



Full wwPDB EM Validation Report ⓘ

Dec 30, 2024 – 02:49 PM EST

PDB ID : 8DG9
EMDB ID : EMD-27419
Title : Cryo-EM Structure of RSV prefusion F trimer in complex with three MxR Fabs
Authors : Rodarte, J.V.; Pancera, M.
Deposited on : 2022-06-23
Resolution : 2.24 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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

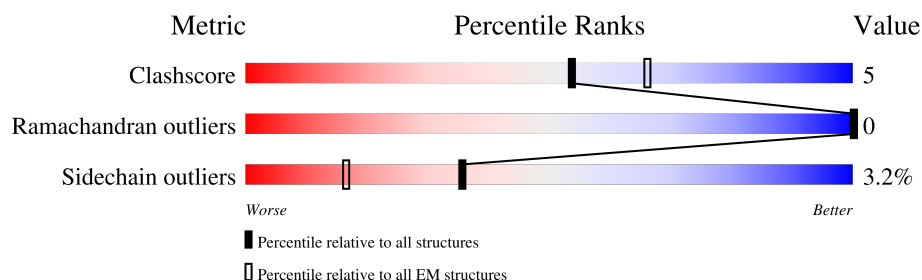
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.24 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	569	
1	B	569	
1	C	569	
2	D	120	
2	F	120	
2	H	120	
3	E	111	
3	G	111	

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Mol	Chain	Length	Quality of chain
3	L	111	<div><div></div><div>81%</div><div>17%</div><div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15450 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 Fusion glycoprotein F0.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	438	Total	C	N	O	S	0	0
			3399	2156	556	665	22		
1	B	438	Total	C	N	O	S	0	0
			3399	2156	556	665	22		
1	C	438	Total	C	N	O	S	0	0
			3399	2156	556	665	22		

- Molecule 2 is a protein called mAb MxR Heavy Chain, VH region.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	120	Total	C	N	O	S	0	0
			906	571	158	173	4		
2	F	120	Total	C	N	O	S	0	0
			906	571	158	173	4		
2	D	120	Total	C	N	O	S	0	0
			906	571	158	173	4		

- Molecule 3 is a protein called mAb MxR Light Chain, VL region.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	111	Total	C	N	O	S	0	0
			817	511	140	164	2		
3	G	111	Total	C	N	O	S	0	0
			817	511	140	164	2		
3	E	111	Total	C	N	O	S	0	0
			817	511	140	164	2		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	

THR
PHE
LEU
GLY
LEU
ASN
ASP
ILE
PHE
GLU
ALA
GLN
LYS
ILE
TRP
GLU
HIS
VAL
GLY
SER
HIS
HIS
HIS
HIS
HIS
HIS

• Molecule 1: Fusion glycoprotein F0

Chain C:  67% 10% 23%

MET
GLU
LEU
LEU
ILE
THR
LEU
LYS
ALA
ASN
ALA
ILE
THR
THR
ILE
LEU
TRP
HIS
VAL
GLY
SER
HIS
HIS
HIS
HIS
HIS
HIS


SER
THR
ALA
PRO
THR
ASN
ASN
ARG
ALA
ARG
GLU
LEU
PRO
ARG
PHE
MET
ASN
TYR
THR
LEU
ASN
ASN
ALA
LYS
LYS
THR
VAL
THR
LEU
SER
LYS
LYS
ARG
LYS
ARG
ARG
F137
L138
L141
K156
G162
K166
F190
L204
P205
L206
L207
ASN
LYS
GLN
SER
C212

S215
V220
T234
P246
N254
N268
K272
L280
Q283
T311
P312
C313
S319
P320
L321
D344
F352
S362
N363
F366
C367
D368
T369
V384
T408
C422
F435
C439
T455
K461
K465
P473
D486
E487
F488

P489
A490
N496
E497
K498
T499
N500
F505
I506
R507
K508
S509
D510
E511
L512
L513
SER
ALA
ILE
GLY
GLY
TYR
ILE
PRO
GLU
ALA
PRO
ARG
ASP
GLY
GLN
ALA
TYR
VAL
ARG
LYS
ASP
GLY
GLU
TRP
VAL
LEU
SER
THR
PHE
LEU
LEU
ASN
ASP
ILE
PHE
GLU
ALA
GLN
LYS
ILE


GLU
TRP
HIS
GLU
GLY
SER
HIS
HIS
HIS
HIS
HIS
HIS
HIS

• Molecule 2: mAb MxR Heavy Chain, VH region

Chain H:  81% 18%


E1
V12
L18
F29
Y32
K33
M34
K43
D61
K64
T68
R71
D72
K75
N76
L78
R83
A84
D85
D86
T87
R84
R88
S100A
K102
S113

• Molecule 2: mAb MxR Heavy Chain, VH region

Chain F:  81% 19%


E1
E6
V12
K13
S17
C22
P28
F29
Y32
K33
M34
I51
R66
R71
N76
S77
L78
M82
L82C
R83
R84
D85
D86
Q105
G106
I107
S113

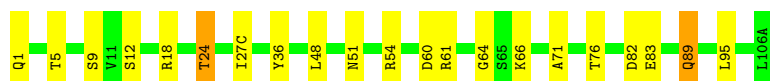
• Molecule 2: mAb MxR Heavy Chain, VH region

Chain D:  86% 12%

E1
V2
S21
C22
F29
K43
D61
K64
T68
R71
K75
N76
S77
L78
Q81
M82
L82C
P100B
K102
S113

• Molecule 3: mAb MxR Light Chain, VL region

Chain L:  81% 17%



- Molecule 3: mAb MxR Light Chain, VL region

Chain G:

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	354922	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	21.136	Depositor
Minimum map value	-13.856	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.368	Depositor
Recommended contour level	2	Depositor
Map size (Å)	395.07837, 395.07837, 395.07837	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.02885, 1.02885, 1.02885	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	0.27	0/3447	0.48	0/4668
1	B	0.27	0/3447	0.47	0/4668
1	C	0.30	0/3447	0.50	0/4668
2	D	0.28	0/925	0.53	0/1247
2	F	0.27	0/925	0.53	0/1247
2	H	0.27	0/925	0.54	0/1247
3	E	0.35	0/836	0.54	0/1141
3	G	0.28	0/836	0.50	0/1141
3	L	0.30	0/836	0.51	0/1141
All	All	0.28	0/15624	0.50	0/21168

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	3399	0	3447	25	0
1	B	3399	0	3448	40	0
1	C	3399	0	3448	33	0
2	D	906	0	889	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	906	0	889	11	0
2	H	906	0	889	9	0
3	E	817	0	788	14	0
3	G	817	0	788	9	0
3	L	817	0	788	11	0
4	A	28	0	26	0	0
4	B	28	0	26	1	0
4	C	28	0	26	1	0
All	All	15450	0	15452	154	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (154) 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:26:GLN:N	1:B:363:ASN:OD1	2.12	0.82
1:A:26:GLN:N	1:A:43:GLY:O	2.27	0.68
1:A:394:LYS:NZ	1:A:489:ASP:OD1	2.27	0.68
2:F:66:ARG:NH1	2:F:86:ASP:OD2	2.27	0.67
2:F:82:MET:HB2	2:F:82(C):LEU:HD21	1.77	0.66
1:B:306:TYR:HB3	1:B:309:ILE:HD11	1.78	0.64
1:B:178:VAL:HG22	1:B:188:LEU:HD23	1.78	0.64
1:C:311:THR:HG21	1:C:344:ASP:O	1.98	0.64
3:E:61:ARG:NH1	3:E:82:ASP:OD2	2.28	0.64
3:L:61:ARG:NH1	3:L:82:ASP:OD2	2.31	0.63
1:C:26:GLN:N	1:C:363:ASN:HD22	1.97	0.62
1:B:321:LEU:HD11	1:B:473:PRO:HB3	1.81	0.62
3:E:27(B):ASN:OD1	3:E:27(C):ILE:N	2.32	0.62
1:B:138:LEU:HB3	1:B:141:LEU:HD12	1.82	0.62
2:F:6:GLU:H	2:F:105:GLN:HE22	1.50	0.60
3:L:5:THR:HB	3:L:24:THR:HG23	1.83	0.60
1:A:138:LEU:HB3	1:A:141:LEU:HD12	1.84	0.59
3:L:18:ARG:HG3	3:L:76:THR:HG22	1.85	0.59
1:A:321:LEU:HD11	1:A:473:PRO:HB3	1.85	0.59
2:H:72:ASP:OD2	2:H:75:LYS:HG3	2.04	0.58
3:L:48:LEU:HD21	3:L:64:GLY:HA3	1.85	0.58
2:F:6:GLU:HB3	2:F:107:ILE:HD13	1.84	0.58
1:C:138:LEU:HB3	1:C:141:LEU:HD12	1.86	0.57
1:B:58:THR:HG23	1:B:296:VAL:HG23	1.86	0.57
3:G:61:ARG:NH1	3:G:82:ASP:OD2	2.27	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:82:MET:HB3	2:D:82(C):LEU:HD21	1.88	0.56
2:F:12:VAL:HG11	2:F:82(C):LEU:HD12	1.88	0.55
1:B:44:TYR:HA	1:B:363:ASN:HD21	1.71	0.55
1:C:246:PRO:HB3	1:C:283:GLN:HA	1.89	0.54
1:A:246:PRO:HB3	1:A:283:GLN:HA	1.90	0.54
1:B:486:ASP:OD1	1:B:486:ASP:N	2.41	0.54
1:B:232:GLU:OE2	1:B:235:ARG:NH2	2.33	0.54
1:B:246:PRO:HB3	1:B:283:GLN:HA	1.90	0.53
1:B:394:LYS:NZ	1:B:489:ASP:OD1	2.32	0.53
1:A:291:ILE:HD11	1:A:293:LYS:HE3	1.90	0.53
3:L:36:TYR:HE2	3:L:89:GLN:HG2	1.74	0.53
1:B:280:ILE:HG21	1:B:366:PHE:CG	2.44	0.53
3:G:85:VAL:HG22	3:G:103:LYS:HG2	1.90	0.53
1:B:76:VAL:HG11	1:B:212:CYS:HB3	1.91	0.52
1:B:268:ASN:O	1:B:272:LYS:HG3	2.10	0.52
1:C:362:SER:HG	1:C:363:ASN:H	1.54	0.52
3:G:1:GLN:HB2	3:G:26:THR:HG21	1.92	0.51
3:E:48:LEU:HD21	3:E:64:GLY:HA3	1.91	0.51
1:C:496:ASN:HB3	4:C:601:NAG:H61	1.93	0.51
1:A:513:LEU:HD12	1:B:512:LEU:HD21	1.93	0.51
1:C:268:ASN:O	1:C:272:LYS:HG3	2.10	0.51
1:C:280:ILE:HG21	1:C:366:PHE:CG	2.45	0.51
1:C:486:ASP:N	1:C:486:ASP:OD1	2.42	0.51
1:B:59:ILE:HG23	1:B:193:LEU:HB3	1.92	0.50
1:A:26:GLN:N	1:A:363:ASN:OD1	2.44	0.50
1:C:362:SER:OG	1:C:363:ASN:N	2.44	0.50
1:A:426:ASN:HD21	1:A:429:ARG:HB2	1.77	0.50
1:A:79:ILE:HG12	1:A:220:VAL:HG22	1.93	0.50
3:G:38:GLN:HG3	3:G:44:PRO:HG3	1.94	0.49
1:B:73:ASP:OD1	1:B:74:ALA:N	2.45	0.49
1:C:422:CYS:HB2	1:C:435:PHE:HB2	1.93	0.49
1:A:37:CYS:SG	1:A:319:SER:HB3	2.52	0.49
1:B:461:LYS:HB2	1:C:156:LYS:HZ3	1.77	0.49
3:G:54:ARG:NH1	3:G:60:ASP:OD1	2.46	0.49
1:B:46:SER:HB2	1:B:48:LEU:HD13	1.94	0.49
1:A:352:PHE:CE2	1:A:367:CYS:HB3	2.48	0.48
1:A:503:LEU:HD23	1:A:506:ILE:HD11	1.95	0.48
1:B:352:PHE:CE2	1:B:367:CYS:HB3	2.48	0.48
3:G:48:LEU:HD21	3:G:64:GLY:HA3	1.94	0.48
1:A:58:THR:HG23	1:A:296:VAL:HG23	1.95	0.48
2:H:12:VAL:HG21	2:H:18:LEU:HG	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:84:ALA:O	2:H:87:THR:HG22	2.14	0.48
3:E:34:HIS:HB2	3:E:89:GLN:HE21	1.79	0.48
1:A:280:ILE:HG21	1:A:366:PHE:CG	2.48	0.48
1:A:486:ASP:N	1:A:486:ASP:OD1	2.45	0.48
1:B:44:TYR:HA	1:B:363:ASN:ND2	2.29	0.47
3:E:34:HIS:HD2	3:E:89:GLN:NE2	2.12	0.47
1:C:79:ILE:HG21	1:C:207:LEU:HD11	1.96	0.47
2:D:2:VAL:HG11	2:D:102:LYS:HG2	1.95	0.47
1:B:73:ASP:HB3	1:B:76:VAL:HG23	1.97	0.47
1:C:497:GLU:O	1:C:500:ASN:HB2	2.15	0.47
3:E:11:VAL:HG13	3:E:104:LEU:HD12	1.95	0.46
1:A:46:SER:HB2	1:A:48:LEU:HD13	1.98	0.46
1:B:56:VAL:HB	1:B:189:THR:HG22	1.96	0.46
1:B:204:LEU:HB3	1:B:205:PRO:HD3	1.97	0.46
1:C:321:LEU:HD11	1:C:473:PRO:HB3	1.97	0.46
1:C:352:PHE:CE2	1:C:367:CYS:HB3	2.50	0.46
3:E:7:PRO:O	3:E:102:THR:OG1	2.25	0.46
1:B:164:VAL:O	1:B:168:LYS:HG3	2.15	0.45
1:C:46:SER:HB3	1:C:313:CYS:SG	2.57	0.45
1:C:75:LYS:HB2	1:C:75:LYS:NZ	2.31	0.45
1:B:465:LYS:HB3	1:B:465:LYS:HE3	1.71	0.45
3:E:89:GLN:HB3	3:E:98:PHE:CD1	2.52	0.45
1:A:461:LYS:HA	1:A:461:LYS:HD2	1.75	0.44
3:L:54:ARG:NH1	3:L:60:ASP:OD1	2.50	0.44
1:C:487:GLU:HB3	1:C:490:ALA:HB2	1.99	0.44
1:B:487:GLU:HB3	1:B:490:ALA:HB2	2.00	0.44
2:D:68:THR:HG23	2:D:81:GLN:HB3	1.98	0.44
3:G:2:SER:O	3:G:2:SER:OG	2.33	0.44
1:C:30:GLU:OE2	1:C:408:THR:OG1	2.21	0.44
2:D:22:CYS:HB3	2:D:78:LEU:HB3	2.00	0.44
2:D:61:ASP:HA	2:D:64:LYS:HE3	2.00	0.44
2:D:75:LYS:HB2	2:D:75:LYS:HE2	1.76	0.44
1:B:455:THR:HG23	1:C:369:THR:HG22	2.00	0.44
1:B:394:LYS:HB3	1:B:394:LYS:HE2	1.77	0.44
2:H:32:TYR:O	2:H:71:ARG:NH2	2.46	0.44
1:B:445:LYS:HD3	1:B:445:LYS:HA	1.53	0.44
1:C:79:ILE:HG12	1:C:220:VAL:HG22	1.98	0.44
1:B:269:ASP:OD1	1:B:272:LYS:NZ	2.50	0.43
2:F:34:MET:HB3	2:F:78:LEU:HD22	2.00	0.43
2:H:94:ARG:HB3	2:H:102:LYS:HB2	2.01	0.43
1:C:46:SER:HB2	1:C:48:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:27:ASN:HA	3:E:28:GLY:HA3	1.99	0.43
1:B:60:GLU:HG3	1:B:191:LYS:HD3	2.01	0.43
2:D:100(B):PRO:HG3	3:E:49:PHE:HB3	2.01	0.43
2:H:61:ASP:HA	2:H:64:LYS:HE3	1.99	0.43
2:D:29:PHE:CD2	2:D:76:ASN:HA	2.53	0.43
3:L:83:GLU:O	3:L:83:GLU:HG3	2.19	0.42
1:B:422:CYS:HB2	1:B:435:PHE:HB2	2.00	0.42
2:F:13:LYS:NZ	2:F:113:SER:O	2.40	0.42
1:C:461:LYS:HA	1:C:461:LYS:HD2	1.86	0.42
1:C:77:LYS:HE2	1:C:81:GLN:OE1	2.19	0.42
3:L:61:ARG:HH12	3:L:82:ASP:CG	2.23	0.42
1:C:93:LEU:HG	1:C:234:THR:HG23	2.01	0.42
3:E:82:ASP:O	3:E:104:LEU:HD23	2.20	0.42
1:C:26:GLN:HG3	1:C:45:LEU:HD11	2.01	0.42
1:C:37:CYS:SG	1:C:319:SER:HB3	2.60	0.42
1:A:426:ASN:HA	1:A:448:ASP:HB2	2.02	0.42
1:B:79:ILE:HG12	1:B:220:VAL:HG22	2.01	0.42
3:G:27(A):SER:OG	3:G:92:ASP:OD2	2.30	0.42
1:B:500:ASN:OD1	4:B:601:NAG:H2	2.20	0.42
1:B:308:VAL:O	1:B:309:ILE:HD13	2.20	0.41
2:F:29:PHE:CD2	2:F:76:ASN:HA	2.54	0.41
1:C:204:LEU:HB3	1:C:205:PRO:HD3	2.02	0.41
1:A:493:SER:O	1:A:497:GLU:HG3	2.20	0.41
3:L:1:GLN:OE1	3:L:1:GLN:N	2.47	0.41
1:B:423:THR:HG21	1:B:431:ILE:HD13	2.03	0.41
2:H:98:ARG:HG2	2:H:100(A):SER:HB3	2.01	0.41
1:B:291:ILE:HD11	1:B:293:LYS:HE3	2.02	0.41
1:C:162:GLY:O	1:C:166:LYS:HD3	2.20	0.41
1:C:506:ILE:HG13	1:C:507:ARG:N	2.35	0.41
1:A:401:ASP:OD1	1:A:401:ASP:N	2.52	0.41
3:G:59:PRO:HB2	3:G:61:ARG:HG3	2.02	0.41
3:L:66:LYS:HG3	3:L:71:ALA:HB2	2.01	0.41
1:B:347:GLY:HA2	2:F:28:PRO:HG2	2.03	0.41
1:A:369:THR:HG22	1:C:455:THR:HB	2.03	0.41
3:L:27(C):ILE:HG23	3:L:66:LYS:HD2	2.02	0.41
3:E:59:PRO:HB2	3:E:61:ARG:HG3	2.02	0.41
2:F:32:TYR:O	2:F:71:ARG:NH2	2.49	0.41
1:C:46:SER:OG	1:C:311:THR:HB	2.21	0.41
1:A:503:LEU:HD23	1:A:503:LEU:HA	1.94	0.40
2:H:29:PHE:CD2	2:H:76:ASN:HA	2.57	0.40
3:E:61:ARG:HB3	3:E:76:THR:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:SER:HA	1:A:473:PRO:HA	2.04	0.40
1:A:268:ASN:HB3	1:A:272:LYS:NZ	2.36	0.40
2:H:34:MET:HB3	2:H:78:LEU:HD22	2.03	0.40
1:B:232:GLU:HG3	1:B:250:TYR:CE1	2.57	0.40
2:F:33:LYS:HG3	2:F:51:ILE:O	2.22	0.40
3:E:78:LEU:HD11	3:E:104:LEU:HD21	2.02	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	430/569 (76%)	424 (99%)	6 (1%)	0	100	100
1	B	430/569 (76%)	423 (98%)	7 (2%)	0	100	100
1	C	430/569 (76%)	422 (98%)	8 (2%)	0	100	100
2	D	118/120 (98%)	113 (96%)	5 (4%)	0	100	100
2	F	118/120 (98%)	112 (95%)	6 (5%)	0	100	100
2	H	118/120 (98%)	115 (98%)	3 (2%)	0	100	100
3	E	109/111 (98%)	104 (95%)	5 (5%)	0	100	100
3	G	109/111 (98%)	103 (94%)	6 (6%)	0	100	100
3	L	109/111 (98%)	102 (94%)	7 (6%)	0	100	100
All	All	1971/2400 (82%)	1918 (97%)	53 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	400/512 (78%)	391 (98%)	9 (2%)	45	52
1	B	400/512 (78%)	391 (98%)	9 (2%)	45	52
1	C	400/512 (78%)	391 (98%)	9 (2%)	45	52
2	D	96/97 (99%)	91 (95%)	5 (5%)	19	18
2	F	96/97 (99%)	92 (96%)	4 (4%)	25	27
2	H	96/97 (99%)	90 (94%)	6 (6%)	15	12
3	E	89/89 (100%)	84 (94%)	5 (6%)	17	16
3	G	89/89 (100%)	85 (96%)	4 (4%)	23	24
3	L	89/89 (100%)	83 (93%)	6 (7%)	13	11
All	All	1755/2094 (84%)	1698 (97%)	57 (3%)	36	39

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	LYS
1	A	96	LEU
1	A	190	PHE
1	A	319	SER
1	A	402	VAL
1	A	451	SER
1	A	455	THR
1	A	465	LYS
1	A	503	LEU
2	H	43	LYS
2	H	68	THR
2	H	71	ARG
2	H	83	ARG
2	H	85	ASP
2	H	113	SER
3	L	9	SER
3	L	12	SER
3	L	24	THR

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Mol	Chain	Res	Type
3	L	51	ASN
3	L	89	GLN
3	L	95	LEU
1	B	190	PHE
1	B	254	ASN
1	B	348	SER
1	B	372	SER
1	B	427	LYS
1	B	439	CYS
1	B	465	LYS
1	B	488	PHE
1	B	500	ASN
2	F	17	SER
2	F	22	CYS
2	F	83	ARG
2	F	85	ASP
3	G	2	SER
3	G	45	LYS
3	G	50	ASP
3	G	95	LEU
1	C	62	SER
1	C	190	PHE
1	C	254	ASN
1	C	384	VAL
1	C	439	CYS
1	C	455	THR
1	C	465	LYS
1	C	488	PHE
1	C	498	LYS
2	D	21	SER
2	D	43	LYS
2	D	68	THR
2	D	71	ARG
2	D	102	LYS
3	E	51	ASN
3	E	70	SER
3	E	89	GLN
3	E	95	LEU
3	E	103	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	363	ASN
1	B	363	ASN
3	E	89	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	$\# Z > 2$
4	NAG	C	601	1	14,14,15	0.33	0	17,19,21	0.34	0
4	NAG	B	601	1	14,14,15	0.53	0	17,19,21	0.50	0
4	NAG	C	602	1	14,14,15	0.31	0	17,19,21	0.55	0
4	NAG	B	602	1	14,14,15	0.22	0	17,19,21	0.40	0
4	NAG	A	5001	1	14,14,15	0.49	0	17,19,21	0.54	0
4	NAG	A	5002	1	14,14,15	0.47	0	17,19,21	0.58	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
4	NAG	C	601	1	-	0/6/23/26	0/1/1/1
4	NAG	B	601	1	-	2/6/23/26	0/1/1/1
4	NAG	C	602	1	-	4/6/23/26	0/1/1/1
4	NAG	B	602	1	-	0/6/23/26	0/1/1/1
4	NAG	A	5001	1	-	0/6/23/26	0/1/1/1
4	NAG	A	5002	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	602	NAG	O5-C5-C6-O6
4	C	602	NAG	C4-C5-C6-O6
4	B	601	NAG	C4-C5-C6-O6
4	B	601	NAG	O5-C5-C6-O6
4	A	5002	NAG	C4-C5-C6-O6
4	C	602	NAG	C3-C2-N2-C7
4	C	602	NAG	C1-C2-N2-C7
4	A	5002	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	601	NAG	1	0
4	B	601	NAG	1	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.

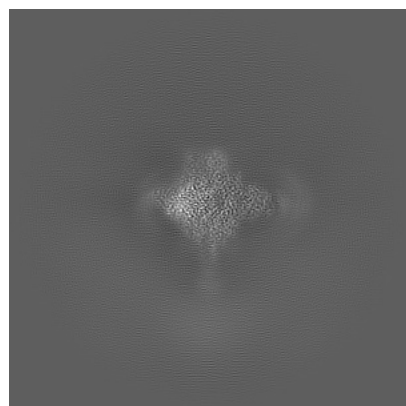
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27419. These allow visual inspection of the internal detail of the map and identification of artifacts.

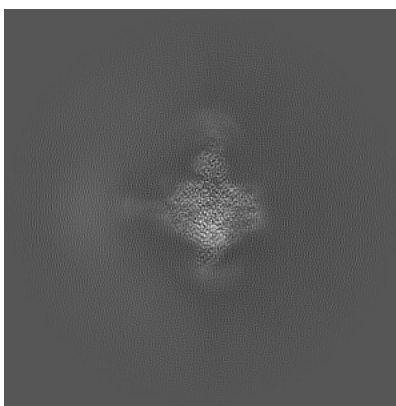
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

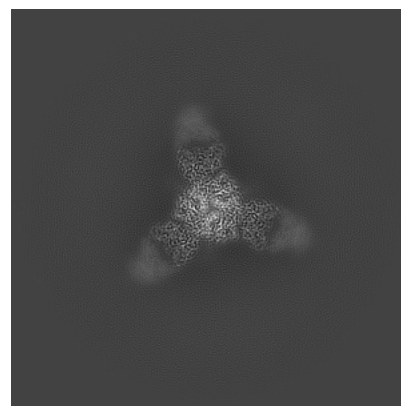
6.1.1 Primary map



X

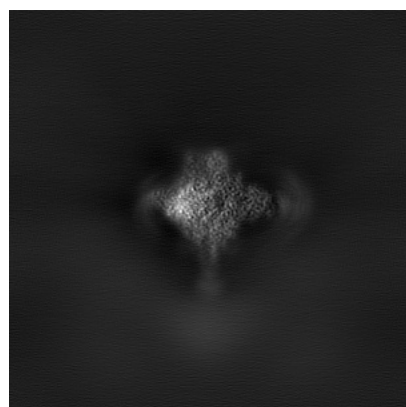


Y

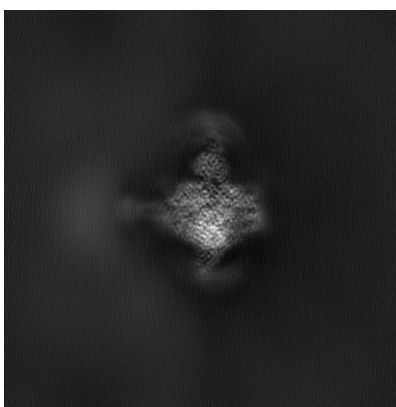


Z

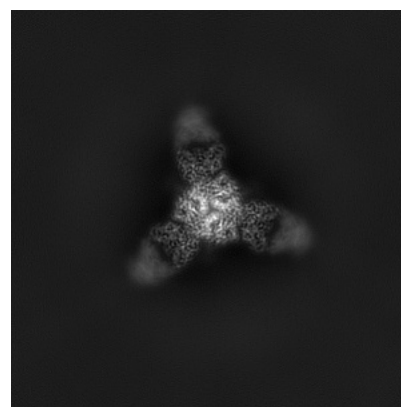
6.1.2 Raw map



X



Y

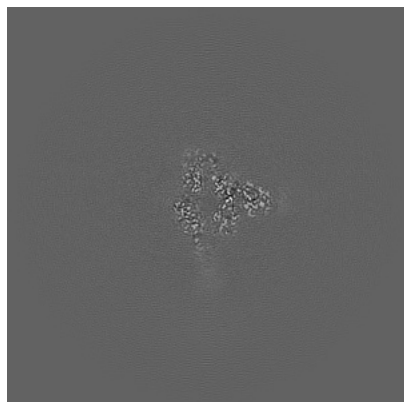


Z

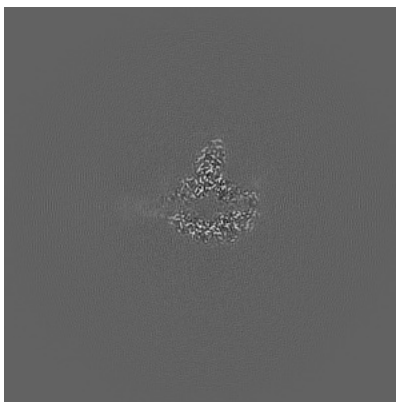
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

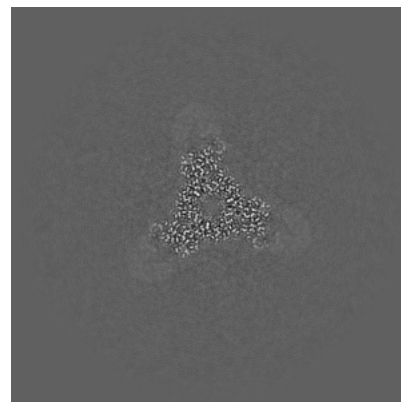
6.2.1 Primary map



X Index: 192

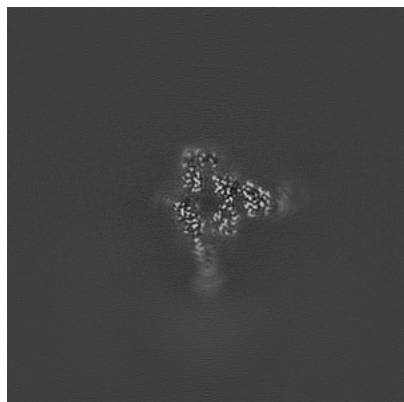


Y Index: 192

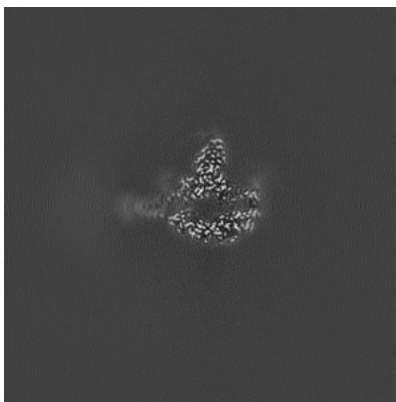


Z Index: 192

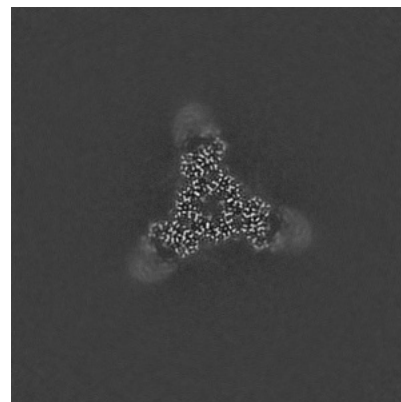
6.2.2 Raw map



X Index: 192



Y Index: 192

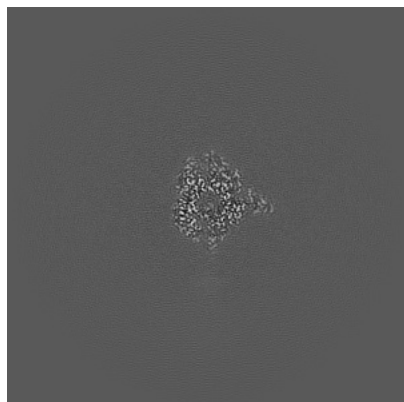


Z Index: 192

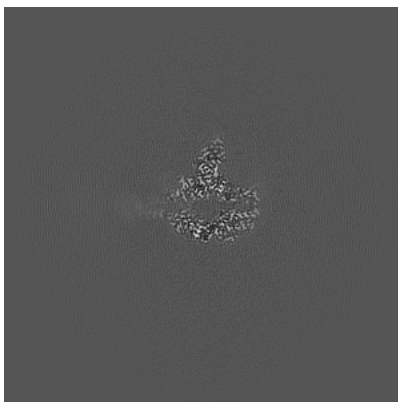
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

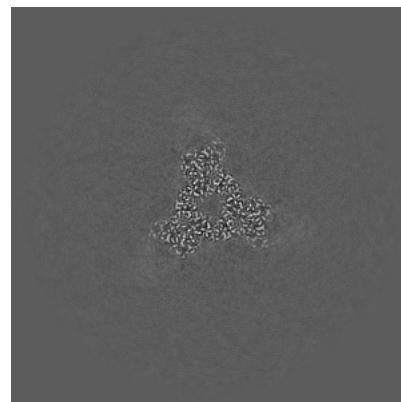
6.3.1 Primary map



X Index: 201

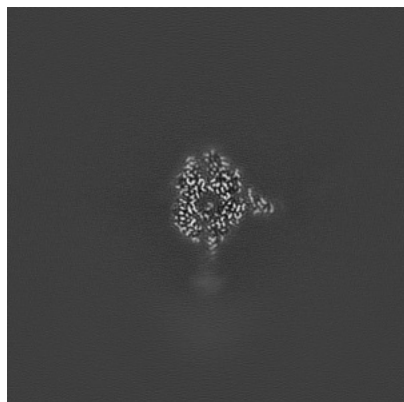


Y Index: 193

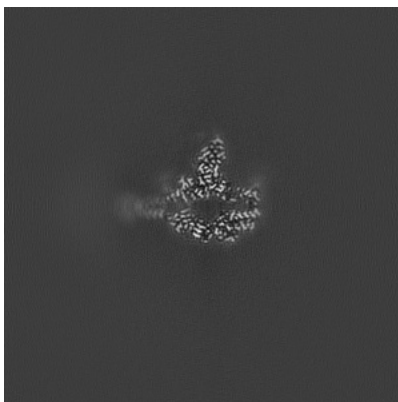


Z Index: 193

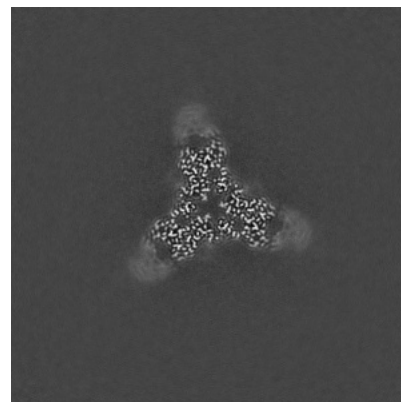
6.3.2 Raw map



X Index: 201



Y Index: 193

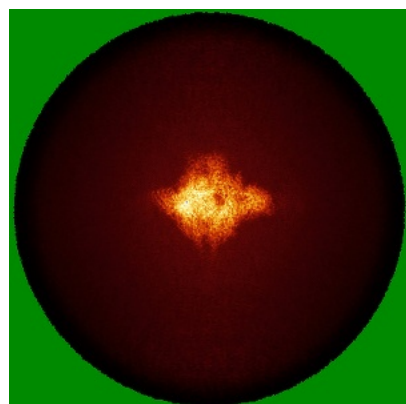


Z Index: 195

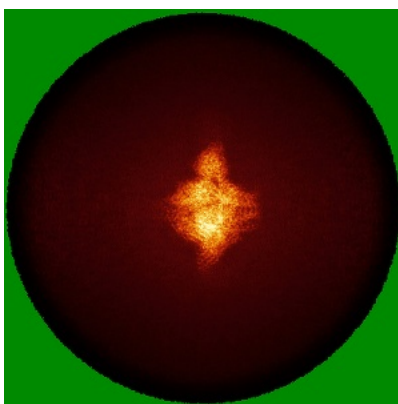
The images above show the largest variance slices of the map in three orthogonal directions.

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

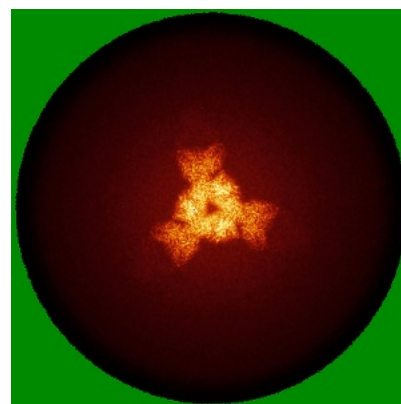
6.4.1 Primary map



X

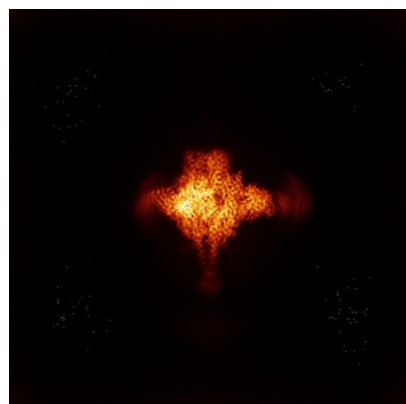


Y

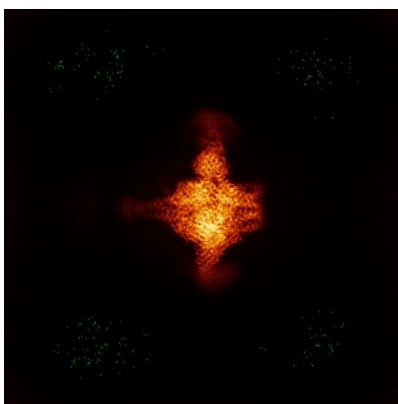


Z

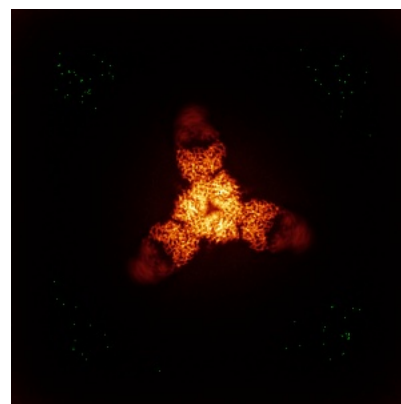
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



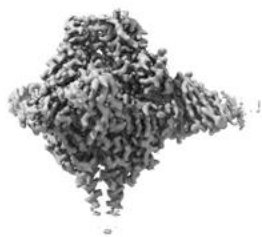
Y



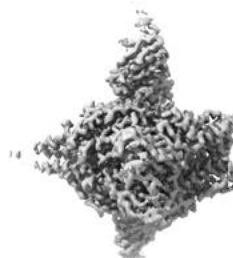
Z

The images above show the 3D surface view of the map at the recommended contour level 2.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

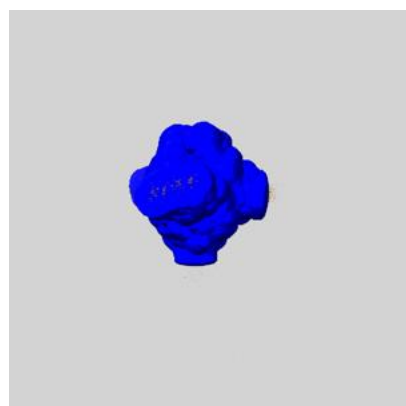
6.6 Mask visualisation [i](#)

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

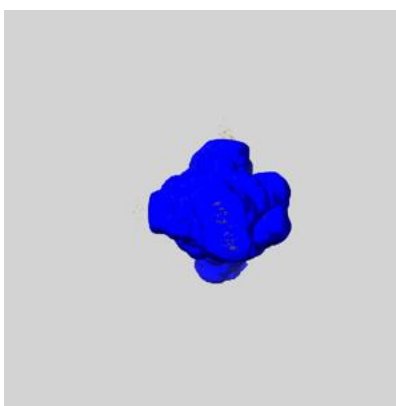
A mask typically either:

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

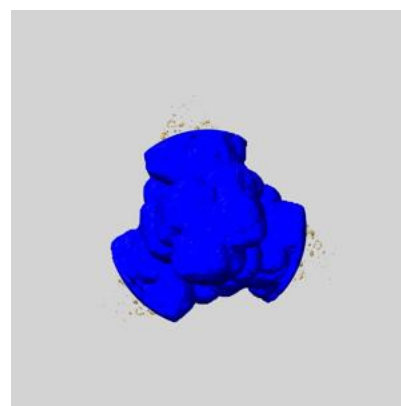
6.6.1 emd_27419_msk_1.map [i](#)



X



Y

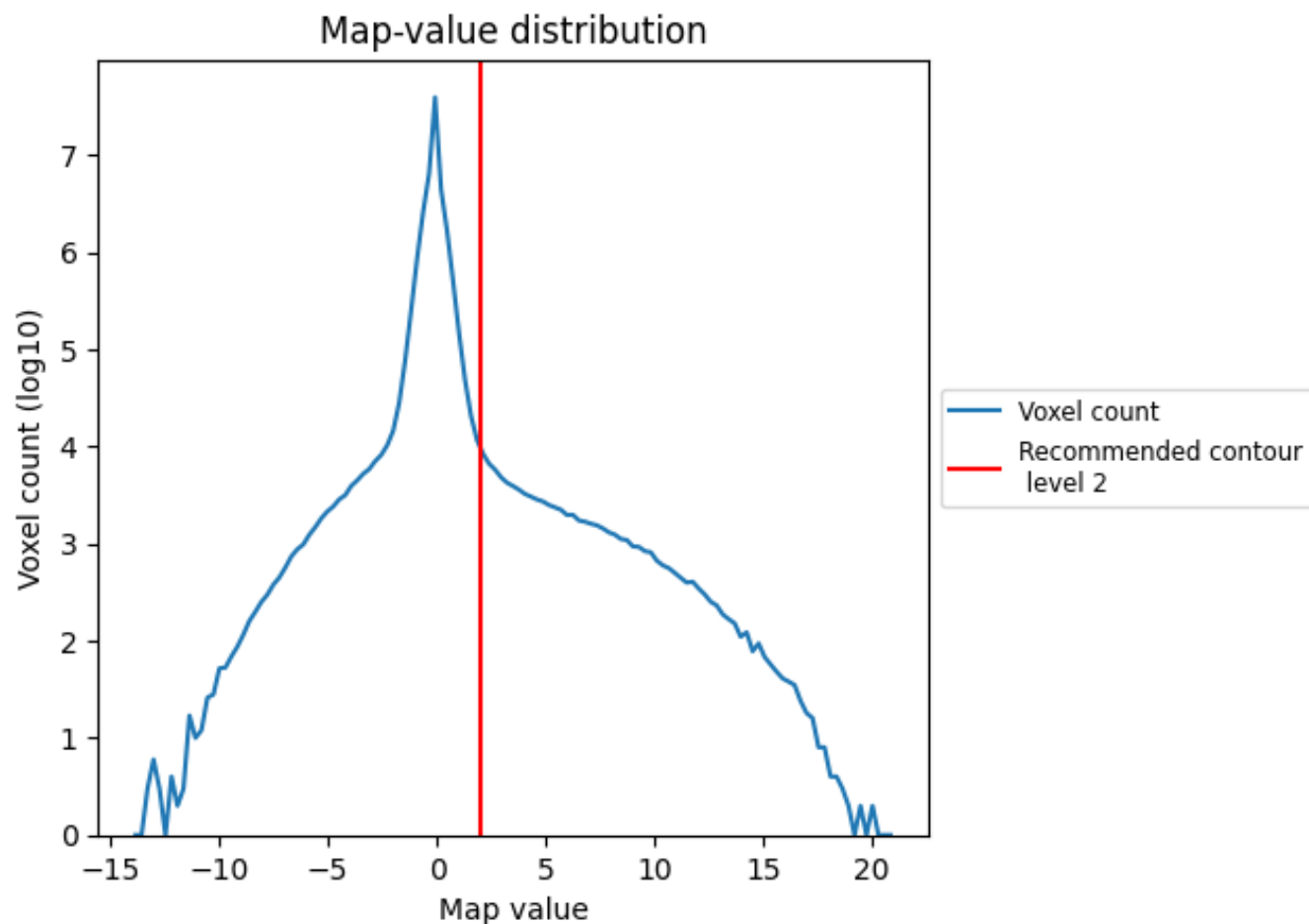


Z

7 Map analysis [i](#)

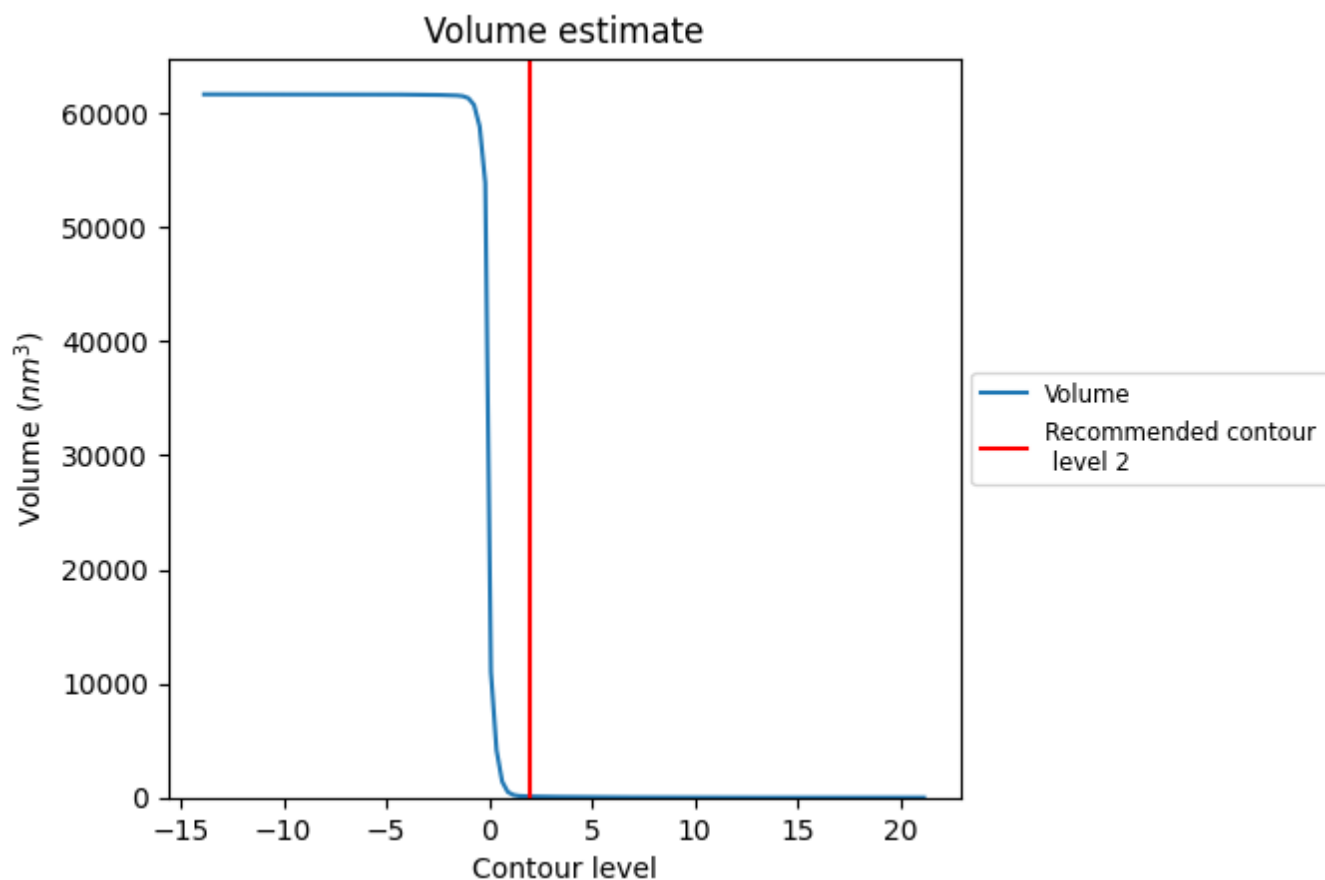
This section contains the results of statistical analysis of the map.

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.

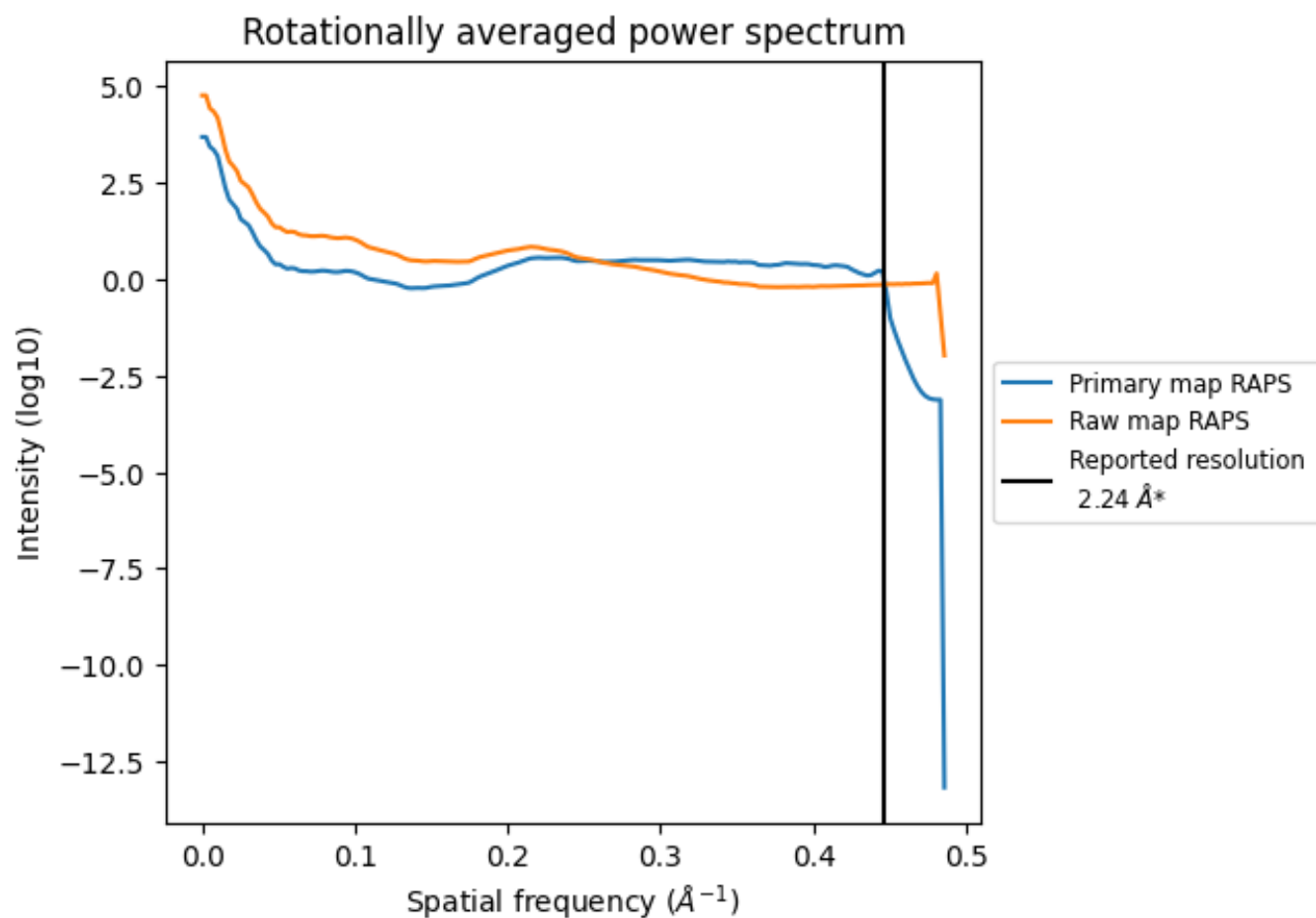
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 95 nm^3 ; this corresponds to an approximate mass of 86 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 ⓘ

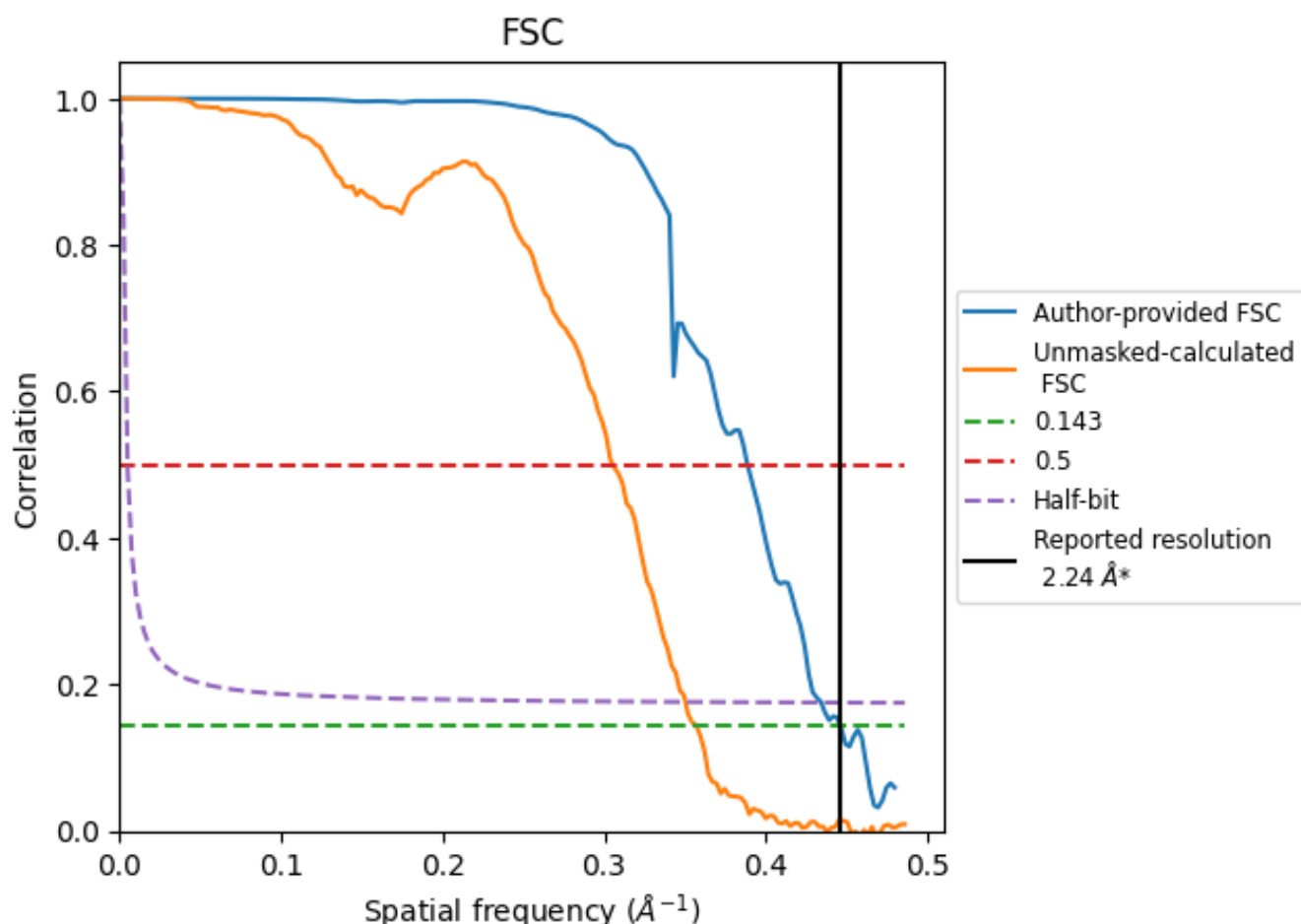


*Reported resolution corresponds to spatial frequency of 0.446 Å⁻¹

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 0.446 Å⁻¹

8.2 Resolution estimates [i](#)

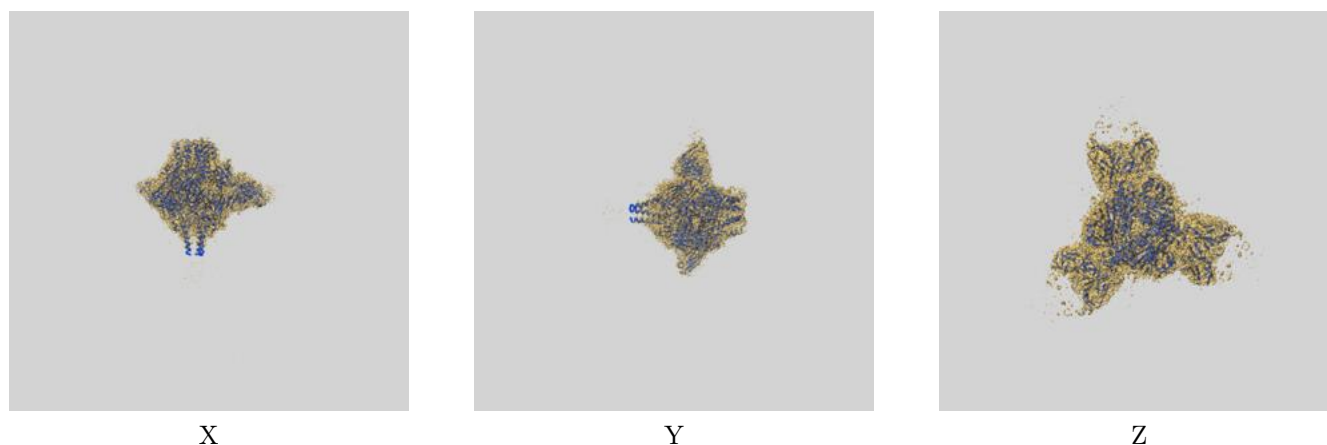
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.24	-	-
Author-provided FSC curve	2.24	2.57	2.30
Unmasked-calculated*	2.80	3.28	2.86

*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 2.80 differs from the reported value 2.24 by more than 10 %

9 Map-model fit [i](#)

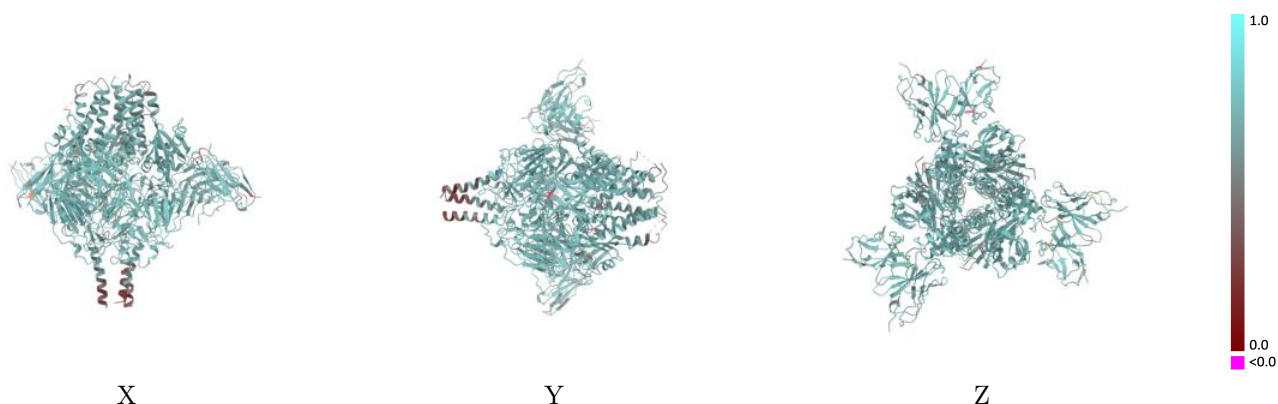
This section contains information regarding the fit between EMDB map EMD-27419 and PDB model 8DG9. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



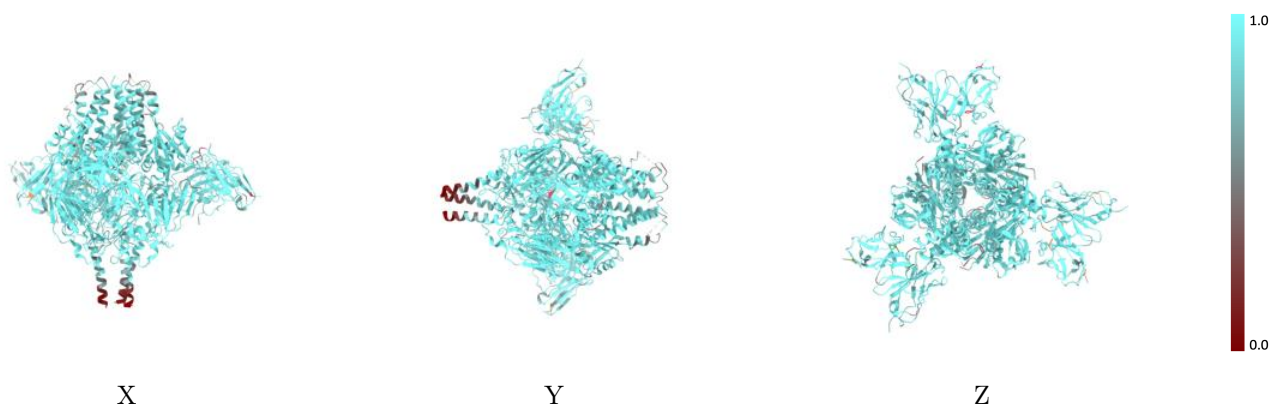
The images above show the 3D surface view of the map at the recommended contour level 2.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



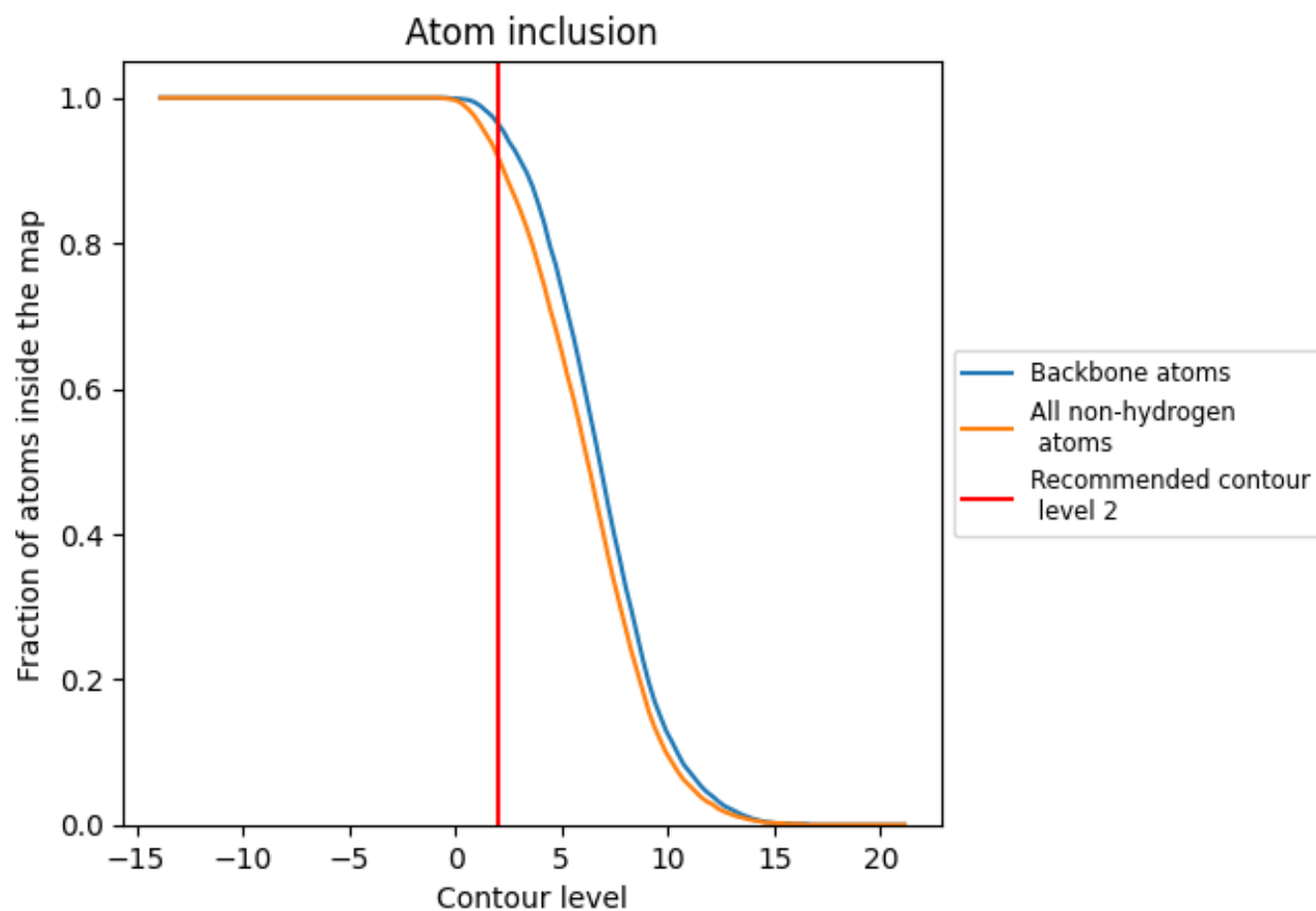
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 92% 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 (2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9200	<div><div></div></div> 0.6760
A	<div><div></div></div> 0.9160	<div><div></div></div> 0.6770
B	<div><div></div></div> 0.9130	<div><div></div></div> 0.6750
C	<div><div></div></div> 0.9160	<div><div></div></div> 0.6790
D	<div><div></div></div> 0.9390	<div><div></div></div> 0.6810
E	<div><div></div></div> 0.9280	<div><div></div></div> 0.6780
F	<div><div></div></div> 0.9290	<div><div></div></div> 0.6780
G	<div><div></div></div> 0.9180	<div><div></div></div> 0.6650
H	<div><div></div></div> 0.9330	<div><div></div></div> 0.6770
L	<div><div></div></div> 0.9280	<div><div></div></div> 0.6700

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