



Full wwPDB EM Validation Report ⓘ

Aug 31, 2026 – 03:45 PM EDT

PDB ID : 9NJS / pdb_00009njs
EMDB ID : EMD-49489
Title : human polycystin-2 with clinical variant D511V
Authors : Wang, Q.; Cao, E.
Deposited on : 2025-02-27
Resolution : 3.10 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:

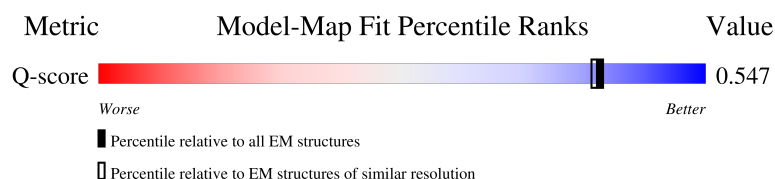
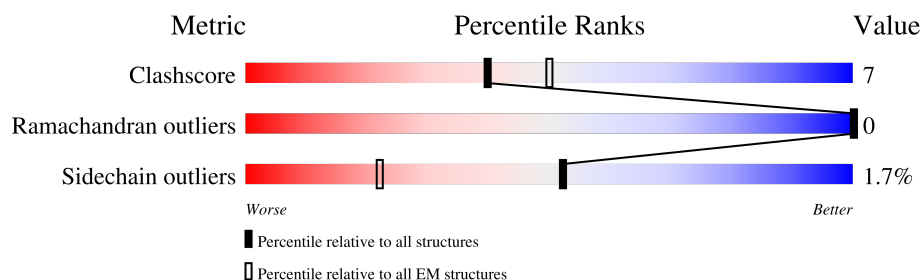
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 3.10 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	14724 (2.60 - 3.60)

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	745	
1	b	745	
1	c	745	
1	d	745	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	b	802	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15636 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 Polycystin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	479	Total	C	N	O	S	0	0
			3867	2562	615	670	20		
1	b	479	Total	C	N	O	S	0	0
			3867	2562	615	670	20		
1	c	479	Total	C	N	O	S	0	0
			3867	2562	615	670	20		
1	d	479	Total	C	N	O	S	0	0
			3867	2562	615	670	20		

There are 24 discrepancies between the modelled and reference sequences:

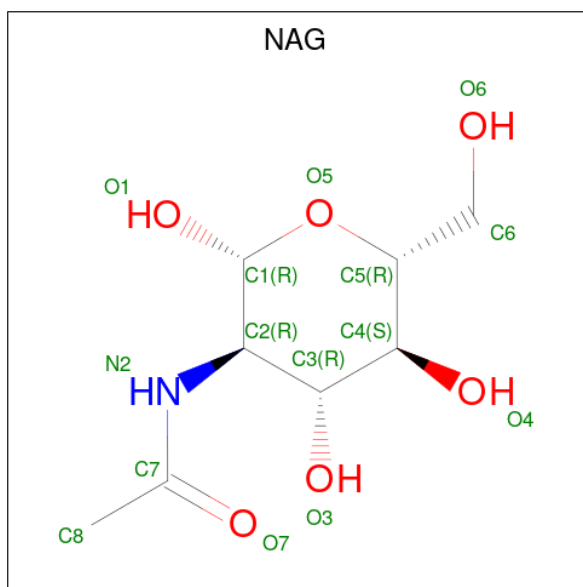
Chain	Residue	Modelled	Actual	Comment	Reference
a	48	GLY	-	expression tag	UNP Q13563
a	49	ALA	-	expression tag	UNP Q13563
a	50	MET	-	expression tag	UNP Q13563
a	51	GLY	-	expression tag	UNP Q13563
a	52	SER	-	expression tag	UNP Q13563
a	511	VAL	ASP	engineered mutation	UNP Q13563
b	48	GLY	-	expression tag	UNP Q13563
b	49	ALA	-	expression tag	UNP Q13563
b	50	MET	-	expression tag	UNP Q13563
b	51	GLY	-	expression tag	UNP Q13563
b	52	SER	-	expression tag	UNP Q13563
b	511	VAL	ASP	engineered mutation	UNP Q13563
c	48	GLY	-	expression tag	UNP Q13563
c	49	ALA	-	expression tag	UNP Q13563
c	50	MET	-	expression tag	UNP Q13563
c	51	GLY	-	expression tag	UNP Q13563
c	52	SER	-	expression tag	UNP Q13563
c	511	VAL	ASP	engineered mutation	UNP Q13563
d	48	GLY	-	expression tag	UNP Q13563
d	49	ALA	-	expression tag	UNP Q13563
d	50	MET	-	expression tag	UNP Q13563
d	51	GLY	-	expression tag	UNP Q13563

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
d	52	SER	-	expression tag	UNP Q13563
d	511	VAL	ASP	engineered mutation	UNP Q13563

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
2	a	1	Total	C	N	O	0
			14	8	1	5	
2	a	1	Total	C	N	O	0
			14	8	1	5	
2	a	1	Total	C	N	O	0
			14	8	1	5	
2	b	1	Total	C	N	O	0
			14	8	1	5	
2	b	1	Total	C	N	O	0
			14	8	1	5	
2	b	1	Total	C	N	O	0
			14	8	1	5	
2	c	1	Total	C	N	O	0
			14	8	1	5	
2	c	1	Total	C	N	O	0
			14	8	1	5	
2	c	1	Total	C	N	O	0
			14	8	1	5	
2	d	1	Total	C	N	O	0
			14	8	1	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
2	d	1	Total	C	N	O	0
			14	8	1	5	
2	d	1	Total	C	N	O	0
			14	8	1	5	

Chain d:

GLY
ALA
GLY
MET
GLY
VAL
SER
GLU
TLE
GLU
MET
ASP
VAL
GLN
GLN
TRP
ARG
TLE
ARG
GLN
GLN
ALA
ALA
ARG
ASP
PRO
PRO
GLY
ALA
ALA
GLY
VAL
SER
ALA
ALA
SER
GLY
PRO
GLY
SER
PRO
LEU
GLY
SER
GLY
CYS
GLY
SER
ARG
GLN
ALA
TRP
GLY
SER
ARG
ASP
ASN
PRO
GLY
PHE
ARG
GLU
GLU
ALA
GLU
GLU
GLU
GLU
VAL
GLU
GLY
PRO

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

VAL
GLY
GLY
ASP
PRO
LEU
HIS
ARG
HIS
LEU
TRP
ARG
PRO
LEU
GLU
GLY
GLN
PRO
PRO
ARG
ARG
VAL
ALA
ALA
TRP
GLY
VAL
ARG
GLY
LEU
VAL
ARG
LEU
GLY
LEU
ARG
GLY
ARG
GLY
LEU
GLY
THR
ARG
LEU
MET
GLU
GLY
SER
SER
THR
ASN
ARG
GLU
LYS
TYR
L217
K218
S219
V220
L221
R222
Y227
L228
L231

L234
T238
M241
Y248
R251
M252
Q255
E266
K281
F282
T283
L287
S298
N299
Q300
T301
E302
S307
F308
I309
N313
L314
V326
R327
N328
G329
S330
I333
R338
D346
S349
S352
P357
N362
G363
W366
I367
I383

Y429
N434
E444
G449
Q458
T468
F471
F485
V489
E490
L493
E494
I495
R496
H501
R504
L510
V511
V512
V519
I524
L535
L536
A552
I561
V566
F567
W570
I571
F576
S584
M590
K595
F600

L609
Q613
L614
F619
V623
F626
G657
F664
M668
I671
L672
L673
M674
F676
L677
A678
I679
T683
K695
ALA
GLU
MET
GLU
LEU
SER
ASP
LEU
ILE
ILE
PHE
THR
LYS
TYR
ASP
GLN
ASP
GLY
ASP
GLN
GLU
LEU
THR
HIS
GLU
HIS
GLN
GLN
MET
ARG
ASN
THR
VAL
ASP
ASP
ILE

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

ARG
GLU
ASP
LEU
ASP
LEU
ASP

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	54727	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	59	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	15.822	Depositor
Minimum map value	-11.659	Depositor
Average map value	-0.012	Depositor
Map value standard deviation	0.347	Depositor
Recommended contour level	1.32	Depositor
Map size (Å)	356.04, 356.04, 356.04	wwPDB
Map dimensions	258, 258, 258	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.38, 1.38, 1.38	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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	0.30	0/3971	0.40	0/5400
1	b	0.38	5/3971 (0.1%)	0.43	0/5400
1	c	0.32	2/3971 (0.1%)	0.45	0/5400
1	d	0.36	2/3971 (0.1%)	0.49	0/5400
All	All	0.34	9/15884 (0.1%)	0.44	0/21600

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	b	334	PRO	C-N	6.73	1.43	1.33
1	c	220	VAL	C-N	6.54	1.42	1.33
1	d	217	LEU	C-N	6.43	1.42	1.33
1	c	224	LEU	C-N	5.86	1.41	1.33
1	d	494	GLU	C-N	-5.50	1.27	1.33
1	b	326	VAL	C-N	-5.35	1.25	1.33
1	b	325	ARG	C-N	-5.28	1.26	1.33
1	b	328	ASN	C-N	-5.04	1.26	1.33
1	b	329	GLY	C-N	5.01	1.40	1.33

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	3867	0	3782	55	0
1	b	3867	0	3783	69	0
1	c	3867	0	3782	55	0
1	d	3867	0	3781	57	0
2	a	42	0	39	1	0
2	b	42	0	39	10	0
2	c	42	0	39	2	0
2	d	42	0	39	7	0
All	All	15636	0	15284	218	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 7.

All (218) 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:d:362:ASN:HB2	2:d:802:NAG:C1	1.47	1.43
1:d:362:ASN:CB	2:d:802:NAG:C1	1.98	1.40
1:b:362:ASN:ND2	2:b:802:NAG:C1	1.93	1.29
1:b:362:ASN:HD21	2:b:802:NAG:C1	1.47	1.28
1:a:375:ASN:ND2	2:a:803:NAG:O5	1.61	1.15
1:b:362:ASN:CG	2:b:802:NAG:C1	2.25	1.10
1:b:362:ASN:ND2	2:b:802:NAG:N2	2.08	0.99
1:b:362:ASN:HD21	2:b:802:NAG:C2	1.76	0.98
1:b:362:ASN:OD1	2:b:802:NAG:C1	2.17	0.92
1:b:362:ASN:ND2	2:b:802:NAG:C2	2.35	0.88
1:d:362:ASN:CG	2:d:802:NAG:C1	2.17	0.87
1:b:362:ASN:HD22	2:b:802:NAG:C7	1.89	0.85
1:a:670:PHE:O	1:a:674:ASN:ND2	2.10	0.83
1:c:674:ASN:HA	1:c:677:LEU:HD13	1.59	0.82
1:b:362:ASN:ND2	2:b:802:NAG:C7	2.42	0.82
1:d:362:ASN:HB2	2:d:802:NAG:O5	1.78	0.82
1:a:677:LEU:HD23	1:b:677:LEU:HD11	1.68	0.75
1:b:670:PHE:O	1:b:674:ASN:ND2	2.15	0.74
1:d:600:PHE:CE1	1:d:675:MET:HG2	2.21	0.74
1:a:600:PHE:CE1	1:a:675:MET:HG2	2.23	0.74
1:d:227:TYR:CD2	1:d:576:PHE:HE2	2.08	0.72
1:d:241:MET:HE3	1:d:241:MET:HA	1.72	0.71
1:c:222:ARG:O	1:c:226:THR:HG22	1.91	0.70
1:a:241:MET:HE3	1:a:241:MET:HA	1.74	0.69
1:b:241:MET:HA	1:b:241:MET:HE3	1.73	0.69
1:c:241:MET:HE3	1:c:241:MET:HA	1.74	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:327:ARG:NH2	1:b:352:SER:HA	2.09	0.67
1:b:375:ASN:OD1	2:b:803:NAG:N2	2.27	0.67
1:b:330:SER:HB3	1:b:346:ASP:HB2	1.75	0.67
1:b:600:PHE:CE1	1:b:675:MET:HG2	2.31	0.65
1:a:600:PHE:CZ	1:a:675:MET:HG2	2.31	0.65
1:d:362:ASN:OD1	1:d:363:GLY:N	2.29	0.65
1:c:248:TYR:O	1:c:252:MET:HG2	1.98	0.64
1:a:675:MET:HE2	1:b:590:MET:HE2	1.80	0.63
1:c:600:PHE:CE1	1:c:675:MET:HG2	2.33	0.63
1:b:359:GLY:O	1:b:361:ARG:NH1	2.32	0.62
1:d:673:LEU:O	1:d:677:LEU:HD13	1.99	0.62
1:c:675:MET:HE2	1:d:590:MET:HE2	1.80	0.62
1:b:327:ARG:HH21	1:b:352:SER:HA	1.65	0.62
1:d:600:PHE:CZ	1:d:675:MET:HG2	2.34	0.61
1:b:335:GLN:HA	1:b:338:ARG:HG3	1.81	0.61
1:d:217:LEU:HA	1:d:220:VAL:HB	1.82	0.61
1:d:248:TYR:O	1:d:252:MET:HG2	2.01	0.61
1:b:248:TYR:O	1:b:252:MET:HG2	2.01	0.59
1:c:343:GLU:OE2	2:c:801:NAG:C1	2.50	0.59
1:c:462:LEU:HD23	1:c:535:LEU:HD12	1.84	0.59
1:d:330:SER:HB3	1:d:346:ASP:HB2	1.83	0.59
1:a:248:TYR:O	1:a:252:MET:HG2	2.03	0.58
1:a:590:MET:HE2	1:d:675:MET:HE2	1.86	0.57
1:b:330:SER:CB	1:b:346:ASP:HB2	2.35	0.57
1:c:585:GLN:HG2	1:c:691:LEU:HD12	1.86	0.56
1:c:671:ILE:HG22	1:c:672:LEU:HD23	1.86	0.56
1:a:585:GLN:HG2	1:a:691:LEU:HD12	1.87	0.56
1:a:468:THR:HA	1:a:471:PHE:HD2	1.69	0.56
1:c:309:ILE:N	1:c:313:ASN:O	2.39	0.56
1:a:668:MET:HE3	1:a:672:LEU:HD12	1.86	0.56
1:d:362:ASN:HB3	2:d:802:NAG:C1	2.22	0.56
1:a:330:SER:HB3	1:a:346:ASP:HB2	1.88	0.56
1:d:234:LEU:O	1:d:238:THR:HG23	2.06	0.56
1:d:327:ARG:HH21	1:d:352:SER:HA	1.71	0.56
1:a:674:ASN:OD1	1:b:677:LEU:HB2	2.06	0.56
1:c:234:LEU:O	1:c:238:THR:HG23	2.06	0.56
1:c:343:GLU:OE1	1:c:343:GLU:HA	2.07	0.55
1:a:309:ILE:N	1:a:313:ASN:O	2.41	0.54
1:b:330:SER:HB3	1:b:346:ASP:CB	2.38	0.54
1:d:664:PHE:O	1:d:668:MET:HB2	2.07	0.54
1:b:309:ILE:N	1:b:313:ASN:O	2.41	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:333:ILE:O	1:d:338:ARG:NH1	2.41	0.54
1:b:609:LEU:O	1:b:613:GLN:HG3	2.08	0.53
1:a:222:ARG:O	1:a:226:THR:HG22	2.08	0.53
1:c:429:TYR:OH	1:c:434:ASN:OD1	2.25	0.53
1:c:664:PHE:O	1:c:668:MET:HB2	2.09	0.53
1:d:668:MET:HE3	1:d:672:LEU:HD12	1.91	0.53
1:a:327:ARG:HH21	1:a:352:SER:HA	1.73	0.53
1:a:664:PHE:O	1:a:668:MET:HB2	2.09	0.52
1:c:600:PHE:CZ	1:c:675:MET:HG2	2.45	0.52
1:c:670:PHE:O	1:c:674:ASN:ND2	2.36	0.52
1:c:668:MET:HE3	1:c:672:LEU:HD12	1.91	0.52
1:d:266:GLU:OE1	1:d:281:LYS:NZ	2.40	0.52
1:d:609:LEU:O	1:d:613:GLN:HG3	2.10	0.51
1:c:434:ASN:HD21	1:c:463:ILE:HB	1.76	0.51
1:c:609:LEU:O	1:c:613:GLN:HG3	2.11	0.51
1:c:251:ARG:O	1:c:255:GLN:HG3	2.10	0.50
1:c:327:ARG:HH21	1:c:352:SER:HA	1.76	0.50
1:a:458:GLN:HG2	1:a:552:ALA:HB1	1.94	0.50
1:a:668:MET:CE	1:a:672:LEU:HD12	2.41	0.50
1:b:375:ASN:OD1	1:b:375:ASN:N	2.45	0.50
1:a:609:LEU:O	1:a:613:GLN:HG3	2.11	0.50
1:b:234:LEU:O	1:b:238:THR:HG23	2.12	0.50
1:c:283:THR:O	1:c:287:LEU:HB3	2.12	0.50
1:d:352:SER:O	1:d:352:SER:OG	2.30	0.50
1:a:234:LEU:O	1:a:238:THR:HG23	2.11	0.49
1:b:434:ASN:ND2	1:b:463:ILE:O	2.45	0.49
1:d:309:ILE:N	1:d:313:ASN:O	2.43	0.49
1:b:283:THR:O	1:b:287:LEU:HB3	2.11	0.49
1:d:251:ARG:O	1:d:255:GLN:HG3	2.12	0.49
1:d:458:GLN:HG2	1:d:552:ALA:HB1	1.93	0.49
1:c:231:LEU:HD21	1:c:570:TRP:CZ3	2.48	0.49
1:b:585:GLN:HG2	1:b:691:LEU:HD12	1.94	0.49
1:d:524:ILE:HD12	1:d:561:ILE:HD12	1.95	0.49
1:c:345:TYR:O	1:c:420:ARG:NH2	2.45	0.49
1:d:671:ILE:HG22	1:d:672:LEU:HD23	1.93	0.49
1:a:429:TYR:OH	1:a:434:ASN:OD1	2.27	0.48
1:c:458:GLN:HG2	1:c:552:ALA:HB1	1.94	0.48
1:d:429:TYR:OH	1:d:434:ASN:OD1	2.26	0.48
1:a:490:GLU:O	1:a:493:LEU:HG	2.14	0.48
1:c:289:ASP:OD1	1:c:399:ARG:NH2	2.46	0.48
1:a:325:ARG:HH12	1:a:416:ASP:HB2	1.79	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:327:ARG:NH2	1:c:352:SER:HA	2.28	0.48
1:b:490:GLU:O	1:b:493:LEU:HG	2.14	0.47
1:b:222:ARG:O	1:b:226:THR:HG22	2.15	0.47
1:c:490:GLU:O	1:c:493:LEU:HG	2.14	0.47
1:d:283:THR:O	1:d:287:LEU:HB3	2.14	0.47
1:a:590:MET:CE	1:d:675:MET:HE2	2.44	0.47
1:a:614:LEU:HD12	1:b:567:PHE:CG	2.48	0.47
1:d:623:VAL:HG21	1:d:626:PHE:HD2	1.80	0.47
1:d:668:MET:CE	1:d:672:LEU:HD12	2.43	0.47
1:a:283:THR:O	1:a:287:LEU:HB3	2.14	0.47
1:b:231:LEU:HD21	1:b:570:TRP:CZ3	2.50	0.47
1:b:458:GLN:HG2	1:b:552:ALA:HB1	1.95	0.47
1:b:604:PHE:HD1	1:b:672:LEU:HB3	1.80	0.47
1:a:231:LEU:HD21	1:a:570:TRP:CZ3	2.50	0.47
1:c:325:ARG:HH12	1:c:416:ASP:HB2	1.80	0.47
1:d:357:PRO:HB3	1:d:367:ILE:HD13	1.97	0.47
1:d:679:ILE:O	1:d:683:THR:HG22	2.15	0.47
1:b:679:ILE:O	1:b:683:THR:HG22	2.15	0.46
1:d:595:LYS:HA	1:d:595:LYS:HD3	1.60	0.46
1:d:231:LEU:HD21	1:d:570:TRP:CZ3	2.50	0.46
1:c:668:MET:CE	1:c:672:LEU:HD12	2.45	0.46
1:a:529:THR:O	1:a:529:THR:HG22	2.16	0.46
1:b:251:ARG:O	1:b:255:GLN:HG3	2.16	0.46
1:b:333:ILE:CG1	1:b:344:CYS:SG	3.04	0.46
1:c:524:ILE:HD12	1:c:561:ILE:HD12	1.97	0.46
1:a:327:ARG:NH2	1:a:352:SER:HA	2.30	0.46
1:b:510:LEU:HD23	1:b:510:LEU:HA	1.80	0.46
1:c:222:ARG:NH2	1:c:486:TYR:OH	2.41	0.46
1:c:595:LYS:HA	1:c:595:LYS:HD3	1.61	0.46
1:a:671:ILE:HG22	1:a:672:LEU:HD23	1.98	0.46
1:d:328:ASN:OD1	2:d:801:NAG:O5	2.34	0.46
1:a:328:ASN:O	1:a:330:SER:N	2.49	0.45
1:c:614:LEU:HD12	1:d:567:PHE:CG	2.51	0.45
1:a:251:ARG:O	1:a:255:GLN:HG3	2.15	0.45
1:c:536:LEU:HD12	1:c:536:LEU:H	1.81	0.45
1:a:567:PHE:CG	1:d:614:LEU:HD12	2.51	0.45
1:a:335:GLN:HA	1:a:338:ARG:HG3	1.98	0.45
1:b:266:GLU:OE2	1:b:281:LYS:NZ	2.45	0.45
1:d:468:THR:HA	1:d:471:PHE:HD2	1.81	0.45
1:c:618:VAL:HG12	1:c:619:PHE:HD1	1.82	0.45
1:d:535:LEU:HD23	1:d:536:LEU:HD13	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:614:LEU:HD12	1:c:567:PHE:CG	2.51	0.44
1:c:308:PHE:CE1	1:c:314:LEU:HB2	2.52	0.44
1:d:366:TRP:HE1	2:d:802:NAG:H82	1.82	0.44
1:a:239:TYR:OH	1:d:613:GLN:OE1	2.34	0.44
1:a:476:CYS:O	1:a:479:ILE:HG22	2.18	0.44
1:b:675:MET:HE2	1:c:590:MET:HE2	1.99	0.44
1:c:377:SER:OG	1:c:378:SER:N	2.51	0.44
1:a:638:ARG:HB3	1:a:643:ASP:HB3	2.00	0.43
1:b:308:PHE:CE1	1:b:314:LEU:HB2	2.53	0.43
1:b:510:LEU:HD11	1:b:571:ILE:HG22	2.00	0.43
1:b:623:VAL:HG21	1:b:626:PHE:HD2	1.82	0.43
1:c:359:GLY:O	1:c:361:ARG:NH1	2.52	0.43
1:b:595:LYS:HD3	1:b:595:LYS:HA	1.67	0.43
1:a:618:VAL:HG12	1:a:619:PHE:HD1	1.83	0.43
1:a:679:ILE:O	1:a:683:THR:HG22	2.18	0.43
1:c:679:ILE:O	1:c:683:THR:HG22	2.19	0.43
1:b:337:LEU:HD22	1:c:429:TYR:CD2	2.54	0.43
1:d:234:LEU:HG	1:d:566:VAL:HG23	2.01	0.42
1:a:475:ALA:HA	1:a:478:ILE:HG12	2.01	0.42
1:b:492:ILE:HD12	1:b:492:ILE:HA	1.93	0.42
1:a:658:PRO:HB3	1:b:634:PHE:CZ	2.54	0.42
1:b:289:ASP:OD1	1:b:399:ARG:NH2	2.45	0.42
1:b:536:LEU:H	1:b:536:LEU:HD12	1.85	0.42
1:a:308:PHE:CE1	1:a:314:LEU:HB2	2.55	0.42
1:a:648:GLU:H	1:a:648:GLU:HG2	1.63	0.42
1:b:383:ILE:HG12	1:b:444:GLU:OE1	2.20	0.42
1:a:289:ASP:OD1	1:a:399:ARG:NH2	2.50	0.42
1:c:383:ILE:HG12	1:c:444:GLU:OE1	2.20	0.42
1:c:475:ALA:HA	1:c:478:ILE:HG12	2.02	0.42
1:b:658:PRO:HB3	1:c:634:PHE:CZ	2.55	0.42
1:d:217:LEU:O	1:d:221:LEU:N	2.45	0.42
1:d:228:LEU:HD23	1:d:228:LEU:HA	1.90	0.42
1:b:232:ILE:HD12	1:b:232:ILE:HA	1.86	0.42
1:b:360:PRO:HB2	1:b:362:ASN:OD1	2.19	0.42
1:b:608:PHE:HA	1:b:668:MET:HE1	2.02	0.42
1:c:510:LEU:HD11	1:c:571:ILE:HG22	2.01	0.41
1:d:510:LEU:HD23	1:d:510:LEU:HA	1.80	0.41
1:a:595:LYS:HA	1:a:595:LYS:HD3	1.59	0.41
1:b:328:ASN:O	1:b:330:SER:N	2.52	0.41
1:c:673:LEU:O	1:c:676:PHE:HB2	2.21	0.41
1:d:308:PHE:CE1	1:d:314:LEU:HB2	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:619:PHE:HE2	1:d:657:GLY:HA2	1.85	0.41
1:b:489:VAL:O	1:b:492:ILE:HG22	2.21	0.41
1:d:510:LEU:HD11	1:d:571:ILE:HG22	2.02	0.41
1:c:532:VAL:HG23	1:c:536:LEU:HD11	2.03	0.41
1:a:264:LYS:H	1:a:264:LYS:HG2	1.54	0.41
1:b:670:PHE:CD1	1:b:670:PHE:N	2.89	0.41
1:a:252:MET:HG3	1:d:449:GLY:O	2.21	0.41
1:a:623:VAL:HG21	1:a:626:PHE:HD2	1.86	0.41
1:a:677:LEU:HD23	1:b:677:LEU:CD1	2.43	0.41
1:b:330:SER:HB2	1:b:346:ASP:H	1.86	0.41
1:b:331:CYS:SG	1:c:432:ASN:HA	2.61	0.41
1:b:345:TYR:O	1:b:420:ARG:NH2	2.53	0.41
1:c:571:ILE:HD13	1:c:571:ILE:HA	1.96	0.41
1:c:623:VAL:HG21	1:c:626:PHE:HD2	1.86	0.41
1:d:227:TYR:CG	1:d:576:PHE:HE2	2.39	0.41
1:d:383:ILE:HG12	1:d:444:GLU:OE1	2.21	0.41
1:b:600:PHE:CZ	1:b:675:MET:HG2	2.56	0.41
1:a:352:SER:O	1:a:352:SER:OG	2.30	0.40
1:a:417:ARG:HE	1:a:417:ARG:HB3	1.70	0.40
1:c:343:GLU:OE2	2:c:801:NAG:H3	2.21	0.40
1:a:593:CYS:SG	1:a:683:THR:HG21	2.62	0.40
1:b:333:ILE:HG12	1:b:344:CYS:SG	2.61	0.40
1:d:490:GLU:O	1:d:493:LEU:HG	2.21	0.40
1:b:309:ILE:HD12	1:b:428:VAL:HG11	2.03	0.40
1:c:604:PHE:HD2	1:c:672:LEU:HB3	1.86	0.40
1:a:524:ILE:HD12	1:a:561:ILE:HD12	2.03	0.40
1:b:232:ILE:O	1:b:236:ILE:HG13	2.22	0.40
1:d:227:TYR:CD2	1:d:576:PHE:CE2	2.98	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	477/745 (64%)	451 (94%)	26 (6%)	0	100	100
1	b	477/745 (64%)	452 (95%)	25 (5%)	0	100	100
1	c	477/745 (64%)	447 (94%)	30 (6%)	0	100	100
1	d	477/745 (64%)	450 (94%)	27 (6%)	0	100	100
All	All	1908/2980 (64%)	1800 (94%)	108 (6%)	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	409/649 (63%)	403 (98%)	6 (2%)	57	75
1	b	409/649 (63%)	401 (98%)	8 (2%)	48	72
1	c	409/649 (63%)	401 (98%)	8 (2%)	48	72
1	d	409/649 (63%)	403 (98%)	6 (2%)	57	75
All	All	1636/2596 (63%)	1608 (98%)	28 (2%)	52	74

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	274	SER
1	a	307	SER
1	a	326	VAL
1	a	349	SER
1	a	416	ASP
1	a	549	GLU
1	b	267	LYS
1	b	274	SER
1	b	307	SER
1	b	326	VAL
1	b	349	SER
1	b	350	VAL
1	b	416	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	b	462	LEU
1	c	307	SER
1	c	326	VAL
1	c	331	CYS
1	c	349	SER
1	c	350	VAL
1	c	510	LEU
1	c	512	VAL
1	c	549	GLU
1	d	307	SER
1	d	326	VAL
1	d	349	SER
1	d	512	VAL
1	d	519	VAL
1	d	584	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	305	ASN
1	b	255	GLN
1	b	305	ASN
1	b	362	ASN
1	b	498	HIS
1	b	557	GLN
1	c	305	ASN
1	c	557	GLN
1	d	305	ASN
1	d	550	HIS
1	d	557	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	a	803	-	14,14,15	0.40	0	17,19,21	0.37	0
2	NAG	a	801	1	14,14,15	0.46	0	17,19,21	0.70	0
2	NAG	c	802	1	14,14,15	0.31	0	17,19,21	0.63	1 (5%)
2	NAG	d	802	-	14,14,15	0.36	0	17,19,21	0.48	0
2	NAG	a	802	1	14,14,15	0.37	0	17,19,21	0.67	1 (5%)
2	NAG	d	801	1	14,14,15	0.66	0	17,19,21	0.72	0
2	NAG	c	803	1	14,14,15	0.19	0	17,19,21	0.63	0
2	NAG	b	802	-	14,14,15	0.35	0	17,19,21	0.60	0
2	NAG	b	801	1	14,14,15	0.44	0	17,19,21	0.83	1 (5%)
2	NAG	b	803	1	14,14,15	0.58	1 (7%)	17,19,21	0.65	1 (5%)
2	NAG	c	801	1	14,14,15	0.21	0	17,19,21	1.05	1 (5%)
2	NAG	d	803	1	14,14,15	0.25	0	17,19,21	0.43	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	a	803	-	-	2/6/23/26	0/1/1/1
2	NAG	a	801	1	-	2/6/23/26	0/1/1/1
2	NAG	c	802	1	-	2/6/23/26	0/1/1/1
2	NAG	d	802	-	-	0/6/23/26	0/1/1/1
2	NAG	a	802	1	-	0/6/23/26	0/1/1/1
2	NAG	d	801	1	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	c	803	1	-	4/6/23/26	0/1/1/1
2	NAG	b	802	-	-	2/6/23/26	0/1/1/1
2	NAG	b	801	1	-	2/6/23/26	0/1/1/1
2	NAG	b	803	1	-	1/6/23/26	0/1/1/1
2	NAG	c	801	1	-	4/6/23/26	0/1/1/1
2	NAG	d	803	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	803	NAG	C1-C2	2.05	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	c	801	NAG	C2-N2-C7	3.38	127.43	122.90
2	b	801	NAG	C1-O5-C5	2.90	116.08	112.19
2	a	802	NAG	C1-O5-C5	2.09	114.99	112.19
2	b	803	NAG	C1-O5-C5	2.04	114.92	112.19
2	c	802	NAG	C1-O5-C5	2.02	114.89	112.19

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	c	801	NAG	C3-C2-N2-C7
2	a	801	NAG	O5-C5-C6-O6
2	a	803	NAG	O5-C5-C6-O6
2	c	801	NAG	O5-C5-C6-O6
2	b	801	NAG	O5-C5-C6-O6
2	b	801	NAG	C4-C5-C6-O6
2	a	803	NAG	C4-C5-C6-O6
2	a	801	NAG	C4-C5-C6-O6
2	c	801	NAG	C4-C5-C6-O6
2	c	803	NAG	O5-C5-C6-O6
2	c	803	NAG	C4-C5-C6-O6
2	d	803	NAG	O5-C5-C6-O6
2	d	803	NAG	C4-C5-C6-O6
2	b	802	NAG	O5-C5-C6-O6
2	b	802	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	b	803	NAG	O5-C5-C6-O6
2	c	802	NAG	C4-C5-C6-O6
2	c	803	NAG	C3-C2-N2-C7
2	c	801	NAG	C1-C2-N2-C7
2	c	803	NAG	C1-C2-N2-C7
2	c	802	NAG	O5-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	a	803	NAG	1	0
2	d	802	NAG	6	0
2	d	801	NAG	1	0
2	b	802	NAG	9	0
2	b	803	NAG	1	0
2	c	801	NAG	2	0

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.

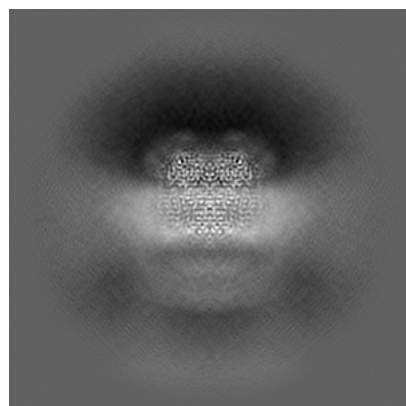
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49489. These allow visual inspection of the internal detail of the map and identification of artifacts.

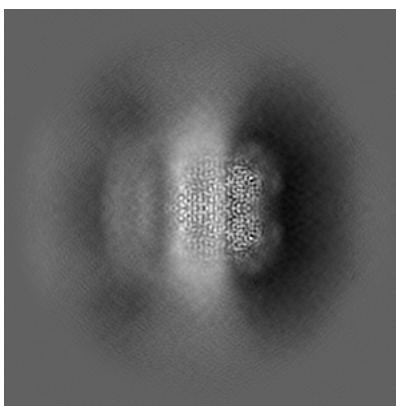
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

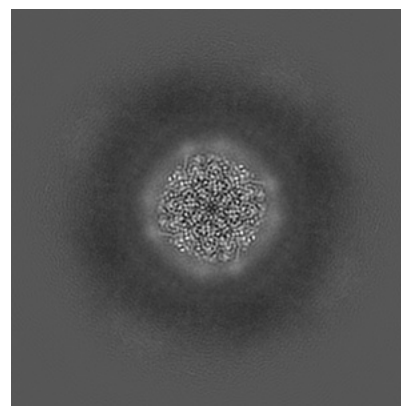
6.1.1 Primary map



X

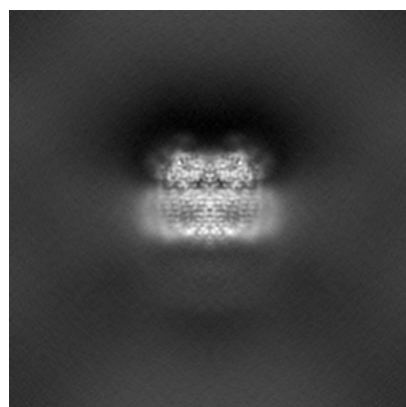


Y

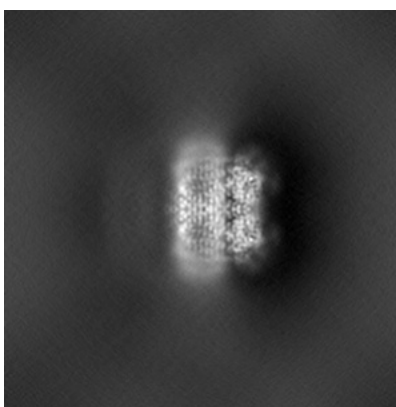


Z

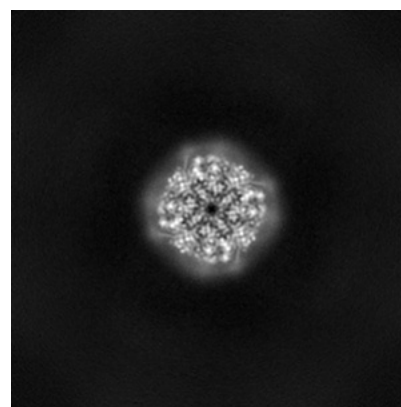
6.1.2 Raw map



X



Y

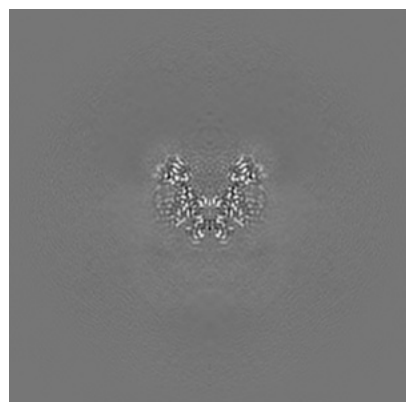


Z

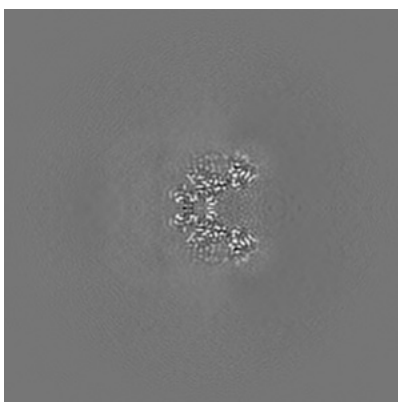
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

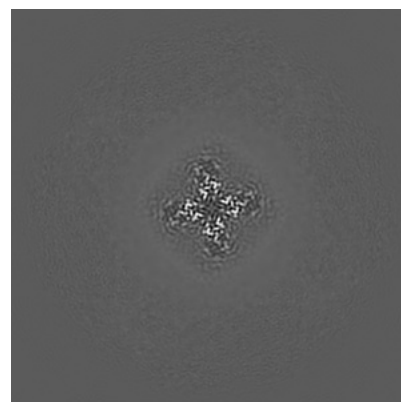
6.2.1 Primary map



X Index: 129

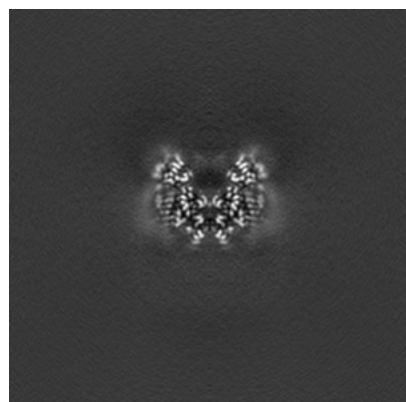


Y Index: 129

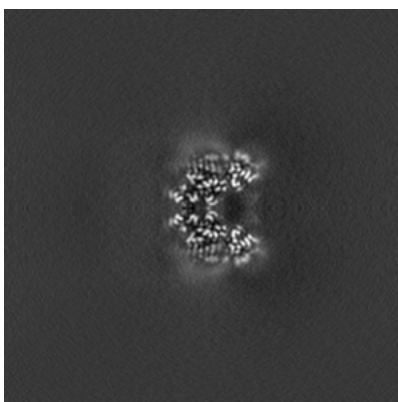


Z Index: 129

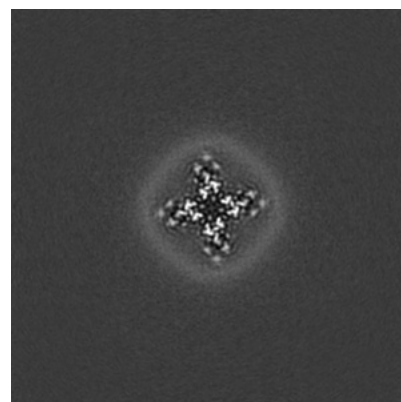
6.2.2 Raw map



X Index: 129



Y Index: 129

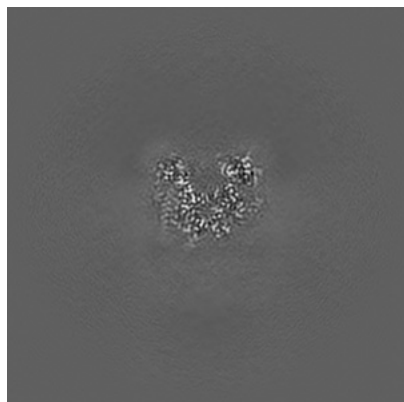


Z Index: 129

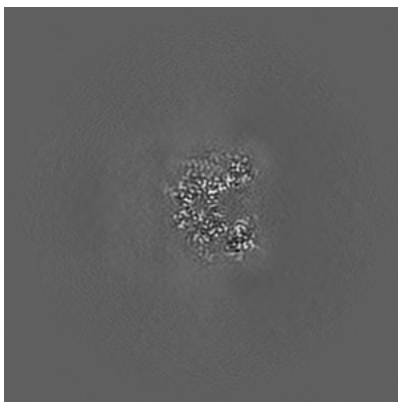
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

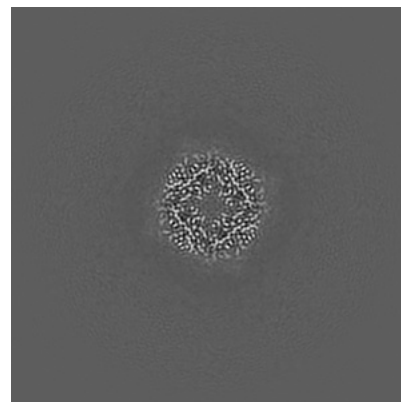
6.3.1 Primary map



X Index: 127

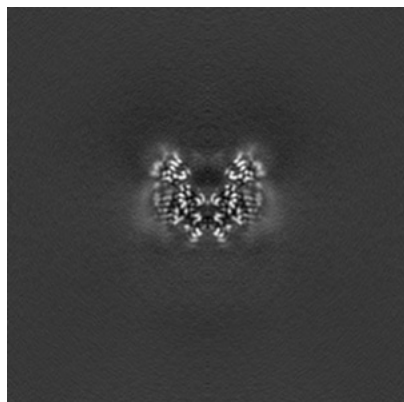


Y Index: 127

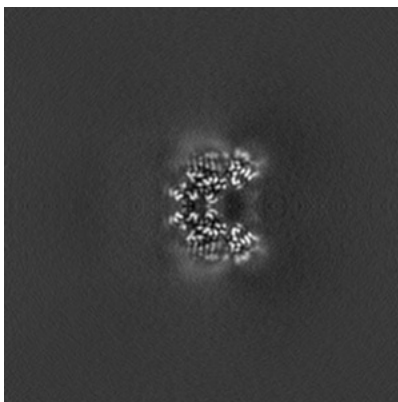


Z Index: 152

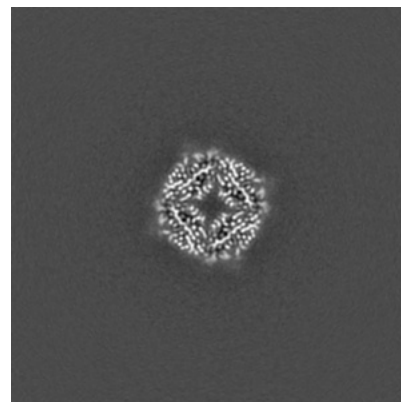
6.3.2 Raw map



X Index: 129



Y Index: 129

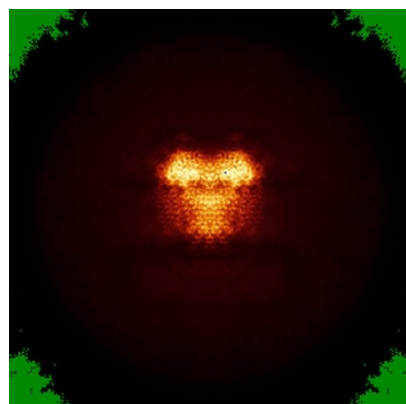


Z Index: 152

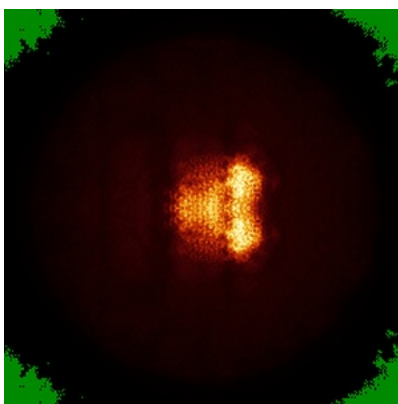
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

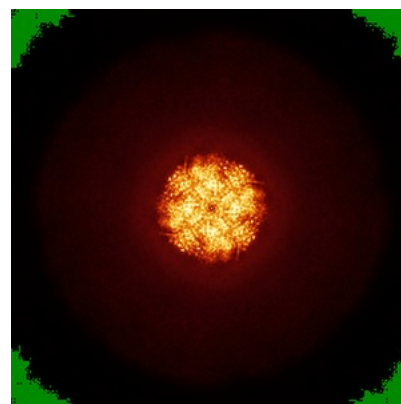
6.4.1 Primary map



X

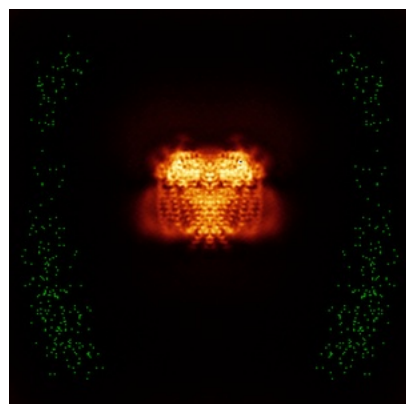


Y

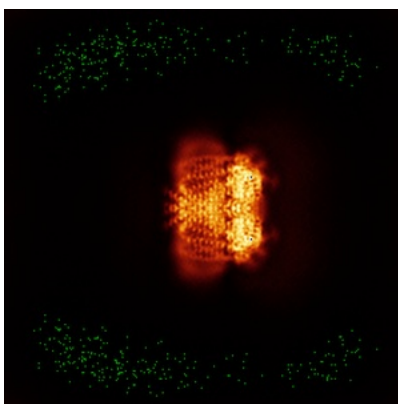


Z

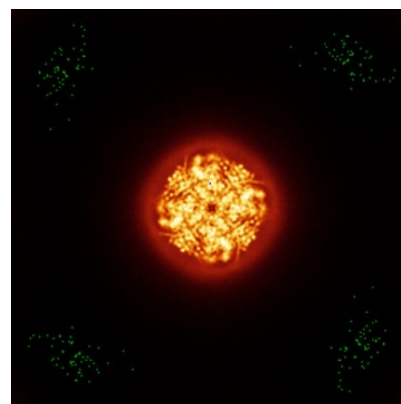
6.4.2 Raw map



X



Y

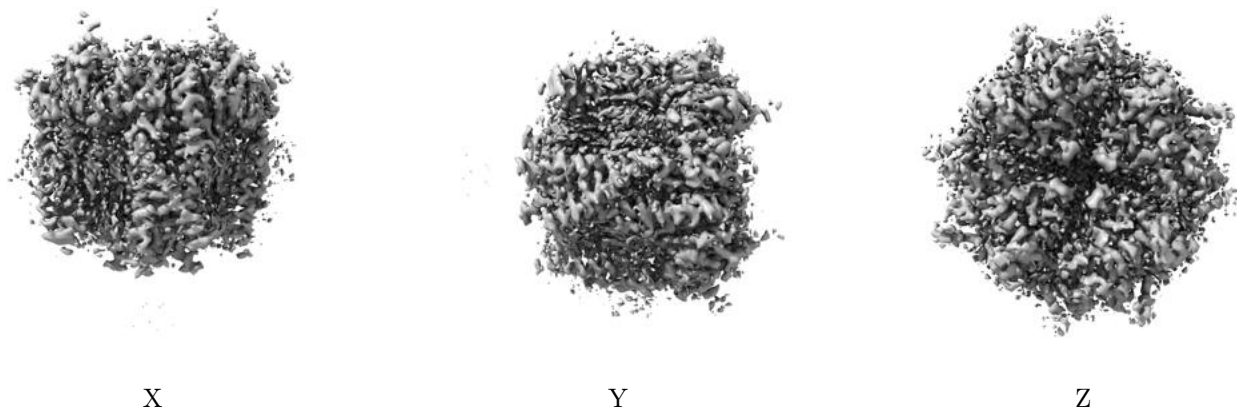


Z

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.

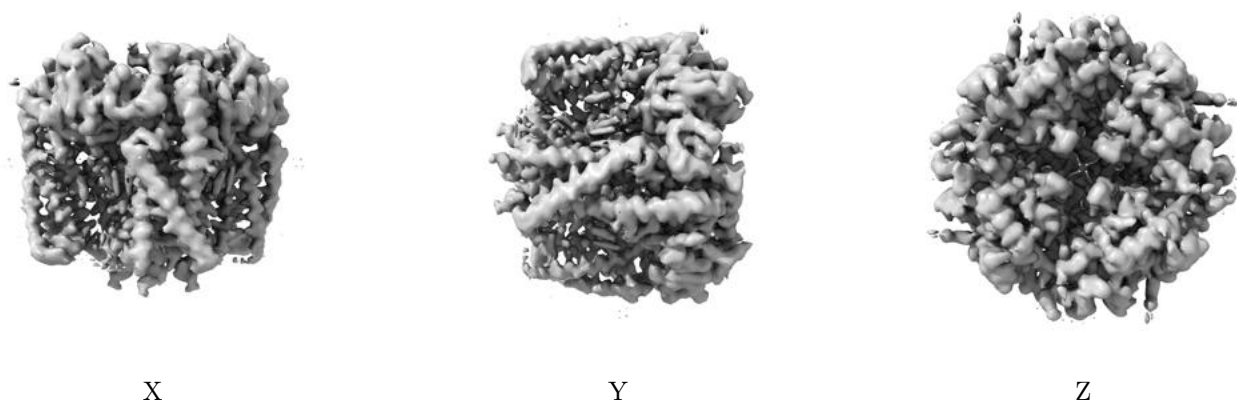
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.32. 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.

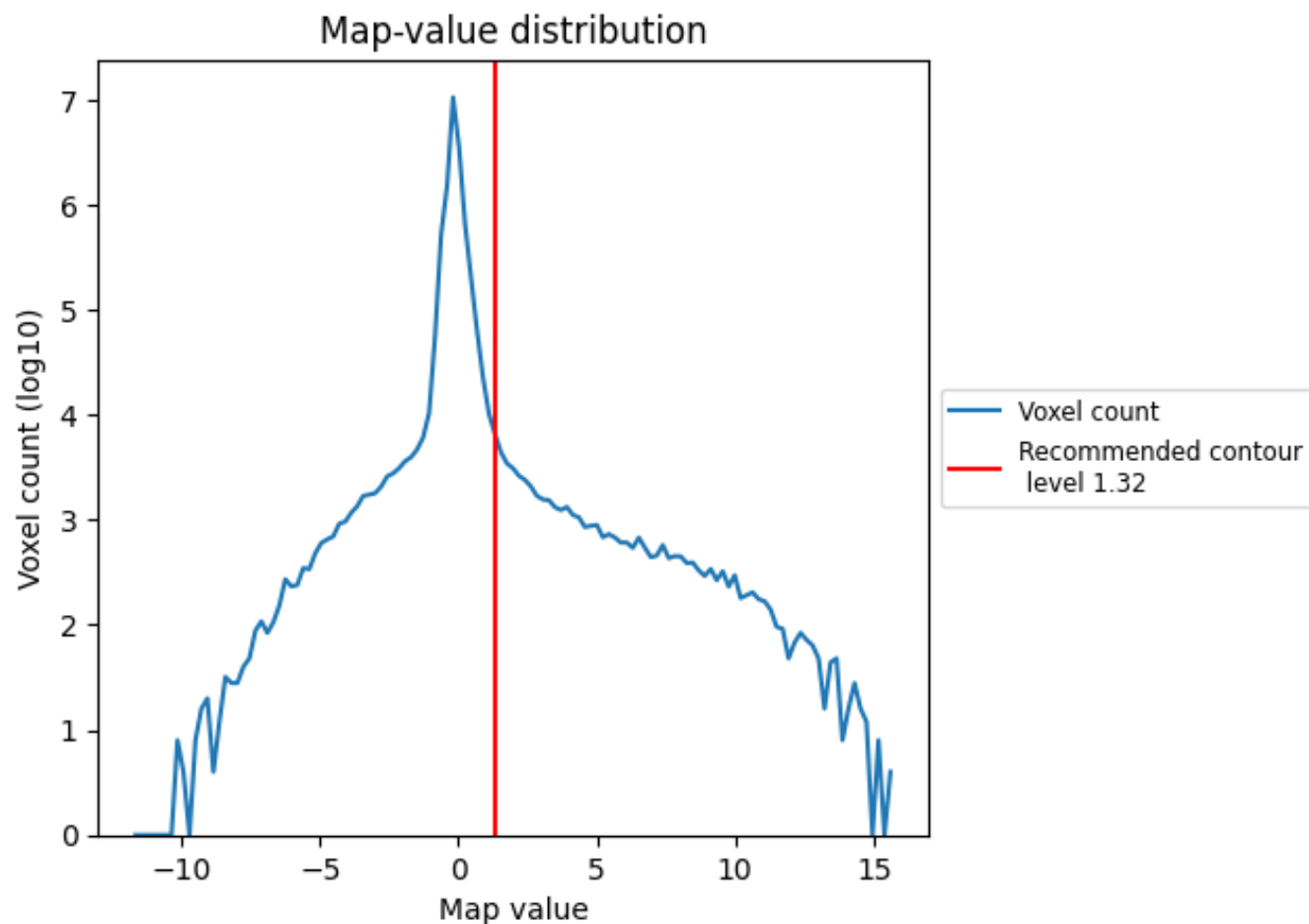
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

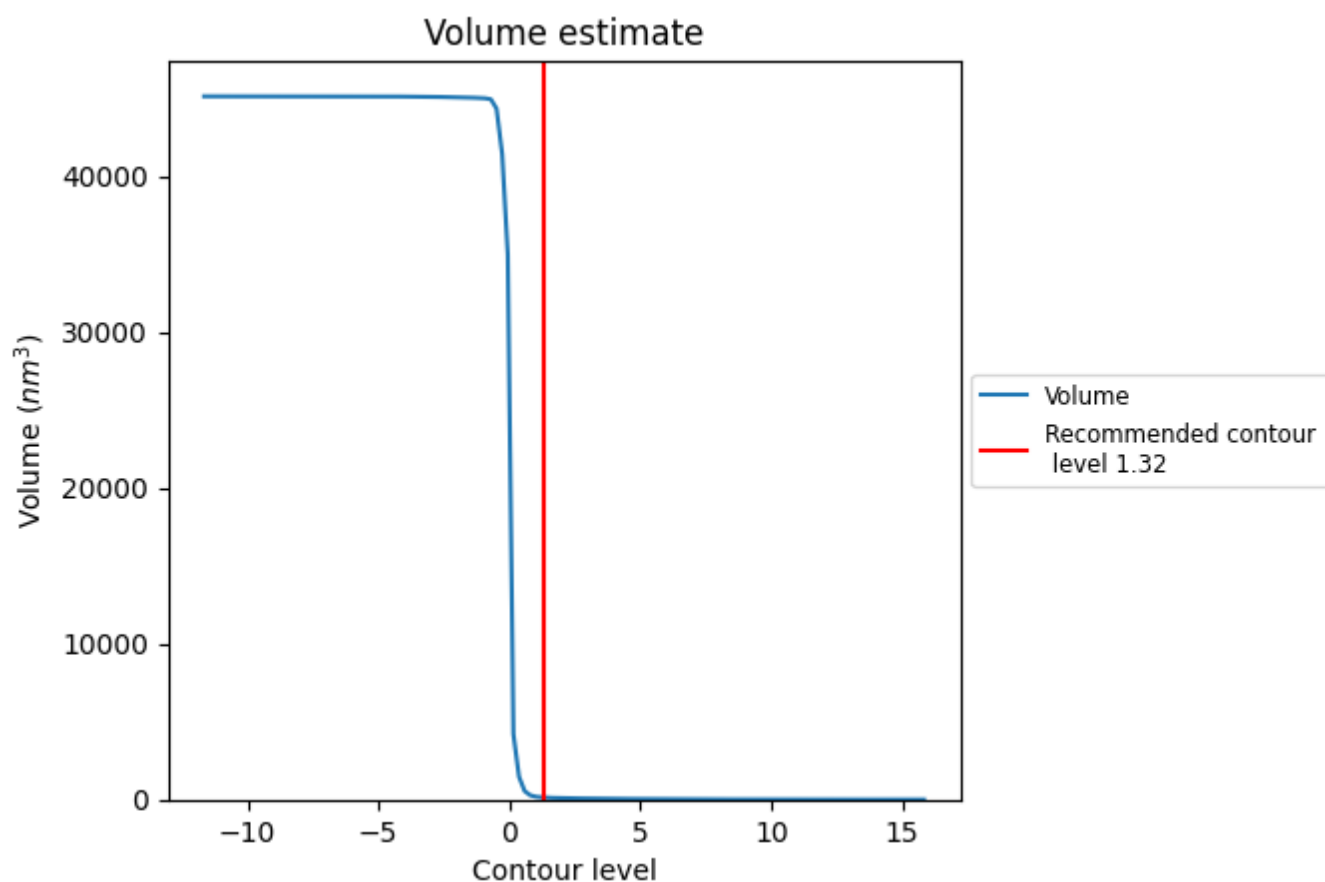
This section contains the results of statistical analysis of the map.

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.

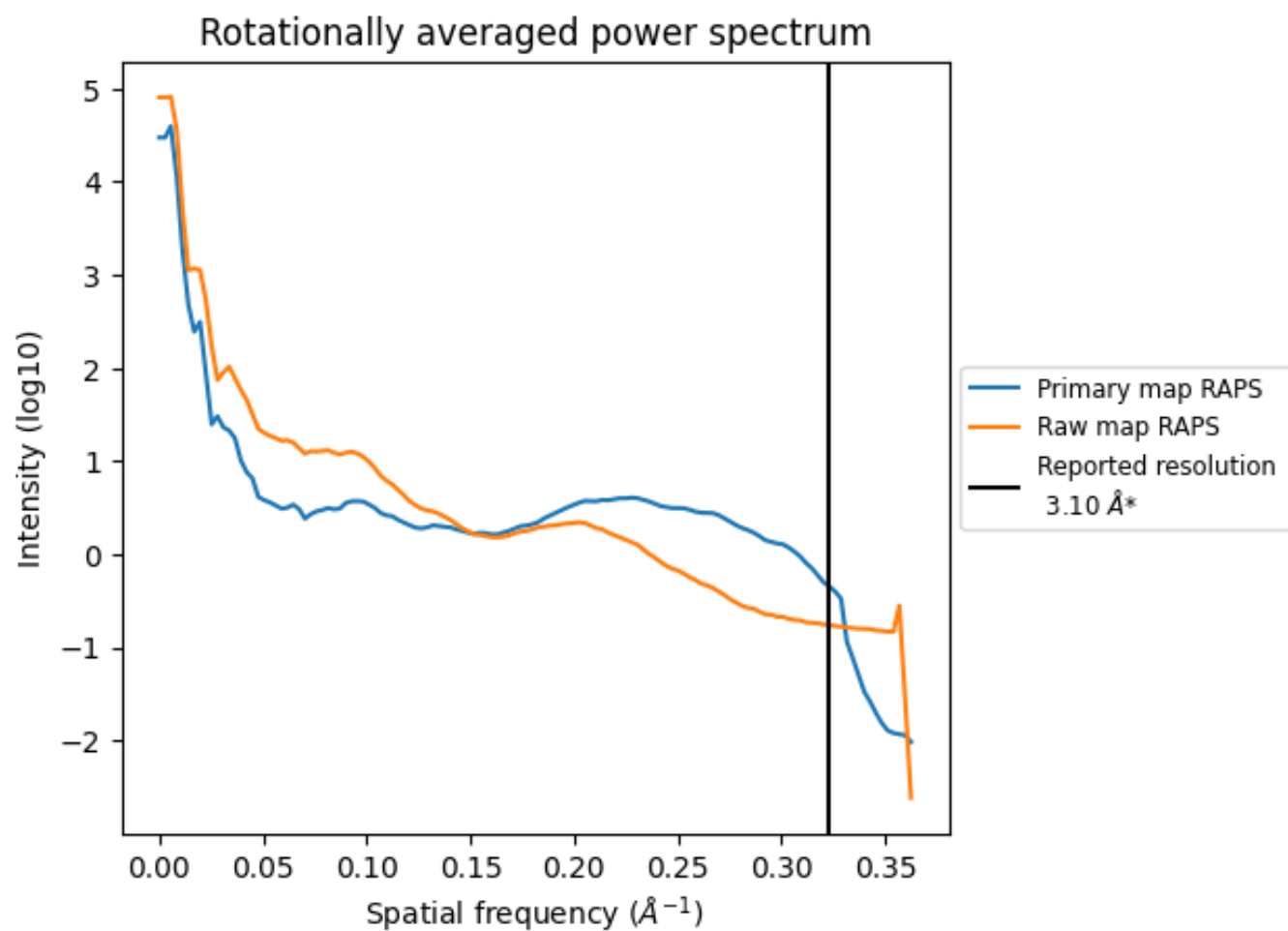
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 134 nm³; this corresponds to an approximate mass of 121 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 ⓘ

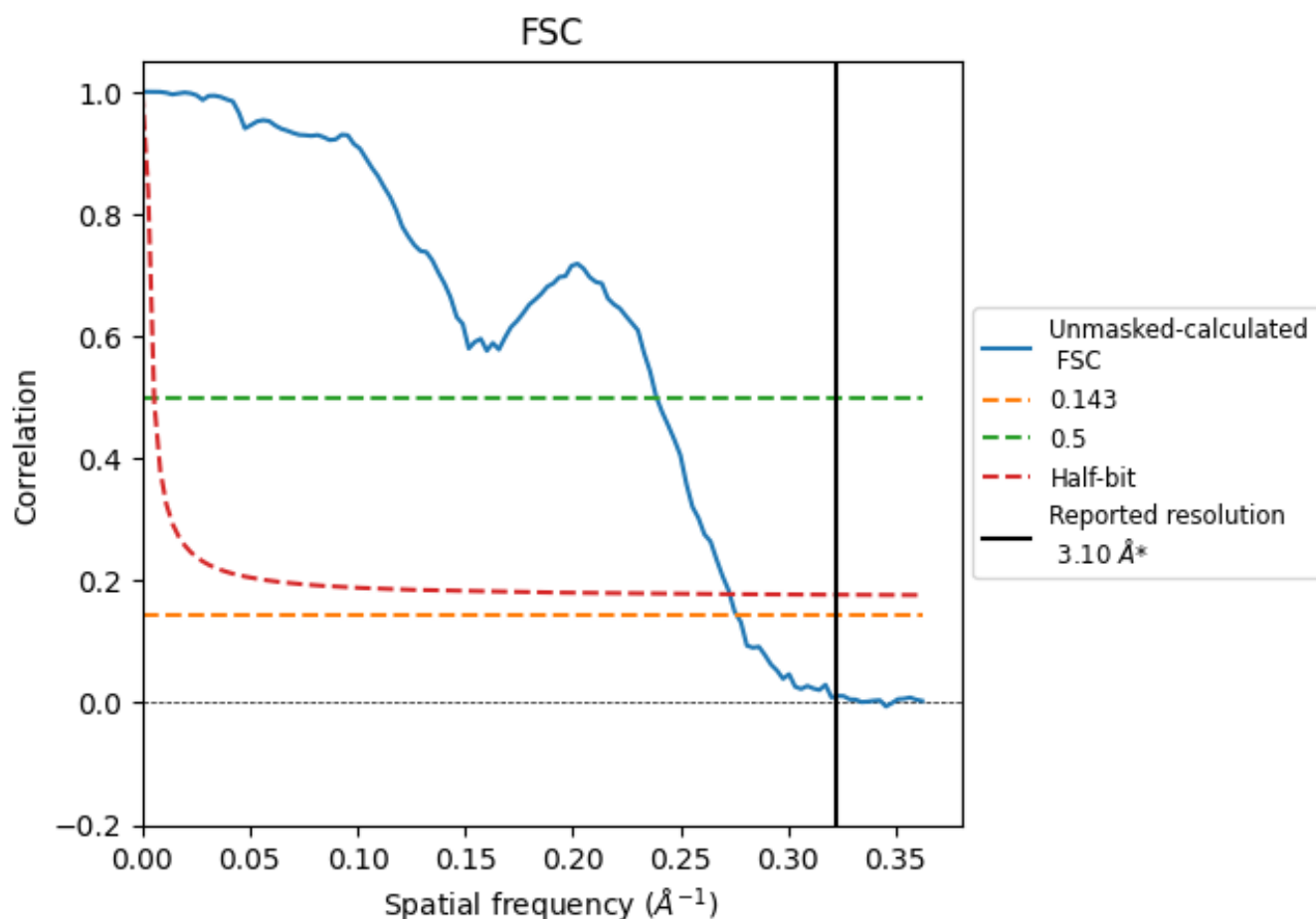


*Reported resolution corresponds to spatial frequency of 0.323 $\text{\AA}^{-1}$

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 $0.323 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

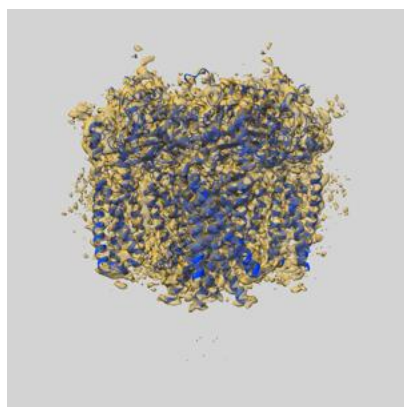
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.62	4.19	3.66

*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 3.62 differs from the reported value 3.1 by more than 10 %

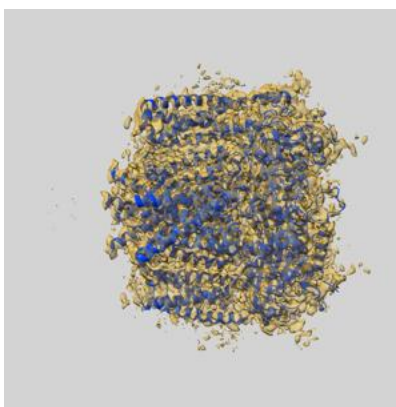
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-49489 and PDB model 9NJS. Per-residue inclusion information can be found in section [3](#) on page [7](#).

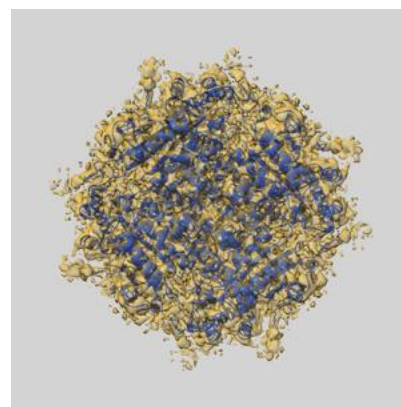
9.1 Map-model overlay [i](#)



X



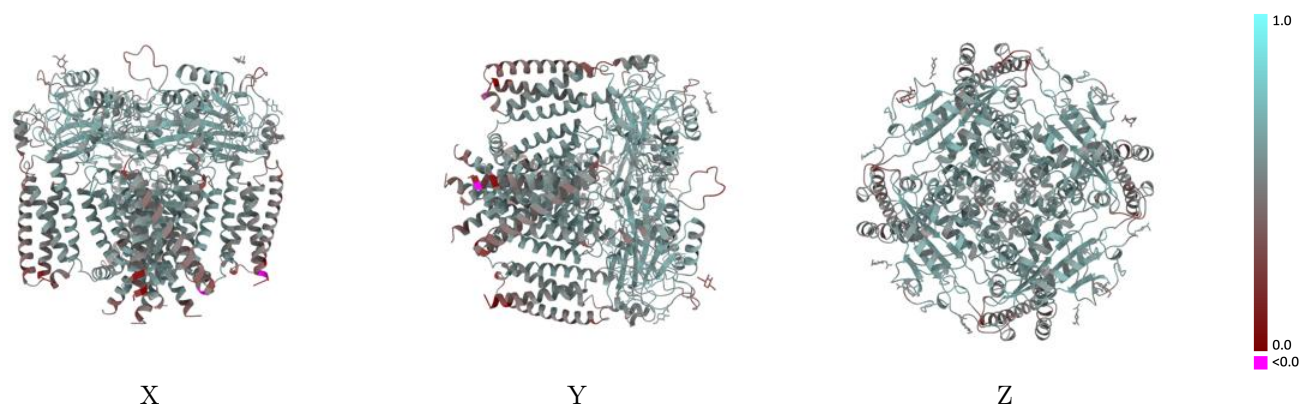
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.32 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](#)



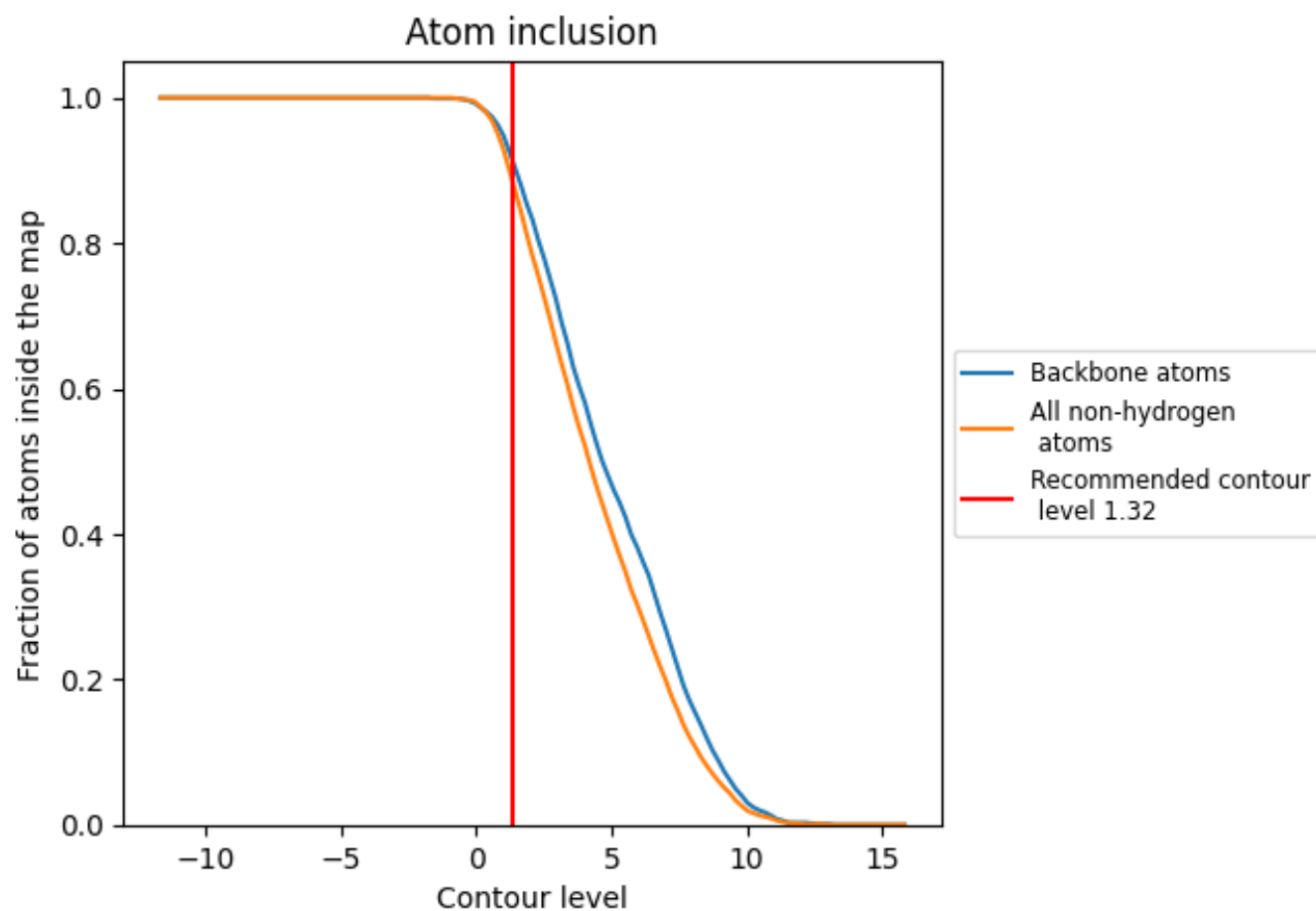
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.32).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 89% 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 (1.32) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8880	0.5470
a	0.8880	0.5460
b	0.8870	0.5450
c	0.8870	0.5450
d	0.8920	0.5510

