



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 11:38 AM UTC

PDB ID : 8C8K / pdb_00008c8k
EMDB ID : EMD-16482
Title : In vitro structure of the Nitrosopumilus maritimus S-layer - Six-fold symmetry (C6)
Authors : von Kuegelgen, A.; Bharat, T.
Deposited on : 2023-01-20
Resolution : 2.87 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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

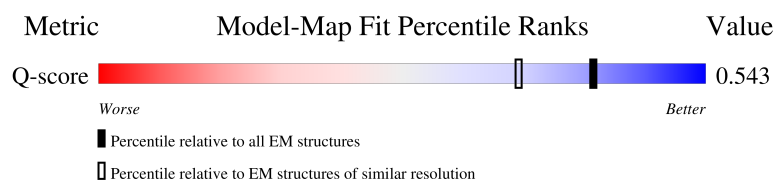
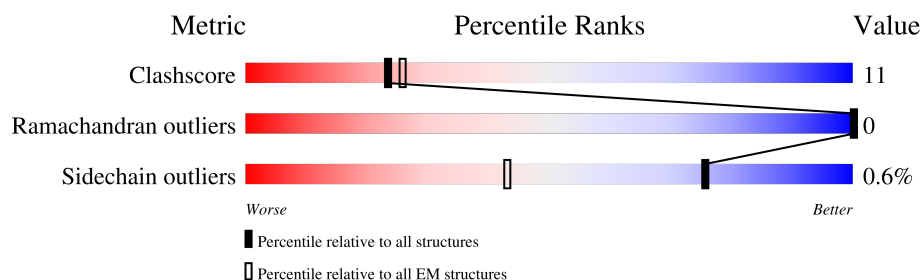
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.87 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12062 (2.37 - 3.37)

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	A	1734	11% . 85%
1	B	1734	11% . 85%
1	C	1734	11% . 85%
1	D	1734	11% . 85%

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Mol	Chain	Length	Quality of chain
1	E	1734	 11% 85%
1	F	1734	 11% 85%

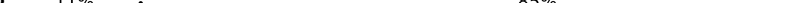
2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11430 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.

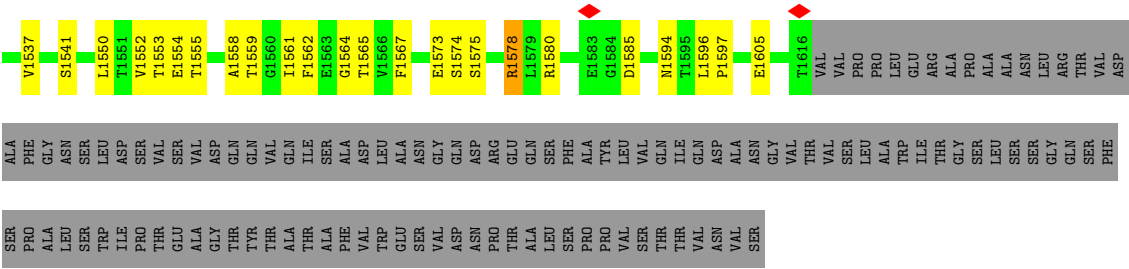
- Molecule 1 is a protein called Cell surface protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	253	Total	C	N	O	S	0	0
			1905	1179	293	432	1		
1	B	253	Total	C	N	O	S	0	0
			1905	1179	293	432	1		
1	C	253	Total	C	N	O	S	0	0
			1905	1179	293	432	1		
1	D	253	Total	C	N	O	S	0	0
			1905	1179	293	432	1		
1	E	253	Total	C	N	O	S	0	0
			1905	1179	293	432	1		
1	F	253	Total	C	N	O	S	0	0
			1905	1179	293	432	1		

Chain B:  11% . 85%







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



[illegible]

- Molecule 1: Cell surface protein

[illegible]





ALA
LEU
SER
TRP
ILE
PRO
THR
GLU
ALA
GLY
THR
TYR
THR
ALA
THR
ALA
PHE
VAL
THR
GLU
SER
VAL
ASP
ASN
PRO
THR
ALA
ALA
LEU
SER
PRO
PRO
VAL
SER
THR
THR
VAL
VAL
ASN
VAL
SER

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	354860	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; RELION refinement with in-built CTF correction. The function is similar to a Wiener filter, so amplitude correction included.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48.5	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.089	Depositor
Minimum map value	-0.044	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.01334	Depositor
Map size ($\text{\AA}$)	349.44, 349.44, 349.44	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.092, 1.092, 1.092	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	0.99	2/1940 (0.1%)	1.07	1/2658 (0.0%)
1	B	0.96	2/1940 (0.1%)	1.07	1/2658 (0.0%)
1	C	0.97	2/1940 (0.1%)	1.06	0/2658
1	D	0.97	2/1940 (0.1%)	1.08	1/2658 (0.0%)
1	E	0.96	3/1940 (0.2%)	1.06	0/2658
1	F	0.97	3/1940 (0.2%)	1.06	0/2658
All	All	0.97	14/11640 (0.1%)	1.07	3/15948 (0.0%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1428	THR	C-O	-8.59	1.13	1.24
1	E	1397	LEU	C-O	-8.34	1.14	1.23
1	B	1397	LEU	C-O	-8.19	1.14	1.23
1	D	1428	THR	C-O	-7.97	1.14	1.24
1	F	1397	LEU	C-O	-7.76	1.14	1.23
1	C	1428	THR	C-O	-7.62	1.15	1.24
1	A	1397	LEU	C-O	-7.20	1.15	1.23
1	C	1397	LEU	C-O	-7.19	1.15	1.23
1	F	1399	ASP	CG-OD1	-6.55	1.12	1.25
1	D	1397	LEU	C-O	-6.44	1.16	1.23
1	F	1428	THR	C-O	-5.88	1.17	1.24
1	B	1428	THR	C-O	-5.51	1.17	1.24
1	E	1399	ASP	CG-OD1	-5.48	1.15	1.25
1	E	1428	THR	C-O	-5.05	1.18	1.24

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1578	ARG	CG-CD-NE	-5.22	100.52	112.00
1	D	1578	ARG	CG-CD-NE	-5.07	100.85	112.00
1	A	1578	ARG	CG-CD-NE	-5.05	100.89	112.00

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	A	1905	0	1738	39	0
1	B	1905	0	1738	41	0
1	C	1905	0	1738	39	0
1	D	1905	0	1738	40	0
1	E	1905	0	1738	42	0
1	F	1905	0	1738	40	0
All	All	11430	0	10428	241	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 11.

All (241) 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:B:1567:PHE:HD2	1:B:1578:ARG:HG3	1.32	0.93
1:E:1567:PHE:HD2	1:E:1578:ARG:HG2	1.41	0.85
1:A:1567:PHE:HD2	1:A:1578:ARG:HG2	1.42	0.84
1:D:1567:PHE:HD2	1:D:1578:ARG:HG2	1.42	0.82
1:E:1567:PHE:CD2	1:E:1578:ARG:HG2	2.15	0.81
1:D:1567:PHE:CD2	1:D:1578:ARG:HG2	2.16	0.80
1:A:1567:PHE:CD2	1:A:1578:ARG:HG2	2.16	0.80
1:F:1567:PHE:CD2	1:F:1578:ARG:HG2	2.21	0.76
1:F:1567:PHE:HD2	1:F:1578:ARG:HG2	1.52	0.73
1:D:1596:LEU:HD12	1:D:1597:PRO:HD2	1.72	0.72
1:C:1596:LEU:HD12	1:C:1597:PRO:HD2	1.72	0.72
1:F:1596:LEU:HD12	1:F:1597:PRO:HD2	1.72	0.72
1:B:1596:LEU:HD12	1:B:1597:PRO:HD2	1.72	0.72
1:A:1596:LEU:HD12	1:A:1597:PRO:HD2	1.72	0.72
1:E:1596:LEU:HD12	1:E:1597:PRO:HD2	1.72	0.72
1:E:1517:VAL:HG22	1:E:1565:THR:HG22	1.74	0.69
1:B:1567:PHE:CD2	1:B:1578:ARG:HG3	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1517:VAL:HG22	1:F:1565:THR:HG22	1.75	0.69
1:A:1517:VAL:HG22	1:A:1565:THR:HG22	1.74	0.69
1:D:1517:VAL:HG22	1:D:1565:THR:HG22	1.74	0.69
1:B:1517:VAL:HG22	1:B:1565:THR:HG22	1.75	0.67
1:C:1517:VAL:HG22	1:C:1565:THR:HG22	1.75	0.67
1:C:1550:LEU:HD21	1:C:1564:GLY:HA3	1.79	0.65
1:D:1550:LEU:HD21	1:D:1564:GLY:HA3	1.80	0.64
1:B:1550:LEU:HD21	1:B:1564:GLY:HA3	1.79	0.64
1:F:1550:LEU:HD21	1:F:1564:GLY:HA3	1.79	0.64
1:A:1550:LEU:HD21	1:A:1564:GLY:HA3	1.80	0.64
1:E:1550:LEU:HD21	1:E:1564:GLY:HA3	1.80	0.64
1:B:1567:PHE:HD2	1:B:1578:ARG:CG	2.11	0.59
1:C:1438:ILE:HB	1:C:1469:LEU:HD23	1.85	0.58
1:B:1438:ILE:HB	1:B:1469:LEU:HD23	1.85	0.58
1:D:1438:ILE:HB	1:D:1469:LEU:HD23	1.85	0.57
1:A:1438:ILE:HB	1:A:1469:LEU:HD23	1.86	0.57
1:C:1499:ASN:N	1:C:1524:ASP:OD2	2.35	0.57
1:D:1537:VAL:O	1:D:1550:LEU:N	2.38	0.57
1:F:1438:ILE:HB	1:F:1469:LEU:HD23	1.85	0.57
1:C:1537:VAL:O	1:C:1550:LEU:N	2.38	0.56
1:E:1537:VAL:O	1:E:1550:LEU:N	2.38	0.56
1:F:1537:VAL:O	1:F:1550:LEU:N	2.38	0.56
1:A:1537:VAL:O	1:A:1550:LEU:N	2.38	0.56
1:E:1438:ILE:HB	1:E:1469:LEU:HD23	1.85	0.56
1:E:1376:TYR:CE1	1:E:1382:VAL:HG12	2.41	0.56
1:D:1369:VAL:HG23	1:D:1490:ILE:HD12	1.87	0.56
1:A:1376:TYR:CE1	1:A:1382:VAL:HG12	2.41	0.56
1:B:1376:TYR:CE1	1:B:1382:VAL:HG12	2.41	0.56
1:F:1376:TYR:CE1	1:F:1382:VAL:HG12	2.41	0.56
1:B:1499:ASN:N	1:B:1524:ASP:OD2	2.34	0.56
1:D:1376:TYR:CE1	1:D:1382:VAL:HG12	2.41	0.55
1:D:1499:ASN:N	1:D:1524:ASP:OD2	2.35	0.55
1:F:1369:VAL:HG23	1:F:1490:ILE:HD12	1.88	0.55
1:C:1376:TYR:CE1	1:C:1382:VAL:HG12	2.41	0.55
1:B:1369:VAL:HG23	1:B:1490:ILE:HD12	1.88	0.55
1:B:1537:VAL:O	1:B:1550:LEU:N	2.38	0.55
1:C:1369:VAL:HG23	1:C:1490:ILE:HD12	1.88	0.55
1:A:1369:VAL:HG23	1:A:1490:ILE:HD12	1.89	0.54
1:E:1369:VAL:HG23	1:E:1490:ILE:HD12	1.88	0.54
1:A:1422:LYS:O	1:A:1423:LEU:HD12	2.08	0.54
1:B:1422:LYS:O	1:B:1423:LEU:HD12	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1422:LYS:O	1:D:1423:LEU:HD12	2.08	0.54
1:C:1422:LYS:O	1:C:1423:LEU:HD12	2.08	0.54
1:F:1422:LYS:O	1:F:1423:LEU:HD12	2.08	0.53
1:A:1499:ASN:N	1:A:1524:ASP:OD2	2.35	0.53
1:E:1422:LYS:O	1:E:1423:LEU:HD12	2.08	0.53
1:B:1573:GLU:O	1:B:1578:ARG:NH1	2.42	0.53
1:B:1372:ASP:OD2	1:B:1383:TYR:HD2	1.92	0.53
1:E:1499:ASN:N	1:E:1524:ASP:OD2	2.35	0.53
1:B:1532:VAL:HG13	1:B:1554:GLU:HB3	1.91	0.53
1:C:1372:ASP:OD2	1:C:1383:TYR:HD2	1.92	0.53
1:F:1499:ASN:N	1:F:1524:ASP:OD2	2.34	0.53
1:C:1532:VAL:HG13	1:C:1554:GLU:HB3	1.90	0.53
1:D:1372:ASP:OD2	1:D:1383:TYR:HD2	1.92	0.53
1:E:1532:VAL:HG13	1:E:1554:GLU:HB3	1.91	0.53
1:A:1372:ASP:OD2	1:A:1383:TYR:HD2	1.92	0.52
1:D:1510:TYR:CE1	1:D:1516:GLY:HA2	2.45	0.52
1:E:1510:TYR:CE1	1:E:1516:GLY:HA2	2.44	0.52
1:F:1574:SER:OG	1:F:1580:ARG:N	2.26	0.52
1:C:1503:VAL:HG22	1:C:1520:VAL:HG23	1.91	0.52
1:D:1503:VAL:HG22	1:D:1520:VAL:HG23	1.91	0.52
1:C:1510:TYR:CE1	1:C:1516:GLY:HA2	2.44	0.52
1:A:1532:VAL:HG13	1:A:1554:GLU:HB3	1.91	0.52
1:A:1503:VAL:HG22	1:A:1520:VAL:HG23	1.91	0.52
1:E:1372:ASP:OD2	1:E:1383:TYR:HD2	1.92	0.52
1:B:1411:VAL:HG12	1:B:1480:VAL:HG22	1.92	0.52
1:F:1510:TYR:CE1	1:F:1516:GLY:HA2	2.44	0.52
1:F:1372:ASP:OD2	1:F:1383:TYR:HD2	1.92	0.52
1:F:1503:VAL:HG22	1:F:1520:VAL:HG23	1.91	0.52
1:B:1510:TYR:CE1	1:B:1516:GLY:HA2	2.45	0.52
1:C:1510:TYR:HE1	1:C:1516:GLY:HA2	1.75	0.52
1:C:1411:VAL:HG12	1:C:1480:VAL:HG22	1.92	0.51
1:C:1473:ASP:OD1	1:C:1474:ASP:N	2.42	0.51
1:F:1532:VAL:HG13	1:F:1554:GLU:HB3	1.90	0.51
1:B:1503:VAL:HG22	1:B:1520:VAL:HG23	1.91	0.51
1:D:1532:VAL:HG13	1:D:1554:GLU:HB3	1.91	0.51
1:A:1446:ASP:OD1	1:A:1453:THR:HA	2.11	0.51
1:A:1411:VAL:HG12	1:A:1480:VAL:HG22	1.92	0.51
1:A:1510:TYR:CE1	1:A:1516:GLY:HA2	2.44	0.51
1:D:1446:ASP:OD1	1:D:1453:THR:HA	2.11	0.51
1:E:1446:ASP:OD1	1:E:1453:THR:HA	2.11	0.51
1:D:1510:TYR:HE1	1:D:1516:GLY:HA2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1574:SER:OG	1:D:1580:ARG:N	2.26	0.51
1:E:1503:VAL:HG22	1:E:1520:VAL:HG23	1.91	0.51
1:E:1574:SER:OG	1:E:1580:ARG:N	2.26	0.51
1:F:1411:VAL:HG12	1:F:1480:VAL:HG22	1.92	0.51
1:C:1446:ASP:OD1	1:C:1453:THR:HA	2.11	0.51
1:D:1411:VAL:HG12	1:D:1480:VAL:HG22	1.92	0.50
1:B:1446:ASP:OD1	1:B:1453:THR:HA	2.11	0.50
1:F:1446:ASP:OD1	1:F:1453:THR:HA	2.11	0.50
1:F:1510:TYR:HE1	1:F:1516:GLY:HA2	1.75	0.50
1:A:1473:ASP:OD1	1:A:1474:ASP:N	2.42	0.50
1:C:1385:THR:HG22	1:C:1434:THR:HG22	1.94	0.50
1:E:1510:TYR:HE1	1:E:1516:GLY:HA2	1.75	0.50
1:A:1510:TYR:HE1	1:A:1516:GLY:HA2	1.76	0.50
1:B:1385:THR:HG22	1:B:1434:THR:HG22	1.94	0.50
1:E:1411:VAL:HG12	1:E:1480:VAL:HG22	1.92	0.50
1:E:1473:ASP:OD1	1:E:1474:ASP:N	2.42	0.50
1:D:1385:THR:HG22	1:D:1434:THR:HG22	1.94	0.49
1:F:1438:ILE:HD12	1:F:1529:PRO:HG2	1.95	0.49
1:A:1574:SER:OG	1:A:1580:ARG:N	2.27	0.49
1:B:1510:TYR:HE1	1:B:1516:GLY:HA2	1.76	0.49
1:B:1438:ILE:HD12	1:B:1529:PRO:HG2	1.95	0.49
1:C:1438:ILE:HD12	1:C:1529:PRO:HG2	1.94	0.49
1:A:1385:THR:HG22	1:A:1434:THR:HG22	1.94	0.49
1:E:1385:THR:HG22	1:E:1434:THR:HG22	1.94	0.48
1:E:1438:ILE:HD12	1:E:1529:PRO:HG2	1.94	0.48
1:F:1385:THR:HG22	1:F:1434:THR:HG22	1.94	0.48
1:A:1438:ILE:HD12	1:A:1529:PRO:HG2	1.95	0.48
1:B:1559:THR:HG23	1:B:1561:ILE:H	1.78	0.48
1:A:1559:THR:HG23	1:A:1561:ILE:H	1.78	0.48
1:F:1559:THR:HG23	1:F:1561:ILE:H	1.78	0.48
1:C:1559:THR:HG23	1:C:1561:ILE:H	1.78	0.48
1:D:1559:THR:HG23	1:D:1561:ILE:H	1.78	0.48
1:D:1473:ASP:OD1	1:D:1474:ASP:N	2.42	0.48
1:E:1559:THR:HG23	1:E:1561:ILE:H	1.78	0.47
1:D:1438:ILE:HD12	1:D:1529:PRO:HG2	1.95	0.47
1:D:1555:THR:OG1	1:D:1559:THR:HG21	2.14	0.47
1:B:1473:ASP:OD1	1:B:1474:ASP:N	2.42	0.47
1:D:1403:GLU:HG2	1:D:1404:THR:HG23	1.97	0.47
1:C:1507:GLU:HB2	1:C:1510:TYR:CE2	2.50	0.47
1:D:1507:GLU:HB2	1:D:1510:TYR:CE2	2.50	0.47
1:E:1403:GLU:HG2	1:E:1404:THR:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1555:THR:OG1	1:E:1559:THR:HG21	2.14	0.47
1:F:1555:THR:OG1	1:F:1559:THR:HG21	2.14	0.47
1:C:1555:THR:OG1	1:C:1559:THR:HG21	2.14	0.47
1:D:1596:LEU:HD12	1:D:1597:PRO:CD	2.44	0.47
1:E:1507:GLU:HB2	1:E:1510:TYR:CE2	2.50	0.47
1:F:1507:GLU:HB2	1:F:1510:TYR:CE2	2.50	0.47
1:B:1507:GLU:HB2	1:B:1510:TYR:CE2	2.50	0.46
1:B:1555:THR:OG1	1:B:1559:THR:HG21	2.14	0.46
1:E:1409:ILE:CD1	1:E:1423:LEU:HD13	2.46	0.46
1:F:1403:GLU:HG2	1:F:1404:THR:HG23	1.97	0.46
1:A:1507:GLU:HB2	1:A:1510:TYR:CE2	2.50	0.46
1:C:1403:GLU:HG2	1:C:1404:THR:HG23	1.97	0.46
1:A:1409:ILE:CD1	1:A:1423:LEU:HD13	2.45	0.46
1:C:1596:LEU:HD12	1:C:1597:PRO:CD	2.44	0.46
1:A:1555:THR:OG1	1:A:1559:THR:HG21	2.14	0.46
1:F:1409:ILE:CD1	1:F:1423:LEU:HD13	2.46	0.46
1:B:1403:GLU:HG2	1:B:1404:THR:HG23	1.97	0.46
1:C:1574:SER:OG	1:C:1580:ARG:N	2.27	0.46
1:D:1409:ILE:CD1	1:D:1423:LEU:HD13	2.45	0.46
1:A:1403:GLU:HG2	1:A:1404:THR:HG23	1.97	0.46
1:E:1596:LEU:HD12	1:E:1597:PRO:CD	2.44	0.46
1:F:1596:LEU:HD12	1:F:1597:PRO:CD	2.44	0.45
1:B:1575:SER:HB3	1:B:1578:ARG:HH21	1.81	0.45
1:C:1409:ILE:CD1	1:C:1423:LEU:HD13	2.46	0.45
1:B:1409:ILE:CD1	1:B:1423:LEU:HD13	2.46	0.45
1:F:1473:ASP:OD1	1:F:1474:ASP:N	2.42	0.45
1:A:1596:LEU:HD12	1:A:1597:PRO:CD	2.44	0.44
1:B:1596:LEU:HD12	1:B:1597:PRO:CD	2.44	0.44
1:C:1594:ASN:HA	1:C:1605:GLU:OE1	2.18	0.44
1:D:1594:ASN:HA	1:D:1605:GLU:OE1	2.18	0.44
1:B:1594:ASN:HA	1:B:1605:GLU:OE1	2.18	0.44
1:B:1379:THR:HA	1:B:1439:LEU:O	2.19	0.43
1:C:1572:ASP:HB3	1:C:1578:ARG:HH12	1.83	0.43
1:F:1517:VAL:HA	1:F:1564:GLY:O	2.18	0.43
1:A:1594:ASN:HA	1:A:1605:GLU:OE1	2.18	0.43
1:C:1379:THR:HA	1:C:1439:LEU:O	2.19	0.43
1:D:1379:THR:HA	1:D:1439:LEU:O	2.19	0.43
1:E:1379:THR:HA	1:E:1439:LEU:O	2.19	0.43
1:F:1541:SER:OG	1:F:1585:ASP:OD1	2.37	0.43
1:B:1574:SER:OG	1:B:1580:ARG:N	2.27	0.43
1:F:1567:PHE:HB3	1:F:1578:ARG:HG2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1594:ASN:HA	1:F:1605:GLU:OE1	2.18	0.43
1:A:1517:VAL:HA	1:A:1564:GLY:O	2.18	0.43
1:E:1517:VAL:HA	1:E:1564:GLY:O	2.18	0.43
1:B:1422:LYS:O	1:B:1465:PRO:HA	2.19	0.43
1:F:1379:THR:HA	1:F:1439:LEU:O	2.19	0.43
1:E:1541:SER:OG	1:E:1585:ASP:OD1	2.37	0.43
1:B:1550:LEU:HD22	1:B:1552:VAL:HG13	2.01	0.43
1:C:1541:SER:OG	1:C:1585:ASP:OD1	2.37	0.43
1:A:1537:VAL:N	1:A:1550:LEU:O	2.47	0.42
1:A:1550:LEU:HD22	1:A:1552:VAL:HG13	2.01	0.42
1:D:1517:VAL:HA	1:D:1564:GLY:O	2.18	0.42
1:E:1594:ASN:HA	1:E:1605:GLU:OE1	2.18	0.42
1:A:1379:THR:HA	1:A:1439:LEU:O	2.19	0.42
1:A:1422:LYS:O	1:A:1465:PRO:HA	2.19	0.42
1:A:1541:SER:OG	1:A:1585:ASP:OD1	2.37	0.42
1:B:1541:SER:OG	1:B:1585:ASP:OD1	2.37	0.42
1:C:1517:VAL:HA	1:C:1564:GLY:O	2.19	0.42
1:C:1550:LEU:HD22	1:C:1552:VAL:HG13	2.01	0.42
1:E:1422:LYS:O	1:E:1465:PRO:HA	2.19	0.42
1:D:1448:ASP:OD2	1:D:1450:ASP:CG	2.63	0.42
1:D:1422:LYS:O	1:D:1465:PRO:HA	2.19	0.42
1:C:1422:LYS:O	1:C:1465:PRO:HA	2.19	0.42
1:B:1517:VAL:HA	1:B:1564:GLY:O	2.18	0.42
1:C:1448:ASP:OD2	1:C:1450:ASP:CG	2.63	0.42
1:F:1422:LYS:O	1:F:1465:PRO:HA	2.19	0.42
1:A:1500:ILE:HG22	1:A:1596:LEU:CD1	2.50	0.41
1:D:1541:SER:OG	1:D:1585:ASP:OD1	2.37	0.41
1:D:1553:THR:O	1:D:1562:PHE:HA	2.20	0.41
1:E:1550:LEU:HD22	1:E:1552:VAL:HG13	2.01	0.41
1:F:1500:ILE:HG22	1:F:1596:LEU:CD1	2.50	0.41
1:F:1550:LEU:HD22	1:F:1552:VAL:HG13	2.02	0.41
1:E:1553:THR:O	1:E:1562:PHE:HA	2.20	0.41
1:D:1480:VAL:O	1:D:1491:VAL:HA	2.21	0.41
1:D:1550:LEU:HD22	1:D:1552:VAL:HG13	2.01	0.41
1:E:1537:VAL:N	1:E:1550:LEU:O	2.48	0.41
1:E:1448:ASP:OD2	1:E:1450:ASP:CG	2.63	0.41
1:E:1500:ILE:HG22	1:E:1596:LEU:CD1	2.51	0.41
1:D:1500:ILE:HG22	1:D:1596:LEU:CD1	2.50	0.41
1:F:1448:ASP:OD2	1:F:1450:ASP:CG	2.63	0.41
1:A:1553:THR:O	1:A:1562:PHE:HA	2.20	0.41
1:F:1480:VAL:O	1:F:1491:VAL:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1553:THR:O	1:F:1562:PHE:HA	2.20	0.41
1:A:1529:PRO:O	1:A:1558:ALA:HB2	2.21	0.41
1:B:1365:PHE:N	1:B:1390:ASP:OD2	2.53	0.41
1:C:1537:VAL:N	1:C:1550:LEU:O	2.47	0.41
1:E:1365:PHE:N	1:E:1390:ASP:OD2	2.53	0.41
1:B:1553:THR:O	1:B:1562:PHE:HA	2.20	0.41
1:C:1553:THR:O	1:C:1562:PHE:HA	2.20	0.41
1:F:1529:PRO:O	1:F:1558:ALA:HB2	2.21	0.41
1:C:1480:VAL:O	1:C:1491:VAL:HA	2.21	0.41
1:B:1529:PRO:O	1:B:1558:ALA:HB2	2.21	0.41
1:E:1529:PRO:O	1:E:1558:ALA:HB2	2.21	0.40
1:D:1409:ILE:HD13	1:D:1423:LEU:HD13	2.04	0.40
1:A:1480:VAL:O	1:A:1491:VAL:HA	2.21	0.40
1:C:1500:ILE:HG22	1:C:1596:LEU:CD1	2.50	0.40
1:C:1529:PRO:O	1:C:1558:ALA:HB2	2.21	0.40
1:D:1529:PRO:O	1:D:1558:ALA:HB2	2.21	0.40
1:E:1409:ILE:HD13	1:E:1423:LEU:HD13	2.04	0.40
1:E:1480:VAL:O	1:E:1491:VAL:HA	2.21	0.40
1:B:1480:VAL:O	1:B:1491:VAL:HA	2.21	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	251/1734 (14%)	245 (98%)	6 (2%)	0	100	100
1	B	251/1734 (14%)	246 (98%)	5 (2%)	0	100	100
1	C	251/1734 (14%)	247 (98%)	4 (2%)	0	100	100
1	D	251/1734 (14%)	246 (98%)	5 (2%)	0	100	100
1	E	251/1734 (14%)	246 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	251/1734 (14%)	247 (98%)	4 (2%)	0	100	100
All	All	1506/10404 (14%)	1477 (98%)	29 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	212/1438 (15%)	210 (99%)	2 (1%)	70	88
1	B	212/1438 (15%)	211 (100%)	1 (0%)	81	93
1	C	212/1438 (15%)	211 (100%)	1 (0%)	81	93
1	D	212/1438 (15%)	210 (99%)	2 (1%)	70	88
1	E	212/1438 (15%)	211 (100%)	1 (0%)	81	93
1	F	212/1438 (15%)	211 (100%)	1 (0%)	81	93
All	All	1272/8628 (15%)	1264 (99%)	8 (1%)	76	92

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

Mol	Chain	Res	Type
1	A	1414	ARG
1	A	1575	SER
1	B	1414	ARG
1	C	1414	ARG
1	D	1414	ARG
1	D	1575	SER
1	E	1414	ARG
1	F	1414	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 [i](#)

There are no chain breaks in this entry.

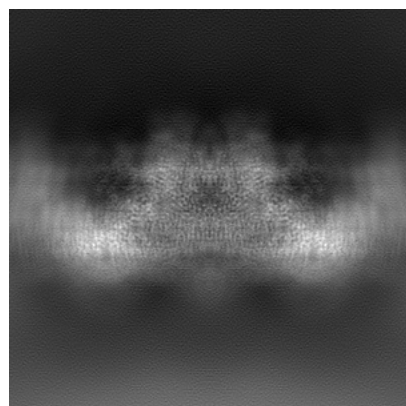
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16482. These allow visual inspection of the internal detail of the map and identification of artifacts.

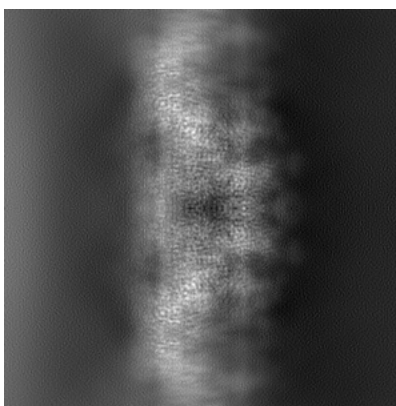
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

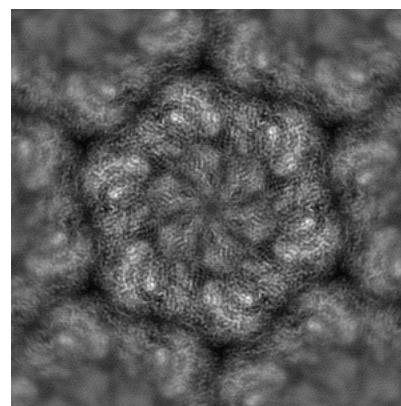
6.1.1 Primary map



X

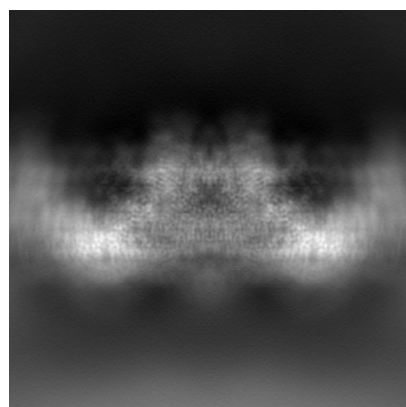


Y

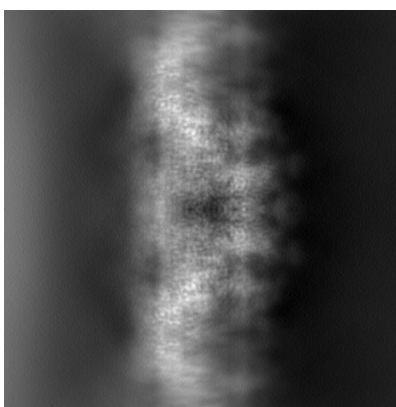


Z

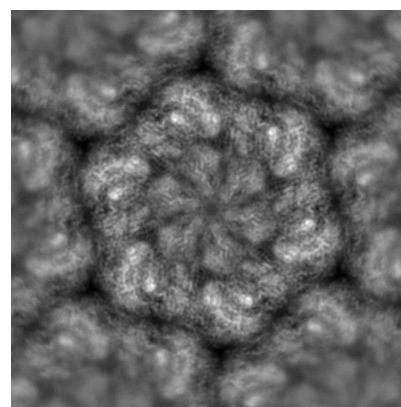
6.1.2 Raw map



X



Y

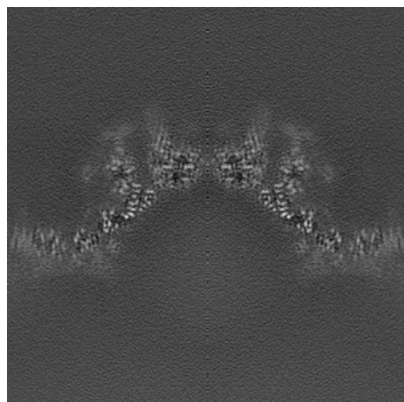


Z

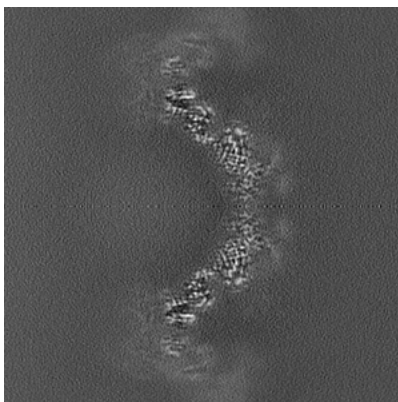
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

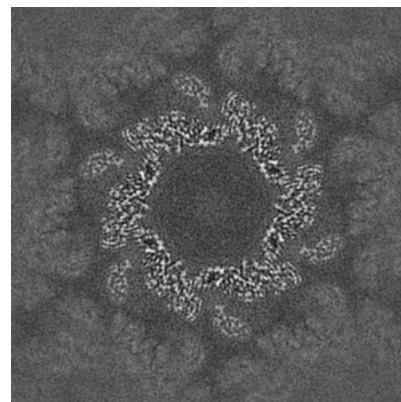
6.2.1 Primary map



X Index: 160

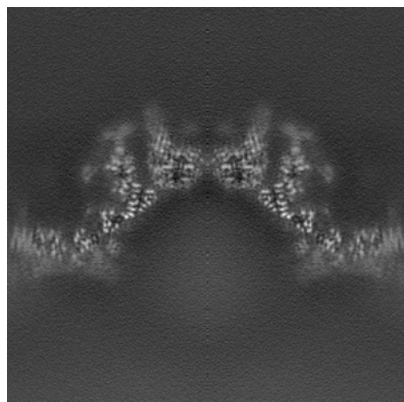


Y Index: 160

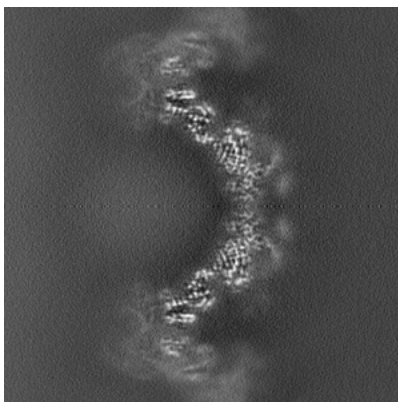


Z Index: 160

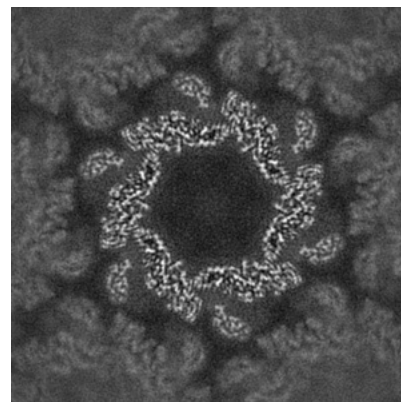
6.2.2 Raw map



X Index: 160



Y Index: 160

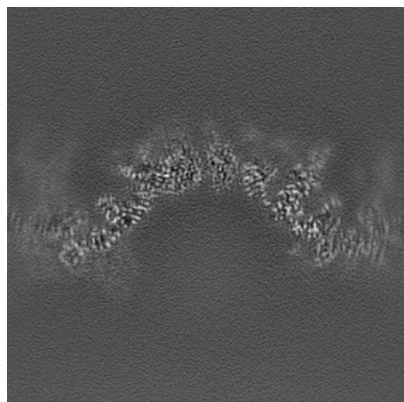


Z Index: 160

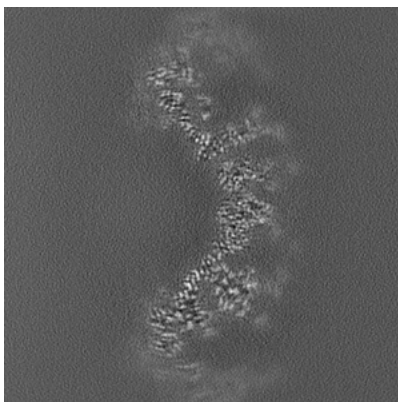
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

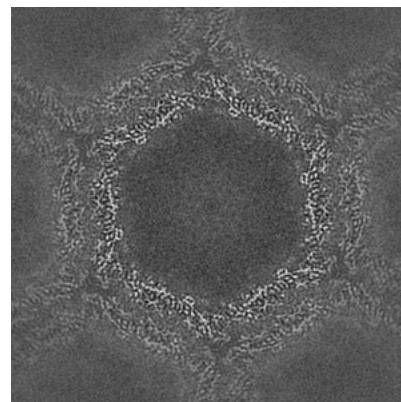
6.3.1 Primary map



X Index: 137

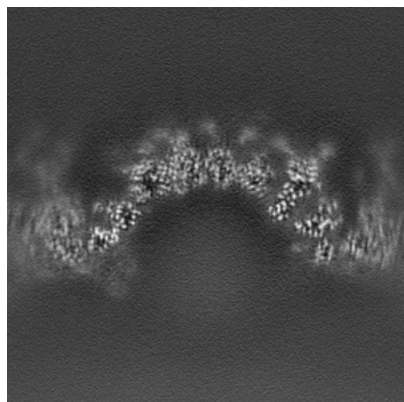


Y Index: 191

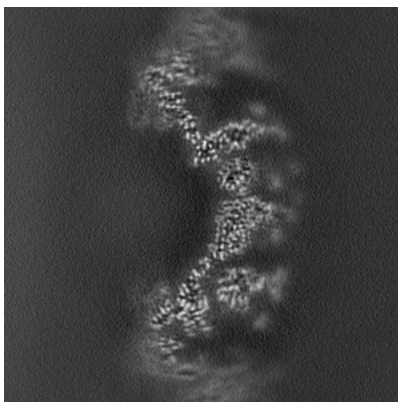


Z Index: 136

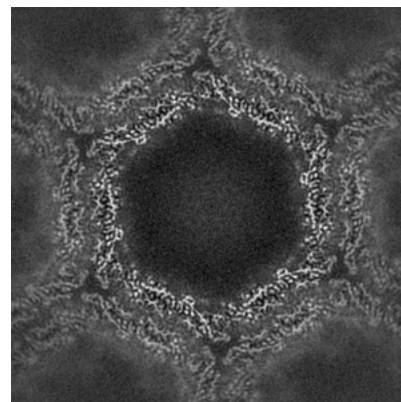
6.3.2 Raw map



X Index: 140



Y Index: 195

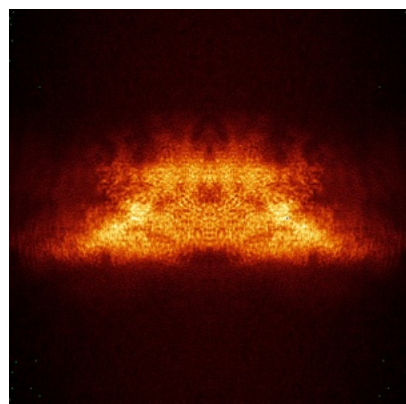


Z Index: 136

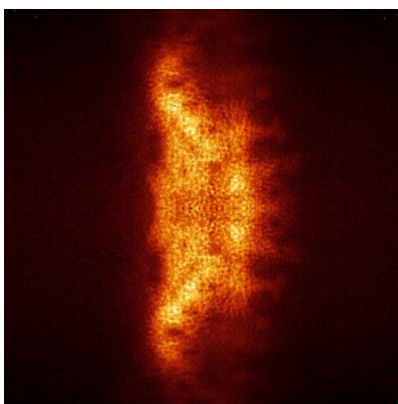
The images above show the largest variance slices of the map in three orthogonal directions.

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

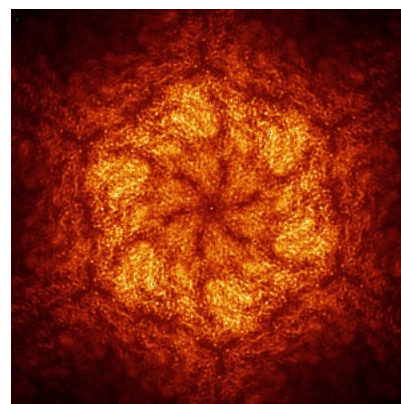
6.4.1 Primary map



X

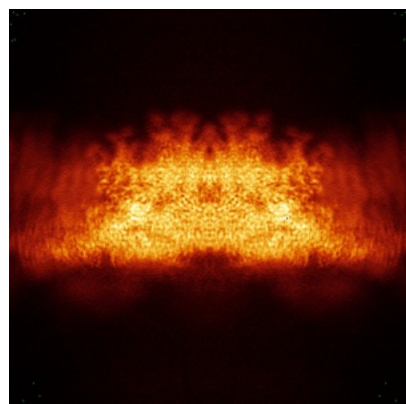


Y

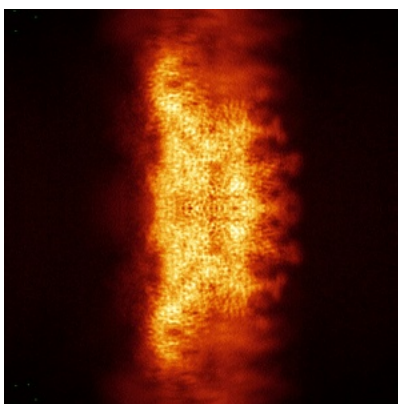


Z

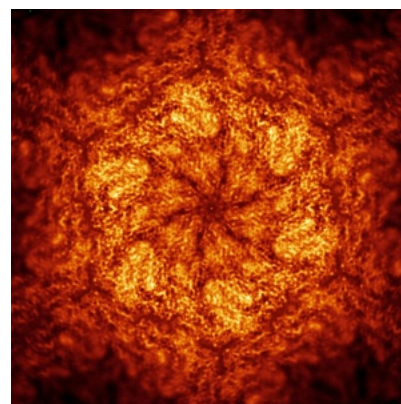
6.4.2 Raw map



X



Y

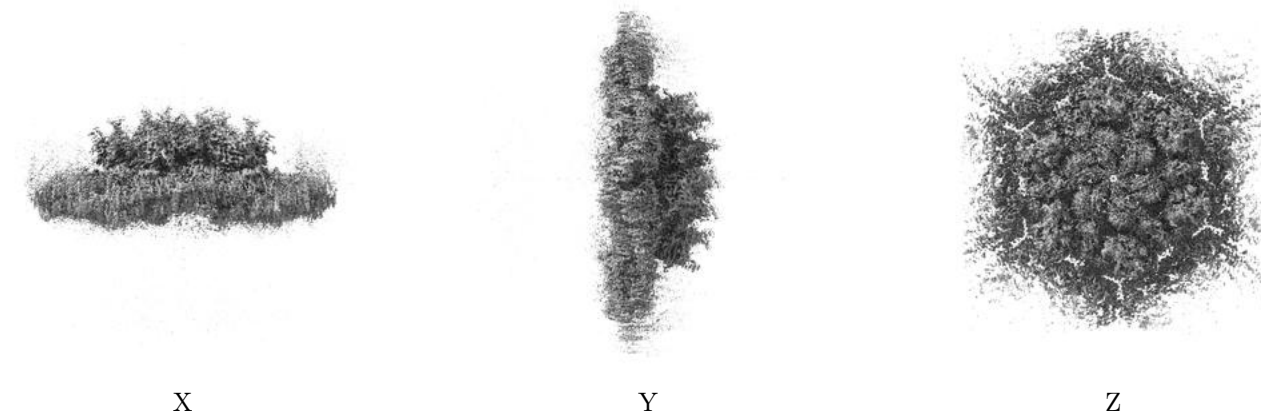


Z

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 0.01334. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

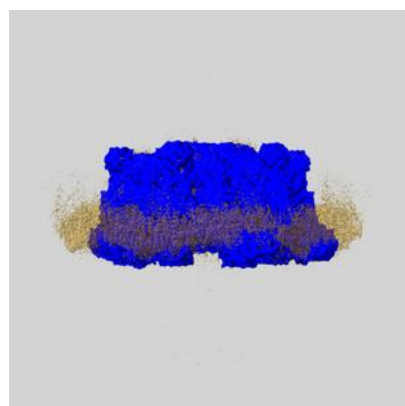
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

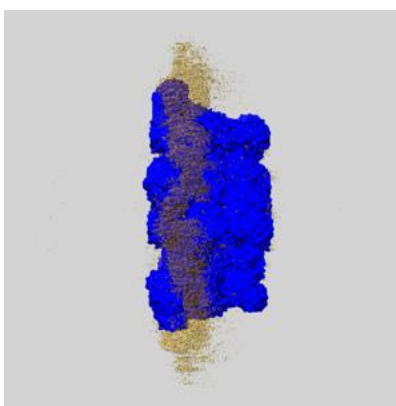
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

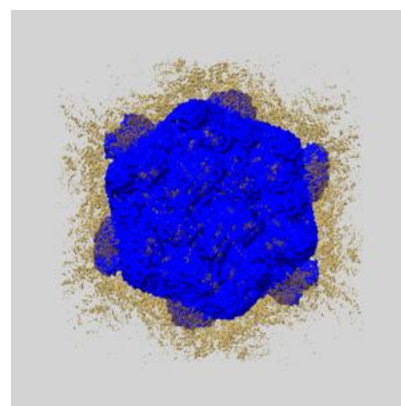
6.6.1 emd_16482_msk_1.map [i](#)



X



Y

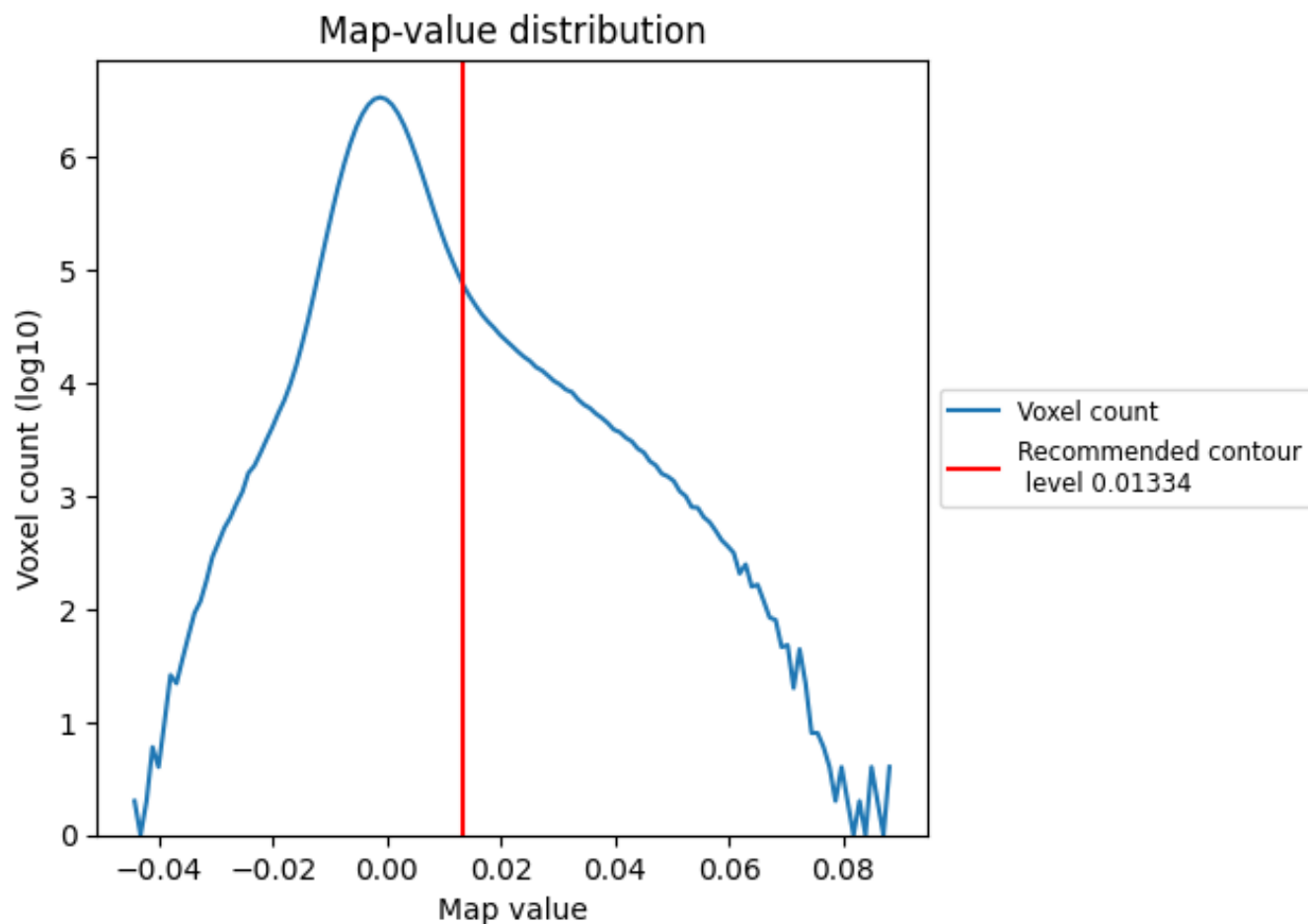


Z

7 Map analysis [i](#)

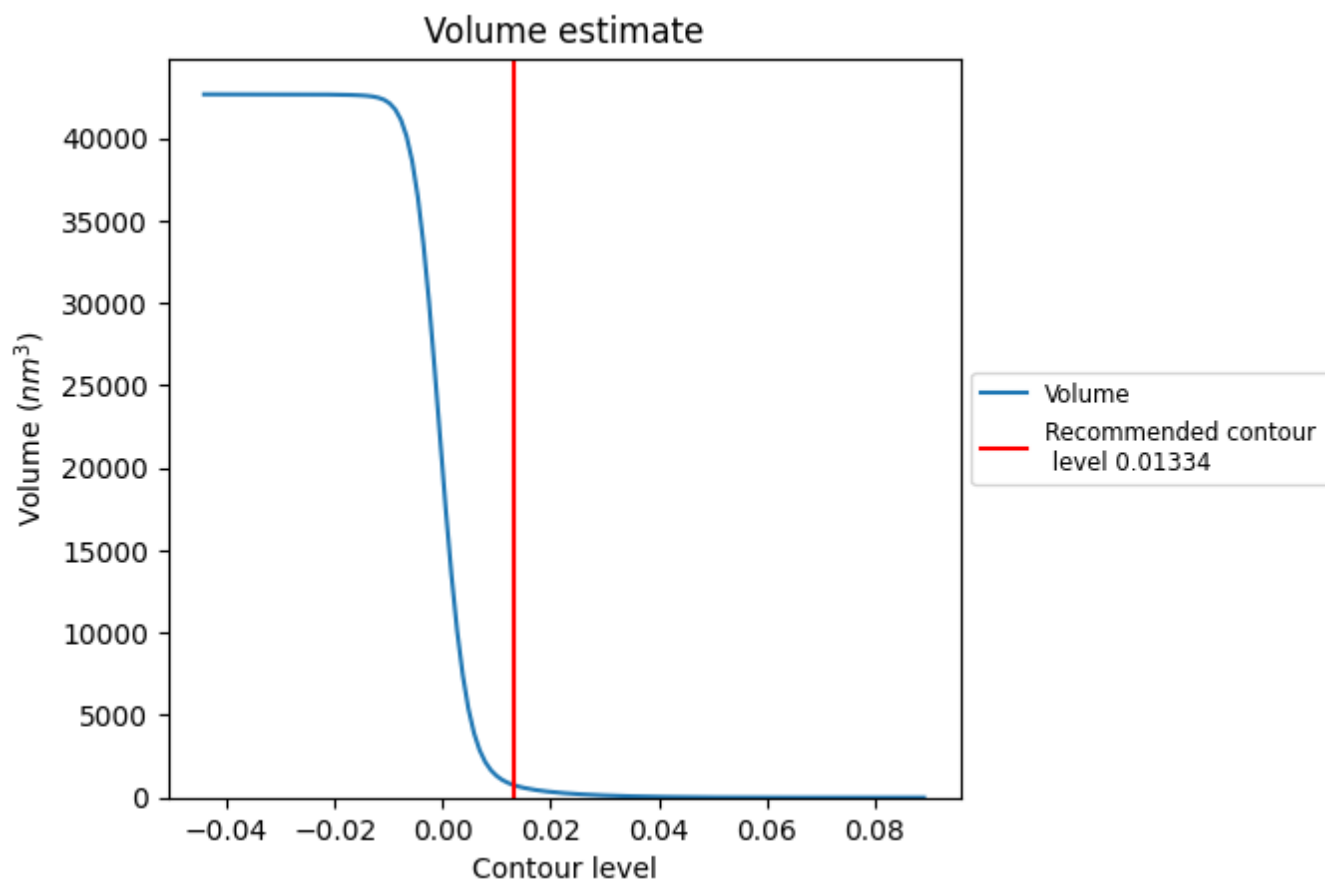
This section contains the results of statistical analysis of the map.

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.

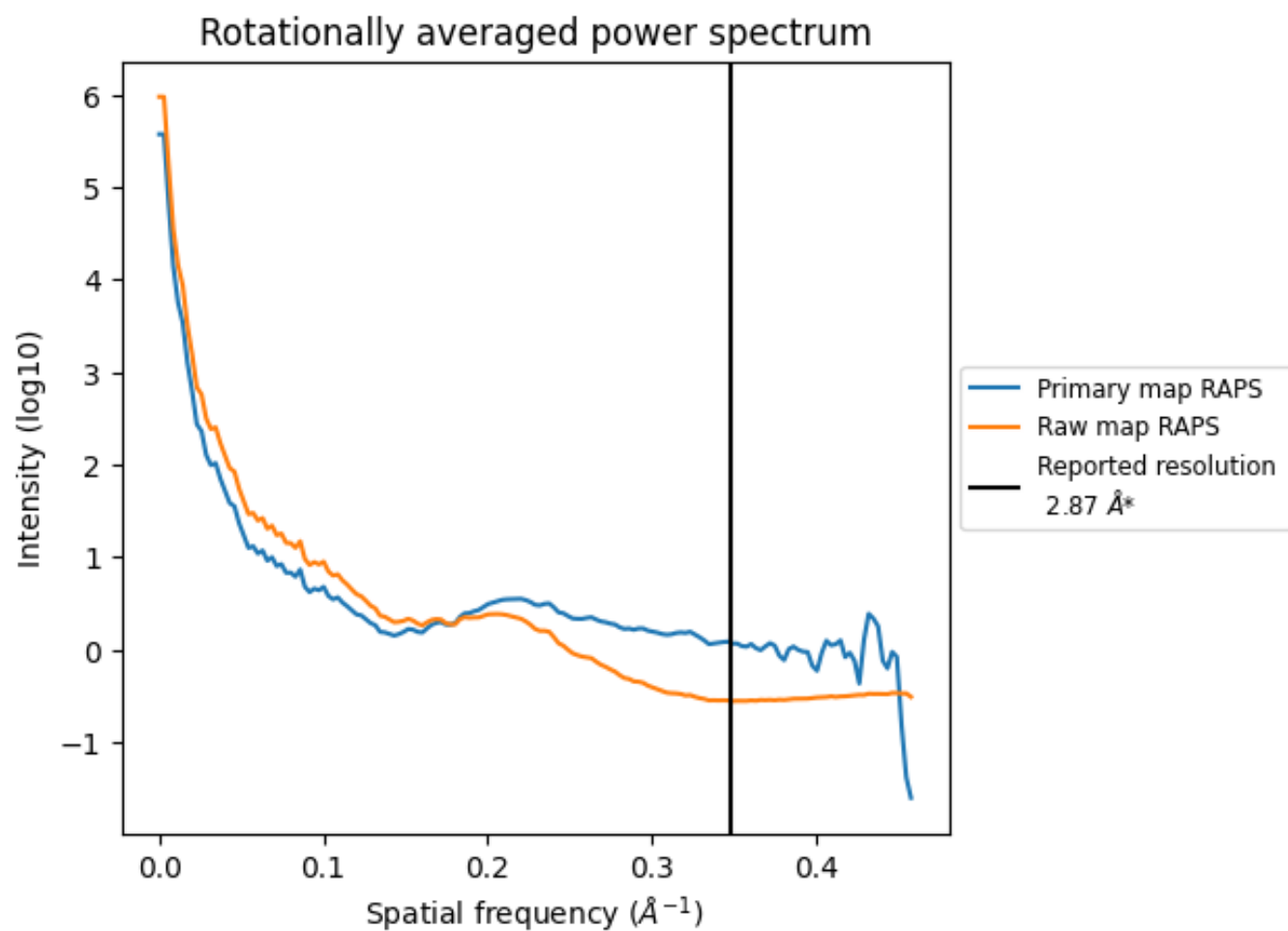
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 741 nm³; this corresponds to an approximate mass of 670 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 ⓘ

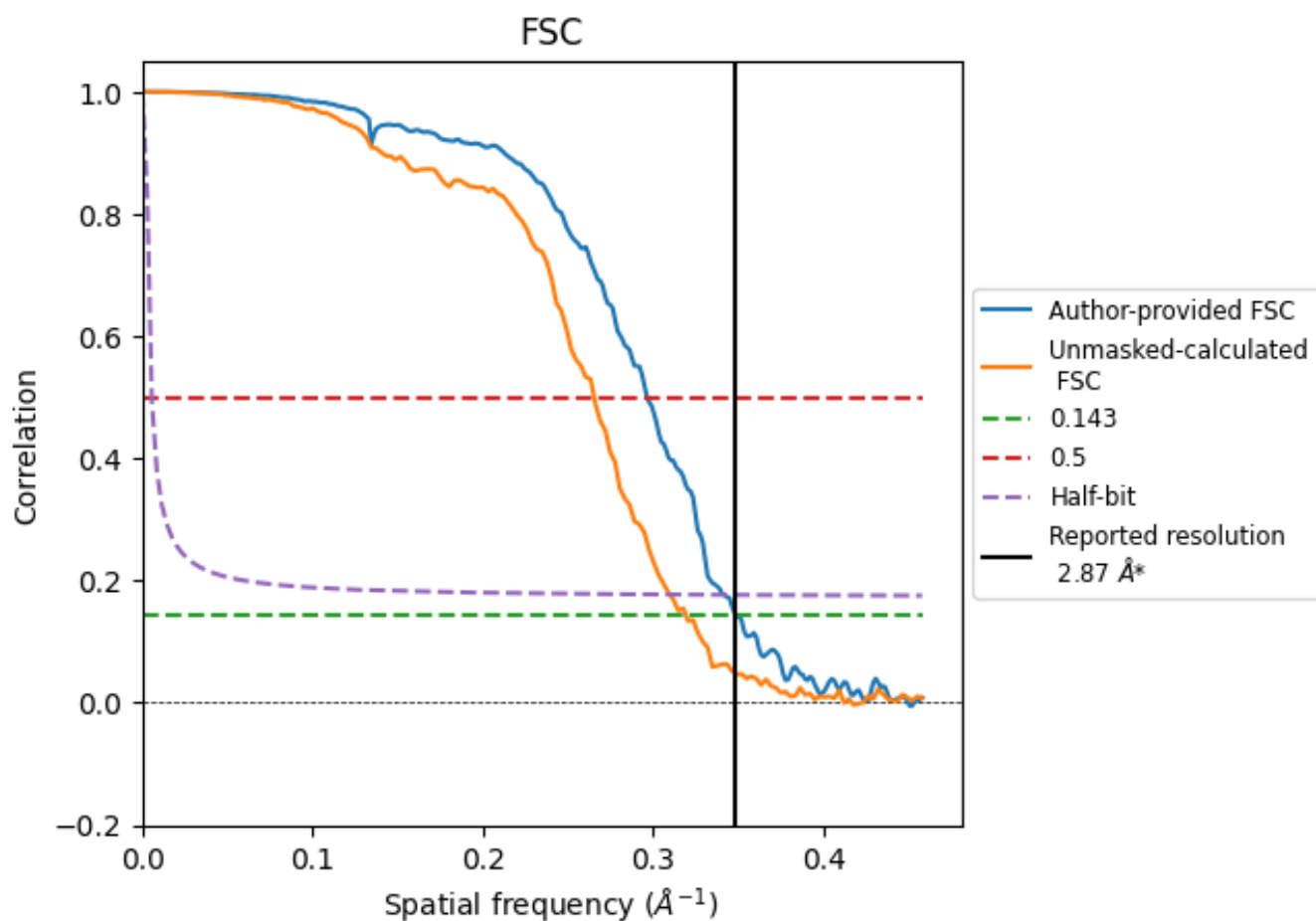


*Reported resolution corresponds to spatial frequency of 0.348 Å⁻¹

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 0.348 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

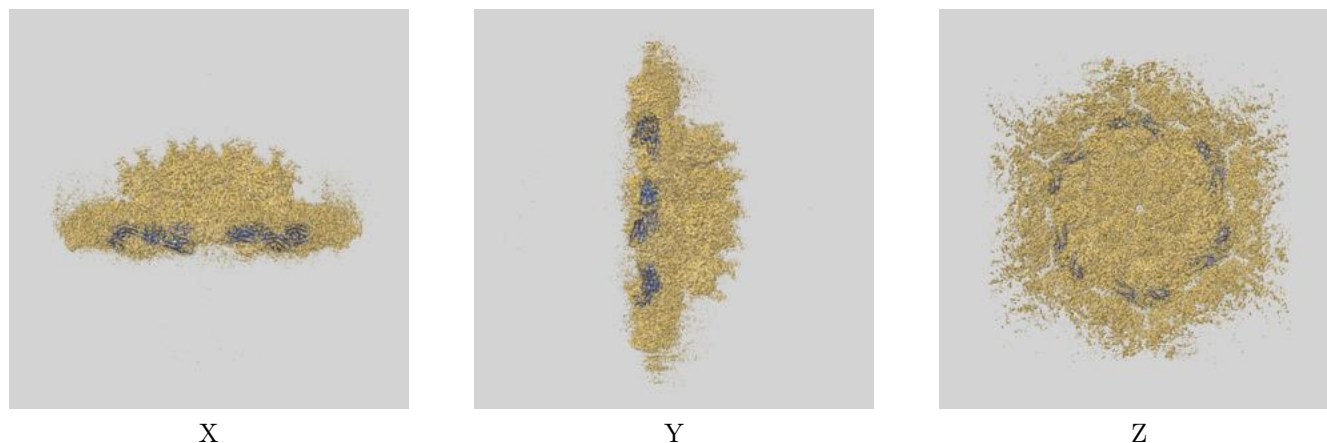
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.87	-	-
Author-provided FSC curve	2.87	3.37	2.92
Unmasked-calculated*	3.13	3.77	3.23

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

9 Map-model fit [i](#)

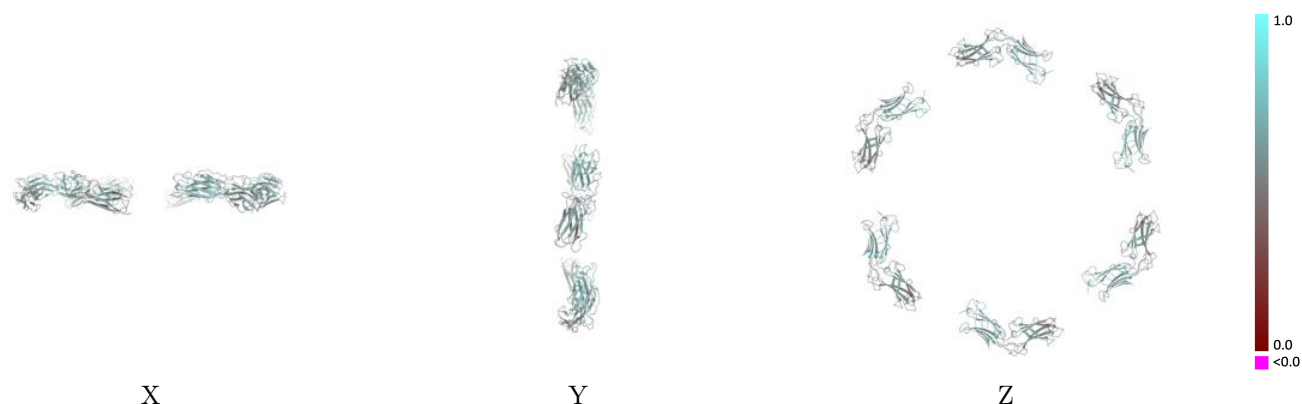
This section contains information regarding the fit between EMDB map EMD-16482 and PDB model 8C8K. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.01334 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](#)



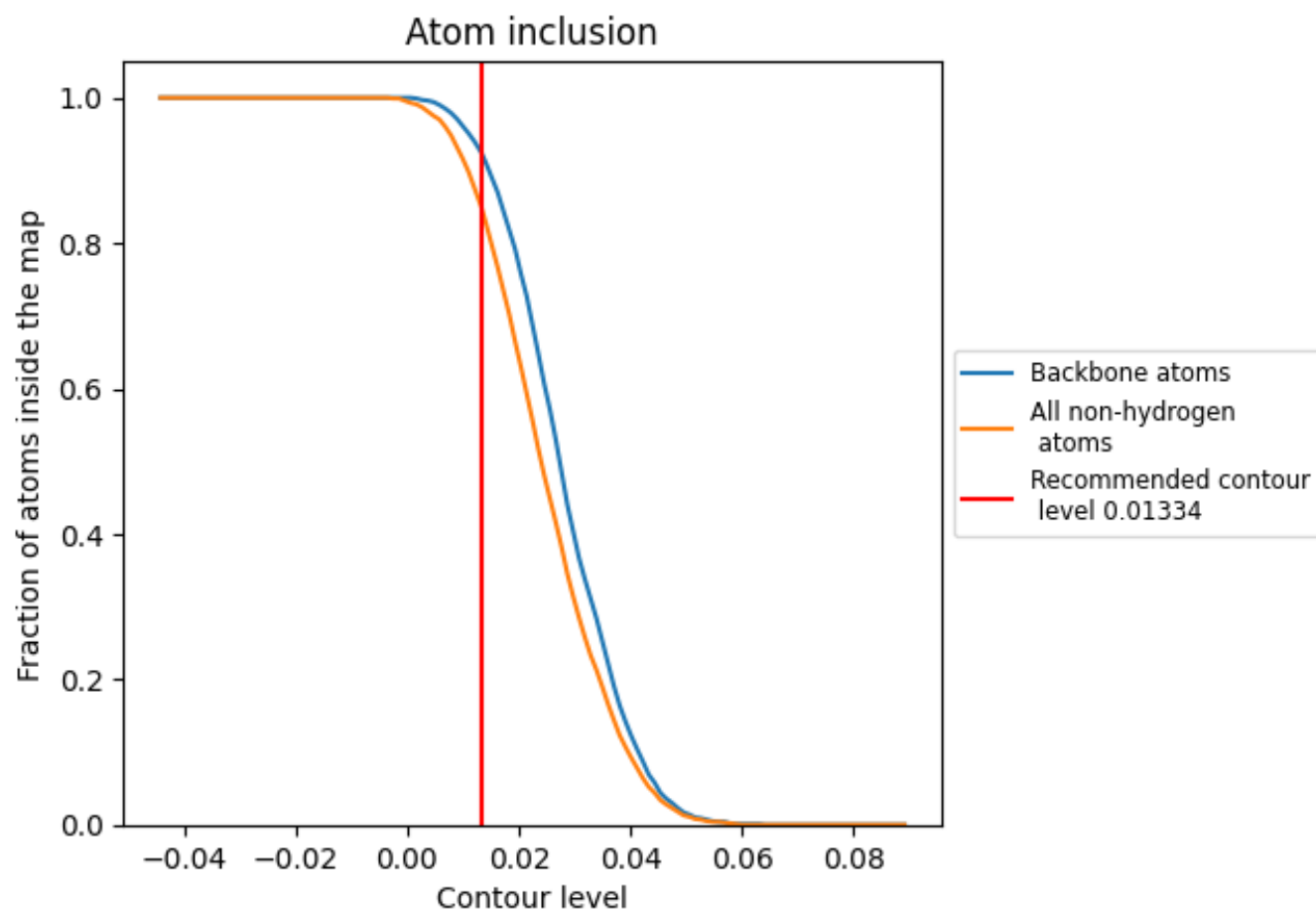
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01334).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% 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 (0.01334) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8490	0.5430
A	0.8540	0.5430
B	0.8470	0.5420
C	0.8460	0.5450
D	0.8520	0.5430
E	0.8480	0.5430
F	0.8460	0.5430

