



## Full wwPDB EM Validation Report ⓘ

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 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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

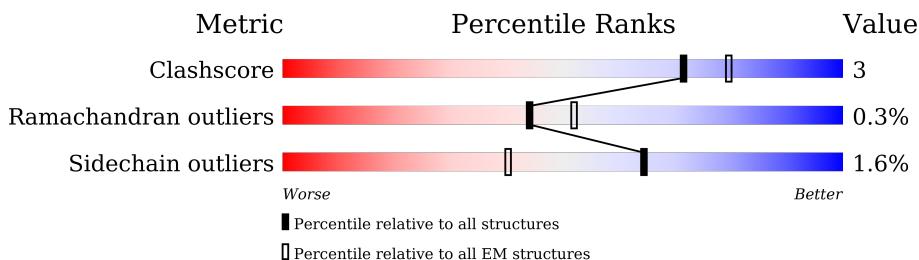
EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 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 3.68 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  $\geq 3$ , 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	284	
2	B	263	
3	C	238	
4	D	68	
5	E	225	

## 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
			Total	C	N	O	S		
1	A	267	2113	1334	371	400	8	0	0

- Molecule 2 is a protein called Capsid protein VP2.

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

- Molecule 3 is a protein called Capsid protein VP3.

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

- Molecule 4 is a protein called Capsid protein VP4.

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

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

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

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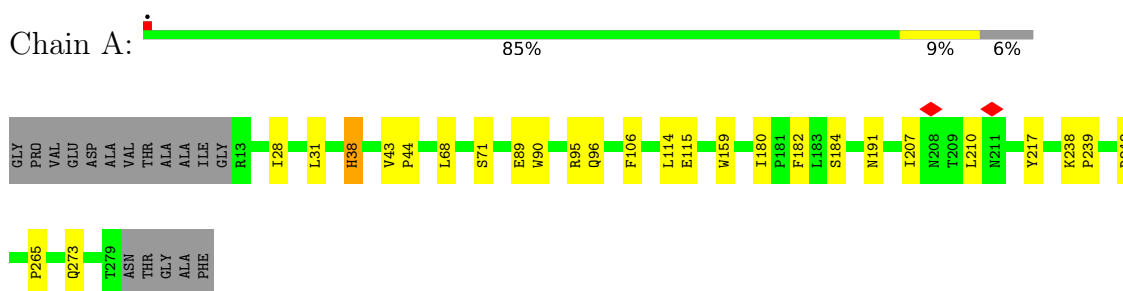
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<b>Chain</b>	<b>Residue</b>	<b>Modelled</b>	<b>Actual</b>	<b>Comment</b>	<b>Reference</b>
E	239	HIS	-	expression tag	UNP P78310
E	240	HIS	-	expression tag	UNP P78310
E	241	HIS	-	expression tag	UNP P78310
E	242	HIS	-	expression tag	UNP P78310
E	243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

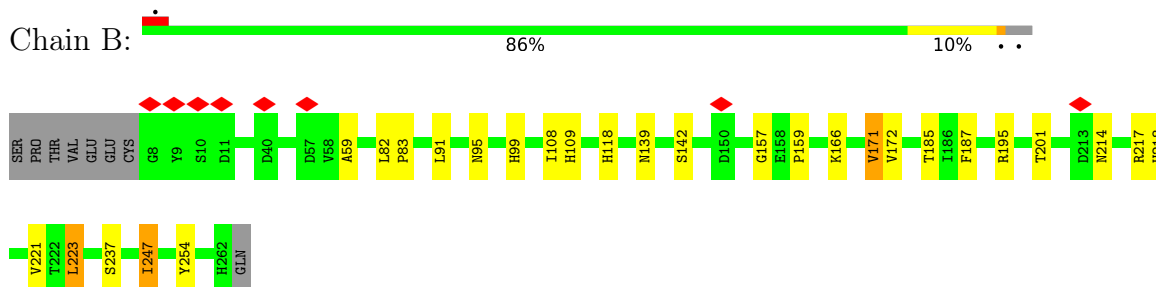
### 3 Residue-property plots [i](#)

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.

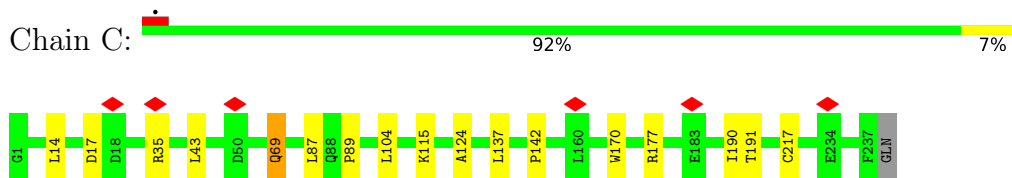
- Molecule 1: Capsid protein VP1



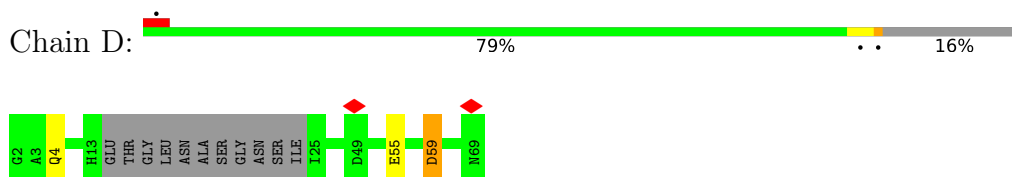
- Molecule 2: Capsid protein VP2



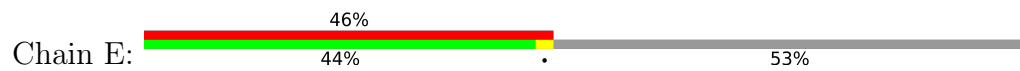
- Molecule 3: Capsid protein VP3



- Molecule 4: Capsid protein VP4



- Molecule 5: Coxsackievirus and adenovirus receptor



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	S95	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	ASN	ALA	SER	GLY	ALA	SER	GLU	TYR	SER	TYR	VAL	GLY	THR	ASP	TYR	SER	SER	GLY	GLU	GLY	ILE	VAL	ARG	ASN	ASP	ASP	PHE	LYS	ILE	SER	LYS	ASP	GLN	CYS	GLU	CYS	PRO	LEU	LYS	GLY	GLY	GLU	LEU	VAL	LEU	PRO	LEU	GLN	TYR	SER	ASN	GLY	LYS	TRP	LYS	ALA	LEU	GLU	HIS	HIS	HIS	HIS	HIS
LYS	ASN	ALA	SER	GLU	TYR	SER	GLY	THR	ASP	TYR	SER	GLY	THR	ASP	TYR	SER	SER	GLY	VAL	ARG	ASN	ASP	ASP	VAL	GLY	SER	LYS	ASP	GLN	CYS	LEU	LEU	ARG	LEU	VAL	VAL	PRO	PRO	ASN	ASN	LYS	ALA	LEU	GLU	HIS	HIS	HIS	HIS	HIS															

## 4 Experimental information

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 ( $e^-/\text{\AA}^2$ )	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 [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	0.55	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 [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	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.

All (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
2:B:82:LEU:HD22	2:B:247:ILE:HD12	1.70	0.72
1:A:191:ASN:O	1:A:207:ILE:HD12	1.90	0.72
1:A:95:ARG:HD3	1:A:207:ILE:HD13	1.73	0.71
1:A:28:ILE:O	1:A:28:ILE:HG13	2.00	0.61
2:B:82:LEU:HD12	2:B:221:VAL:HG13	1.84	0.60
2:B:59:ALA:HB1	2:B:91:LEU:HD12	1.86	0.57
2:B:109:HIS:CD2	2:B:201:THR:OG1	2.49	0.55
1:A:114:LEU:HB2	1:A:180:ILE:HB	1.88	0.55
1:A:159:TRP:CH2	1:A:217:TYR:HB3	2.43	0.53
1:A:248:ARG:HG3	2:B:187:PHE:HZ	1.74	0.53
1:A:71:SER:HA	1:A:238:LYS:HB3	1.93	0.51
1:A:90:TRP:HE1	1:A:96:GLN:HG3	1.75	0.50
2:B:157:GLY:HA2	2:B:172:VAL:HG12	1.94	0.50
1:A:182:PHE:CZ	1:A:184:SER:HB3	2.48	0.49
1:A:265:PRO:HG2	2:B:159:PRO:HB3	1.93	0.49
3:C:137:LEU:HD22	3:C:177:ARG:HH22	1.77	0.47
2:B:82:LEU:HD21	2:B:223:LEU:HB2	1.97	0.47
3:C:89:PRO:HB2	3:C:104:LEU:HD22	1.96	0.47
3:C:87:LEU:HD13	3:C:190:ILE:HD11	1.97	0.46
2:B:82:LEU:CD1	2:B:108:ILE:HD11	2.33	0.45
5:E:54:ASP:HB2	5:E:123:LYS:HB3	1.98	0.45
2:B:214:ASN:HB3	2:B:217:ARG:HB2	1.98	0.45
1:A:115:GLU:HB3	1:A:238:LYS:HG3	1.99	0.44
1:A:43:VAL:HB	1:A:44:PRO:HD2	1.98	0.44
2:B:142:SER:HB2	2:B:166:LYS:HD2	2.00	0.44
2:B:99:HIS:CG	2:B:254:TYR:HB3	2.53	0.44
4:D:59:ASP:N	4:D:59:ASP:OD1	2.50	0.44
1:A:89:GLU:O	1:A:89:GLU:CG	2.62	0.43
2:B:95:ASN:HB3	2:B:254:TYR:CD2	2.53	0.43
2:B:118:HIS:CE1	2:B:237:SER:HB3	2.53	0.43
1:A:273:GLN:HA	1:A:273:GLN:OE1	2.18	0.43
3:C:69:GLN:H	3:C:69:GLN:HG3	1.67	0.43
3:C:170:TRP:CH2	3:C:177:ARG:HG3	2.54	0.43
3:C:115:LYS:HG3	3:C:217:CYS:SG	2.59	0.42
1:A:68:LEU:O	1:A:239:PRO:HD2	2.19	0.42
2:B:195:ARG:HB2	3:C:124:ALA:HA	2.02	0.42
3:C:14:LEU:HD23	3:C:17:ASP:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:139:ASN:HB2	5:E:24:THR:HA	2.01	0.42
1:A:38:HIS:CD2	4:D:55:GLU:HG3	2.54	0.41
1:A:89:GLU:OE1	1:A:89:GLU:N	2.54	0.41
2:B:82:LEU:HB2	2:B:83:PRO:HD3	2.02	0.41
2:B:108:ILE:HG21	2:B:223:LEU:HG	2.03	0.41
1:A:95:ARG:CD	1:A:207:ILE:HG21	2.52	0.40
3:C:142:PRO:HG2	3:C:191:THR:HG21	2.03	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	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

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	HIS
1	A	210	LEU
2	B	171	VAL
2	B	218	HIS
2	B	223	LEU
2	B	247	ILE
3	C	35	ARG
3	C	43	LEU
3	C	69	GLN
4	D	4	GLN
4	D	59	ASP
5	E	92	HIS
5	E	128	VAL

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	38	HIS
1	A	125	GLN
2	B	30	ASN
2	B	109	HIS
2	B	169	GLN

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Mol	Chain	Res	Type
3	C	56	GLN
3	C	69	GLN
4	D	4	GLN
5	E	50	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.

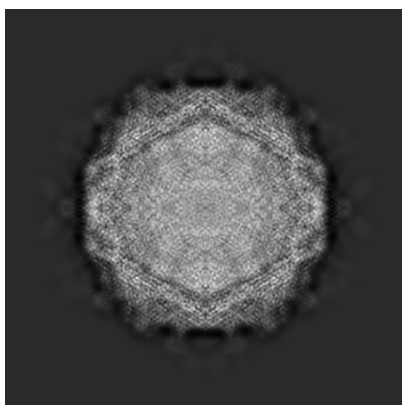
## 6 Map visualisation [i](#)

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.

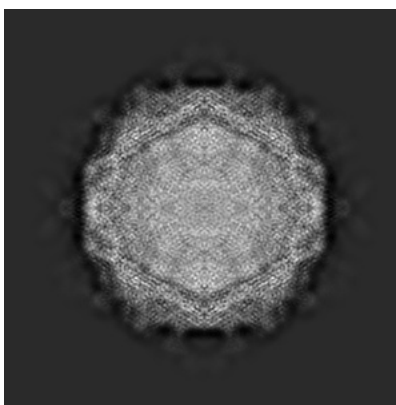
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

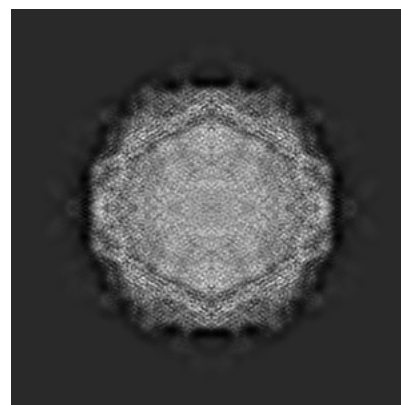
#### 6.1.1 Primary map



X



Y

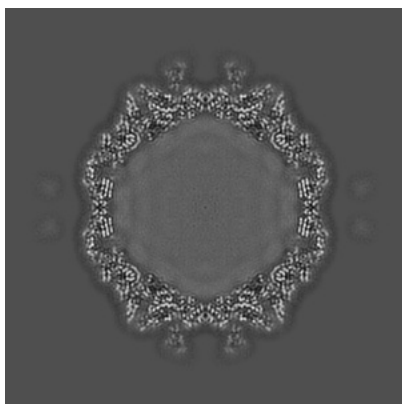


Z

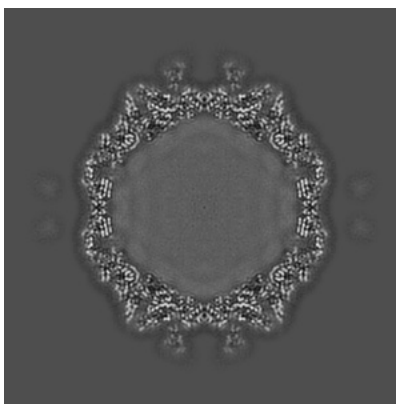
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

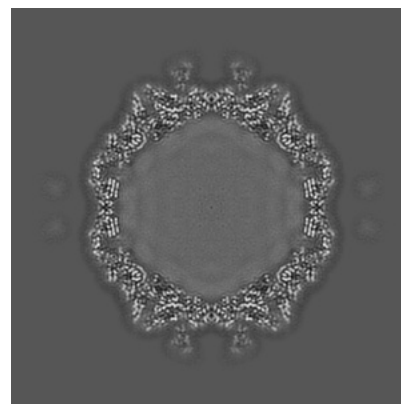
#### 6.2.1 Primary map



X Index: 216



Y Index: 216

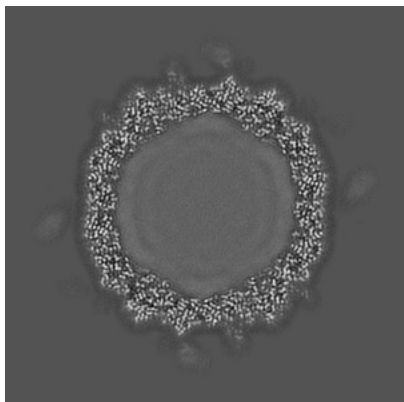


Z Index: 216

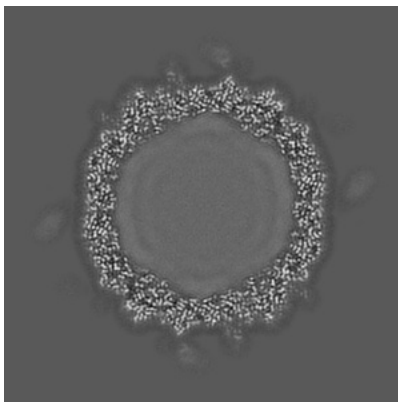
The images above show central slices of the map in three orthogonal directions.

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

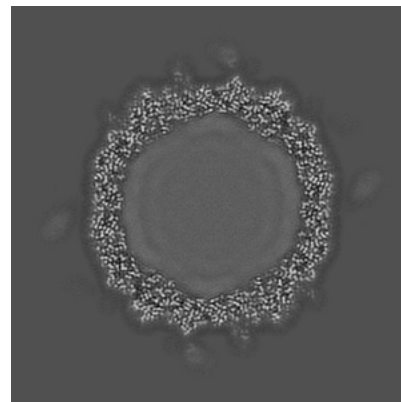
### 6.3.1 Primary map



X Index: 203



Y Index: 203

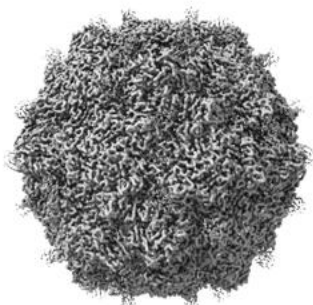


Z Index: 203

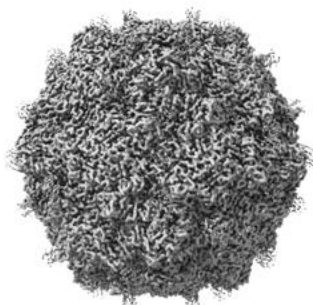
The images above show the largest variance slices of the map in three orthogonal directions.

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

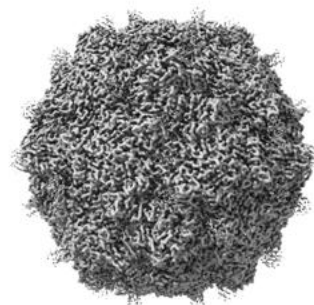
### 6.4.1 Primary map



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.

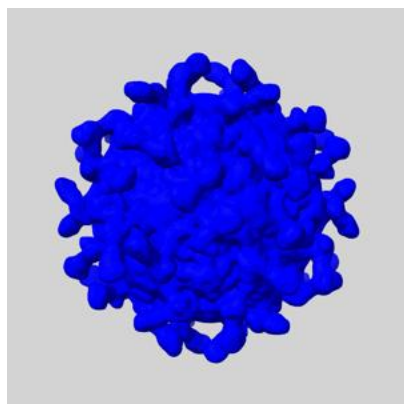
## 6.5 Mask visualisation [i](#)

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

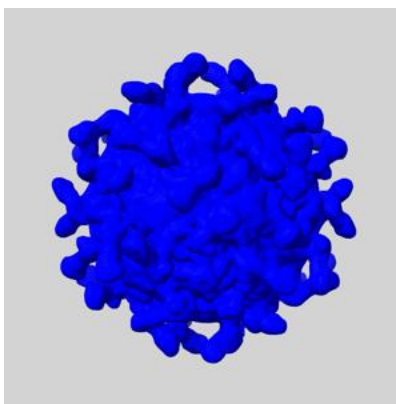
A mask typically either:

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

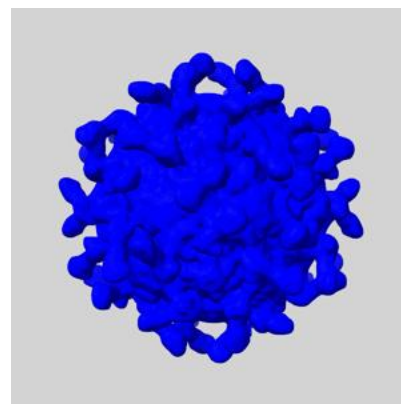
### 6.5.1 emd\_32209\_msk\_1.map [i](#)



X



Y

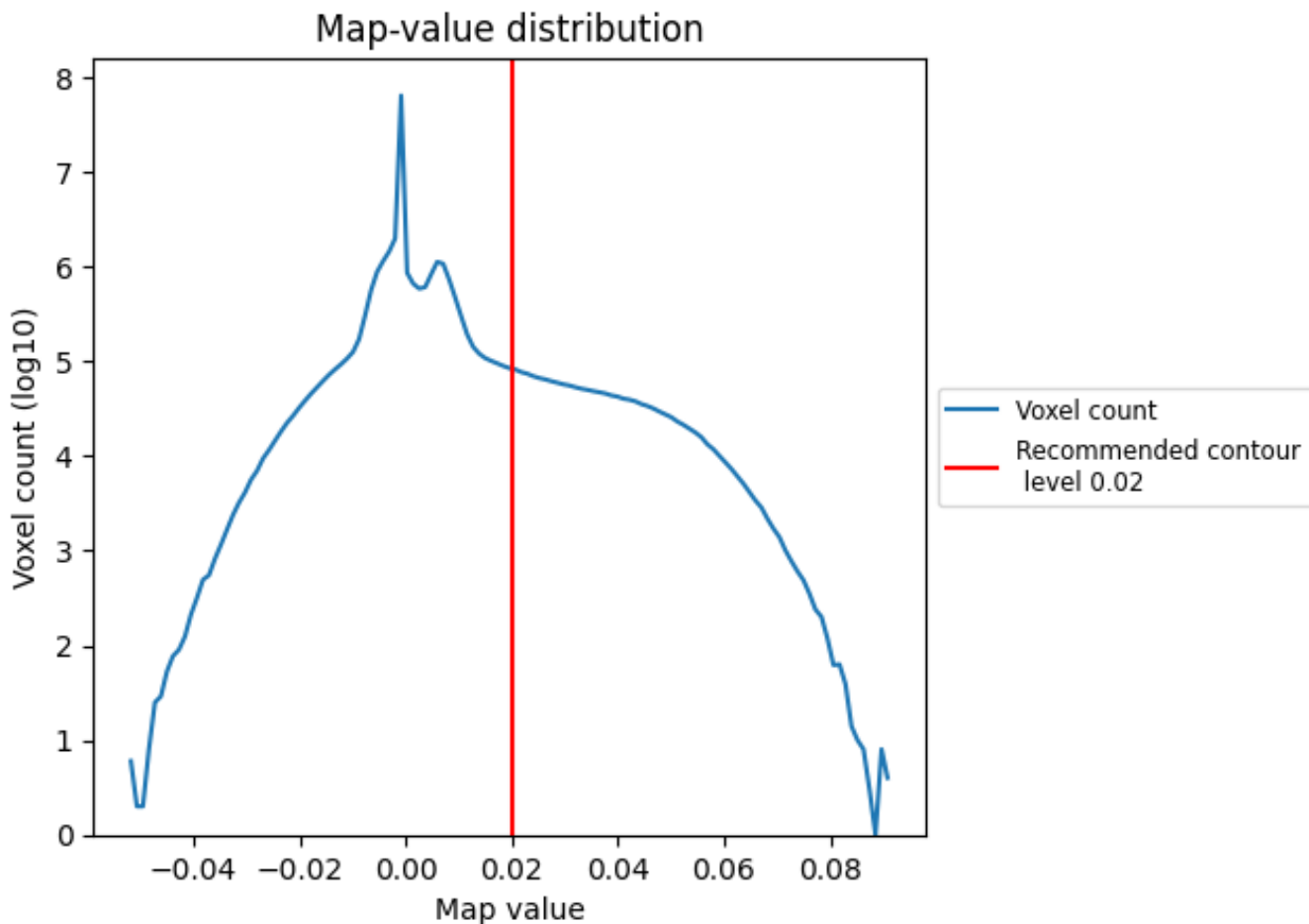


Z

## 7 Map analysis [i](#)

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

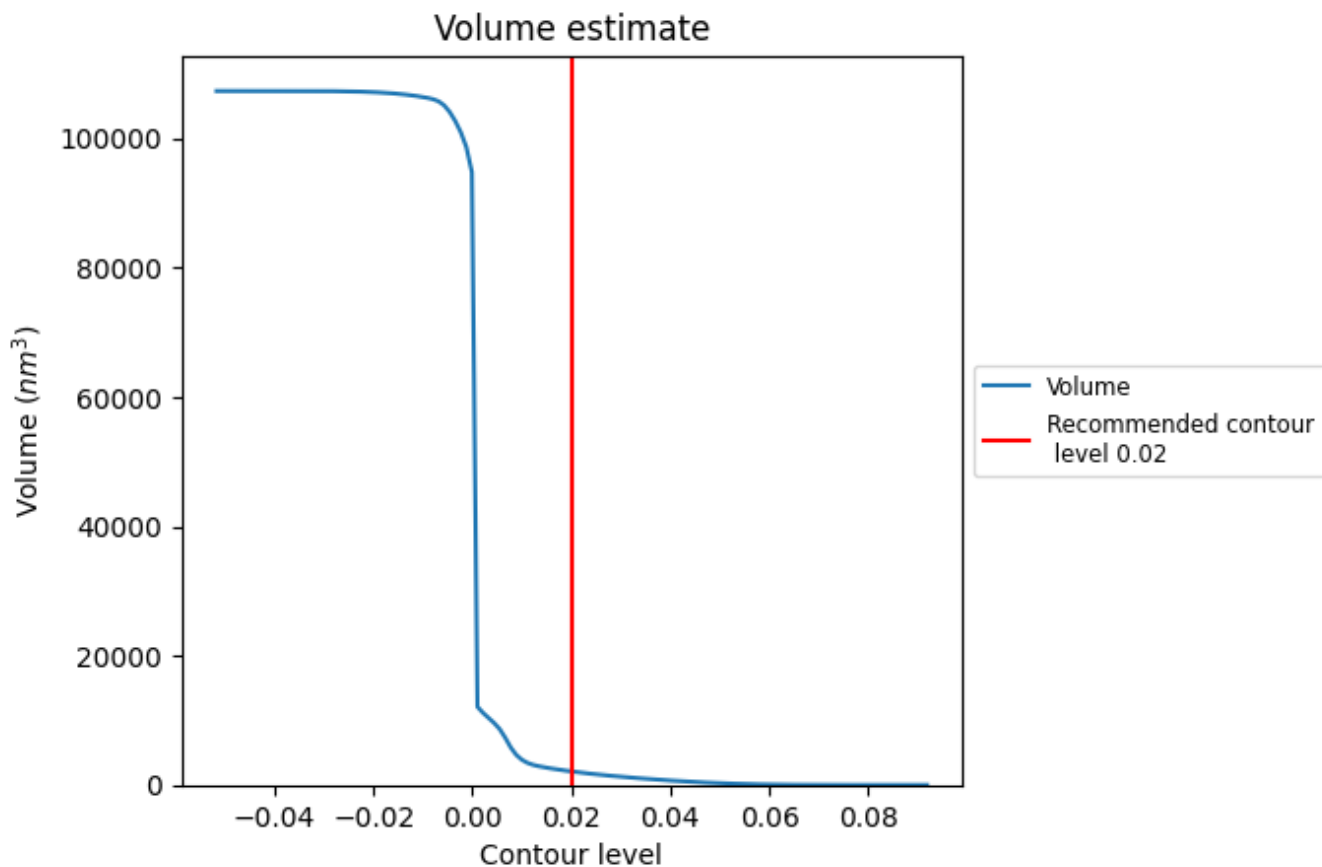
### 7.1 Map-value distribution [i](#)



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.



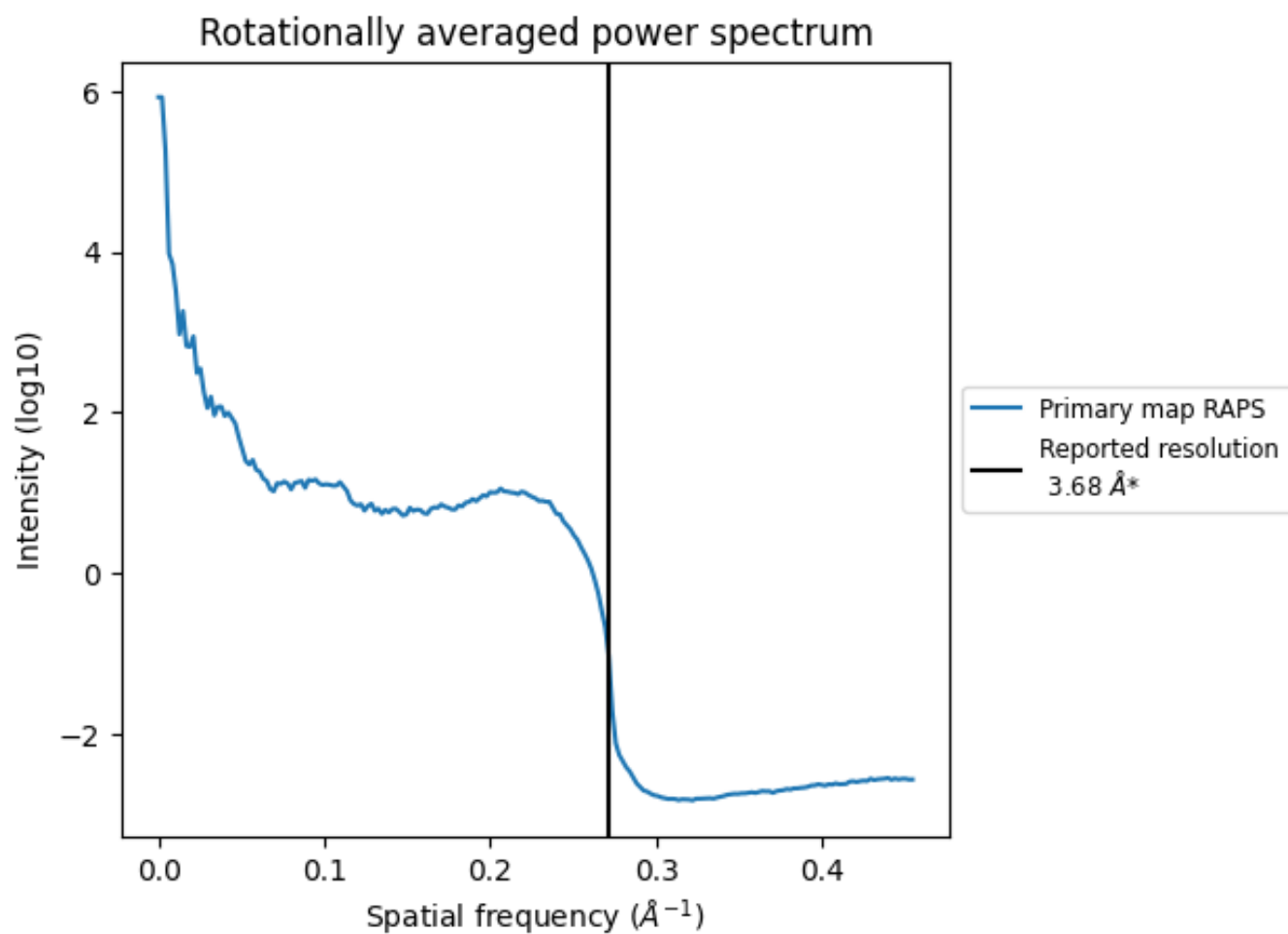
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2095 nm<sup>3</sup>; 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](#)

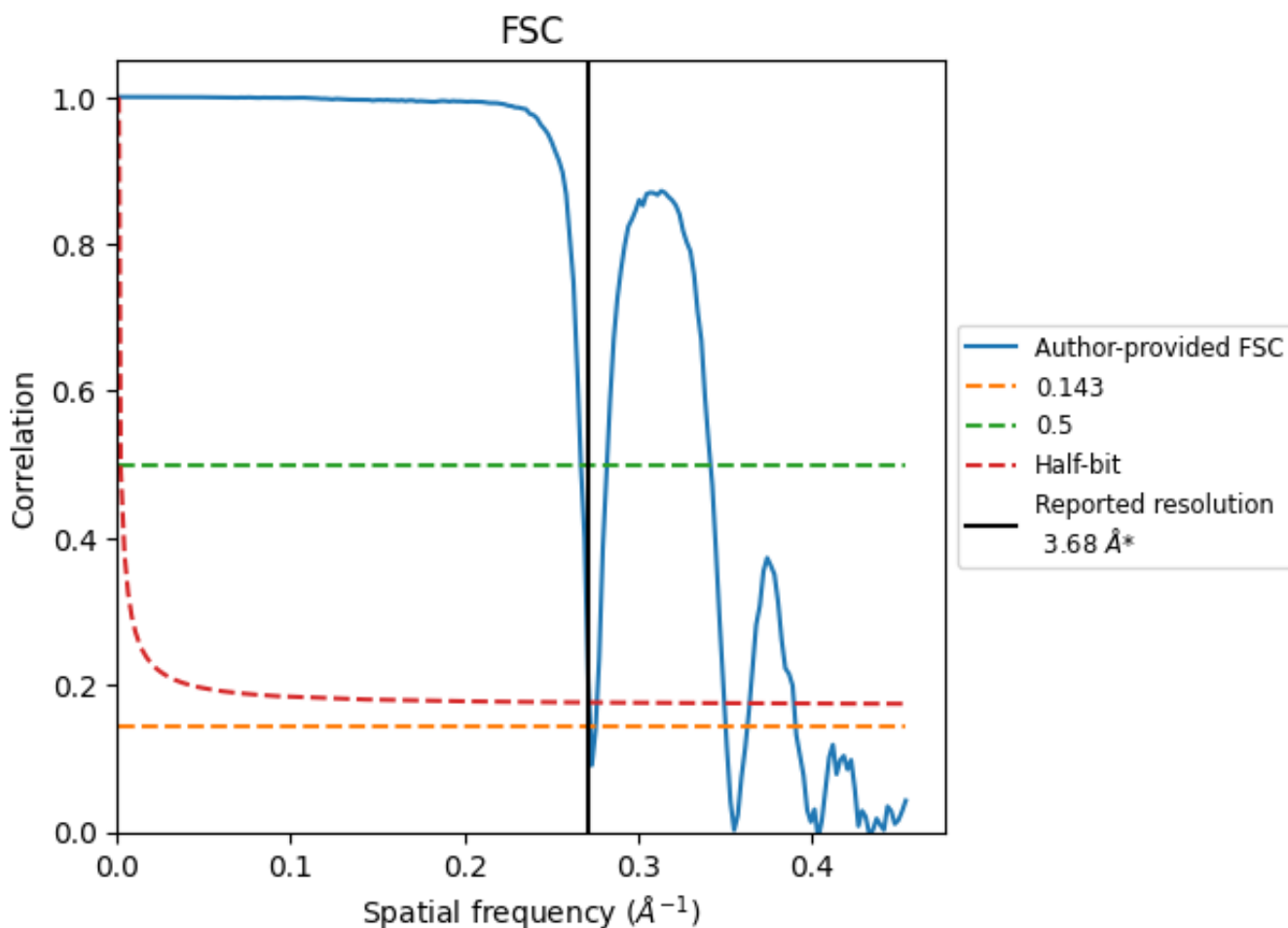


\*Reported resolution corresponds to spatial frequency of 0.272 Å<sup>-1</sup>

## 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 0.272 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	3.68	-	-
Author-provided FSC curve	3.67	3.74	3.68
Unmasked-calculated*	-	-	-

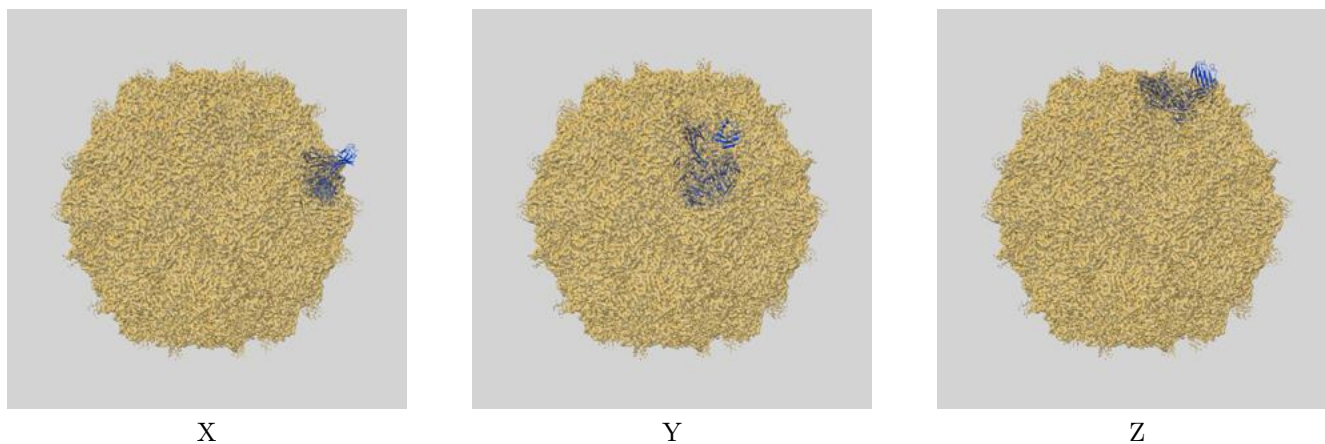
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

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

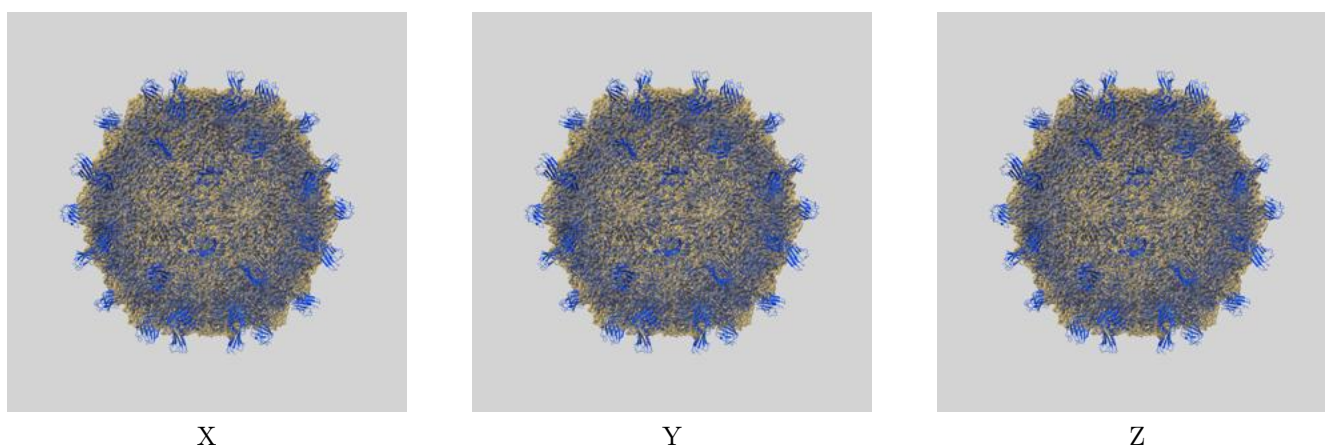
This section contains information regarding the fit between EMDB map EMD-32209 and PDB model 7VYM. Per-residue inclusion information can be found in section 3 on page 5.

### 9.1 Map-model overlays

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

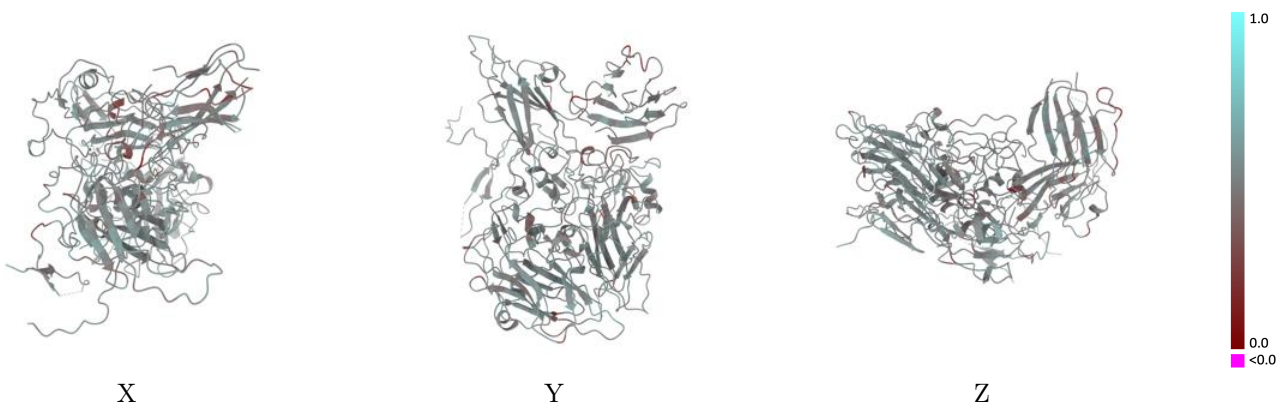


#### 9.1.2 Map-model assembly overlay [i](#)



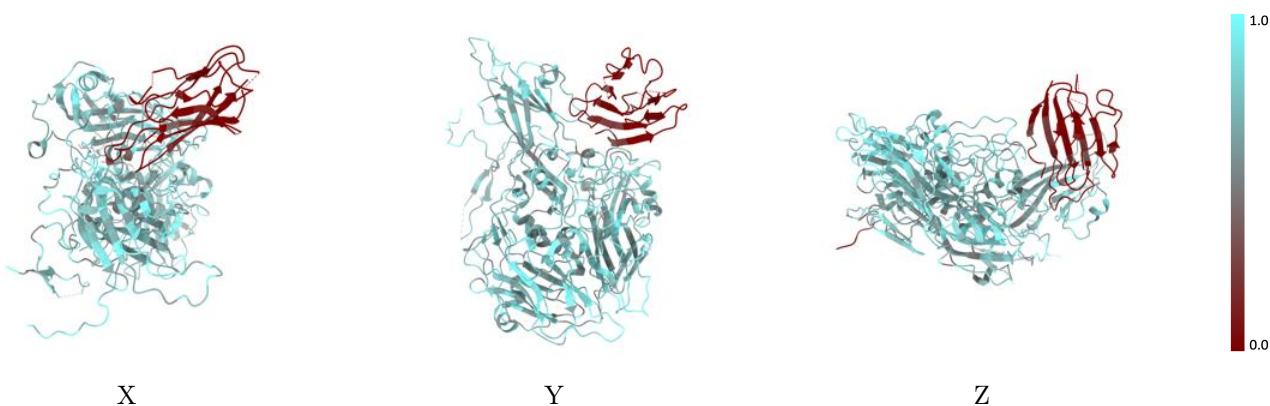
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



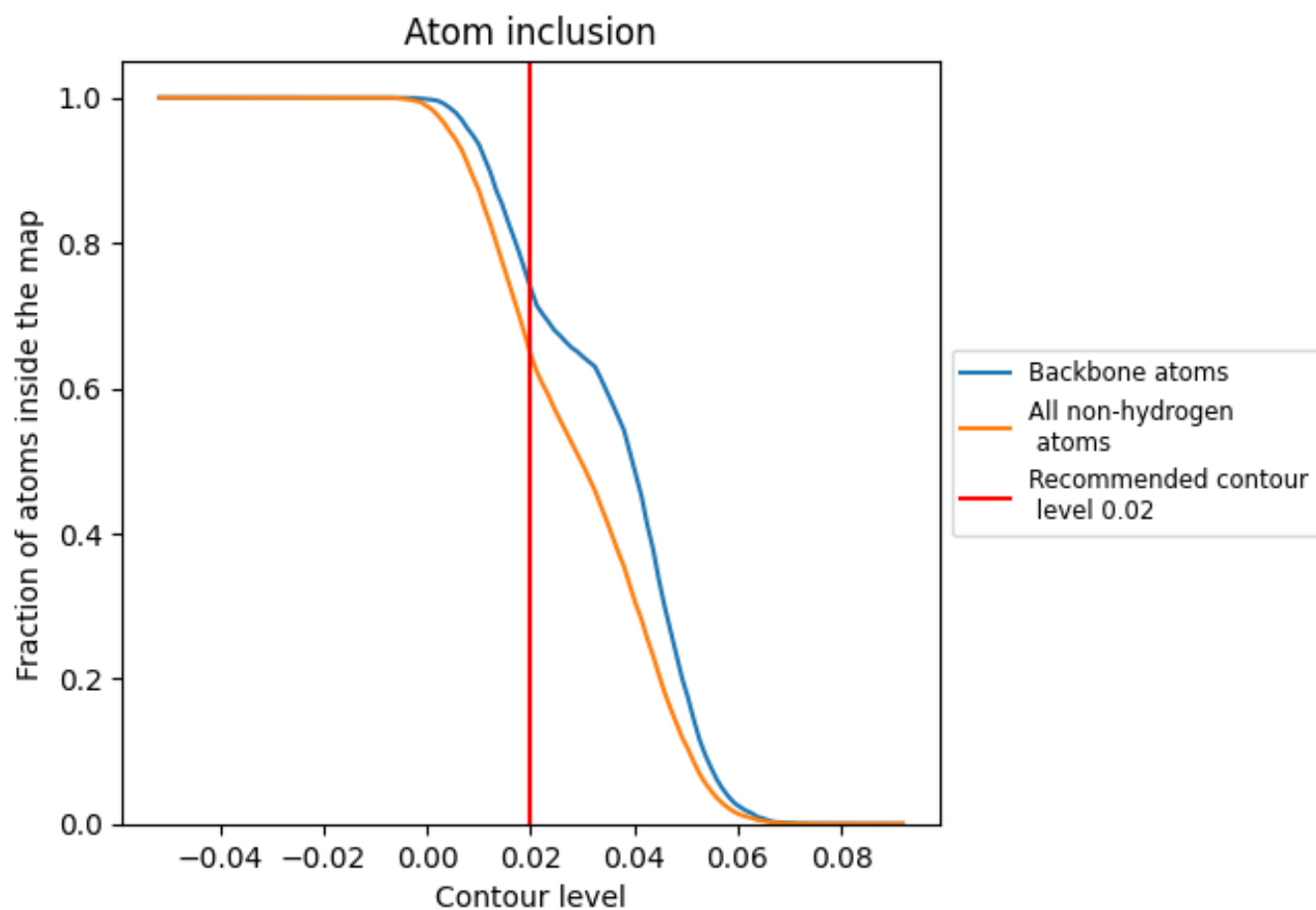
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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













## 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

