



Full wwPDB EM Validation Report ⓘ

May 13, 2025 – 04:17 AM EDT

PDB ID : 8DYX / pdb_00008dyx
EMDB ID : EMD-27785
Title : Cryo-EM structure of 311 Fab in complex with recombinant shortened Plasmodium falciparum circumsporozoite protein (rsCSP)
Authors : Martin, G.M.; Ward, A.B.
Deposited on : 2022-08-05
Resolution : 3.00 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

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>.

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) : 2.43.1

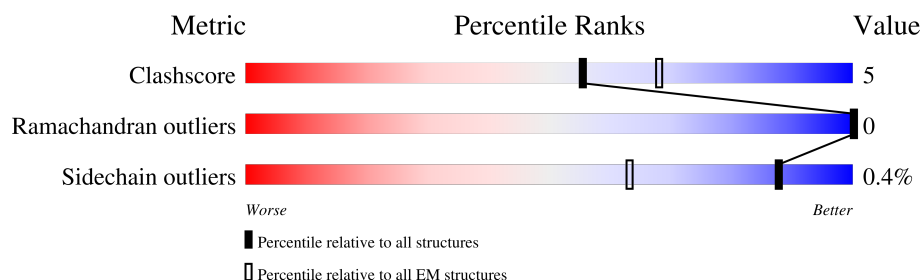
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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.



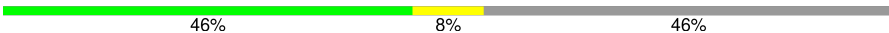



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 ≥ 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	I	278	
2	A	225	
2	C	225	
2	E	225	
2	H	225	
2	M	225	
2	O	225	
2	Q	225	

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Mol	Chain	Length	Quality of chain
2	S	225	
2	U	225	
2	W	225	
2	Y	225	
3	B	218	
3	D	218	
3	F	218	
3	L	218	
3	N	218	
3	P	218	
3	R	218	
3	T	218	
3	V	218	
3	X	218	
3	Z	218	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20030 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 Circumsporozoite protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	I	90	Total	C	N	O	0	0
			637	367	131	139		

- Molecule 2 is a protein called 311 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	121	Total	C	N	O	S	0	0
			946	599	163	180	4		
2	A	121	Total	C	N	O	S	0	0
			946	599	163	180	4		
2	C	121	Total	C	N	O	S	0	0
			946	599	163	180	4		
2	E	121	Total	C	N	O	S	0	0
			946	599	163	180	4		
2	M	121	Total	C	N	O	S	0	0
			946	599	163	180	4		
2	O	121	Total	C	N	O	S	0	0
			946	599	163	180	4		
2	Q	121	Total	C	N	O	S	0	0
			946	599	163	180	4		
2	S	121	Total	C	N	O	S	0	0
			946	599	163	180	4		
2	U	121	Total	C	N	O	S	0	0
			946	599	163	180	4		
2	W	121	Total	C	N	O	S	0	0
			946	599	163	180	4		
2	Y	121	Total	C	N	O	S	0	0
			946	599	163	180	4		

- Molecule 3 is a protein called 311 light chain.

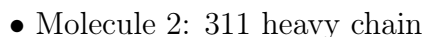
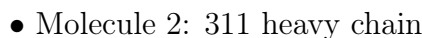
Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	112	Total	C	N	O	S	0	0
			817	510	140	165	2		

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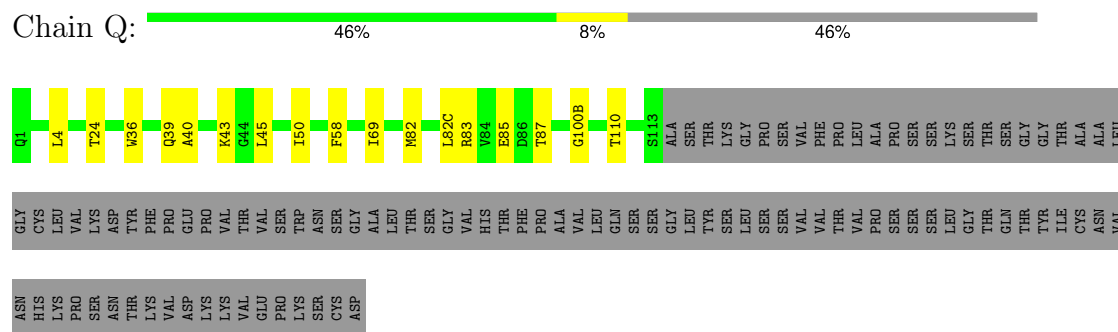
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Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	112	Total 817	C 510	N 140	O 165	S 2	0	0
3	D	112	Total 817	C 510	N 140	O 165	S 2	0	0
3	F	112	Total 817	C 510	N 140	O 165	S 2	0	0
3	N	112	Total 817	C 510	N 140	O 165	S 2	0	0
3	P	112	Total 817	C 510	N 140	O 165	S 2	0	0
3	R	112	Total 817	C 510	N 140	O 165	S 2	0	0
3	T	112	Total 817	C 510	N 140	O 165	S 2	0	0
3	V	112	Total 817	C 510	N 140	O 165	S 2	0	0
3	X	112	Total 817	C 510	N 140	O 165	S 2	0	0
3	Z	112	Total 817	C 510	N 140	O 165	S 2	0	0

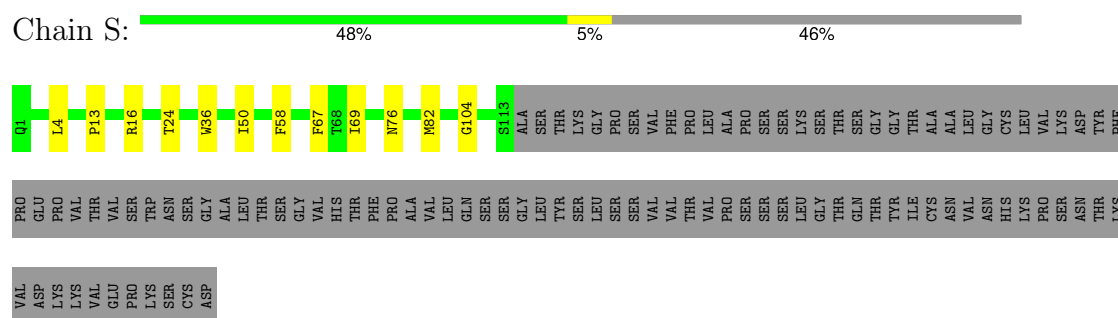
- Molecule 1: Circumsporozoite protein



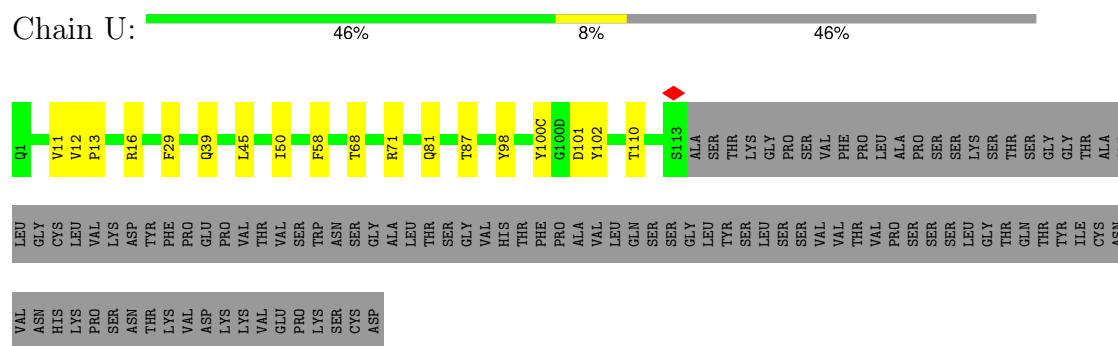
● Molecule 2: 311 heavy chain



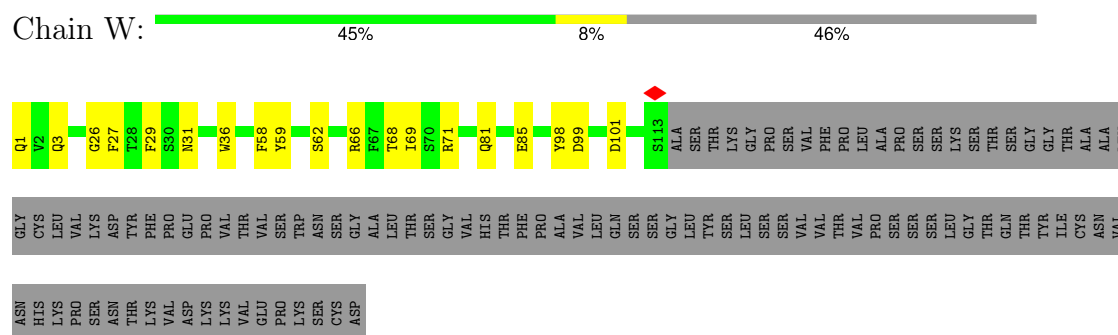
● Molecule 2: 311 heavy chain



● Molecule 2: 311 heavy chain



● Molecule 2: 311 heavy chain



● Molecule 2: 311 heavy chain

THR
HIS
GLY
GLY
SER
THR
VAL
GLY
LYS
THR
VAL
VAL
ALA
PRO
GLY
CYS
SER

• Molecule 3: 311 light chain



GLN
S2
P7
T24
N27B
Y31
L39
T42
R54
F62
G77
L78
Q79
A80
A84
Q89
T102
K103
L104
T105
V106
L106A
G107
GLN
PRO
LYS
ALA
ALA
PRO
SER
VAL
THR
LEU
PHE
PRO
PRO
SER
SER
GLY
GLY
LEU
TRP
GLN
ALA
ASN
LYS
THR
LEU
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VAL
CYS
LEU
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VAL
ASP
PHE
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GLY
ALA
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ALA
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GLY
SER
THR
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GLY
LYS
THR
VAL
ALA
PRO
CYS
SER

CYS
ARG
VAL
THR
HIS
GLY
SER
THR
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GLY
LYS
THR
VAL
ALA
PRO
GLY
CYS
SER

• Molecule 3: 311 light chain



GLN
S2
V3
P55
V58
R61
D82
D85
Y91
D92
S95A
G107
GLN
PRO
LYS
ALA
ALA
PRO
SER
VAL
THR
THR
PHE
PRO
SER
SER
GLY
LEU
TRP
GLN
LEU
GLN
TRP
LYS
ALA
HIS
ARG
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TYR
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CYS
VAL
VAL
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TRP
LYS
ALA
ASP
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PHE
TYR
PRO
GLY
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LYS
THR
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ALA

PRO
ALA
GLY
CYS
SER

• Molecule 3: 311 light chain



GLN
S2
P7
T18
L39
T42
R61
D82
Q89
T102
G107
GLN
PRO
LYS
ALA
ALA
PRO
SER
VAL
THR
THR
PHE
PRO
PRO
SER
SER
GLY
GLY
LEU
TRP
LYS
ALA
HIS
ARG
SER
TYR
SER
CYS
VAL
VAL
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PHE
TYR
PRO
GLY
ALA
VAL
THR
VAL
ALA

TRP
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ALA
ASP
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LYS
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LYS
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ASN
ASN
LYS
TYR
ALA
ALA
SER
SER
TYR
LEU
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GLY
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LYS
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SER
TYR
SER
CYS
VAL
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GLY
PHE
TYR
PRO
GLY
VAL
LYS
THR
VAL
ALA

PRO
ALA
GLY
CYS
SER

• Molecule 3: 311 light chain



GLN
S2
A14
Q17
T18
L39
T42
A84
D85
Q89
S90
R94
G107
GLN
PRO
LYS
ALA
ALA
PRO
SER
VAL
THR
THR
PHE
PRO
PRO
SER
SER
GLY
GLY
LEU
TRP
LYS
ALA
HIS
ARG
SER
TYR
SER
CYS
VAL
VAL
THR
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ASP
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ALA
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TYR
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GLY
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LYS
SER
HIS
ARG
SER
TYR
SER
CYS
ARG
VAL
VAL
THR
HIS
GLY
ASP
PHE
TYR
PRO
GLY
VAL
GLY
LYS
THR
VAL

ALA
PRO
ALA
GLY
CYS
SER

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

THR HIS GLU GLY SER THR VAL GLU LYS THR VAL ALA TRP PRO ALA GLU CYS SER

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	399027	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.147	Depositor
Minimum map value	-0.082	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	226.59999, 226.59999, 226.59999	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	Depositor

5 Model quality

5.1 Standard geometry

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	I	0.20	0/659	0.39	0/931
2	A	0.10	0/971	0.30	0/1320
2	C	0.12	0/971	0.32	0/1320
2	E	0.14	0/971	0.32	0/1320
2	H	0.15	0/971	0.34	0/1320
2	M	0.15	0/971	0.34	0/1320
2	O	0.15	0/971	0.34	0/1320
2	Q	0.14	0/971	0.32	0/1320
2	S	0.14	0/971	0.31	0/1320
2	U	0.13	0/971	0.32	0/1320
2	W	0.12	0/971	0.31	0/1320
2	Y	0.11	0/971	0.31	0/1320
3	B	0.10	0/836	0.30	0/1139
3	D	0.13	0/836	0.35	0/1139
3	F	0.15	0/836	0.36	0/1139
3	L	0.14	0/836	0.36	0/1139
3	N	0.16	0/836	0.36	0/1139
3	P	0.15	0/836	0.36	0/1139
3	R	0.13	0/836	0.37	0/1139
3	T	0.14	0/836	0.37	0/1139
3	V	0.14	0/836	0.37	0/1139
3	X	0.12	0/836	0.35	0/1139
3	Z	0.10	0/836	0.30	0/1139
All	All	0.14	0/20536	0.34	0/27980

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 ⓘ

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	I	637	0	544	9	0
2	A	946	0	894	12	0
2	C	946	0	894	14	0
2	E	946	0	894	13	0
2	H	946	0	894	10	0
2	M	946	0	894	6	0
2	O	946	0	894	10	0
2	Q	946	0	894	10	0
2	S	946	0	894	7	0
2	U	946	0	894	10	0
2	W	946	0	894	15	0
2	Y	946	0	894	14	0
3	B	817	0	785	8	0
3	D	817	0	785	9	0
3	F	817	0	785	9	0
3	L	817	0	785	5	0
3	N	817	0	785	5	0
3	P	817	0	785	6	0
3	R	817	0	785	8	0
3	T	817	0	785	10	0
3	V	817	0	785	9	0
3	X	817	0	785	6	0
3	Z	817	0	785	9	0
All	All	20030	0	19013	187	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 (187) 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:M:16:ARG:NH2	3:T:18:THR:O	2.16	0.78
2:E:85:GLU:OE2	2:E:85:GLU:N	2.20	0.74
3:X:39:LEU:HB2	3:X:42:THR:HG22	1.69	0.73
3:B:39:LEU:HB2	3:B:42:THR:HG22	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:6:GLN:HE22	3:T:88:CYS:H	1.39	0.71
3:Z:39:LEU:HB2	3:Z:42:THR:HG22	1.76	0.67
2:E:16:ARG:NH2	3:R:18:THR:O	2.28	0.67
3:F:78:LEU:HD11	3:F:104:LEU:HD21	1.76	0.66
2:Y:34:MET:HE1	2:Y:92:CYS:HB2	1.76	0.66
3:V:54:ARG:HD3	3:V:58:VAL:HG12	1.78	0.65
3:D:39:LEU:HB2	3:D:42:THR:HG22	1.79	0.64
3:V:39:LEU:HB2	3:V:42:THR:HG22	1.80	0.63
3:R:39:LEU:HB2	3:R:42:THR:HG22	1.81	0.61
2:C:50:ILE:HG22	2:C:58:PHE:HB2	1.82	0.61
2:W:29:PHE:O	2:W:71:ARG:NH2	2.34	0.60
2:O:82:MET:HE2	2:O:82(C):LEU:HD21	1.84	0.60
3:L:18:THR:O	2:C:16:ARG:NH2	2.35	0.60
2:Y:47:TRP:HZ2	2:Y:50:ILE:HG22	1.67	0.59
2:S:13:PRO:HG2	2:S:16:ARG:HE	1.66	0.59
2:S:24:THR:OG1	2:S:76:ASN:O	2.20	0.59
2:E:13:PRO:HG2	2:E:16:ARG:HD3	1.85	0.59
2:A:35:HIS:CE1	2:A:50:ILE:HD12	2.37	0.58
3:X:47:LEU:HD23	3:X:48:ILE:HG13	1.86	0.57
1:I:126:VAL:HG22	2:E:52(A):TYR:CD2	2.39	0.57
3:B:31:TYR:O	3:B:66:LYS:NZ	2.38	0.57
2:C:4:LEU:HD22	2:C:24:THR:HG22	1.87	0.56
2:C:41:PRO:O	2:C:43:LYS:NZ	2.38	0.56
3:V:27(A):SER:OG	3:V:92:ASP:OD1	2.24	0.56
3:V:103:LYS:NZ	3:V:104:LEU:O	2.39	0.56
2:W:68:THR:HB	2:W:81:GLN:HB3	1.88	0.56
3:Z:31:TYR:O	3:Z:66:LYS:NZ	2.39	0.56
2:O:100(B):GLY:O	3:P:89:GLN:NE2	2.34	0.55
2:A:47:TRP:HZ2	2:A:50:ILE:HG22	1.71	0.55
1:I:106:ALA:HB3	2:A:52:TRP:HZ2	1.72	0.54
2:O:101:ASP:N	2:O:101:ASP:OD1	2.39	0.54
2:H:87:THR:HG23	2:H:110:THR:HA	1.90	0.54
3:F:39:LEU:HB2	3:F:42:THR:HG22	1.90	0.54
2:Y:37:VAL:O	2:Y:91:TYR:N	2.33	0.54
2:Q:50:ILE:HG22	2:Q:58:PHE:HB2	1.90	0.54
2:W:36:TRP:HD1	2:W:69:ILE:HD12	1.72	0.54
3:N:95(A):SER:O	3:N:95(A):SER:OG	2.26	0.54
1:I:105:ASN:ND2	2:A:100:THR:O	2.30	0.54
2:O:82(B):SER:O	2:O:82(B):SER:OG	2.26	0.53
2:C:100(A):SER:HB3	3:D:32:ASP:HB2	1.90	0.53
2:O:35:HIS:CE1	2:O:50:ILE:HD12	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:68:THR:O	2:W:81:GLN:N	2.38	0.53
2:H:35:HIS:CE1	2:H:50:ILE:HD12	2.44	0.53
2:C:35:HIS:CE1	2:C:50:ILE:HD12	2.45	0.52
3:B:27(B):ASN:OD1	3:B:27(C):ILE:N	2.42	0.52
3:F:7:PRO:O	3:F:102:THR:OG1	2.25	0.52
3:N:61:ARG:NH2	3:N:82:ASP:OD1	2.43	0.52
2:U:39:GLN:HB2	2:U:45:LEU:HD23	1.92	0.52
2:S:13:PRO:HG2	2:S:16:ARG:HH21	1.75	0.52
2:U:68:THR:HB	2:U:81:GLN:HB3	1.91	0.52
3:F:77:GLY:O	3:F:79:GLN:NE2	2.35	0.51
3:Z:27(B):ASN:OD1	3:Z:27(C):ILE:N	2.40	0.51
3:V:39:LEU:HD23	3:V:84:ALA:HB2	1.90	0.51
2:U:11:VAL:HG12	2:U:110:THR:HB	1.91	0.51
2:C:101:ASP:N	2:C:101:ASP:OD1	2.33	0.51
2:M:24:THR:OG1	2:M:76:ASN:O	2.27	0.51
2:M:101:ASP:OD1	2:M:101:ASP:N	2.43	0.51
3:T:44:PRO:O	3:T:45:LYS:NZ	2.38	0.50
3:T:6:GLN:NE2	3:T:88:CYS:SG	2.83	0.50
2:U:50:ILE:HG22	2:U:58:PHE:HB2	1.94	0.50
3:L:42:THR:OG1	3:L:43:ALA:N	2.43	0.50
2:Q:87:THR:HG23	2:Q:110:THR:HA	1.94	0.50
2:U:87:THR:HG23	2:U:110:THR:HA	1.94	0.50
2:O:87:THR:HG23	2:O:110:THR:HA	1.93	0.49
2:C:67:PHE:CE1	2:C:82:MET:HB3	2.47	0.49
2:E:6:GLU:OE2	2:E:106:GLY:N	2.37	0.49
2:U:29:PHE:O	2:U:71:ARG:NH2	2.45	0.49
2:E:47:TRP:HZ2	2:E:50:ILE:HG22	1.77	0.49
1:I:176:PRO:HB3	2:W:58:PHE:CD2	2.48	0.48
3:L:54:ARG:HD2	3:L:58:VAL:HG12	1.95	0.48
2:W:62:SER:O	2:W:66:ARG:NH1	2.46	0.48
2:A:16:ARG:NH2	3:P:18:THR:O	2.46	0.48
2:Y:35:HIS:CE1	2:Y:50:ILE:HD12	2.48	0.48
1:I:129:ASN:ND2	2:M:100:THR:O	2.38	0.48
2:H:36:TRP:HD1	2:H:69:ILE:HD12	1.77	0.47
1:I:118:VAL:HG22	2:C:52(A):TYR:CD2	2.49	0.47
2:H:98:TYR:OH	3:R:94:ARG:NH1	2.47	0.47
2:A:16:ARG:NH2	3:P:18:THR:H	2.13	0.47
3:B:28:GLY:HA3	3:B:69:THR:HG22	1.95	0.47
2:E:35:HIS:CE1	2:E:50:ILE:HD12	2.50	0.47
2:Q:100(B):GLY:O	3:R:89:GLN:NE2	2.42	0.47
1:I:113:ASN:CG	1:I:113:ASN:O	2.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:101:ASP:N	2:W:101:ASP:OD1	2.45	0.47
2:E:100(B):GLY:O	3:F:89:GLN:NE2	2.42	0.46
3:P:39:LEU:HB2	3:P:42:THR:OG1	2.16	0.46
2:S:67:PHE:CE1	2:S:82:MET:HB3	2.50	0.46
3:N:55:PRO:HD2	3:N:58:VAL:HG21	1.97	0.46
2:A:4:LEU:HB2	2:A:104:GLY:HA2	1.96	0.46
2:M:12:VAL:HG11	2:M:82(C):LEU:HD13	1.96	0.46
2:O:6:GLU:OE1	2:O:106:GLY:N	2.43	0.46
2:E:3:GLN:OE1	2:E:25:SER:OG	2.33	0.46
3:L:18:THR:H	2:C:16:ARG:NH2	2.14	0.46
3:D:25:GLY:HA3	3:D:27(C):ILE:HD12	1.97	0.46
2:O:18:LEU:HD12	2:O:19:ARG:H	1.80	0.46
2:U:12:VAL:HG23	2:U:16:ARG:HH21	1.81	0.46
2:E:87:THR:HG23	2:E:110:THR:HA	1.98	0.46
3:F:54:ARG:NH1	3:F:62:PHE:O	2.49	0.46
2:W:59:TYR:CE2	2:W:69:ILE:HG22	2.52	0.45
2:H:4:LEU:HD22	2:H:24:THR:HG22	1.97	0.45
2:H:50:ILE:HG22	2:H:58:PHE:HB2	1.98	0.45
3:D:27(B):ASN:O	3:D:31:TYR:HB2	2.17	0.45
3:D:37:GLN:HG3	3:D:86:TYR:HE1	1.81	0.45
2:O:50:ILE:HG22	2:O:58:PHE:HB2	1.97	0.45
2:W:99:ASP:OD2	3:Z:94:ARG:NH2	2.49	0.45
2:Y:39:GLN:HB2	2:Y:45:LEU:HD23	1.98	0.45
2:C:20:LEU:HD22	2:C:107:THR:HG21	1.98	0.45
3:P:7:PRO:O	3:P:102:THR:OG1	2.22	0.45
3:B:14:ALA:O	3:B:17:GLN:HG2	2.17	0.45
2:S:4:LEU:HB2	2:S:104:GLY:HA2	1.99	0.45
3:F:80:ALA:HA	3:F:106:VAL:HG11	1.99	0.44
2:Q:82:MET:HE2	2:Q:82(C):LEU:HD21	1.98	0.44
2:S:36:TRP:HD1	2:S:69:ILE:HD12	1.82	0.44
3:V:11:VAL:HG23	3:V:104:LEU:HD13	1.99	0.44
3:D:14:ALA:O	3:D:17:GLN:HG2	2.17	0.44
2:M:36:TRP:HD1	2:M:69:ILE:HD12	1.81	0.44
3:T:6:GLN:NE2	3:T:88:CYS:H	2.11	0.44
2:A:67:PHE:CE1	2:A:82:MET:HG2	2.52	0.44
2:W:85:GLU:OE1	2:W:85:GLU:N	2.30	0.44
3:X:47:LEU:HA	3:X:58:VAL:HG21	1.99	0.43
3:R:14:ALA:O	3:R:17:GLN:HG2	2.18	0.43
2:U:13:PRO:HD2	2:U:16:ARG:NH2	2.33	0.43
3:V:27(B):ASN:OD1	3:V:27(C):ILE:N	2.49	0.43
2:H:24:THR:OG1	2:H:76:ASN:O	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:83:ARG:HB2	2:Q:85:GLU:HG2	1.99	0.43
2:W:31:ASN:ND2	2:Y:57:ASN:O	2.46	0.43
3:X:14:ALA:O	3:X:17:GLN:HG2	2.17	0.43
3:B:37:GLN:HB2	3:B:47:LEU:HD22	2.00	0.43
2:E:36:TRP:HD1	2:E:69:ILE:HD12	1.84	0.43
2:O:36:TRP:HD1	2:O:69:ILE:HD12	1.83	0.43
3:T:14:ALA:O	3:T:17:GLN:HG2	2.18	0.43
2:H:82(C):LEU:HD23	2:H:82(C):LEU:HA	1.90	0.43
2:Y:101:ASP:HA	3:Z:46:LEU:HD22	2.01	0.43
3:Z:14:ALA:O	3:Z:17:GLN:HG2	2.19	0.43
2:Q:4:LEU:HG	2:Q:24:THR:HG22	1.99	0.43
2:Q:39:GLN:HB2	2:Q:45:LEU:HD23	2.00	0.43
3:L:19:VAL:HG21	3:L:104:LEU:HD11	2.01	0.43
2:W:98:TYR:CE1	3:Z:94:ARG:HD3	2.53	0.43
3:R:89:GLN:HG2	3:R:90:SER:N	2.33	0.42
2:A:101:ASP:OD1	2:A:101:ASP:N	2.53	0.42
2:Y:45:LEU:HD11	3:Z:44:PRO:HG2	2.01	0.42
3:F:39:LEU:HD23	3:F:84:ALA:HB2	2.01	0.42
2:Y:12:VAL:HG11	2:Y:82(C):LEU:HD13	2.02	0.42
2:H:42:GLY:C	2:H:43:LYS:HD3	2.44	0.42
2:Q:40:ALA:HB3	2:Q:43:LYS:HD3	2.00	0.42
2:U:101:ASP:OD1	2:U:102:TYR:N	2.52	0.42
2:H:98:TYR:O	3:R:94:ARG:HG2	2.20	0.42
2:Q:40:ALA:HB3	2:Q:43:LYS:HB2	2.02	0.42
2:E:39:GLN:HB2	2:E:45:LEU:HD23	2.02	0.42
3:V:14:ALA:N	3:V:17:GLN:OE1	2.49	0.41
3:X:95(A):SER:O	3:X:95(A):SER:OG	2.34	0.41
3:P:61:ARG:NH1	3:P:82:ASP:OD2	2.53	0.41
3:R:39:LEU:HD23	3:R:84:ALA:HB2	2.02	0.41
3:T:39:LEU:HD23	3:T:84:ALA:HB2	2.01	0.41
3:V:14:ALA:O	3:V:17:GLN:HG2	2.19	0.41
2:Y:34:MET:SD	2:Y:78:LEU:HD22	2.61	0.41
2:Y:94:ARG:NH2	2:Y:101:ASP:OD2	2.37	0.41
2:A:37:VAL:HG11	2:A:103:TRP:CZ3	2.55	0.41
3:Z:38:GLN:HA	3:Z:44:PRO:HA	2.03	0.41
1:I:129:ASN:HB2	3:N:91:TYR:CE1	2.56	0.41
2:C:47:TRP:CZ3	3:D:95(B):GLY:HA2	2.56	0.41
2:U:98:TYR:HB2	2:U:100(C):TYR:HE1	1.86	0.41
1:I:181:ASN:O	1:I:183:ASN:N	2.47	0.41
2:E:53:ASP:OD2	2:E:53:ASP:N	2.45	0.41
3:F:27(B):ASN:O	3:F:31:TYR:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:3:VAL:HG11	3:N:92:ASP:OD2	2.21	0.41
2:Q:36:TRP:HD1	2:Q:69:ILE:HD12	1.86	0.41
2:S:50:ILE:HG22	2:S:58:PHE:HB2	2.03	0.41
2:C:94:ARG:NH2	2:C:101:ASP:OD2	2.45	0.41
2:W:1:GLN:HG2	2:W:3:GLN:HE21	1.86	0.41
3:X:27(A):SER:HA	3:X:93:ARG:NH2	2.36	0.41
2:Y:71:ARG:HB3	2:Y:78:LEU:HD12	2.03	0.41
2:A:98:TYR:CD2	2:A:99:ASP:HB2	2.56	0.40
3:D:37:GLN:HG3	3:D:86:TYR:CE1	2.56	0.40
2:A:45:LEU:HD21	3:B:44:PRO:HG2	2.03	0.40
2:C:24:THR:OG1	2:C:76:ASN:O	2.39	0.40
2:W:27:PHE:HA	2:Y:64:GLU:HG2	2.03	0.40
3:B:46:LEU:HD12	3:B:47:LEU:H	1.86	0.40
3:D:61:ARG:NH2	3:D:82:ASP:OD1	2.53	0.40
3:T:3:VAL:HG11	3:T:92:ASP:OD1	2.21	0.40
2:W:1:GLN:O	2:W:26:GLY:HA3	2.21	0.40
3:T:84:ALA:HB3	3:T:86:TYR:HE1	1.86	0.40
3:T:12:SER:OG	3:T:105:THR:O	2.30	0.40
2:Y:53:ASP:N	2:Y:53:ASP:OD1	2.49	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	I	88/278 (32%)	80 (91%)	8 (9%)	0	100	100
2	A	119/225 (53%)	117 (98%)	2 (2%)	0	100	100
2	C	119/225 (53%)	117 (98%)	2 (2%)	0	100	100
2	E	119/225 (53%)	117 (98%)	2 (2%)	0	100	100
2	H	119/225 (53%)	117 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	M	119/225 (53%)	117 (98%)	2 (2%)	0	100	100
2	O	119/225 (53%)	116 (98%)	3 (2%)	0	100	100
2	Q	119/225 (53%)	117 (98%)	2 (2%)	0	100	100
2	S	119/225 (53%)	115 (97%)	4 (3%)	0	100	100
2	U	119/225 (53%)	117 (98%)	2 (2%)	0	100	100
2	W	119/225 (53%)	116 (98%)	3 (2%)	0	100	100
2	Y	119/225 (53%)	117 (98%)	2 (2%)	0	100	100
3	B	110/218 (50%)	108 (98%)	2 (2%)	0	100	100
3	D	110/218 (50%)	107 (97%)	3 (3%)	0	100	100
3	F	110/218 (50%)	107 (97%)	3 (3%)	0	100	100
3	L	110/218 (50%)	106 (96%)	4 (4%)	0	100	100
3	N	110/218 (50%)	104 (94%)	6 (6%)	0	100	100
3	P	110/218 (50%)	106 (96%)	4 (4%)	0	100	100
3	R	110/218 (50%)	107 (97%)	3 (3%)	0	100	100
3	T	110/218 (50%)	107 (97%)	3 (3%)	0	100	100
3	V	110/218 (50%)	107 (97%)	3 (3%)	0	100	100
3	X	110/218 (50%)	108 (98%)	2 (2%)	0	100	100
3	Z	110/218 (50%)	108 (98%)	2 (2%)	0	100	100
All	All	2607/5151 (51%)	2538 (97%)	69 (3%)	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	I	71/240 (30%)	71 (100%)	0	100	100
2	A	98/188 (52%)	98 (100%)	0	100	100
2	C	98/188 (52%)	98 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	98/188 (52%)	98 (100%)	0	100	100
2	H	98/188 (52%)	98 (100%)	0	100	100
2	M	98/188 (52%)	98 (100%)	0	100	100
2	O	98/188 (52%)	94 (96%)	4 (4%)	26	60
2	Q	98/188 (52%)	98 (100%)	0	100	100
2	S	98/188 (52%)	98 (100%)	0	100	100
2	U	98/188 (52%)	98 (100%)	0	100	100
2	W	98/188 (52%)	98 (100%)	0	100	100
2	Y	98/188 (52%)	98 (100%)	0	100	100
3	B	88/179 (49%)	88 (100%)	0	100	100
3	D	88/179 (49%)	88 (100%)	0	100	100
3	F	88/179 (49%)	87 (99%)	1 (1%)	70	87
3	L	88/179 (49%)	88 (100%)	0	100	100
3	N	88/179 (49%)	87 (99%)	1 (1%)	70	87
3	P	88/179 (49%)	88 (100%)	0	100	100
3	R	88/179 (49%)	87 (99%)	1 (1%)	70	87
3	T	88/179 (49%)	88 (100%)	0	100	100
3	V	88/179 (49%)	87 (99%)	1 (1%)	70	87
3	X	88/179 (49%)	88 (100%)	0	100	100
3	Z	88/179 (49%)	88 (100%)	0	100	100
All	All	2117/4277 (50%)	2109 (100%)	8 (0%)	88	95

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

Mol	Chain	Res	Type
3	F	24	THR
3	N	85	ASP
2	O	82	MET
2	O	82(A)	ASN
2	O	82(B)	SER
2	O	82(C)	LEU
3	R	85	ASP
3	V	65	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19)

such sidechains are listed below:

Mol	Chain	Res	Type
1	I	185	ASN
2	H	39	GLN
3	L	37	GLN
3	L	38	GLN
2	C	39	GLN
3	D	38	GLN
3	F	37	GLN
2	M	39	GLN
3	N	38	GLN
3	N	53	ASN
2	O	39	GLN
3	P	17	GLN
3	P	38	GLN
2	Q	39	GLN
2	Q	76	ASN
2	S	76	ASN
3	T	6	GLN
3	V	34	HIS
2	W	105	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

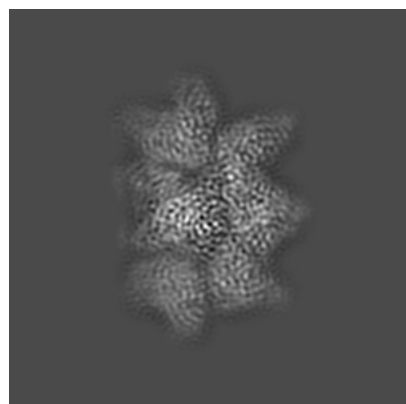
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27785. These allow visual inspection of the internal detail of the map and identification of artifacts.

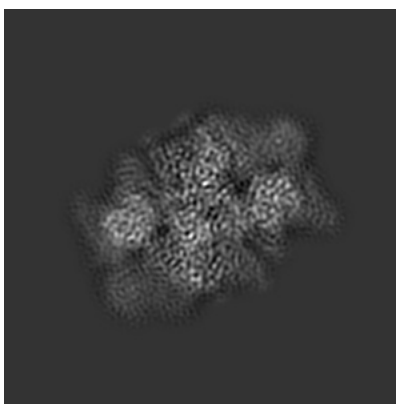
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

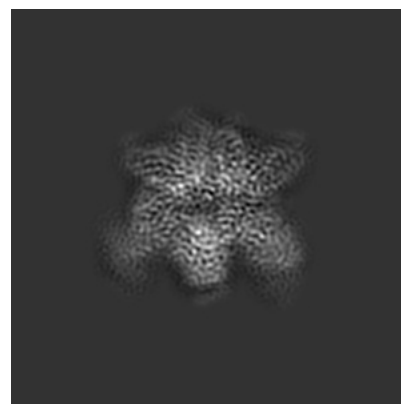
6.1.1 Primary map



X

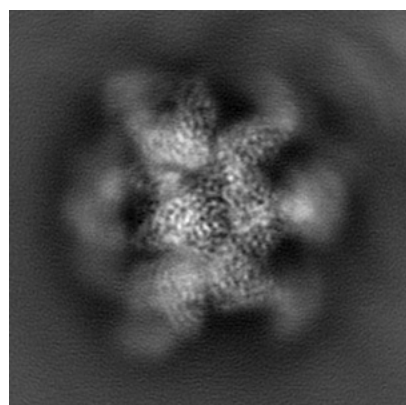


Y

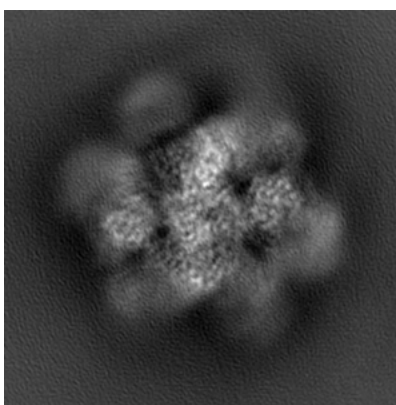


Z

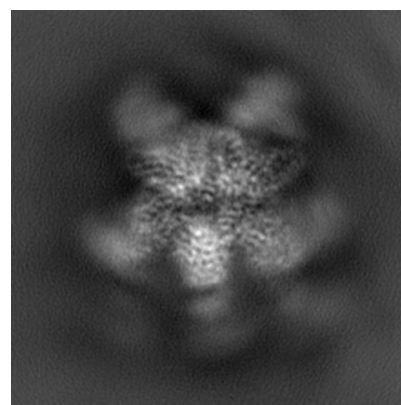
6.1.2 Raw map



X



Y

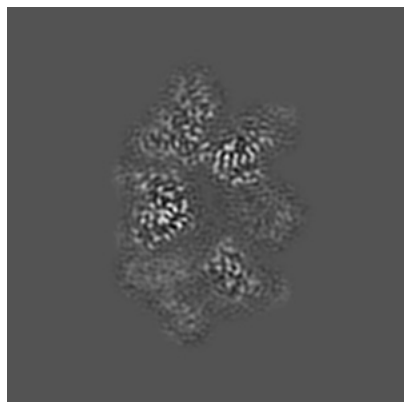


Z

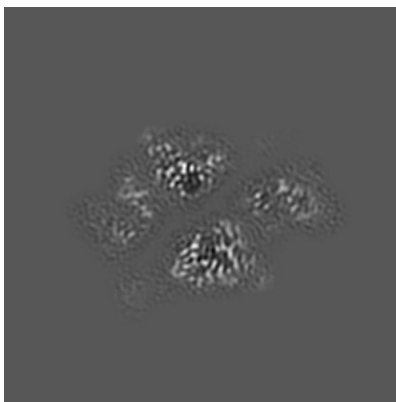
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

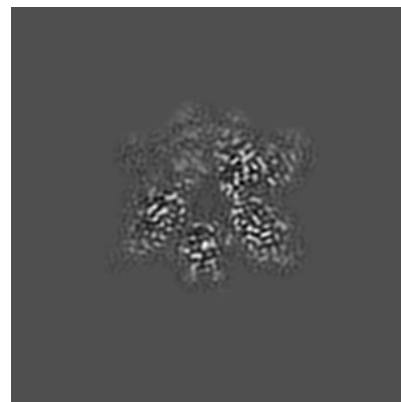
6.2.1 Primary map



X Index: 110

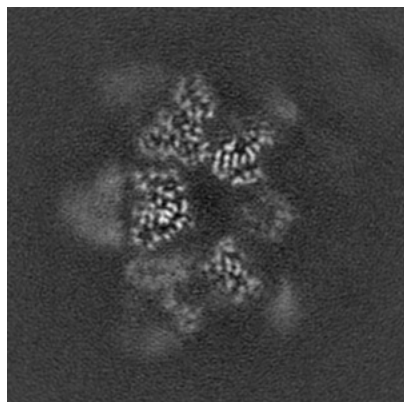


Y Index: 110

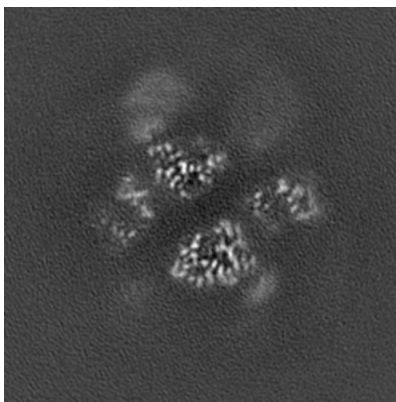


Z Index: 110

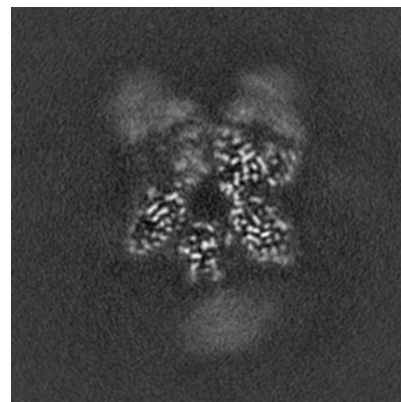
6.2.2 Raw map



X Index: 110



Y Index: 110

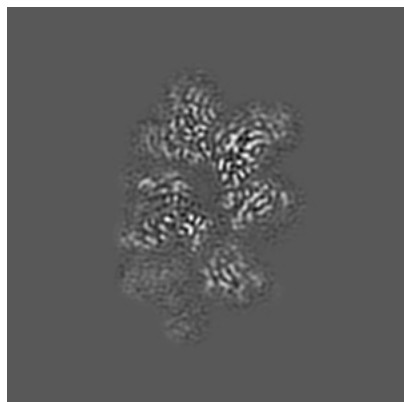


Z Index: 110

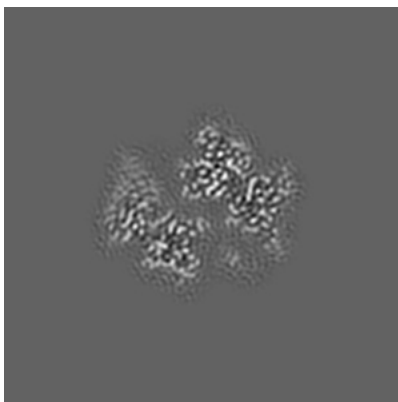
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

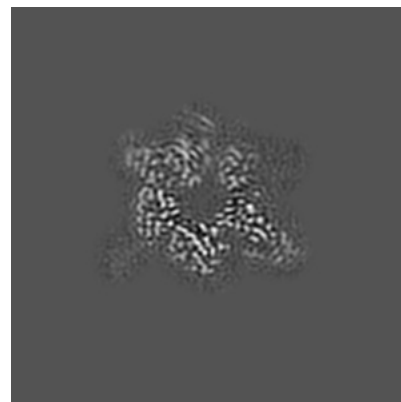
6.3.1 Primary map



X Index: 115

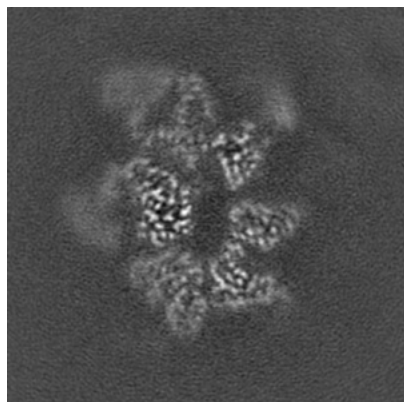


Y Index: 127

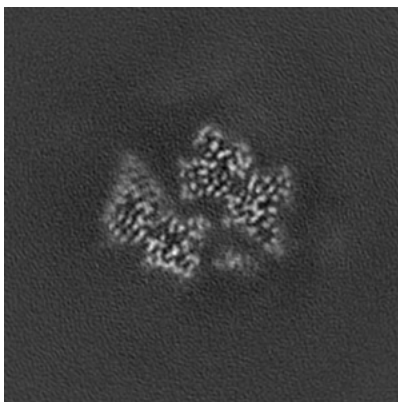


Z Index: 103

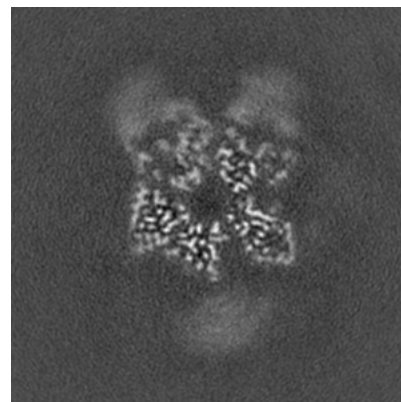
6.3.2 Raw map



X Index: 103



Y Index: 126

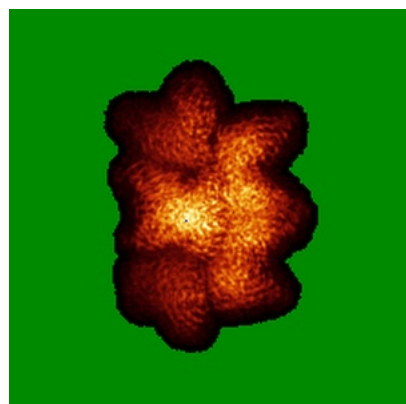


Z Index: 107

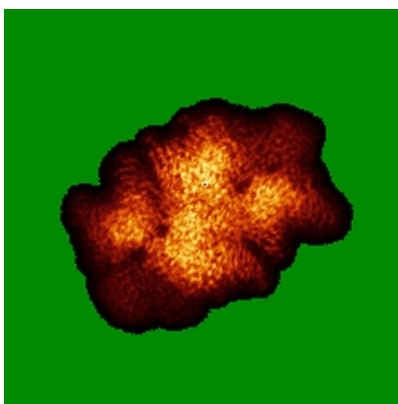
The images above show the largest variance slices of the map in three orthogonal directions.

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

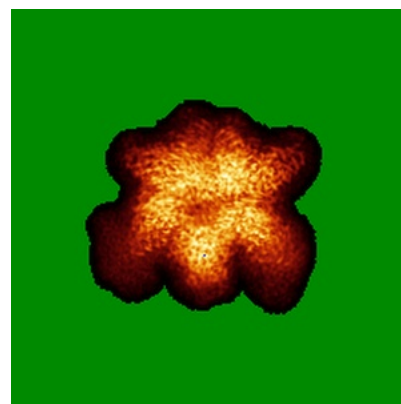
6.4.1 Primary map



X

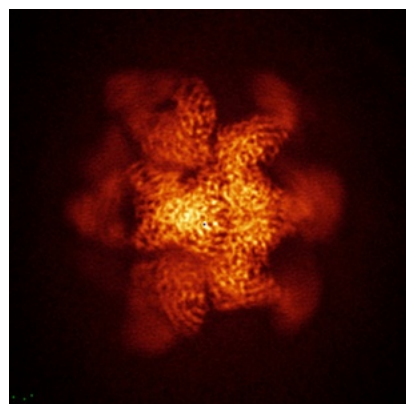


Y

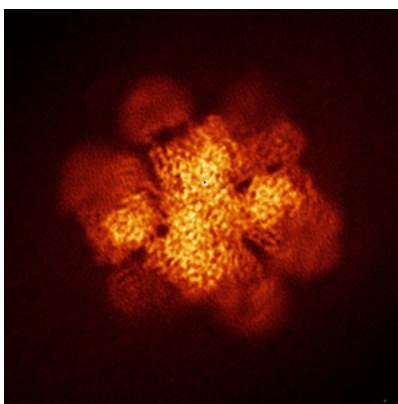


Z

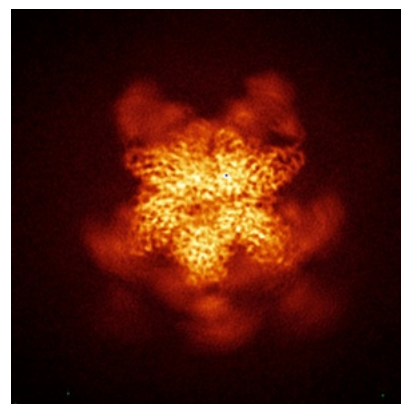
6.4.2 Raw map



X



Y

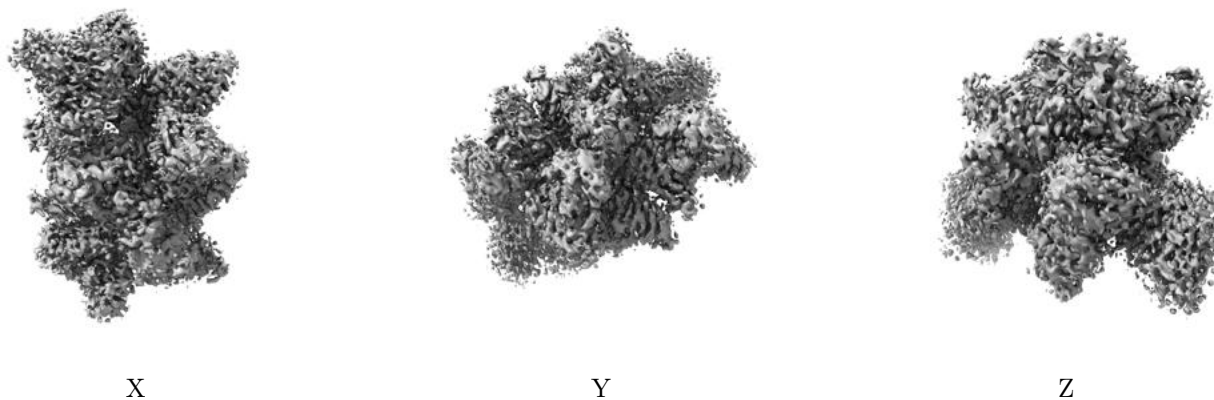


Z

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.

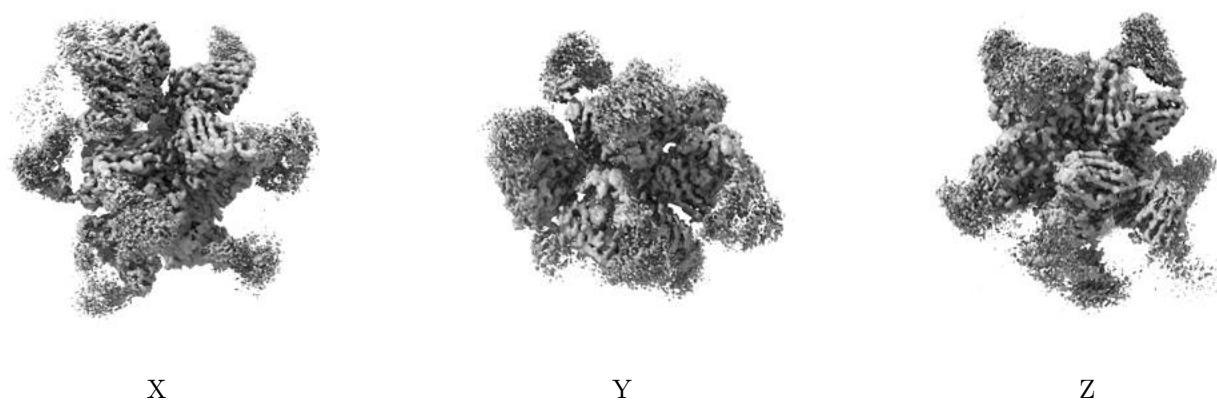
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. 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.

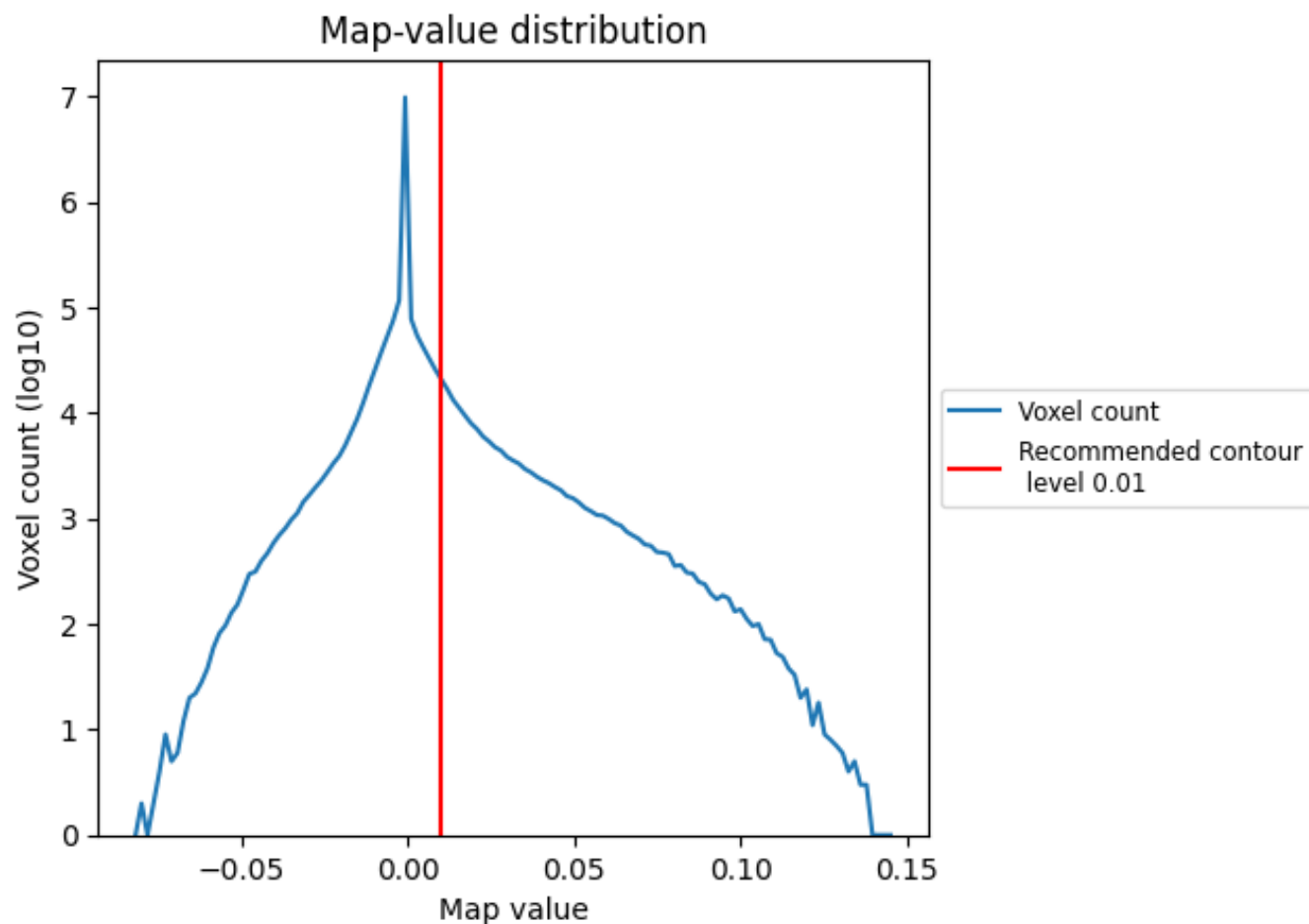
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

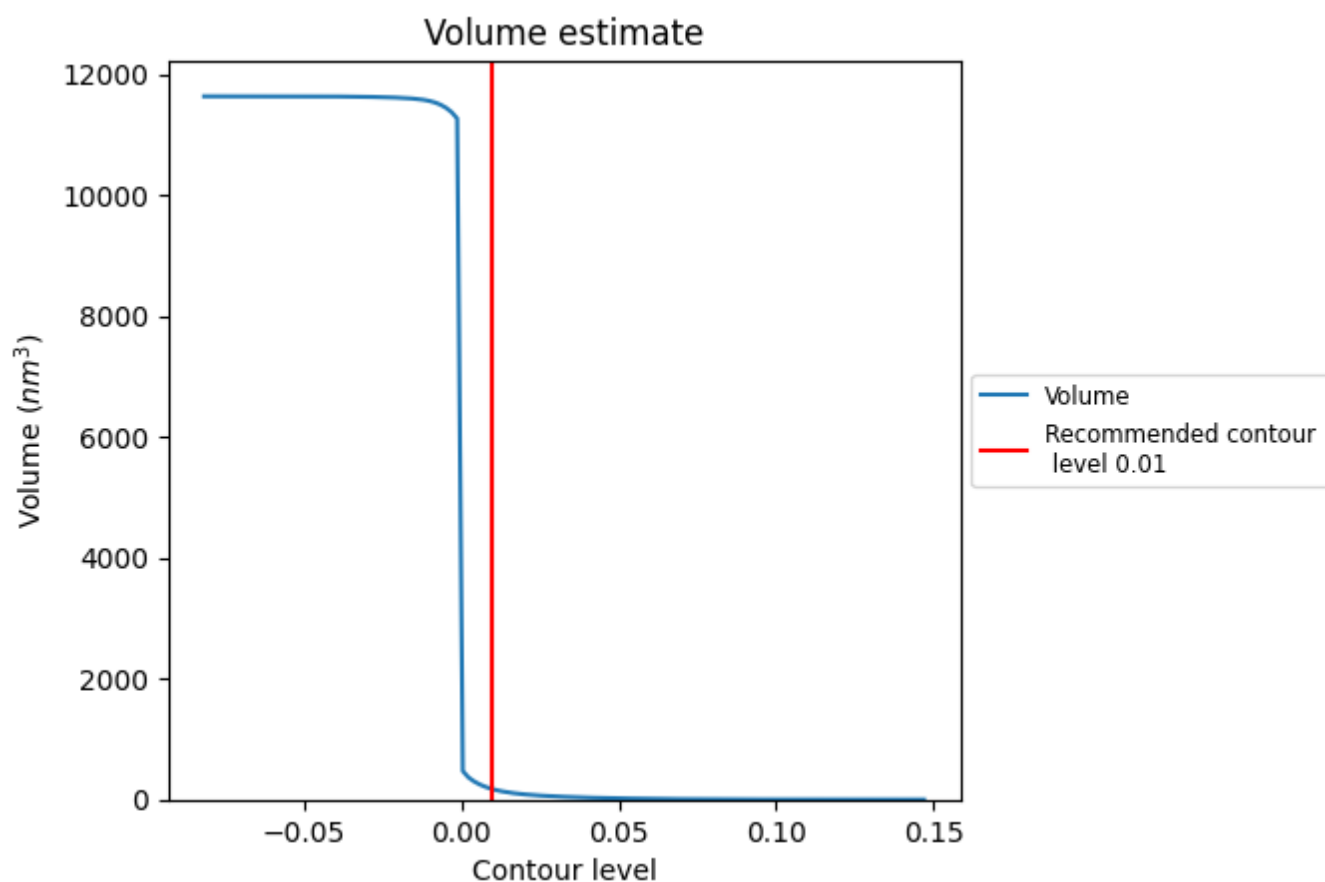
This section contains the results of statistical analysis of the map.

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.

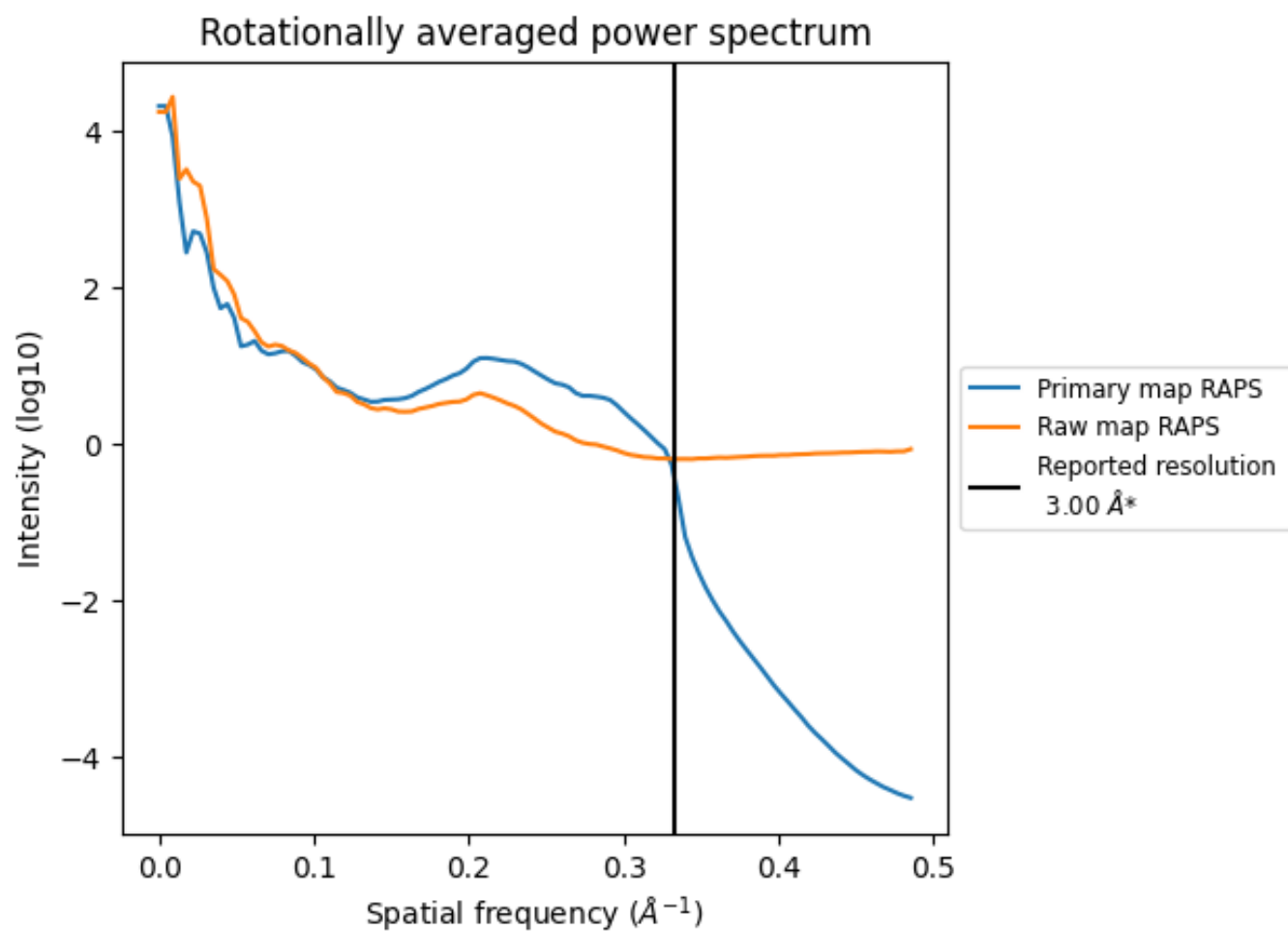
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 172 nm³; this corresponds to an approximate mass of 155 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 ⓘ

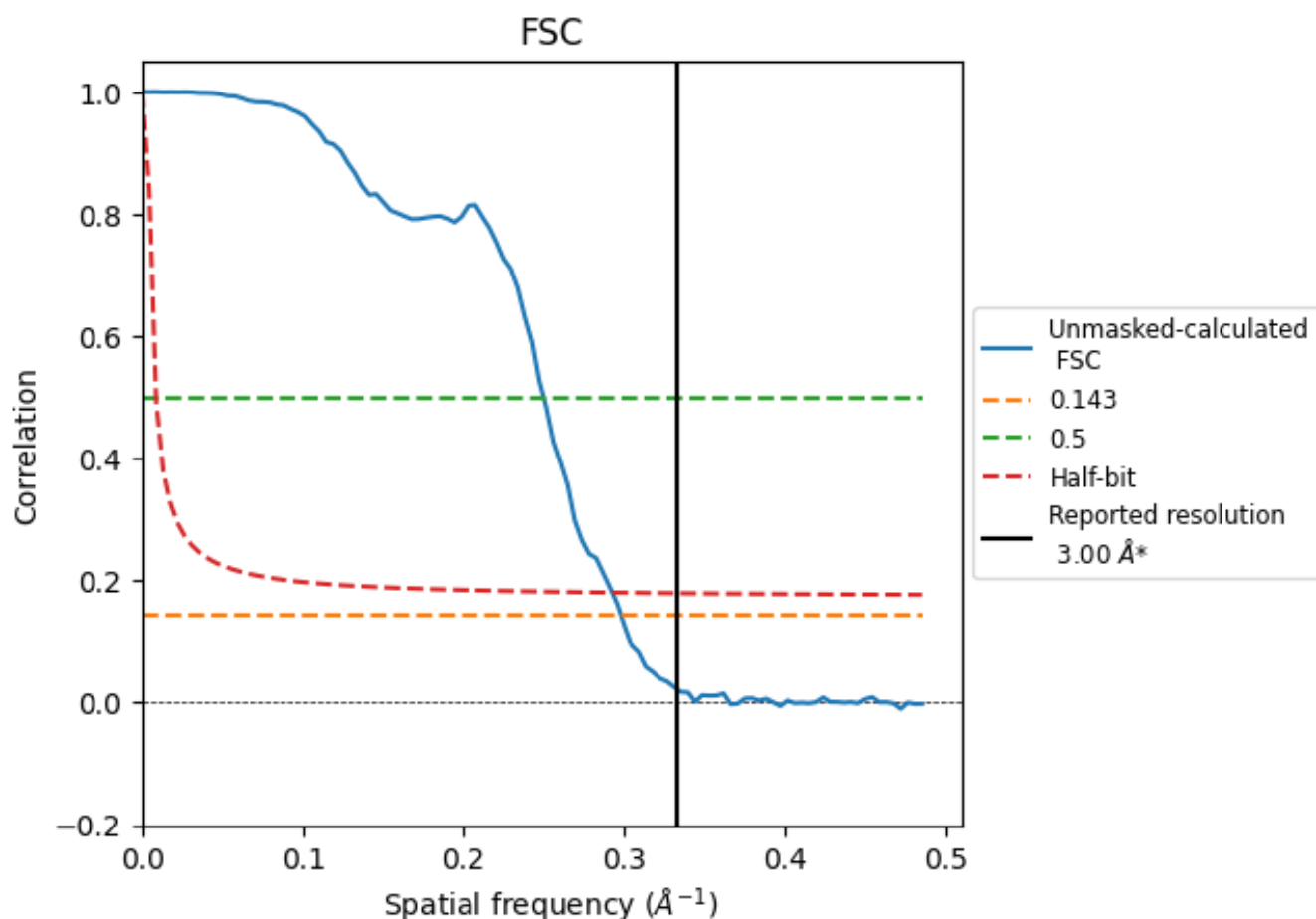


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

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 0.333 \AA^{-1}

8.2 Resolution estimates [i](#)

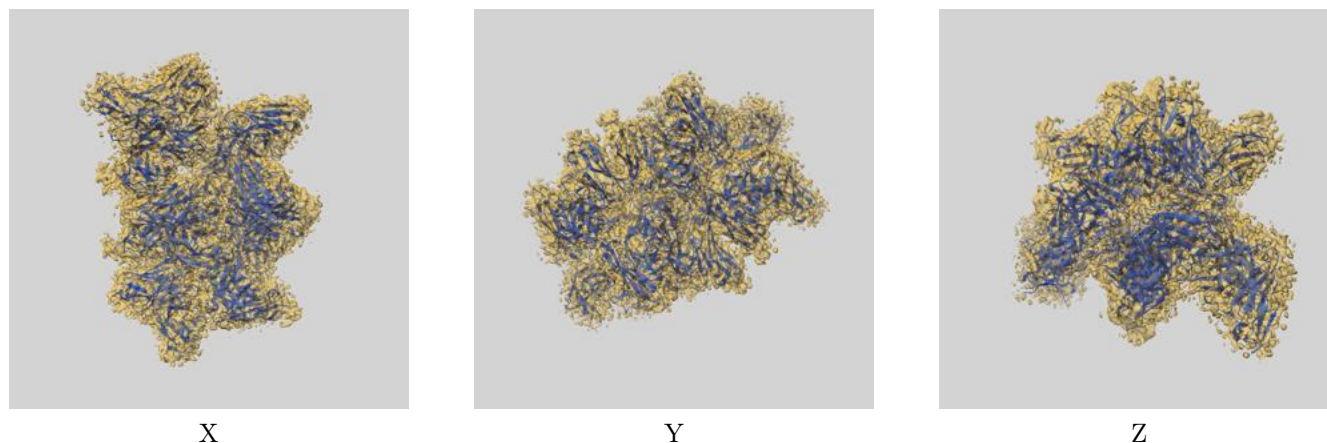
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.36	4.00	3.42

*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 3.36 differs from the reported value 3.0 by more than 10 %

9 Map-model fit [i](#)

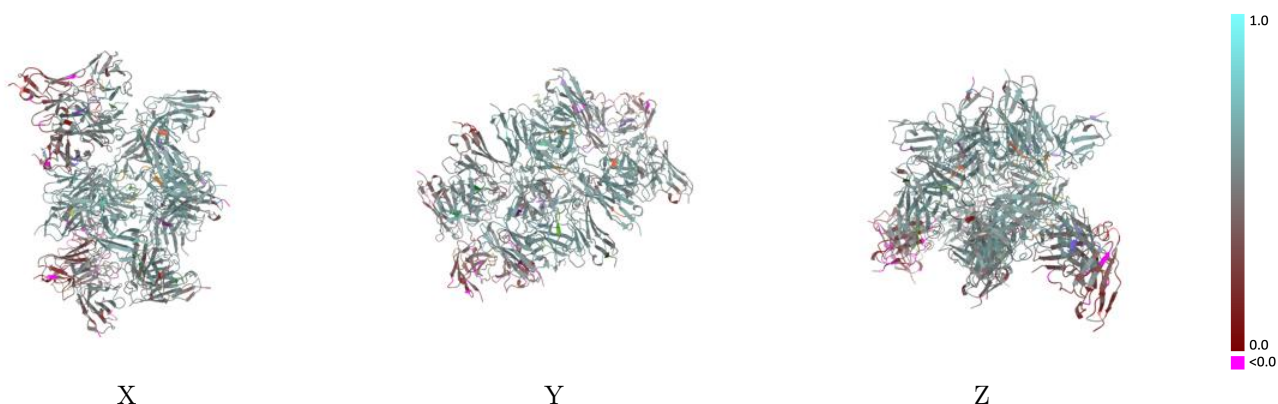
This section contains information regarding the fit between EMDB map EMD-27785 and PDB model 8DYX. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



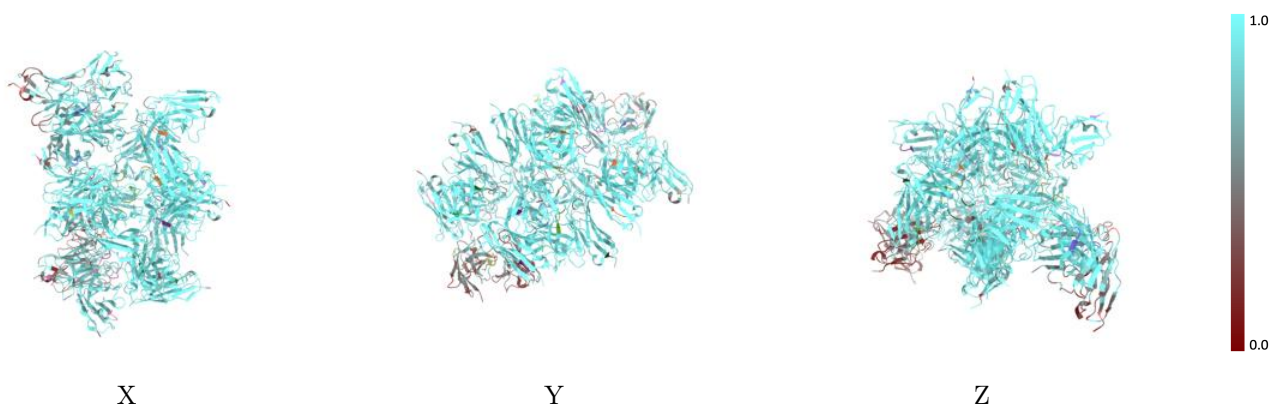
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



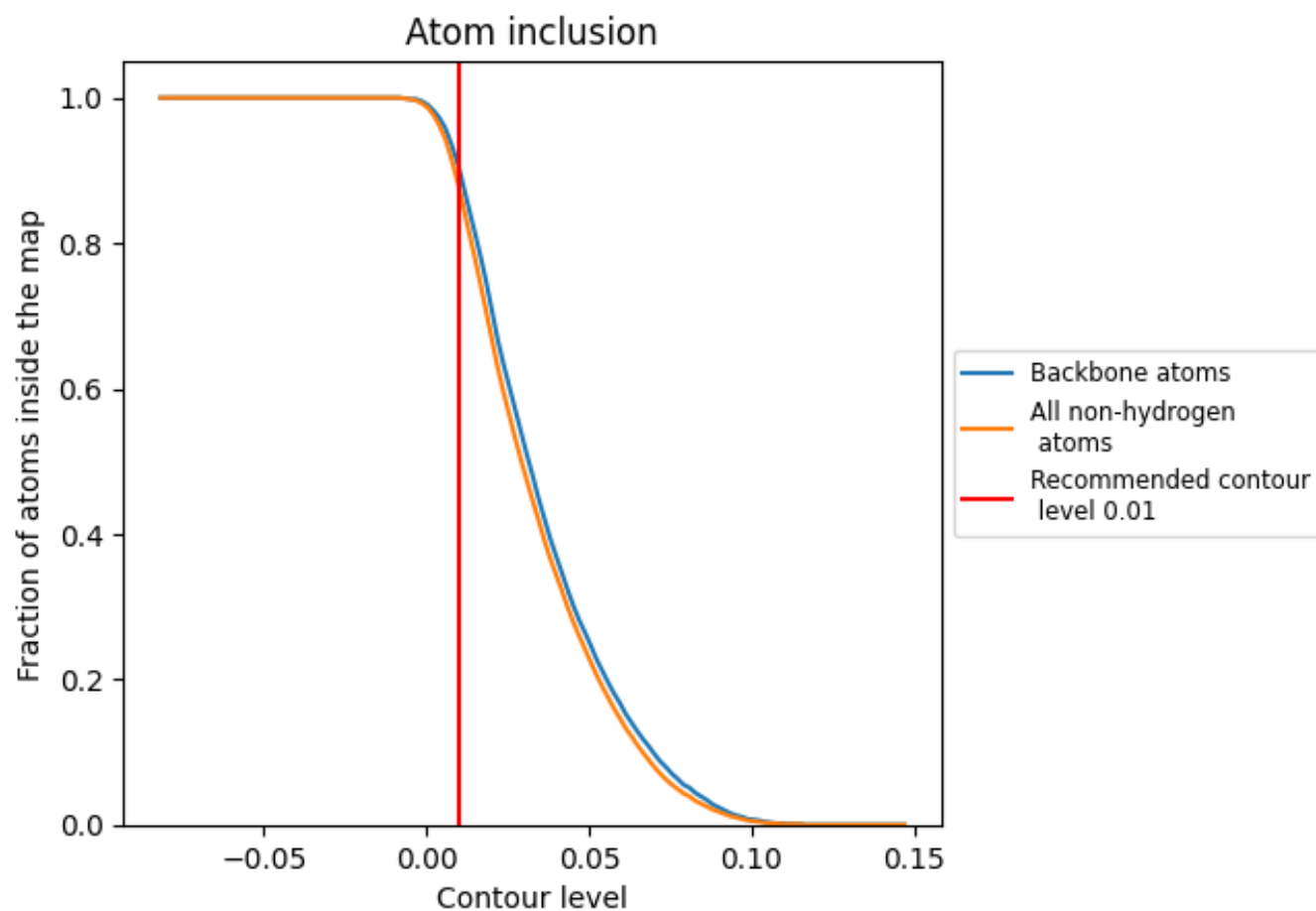
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

















































9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 88% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8770	 0.5140
A	 0.7580	 0.4200
B	 0.7000	 0.3450
C	 0.9220	 0.5460
D	 0.8930	 0.5210
E	 0.9690	 0.5890
F	 0.9550	 0.5630
H	 0.9780	 0.6080
I	 0.9170	 0.5510
L	 0.9530	 0.5660
M	 0.9790	 0.6060
N	 0.9710	 0.5830
O	 0.9750	 0.6080
P	 0.9740	 0.5880
Q	 0.9840	 0.6010
R	 0.9430	 0.5570
S	 0.9690	 0.5840
T	 0.9290	 0.5270
U	 0.9560	 0.5580
V	 0.8880	 0.4890
W	 0.9060	 0.4870
X	 0.8180	 0.4120
Y	 0.4570	 0.2630
Z	 0.3610	 0.2290

