



wwPDB EM Validation Summary Report ⓘ

Apr 5, 2026 – 04:32 PM UTC

PDB ID : 9UAQ / pdb_00009uaq
EMDB ID : EMD-63989
Title : CryoEM structure of GFP-like protein from Aequorea coerulescens with Trim-body
Authors : Song, J.Y.; Wang, W.
Deposited on : 2025-04-01
Resolution : 2.29 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

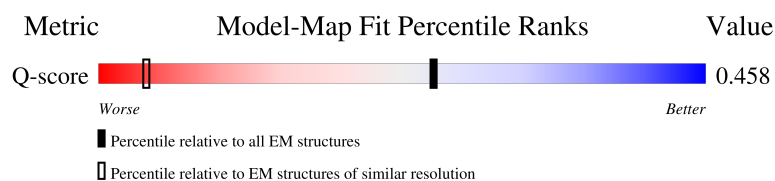
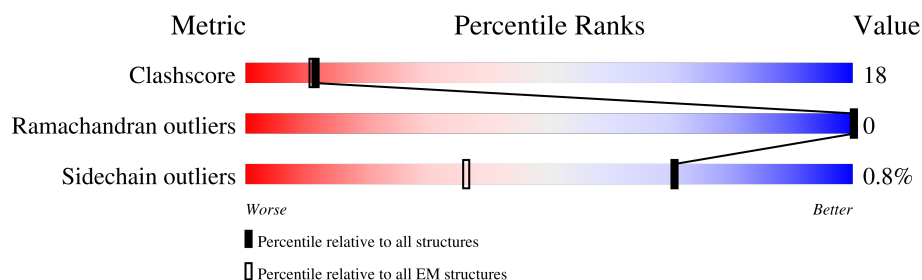
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.29 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.



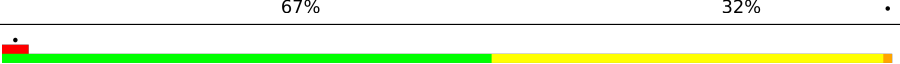
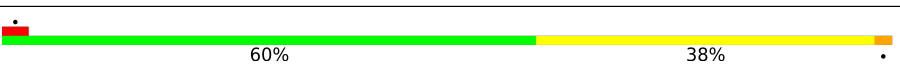
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3699 (1.79 - 2.79)

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	320	 69% 29%
1	B	320	 75% 25%
1	C	320	 68% 32%
2	D	233	 70% 29%

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Mol	Chain	Length	Quality of chain
2	E	233	 5% 70% 30%
2	F	233	 2% 65% 32% 1%
3	G	225	 2% 67% 32% 1%
3	H	225	 2% 55% 44% 1%
3	I	225	 2% 60% 38% 1%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 18042 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 H3-PrAC-5350A,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	319	Total	C	N	O	S	0	0
			2424	1545	414	455	10		
1	B	319	Total	C	N	O	S	0	0
			2424	1545	414	455	10		
1	C	320	Total	C	N	O	S	0	0
			2433	1550	415	458	10		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	141	ILE	LYS	conflict	UNP Q9WXS1
A	145	VAL	LEU	conflict	UNP Q9WXS1
A	149	ALA	GLU	conflict	UNP Q9WXS1
A	170	ALA	GLU	conflict	UNP Q9WXS1
A	173	VAL	PHE	conflict	UNP Q9WXS1
B	141	ILE	LYS	conflict	UNP Q9WXS1
B	145	VAL	LEU	conflict	UNP Q9WXS1
B	149	ALA	GLU	conflict	UNP Q9WXS1
B	170	ALA	GLU	conflict	UNP Q9WXS1
B	173	VAL	PHE	conflict	UNP Q9WXS1
C	141	ILE	LYS	conflict	UNP Q9WXS1
C	145	VAL	LEU	conflict	UNP Q9WXS1
C	149	ALA	GLU	conflict	UNP Q9WXS1
C	170	ALA	GLU	conflict	UNP Q9WXS1
C	173	VAL	PHE	conflict	UNP Q9WXS1

- Molecule 2 is a protein called GFP-nanobody-TAIL.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	232	Total	C	N	O	S	0	0
			1790	1142	302	341	5		

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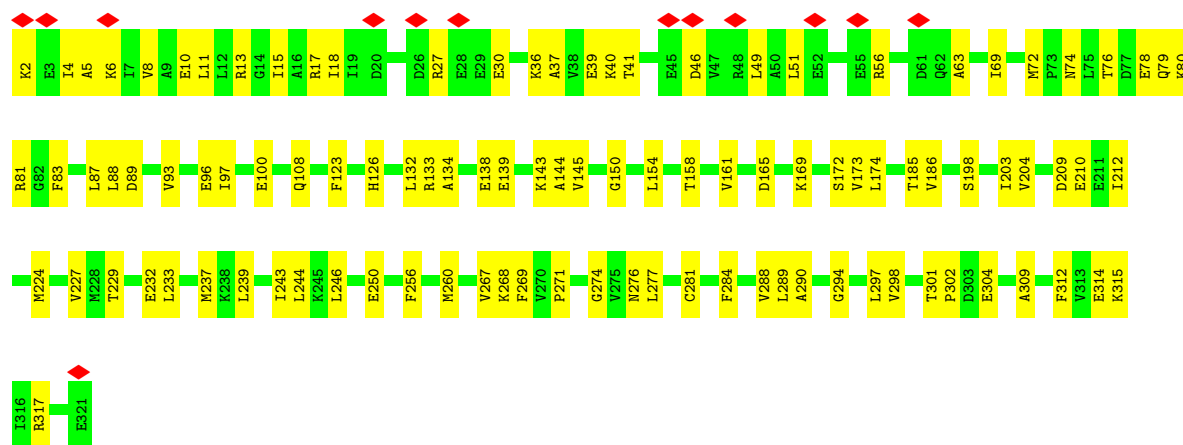
Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	232	Total	C	N	O	S	0	0
			1790	1142	302	341	5		
2	F	233	Total	C	N	O	S	0	0
			1799	1147	303	344	5		

- Molecule 3 is a protein called Green fluorescent protein.

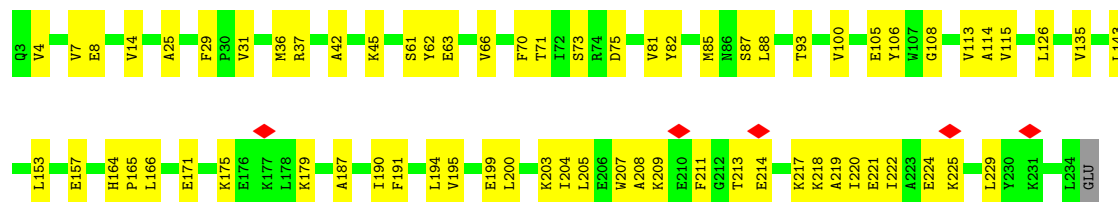
Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	225	Total	C	N	O	S	0	0
			1794	1141	300	346	7		
3	H	225	Total	C	N	O	S	0	0
			1794	1141	300	346	7		
3	I	225	Total	C	N	O	S	0	0
			1794	1141	300	346	7		

There are 24 discrepancies between the modelled and reference sequences:

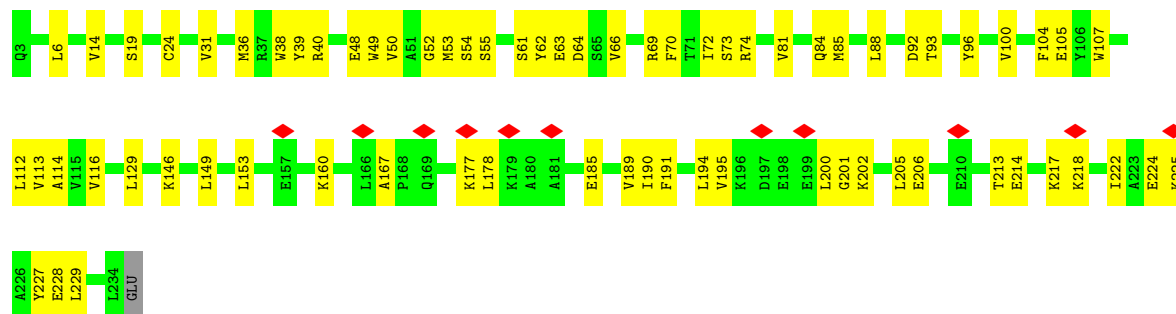
Chain	Residue	Modelled	Actual	Comment	Reference
G	12	ILE	VAL	conflict	UNP Q6YGZ0
G	65	LEU	PHE	conflict	UNP Q6YGZ0
G	66	GYS	SER	chromophore	UNP Q6YGZ0
G	66	GYS	TYR	chromophore	UNP Q6YGZ0
G	66	GYS	GLY	chromophore	UNP Q6YGZ0
G	102	GLU	LYS	conflict	UNP Q6YGZ0
G	207	ALA	THR	conflict	UNP Q6YGZ0
G	223	GLY	GLU	conflict	UNP Q6YGZ0
H	12	ILE	VAL	conflict	UNP Q6YGZ0
H	65	LEU	PHE	conflict	UNP Q6YGZ0
H	66	GYS	SER	chromophore	UNP Q6YGZ0
H	66	GYS	TYR	chromophore	UNP Q6YGZ0
H	66	GYS	GLY	chromophore	UNP Q6YGZ0
H	102	GLU	LYS	conflict	UNP Q6YGZ0
H	207	ALA	THR	conflict	UNP Q6YGZ0
H	223	GLY	GLU	conflict	UNP Q6YGZ0
I	12	ILE	VAL	conflict	UNP Q6YGZ0
I	65	LEU	PHE	conflict	UNP Q6YGZ0
I	66	GYS	SER	chromophore	UNP Q6YGZ0
I	66	GYS	TYR	chromophore	UNP Q6YGZ0
I	66	GYS	GLY	chromophore	UNP Q6YGZ0
I	102	GLU	LYS	conflict	UNP Q6YGZ0
I	207	ALA	THR	conflict	UNP Q6YGZ0
I	223	GLY	GLU	conflict	UNP Q6YGZ0



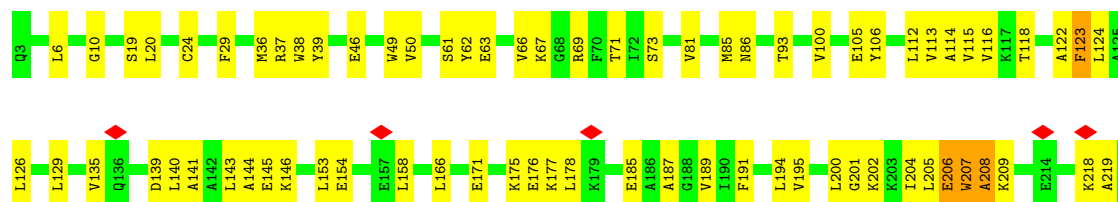
- Molecule 2: GFP-nanobody-TAIL

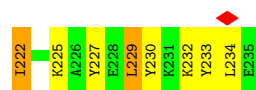


- Molecule 2: GFP-nanobody-TAIL

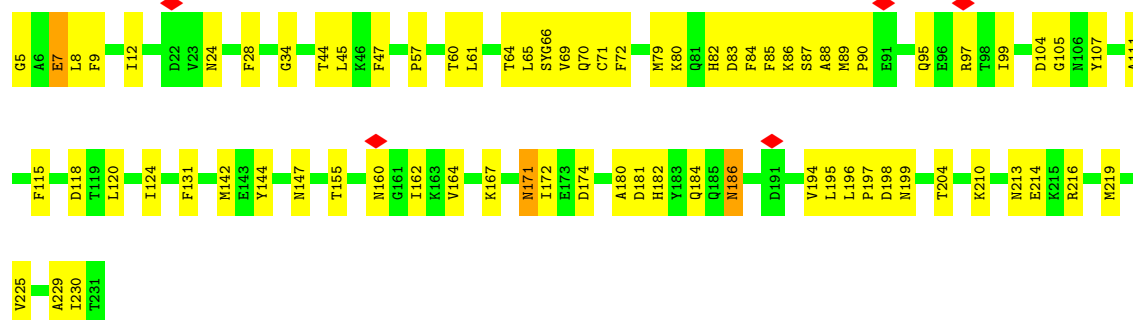


- Molecule 2: GFP-nanobody-TAIL

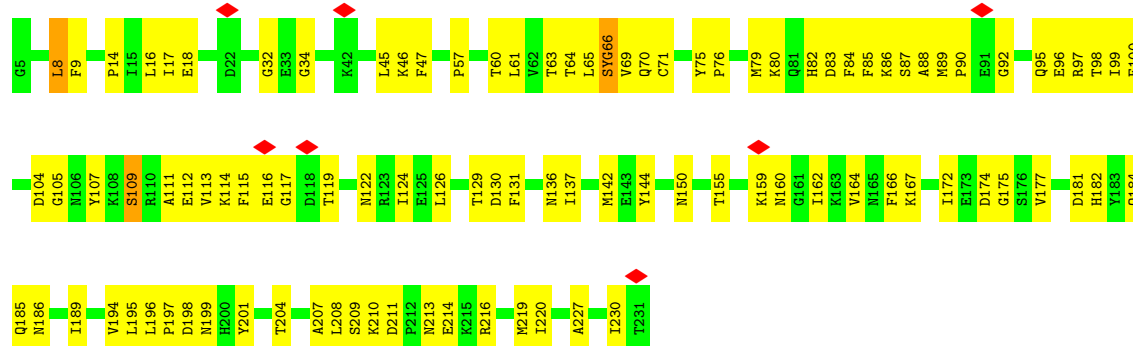




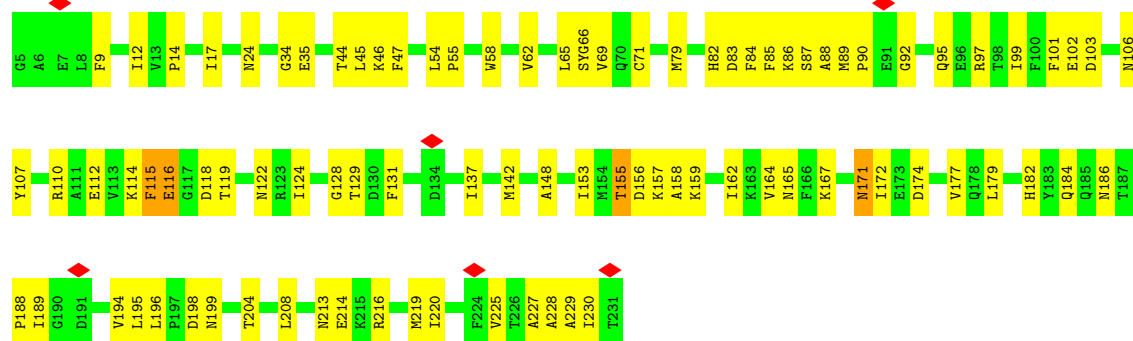
• Molecule 3: Green fluorescent protein



• Molecule 3: Green fluorescent protein



• Molecule 3: Green fluorescent protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1209700	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.575	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	264.96, 264.96, 264.96	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.91999996, 0.91999996, 0.91999996	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GYS

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	0.28	0/2457	0.54	2/3309 (0.1%)
1	B	0.27	0/2457	0.45	1/3309 (0.0%)
1	C	0.26	0/2466	0.42	0/3321
2	D	0.26	0/1822	0.44	0/2462
2	E	0.29	0/1822	0.60	2/2462 (0.1%)
2	F	0.36	1/1831 (0.1%)	0.76	8/2474 (0.3%)
3	G	0.38	0/1814	0.64	2/2454 (0.1%)
3	H	0.35	0/1814	0.66	3/2454 (0.1%)
3	I	0.37	0/1814	0.75	5/2454 (0.2%)
All	All	0.31	1/18297 (0.0%)	0.58	23/24699 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	207	TRP	CA-C	5.70	1.60	1.52

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	208	ALA	N-CA-C	10.23	123.70	111.33
3	I	158	ALA	N-CA-C	-9.94	99.03	111.75
3	I	118	ASP	N-CA-C	-9.40	100.39	112.23
2	E	48	GLU	N-CA-C	8.37	123.12	109.72
2	F	206	GLU	N-CA-C	-6.99	103.59	111.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2424	0	2533	77	0
1	B	2424	0	2533	59	0
1	C	2433	0	2539	84	0
2	D	1790	0	1799	59	0
2	E	1790	0	1799	73	0
2	F	1799	0	1805	73	0
3	G	1794	0	1722	69	0
3	H	1794	0	1722	97	0
3	I	1794	0	1722	100	0
All	All	18042	0	18174	644	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 18.

The worst 5 of 644 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:E:85:MET:HE1	2:E:96:TYR:CE2	2.09	0.88
3:I:164:VAL:HB	3:I:184:GLN:HB3	1.54	0.86
2:F:112:LEU:CD2	2:F:129:LEU:HG	2.09	0.82
1:A:185:THR:HG22	1:A:185:THR:O	1.79	0.82
1:C:89:ASP:HB2	2:F:73:SER:HB3	1.64	0.80

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	317/320 (99%)	313 (99%)	4 (1%)	0	100	100
1	B	317/320 (99%)	311 (98%)	6 (2%)	0	100	100
1	C	318/320 (99%)	312 (98%)	6 (2%)	0	100	100
2	D	230/233 (99%)	226 (98%)	4 (2%)	0	100	100
2	E	230/233 (99%)	225 (98%)	5 (2%)	0	100	100
2	F	231/233 (99%)	228 (99%)	3 (1%)	0	100	100
3	G	220/225 (98%)	217 (99%)	3 (1%)	0	100	100
3	H	220/225 (98%)	214 (97%)	6 (3%)	0	100	100
3	I	220/225 (98%)	217 (99%)	3 (1%)	0	100	100
All	All	2303/2334 (99%)	2263 (98%)	40 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	258/259 (100%)	252 (98%)	6 (2%)	44	63
1	B	258/259 (100%)	257 (100%)	1 (0%)	84	92
1	C	259/259 (100%)	259 (100%)	0	100	100
2	D	182/183 (100%)	182 (100%)	0	100	100
2	E	182/183 (100%)	182 (100%)	0	100	100
2	F	183/183 (100%)	180 (98%)	3 (2%)	55	73
3	G	193/193 (100%)	190 (98%)	3 (2%)	55	73
3	H	193/193 (100%)	192 (100%)	1 (0%)	81	90
3	I	193/193 (100%)	191 (99%)	2 (1%)	68	82
All	All	1901/1905 (100%)	1885 (99%)	16 (1%)	70	86

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	I	171	ASN
3	H	213	ASN
2	F	116	VAL
3	G	186	ASN
2	F	115	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	192	GLN
3	I	70	GLN
3	I	184	GLN
3	I	95	GLN
1	B	276	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

3 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GYS	G	66	3	20,22,23	0.86	0	25,30,32	1.22	2 (8%)
3	GYS	I	66	3	20,22,23	0.86	0	25,30,32	1.21	2 (8%)
3	GYS	H	66	3	20,22,23	0.86	0	25,30,32	1.22	2 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GYS	G	66	3	-	1/10/29/30	0/2/2/2
3	GYS	I	66	3	-	1/10/29/30	0/2/2/2
3	GYS	H	66	3	-	1/10/29/30	0/2/2/2

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	66	GYS	CA1-C1-N3	-3.07	120.84	124.84
3	H	66	GYS	CA1-C1-N3	-3.07	120.85	124.84
3	I	66	GYS	CA1-C1-N3	-3.06	120.86	124.84
3	I	66	GYS	N3-C1-N2	2.12	113.15	111.48
3	G	66	GYS	N3-C1-N2	2.09	113.13	111.48

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	66	GYS	N1-CA1-CB1-OG1
3	H	66	GYS	N1-CA1-CB1-OG1
3	I	66	GYS	N1-CA1-CB1-OG1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	66	GYS	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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 ⓘ

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63989. These allow visual inspection of the internal detail of the map and identification of artifacts.

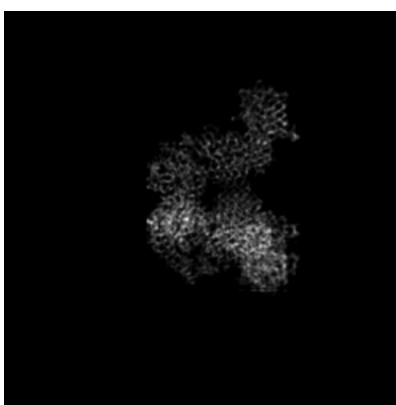
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

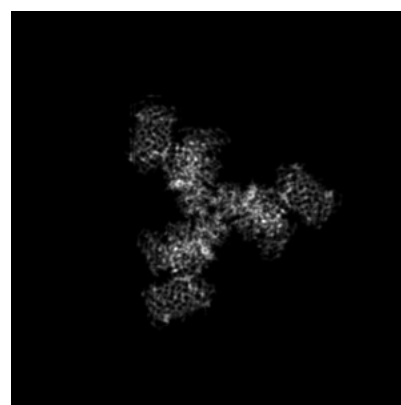
6.1.1 Primary map



X



Y

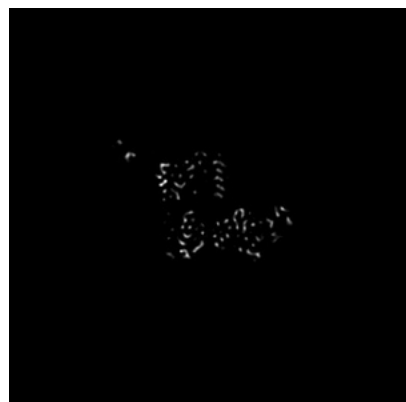


Z

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

6.2 Central slices [i](#)

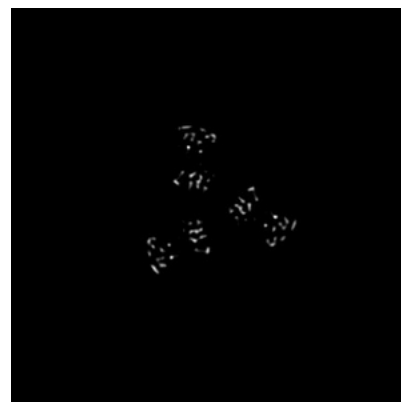
6.2.1 Primary map



X Index: 144



Y Index: 144



Z Index: 144

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

6.3 Largest variance slices [i](#)

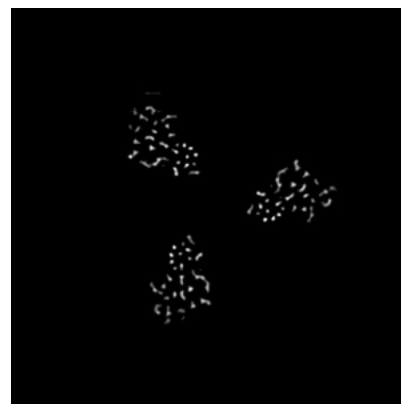
6.3.1 Primary map



X Index: 128



Y Index: 153

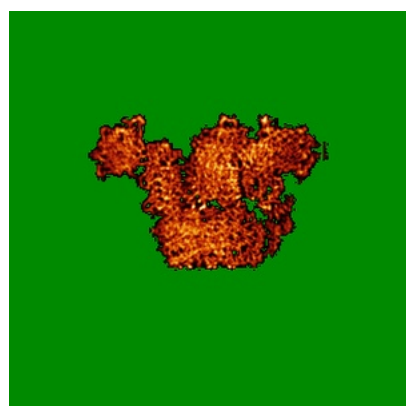


Z Index: 187

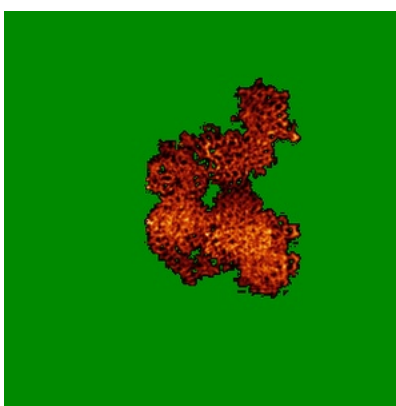
The images above show the largest variance slices of the map in three orthogonal directions.

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

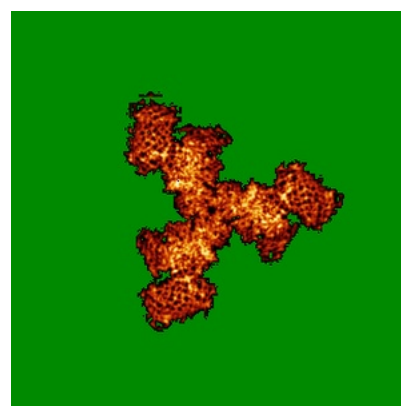
6.4.1 Primary map



X



Y

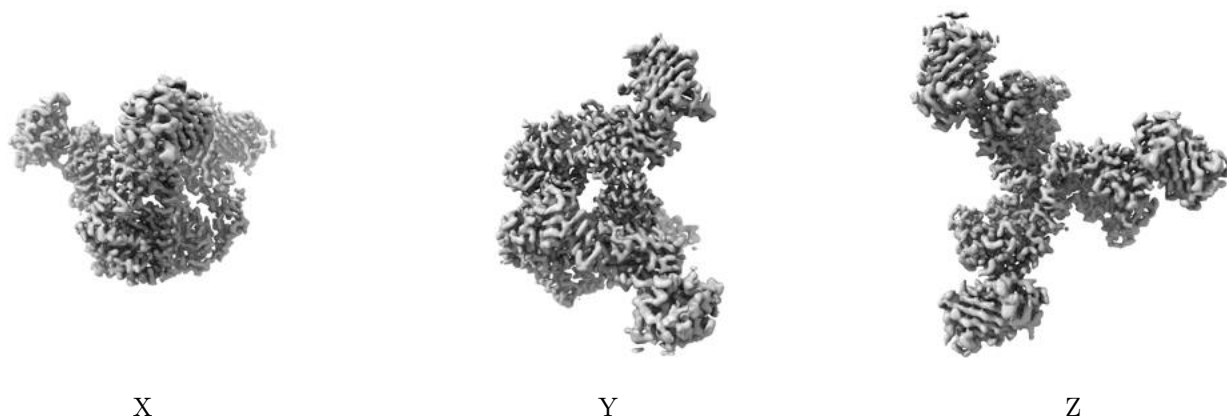


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

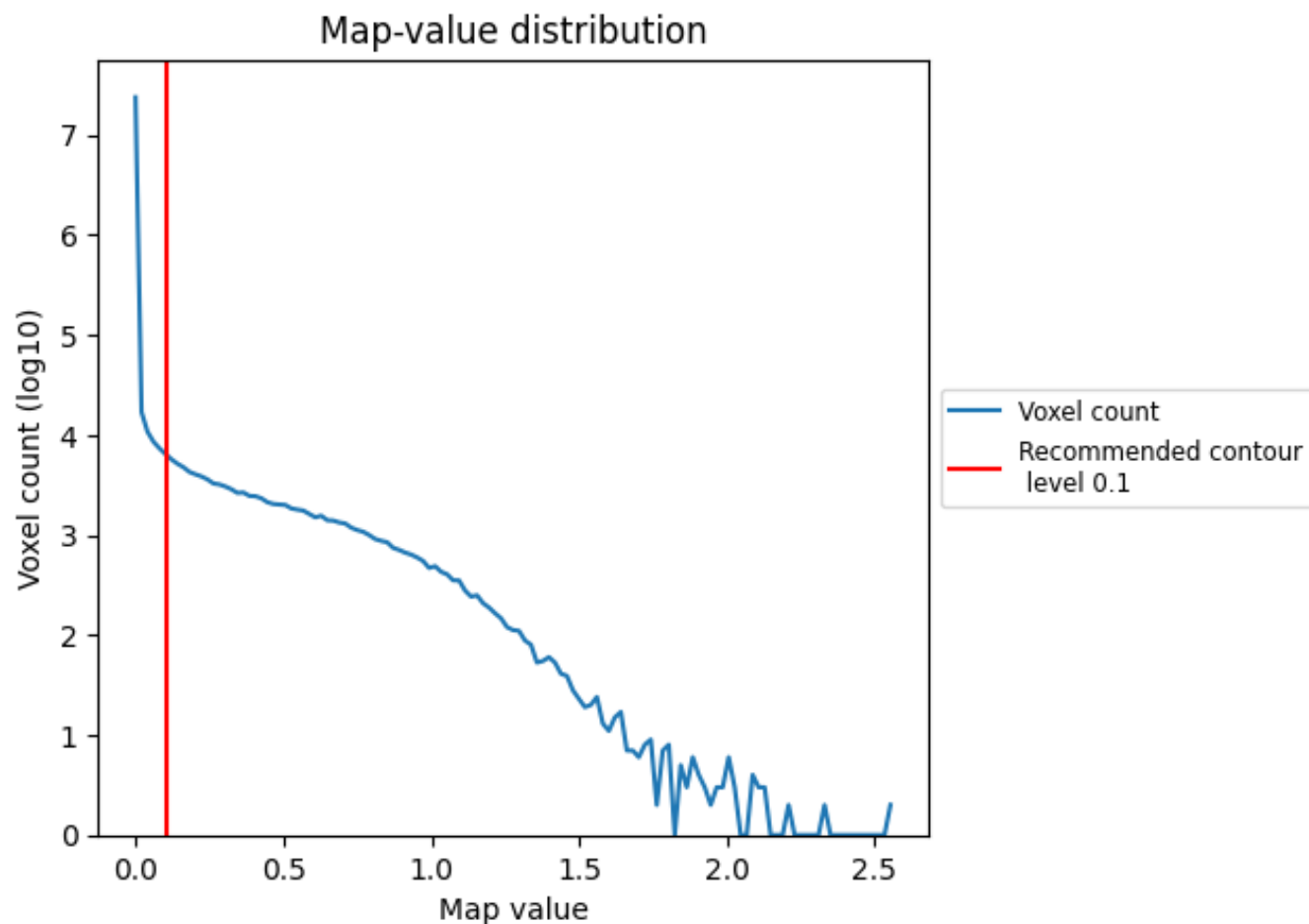
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

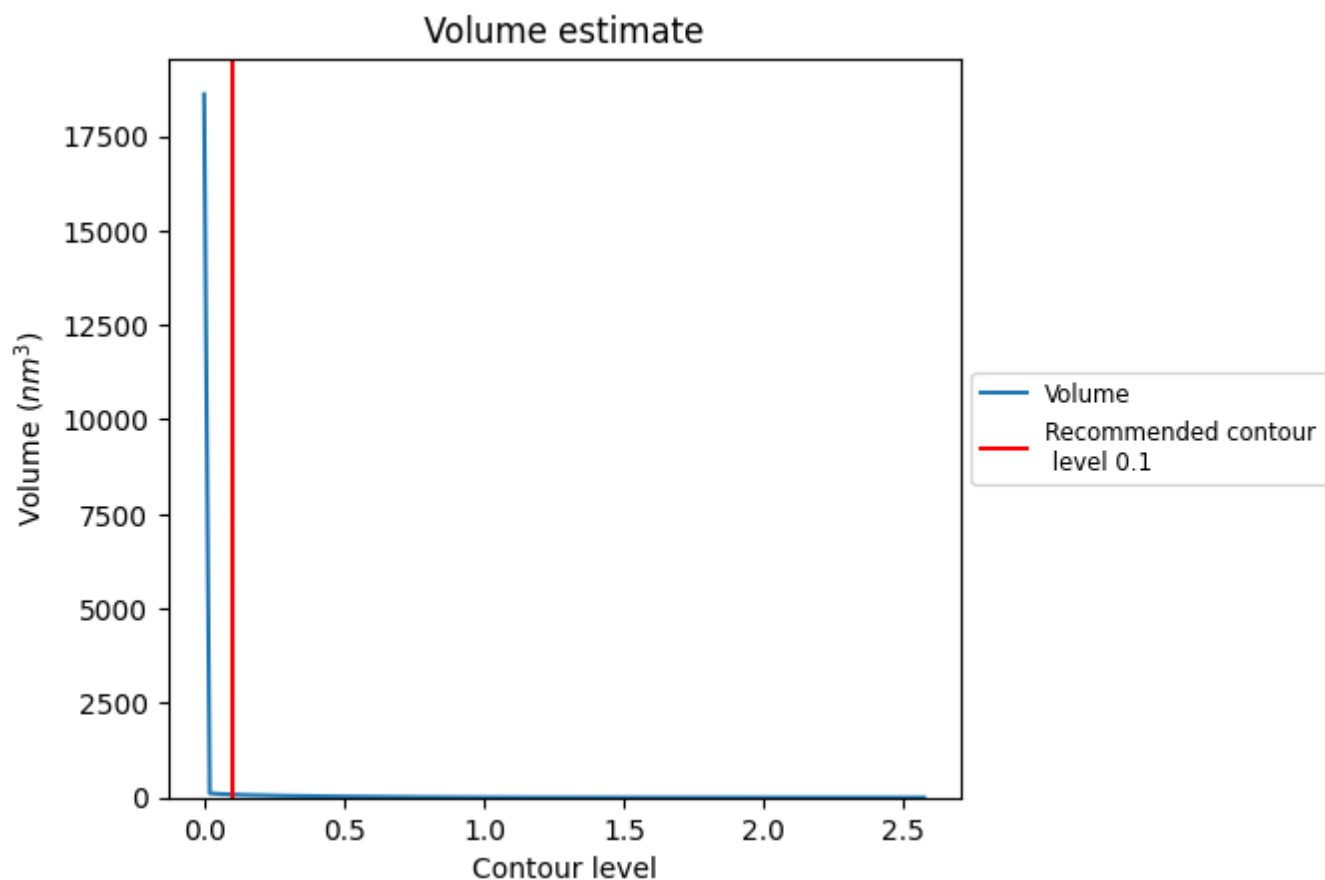
This section contains the results of statistical analysis of the map.

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.

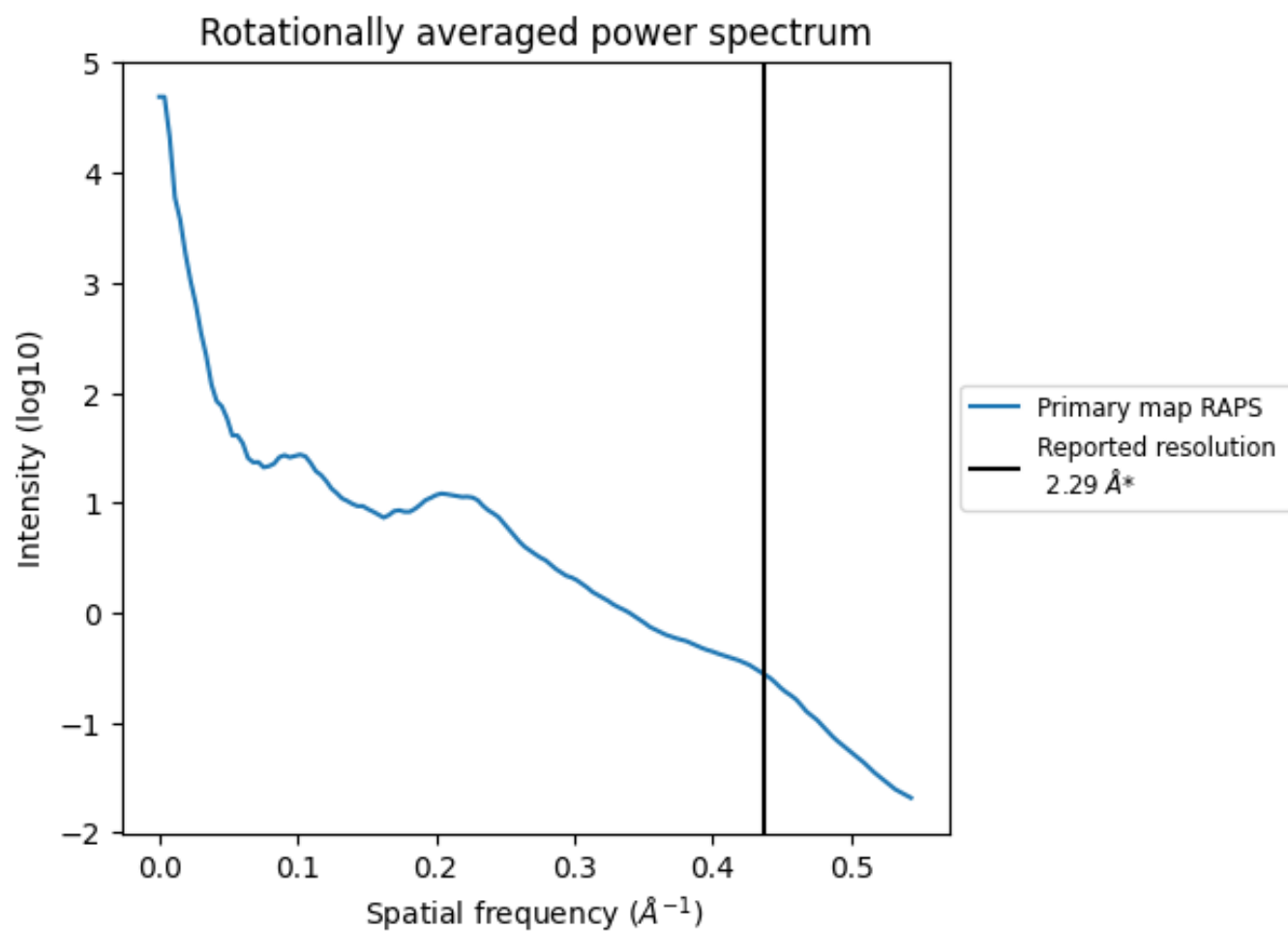
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 80 nm³; this corresponds to an approximate mass of 72 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 0.437 Å⁻¹

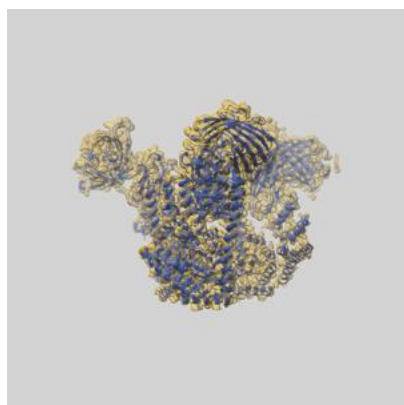
8 Fourier-Shell correlation

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

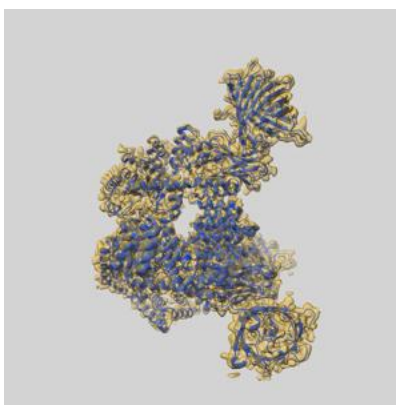
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-63989 and PDB model 9UAQ. Per-residue inclusion information can be found in section [3](#) on page [6](#).

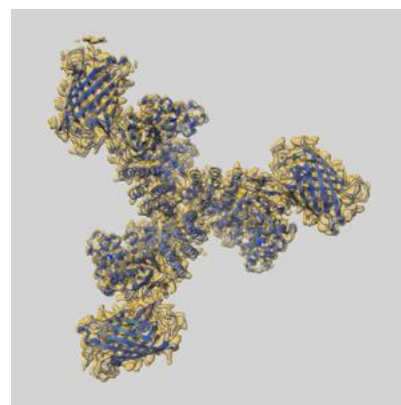
9.1 Map-model overlay [i](#)



X



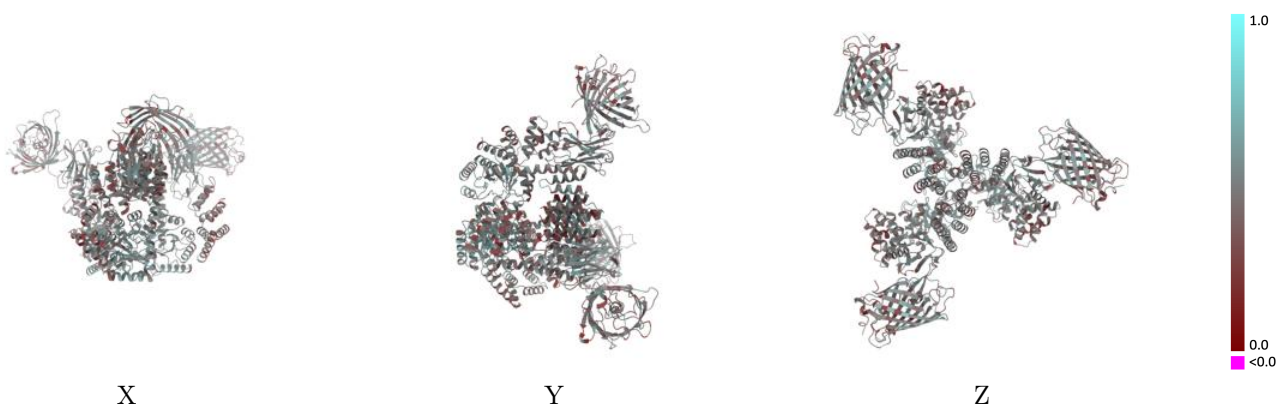
Y



Z

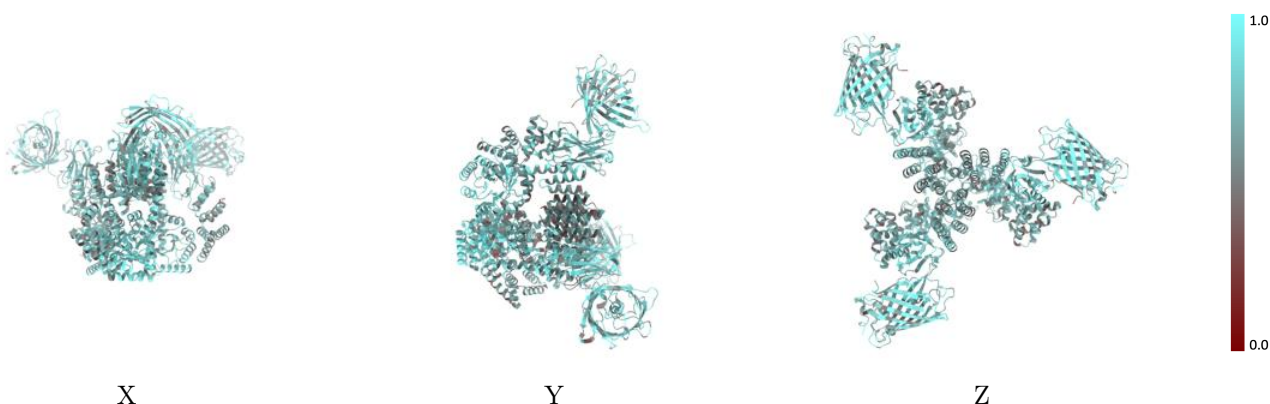
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



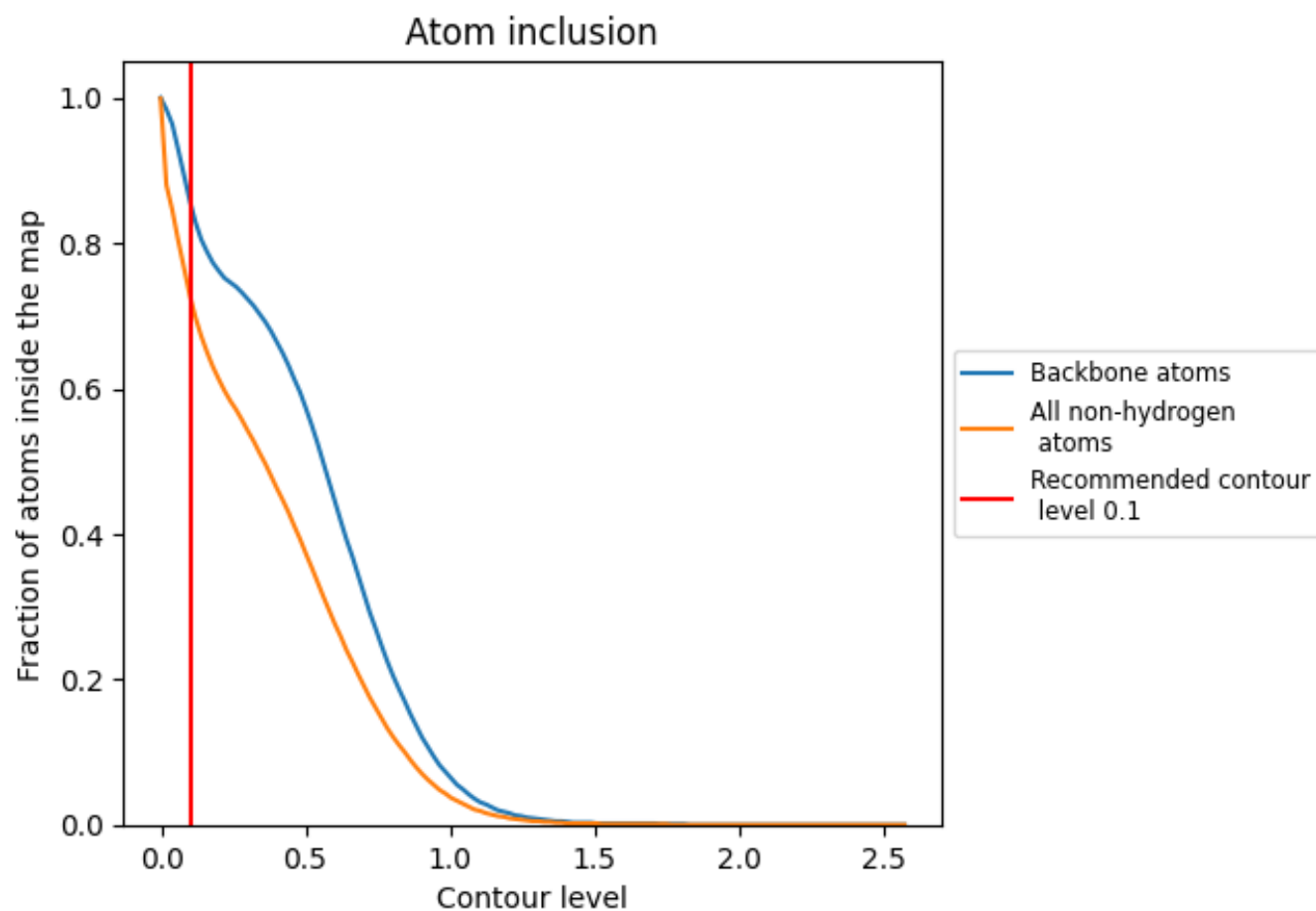
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 73% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7270	0.4580
A	0.7390	0.4850
B	0.7390	0.4910
C	0.7410	0.4860
D	0.7200	0.4440
E	0.7040	0.4460
F	0.7170	0.4470
G	0.7250	0.4280
H	0.7210	0.4390
I	0.7260	0.4290

