



## Full wwPDB EM Validation Report ⓘ

Apr 26, 2023 – 12:44 PM JST

PDB ID : 7F94  
EMDB ID : EMD-31497  
Title : Structure of C-terminal truncated connexin43/Cx43/GJA1 gap junction inter-cellular channel with two conformationally different hemichannels  
Authors : Lee, H.J.; Cha, H.J.; Jeong, H.; Lee, S.N.; Lee, C.W.; Woo, J.S.  
Deposited on : 2021-07-03  
Resolution : 3.60 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:

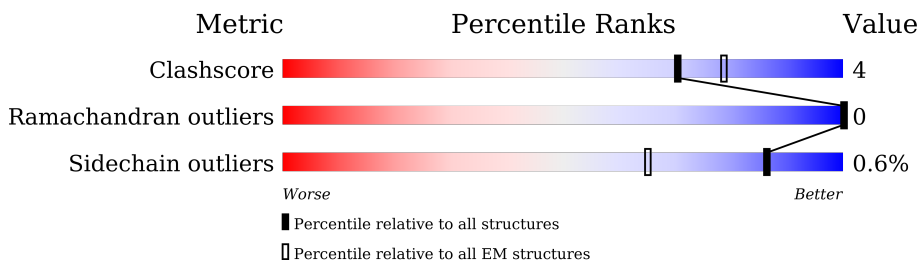
EMDB validation analysis : 0.0.1.dev50  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.32.2

# 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 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



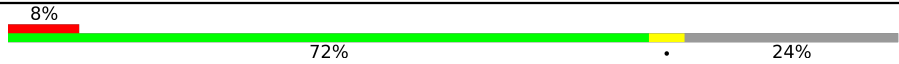

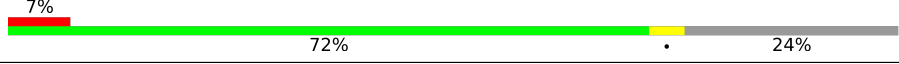
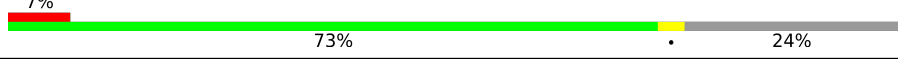
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	257	
1	B	257	
1	C	257	
1	D	257	
1	E	257	
1	F	257	
1	G	257	
1	H	257	

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Mol	Chain	Length	Quality of chain
1	I	257	
1	J	257	
1	K	257	
1	L	257	

## 2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 19128 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.

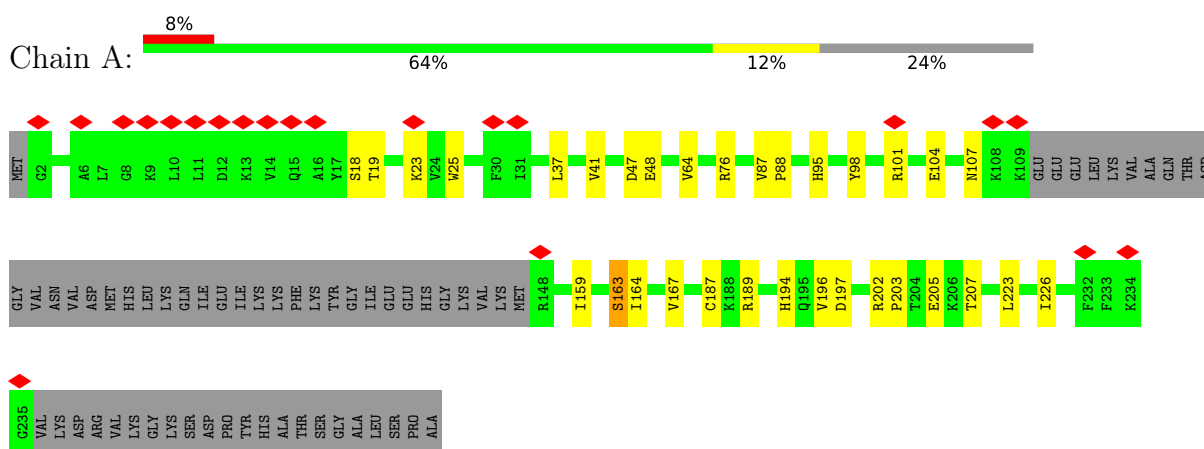
- Molecule 1 is a protein called A C-terminal deletion mutant of gap junction alpha-1 protein (Cx43-M257).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	196	1594	1065	254	267	8	0	0
1	G	196	1594	1065	254	267	8	0	0
1	B	196	1594	1065	254	267	8	0	0
1	L	196	1594	1065	254	267	8	0	0
1	C	196	1594	1065	254	267	8	0	0
1	K	196	1594	1065	254	267	8	0	0
1	D	196	1594	1065	254	267	8	0	0
1	J	196	1594	1065	254	267	8	0	0
1	E	196	1594	1065	254	267	8	0	0
1	I	196	1594	1065	254	267	8	0	0
1	F	196	1594	1065	254	267	8	0	0
1	H	196	1594	1065	254	267	8	0	0

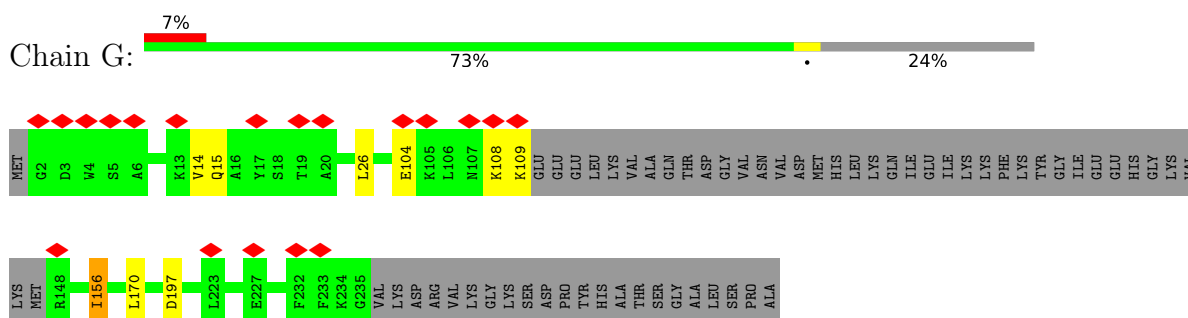
### 3 Residue-property plots

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.

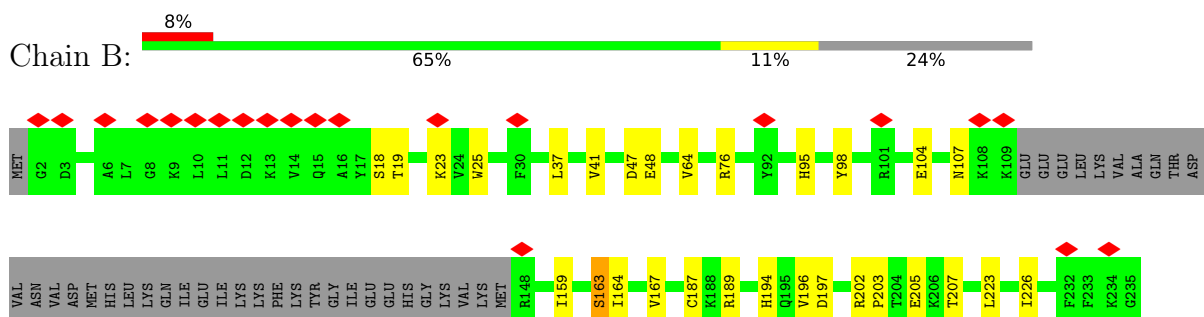
- Molecule 1: A C-terminal deletion mutant of gap junction alpha-1 protein (Cx43-M257)



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VAL  
LYS  
ASP  
ARG  
VAL  
VAL  
LYS  
GLY  
LYS  
SER  
SER  
ASP  
PRO  
TYR  
HIS  
ALA  
THR  
SER  
SER  
GLY  
ALA  
LEU  
SER  
PRO  
ALA

- Molecule 1: A C-terminal deletion mutant of gap junction alpha-1 protein (Cx43-M257)

Chain L: 7% 73% 24%

MET G2 D3 W4 S5 A6 L11 V14 Q15 T19 A20 R53 L93 E104 K105 L106 M107 K108 K109  
GLU  
LEU  
LYS  
VAL  
ALA  
GLN  
THR  
ASP  
GLY  
VAL  
ASN  
VAL  
ASP  
MET  
HIS  
LEU  
GLN  
ILE  
ILE  
LYS  
PHE  
LYS  
TYR  
GLY  
ILE  
GLU  
GLY  
LYS

VAL  
LYS  
MET  
R148  
I156  
D197  
L223  
E227  
F232  
F233  
K234  
G235  
VAL  
LYS  
ASP  
ARG  
VAL  
LYS  
GLY  
LYS  
SER  
ASP  
PRO  
TYR  
HIS  
ALA  
THR  
SER  
GLY  
ALA  
LEU  
SER  
PRO  
ALA

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Chain C: 8% 65% 11% 24%

MET G2 A6 L7 G8 K9 L10 L11 L12 D12 K13 V14 Q15 A16 V17 S18 T19 K23 K24 W25 F30 L37 V41 D47 E48 V64 R76 H95 Y98 R101 E104 M107 K108 K109  
GLU  
GLU  
LYS  
LYS  
VAL  
VAL  
ALA  
THR  
SER  
GLY  
VAL  
ASN  
VAL  
ASP  
MET  
HIS  
LEU  
GLN  
ILE  
ILE  
LYS  
PHE  
LYS  
TYR  
GLY  
VAL  
ASN  
VAL

ASP  
MET  
HIS  
LEU  
LYS  
GLN  
ILE  
GLU  
ILE  
LYS  
LYS  
PHE  
LYS  
TYR  
GLY  
ILE  
GLU  
GLU  
HIS  
GLY  
VAL  
VAL  
LYS  
MET  
R148  
I159  
S163  
I164  
V167  
C187  
K188  
R189  
H194  
Q195  
V196  
D197  
R202  
P203  
T204  
E205  
K206  
T207  
L223  
L226  
F232  
F233  
K234  
G235  
VAL  
ASP

ARG  
VAL  
GLY  
LYS  
SER  
ASP  
PRO  
TYR  
HIS  
ALA  
THR  
SER  
GLY  
ALA  
LEU  
SER  
PRO  
ALA

- Molecule 1: A C-terminal deletion mutant of gap junction alpha-1 protein (Cx43-M257)

Chain K: 7% 72% 24%

MET G2 D3 W4 S5 A6 V14 Q15 A16 Y17 S18 T19 A20 L26 D47 R53 M63 L93 E104 K105 L106 M107 K108 K109  
GLU  
GLU  
LEU  
LYS  
VAL  
GLN  
THR  
ASP  
VAL  
VAL  
ASN  
TYR  
HIS  
ALA  
THR  
SER  
GLY  
ALA  
LEU  
SER  
PRO  
ALA

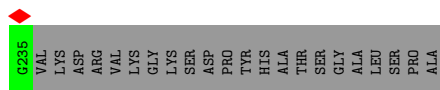
ILE  
GLU  
GLU  
HIS  
GLY  
LYS  
VAL  
LYS  
MET  
R148  
I156  
D197  
L223  
E227  
F233  
K234  
G235  
VAL  
LYS  
ASP  
ARG  
VAL  
LYS  
GLY  
LYS  
SER  
ASP  
PRO  
TYR  
HIS  
ALA  
THR  
SER  
GLY  
ALA  
LEU  
SER  
PRO  
ALA

- Molecule 1: A C-terminal deletion mutant of gap junction alpha-1 protein (Cx43-M257)

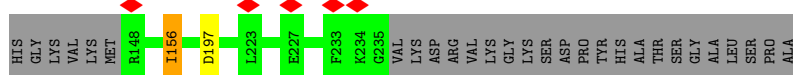
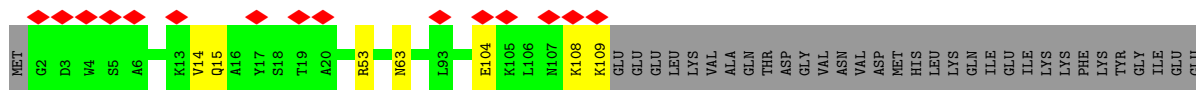
Chain D: 8% 64% 12% 24%

MET G2 A6 L7 G8 K9 L10 L11 L12 D12 K13 V14 Q15 A16 V17 S18 T19 K23 K24 W25 F30 I31 L37 V41 D47 E48 V64 R76 V87 P88 H95 Y98 R101 E104 M107 K108 K109  
GLU  
GLU  
LEU  
LYS  
VAL  
VAL  
ALA  
GLN  
THR  
ASP

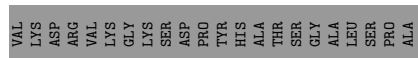
GLY  
VAL  
ASN  
VAL  
VAL  
MET  
HIS  
LEU  
GLN  
ILE  
ILE  
GLU  
LYS  
PHE  
LYS  
TYR  
GLY  
ILE  
GLU  
HIS  
GLY  
LYS  
VAL  
LYS  
MET  
R148  
I159  
S163  
I164  
V167  
C187  
K188  
R189  
H194  
Q195  
V196  
D197  
R202  
P203  
T204  
E205  
K206  
T207  
L223  
L226  
F232  
F233  
K234



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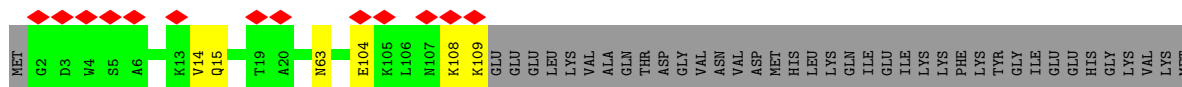
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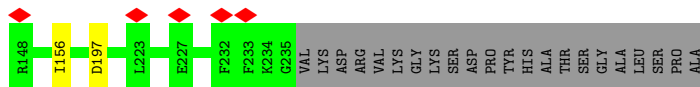


LYS  
ASP  
ARG  
VAL  
LYS  
GLY  
LYS  
SER  
ASP  
PRO  
TYR  
HIS  
ALA  
THR  
SER  
GLY  
ALA  
LEU  
SER  
PRO  
ALA

- Molecule 1: A C-terminal deletion mutant of gap junction alpha-1 protein (Cx43-M257)

Chain H:  7% 73% 24%

  
MET G2 D3 W4 S5 A6 K13 V14 Q15 T19 A20 N63 E104 K105 L106 N107 K108 K109  
GLU  
GLU  
LEU  
LEU  
LYS  
VAL  
VAL  
ALA  
GLN  
THR  
ASP  
GLY  
VAL  
ASN  
VAL  
VAL  
ASP  
MET  
HIS  
LEU  
LYS  
GLN  
GLN  
ILE  
ILE  
GLU  
ILE  
LYS  
PHE  
LYS  
TYR  
GLY  
ILE  
GLU  
HIS  
GLY  
LYS  
VAL  
LYS  
MET

  
R148 I156 D197 L223 E227 F232 F233 K234 G235  
VAL  
LYS  
ASP  
ARG  
VAL  
LYS  
GLY  
LYS  
SER  
ASP  
PRO  
TYR  
HIS  
ALA  
THR  
SER  
GLY  
ALA  
LEU  
SER  
PRO  
ALA



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	7446	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.043	Depositor
Minimum map value	-0.019	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	270.0, 270.0, 270.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.675, 0.675, 0.675	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	0.35	0/1637	0.51	0/2218
1	B	0.36	0/1637	0.51	0/2218
1	C	0.36	0/1637	0.51	0/2218
1	D	0.35	0/1637	0.51	0/2218
1	E	0.36	0/1637	0.51	0/2218
1	F	0.35	0/1637	0.51	0/2218
1	G	0.36	0/1637	0.53	0/2218
1	H	0.36	0/1637	0.53	0/2218
1	I	0.36	0/1637	0.53	0/2218
1	J	0.36	0/1637	0.53	0/2218
1	K	0.36	0/1637	0.53	0/2218
1	L	0.36	0/1637	0.53	0/2218
All	All	0.36	0/19644	0.52	0/26616

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1594	0	1626	21	0
1	B	1594	0	1626	19	0
1	C	1594	0	1626	20	0
1	D	1594	0	1626	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1594	0	1626	20	0
1	F	1594	0	1626	20	0
1	G	1594	0	1626	7	0
1	H	1594	0	1626	5	0
1	I	1594	0	1626	7	0
1	J	1594	0	1626	7	0
1	K	1594	0	1626	8	0
1	L	1594	0	1626	7	0
All	All	19128	0	19512	140	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (140) 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:L:14:VAL:HG13	1:L:15:GLN:HG3	1.85	0.58
1:J:14:VAL:HG13	1:J:15:GLN:HG3	1.85	0.58
1:E:37:LEU:HA	1:E:41:VAL:HB	1.85	0.58
1:K:14:VAL:HG13	1:K:15:GLN:HG3	1.85	0.58
1:G:14:VAL:HG13	1:G:15:GLN:HG3	1.85	0.58
1:F:37:LEU:HA	1:F:41:VAL:HB	1.85	0.58
1:D:37:LEU:HA	1:D:41:VAL:HB	1.86	0.58
1:I:14:VAL:HG13	1:I:15:GLN:HG3	1.85	0.57
1:A:37:LEU:HA	1:A:41:VAL:HB	1.86	0.57
1:B:37:LEU:HA	1:B:41:VAL:HB	1.85	0.57
1:C:37:LEU:HA	1:C:41:VAL:HB	1.85	0.57
1:H:14:VAL:HG13	1:H:15:GLN:HG3	1.85	0.57
1:F:197:ASP:N	1:F:197:ASP:OD1	2.38	0.56
1:A:197:ASP:N	1:A:197:ASP:OD1	2.38	0.56
1:E:95:HIS:O	1:E:98:TYR:HB3	2.06	0.56
1:D:95:HIS:O	1:D:98:TYR:HB3	2.06	0.56
1:A:95:HIS:O	1:A:98:TYR:HB3	2.06	0.56
1:B:95:HIS:O	1:B:98:TYR:HB3	2.06	0.56
1:C:95:HIS:O	1:C:98:TYR:HB3	2.06	0.56
1:E:197:ASP:N	1:E:197:ASP:OD1	2.38	0.56
1:A:76:ARG:NH1	1:B:205:GLU:OE2	2.39	0.55
1:B:76:ARG:NH1	1:C:205:GLU:OE2	2.39	0.55
1:A:194:HIS:NE2	1:J:197:ASP:OD1	2.37	0.55
1:E:76:ARG:NH1	1:F:205:GLU:OE2	2.39	0.55
1:F:95:HIS:O	1:F:98:TYR:HB3	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:LEU:HA	1:C:226:ILE:HD12	1.90	0.54
1:A:223:LEU:HA	1:A:226:ILE:HD12	1.90	0.54
1:B:223:LEU:HA	1:B:226:ILE:HD12	1.90	0.54
1:K:197:ASP:OD1	1:F:194:HIS:NE2	2.37	0.54
1:F:223:LEU:HA	1:F:226:ILE:HD12	1.90	0.54
1:D:223:LEU:HA	1:D:226:ILE:HD12	1.90	0.54
1:F:47:ASP:OD1	1:F:47:ASP:N	2.42	0.53
1:C:197:ASP:N	1:C:197:ASP:OD1	2.38	0.53
1:E:223:LEU:HA	1:E:226:ILE:HD12	1.90	0.53
1:F:203:PRO:O	1:F:207:THR:OG1	2.27	0.53
1:A:47:ASP:OD1	1:A:47:ASP:N	2.42	0.53
1:B:203:PRO:O	1:B:207:THR:OG1	2.27	0.53
1:E:47:ASP:OD1	1:E:47:ASP:N	2.42	0.53
1:A:203:PRO:O	1:A:207:THR:OG1	2.27	0.53
1:B:197:ASP:N	1:B:197:ASP:OD1	2.38	0.53
1:C:203:PRO:O	1:C:207:THR:OG1	2.27	0.53
1:A:205:GLU:OE2	1:F:76:ARG:NH1	2.42	0.53
1:D:197:ASP:OD1	1:D:197:ASP:N	2.38	0.52
1:D:47:ASP:N	1:D:47:ASP:OD1	2.42	0.52
1:D:187:CYS:HB3	1:D:196:VAL:HG23	1.93	0.51
1:C:76:ARG:NH1	1:D:205:GLU:OE2	2.43	0.51
1:D:203:PRO:O	1:D:207:THR:OG1	2.27	0.51
1:C:187:CYS:HB3	1:C:196:VAL:HG23	1.93	0.51
1:E:187:CYS:HB3	1:E:196:VAL:HG23	1.93	0.51
1:B:187:CYS:HB3	1:B:196:VAL:HG23	1.93	0.50
1:C:47:ASP:OD1	1:C:47:ASP:N	2.42	0.50
1:K:104:GLU:O	1:K:108:LYS:NZ	2.38	0.50
1:F:187:CYS:HB3	1:F:196:VAL:HG23	1.93	0.50
1:B:47:ASP:OD1	1:B:47:ASP:N	2.42	0.49
1:A:187:CYS:HB3	1:A:196:VAL:HG23	1.93	0.49
1:B:48:GLU:OE2	1:C:202:ARG:NH1	2.43	0.49
1:G:104:GLU:O	1:G:108:LYS:NZ	2.38	0.49
1:D:18:SER:OG	1:D:19:THR:N	2.46	0.49
1:D:76:ARG:NH1	1:E:205:GLU:OE2	2.45	0.49
1:F:18:SER:OG	1:F:19:THR:N	2.46	0.48
1:A:18:SER:OG	1:A:19:THR:N	2.46	0.48
1:E:18:SER:OG	1:E:19:THR:N	2.46	0.48
1:E:203:PRO:O	1:E:207:THR:OG1	2.27	0.48
1:B:18:SER:OG	1:B:19:THR:N	2.46	0.48
1:C:18:SER:OG	1:C:19:THR:N	2.46	0.48
1:L:104:GLU:O	1:L:108:LYS:NZ	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:HIS:NE2	1:I:197:ASP:OD1	2.43	0.47
1:A:18:SER:O	1:A:23:LYS:NZ	2.48	0.47
1:E:18:SER:O	1:E:23:LYS:NZ	2.48	0.47
1:F:18:SER:O	1:F:23:LYS:NZ	2.48	0.47
1:B:18:SER:O	1:B:23:LYS:NZ	2.48	0.47
1:C:48:GLU:OE2	1:D:202:ARG:NH1	2.46	0.47
1:C:18:SER:O	1:C:23:LYS:NZ	2.48	0.46
1:D:18:SER:O	1:D:23:LYS:NZ	2.48	0.46
1:L:197:ASP:OD1	1:E:194:HIS:NE2	2.43	0.46
1:J:156:ILE:H	1:J:156:ILE:HG12	1.35	0.46
1:D:159:ILE:O	1:D:163:SER:OG	2.34	0.46
1:L:156:ILE:H	1:L:156:ILE:HG12	1.35	0.45
1:F:159:ILE:O	1:F:163:SER:OG	2.34	0.45
1:A:48:GLU:OE2	1:B:202:ARG:NH1	2.46	0.45
1:A:159:ILE:O	1:A:163:SER:OG	2.34	0.45
1:C:194:HIS:NE2	1:H:197:ASP:OD1	2.44	0.45
1:K:156:ILE:H	1:K:156:ILE:HG12	1.35	0.45
1:C:64:VAL:HB	1:C:189:ARG:HD3	1.99	0.45
1:D:64:VAL:HB	1:D:189:ARG:HD3	1.99	0.45
1:E:64:VAL:HB	1:E:189:ARG:HD3	1.99	0.45
1:B:64:VAL:HB	1:B:189:ARG:HD3	1.99	0.45
1:I:109:LYS:HE2	1:I:109:LYS:HB2	1.89	0.45
1:C:159:ILE:O	1:C:163:SER:OG	2.34	0.44
1:F:64:VAL:HB	1:F:189:ARG:HD3	1.99	0.44
1:A:64:VAL:HB	1:A:189:ARG:HD3	1.99	0.44
1:H:109:LYS:HE2	1:H:109:LYS:HB2	1.88	0.44
1:J:109:LYS:HE2	1:J:109:LYS:HB2	1.89	0.44
1:G:156:ILE:H	1:G:156:ILE:HG12	1.35	0.44
1:L:53:ARG:NH1	1:K:63:ASN:OD1	2.51	0.44
1:B:159:ILE:O	1:B:163:SER:OG	2.34	0.44
1:A:202:ARG:NH1	1:F:48:GLU:OE2	2.45	0.43
1:K:53:ARG:NH1	1:J:63:ASN:OD1	2.51	0.43
1:E:48:GLU:OE2	1:F:202:ARG:NH1	2.46	0.43
1:C:25:TRP:HB2	1:C:223:LEU:HD22	2.01	0.43
1:F:25:TRP:HB2	1:F:223:LEU:HD22	2.01	0.43
1:G:197:ASP:OD1	1:D:194:HIS:NE2	2.45	0.43
1:B:25:TRP:HB2	1:B:223:LEU:HD22	2.01	0.43
1:A:25:TRP:HB2	1:A:223:LEU:HD22	2.01	0.43
1:L:234:LYS:HA	1:L:234:LYS:HD3	1.87	0.43
1:J:53:ARG:NH1	1:I:63:ASN:OD1	2.51	0.43
1:I:104:GLU:O	1:I:108:LYS:NZ	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:GLU:O	1:A:107:ASN:HB2	2.19	0.43
1:C:104:GLU:O	1:C:107:ASN:HB2	2.19	0.43
1:D:104:GLU:O	1:D:107:ASN:HB2	2.19	0.43
1:F:104:GLU:O	1:F:107:ASN:HB2	2.19	0.43
1:E:25:TRP:HB2	1:E:223:LEU:HD22	2.01	0.43
1:D:25:TRP:HB2	1:D:223:LEU:HD22	2.01	0.42
1:D:48:GLU:OE2	1:E:202:ARG:NH1	2.49	0.42
1:E:104:GLU:O	1:E:107:ASN:HB2	2.19	0.42
1:B:104:GLU:O	1:B:107:ASN:HB2	2.19	0.42
1:K:47:ASP:OD1	1:K:47:ASP:N	2.43	0.42
1:L:11:LEU:HD23	1:L:11:LEU:HA	1.93	0.42
1:E:159:ILE:O	1:E:163:SER:OG	2.34	0.42
1:E:164:ILE:HA	1:E:167:VAL:HG12	2.02	0.42
1:F:164:ILE:HA	1:F:167:VAL:HG12	2.02	0.42
1:K:26:LEU:HD23	1:K:26:LEU:HA	1.93	0.42
1:C:101:ARG:O	1:C:104:GLU:HB2	2.20	0.41
1:A:164:ILE:HA	1:A:167:VAL:HG12	2.02	0.41
1:D:101:ARG:O	1:D:104:GLU:HB2	2.20	0.41
1:D:164:ILE:HA	1:D:167:VAL:HG12	2.02	0.41
1:I:162:LYS:HE2	1:I:162:LYS:HB3	1.91	0.41
1:H:104:GLU:O	1:H:108:LYS:NZ	2.38	0.41
1:G:26:LEU:HD23	1:G:26:LEU:HA	1.93	0.41
1:G:170:LEU:HD23	1:G:170:LEU:HA	1.93	0.41
1:E:101:ARG:O	1:E:104:GLU:HB2	2.20	0.41
1:A:101:ARG:O	1:A:104:GLU:HB2	2.20	0.40
1:B:164:ILE:HA	1:B:167:VAL:HG12	2.02	0.40
1:C:164:ILE:HA	1:C:167:VAL:HG12	2.02	0.40
1:I:53:ARG:NH1	1:H:63:ASN:OD1	2.54	0.40
1:F:218:LEU:HD23	1:F:218:LEU:HA	1.95	0.40
1:J:104:GLU:O	1:J:108:LYS:NZ	2.38	0.40
1:A:87:VAL:HG23	1:A:88:PRO:HD3	2.04	0.40
1:G:109:LYS:HE2	1:G:109:LYS:HB2	1.88	0.40
1:D:87:VAL:HG23	1:D:88:PRO:HD3	2.04	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	192/257 (75%)	180 (94%)	12 (6%)	0	100	100
1	B	192/257 (75%)	180 (94%)	12 (6%)	0	100	100
1	C	192/257 (75%)	180 (94%)	12 (6%)	0	100	100
1	D	192/257 (75%)	180 (94%)	12 (6%)	0	100	100
1	E	192/257 (75%)	180 (94%)	12 (6%)	0	100	100
1	F	192/257 (75%)	180 (94%)	12 (6%)	0	100	100
1	G	192/257 (75%)	186 (97%)	6 (3%)	0	100	100
1	H	192/257 (75%)	186 (97%)	6 (3%)	0	100	100
1	I	192/257 (75%)	187 (97%)	5 (3%)	0	100	100
1	J	192/257 (75%)	187 (97%)	5 (3%)	0	100	100
1	K	192/257 (75%)	187 (97%)	5 (3%)	0	100	100
1	L	192/257 (75%)	187 (97%)	5 (3%)	0	100	100
All	All	2304/3084 (75%)	2200 (96%)	104 (4%)	0	100	100

There are no Ramachandran outliers to report.

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	175/227 (77%)	174 (99%)	1 (1%)	86	94
1	B	175/227 (77%)	174 (99%)	1 (1%)	86	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	175/227 (77%)	174 (99%)	1 (1%)	86	94
1	D	175/227 (77%)	174 (99%)	1 (1%)	86	94
1	E	175/227 (77%)	174 (99%)	1 (1%)	86	94
1	F	175/227 (77%)	174 (99%)	1 (1%)	86	94
1	G	175/227 (77%)	174 (99%)	1 (1%)	86	94
1	H	175/227 (77%)	174 (99%)	1 (1%)	86	94
1	I	175/227 (77%)	174 (99%)	1 (1%)	86	94
1	J	175/227 (77%)	174 (99%)	1 (1%)	86	94
1	K	175/227 (77%)	174 (99%)	1 (1%)	86	94
1	L	175/227 (77%)	174 (99%)	1 (1%)	86	94
All	All	2100/2724 (77%)	2088 (99%)	12 (1%)	86	94

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	163	SER
1	G	156	ILE
1	B	163	SER
1	L	156	ILE
1	C	163	SER
1	K	156	ILE
1	D	163	SER
1	J	156	ILE
1	E	163	SER
1	I	156	ILE
1	F	163	SER
1	H	156	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	49	GLN
1	L	49	GLN
1	K	49	GLN
1	J	49	GLN
1	I	49	GLN
1	H	49	GLN



### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no 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.

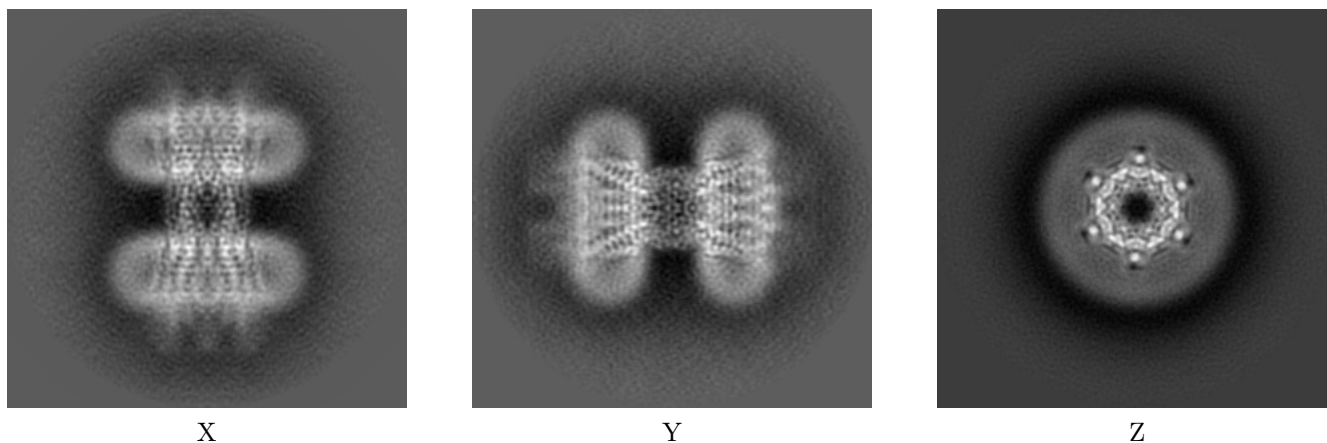
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31497. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

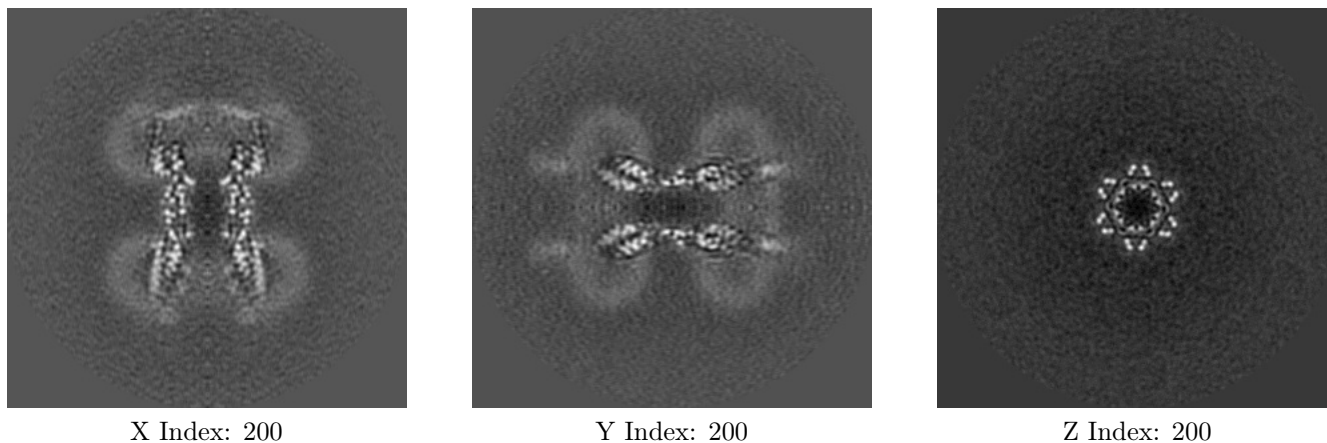
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

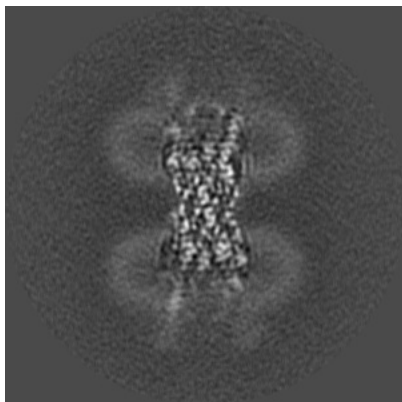
#### 6.2.1 Primary map



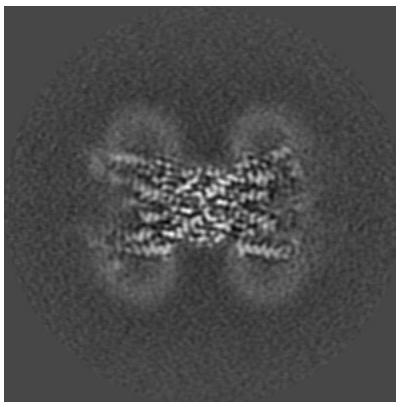
The images above show central slices of the map in three orthogonal directions.

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

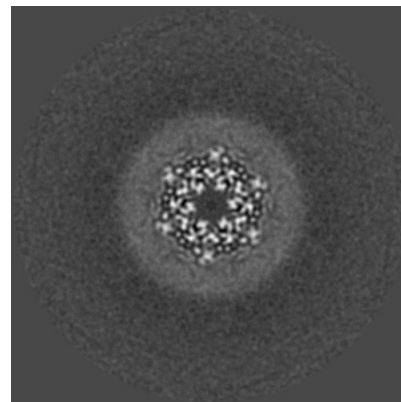
### 6.3.1 Primary map



X Index: 174



Y Index: 178

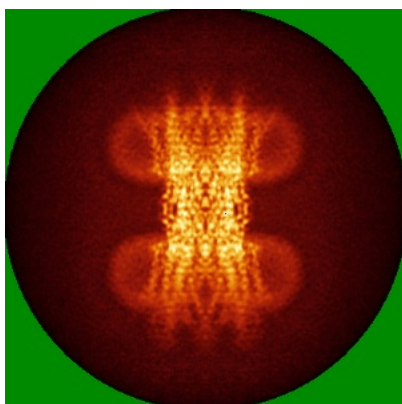


Z Index: 161

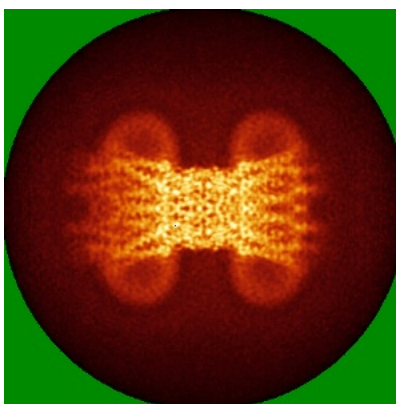
The images above show the largest variance slices of the map in three orthogonal directions.

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

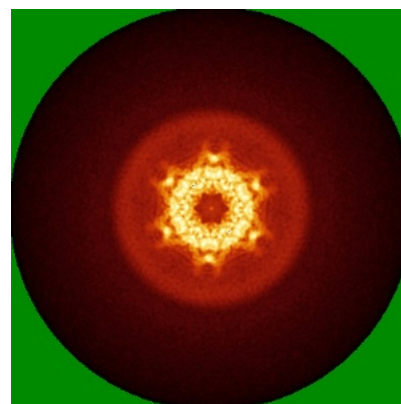
### 6.4.1 Primary map



X



Y

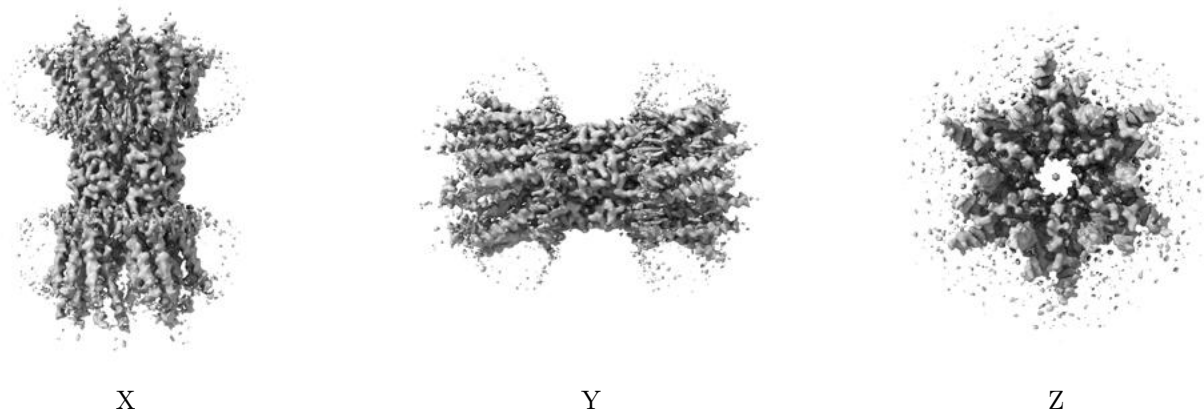


Z

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 0.008. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

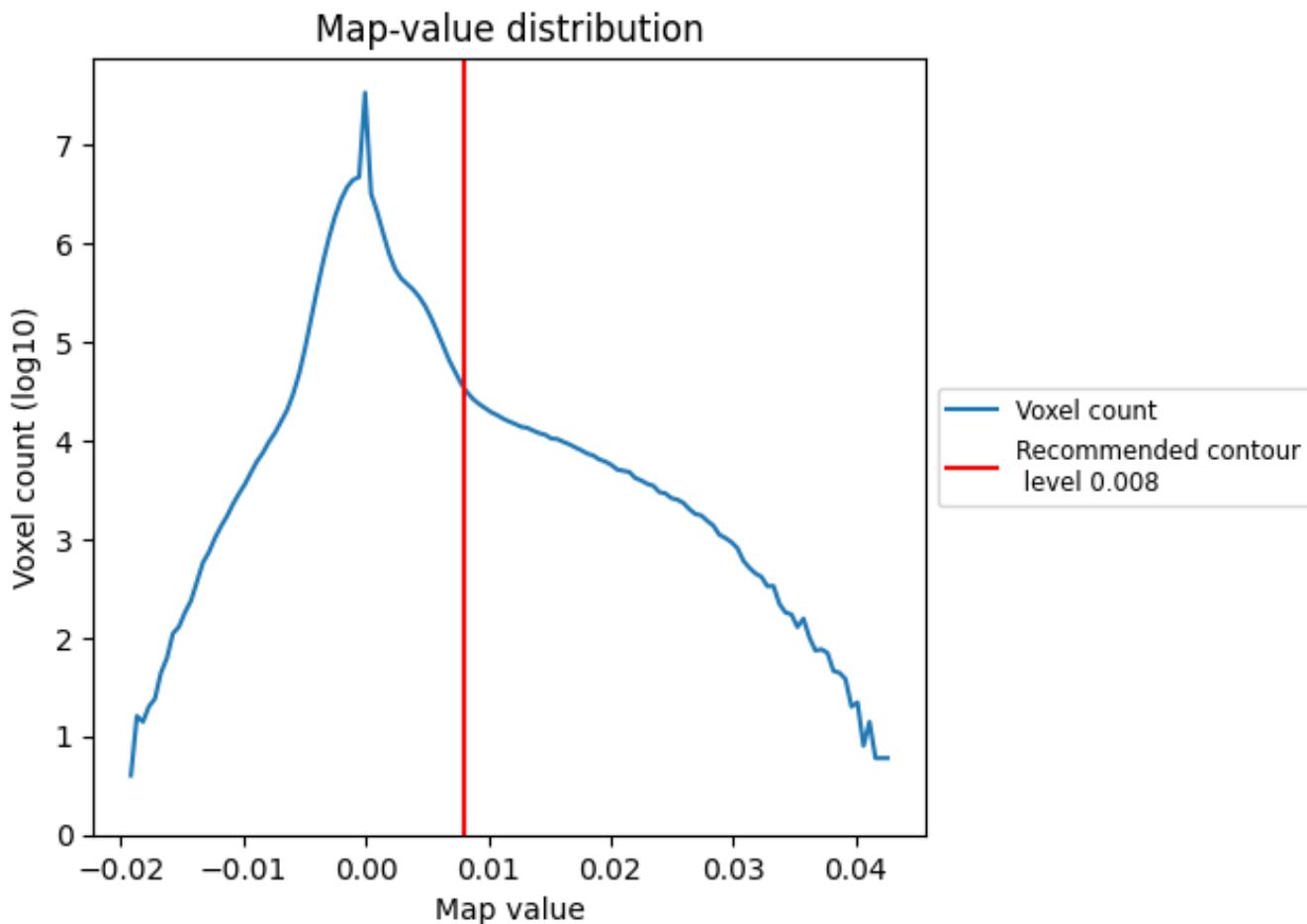
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

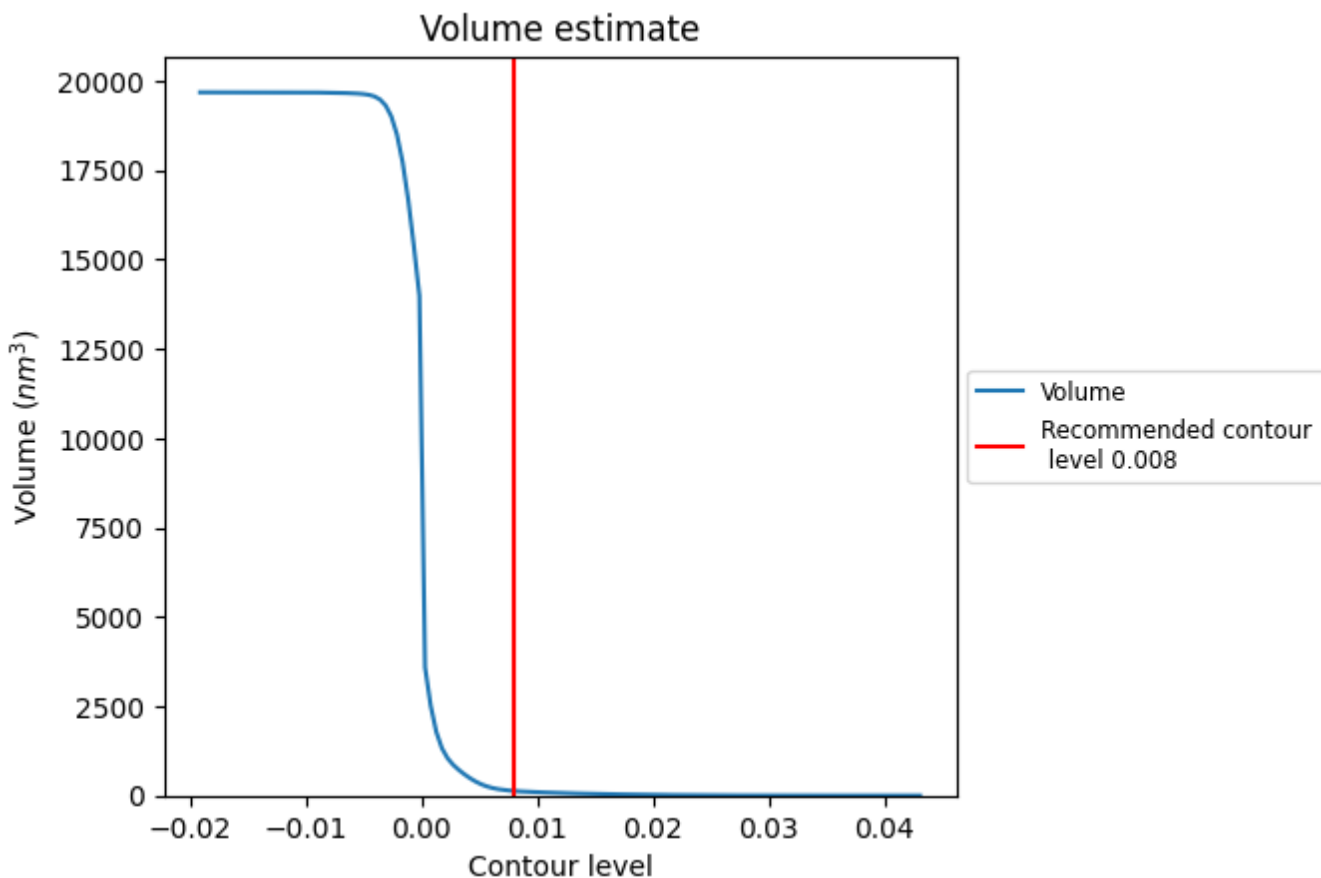
This section contains the results of statistical analysis of the map.

### 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.

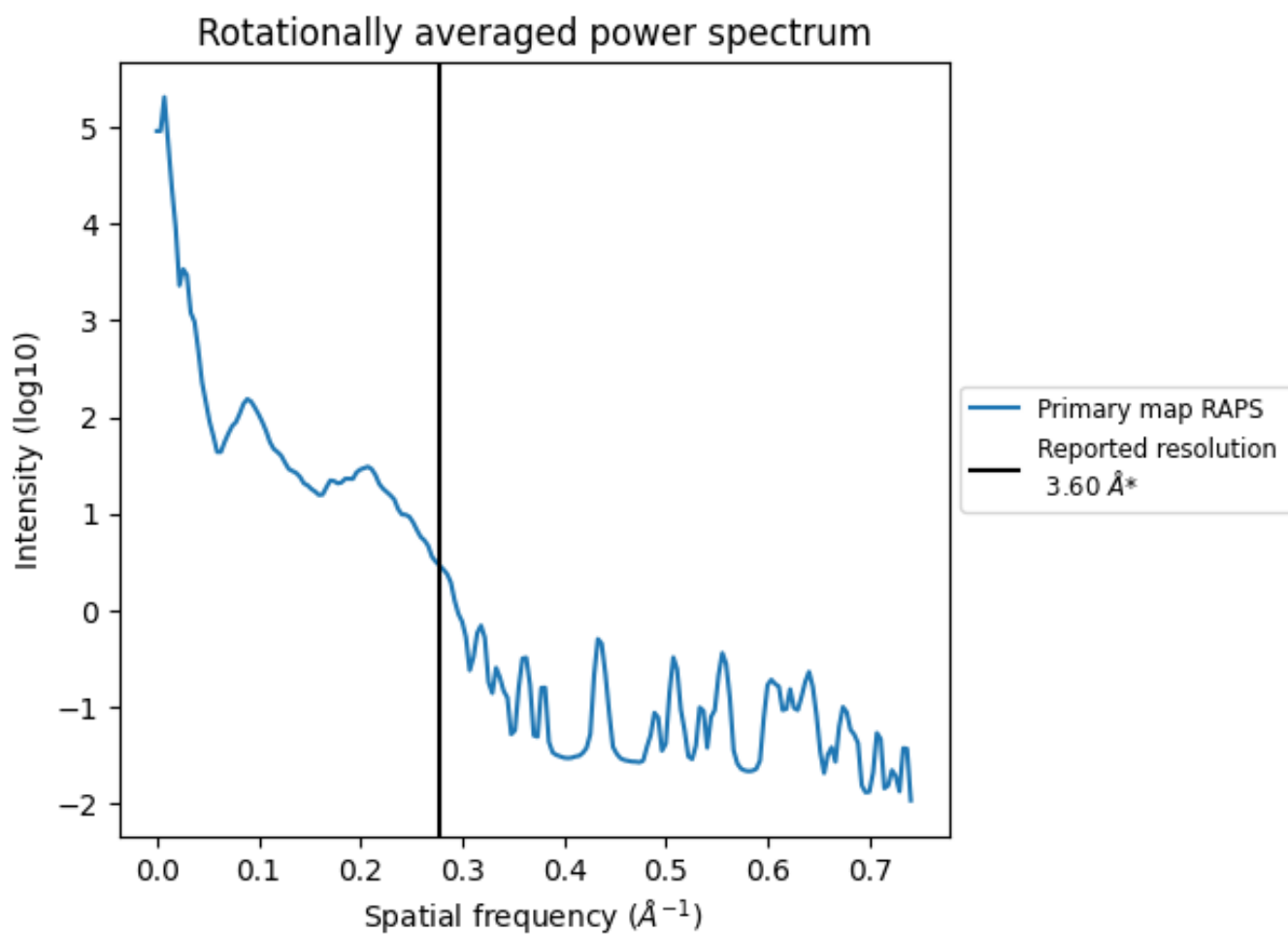
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 129 nm<sup>3</sup>; this corresponds to an approximate mass of 116 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

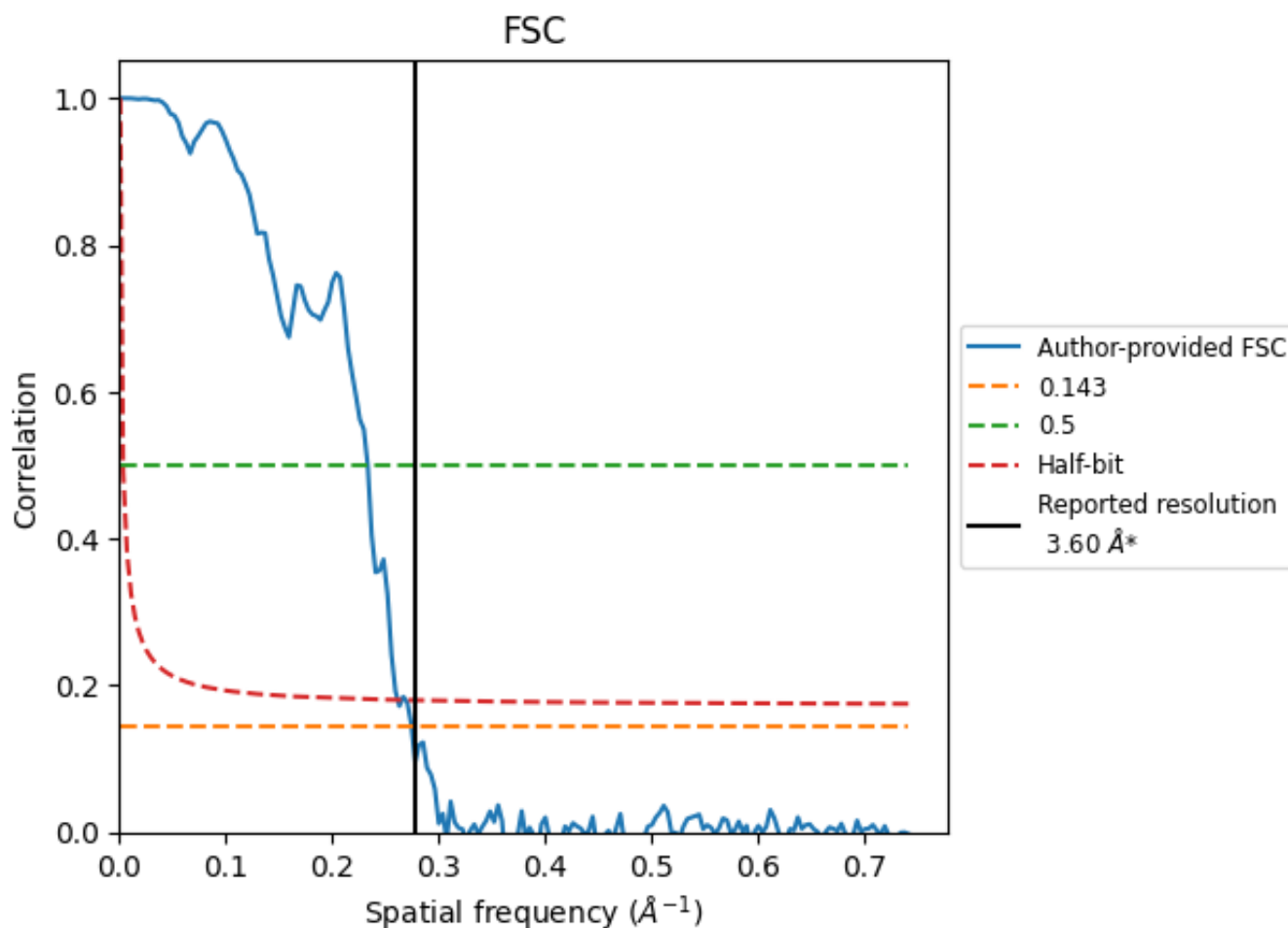


\*Reported resolution corresponds to spatial frequency of 0.278 Å<sup>-1</sup>

## 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 0.278 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

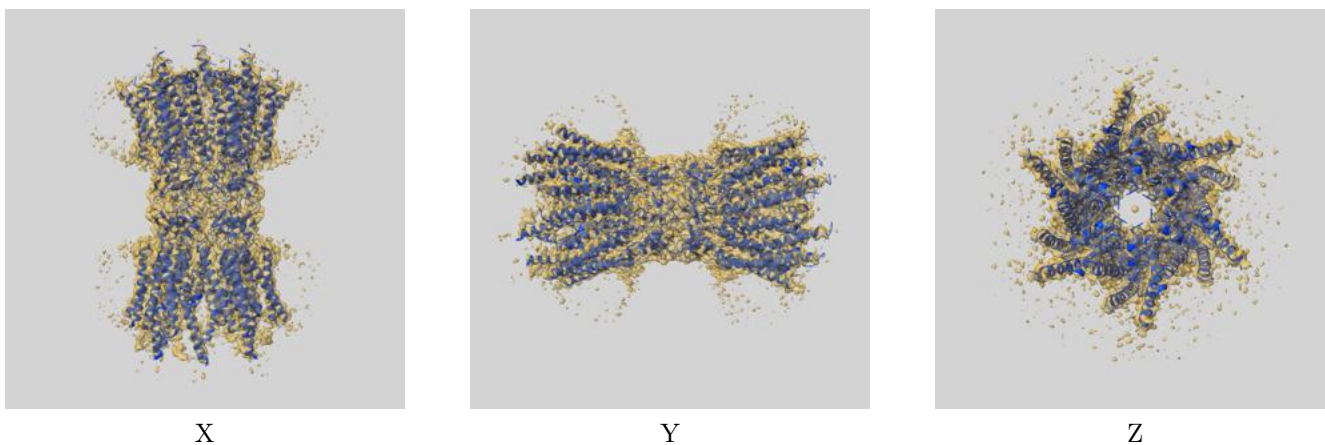
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.64	4.29	3.83
Unmasked-calculated*	-	-	-

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

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

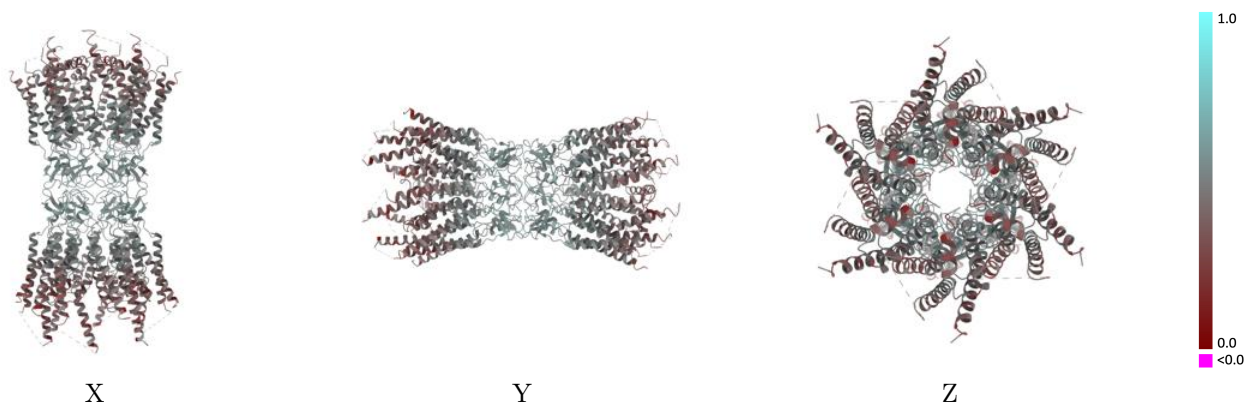
This section contains information regarding the fit between EMDB map EMD-31497 and PDB model 7F94. Per-residue inclusion information can be found in section 3 on page 5.

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



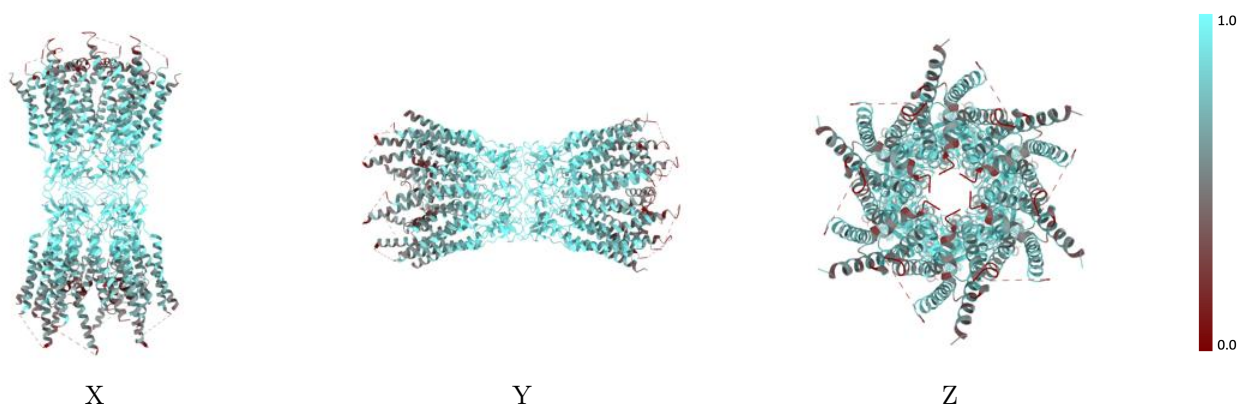
The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



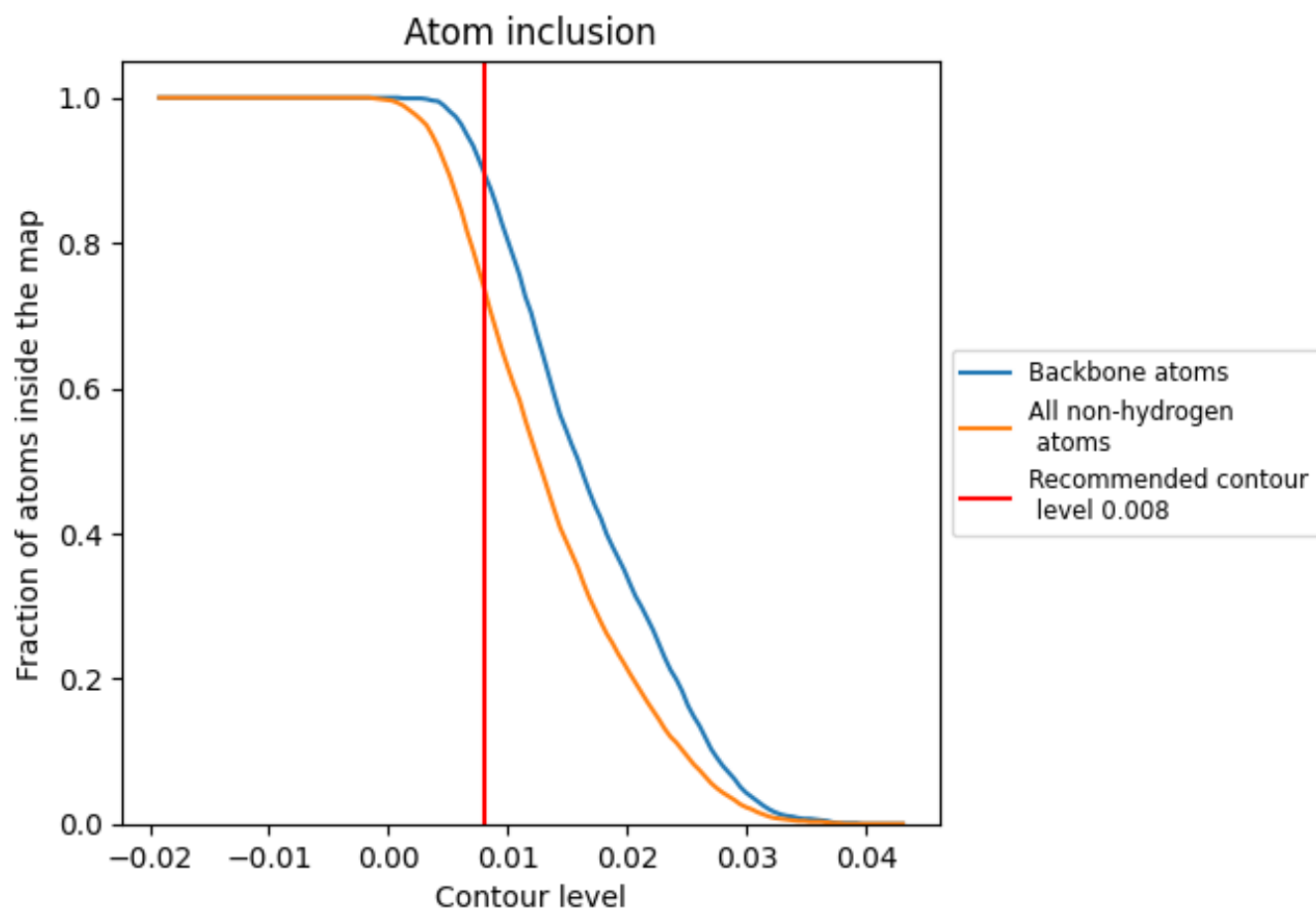
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.008).



























## 9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 74% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7390	 0.4560
A	 0.7300	 0.4500
B	 0.7280	 0.4520
C	 0.7300	 0.4540
D	 0.7300	 0.4520
E	 0.7290	 0.4510
F	 0.7300	 0.4510
G	 0.7490	 0.4590
H	 0.7510	 0.4600
I	 0.7470	 0.4600
J	 0.7470	 0.4590
K	 0.7470	 0.4600
L	 0.7480	 0.4610

