



wwPDB EM Validation Summary Report ⓘ

Nov 21, 2022 – 07:06 PM JST

PDB ID : 7DAG
EMDB ID : EMD-30625
Title : Vibrio cholera aldehyde-alcohol dehydrogenase
Authors : Cho, S.; Cho, C.; Song, J.; Kim, G.
Deposited on : 2020-10-16
Resolution : 4.37 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

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

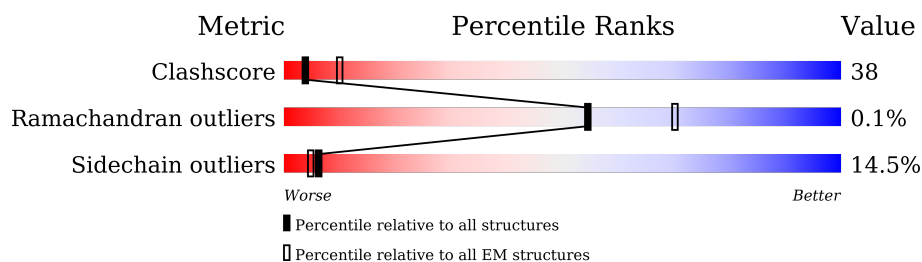
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.37 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	A	894	<div> <div>71%</div> <div>36% 50% 10% ..</div> </div>
1	B	894	<div> <div>55%</div> <div>36% 50% 10% ..</div> </div>
1	C	894	<div> <div>13%</div> <div>36% 49% 10% ..</div> </div>
1	D	894	<div> <div>12%</div> <div>36% 49% 10% ..</div> </div>
1	E	894	<div> <div>31%</div> <div>36% 50% 10% ..</div> </div>
1	F	894	<div> <div>38%</div> <div>36% 49% 10% ..</div> </div>
1	G	894	<div> <div>40%</div> <div>20% 26% 53%</div> </div>
1	H	894	<div> <div>48%</div> <div>28% 22% 50%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 45976 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.

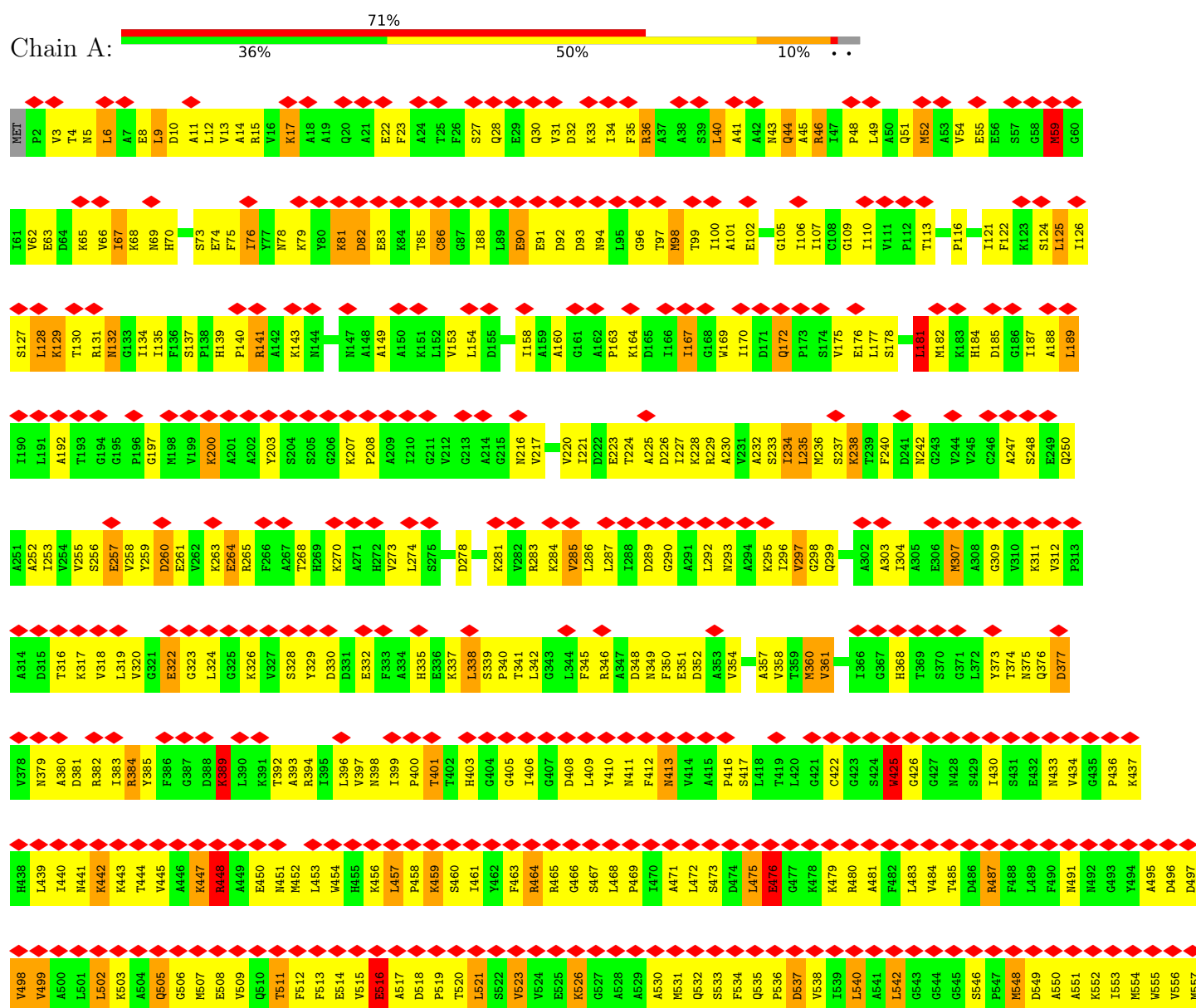
- Molecule 1 is a protein called Aldehyde-alcohol dehydrogenase.

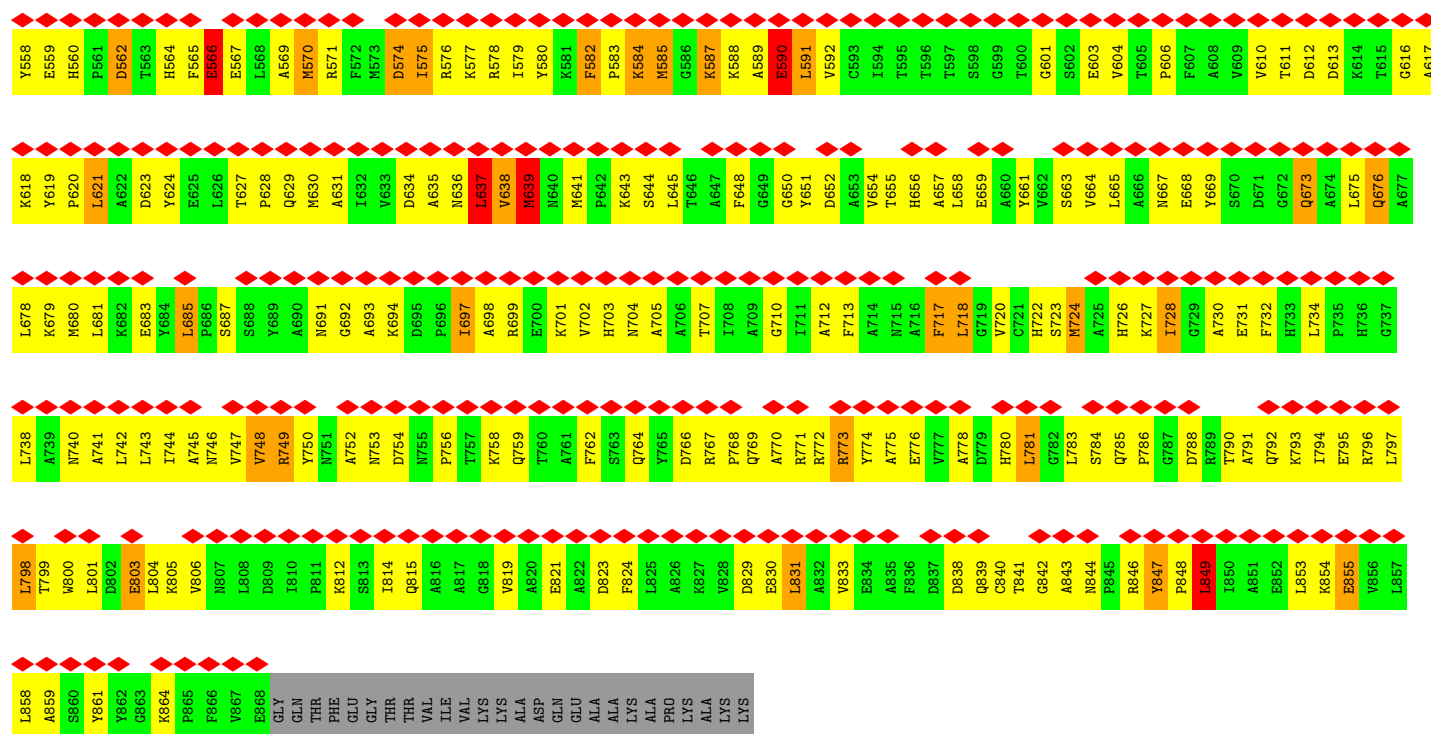
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	867	Total	C	N	O	S	0	0
			6568	4174	1119	1246	29		
1	B	867	Total	C	N	O	S	0	0
			6568	4174	1119	1246	29		
1	C	867	Total	C	N	O	S	0	0
			6568	4174	1119	1246	29		
1	D	867	Total	C	N	O	S	0	0
			6568	4174	1119	1246	29		
1	E	867	Total	C	N	O	S	0	0
			6568	4174	1119	1246	29		
1	F	867	Total	C	N	O	S	0	0
			6568	4174	1119	1246	29		
1	G	419	Total	C	N	O	S	0	0
			3250	2078	547	608	17		
1	H	448	Total	C	N	O	S	0	0
			3318	2096	572	638	12		

3 Residue-property plots

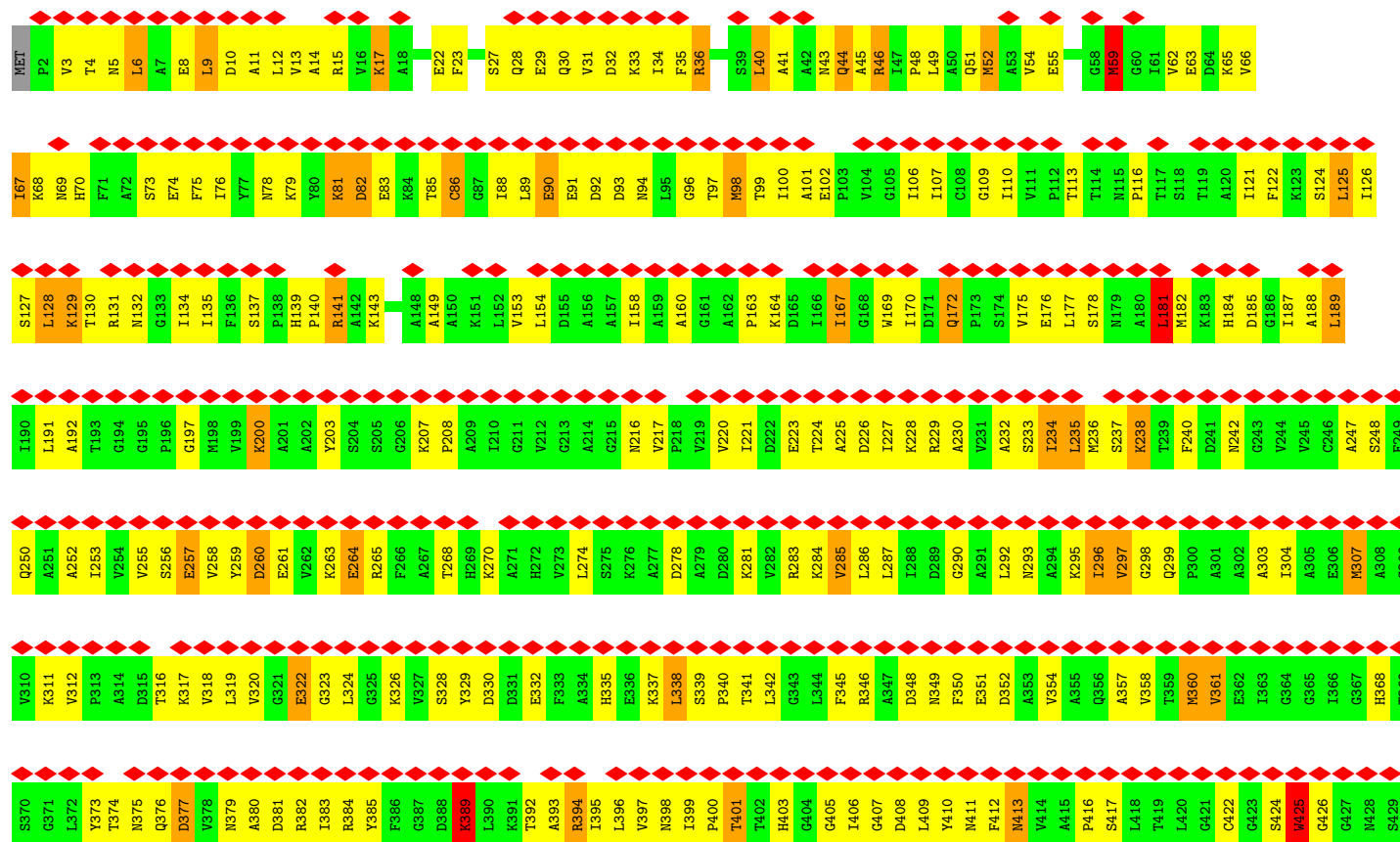
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

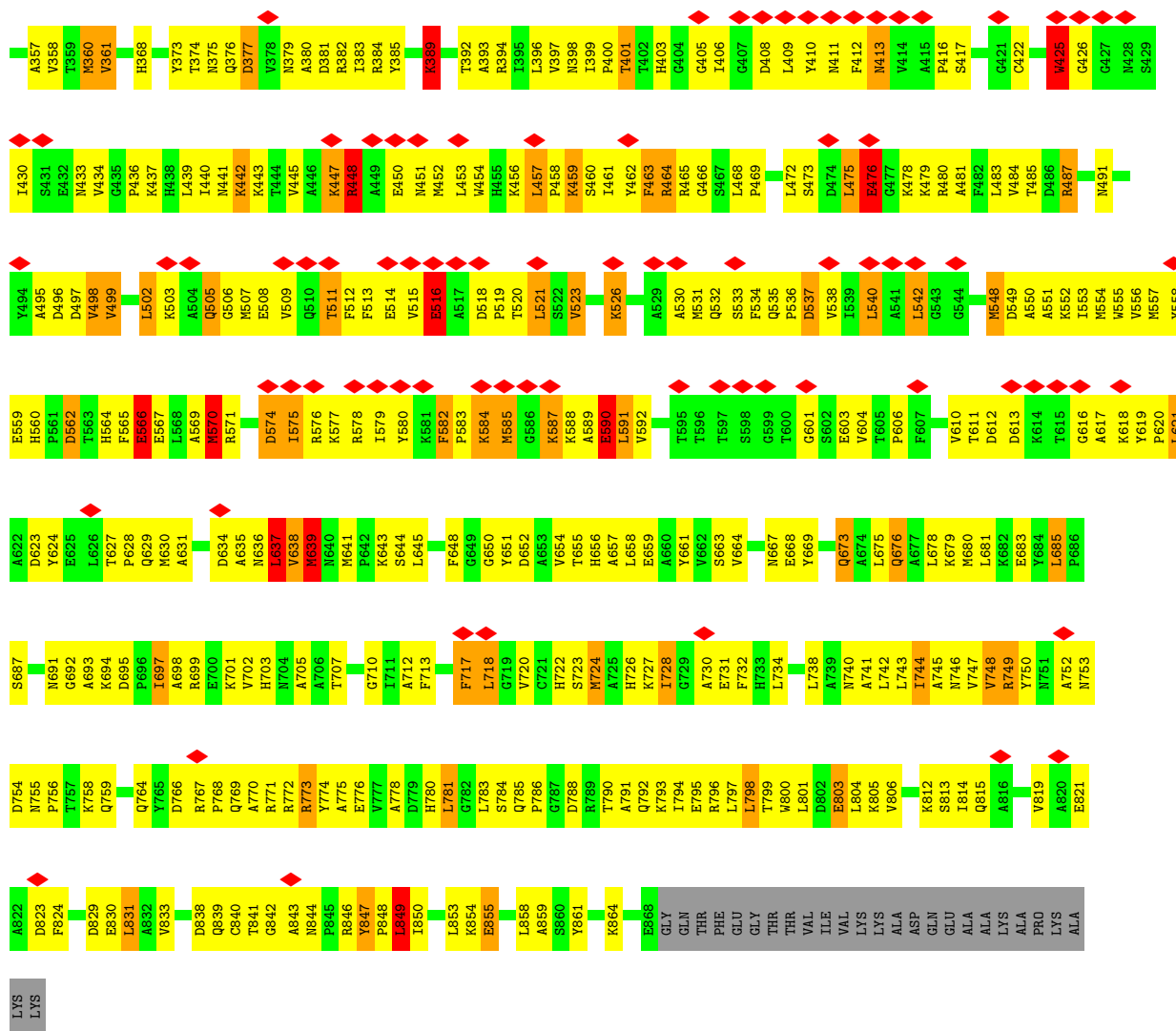
• Molecule 1: Aldehyde-alcohol dehydrogenase



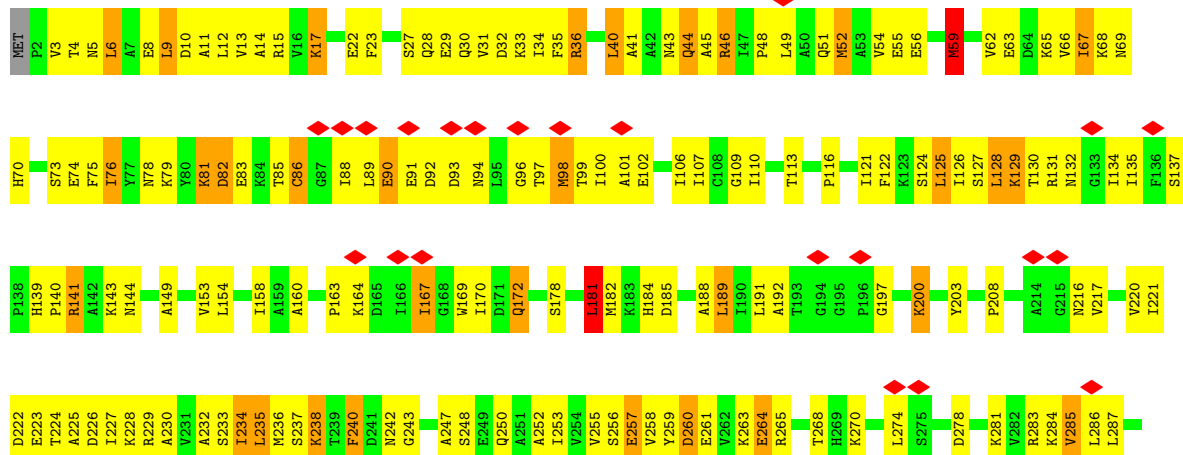


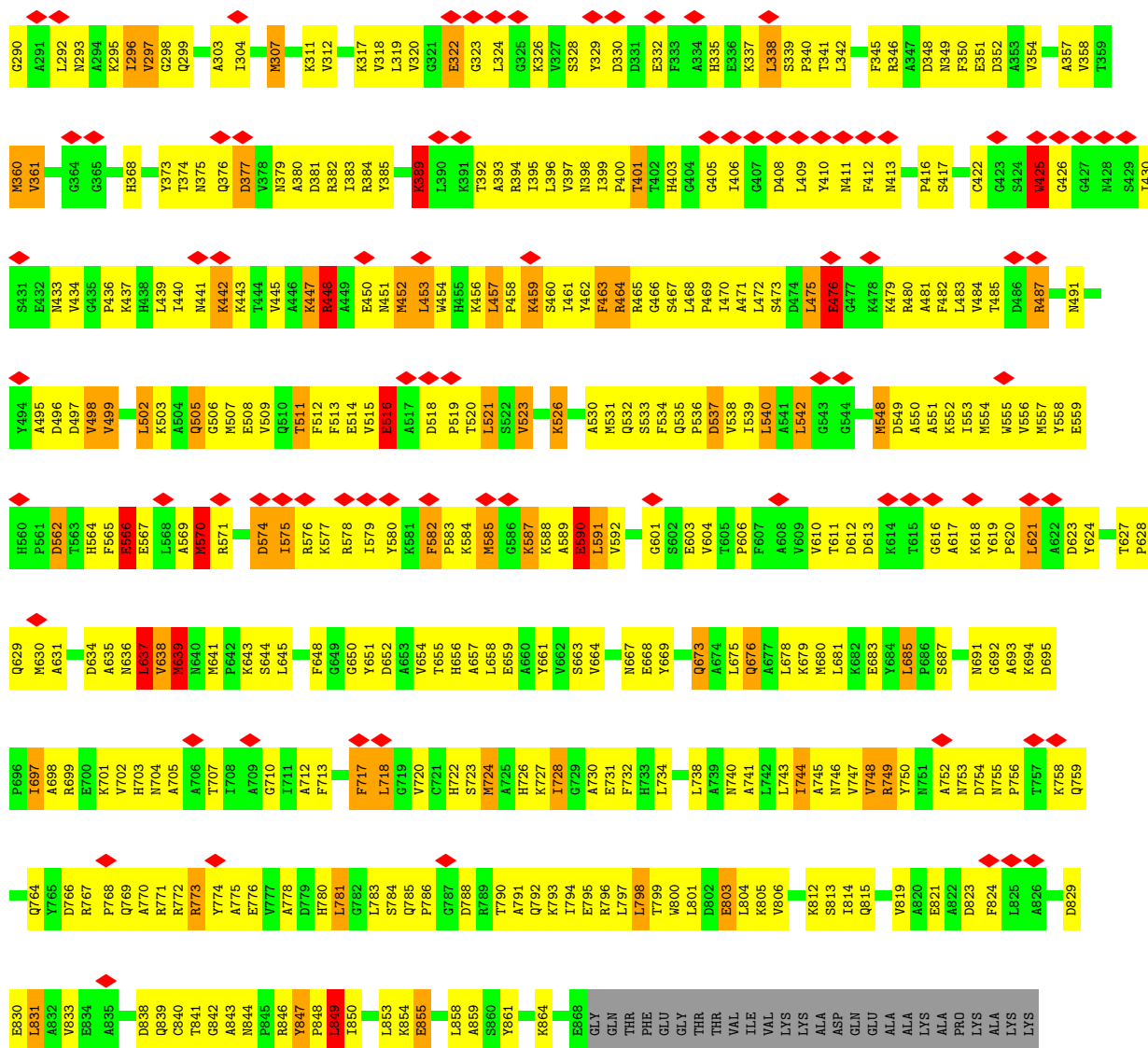
• Molecule 1: Aldehyde-alcohol dehydrogenase



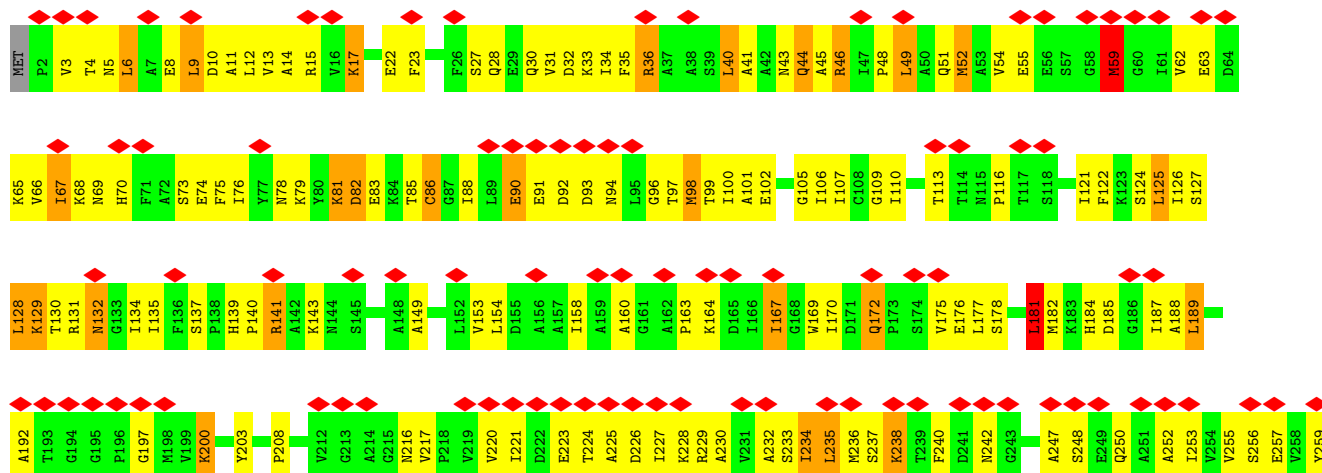


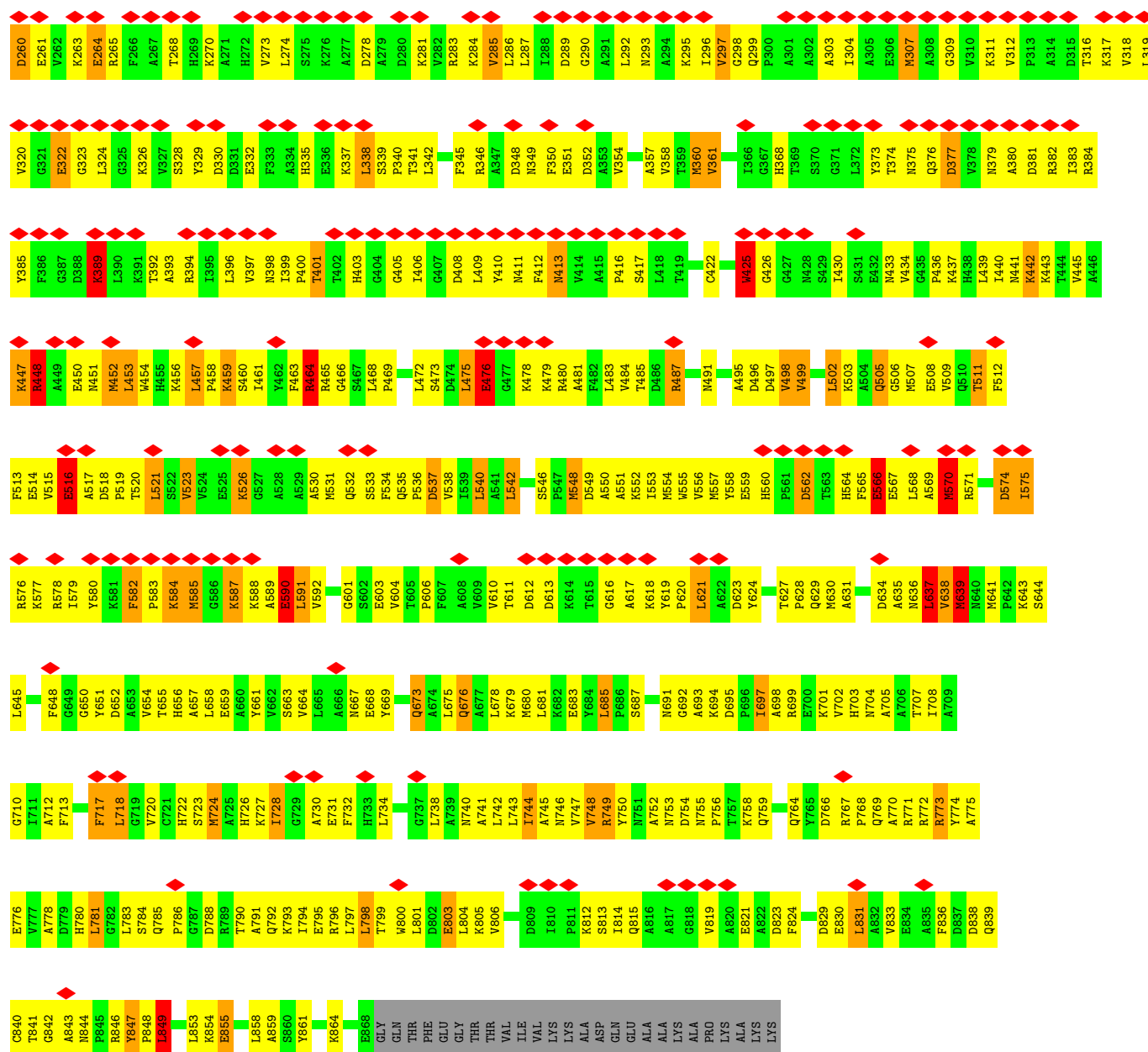
• Molecule 1: Aldehyde-alcohol dehydrogenase



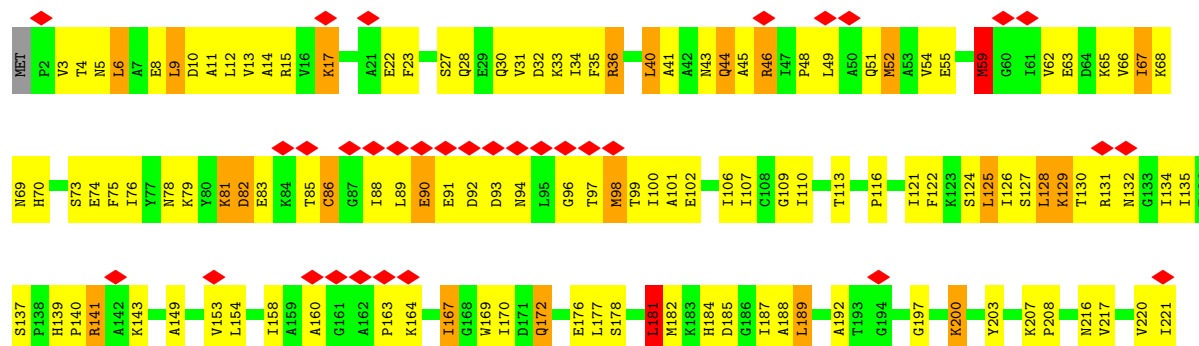


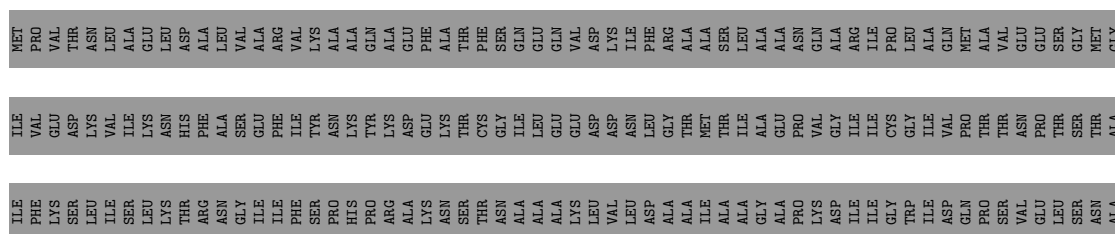
• Molecule 1: Aldehyde-alcohol dehydrogenase





● Molecule 1: Aldehyde-alcohol dehydrogenase





- Molecule 1: Aldehyde-alcohol dehydrogenase

	I61	P2	V3	T4	N5	L6	A7	E8	L9	D10	A11	L12	V13	A14	R15	V16	K17	A18	A19	Q20	A21	E22	F23	A24	T25	F26	S27	Q28	E29	Q30	V31	D32	K33	T34	F35	R36	A37	A38	S39	L40	A41	A42	M43	Q44	A45	R46	I47	P48	L49	A50	Q51	M52	A53	V54	E55	E56	S57	G58	M59	A60
	V62	E63	D64	K65	V66	I67	K68	N69	H70	F71	A72	S73	E74	F75	I76	Y77	N78	K79	Y80	K81	D82	E83	K84	T85	C86	G87	I88	L89	E90	E91	D92	D93	N94	L95	G96	T97	M98	T99	I100	A101	E102	P103	V104	G105	I106	I107	C108	G109	I110	V111	P112	T113	T114	N115	P116	T117	L118	A119	A120	



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	62417	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.932	Depositor
Minimum map value	-0.331	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.066	Depositor
Recommended contour level	0.31	Depositor
Map size (Å)	293.41998, 293.41998, 293.41998	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.863, 0.863, 0.863	Depositor

5 Model quality

5.1 Standard geometry

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	0.42	2/6693 (0.0%)	0.79	21/9077 (0.2%)
1	B	0.42	2/6693 (0.0%)	0.79	21/9077 (0.2%)
1	C	0.42	2/6693 (0.0%)	0.79	21/9077 (0.2%)
1	D	0.42	2/6693 (0.0%)	0.79	21/9077 (0.2%)
1	E	0.42	2/6693 (0.0%)	0.79	21/9077 (0.2%)
1	F	0.42	2/6693 (0.0%)	0.79	21/9077 (0.2%)
1	G	0.37	2/3322 (0.1%)	0.65	7/4505 (0.2%)
1	H	0.30	0/3370	0.54	2/4569 (0.0%)
All	All	0.41	14/46850 (0.0%)	0.76	135/63536 (0.2%)

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	6
1	B	0	6
1	C	0	6
1	D	0	6
1	E	0	6
1	F	0	6
1	G	0	1
All	All	0	37

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	590	GLU	CG-CD	-6.96	1.41	1.51
1	F	425	TRP	CB-CG	6.14	1.61	1.50
1	D	425	TRP	CB-CG	6.13	1.61	1.50
1	E	425	TRP	CB-CG	6.12	1.61	1.50
1	B	425	TRP	CB-CG	6.11	1.61	1.50

The worst 5 of 135 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	464	ARG	NE-CZ-NH1	-13.38	113.61	120.30
1	C	464	ARG	CB-CG-CD	12.30	143.58	111.60
1	D	464	ARG	CB-CG-CD	12.28	143.54	111.60
1	E	464	ARG	CB-CG-CD	12.28	143.52	111.60
1	F	464	ARG	CB-CG-CD	12.27	143.51	111.60

There are no chirality outliers.

5 of 37 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	295	LYS	Peptide
1	A	425	TRP	Peptide
1	A	447	LYS	Peptide
1	A	59	MET	Peptide
1	A	90	GLU	Sidechain

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	6568	0	6618	540	0
1	B	6568	0	6618	555	0
1	C	6568	0	6618	525	0
1	D	6568	0	6618	519	0
1	E	6568	0	6618	529	0
1	F	6568	0	6618	523	0
1	G	3250	0	3233	249	0
1	H	3318	0	3384	179	0
All	All	45976	0	46325	3511	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 38.

The worst 5 of 3511 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:F:452:MET:HA	1:G:464:ARG:HH12	1.11	1.12
1:D:567:GLU:O	1:D:571:ARG:HB3	1.64	0.98
1:E:75:PHE:O	1:E:79:LYS:HB2	1.63	0.98
1:B:567:GLU:O	1:B:571:ARG:HB3	1.64	0.98
1:C:567:GLU:O	1:C:571:ARG:HB3	1.64	0.98

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	865/894 (97%)	770 (89%)	94 (11%)	1 (0%)	51	85
1	B	865/894 (97%)	770 (89%)	94 (11%)	1 (0%)	51	85
1	C	865/894 (97%)	772 (89%)	92 (11%)	1 (0%)	51	85
1	D	865/894 (97%)	771 (89%)	93 (11%)	1 (0%)	51	85
1	E	865/894 (97%)	771 (89%)	93 (11%)	1 (0%)	51	85
1	F	865/894 (97%)	770 (89%)	94 (11%)	1 (0%)	51	85
1	G	417/894 (47%)	380 (91%)	37 (9%)	0	100	100
1	H	446/894 (50%)	421 (94%)	25 (6%)	0	100	100
All	All	6053/7152 (85%)	5425 (90%)	622 (10%)	6 (0%)	54	85

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	448	ARG
1	B	448	ARG
1	C	448	ARG
1	D	448	ARG
1	E	448	ARG

5.3.2 Protein sidechains ⓘ

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	687/707 (97%)	571 (83%)	116 (17%)	2	13
1	B	687/707 (97%)	572 (83%)	115 (17%)	2	14
1	C	687/707 (97%)	571 (83%)	116 (17%)	2	13
1	D	687/707 (97%)	572 (83%)	115 (17%)	2	14
1	E	687/707 (97%)	571 (83%)	116 (17%)	2	13
1	F	687/707 (97%)	572 (83%)	115 (17%)	2	14
1	G	338/707 (48%)	337 (100%)	1 (0%)	92	95
1	H	349/707 (49%)	347 (99%)	2 (1%)	86	92
All	All	4809/5656 (85%)	4113 (86%)	696 (14%)	6	18

5 of 696 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	9	LEU
1	E	823	ASP
1	E	82	ASP
1	E	6	LEU
1	E	457	LEU

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	D	560	HIS
1	G	736	HIS
1	E	172	GLN
1	G	722	HIS
1	H	179	ASN

5.3.3 RNA ⓘ

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.

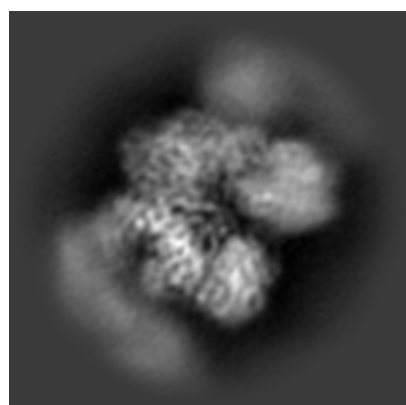
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30625. These allow visual inspection of the internal detail of the map and identification of artifacts.

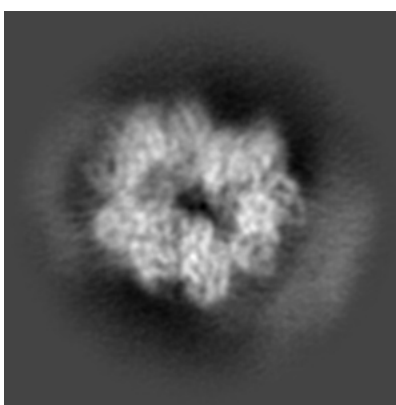
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

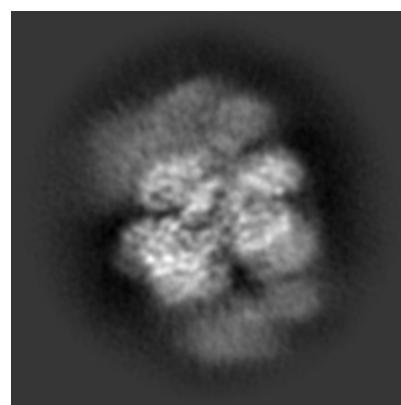
6.1.1 Primary map



X



Y

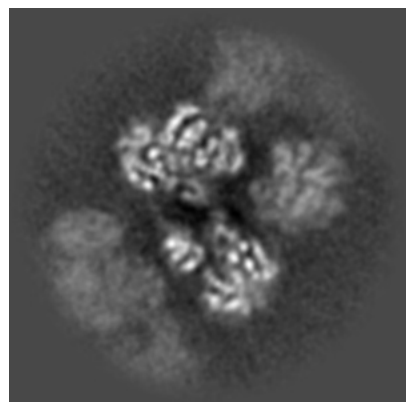


Z

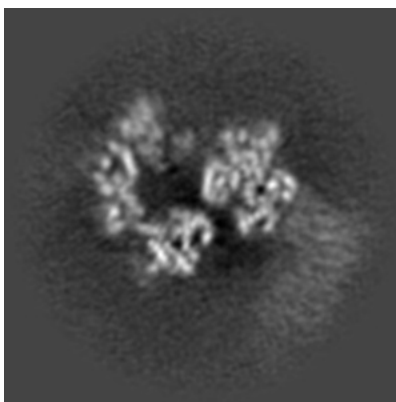
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

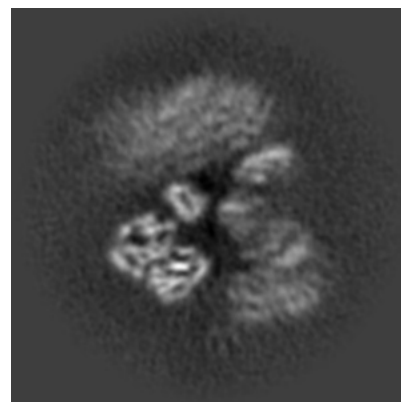
6.2.1 Primary map



X Index: 170



Y Index: 170

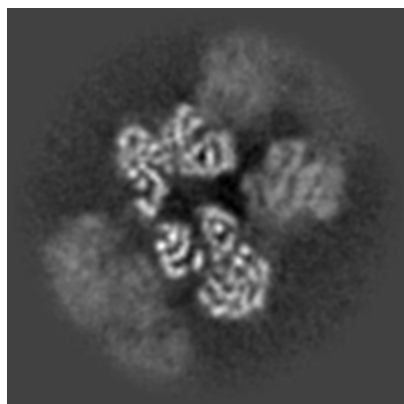


Z Index: 170

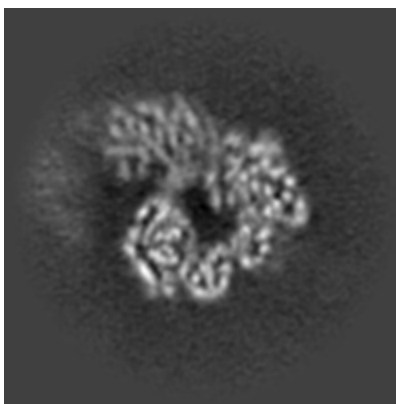
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

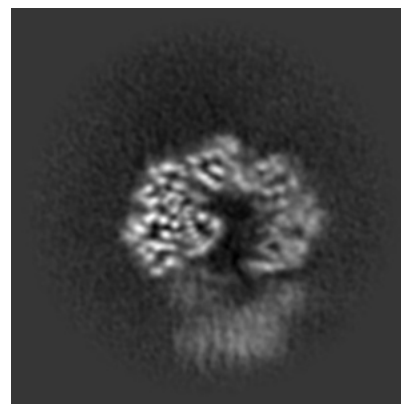
6.3.1 Primary map



X Index: 162



Y Index: 149

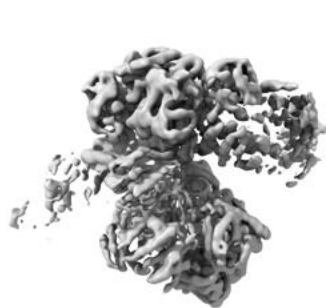


Z Index: 125

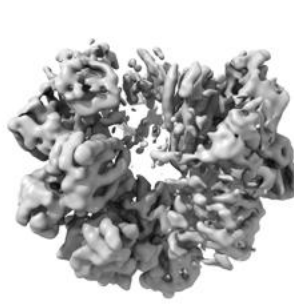
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

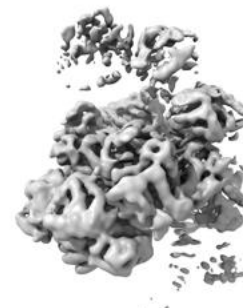
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.31. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

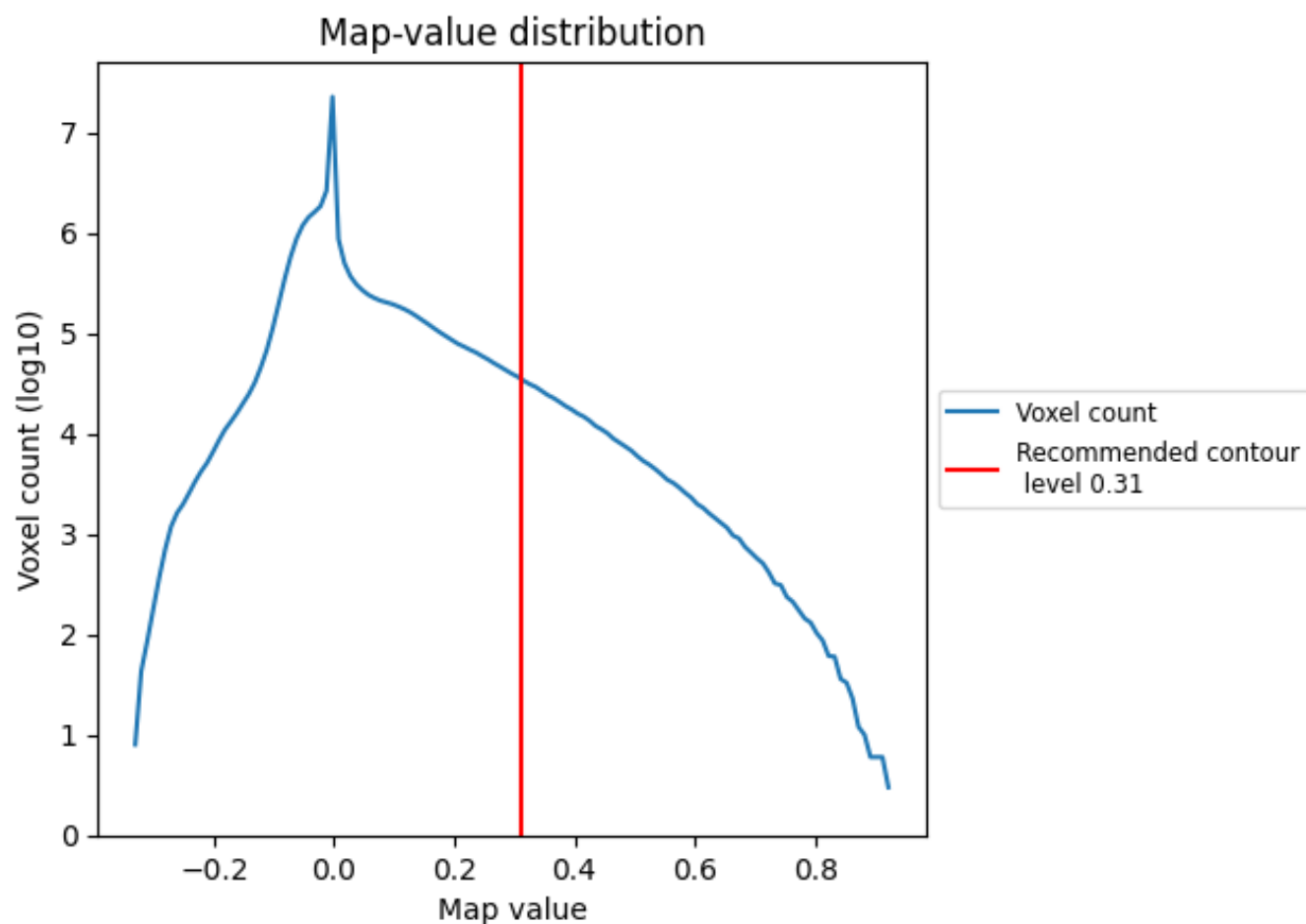
6.5 Mask visualisation

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

7 Map analysis [i](#)

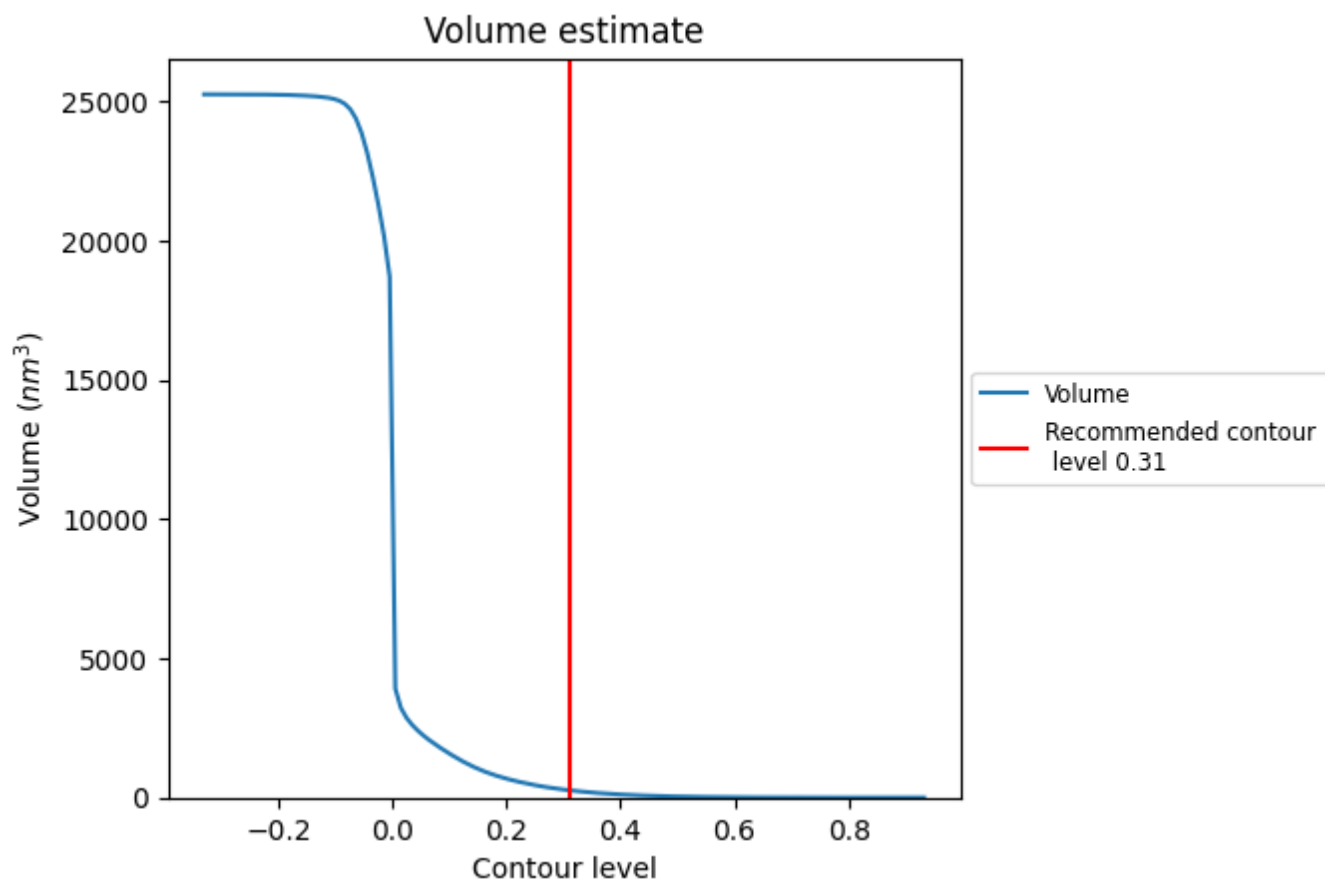
This section contains the results of statistical analysis of the map.

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.

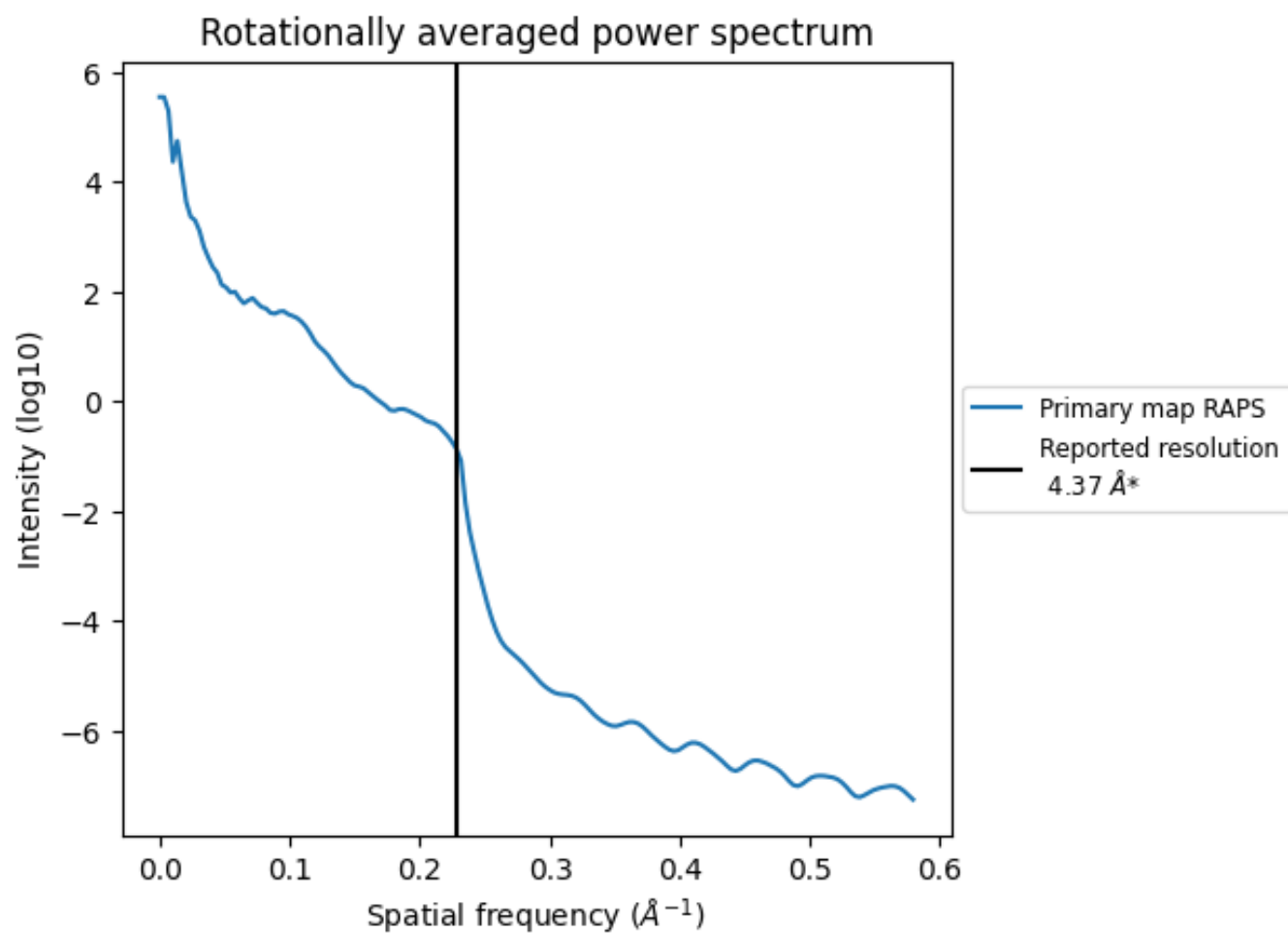
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 262 nm³; this corresponds to an approximate mass of 237 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.229 Å⁻¹

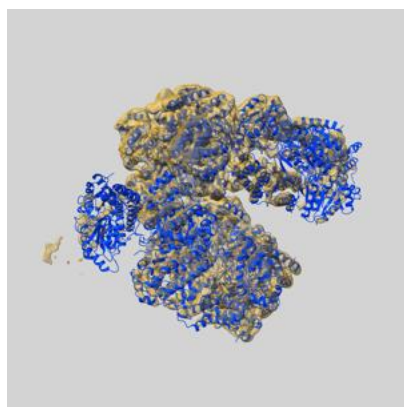
8 Fourier-Shell correlation

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

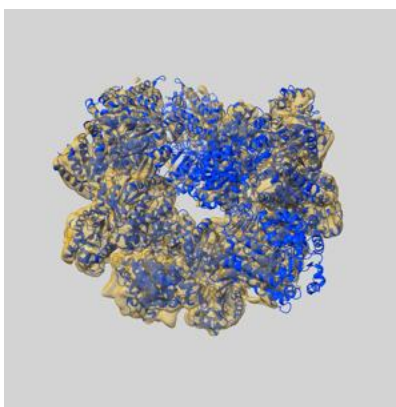
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30625 and PDB model 7DAG. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

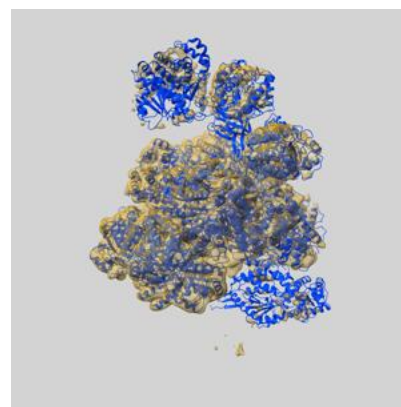
9.1 Map-model overlay [i](#)



X



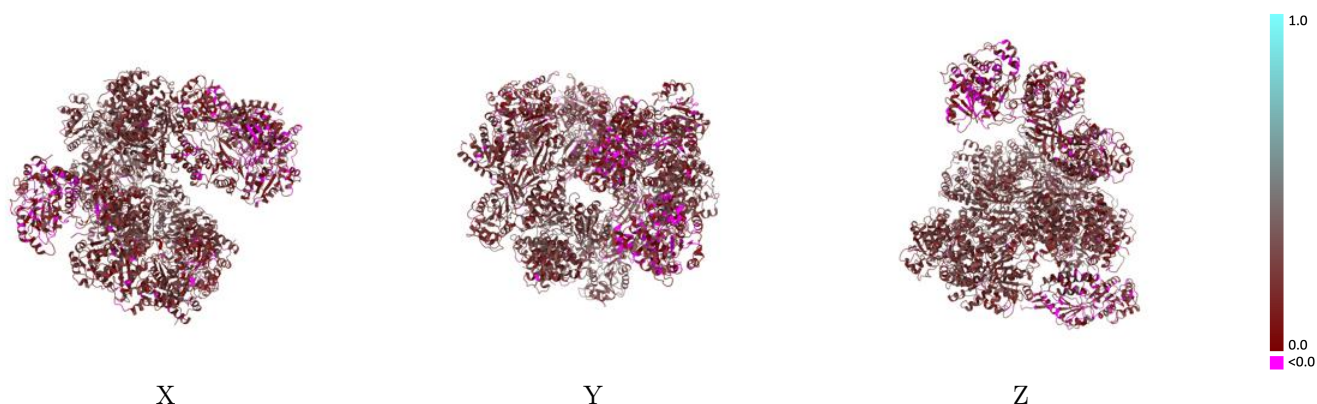
Y



Z

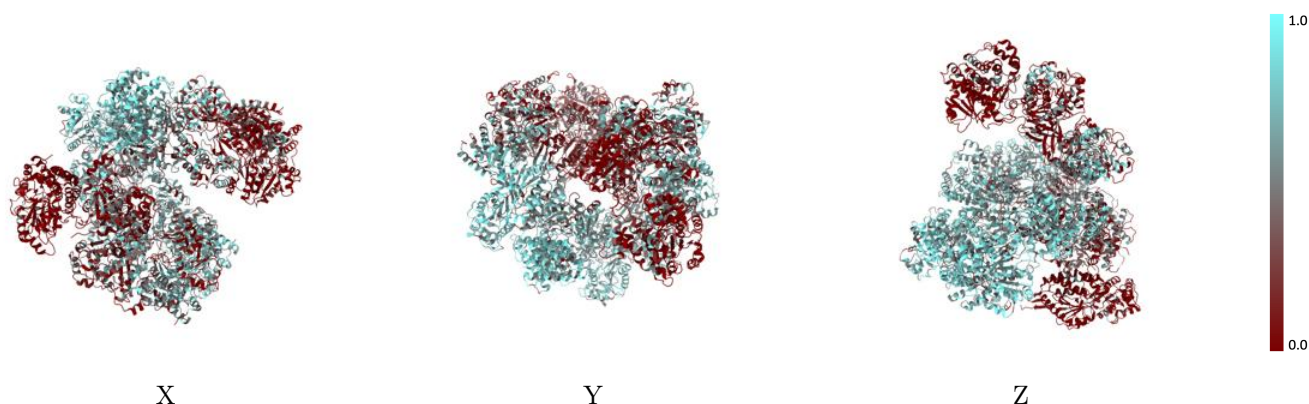
The images above show the 3D surface view of the map at the recommended contour level 0.31 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



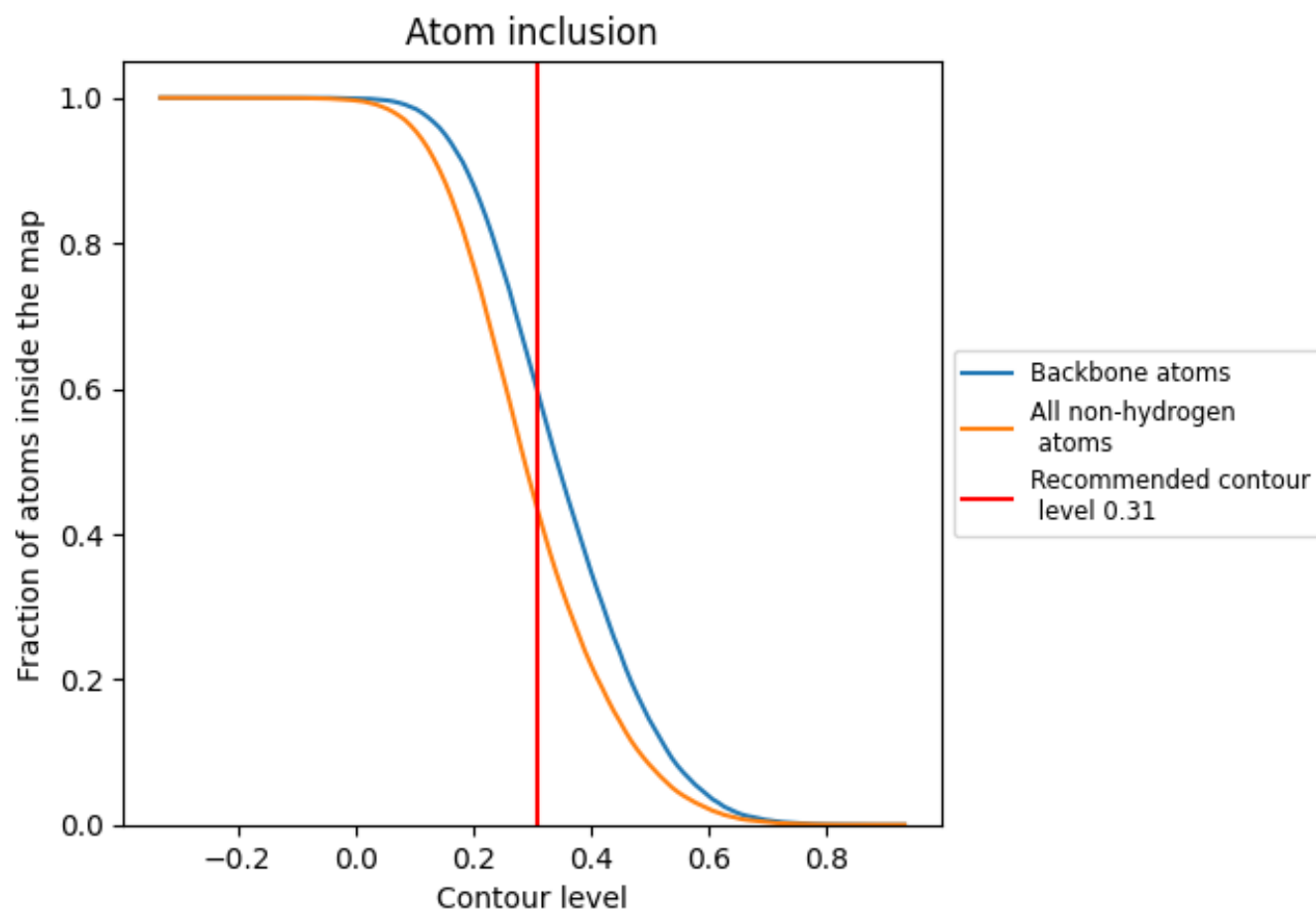
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.31).

9.4 Atom inclusion [i](#)



At the recommended contour level, 59% of all backbone atoms, 43% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.31) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4312	<div></div> 0.1970
A	<div></div> 0.2296	<div></div> 0.1290
B	<div></div> 0.3545	<div></div> 0.1930
C	<div></div> 0.6613	<div></div> 0.2430
D	<div></div> 0.6823	<div></div> 0.2390
E	<div></div> 0.5315	<div></div> 0.2110
F	<div></div> 0.4650	<div></div> 0.2120
G	<div></div> 0.1492	<div></div> 0.1980
H	<div></div> 0.0405	<div></div> 0.1080

1.0

0.0

<0.0