



Full wwPDB EM Validation Report ⓘ

May 8, 2023 – 01:17 PM EDT

PDB ID : 8GBS
EMDB ID : EMD-29921
Title : Integrative model of the native Ana GV shell
Authors : Dutka, P.; Metskas, L.A.; Hurt, R.C.; Salahshoor, H.; Wang, T.U.; Malounda, D.; Lu, G.; Chou, T.F.; Shapiro, M.G.; Jensen, J.J.
Deposited on : 2023-02-28
Resolution : 8.00 Å(reported)
Based on initial model : 7R1C

This is a Full wwPDB EM Validation 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.dev50
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) : 2.32.2

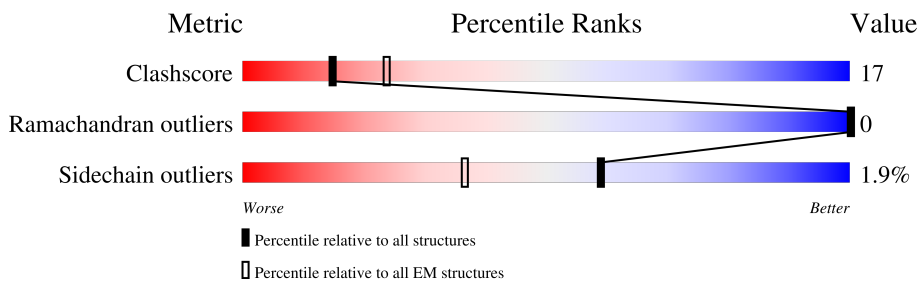
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 8.00 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 ≥ 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	A1	71	
1	A2	71	
1	A3	71	
1	A4	71	
2	C	33	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2121 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 Gas vesicle structural protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	A1	65	489	312	80	97	0	0
1	A2	65	489	312	80	97	0	0
1	A4	65	489	312	80	97	0	0
1	A3	65	489	312	80	97	0	0

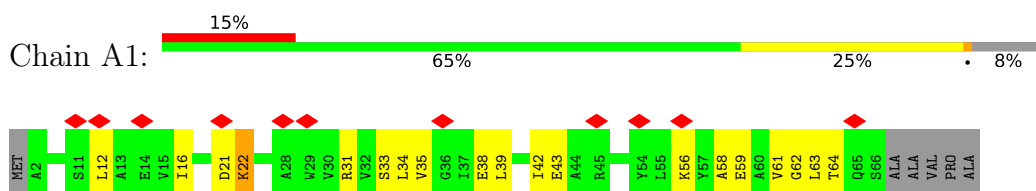
- Molecule 2 is a protein called Gas vesicle protein C.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	C	33	165	99	33	33	0	0

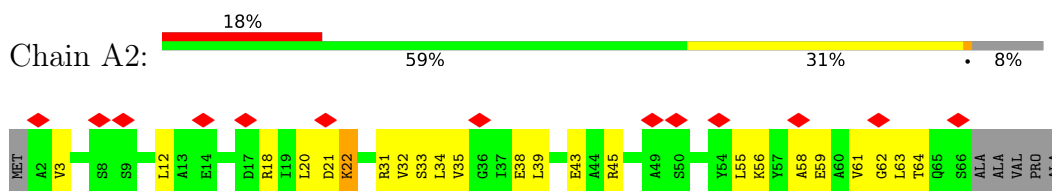
3 Residue-property plots [i](#)

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.

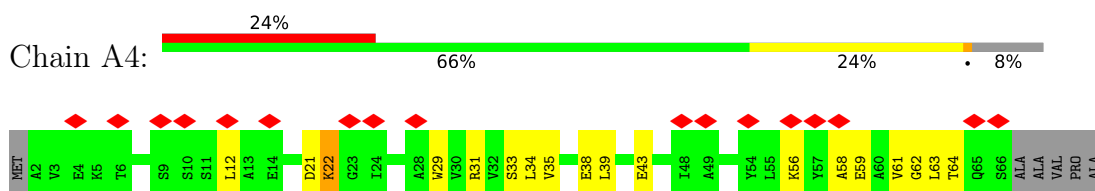
- Molecule 1: Gas vesicle structural protein



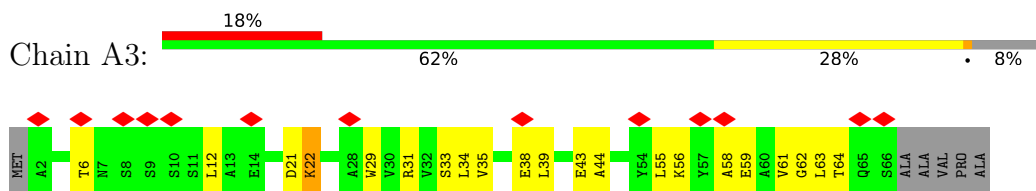
- Molecule 1: Gas vesicle structural protein



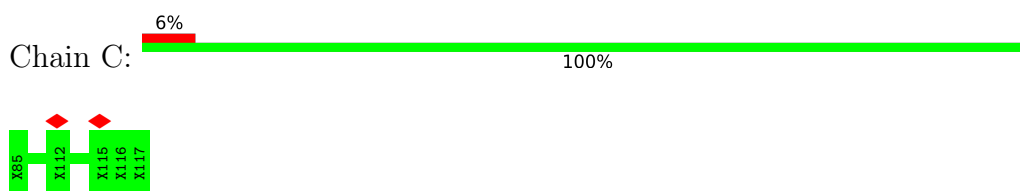
- Molecule 1: Gas vesicle structural protein



- Molecule 1: Gas vesicle structural protein



- Molecule 2: Gas vesicle protein C



4 Experimental information

Property	Value	Source
EM reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, Not provided	
Number of tilted images used	5874	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum voxel value	1.410	Depositor
Minimum voxel value	-0.796	Depositor
Average voxel value	0.019	Depositor
Voxel value standard deviation	0.116	Depositor
Recommended contour level	0.638	Depositor
Tomogram size (\AA)	300.286, 300.286, 300.286	wwPDB
Tomogram dimensions	178, 178, 178	wwPDB
Tomogram angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Grid spacing (\AA)	1.687, 1.687, 1.687	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	A1	0.24	0/492	0.54	0/668
1	A2	0.24	0/492	0.54	0/668
1	A3	0.24	0/492	0.54	0/668
1	A4	0.24	0/492	0.54	0/668
All	All	0.24	0/1968	0.54	0/2672

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	A1	489	0	511	16	0
1	A2	489	0	511	22	0
1	A3	489	0	511	25	0
1	A4	489	0	511	20	0
2	C	165	0	35	0	0
All	All	2121	0	2079	71	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 17.

All (71) 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:A4:56:LYS:HZ3	1:A3:55:LEU:HD11	1.31	0.92
1:A4:56:LYS:NZ	1:A3:55:LEU:HD11	2.08	0.67
1:A2:34:LEU:HD12	1:A2:35:VAL:HG12	1.85	0.59
1:A1:34:LEU:HD12	1:A1:35:VAL:HG12	1.85	0.59
1:A3:34:LEU:HD12	1:A3:35:VAL:HG12	1.85	0.59
1:A2:55:LEU:HD11	1:A3:56:LYS:HZ3	1.68	0.59
1:A4:34:LEU:HD12	1:A4:35:VAL:HG12	1.85	0.59
1:A1:58:ALA:HB1	1:A1:63:LEU:HB2	1.86	0.58
1:A3:58:ALA:HB1	1:A3:63:LEU:HB2	1.86	0.58
1:A2:58:ALA:HB1	1:A2:63:LEU:HB2	1.86	0.58
1:A4:58:ALA:HB1	1:A4:63:LEU:HB2	1.86	0.58
1:A1:33:SER:HA	1:A1:38:GLU:HA	1.87	0.57
1:A2:45:ARG:HG2	1:A3:29:TRP:CZ2	2.40	0.57
1:A1:21:ASP:OD1	1:A1:22:LYS:N	2.39	0.56
1:A2:21:ASP:OD1	1:A2:22:LYS:N	2.39	0.56
1:A4:21:ASP:OD1	1:A4:22:LYS:N	2.39	0.56
1:A3:21:ASP:OD1	1:A3:22:LYS:N	2.39	0.56
1:A2:33:SER:HA	1:A2:38:GLU:HA	1.87	0.55
1:A3:33:SER:HA	1:A3:38:GLU:HA	1.87	0.54
1:A4:33:SER:HA	1:A4:38:GLU:HA	1.87	0.54
1:A4:56:LYS:HZ2	1:A3:55:LEU:HD21	1.72	0.54
1:A1:31:ARG:HH12	1:A1:43:GLU:HB3	1.75	0.52
1:A4:59:GLU:HB3	1:A4:64:THR:HB	1.91	0.52
1:A3:59:GLU:HB3	1:A3:64:THR:HB	1.91	0.51
1:A2:59:GLU:HB3	1:A2:64:THR:HB	1.91	0.51
1:A1:59:GLU:HB3	1:A1:64:THR:HB	1.91	0.51
1:A4:31:ARG:HH12	1:A4:43:GLU:HB3	1.75	0.51
1:A3:31:ARG:HH12	1:A3:43:GLU:HB3	1.75	0.51
1:A2:3:VAL:HG21	1:A3:6:THR:HG22	1.93	0.51
1:A2:31:ARG:HH12	1:A2:43:GLU:HB3	1.75	0.50
1:A2:61:VAL:HG23	1:A2:63:LEU:HD23	1.95	0.49
1:A3:61:VAL:HG23	1:A3:63:LEU:HD23	1.94	0.49
1:A4:61:VAL:HG23	1:A4:63:LEU:HD23	1.95	0.49
1:A1:61:VAL:HG23	1:A1:63:LEU:HD23	1.94	0.49
1:A2:20:LEU:HG	1:A3:22:LYS:HZ3	1.79	0.47
1:A4:39:LEU:HD23	1:A4:39:LEU:H	1.79	0.47
1:A3:39:LEU:HD23	1:A3:39:LEU:H	1.79	0.47
1:A2:39:LEU:HD23	1:A2:39:LEU:H	1.79	0.47
1:A1:39:LEU:H	1:A1:39:LEU:HD23	1.79	0.46
1:A4:58:ALA:O	1:A4:63:LEU:N	2.48	0.46
1:A3:58:ALA:O	1:A3:63:LEU:N	2.48	0.46
1:A1:58:ALA:O	1:A1:63:LEU:N	2.48	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:16:ILE:HD12	1:A2:18:ARG:HH12	1.81	0.45
1:A2:20:LEU:HG	1:A3:22:LYS:NZ	2.31	0.45
1:A1:12:LEU:H	1:A1:12:LEU:HD23	1.82	0.45
1:A4:12:LEU:H	1:A4:12:LEU:HD23	1.82	0.44
1:A1:58:ALA:O	1:A1:62:GLY:N	2.50	0.44
1:A2:58:ALA:O	1:A2:62:GLY:N	2.50	0.44
1:A3:58:ALA:O	1:A3:62:GLY:N	2.50	0.44
1:A3:12:LEU:H	1:A3:12:LEU:HD23	1.82	0.44
1:A4:58:ALA:O	1:A4:62:GLY:N	2.50	0.44
1:A4:56:LYS:HE3	1:A4:56:LYS:HB3	1.82	0.44
1:A2:58:ALA:O	1:A2:63:LEU:N	2.48	0.44
1:A3:56:LYS:HE3	1:A3:56:LYS:HB3	1.82	0.44
1:A2:12:LEU:H	1:A2:12:LEU:HD23	1.82	0.44
1:A4:58:ALA:HA	1:A4:61:VAL:HG22	2.02	0.42
1:A3:58:ALA:HA	1:A3:61:VAL:HG22	2.02	0.42
1:A1:34:LEU:HD23	1:A1:39:LEU:HD22	2.02	0.41
1:A4:56:LYS:NZ	1:A3:55:LEU:HD21	2.34	0.41
1:A4:29:TRP:CH2	1:A3:44:ALA:HA	2.55	0.41
1:A2:34:LEU:HD23	1:A2:39:LEU:HD22	2.03	0.41
1:A2:58:ALA:HA	1:A2:61:VAL:HG22	2.02	0.41
1:A3:34:LEU:HD23	1:A3:39:LEU:HD22	2.02	0.41
1:A4:34:LEU:HD23	1:A4:39:LEU:HD22	2.02	0.41
1:A1:56:LYS:HA	1:A1:59:GLU:HG2	2.03	0.41
1:A4:56:LYS:HA	1:A4:59:GLU:HG2	2.03	0.41
1:A1:42:ILE:HD12	1:A2:32:VAL:HG22	2.02	0.41
1:A2:56:LYS:HA	1:A2:59:GLU:HG2	2.03	0.41
1:A3:56:LYS:HA	1:A3:59:GLU:HG2	2.03	0.40
1:A1:58:ALA:HA	1:A1:61:VAL:HG22	2.02	0.40
1:A2:56:LYS:HB3	1:A2:56:LYS:HE3	1.82	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	A1	63/71 (89%)	61 (97%)	2 (3%)	0	100	100
1	A2	63/71 (89%)	61 (97%)	2 (3%)	0	100	100
1	A3	63/71 (89%)	61 (97%)	2 (3%)	0	100	100
1	A4	63/71 (89%)	61 (97%)	2 (3%)	0	100	100
All	All	252/284 (89%)	244 (97%)	8 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	A1	53/57 (93%)	52 (98%)	1 (2%)	57	75
1	A2	53/57 (93%)	52 (98%)	1 (2%)	57	75
1	A3	53/57 (93%)	52 (98%)	1 (2%)	57	75
1	A4	53/57 (93%)	52 (98%)	1 (2%)	57	75
All	All	212/228 (93%)	208 (98%)	4 (2%)	59	75

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A1	22	LYS
1	A2	22	LYS
1	A4	22	LYS
1	A3	22	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A2	7	ASN
1	A3	7	ASN

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](#)

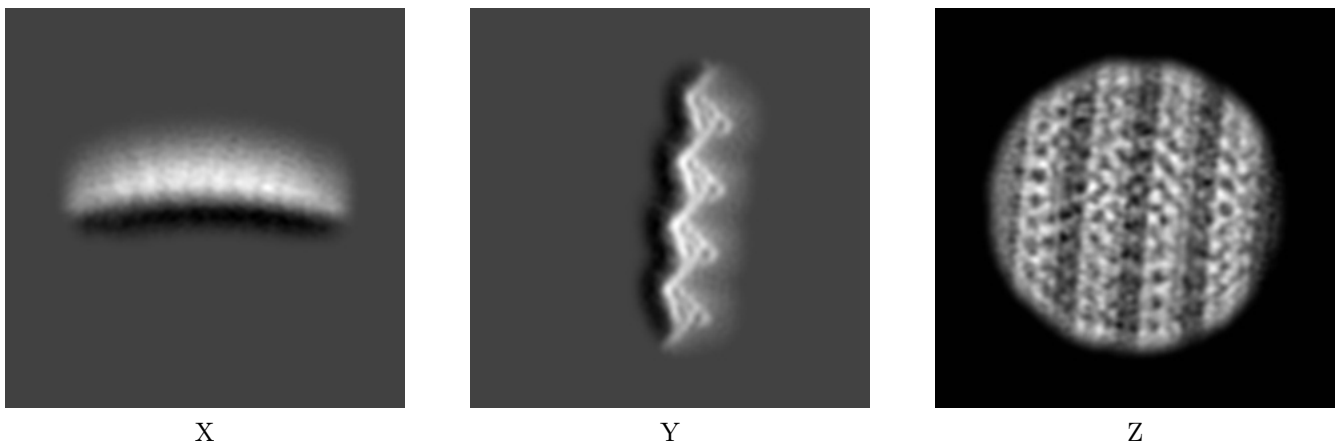
There are no chain breaks in this entry.

6 Tomogram visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29921. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

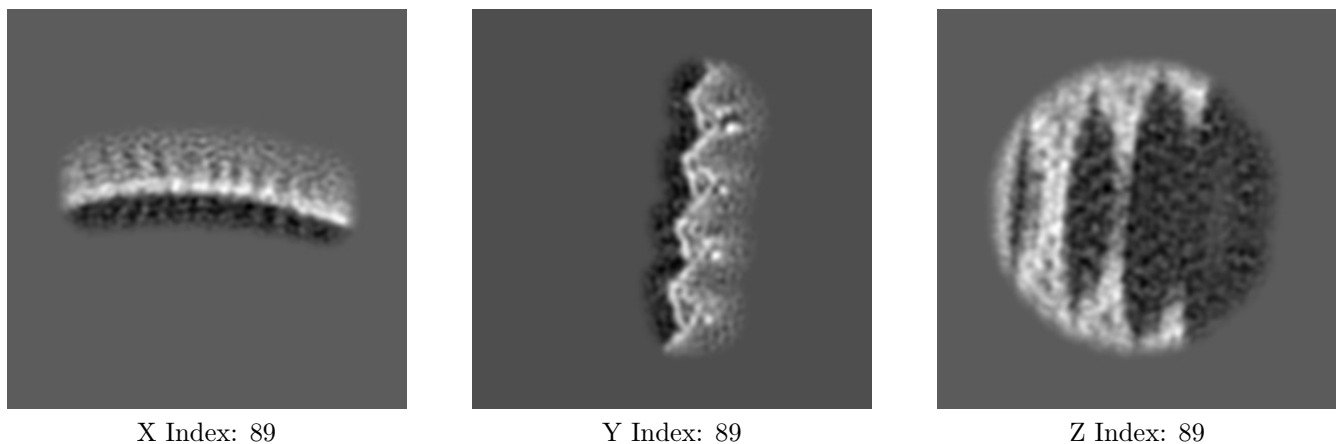
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)



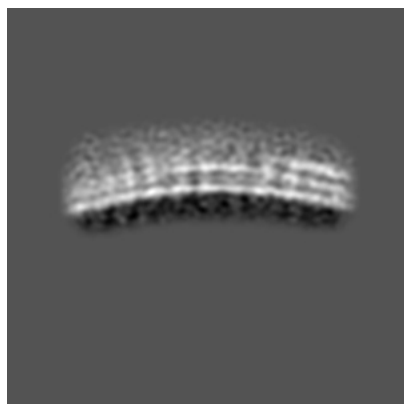
The images above show the tomogram projected in three orthogonal directions.

6.2 Central slices [i](#)

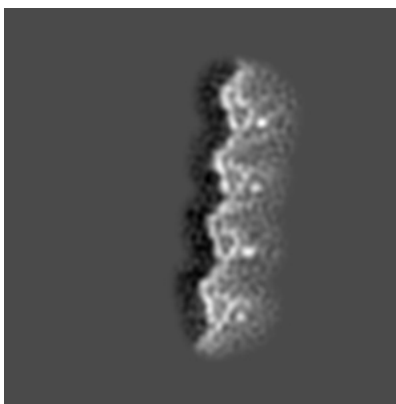


The images above show central slices of the tomogram in three orthogonal directions.

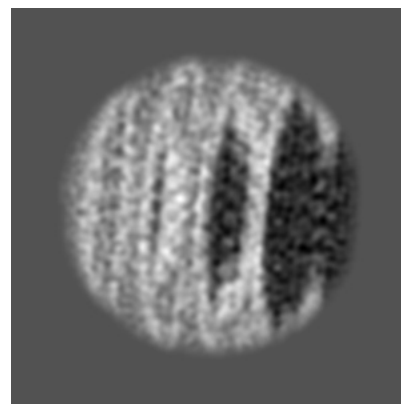
6.3 Largest variance slices [i](#)



X Index: 102



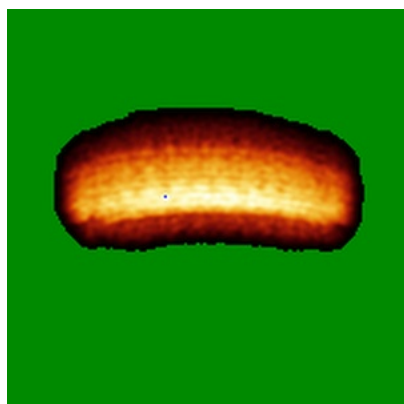
Y Index: 96



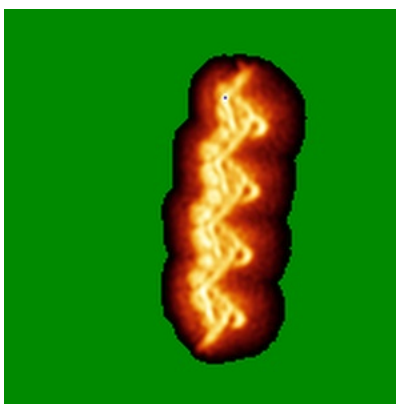
Z Index: 94

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

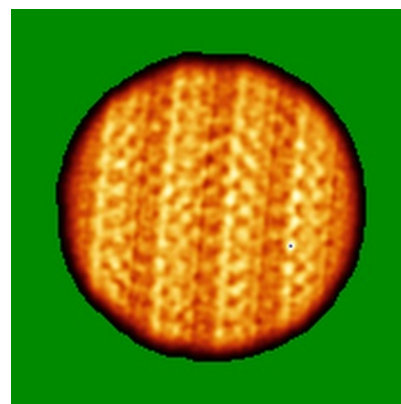
6.4 Orthogonal standard-deviation projections (False-color) [i](#)



X



Y



Z

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

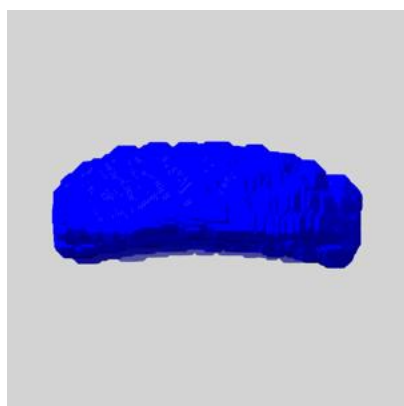
6.5 Mask visualisation [i](#)

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

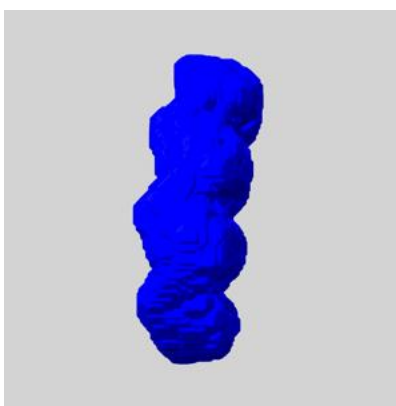
A mask typically either:

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

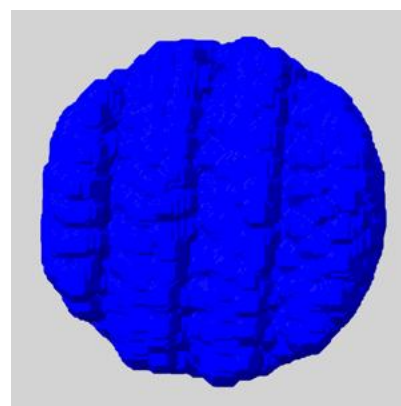
6.5.1 emd_29921_msk_1.map [i](#)



X



Y

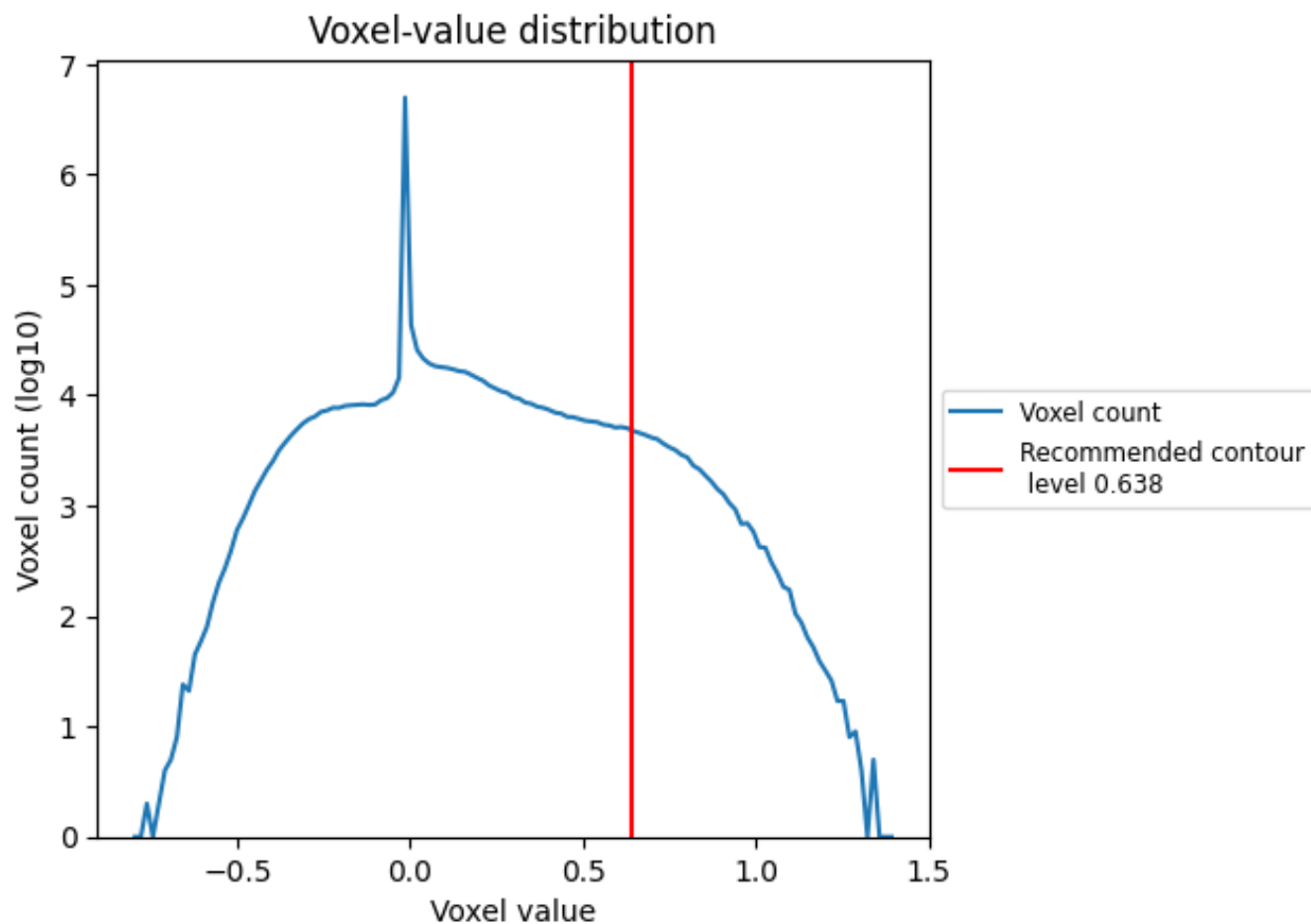


Z

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.

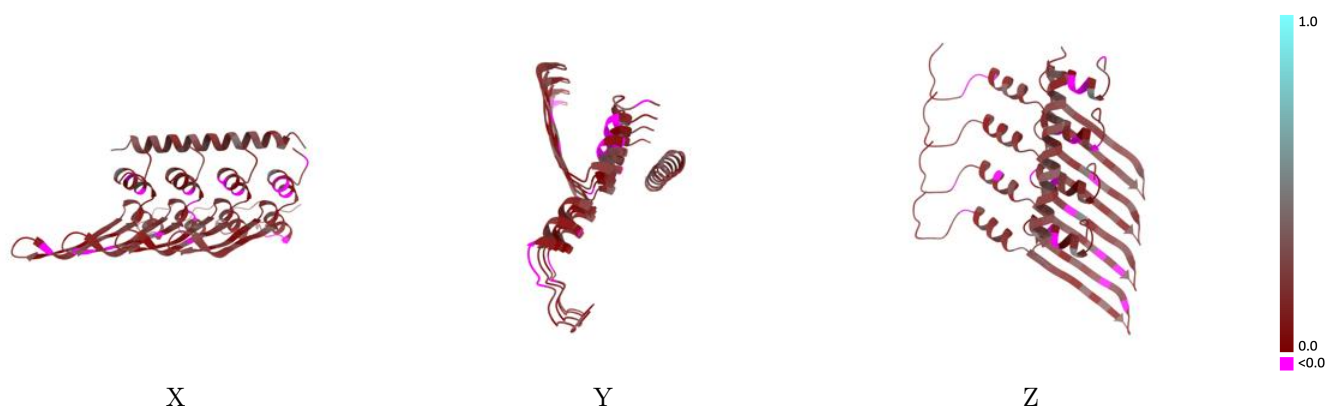
8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-29921 and PDB model 8GBS. 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](#)

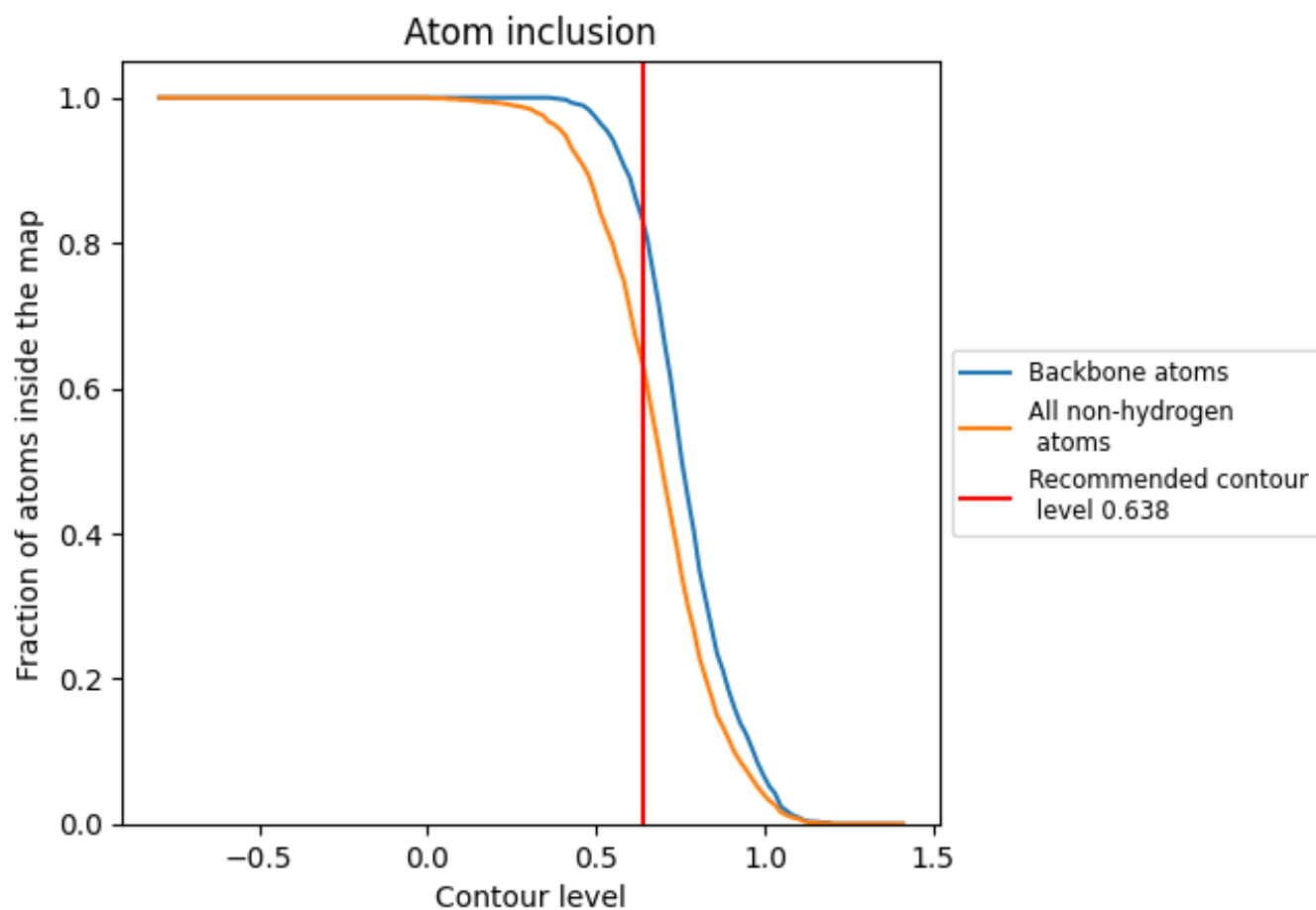


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 63% 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 (0.638) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6330	 0.1600
A1	 0.6150	 0.1480
A2	 0.6330	 0.1560
A3	 0.6060	 0.1510
A4	 0.6000	 0.1470
C	 0.8610	 0.2730

