



## wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 02:09 PM EST

PDB ID : 3J17  
EMDB ID : EMD-5376  
Title : Structure of a transcribing cypovirus by cryo-electron microscopy  
Authors : Yang, C.; Ji, G.; Liu, H.; Zhang, K.; Liu, G.; Sun, F.; Zhu, P.; Cheng, L.  
Deposited on : 2011-12-25  
Resolution : 4.10 Å(reported)

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

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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  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
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

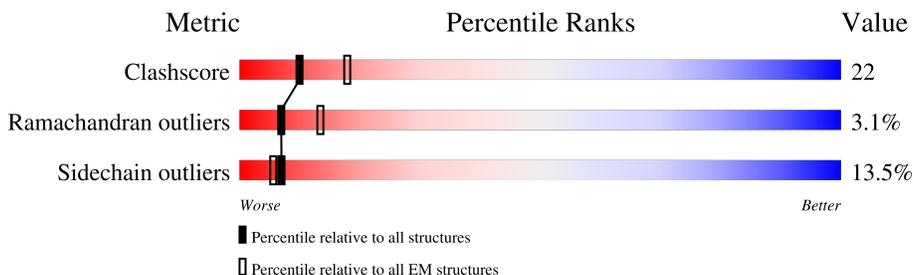
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.10 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	1058	
2	B	1333	
2	C	1333	
3	D	448	
3	E	448	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 32047 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 Structural protein VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	N	O	P			S
1	A	1047	8372	5304	1444	1579	1	44	0	0

- Molecule 2 is a protein called VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1180	9317	5889	1621	1771	36	0	0
2	C	1244	9806	6191	1704	1873	38	0	0

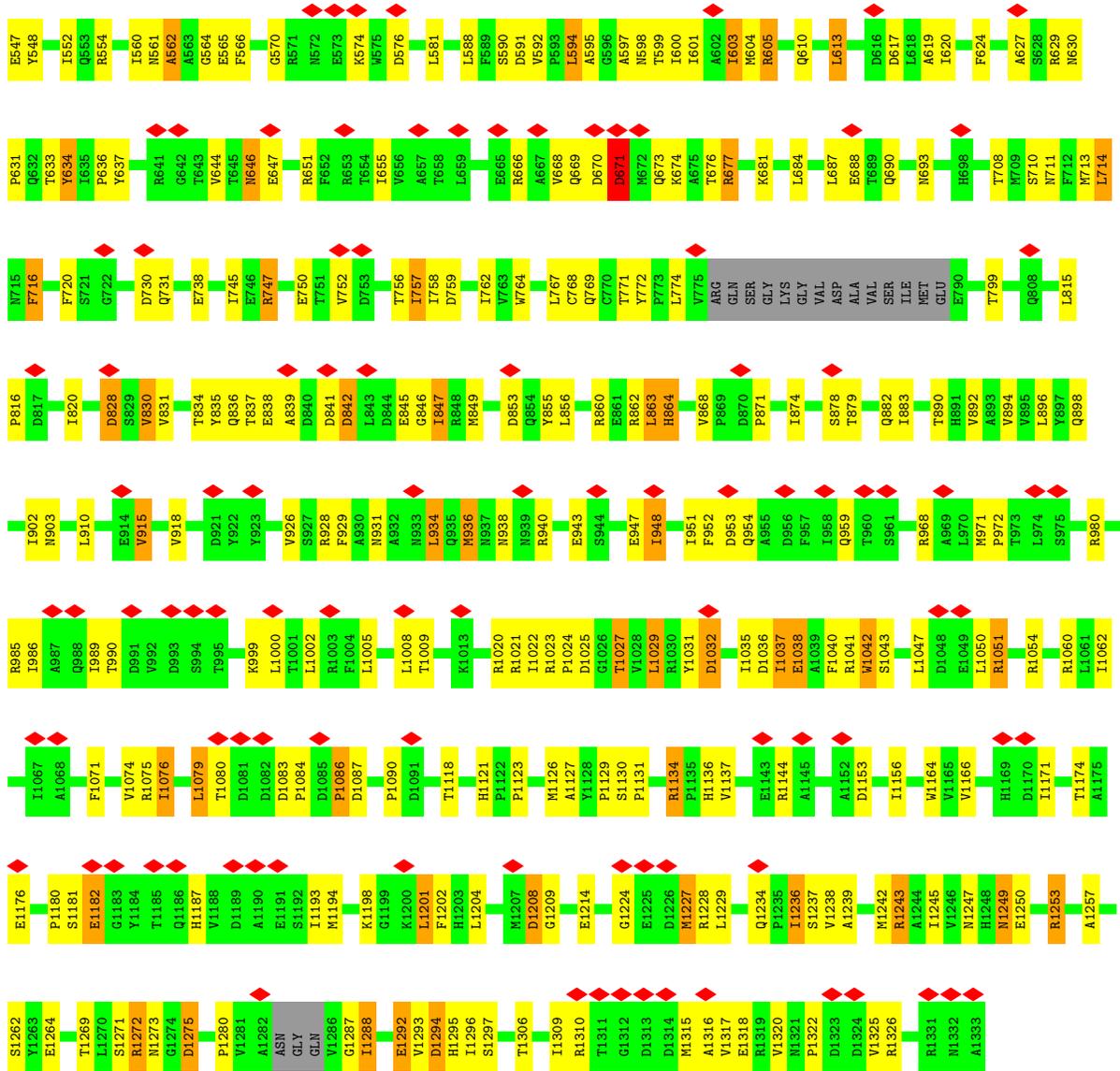
- Molecule 3 is a protein called Structural protein VP5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	291	2276	1446	398	424	8	0	0
3	E	291	2276	1446	398	424	8	0	0

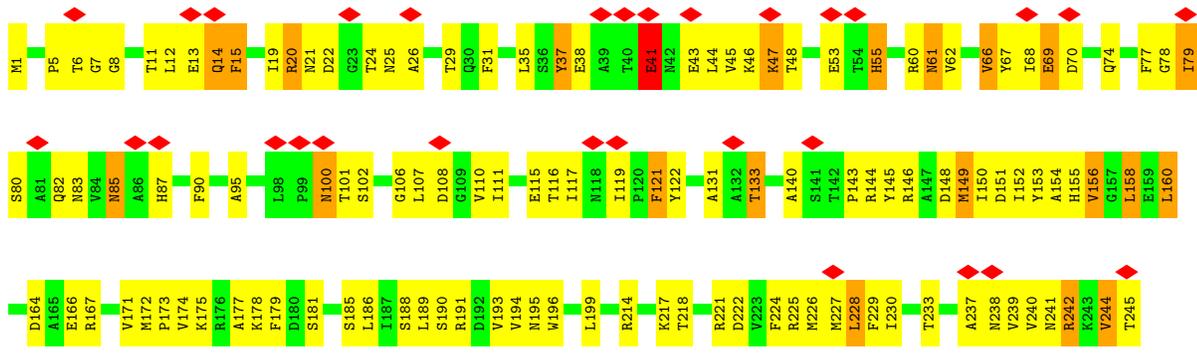
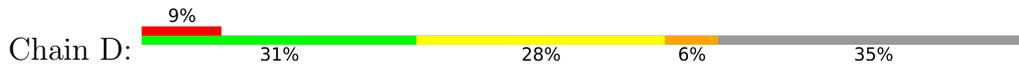








• Molecule 3: Structural protein VP5





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	8000	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	each image	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	22	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	125390	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor
Maximum map value	15.127	Depositor
Minimum map value	-10.037	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.002	Depositor
Recommended contour level	2.6	Depositor
Map size ( $\text{\AA}$ )	861.12, 861.12, 430.56	wwPDB
Map dimensions	720, 720, 360	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.196, 1.196, 1.196	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: GPL

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	0.41	0/8520	0.59	1/11599 (0.0%)
2	B	0.35	0/9508	0.54	1/12941 (0.0%)
2	C	0.35	0/10006	0.55	4/13622 (0.0%)
3	D	0.37	0/2322	0.64	2/3156 (0.1%)
3	E	0.37	0/2322	0.74	5/3156 (0.2%)
All	All	0.37	0/32678	0.58	13/44474 (0.0%)

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	59	ALA	CB-CA-C	-11.46	92.91	110.10
3	E	60	ARG	N-CA-CB	-7.76	96.63	110.60
3	D	7	GLY	N-CA-C	-6.60	96.61	113.10
3	E	263	ALA	N-CA-C	-5.96	94.91	111.00
1	A	535	LEU	CA-CB-CG	5.56	128.08	115.30

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	8372	0	8310	421	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	9317	0	9234	336	0
2	C	9806	0	9713	336	0
3	D	2276	0	2271	227	0
3	E	2276	0	2277	252	0
All	All	32047	0	31805	1392	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 22.

The worst 5 of 1392 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:194:HIS:CE1	3:D:146:ARG:NH1	1.74	1.53
2:B:271:THR:CG2	2:C:237:VAL:HG23	1.34	1.53
3:E:46:LYS:HD3	3:E:155:HIS:CE1	1.49	1.45
3:E:53:GLU:HG2	3:E:145:TYR:CD1	1.57	1.37
2:B:271:THR:HG21	2:C:237:VAL:CG2	1.54	1.36

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	1038/1058 (98%)	813 (78%)	161 (16%)	64 (6%)	1	19
2	B	1172/1333 (88%)	958 (82%)	186 (16%)	28 (2%)	6	35
2	C	1238/1333 (93%)	1018 (82%)	192 (16%)	28 (2%)	6	36
3	D	289/448 (64%)	253 (88%)	33 (11%)	3 (1%)	15	52
3	E	289/448 (64%)	254 (88%)	34 (12%)	1 (0%)	41	75
All	All	4026/4620 (87%)	3296 (82%)	606 (15%)	124 (3%)	7	31

5 of 124 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	49	HIS
1	A	72	PHE
1	A	255	ARG
1	A	282	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	932/942 (99%)	778 (84%)	154 (16%)	2	14
2	B	1029/1155 (89%)	920 (89%)	109 (11%)	6	27
2	C	1085/1155 (94%)	950 (88%)	135 (12%)	4	22
3	D	240/379 (63%)	205 (85%)	35 (15%)	3	18
3	E	240/379 (63%)	198 (82%)	42 (18%)	2	12
All	All	3526/4010 (88%)	3051 (86%)	475 (14%)	7	20

5 of 475 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	1049	GLU
3	E	53	GLU
2	C	339	LEU
3	E	35	LEU
3	E	289	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 94 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	297	ASN
2	C	854	GLN
2	C	311	ASN
2	C	646	ASN

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Mol	Chain	Res	Type
2	C	959	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](#)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	GPL	A	234	1	29,34,35	2.41	2 (6%)	29,49,51	1.53	4 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	GPL	A	234	1	-	6/15/37/39	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	234	GPL	P-NZ	11.92	1.74	1.61
1	A	234	GPL	C6-N1	-2.45	1.34	1.37

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	GPL	P-NZ-CE	-5.04	117.47	124.67
1	A	234	GPL	C3'-C2'-C1'	2.92	105.38	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	GPL	C5-C6-N1	2.54	118.44	113.95
1	A	234	GPL	C8-N7-C5	2.47	107.69	102.99

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	234	GPL	N-CA-CB-CG
1	A	234	GPL	CG-CD-CE-NZ
1	A	234	GPL	C5'-O5'-P-O1P
1	A	234	GPL	CE-NZ-P-O1P
1	A	234	GPL	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	234	GPL	1	0

## 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.

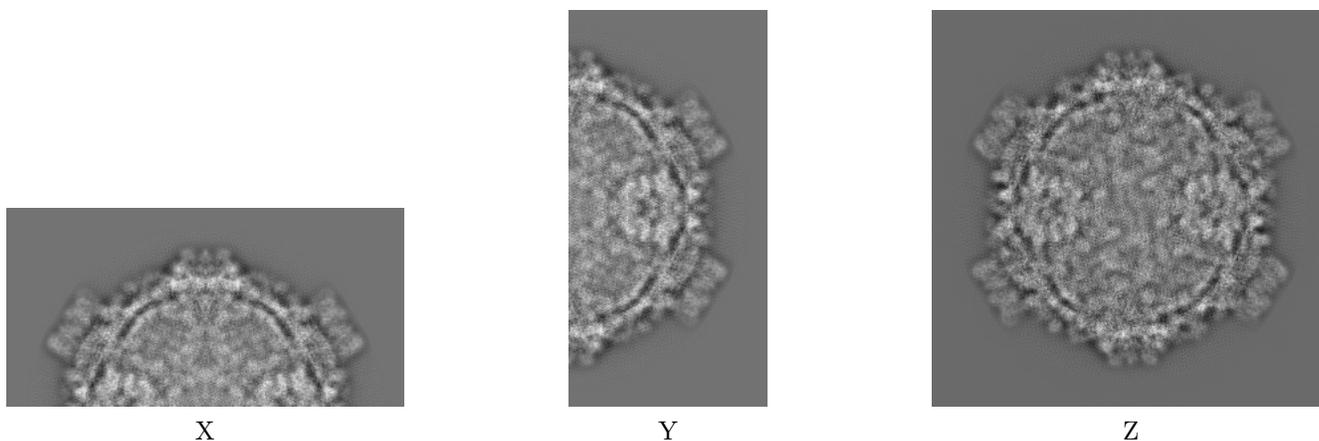
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5376. 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](#)

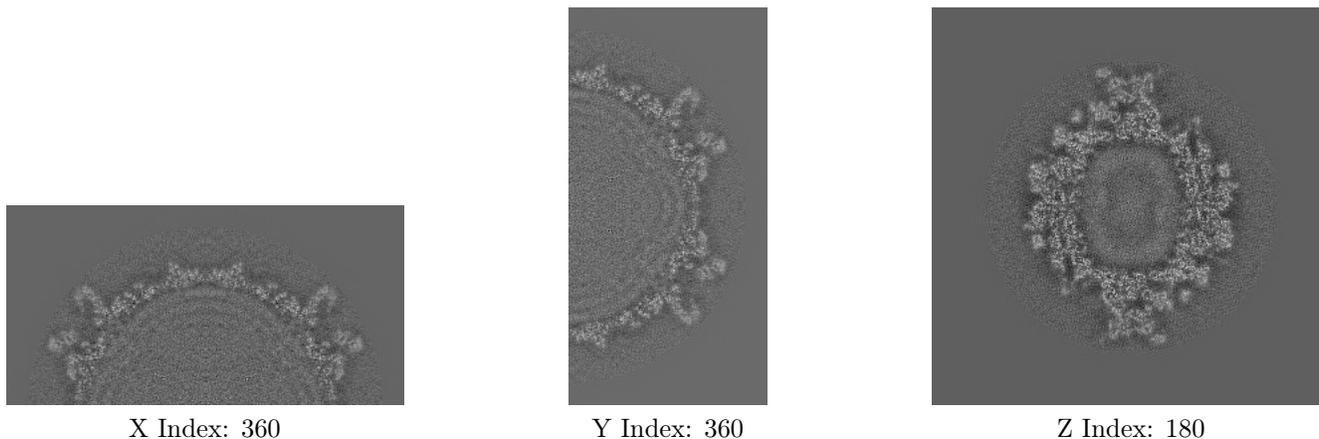
#### 6.1.1 Primary map



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

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

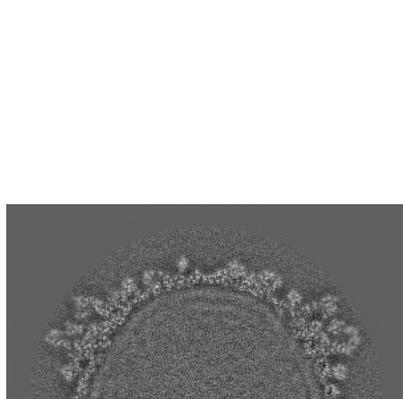
#### 6.2.1 Primary map



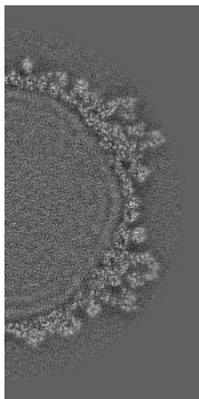
The images above show central slices of the map in three orthogonal directions.

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

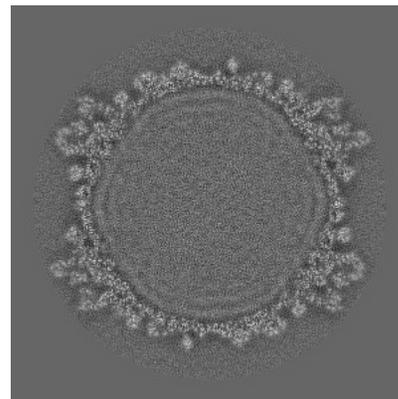
### 6.3.1 Primary map



X Index: 336



Y Index: 384



Z Index: 24

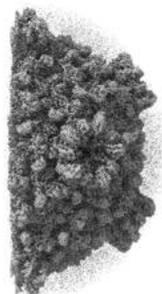
The images above show the largest variance slices of the map in three orthogonal directions.

## 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 2.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

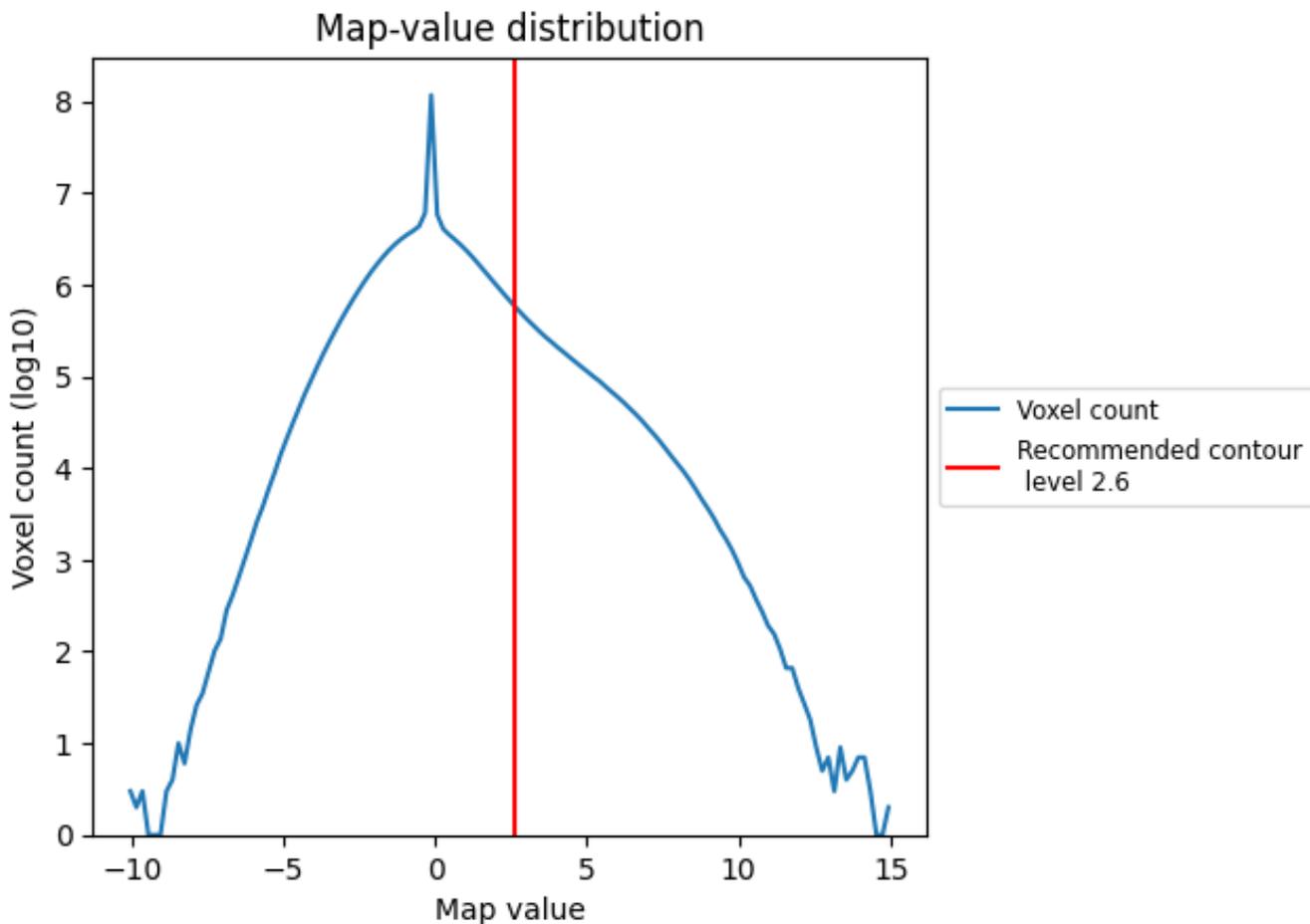
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

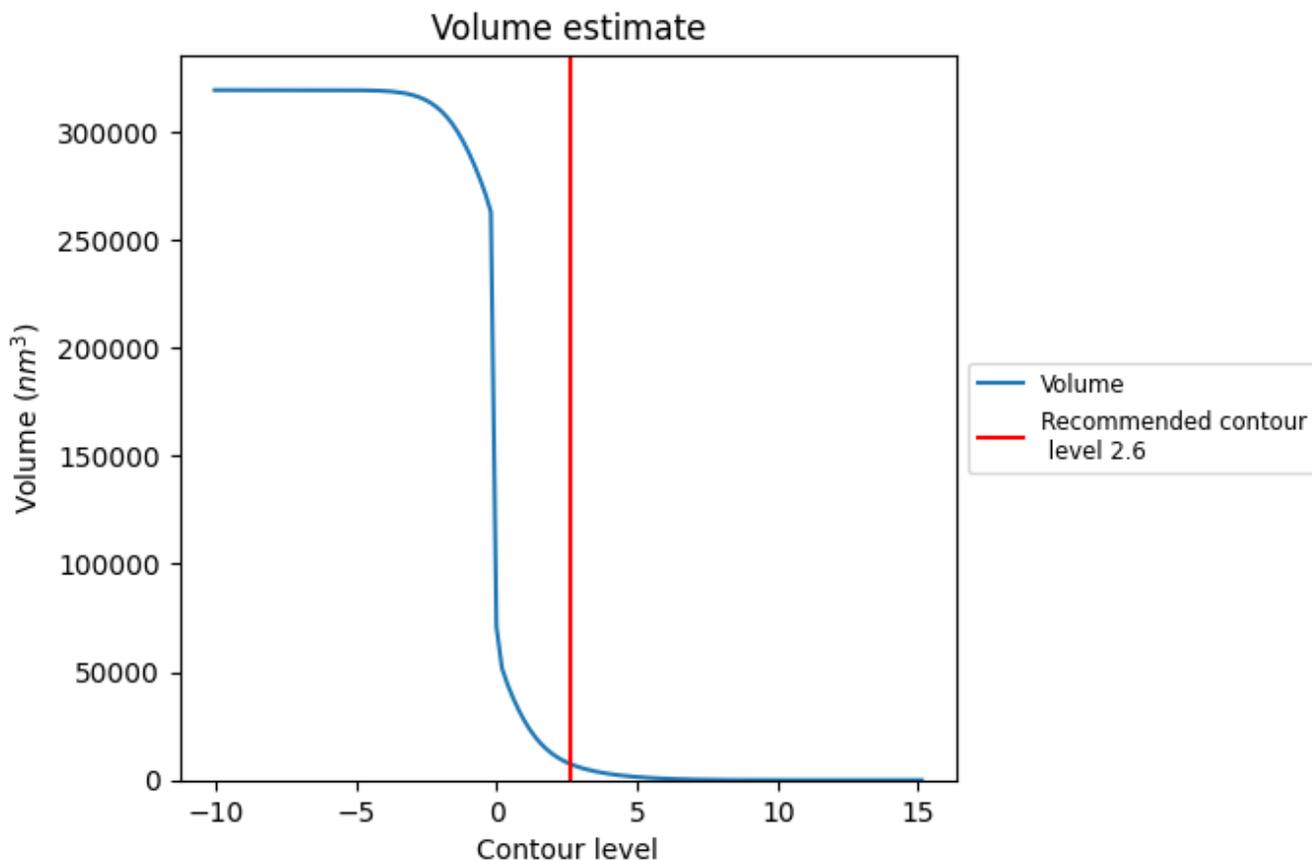
This section contains the results of statistical analysis of the map.

### 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 7585 nm<sup>3</sup>; this corresponds to an approximate mass of 6852 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](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

## 8 Fourier-Shell correlation

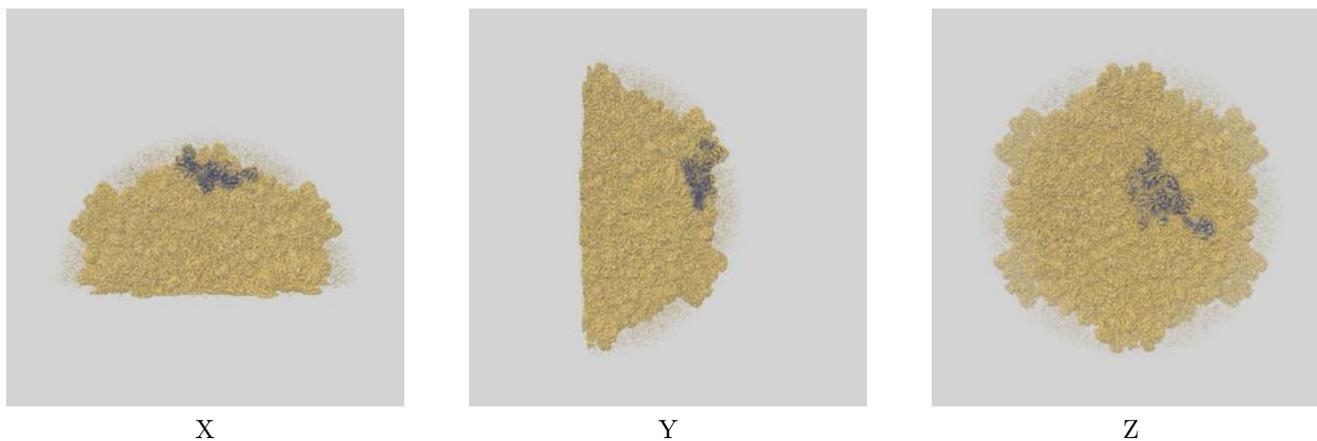
This section was not generated. No FSC curve or half-maps provided.

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

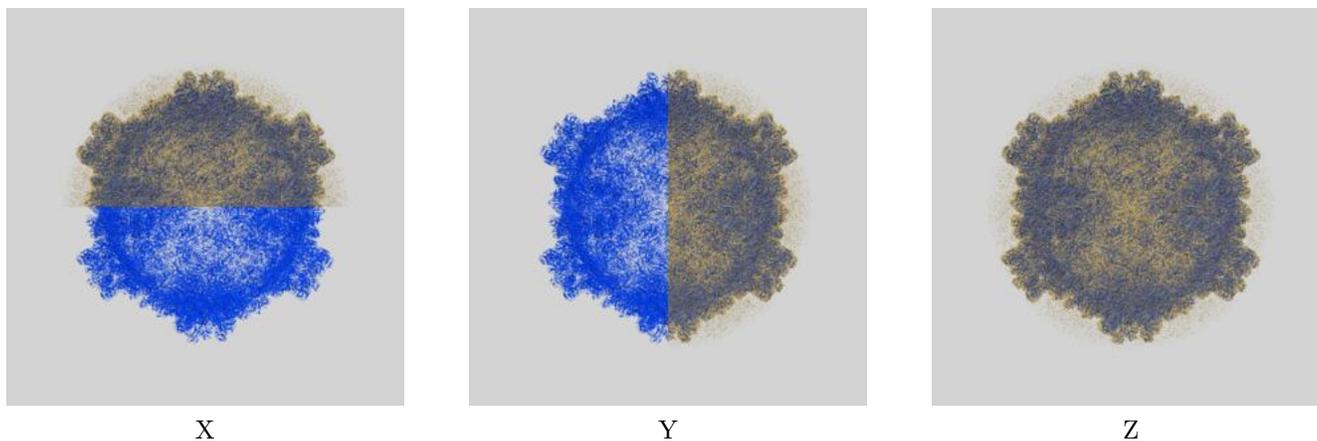
This section contains information regarding the fit between EMDB map EMD-5376 and PDB model 3J17. Per-residue inclusion information can be found in section 3 on page 4.

### 9.1 Map-model overlays

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

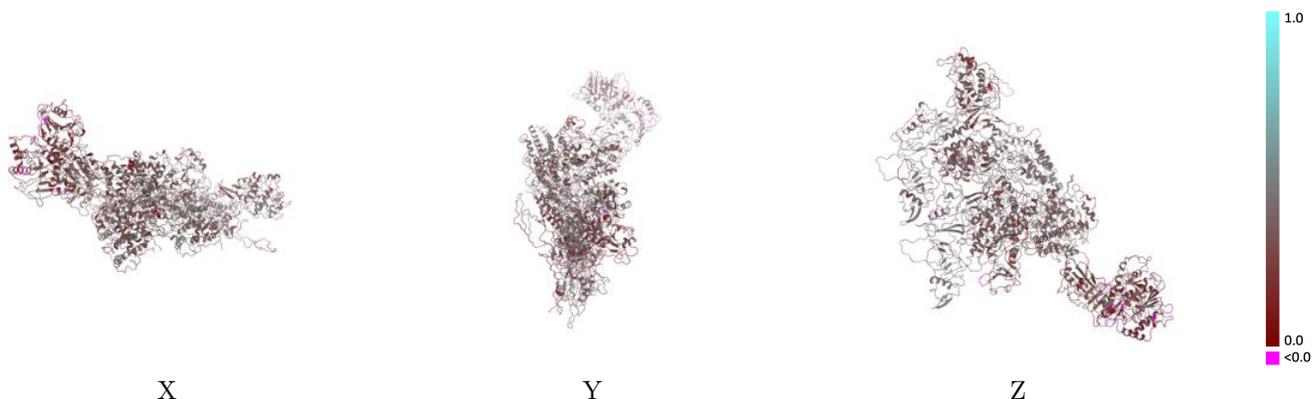


#### 9.1.2 Map-model assembly overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 2.6 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](#)



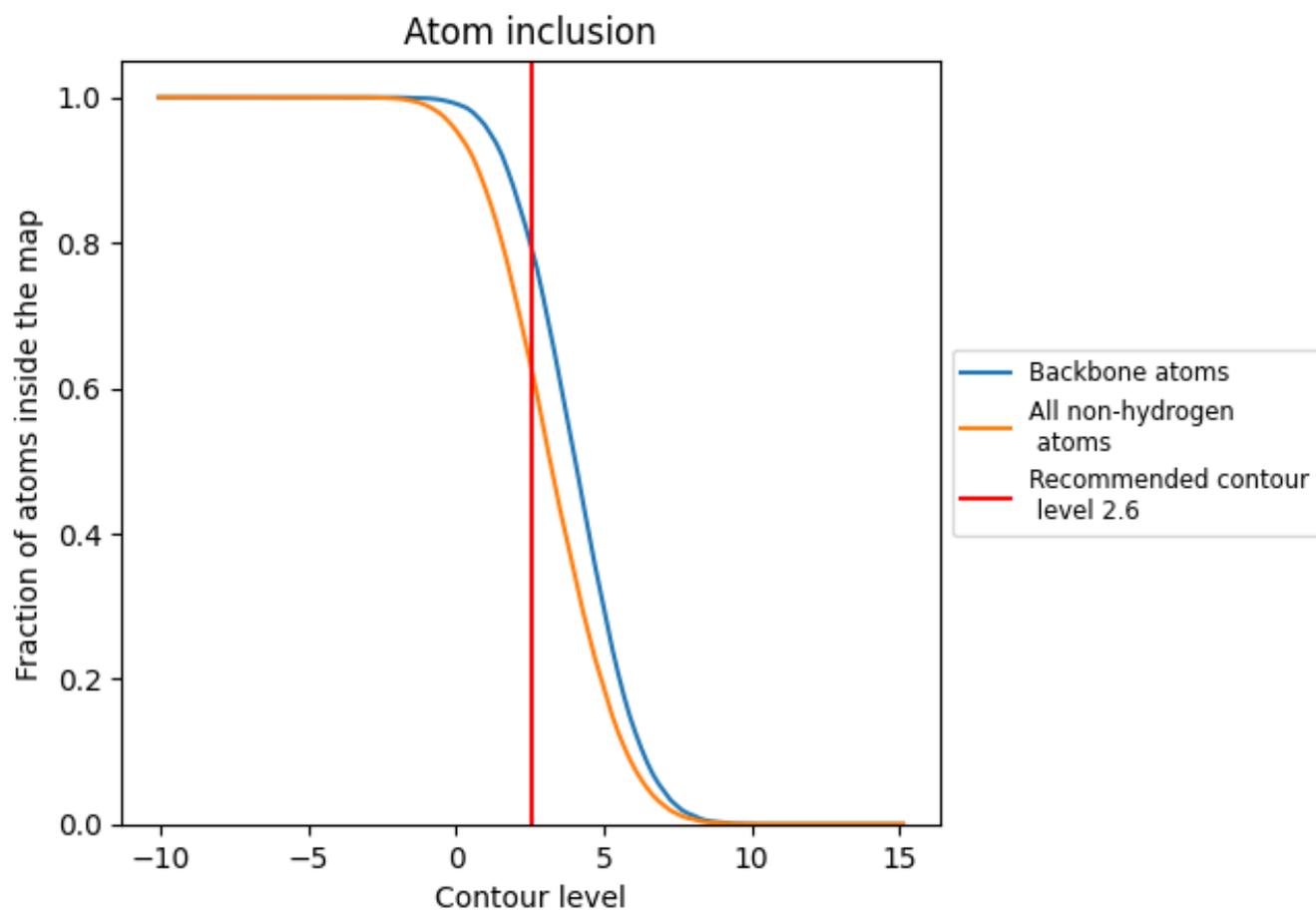
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.6).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 62% 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 (2.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6195	 0.3550
A	 0.5525	 0.3190
B	 0.6200	 0.3700
C	 0.6507	 0.3760
D	 0.6431	 0.3500
E	 0.7052	 0.3340

