



wwPDB EM Validation Summary Report ⓘ

Dec 17, 2022 – 04:42 pm GMT

PDB ID : 6ZTY
EMDB ID : EMD-22164
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

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>.

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

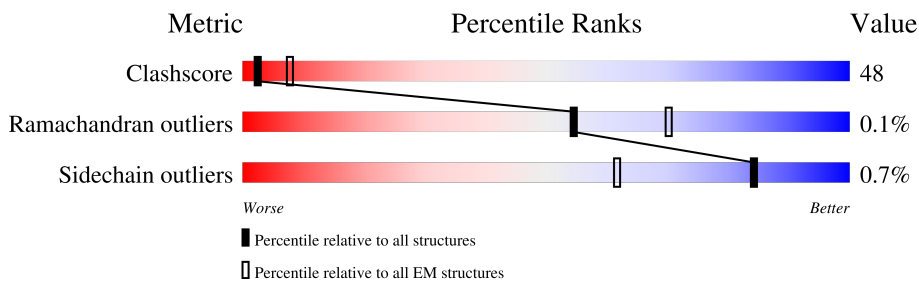
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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 ≥ 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	H	641	88% 28% 71%
1	I	641	88% 30% 69%
1	J	641	89% 29% 71%
2	U	365	68% 33% 65%
2	V	365	74% 33% 67%
2	W	365	73% 28% 72%

2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 23268 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 Outer capsid protein mu-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	H	641	4871	3091	807	954	19	0	0
1	I	641	4871	3091	807	954	19	0	0
1	J	641	4871	3091	807	954	19	0	0

There are 81 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	?	-	PRO	deletion	UNP P11077
H	?	-	GLU	deletion	UNP P11077
H	?	-	THR	deletion	UNP P11077
H	?	-	ALA	deletion	UNP P11077
H	?	-	ILE	deletion	UNP P11077
H	?	-	ILE	deletion	UNP P11077
H	?	-	ASN	deletion	UNP P11077
H	?	-	THR	deletion	UNP P11077
H	?	-	ASP	deletion	UNP P11077
H	?	-	ASN	deletion	UNP P11077
H	?	-	SER	deletion	UNP P11077
H	?	-	SER	deletion	UNP P11077
H	?	-	GLY	deletion	UNP P11077
H	?	-	ALA	deletion	UNP P11077
H	?	-	VAL	deletion	UNP P11077
H	?	-	PRO	deletion	UNP P11077
H	?	-	SER	deletion	UNP P11077
H	?	-	GLU	deletion	UNP P11077
H	?	-	SER	deletion	UNP P11077
H	?	-	ALA	deletion	UNP P11077
H	?	-	LEU	deletion	UNP P11077
H	?	-	VAL	deletion	UNP P11077
H	?	-	PRO	deletion	UNP P11077
H	?	-	TYR	deletion	UNP P11077

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Chain	Residue	Modelled	Actual	Comment	Reference
H	?	-	ASN	deletion	UNP P11077
H	344	LEU	PRO	conflict	UNP P11077
H	359	PHE	LEU	conflict	UNP P11077
I	?	-	PRO	deletion	UNP P11077
I	?	-	GLU	deletion	UNP P11077
I	?	-	THR	deletion	UNP P11077
I	?	-	ALA	deletion	UNP P11077
I	?	-	ILE	deletion	UNP P11077
I	?	-	ILE	deletion	UNP P11077
I	?	-	ASN	deletion	UNP P11077
I	?	-	THR	deletion	UNP P11077
I	?	-	ASP	deletion	UNP P11077
I	?	-	ASN	deletion	UNP P11077
I	?	-	SER	deletion	UNP P11077
I	?	-	SER	deletion	UNP P11077
I	?	-	GLY	deletion	UNP P11077
I	?	-	ALA	deletion	UNP P11077
I	?	-	VAL	deletion	UNP P11077
I	?	-	PRO	deletion	UNP P11077
I	?	-	SER	deletion	UNP P11077
I	?	-	GLU	deletion	UNP P11077
I	?	-	SER	deletion	UNP P11077
I	?	-	ALA	deletion	UNP P11077
I	?	-	LEU	deletion	UNP P11077
I	?	-	VAL	deletion	UNP P11077
I	?	-	PRO	deletion	UNP P11077
I	?	-	TYR	deletion	UNP P11077
I	?	-	ASN	deletion	UNP P11077
I	344	LEU	PRO	conflict	UNP P11077
I	359	PHE	LEU	conflict	UNP P11077
J	?	-	PRO	deletion	UNP P11077
J	?	-	GLU	deletion	UNP P11077
J	?	-	THR	deletion	UNP P11077
J	?	-	ALA	deletion	UNP P11077
J	?	-	ILE	deletion	UNP P11077
J	?	-	ILE	deletion	UNP P11077
J	?	-	ASN	deletion	UNP P11077
J	?	-	THR	deletion	UNP P11077
J	?	-	ASP	deletion	UNP P11077
J	?	-	ASN	deletion	UNP P11077
J	?	-	SER	deletion	UNP P11077
J	?	-	SER	deletion	UNP P11077

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Chain	Residue	Modelled	Actual	Comment	Reference
J	?	-	GLY	deletion	UNP P11077
J	?	-	ALA	deletion	UNP P11077
J	?	-	VAL	deletion	UNP P11077
J	?	-	PRO	deletion	UNP P11077
J	?	-	SER	deletion	UNP P11077
J	?	-	GLU	deletion	UNP P11077
J	?	-	SER	deletion	UNP P11077
J	?	-	ALA	deletion	UNP P11077
J	?	-	LEU	deletion	UNP P11077
J	?	-	VAL	deletion	UNP P11077
J	?	-	PRO	deletion	UNP P11077
J	?	-	TYR	deletion	UNP P11077
J	?	-	ASN	deletion	UNP P11077
J	344	LEU	PRO	conflict	UNP P11077
J	359	PHE	LEU	conflict	UNP P11077

- Molecule 2 is a protein called Outer capsid protein sigma-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	U	365	2885	1818	508	531	28	0	0
2	V	365	2885	1818	508	531	28	0	0
2	W	365	2885	1818	508	531	28	0	0

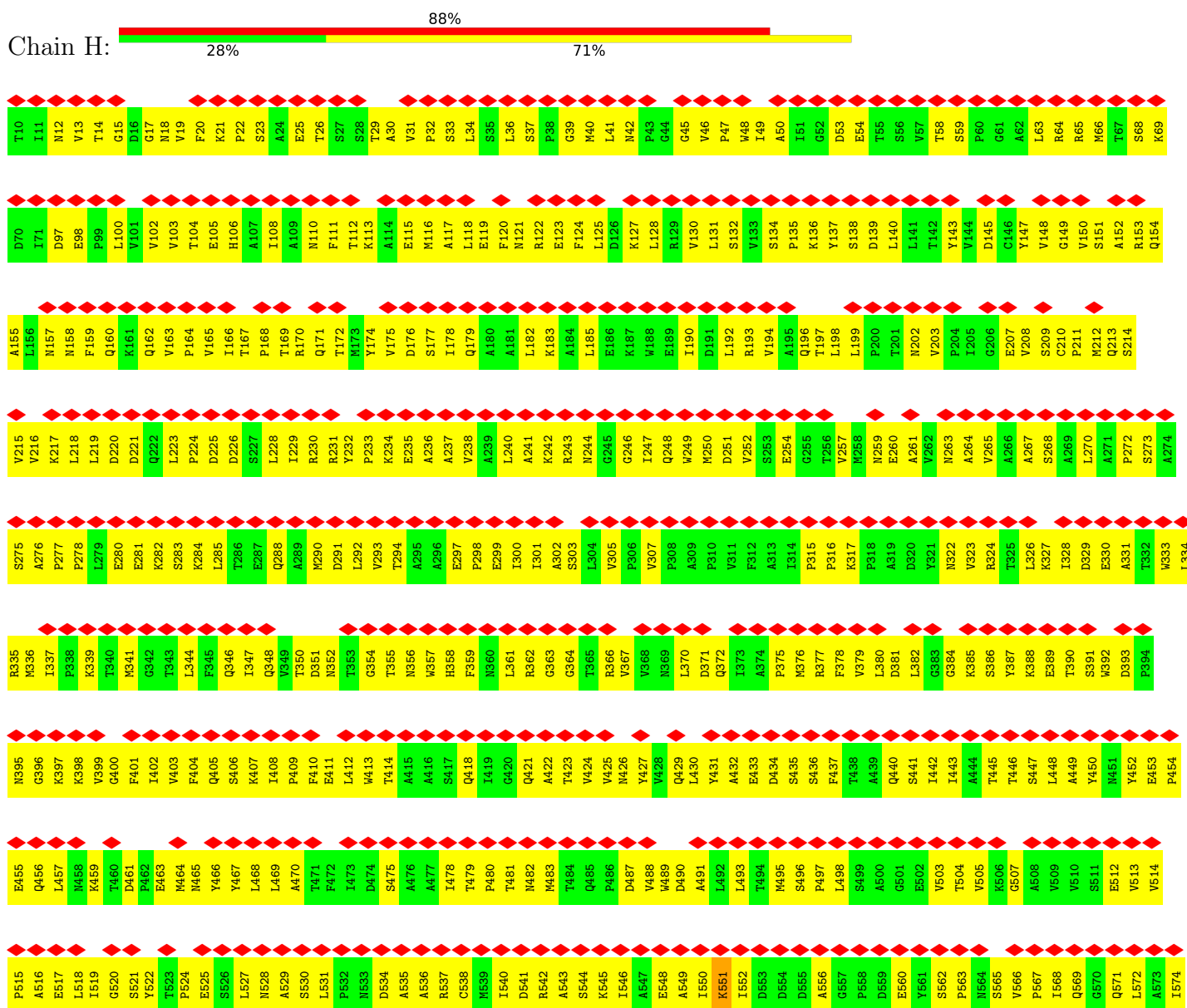
There are 6 discrepancies between the modelled and reference sequences:

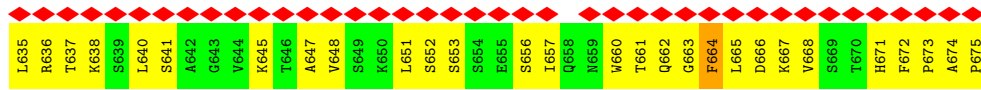
Chain	Residue	Modelled	Actual	Comment	Reference
U	104	CYS	ALA	conflict	UNP P07939
U	325	ASN	ASP	conflict	UNP P07939
V	104	CYS	ALA	conflict	UNP P07939
V	325	ASN	ASP	conflict	UNP P07939
W	104	CYS	ALA	conflict	UNP P07939
W	325	ASN	ASP	conflict	UNP P07939

3 Residue-property plots

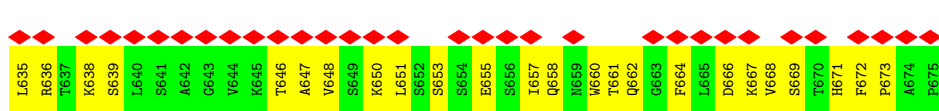
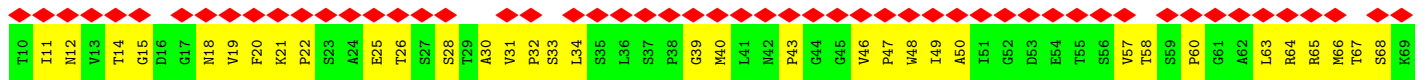
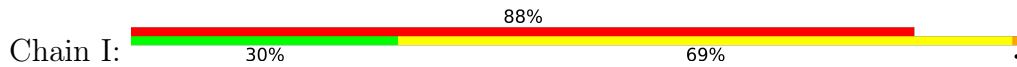
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

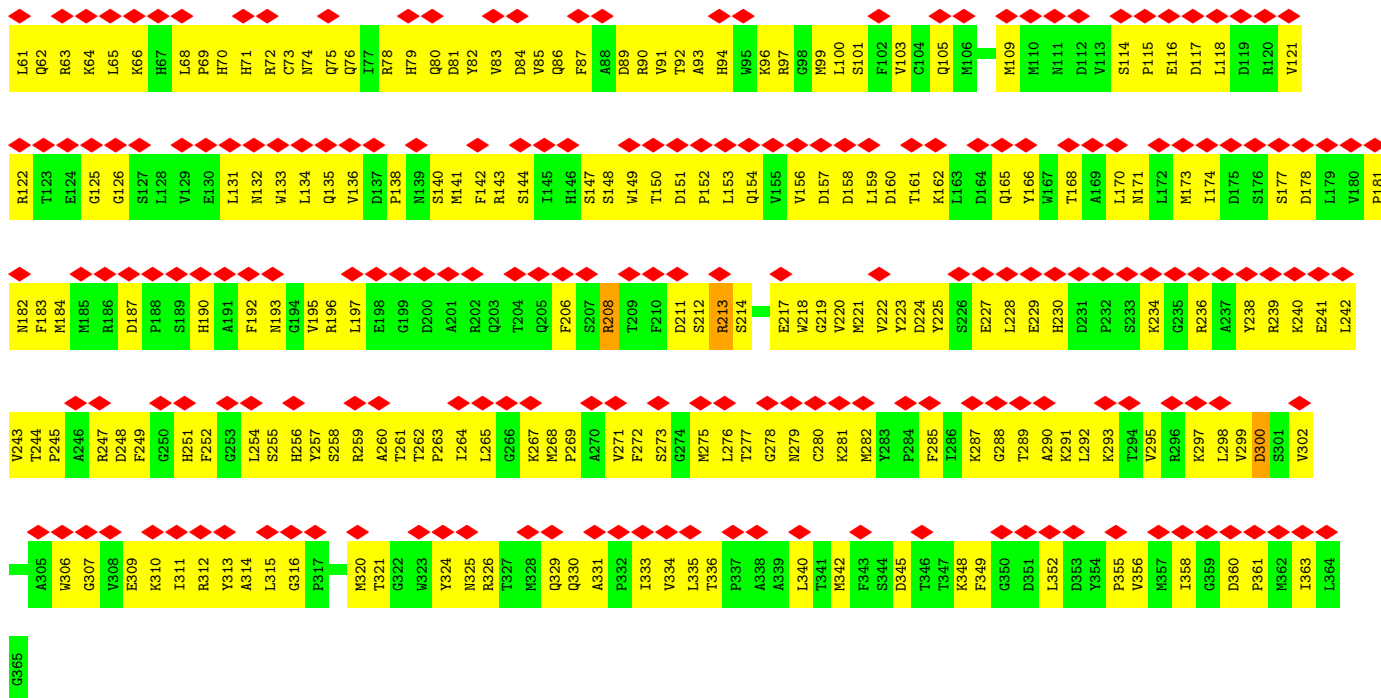
- Molecule 1: Outer capsid protein mu-1



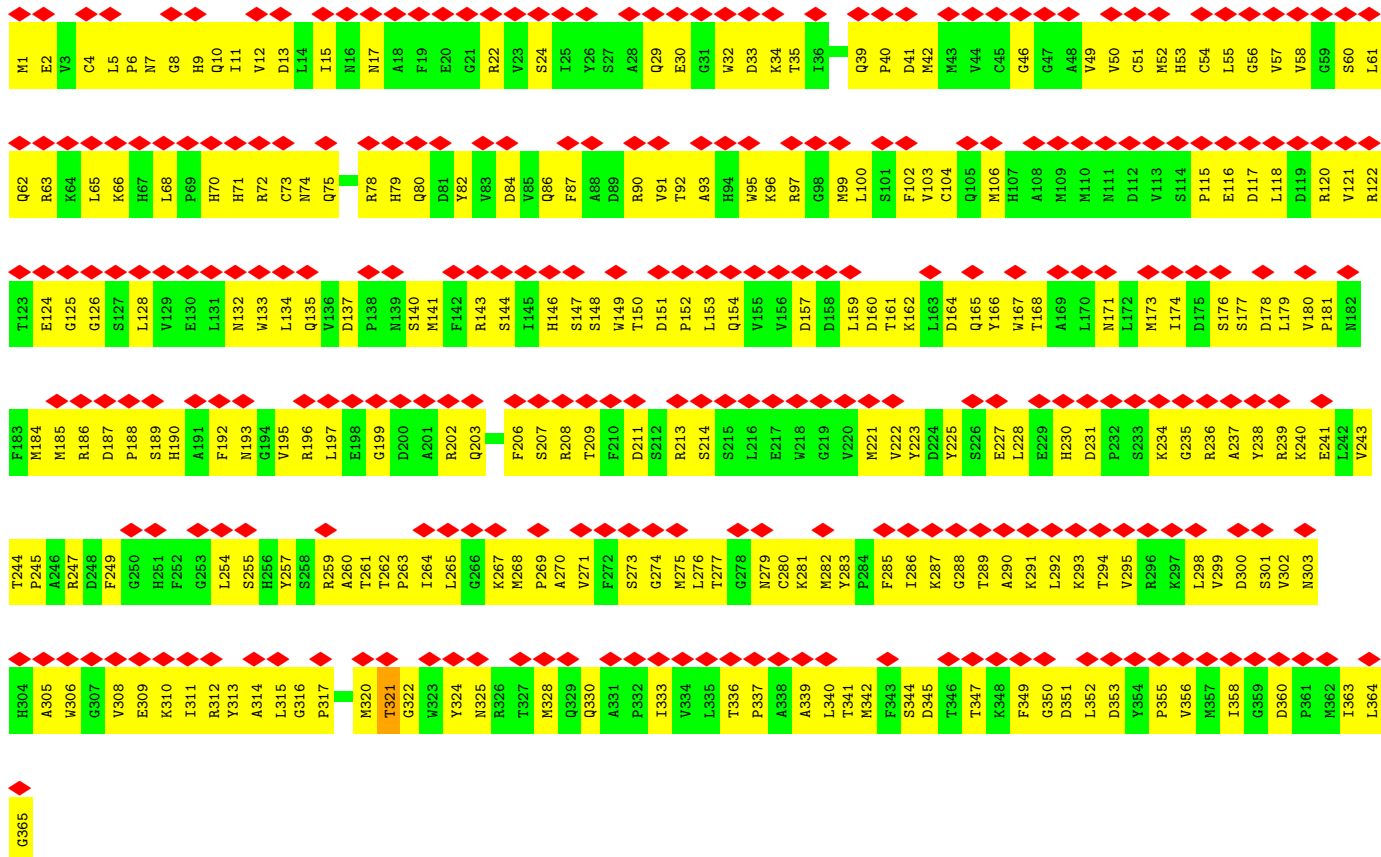
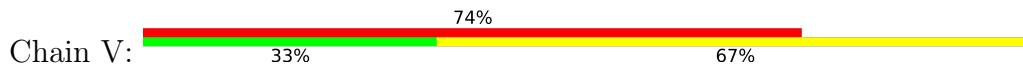


• Molecule 1: Outer capsid protein mu-1

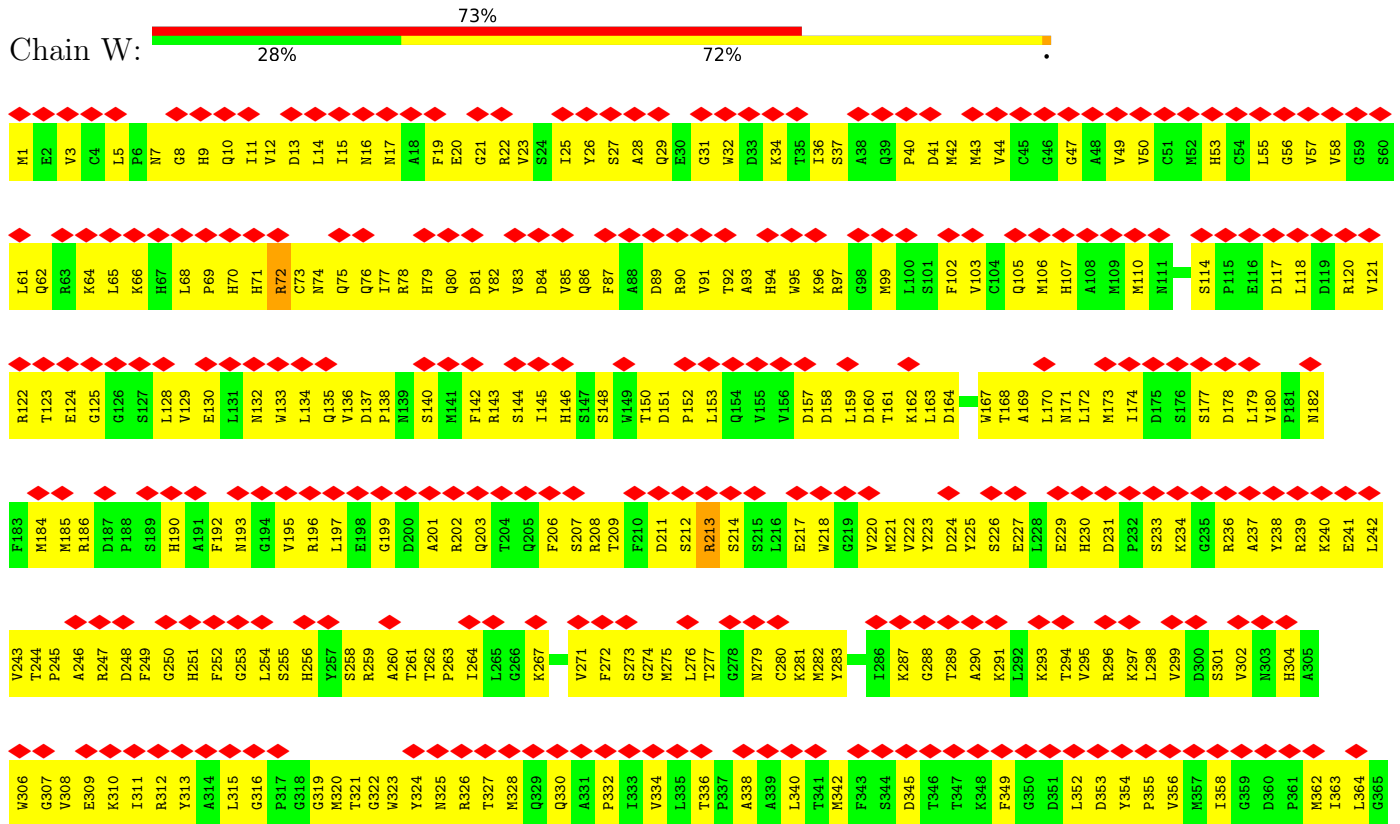




• Molecule 2: Outer capsid protein sigma-3



• Molecule 2: Outer capsid protein sigma-3



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	8.877	Depositor
Minimum voxel value	-5.347	Depositor
Average voxel value	0.049	Depositor
Voxel value standard deviation	0.457	Depositor
Recommended contour level	2.8	Depositor
Tomogram size (\AA)	460.8, 460.8, 460.8	wwPDB
Tomogram dimensions	256, 256, 256	wwPDB
Tomogram angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Grid spacing (\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	H	0.35	0/4971	0.51	0/6787
1	I	0.36	0/4971	0.52	0/6787
1	J	0.36	0/4971	0.51	0/6787
2	U	0.36	0/2957	0.50	0/4005
2	V	0.35	0/2957	0.48	0/4005
2	W	0.35	0/2957	0.49	0/4005
All	All	0.36	0/23784	0.51	0/32376

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	H	4871	0	4900	517	0
1	I	4871	0	4900	527	0
1	J	4871	0	4900	543	0
2	U	2885	0	2816	267	0
2	V	2885	0	2816	250	0
2	W	2885	0	2816	281	0
All	All	23268	0	23148	2224	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 48.

The worst 5 of 2224 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)
2:V:271:VAL:O	2:V:282:MET:HA	1.45	1.15
1:H:406:SER:O	1:H:465:ASN:HB2	1.55	1.06
2:W:271:VAL:O	2:W:282:MET:HA	1.60	1.01
1:J:406:SER:O	1:J:465:ASN:HB2	1.59	1.00
1:J:19:VAL:HB	1:J:248:GLN:HB2	1.46	0.97

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	H	637/641 (99%)	571 (90%)	65 (10%)	1 (0%)	47	47
1	I	637/641 (99%)	578 (91%)	58 (9%)	1 (0%)	47	47
1	J	637/641 (99%)	570 (90%)	67 (10%)	0	100	100
2	U	363/365 (100%)	321 (88%)	42 (12%)	0	100	100
2	V	363/365 (100%)	331 (91%)	32 (9%)	0	100	100
2	W	363/365 (100%)	329 (91%)	34 (9%)	0	100	100
All	All	3000/3018 (99%)	2700 (90%)	298 (10%)	2 (0%)	54	51

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	233	PRO
1	I	233	PRO

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	H	541/541 (100%)	539 (100%)	2 (0%)	91	91
1	I	541/541 (100%)	537 (99%)	4 (1%)	84	84
1	J	541/541 (100%)	539 (100%)	2 (0%)	91	91
2	U	317/317 (100%)	312 (98%)	5 (2%)	62	62
2	V	317/317 (100%)	316 (100%)	1 (0%)	92	92
2	W	317/317 (100%)	314 (99%)	3 (1%)	78	78
All	All	2574/2574 (100%)	2557 (99%)	17 (1%)	84	84

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

Mol	Chain	Res	Type
2	W	14	LEU
2	W	213	ARG
1	J	551	LYS
2	U	17	ASN
2	U	29	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 63 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	346	GLN
2	V	279	ASN
2	U	16	ASN
2	V	171	ASN
2	W	79	HIS

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	I	1
1	H	1
1	J	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	71:ILE	C	97:ASP	N	13.75
1	H	71:ILE	C	97:ASP	N	12.23
1	J	71:ILE	C	97:ASP	N	10.83

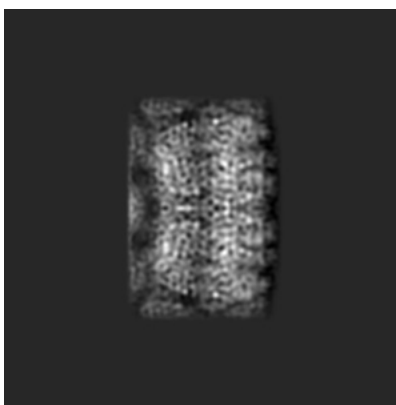
6 Tomogram visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22164. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

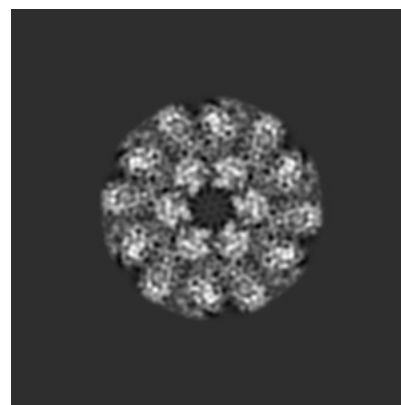
6.1 Orthogonal projections [i](#)



X



Y



Z

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

6.2 Central slices [i](#)



X Index: 128



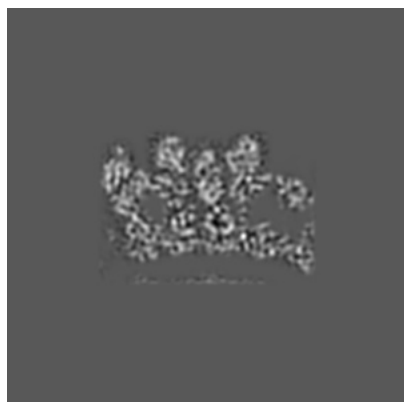
Y Index: 128



Z Index: 128

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

6.3 Largest variance slices [i](#)



X Index: 147



Y Index: 100



Z Index: 141

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

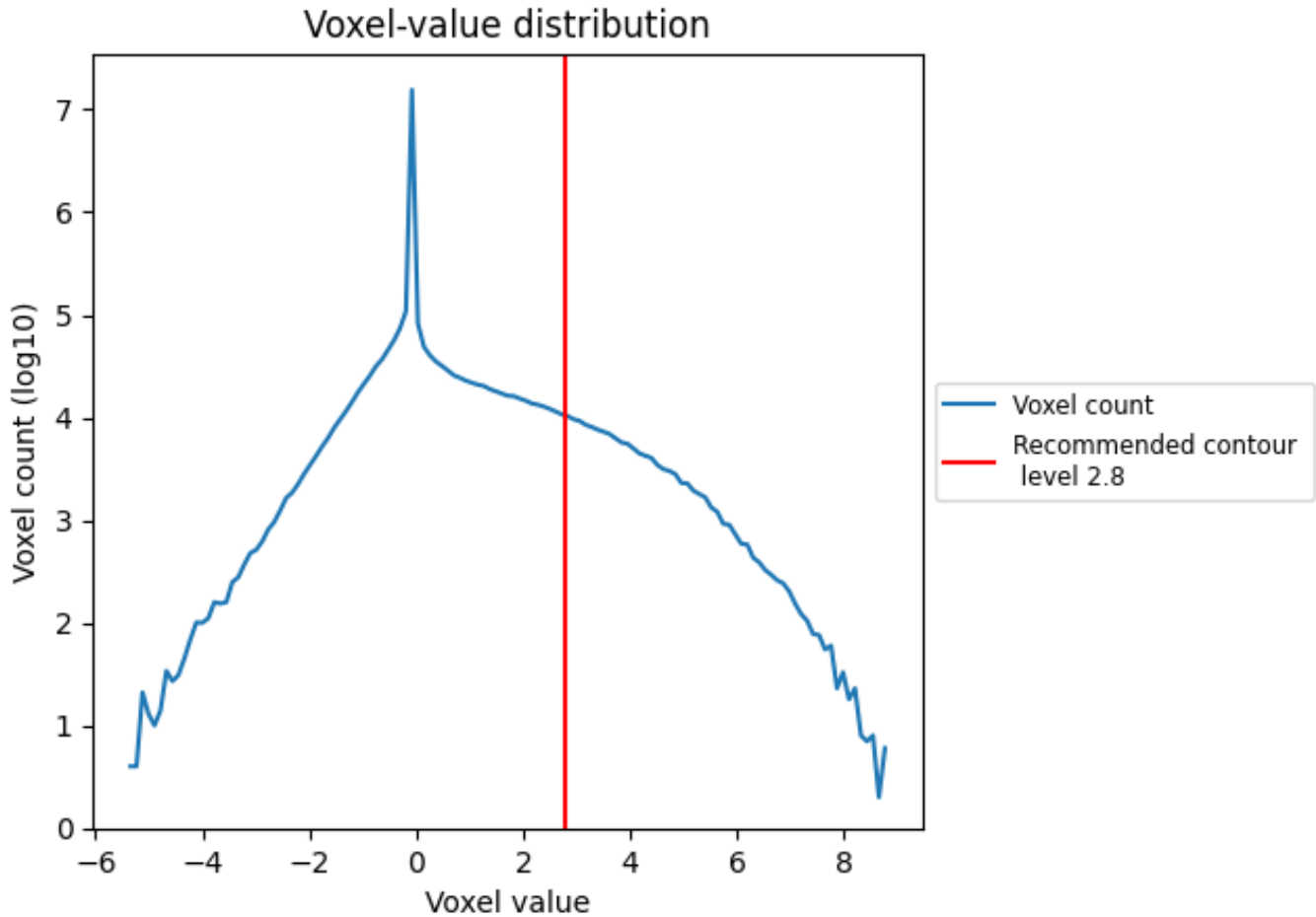
6.4 Mask visualisation [i](#)

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.

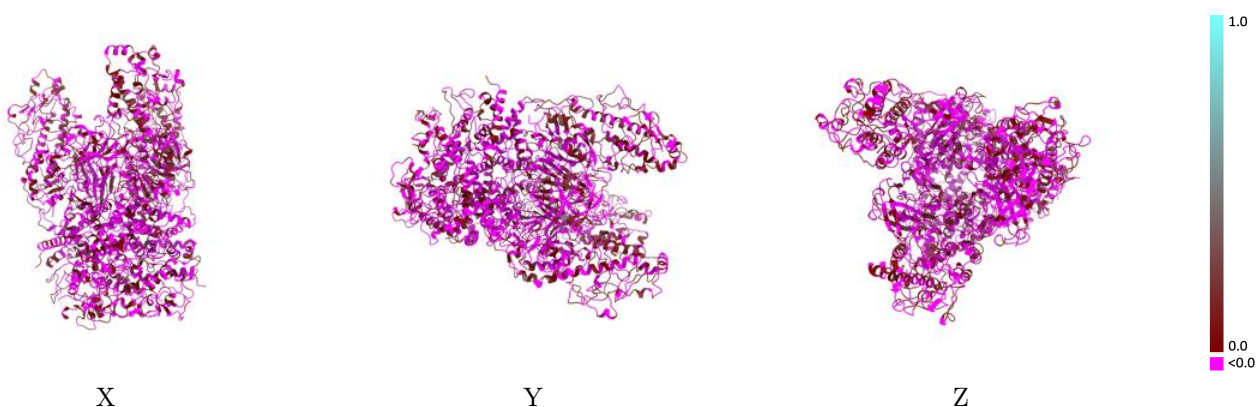
8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22164 and PDB model 6ZTY. Per-residue inclusion information can be found in section 3 on page 6.

8.1 Map-model overlay [i](#)

This section was not generated.

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

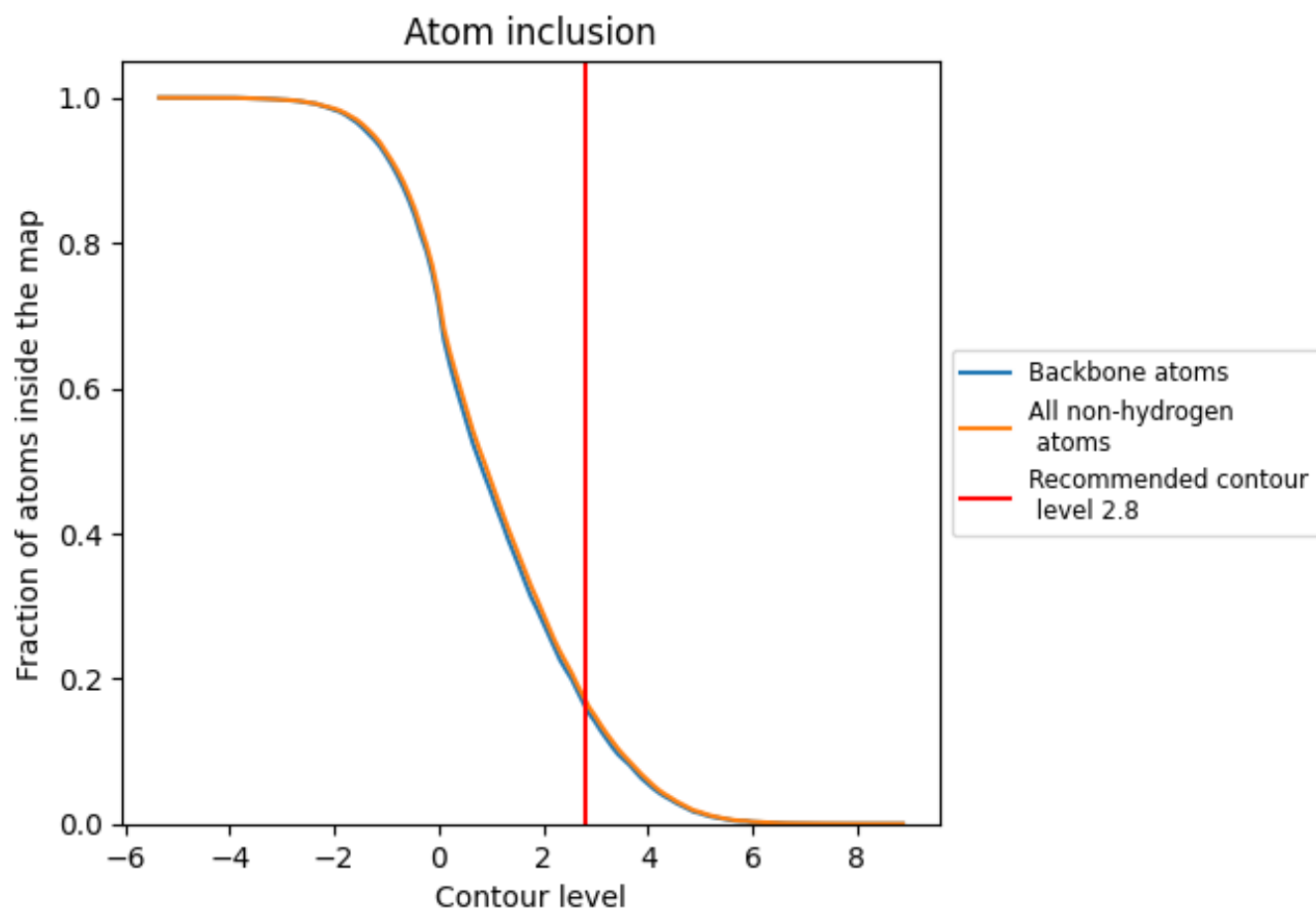


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 16% of all backbone atoms, 17% 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 (2.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.1705	 -0.0310
H	 0.1215	 -0.0480
I	 0.1224	 -0.0500
J	 0.1180	 -0.0490
U	 0.2790	 0.0190
V	 0.2461	 -0.0140
W	 0.2411	 -0.0030

