LEU:HD22	2:B:1093:ILE:HD12	1.96	0.48
3:D:1235:ARG:NH1	3:D:1256:MET:HG3	2.29	0.48
1:A:1022:LEU:HA	1:A:1025:LYS:HB2	1.95	0.48
3:D:449:MET:HA	3:D:452:ARG:HB2	1.95	0.48
1:A:124:ASN:OD1	1:A:128:GLN:NE2	2.45	0.48
3:D:1217:ILE:HG22	3:D:1219:ALA:H	1.79	0.47
3:D:100:VAL:HG22	3:D:110:ARG:HA	1.96	0.47
6:G:528:PRO:HD3	6:G:539:ARG:HD2	1.95	0.47
1:A:217:TYR:HD2	1:A:984:ASN:HD22	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:440:VAL:O	6:G:443:CYS:HB2	2.14	0.47
1:A:162:LEU:O	1:A:166:GLU:HB2	2.14	0.47
3:D:427:VAL:HA	3:D:439:LEU:HD13	1.95	0.47
6:G:468:LEU:HD21	6:G:506:ARG:HB2	1.96	0.47
2:B:167:ILE:HD12	2:B:177:VAL:HG12	1.97	0.47
3:D:590:ASP:HB2	3:D:595:VAL:HG11	1.96	0.47
3:D:1098:LYS:HG2	3:D:1101:LYS:HZ3	1.79	0.47
1:A:909:LYS:HD3	2:B:1018:LEU:HD22	1.97	0.47
2:B:315:ILE:HA	2:B:318:LYS:HD2	1.97	0.47
3:D:625:VAL:HG11	3:D:681:LEU:HD22	1.96	0.47
3:D:834:ARG:NH1	3:D:856:TYR:OH	2.48	0.47
3:D:1051:MET:O	3:D:1055:HIS:ND1	2.44	0.47
3:D:1236:ASP:OD1	3:D:1236:ASP:N	2.46	0.47
2:B:319:LYS:NZ	2:B:1072:ILE:O	2.48	0.47
2:B:1136:MET:HA	2:B:1139:PHE:HB3	1.96	0.47
3:D:466:SER:O	3:D:470:HIS:ND1	2.48	0.47
3:D:1069:HIS:O	3:D:1074:LYS:NZ	2.48	0.47
3:D:242:CYS:HA	3:D:245:VAL:HG22	1.97	0.47
3:D:1112:ARG:NH1	3:D:1153:GLU:O	2.42	0.47
4:H:329:LYS:O	6:G:393:ARG:NH2	2.48	0.47
3:D:629:MET:HB3	3:D:684:TYR:HE1	1.80	0.46
4:H:17:ASP:O	4:H:21:ASN:N	2.47	0.46
6:G:528:PRO:HB2	6:G:531:GLN:HB2	1.96	0.46
3:D:674:LEU:HD22	3:D:681:LEU:HD11	1.96	0.46
3:D:1135:ASP:N	3:D:1135:ASP:OD1	2.48	0.46
3:D:1254:TYR:CZ	3:D:1258:LYS:HD2	2.51	0.46
6:G:397:ILE:HD11	6:G:427:LEU:HD11	1.97	0.46
3:D:918:VAL:HG13	4:H:190:GLY:HA3	1.96	0.46
6:G:528:PRO:HG2	6:G:536:TRP:HD1	1.80	0.46
3:D:653:HIS:O	3:D:657:PHE:N	2.48	0.46
6:G:217:ILE:HG22	6:G:221:LYS:HE3	1.98	0.46
2:B:324:GLN:HA	2:B:327:ILE:HG12	1.96	0.46
2:B:1154:THR:HB	2:B:1181:PRO:HG3	1.97	0.46
3:D:1146:PHE:CZ	3:D:1223:LEU:HG	2.51	0.46
3:D:1208:LEU:O	3:D:1212:LEU:HB2	2.16	0.46
1:A:161:ILE:HA	1:A:164:MET:HG3	1.98	0.46
2:B:105:HIS:ND1	2:B:1261:ARG:HG2	2.31	0.46
2:B:128:PHE:HB3	2:B:187:ARG:HH12	1.80	0.46
2:B:327:ILE:HG22	2:B:1036:HIS:CE1	2.51	0.46
3:D:11:LEU:O	3:D:15:CYS:N	2.47	0.46
3:D:785:LEU:HD23	3:D:790:TRP:HZ3	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:ARG:NH1	1:A:113:ASN:O	2.49	0.46
1:A:117:ILE:HG12	1:A:122:ALA:HB2	1.96	0.46
2:B:1043:SER:HB3	2:B:1052:ILE:HG13	1.98	0.46
3:D:98:GLN:HA	3:D:101:HIS:HD2	1.79	0.46
3:D:390:TYR:HE1	3:D:419:LEU:HD11	1.81	0.45
4:H:166:TYR:HA	4:H:172:VAL:HA	1.98	0.45
4:H:189:ARG:NH2	4:H:201:PRO:O	2.47	0.45
3:D:147:LEU:HB3	3:D:249:LEU:HD11	1.99	0.45
2:B:202:LYS:NZ	2:B:203:LYS:O	2.49	0.45
2:B:1266:TYR:HB3	4:H:557:LEU:HD23	1.98	0.45
3:D:760:CYS:O	3:D:764:HIS:ND1	2.50	0.45
1:A:911:LYS:HD2	1:A:911:LYS:HA	1.75	0.45
2:B:88:VAL:HG23	2:B:161:GLU:HB2	1.98	0.45
2:B:91:ASN:HB2	2:B:158:CYS:HA	1.97	0.45
3:D:368:SER:HA	3:D:371:ARG:HE	1.82	0.45
6:G:255:GLN:H	6:G:258:LEU:HD12	1.82	0.45
6:G:388:PRO:O	6:G:393:ARG:NH2	2.49	0.45
2:B:235:ILE:HA	2:B:238:MET:HG3	1.99	0.45
3:D:707:ILE:O	3:D:710:THR:OG1	2.29	0.45
2:B:120:SER:HA	2:B:123:ILE:HG22	1.98	0.45
3:D:258:GLU:HA	3:D:333:GLN:HG2	1.98	0.45
3:D:1249:ALA:O	3:D:1252:LEU:HB2	2.16	0.45
2:B:1219:ASP:OD1	2:B:1219:ASP:N	2.48	0.45
3:D:208:ASP:OD1	3:D:208:ASP:N	2.49	0.45
3:D:282:TYR:HB2	3:D:337:PHE:HE1	1.82	0.45
2:B:102:GLY:HA2	4:H:573:LEU:HD11	1.98	0.45
2:B:212:LEU:O	2:B:216:HIS:ND1	2.45	0.45
3:D:331:ARG:NH1	3:D:373:PHE:O	2.49	0.45
4:H:361:ASP:O	6:G:552:ARG:NH1	2.49	0.45
6:G:301:PRO:O	6:G:304:SER:OG	2.32	0.45
1:A:106:GLN:HE22	1:A:116:LEU:HB2	1.82	0.45
3:D:611:PRO:HG2	3:D:612:ARG:HG3	1.99	0.45
4:H:550:CYS:HA	4:H:553:MET:HG2	1.99	0.45
2:B:260:CYS:HA	2:B:1131:ARG:HE	1.82	0.45
3:D:715:SER:O	3:D:719:TRP:N	2.48	0.45
3:D:751:ASN:O	3:D:754:THR:OG1	2.33	0.45
3:D:984:SER:HB2	3:D:1020:ARG:HD2	1.99	0.45
1:A:153:VAL:HA	1:A:156:MET:HG2	2.00	0.44
3:D:671:LEU:HD13	3:D:717:PRO:HB2	1.98	0.44
3:D:942:ILE:HG13	3:D:943:PRO:HD3	1.99	0.44
2:B:328:TYR:CG	2:B:1063:LEU:HD23	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:15:ILE:HD12	4:H:71:VAL:HG23	1.99	0.44
3:D:562:LEU:HA	3:D:565:LEU:HG	1.99	0.44
3:D:990:SER:O	3:D:995:ARG:NH2	2.50	0.44
4:H:337:TYR:HB3	6:G:469:HIS:HB2	1.98	0.44
6:G:212:GLU:HA	6:G:215:ILE:HD12	2.00	0.44
1:A:962:PRO:HD2	2:B:1035:TRP:CZ2	2.52	0.44
2:B:1070:ASP:OD1	2:B:1070:ASP:N	2.47	0.44
2:B:1261:ARG:NH1	2:B:1278:ASN:OD1	2.51	0.44
1:A:136:LEU:HG	1:A:141:PRO:HD3	1.99	0.44
3:D:866:LEU:O	4:H:166:TYR:OH	2.34	0.44
3:D:238:CYS:O	3:D:242:CYS:SG	2.75	0.44
3:D:457:ALA:HB3	3:D:460:VAL:HB	1.99	0.44
3:D:1108:THR:O	3:D:1112:ARG:N	2.48	0.44
6:G:172:ARG:HA	6:G:209:MET:HE1	1.98	0.44
3:D:799:VAL:HG21	3:D:862:ASP:HB3	1.99	0.44
3:D:955:VAL:O	3:D:959:ASN:ND2	2.51	0.44
1:A:1130:MET:HE3	1:A:1130:MET:HB3	1.85	0.44
3:D:103:LYS:O	3:D:110:ARG:NH2	2.51	0.44
3:D:996:LYS:HB3	3:D:1032:ILE:HG12	1.99	0.44
3:D:1071:LYS:HE2	3:D:1071:LYS:HB3	1.84	0.44
3:D:1194:LYS:HB3	3:D:1194:LYS:HE3	1.88	0.44
1:A:210:LEU:HD22	1:A:990:VAL:HG11	2.00	0.43
2:B:147:HIS:CD2	2:B:152:HIS:HB3	2.53	0.43
3:D:1129:ASP:HB3	3:D:1131:ILE:HG13	2.00	0.43
4:H:199:MET:HE3	4:H:199:MET:HB3	1.76	0.43
4:H:541:VAL:HB	4:H:549:VAL:HG22	2.00	0.43
1:A:1085:LEU:O	1:A:1090:ARG:NH2	2.47	0.43
3:D:1068:LYS:HE2	3:D:1068:LYS:HB2	1.86	0.43
6:G:528:PRO:O	6:G:536:TRP:NE1	2.51	0.43
3:D:428:ASP:HB3	3:D:431:LEU:HD12	2.01	0.43
6:G:435:ASP:OD1	6:G:435:ASP:N	2.50	0.43
6:G:535:VAL:HA	6:G:538:GLU:HG3	2.01	0.43
1:A:232:ARG:HA	1:A:235:ILE:HB	1.98	0.43
2:B:1145:LYS:HA	2:B:1148:GLU:HG2	2.01	0.43
3:D:345:LEU:O	3:D:347:GLU:N	2.51	0.43
6:G:449:ASP:OD1	6:G:449:ASP:N	2.52	0.43
1:A:933:LYS:NZ	1:A:937:ASP:OD1	2.51	0.43
1:A:947:LEU:HD22	1:A:951:PRO:HG3	1.99	0.43
3:D:13:PRO:HA	3:D:45:GLU:HG2	2.01	0.43
3:D:1139:SER:HB2	3:D:1218:PRO:HD2	1.99	0.43
4:H:325:SER:HB2	6:G:342:ARG:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:470:ASP:O	6:G:476:ARG:NH1	2.52	0.43
1:A:207:ILE:HD11	1:A:997:ARG:HH21	1.83	0.43
1:A:33:LEU:HB2	1:A:36:SER:HB2	2.00	0.43
1:A:988:MET:O	1:A:992:THR:OG1	2.20	0.43
2:B:1259:SER:OG	2:B:1261:ARG:O	2.34	0.43
1:A:1146:LYS:HB2	1:A:1149:MET:HE1	2.00	0.42
2:B:1262:LEU:HB2	2:B:1277:VAL:HG23	2.02	0.42
6:G:482:MET:HE2	6:G:482:MET:HB2	1.86	0.42
2:B:294:GLU:HG3	2:B:295:LYS:HD3	2.00	0.42
2:B:269:VAL:O	2:B:273:ARG:HG3	2.18	0.42
3:D:775:ASP:OD1	3:D:776:LYS:N	2.52	0.42
3:D:1215:ASN:HB3	3:D:1217:ILE:HG13	2.01	0.42
1:A:1095:LEU:HA	1:A:1098:ILE:HG12	2.00	0.42
2:B:1039:ILE:HB	2:B:1052:ILE:HG23	2.00	0.42
1:A:1072:VAL:O	1:A:1079:LYS:N	2.53	0.42
3:D:710:THR:HG22	3:D:719:TRP:HE1	1.85	0.42
4:H:365:TRP:HZ2	6:G:556:GLN:HB2	1.84	0.42
2:B:146:ILE:HG22	2:B:147:HIS:N	2.34	0.42
6:G:207:LYS:HA	6:G:210:LEU:HD12	2.00	0.42
6:G:325:GLU:HG3	6:G:329:ARG:HH21	1.84	0.42
1:A:4:LYS:HB2	1:A:4:LYS:HE2	1.83	0.42
6:G:507:LEU:HD13	6:G:507:LEU:HA	1.80	0.42
2:B:268:LYS:HA	2:B:1124:TYR:CE1	2.54	0.42
3:D:936:ASP:OD1	3:D:937:LEU:N	2.53	0.42
4:H:336:PRO:HG3	6:G:431:THR:HG22	2.02	0.42
6:G:290:MET:SD	6:G:334:ILE:HD12	2.60	0.42
6:G:334:ILE:H	6:G:334:ILE:HG12	1.69	0.42
6:G:480:VAL:HG11	6:G:518:LEU:HD22	2.02	0.42
2:B:126:MET:HA	2:B:129:VAL:HG22	2.01	0.42
2:B:99:LYS:HA	2:B:99:LYS:HD3	1.86	0.42
3:D:382:LEU:HD11	3:D:390:TYR:HD1	1.84	0.41
3:D:675:THR:HG22	3:D:717:PRO:HG3	2.02	0.41
4:H:524:LEU:HD23	4:H:527:ARG:HE	1.85	0.41
6:G:210:LEU:HD22	6:G:232:LEU:HD11	2.02	0.41
2:B:110:CYS:HB3	2:B:112:ILE:HG23	2.02	0.41
3:D:38:LEU:CD2	3:D:39:ASP:H	2.33	0.41
4:H:513:VAL:O	4:H:551:ARG:NH1	2.53	0.41
1:A:234:TYR:CG	1:A:957:PHE:HB3	2.55	0.41
3:D:384:LYS:HA	3:D:384:LYS:HD3	1.85	0.41
3:D:621:LEU:HA	3:D:624:VAL:HG22	2.01	0.41
1:A:12:LYS:HB2	1:A:12:LYS:HE3	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:170:LYS:NZ	2:B:174:ASP:OD2	2.51	0.41
3:D:550:ILE:HD13	3:D:587:GLN:HE21	1.84	0.41
3:D:553:GLU:O	3:D:558:ARG:NH2	2.53	0.41
3:D:803:GLN:HB2	3:D:866:LEU:HD11	2.02	0.41
3:D:1225:HIS:O	3:D:1228:ARG:HG3	2.20	0.41
1:A:1:MET:HE2	1:A:1108:PRO:HB2	2.01	0.41
2:B:1056:SER:HB2	2:B:1063:LEU:HD11	2.02	0.41
3:D:1220:LEU:HA	3:D:1223:LEU:HB2	2.01	0.41
4:H:567:ILE:HG23	4:H:580:MET:HB2	2.03	0.41
1:A:234:TYR:HE1	1:A:954:ALA:HA	1.85	0.41
2:B:1091:GLY:O	2:B:1095:GLU:HB2	2.20	0.41
3:D:600:LEU:HD12	3:D:603:LEU:HD11	2.03	0.41
4:H:528:PHE:CE2	4:H:582:LEU:HB2	2.55	0.41
6:G:197:ASP:HB3	6:G:200:LEU:HG	2.02	0.41
2:B:146:ILE:HD13	2:B:155:ILE:O	2.20	0.41
3:D:1065:ASN:HB2	3:D:1088:LYS:HE2	2.02	0.41
6:G:170:LEU:HG	6:G:186:LEU:HD21	2.01	0.41
1:A:172:ARG:HG2	1:A:173:MET:N	2.36	0.41
2:B:1271:ILE:O	2:B:1273:LYS:NZ	2.53	0.41
3:D:325:SER:HA	3:D:328:ILE:HD12	2.03	0.41
3:D:338:ILE:HA	3:D:341:LEU:HD12	2.02	0.41
3:D:388:GLY:HA2	3:D:431:LEU:HD21	2.03	0.41
3:D:630:ASP:O	3:D:636:GLN:NE2	2.53	0.41
3:D:1092:ASN:OD1	3:D:1095:ARG:NH1	2.52	0.41
6:G:495:TRP:HA	6:G:500:MET:HE3	2.02	0.41
1:A:1105:LYS:HA	1:A:1105:LYS:HD2	1.95	0.41
2:B:129:VAL:HG12	2:B:187:ARG:HD3	2.02	0.41
2:B:260:CYS:O	2:B:264:ASN:N	2.53	0.41
3:D:735:SER:HA	3:D:738:ILE:HD12	2.03	0.41
3:D:47:ILE:O	3:D:48:GLU:C	2.63	0.41
2:B:119:LYS:HE2	2:B:119:LYS:HB2	1.91	0.40
3:D:239:VAL:O	3:D:243:ILE:HB	2.20	0.40
3:D:1192:VAL:HA	3:D:1195:ARG:HG2	2.03	0.40
1:A:193:LYS:HA	1:A:1004:LYS:HD3	2.03	0.40
2:B:315:ILE:HD13	2:B:1078:LEU:HB3	2.02	0.40
2:B:1144:ASN:HA	2:B:1147:LYS:HG2	2.02	0.40
2:B:1228:LYS:HG2	4:H:506:LEU:HD13	2.03	0.40
3:D:401:SER:OG	3:D:402:ARG:NH1	2.54	0.40
3:D:820:LEU:HD21	3:D:866:LEU:HD12	2.04	0.40
3:D:1194:LYS:HD2	3:D:1234:TYR:CZ	2.57	0.40
6:G:487:LYS:HE3	6:G:487:LYS:HB2	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:ARG:HH21	1:A:124:ASN:HB2	1.87	0.40
1:A:988:MET:O	1:A:992:THR:N	2.51	0.40
3:D:354:ARG:HH21	3:D:396:TRP:HB2	1.87	0.40
3:D:753:ASN:O	3:D:757:HIS:ND1	2.55	0.40
3:D:1118:LYS:HD2	3:D:1118:LYS:HA	1.91	0.40
4:H:66:VAL:HG23	4:H:69:LYS:H	1.87	0.40
1:A:919:LYS:O	1:A:923:GLU:HB2	2.22	0.40
3:D:240:GLN:O	3:D:244:GLU:HB2	2.21	0.40
3:D:382:LEU:HD12	3:D:385:LEU:HD12	2.04	0.40
3:D:465:LEU:HD11	3:D:549:ARG:HG3	2.03	0.40
3:D:991:ASP:HA	3:D:992:PRO:HD3	1.97	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	509/1197 (42%)	497 (98%)	12 (2%)	0	100	100
2	B	523/1305 (40%)	507 (97%)	16 (3%)	0	100	100
3	D	1103/1498 (74%)	1078 (98%)	25 (2%)	0	100	100
4	H	240/640 (38%)	231 (96%)	9 (4%)	0	100	100
5	M	3/652 (0%)	3 (100%)	0	0	100	100
6	G	429/1143 (38%)	424 (99%)	5 (1%)	0	100	100
All	All	2807/6435 (44%)	2740 (98%)	67 (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	A	452/1040 (44%)	449 (99%)	3 (1%)	81	87
2	B	483/1165 (42%)	482 (100%)	1 (0%)	92	94
3	D	1014/1345 (75%)	1012 (100%)	2 (0%)	92	94
4	H	228/548 (42%)	227 (100%)	1 (0%)	89	91
5	M	5/549 (1%)	5 (100%)	0	100	100
6	G	394/1035 (38%)	392 (100%)	2 (0%)	86	89
All	All	2576/5682 (45%)	2567 (100%)	9 (0%)	90	92

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	173	MET
1	A	1099	LEU
1	A	1130	MET
2	B	146	ILE
3	D	38	LEU
3	D	1223	LEU
4	H	199	MET
6	G	443	CYS
6	G	507	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	56	GLN
1	A	69	ASN
1	A	106	GLN
1	A	229	HIS
1	A	257	GLN
1	A	916	ASN
1	A	920	HIS

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Mol	Chain	Res	Type
1	A	961	ASN
2	B	223	ASN
2	B	229	GLN
2	B	234	GLN
2	B	320	ASN
2	B	1075	GLN
2	B	1245	GLN
3	D	240	GLN
3	D	435	HIS
3	D	704	ASN
3	D	786	ASN
3	D	880	GLN
3	D	982	ASN
3	D	1182	GLN
3	D	1185	GLN
3	D	1225	HIS
3	D	1247	GLN
4	H	558	GLN
6	G	283	ASN
6	G	349	ASN
6	G	377	GLN
6	G	454	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](#)

There are no ligands in this entry.

## 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.

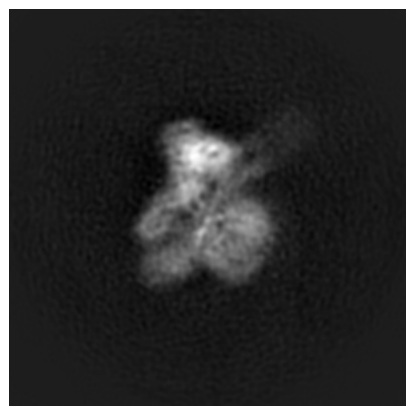
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50201. These allow visual inspection of the internal detail of the map and identification of artifacts.

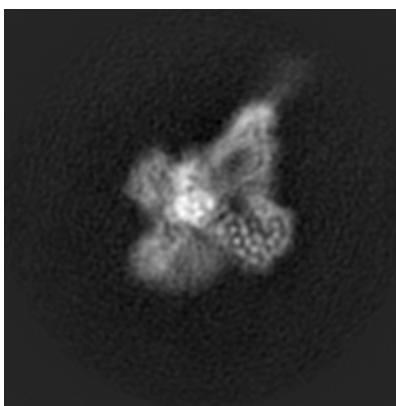
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

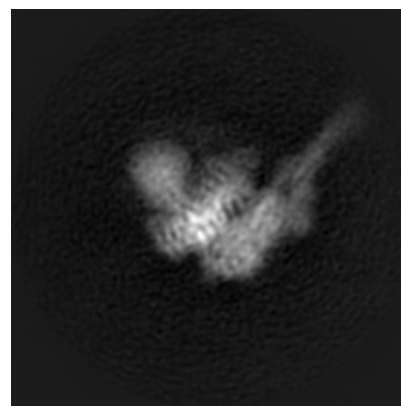
#### 6.1.1 Primary map



X

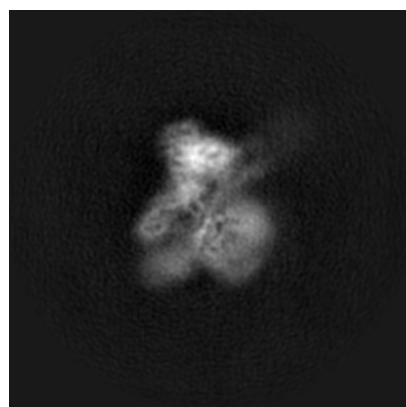


Y

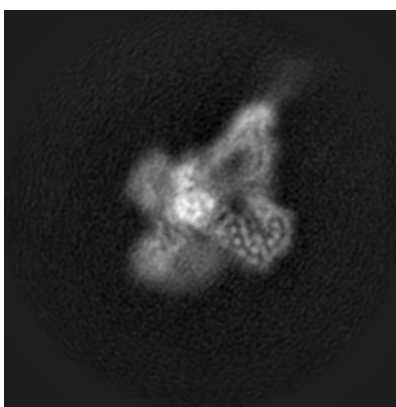


Z

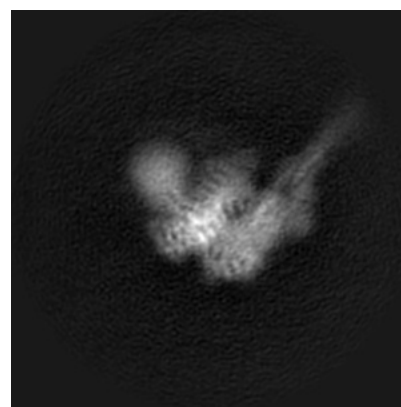
#### 6.1.2 Raw map



X



Y

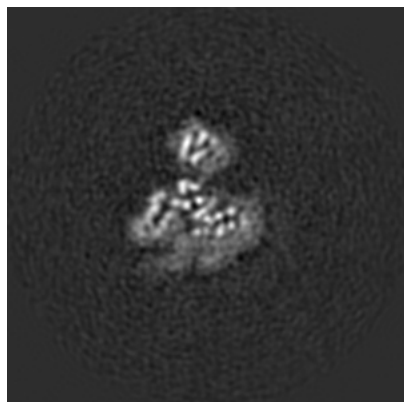


Z

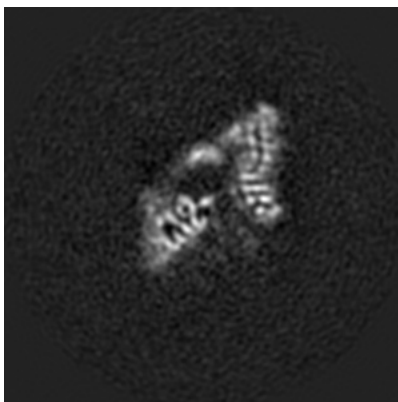
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

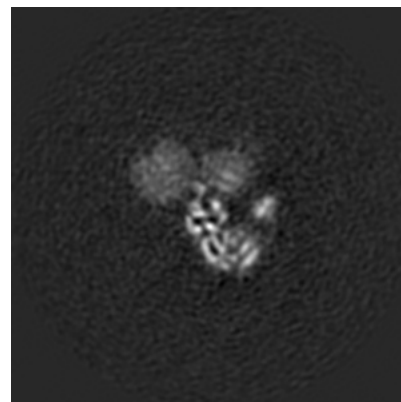
### 6.2.1 Primary map



X Index: 80

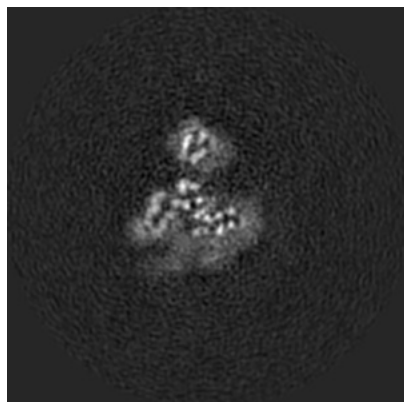


Y Index: 80

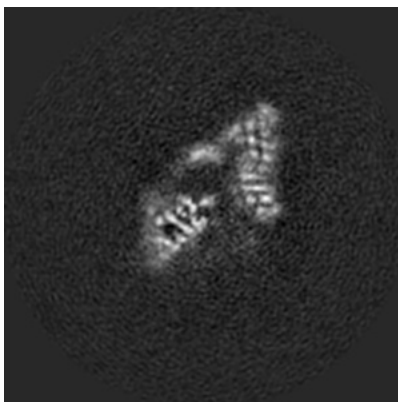


Z Index: 80

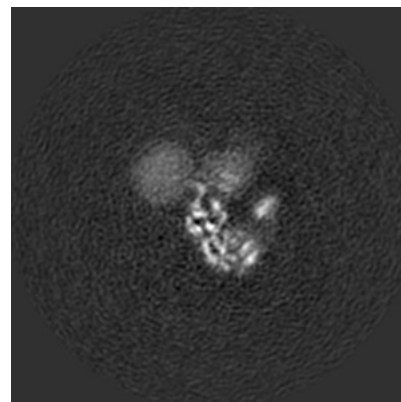
### 6.2.2 Raw map



X Index: 80



Y Index: 80

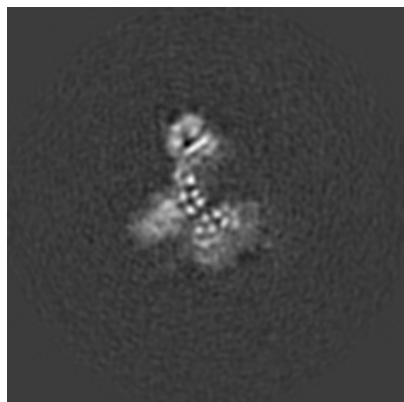


Z Index: 80

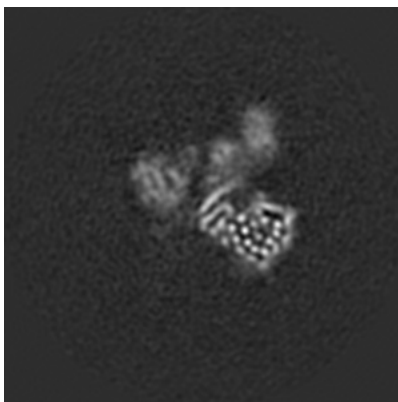
The images above show central slices of the map in three orthogonal directions.

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

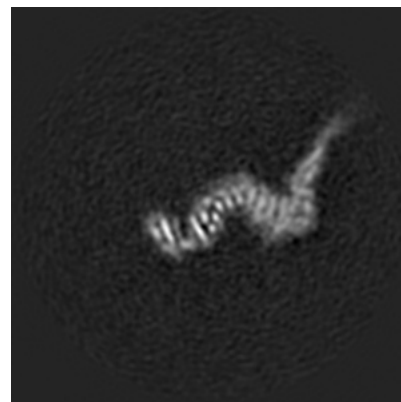
### 6.3.1 Primary map



X Index: 77

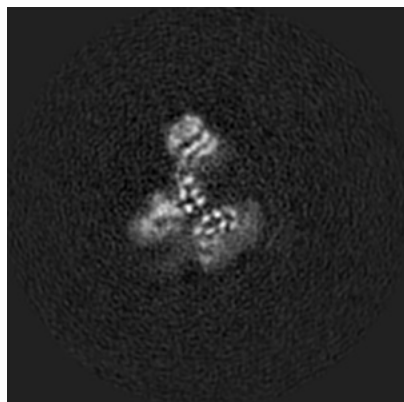


Y Index: 71

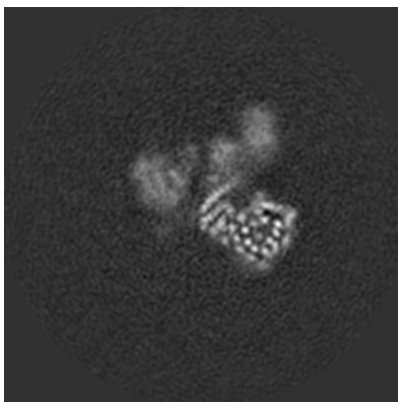


Z Index: 104

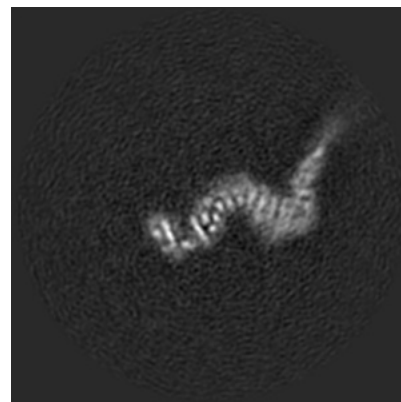
### 6.3.2 Raw map



X Index: 78



Y Index: 71

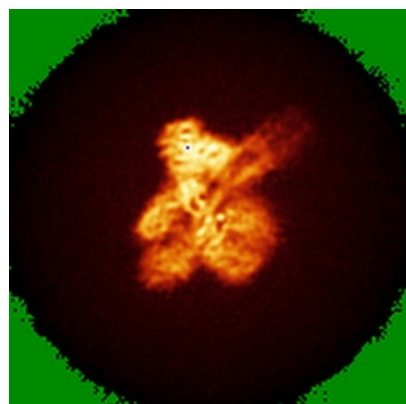


Z Index: 104

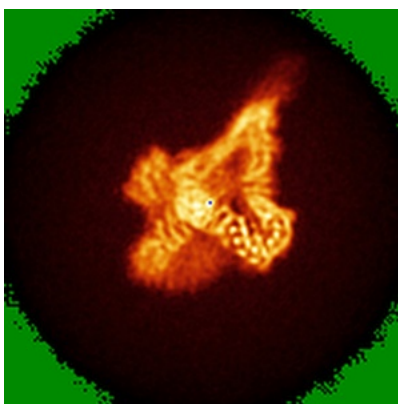
The images above show the largest variance slices of the map in three orthogonal directions.

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

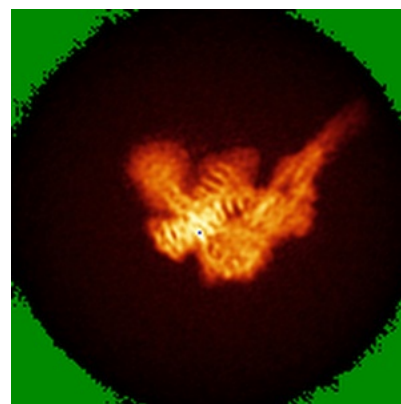
### 6.4.1 Primary map



X

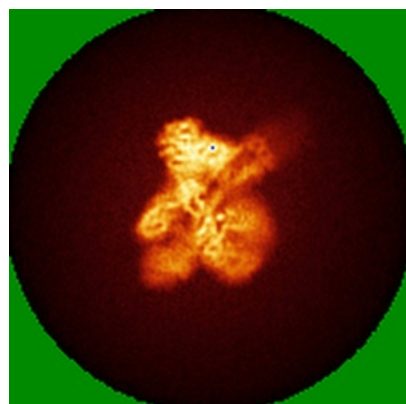


Y

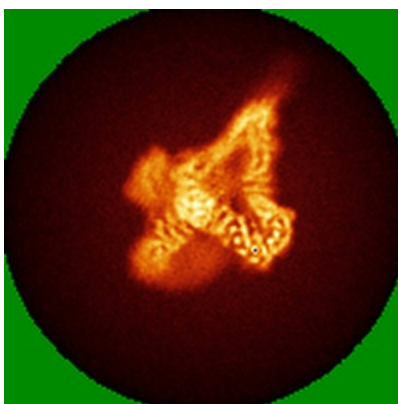


Z

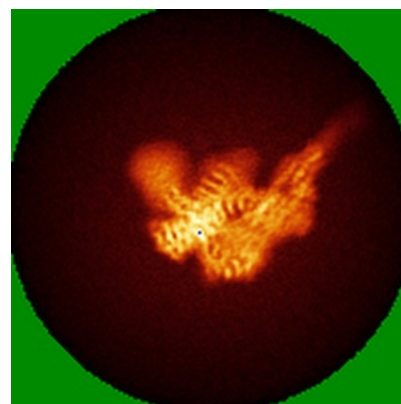
### 6.4.2 Raw map



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.



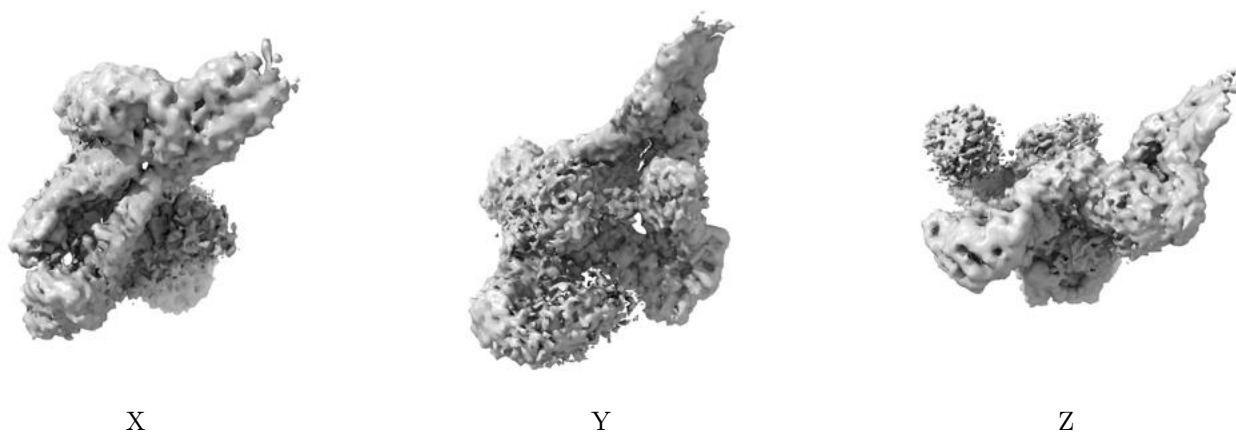
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0248. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

## 6.6 Mask visualisation [i](#)

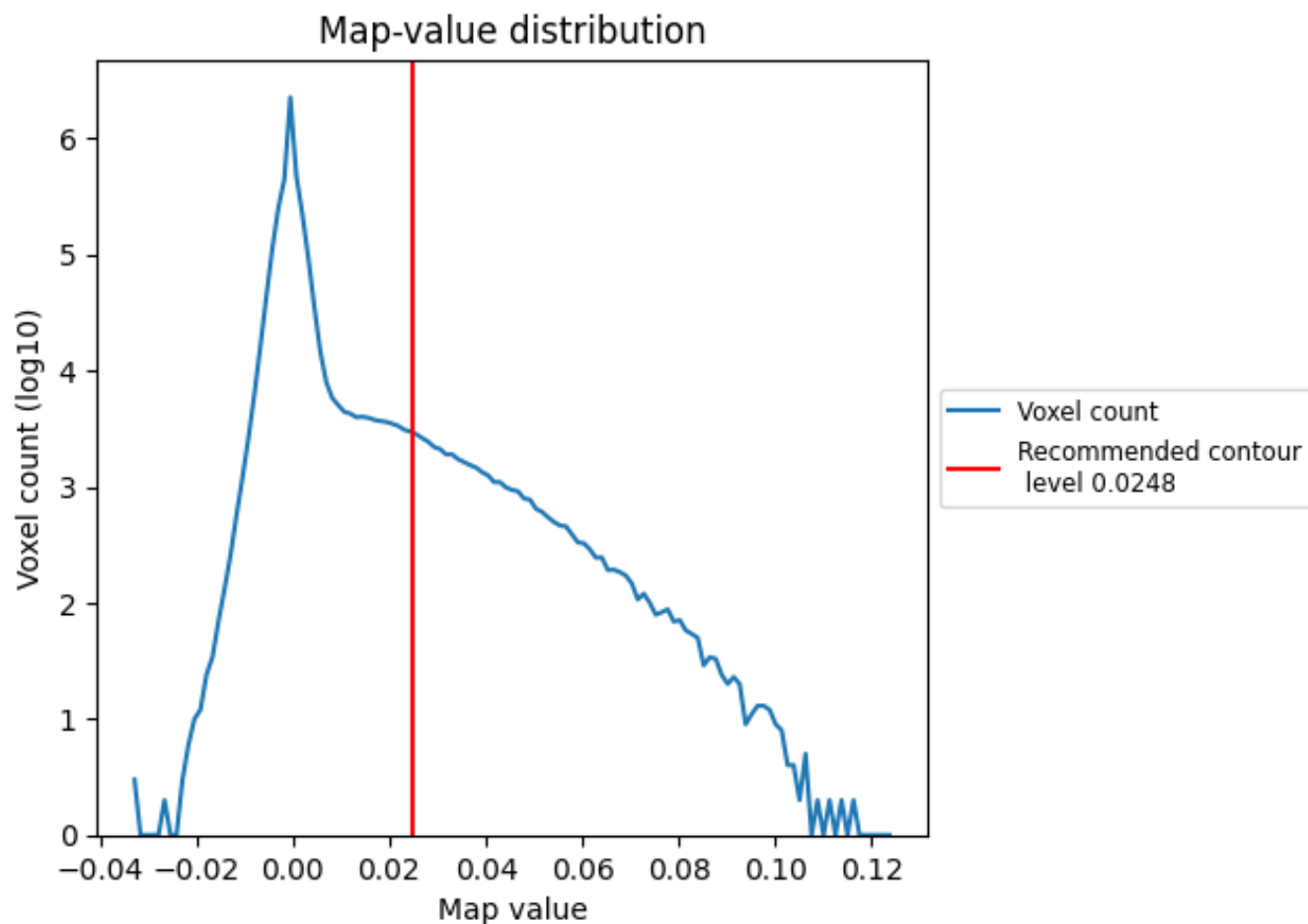
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

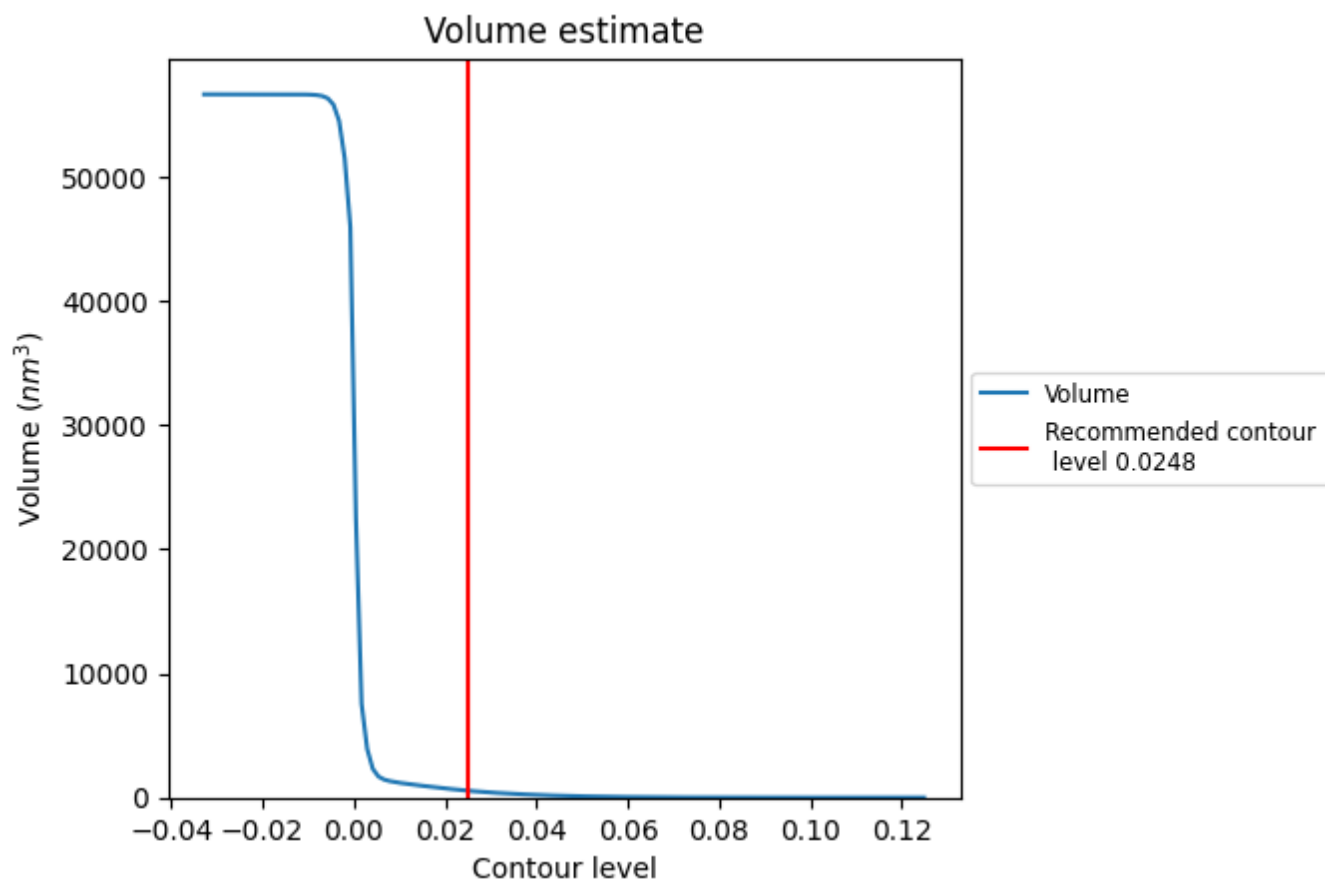
This section contains the results of statistical analysis of the map.

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



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

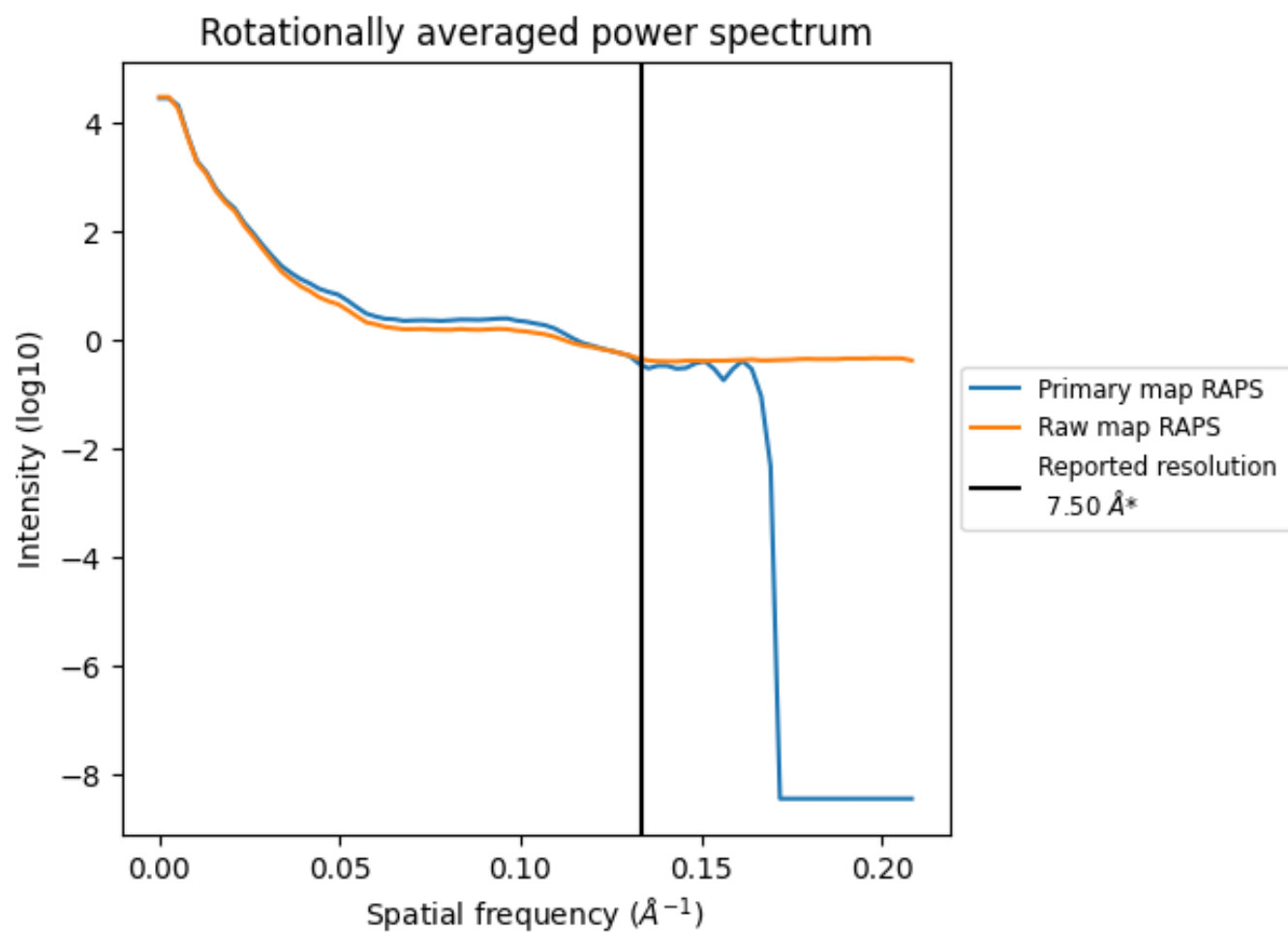
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 560 nm<sup>3</sup>; this corresponds to an approximate mass of 506 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 ⓘ

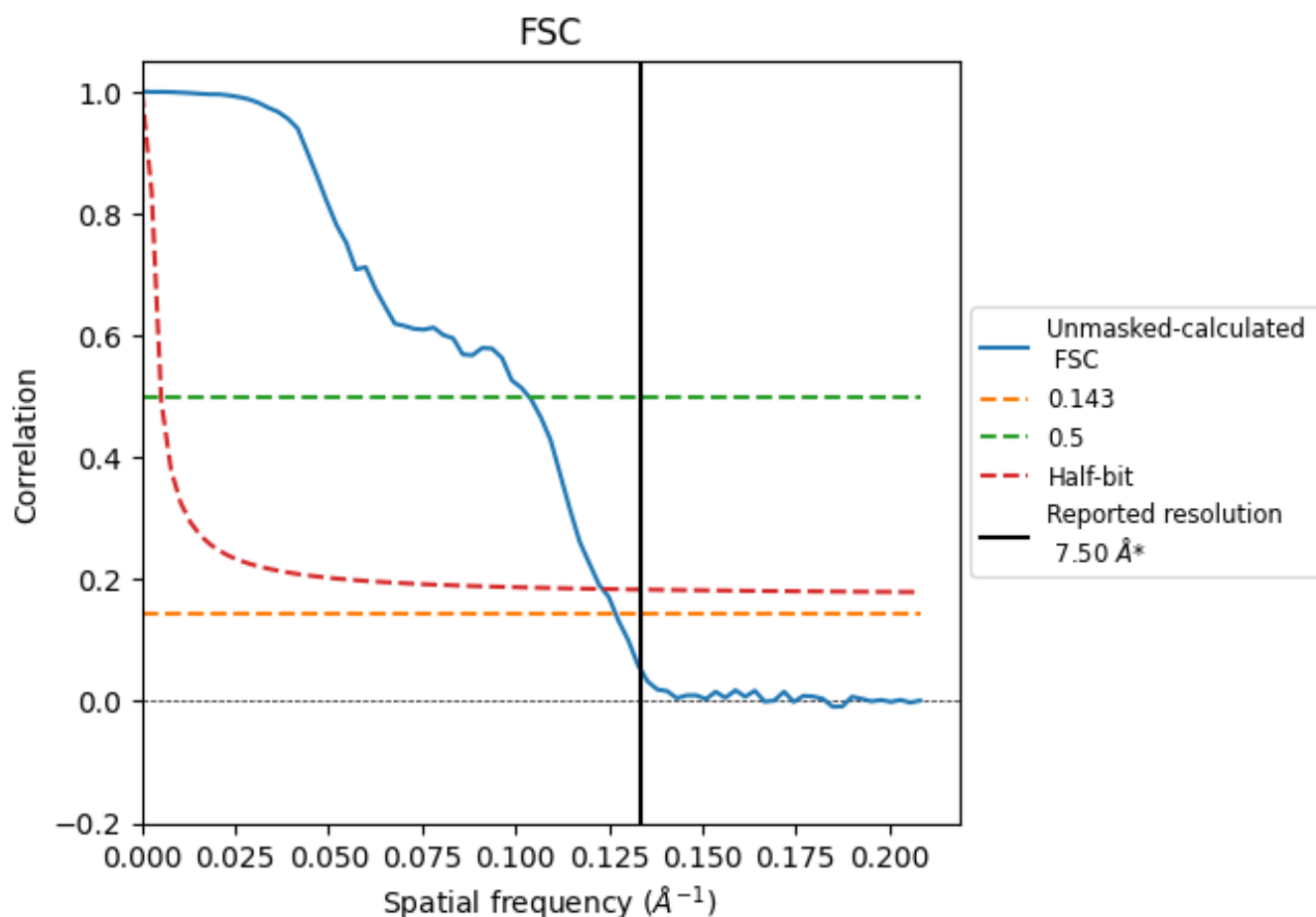


\*Reported resolution corresponds to spatial frequency of 0.133 Å<sup>-1</sup>

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

## 8.2 Resolution estimates [i](#)

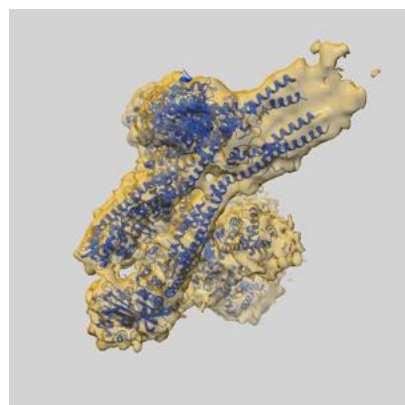
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.89	9.66	8.11

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

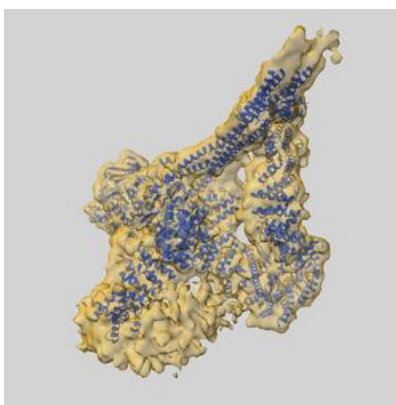
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-50201 and PDB model 9F5W. Per-residue inclusion information can be found in section [3](#) on page [6](#).

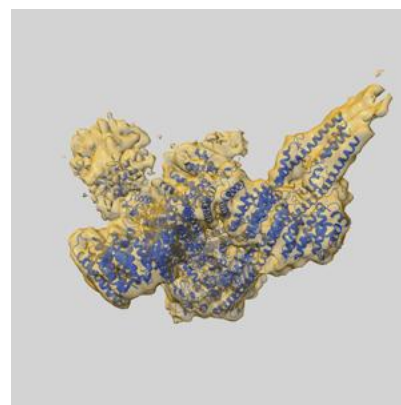
### 9.1 Map-model overlay [i](#)



X



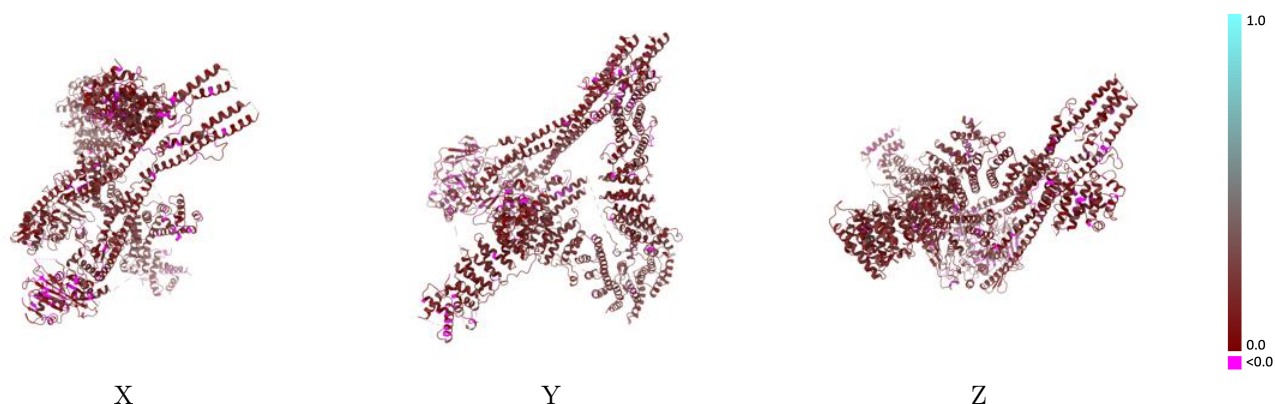
Y



Z

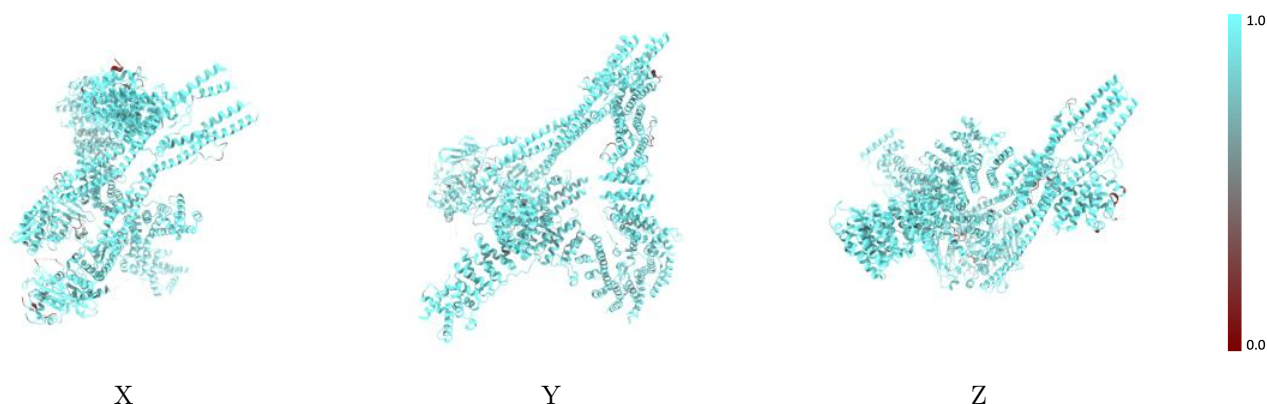
The images above show the 3D surface view of the map at the recommended contour level 0.0248 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



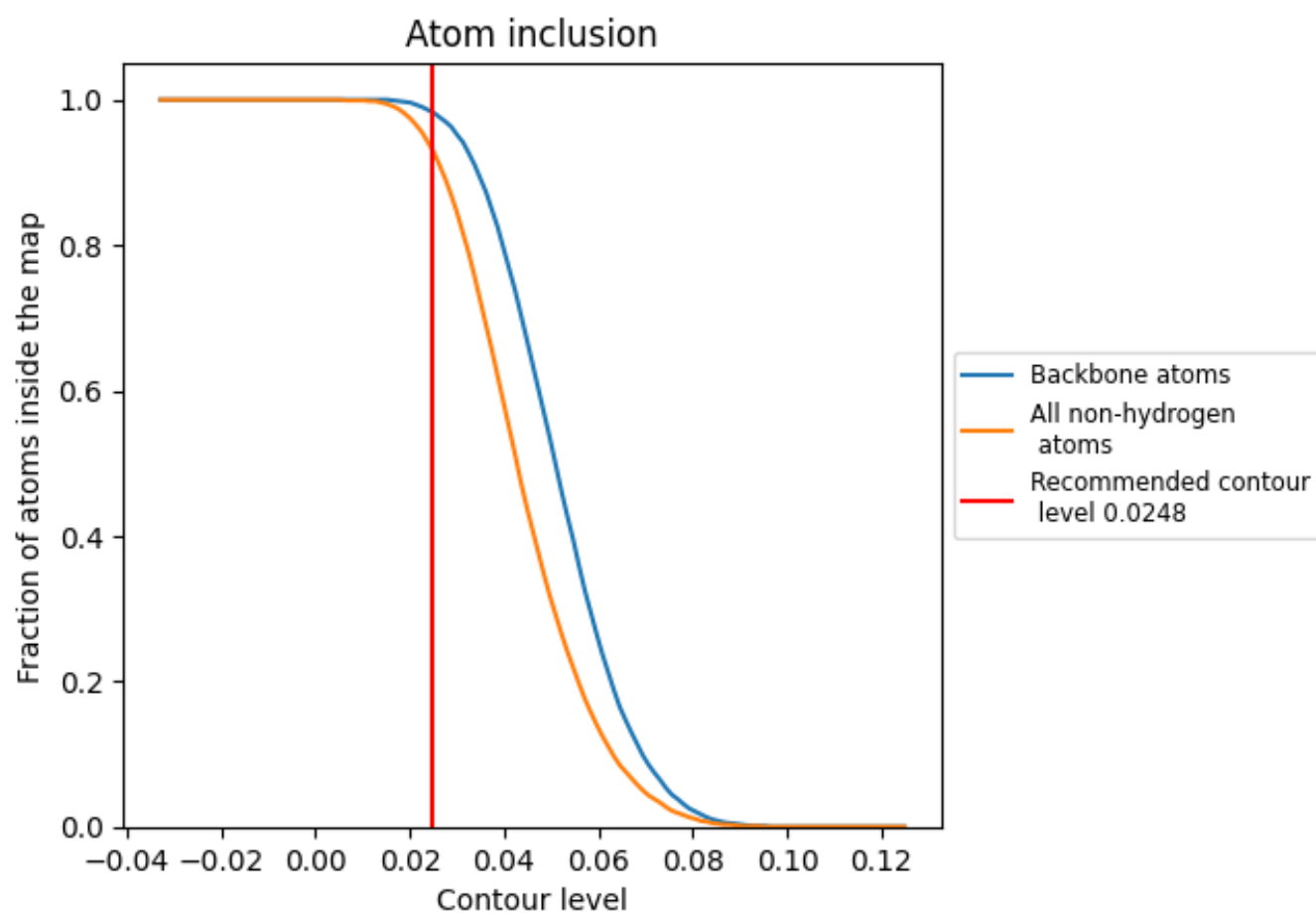
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0248).

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 98% of all backbone atoms, 93% 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 (0.0248) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.9320</div>	<div><div></div>0.1550</div>
A	<div><div></div>0.9390</div>	<div><div></div>0.1600</div>
B	<div><div></div>0.9320</div>	<div><div></div>0.1340</div>
D	<div><div></div>0.9340</div>	<div><div></div>0.1630</div>
G	<div><div></div>0.9380</div>	<div><div></div>0.1560</div>
H	<div><div></div>0.8970</div>	<div><div></div>0.1580</div>
M	<div><div></div>0.9790</div>	<div><div></div>0.0820</div>

1.0

0.0

<0.0