



Full wwPDB EM Validation Report ⓘ

Dec 10, 2022 – 01:30 pm GMT

PDB ID : 6QPC
EMDB ID : EMD-4613
Title : Cryo-EM structure of calcium-bound mTMEM16F lipid scramblase in nanodisc
Authors : Alvadia, C.; Lim, N.K.; Clerico Mosina, V.; Oostergetel, G.T.; Dutzler, R.; Paulino, C.
Deposited on : 2019-02-13
Resolution : 3.50 Å (reported)
Based on initial model : ?

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.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

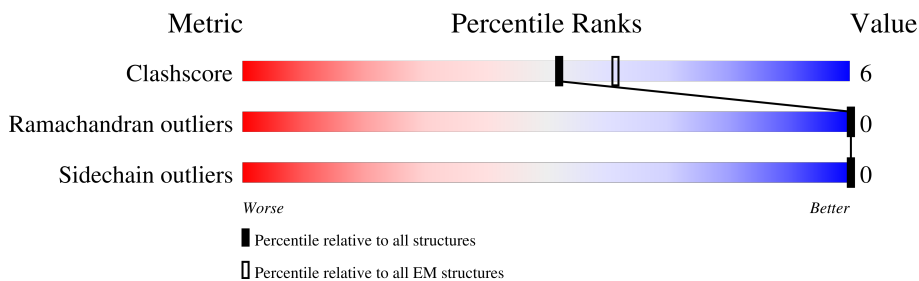
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	911	
1	B	911	

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
3	P1O	A	1003	X	-	-	-
3	P1O	B	1003	X	-	-	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9140 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.

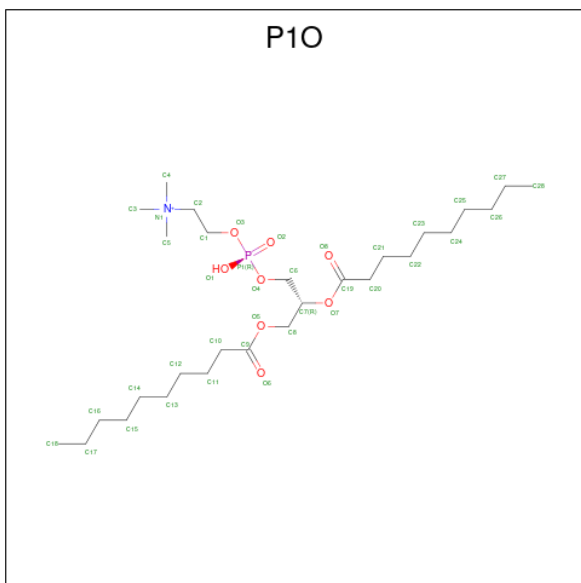
- Molecule 1 is a protein called Anoctamin-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	577	Total 4530	C 2992	N 726	O 781	S 31	0	0
1	B	577	Total 4530	C 2992	N 726	O 781	S 31	0	0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
2	A	2	Total Ca 2 2	0
2	B	2	Total Ca 2 2	0

- Molecule 3 is 1,2-DIDECANOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: P1O) (formula: C₂₈H₅₇NO₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	A	1	38	28	1	8	1	0
3	B	1	38	28	1	8	1	0

Chain B:  53% 10% 37%

MET
GLN
MET
MET
THR
THR
ARG
LYS
VAL
LEU
LEU
LEU
LEU
MET
MET
GLU
LEU
GLU
GLU
ASP
ASP
ASP
GLU
ASP
GLY
GLY
VAL
ILE
VAL
LEU
LEU
GLU
GLN
GLN
GLN
ASP
PHE
THR
GLY
PHE
THR
LEU
LEU
LEU
GLN
GLN
ASP
PHE
PHE
THR
PRO
GLU
PHE
GLU
GLU
ASP
PHE
ASN
GLY
PRO
PRO
ASP

SER
LEU
PHE
PHE
LYS
THR
THR
GLN
GLN
LEU
LEU
ILE
ILE
PHE
PHE
ILE
ILE
VAL
VAL
TYR
TYR
PHE
GLU
ASP
GLU
SER
SER
GLY
LYS
LYS
LYS
GLU
GLU
ASP
ASP
C107
HIS
GLY
LEU
LEU
GLN
LEU
GLU
ALA
ALA
R115
R116
D120
D121
D124
C136
T137
Y138
A139
E140
F147

LEU
LYS
PRO
ASN
ASP
LEU
THR
THR
SER
SER
ASN
PHE
PHE
ASN
ASN
LEU
LEU
TYR
THR
THR
LYS
VAL
ARG
GLY
VAL
VAL
ASN
ASN
SER
SER
VAL
VAL
PRO
VAL
ILE
LYS
PRO
GLU
GLN
GLU
PHE
PHE
PHE
GLY
LEU
LYS
SER
ARG
MET
ASP
ASP
PHE
TYR
ILE
LEU
ASP
ARG
ASP
S202
Y214

SER
ARG
VAL
LYS
TYR
VAL
MET
ASN
ASN
VAL
ASN
ASN
PHE
GLY
ILE
ILE
R235
R252
S257
GLU
ASP
ILE
SER
CYS
PRO
S264
Y270
W273
A274
P284
L285
D286
L287
I288
R289
G293
E294
Q328
S334
V337
D341
I342
T346
P350
Q351
R354

L355
C356
F357
F358
L361
N362
I363
T364
C365
E366
S367
S368
K369
K370
L373
F374
D375
M386
T391
R399
E405
GLU
TRP
ASP
THR
VAL
GLU
LEU
GLN
GLN
GLU
GLU
GLN
ALA
ARG
PRO
GLU
TYR
ALA
ALA
CYS
ASN
VAL
VAL
ASN
ASN
GLU
ILE
ILE
GLU
GLU

GLU
GLU
ARG
ILE
PHE
THR
THR
CYS
GLY
LYS
CYS
ILE
ARG
VAL
THR
LEU
CYS
ALA
SER
ALA
VAL
F461
F462
W463
S470
I474
R478
V481
F482
I483
V484
F485
S486
T487
THR
LEU
PRO
LYS
ASN
PRO
ASN
GLY
THR
ASP
PRO
ILE
GLN
LYS
TYR
L503
A508
T512

S517
L524
Y527
Y528
E529
K530
V531
M534
E538
E539
P541
H542
T543
Q544
V561
S565
S566
Y569
K574
L587
K590
E594
E595
G601
L602
E604
L605
T606
T607
Q608
K616
N620
K638
ARG
VAL
GLY
SER
GLU
LYS
ILE
T647

Q652
M659
G660
K661
L662
G663
Y666
L669
V682
A683
S684
F685
P686
A692
N696
E699
I700
R701
W702
K718
H742
I743
A745
F746
H750
R753
W755
S759
F760
S761
T764
GLY
ASP
HIS
THR
TYR
TYR
T772
N785
I786
T787
ASP
PHE

LYS
ASN
THR
ASP
LYS
GLU
ASN
PRO
TYR
ILE
ILE
GLY
GLY
ASN
TYR
THR
THR
L540
LEU
SER
C807
R808
P816
G817
H818
I832
K835
K850
Y855
V860
S861
LYS
ILE
THR
LYS
SER
LYS
ILE
LYS
ARG
GLU
LYS
TYR
LEU
THR
GLN
LYS
LEU
LEU
HIS
GLU
SER
SER
HIS
LEU
LYS
ASP
LEU

THR
LYS
ASN
MET
GLY
ILE
ALA
GLU
ARG
GLY
THR
VAL
ASP
SER
VAL
PRO
LYS
LEU
GLU

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	186487	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	52	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	49407	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.283	Depositor
Minimum map value	-0.169	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	259.072, 259.072, 259.072	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.012, 1.012, 1.012	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, P1O

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	0.42	0/4649	0.55	0/6322
1	B	0.42	0/4649	0.55	0/6322
All	All	0.42	0/9298	0.55	0/12644

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	354	ARG	Peptide
1	A	356	CYS	Peptide
1	B	354	ARG	Peptide
1	B	356	CYS	Peptide

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	4530	0	4327	50	0
1	B	4530	0	4327	52	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	38	0	54	0	0
3	B	38	0	54	0	0
All	All	9140	0	8762	102	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 6.

All (102) 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:616:LYS:O	1:B:620:ASN:HB2	1.87	0.75
1:A:616:LYS:O	1:A:620:ASN:HB2	1.87	0.75
1:B:481:VAL:HG21	1:B:517:SER:HB3	1.76	0.68
1:A:481:VAL:HG21	1:A:517:SER:HB3	1.76	0.66
1:A:375:ASP:O	1:A:753:ARG:NH1	2.32	0.63
1:B:375:ASP:O	1:B:753:ARG:NH1	2.32	0.63
1:B:647:THR:HG23	1:B:652:GLN:HE21	1.66	0.60
1:A:692:ALA:O	1:A:696:ASN:ND2	2.31	0.59
1:A:647:THR:HG23	1:A:652:GLN:HE21	1.66	0.59
1:A:116:ARG:HA	1:A:124:VAL:HA	1.85	0.59
1:B:116:ARG:HA	1:B:124:VAL:HA	1.85	0.58
1:B:284:PRO:HB2	1:B:287:LEU:HB3	1.85	0.58
1:A:270:TYR:HA	1:A:274:ALA:HB3	1.86	0.57
1:B:270:TYR:HA	1:B:274:ALA:HB3	1.86	0.57
1:B:273:TRP:O	1:B:701:ARG:NH1	2.37	0.57
1:A:284:PRO:HB2	1:A:287:LEU:HB3	1.85	0.57
1:A:273:TRP:O	1:A:701:ARG:NH1	2.37	0.57
1:A:366:GLU:O	1:A:370:LYS:NZ	2.37	0.57
1:A:478:ARG:NH2	1:A:604:GLU:OE2	2.37	0.57
1:B:366:GLU:O	1:B:370:LYS:NZ	2.37	0.57
1:B:478:ARG:NH2	1:B:604:GLU:OE2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:761:SER:HG	1:B:772:THR:N	2.04	0.56
1:A:399:ARG:NH1	1:A:860:VAL:O	2.40	0.55
1:A:761:SER:HG	1:A:772:THR:N	2.05	0.55
1:B:399:ARG:NH1	1:B:860:VAL:O	2.40	0.54
1:A:566:SER:OG	1:A:608:GLN:NE2	2.42	0.53
1:A:362:ASN:O	1:A:365:CYS:HB3	2.09	0.53
1:B:362:ASN:O	1:B:365:CYS:HB3	2.09	0.53
1:A:346:ILE:O	1:A:808:ARG:NH2	2.42	0.53
1:B:566:SER:OG	1:B:608:GLN:NE2	2.42	0.53
1:B:346:ILE:O	1:B:808:ARG:NH2	2.42	0.52
1:B:659:MET:HG2	1:B:663:GLY:HA2	1.91	0.52
1:A:524:LEU:HG	1:A:528:TYR:CE2	2.45	0.52
1:A:659:MET:HG2	1:A:663:GLY:HA2	1.91	0.52
1:B:785:ASN:HB2	1:B:816:PRO:HB3	1.91	0.52
1:A:785:ASN:HB2	1:A:816:PRO:HB3	1.91	0.51
1:B:524:LEU:HG	1:B:528:TYR:CE2	2.45	0.51
1:A:524:LEU:HD11	1:A:528:TYR:CZ	2.45	0.51
1:B:524:LEU:HD11	1:B:528:TYR:CZ	2.46	0.51
1:B:692:ALA:O	1:B:696:ASN:ND2	2.31	0.51
1:A:561:VAL:O	1:A:565:SER:OG	2.18	0.51
1:B:364:THR:O	1:B:368:SER:N	2.44	0.50
1:B:481:VAL:HA	1:B:484:VAL:HG22	1.94	0.50
1:A:328:GLN:HE21	1:A:373:ILE:HG13	1.77	0.49
1:B:328:GLN:HE21	1:B:373:ILE:HG13	1.77	0.49
1:A:481:VAL:HA	1:A:484:VAL:HG22	1.94	0.48
1:B:386:MET:HG3	1:B:682:VAL:HG21	1.95	0.48
1:B:531:VAL:HA	1:B:534:MET:HE2	1.96	0.48
1:A:364:THR:O	1:A:368:SER:N	2.44	0.48
1:B:606:THR:HG23	1:B:685:PHE:HB3	1.96	0.48
1:A:386:MET:HG3	1:A:682:VAL:HG21	1.96	0.48
1:B:699:GLU:HA	1:B:702:VAL:HG12	1.96	0.48
1:A:606:THR:HG23	1:A:685:PHE:HB3	1.96	0.47
1:A:699:GLU:HA	1:A:702:VAL:HG12	1.96	0.47
1:B:350:PRO:HD3	1:B:358:PHE:HB3	1.96	0.46
1:B:351:GLN:HB3	1:B:595:GLU:HB2	1.97	0.46
1:B:602:LEU:HD11	1:B:684:SER:HA	1.97	0.46
1:B:755:VAL:O	1:B:759:SER:HB3	2.16	0.46
1:A:602:LEU:HD11	1:A:684:SER:HA	1.97	0.46
1:A:350:PRO:HD3	1:A:358:PHE:HB3	1.96	0.46
1:A:755:VAL:O	1:A:759:SER:HB3	2.15	0.46
1:A:285:LEU:HA	1:A:288:ILE:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:508:ALA:O	1:B:512:THR:OG1	2.29	0.45
1:B:530:LYS:HA	1:B:530:LYS:HD3	1.81	0.45
1:A:351:GLN:HB3	1:A:595:GLU:HB2	1.97	0.45
1:A:470:SER:O	1:A:474:ILE:HG12	2.17	0.45
1:B:285:LEU:HA	1:B:288:ILE:HG22	1.99	0.45
1:B:470:SER:O	1:B:474:ILE:HG12	2.17	0.45
1:B:569:TYR:OH	1:B:594:GLU:OE1	2.34	0.44
1:A:294:GLU:HG3	1:A:718:LYS:HG2	2.00	0.44
1:A:531:VAL:HA	1:A:534:MET:HE2	1.98	0.44
1:B:744:ILE:HG23	1:B:750:MET:HE3	2.00	0.44
1:A:569:TYR:OH	1:A:594:GLU:OE1	2.34	0.44
1:B:294:GLU:HB2	1:B:718:LYS:HA	2.00	0.44
1:B:294:GLU:HG3	1:B:718:LYS:HG2	2.00	0.43
1:A:294:GLU:HB2	1:A:718:LYS:HA	2.00	0.43
1:A:684:SER:OG	1:A:685:PHE:N	2.51	0.43
1:B:289:ARG:NH1	1:B:294:GLU:OE2	2.39	0.43
1:A:753:ARG:H	1:A:753:ARG:HG2	1.68	0.43
1:B:742:MET:O	1:B:746:PHE:HB2	2.19	0.43
1:A:742:MET:O	1:A:746:PHE:HB2	2.19	0.43
1:B:391:THR:OG1	1:B:850:LYS:HG2	2.19	0.43
1:B:832:ILE:HA	1:B:835:LYS:HD2	2.01	0.43
1:A:334:SER:HA	1:A:337:VAL:HG22	2.01	0.43
1:A:744:ILE:HG23	1:A:750:MET:HE3	2.01	0.42
1:B:561:VAL:O	1:B:565:SER:OG	2.18	0.42
1:B:745:ALA:O	1:B:835:LYS:NZ	2.40	0.42
1:A:391:THR:OG1	1:A:850:LYS:HG2	2.19	0.42
1:B:334:SER:HA	1:B:337:VAL:HG22	2.01	0.42
1:B:684:SER:OG	1:B:685:PHE:N	2.51	0.42
1:B:753:ARG:H	1:B:753:ARG:HG2	1.68	0.42
1:A:784:PHE:HB2	1:A:809:TYR:CE2	2.55	0.42
1:B:685:PHE:HA	1:B:686:PRO:HD3	1.89	0.42
1:A:832:ILE:HA	1:A:835:LYS:HD2	2.01	0.41
1:A:289:ARG:NH1	1:A:294:GLU:OE2	2.39	0.41
1:B:527:ILE:O	1:B:531:VAL:HG12	2.20	0.41
1:A:666:TYR:O	1:A:669:LEU:HB3	2.21	0.41
1:A:478:ARG:HE	1:A:570:ILE:HD11	1.86	0.40
1:B:574:LYS:NZ	1:B:601:CYS:SG	2.87	0.40
1:B:666:TYR:O	1:B:669:LEU:HB3	2.21	0.40
1:A:530:LYS:HA	1:A:530:LYS:HD3	1.81	0.40
1:A:527:ILE:O	1:A:531:VAL:HG12	2.20	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	555/911 (61%)	541 (98%)	14 (2%)	0	100	100
1	B	555/911 (61%)	541 (98%)	14 (2%)	0	100	100
All	All	1110/1822 (61%)	1082 (98%)	28 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	454/827 (55%)	454 (100%)	0	100	100
1	B	454/827 (55%)	454 (100%)	0	100	100
All	All	908/1654 (55%)	908 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	328	GLN
1	A	549	ASN
1	A	608	GLN
1	A	695	ASN
1	A	730	GLN
1	B	328	GLN

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Mol	Chain	Res	Type
1	B	549	ASN
1	B	608	GLN
1	B	695	ASN
1	B	730	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z > 2$
3	P1O	B	1003	1	37,37,37	1.45	6 (16%)	43,45,45	0.91	3 (6%)
3	P1O	A	1003	1	37,37,37	1.45	6 (16%)	43,45,45	0.91	3 (6%)

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
3	P1O	B	1003	1	1/1/5/5	19/41/41/41	-
3	P1O	A	1003	1	1/1/5/5	19/41/41/41	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1003	P1O	P1-O3	4.49	1.77	1.59
3	B	1003	P1O	P1-O3	4.49	1.77	1.59
3	A	1003	P1O	C20-C19	2.77	1.58	1.50
3	B	1003	P1O	C20-C19	2.75	1.58	1.50
3	B	1003	P1O	C2-C1	2.57	1.59	1.51
3	A	1003	P1O	C2-C1	2.53	1.59	1.51
3	A	1003	P1O	P1-O4	2.35	1.68	1.59
3	B	1003	P1O	P1-O4	2.32	1.68	1.59
3	B	1003	P1O	O7-C19	2.28	1.40	1.34
3	A	1003	P1O	O7-C19	2.25	1.40	1.34
3	B	1003	P1O	O3-C1	-2.24	1.35	1.44
3	A	1003	P1O	O3-C1	-2.22	1.35	1.44

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1003	P1O	O7-C19-C20	3.06	118.09	111.50
3	B	1003	P1O	O7-C19-C20	3.05	118.08	111.50
3	A	1003	P1O	O1-P1-O2	2.17	122.98	112.24
3	B	1003	P1O	O1-P1-O2	2.17	122.97	112.24
3	B	1003	P1O	O5-C9-C10	2.12	118.57	111.91
3	A	1003	P1O	O5-C9-C10	2.11	118.54	111.91

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1003	P1O	C7
3	B	1003	P1O	C7

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1003	P1O	C1-O3-P1-O1
3	A	1003	P1O	O3-C1-C2-N1
3	B	1003	P1O	C1-O3-P1-O1
3	B	1003	P1O	O3-C1-C2-N1

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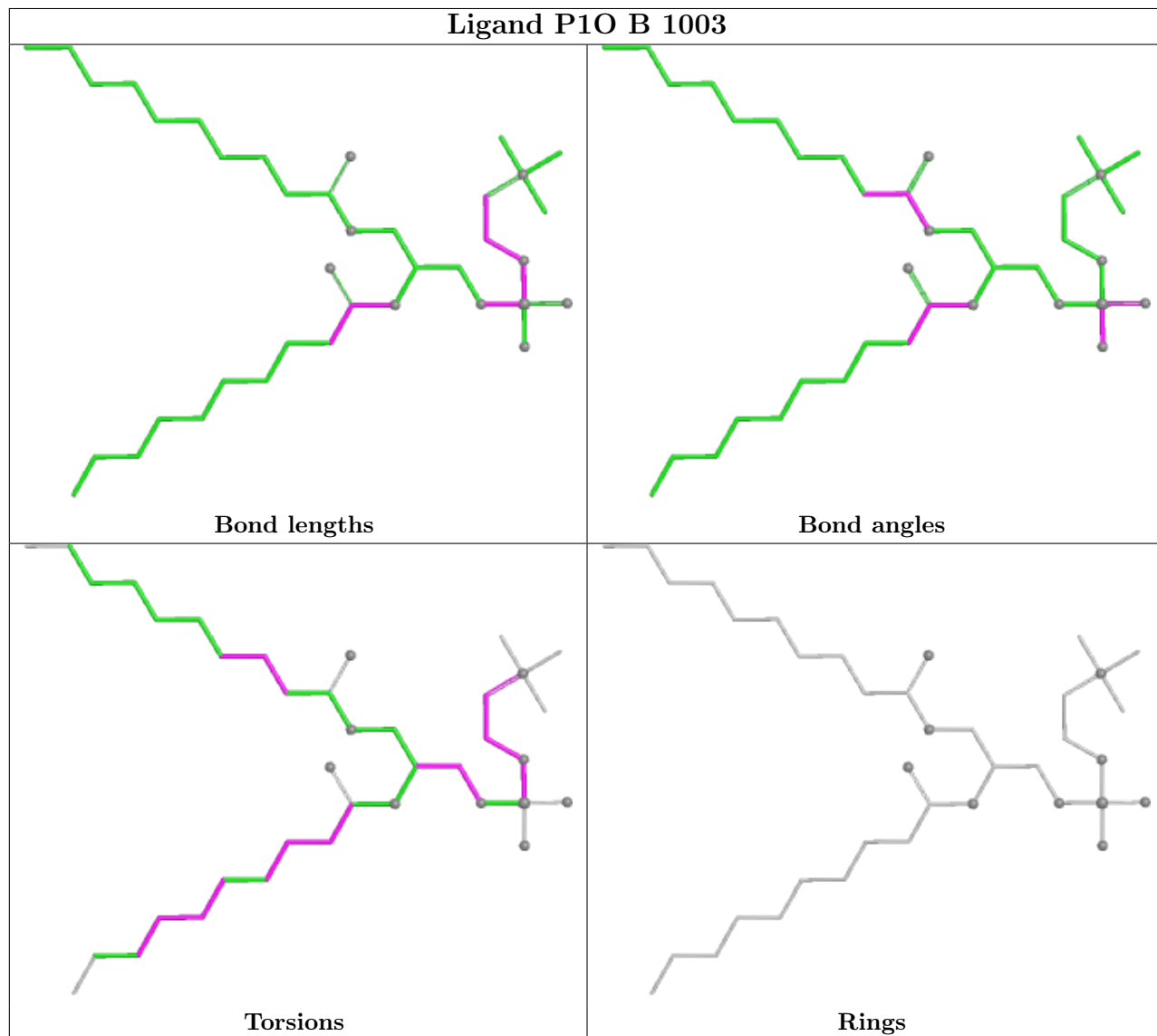
Mol	Chain	Res	Type	Atoms
3	A	1003	P1O	C24-C25-C26-C27
3	B	1003	P1O	C24-C25-C26-C27
3	A	1003	P1O	C1-C2-N1-C4
3	B	1003	P1O	C1-C2-N1-C4
3	A	1003	P1O	C9-C10-C11-C12
3	B	1003	P1O	C9-C10-C11-C12
3	A	1003	P1O	C1-C2-N1-C5
3	B	1003	P1O	C1-C2-N1-C5
3	A	1003	P1O	C1-O3-P1-O4
3	B	1003	P1O	C1-O3-P1-O4
3	A	1003	P1O	C20-C21-C22-C23
3	B	1003	P1O	C20-C21-C22-C23
3	A	1003	P1O	C19-C20-C21-C22
3	B	1003	P1O	C19-C20-C21-C22
3	A	1003	P1O	C1-C2-N1-C3
3	B	1003	P1O	C1-C2-N1-C3
3	B	1003	P1O	O4-C6-C7-C8
3	A	1003	P1O	O4-C6-C7-C8
3	A	1003	P1O	O4-C6-C7-O7
3	B	1003	P1O	O4-C6-C7-O7
3	A	1003	P1O	C22-C23-C24-C25
3	B	1003	P1O	C22-C23-C24-C25
3	A	1003	P1O	C2-C1-O3-P1
3	B	1003	P1O	C2-C1-O3-P1
3	B	1003	P1O	C23-C24-C25-C26
3	A	1003	P1O	C23-C24-C25-C26
3	A	1003	P1O	C7-C6-O4-P1
3	B	1003	P1O	C7-C6-O4-P1
3	A	1003	P1O	C10-C11-C12-C13
3	B	1003	P1O	C10-C11-C12-C13
3	A	1003	P1O	O7-C19-C20-C21
3	B	1003	P1O	O7-C19-C20-C21
3	A	1003	P1O	O8-C19-C20-C21
3	B	1003	P1O	O8-C19-C20-C21

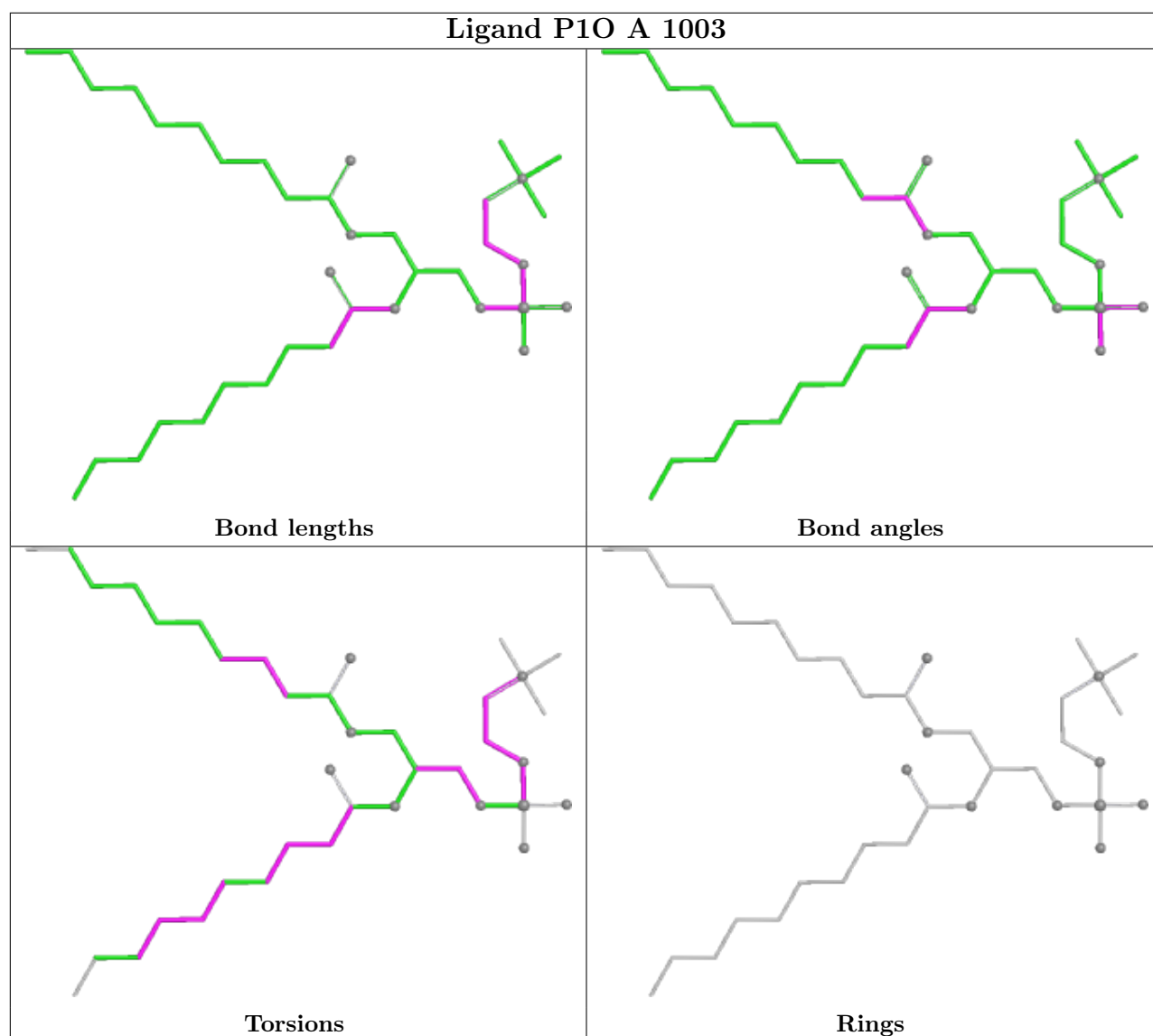
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	815:PRO	C	816:PRO	N	3.10
1	B	815:PRO	C	816:PRO	N	3.10

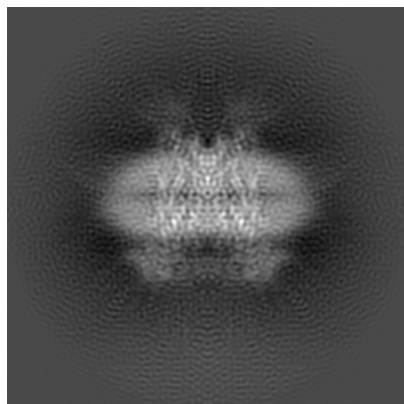
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4613. These allow visual inspection of the internal detail of the map and identification of artifacts.

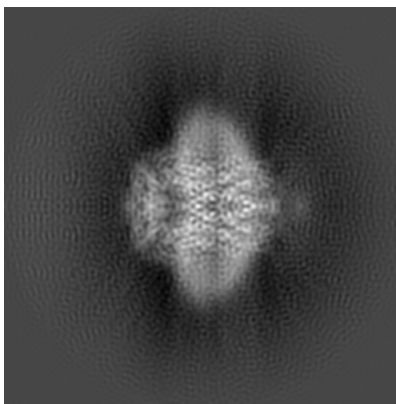
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

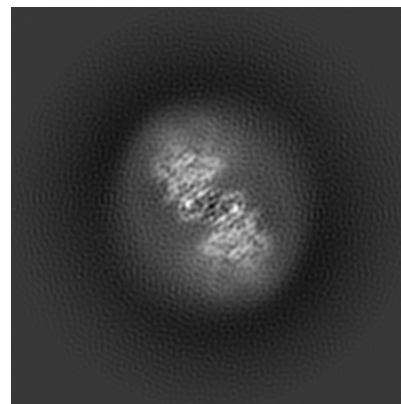
6.1.1 Primary map



X

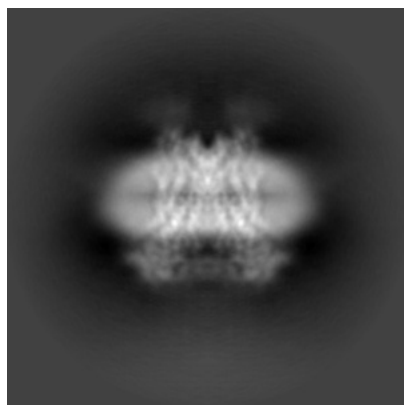


Y

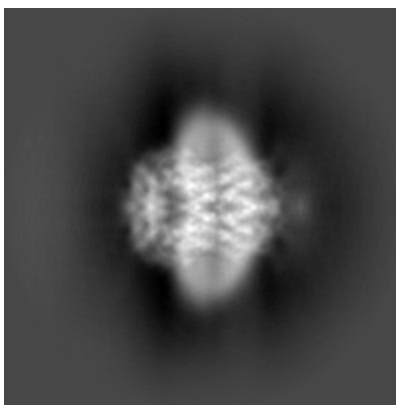


Z

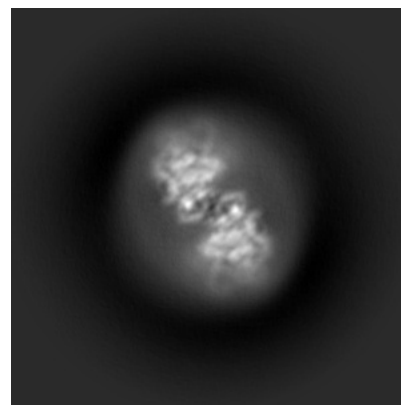
6.1.2 Raw map



X



Y

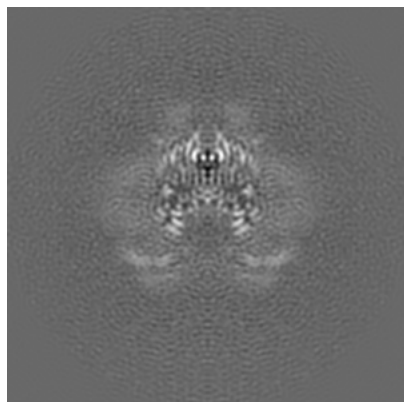


Z

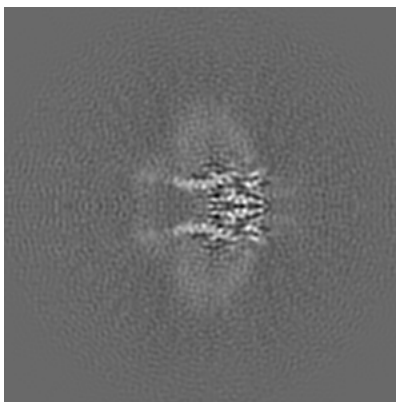
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

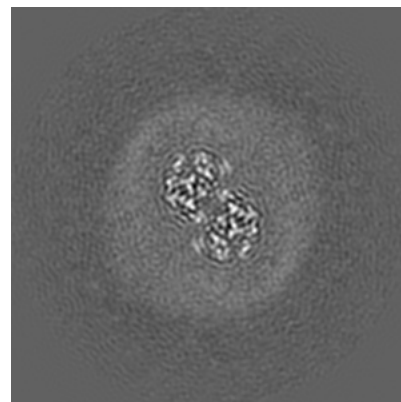
6.2.1 Primary map



X Index: 128

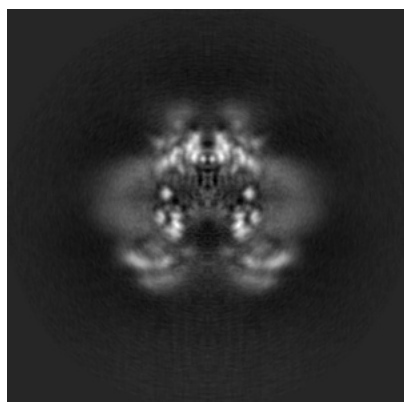


Y Index: 128

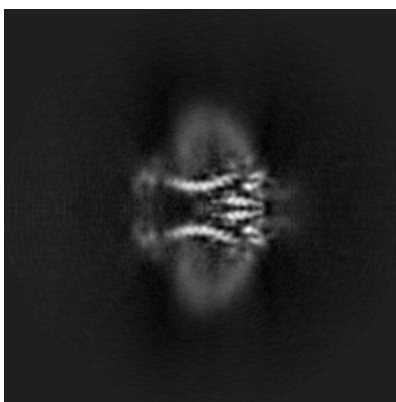


Z Index: 128

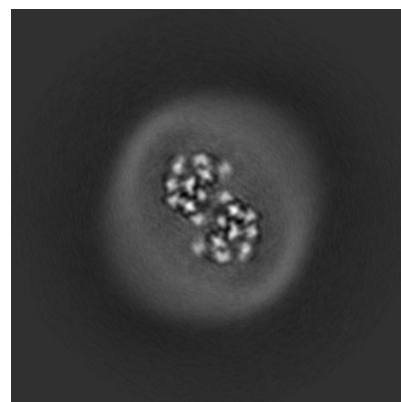
6.2.2 Raw map



X Index: 128



Y Index: 128

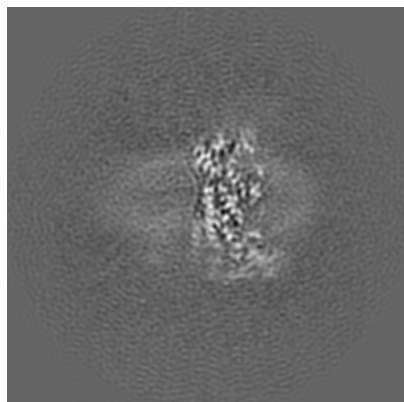


Z Index: 128

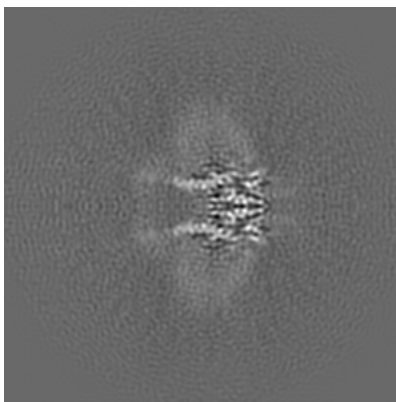
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

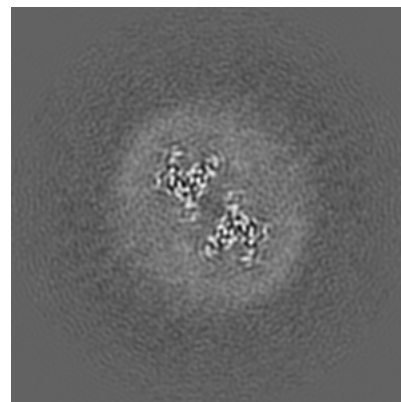
6.3.1 Primary map



X Index: 113

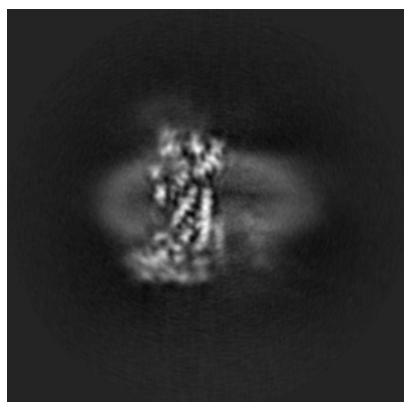


Y Index: 128

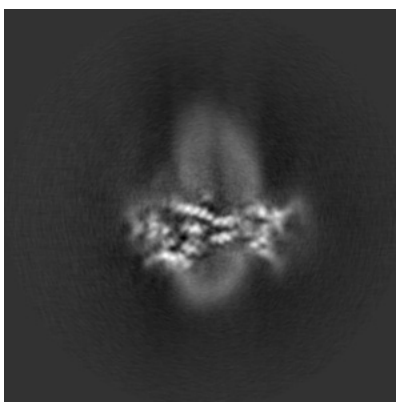


Z Index: 119

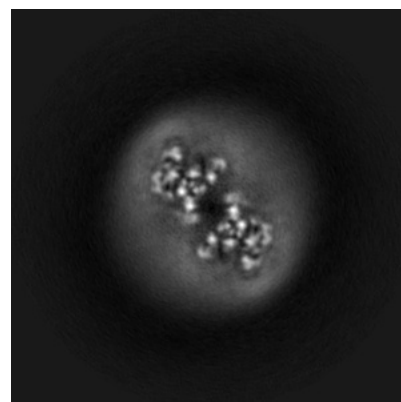
6.3.2 Raw map



X Index: 143



Y Index: 148



Z Index: 117

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

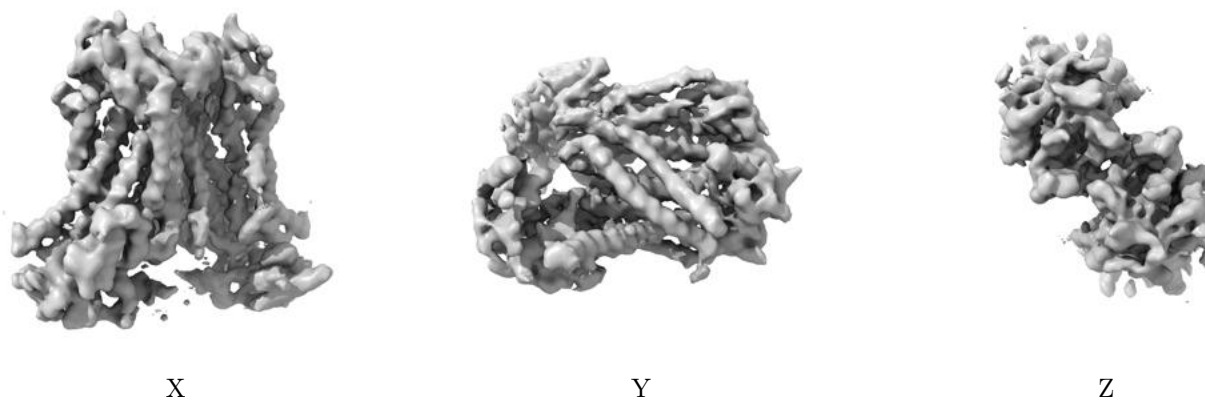
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

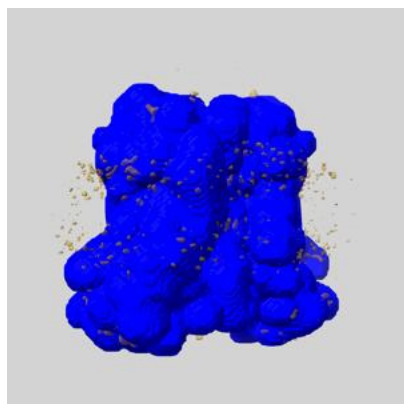
6.5 Mask visualisation [i](#)

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

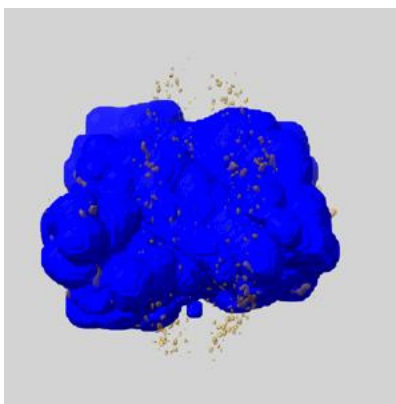
A mask typically either:

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

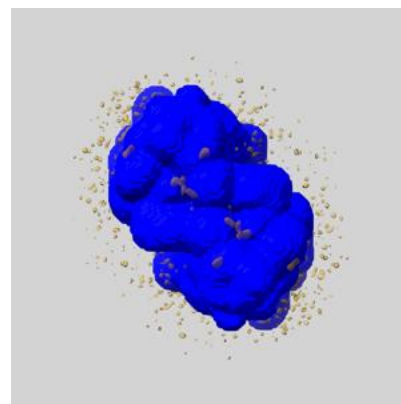
6.5.1 emd_4613_msk_1.map [i](#)



X



Y

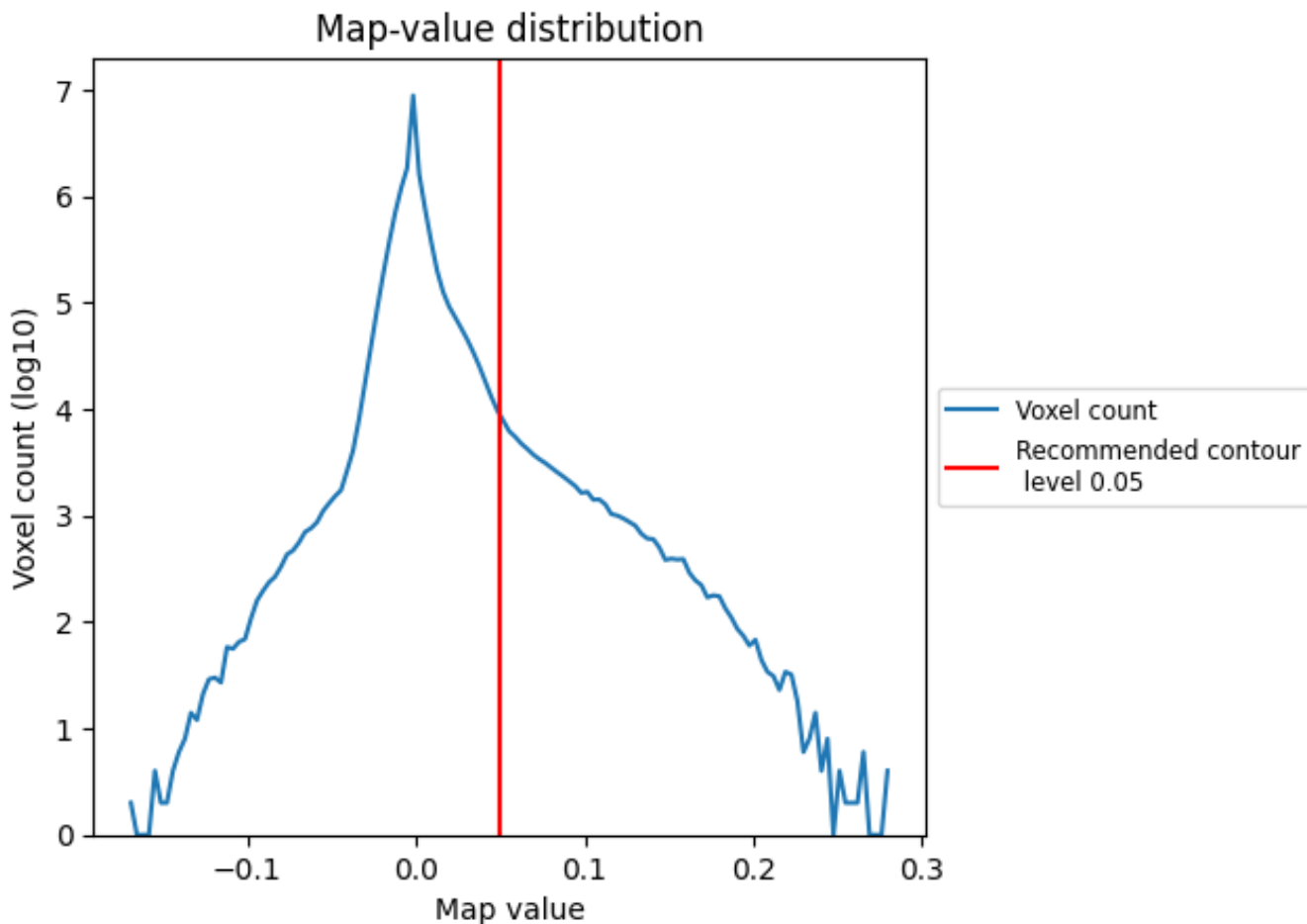


Z

7 Map analysis [i](#)

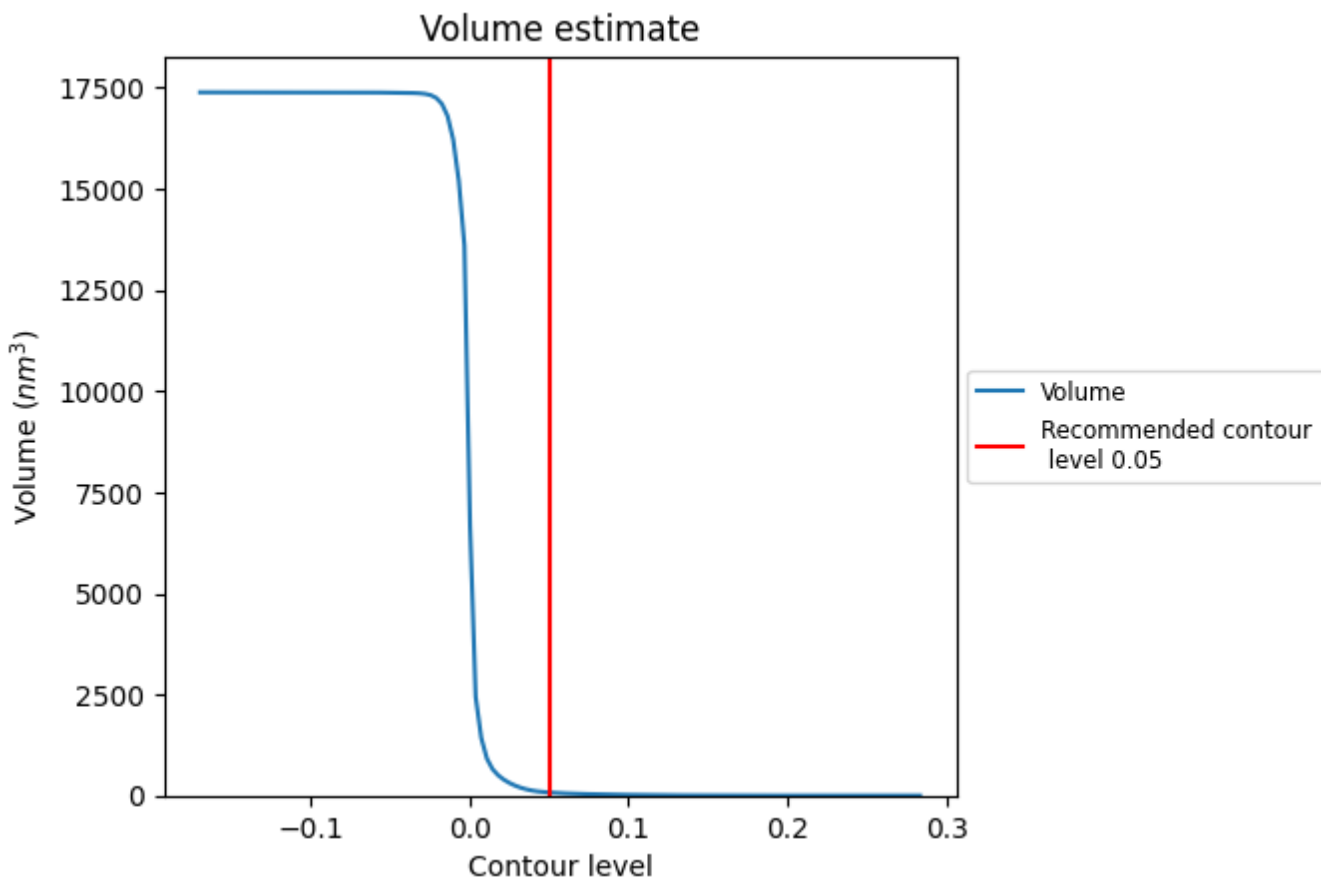
This section contains the results of statistical analysis of the map.

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.

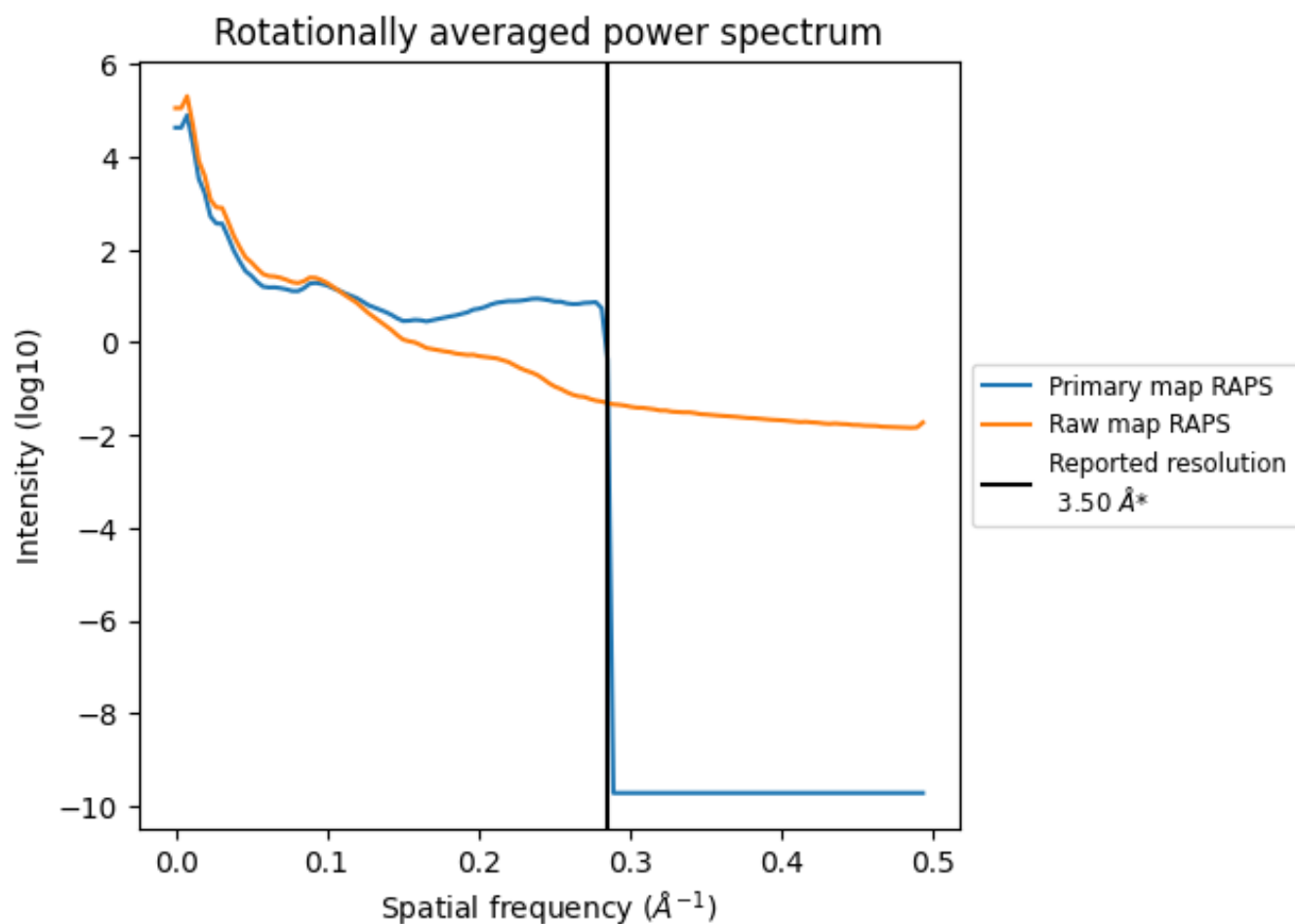
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 75 nm³; this corresponds to an approximate mass of 68 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

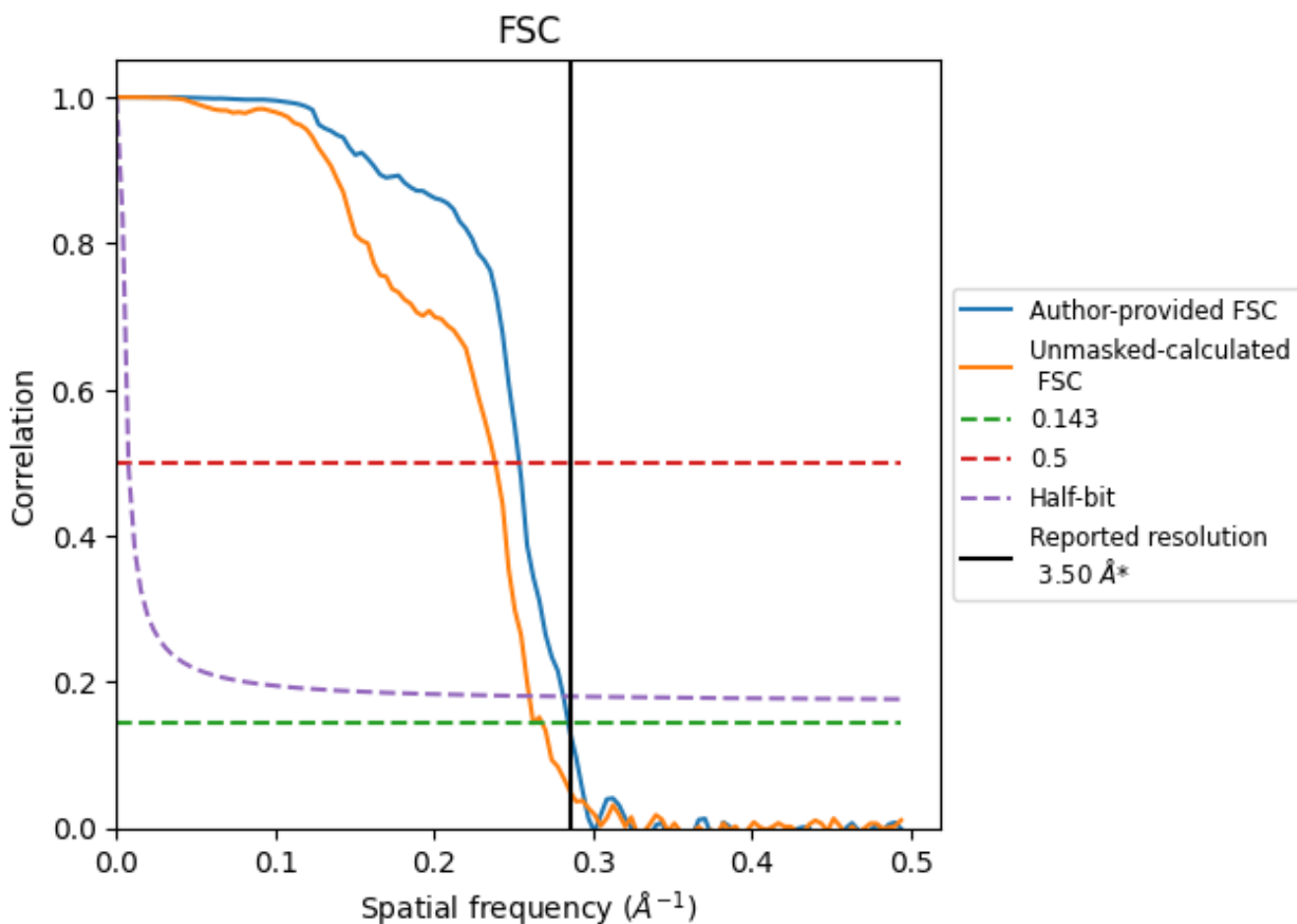


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

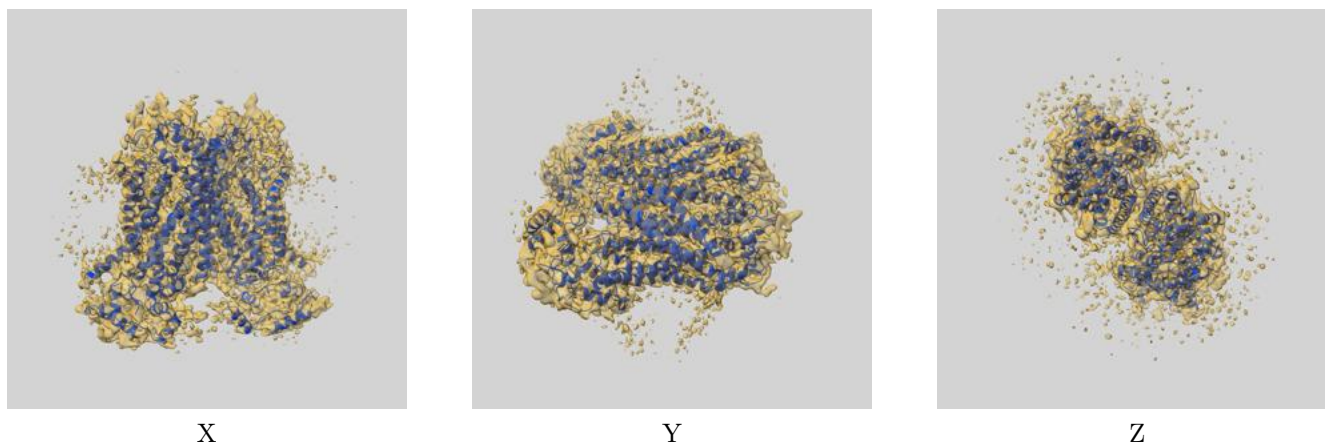
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.51	3.94	3.55
Unmasked-calculated*	3.73	4.19	3.85

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

9 Map-model fit [i](#)

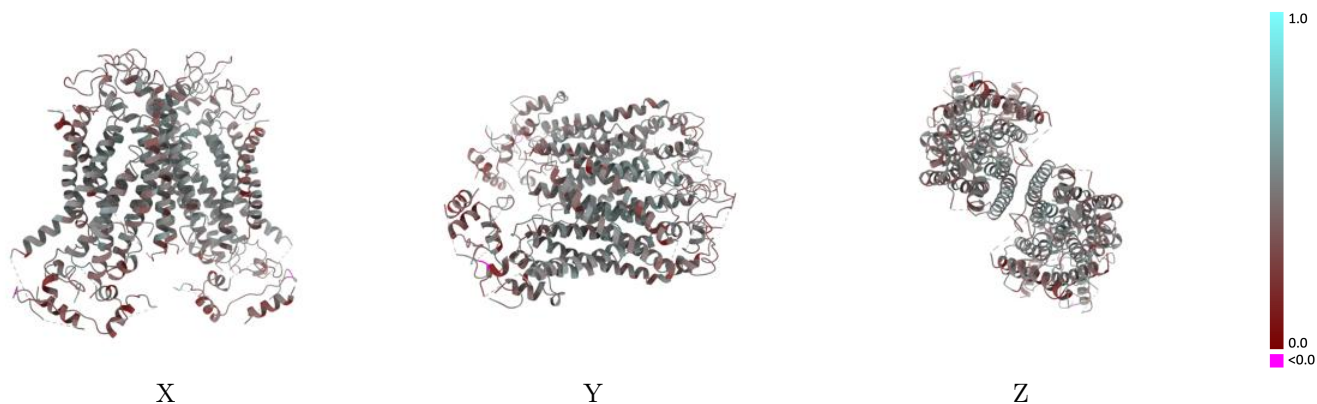
This section contains information regarding the fit between EMDB map EMD-4613 and PDB model 6QPC. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



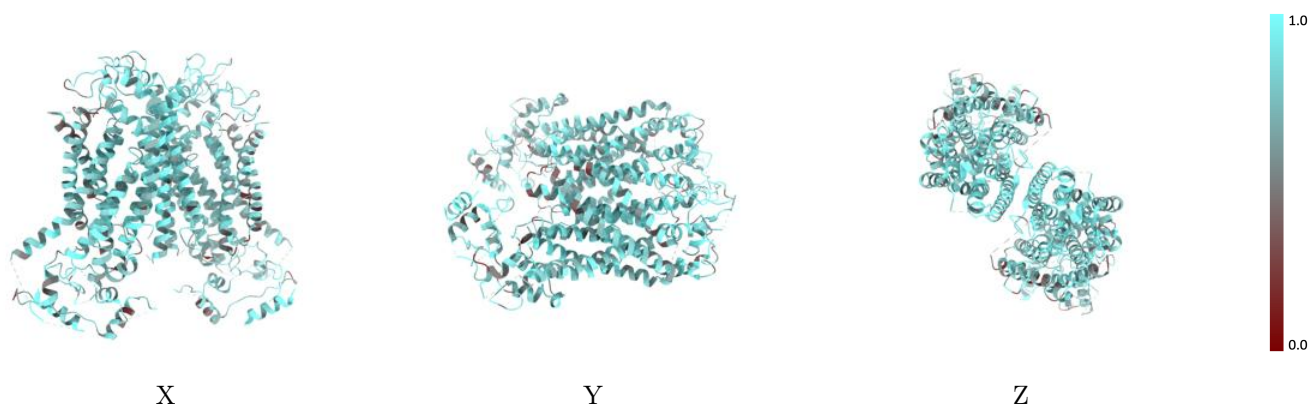
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



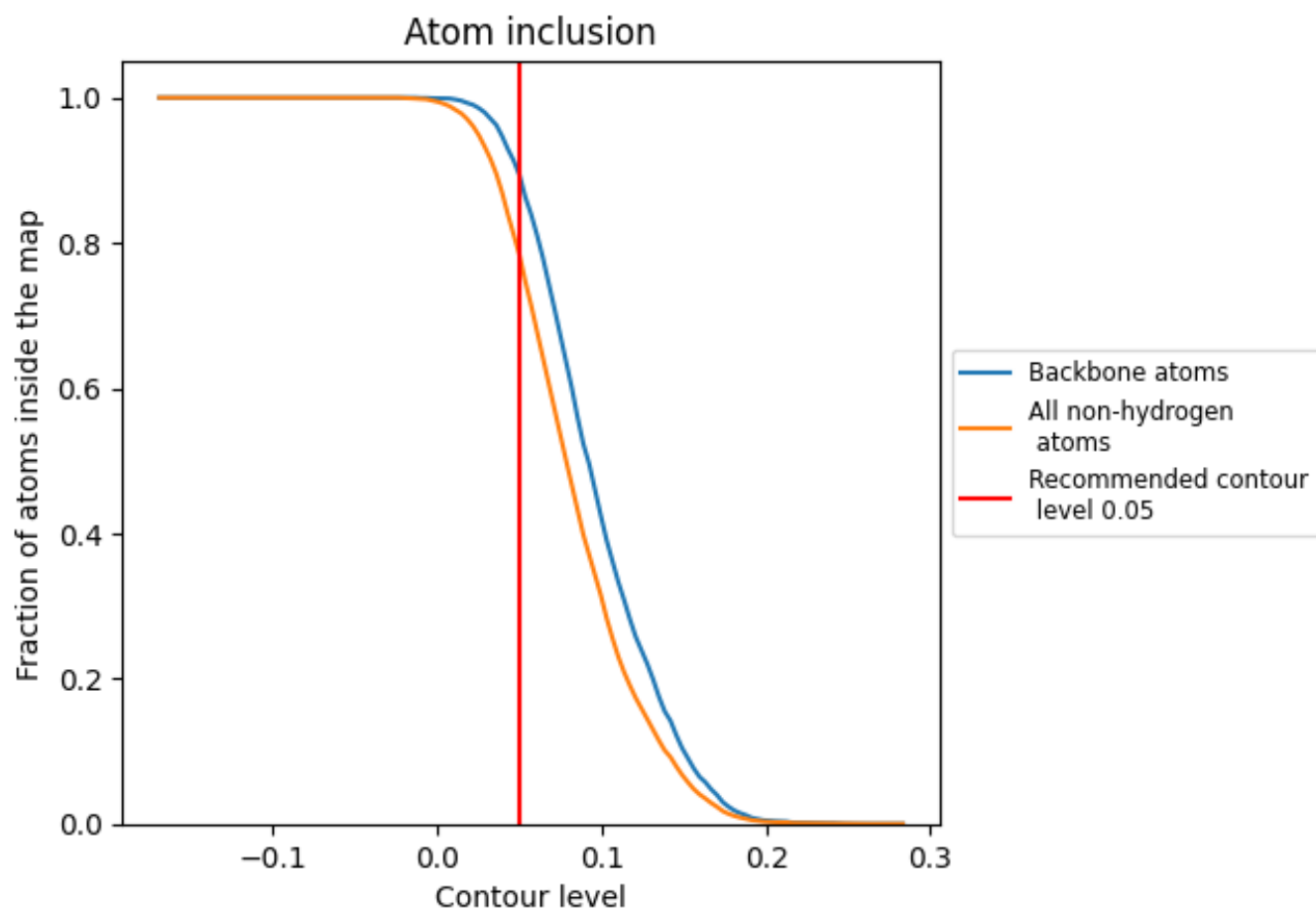
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).



9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 78% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7824	 0.4400
A	 0.7826	 0.4390
B	 0.7821	 0.4400

