



## wwPDB EM Validation Summary Report ⓘ

Dec 10, 2022 – 08:12 am GMT

PDB ID : 5A9E  
EMDB ID : EMD-3101  
Title : Cryo-electron tomography and subtomogram averaging of Rous-Sarcoma-Virus deltaMBD virus-like particles  
Authors : Schur, F.K.M.; Dick, R.A.; Hagen, W.J.H.; Vogt, V.M.; Briggs, J.A.G.  
Deposited on : 2015-07-21  
Resolution : 7.70 Å(reported)

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>.

---

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

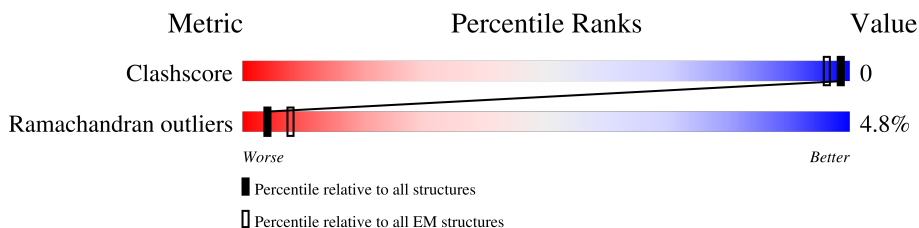
EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 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 7.70 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

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	495	 5% 46% 5% • 48%
1	B	495	 5% 46% • • 48%
1	C	495	 5% 47% • • 48%
1	D	495	 5% 45% 6% • 48%
1	E	495	 6% 46% • • 48%
1	F	495	 5% 46% 5% 48%
1	G	495	 6% 46% 5% • 48%
1	H	495	 7% 46% 5% • 48%
1	I	495	 7% 46% 5% • 48%

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	J	495	<p>7% 45% 6% 48%</p>
1	K	495	<p>6% 44% 6% 48%</p>
1	L	495	<p>7% 45% 5% 48%</p>
1	M	495	<p>5% 40% 5% 56%</p>
1	N	495	<p>5% 40% 5% 56%</p>
1	O	495	<p>5% 41% 5% 56%</p>
1	P	495	<p>5% 41% 5% 56%</p>
1	Q	495	<p>5% 40% 5% 56%</p>
1	R	495	<p>5% 40% 5% 56%</p>

## 2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 17406 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 DELTAMBD GAG PROTEIN.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	A	255	1019	510	255	254	0	0
1	B	255	1019	510	255	254	0	0
1	C	255	1019	510	255	254	0	0
1	D	255	1019	510	255	254	0	0
1	E	255	1019	510	255	254	0	0
1	F	255	1019	510	255	254	0	0
1	G	255	1019	510	255	254	0	0
1	H	255	1019	510	255	254	0	0
1	I	255	1019	510	255	254	0	0
1	J	255	1019	510	255	254	0	0
1	K	255	1019	510	255	254	0	0
1	L	255	1019	510	255	254	0	0
1	M	216	863	432	216	215	0	0
1	N	216	863	432	216	215	0	0
1	O	216	863	432	216	215	0	0
1	P	216	863	432	216	215	0	0
1	Q	216	863	432	216	215	0	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
1	R	216	Total 863	C 432	N 216	O 215	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	83	SER	-	expression tag	UNP P03322
A	573	GLN	PRO	conflict	UNP P03322
B	83	SER	-	expression tag	UNP P03322
B	573	GLN	PRO	conflict	UNP P03322
C	83	SER	-	expression tag	UNP P03322
C	573	GLN	PRO	conflict	UNP P03322
D	83	SER	-	expression tag	UNP P03322
D	573	GLN	PRO	conflict	UNP P03322
E	83	SER	-	expression tag	UNP P03322
E	573	GLN	PRO	conflict	UNP P03322
F	83	SER	-	expression tag	UNP P03322
F	573	GLN	PRO	conflict	UNP P03322
G	83	SER	-	expression tag	UNP P03322
G	573	GLN	PRO	conflict	UNP P03322
H	83	SER	-	expression tag	UNP P03322
H	573	GLN	PRO	conflict	UNP P03322
I	83	SER	-	expression tag	UNP P03322
I	573	GLN	PRO	conflict	UNP P03322
J	83	SER	-	expression tag	UNP P03322
J	573	GLN	PRO	conflict	UNP P03322
K	83	SER	-	expression tag	UNP P03322
K	573	GLN	PRO	conflict	UNP P03322
L	83	SER	-	expression tag	UNP P03322
L	573	GLN	PRO	conflict	UNP P03322
M	83	SER	-	expression tag	UNP P03322
M	573	GLN	PRO	conflict	UNP P03322
N	83	SER	-	expression tag	UNP P03322
N	573	GLN	PRO	conflict	UNP P03322
O	83	SER	-	expression tag	UNP P03322
O	573	GLN	PRO	conflict	UNP P03322
P	83	SER	-	expression tag	UNP P03322
P	573	GLN	PRO	conflict	UNP P03322
Q	83	SER	-	expression tag	UNP P03322
Q	573	GLN	PRO	conflict	UNP P03322
R	83	SER	-	expression tag	UNP P03322
R	573	GLN	PRO	conflict	UNP P03322



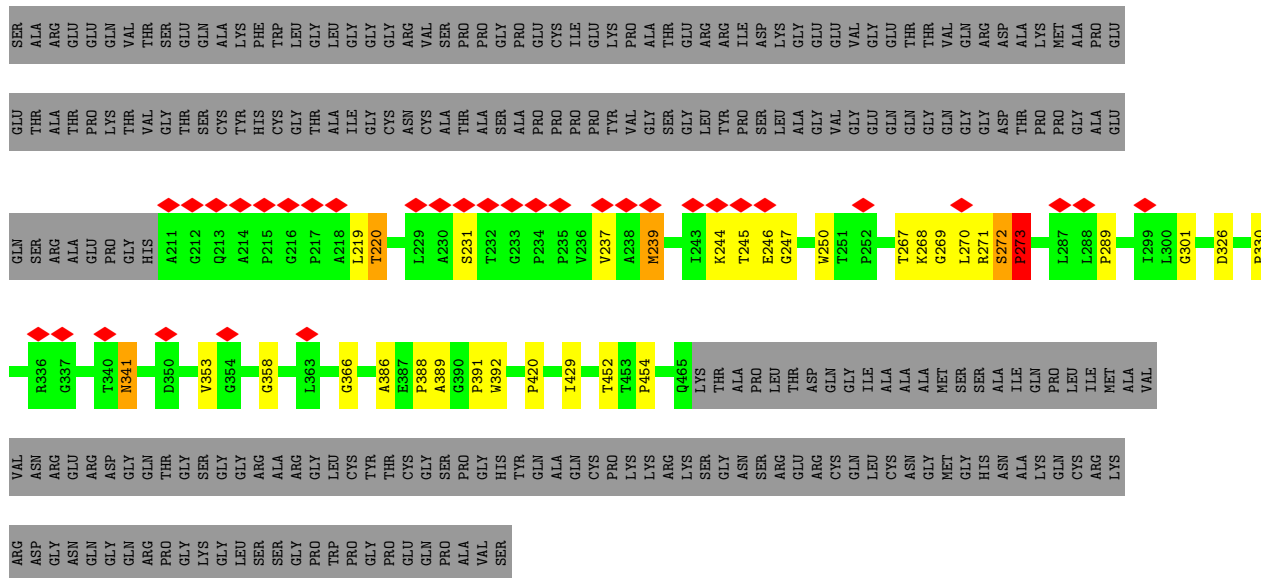




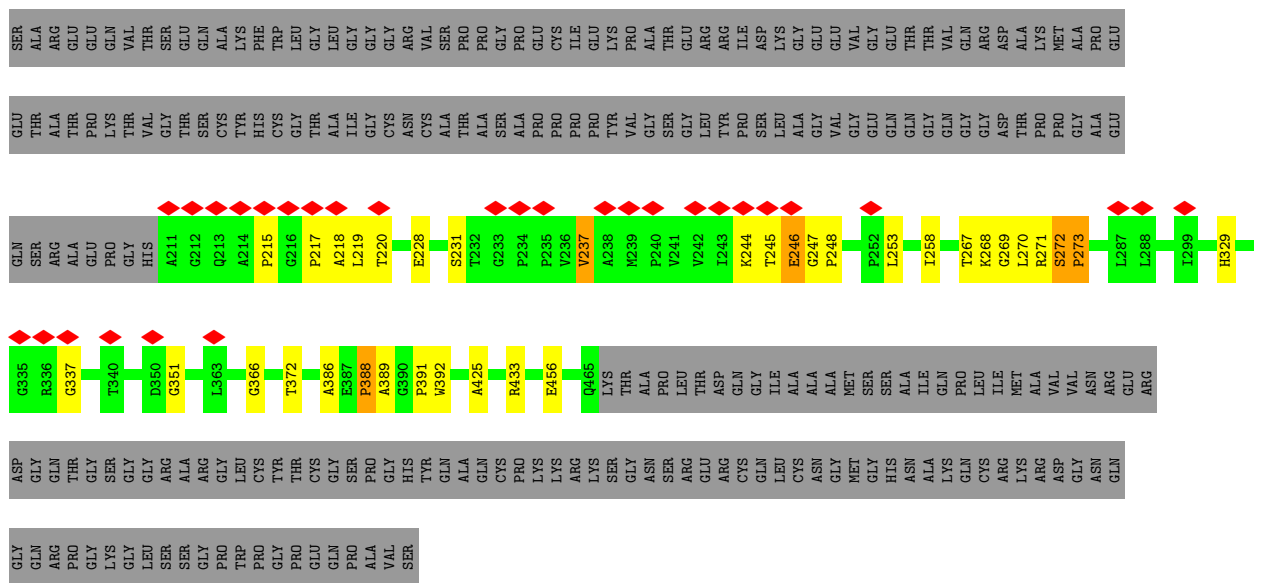
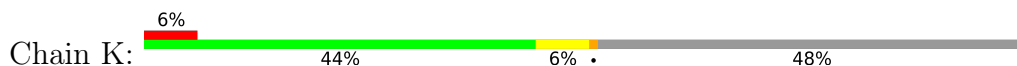




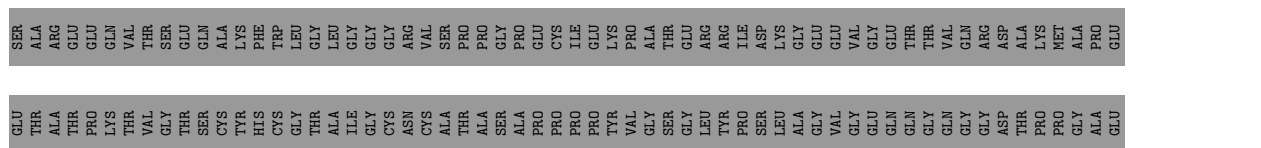
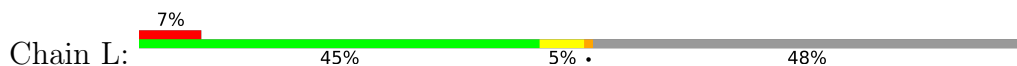
• Molecule 1: DELTAMBD GAG PROTEIN



• Molecule 1: DELTAMBD GAG PROTEIN



• Molecule 1: DELTAMBD GAG PROTEIN









## 4 Experimental information

Property	Value	Source
EM reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of tilted images used	8375	Depositor
Resolution determination method	Not provided	
CTF correction method	PHASE-FLIPPING OF INDIVIDUAL MICROGRAPHS	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	34	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	81000	Depositor
Image detector	GATAN MULTISCAN	Depositor
Maximum voxel value	8.247	Depositor
Minimum voxel value	-6.577	Depositor
Average voxel value	-0.000	Depositor
Voxel value standard deviation	0.761	Depositor
Recommended contour level	2.0	Depositor
Tomogram size ( $\text{\AA}$ )	248.4, 248.4, 248.4	wwPDB
Tomogram dimensions	120, 120, 120	wwPDB
Tomogram angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Grid spacing ( $\text{\AA}$ )	2.07, 2.07, 2.07	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	1.43	1/1018 (0.1%)	1.70	8/1271 (0.6%)
1	B	1.40	2/1018 (0.2%)	1.62	3/1271 (0.2%)
1	C	1.45	0/1018	1.64	3/1271 (0.2%)
1	D	1.44	4/1018 (0.4%)	1.73	14/1271 (1.1%)
1	E	1.44	3/1018 (0.3%)	1.60	4/1271 (0.3%)
1	F	1.46	1/1018 (0.1%)	1.70	9/1271 (0.7%)
1	G	1.44	0/1018	1.72	6/1271 (0.5%)
1	H	1.51	1/1018 (0.1%)	1.63	5/1271 (0.4%)
1	I	1.49	2/1018 (0.2%)	1.68	7/1271 (0.6%)
1	J	1.50	5/1018 (0.5%)	1.70	7/1271 (0.6%)
1	K	1.47	4/1018 (0.4%)	1.69	14/1271 (1.1%)
1	L	1.49	2/1018 (0.2%)	1.67	4/1271 (0.3%)
1	M	1.47	1/862 (0.1%)	1.65	6/1076 (0.6%)
1	N	1.42	2/862 (0.2%)	1.66	7/1076 (0.7%)
1	O	1.47	3/862 (0.3%)	1.63	2/1076 (0.2%)
1	P	1.39	0/862	1.62	6/1076 (0.6%)
1	Q	1.49	3/862 (0.3%)	1.65	5/1076 (0.5%)
1	R	1.42	2/862 (0.2%)	1.57	2/1076 (0.2%)
All	All	1.46	36/17388 (0.2%)	1.66	112/21708 (0.5%)

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	11
1	B	0	10
1	C	0	10
1	D	0	9
1	E	0	12
1	F	0	11
1	G	0	13

*Continued on next page...*

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	11
1	I	0	9
1	J	0	13
1	K	0	11
1	L	0	11
1	M	0	3
1	N	0	4
1	O	0	5
1	P	0	4
1	Q	0	6
1	R	0	5
All	All	0	158

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	390	GLY	CA-C	-6.71	1.41	1.51
1	R	437	GLN	C-N	6.15	1.46	1.34
1	A	301	GLY	C-N	-6.07	1.22	1.34
1	J	326	ASP	C-N	-6.00	1.22	1.34
1	Q	333	GLY	CA-C	-5.99	1.42	1.51

The worst 5 of 112 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	389	ALA	C-N-CA	7.78	138.63	122.30
1	H	217	PRO	C-N-CA	7.34	140.04	121.70
1	N	414	VAL	O-C-N	-7.06	111.41	122.70
1	P	330	PRO	N-CA-C	6.85	129.91	112.10
1	D	337	GLY	O-C-N	-6.65	112.06	122.70

There are no chirality outliers.

5 of 158 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	219	LEU	Peptide
1	A	220	THR	Peptide
1	A	221	ASP	Peptide
1	A	244	LYS	Peptide
1	A	245	THR	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	1019	0	266	1	0
1	B	1019	0	266	1	0
1	C	1019	0	266	0	0
1	D	1019	0	266	0	0
1	E	1019	0	266	0	0
1	F	1019	0	266	0	0
1	G	1019	0	266	0	0
1	H	1019	0	266	0	0
1	I	1019	0	266	0	0
1	J	1019	0	266	0	0
1	K	1019	0	266	0	0
1	L	1019	0	266	0	0
1	M	863	0	225	0	0
1	N	863	0	225	0	0
1	O	863	0	225	0	0
1	P	863	0	225	0	0
1	Q	863	0	225	0	0
1	R	863	0	225	0	0
All	All	17406	0	4542	2	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 0.

All (2) 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:382:VAL:C	1:B:384:ARG:H	2.21	0.43
1:A:351:GLY:O	1:A:358:GLY:HA3	2.20	0.42

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	253/495 (51%)	210 (83%)	28 (11%)	15 (6%)	1	17
1	B	253/495 (51%)	216 (85%)	25 (10%)	12 (5%)	2	21
1	C	253/495 (51%)	218 (86%)	20 (8%)	15 (6%)	1	17
1	D	253/495 (51%)	220 (87%)	22 (9%)	11 (4%)	2	22
1	E	253/495 (51%)	224 (88%)	18 (7%)	11 (4%)	2	22
1	F	253/495 (51%)	222 (88%)	20 (8%)	11 (4%)	2	22
1	G	253/495 (51%)	221 (87%)	17 (7%)	15 (6%)	1	17
1	H	253/495 (51%)	212 (84%)	27 (11%)	14 (6%)	2	19
1	I	253/495 (51%)	218 (86%)	20 (8%)	15 (6%)	1	17
1	J	253/495 (51%)	218 (86%)	19 (8%)	16 (6%)	1	17
1	K	253/495 (51%)	224 (88%)	16 (6%)	13 (5%)	2	19
1	L	253/495 (51%)	214 (85%)	22 (9%)	17 (7%)	1	15
1	M	214/495 (43%)	190 (89%)	17 (8%)	7 (3%)	4	26
1	N	214/495 (43%)	188 (88%)	17 (8%)	9 (4%)	3	22
1	O	214/495 (43%)	195 (91%)	11 (5%)	8 (4%)	3	24
1	P	214/495 (43%)	191 (89%)	18 (8%)	5 (2%)	6	34
1	Q	214/495 (43%)	188 (88%)	19 (9%)	7 (3%)	4	26
1	R	214/495 (43%)	191 (89%)	15 (7%)	8 (4%)	3	24
All	All	4320/8910 (48%)	3760 (87%)	351 (8%)	209 (5%)	4	21

5 of 209 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	246	GLU
1	A	267	THR
1	A	271	ARG
1	A	273	PRO

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	327	PRO

### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 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.

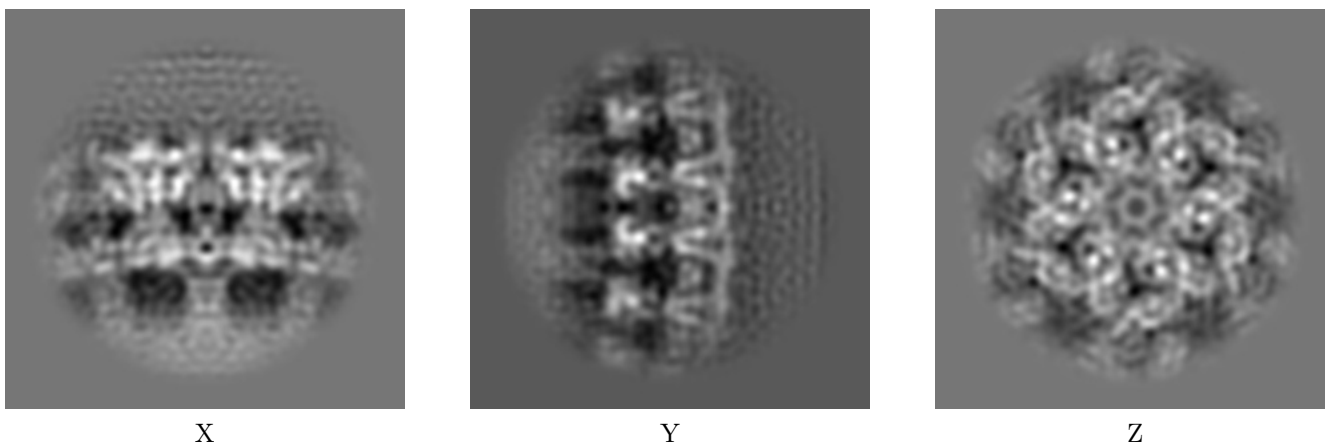
### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Tomogram visualisation [i](#)

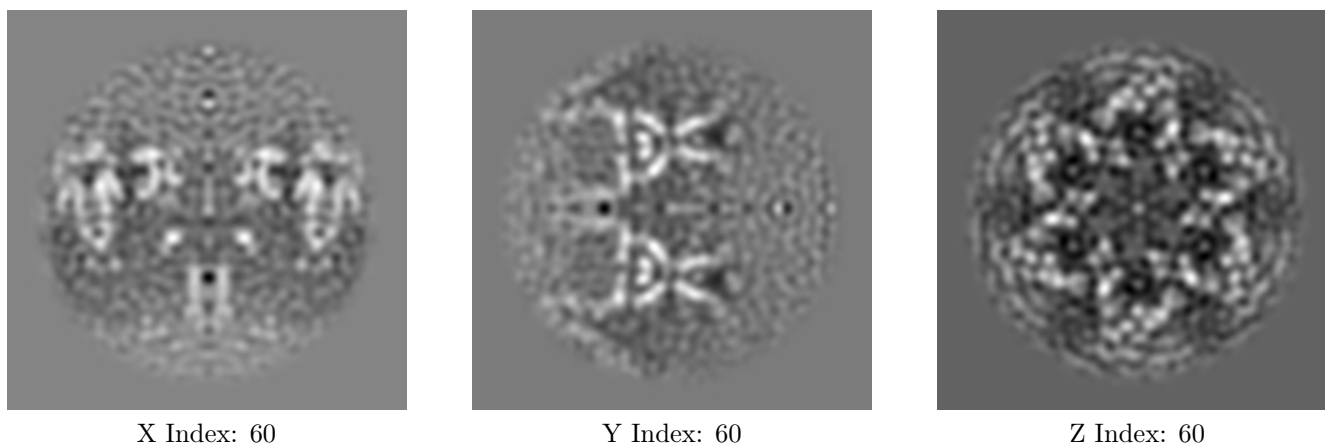
This section contains visualisations of the EMDB entry EMD-3101. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

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



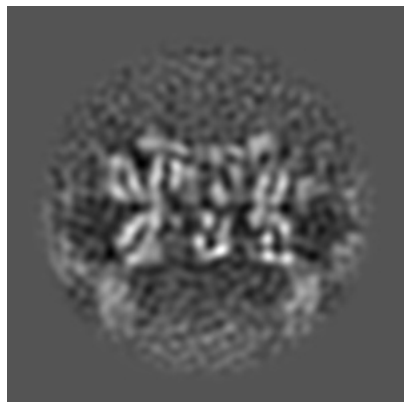
The images above show the tomogram projected in three orthogonal directions.

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

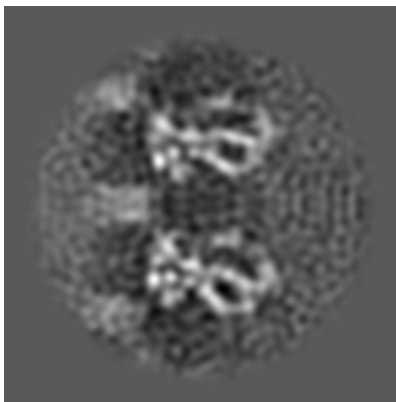


The images above show central slices of the tomogram in three orthogonal directions.

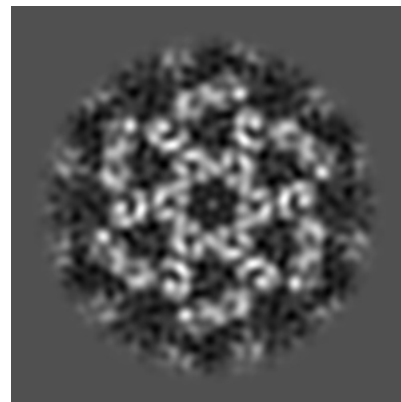
### 6.3 Largest variance slices [i](#)



X Index: 47



Y Index: 57



Z Index: 50

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

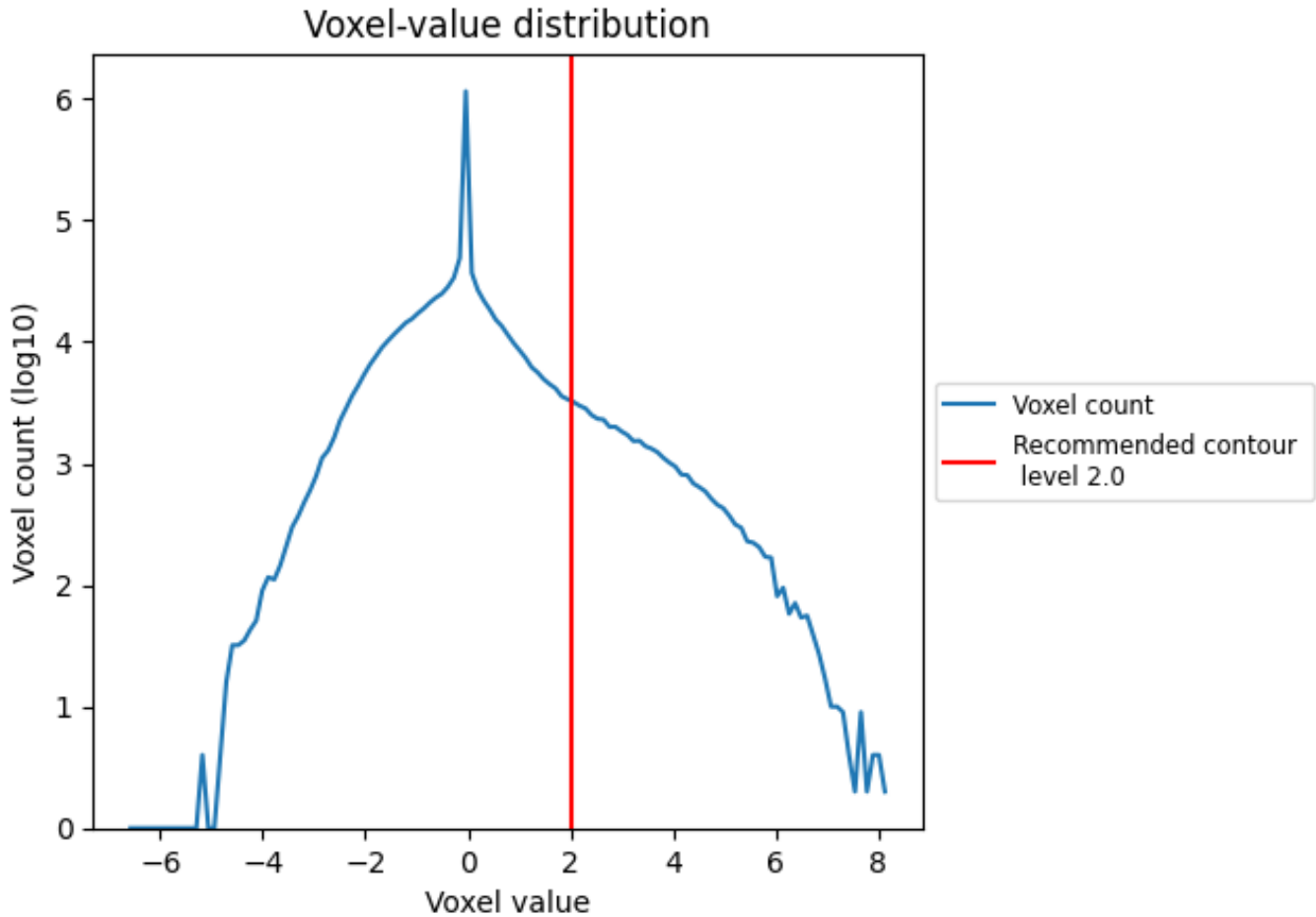
### 6.4 Mask visualisation [i](#)

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.

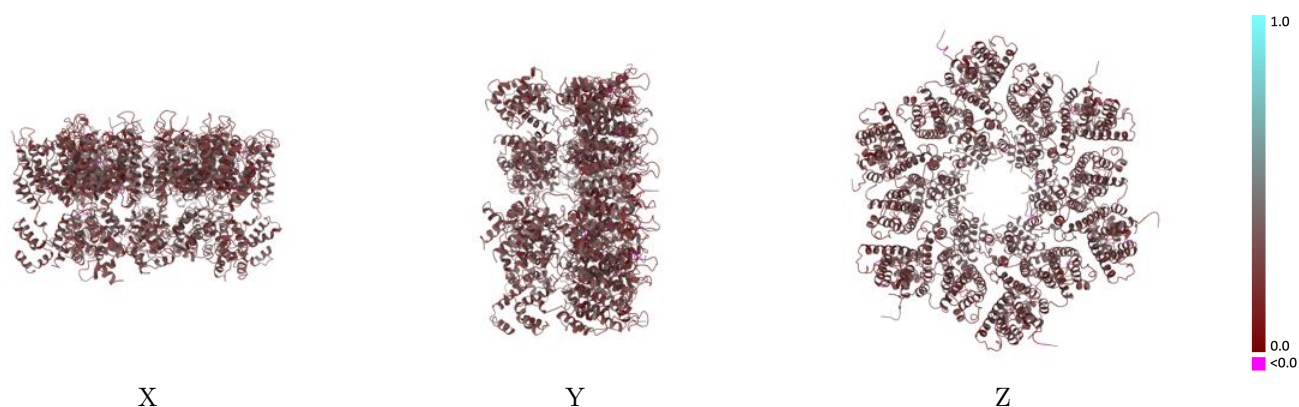
## 8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3101 and PDB model 5A9E. 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](#)

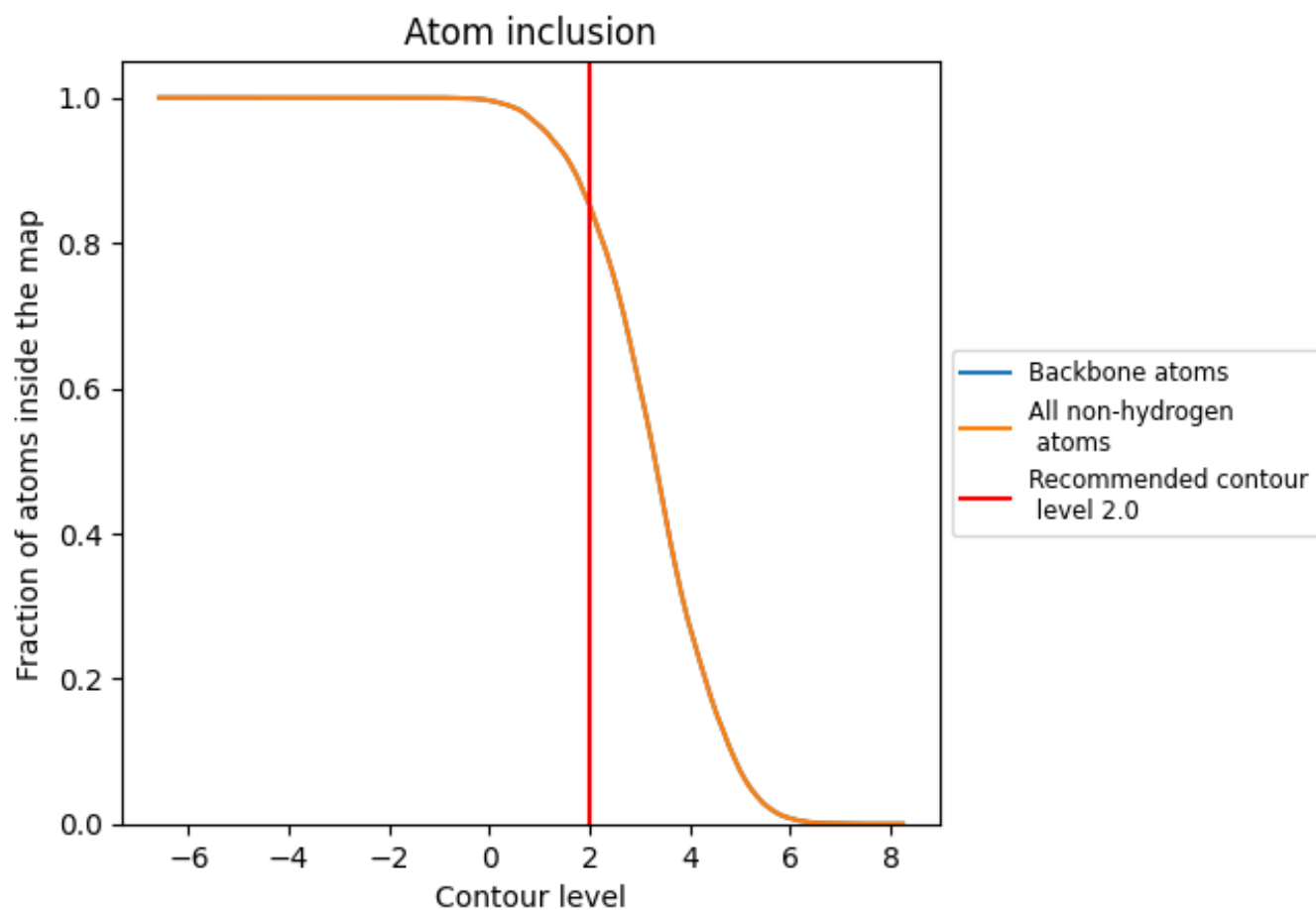


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 85% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.



## 8.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (2.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8522	 0.2840
A	 0.8754	 0.2960
B	 0.8675	 0.2980
C	 0.8763	 0.2960
D	 0.8665	 0.2920
E	 0.8665	 0.2920
F	 0.8665	 0.2930
G	 0.8351	 0.2850
H	 0.8391	 0.2810
I	 0.8283	 0.2790
J	 0.8371	 0.2800
K	 0.8400	 0.2860
L	 0.8381	 0.2760
M	 0.8436	 0.2780
N	 0.8343	 0.2730
O	 0.8679	 0.2750
P	 0.8563	 0.2740
Q	 0.8447	 0.2750
R	 0.8552	 0.2710

