



wwPDB EM Validation Summary Report ⓘ

May 14, 2025 – 08:44 AM EDT

PDB ID : 8DYW / pdb_00008dyw
EMDB ID : EMD-27784
Title : Cryo-EM structure of 239 Fab in complex with recombinant shortened Plasmodium falciparum circumsporozoite protein (rsCSP)
Authors : Martin, G.M.; Ward, A.B.
Deposited on : 2022-08-05
Resolution : 3.72 Å(reported)

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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

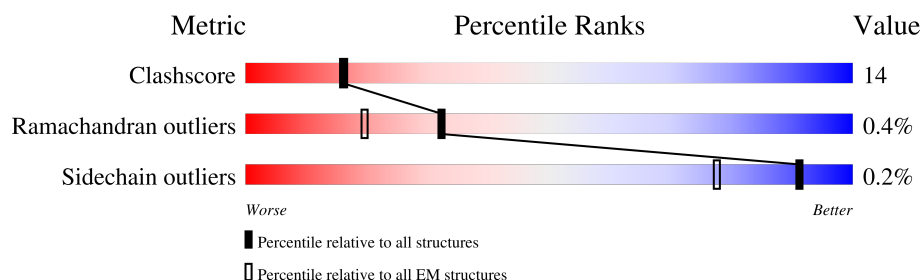
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.72 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	B	215	
2	D	215	
2	F	215	
2	L	215	
2	N	215	
2	P	215	
2	R	215	

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Mol	Chain	Length	Quality of chain
2	T	215	 32%18%50%
2	V	215	 32%19%50%
2	X	215	 33%16%50%
3	A	450	 18%9%73%
3	C	450	 18%9%73%
3	E	450	 19%7%73%
3	H	450	 20%7%73%
3	M	450	 18%8%73%
3	O	450	 18%9%73%
3	Q	450	 17%9%73%
3	S	450	 16%11%73%
3	U	450	 16%11%73%
3	W	450	 12%14%13%73%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18494 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	80	Total	C	N	O	0	0
			564	324	117	123		

- Molecule 2 is a protein called 239 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	108	Total	C	N	O	S	0	0
			833	521	143	166	3		
2	B	108	Total	C	N	O	S	0	0
			833	521	143	166	3		
2	D	108	Total	C	N	O	S	0	0
			833	521	143	166	3		
2	F	108	Total	C	N	O	S	0	0
			833	521	143	166	3		
2	N	108	Total	C	N	O	S	0	0
			833	521	143	166	3		
2	P	108	Total	C	N	O	S	0	0
			833	521	143	166	3		
2	R	108	Total	C	N	O	S	0	0
			833	521	143	166	3		
2	T	108	Total	C	N	O	S	0	0
			833	521	143	166	3		
2	V	108	Total	C	N	O	S	0	0
			833	521	143	166	3		
2	X	108	Total	C	N	O	S	0	0
			833	521	143	166	3		

- Molecule 3 is a protein called 239 Fab heavy chain.

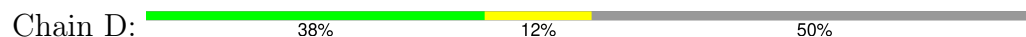
Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	121	Total	C	N	O	S	0	0
			960	604	174	178	4		
3	A	121	Total	C	N	O	S	0	0
			960	604	174	178	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	121	Total 960	C 604	N 174	O 178	S 4	0	0
3	E	121	Total 960	C 604	N 174	O 178	S 4	0	0
3	M	121	Total 960	C 604	N 174	O 178	S 4	0	0
3	O	121	Total 960	C 604	N 174	O 178	S 4	0	0
3	Q	121	Total 960	C 604	N 174	O 178	S 4	0	0
3	S	121	Total 960	C 604	N 174	O 178	S 4	0	0
3	U	121	Total 960	C 604	N 174	O 178	S 4	0	0
3	W	121	Total 960	C 604	N 174	O 178	S 4	0	0

- Molecule 2: 239 Fab light chain



TYR	GLU	LYS	HIS	LYS	VAL	TYR	CYS	GLU	VAL	THR	HIS	GLN	GLY	LEU	SER	SER	PRO	VAL	THR	LYS	SER	PHE	ASN	ARG	GLY	GLU	CYS														
D1	T5	O6	S7	P8	L11	R18	C23	S26	Q27	L33	Q38	K39	P44	Y55	R56	F71	D81	Y91	N92	R95A	Q100	G101	T102	I106	K107	ARG	THR	VAL	ALA	ALA	PRO	SER	VAL	PHE	ILE	PHE	PRO	SER	ASP	GLU	GLN

- Molecule 2: 239 Fab light chain



HIS	THR	D1
LYS	ALA	I2
VAL	SER	Q3
TYR	VAL	Q6
ALA	VAL	Q6
CYS	CYS	S26
GLU	LEU	S26
VAL	LEU	S26
THR	ASN	Q37
HIS	ASN	Q38
GLN	PHE	K39
LEU	THR	K42
GLY	PRO	K42
SER	ARG	L46
SER	GLU	L47
PRO	ALA	L47
VAL	LYS	R56
THR	VAL	R56
LYS	GLN	R61
SER	THR	F62
SER	PHE	F62
PHE	LYS	F62
ASN	VAL	L78
ARG	ASP	L78
GLY	ASN	D82
GLU	ALA	D82
CYS	LEU	F83
	GLN	A84
	SER	T85
	GLY	Y86
	ASN	Y86
	SER	H90
	GLN	H90
	GLU	S95
	SER	S95
	VAL	R95A
	THR	T102
	GLU	T106
	GLN	T106
	ASP	K107
	SER	ARG
	LYS	THR
	ASP	VAL
	SER	ALA
	THR	ALA
	TVR	PRO
	SER	SER
	LEU	VAL
	SER	PHE
	THR	ILE
	THR	PRO
	LEU	PRO
	THR	PRO
	LEU	SER
	LYS	ASP
	LYS	GLN
	ALA	GLN
	ASP	LYS
	TVR	LEU
	GLU	SER

- Molecule 2: 239 Fab light chain



LYS	ALA	D1
VAL	SER	I2
TYR	VAL	Q3
ALA	VAL	M4
CYS	CYS	T5
GLU	LEU	Q6
THR	LEU	S26
VAL	ASN	ASN
HIS	PHE	L33
GLN	TYR	Y36
GLY	PRO	ARG
LEU	ARG	K39
SER	GLU	L46
SER	ALA	L47
PRO	LYS	A61
PRO	VAL	R56
VAL	GLN	G57
THR	LYS	Y58
LYS	TRP	R61
SER	THR	D82
PHE	LYS	H90
ASN	GLN	Y91
GLY	GLY	N92
ASN	GLU	F98
ARG	SER	G99
GLY	VAL	Q100
GLU	THR	I106
CYS	GLN	K107
	ASP	ARG
	SER	THR
	SER	VAL
	ASP	ALA
	SER	ALA
	THR	PRO
	TYR	SER
	SER	VAL
	LEU	PHE
	SER	ILE
	THR	PHE
	LEU	PRO
	THR	PRO
	THR	SER
	SER	ASP
	LYS	GLU
	ALA	GLN
	ASP	LEU
	TYR	LYS
	THR	GLY
	LYS	

- Molecule 2: 239 Fab light chain



ALA	D1
SER	I2
VAL	Q3
VAL	M4
CYS	T5
LEU	Q6
LEU	S7
ASN	
ASN	T10
PHE	L11
THR	
PRO	T22
ARG	C23
GLU	R24
ALA	A25
LYS	
VAL	L33
GLN	A34
TRP	
LYS	L47
VAL	I48
ASP	
ASN	V68
ALA	
LEU	T72
GLN	
SER	C88
GLY	Q89
ASN	H90
SER	T91
GLN	N92
GLU	
SER	S95
VAL	R95A
THR	
GLU	F98
GLN	
ASP	K107
SER	ARG
LYS	THR
ASP	VAL
SER	ALA
THR	ALA
TYR	PRO
SER	SER
LEU	VAL
SER	PHE
SER	ILE
THR	PHE
LEU	PRO
THR	PRO
LEU	SER
SER	ASP
LYS	GLU
ALA	GLN
ASP	LEU
TYR	LYS
GLY	SER
LYS	GLY

[illegible]

- Molecule 3: 239 Fab heavy chain

Chain C: 18% 9% 73%

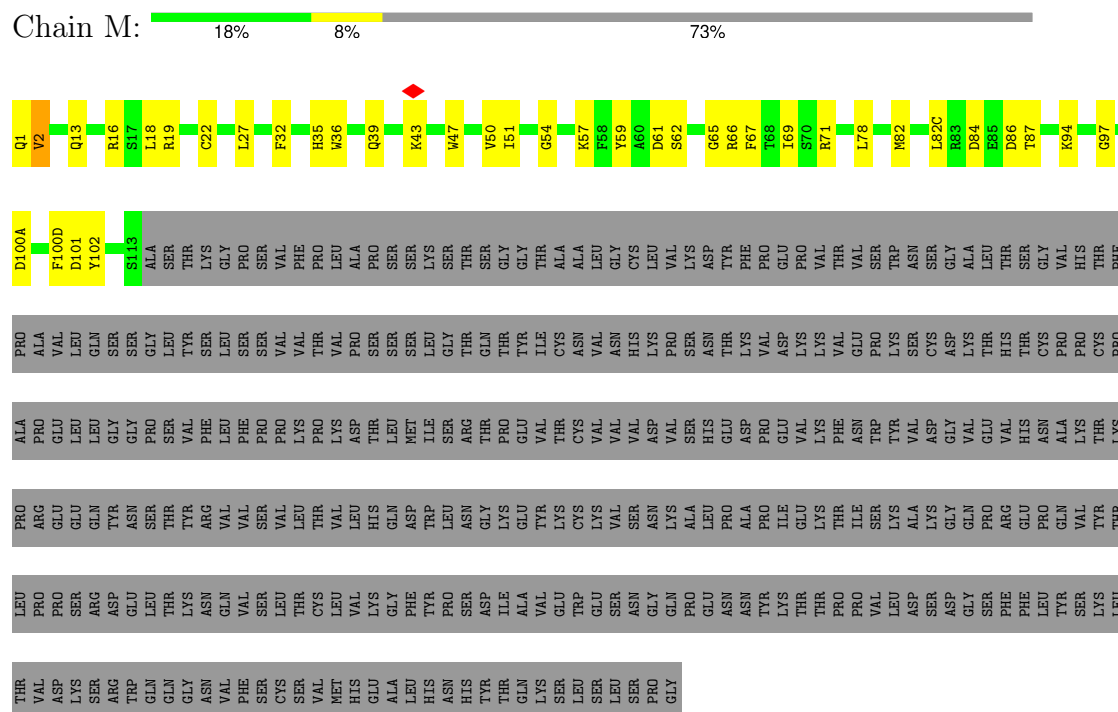
[illegible]

- Molecule 3: 239 Fab heavy chain

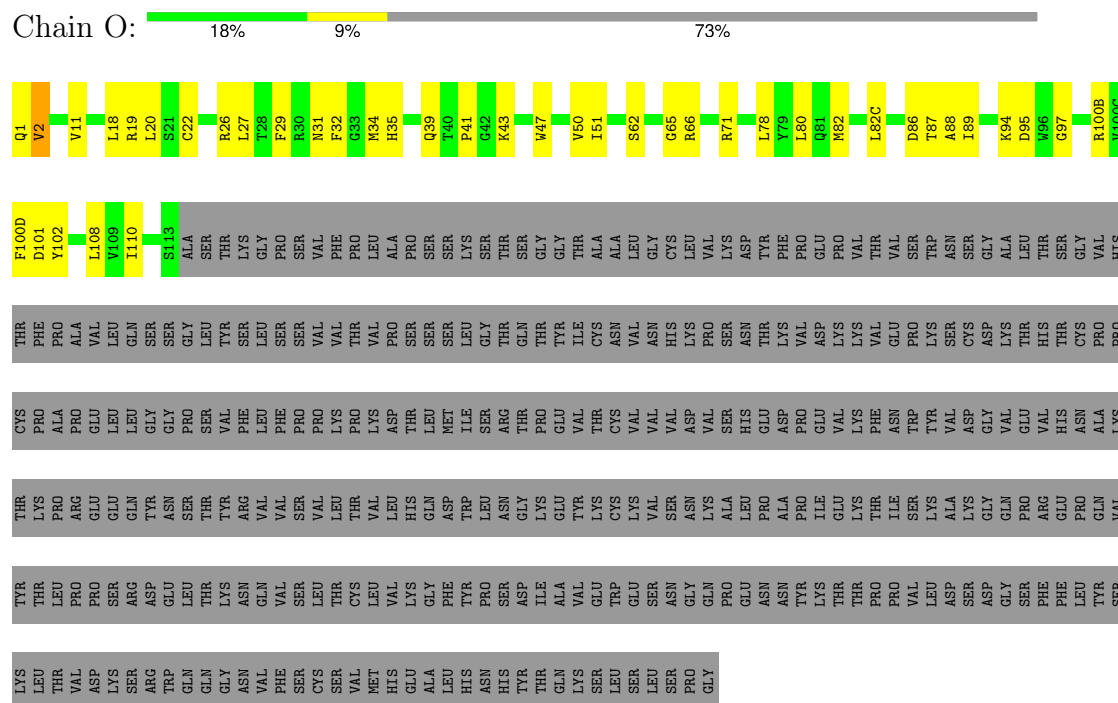
Chain E: 19% 7% 73%

VAL	PHE	SER	SER	CYS	SER	VAL	VAL	GLN	VAL	VAL	LEU	LEU	LEU	VAL	GLY	PRO	Q1
SER	SER	SER	THR	THR	LEU	VAL	SER	SER	SER	VAL	PHE	SER	PRO	VAL	SER	THR	V2
SER	VAL	VAL	THR	THR	LEU	THR	THR	THR	LEU	VAL	VAL	VAL	PRO	THR	PHE	VAL	E6
MET	VAL	VAL	CYS	THR	VAL	VAL	VAL	CYS	THR	VAL	PRO	PRO	ASP	THR	PRO	PRO	R26
HIS	HIS	GLY	VAL	VAL	LEU	LEU	LEU	VAL	HIS	VAL	LYS	ASP	THR	ALA	ALA	LEU	L27
ALA	ALA	GLY	GLY	GLY	GLN	GLN	GLN	GLY	THR	THR	LEU	THR	SER	SER	SER	PRO	N31
LEU	LEU	PHE	THR	THR	THR	THR	THR	THR	THR	ASP	MET	MET	SER	SER	SER	SER	F32
HIS	HIS	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	H35
ASN	ASN	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	LEU	SER	SER	GLY	SER	THR	THR	R38
THR	THR	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	GLY	ARG	THR	GLN	SER	SER	GLY	Q39
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	GLY	THR	THR	GLY	GLY	THR	E46
GLN	GLN	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	GLY	VAL	ILE	THR	THR	THR	THR	W47
LYS	LYS	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	THR	SER	THR	CYS	ALA	ALA	ALA	V50
SER	SER	THR	THR	THR	THR	THR	THR	THR	THR	CYS	ARG	CYS	ASN	VAL	VAL	LEU	K57
SER	SER	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	VAL	VAL	VAL	HIS	THR	CYS	THR	G65
PRO	PRO	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ASP	ASP	VAL	PRO	VAL	VAL	VAL	R66
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	VAL	SER	SER	ASN	ASN	LYS	LYS	R71
										HIS	SER	SER	ASN	ASN	PHE	THR	K75
										GLY	GLY	PRO	GLY	VAL	PRO	PRO	R76
										ILE	THR	GLY	VAL	ASP	GLY	THR	T77
										VAL	THR	VAL	LYS	LYS	VAL	VAL	M82
										THR	PHE	VAL	VAL	THR	THR	THR	L82C
										ILE	SER	ASN	GLY	VAL	VAL	SER	D86
										SER	THR	THR	PRO	THR	TRP	TRP	T87
										LYS	THR	LYS	LYS	LYS	ASN	ASN	A88
										VAL	VAL	VAL	CYS	CYS	SER	SER	I89
										GLY	GLY	GLY	ASP	GLY	GLY	ALA	A93
										GLN	VAL	VAL	VAL	THR	LEU	LEU	A94
										PRO	GLY	THR	THR	HIS	THR	SER	R100B
										ARG	VAL	VAL	THR	THR	SER	SER	V100C
										GLY	GLY	ASN	CYS	VAL	GLY	VAL	F100D
										PRO	ALA	ALA	PRO	HIS	HIS	HIS	D101
										VAL	VAL	LYS	PRO	THR	THR	THR	Y102
										THR	THR	THR	CYS	PRO	PHE	PHE	T107
										LYS	LYS	VAL	ALA	PRO	PRO	ALA	L108
										PRO	ARG	ARG	PRO	GLY	VAL	VAL	Y109
										PRO	GLY	GLY	GLY	GLN	GLN	GLN	I110
										ARG	THR	THR	THR	SER	SER	SER	S113
										ASP	GLY	ASN	GLY	GLY	GLY	GLY	ALA
										LEU	THR	SER	THR	SER	LEU	SER	SER
										THR	THR	THR	THR	THR	THR	THR	THR
										GLY	ASN	VAL	PHE	SER	THR	LYS	LYS

- Molecule 3: 239 Fab heavy chain



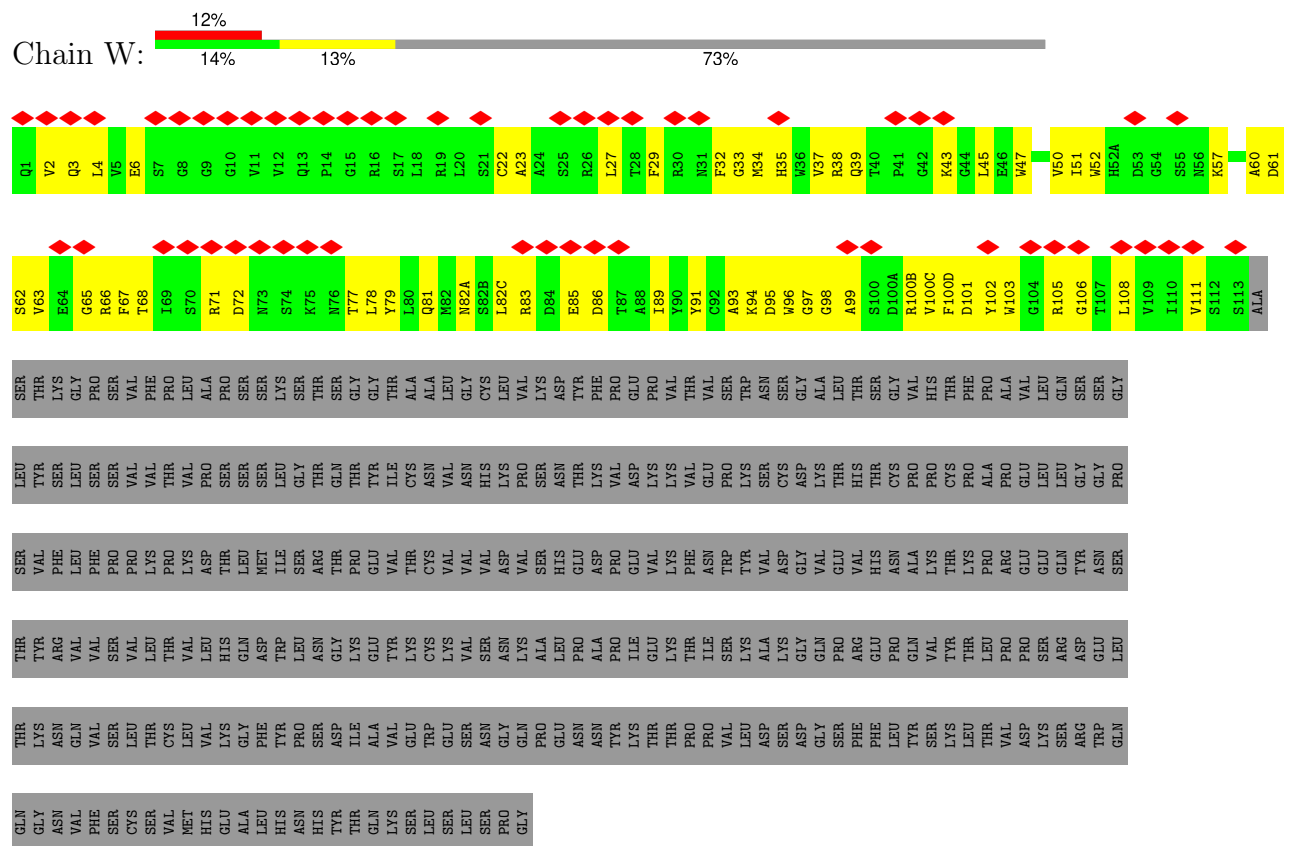
- Molecule 3: 239 Fab heavy chain



- Molecule 3: 239 Fab heavy chain



- Molecule 3: 239 Fab heavy chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	227439	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.464	Depositor
Minimum map value	-1.767	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.150	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	253.0, 253.0, 253.0	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.15, 1.15, 1.15	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	I	0.18	0/583	0.35	0/823
2	B	0.13	0/851	0.39	0/1155
2	D	0.16	0/851	0.43	0/1155
2	F	0.14	0/851	0.44	2/1155 (0.2%)
2	L	0.12	0/851	0.35	0/1155
2	N	0.14	0/851	0.38	0/1155
2	P	0.13	0/851	0.37	0/1155
2	R	0.13	0/851	0.38	0/1155
2	T	0.17	0/851	0.50	0/1155
2	V	0.15	0/851	0.47	0/1155
2	X	0.14	0/851	0.40	0/1155
3	A	0.50	2/983 (0.2%)	0.93	4/1330 (0.3%)
3	C	0.14	0/983	0.42	0/1330
3	E	0.14	0/983	0.36	0/1330
3	H	0.16	0/983	0.44	0/1330
3	M	0.15	0/983	0.39	0/1330
3	O	0.14	0/983	0.36	0/1330
3	Q	0.17	0/983	0.47	0/1330
3	S	0.15	0/983	0.43	0/1330
3	U	0.16	0/983	0.48	0/1330
3	W	0.17	0/983	0.51	0/1330
All	All	0.19	2/18923 (0.0%)	0.46	6/25673 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	41	PRO	CB-CG	-10.93	0.94	1.49
3	A	41	PRO	CG-CD	-9.89	1.17	1.50

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	41	PRO	N-CD-CG	-17.55	76.87	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	41	PRO	CA-CB-CG	-16.73	72.71	104.50
3	A	41	PRO	CB-CG-CD	15.23	154.84	106.10
3	A	41	PRO	CA-N-CD	-8.57	100.00	112.00
2	F	38	GLN	CA-C-N	-5.20	112.78	120.68

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	564	0	484	35	0
2	B	833	0	810	22	0
2	D	833	0	810	18	0
2	F	833	0	810	17	0
2	L	833	0	810	14	0
2	N	833	0	810	13	0
2	P	833	0	810	17	0
2	R	833	0	810	22	0
2	T	833	0	810	29	0
2	V	833	0	810	33	0
2	X	833	0	810	29	0
3	A	960	0	922	30	0
3	C	960	0	922	29	0
3	E	960	0	922	23	0
3	H	960	0	922	21	0
3	M	960	0	922	28	0
3	O	960	0	922	27	0
3	Q	960	0	922	34	0
3	S	960	0	922	44	0
3	U	960	0	922	49	0
3	W	960	0	922	53	0
All	All	18494	0	17804	510	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 14.

The worst 5 of 510 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)
3:E:82:MET:HB3	3:E:82(C):LEU:HD11	1.58	0.84
2:X:6:GLN:NE2	2:X:88:CYS:SG	2.52	0.82
3:W:33:GLY:HA2	3:W:71:ARG:HH22	1.45	0.82
2:B:6:GLN:HE21	2:B:100:GLN:HG2	1.46	0.80
2:F:3:GLN:HE21	2:F:26:SER:HB3	1.46	0.80

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	78/278 (28%)	67 (86%)	11 (14%)	0	100	100
2	B	106/215 (49%)	103 (97%)	3 (3%)	0	100	100
2	D	106/215 (49%)	102 (96%)	4 (4%)	0	100	100
2	F	106/215 (49%)	103 (97%)	3 (3%)	0	100	100
2	L	106/215 (49%)	103 (97%)	3 (3%)	0	100	100
2	N	106/215 (49%)	102 (96%)	4 (4%)	0	100	100
2	P	106/215 (49%)	102 (96%)	4 (4%)	0	100	100
2	R	106/215 (49%)	103 (97%)	3 (3%)	0	100	100
2	T	106/215 (49%)	99 (93%)	7 (7%)	0	100	100
2	V	106/215 (49%)	103 (97%)	3 (3%)	0	100	100
2	X	106/215 (49%)	100 (94%)	6 (6%)	0	100	100
3	A	119/450 (26%)	114 (96%)	4 (3%)	1 (1%)	16	49
3	C	119/450 (26%)	112 (94%)	6 (5%)	1 (1%)	16	49
3	E	119/450 (26%)	117 (98%)	1 (1%)	1 (1%)	16	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	H	119/450 (26%)	116 (98%)	2 (2%)	1 (1%)	16	49
3	M	119/450 (26%)	116 (98%)	2 (2%)	1 (1%)	16	49
3	O	119/450 (26%)	117 (98%)	1 (1%)	1 (1%)	16	49
3	Q	119/450 (26%)	114 (96%)	4 (3%)	1 (1%)	16	49
3	S	119/450 (26%)	114 (96%)	4 (3%)	1 (1%)	16	49
3	U	119/450 (26%)	112 (94%)	6 (5%)	1 (1%)	16	49
3	W	119/450 (26%)	114 (96%)	4 (3%)	1 (1%)	16	49
All	All	2328/6928 (34%)	2233 (96%)	85 (4%)	10 (0%)	32	62

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	Q	2	VAL
3	H	2	VAL
3	C	2	VAL
3	O	2	VAL
3	A	2	VAL

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	62/240 (26%)	62 (100%)	0	100	100
2	B	93/189 (49%)	93 (100%)	0	100	100
2	D	93/189 (49%)	93 (100%)	0	100	100
2	F	93/189 (49%)	92 (99%)	1 (1%)	70	80
2	L	93/189 (49%)	92 (99%)	1 (1%)	70	80
2	N	93/189 (49%)	93 (100%)	0	100	100
2	P	93/189 (49%)	93 (100%)	0	100	100
2	R	93/189 (49%)	92 (99%)	1 (1%)	70	80
2	T	93/189 (49%)	93 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	V	93/189 (49%)	93 (100%)	0	100	100
2	X	93/189 (49%)	92 (99%)	1 (1%)	70	80
3	A	101/399 (25%)	101 (100%)	0	100	100
3	C	101/399 (25%)	101 (100%)	0	100	100
3	E	101/399 (25%)	100 (99%)	1 (1%)	73	82
3	H	101/399 (25%)	101 (100%)	0	100	100
3	M	101/399 (25%)	101 (100%)	0	100	100
3	O	101/399 (25%)	101 (100%)	0	100	100
3	Q	101/399 (25%)	101 (100%)	0	100	100
3	S	101/399 (25%)	101 (100%)	0	100	100
3	U	101/399 (25%)	101 (100%)	0	100	100
3	W	101/399 (25%)	101 (100%)	0	100	100
All	All	2002/6120 (33%)	1997 (100%)	5 (0%)	91	95

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	3	GLN
2	F	78	LEU
3	E	1	GLN
2	R	33	LEU
2	X	50	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
3	U	82(A)	ASN
2	X	90	HIS
2	X	50	GLN
3	W	3	GLN
2	F	37	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

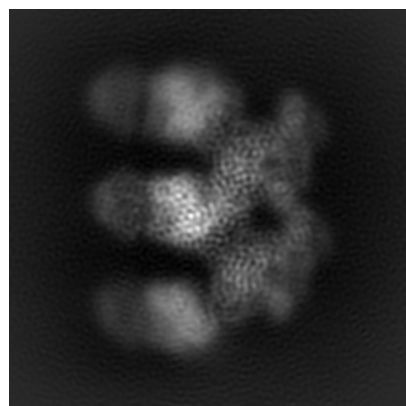
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27784. These allow visual inspection of the internal detail of the map and identification of artifacts.

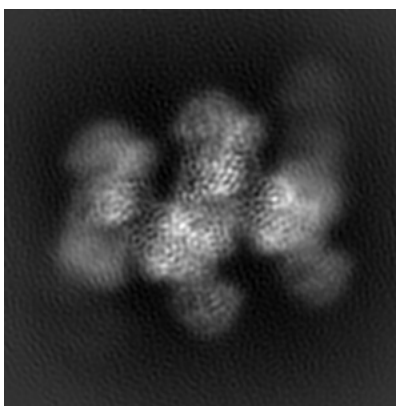
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

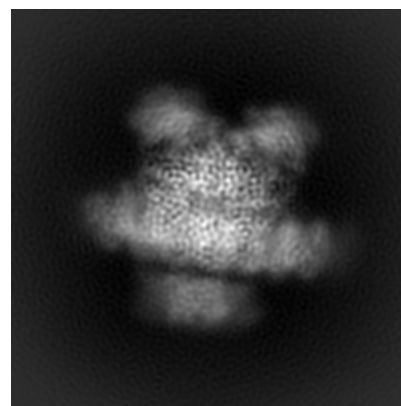
6.1.1 Primary map



X

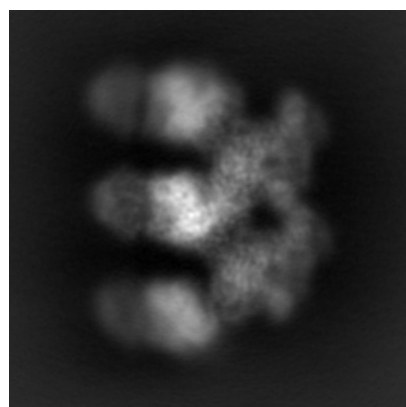


Y

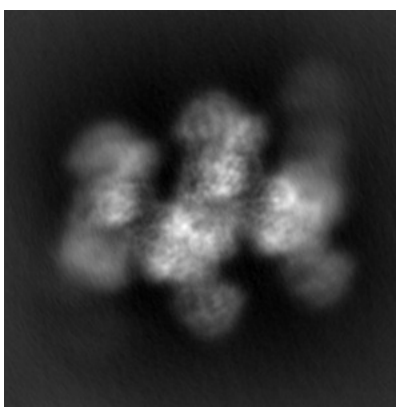


Z

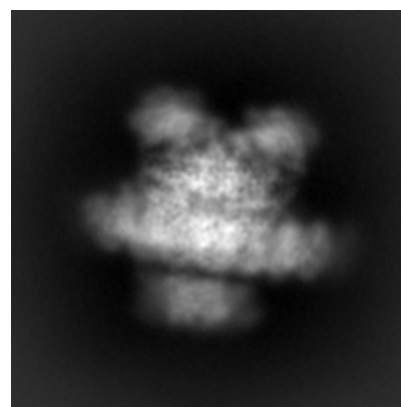
6.1.2 Raw map



X



Y

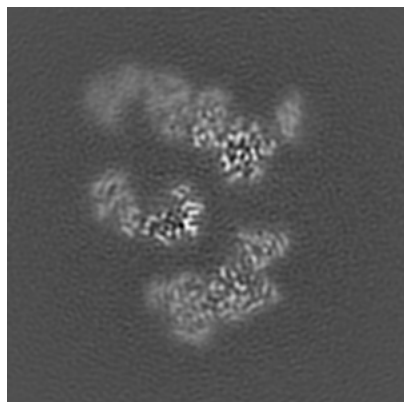


Z

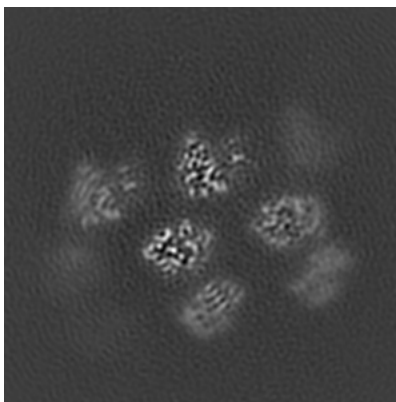
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

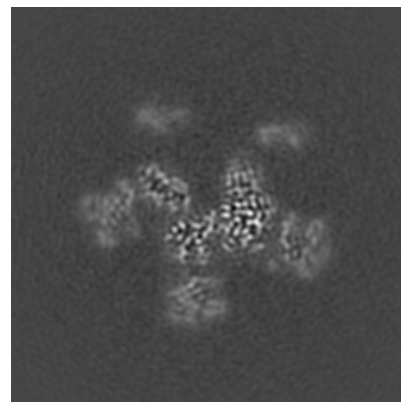
6.2.1 Primary map



X Index: 110

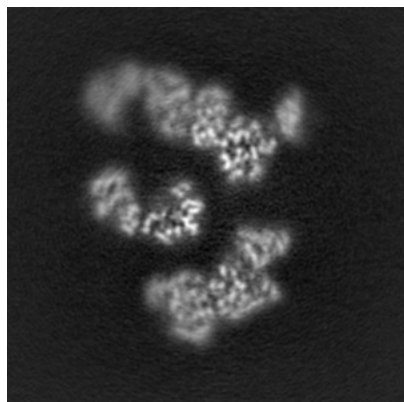


Y Index: 110

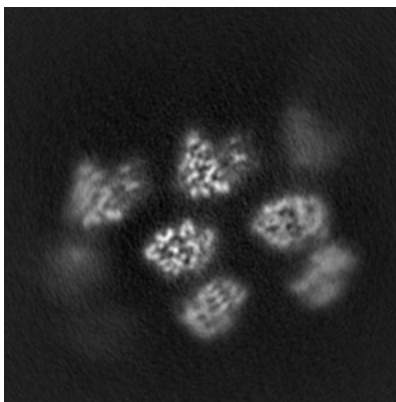


Z Index: 110

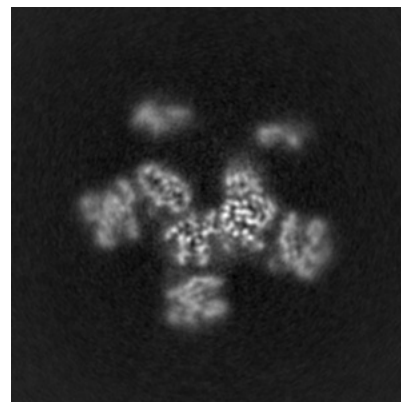
6.2.2 Raw map



X Index: 110



Y Index: 110

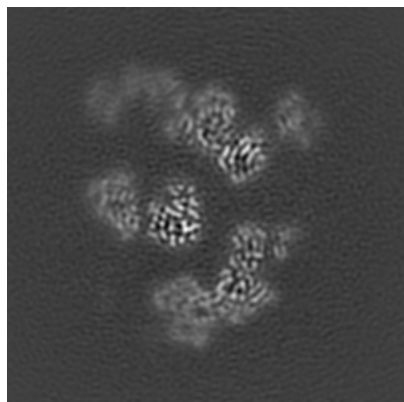


Z Index: 110

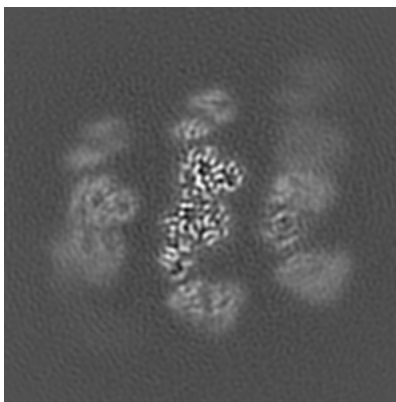
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

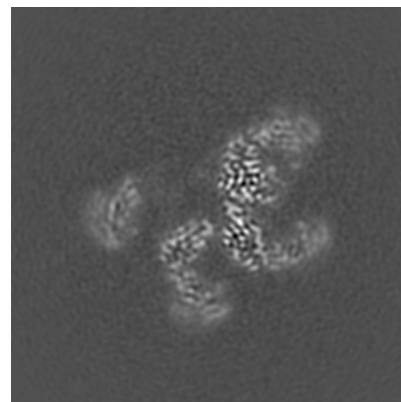
6.3.1 Primary map



X Index: 106

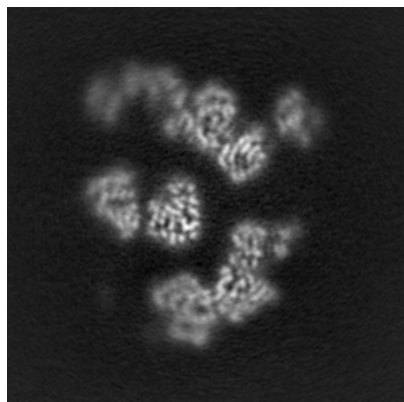


Y Index: 99

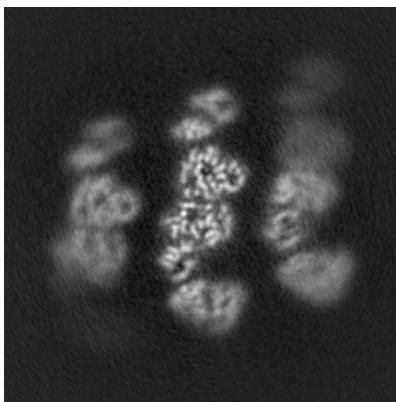


Z Index: 120

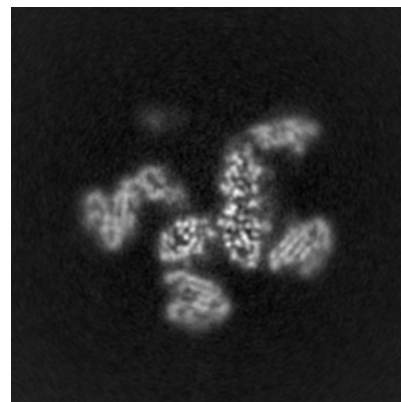
6.3.2 Raw map



X Index: 106



Y Index: 99

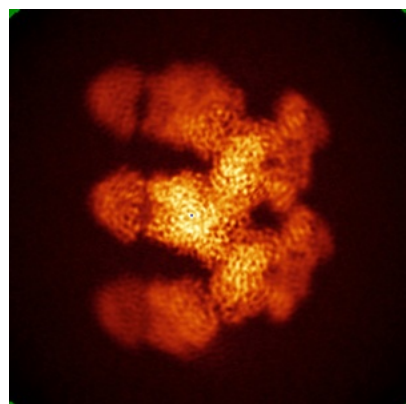


Z Index: 116

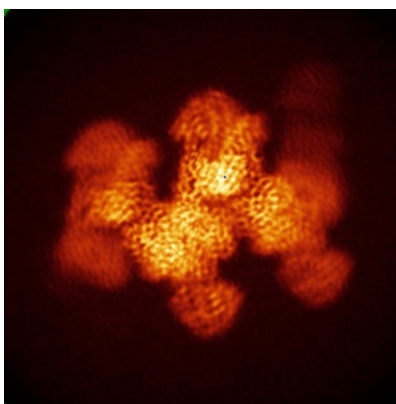
The images above show the largest variance slices of the map in three orthogonal directions.

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

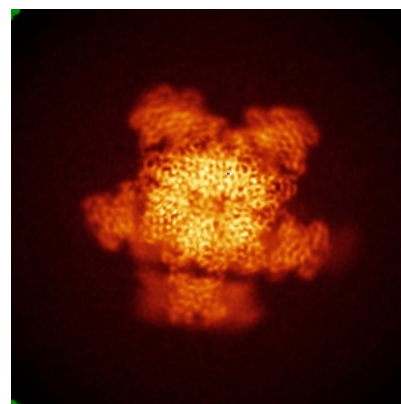
6.4.1 Primary map



X

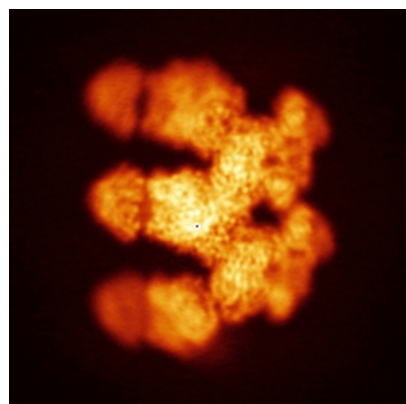


Y

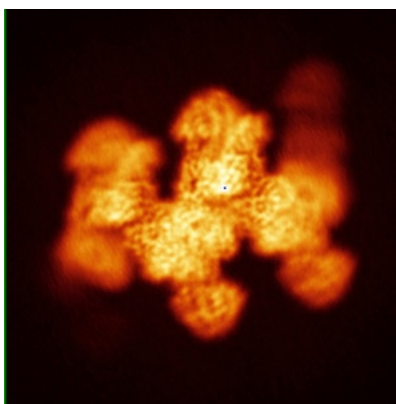


Z

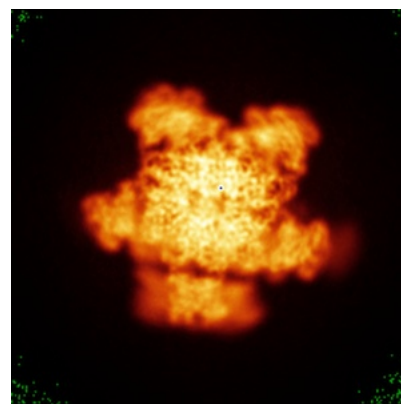
6.4.2 Raw map



X



Y

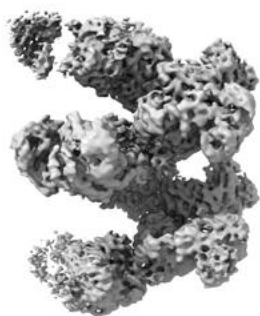


Z

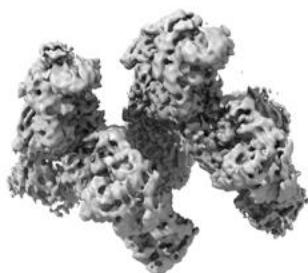
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

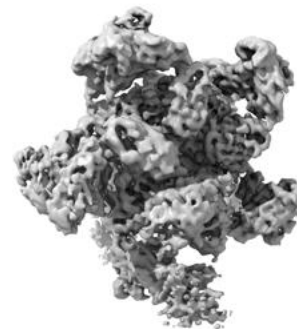
6.5.1 Primary map



X



Y



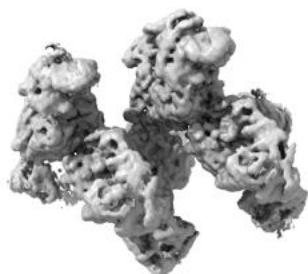
Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

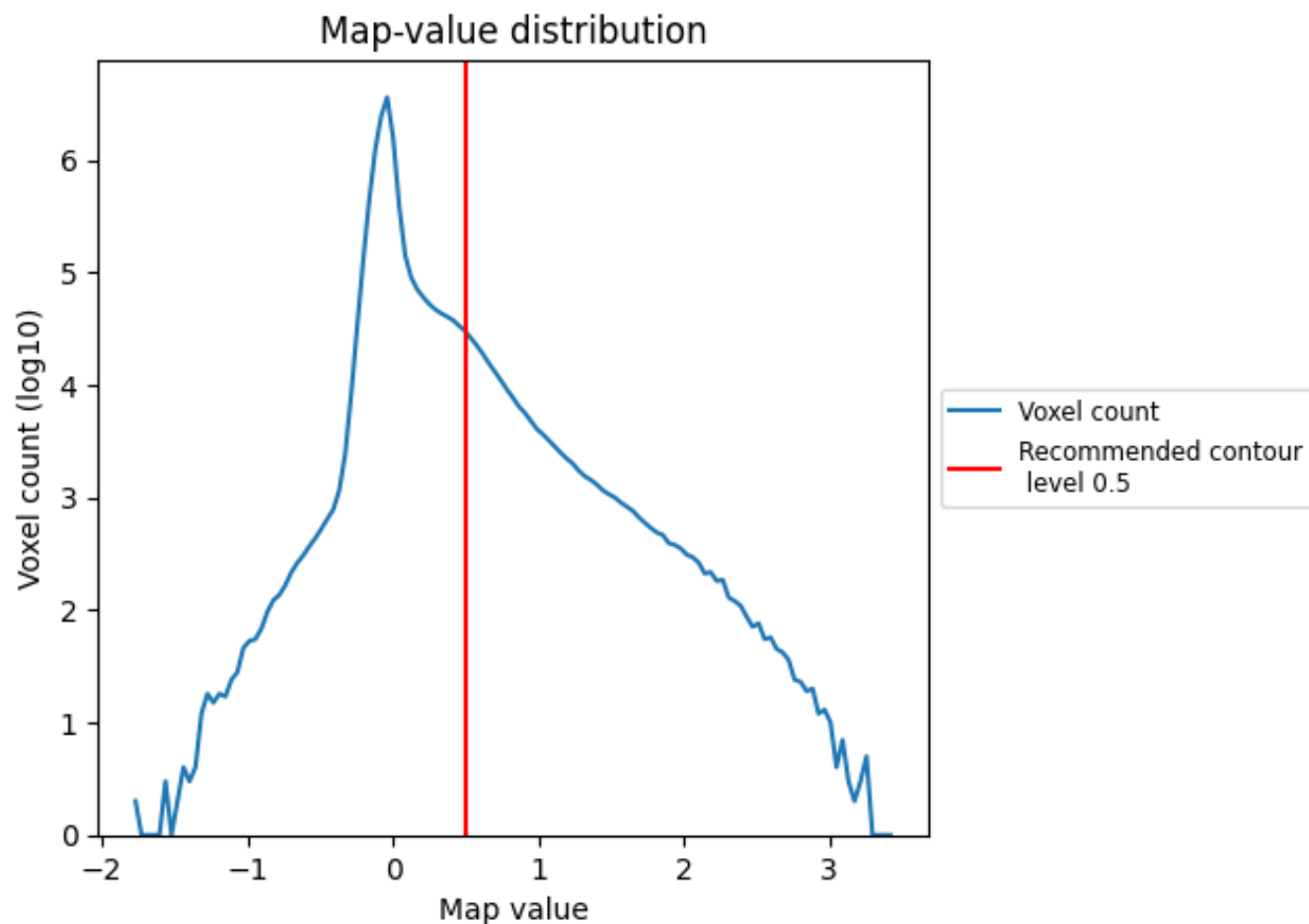
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

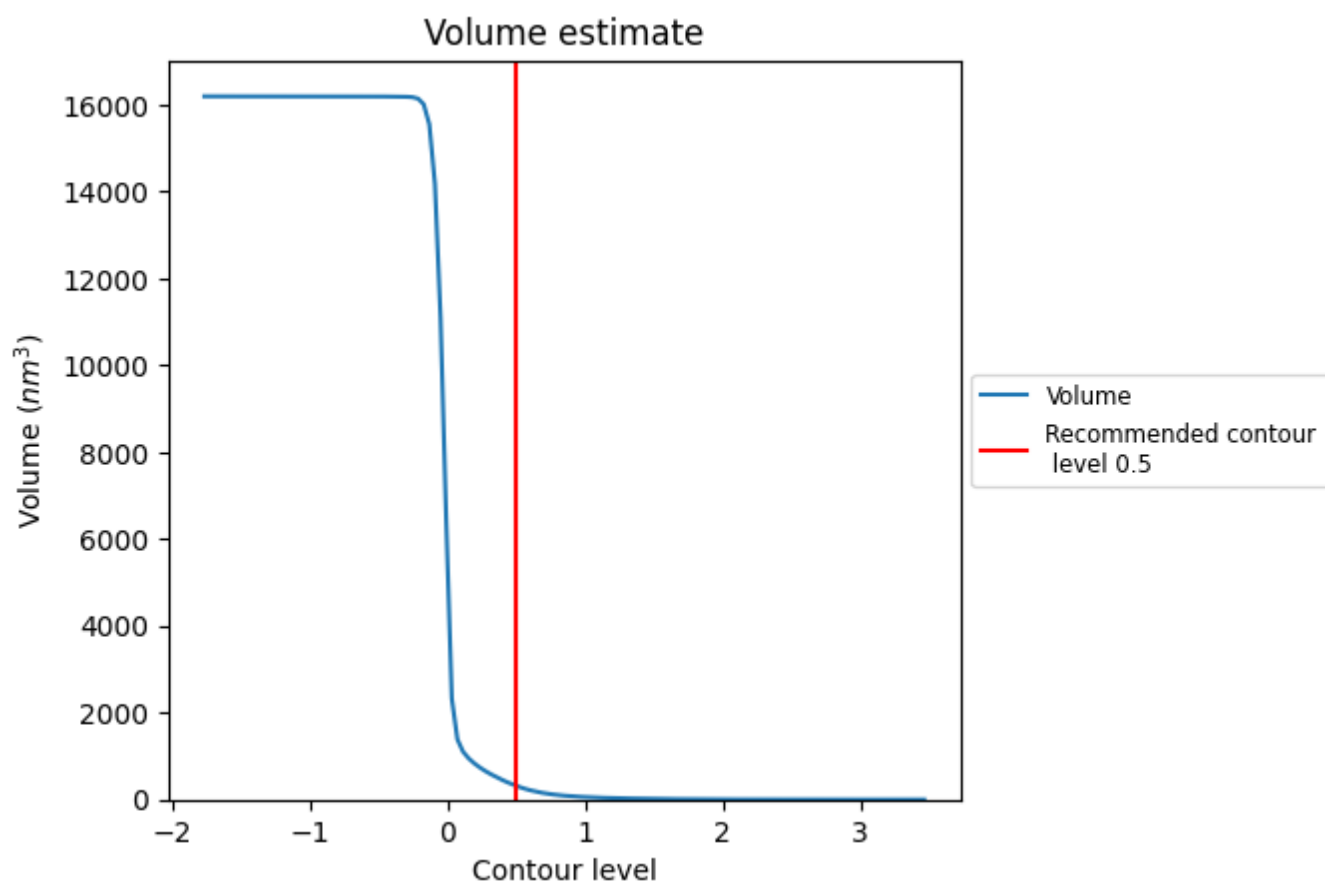
This section contains the results of statistical analysis of the map.

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.

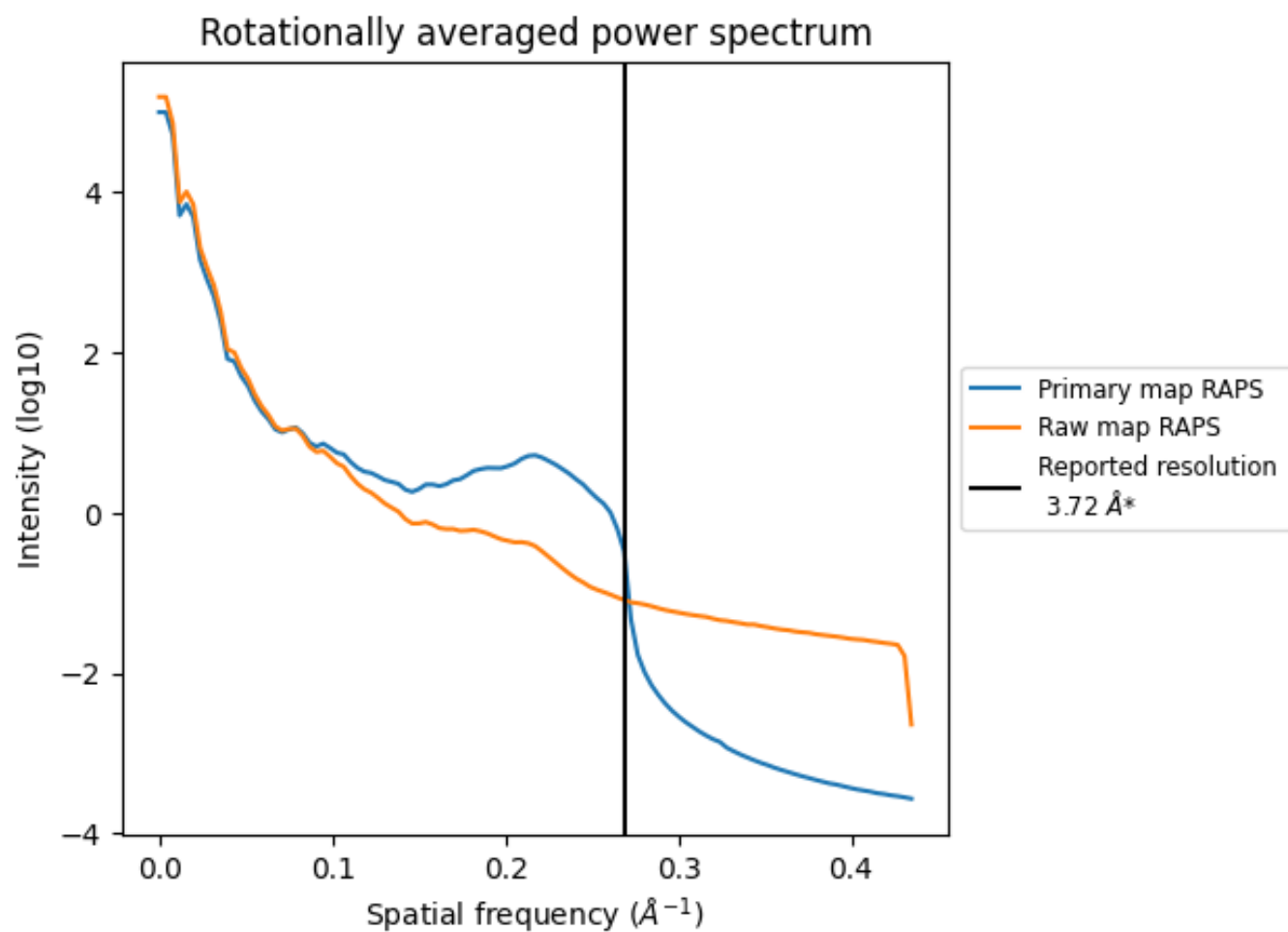
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 316 nm³; this corresponds to an approximate mass of 286 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 ⓘ

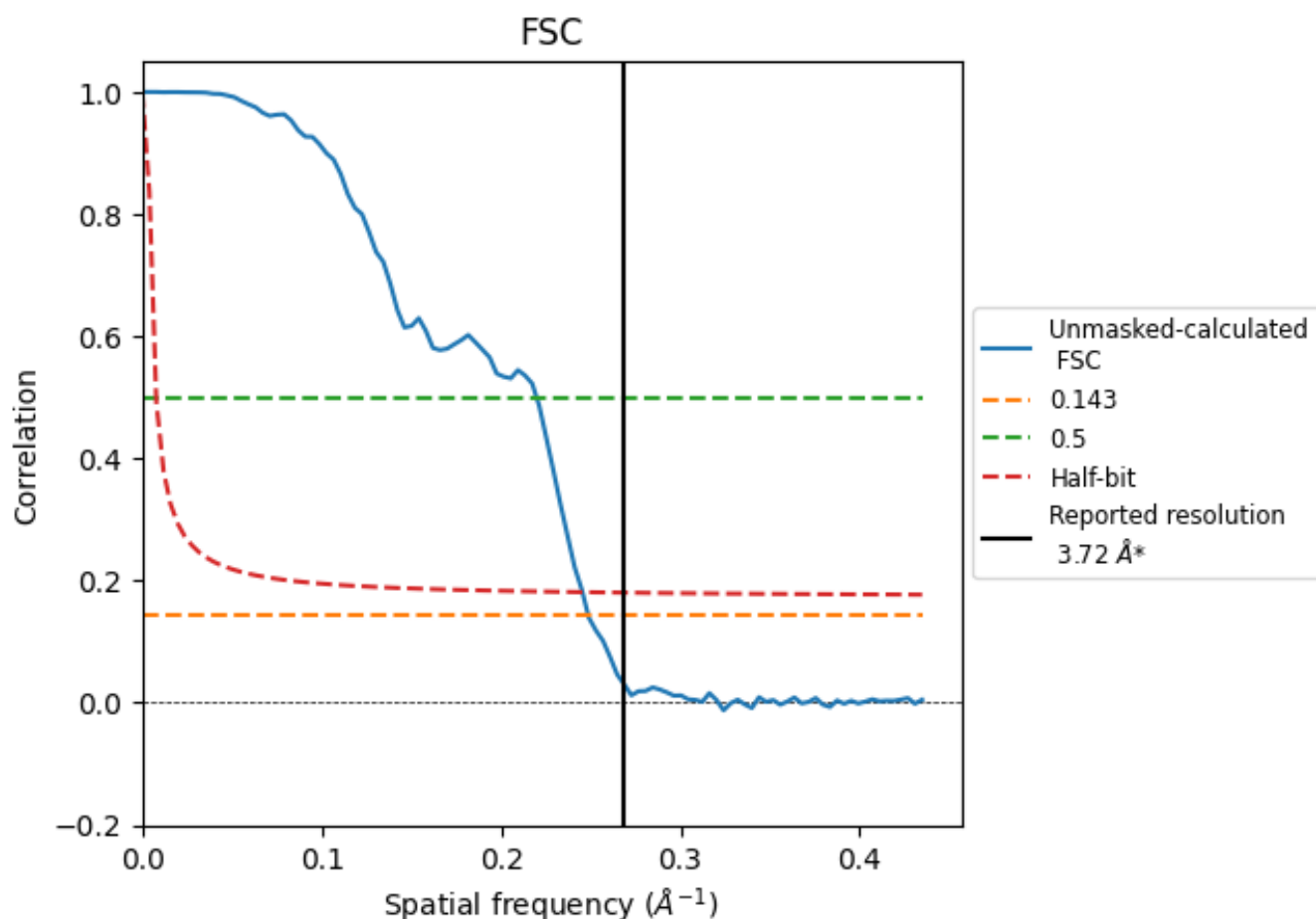


*Reported resolution corresponds to spatial frequency of 0.269 Å⁻¹

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 0.269 \AA^{-1}

8.2 Resolution estimates [i](#)

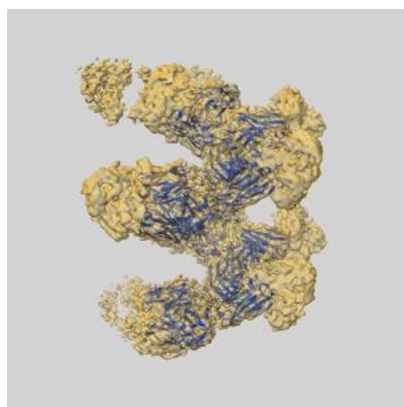
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.72	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.02	4.55	4.07

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

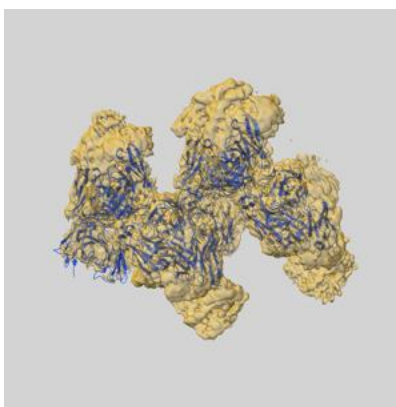
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-27784 and PDB model 8DYW. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

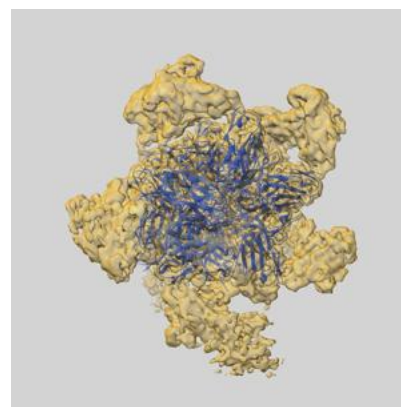
9.1 Map-model overlay [i](#)



X



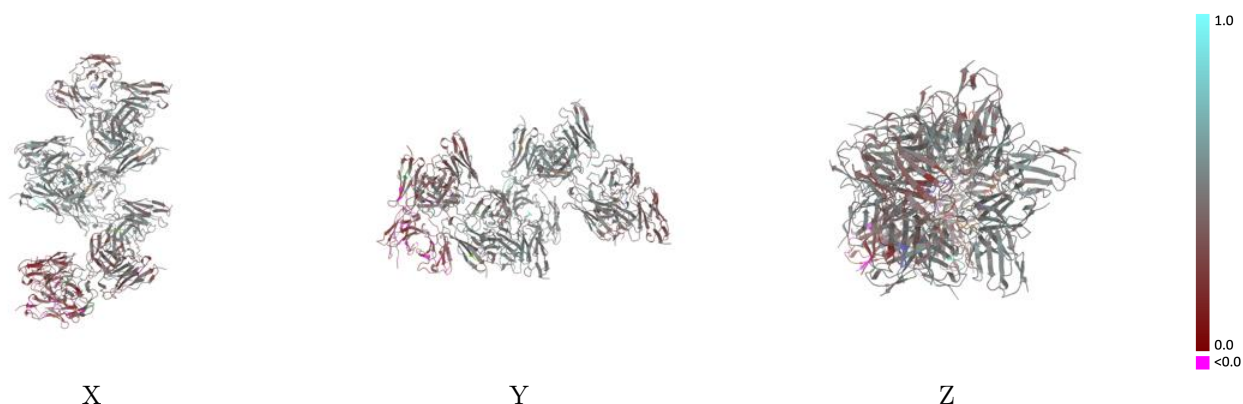
Y



Z

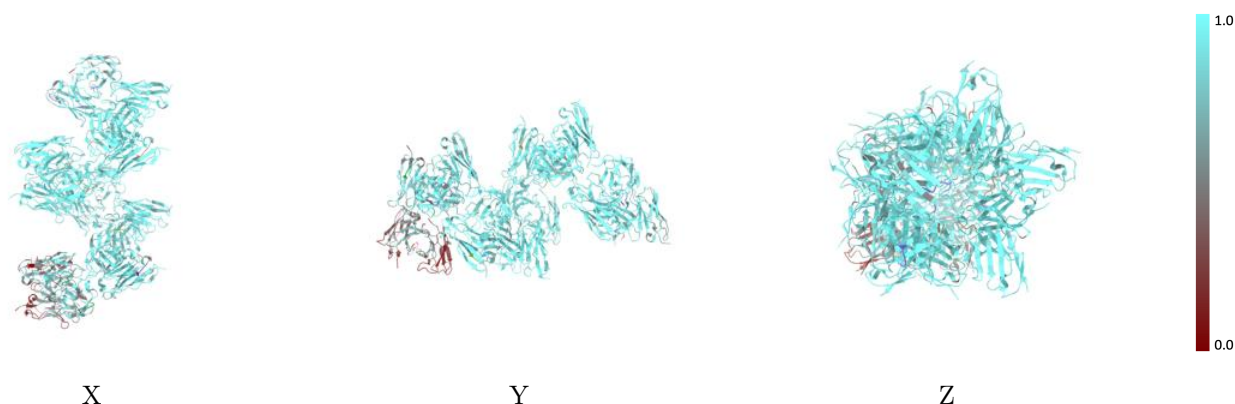
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



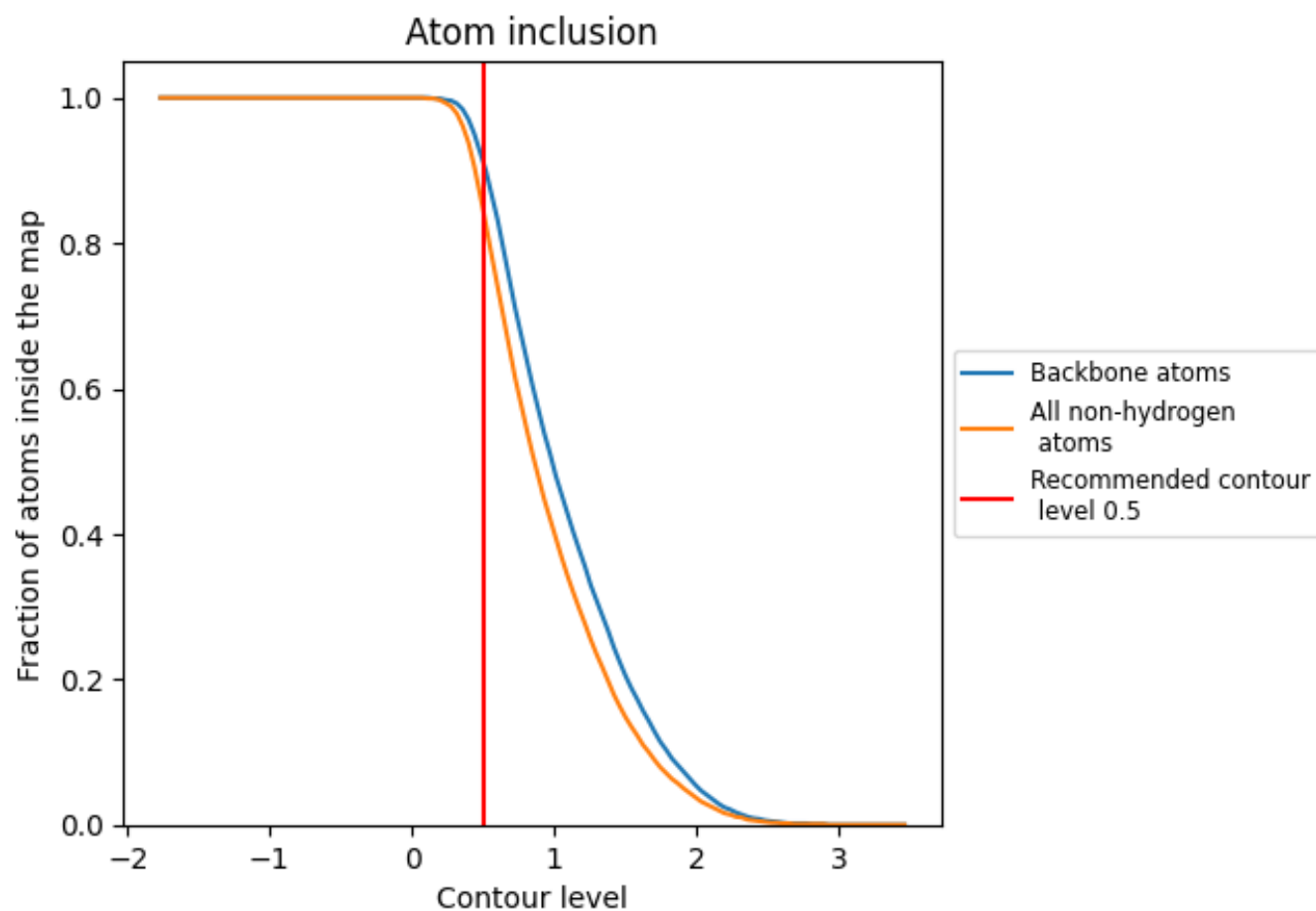
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).













































9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8470	 0.4240
A	 0.8780	 0.4100
B	 0.8320	 0.3790
C	 0.9290	 0.4680
D	 0.9130	 0.4580
E	 0.9420	 0.5000
F	 0.9220	 0.4900
H	 0.9270	 0.4980
I	 0.9450	 0.4320
L	 0.9320	 0.4820
M	 0.9510	 0.5050
N	 0.9410	 0.5020
O	 0.9510	 0.5040
P	 0.9410	 0.4910
Q	 0.9070	 0.4630
R	 0.9000	 0.4520
S	 0.8740	 0.4140
T	 0.8720	 0.4120
U	 0.7740	 0.3240
V	 0.7590	 0.3270
W	 0.4200	 0.1930
X	 0.3030	 0.1930

