Full wwPDB EM Validation Report (i)

Nov 20, 2022 – 05:12 am GMT

PDB ID	:	6H2B
EMDB ID	:	EMD-0129
Title	:	Structure of the Macrobrachium rosenbergii Nodavirus
Authors	:	Ho, K.H.; Gabrielsen, M.; Beh, P.L.; Kueh, C.L.; Thong, Q.X.; Streetley, J.; Tan, W.S.; Bhella, D.
Deposited on	:	2018-07-13
Resolution	:	3.28 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 (i) 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 (i)) were used in the production of this report:

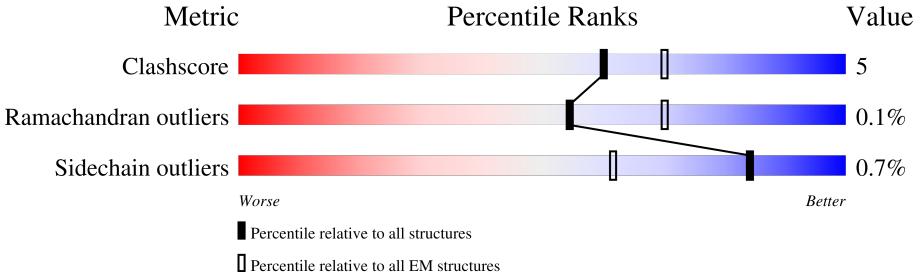
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.28 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	371	14% 73% 12% 15%
1	B	371	14% 73% 12% 15%
1	C	371	23% 82% 10% 8%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 15252 atoms, of which 7582 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.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	316	4947	1575	2458	421	486	7	0	0
1	B	317	4958	1578	2463	422	488	7	0	0
1	C	341	5341	1698	2661	455	520	7	0	0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

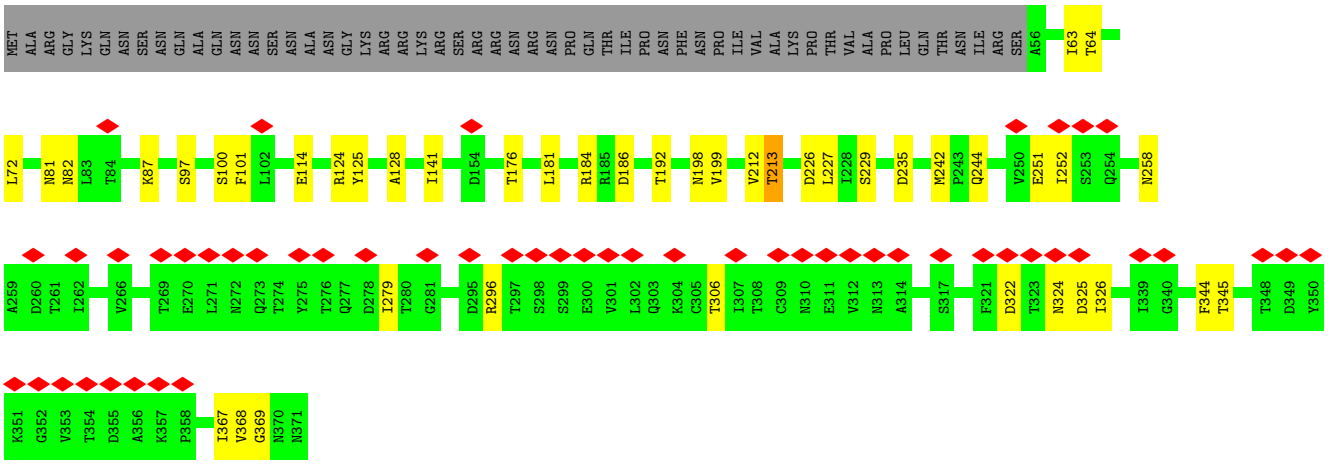
Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
2	A	3	3	3	0
2	B	1	1	1	0
2	C	2	2	2	0

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.

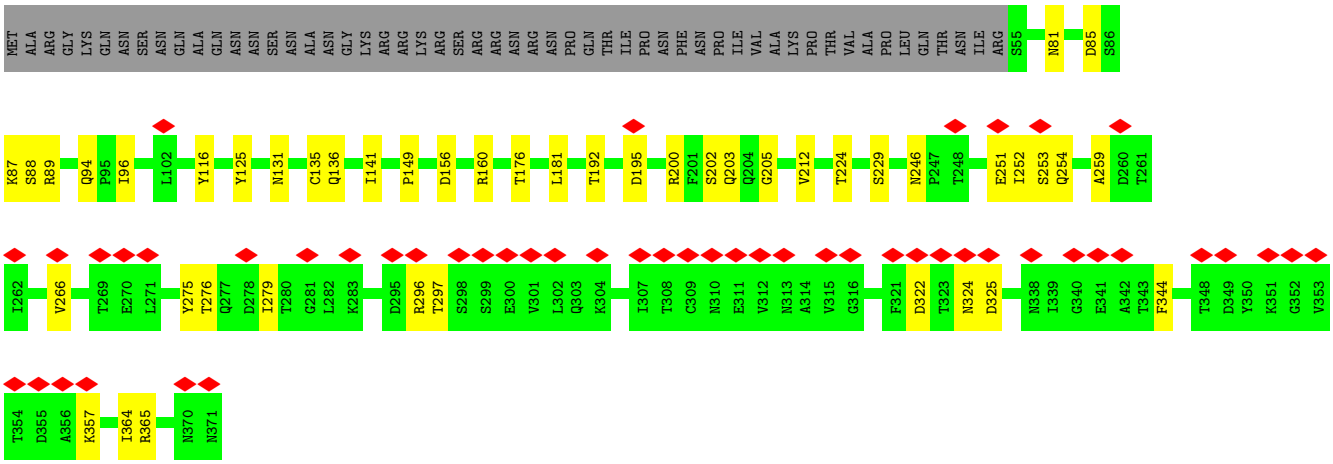
- Molecule 1: Capsid protein

Chain A:



- Molecule 1: Capsid protein

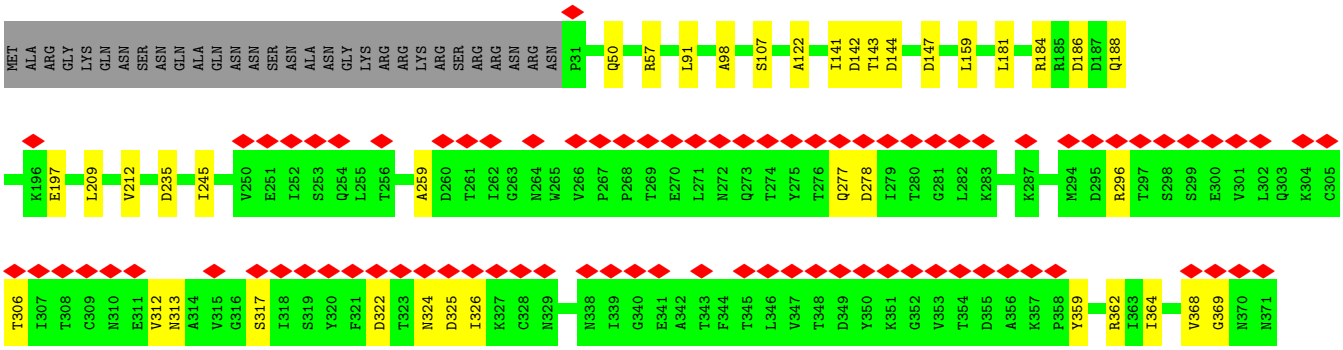
Chain B:



- Molecule 1: Capsid protein

Chain C:

23%
82%
10%
8%


MET ALA ARG GLY LYS GLN ASN SER ASN GLN ALA GLN ASN ASN SER ASN ALA ASN GLY LYS ARG ARG LYS ARG SER ARG ARG ASN ARG ASN P31 Q50 R57 L91 A98 S107 A122 I141 D142 T143 D144 D147 L159 L181 R184 R185 D186 D187 Q188
K196 E197 L209 V212 D235 I245 V250 E251 I252 S253 Q254 L255 T256 A259 D260 T261 I262 G263 N264 W265 V266 P267 P268 T269 E270 L271 N272 Q273 T274 Y275 T276 Q277 D278 I279 T280 G281 L282 K283 K287 M294 D295 R296 T297 S298 S299 E300 V301 L302 Q303 K304 C305
T306 I307 T308 C309 N310 E311 V312 N313 A314 V315 G316 S317 I318 S319 Y320 F321 D322 T323 N324 D325 I326 K327 C328 N329 N338 I339 G340 E341 A342 T343 F344 T345 L346 V347 T348 D349 Y350 K351 G352 V353 T354 D355 A356 K357 P358 Y359 R362 I363 I364 V368 G369 N370 N371

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	40883	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 ($e^-/Å^2$)	36	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	47170	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.159	Depositor
Minimum map value	-0.088	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	542.72, 542.72, 542.72	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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: CA

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	0.52	0/2539	0.63	0/3467
1	B	0.52	0/2545	0.61	0/3475
1	C	0.49	0/2736	0.62	0/3740
All	All	0.51	0/7820	0.62	0/10682

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	2489	2458	2458	28	0
1	B	2495	2463	2463	25	0
1	C	2680	2661	2661	23	0
2	A	3	0	0	0	0
2	B	1	0	0	0	0
2	C	2	0	0	0	0
All	All	7670	7582	7582	71	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 (71) 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:296:ARG:NH2	1:A:322:ASP:OD2	2.18	0.77
1:B:81:ASN:OD1	1:B:224:THR:OG1	2.03	0.76
1:C:306:THR:O	1:C:317:SER:OG	2.06	0.74
1:B:276:THR:OG1	1:B:344:PHE:O	2.04	0.73
1:B:87:LYS:NZ	1:B:149:PRO:O	2.22	0.73
1:A:124:ARG:NH1	1:A:235:ASP:OD2	2.22	0.72
1:C:144:ASP:HB3	1:C:147:ASP:OD1	1.92	0.70
1:C:98:ALA:O	1:C:107:SER:OG	2.08	0.68
1:A:306:THR:OG1	1:A:345:THR:O	2.07	0.67
1:B:116:TYR:OH	1:B:202:SER:O	2.13	0.67
1:C:322:ASP:OD2	1:C:359:TYR:OH	2.12	0.66
1:C:184:ARG:NH2	1:C:186:ASP:OD2	2.30	0.64
1:C:159:LEU:HD13	1:C:212:VAL:HG23	1.80	0.63
1:B:156:ASP:OD2	1:B:160:ARG:NH2	2.34	0.61
1:C:277:GLN:NE2	1:C:278:ASP:O	2.36	0.59
1:A:141:ILE:HG21	1:A:181:LEU:HD23	1.86	0.57
1:A:97:SER:OG	1:A:100:SER:OG	2.20	0.57
1:B:125:TYR:OH	1:B:229:SER:O	2.10	0.57
1:A:184:ARG:NE	1:A:186:ASP:OD1	2.36	0.56
1:A:97:SER:HG	1:A:100:SER:HG	1.52	0.55
1:C:184:ARG:NH1	1:C:188:GLN:OE1	2.38	0.55
1:B:200:ARG:NH2	1:C:197:GLU:OE1	2.40	0.54
1:B:89:ARG:NH1	1:B:212:VAL:O	2.41	0.54
1:B:266:VAL:O	1:B:275:TYR:OH	2.25	0.53
1:B:131:ASN:O	1:C:50:GLN:NE2	2.42	0.53
1:A:63:ILE:O	1:A:64:THR:OG1	2.27	0.51
1:A:114:GLU:OE1	1:C:143:THR:OG1	2.28	0.51
1:C:122:ALA:HB3	1:C:235:ASP:OD1	2.12	0.50
1:B:125:TYR:O	1:B:176:THR:OG1	2.16	0.50
1:A:212:VAL:HG12	1:A:213:THR:H	1.76	0.50
1:B:252:ILE:O	1:B:253:SER:OG	2.20	0.50
1:A:368:VAL:HG22	1:A:369:GLY:H	1.76	0.50
1:B:192:THR:OG1	1:B:246:ASN:ND2	2.46	0.49
1:A:81:ASN:OD1	1:A:82:ASN:N	2.46	0.48
1:A:242:MET:SD	1:C:143:THR:OG1	2.62	0.48
1:B:297:THR:O	1:B:357:LYS:NZ	2.35	0.47
1:C:368:VAL:HG22	1:C:369:GLY:H	1.79	0.47
1:A:226:ASP:OD1	1:A:227:LEU:N	2.48	0.46
1:A:114:GLU:O	1:A:192:THR:N	2.49	0.45
1:A:198:ASN:OD1	1:A:199:VAL:N	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:ASN:OD1	1:B:325:ASP:N	2.50	0.45
1:C:91:LEU:HD11	1:C:209:LEU:HD23	1.99	0.45
1:B:296:ARG:NH2	1:B:322:ASP:OD2	2.50	0.45
1:C:324:ASN:OD1	1:C:325:ASP:N	2.49	0.44
1:A:279:ILE:HD12	1:A:344:PHE:CE2	2.53	0.44
1:C:141:ILE:HG21	1:C:181:LEU:HD23	2.00	0.44
1:B:135:CYS:SG	1:B:136:GLN:N	2.91	0.44
1:B:251:GLU:OE2	1:B:254:GLN:NE2	2.51	0.44
1:A:184:ARG:NH2	1:A:186:ASP:OD2	2.50	0.43
1:A:128:ALA:N	1:A:229:SER:O	2.47	0.43
1:B:141:ILE:HG21	1:B:181:LEU:HD13	1.99	0.43
1:C:259:ALA:HB2	1:C:364:ILE:HG22	2.01	0.43
1:C:144:ASP:CB	1:C:147:ASP:OD1	2.62	0.42
1:C:245:ILE:HG23	1:C:245:ILE:O	2.19	0.42
1:A:279:ILE:HD12	1:A:344:PHE:HE2	1.84	0.42
1:B:279:ILE:HD12	1:B:344:PHE:HE2	1.84	0.42
1:A:324:ASN:OD1	1:A:325:ASP:N	2.53	0.42
1:A:325:ASP:OD1	1:A:326:ILE:N	2.53	0.42
1:B:259:ALA:HB2	1:B:364:ILE:HG22	2.02	0.41
1:A:125:TYR:O	1:A:176:THR:OG1	2.29	0.41
1:B:141:ILE:HG21	1:B:181:LEU:CD1	2.51	0.41
1:C:325:ASP:OD1	1:C:326:ILE:N	2.53	0.41
1:B:96:ILE:HG22	1:B:205:GLY:C	2.41	0.41
1:B:195:ASP:OD2	1:B:203:GLN:NE2	2.48	0.41
1:A:114:GLU:OE2	1:C:142:ASP:OD1	2.39	0.41
1:C:312:VAL:HG23	1:C:313:ASN:N	2.36	0.41
1:A:72:LEU:HD22	1:A:101:PHE:CE1	2.56	0.40
1:A:114:GLU:HG3	1:A:244:GLN:HG2	2.03	0.40
1:A:251:GLU:HG2	1:A:252:ILE:HD12	2.03	0.40
1:A:258:ASN:HB2	1:A:367:ILE:HD11	2.02	0.40
1:B:85:ASP:OD1	1:B:88:SER: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	314/371 (85%)	271 (86%)	42 (13%)	1 (0%)	41	72
1	B	315/371 (85%)	270 (86%)	45 (14%)	0	100	100
1	C	339/371 (91%)	302 (89%)	37 (11%)	0	100	100
All	All	968/1113 (87%)	843 (87%)	124 (13%)	1 (0%)	54	82

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	213	THR

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	282/330 (86%)	281 (100%)	1 (0%)	91	95
1	B	283/330 (86%)	281 (99%)	2 (1%)	84	90
1	C	305/330 (92%)	302 (99%)	3 (1%)	76	85
All	All	870/990 (88%)	864 (99%)	6 (1%)	84	90

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	LYS
1	B	94	GLN
1	B	365	ARG
1	C	57	ARG
1	C	296	ARG
1	C	362	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

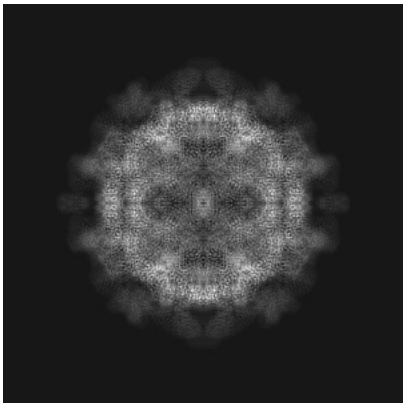
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-0129. These allow visual inspection of the internal detail of the map and identification of artifacts.

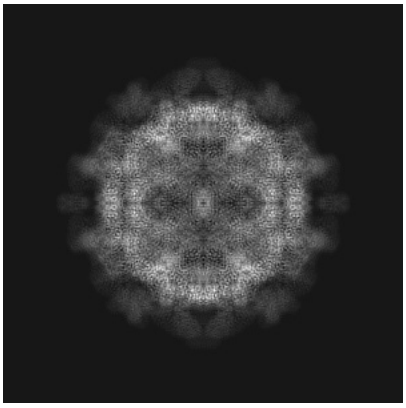
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

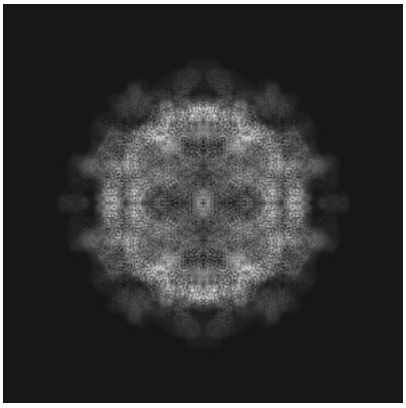
6.1.1 Primary map



X



Y

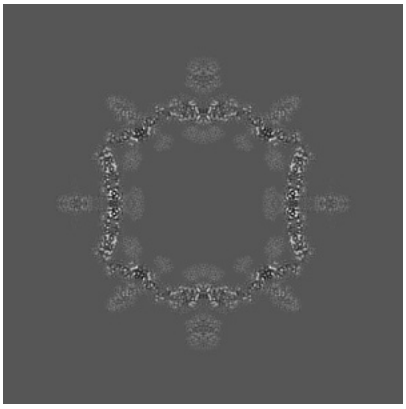


Z

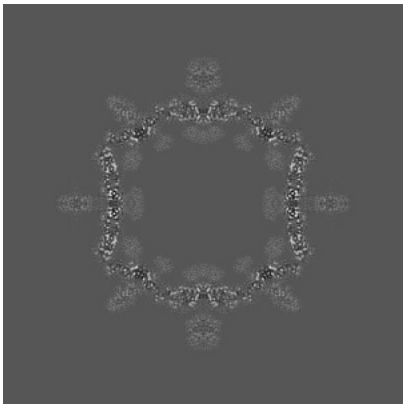
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

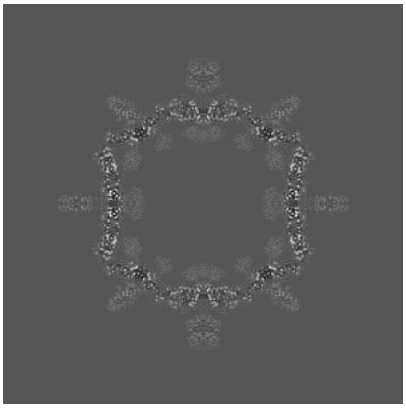
6.2.1 Primary map



X Index: 256



Y Index: 256

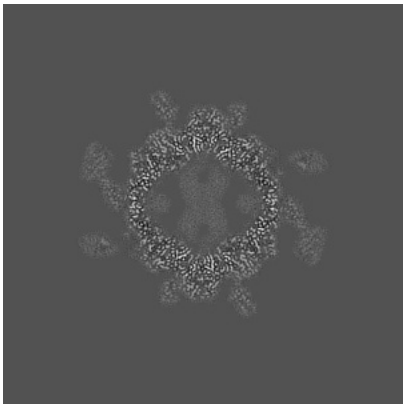


Z Index: 256

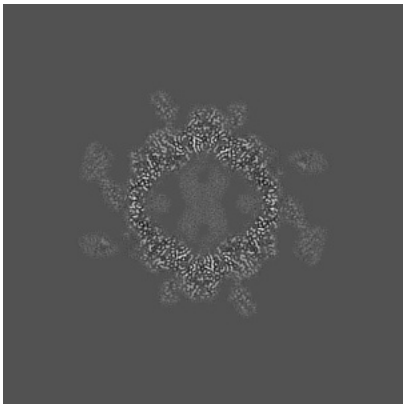
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

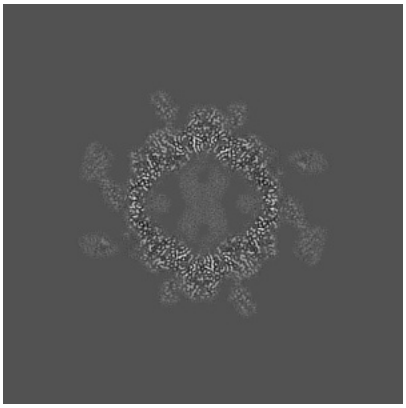
6.3.1 Primary map



X Index: 344



Y Index: 344

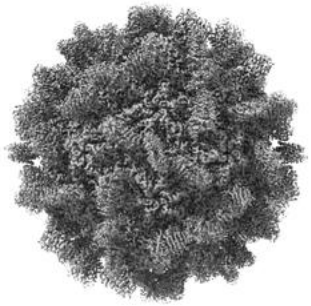


Z Index: 344

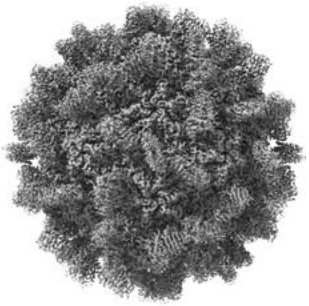
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

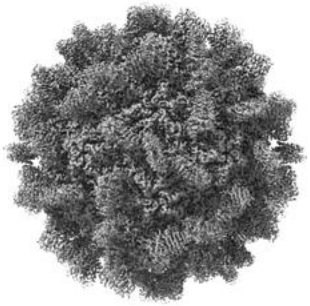
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

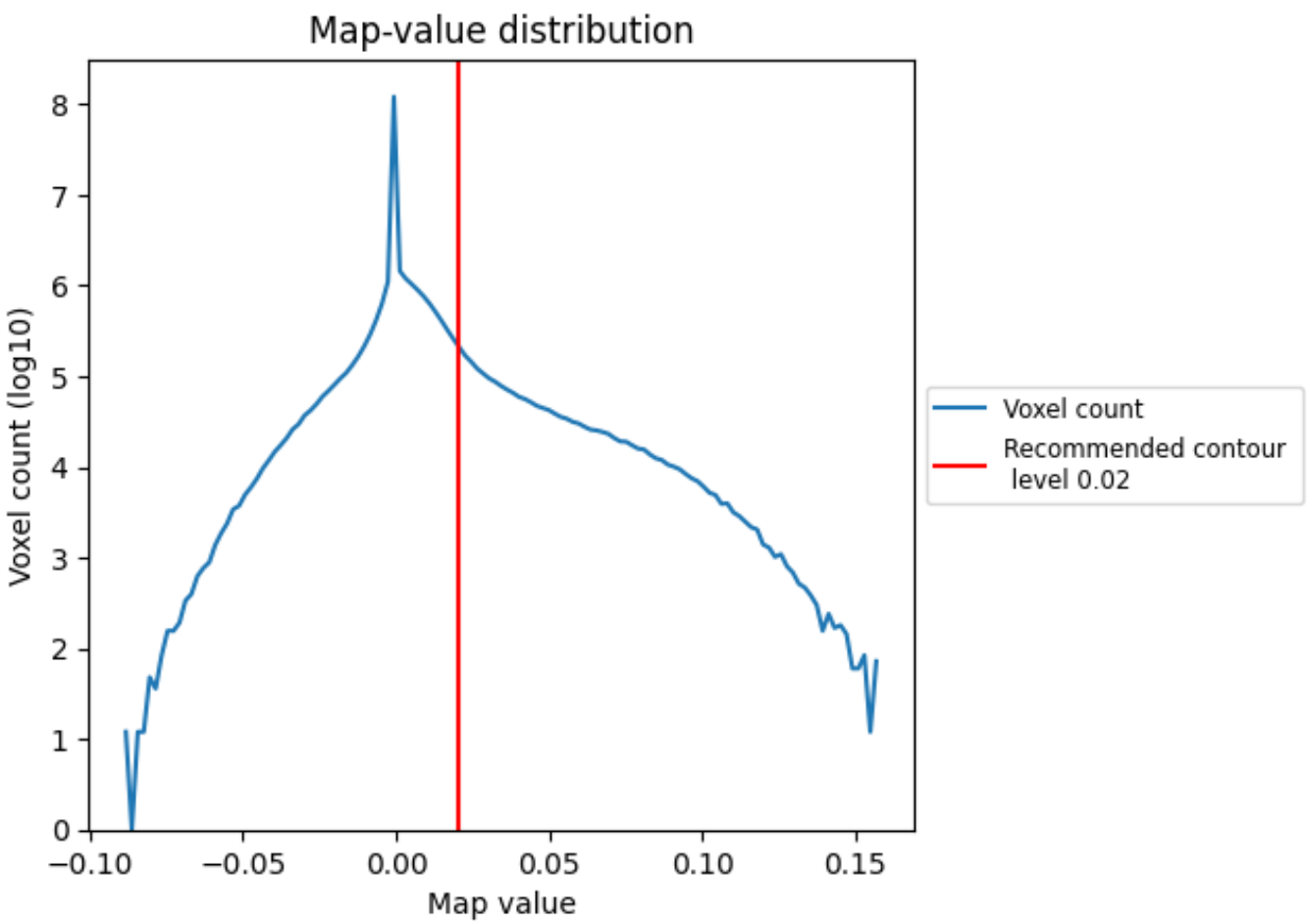
6.5 Mask visualisation (i)

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

7 Map analysis (i)

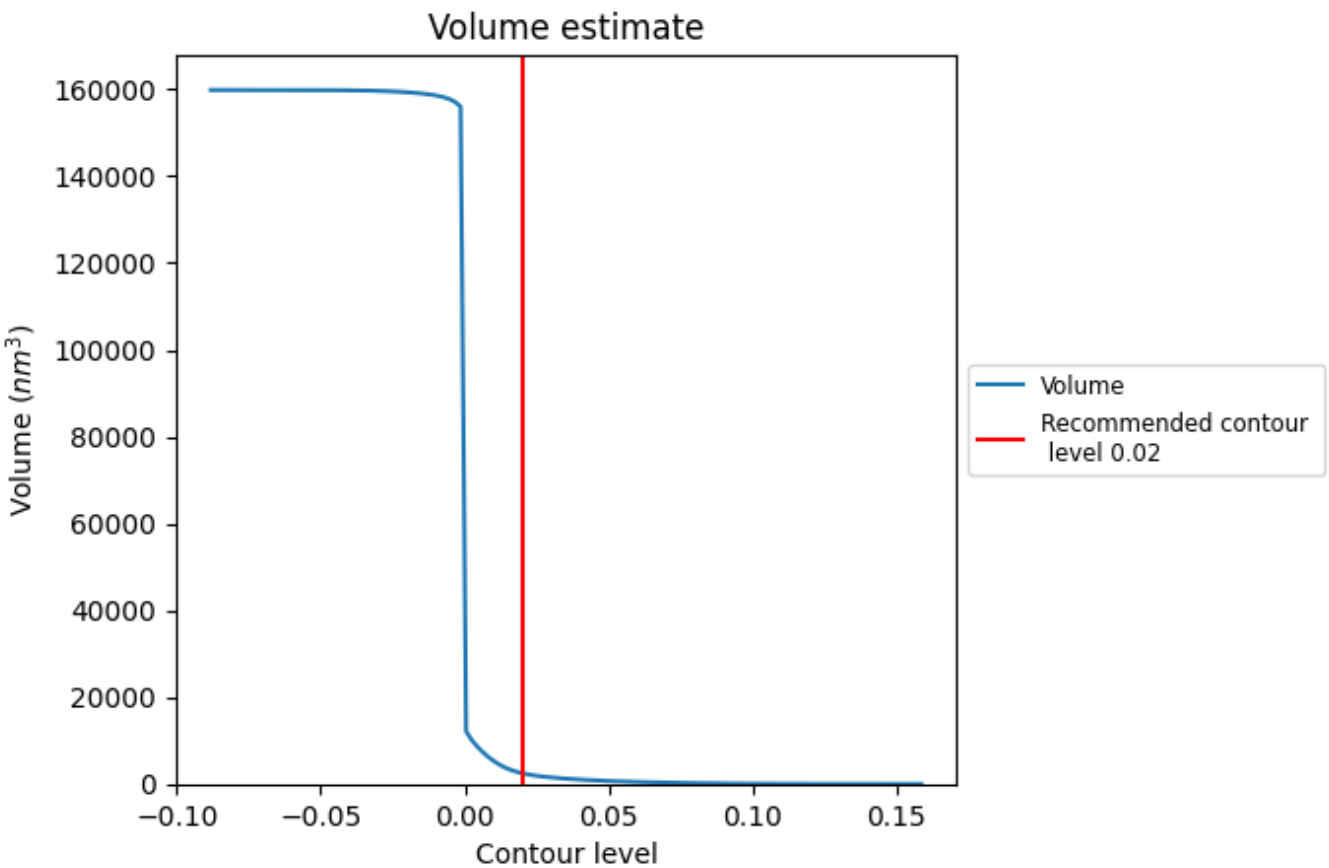
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

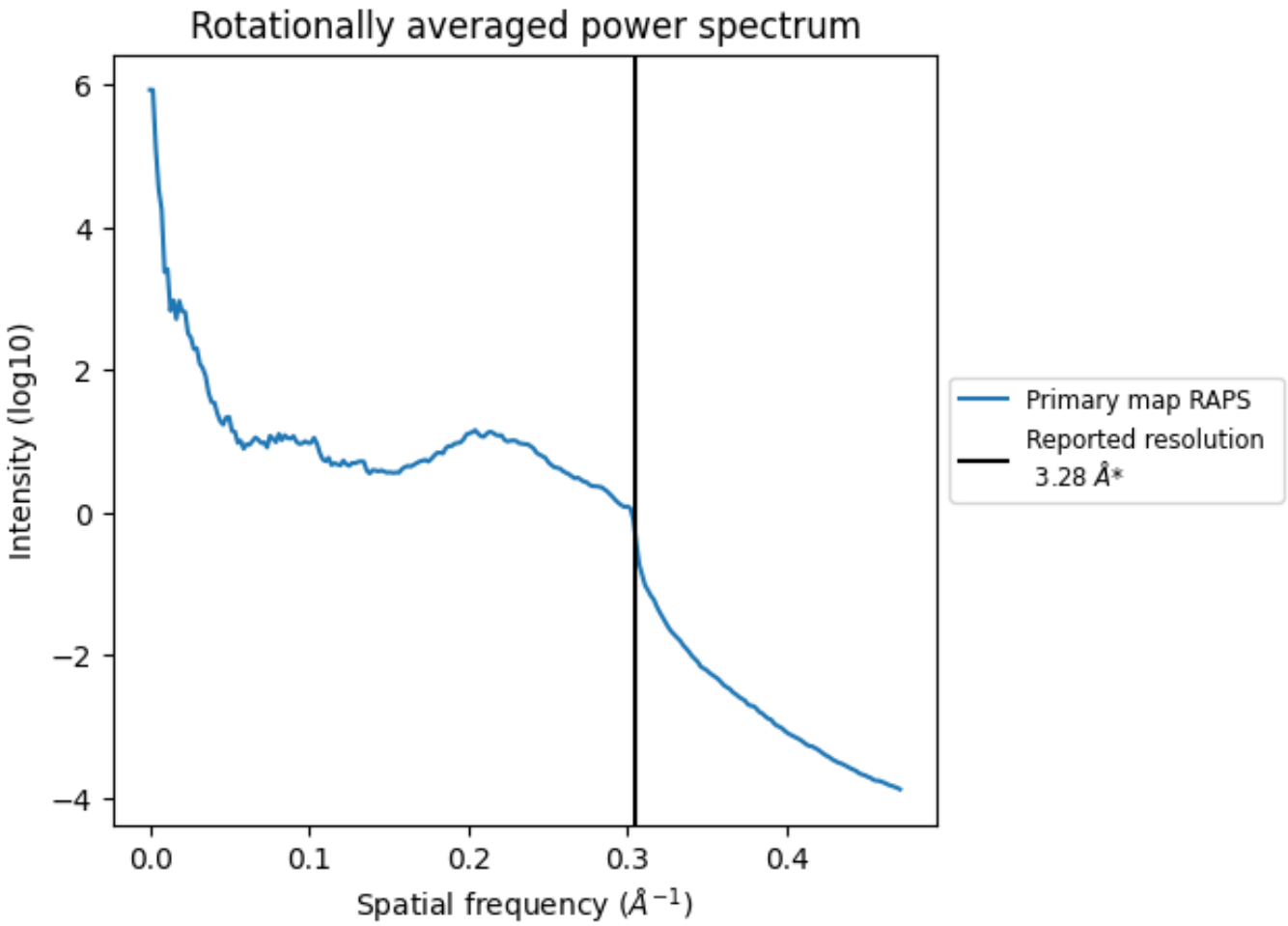
7.2 Volume estimate (i)



The volume at the recommended contour level is 2471 nm^3; this corresponds to an approximate mass of 2232 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)

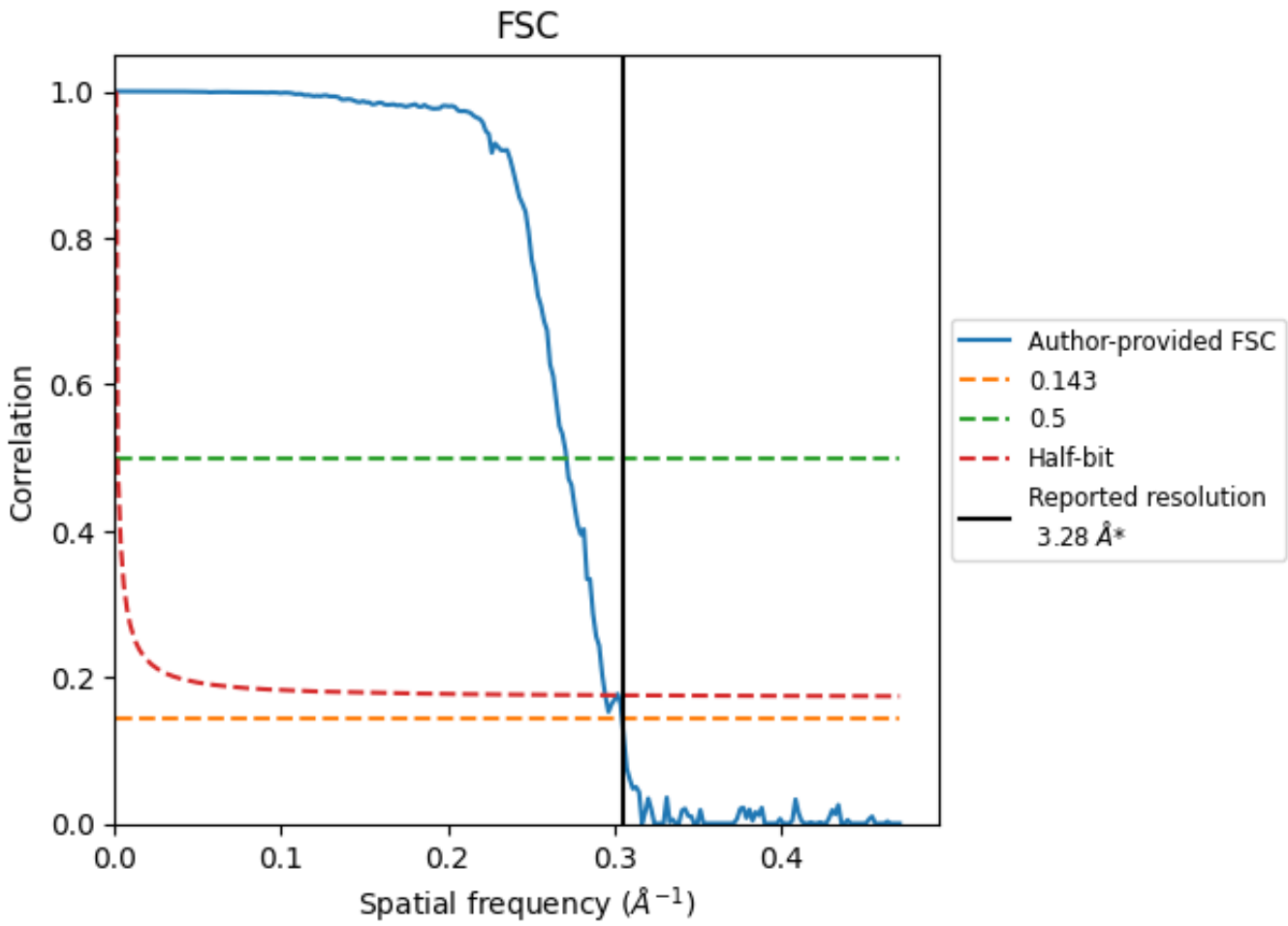


*Reported resolution corresponds to spatial frequency of 0.305 Å^{-1}

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 0.305 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.28	-	-
Author-provided FSC curve	3.28	3.69	3.39
Unmasked-calculated*	-	-	-

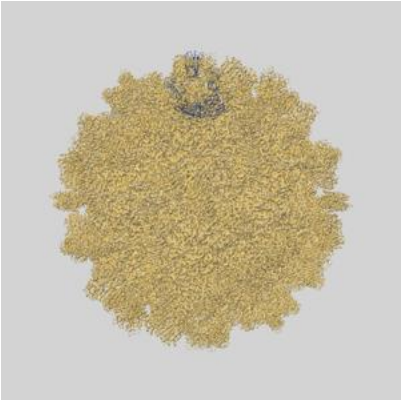
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit (i)

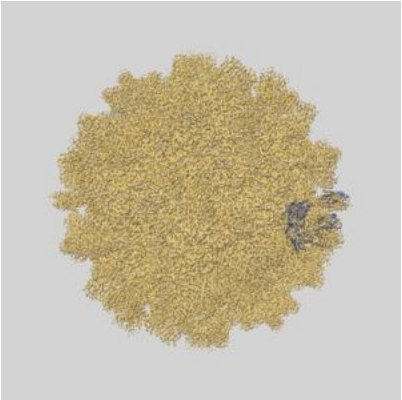
This section contains information regarding the fit between EMDB map EMD-0129 and PDB model 6H2B. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlays

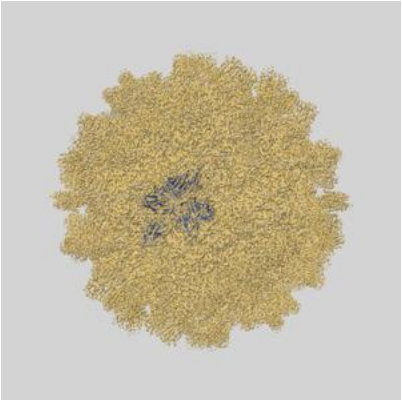
9.1.1 Map-model overlay (i)



X

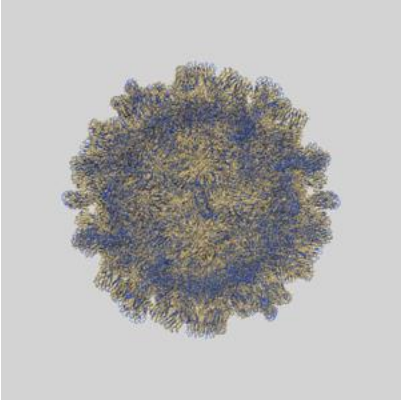


Y

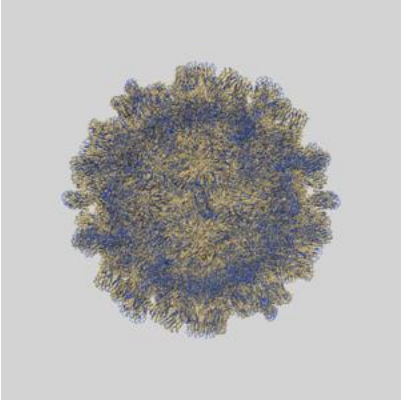


Z

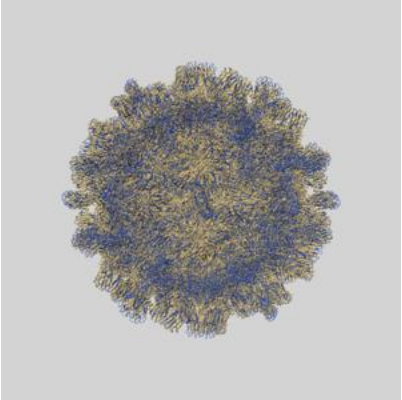
9.1.2 Map-model assembly overlay (i)



X



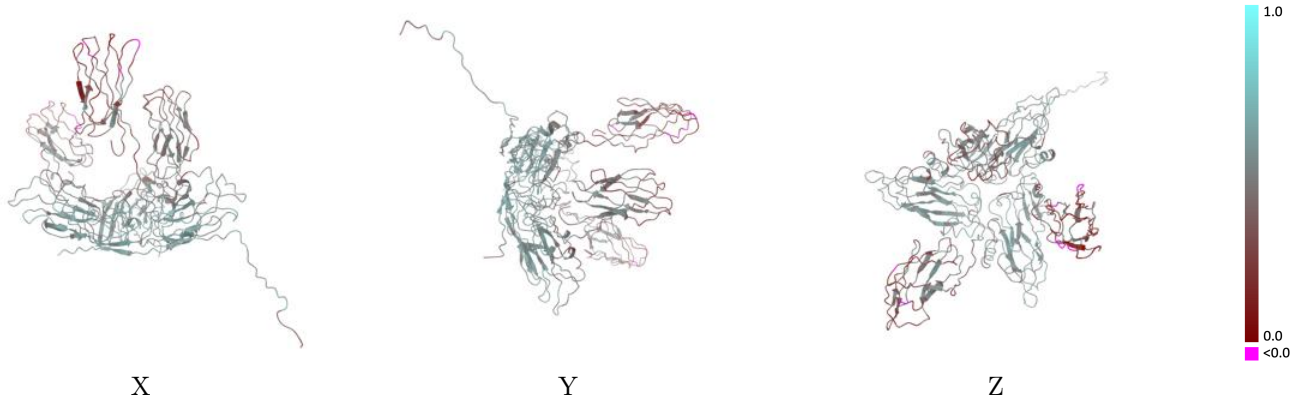
Y



Z

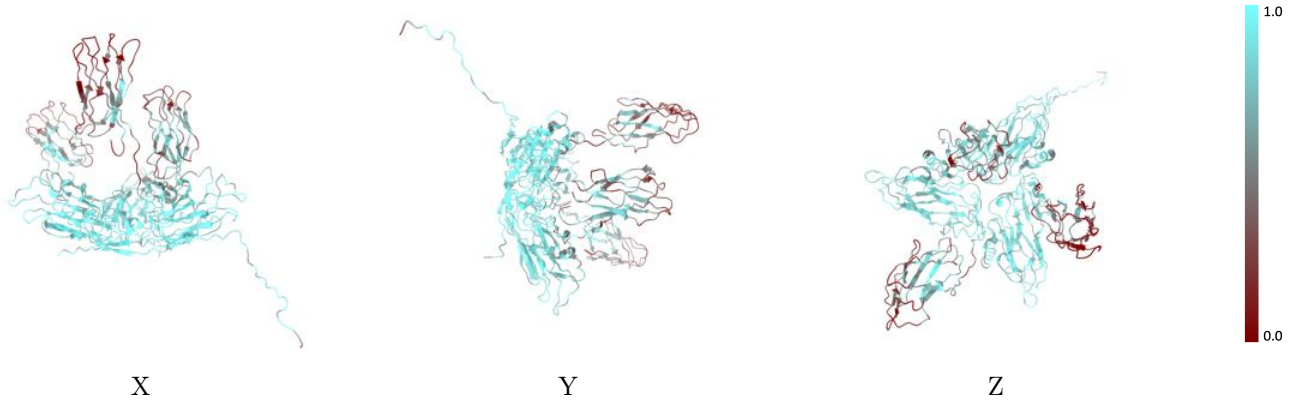
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



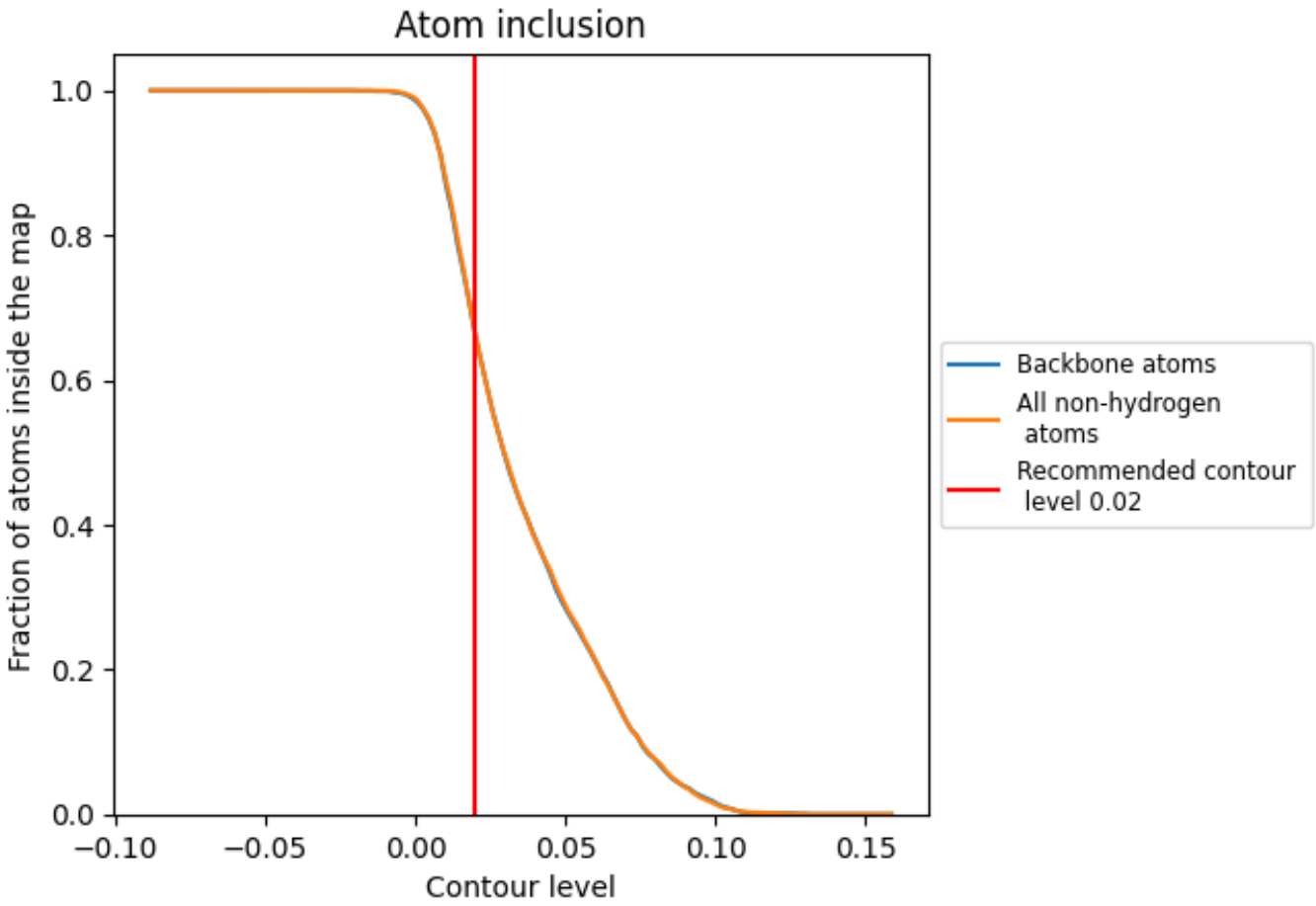
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 66% of all backbone atoms, 66% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6623	0.4610
A	0.6867	0.4660
B	0.7044	0.4820
C	0.6304	0.4380