



## Full wwPDB EM Validation Report ⓘ

Mar 14, 2023 – 03:39 pm GMT

PDB ID : 8GZ7  
EMDB ID : EMD-34391  
Title : Octahedral supramolecular assembly of the bicomponent gamma-hemolysin octameric pore complexes from *Staphylococcus aureus* Newman.  
Authors : Mishra, S.; Roy, A.; Dutta, S.  
Deposited on : 2022-09-26  
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.32.1

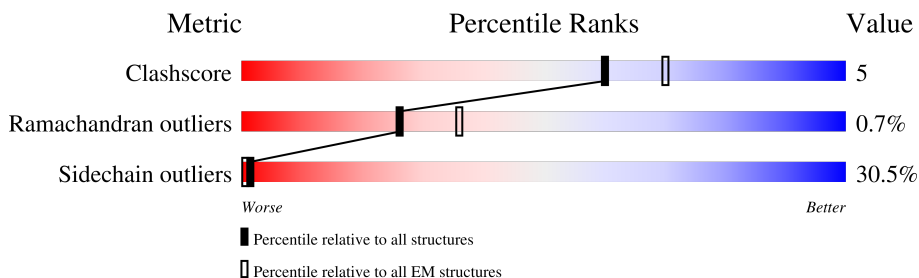
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.50 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	271	
1	C	271	
1	E	271	
1	G	271	
2	B	265	
2	D	265	
2	F	265	
2	H	265	

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 17474 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 Gamma-hemolysin component B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	270	2212	1404	379	426	3	0	0
1	C	270	2212	1404	379	426	3	0	0
1	E	270	2212	1404	379	426	3	0	0
1	G	270	2212	1404	379	426	3	0	0

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASP	deletion	UNP P0A077
A	?	-	ILE	deletion	UNP P0A077
A	?	-	SER	deletion	UNP P0A077
A	?	-	ILE	deletion	UNP P0A077
A	?	-	SER	deletion	UNP P0A077
A	?	-	ASN	deletion	UNP P0A077
A	?	-	GLY	deletion	UNP P0A077
A	?	-	LEU	deletion	UNP P0A077
A	?	-	SER	deletion	UNP P0A077
A	?	-	GLY	deletion	UNP P0A077
A	?	-	GLY	deletion	UNP P0A077
A	?	-	LEU	deletion	UNP P0A077
A	?	-	ASN	deletion	UNP P0A077
A	?	-	GLY	deletion	UNP P0A077
C	?	-	ASP	deletion	UNP P0A077
C	?	-	ILE	deletion	UNP P0A077
C	?	-	SER	deletion	UNP P0A077
C	?	-	ILE	deletion	UNP P0A077
C	?	-	SER	deletion	UNP P0A077
C	?	-	ASN	deletion	UNP P0A077
C	?	-	GLY	deletion	UNP P0A077
C	?	-	LEU	deletion	UNP P0A077

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	SER	deletion	UNP P0A077
C	?	-	GLY	deletion	UNP P0A077
C	?	-	GLY	deletion	UNP P0A077
C	?	-	LEU	deletion	UNP P0A077
C	?	-	ASN	deletion	UNP P0A077
C	?	-	GLY	deletion	UNP P0A077
E	?	-	ASP	deletion	UNP P0A077
E	?	-	ILE	deletion	UNP P0A077
E	?	-	SER	deletion	UNP P0A077
E	?	-	ILE	deletion	UNP P0A077
E	?	-	SER	deletion	UNP P0A077
E	?	-	ASN	deletion	UNP P0A077
E	?	-	GLY	deletion	UNP P0A077
E	?	-	LEU	deletion	UNP P0A077
E	?	-	SER	deletion	UNP P0A077
E	?	-	GLY	deletion	UNP P0A077
E	?	-	GLY	deletion	UNP P0A077
E	?	-	LEU	deletion	UNP P0A077
E	?	-	ASN	deletion	UNP P0A077
E	?	-	GLY	deletion	UNP P0A077
G	?	-	ASP	deletion	UNP P0A077
G	?	-	ILE	deletion	UNP P0A077
G	?	-	SER	deletion	UNP P0A077
G	?	-	ILE	deletion	UNP P0A077
G	?	-	SER	deletion	UNP P0A077
G	?	-	ASN	deletion	UNP P0A077
G	?	-	GLY	deletion	UNP P0A077
G	?	-	LEU	deletion	UNP P0A077
G	?	-	SER	deletion	UNP P0A077
G	?	-	GLY	deletion	UNP P0A077
G	?	-	GLY	deletion	UNP P0A077
G	?	-	LEU	deletion	UNP P0A077
G	?	-	ASN	deletion	UNP P0A077
G	?	-	GLY	deletion	UNP P0A077

- Molecule 2 is a protein called Gamma-hemolysin component A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	264	Total	C	N	O	S	0	0
			2155	1374	371	407	3		
2	D	264	Total	C	N	O	S	0	0
			2155	1374	371	407	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	264	Total	C	N	O	S	0	0
			2155	1374	371	407	3		
2	H	264	Total	C	N	O	S	1	0
			2161	1379	372	407	3		

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLY	deletion	UNP P0A074
B	?	-	ASN	deletion	UNP P0A074
B	?	-	PHE	deletion	UNP P0A074
B	?	-	GLN	deletion	UNP P0A074
B	?	-	SER	deletion	UNP P0A074
B	?	-	ALA	deletion	UNP P0A074
B	?	-	PRO	deletion	UNP P0A074
B	?	-	SER	deletion	UNP P0A074
B	?	-	ILE	deletion	UNP P0A074
B	?	-	GLY	deletion	UNP P0A074
B	?	-	GLY	deletion	UNP P0A074
B	?	-	SER	deletion	UNP P0A074
B	?	-	GLY	deletion	UNP P0A074
D	?	-	GLY	deletion	UNP P0A074
D	?	-	ASN	deletion	UNP P0A074
D	?	-	PHE	deletion	UNP P0A074
D	?	-	GLN	deletion	UNP P0A074
D	?	-	SER	deletion	UNP P0A074
D	?	-	ALA	deletion	UNP P0A074
D	?	-	PRO	deletion	UNP P0A074
D	?	-	SER	deletion	UNP P0A074
D	?	-	ILE	deletion	UNP P0A074
D	?	-	GLY	deletion	UNP P0A074
D	?	-	GLY	deletion	UNP P0A074
D	?	-	SER	deletion	UNP P0A074
D	?	-	GLY	deletion	UNP P0A074
F	?	-	GLY	deletion	UNP P0A074
F	?	-	ASN	deletion	UNP P0A074
F	?	-	PHE	deletion	UNP P0A074
F	?	-	GLN	deletion	UNP P0A074
F	?	-	SER	deletion	UNP P0A074
F	?	-	ALA	deletion	UNP P0A074
F	?	-	PRO	deletion	UNP P0A074
F	?	-	SER	deletion	UNP P0A074

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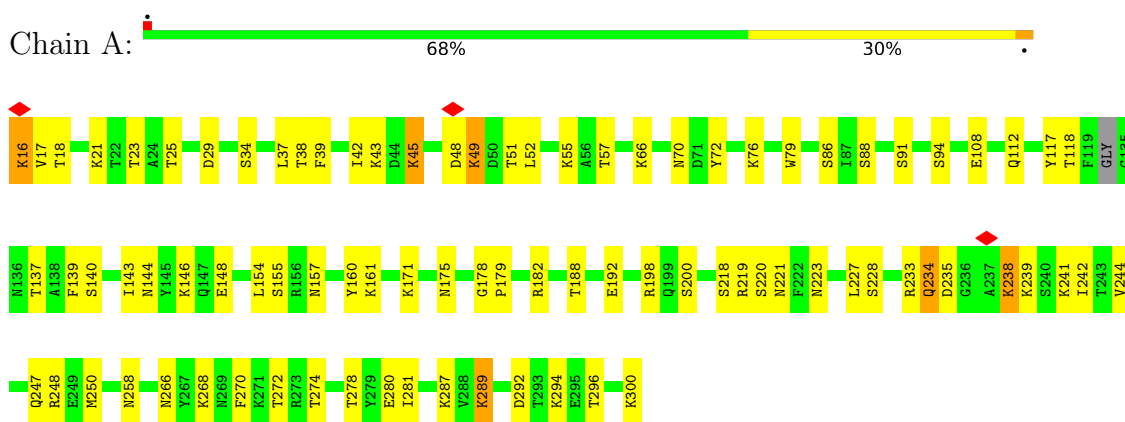
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Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	ILE	deletion	UNP P0A074
F	?	-	GLY	deletion	UNP P0A074
F	?	-	GLY	deletion	UNP P0A074
F	?	-	SER	deletion	UNP P0A074
F	?	-	GLY	deletion	UNP P0A074
H	?	-	GLY	deletion	UNP P0A074
H	?	-	ASN	deletion	UNP P0A074
H	?	-	PHE	deletion	UNP P0A074
H	?	-	GLN	deletion	UNP P0A074
H	?	-	SER	deletion	UNP P0A074
H	?	-	ALA	deletion	UNP P0A074
H	?	-	PRO	deletion	UNP P0A074
H	?	-	SER	deletion	UNP P0A074
H	?	-	ILE	deletion	UNP P0A074
H	?	-	GLY	deletion	UNP P0A074
H	?	-	GLY	deletion	UNP P0A074
H	?	-	SER	deletion	UNP P0A074
H	?	-	GLY	deletion	UNP P0A074

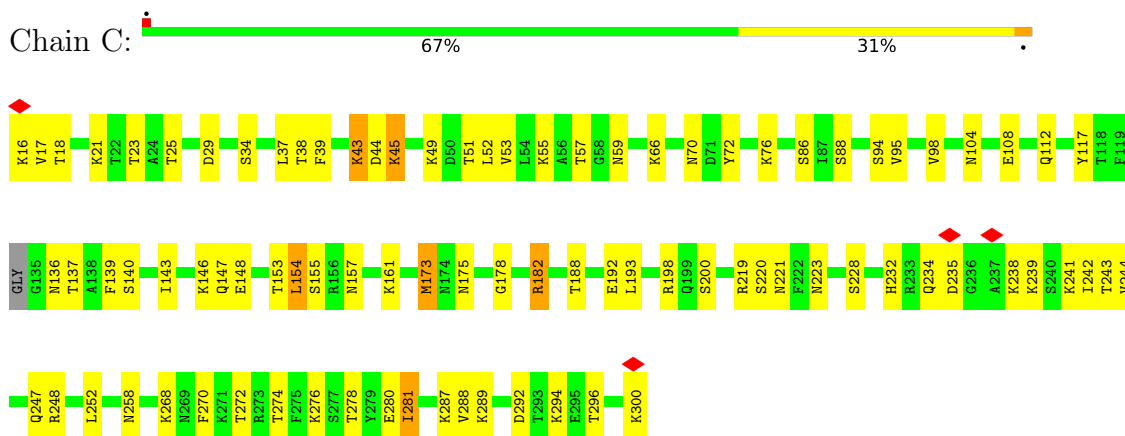
### 3 Residue-property plots

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.

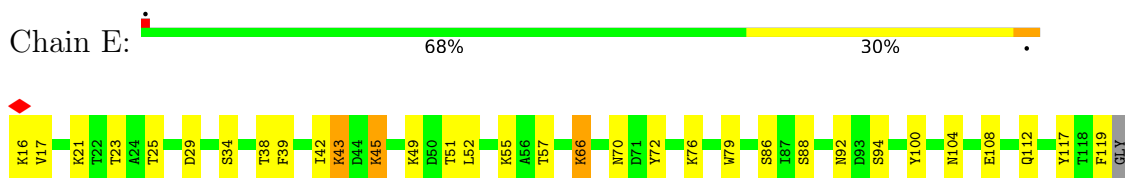
- Molecule 1: Gamma-hemolysin component B

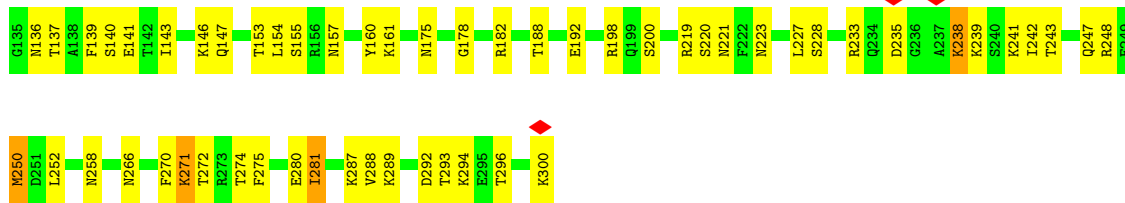


- Molecule 1: Gamma-hemolysin component B

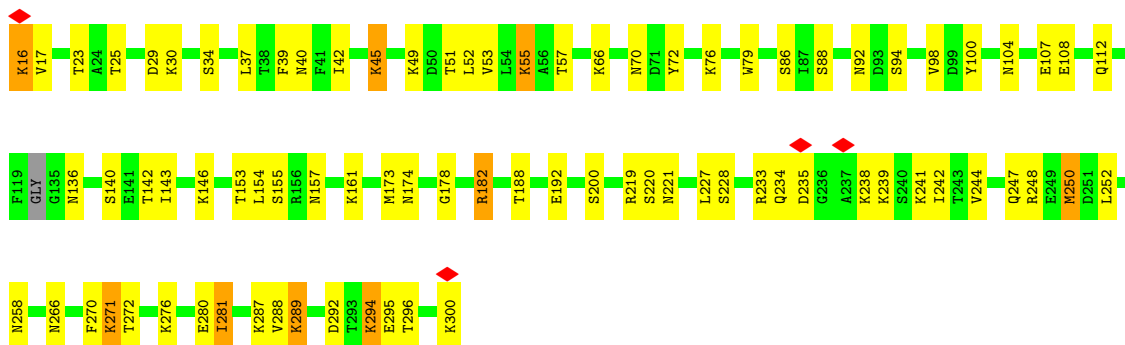


- Molecule 1: Gamma-hemolysin component B

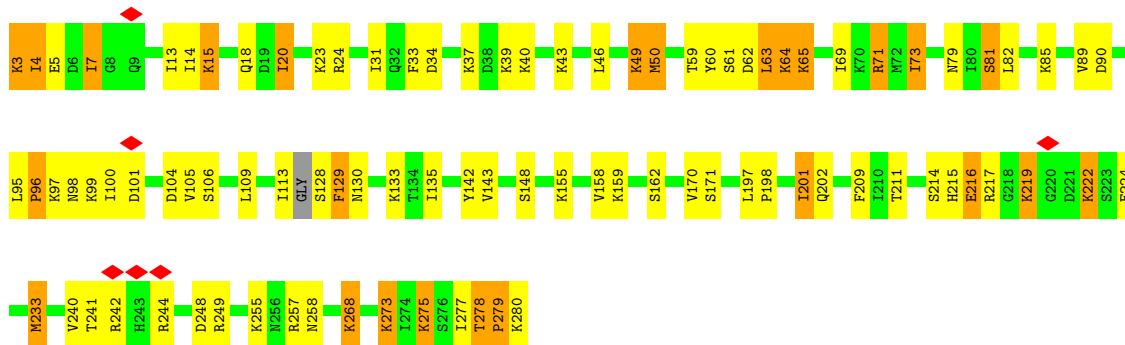




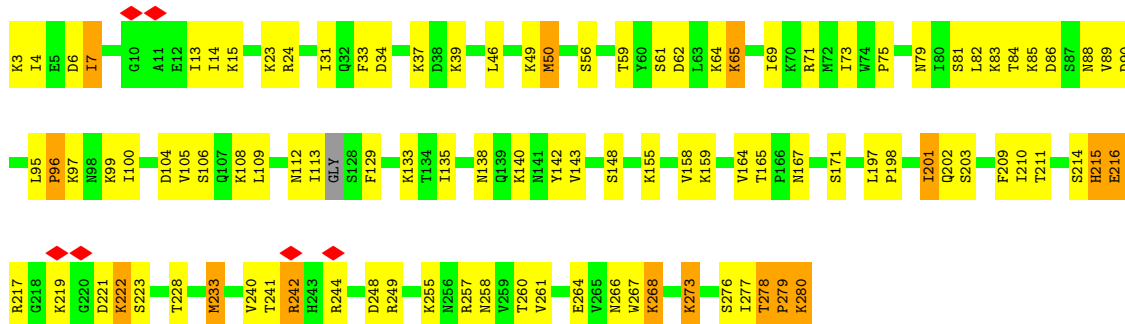
• Molecule 1: Gamma-hemolysin component B



• Molecule 2: Gamma-hemolysin component A

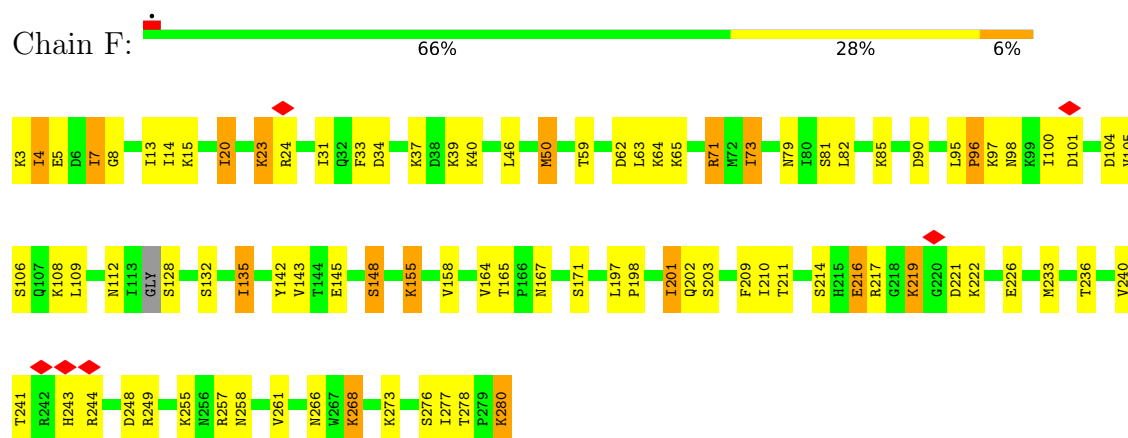


• Molecule 2: Gamma-hemolysin component A

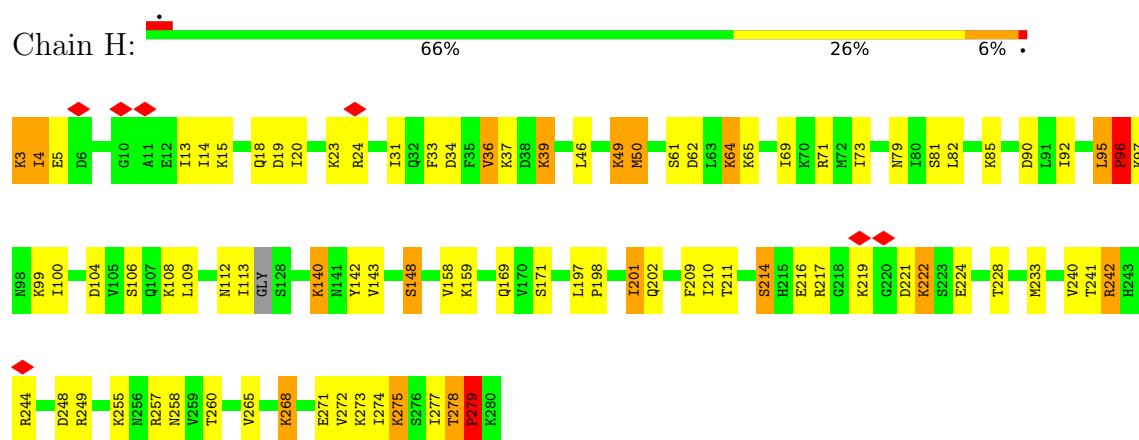




- Molecule 2: Gamma-hemolysin component A



- Molecule 2: Gamma-hemolysin component A



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	11634	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	3500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.676	Depositor
Minimum map value	-1.570	Depositor
Average map value	0.017	Depositor
Map value standard deviation	0.132	Depositor
Recommended contour level	0.427	Depositor
Map size ( $\text{\AA}$ )	368.0, 368.0, 368.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.92, 0.92, 0.92	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	0.58	0/2268	0.69	0/3065
1	C	0.58	0/2268	0.69	0/3065
1	E	0.58	0/2268	0.69	0/3065
1	G	0.58	0/2268	0.69	0/3065
2	B	0.60	0/2203	0.72	0/2973
2	D	0.60	0/2203	0.71	0/2973
2	F	0.60	0/2203	0.72	0/2973
2	H	0.67	2/2212 (0.1%)	0.79	6/2984 (0.2%)
All	All	0.60	2/17893 (0.0%)	0.71	6/24163 (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
1	A	0	1
1	C	0	1
1	E	0	1
1	G	0	1
2	B	0	2
2	D	0	2
2	F	0	1
2	H	0	2
All	All	0	11

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	3[A]	LYS	C-O	9.37	1.41	1.23
2	H	3[B]	LYS	C-O	9.37	1.41	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	3[A]	LYS	CA-C-O	7.18	135.18	120.10
2	H	3[B]	LYS	CA-C-O	7.18	135.18	120.10
2	H	3[A]	LYS	N-CA-C	6.32	128.05	111.00
2	H	3[B]	LYS	N-CA-C	6.32	128.05	111.00
2	H	279	PRO	CA-N-CD	-5.14	104.31	111.50
2	H	96	PRO	N-CA-C	5.03	125.19	112.10

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	178	GLY	Peptide
2	B	278	THR	Peptide
2	B	95	LEU	Peptide
1	C	178	GLY	Peptide
2	D	278	THR	Peptide
2	D	95	LEU	Peptide
1	E	178	GLY	Peptide
2	F	95	LEU	Peptide
1	G	178	GLY	Peptide
2	H	278	THR	Peptide
2	H	95	LEU	Peptide

## 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	2212	0	2113	32	0
1	C	2212	0	2113	14	0
1	E	2212	0	2113	15	0
1	G	2212	0	2113	17	0
2	B	2155	0	2147	31	0
2	D	2155	0	2147	22	0
2	F	2155	0	2147	19	0
2	H	2161	0	2159	23	0
All	All	17474	0	17052	161	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 (161) 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:49:LYS:CA	1:A:234:GLN:NE2	1.96	1.26
1:A:49:LYS:HA	1:A:234:GLN:NE2	1.50	1.21
1:A:233:ARG:NH2	1:A:235:ASP:OD1	1.77	1.18
1:A:235:ASP:OD1	1:A:235:ASP:O	1.69	1.10
1:A:49:LYS:N	1:A:234:GLN:HE22	1.52	1.08
1:A:49:LYS:CA	1:A:234:GLN:HE22	1.59	1.06
1:A:49:LYS:N	1:A:234:GLN:NE2	2.06	1.03
1:A:48:ASP:C	1:A:234:GLN:NE2	2.13	1.02
2:B:128:SER:C	2:B:129:PHE:HD2	1.64	1.00
1:A:49:LYS:HA	1:A:234:GLN:HE21	1.24	0.91
2:D:198:PRO:HG2	2:D:201:ILE:HG13	1.55	0.88
1:A:48:ASP:O	1:A:234:GLN:NE2	2.07	0.87
2:B:198:PRO:HG2	2:B:201:ILE:HG13	1.58	0.85
2:F:198:PRO:HG2	2:F:201:ILE:HG13	1.56	0.85
2:H:198:PRO:HG2	2:H:201:ILE:HG13	1.58	0.84
2:B:128:SER:C	2:B:129:PHE:CD2	2.54	0.75
1:A:37:LEU:HD21	1:A:244:VAL:HG21	1.72	0.71
1:C:37:LEU:HD21	1:C:244:VAL:HG21	1.72	0.70
1:G:37:LEU:HD21	1:G:244:VAL:HG21	1.73	0.70
1:A:233:ARG:CZ	1:A:235:ASP:OD1	2.41	0.68
1:A:233:ARG:NH2	1:A:235:ASP:CG	2.47	0.67
1:A:233:ARG:HH21	1:A:235:ASP:CG	1.97	0.66
2:B:129:PHE:HD2	2:B:129:PHE:N	1.94	0.65
1:G:39:PHE:HB3	1:G:52:LEU:HD11	1.79	0.64
1:A:39:PHE:HB3	1:A:52:LEU:HD11	1.82	0.61
1:A:49:LYS:C	1:A:234:GLN:HE22	2.03	0.61
1:E:39:PHE:HB3	1:E:52:LEU:HD11	1.84	0.59
1:C:39:PHE:HB3	1:C:52:LEU:HD11	1.85	0.58
1:A:49:LYS:CA	1:A:234:GLN:HE21	1.92	0.57
1:A:247:GLN:HB2	1:A:274:THR:HG23	1.87	0.56
2:B:129:PHE:CD2	2:B:129:PHE:N	2.67	0.56
1:A:48:ASP:C	1:A:234:GLN:HE21	1.95	0.55
1:E:247:GLN:HB2	1:E:274:THR:HG23	1.87	0.55
1:A:235:ASP:OD1	1:A:235:ASP:C	2.44	0.55
1:G:250:MET:HE3	1:G:271:LYS:HB2	1.90	0.54
1:G:79:TRP:HE1	1:G:266:ASN:HD21	1.55	0.53
1:G:227:LEU:HG	2:H:4:ILE:HD11	1.89	0.53
2:H:50:MET:HG3	2:H:209:PHE:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:128:SER:O	2:B:129:PHE:CD2	2.62	0.53
2:H:33:PHE:HB3	2:H:46:LEU:HD11	1.90	0.53
1:E:250:MET:HE3	1:E:271:LYS:HB2	1.91	0.52
1:G:55:LYS:HB2	2:H:4:ILE:HG21	1.92	0.52
2:B:33:PHE:HB3	2:B:46:LEU:HD11	1.91	0.52
2:F:33:PHE:HB3	2:F:46:LEU:HD11	1.91	0.51
2:D:33:PHE:HB3	2:D:46:LEU:HD11	1.92	0.51
1:C:247:GLN:HB2	1:C:274:THR:HG23	1.92	0.51
2:B:71:ARG:HD2	2:B:73:ILE:HG12	1.92	0.50
2:B:13:ILE:HG23	2:B:34:ASP:HB3	1.94	0.49
1:E:119:PHE:HB2	2:D:129:PHE:HB2	1.94	0.49
1:C:289:LYS:HE3	1:C:289:LYS:HB3	1.57	0.49
2:D:13:ILE:HG23	2:D:34:ASP:HB3	1.96	0.48
1:A:79:TRP:HE1	1:A:266:ASN:HD21	1.61	0.48
2:F:71:ARG:HD2	2:F:73:ILE:HG12	1.95	0.48
1:E:79:TRP:HE1	1:E:266:ASN:HD21	1.61	0.48
1:G:287:LYS:HB2	1:G:287:LYS:HE2	1.63	0.48
2:H:275:LYS:HA	2:H:275:LYS:HD2	1.44	0.48
2:B:3:LYS:HB2	2:B:3:LYS:HE2	1.51	0.47
2:H:13:ILE:HG23	2:H:34:ASP:HB3	1.96	0.47
2:D:216:GLU:H	2:D:216:GLU:HG2	1.55	0.47
2:B:50:MET:HG3	2:B:209:PHE:HB2	1.97	0.47
2:F:142:TYR:HB3	2:F:158:VAL:HG12	1.96	0.47
1:C:59:ASN:HD22	1:C:223:ASN:HD21	1.63	0.47
1:A:16:LYS:HB2	1:A:16:LYS:HE2	1.44	0.47
1:G:40:ASN:HD21	2:H:5:GLU:HB2	1.79	0.47
2:H:268:LYS:HB3	2:H:268:LYS:HE3	1.38	0.47
2:D:84:THR:HG22	2:D:86:ASP:H	1.79	0.47
2:H:142:TYR:HB3	2:H:158:VAL:HG12	1.97	0.47
1:G:294:LYS:HB3	1:G:294:LYS:HE2	1.37	0.46
2:H:242:ARG:HA	2:H:242:ARG:HD2	1.55	0.46
2:H:92:ILE:HD13	2:H:214:SER:HB3	1.97	0.46
2:B:219:LYS:HE2	2:B:219:LYS:HB2	1.41	0.46
1:E:104:ASN:HD21	2:D:203:SER:HB3	1.80	0.46
2:B:65:LYS:H	2:B:65:LYS:HG2	1.49	0.46
2:H:49:LYS:HE3	2:H:49:LYS:HB2	1.59	0.46
2:D:50:MET:HG3	2:D:209:PHE:HB2	1.98	0.46
2:D:242:ARG:HA	2:D:242:ARG:HD2	1.62	0.46
1:A:16:LYS:HD3	1:A:45:LYS:HE2	1.98	0.45
1:A:49:LYS:C	1:A:234:GLN:NE2	2.63	0.45
2:H:64:LYS:HE3	2:H:64:LYS:HB3	1.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:275:LYS:HA	2:B:275:LYS:HD2	1.46	0.45
1:C:43:LYS:HD3	1:C:43:LYS:HA	1.58	0.45
1:E:221:ASN:HD21	2:F:148:SER:HA	1.82	0.45
2:D:65:LYS:HD3	2:D:65:LYS:HA	1.42	0.45
2:D:142:TYR:HB3	2:D:158:VAL:HG12	1.98	0.45
2:D:233:MET:HE3	2:D:233:MET:HB3	1.62	0.45
2:B:20:ILE:HD12	2:B:20:ILE:HA	1.70	0.45
2:H:20:ILE:HD12	2:H:274:ILE:HD13	1.99	0.45
2:H:140:LYS:HB3	2:H:140:LYS:HE3	1.48	0.45
1:A:234:GLN:H	1:A:234:GLN:HG2	1.53	0.45
2:D:222:LYS:HB2	2:D:222:LYS:HE2	1.34	0.44
1:C:173:MET:HE3	1:C:173:MET:HB3	1.73	0.44
2:F:20:ILE:HD13	2:F:20:ILE:HA	1.69	0.44
1:C:95:VAL:HG22	1:C:232:HIS:HB2	1.98	0.44
1:G:221:ASN:HD21	2:H:148:SER:HA	1.82	0.44
2:B:142:TYR:HB3	2:B:158:VAL:HG12	1.98	0.44
1:A:287:LYS:HB2	1:A:287:LYS:HE2	1.65	0.44
2:B:15:LYS:H	2:B:15:LYS:HG2	1.68	0.44
2:B:222:LYS:HE3	2:B:222:LYS:HB2	1.65	0.44
2:D:280:LYS:HD3	2:D:280:LYS:HA	1.81	0.44
1:E:223:ASN:ND2	2:F:98:ASN:HB2	2.33	0.43
1:E:287:LYS:HB2	1:E:287:LYS:HE2	1.65	0.43
2:F:63:LEU:HD23	2:F:63:LEU:HA	1.85	0.43
2:F:219:LYS:HE2	2:F:219:LYS:HB2	1.71	0.43
2:H:222:LYS:HB2	2:H:222:LYS:HE2	1.41	0.43
1:C:287:LYS:HB2	1:C:287:LYS:HE2	1.64	0.43
2:B:105:VAL:HG22	2:B:135:ILE:HG23	2.01	0.43
2:F:50:MET:HG3	2:F:209:PHE:HB2	2.00	0.43
1:E:45:LYS:H	1:E:45:LYS:HG2	1.50	0.43
1:G:104:ASN:HD21	2:F:203:SER:HB3	1.83	0.43
2:B:89:VAL:HG22	2:B:215:HIS:HB2	1.99	0.43
1:A:171:LYS:HB3	1:A:179:PRO:HB3	1.99	0.43
1:A:221:ASN:HD21	2:B:148:SER:HA	1.84	0.43
2:B:7:ILE:H	2:B:7:ILE:HG12	1.75	0.43
2:B:216:GLU:H	2:B:216:GLU:HG2	1.55	0.43
2:B:273:LYS:HB3	2:B:273:LYS:HE3	1.31	0.43
2:B:268:LYS:HB3	2:B:268:LYS:HE3	1.53	0.43
1:G:16:LYS:HB2	1:G:16:LYS:HE3	1.70	0.43
1:C:45:LYS:H	1:C:45:LYS:HG2	1.42	0.43
1:G:107:GLU:H	1:G:107:GLU:HG2	1.67	0.43
2:B:64:LYS:HE3	2:B:64:LYS:HB3	1.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:13:ILE:HG23	2:F:34:ASP:HB3	2.00	0.42
1:A:238:LYS:H	1:A:238:LYS:HG3	1.43	0.42
1:E:238:LYS:H	1:E:238:LYS:HG3	1.37	0.42
2:B:49:LYS:HB2	2:B:49:LYS:HE2	1.40	0.42
2:F:216:GLU:H	2:F:216:GLU:HG2	1.57	0.42
1:C:281:ILE:HG23	1:C:288:VAL:HG22	2.01	0.42
1:E:66:LYS:H	1:E:66:LYS:HG3	1.50	0.42
2:F:268:LYS:HE3	2:F:268:LYS:HB3	1.63	0.42
1:C:104:ASN:OD1	1:C:154:LEU:HB2	2.20	0.42
1:E:281:ILE:HG23	1:E:288:VAL:HG22	2.01	0.42
1:C:182:ARG:H	1:C:182:ARG:HG3	1.58	0.42
2:B:63:LEU:HD22	2:B:63:LEU:HA	1.71	0.42
2:B:233:MET:HE3	2:B:233:MET:HB3	1.71	0.42
2:H:13:ILE:HG12	2:H:36:VAL:HG13	2.01	0.42
2:D:268:LYS:HE3	2:D:268:LYS:HB3	1.63	0.41
2:D:89:VAL:HG22	2:D:215:HIS:HB2	2.01	0.41
1:A:289:LYS:HB3	1:A:289:LYS:HE2	1.41	0.41
1:G:182:ARG:H	1:G:182:ARG:HG3	1.58	0.41
2:D:273:LYS:HE3	2:D:273:LYS:HB3	1.57	0.41
2:H:265:VAL:HG22	2:H:272:VAL:HG22	2.02	0.41
2:D:261:VAL:HG22	2:D:277:ILE:HG23	2.02	0.41
2:F:155:LYS:HB3	2:F:155:LYS:HE3	1.76	0.41
2:H:49:LYS:HG3	2:H:210:ILE:HG12	2.02	0.41
1:A:45:LYS:H	1:A:45:LYS:HG2	1.59	0.41
1:C:221:ASN:HD21	2:D:148:SER:HA	1.86	0.41
1:G:45:LYS:H	1:G:45:LYS:HG2	1.39	0.41
2:D:140:LYS:HB2	2:D:140:LYS:HE2	1.76	0.41
1:G:281:ILE:HG23	1:G:288:VAL:HG22	2.02	0.41
1:G:289:LYS:HB3	1:G:289:LYS:HE2	1.49	0.41
2:F:23:LYS:H	2:F:23:LYS:HG2	1.42	0.41
2:F:105:VAL:HG22	2:F:135:ILE:HG23	2.03	0.41
1:E:43:LYS:HA	1:E:43:LYS:HD3	1.76	0.41
2:B:81:SER:HB2	2:B:155:LYS:HD2	2.02	0.41
1:A:223:ASN:ND2	2:B:98:ASN:HB2	2.36	0.40
1:E:275:PHE:HE1	1:E:293:THR:HB	1.86	0.40
2:F:280:LYS:HD3	2:F:280:LYS:HA	1.69	0.40
2:D:223:SER:HB2	2:D:267:TRP:HE1	1.87	0.40
2:H:95:LEU:HA	2:H:95:LEU:HD23	1.84	0.40
2:D:56:SER:HB2	2:D:75:PRO:HG3	2.03	0.40
2:F:261:VAL:HG22	2:F:277:ILE:HG23	2.04	0.40
2:H:39:LYS:H	2:H:39:LYS:HG3	1.39	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	266/271 (98%)	253 (95%)	12 (4%)	1 (0%)	34	72
1	C	266/271 (98%)	247 (93%)	19 (7%)	0	100	100
1	E	266/271 (98%)	253 (95%)	12 (4%)	1 (0%)	34	72
1	G	266/271 (98%)	251 (94%)	14 (5%)	1 (0%)	34	72
2	B	260/265 (98%)	239 (92%)	18 (7%)	3 (1%)	13	50
2	D	260/265 (98%)	240 (92%)	17 (6%)	3 (1%)	13	50
2	F	260/265 (98%)	241 (93%)	15 (6%)	4 (2%)	10	45
2	H	260/265 (98%)	243 (94%)	15 (6%)	2 (1%)	19	58
All	All	2104/2144 (98%)	1967 (94%)	122 (6%)	15 (1%)	26	61

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	96	PRO
2	B	279	PRO
2	D	96	PRO
2	F	7	ILE
2	H	96	PRO
2	H	279	PRO
2	D	279	PRO
2	F	96	PRO
1	E	175	ASN
2	D	7	ILE
2	F	4	ILE
1	A	175	ASN
2	F	8	GLY
1	G	174	ASN

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Mol	Chain	Res	Type
2	B	4	ILE

### 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	240/240 (100%)	171 (71%)	69 (29%)	0	2
1	C	240/240 (100%)	167 (70%)	73 (30%)	0	2
1	E	240/240 (100%)	169 (70%)	71 (30%)	0	2
1	G	240/240 (100%)	172 (72%)	68 (28%)	0	3
2	B	239/239 (100%)	163 (68%)	76 (32%)	0	2
2	D	239/239 (100%)	158 (66%)	81 (34%)	0	1
2	F	239/239 (100%)	165 (69%)	74 (31%)	0	2
2	H	240/239 (100%)	167 (70%)	73 (30%)	0	2
All	All	1917/1916 (100%)	1332 (70%)	585 (30%)	1	2

All (585) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LYS
1	A	17	VAL
1	A	18	THR
1	A	21	LYS
1	A	23	THR
1	A	25	THR
1	A	29	ASP
1	A	34	SER
1	A	38	THR
1	A	42	ILE
1	A	43	LYS
1	A	45	LYS
1	A	49	LYS
1	A	51	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	55	LYS
1	A	57	THR
1	A	66	LYS
1	A	70	ASN
1	A	72	TYR
1	A	76	LYS
1	A	86	SER
1	A	88	SER
1	A	91	SER
1	A	94	SER
1	A	108	GLU
1	A	112	GLN
1	A	117	TYR
1	A	118	THR
1	A	137	THR
1	A	139	PHE
1	A	140	SER
1	A	143	ILE
1	A	144	ASN
1	A	146	LYS
1	A	148	GLU
1	A	154	LEU
1	A	155	SER
1	A	157	ASN
1	A	160	TYR
1	A	161	LYS
1	A	182	ARG
1	A	188	THR
1	A	192	GLU
1	A	198	ARG
1	A	200	SER
1	A	218	SER
1	A	219	ARG
1	A	220	SER
1	A	227	LEU
1	A	228	SER
1	A	234	GLN
1	A	238	LYS
1	A	239	LYS
1	A	241	LYS
1	A	242	ILE
1	A	248	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	250	MET
1	A	258	ASN
1	A	268	LYS
1	A	270	PHE
1	A	272	THR
1	A	278	THR
1	A	280	GLU
1	A	281	ILE
1	A	289	LYS
1	A	292	ASP
1	A	294	LYS
1	A	296	THR
1	A	300	LYS
1	C	16	LYS
1	C	17	VAL
1	C	18	THR
1	C	21	LYS
1	C	23	THR
1	C	25	THR
1	C	29	ASP
1	C	34	SER
1	C	38	THR
1	C	43	LYS
1	C	44	ASP
1	C	45	LYS
1	C	49	LYS
1	C	51	THR
1	C	53	VAL
1	C	55	LYS
1	C	57	THR
1	C	66	LYS
1	C	70	ASN
1	C	72	TYR
1	C	76	LYS
1	C	86	SER
1	C	88	SER
1	C	94	SER
1	C	98	VAL
1	C	108	GLU
1	C	112	GLN
1	C	117	TYR
1	C	136	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	137	THR
1	C	139	PHE
1	C	140	SER
1	C	143	ILE
1	C	146	LYS
1	C	147	GLN
1	C	148	GLU
1	C	153	THR
1	C	154	LEU
1	C	155	SER
1	C	157	ASN
1	C	161	LYS
1	C	173	MET
1	C	175	ASN
1	C	182	ARG
1	C	188	THR
1	C	192	GLU
1	C	193	LEU
1	C	198	ARG
1	C	200	SER
1	C	219	ARG
1	C	220	SER
1	C	228	SER
1	C	234	GLN
1	C	235	ASP
1	C	238	LYS
1	C	239	LYS
1	C	241	LYS
1	C	242	ILE
1	C	243	THR
1	C	248	ARG
1	C	252	LEU
1	C	258	ASN
1	C	268	LYS
1	C	270	PHE
1	C	272	THR
1	C	276	LYS
1	C	278	THR
1	C	280	GLU
1	C	281	ILE
1	C	292	ASP
1	C	294	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	296	THR
1	C	300	LYS
1	E	16	LYS
1	E	17	VAL
1	E	21	LYS
1	E	23	THR
1	E	25	THR
1	E	29	ASP
1	E	34	SER
1	E	38	THR
1	E	42	ILE
1	E	43	LYS
1	E	45	LYS
1	E	49	LYS
1	E	51	THR
1	E	55	LYS
1	E	57	THR
1	E	66	LYS
1	E	70	ASN
1	E	72	TYR
1	E	76	LYS
1	E	86	SER
1	E	88	SER
1	E	92	ASN
1	E	94	SER
1	E	100	TYR
1	E	108	GLU
1	E	112	GLN
1	E	117	TYR
1	E	136	ASN
1	E	137	THR
1	E	139	PHE
1	E	140	SER
1	E	141	GLU
1	E	143	ILE
1	E	146	LYS
1	E	147	GLN
1	E	153	THR
1	E	154	LEU
1	E	155	SER
1	E	157	ASN
1	E	160	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	E	161	LYS
1	E	182	ARG
1	E	188	THR
1	E	192	GLU
1	E	198	ARG
1	E	200	SER
1	E	219	ARG
1	E	220	SER
1	E	227	LEU
1	E	228	SER
1	E	233	ARG
1	E	235	ASP
1	E	238	LYS
1	E	239	LYS
1	E	241	LYS
1	E	242	ILE
1	E	243	THR
1	E	248	ARG
1	E	250	MET
1	E	252	LEU
1	E	258	ASN
1	E	270	PHE
1	E	271	LYS
1	E	272	THR
1	E	280	GLU
1	E	281	ILE
1	E	289	LYS
1	E	292	ASP
1	E	294	LYS
1	E	296	THR
1	E	300	LYS
1	G	16	LYS
1	G	17	VAL
1	G	23	THR
1	G	25	THR
1	G	29	ASP
1	G	30	LYS
1	G	34	SER
1	G	42	ILE
1	G	45	LYS
1	G	49	LYS
1	G	51	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	G	53	VAL
1	G	55	LYS
1	G	57	THR
1	G	66	LYS
1	G	70	ASN
1	G	72	TYR
1	G	76	LYS
1	G	86	SER
1	G	88	SER
1	G	92	ASN
1	G	94	SER
1	G	98	VAL
1	G	100	TYR
1	G	108	GLU
1	G	112	GLN
1	G	136	ASN
1	G	140	SER
1	G	142	THR
1	G	143	ILE
1	G	146	LYS
1	G	153	THR
1	G	154	LEU
1	G	155	SER
1	G	157	ASN
1	G	161	LYS
1	G	173	MET
1	G	182	ARG
1	G	188	THR
1	G	192	GLU
1	G	200	SER
1	G	219	ARG
1	G	220	SER
1	G	228	SER
1	G	233	ARG
1	G	234	GLN
1	G	235	ASP
1	G	238	LYS
1	G	239	LYS
1	G	241	LYS
1	G	242	ILE
1	G	247	GLN
1	G	248	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	G	250	MET
1	G	252	LEU
1	G	258	ASN
1	G	270	PHE
1	G	271	LYS
1	G	272	THR
1	G	276	LYS
1	G	280	GLU
1	G	281	ILE
1	G	289	LYS
1	G	292	ASP
1	G	294	LYS
1	G	295	GLU
1	G	296	THR
1	G	300	LYS
2	B	3	LYS
2	B	4	ILE
2	B	5	GLU
2	B	7	ILE
2	B	14	ILE
2	B	15	LYS
2	B	18	GLN
2	B	20	ILE
2	B	23	LYS
2	B	24	ARG
2	B	31	ILE
2	B	37	LYS
2	B	39	LYS
2	B	40	LYS
2	B	43	LYS
2	B	49	LYS
2	B	50	MET
2	B	59	THR
2	B	60	TYR
2	B	61	SER
2	B	62	ASP
2	B	63	LEU
2	B	64	LYS
2	B	65	LYS
2	B	69	ILE
2	B	71	ARG
2	B	73	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	79	ASN
2	B	81	SER
2	B	82	LEU
2	B	85	LYS
2	B	90	ASP
2	B	96	PRO
2	B	97	LYS
2	B	99	LYS
2	B	100	ILE
2	B	101	ASP
2	B	104	ASP
2	B	106	SER
2	B	109	LEU
2	B	113	ILE
2	B	129	PHE
2	B	130	ASN
2	B	133	LYS
2	B	143	VAL
2	B	159	LYS
2	B	162	SER
2	B	170	VAL
2	B	171	SER
2	B	197	LEU
2	B	201	ILE
2	B	202	GLN
2	B	211	THR
2	B	214	SER
2	B	216	GLU
2	B	217	ARG
2	B	219	LYS
2	B	222	LYS
2	B	224	GLU
2	B	233	MET
2	B	240	VAL
2	B	241	THR
2	B	242	ARG
2	B	244	ARG
2	B	248	ASP
2	B	249	ARG
2	B	255	LYS
2	B	257	ARG
2	B	258	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	268	LYS
2	B	273	LYS
2	B	275	LYS
2	B	277	ILE
2	B	278	THR
2	B	279	PRO
2	B	280	LYS
2	D	3	LYS
2	D	4	ILE
2	D	6	ASP
2	D	7	ILE
2	D	14	ILE
2	D	15	LYS
2	D	23	LYS
2	D	24	ARG
2	D	31	ILE
2	D	37	LYS
2	D	39	LYS
2	D	49	LYS
2	D	50	MET
2	D	59	THR
2	D	61	SER
2	D	62	ASP
2	D	64	LYS
2	D	65	LYS
2	D	69	ILE
2	D	71	ARG
2	D	73	ILE
2	D	79	ASN
2	D	81	SER
2	D	82	LEU
2	D	83	LYS
2	D	85	LYS
2	D	88	ASN
2	D	90	ASP
2	D	96	PRO
2	D	97	LYS
2	D	99	LYS
2	D	100	ILE
2	D	104	ASP
2	D	105	VAL
2	D	106	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	D	108	LYS
2	D	109	LEU
2	D	112	ASN
2	D	113	ILE
2	D	133	LYS
2	D	135	ILE
2	D	138	ASN
2	D	143	VAL
2	D	155	LYS
2	D	159	LYS
2	D	164	VAL
2	D	165	THR
2	D	167	ASN
2	D	171	SER
2	D	197	LEU
2	D	201	ILE
2	D	202	GLN
2	D	210	ILE
2	D	211	THR
2	D	214	SER
2	D	215	HIS
2	D	216	GLU
2	D	217	ARG
2	D	219	LYS
2	D	221	ASP
2	D	222	LYS
2	D	228	THR
2	D	233	MET
2	D	240	VAL
2	D	241	THR
2	D	242	ARG
2	D	244	ARG
2	D	248	ASP
2	D	249	ARG
2	D	255	LYS
2	D	257	ARG
2	D	258	ASN
2	D	260	THR
2	D	264	GLU
2	D	266	ASN
2	D	268	LYS
2	D	273	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	D	276	SER
2	D	278	THR
2	D	279	PRO
2	D	280	LYS
2	F	3	LYS
2	F	4	ILE
2	F	5	GLU
2	F	7	ILE
2	F	14	ILE
2	F	15	LYS
2	F	20	ILE
2	F	23	LYS
2	F	24	ARG
2	F	31	ILE
2	F	37	LYS
2	F	39	LYS
2	F	40	LYS
2	F	50	MET
2	F	59	THR
2	F	62	ASP
2	F	64	LYS
2	F	65	LYS
2	F	71	ARG
2	F	73	ILE
2	F	79	ASN
2	F	81	SER
2	F	82	LEU
2	F	85	LYS
2	F	90	ASP
2	F	96	PRO
2	F	97	LYS
2	F	100	ILE
2	F	101	ASP
2	F	104	ASP
2	F	106	SER
2	F	108	LYS
2	F	109	LEU
2	F	112	ASN
2	F	128	SER
2	F	132	SER
2	F	135	ILE
2	F	143	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	F	145	GLU
2	F	148	SER
2	F	155	LYS
2	F	164	VAL
2	F	165	THR
2	F	167	ASN
2	F	171	SER
2	F	197	LEU
2	F	201	ILE
2	F	202	GLN
2	F	210	ILE
2	F	211	THR
2	F	214	SER
2	F	216	GLU
2	F	217	ARG
2	F	219	LYS
2	F	221	ASP
2	F	222	LYS
2	F	226	GLU
2	F	233	MET
2	F	236	THR
2	F	240	VAL
2	F	241	THR
2	F	243	HIS
2	F	244	ARG
2	F	248	ASP
2	F	249	ARG
2	F	255	LYS
2	F	257	ARG
2	F	258	ASN
2	F	266	ASN
2	F	268	LYS
2	F	273	LYS
2	F	276	SER
2	F	278	THR
2	F	280	LYS
2	H	3[A]	LYS
2	H	3[B]	LYS
2	H	4	ILE
2	H	14	ILE
2	H	15	LYS
2	H	18	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	H	19	ASP
2	H	23	LYS
2	H	24	ARG
2	H	31	ILE
2	H	36	VAL
2	H	37	LYS
2	H	39	LYS
2	H	49	LYS
2	H	50	MET
2	H	61	SER
2	H	62	ASP
2	H	64	LYS
2	H	65	LYS
2	H	69	ILE
2	H	71	ARG
2	H	73	ILE
2	H	79	ASN
2	H	81	SER
2	H	82	LEU
2	H	85	LYS
2	H	90	ASP
2	H	96	PRO
2	H	97	LYS
2	H	99	LYS
2	H	100	ILE
2	H	104	ASP
2	H	106	SER
2	H	108	LYS
2	H	109	LEU
2	H	112	ASN
2	H	113	ILE
2	H	140	LYS
2	H	143	VAL
2	H	148	SER
2	H	159	LYS
2	H	169	GLN
2	H	171	SER
2	H	197	LEU
2	H	201	ILE
2	H	202	GLN
2	H	211	THR
2	H	214	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	H	216	GLU
2	H	217	ARG
2	H	219	LYS
2	H	221	ASP
2	H	222	LYS
2	H	224	GLU
2	H	228	THR
2	H	233	MET
2	H	240	VAL
2	H	241	THR
2	H	242	ARG
2	H	244	ARG
2	H	248	ASP
2	H	249	ARG
2	H	255	LYS
2	H	257	ARG
2	H	258	ASN
2	H	260	THR
2	H	268	LYS
2	H	271	GLU
2	H	273	LYS
2	H	275	LYS
2	H	277	ILE
2	H	278	THR
2	H	279	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	104	ASN
1	A	113	ASN
1	A	223	ASN
1	A	234	GLN
1	A	266	ASN
1	C	59	ASN
1	C	147	GLN
1	C	175	ASN
1	C	206	GLN
1	E	223	ASN
1	E	266	ASN
1	G	40	ASN
1	G	84	ASN

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Mol	Chain	Res	Type
1	G	247	GLN
1	G	266	ASN
1	G	298	ASN
2	B	206	ASN
2	D	88	ASN
2	D	215	HIS
2	D	266	ASN
2	F	266	ASN
2	H	141	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 monosaccharides 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.

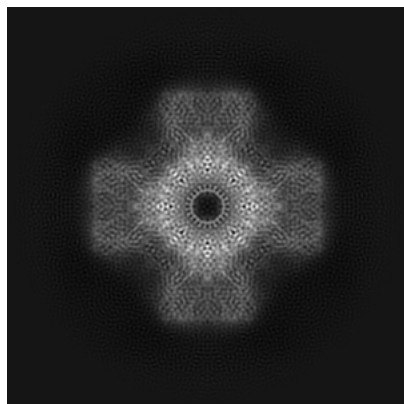
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34391. These allow visual inspection of the internal detail of the map and identification of artifacts.

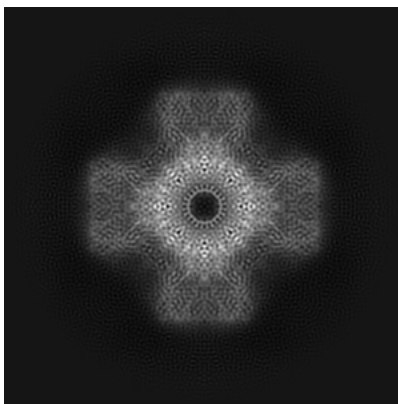
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

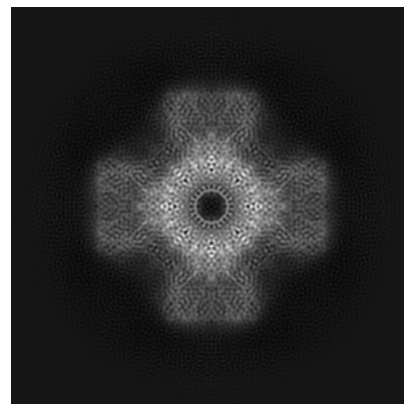
#### 6.1.1 Primary map



X

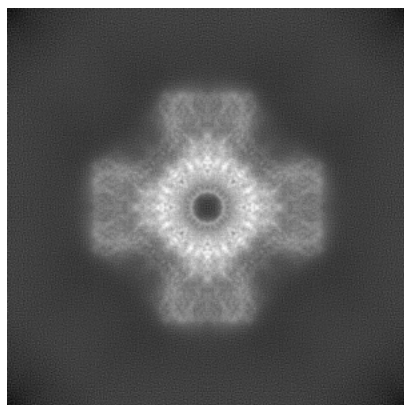


Y

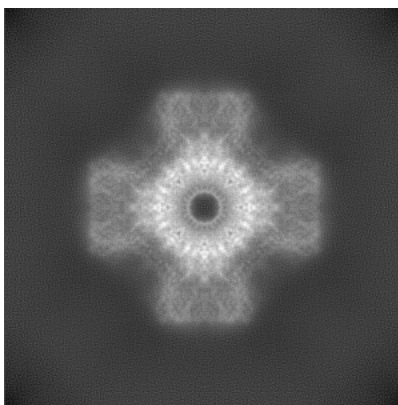


Z

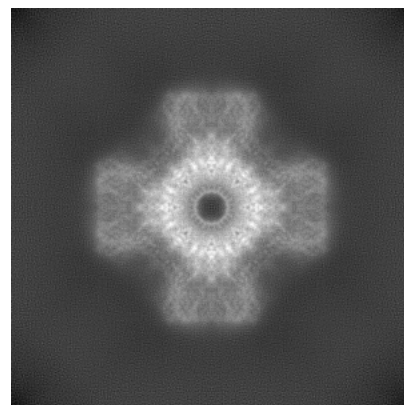
#### 6.1.2 Raw map



X



Y

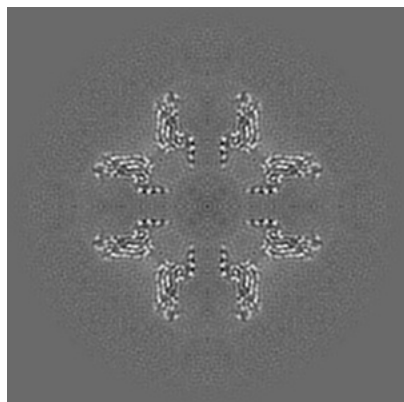


Z

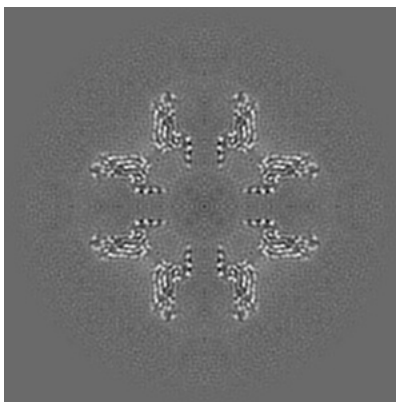
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

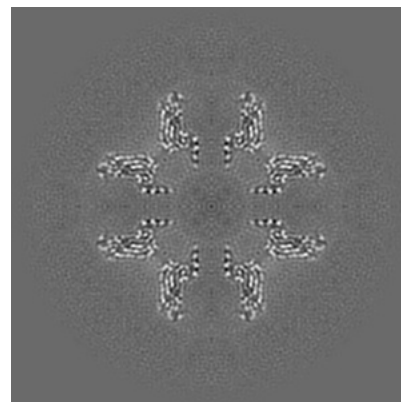
### 6.2.1 Primary map



X Index: 200

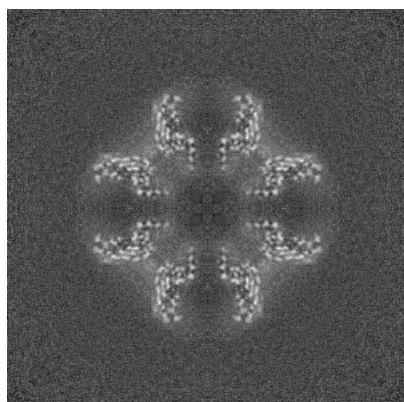


Y Index: 200

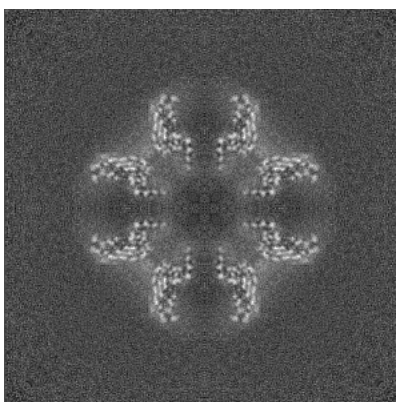


Z Index: 200

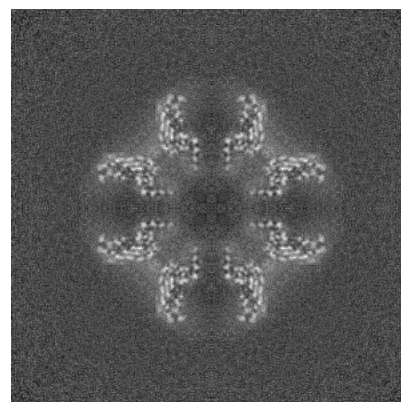
### 6.2.2 Raw map



X Index: 200



Y Index: 200

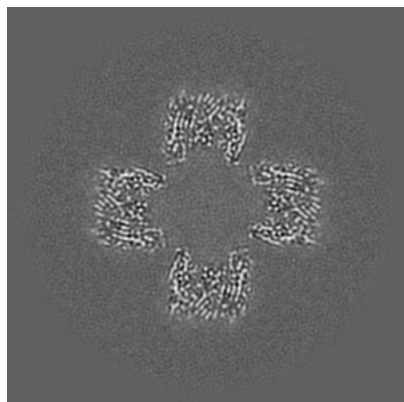


Z Index: 200

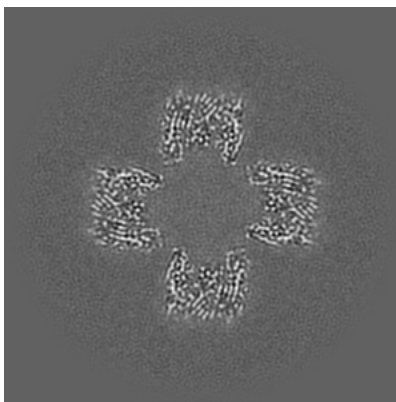
The images above show central slices of the map in three orthogonal directions.

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

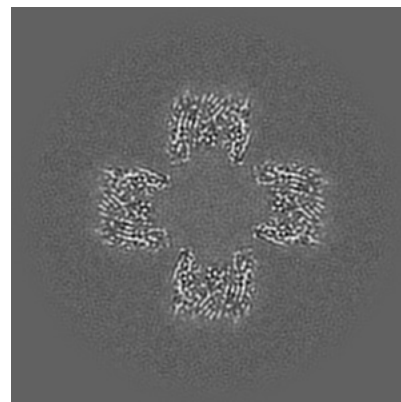
### 6.3.1 Primary map



X Index: 168

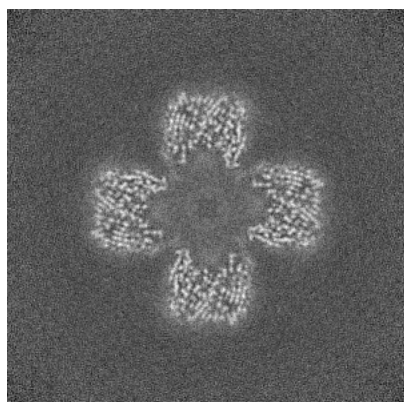


Y Index: 168

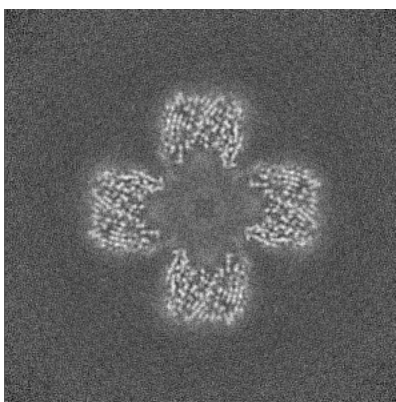


Z Index: 168

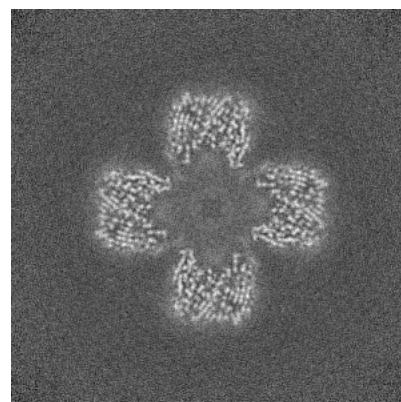
### 6.3.2 Raw map



X Index: 167



Y Index: 167

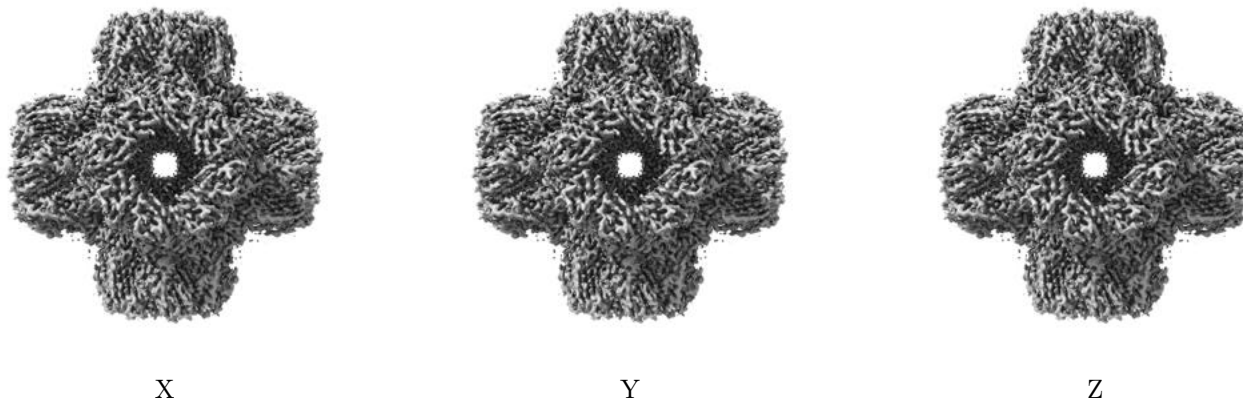


Z Index: 167

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

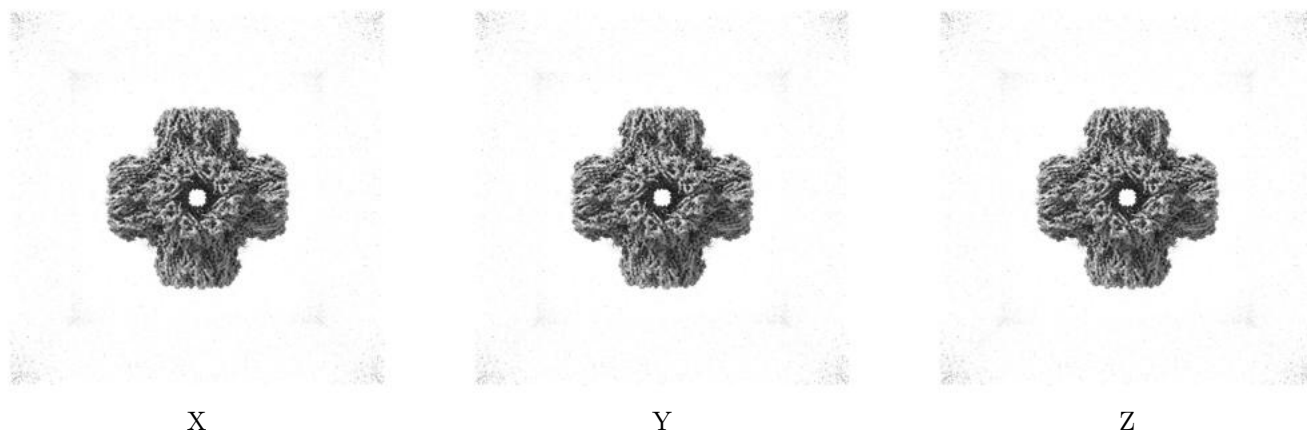
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.427. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 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.

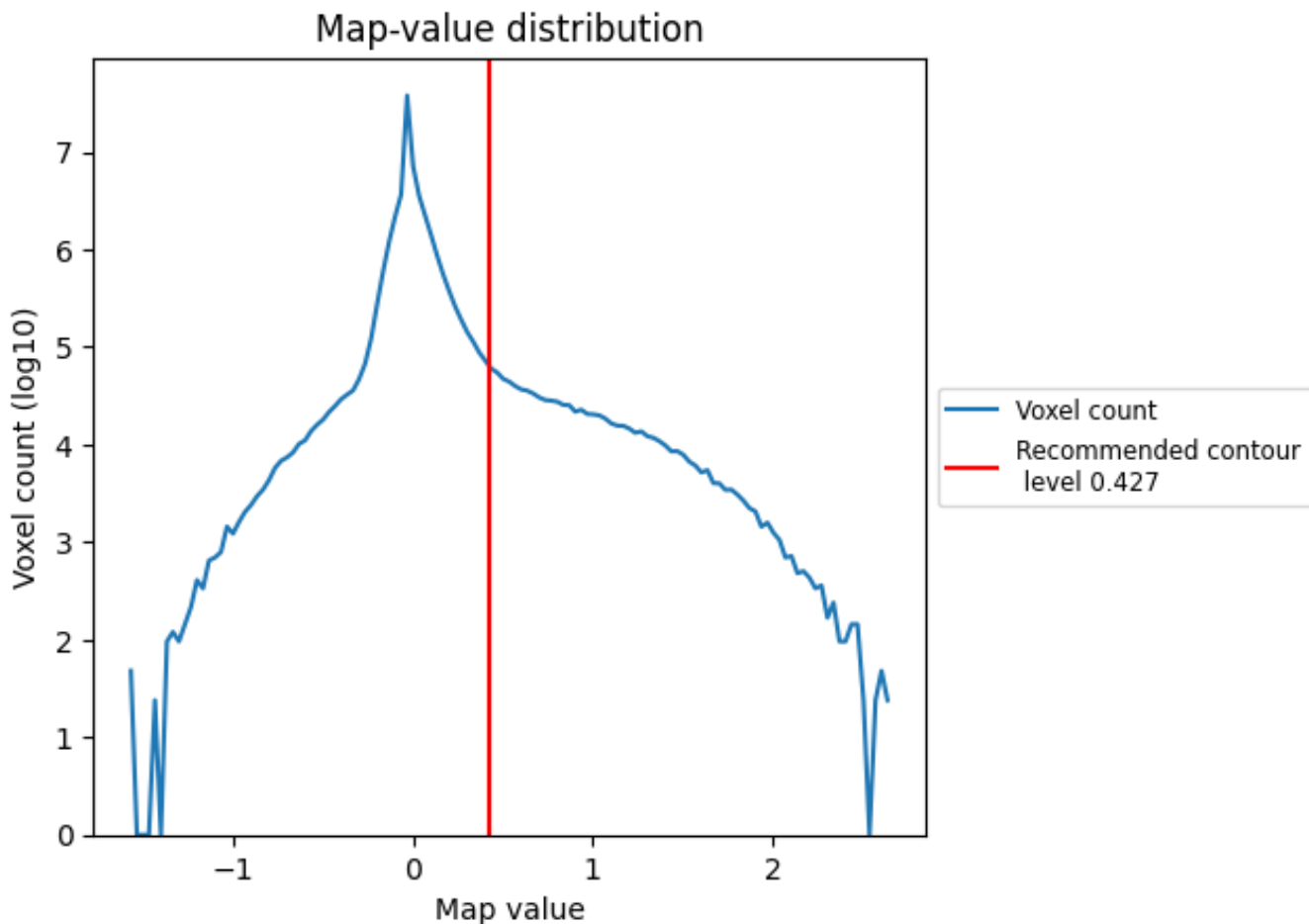
## 6.5 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

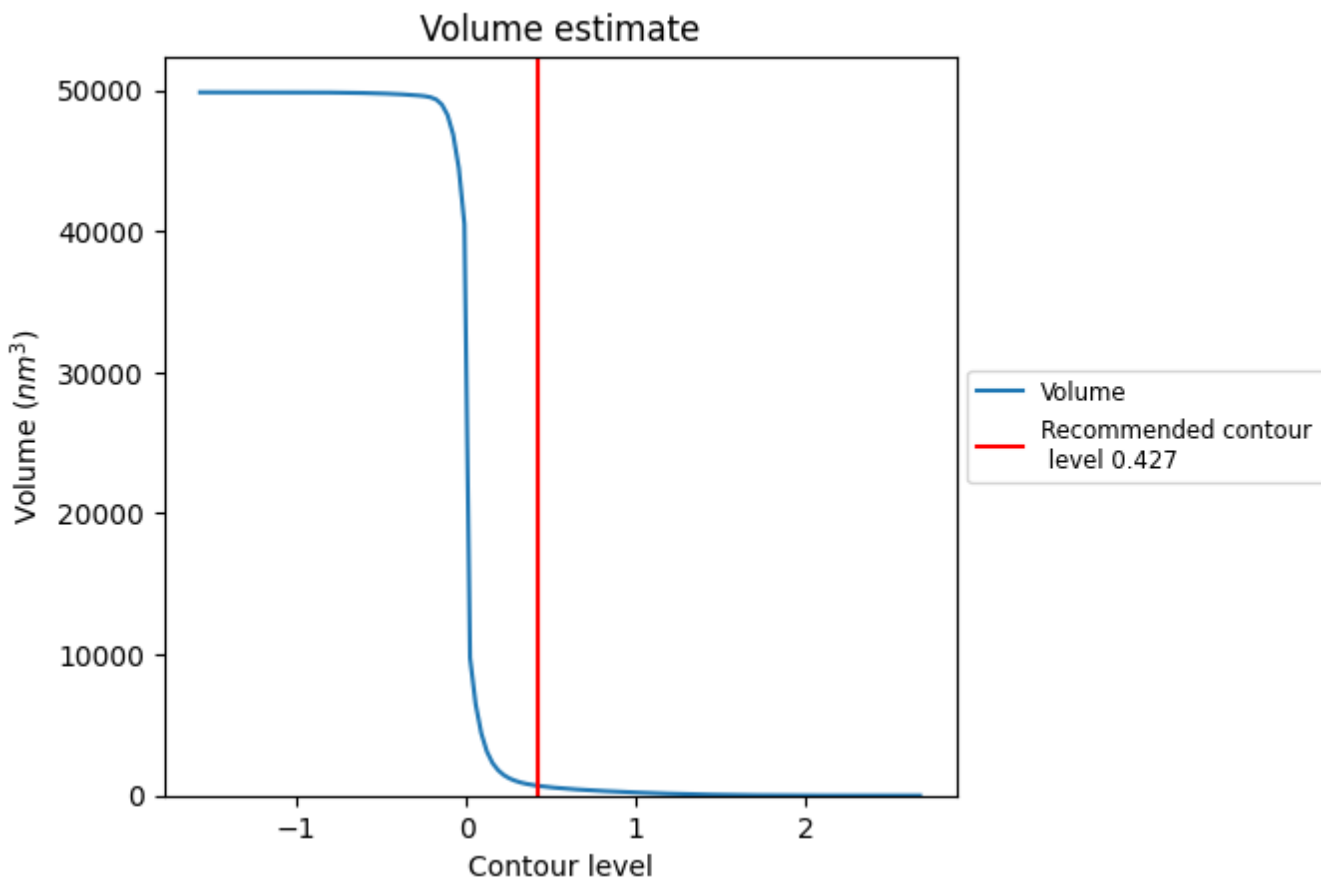
This section contains the results of statistical analysis of the map.

### 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.

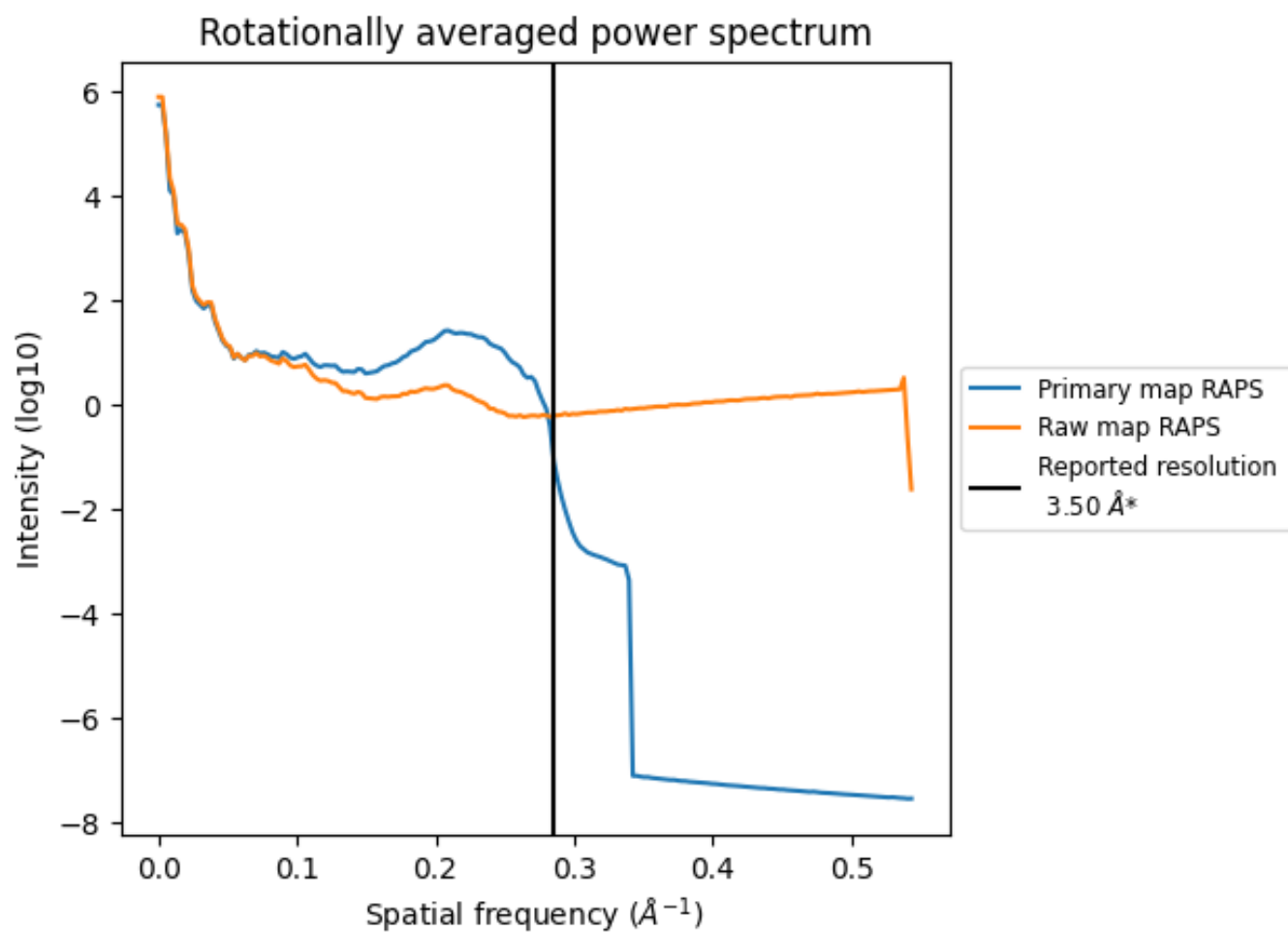
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 683 nm<sup>3</sup>; this corresponds to an approximate mass of 617 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



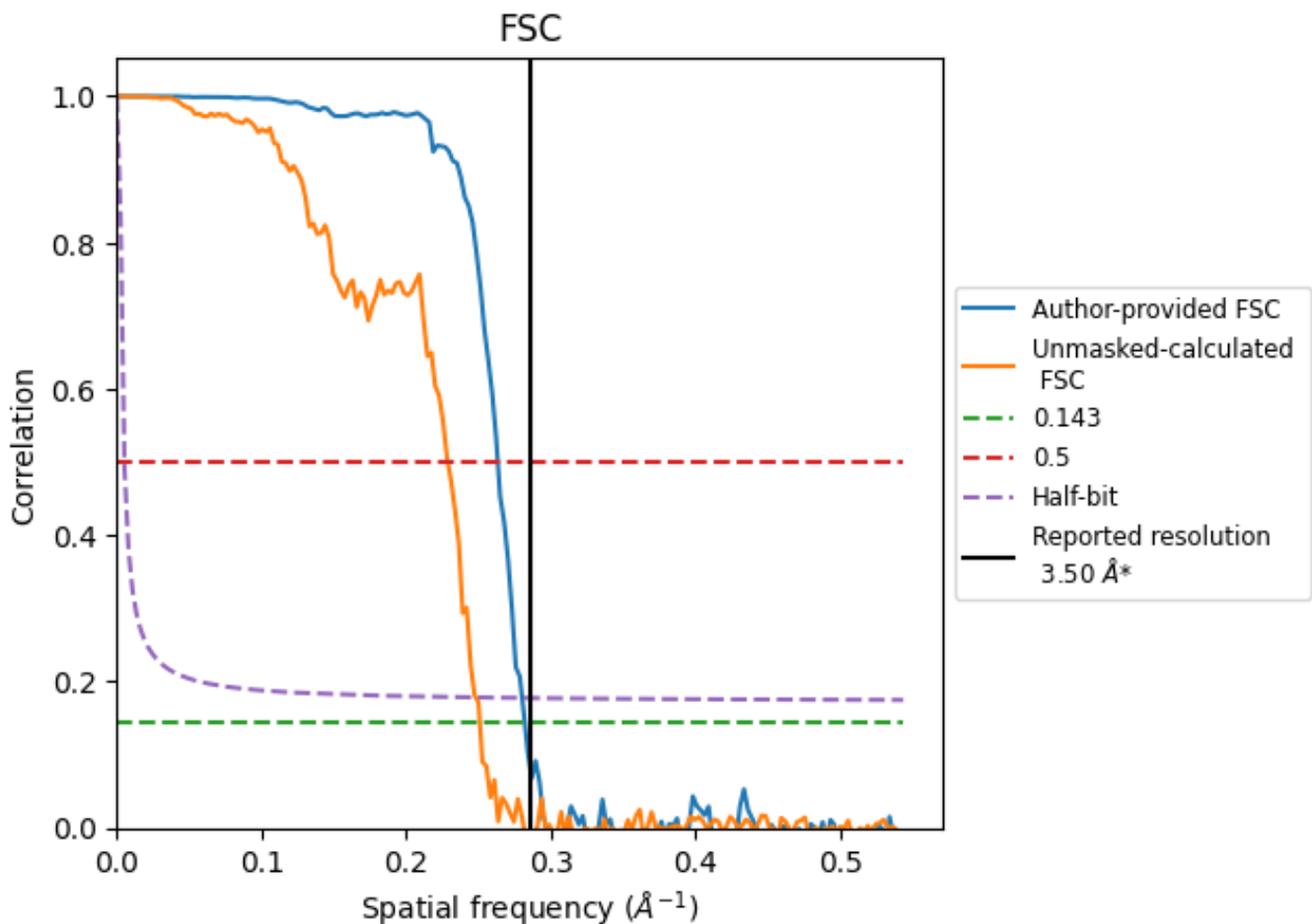
\*Reported resolution corresponds to spatial frequency of 0.286 Å<sup>-1</sup>



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

## 8.2 Resolution estimates [i](#)

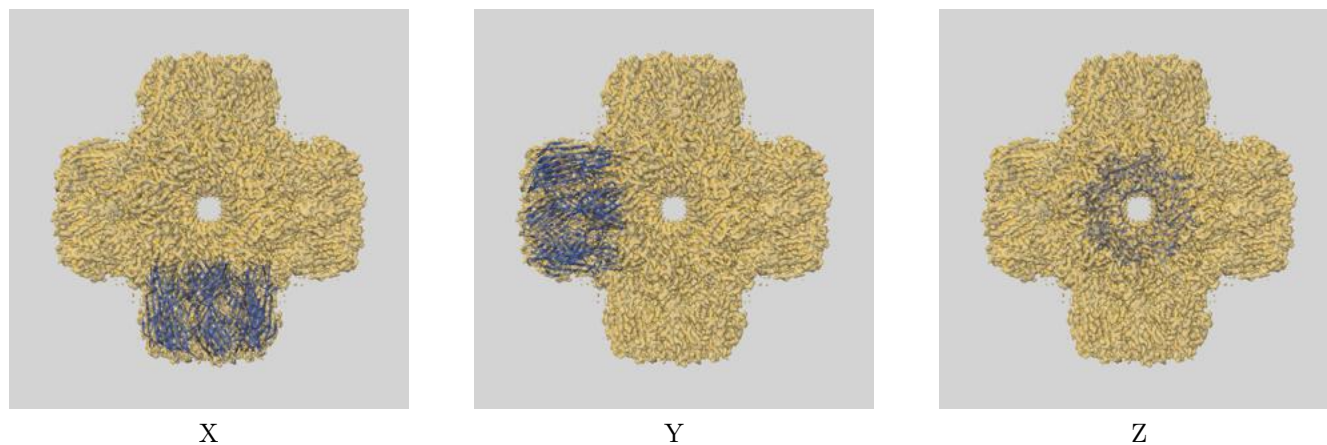
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.55	3.80	3.57
Unmasked-calculated*	3.99	4.37	4.03

\*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 3.99 differs from the reported value 3.5 by more than 10 %

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

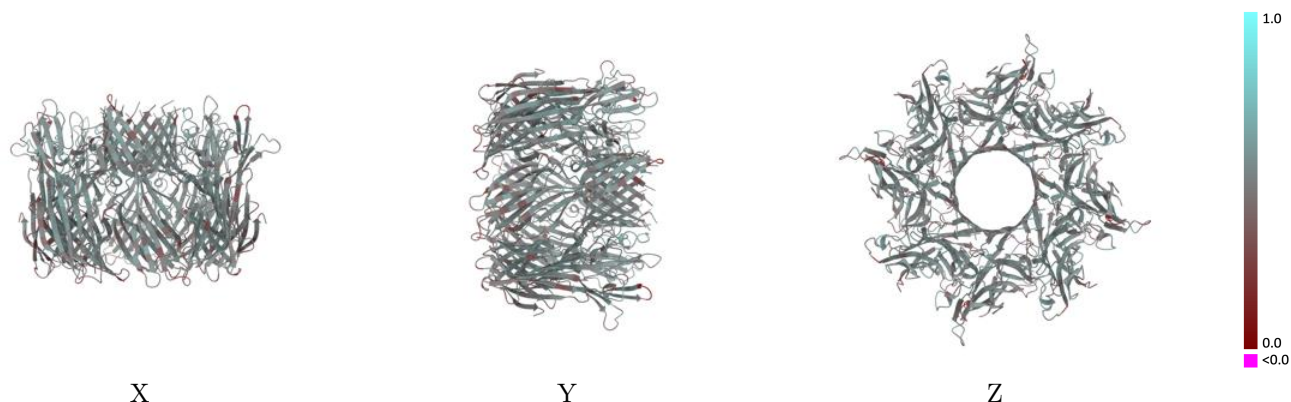
This section contains information regarding the fit between EMDB map EMD-34391 and PDB model 8GZ7. Per-residue inclusion information can be found in section 3 on page 7.

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



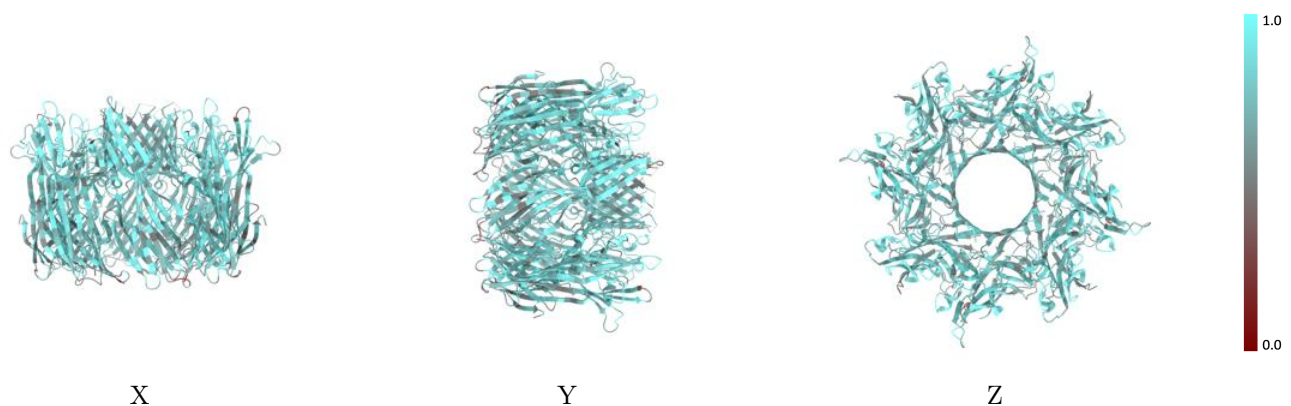
The images above show the 3D surface view of the map at the recommended contour level 0.427 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



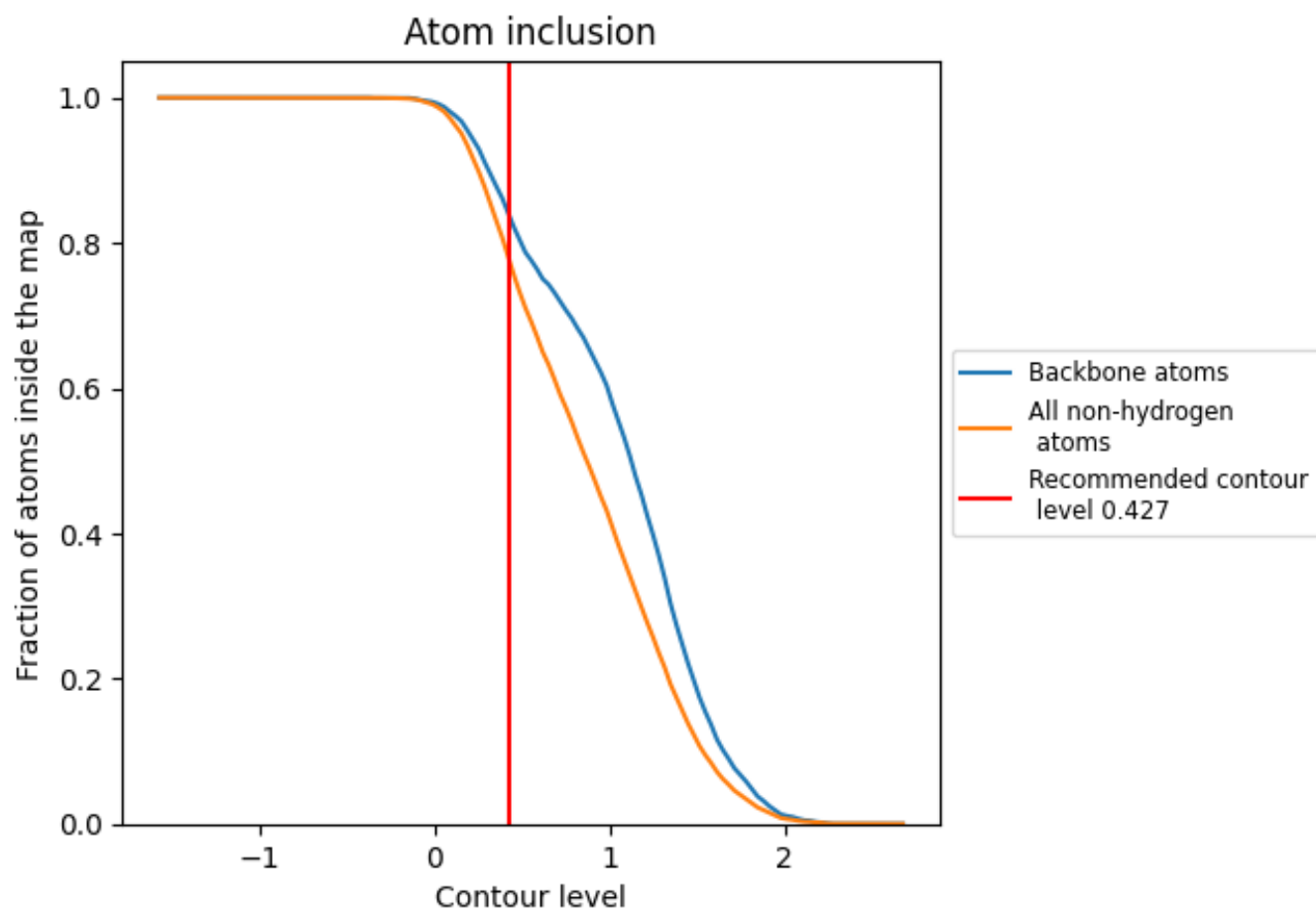
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.427).



















## 9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 78% 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 (0.427) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7771	 0.4910
A	 0.7876	 0.5010
B	 0.7705	 0.4850
C	 0.7871	 0.4980
D	 0.7672	 0.4810
E	 0.7857	 0.4960
F	 0.7662	 0.4820
G	 0.7816	 0.4970
H	 0.7705	 0.4850

