



## Full wwPDB EM Validation Report ⓘ

Dec 22, 2022 – 06:07 pm GMT

PDB ID : 8ACH  
EMDB ID : EMD-15348  
Title : Nudaurelia capensis omega virus maturation intermediate captured at pH5.6  
(insect cell expressed VLPs): large class from symmetry expansion  
Authors : Castells-Graells, R.; Hesketh, E.L.; Johnson, J.E.; Ranson, N.A.; Lawson,  
D.M.; Lomonosoff, G.P.  
Deposited on : 2022-07-05  
Resolution : 3.91 Å (reported)  
Based on initial model : 8AC6

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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  
MolProbity : 4.02b-467  
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

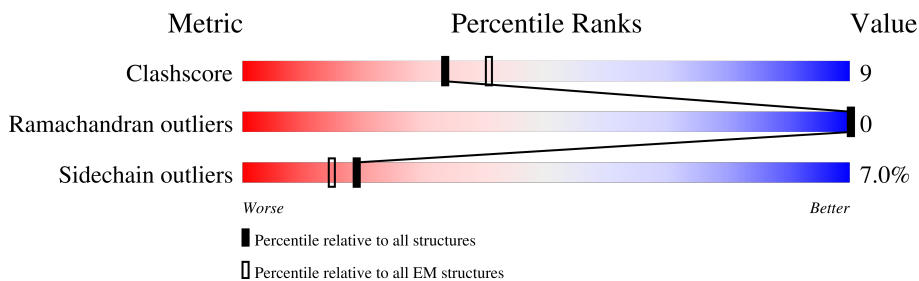
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.91 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  $\geq 3$ , 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	644	
1	B	644	
1	C	644	
1	D	644	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 16450 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 p70.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	536	4103	2606	682	803	12	0	0
1	B	538	4116	2613	685	806	12	0	0
1	C	538	4116	2613	685	806	12	0	0
1	D	538	4115	2614	685	804	12	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	ARG	HIS	conflict	UNP Q4TVS9
A	204	THR	ALA	conflict	UNP Q4TVS9
A	576	LEU	SER	conflict	UNP Q4TVS9
B	37	ARG	HIS	conflict	UNP Q4TVS9
B	204	THR	ALA	conflict	UNP Q4TVS9
B	576	LEU	SER	conflict	UNP Q4TVS9
C	37	ARG	HIS	conflict	UNP Q4TVS9
C	204	THR	ALA	conflict	UNP Q4TVS9
C	576	LEU	SER	conflict	UNP Q4TVS9
D	37	ARG	HIS	conflict	UNP Q4TVS9
D	204	THR	ALA	conflict	UNP Q4TVS9
D	576	LEU	SER	conflict	UNP Q4TVS9







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	96960	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 ( $e^-/\text{\AA}^2$ )	49.1	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.100	Depositor
Minimum map value	-0.048	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	766.80194, 766.80194, 766.80194	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.49766, 1.49766, 1.49766	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.25	0/4211	0.47	0/5769
1	B	0.25	0/4224	0.47	0/5786
1	C	0.25	0/4224	0.47	0/5786
1	D	0.26	0/4223	0.47	0/5785
All	All	0.25	0/16882	0.47	0/23126

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	4103	0	3949	59	0
1	B	4116	0	3960	82	0
1	C	4116	0	3960	70	0
1	D	4115	0	3965	91	0
All	All	16450	0	15834	294	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 9.

All (294) 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:A:185:VAL:O	1:A:189:ASN:ND2	2.09	0.85
1:D:482:PHE:O	1:D:484:ARG:NH2	2.10	0.85
1:C:533:ASN:ND2	1:D:223:ASP:OD2	2.11	0.83
1:C:461:ASN:ND2	1:C:463:VAL:O	2.12	0.82
1:B:133:GLU:OE1	1:B:214:ARG:NH1	2.13	0.81
1:A:433:GLN:O	1:A:437:ASN:ND2	2.13	0.81
1:B:460:ARG:NH1	1:B:502:MET:O	2.14	0.81
1:A:284:HIS:NE2	1:A:349:MET:SD	2.53	0.80
1:B:151:SER:OG	1:B:172:ASN:OD1	2.00	0.80
1:D:288:VAL:O	1:D:404:ASN:ND2	2.15	0.79
1:B:94:LYS:NZ	1:B:102:THR:OG1	2.18	0.76
1:C:199:SER:O	1:C:201:GLN:NE2	2.18	0.76
1:B:324:GLN:N	1:B:324:GLN:OE1	2.20	0.75
1:A:135:CYS:SG	1:A:514:LYS:NZ	2.60	0.75
1:B:199:SER:OG	1:B:201:GLN:OE1	2.04	0.74
1:D:75:ARG:O	1:D:75:ARG:NH1	2.22	0.73
1:D:370:THR:OG1	1:D:387:THR:OG1	2.05	0.73
1:A:73:GLU:N	1:A:73:GLU:OE1	2.22	0.72
1:D:317:TRP:NE1	1:D:337:GLY:O	2.21	0.72
1:D:199:SER:O	1:D:201:GLN:NE2	2.23	0.72
1:D:433:GLN:O	1:D:437:ASN:ND2	2.22	0.72
1:C:604:THR:O	1:C:608:ASN:ND2	2.23	0.71
1:D:499:ASP:OD1	1:D:500:VAL:N	2.23	0.71
1:B:290:ARG:NH2	1:B:376:GLY:O	2.24	0.70
1:D:176:SER:OG	1:D:178:ASP:OD1	2.09	0.70
1:D:313:GLY:O	1:D:316:ALA:HB2	1.92	0.70
1:A:257:GLN:OE1	1:A:257:GLN:N	2.24	0.70
1:B:161:ARG:NH1	1:B:221:THR:O	2.24	0.69
1:B:510:ARG:NH1	1:D:132:ASN:OD1	2.24	0.69
1:B:590:GLU:N	1:B:590:GLU:OE1	2.26	0.69
1:B:257:GLN:N	1:B:257:GLN:OE1	2.26	0.69
1:D:133:GLU:OE2	1:D:216:ARG:NE	2.26	0.69
1:C:590:GLU:N	1:C:590:GLU:OE1	2.25	0.68
1:A:247:CYS:SG	1:A:452:SER:OG	2.50	0.68
1:A:460:ARG:NH2	1:A:502:MET:O	2.27	0.68
1:A:309:SER:O	1:A:340:THR:N	2.26	0.68
1:D:290:ARG:NH1	1:D:380:THR:O	2.26	0.68
1:D:284:HIS:O	1:D:301:TRP:NE1	2.26	0.68
1:B:373:GLN:NE2	1:B:375:GLY:O	2.28	0.67
1:B:265:TYR:OH	1:B:437:ASN:ND2	2.27	0.67
1:D:438:ASN:ND2	1:D:442:GLU:OE2	2.27	0.67
1:A:362:PHE:O	1:A:390:THR:OG1	2.12	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:461:ASN:ND2	1:B:500:VAL:O	2.28	0.66
1:A:148:ALA:O	1:A:514:LYS:N	2.29	0.66
1:D:112:SER:OG	1:D:241:THR:OG1	2.14	0.65
1:B:317:TRP:CD2	1:B:339:ILE:HD11	2.32	0.65
1:D:431:PHE:O	1:D:435:ALA:N	2.29	0.65
1:C:123:VAL:HG12	1:C:540:ALA:HB2	1.78	0.65
1:B:453:TYR:N	1:B:565:TYR:O	2.29	0.64
1:D:438:ASN:OD1	1:D:441:ILE:N	2.30	0.64
1:C:433:GLN:O	1:C:437:ASN:ND2	2.30	0.64
1:B:304:MET:O	1:B:325:PHE:N	2.31	0.64
1:C:161:ARG:NH2	1:C:495:ARG:O	2.30	0.64
1:B:194:ARG:NH2	1:B:226:ASP:OD1	2.30	0.63
1:D:131:TYR:O	1:D:520:THR:OG1	2.10	0.63
1:B:434:THR:O	1:B:437:ASN:ND2	2.30	0.63
1:C:328:ARG:NH2	1:C:329:HIS:O	2.32	0.63
1:D:453:TYR:N	1:D:565:TYR:O	2.30	0.63
1:C:478:THR:OG1	1:C:484:ARG:NH1	2.33	0.62
1:B:433:GLN:OE1	1:C:533:ASN:ND2	2.32	0.62
1:B:333:ASP:OD1	1:B:334:ALA:N	2.32	0.62
1:C:248:GLU:OE1	1:C:249:ALA:N	2.32	0.62
1:C:153:SER:OG	1:C:167:VAL:O	2.13	0.61
1:C:192:SER:OG	1:C:195:ASP:OD2	2.14	0.61
1:C:123:VAL:HG11	1:C:536:PHE:HB3	1.82	0.61
1:B:226:ASP:N	1:B:229:GLU:OE2	2.34	0.61
1:B:538:GLN:OE1	1:B:538:GLN:N	2.32	0.61
1:A:535:PRO:O	1:A:538:GLN:NE2	2.34	0.61
1:C:463:VAL:O	1:C:465:GLN:NE2	2.34	0.60
1:A:273:THR:OG1	1:A:419:SER:O	2.16	0.60
1:C:496:ASP:OD1	1:C:497:SER:N	2.34	0.60
1:B:530:THR:HB	1:B:534:THR:HG21	1.83	0.60
1:D:108:VAL:O	1:D:111:TYR:OH	2.14	0.60
1:A:103:GLU:OE1	1:A:103:GLU:N	2.34	0.60
1:D:531:ASN:ND2	1:D:532:VAL:O	2.34	0.60
1:B:443:GLN:O	1:B:443:GLN:NE2	2.35	0.59
1:A:81:LYS:NZ	1:A:586:VAL:O	2.35	0.59
1:D:275:ASN:ND2	1:D:416:THR:OG1	2.35	0.59
1:D:601:ASN:O	1:D:604:THR:OG1	2.19	0.59
1:D:423:GLU:N	1:D:423:GLU:OE1	2.35	0.59
1:D:412:ASP:OD1	1:D:413:ALA:N	2.36	0.59
1:B:353:ASP:O	1:B:357:ASN:N	2.36	0.59
1:D:422:SER:O	1:D:476:SER:N	2.33	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:373:GLN:OE1	1:D:374:THR:N	2.36	0.59
1:A:250:ASN:N	1:A:517:SER:O	2.34	0.59
1:A:290:ARG:NH1	1:A:380:THR:O	2.35	0.58
1:D:246:THR:HG1	1:D:453:TYR:HD1	1.50	0.58
1:D:577:ALA:O	1:D:581:ASN:ND2	2.36	0.58
1:B:569:ASP:OD1	1:B:570:ASN:N	2.37	0.58
1:D:350:GLN:NE2	1:D:359:TRP:O	2.35	0.58
1:D:372:GLY:O	1:D:385:THR:N	2.36	0.58
1:C:589:SER:OG	1:C:590:GLU:OE1	2.22	0.58
1:C:234:THR:HB	1:C:534:THR:HG23	1.85	0.58
1:C:410:ASN:ND2	1:C:412:ASP:OD1	2.36	0.58
1:D:85:ASP:OD2	1:D:88:SER:N	2.37	0.57
1:A:593:THR:OG1	1:B:549:GLU:OE2	2.22	0.57
1:B:290:ARG:NE	1:B:294:ALA:O	2.37	0.57
1:B:530:THR:CB	1:B:534:THR:HG21	2.34	0.57
1:C:582:MET:SD	1:C:602:GLN:NE2	2.77	0.57
1:C:190:LEU:HD23	1:C:191:ALA:H	1.70	0.57
1:B:184:ILE:HD11	1:B:426:LEU:HD11	1.86	0.57
1:C:460:ARG:NH1	1:C:499:ASP:O	2.37	0.57
1:C:194:ARG:NH1	1:C:222:TYR:O	2.38	0.57
1:D:172:ASN:OD1	1:D:510:ARG:NH1	2.36	0.57
1:B:577:ALA:O	1:B:581:ASN:ND2	2.38	0.56
1:D:194:ARG:NH2	1:D:222:TYR:O	2.38	0.56
1:A:386:ILE:N	1:A:393:LEU:O	2.37	0.56
1:B:116:ASP:OD2	1:B:239:ARG:NH1	2.38	0.56
1:A:194:ARG:NH1	1:A:222:TYR:O	2.39	0.56
1:A:290:ARG:NH2	1:A:293:ILE:O	2.39	0.56
1:D:426:LEU:HD11	1:D:477:PHE:HB3	1.87	0.56
1:B:236:SER:O	1:B:469:ALA:N	2.39	0.56
1:D:275:ASN:OD1	1:D:276:ALA:N	2.39	0.56
1:D:353:ASP:O	1:D:357:ASN:N	2.39	0.56
1:B:549:GLU:OE1	1:B:549:GLU:N	2.37	0.55
1:B:265:TYR:O	1:B:504:THR:N	2.39	0.55
1:D:428:PRO:O	1:D:434:THR:OG1	2.24	0.55
1:A:159:MET:HB2	1:A:162:THR:HG22	1.88	0.55
1:B:86:GLN:N	1:B:86:GLN:OE1	2.39	0.55
1:C:226:ASP:OD2	1:C:228:THR:OG1	2.22	0.55
1:D:443:GLN:OE1	1:D:443:GLN:N	2.39	0.55
1:A:486:LEU:HD12	1:A:486:LEU:O	2.07	0.55
1:B:172:ASN:O	1:B:510:ARG:NH2	2.40	0.55
1:B:320:ASP:OD1	1:B:320:ASP:N	2.40	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:GLU:OE1	1:B:229:GLU:N	2.38	0.54
1:C:122:SER:OG	1:C:528:GLY:O	2.23	0.54
1:C:123:VAL:HG13	1:C:530:THR:HG23	1.90	0.54
1:A:227:PRO:O	1:A:233:ARG:NH2	2.41	0.54
1:A:516:CYS:SG	1:A:517:SER:N	2.81	0.54
1:D:120:LYS:O	1:D:543:GLY:N	2.39	0.54
1:D:314:ASP:N	1:D:315:PRO:O	2.41	0.53
1:C:547:ASN:ND2	1:C:549:GLU:OE1	2.42	0.53
1:A:384:ILE:N	1:A:395:ILE:O	2.37	0.53
1:D:260:TRP:NE1	1:D:445:LEU:O	2.43	0.52
1:C:237:ASP:OD1	1:C:469:ALA:N	2.42	0.52
1:A:199:SER:O	1:A:201:GLN:NE2	2.42	0.52
1:C:172:ASN:O	1:C:172:ASN:ND2	2.43	0.52
1:C:569:ASP:OD1	1:C:570:ASN:N	2.43	0.52
1:A:465:GLN:N	1:A:501:ASN:OD1	2.38	0.51
1:B:530:THR:OG1	1:B:534:THR:HG21	2.10	0.51
1:B:339:ILE:N	1:B:371:PHE:O	2.42	0.51
1:B:433:GLN:OE1	1:C:532:VAL:HG22	2.11	0.51
1:A:257:GLN:NE2	1:A:511:SER:O	2.44	0.51
1:D:169:ASN:OD1	1:D:173:LYS:N	2.41	0.51
1:B:230:GLY:O	1:B:232:LEU:N	2.44	0.51
1:D:290:ARG:NH2	1:D:293:ILE:O	2.40	0.51
1:C:265:TYR:N	1:C:504:THR:O	2.44	0.51
1:D:430:THR:O	1:D:434:THR:N	2.40	0.51
1:A:173:LYS:NZ	1:A:208:ASP:OD2	2.45	0.50
1:B:446:VAL:O	1:B:450:LEU:N	2.43	0.50
1:B:254:LEU:HD23	1:B:255:VAL:HG13	1.93	0.50
1:A:269:PRO:HB3	1:A:498:LEU:HD13	1.92	0.50
1:B:126:GLU:OE1	1:B:127:ILE:N	2.44	0.50
1:B:264:HIS:NE2	1:B:455:VAL:O	2.45	0.50
1:C:232:LEU:HD12	1:C:234:THR:HG23	1.92	0.50
1:A:340:THR:HA	1:A:370:THR:HG22	1.94	0.49
1:B:320:ASP:OD2	1:B:326:GLN:NE2	2.44	0.49
1:C:197:VAL:HG11	1:C:217:VAL:HG22	1.95	0.49
1:D:496:ASP:OD1	1:D:497:SER:N	2.42	0.49
1:B:85:ASP:OD2	1:B:88:SER:N	2.41	0.49
1:A:440:LYS:NZ	1:A:559:THR:O	2.45	0.49
1:B:516:CYS:SG	1:B:517:SER:N	2.86	0.49
1:B:358:GLU:OE1	1:B:359:TRP:N	2.46	0.49
1:D:177:LEU:O	1:D:181:ASN:ND2	2.40	0.48
1:D:289:THR:HG23	1:D:402:ALA:HB2	1.95	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:398:THR:O	1:D:401:SER:OG	2.29	0.48
1:A:496:ASP:OD1	1:A:497:SER:N	2.41	0.48
1:C:143:ILE:N	1:C:144:PRO:CD	2.77	0.48
1:B:348:THR:N	1:B:410:ASN:OD1	2.47	0.48
1:D:532:VAL:O	1:D:533:ASN:HB3	2.14	0.48
1:B:362:PHE:O	1:B:390:THR:OG1	2.26	0.48
1:B:560:ARG:NH2	1:B:604:THR:OG1	2.47	0.48
1:B:395:ILE:HB	1:B:406:ILE:HD11	1.96	0.47
1:D:524:GLN:OE1	1:D:525:GLY:N	2.46	0.47
1:A:198:ASP:OD1	1:A:222:TYR:OH	2.28	0.47
1:D:426:LEU:HD12	1:D:426:LEU:N	2.29	0.47
1:C:276:ALA:HB2	1:C:418:ALA:HB2	1.96	0.47
1:C:280:SER:OG	1:C:411:LEU:O	2.31	0.47
1:D:74:PHE:O	1:D:77:TRP:NE1	2.46	0.47
1:D:353:ASP:N	1:D:358:GLU:O	2.36	0.47
1:A:123:VAL:HG21	1:A:530:THR:HG23	1.97	0.47
1:C:134:GLU:OE2	1:C:214:ARG:NH2	2.48	0.47
1:C:454:LEU:HD11	1:C:507:CYS:HB2	1.95	0.47
1:C:545:LEU:HD23	1:C:545:LEU:H	1.78	0.47
1:D:138:VAL:HG13	1:D:170:VAL:HG21	1.95	0.47
1:D:483:ASP:OD1	1:D:483:ASP:N	2.48	0.47
1:D:91:TRP:O	1:D:95:TYR:N	2.40	0.46
1:C:84:ILE:HD12	1:C:84:ILE:O	2.15	0.46
1:A:284:HIS:O	1:A:301:TRP:NE1	2.38	0.46
1:A:538:GLN:OE1	1:A:538:GLN:N	2.39	0.46
1:C:435:ALA:HA	1:C:441:ILE:HD13	1.96	0.46
1:C:498:LEU:HD23	1:C:499:ASP:N	2.30	0.46
1:A:398:THR:O	1:A:401:SER:OG	2.21	0.46
1:B:433:GLN:O	1:C:532:VAL:HG21	2.15	0.46
1:C:275:ASN:HB3	1:C:277:VAL:HG12	1.98	0.46
1:A:73:GLU:O	1:A:77:TRP:NE1	2.48	0.46
1:B:149:GLN:NE2	1:D:515:SER:O	2.49	0.46
1:D:566:GLY:N	1:D:569:ASP:OD2	2.38	0.46
1:A:115:PRO:HG3	1:A:550:ILE:HD11	1.97	0.46
1:A:509:PHE:HB3	1:A:512:LEU:HD11	1.98	0.46
1:B:239:ARG:N	1:B:527:GLU:O	2.42	0.46
1:C:386:ILE:N	1:C:393:LEU:O	2.47	0.46
1:B:241:THR:N	1:B:525:GLY:O	2.49	0.45
1:C:322:THR:O	1:C:324:GLN:NE2	2.49	0.45
1:A:248:GLU:N	1:A:248:GLU:OE1	2.49	0.45
1:B:127:ILE:HG21	1:B:218:LEU:HD23	1.98	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:HIS:NE2	1:B:333:ASP:O	2.48	0.45
1:A:602:GLN:NE2	1:B:73:GLU:OE1	2.49	0.45
1:C:190:LEU:HD23	1:C:191:ALA:N	2.30	0.45
1:B:131:TYR:HH	1:B:219:HIS:CD2	2.35	0.45
1:B:218:LEU:N	1:B:218:LEU:HD12	2.32	0.45
1:C:229:GLU:OE1	1:C:230:GLY:N	2.49	0.45
1:C:352:PHE:HA	1:C:359:TRP:HA	1.99	0.45
1:B:247:CYS:O	1:B:452:SER:N	2.48	0.45
1:B:587:LEU:HD13	1:B:588:LYS:N	2.31	0.45
1:C:420:ASN:ND2	1:C:420:ASN:O	2.49	0.45
1:D:465:GLN:NE2	1:D:466:LEU:O	2.50	0.45
1:D:466:LEU:HD12	1:D:466:LEU:O	2.16	0.45
1:D:293:ILE:HD12	1:D:293:ILE:H	1.82	0.45
1:B:297:VAL:HG23	1:B:317:TRP:CH2	2.52	0.45
1:B:407:ASN:OD1	1:B:408:PHE:N	2.50	0.45
1:D:227:PRO:O	1:D:231:LEU:N	2.50	0.44
1:D:289:THR:HG23	1:D:402:ALA:CB	2.48	0.44
1:D:381:ASN:HB3	1:D:396:LEU:HD11	1.99	0.44
1:B:86:GLN:HA	1:B:89:ILE:HG22	1.99	0.44
1:B:226:ASP:O	1:B:230:GLY:N	2.47	0.44
1:C:280:SER:HA	1:C:413:ALA:HA	2.00	0.44
1:D:174:GLU:OE2	1:D:432:GLY:N	2.37	0.44
1:A:172:ASN:O	1:A:510:ARG:NH2	2.46	0.43
1:A:208:ASP:OD1	1:A:210:THR:OG1	2.26	0.43
1:A:241:THR:OG1	1:A:525:GLY:O	2.28	0.43
1:A:351:TYR:OH	1:A:353:ASP:OD1	2.32	0.43
1:B:112:SER:O	1:B:241:THR:HG21	2.18	0.43
1:C:155:ILE:O	1:C:165:PHE:N	2.40	0.43
1:C:248:GLU:O	1:C:519:VAL:N	2.47	0.43
1:C:189:ASN:N	1:C:189:ASN:OD1	2.51	0.43
1:C:386:ILE:N	1:C:386:ILE:HD12	2.33	0.43
1:D:288:VAL:HG23	1:D:404:ASN:HD22	1.84	0.43
1:B:155:ILE:HD12	1:B:155:ILE:N	2.34	0.43
1:D:370:THR:O	1:D:387:THR:OG1	2.36	0.43
1:D:454:LEU:N	1:D:454:LEU:HD12	2.34	0.43
1:C:131:TYR:O	1:C:520:THR:OG1	2.36	0.43
1:C:143:ILE:HG13	1:C:144:PRO:HD3	2.01	0.43
1:D:317:TRP:HB2	1:D:327:TRP:CE3	2.53	0.43
1:D:81:LYS:HA	1:D:587:LEU:HA	2.01	0.43
1:D:161:ARG:O	1:D:218:LEU:HD12	2.19	0.43
1:D:498:LEU:HD23	1:D:499:ASP:N	2.33	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:GLU:N	1:A:134:GLU:OE1	2.51	0.43
1:A:482:PHE:O	1:A:484:ARG:N	2.52	0.42
1:A:237:ASP:OD1	1:A:237:ASP:N	2.52	0.42
1:D:152:LEU:HA	1:D:168:ALA:HA	2.01	0.42
1:A:169:ASN:ND2	1:A:210:THR:OG1	2.52	0.42
1:D:84:ILE:O	1:D:84:ILE:HD12	2.19	0.42
1:D:494:ILE:N	1:D:494:ILE:HD12	2.34	0.42
1:C:85:ASP:OD2	1:C:88:SER:N	2.41	0.42
1:B:173:LYS:NZ	1:B:210:THR:OG1	2.44	0.42
1:D:287:ASN:ND2	1:D:289:THR:OG1	2.53	0.42
1:A:299:LEU:N	1:A:327:TRP:O	2.42	0.42
1:C:217:VAL:HG21	1:C:222:TYR:CD1	2.55	0.42
1:D:384:ILE:HD12	1:D:384:ILE:N	2.34	0.42
1:B:479:ASN:N	1:B:479:ASN:OD1	2.52	0.42
1:D:286:PHE:HA	1:D:301:TRP:HA	2.02	0.42
1:A:145:LEU:HD13	1:A:145:LEU:O	2.20	0.42
1:B:544:LEU:N	1:B:544:LEU:HD23	2.35	0.42
1:C:239:ARG:N	1:C:527:GLU:O	2.52	0.42
1:B:386:ILE:O	1:B:393:LEU:N	2.53	0.42
1:C:384:ILE:N	1:C:384:ILE:HD12	2.35	0.42
1:D:161:ARG:NH1	1:D:224:LEU:O	2.49	0.42
1:D:317:TRP:NE1	1:D:335:PRO:HB2	2.34	0.42
1:A:445:LEU:H	1:A:445:LEU:HD12	1.84	0.42
1:D:429:LEU:O	1:D:508:HIS:NE2	2.53	0.42
1:A:195:ASP:OD2	1:A:328:ARG:NE	2.52	0.41
1:A:530:THR:HG21	1:A:536:PHE:HB2	2.02	0.41
1:C:172:ASN:O	1:C:510:ARG:NH2	2.53	0.41
1:C:354:THR:O	1:C:357:ASN:ND2	2.53	0.41
1:B:364:ASN:N	1:B:367:ASP:OD2	2.54	0.41
1:D:440:LYS:HG3	1:D:562:THR:HG22	2.02	0.41
1:A:208:ASP:CG	1:A:210:THR:HG1	2.21	0.41
1:A:353:ASP:N	1:A:358:GLU:O	2.41	0.41
1:C:387:THR:HA	1:C:392:THR:HG23	2.03	0.41
1:D:175:ILE:HD11	1:D:430:THR:N	2.35	0.41
1:B:195:ASP:N	1:B:195:ASP:OD1	2.54	0.41
1:D:435:ALA:HB3	1:D:436:PRO:HD3	2.03	0.41
1:D:557:LEU:HD21	1:D:600:GLY:HA3	2.02	0.41
1:B:496:ASP:OD1	1:B:497:SER:N	2.47	0.41
1:D:283:VAL:HA	1:D:409:ARG:HA	2.02	0.41
1:B:114:ILE:HG13	1:B:241:THR:HG22	2.03	0.40
1:C:264:HIS:O	1:C:438:ASN:ND2	2.54	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:TYR:O	1:D:159:MET:N	2.53	0.40
1:B:274:GLN:OE1	1:B:274:GLN:N	2.47	0.40
1:C:122:SER:O	1:C:540:ALA:HB1	2.22	0.40
1:C:270:ILE:N	1:C:270:ILE:HD12	2.37	0.40
1:C:82:LEU:N	1:C:586:VAL:O	2.41	0.40
1:D:301:TRP:O	1:D:324:GLN:HA	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	534/644 (83%)	509 (95%)	25 (5%)	0	100	100
1	B	536/644 (83%)	516 (96%)	20 (4%)	0	100	100
1	C	536/644 (83%)	517 (96%)	19 (4%)	0	100	100
1	D	536/644 (83%)	492 (92%)	44 (8%)	0	100	100
All	All	2142/2576 (83%)	2034 (95%)	108 (5%)	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	444/527 (84%)	416 (94%)	28 (6%)	18	47
1	B	445/527 (84%)	418 (94%)	27 (6%)	18	48
1	C	445/527 (84%)	414 (93%)	31 (7%)	15	44
1	D	445/527 (84%)	407 (92%)	38 (8%)	10	39
All	All	1779/2108 (84%)	1655 (93%)	124 (7%)	19	44

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	ARG
1	A	77	TRP
1	A	79	ARG
1	A	85	ASP
1	A	111	TYR
1	A	123	VAL
1	A	140	ASP
1	A	145	LEU
1	A	160	PHE
1	A	233	ARG
1	A	239	ARG
1	A	274	GLN
1	A	367	ASP
1	A	373	GLN
1	A	410	ASN
1	A	412	ASP
1	A	437	ASN
1	A	443	GLN
1	A	472	PHE
1	A	482	PHE
1	A	486	LEU
1	A	491	PHE
1	A	536	PHE
1	A	541	HIS
1	A	544	LEU
1	A	546	LYS
1	A	565	TYR
1	A	597	LYS
1	B	75	ARG
1	B	81	LYS
1	B	113	LYS
1	B	182	ASP
1	B	190	LEU

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	201	GLN
1	B	232	LEU
1	B	255	VAL
1	B	270	ILE
1	B	284	HIS
1	B	286	PHE
1	B	293	ILE
1	B	370	THR
1	B	409	ARG
1	B	430	THR
1	B	437	ASN
1	B	442	GLU
1	B	443	GLN
1	B	447	LYS
1	B	465	GLN
1	B	479	ASN
1	B	484	ARG
1	B	498	LEU
1	B	536	PHE
1	B	546	LYS
1	B	578	PHE
1	B	587	LEU
1	C	81	LYS
1	C	85	ASP
1	C	106	ARG
1	C	110	GLU
1	C	129	GLU
1	C	131	TYR
1	C	134	GLU
1	C	189	ASN
1	C	190	LEU
1	C	214	ARG
1	C	219	HIS
1	C	229	GLU
1	C	232	LEU
1	C	248	GLU
1	C	257	GLN
1	C	284	HIS
1	C	314	ASP
1	C	324	GLN
1	C	328	ARG
1	C	350	GLN

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	351	TYR
1	C	431	PHE
1	C	443	GLN
1	C	453	TYR
1	C	461	ASN
1	C	514	LYS
1	C	530	THR
1	C	532	VAL
1	C	544	LEU
1	C	547	ASN
1	C	565	TYR
1	D	75	ARG
1	D	77	TRP
1	D	81	LYS
1	D	84	ILE
1	D	111	TYR
1	D	113	LYS
1	D	120	LYS
1	D	121	PHE
1	D	127	ILE
1	D	128	ARG
1	D	134	GLU
1	D	175	ILE
1	D	186	TRP
1	D	201	GLN
1	D	218	LEU
1	D	224	LEU
1	D	226	ASP
1	D	243	LYS
1	D	274	GLN
1	D	317	TRP
1	D	329	HIS
1	D	352	PHE
1	D	373	GLN
1	D	381	ASN
1	D	404	ASN
1	D	409	ARG
1	D	440	LYS
1	D	447	LYS
1	D	465	GLN
1	D	466	LEU
1	D	484	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	539	PHE
1	D	549	GLU
1	D	551	LEU
1	D	560	ARG
1	D	576	LEU
1	D	583	LEU
1	D	592	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	189	ASN
1	A	461	ASN
1	A	465	GLN
1	B	132	ASN
1	B	284	HIS
1	B	420	ASN
1	B	437	ASN
1	B	443	GLN
1	B	609	GLN
1	C	250	ASN
1	C	326	GLN
1	C	357	ASN
1	C	381	ASN
1	C	404	ASN
1	C	420	ASN
1	C	433	GLN
1	C	437	ASN
1	C	461	ASN
1	C	533	ASN
1	C	541	HIS
1	C	547	ASN
1	C	609	GLN
1	D	219	HIS
1	D	350	GLN
1	D	360	ASN
1	D	404	ASN
1	D	433	GLN
1	D	608	ASN

### 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](#)

There are no ligands in this entry.

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

There are no such residues in this entry.

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

There are no chain breaks in this entry.

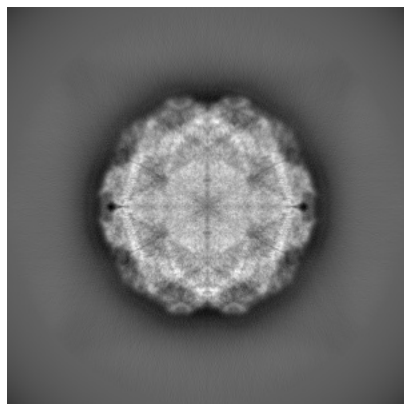
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15348. These allow visual inspection of the internal detail of the map and identification of artifacts.

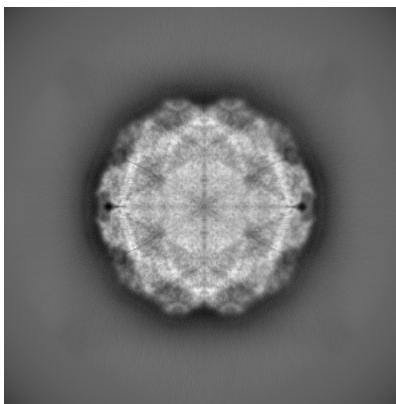
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

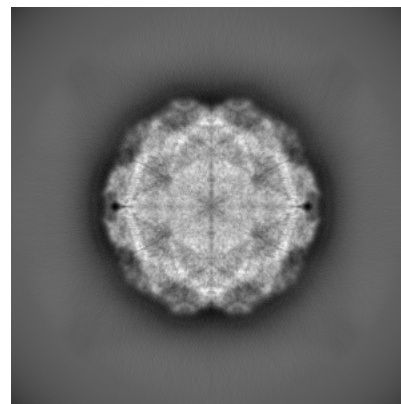
#### 6.1.1 Primary map



X

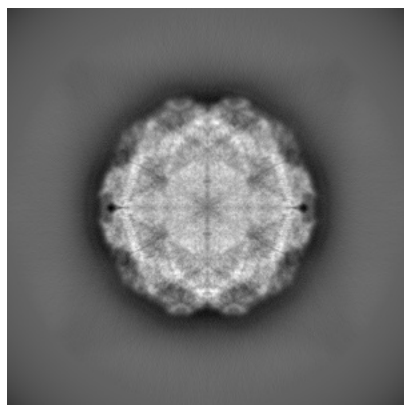


Y

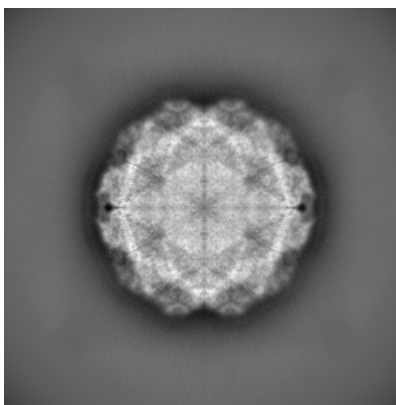


Z

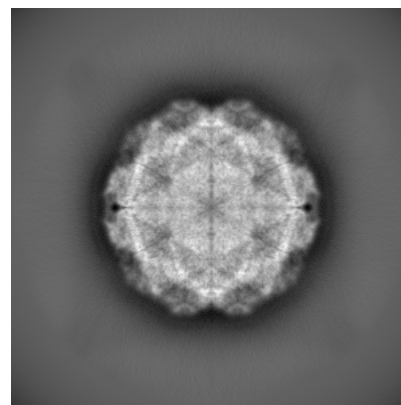
#### 6.1.2 Raw map



X



Y

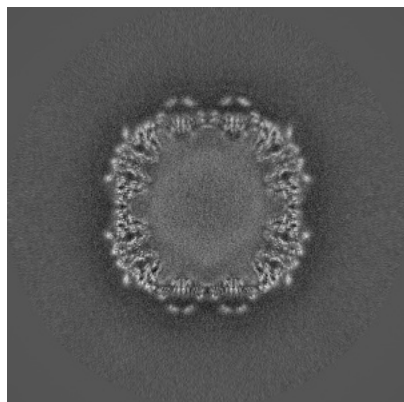


Z

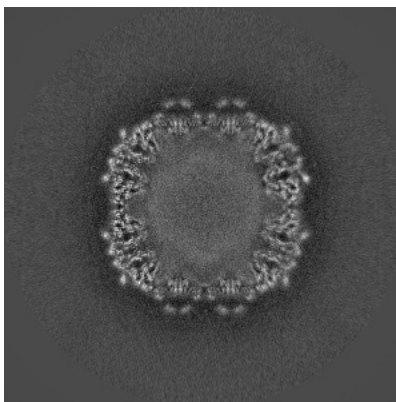
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

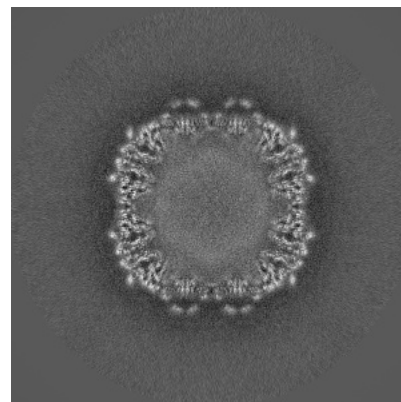
### 6.2.1 Primary map



X Index: 256

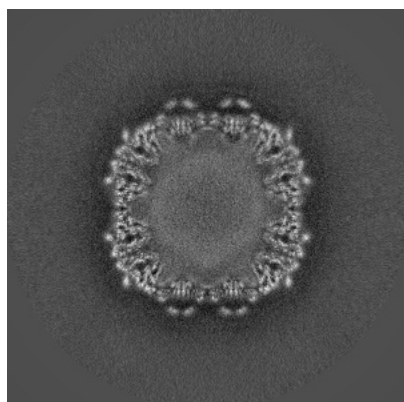


Y Index: 256

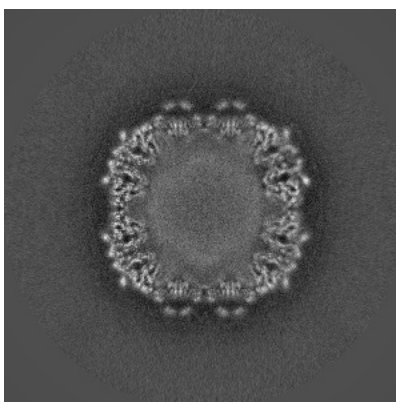


Z Index: 256

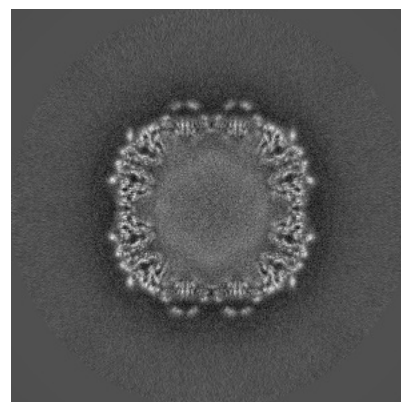
### 6.2.2 Raw map



X Index: 256



Y Index: 256

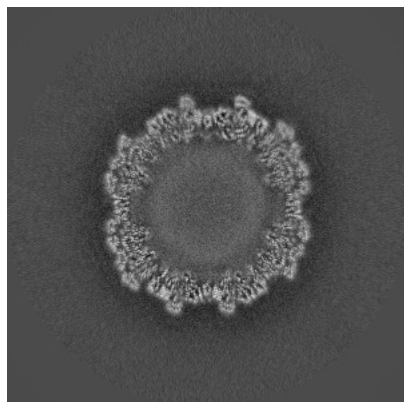


Z Index: 256

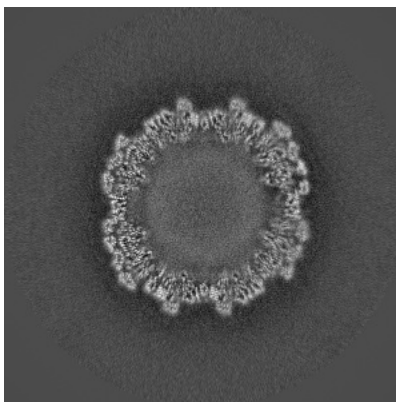
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

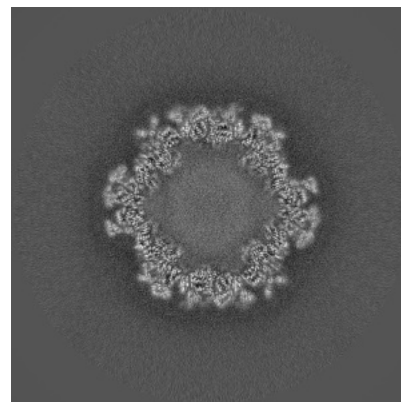
### 6.3.1 Primary map



X Index: 267

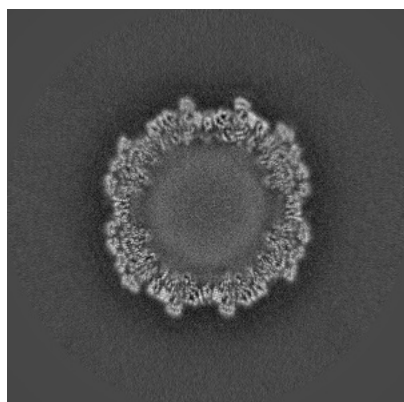


Y Index: 267

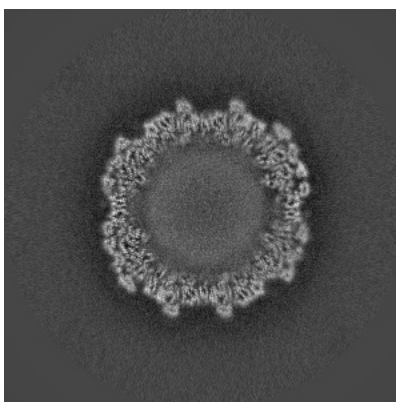


Z Index: 210

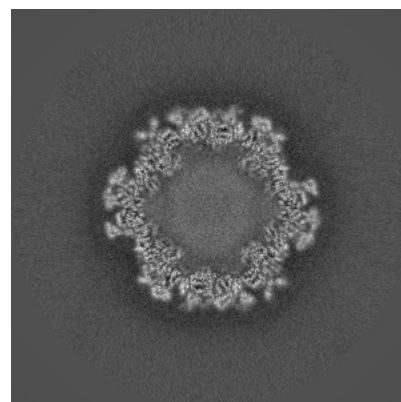
### 6.3.2 Raw map



X Index: 267



Y Index: 268



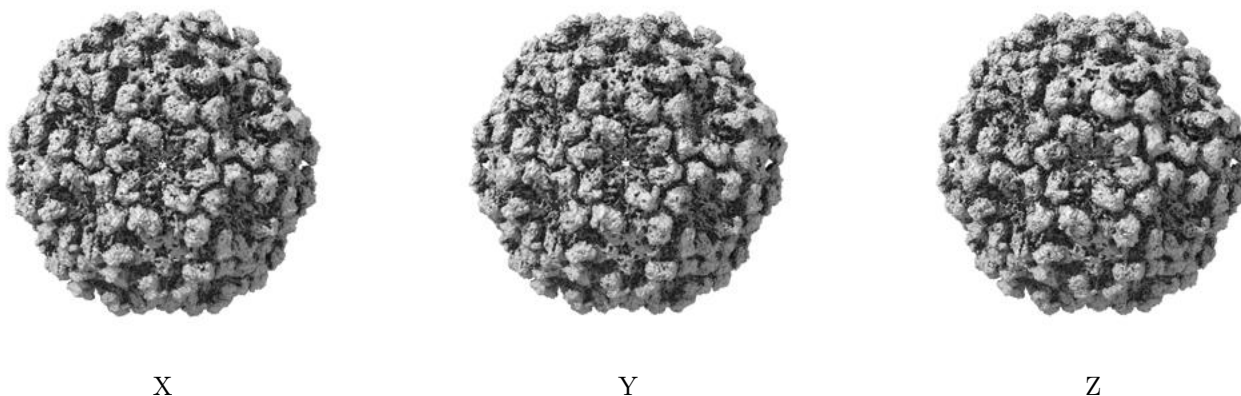
Z Index: 210

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



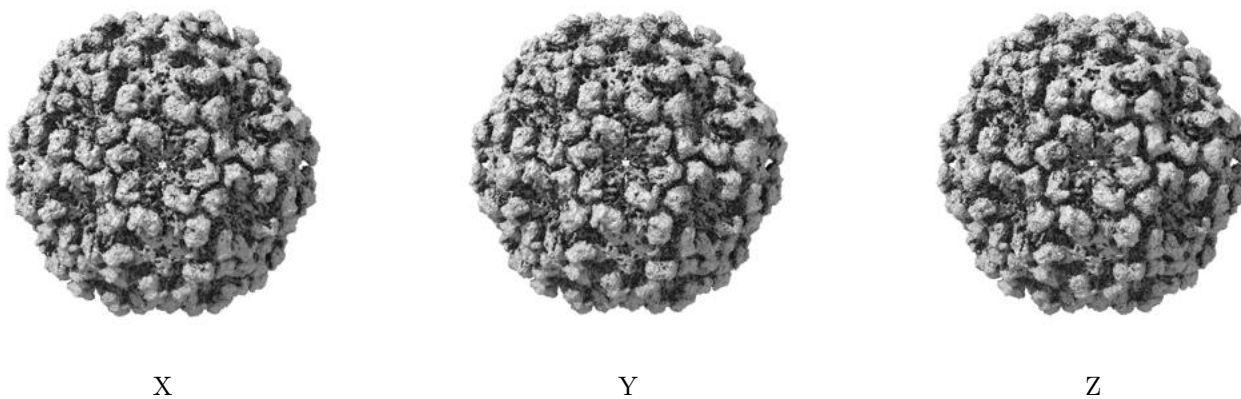
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. 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.

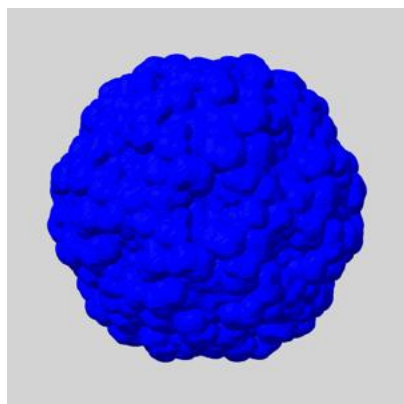
## 6.5 Mask visualisation [i](#)

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

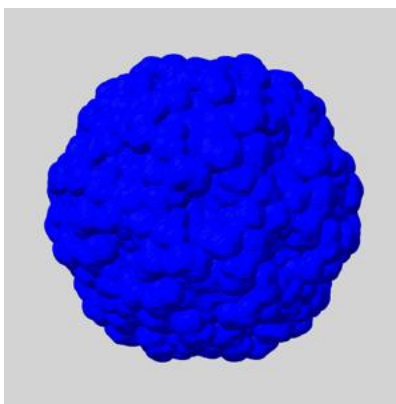
A mask typically either:

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

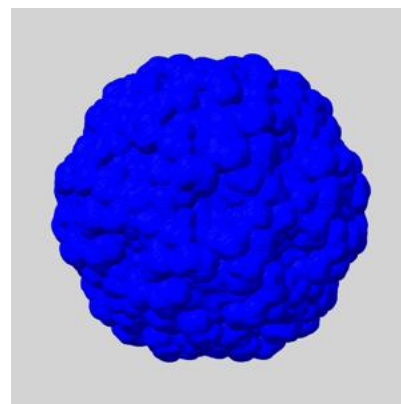
### 6.5.1 emd\_15348\_msk\_1.map [i](#)



X



Y

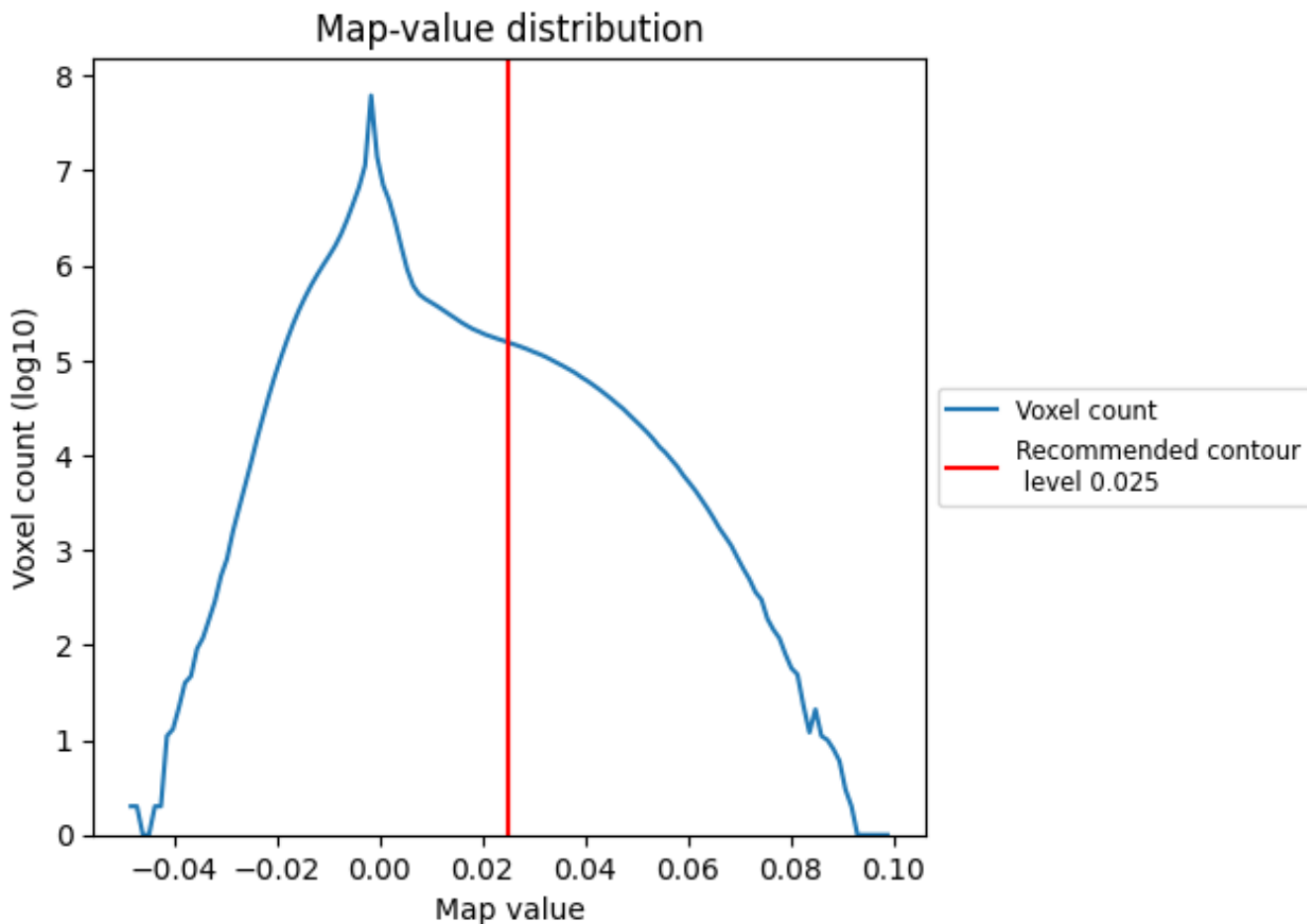


Z

## 7 Map analysis [i](#)

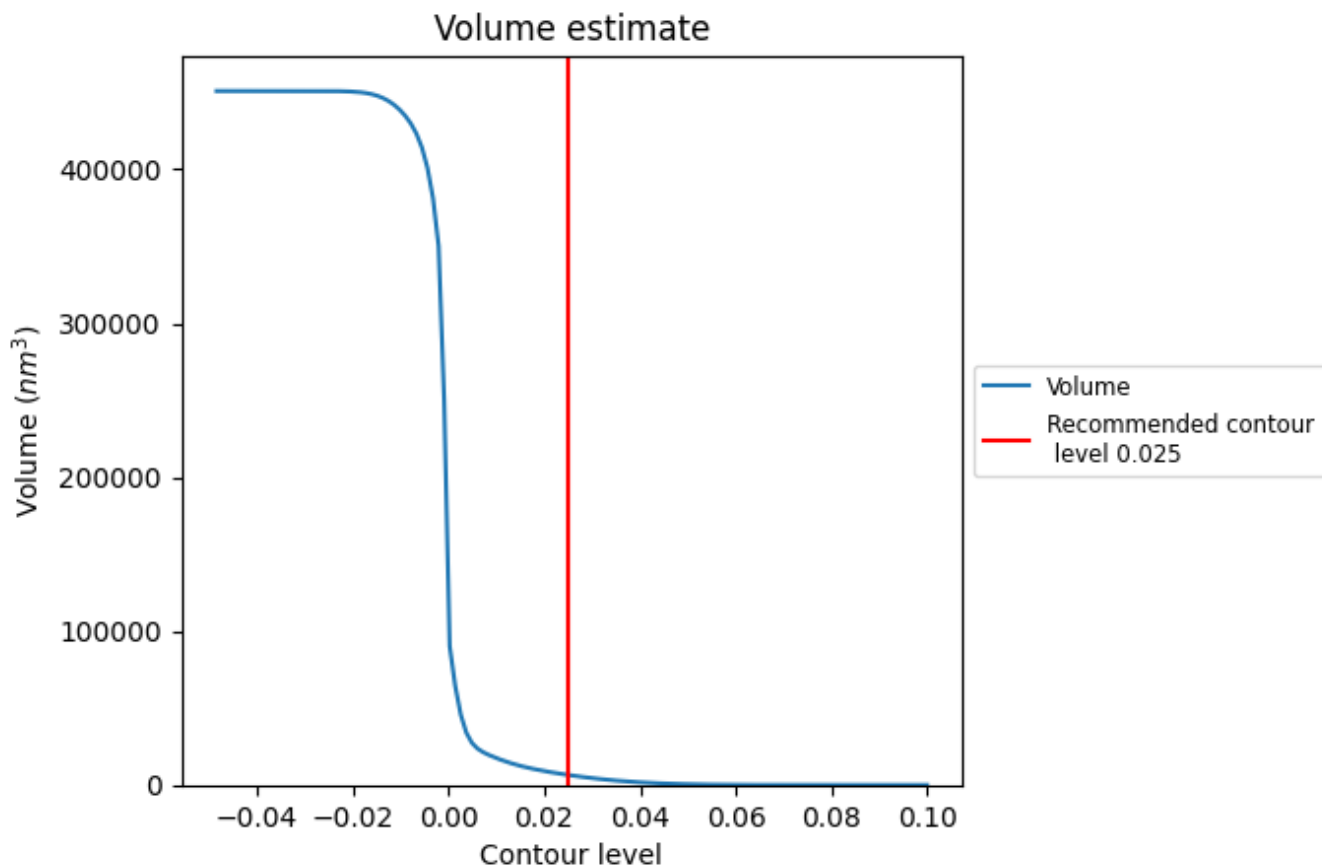
This section contains the results of statistical analysis of the map.

### 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.

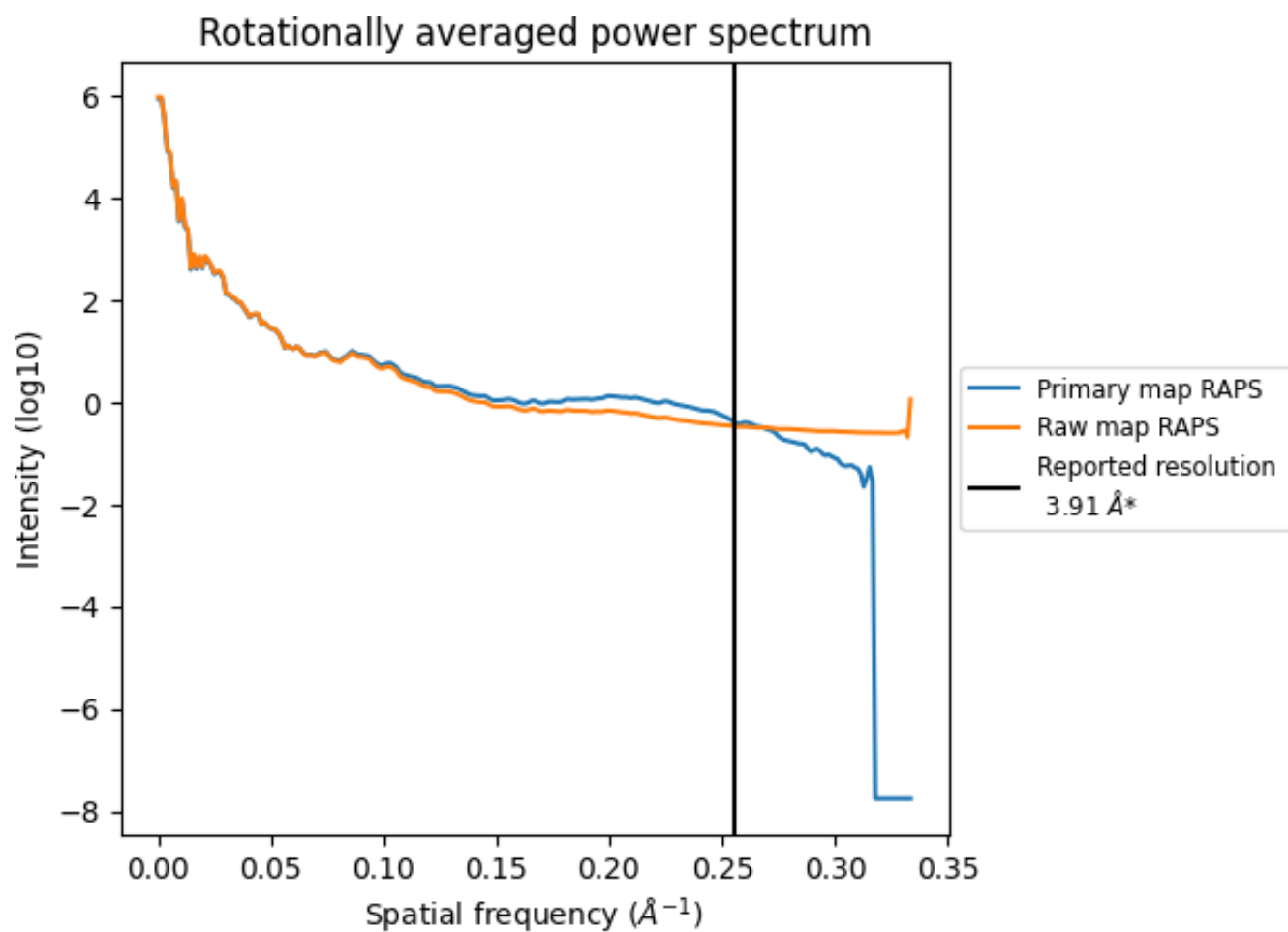
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 6490 nm<sup>3</sup>; this corresponds to an approximate mass of 5863 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

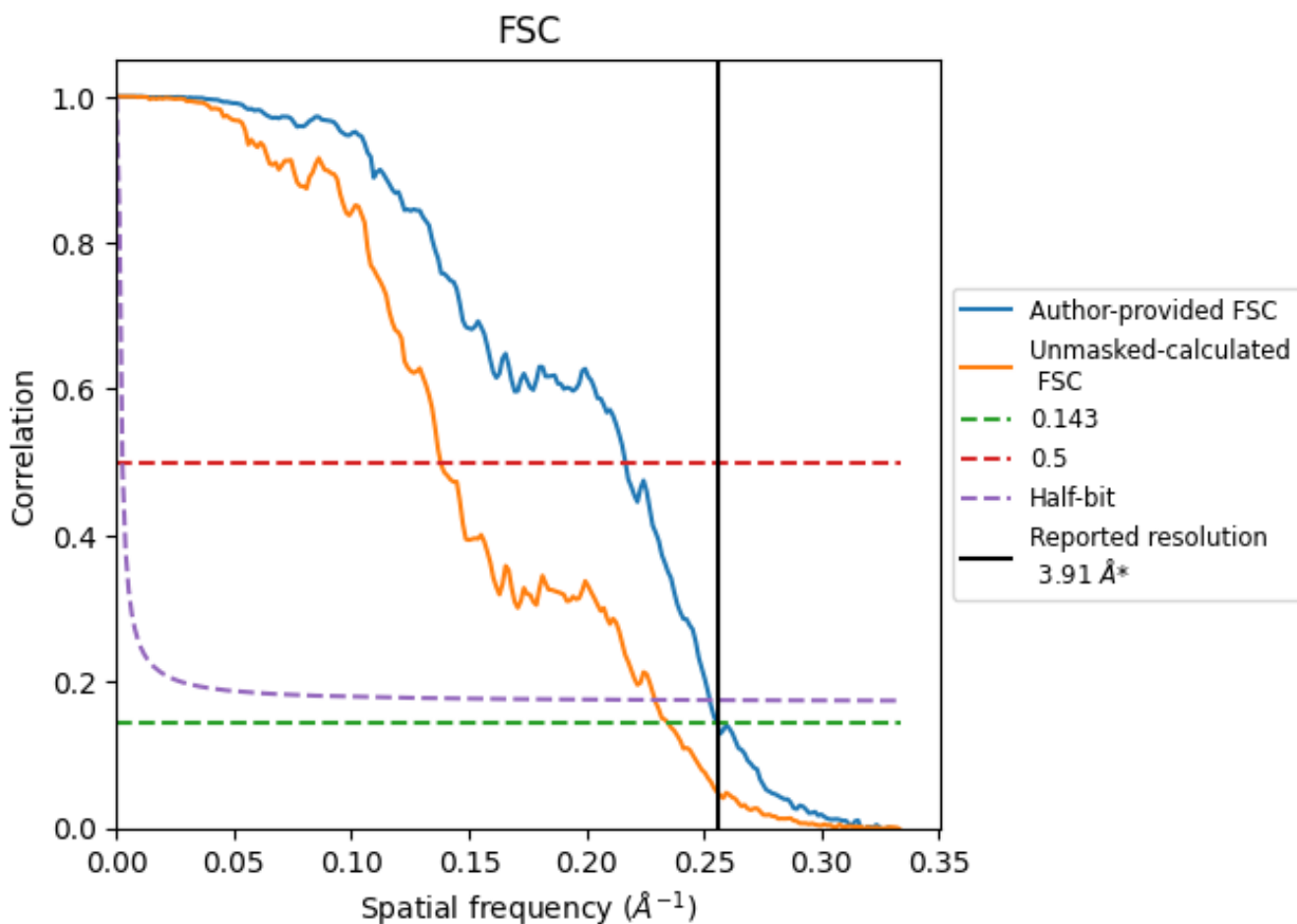


\*Reported resolution corresponds to spatial frequency of 0.256 Å<sup>-1</sup>

## 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 0.256 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.91	-	-
Author-provided FSC curve	3.91	4.62	3.96
Unmasked-calculated*	4.26	7.25	4.36

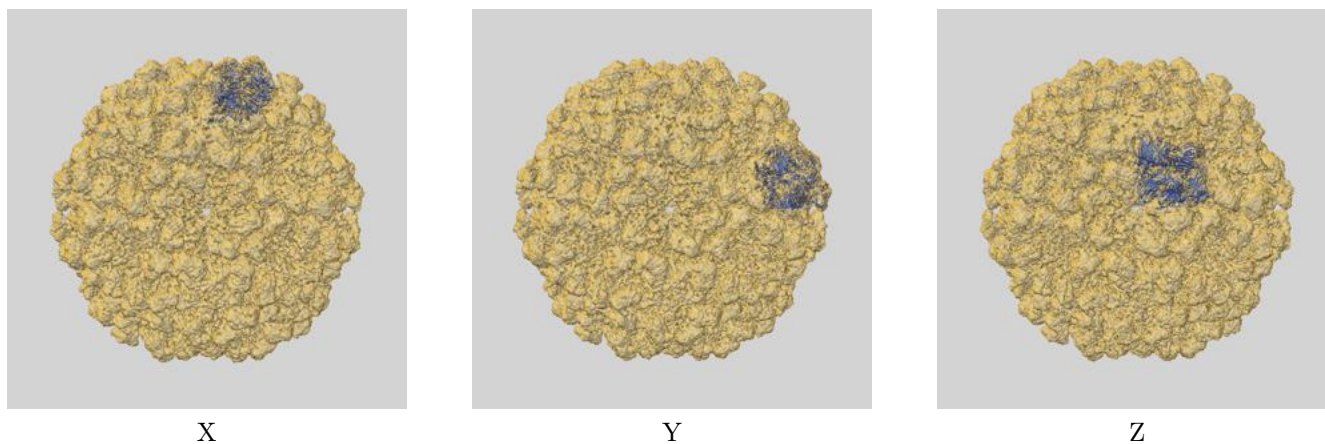
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

## 9 Map-model fit [i](#)

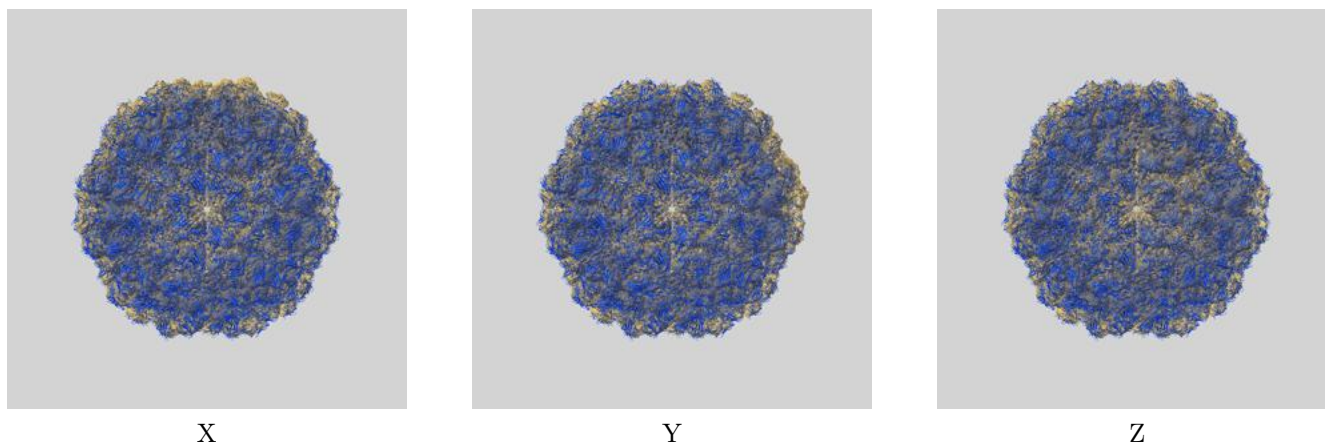
This section contains information regarding the fit between EMDB map EMD-15348 and PDB model 8ACH. Per-residue inclusion information can be found in section 3 on page 4.

### 9.1 Map-model overlays

#### 9.1.1 Map-model overlay [i](#)



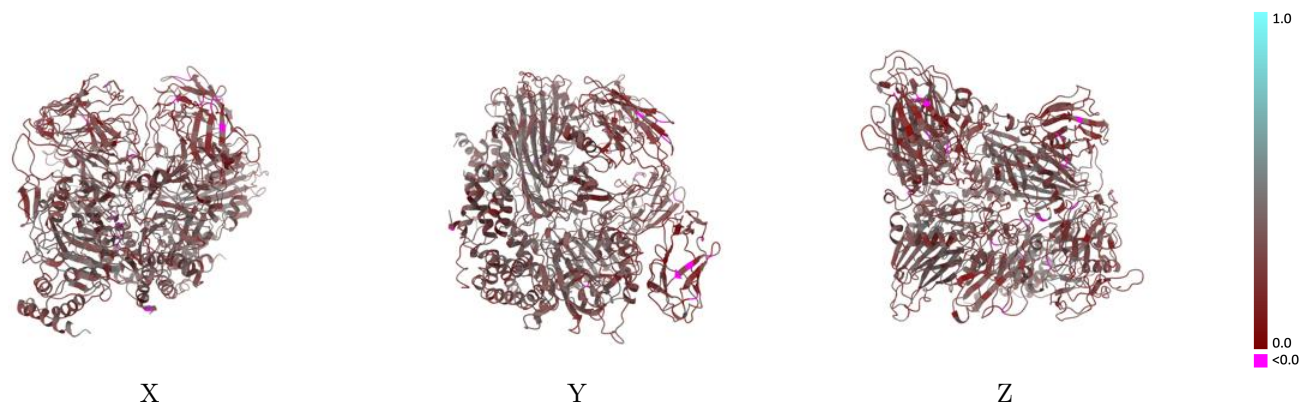
#### 9.1.2 Map-model assembly overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.025 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.

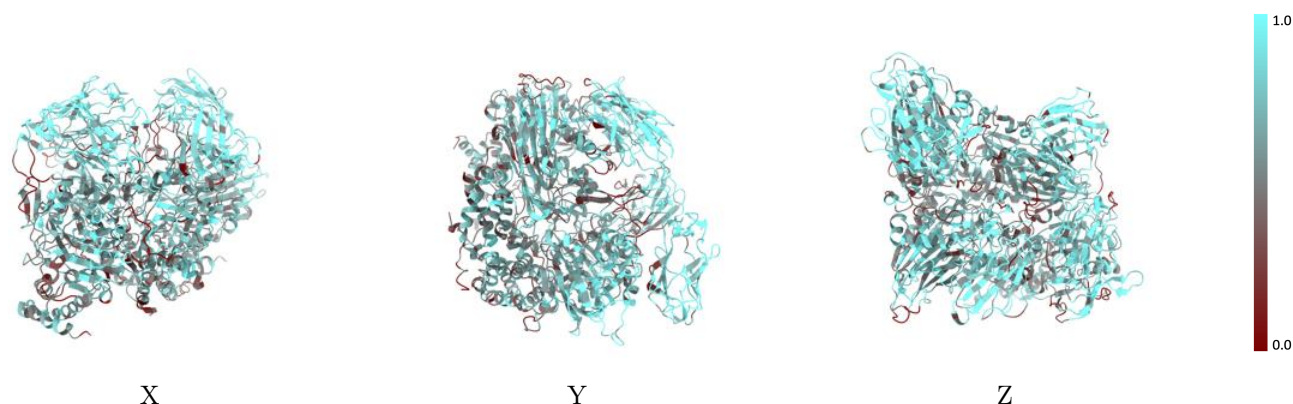


## 9.2 Q-score mapped to coordinate model [i](#)



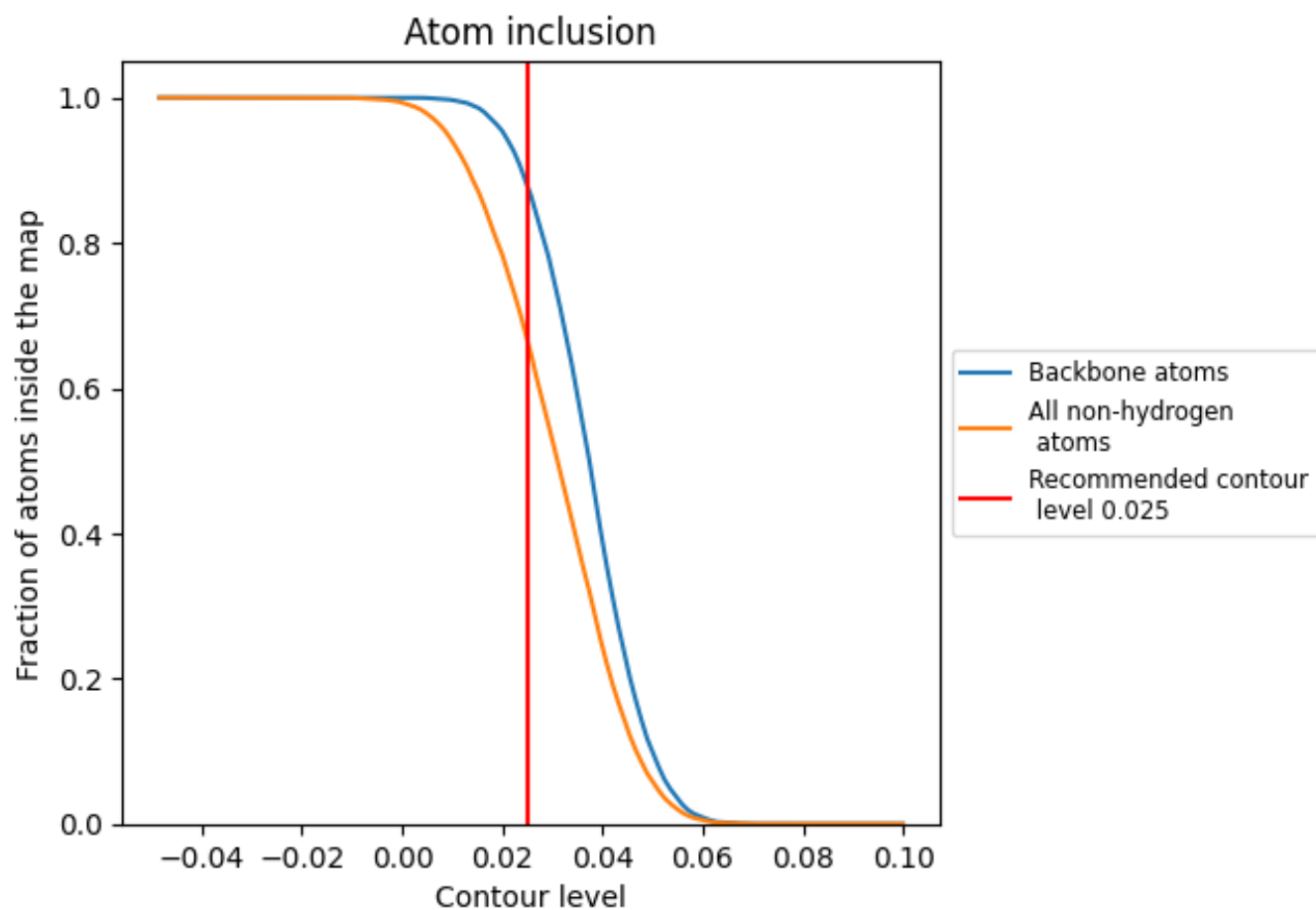
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).


## 9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 67% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6666	 0.3020
A	 0.6869	 0.2880
B	 0.6536	 0.2970
C	 0.6738	 0.3110
D	 0.6522	 0.3130

