Full wwPDB EM Validation Report ⓘ

May 20, 2025 – 03:19 AM EDT

PDB ID	:	9EAN / pdb_00009ean
EMDB ID	:	EMD-47837
Title	:	Murine norovirus allosteric escape mutant D348E
Authors	:	Smith, T.J.; Sherman, M.
Deposited on	:	2024-11-11
Resolution	:	2.40 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:

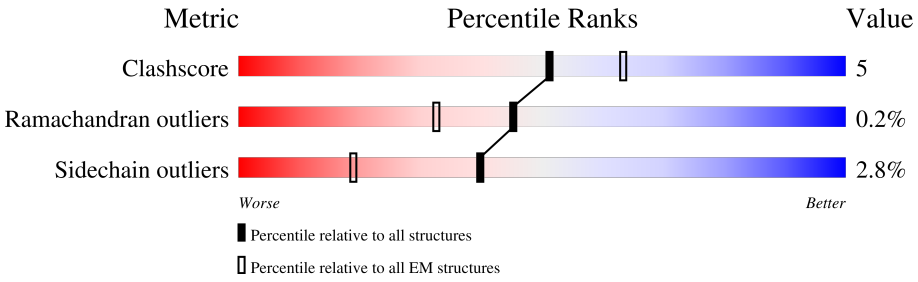
EMDB validation analysis	:	0.0.1.dev118
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 2.40 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 <=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	540	84% 85% 10% 5%
1	B	540	85% 80% 15% • •
1	C	540	83% 79% 13% • 7%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 11798 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 Capsid protein VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	515	Total	C	N	O	S	0	0
			3953	2547	651	739	16		
1	B	516	Total	C	N	O	S	0	0
			3963	2553	652	742	16		
1	C	504	Total	C	N	O	S	0	0
			3882	2503	639	724	16		

There are 6 discrepancies between the modelled and reference sequences:

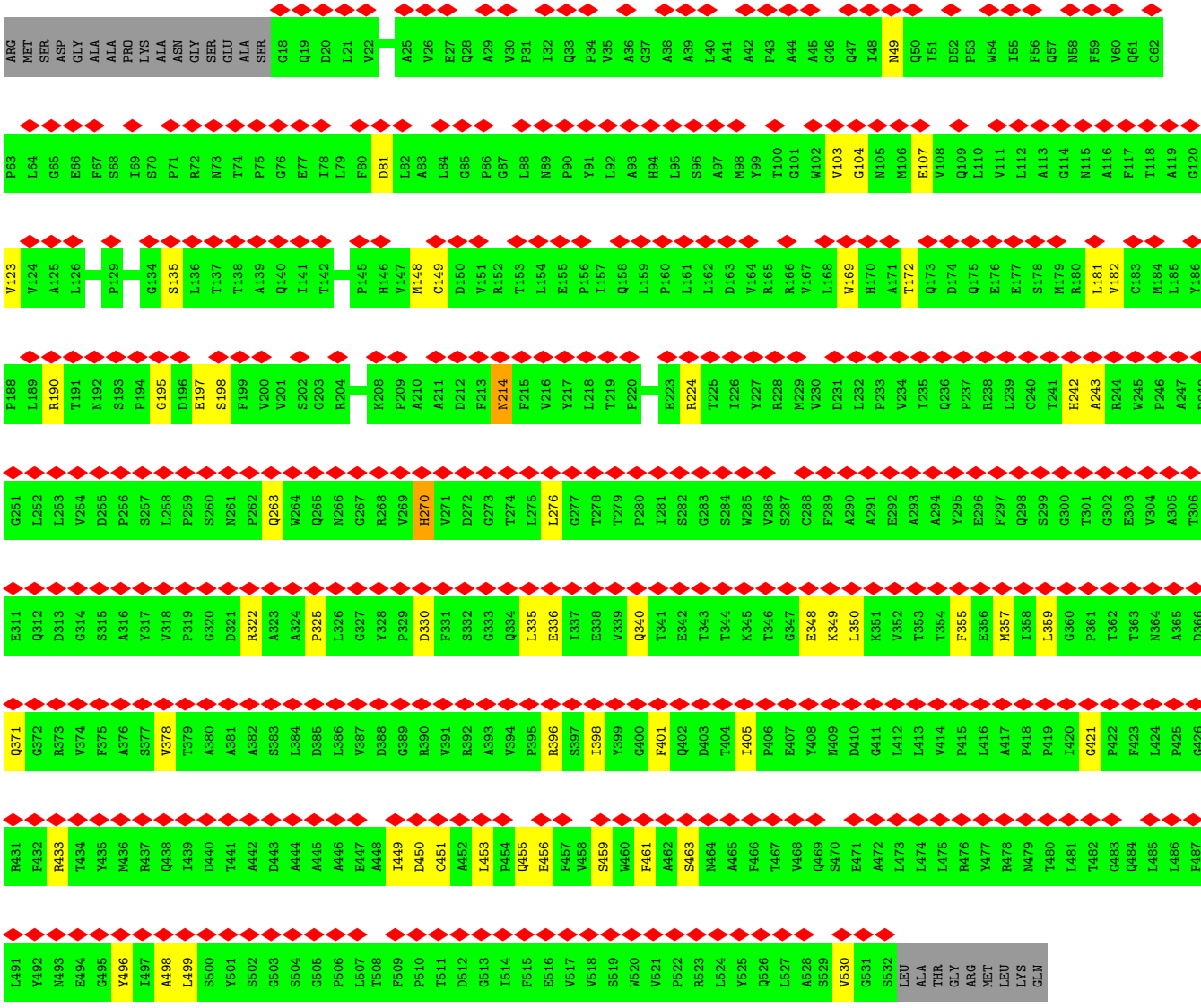
Chain	Residue	Modelled	Actual	Comment	Reference
A	296	GLU	LYS	variant	UNP Q80J94
A	348	GLU	ASP	variant	UNP Q80J94
B	296	GLU	LYS	variant	UNP Q80J94
B	348	GLU	ASP	variant	UNP Q80J94
C	296	GLU	LYS	variant	UNP Q80J94
C	348	GLU	ASP	variant	UNP Q80J94

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

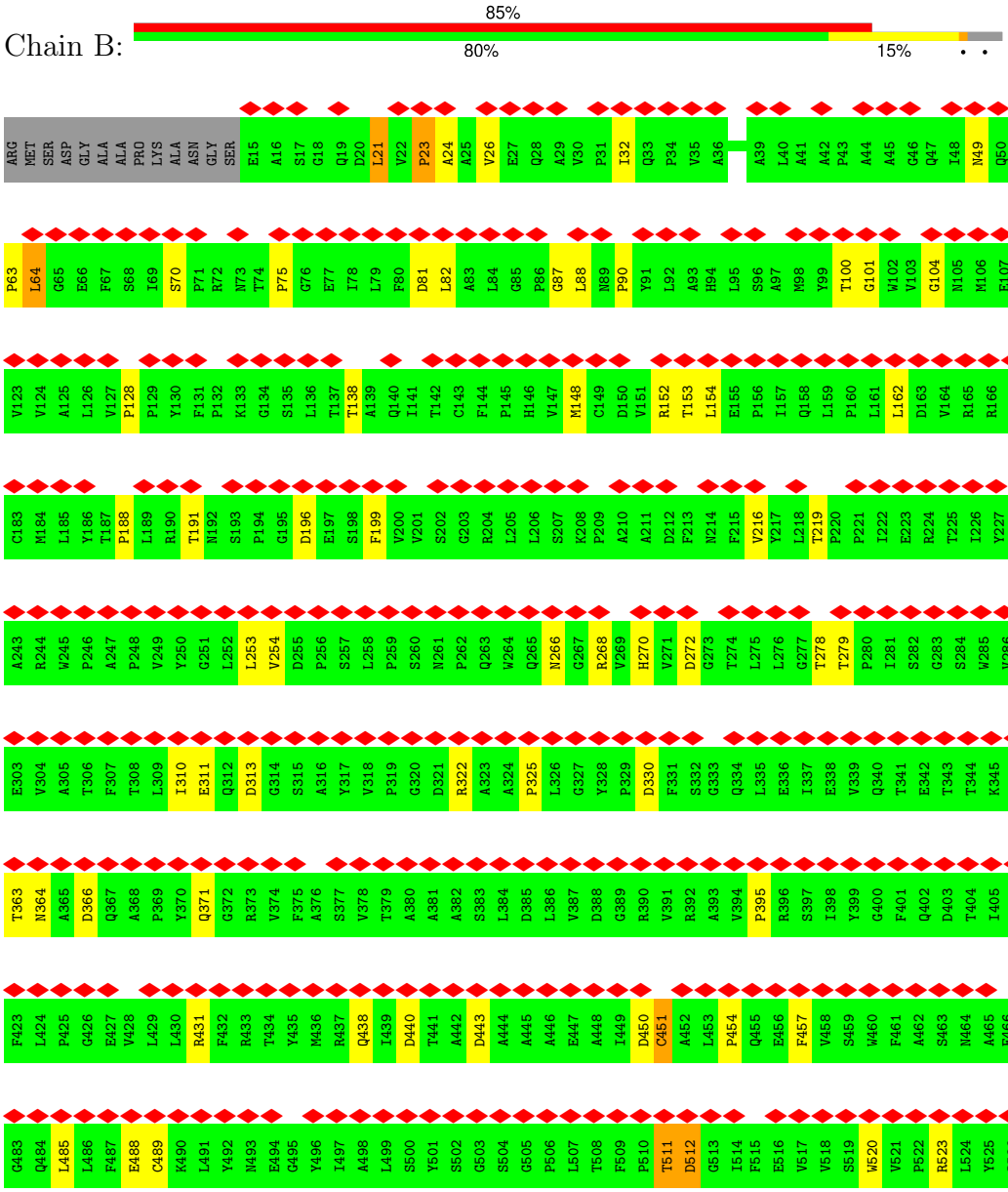
• Molecule 1: Capsid protein VP1

Chain A:



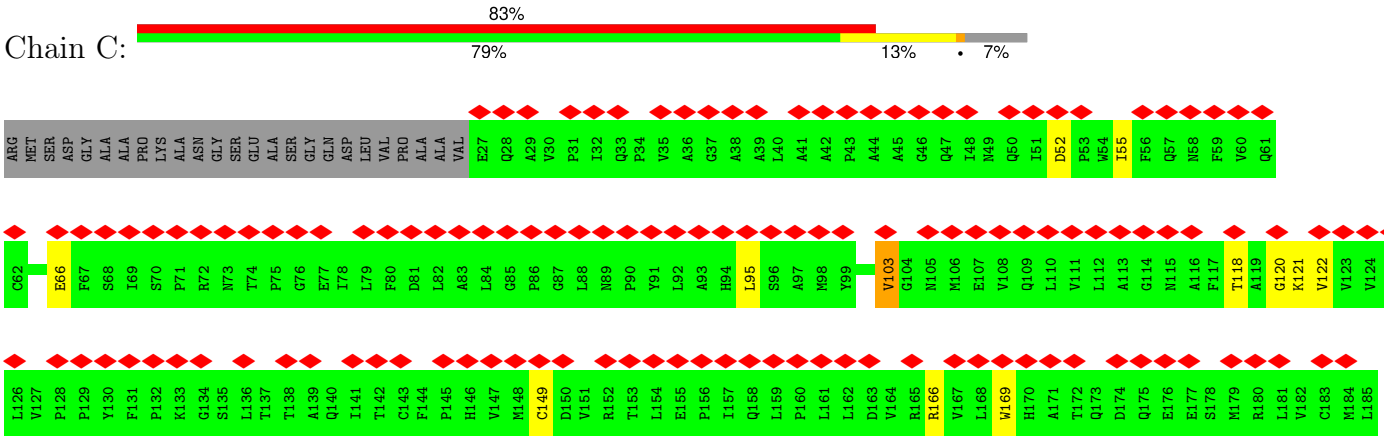
• Molecule 1: Capsid protein VP1

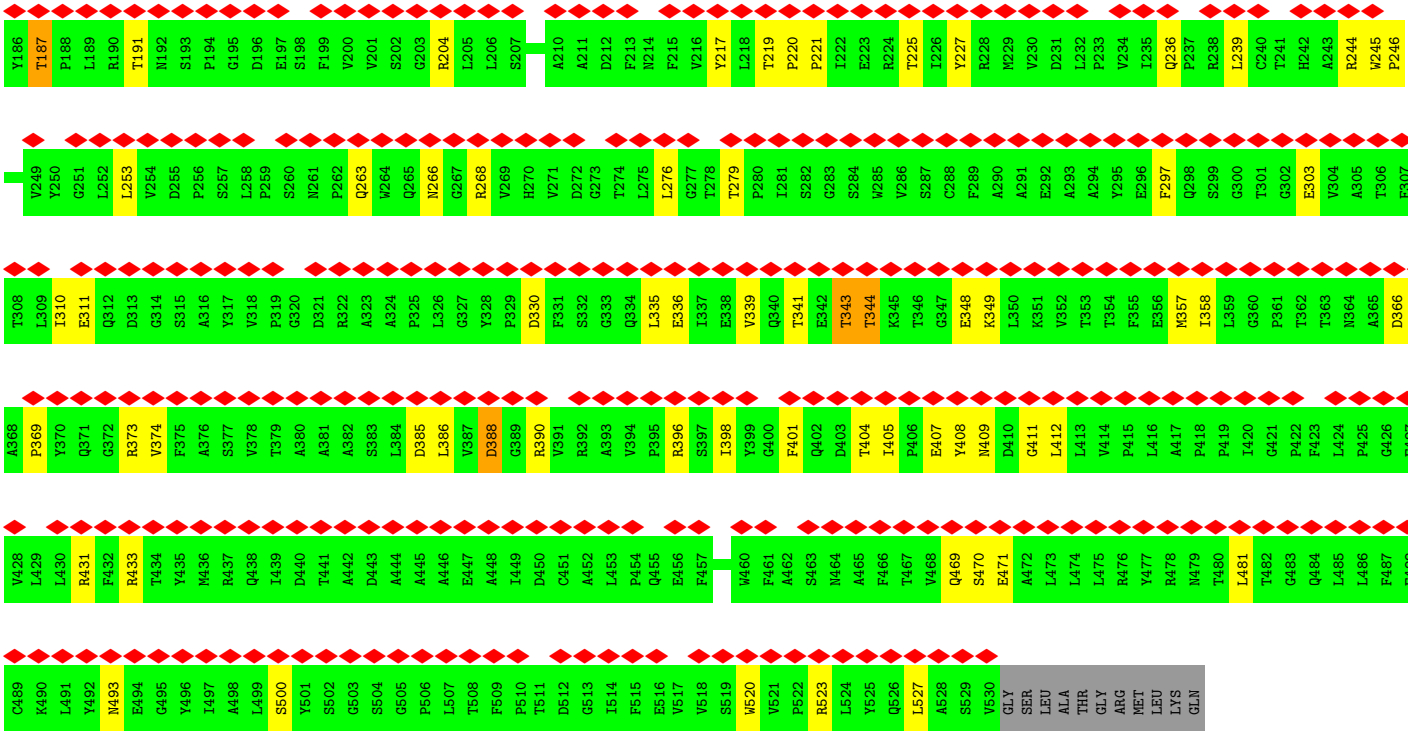
Chain B:



• Molecule 1: Capsid protein VP1

Chain C:




Y186 T187 P188 L189 R190 T191 N192 S193 P194 G195 D196 E197 S198 F199 V200 V201 S202 G203 R204 L205 L206 S207
A210 A211 D212 F213 N214 F215 V216 Y217 L218 T219 P220 P221 I222 E223 R224 T225 I226 Y227 R228 M229 V230 D231 L232 P233 V234 I235 Q236 P237 R238 L239 C240 T241 H242 A243 R244 W245 P246
V249 Y250 G251 L252 L253 V254 D255 P256 S257 L258 P259 S260 N261 P262 Q263 W264 Q265 N266 G267 R268 V269 H270 V271 D272 G273 T274 L275 L276 G277 T278 T279 P280 I281 S282 G283 S284 W285 V286 S287 C288 F289 A290 A291 E292 A293 A294 Y295 E296 F297 Q298 S299 G300 T301 G302 E303 V304 A305 T306 F307
T308 L309 I310 E311 Q312 D313 G314 S315 A316 Y317 V318 P319 G320 D321 R322 A323 A324 P325 L326 G327 Y328 P329 D330 F331 S332 G333 Q334 L335 E336 I337 E338 V339 Q340 T341 E342 T343 T344 K345 T346 G347 E348 K349 L350 K351 V352 T353 T354 F355 E356 M357 I358 L359 G360 P361 T362 T363 N364 A365 D366 Q367
A368 P369 Y370 Q371 G372 R373 V374 F375 A376 S377 V378 T379 A380 A381 A382 S383 L384 D385 L386 V387 D388 G389 R390 V391 R392 A393 V394 P395 R396 S397 I398 Y399 G400 F401 Q402 D403 T404 I405 P406 E407 Y408 N409 D410 G411 L412 L413 V414 P415 L416 A417 P418 P419 I420 G421 P422 F423 L424 P425 G426 E427
V428 L429 L430 R431 F432 R433 T434 Y435 M436 R437 Q438 I439 D440 T441 A442 D443 A444 A445 A446 E447 A448 I449 D450 C451 A452 L453 P454 Q455 E456 F457
W460 F461 A462 S463 N464 A465 F466 T467 V468 Q469 S470 E471 A472 L473 L474 L475 R476 Y477 R478 N479 T480 L481 T482 G483 Q484 L485 L486 F487 E488
C489 K490 L491 Y492 N493 E494 G495 Y496 I497 A498 L499 S500 Y501 S502 G503 S504 G505 P506 L507 T508 F509 P510 T511 D512 G513 I514 F515 E516 V517 V518 S519 W520 V521 P522 R523 L524 Y525 Q526 L527 A528 S529 V530
GLY SER LEU ALA THR GLY ARG MET LEU LYS GLN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	187851	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.844	Depositor
Minimum map value	-2.220	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.154	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	594.0, 594.0, 594.0	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

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	0.24	0/4062	0.47	1/5570 (0.0%)
1	B	0.26	0/4072	0.51	1/5584 (0.0%)
1	C	0.25	0/3990	0.48	0/5470
All	All	0.25	0/12124	0.49	2/16624 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	104	GLY	N-CA-C	6.09	118.63	111.63
1	B	104	GLY	N-CA-C	5.52	117.98	111.63

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3953	0	3899	30	0
1	B	3963	0	3907	48	0
1	C	3882	0	3826	50	0
All	All	11798	0	11632	125	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 (125) 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:49:ASN:ND2	1:B:216:VAL:O	2.09	0.85
1:C:225:THR:HG22	1:C:227:TYR:H	1.42	0.84
1:B:191:THR:HG21	1:B:199:PHE:H	1.50	0.74
1:C:268:ARG:H	1:C:279:THR:HG21	1.50	0.73
1:A:499:LEU:HD23	1:A:530:VAL:HG11	1.68	0.73
1:C:266:ASN:HA	1:C:279:THR:HG22	1.72	0.72
1:C:244:ARG:NH1	1:C:330:ASP:OD2	2.25	0.70
1:B:270:HIS:ND1	1:B:272:ASP:OD1	2.26	0.69
1:B:322:ARG:HH21	1:B:325:PRO:HA	1.58	0.69
1:C:266:ASN:ND2	1:C:330:ASP:OD1	2.27	0.68
1:B:268:ARG:H	1:B:279:THR:HG21	1.60	0.66
1:B:101:GLY:H	1:B:172:THR:HG23	1.59	0.65
1:B:238:ARG:NH1	1:B:512:ASP:HB3	2.10	0.65
1:B:101:GLY:HA2	1:B:170:HIS:O	1.97	0.65
1:A:427:GLU:HG2	1:A:498:ALA:HB1	1.79	0.64
1:C:366:ASP:O	1:C:373:ARG:NH1	2.30	0.64
1:B:236:GLN:HB2	1:B:239:LEU:HD12	1.78	0.63
1:C:358:ILE:O	1:C:367:GLN:NE2	2.26	0.62
1:C:335:LEU:HB3	1:C:398:ILE:HD12	1.81	0.62
1:B:471:GLU:HG3	1:B:523:ARG:HG3	1.81	0.62
1:C:336:GLU:HG2	1:C:396:ARG:HB3	1.82	0.62
1:B:21:LEU:HG	1:B:152:ARG:HB3	1.81	0.61
1:B:266:ASN:HA	1:B:279:THR:HG22	1.81	0.61
1:B:100:THR:HG23	1:B:219:THR:HG21	1.83	0.60
1:C:120:GLY:HA2	1:C:187:THR:HG22	1.84	0.60
1:C:297:PHE:HA	1:C:303:GLU:HA	1.84	0.60
1:A:224:ARG:NH1	1:A:463:SER:O	2.35	0.59
1:C:341:THR:HB	1:C:386:LEU:HD22	1.86	0.58
1:B:24:ALA:HB1	1:B:26:VAL:HG23	1.85	0.58
1:C:398:ILE:HG12	1:C:401:PHE:HB2	1.85	0.57
1:B:81:ASP:OD2	1:B:81:ASP:N	2.40	0.54
1:C:263:GLN:HB3	1:C:405:ILE:HD11	1.89	0.54
1:C:388:ASP:OD1	1:C:388:ASP:N	2.37	0.54
1:A:243:ALA:HB3	1:A:451:CYS:SG	2.48	0.53
1:C:66:GLU:HB3	1:C:204:ARG:HD3	1.89	0.53
1:B:242:HIS:CE1	1:B:451:CYS:HB3	2.43	0.53
1:B:21:LEU:C	1:B:23:PRO:HD2	2.34	0.53
1:A:398:ILE:HG12	1:A:401:PHE:HB2	1.90	0.52
1:C:470:SER:OG	1:C:471:GLU:N	2.42	0.52
1:C:390:ARG:O	1:C:390:ARG:HG3	2.10	0.51
1:A:371:GLN:HG2	1:C:412:LEU:HD23	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:THR:OG1	1:B:364:ASN:N	2.44	0.50
1:B:366:ASP:OD1	1:B:366:ASP:N	2.37	0.50
1:A:123:VAL:HG22	1:A:148:MET:HE2	1.94	0.50
1:B:63:PRO:HD3	1:B:90:PRO:HD3	1.92	0.50
1:B:21:LEU:HD11	1:B:116:ALA:HA	1.94	0.50
1:B:313:ASP:OD1	1:B:313:ASP:N	2.42	0.50
1:C:405:ILE:HD12	1:C:405:ILE:H	1.77	0.50
1:B:310:ILE:HD12	1:B:311:GLU:O	2.13	0.49
1:A:355:PHE:CE2	1:A:378:VAL:HB	2.47	0.49
1:B:454:PRO:HD2	1:B:457:PHE:CD2	2.47	0.49
1:A:433:ARG:NH2	1:A:450:ASP:OD2	2.36	0.49
1:A:330:ASP:OD1	1:A:330:ASP:N	2.46	0.48
1:A:81:ASP:HA	1:A:181:LEU:O	2.13	0.48
1:C:121:LYS:HB2	1:C:187:THR:HB	1.96	0.48
1:A:195:GLY:HA2	1:A:197:GLU:HG3	1.96	0.48
1:C:103:VAL:HG13	1:C:169:TRP:HA	1.95	0.48
1:B:128:PRO:HA	1:B:179:MET:HE2	1.95	0.48
1:A:242:HIS:HE1	1:A:449:ILE:HG12	1.79	0.48
1:B:454:PRO:HD2	1:B:457:PHE:HD2	1.79	0.47
1:C:369:PRO:HD2	1:C:408:TYR:HA	1.96	0.47
1:C:253:LEU:HD11	1:C:433:ARG:NH1	2.30	0.47
1:C:407:GLU:OE1	1:C:411:GLY:HA2	2.15	0.47
1:C:217:TYR:O	1:C:219:THR:HG23	2.15	0.47
1:A:357:MET:HE2	1:A:359:LEU:HD23	1.97	0.47
1:A:459:SER:C	1:A:461:PHE:H	2.21	0.47
1:C:236:GLN:HB2	1:C:239:LEU:HD12	1.97	0.47
1:A:455:GLN:O	1:A:456:GLU:HB2	2.15	0.46
1:B:488:GLU:HG3	1:B:527:LEU:HD22	1.97	0.46
1:A:340:GLN:HE21	1:A:350:LEU:HB2	1.80	0.46
1:B:64:LEU:HD12	1:B:64:LEU:O	2.16	0.46
1:C:310:ILE:HD13	1:C:390:ARG:NH1	2.32	0.45
1:A:198:SER:O	1:A:198:SER:OG	2.26	0.45
1:C:236:GLN:HB2	1:C:239:LEU:CD1	2.47	0.45
1:C:471:GLU:HG2	1:C:523:ARG:HB2	1.99	0.45
1:B:431:ARG:HB3	1:B:450:ASP:HB3	1.99	0.45
1:A:349:LYS:HD2	1:A:349:LYS:HA	1.54	0.44
1:B:23:PRO:O	1:B:153:THR:HG23	2.18	0.44
1:B:82:LEU:HB3	1:B:88:LEU:HD21	1.99	0.44
1:B:469:GLN:HB2	1:B:520:TRP:CE2	2.52	0.44
1:B:330:ASP:OD1	1:B:330:ASP:N	2.48	0.44
1:C:253:LEU:HD23	1:C:431:ARG:HG3	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:481:LEU:H	1:C:481:LEU:HD23	1.82	0.44
1:C:385:ASP:OD1	1:C:385:ASP:N	2.48	0.44
1:B:81:ASP:HA	1:B:181:LEU:O	2.17	0.44
1:B:478:ARG:HB2	1:B:485:LEU:HD23	2.00	0.44
1:B:238:ARG:HH11	1:B:512:ASP:HB3	1.80	0.44
1:C:52:ASP:HB3	1:C:55:ILE:HG13	1.99	0.44
1:B:440:ASP:OD2	1:B:443:ASP:HB3	2.18	0.44
1:C:245:TRP:CD2	1:C:246:PRO:HD2	2.53	0.43
1:C:310:ILE:HG13	1:C:311:GLU:N	2.34	0.43
1:C:500:SER:O	1:C:500:SER:OG	2.36	0.43
1:B:196:ASP:OD2	1:B:196:ASP:C	2.61	0.43
1:B:253:LEU:HG	1:B:254:VAL:N	2.33	0.43
1:C:118:THR:HG22	1:C:191:THR:HG21	2.00	0.43
1:A:336:GLU:OE2	1:A:396:ARG:NE	2.37	0.43
1:B:23:PRO:HD3	1:B:154:LEU:HB2	2.01	0.43
1:B:278:THR:HA	1:B:322:ARG:HD2	2.01	0.43
1:C:469:GLN:HB2	1:C:520:TRP:CD2	2.54	0.43
1:A:405:ILE:HD13	1:A:405:ILE:HA	1.87	0.42
1:B:63:PRO:HG2	1:B:87:GLY:O	2.19	0.42
1:B:110:LEU:HG	1:B:112:LEU:HD22	2.01	0.42
1:B:475:LEU:HB2	1:B:489:CYS:SG	2.59	0.42
1:C:500:SER:HB3	1:C:527:LEU:HB2	2.01	0.42
1:A:421:GLY:O	1:A:496:TYR:OH	2.34	0.42
1:B:287:SER:O	1:B:395:PRO:HD3	2.19	0.41
1:C:407:GLU:HG3	1:C:409:ASN:O	2.20	0.41
1:B:75:PRO:HG3	1:B:188:PRO:HD3	2.01	0.41
1:C:336:GLU:OE1	1:C:336:GLU:N	2.53	0.41
1:C:405:ILE:HD12	1:C:405:ILE:N	2.33	0.41
1:A:355:PHE:CD2	1:A:378:VAL:HB	2.54	0.41
1:A:49:ASN:O	1:A:214:ASN:HB2	2.21	0.41
1:A:169:TRP:O	1:C:166:ARG:HD2	2.20	0.41
1:B:237:PRO:HB2	1:B:511:THR:HG22	2.03	0.41
1:A:322:ARG:HH12	1:A:325:PRO:HA	1.85	0.41
1:B:32:ILE:HG12	1:B:162:LEU:CD1	2.51	0.41
1:C:276:LEU:O	1:C:279:THR:HG23	2.21	0.41
1:C:343:THR:N	1:C:349:LYS:O	2.53	0.41
1:A:453:LEU:HD23	1:A:453:LEU:HA	1.94	0.40
1:A:81:ASP:HB2	1:A:182:VAL:HG22	2.02	0.40
1:A:169:TRP:CE2	1:C:166:ARG:HG2	2.56	0.40
1:C:310:ILE:HG13	1:C:311:GLU:O	2.22	0.40
1:A:270:HIS:ND1	1:A:276:LEU:HD11	2.37	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:PRO:HA	1:C:221:PRO:HD3	1.91	0.40
1:C:343:THR:OG1	1:C:344:THR:N	2.55	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	513/540 (95%)	488 (95%)	24 (5%)	1 (0%)	44	59
1	B	514/540 (95%)	484 (94%)	29 (6%)	1 (0%)	44	59
1	C	502/540 (93%)	470 (94%)	31 (6%)	1 (0%)	44	59
All	All	1529/1620 (94%)	1442 (94%)	84 (6%)	3 (0%)	45	59

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	23	PRO
1	C	348	GLU
1	A	348	GLU

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	426/443 (96%)	416 (98%)	10 (2%)	45	66
1	B	427/443 (96%)	415 (97%)	12 (3%)	38	59
1	C	418/443 (94%)	405 (97%)	13 (3%)	35	56
All	All	1271/1329 (96%)	1236 (97%)	35 (3%)	40	59

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	VAL
1	A	107	GLU
1	A	135	SER
1	A	149	CYS
1	A	172	THR
1	A	190	ARG
1	A	214	ASN
1	A	263	GLN
1	A	270	HIS
1	A	335	LEU
1	B	21	LEU
1	B	64	LEU
1	B	70	SER
1	B	138	THR
1	B	148	MET
1	B	174	ASP
1	B	371	GLN
1	B	438	GLN
1	B	451	CYS
1	B	511	THR
1	B	512	ASP
1	B	529	SER
1	C	95	LEU
1	C	103	VAL
1	C	122	VAL
1	C	149	CYS
1	C	187	THR
1	C	339	VAL
1	C	343	THR
1	C	344	THR
1	C	357	MET
1	C	374	VAL
1	C	388	ASP
1	C	404	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	493	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	58	ASN
1	A	261	ASN
1	A	340	GLN
1	B	236	GLN
1	B	438	GLN
1	C	57	GLN
1	C	89	ASN
1	C	469	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)

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.

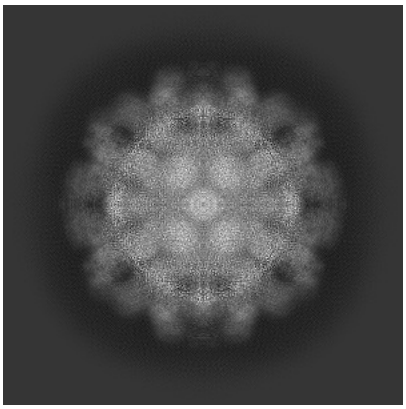
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-47837. These allow visual inspection of the internal detail of the map and identification of artifacts.

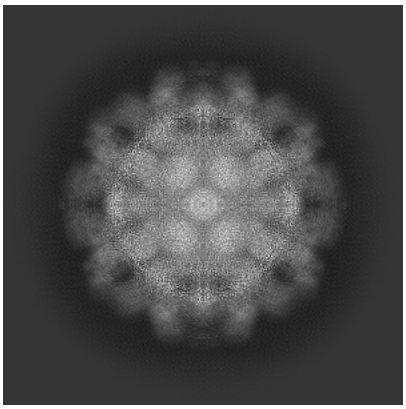
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

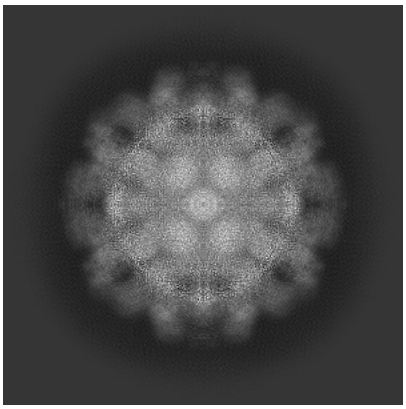
6.1.1 Primary map



X

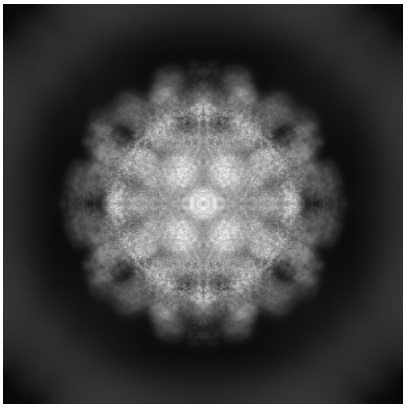


Y

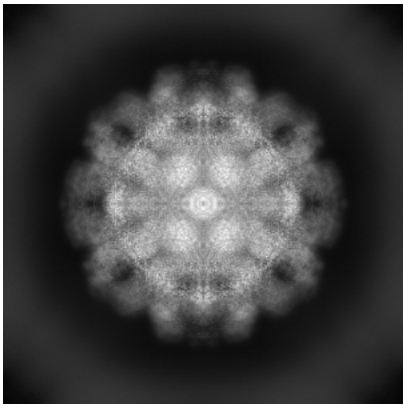


Z

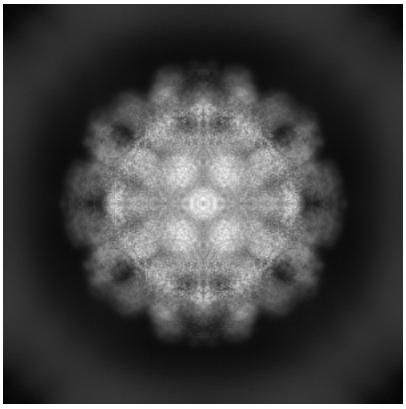
6.1.2 Raw map



X



Y

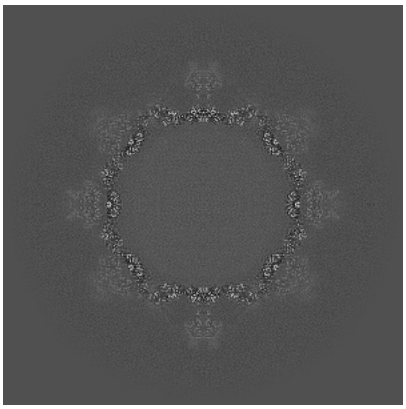


Z

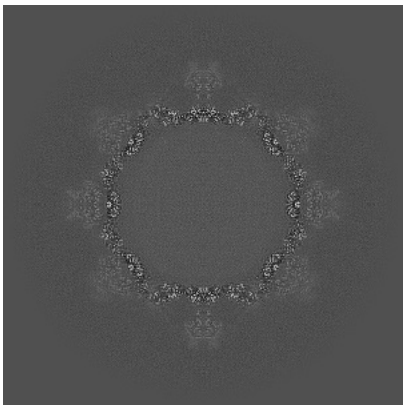
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

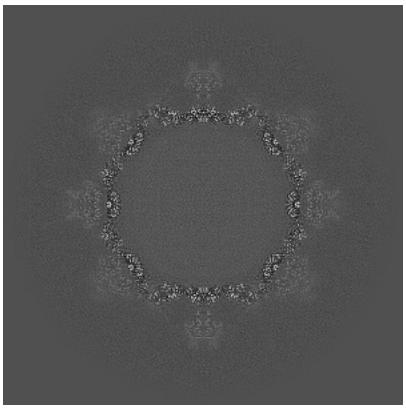
6.2.1 Primary map



X Index: 270

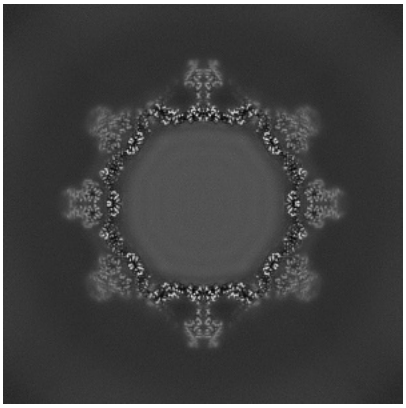


Y Index: 270

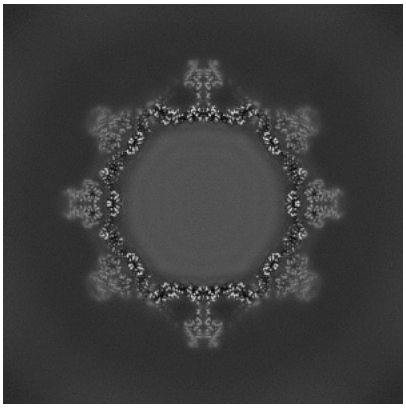


Z Index: 270

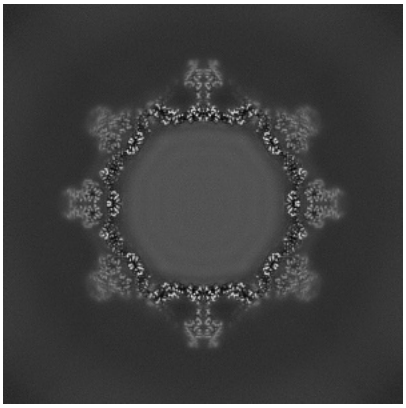
6.2.2 Raw map



X Index: 270



Y Index: 270

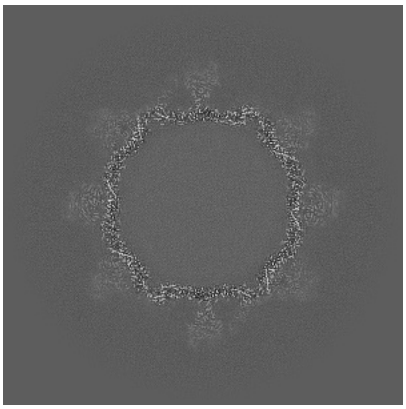


Z Index: 270

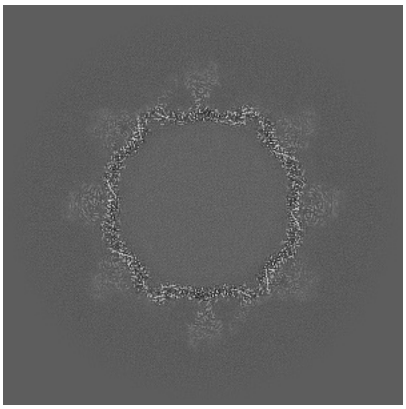
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

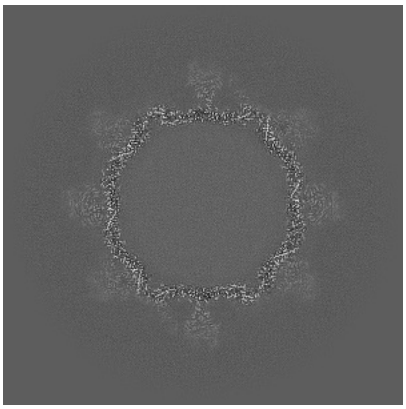
6.3.1 Primary map



X Index: 275

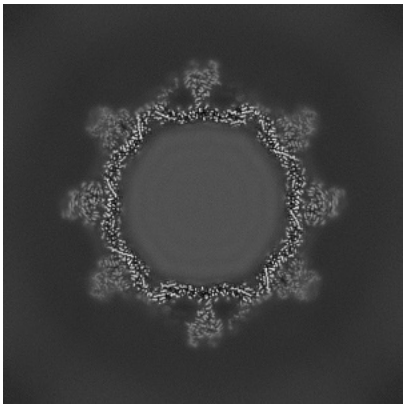


Y Index: 275

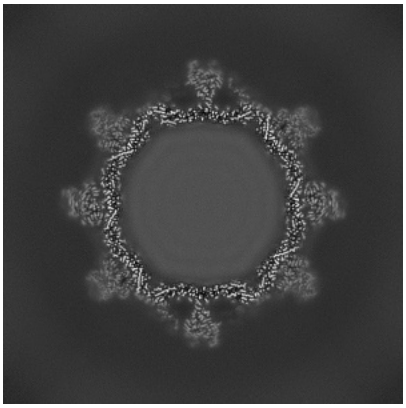


Z Index: 265

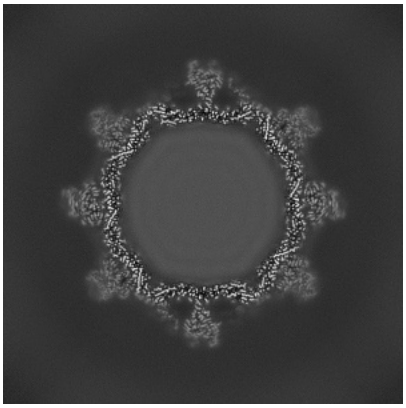
6.3.2 Raw map



X Index: 275



Y Index: 265

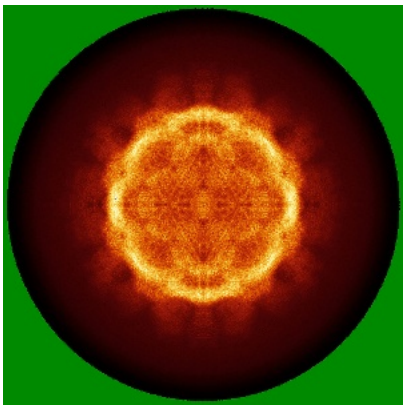


Z Index: 265

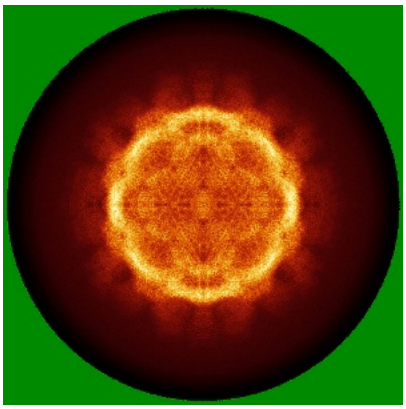
The images above show the largest variance slices of the map in three orthogonal directions.

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

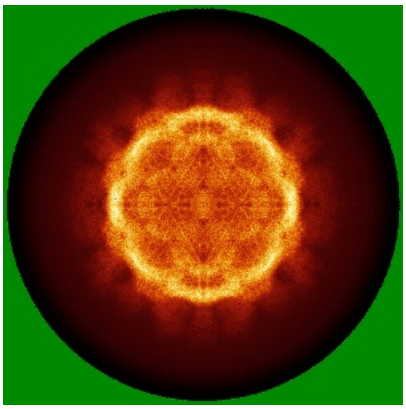
6.4.1 Primary map



X

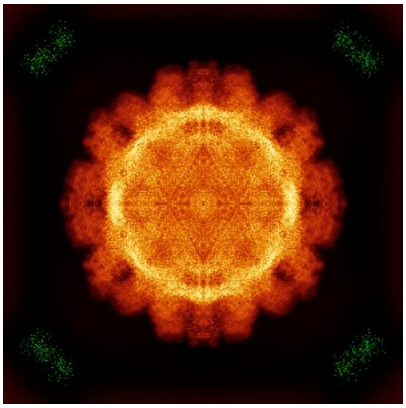


Y

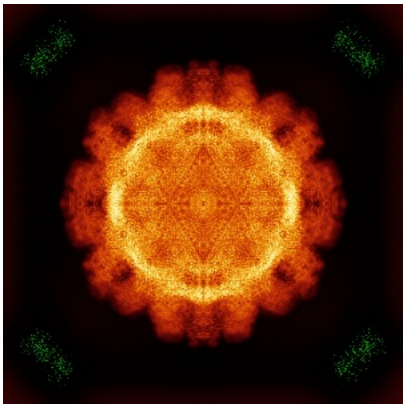


Z

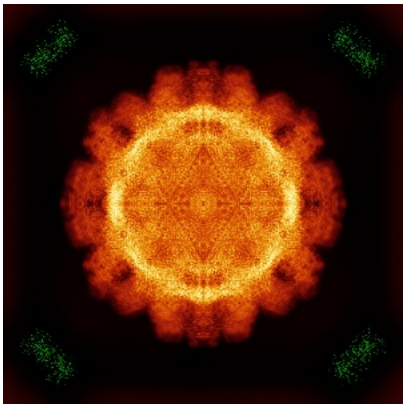
6.4.2 Raw map



X



Y

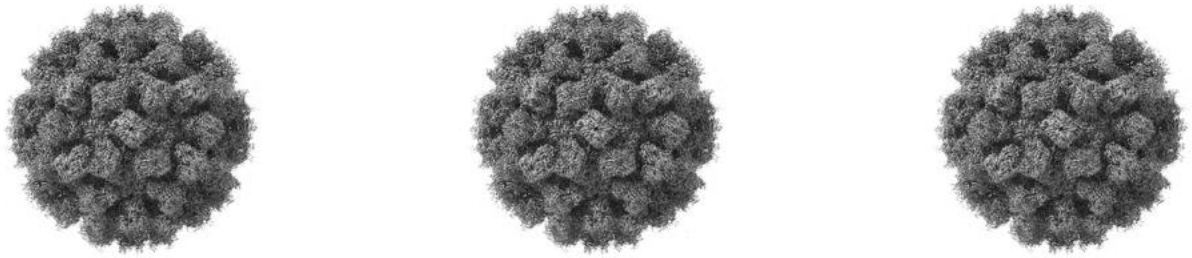


Z

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)

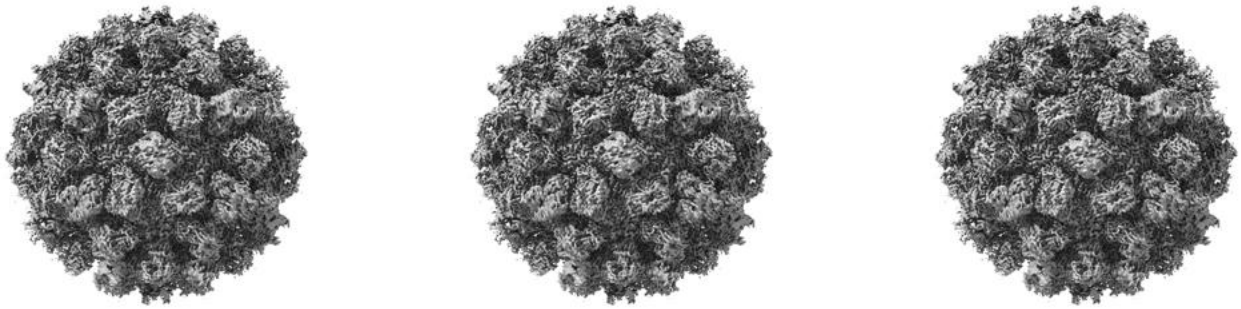
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.35. 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.

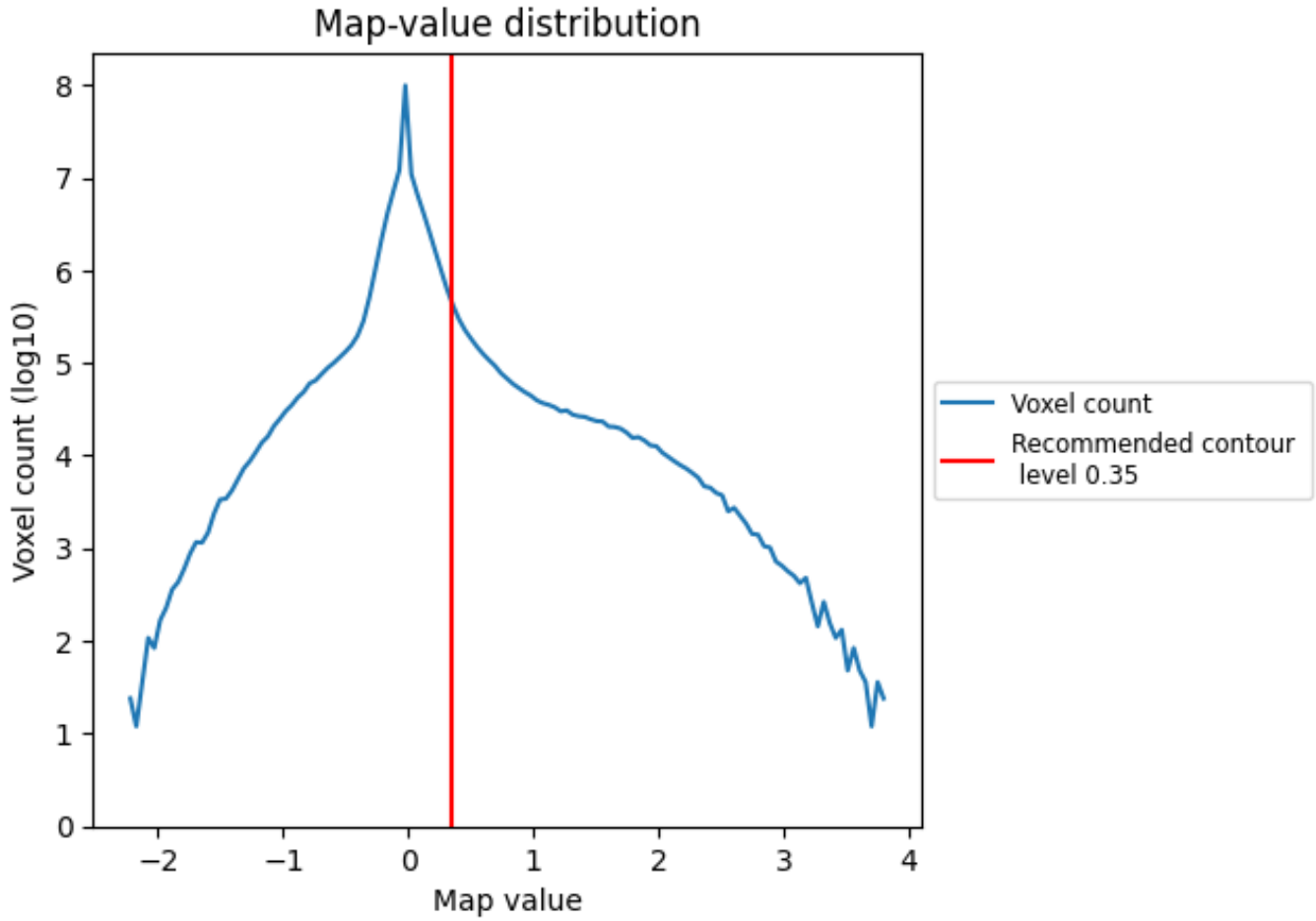
6.6 Mask visualisation (i)

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

7 Map analysis

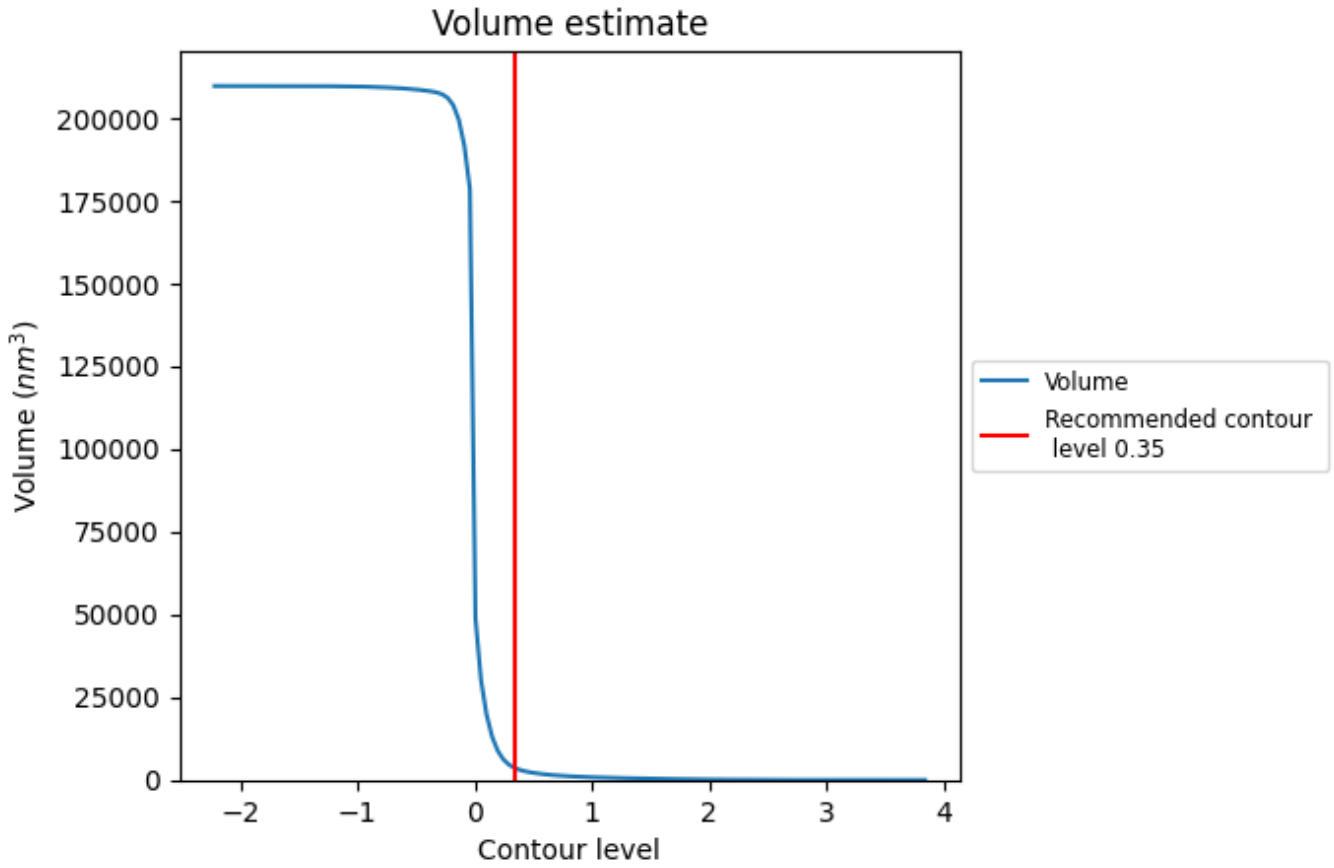
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

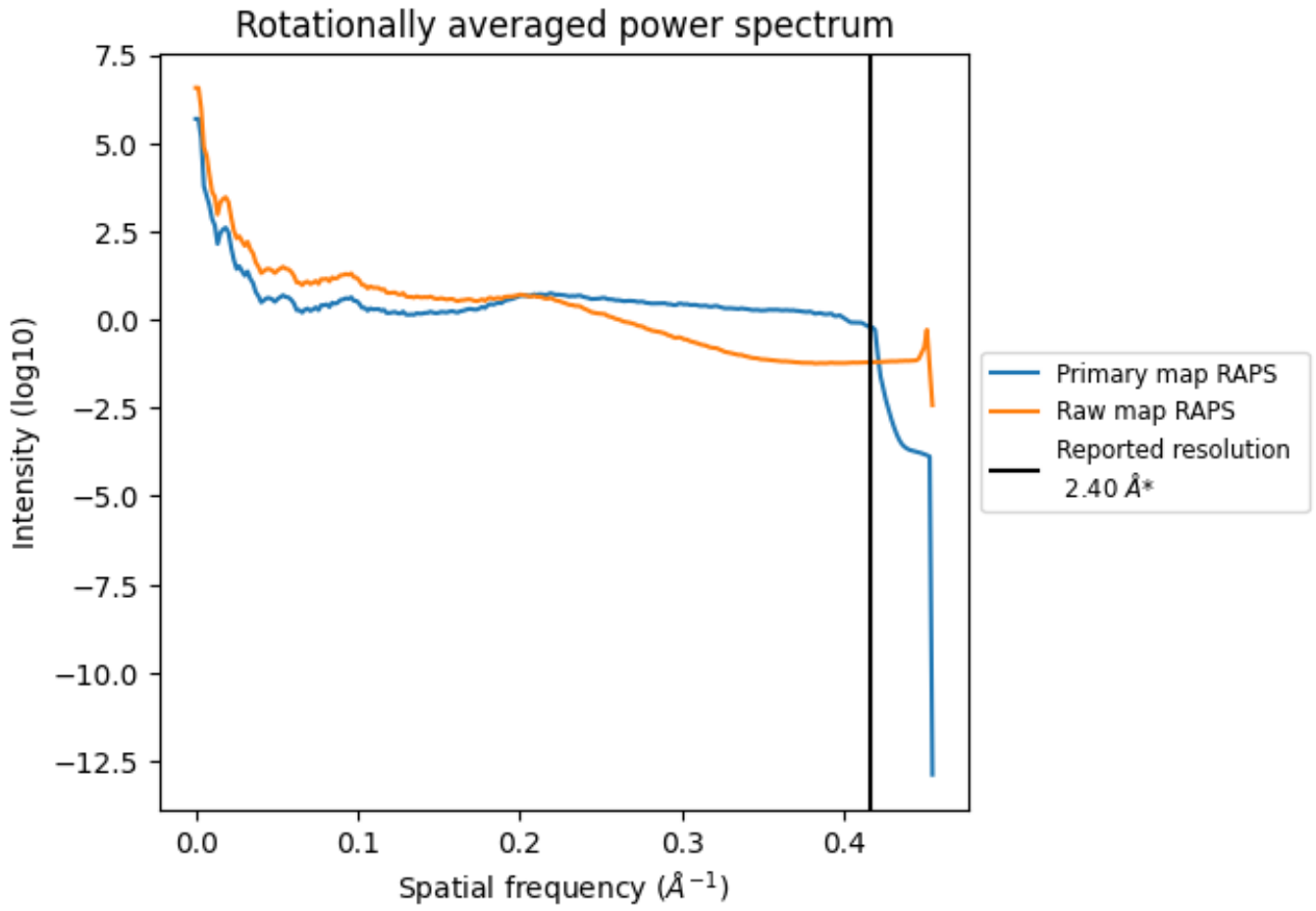
7.2 Volume estimate



The volume at the recommended contour level is 3529 nm^3; this corresponds to an approximate mass of 3188 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)

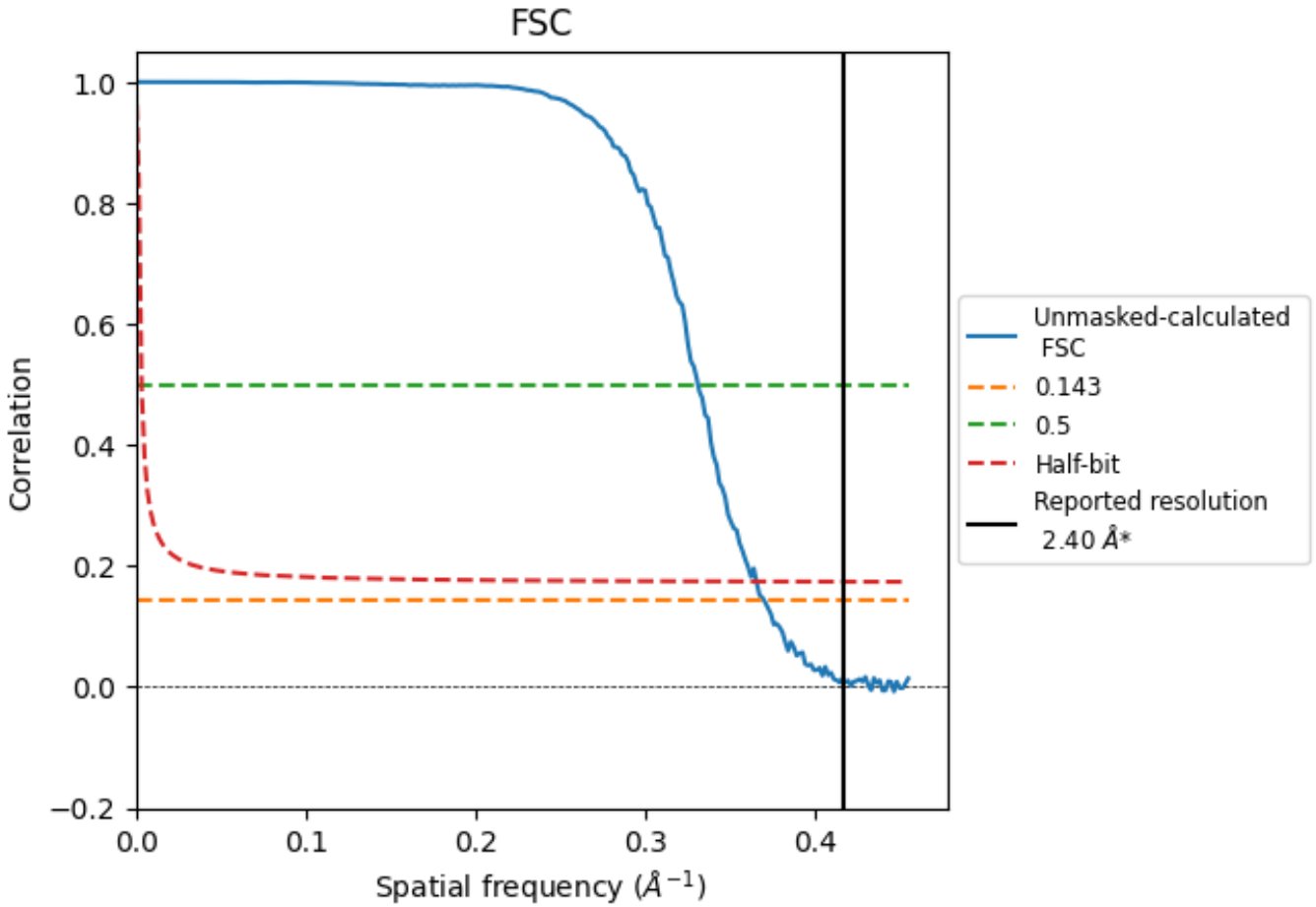


*Reported resolution corresponds to spatial frequency of 0.417 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.417 Å^{-1}

8.2 Resolution estimates (i)

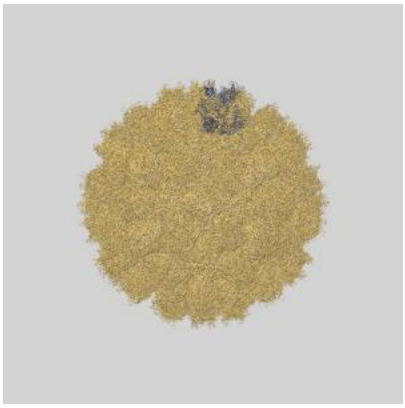
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.71	3.02	2.74

*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 2.71 differs from the reported value 2.4 by more than 10 %

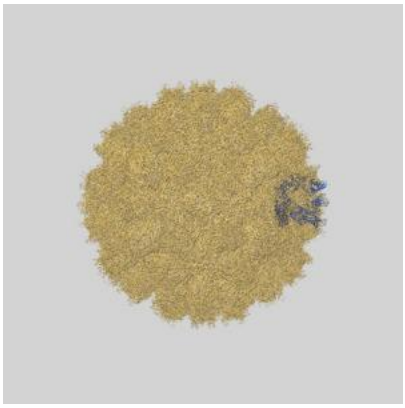
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-47837 and PDB model 9EAN. Per-residue inclusion information can be found in section 3 on page 4.

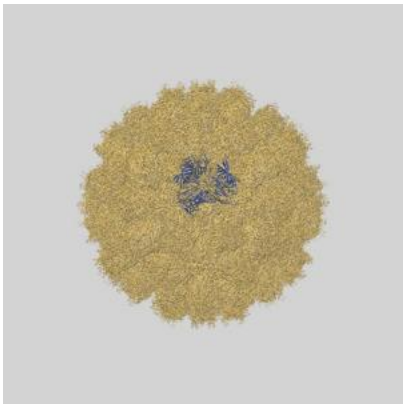
9.1 Map-model overlay



X



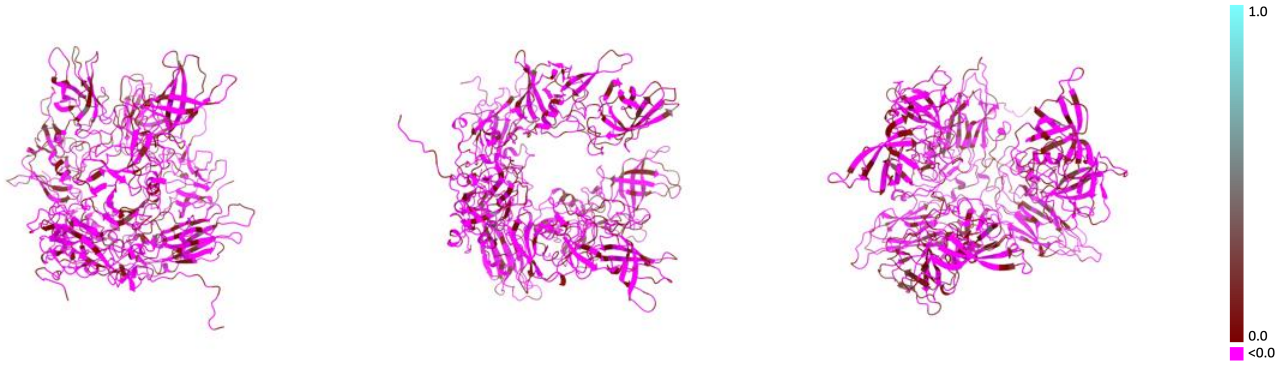
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.35 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.

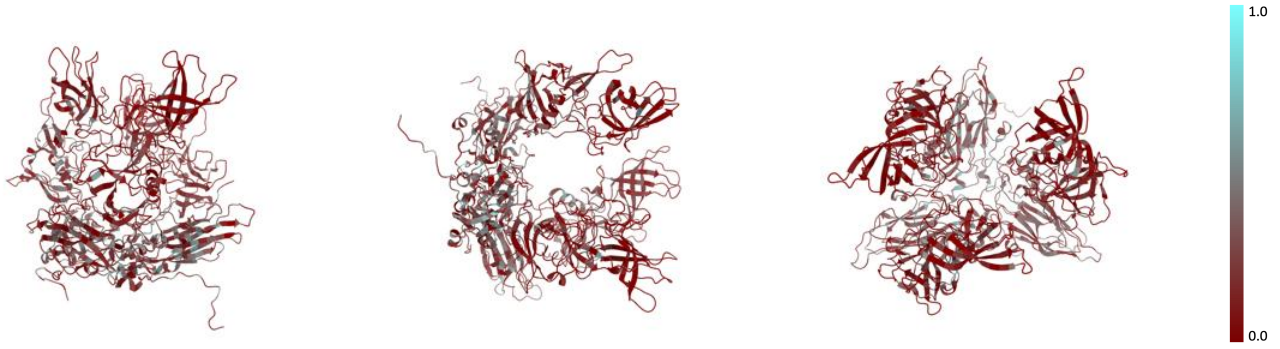
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

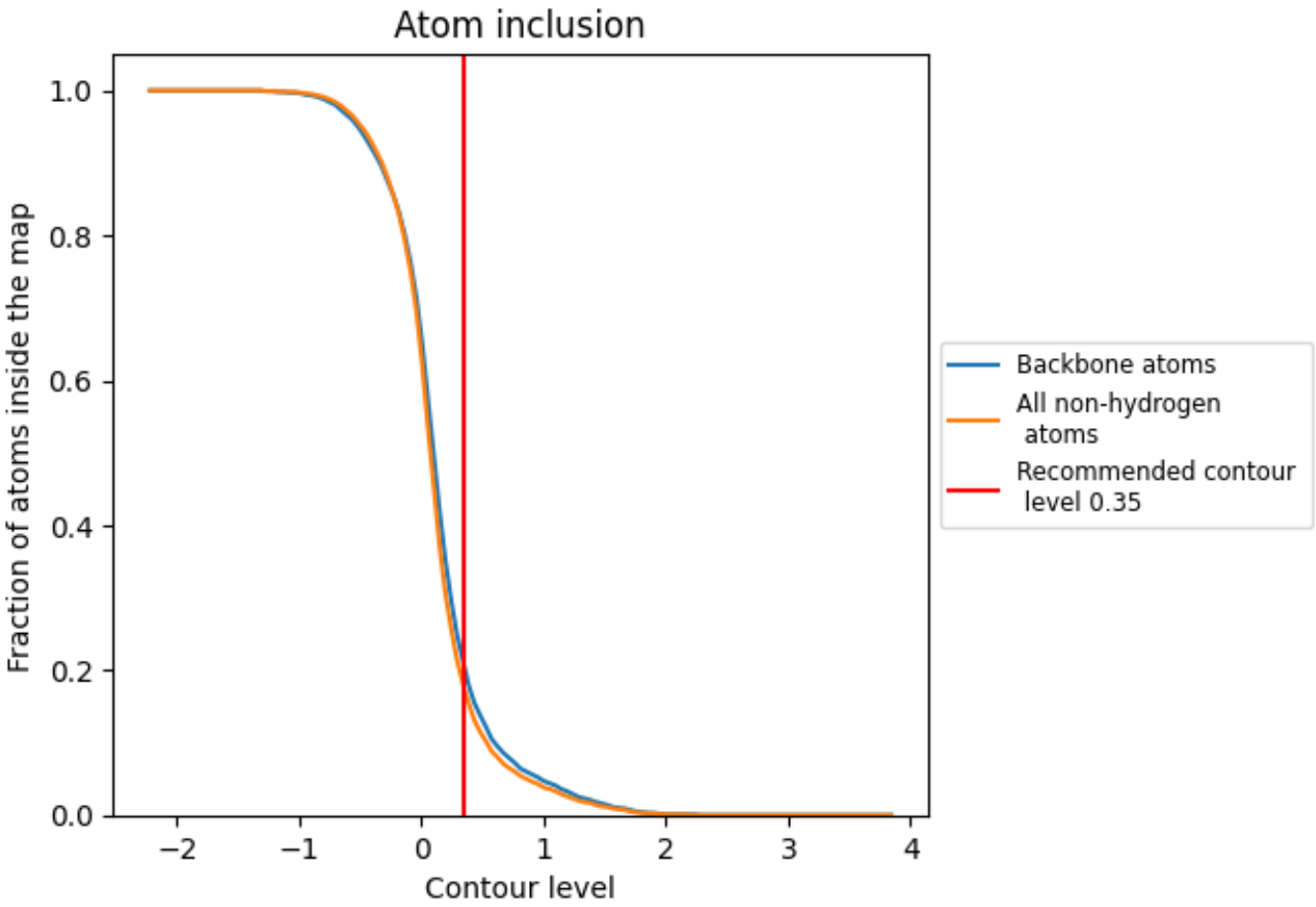
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.35).

9.4 Atom inclusion (i)



At the recommended contour level, 21% of all backbone atoms, 18% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.1750	-0.0780
A	0.1660	-0.0910
B	0.1690	-0.0820
C	0.1920	-0.0590