wwPDB EM Validation Summary Report (i)

Nov 29, 2022 – 06:17 AM JST

PDB ID	:	7VYM
EMDB ID	:	EMD-32209
Title	:	Coxsackievirus B3 at pH7.4 (VP3-234E) incubation with coxsackievirus and adenovirus receptor for 10min
Authors	:	Wang, Q.L.; Liu, C.C.
Deposited on	:	2021-11-14
Resolution	:	3.68 Å(reported)
Based on initial model	:	1COV

This is a wwPDB EM Validation Summary 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:

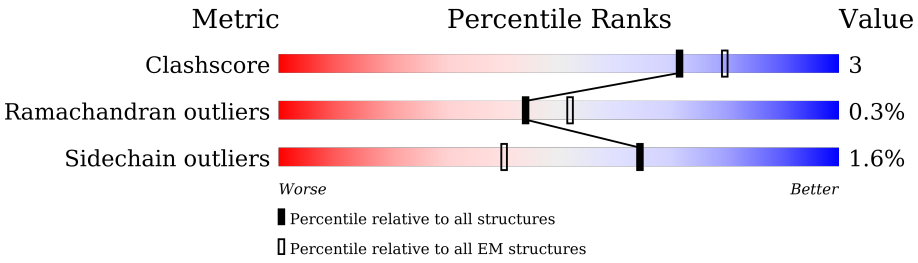
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.68 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	284	85% 9% 6%
2	B	263	86% 10%
3	C	238	92% 7%
4	D	68	79% 16%
5	E	225	46% 44% 53%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7162 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	267	Total	C	N	O	S	0	0
			2113	1334	371	400	8		

- Molecule 2 is a protein called Capsid protein VP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	255	Total	C	N	O	S	0	0
			1963	1242	333	373	15		

- Molecule 3 is a protein called Capsid protein VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	237	Total	C	N	O	S	0	0
			1822	1164	292	348	18		

- Molecule 4 is a protein called Capsid protein VP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	57	Total	C	N	O	S	0	0
			441	275	77	88	1		

- Molecule 5 is a protein called Coxsackievirus and adenovirus receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	105	Total	C	N	O	S	0	0
			823	529	131	160	3		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	20	MET	-	initiating methionine	UNP P78310
E	237	LEU	-	expression tag	UNP P78310
E	238	GLU	-	expression tag	UNP P78310

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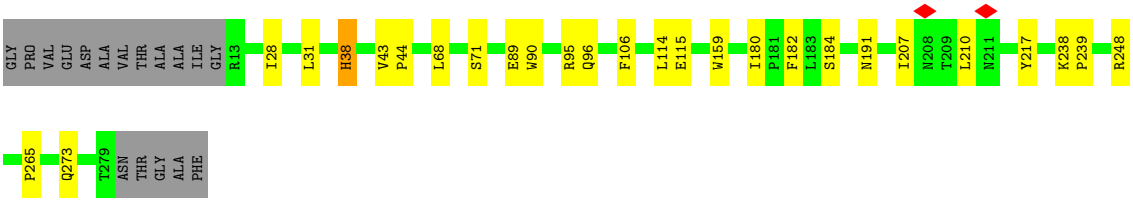
Chain	Residue	Modelled	Actual	Comment	Reference
E	239	HIS	-	expression tag	UNP P78310
E	240	HIS	-	expression tag	UNP P78310
E	241	HIS	-	expression tag	UNP P78310
E	242	HIS	-	expression tag	UNP P78310
E	243	HIS	-	expression tag	UNP P78310
E	244	HIS	-	expression tag	UNP P78310

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.

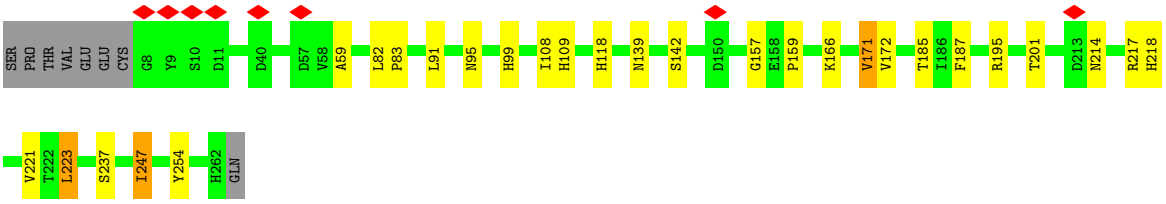
- Molecule 1: Capsid protein VP1

Chain A:



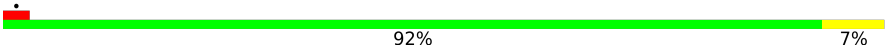
- Molecule 2: Capsid protein VP2

Chain B:



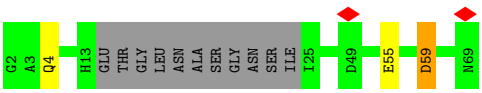
- Molecule 3: Capsid protein VP3

Chain C:



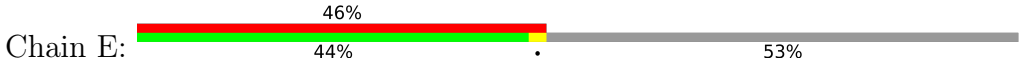
- Molecule 4: Capsid protein VP4

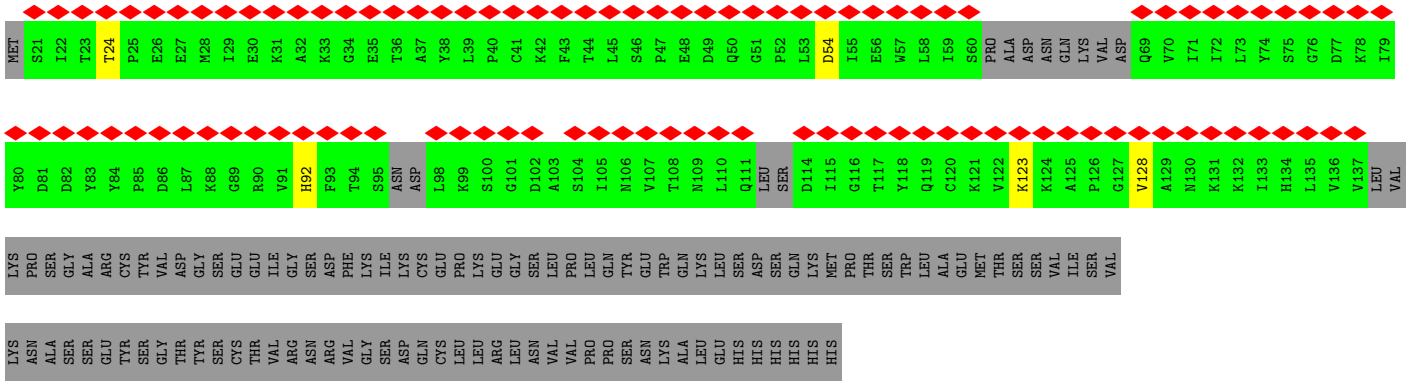
Chain D:



- Molecule 5: Coxsackievirus and adenovirus receptor

Chain E:


46%
44%
53%


MET S21 I22 T23 T24 P25 E26 E27 M28 I29 E30 K31 A32 K33 G34 E35 T36 A37 Y38 L39 P40 C41 K42 F43 T44 L45 S46 P47 E48 D49 Q50 G51 P52 L53 D54 I55 E56 W57 L58 I59 S60 PRO ALA ASP ASN GLN LYS VAL ASP Q69 V70 I71 I72 L73 Y74 S75 G76 D77 K78 I79
Y80 D81 D82 Y83 Y84 P85 D86 L87 K88 G89 R90 V91 H92 F93 T94 S96 ASN ASP L98 K99 S100 G101 D102 A103 S104 I105 N106 V107 T108 N109 L110 Q111 LEU SER D114 I115 G116 T117 Y118 Q119 C120 K121 V122 K123 K124 A125 P126 G127 V128 A129 N130 K131 K132 I133 H134 L135 V136 V137 LEU VAL
LYS PRO SER GLY ALA ARG CYS TYR VAL ASP GLY SER GLU GLU ILE GLY SER ASP PHE LYS ILE LYS CYS GLU PRO LYS GLU GLY SER LEU PRO LEU GLN TYR GLU TRP GLN LYS LEU SER ASP SER GLN LYS MET PRO THR SER TRP LEU ALA GLU MET THR SER SER VAL ILE SER VAL
LYS ASN ALA SER SER GLU TYR SER GLY THR TYR SER CYS THR VAL ARG ASN ARG VAL GLY SER ASP GLN CYS LEU LEU ARG LEU ASN VAL VAL PRO PRO SER ASN LYS ALA LEU GLU HIS HIS HIS HIS HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	54522	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.092	Depositor
Minimum map value	-0.052	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	475.2, 475.2, 475.2	wwPDB
Map dimensions	432, 432, 432	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	0.55	0/2171	0.61	0/2961
2	B	0.55	0/2015	0.63	0/2758
3	C	0.51	0/1871	0.55	0/2550
4	D	0.53	0/449	0.60	0/605
5	E	0.48	0/837	0.57	0/1130
All	All	0.53	0/7343	0.59	0/10004

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

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	2113	0	2054	21	0
2	B	1963	0	1892	20	0
3	C	1822	0	1758	9	0
4	D	441	0	426	2	0
5	E	823	0	827	2	0
All	All	7162	0	6957	49	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 3.

The worst 5 of 49 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:28:ILE:HD12	1:A:31:LEU:HB2	1.32	1.11
2:B:82:LEU:HD11	2:B:108:ILE:HD11	1.48	0.94
2:B:109:HIS:HD2	2:B:201:THR:OG1	1.57	0.86
1:A:28:ILE:HD12	1:A:31:LEU:CB	2.10	0.81
1:A:89:GLU:O	1:A:89:GLU:HG2	1.83	0.77

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	265/284 (93%)	248 (94%)	16 (6%)	1 (0%)	34 69
2	B	253/263 (96%)	238 (94%)	13 (5%)	2 (1%)	19 56
3	C	235/238 (99%)	223 (95%)	12 (5%)	0	100 100
4	D	53/68 (78%)	51 (96%)	2 (4%)	0	100 100
5	E	97/225 (43%)	94 (97%)	3 (3%)	0	100 100
All	All	903/1078 (84%)	854 (95%)	46 (5%)	3 (0%)	44 74

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	PHE
2	B	185	THR
2	B	171	VAL

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	234/244 (96%)	232 (99%)	2 (1%)	78 88
2	B	215/223 (96%)	211 (98%)	4 (2%)	57 76
3	C	205/206 (100%)	202 (98%)	3 (2%)	65 81
4	D	47/55 (86%)	45 (96%)	2 (4%)	29 58
5	E	93/202 (46%)	91 (98%)	2 (2%)	52 72
All	All	794/930 (85%)	781 (98%)	13 (2%)	64 79

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	43	LEU
3	C	69	GLN
5	E	128	VAL
4	D	59	ASP
5	E	92	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	4	GLN
5	E	50	GLN
2	B	109	HIS
2	B	169	GLN
3	C	56	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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.

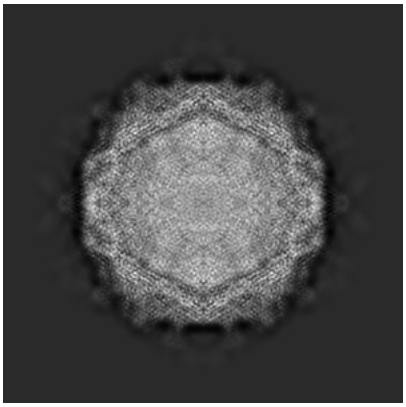
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-32209. These allow visual inspection of the internal detail of the map and identification of artifacts.

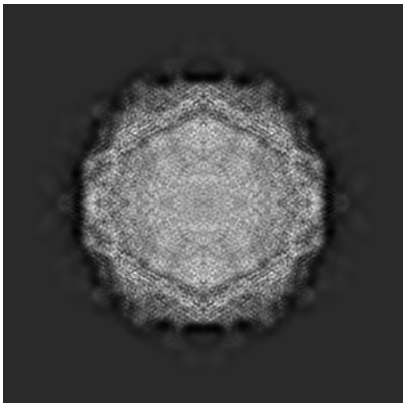
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

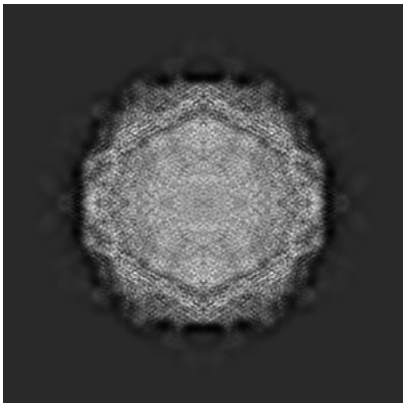
6.1.1 Primary map



X



Y

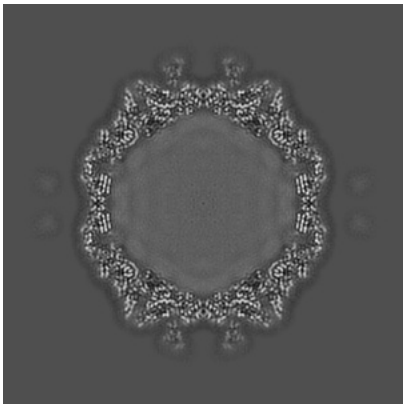


Z

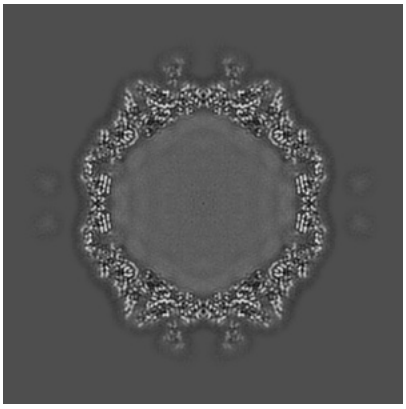
The images above show the map projected in three orthogonal directions.

6.2 Central slices

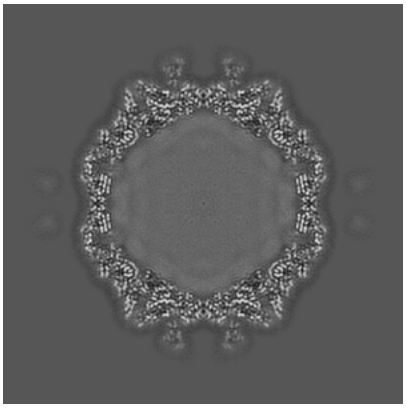
6.2.1 Primary map



X Index: 216



Y Index: 216

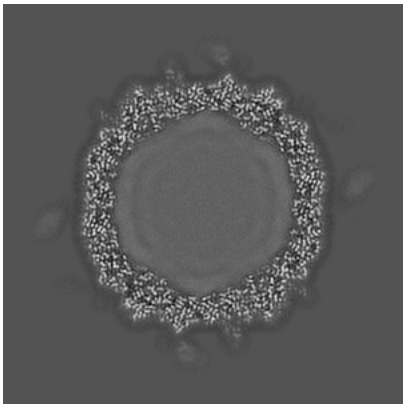


Z Index: 216

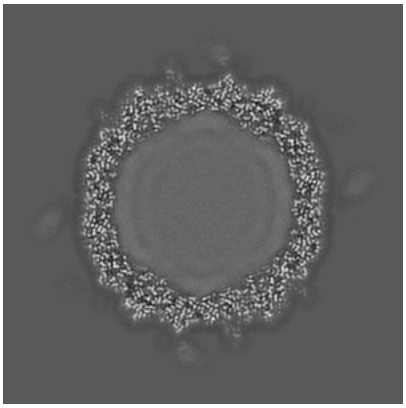
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

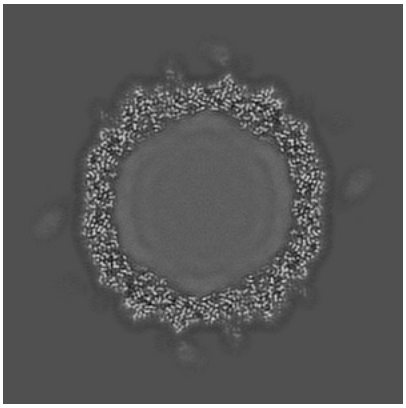
6.3.1 Primary map



X Index: 203



Y Index: 203

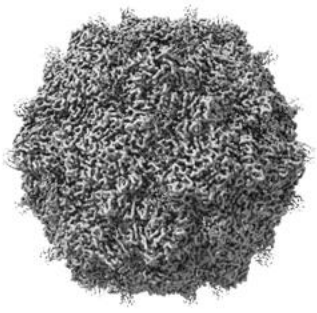


Z Index: 203

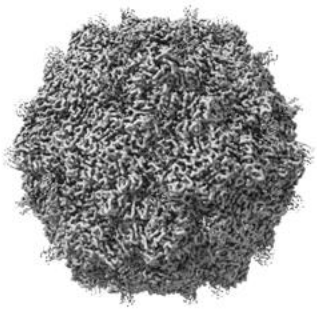
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

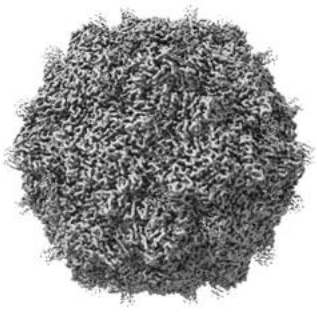
6.4.1 Primary map



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.

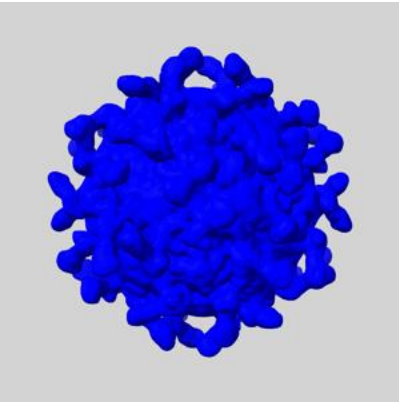
6.5 Mask visualisation (i)

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

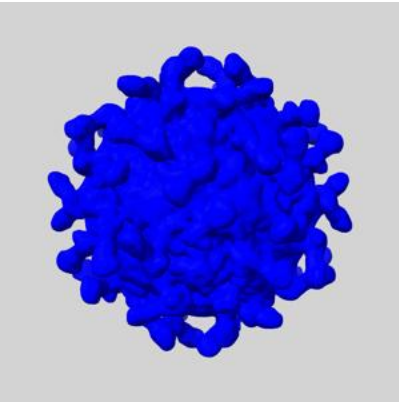
A mask typically either:

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

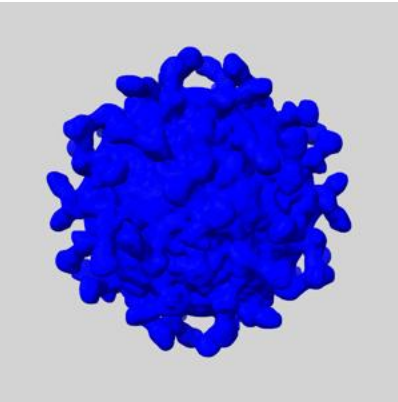
6.5.1 emd_32209_msk_1.map (i)



X



Y

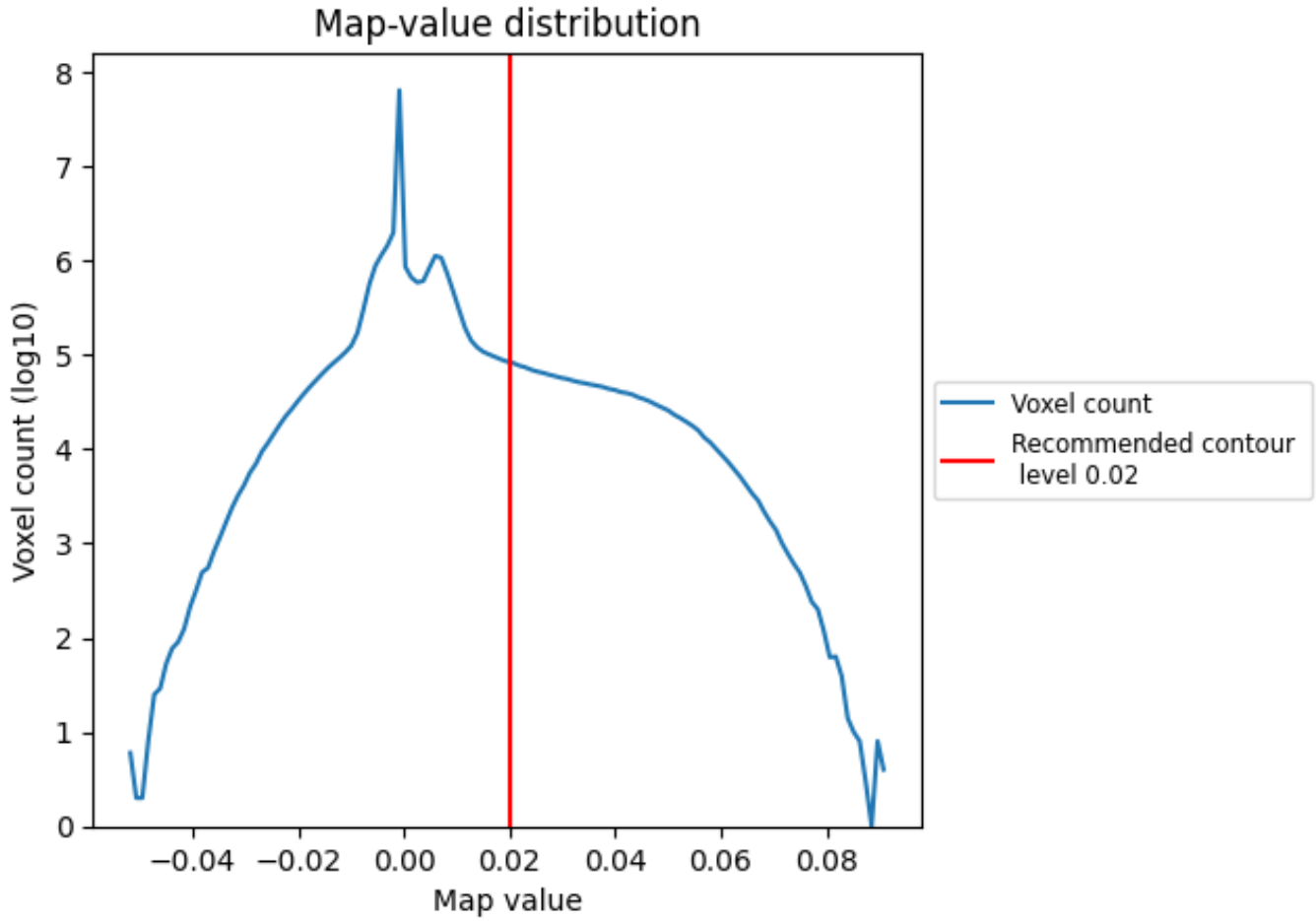


Z

7 Map analysis

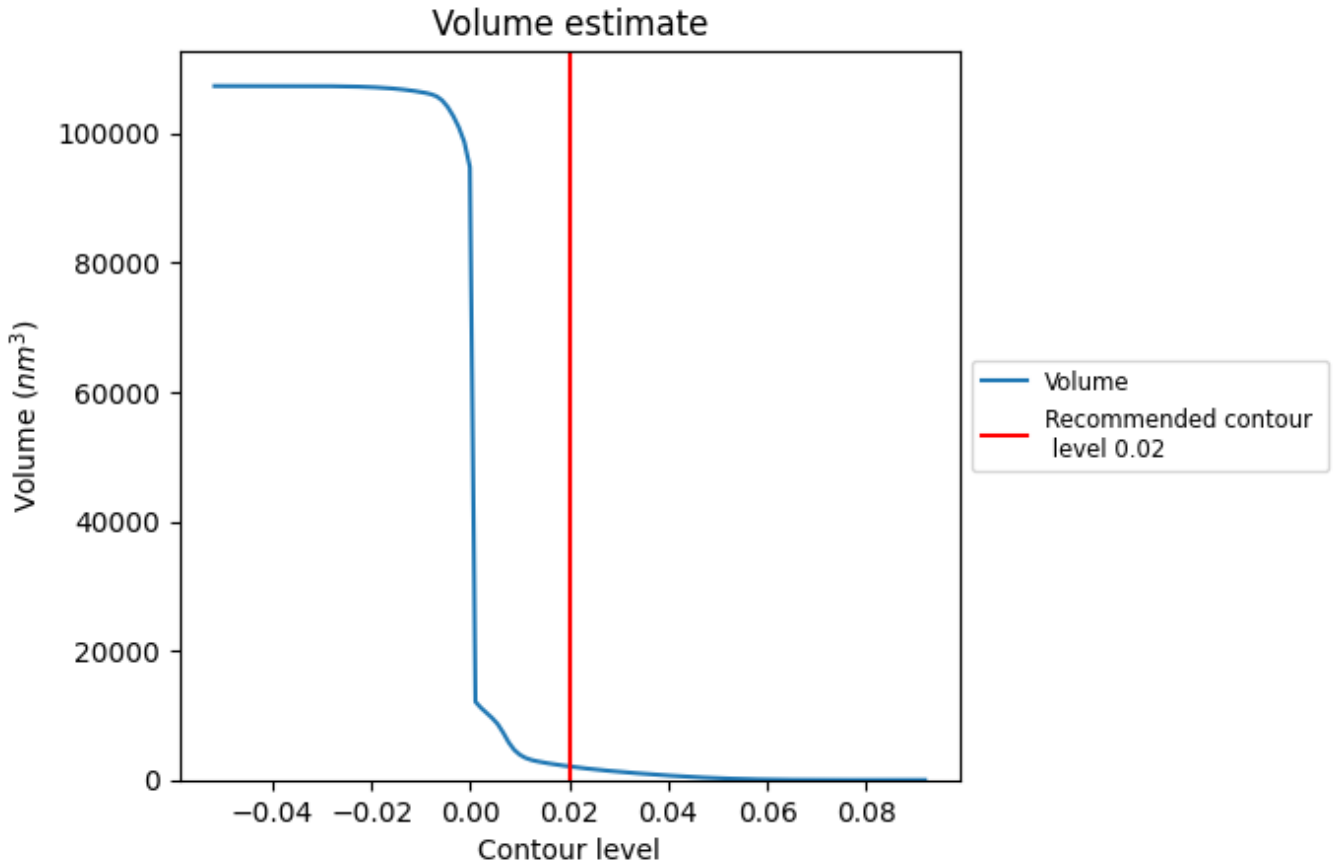
This section contains the results of statistical analysis of the map.

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.

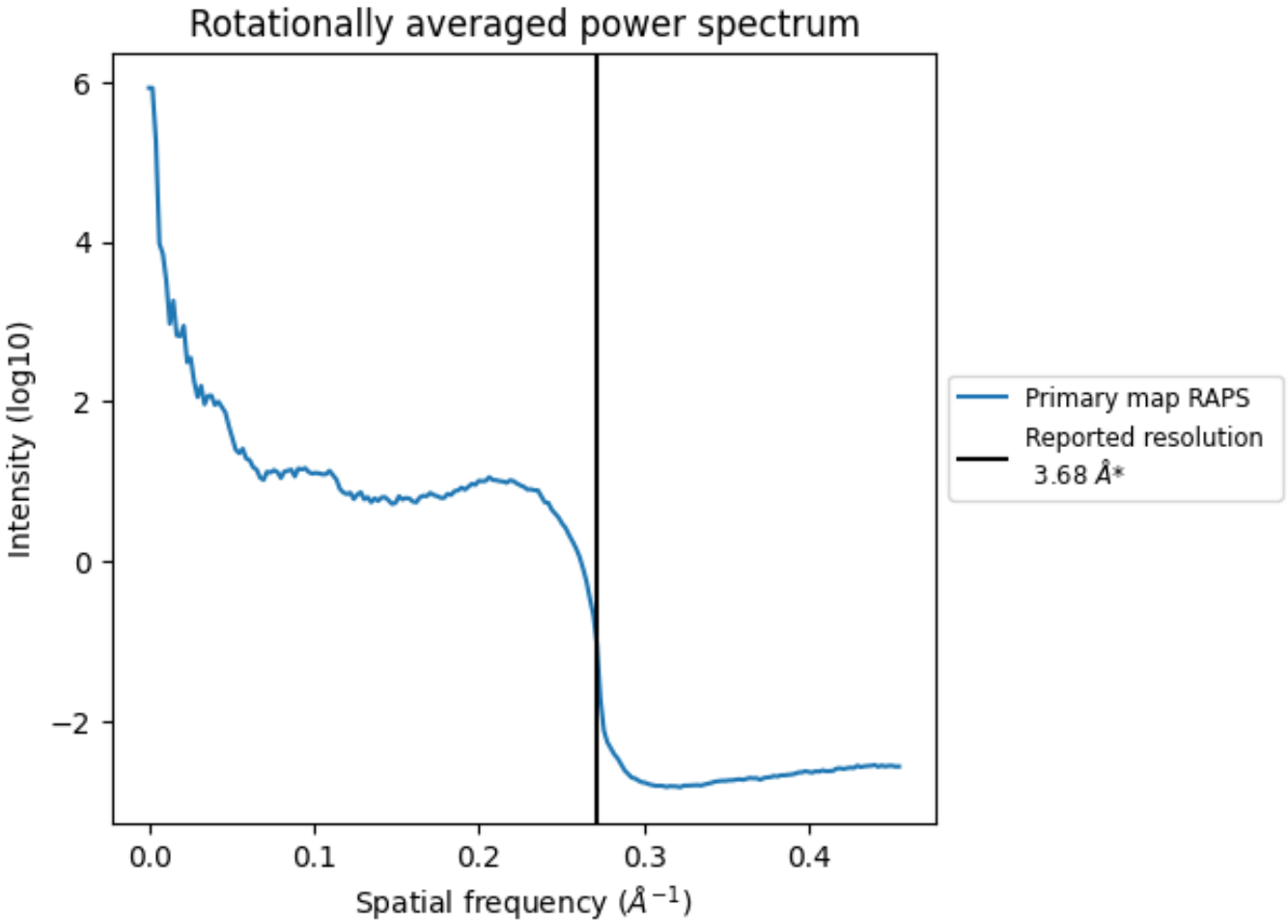
7.2 Volume estimate (i)



The volume at the recommended contour level is 2095 nm^3; this corresponds to an approximate mass of 1892 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)

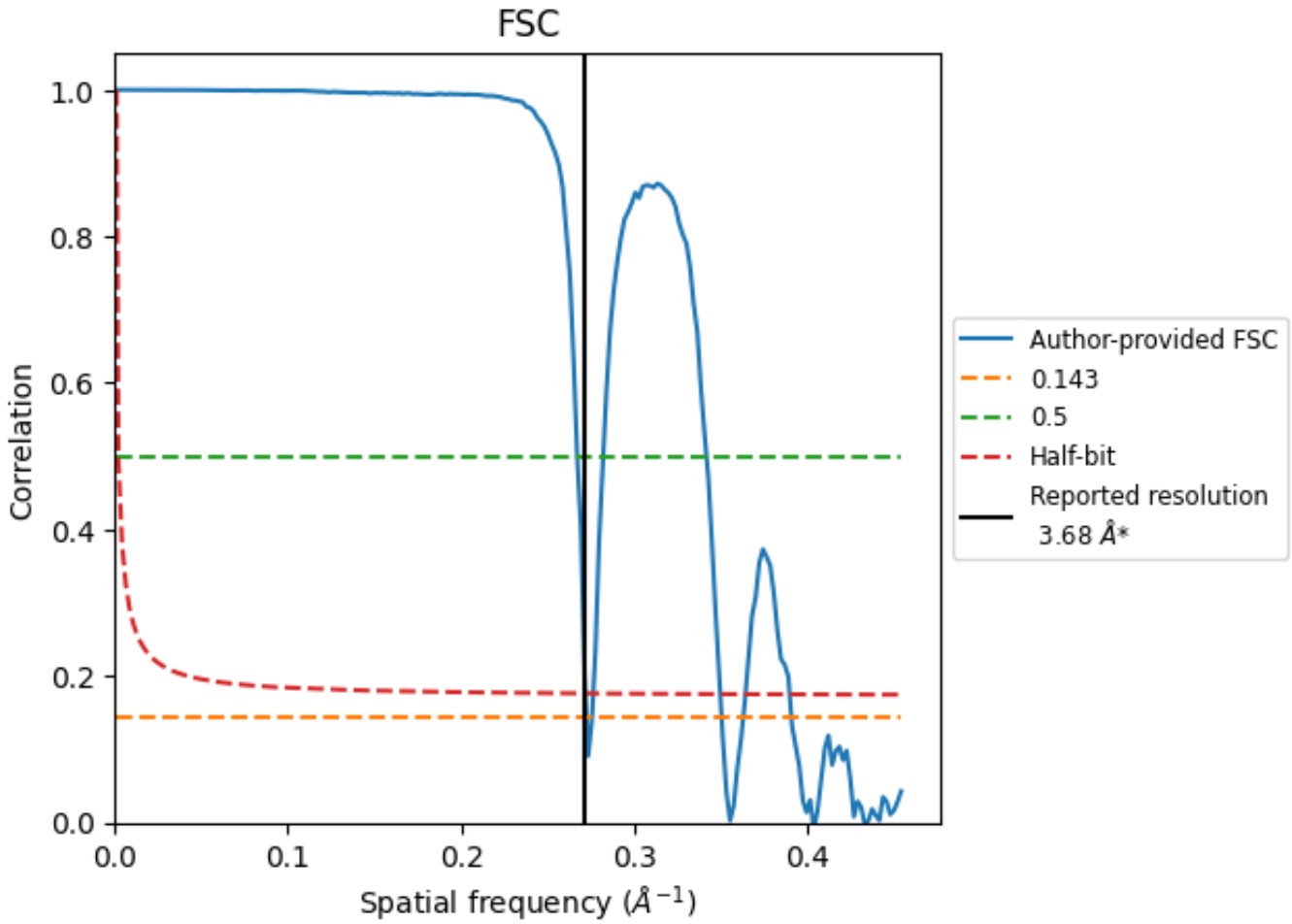


*Reported resolution corresponds to spatial frequency of 0.272 $Å^{-1}$

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 0.272 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.68	-	-
Author-provided FSC curve	3.67	3.74	3.68
Unmasked-calculated*	-	-	-

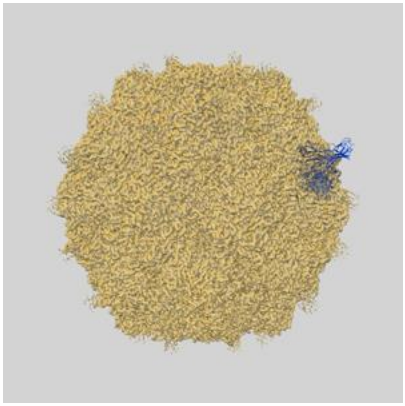
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit

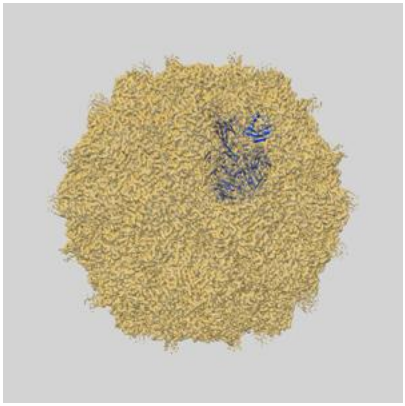
This section contains information regarding the fit between EMDB map EMD-32209 and PDB model 7VYM. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlays

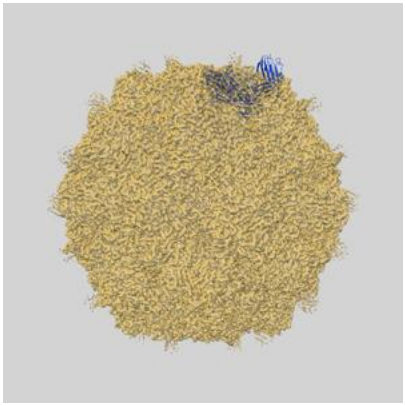
9.1.1 Map-model overlay



X

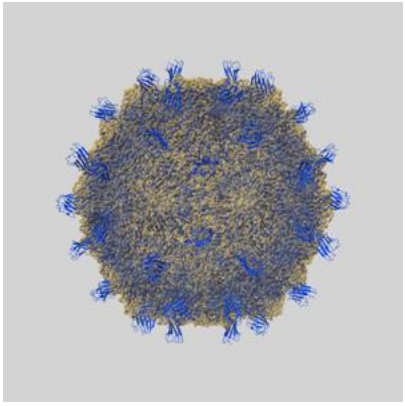


Y

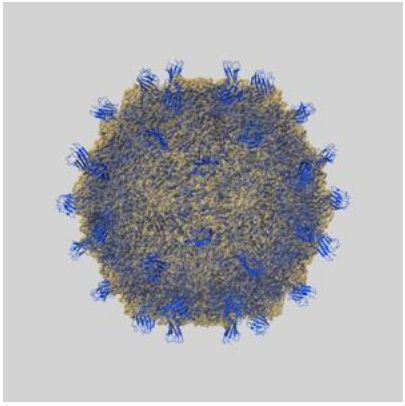


Z

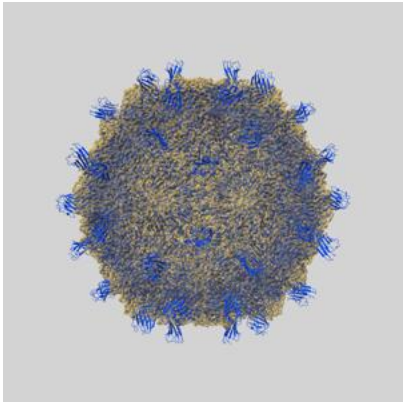
9.1.2 Map-model assembly overlay



X



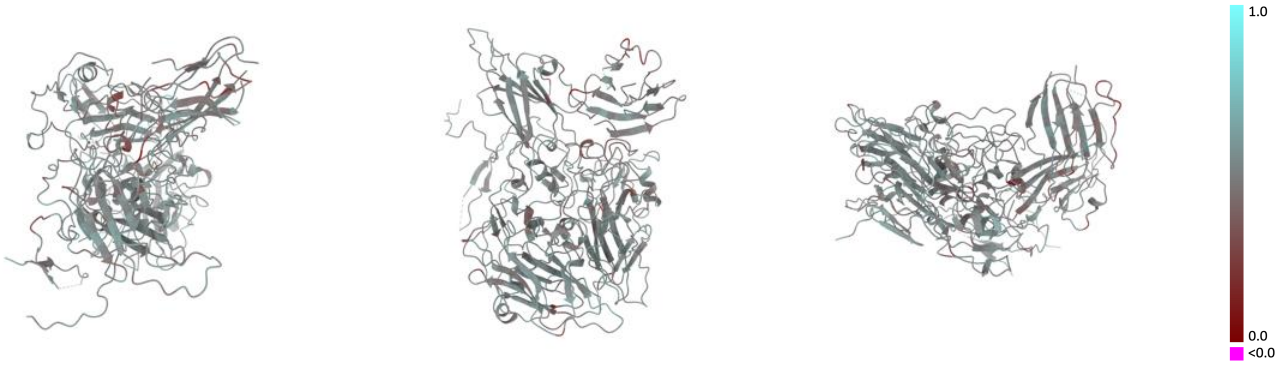
Y



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.

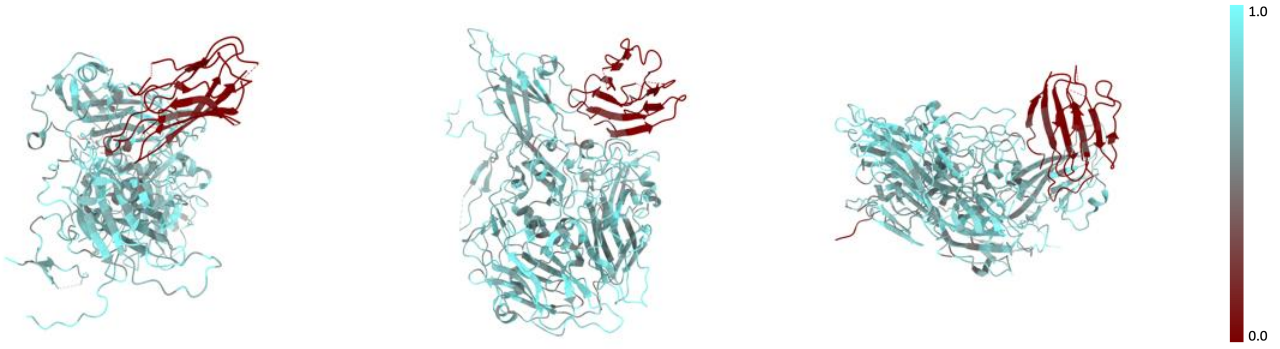
9.2 Q-score mapped to coordinate model



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.

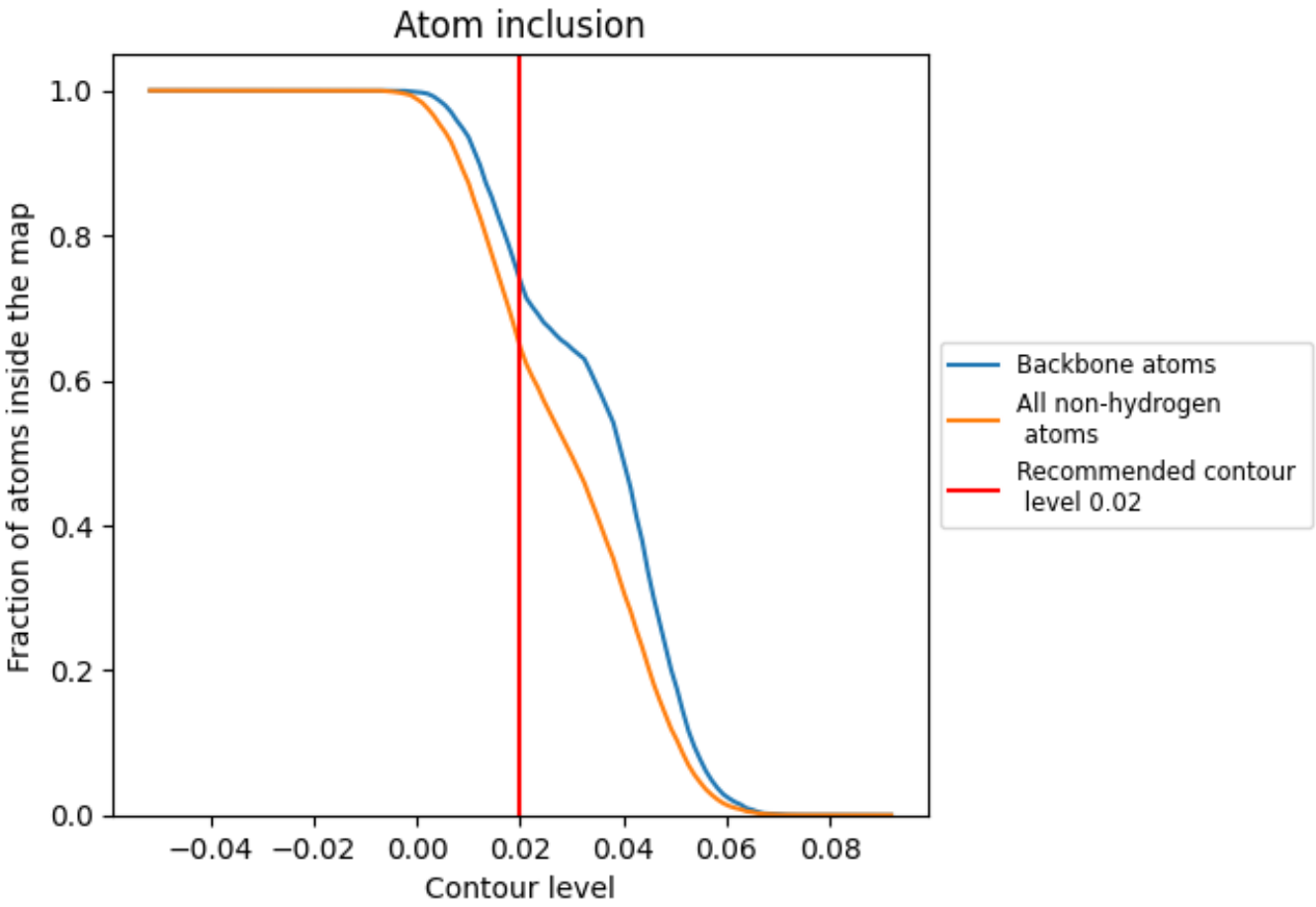
9.3 Atom inclusion mapped to coordinate model



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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 65% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6463	0.4960
A	0.7237	0.4980
B	0.7273	0.5010
C	0.7394	0.5050
D	0.6399	0.5010
E	0.0565	0.4570