



## wwPDB EM Validation Summary Report ⓘ

Dec 17, 2022 – 04:41 pm GMT

PDB ID : 6ZTS  
EMDB ID : EMD-22165  
Title : Assembly intermediates of orthoreovirus captured in the cell  
Authors : Sutton, G.C.; Stuart, D.I.  
Deposited on : 2020-07-20  
Resolution : Not provided

This is a wwPDB EM Validation Summary 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

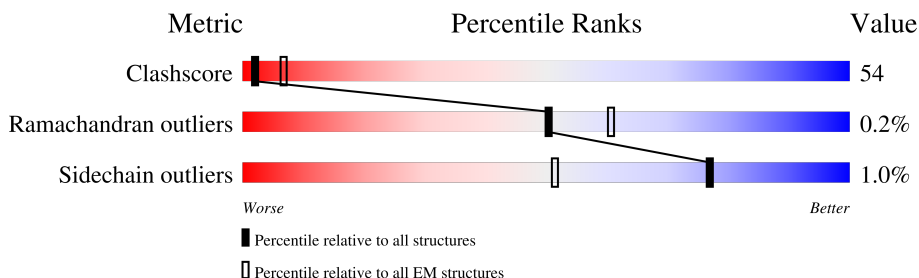
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is unknown.

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	975	<p>21% (red), 28% (green), 70% (yellow), . (grey)</p>
1	B	975	<p>15% (red), 26% (green), 72% (yellow), .. (grey)</p>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 15341 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.

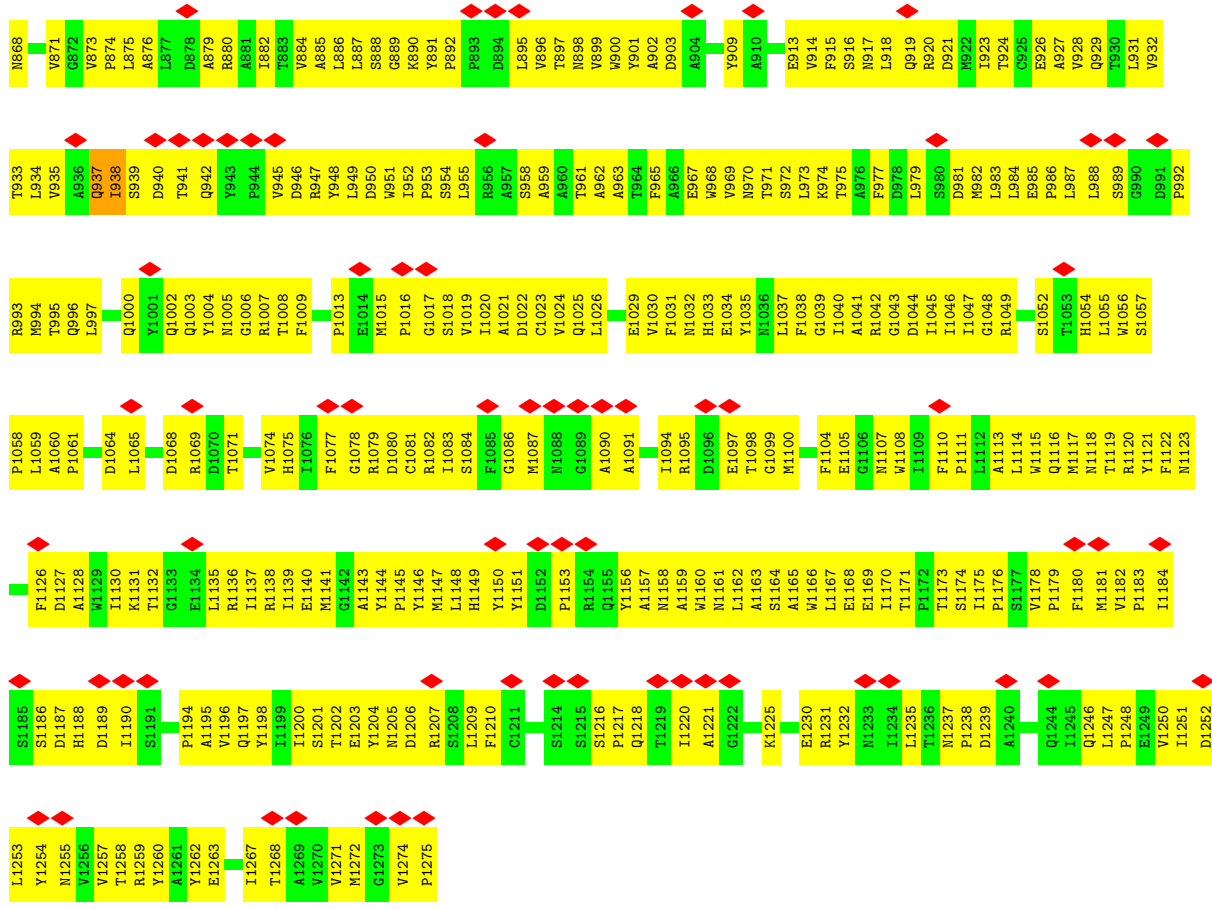
- Molecule 1 is a protein called Lambda-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	974	7696	4911	1304	1432	49	0	0
1	B	967	7645	4883	1296	1417	49	0	0

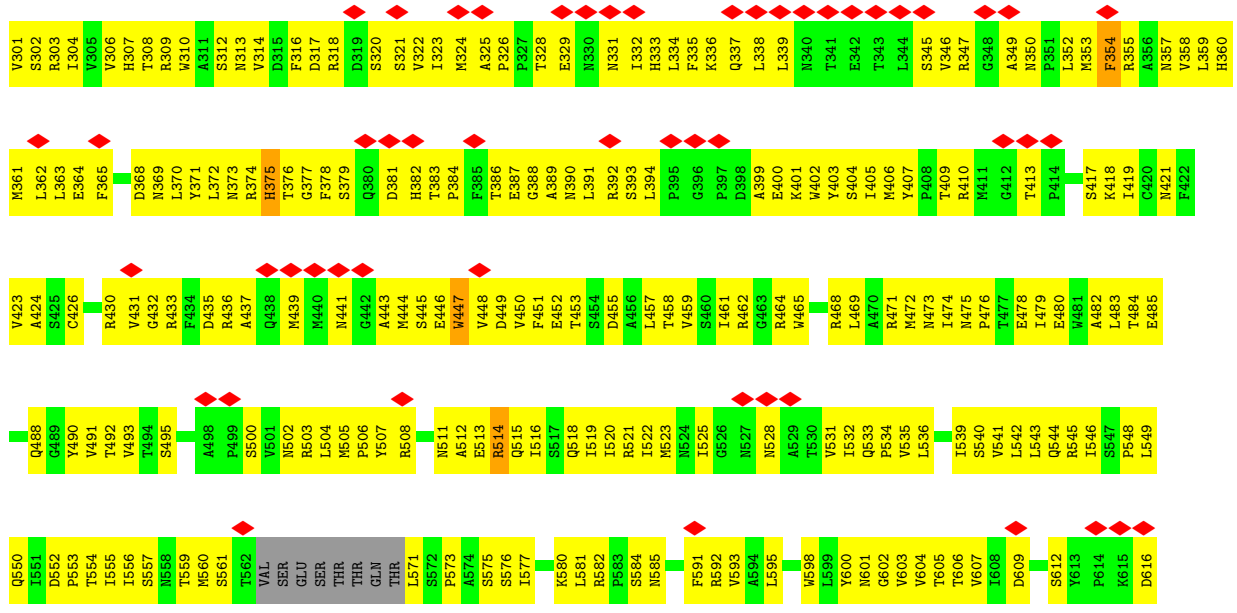
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	336	LYS	ARG	conflict	UNP A0A023VYS9
A	507	TYR	ARG	conflict	UNP A0A023VYS9
A	973	LEU	MET	conflict	UNP A0A023VYS9
A	1010	ASP	ASN	conflict	UNP A0A023VYS9
A	1163	ALA	THR	conflict	UNP A0A023VYS9
B	336	LYS	ARG	conflict	UNP A0A023VYS9
B	507	TYR	ARG	conflict	UNP A0A023VYS9
B	973	LEU	MET	conflict	UNP A0A023VYS9
B	1010	ASP	ASN	conflict	UNP A0A023VYS9
B	1163	ALA	THR	conflict	UNP A0A023VYS9





• Molecule 1: Lambda-1





## 4 Experimental information

Property	Value	Source
EM reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, Not provided	
Number of tilted images used	41	Depositor
Resolution determination method	Not provided	
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum voxel value	10.927	Depositor
Minimum voxel value	-5.906	Depositor
Average voxel value	0.059	Depositor
Voxel value standard deviation	0.498	Depositor
Recommended contour level	3.0	Depositor
Tomogram size ( $\text{\AA}$ )	696.6, 696.6, 696.6	wwPDB
Tomogram dimensions	387, 387, 387	wwPDB
Tomogram angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Grid spacing ( $\text{\AA}$ )	1.8, 1.8, 1.8	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	0.40	0/7902	0.57	1/10819 (0.0%)
1	B	0.39	0/7850	0.54	0/10746
All	All	0.39	0/15752	0.55	1/21565 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
1	B	0	1
All	All	0	8

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	825	MET	C-N-CA	10.24	147.29	121.70

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	334	LEU	Peptide
1	A	352	LEU	Peptide
1	A	582	ARG	Peptide
1	A	822	ILE	Peptide
1	A	823	ALA	Peptide



## 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	7696	0	7604	825	0
1	B	7645	0	7559	815	0
All	All	15341	0	15163	1634	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 54.

The worst 5 of 1634 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:GLU:HA	1:B:1261:ALA:H	1.24	1.02
1:B:511:ASN:HA	1:B:514:ARG:HH21	1.25	1.00
1:A:847:VAL:H	1:A:871:VAL:HG11	1.23	0.98
1:A:929:GLN:HB2	1:A:1015:MET:HG2	1.43	0.97
1:A:449:ASP:HA	1:A:1257:VAL:O	1.67	0.95

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	972/975 (100%)	783 (81%)	187 (19%)	2 (0%)	47	47
1	B	963/975 (99%)	806 (84%)	156 (16%)	1 (0%)	51	51
All	All	1935/1950 (99%)	1589 (82%)	343 (18%)	3 (0%)	50	47

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1111	PRO
1	A	1161	ASN
1	A	582	ARG

### 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	861/862 (100%)	852 (99%)	9 (1%)	76	76
1	B	854/862 (99%)	846 (99%)	8 (1%)	78	78
All	All	1715/1724 (100%)	1698 (99%)	17 (1%)	77	76

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	720	ARG
1	B	1212	THR
1	A	842	ARG
1	A	851	ARG
1	B	354	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	852	GLN
1	B	1088	ASN
1	B	917	ASN
1	B	942	GLN
1	B	1116	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.

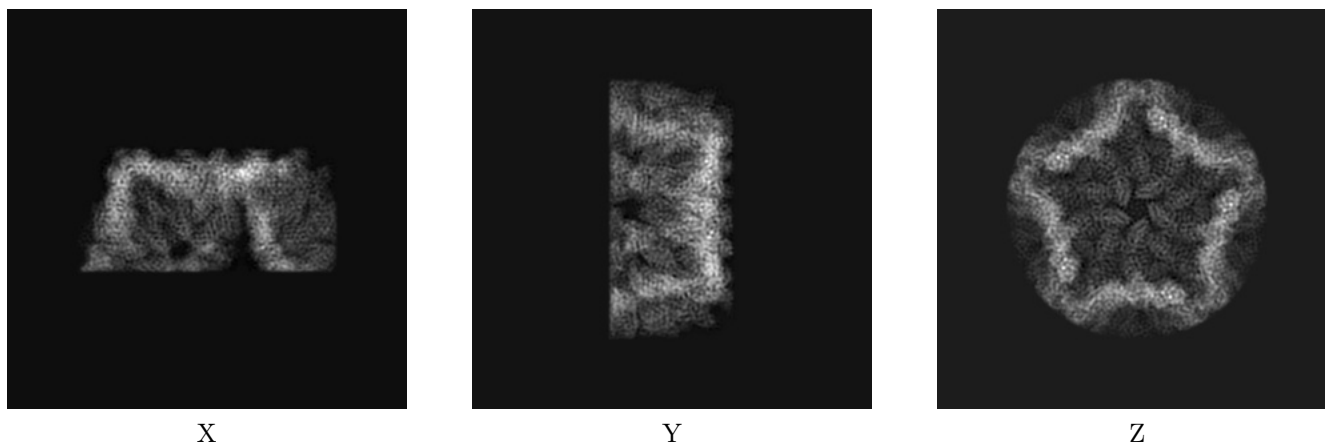
## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Tomogram visualisation [i](#)

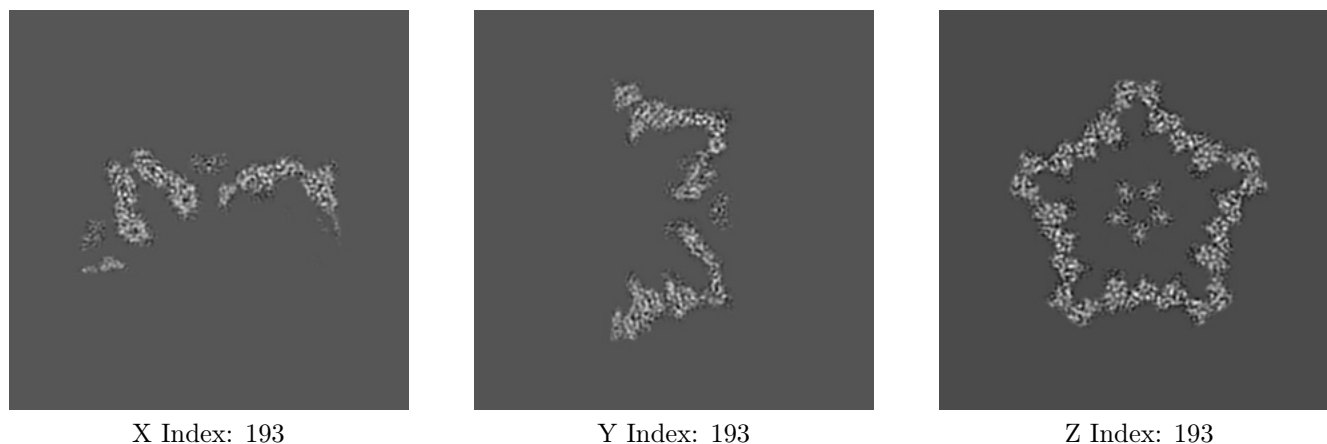
This section contains visualisations of the EMDB entry EMD-22165. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

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



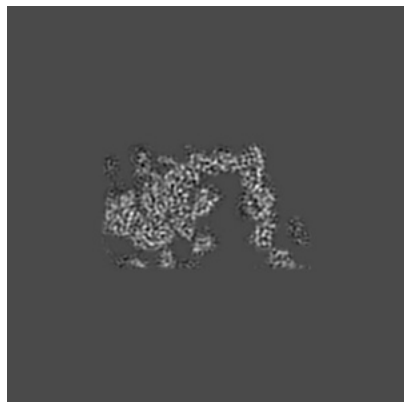
The images above show the tomogram projected in three orthogonal directions.

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

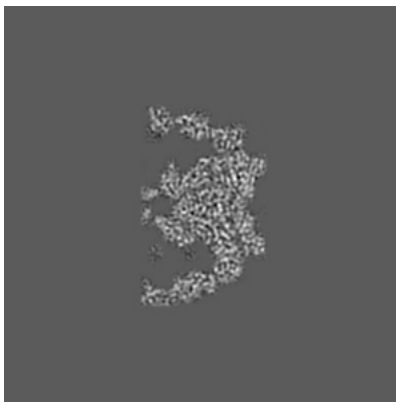


The images above show central slices of the tomogram in three orthogonal directions.

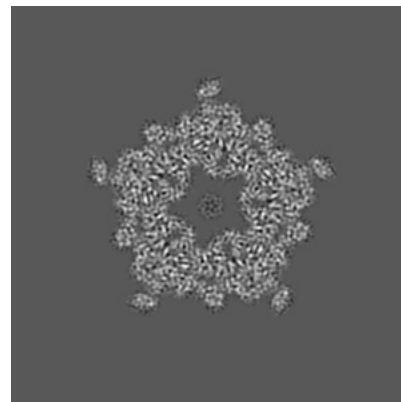
### 6.3 Largest variance slices [i](#)



X Index: 117



Y Index: 112



Z Index: 230

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

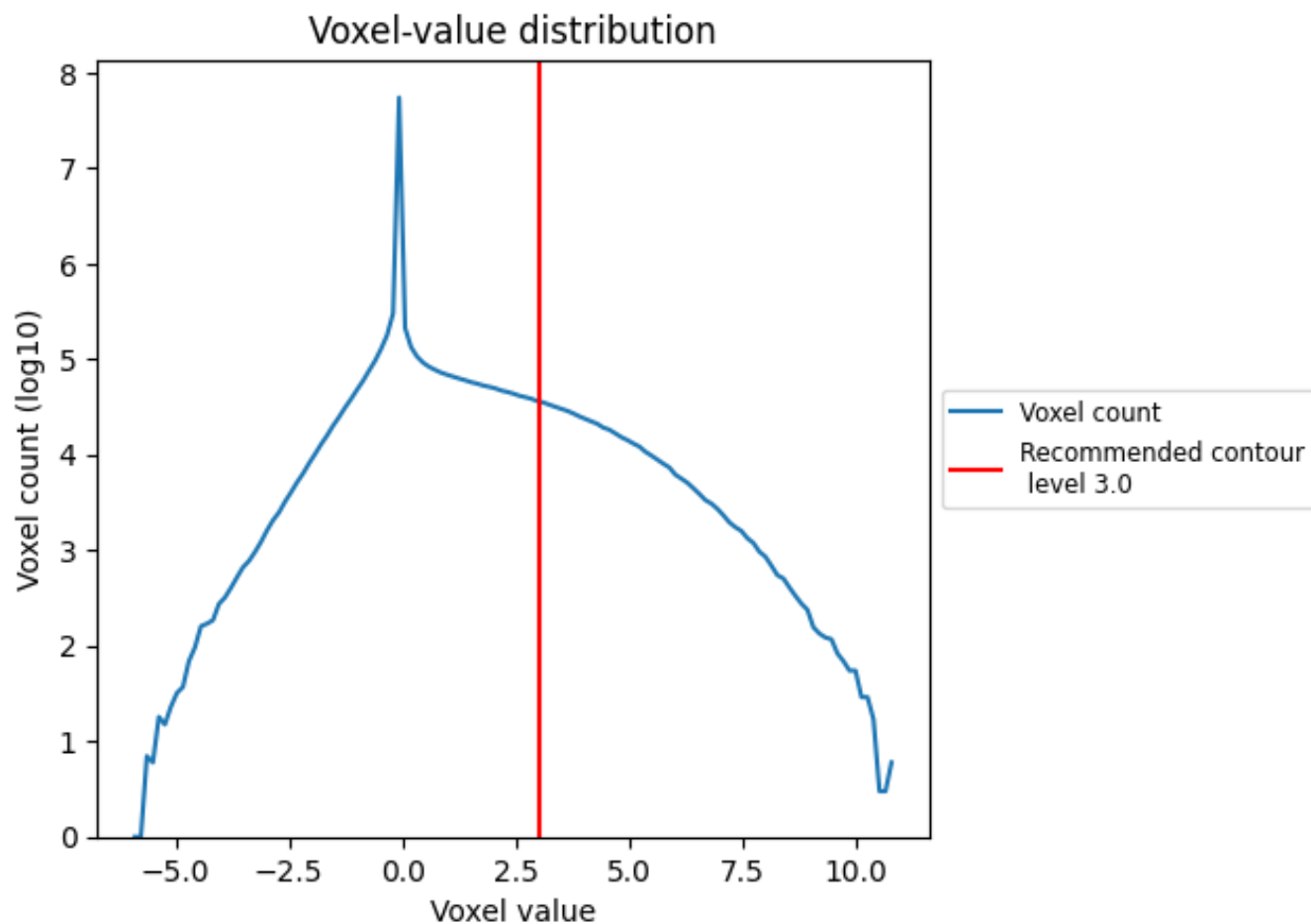
### 6.4 Mask visualisation [i](#)

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

## 7 Tomogram analysis [i](#)

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

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



The voxel-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic.

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

This section contains information regarding the fit between EMDB map EMD-22165 and PDB model 6ZTS. Per-residue inclusion information can be found in section 3 on page 4.

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

This section was not generated.

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

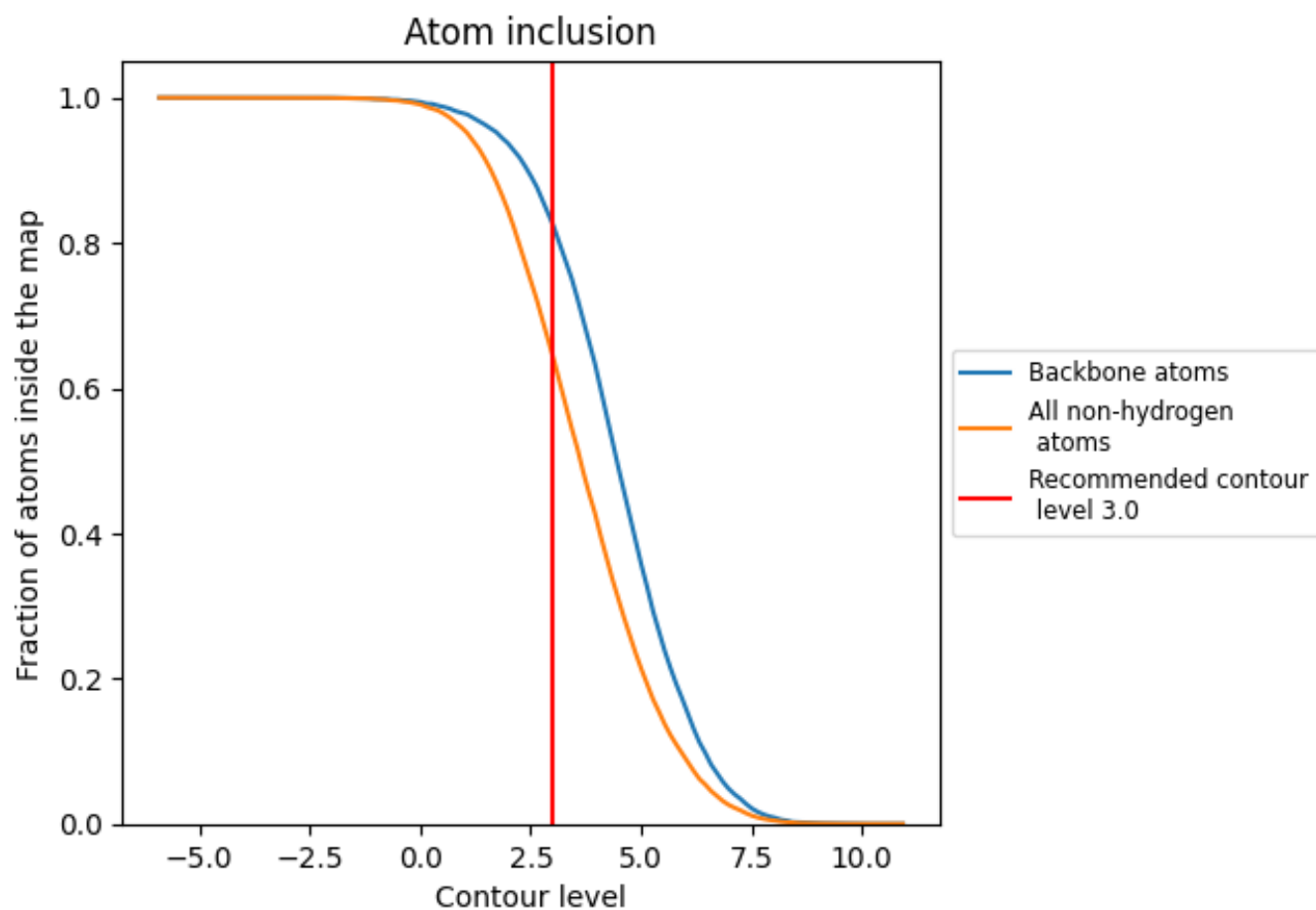


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

### 8.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

## 8.4 Atom inclusion [i](#)








At the recommended contour level, 83% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.



## 8.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (3.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6448	 0.2160
A	 0.6346	 0.2110
B	 0.6550	 0.2220

