



wwPDB EM Validation Summary Report ⓘ

Oct 28, 2024 – 05:37 am GMT

PDB ID : 8AFM
EMDB ID : EMD-15402
Title : Cryo-EM structure of crescentin filaments (wildtype, C2 symmetry and small box)
Authors : Liu, Y.; Lowe, J.
Deposited on : 2022-07-18
Resolution : 4.80 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.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

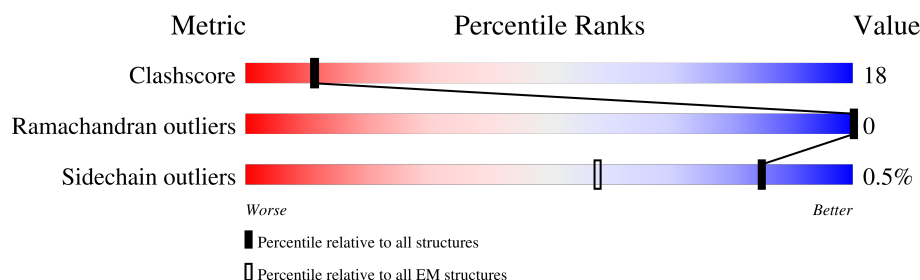
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.80 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	457	
1	B	457	
1	E	457	
1	F	457	
1	G	457	
1	H	457	
1	K	457	
1	L	457	

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Mol	Chain	Length	Quality of chain
2	C	907	 7% 5% 88%
2	D	907	 7% 5% 88%
2	I	907	 7% 6% 88%
2	J	907	 8% . 88%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7842 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 Crescentin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	77	Total	C	N	O	S	0	0
			605	361	124	118	2		
1	B	77	Total	C	N	O	S	0	0
			605	361	124	118	2		
1	E	68	Total	C	N	O		0	0
			518	308	99	111			
1	F	59	Total	C	N	O		0	0
			455	269	89	97			
1	G	77	Total	C	N	O	S	0	0
			605	361	124	118	2		
1	H	77	Total	C	N	O	S	0	0
			605	361	124	118	2		
1	K	68	Total	C	N	O		0	0
			518	308	99	111			
1	L	59	Total	C	N	O		0	0
			455	269	89	97			

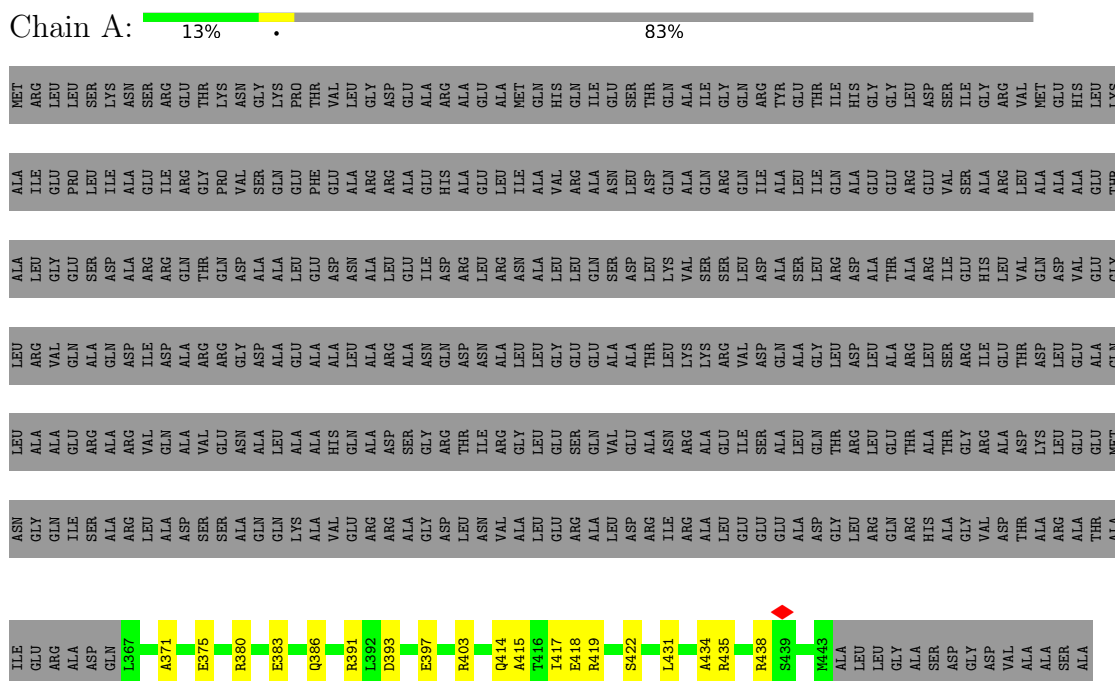
- Molecule 2 is a protein called Crescentin-specific megabody MB13.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	112	Total	C	N	O	S	0	0
			869	539	155	170	5		
2	C	112	Total	C	N	O	S	0	0
			869	539	155	170	5		
2	J	112	Total	C	N	O	S	0	0
			869	539	155	170	5		
2	I	112	Total	C	N	O	S	0	0
			869	539	155	170	5		

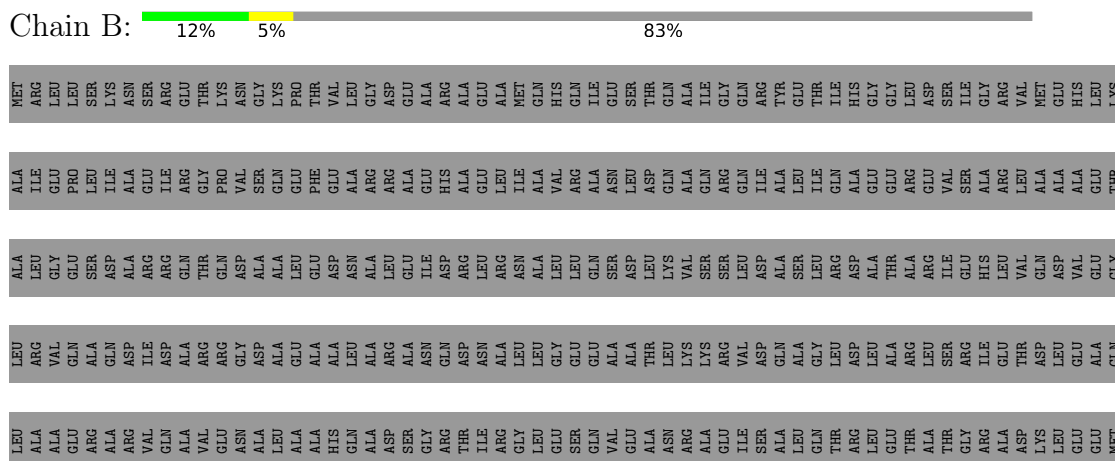
3 Residue-property plots

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.

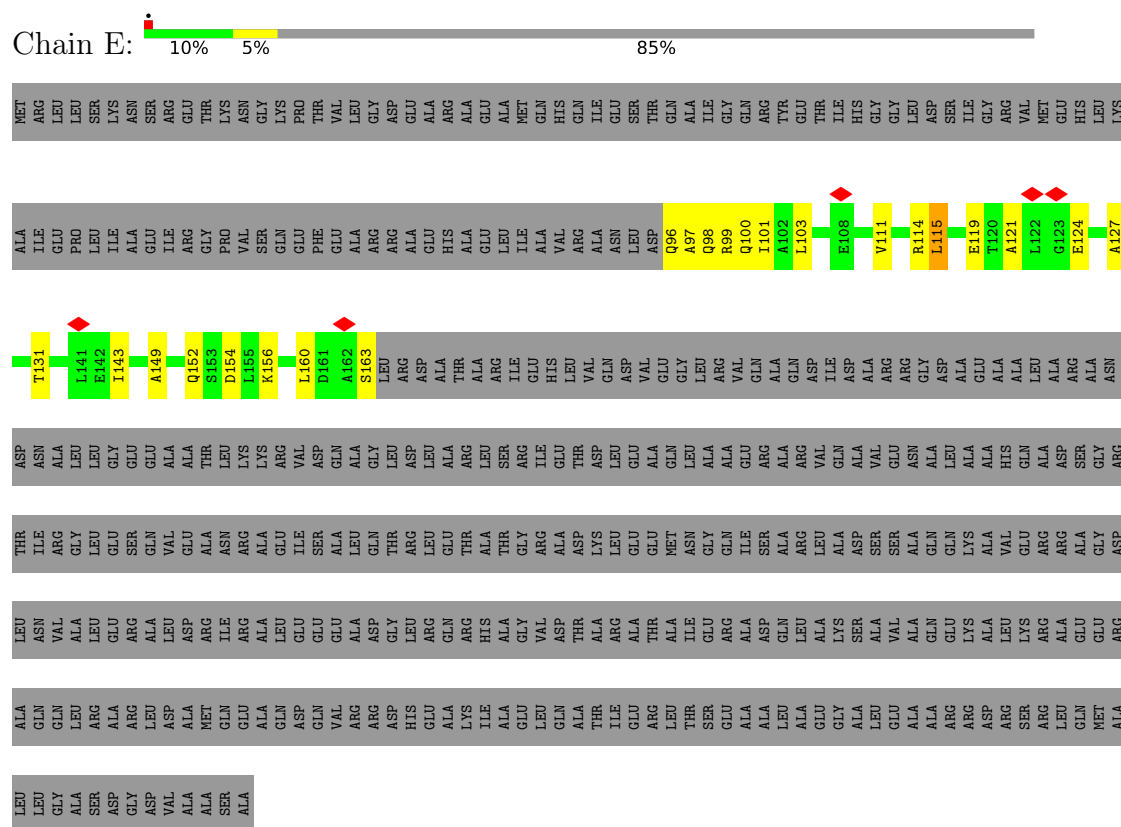
• Molecule 1: Crescentin



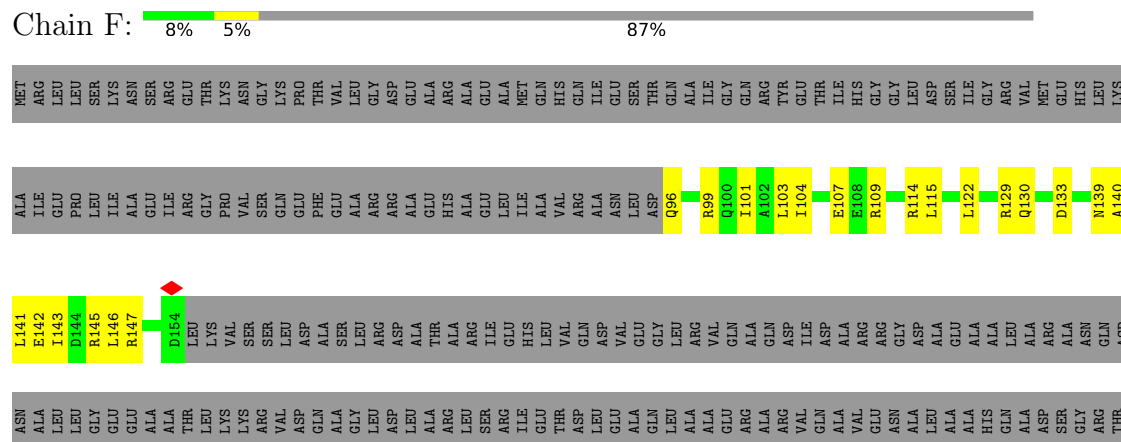
• Molecule 1: Crescentin



- Molecule 1: Crescentin



- Molecule 1: Crescentin



LEU	GLN	ASN	TLE
GLY	GLN	VAL	ARG
ALA	LEU	ALA	GLY
SER	ARG	GLU	LEU
ASP	ALA	LEU	GLU
GLY	ARG	ARG	SER
ASP	LEU	LEU	GLN
VAL	ASP	LEU	VAL
ALA	ALA	ASP	GLU
ALA	MET	ALA	ALA
SER	GLN	TLE	ASN
ALA	GLU	ARG	ARG
	ALA	ALA	ALA
	GLN	LEU	TLE
	ASP	GLU	GLY
	GLN	GLU	SER
	VAL	GLU	ALA
	ARG	ALA	LEU
	ARG	ASP	GLN
	ASP	GLY	GLN
	HIS	LEU	ARG
	GLU	ARG	LEU
	ALA	GLN	GLU
	LYS	ARG	THR
	TLE	HIS	ALA
	GLU	GLY	THR
	LEU	VAL	ARG
	GLN	ASP	ALA
	ALA	THR	ASP
	TLE	ALA	LYS
	GLU	ARG	LEU
	ARG	THR	GLU
	LEU	TLE	MET
	THR	ALA	ASN
	SER	GLU	GLY
	GLU	ARG	TLE
	ALA	ALA	GLN
	LEU	ASP	SER
	LEU	VAL	SER
	ALA	ALA	ALA
	ALA	GLN	ALA
	GLY	LYS	LEU
	LEU	SER	ASP
	ALA	ALA	LEU
	GLU	VAL	ARG
	ALA	ALA	GLN
	ARG	GLN	GLN
	ASP	ALA	LYS
	GLY	LEU	VAL
	ARG	LEU	VAL
	ASP	LYS	GLU
	SER	LYS	GLU
	ARG	ARG	ARG
	LEU	ALA	ARG
	GLN	GLU	GLY
	MET	GLU	GLY
	ALA	ARG	ASP
	THR	ALA	THR

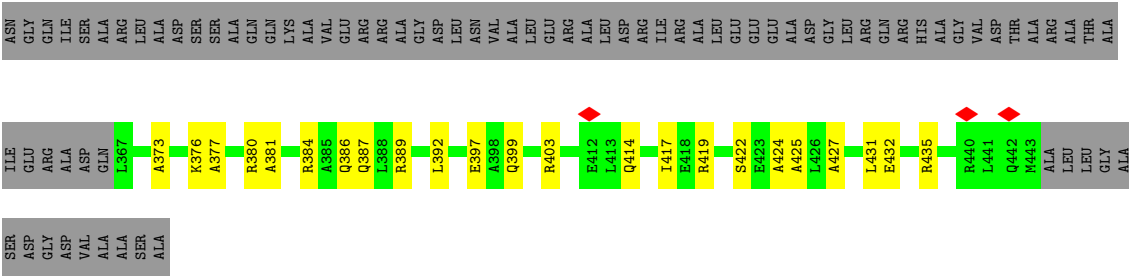
- Molecule 1: Crescentin



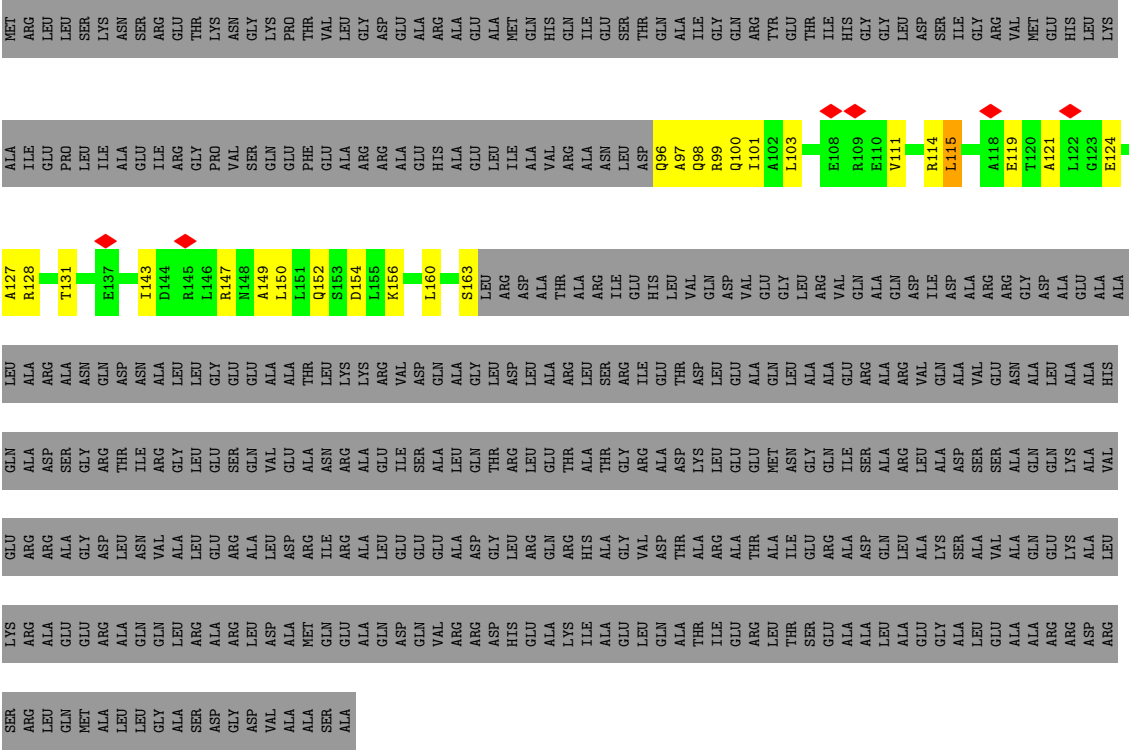
ALA	ILE	ASN	LEU	LEU	LEU	ALA	ARG	ILE	ALA	MET
	GLU	GLY	ALA	ALA	GLN	VAL	VAL	GLY	GLU	ARG
	ARG	GLN	ALA	GLU	GLN	GLN	GLN	GLU	PRO	LEU
	ALA	ILE	ARG	ARG	ALA	GLN	ALA	SER	LEU	SER
	ASP	SER	ALA	ALA	ALA	GLN	ASP	ASP	ILE	LYS
	GLN	ALA	ARG	ARG	GLN	ASP	ASP	ALA	ASN	ASN
	367	LEU	VAL	VAL	ALA	ALA	ALA	GLN	ARG	ARG
	371	ASP	ALA	ALA	ALA	ALA	ARG	THR	GLY	THR
	375	SER	GLU	GLU	GLU	ARG	ARG	GLN	PRO	LYS
	380	SER	GLU	ASN	GLY	GLN	GLY	ASN	VAL	ASN
	383	GLN	ALA	ALA	ASP	ALA	ASP	ALA	SER	GLY
	386	LYS	ALA	LEU	GLU	LEU	GLU	ALA	GLN	LYS
	391	VAL	HIS	HIS	ALA	ALA	ALA	ASP	GLU	THR
	392	ARG	GLN	GLN	ALA	ALA	ALA	ALA	ARG	LEU
	393	ARG	ASP	ASP	ARG	ARG	ARG	LEU	ARG	ASP
	397	ALA	SER	SER	ALA	ALA	ALA	GLU	ALA	GLU
	403	GLY	GLY	GLY	ASN	ILE	ASN	ILE	HIS	ARG
	407	ASP	ARG	LEU	GLN	GLY	GLN	VAL	GLU	VAL
	414	LEU	LEU	LEU	ALA	GLY	LEU	ALA	ALA	ALA
	415	LEU	GLU	GLU	GLY	GLY	LEU	LEU	VAL	GLY
	416	ARG	SER	SER	ALA	GLN	LYS	ARG	ARG	GLN
	417	ALA	GLN	GLN	ALA	GLU	SER	ALA	ILE	GLN
	418	LEU	VAL	VAL	ALA	ALA	SER	ASN	GLU	GLY
	419	ASP	GLU	GLU	ALA	THR	LEU	ASP	LEU	SER
	422	ARG	ALA	ALA	THR	LEU	LEU	LYS	ASN	THR
	431	ILE	ASN	ASN	LYS	LEU	LYS	VAL	GLN	GLN
	434	ARG	ALA	ALA	LYS	VAL	SER	ALA	ALA	ILE
	435	LEU	ALA	ALA	LYS	SER	SER	ARG	GLN	GLY
	436	GLU	GLU	ILE	VAL	VAL	ARG	LEU	GLN	GLN
	437	GLU	SER	SER	ASP	ASP	ASP	ASP	ILE	GLY
	438	ALA	ALA	ALA	GLU	ALA	ALA	SER	ALA	TYR
	439	GLY	THR	THR	LEU	LEU	ARG	ASP	LEU	GLY
	443	ARG	LEU	LEU	GLY	THR	ALA	ALA	GLY	GLY
	443	GLN	GLU	GLU	ALA	THR	THR	THR	GLU	GLY
	ALA	ARG	ALA	ALA	ARG	ALA	ALA	ARG	LEU	LEU
	LEU	HIS	THR	THR	LEU	LEU	LEU	GLU	ARG	ASP
	LEU	ALA	ALA	ALA	SER	ILE	ILE	VAL	VAL	GLY
	GLY	GLY	GLY	GLY	GLY	ILE	GLY	SER	ILE	ILE
	ALA	VAL	ARG	ARG	ILE	HIS	HIS	ALA	GLY	ARG
	SER	ASP	ALA	ALA	GLU	LEU	LEU	ARG	ARG	VAL
	ASP	THR	ASP	ASP	THR	THR	THR	VAL	LEU	VAL
	GLY	ALA	LYS	LYS	ASP	GLN	GLN	ASP	ALA	GLU
	ASP	ARG	GLU	GLU	LEU	LEU	LEU	VAL	ALA	HIS
	VAL	ALA	LEU	LEU	GLU	GLU	GLU	VAL	ALA	GLY
	ALA	THR	ALA	ALA	GLU	GLU	GLN	GLU	THR	LYS
	ALA	ALA	MET	MET	ALA	ALA	ALA	GLY	THR	ALA

- Molecule 1: Crescentin

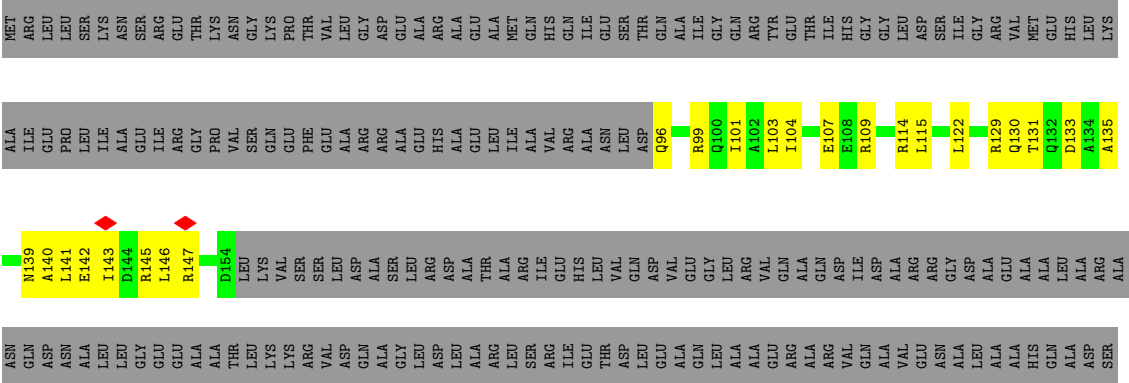
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● Molecule 1: Crescentin

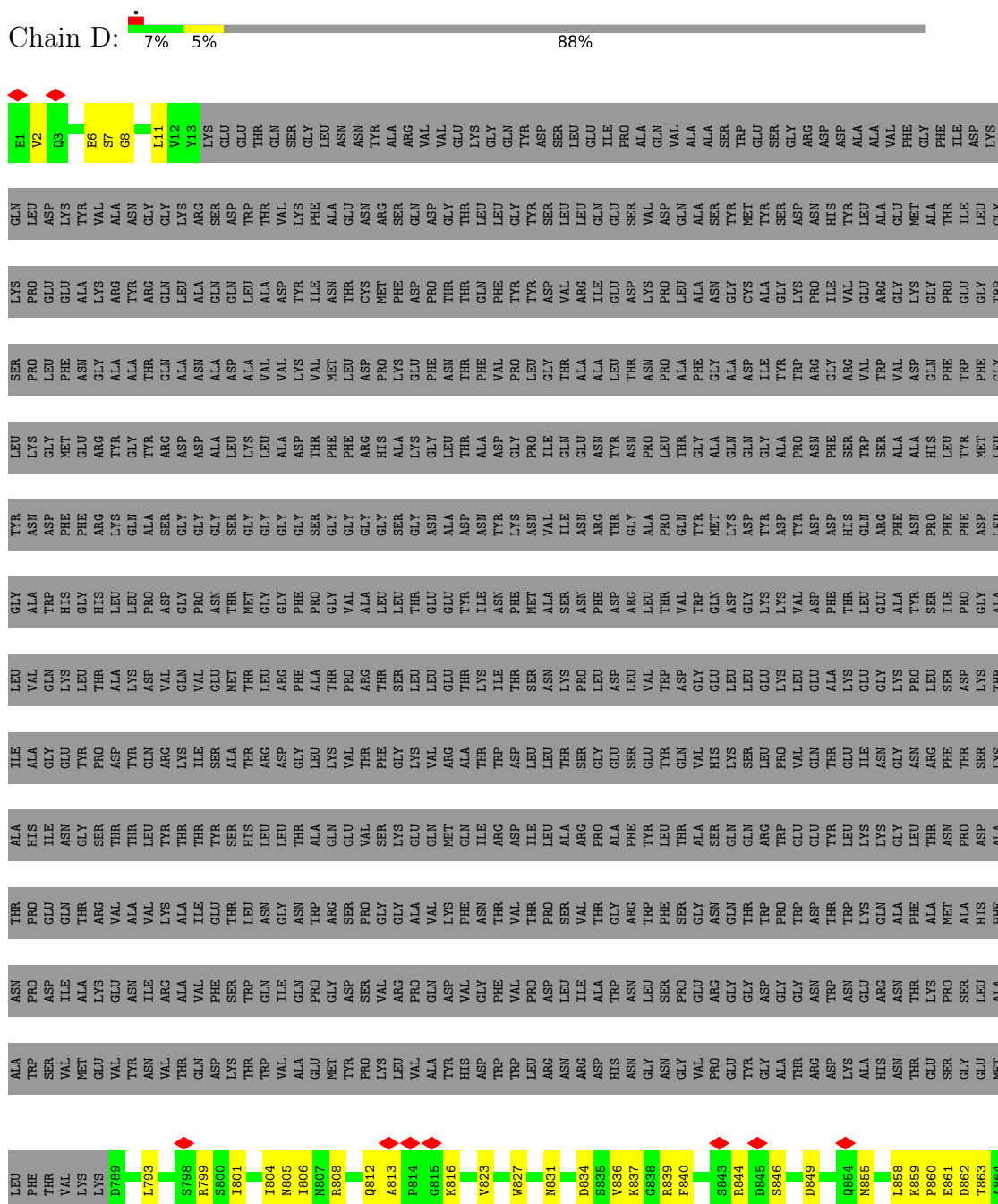


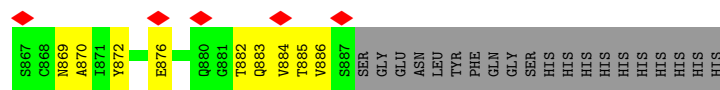
● Molecule 1: Crescentin



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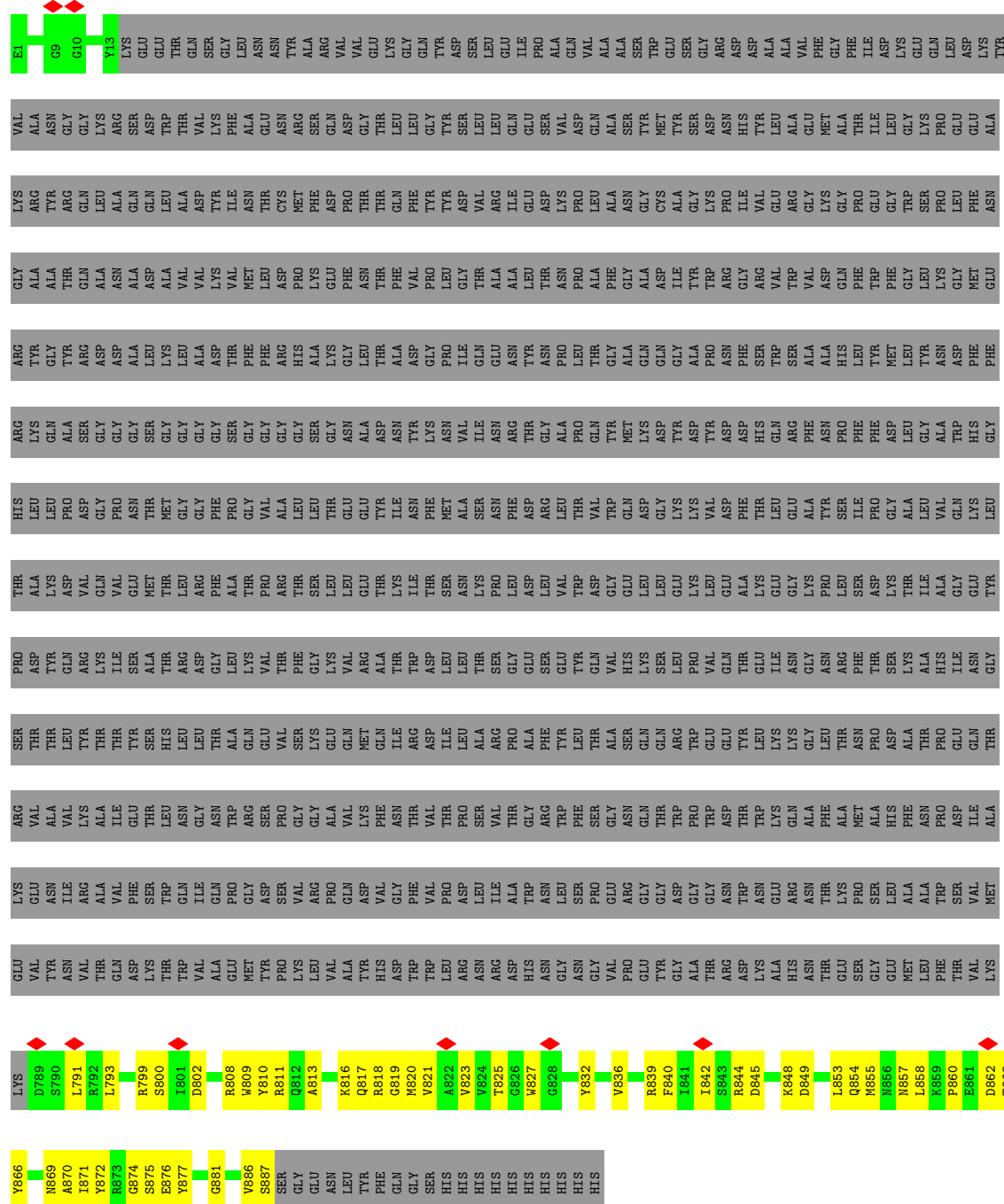
- Molecule 2: Crescentin-specific megabody MB13





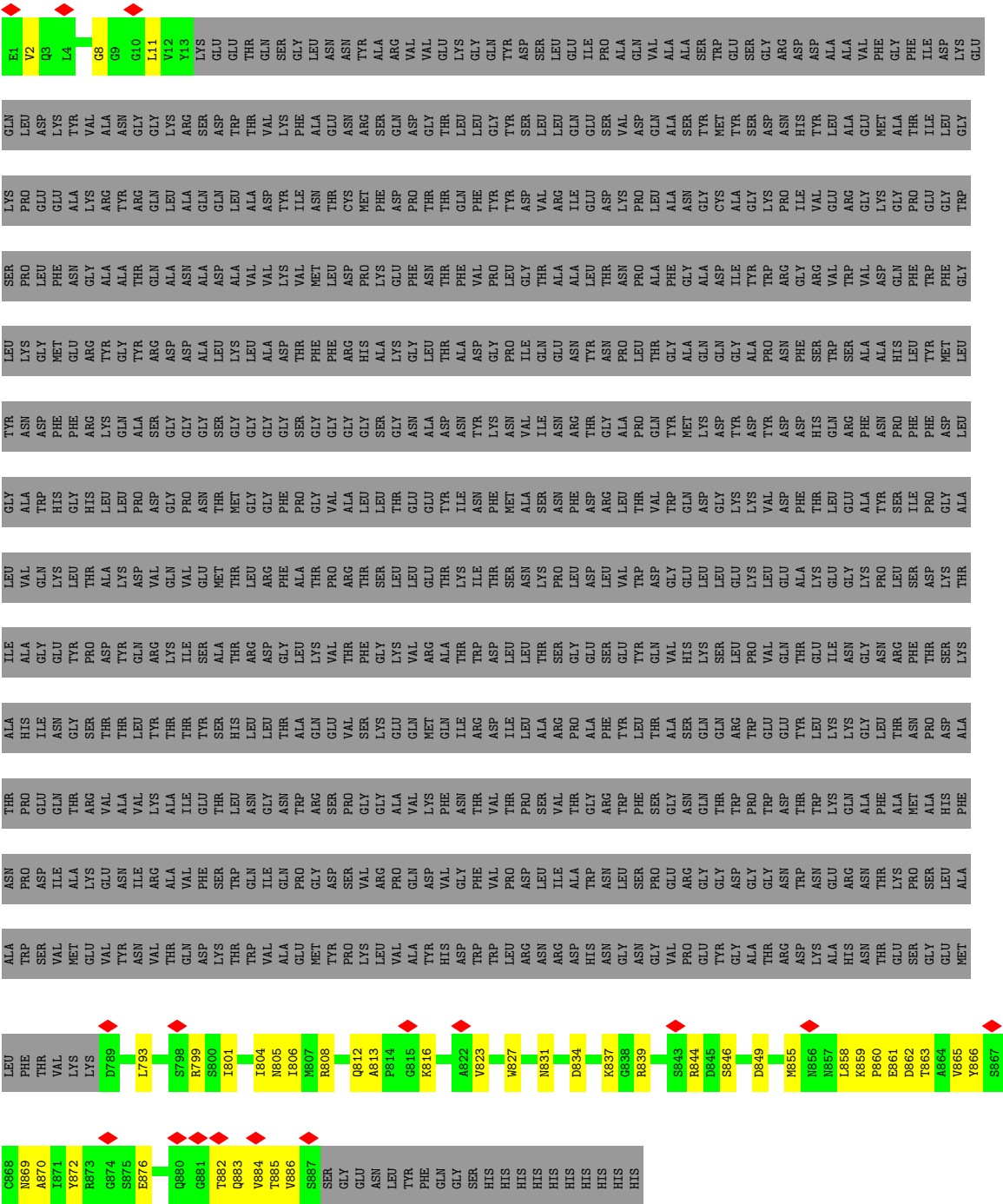
• Molecule 2: Crescentin-specific megabody MB13

Chain C: 7% 5% 88%

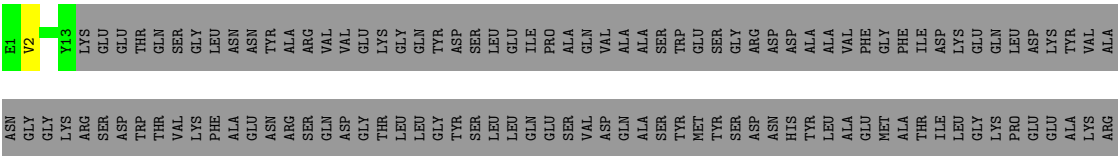


• Molecule 2: Crescentin-specific megabody MB13

Chain J: 8% 88%



● Molecule 2: Crescentin-specific megabody MB13





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	550575	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 ($e^-/\text{\AA}^2$)	34	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.908	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.046	Depositor
Map size (Å)	432.0, 432.0, 432.0	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.728, 1.728, 1.728	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	0.25	0/605	0.40	0/806
1	B	0.26	0/605	0.42	0/806
1	E	0.28	0/517	0.44	0/696
1	F	0.24	0/454	0.42	0/611
1	G	0.25	0/605	0.40	0/806
1	H	0.26	0/605	0.42	0/806
1	K	0.28	0/517	0.44	0/696
1	L	0.24	0/454	0.42	0/611
2	C	0.31	0/883	0.55	0/1192
2	D	0.31	0/883	0.53	0/1192
2	I	0.31	0/883	0.55	0/1192
2	J	0.31	0/883	0.53	0/1192
All	All	0.28	0/7894	0.48	0/10606

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	A	605	0	620	20	0
1	B	605	0	620	18	0
1	E	518	0	515	28	0
1	F	455	0	447	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	605	0	620	20	0
1	H	605	0	620	18	0
1	K	518	0	515	28	0
1	L	455	0	447	19	0
2	C	869	0	846	37	0
2	D	869	0	846	34	0
2	I	869	0	846	39	0
2	J	869	0	846	32	0
All	All	7842	0	7788	276	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 276 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:K:111:VAL:HA	1:K:115:LEU:HB2	1.29	1.14
1:E:111:VAL:HA	1:E:115:LEU:HB2	1.29	1.10
1:K:111:VAL:HB	1:K:115:LEU:HD12	1.49	0.95
1:E:111:VAL:HB	1:E:115:LEU:HD12	1.49	0.92
1:K:111:VAL:CA	1:K:115:LEU:HB2	2.00	0.91

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	75/457 (16%)	72 (96%)	3 (4%)	0	100	100
1	B	75/457 (16%)	73 (97%)	2 (3%)	0	100	100
1	E	66/457 (14%)	64 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	57/457 (12%)	57 (100%)	0	0	100	100
1	G	75/457 (16%)	72 (96%)	3 (4%)	0	100	100
1	H	75/457 (16%)	73 (97%)	2 (3%)	0	100	100
1	K	66/457 (14%)	64 (97%)	2 (3%)	0	100	100
1	L	57/457 (12%)	57 (100%)	0	0	100	100
2	C	108/907 (12%)	88 (82%)	20 (18%)	0	100	100
2	D	108/907 (12%)	95 (88%)	13 (12%)	0	100	100
2	I	108/907 (12%)	89 (82%)	19 (18%)	0	100	100
2	J	108/907 (12%)	94 (87%)	14 (13%)	0	100	100
All	All	978/7284 (13%)	898 (92%)	80 (8%)	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	58/345 (17%)	58 (100%)	0	100	100
1	B	58/345 (17%)	58 (100%)	0	100	100
1	E	53/345 (15%)	51 (96%)	2 (4%)	28	49
1	F	45/345 (13%)	45 (100%)	0	100	100
1	G	58/345 (17%)	58 (100%)	0	100	100
1	H	58/345 (17%)	58 (100%)	0	100	100
1	K	53/345 (15%)	51 (96%)	2 (4%)	28	49
1	L	45/345 (13%)	45 (100%)	0	100	100
2	C	94/749 (13%)	94 (100%)	0	100	100
2	D	94/749 (13%)	94 (100%)	0	100	100
2	I	94/749 (13%)	94 (100%)	0	100	100
2	J	94/749 (13%)	94 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	804/5756 (14%)	800 (100%)	4 (0%)	85	90

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

Mol	Chain	Res	Type
1	E	114	ARG
1	E	115	LEU
1	K	114	ARG
1	K	115	LEU

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

Mol	Chain	Res	Type
2	C	854	GLN
2	I	854	GLN

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 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.

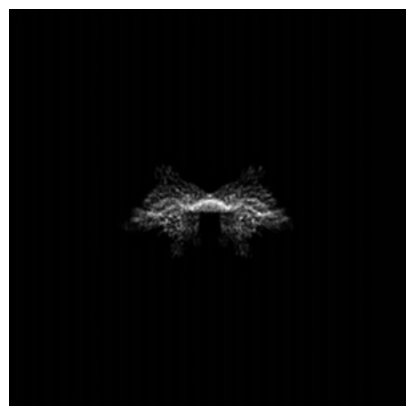
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15402. These allow visual inspection of the internal detail of the map and identification of artifacts.

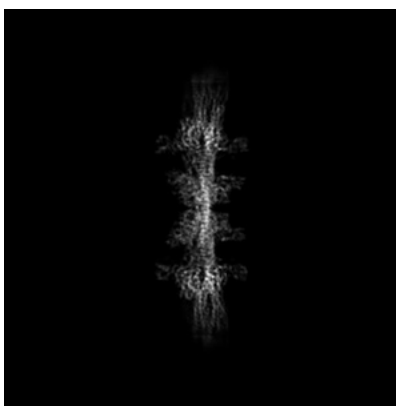
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

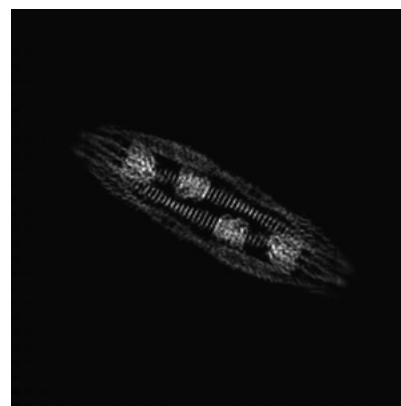
6.1.1 Primary map



X

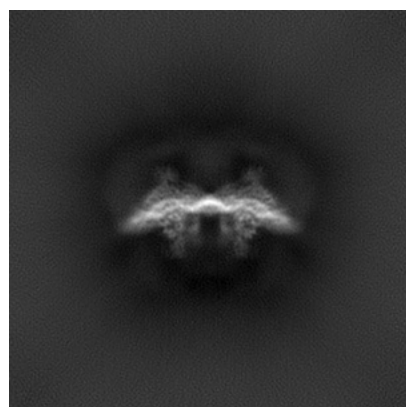


Y

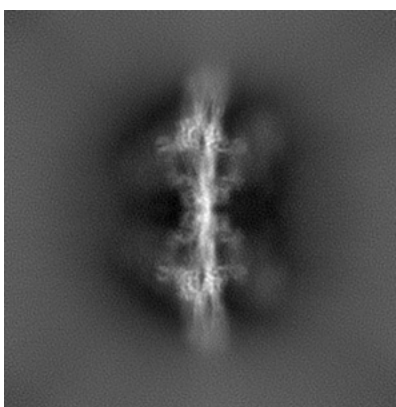


Z

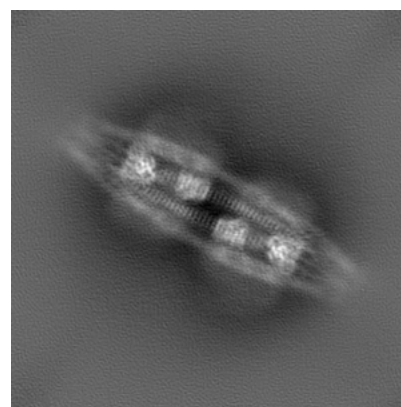
6.1.2 Raw map



X



Y

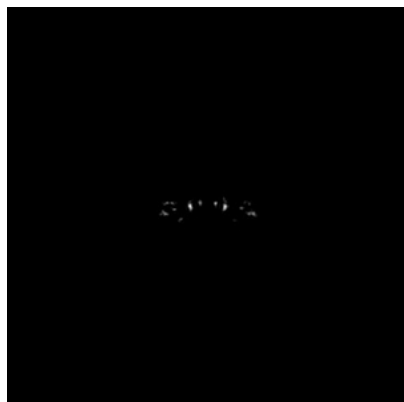


Z

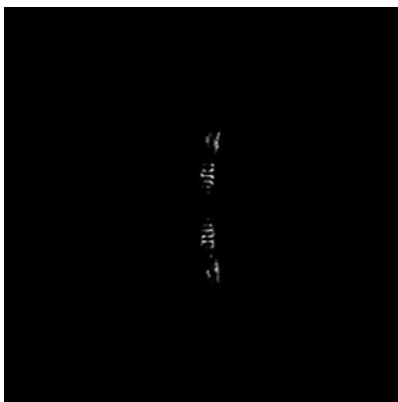
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 125

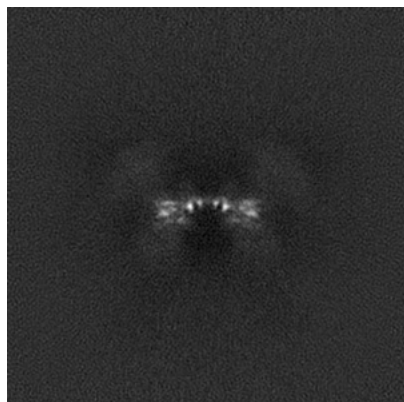


Y Index: 125

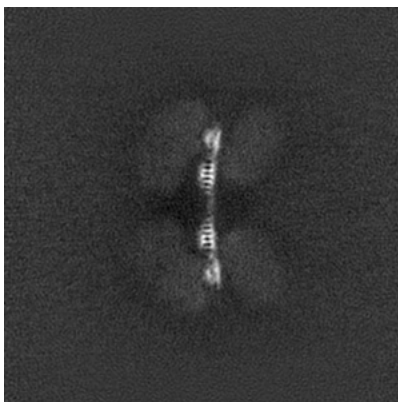


Z Index: 125

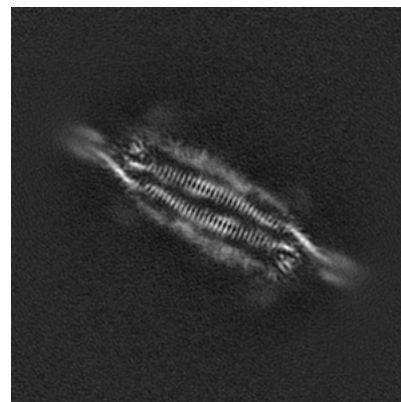
6.2.2 Raw map



X Index: 125



Y Index: 125



Z Index: 125

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: 82

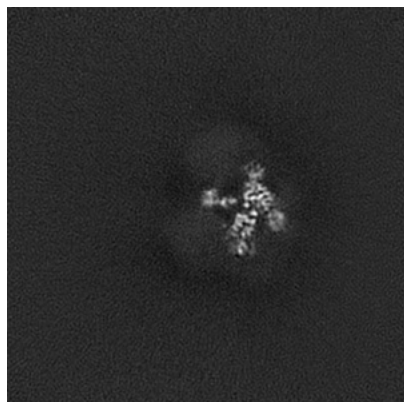


Y Index: 144

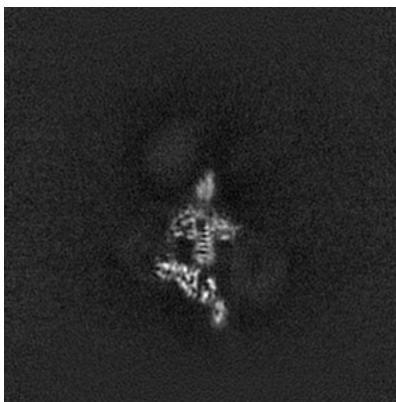


Z Index: 126

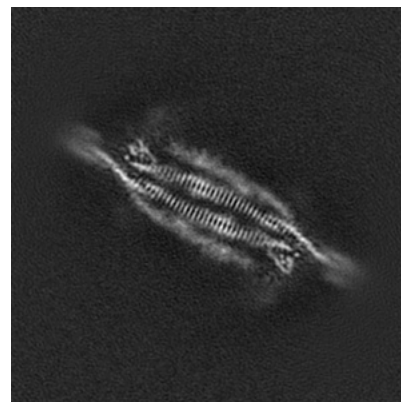
6.3.2 Raw map



X Index: 82



Y Index: 144

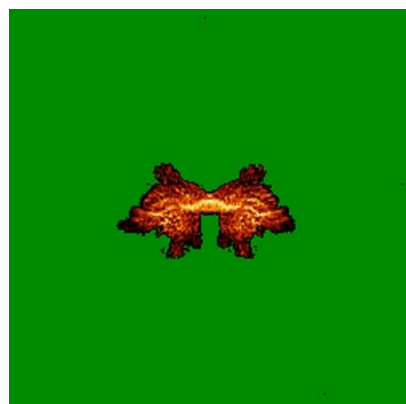


Z Index: 126

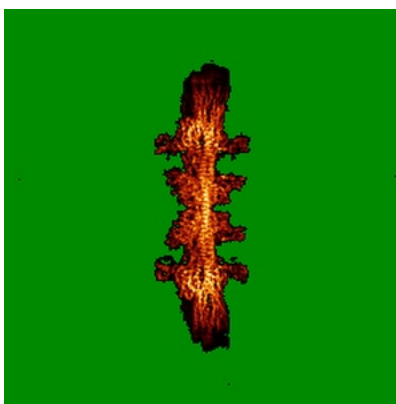
The images above show the largest variance slices of the map in three orthogonal directions.

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

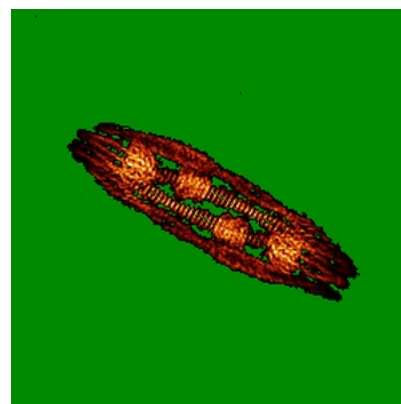
6.4.1 Primary map



X

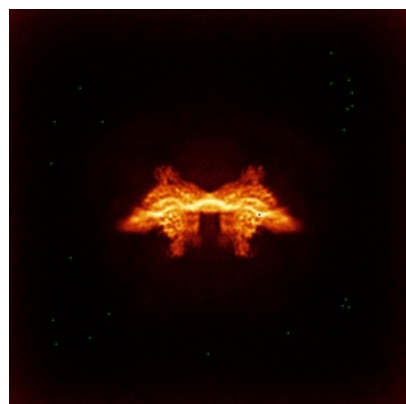


Y

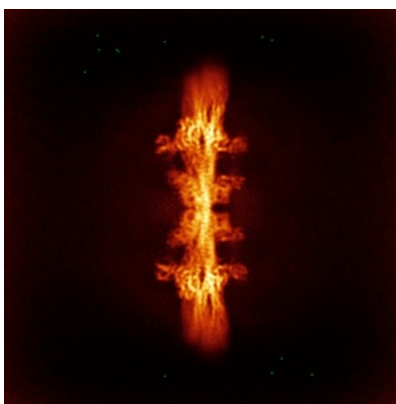


Z

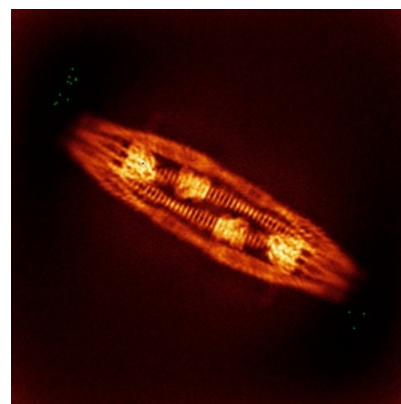
6.4.2 Raw map



X



Y

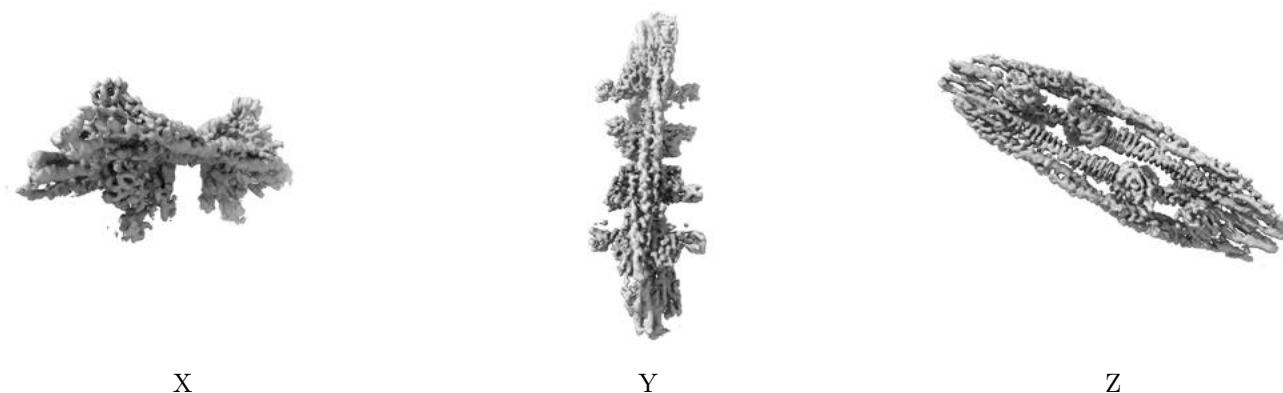


Z

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.

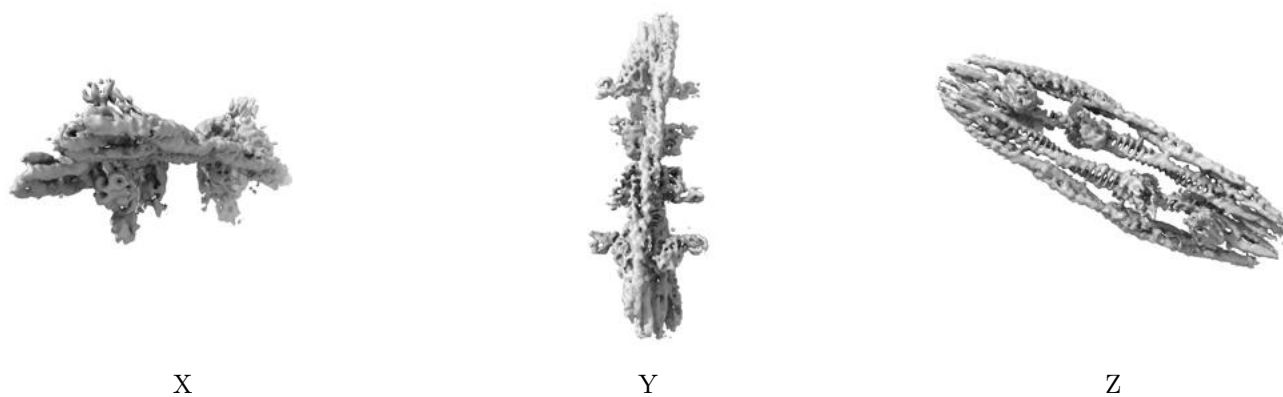
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.046. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

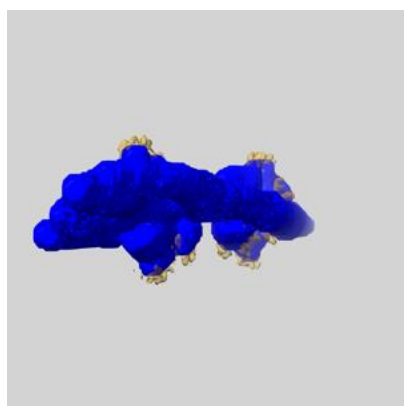
6.6 Mask visualisation [i](#)

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

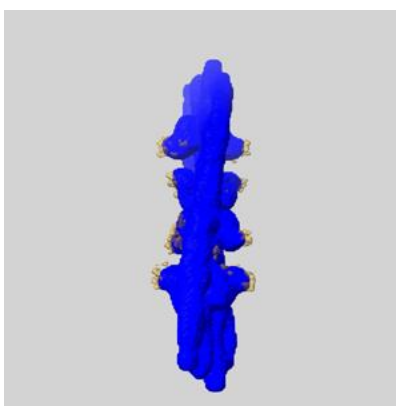
A mask typically either:

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

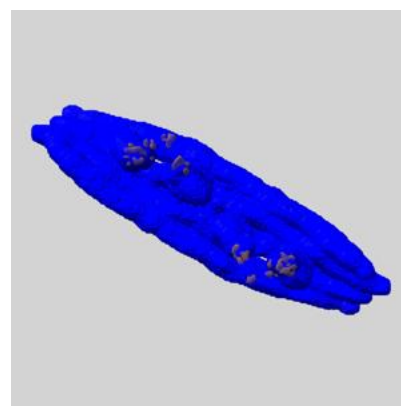
6.6.1 emd_15402_msk_1.map [i](#)



X



Y

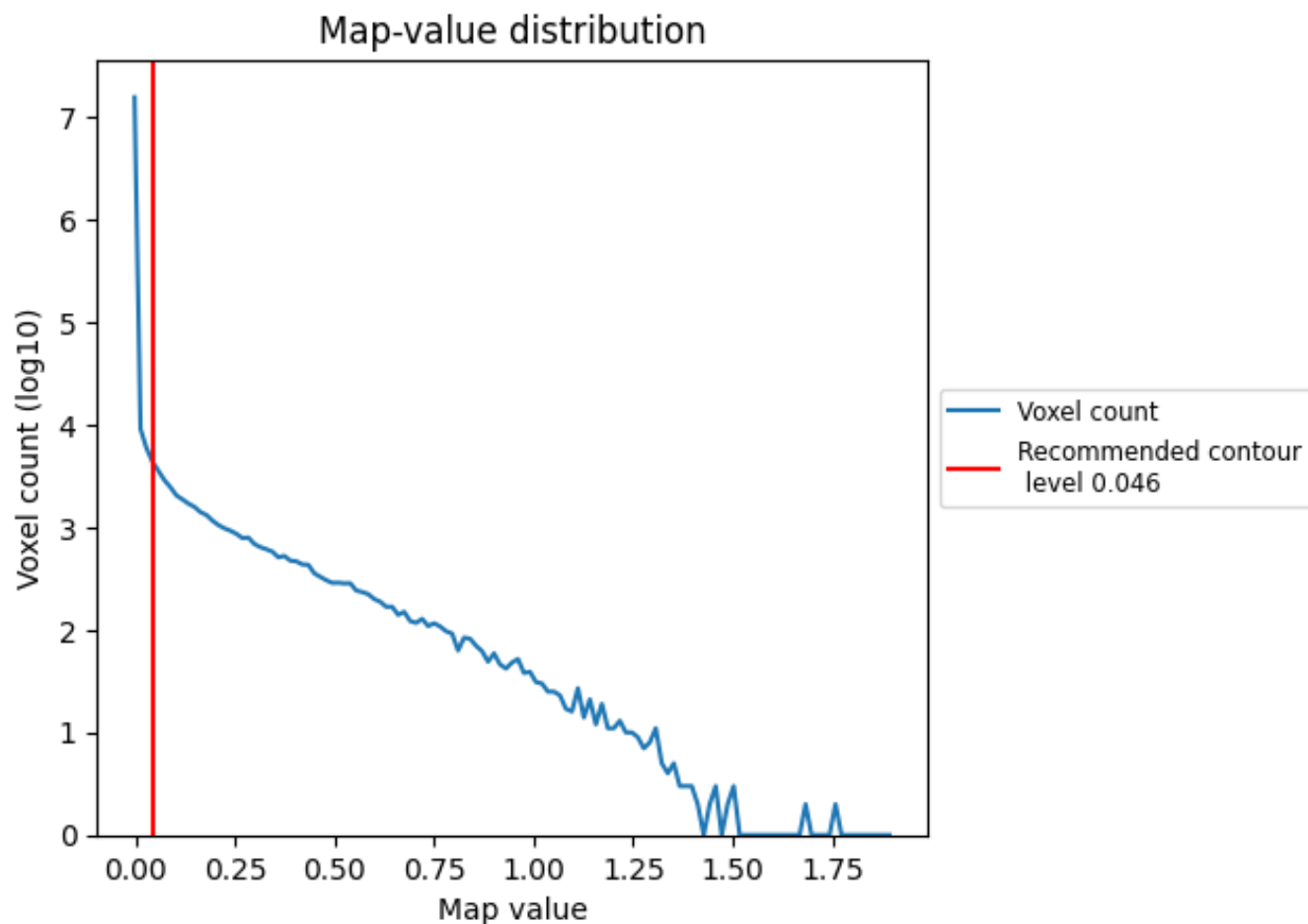


Z

7 Map analysis ⓘ

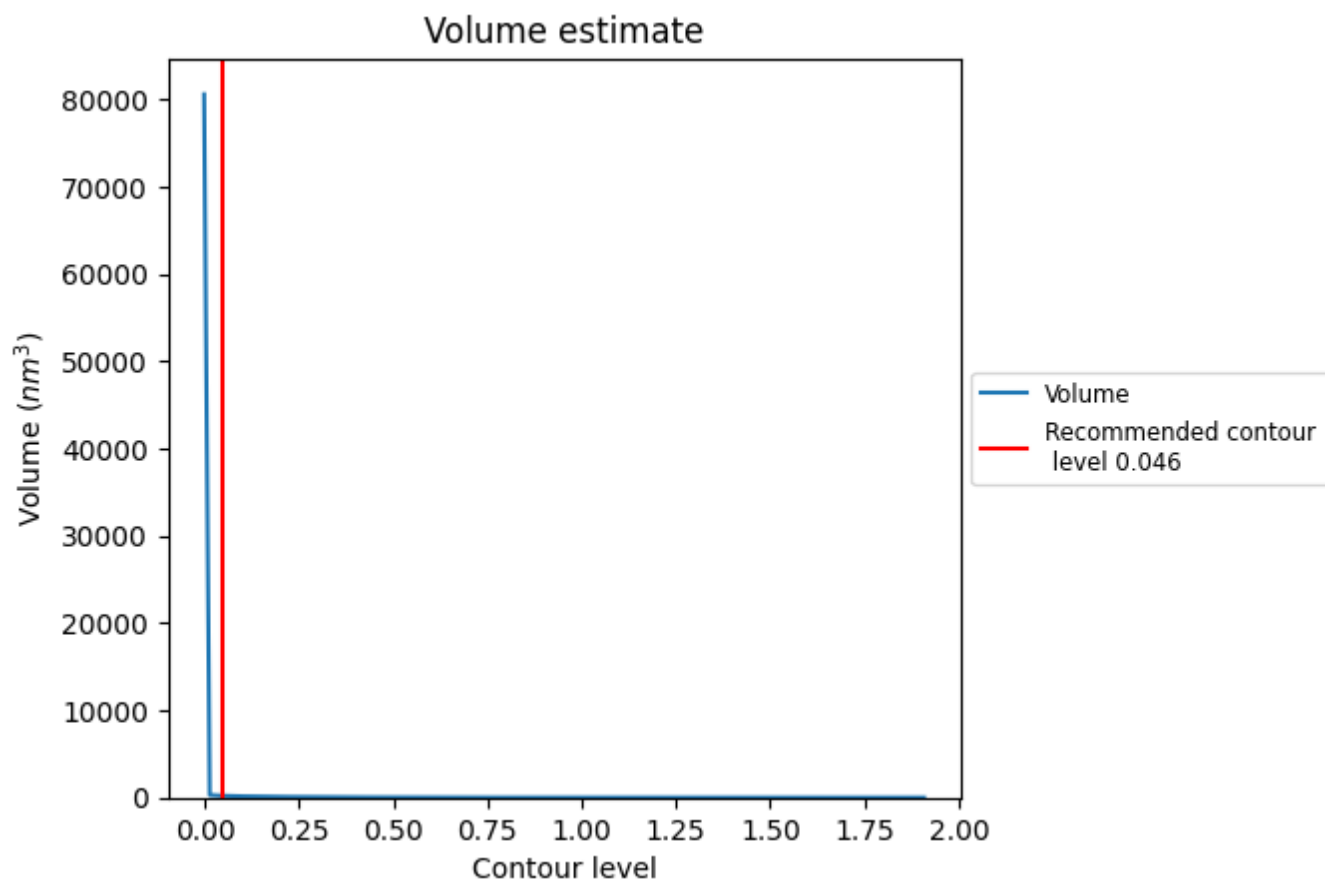
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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.

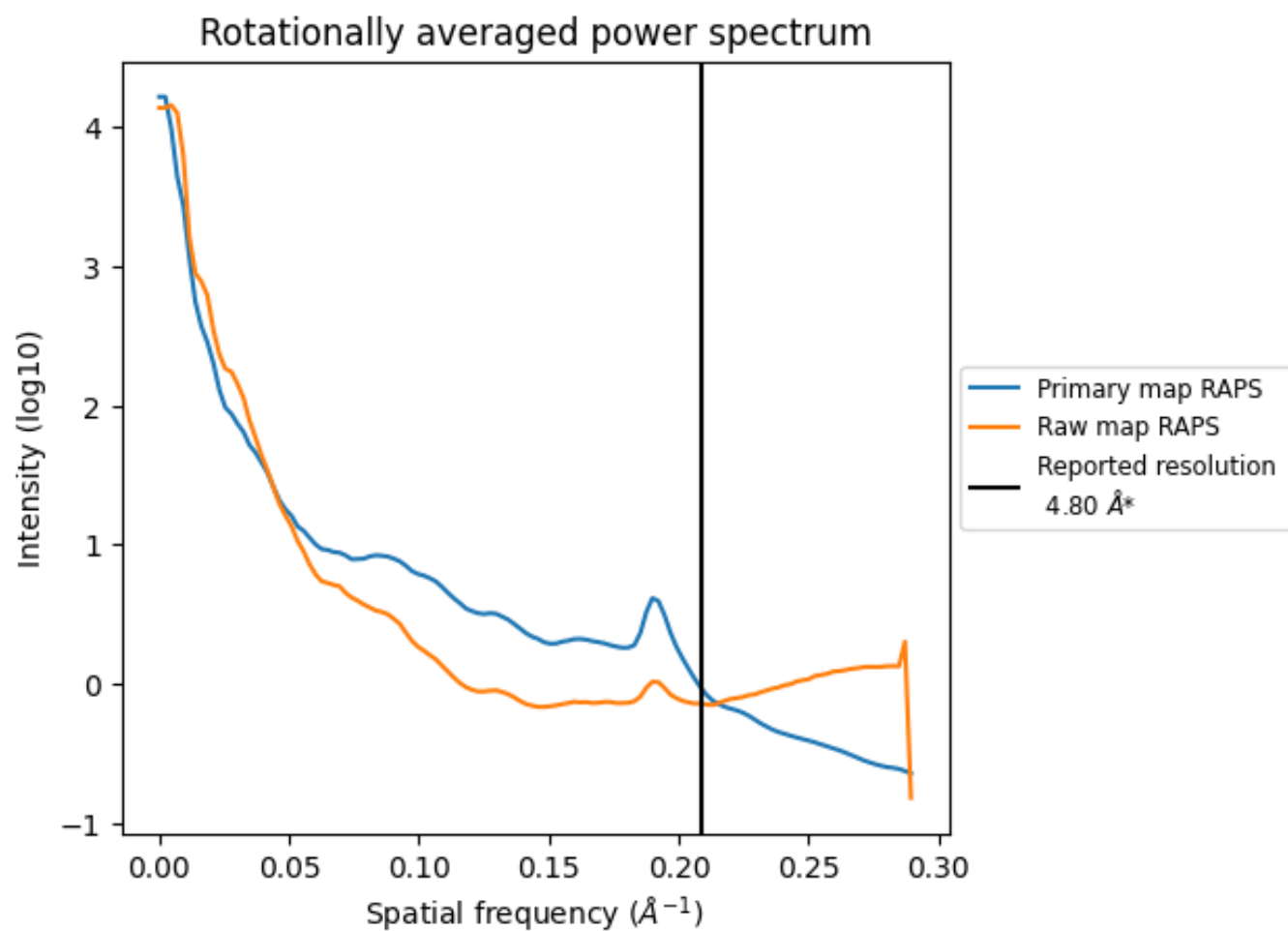
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 207 nm³; this corresponds to an approximate mass of 187 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 ⓘ

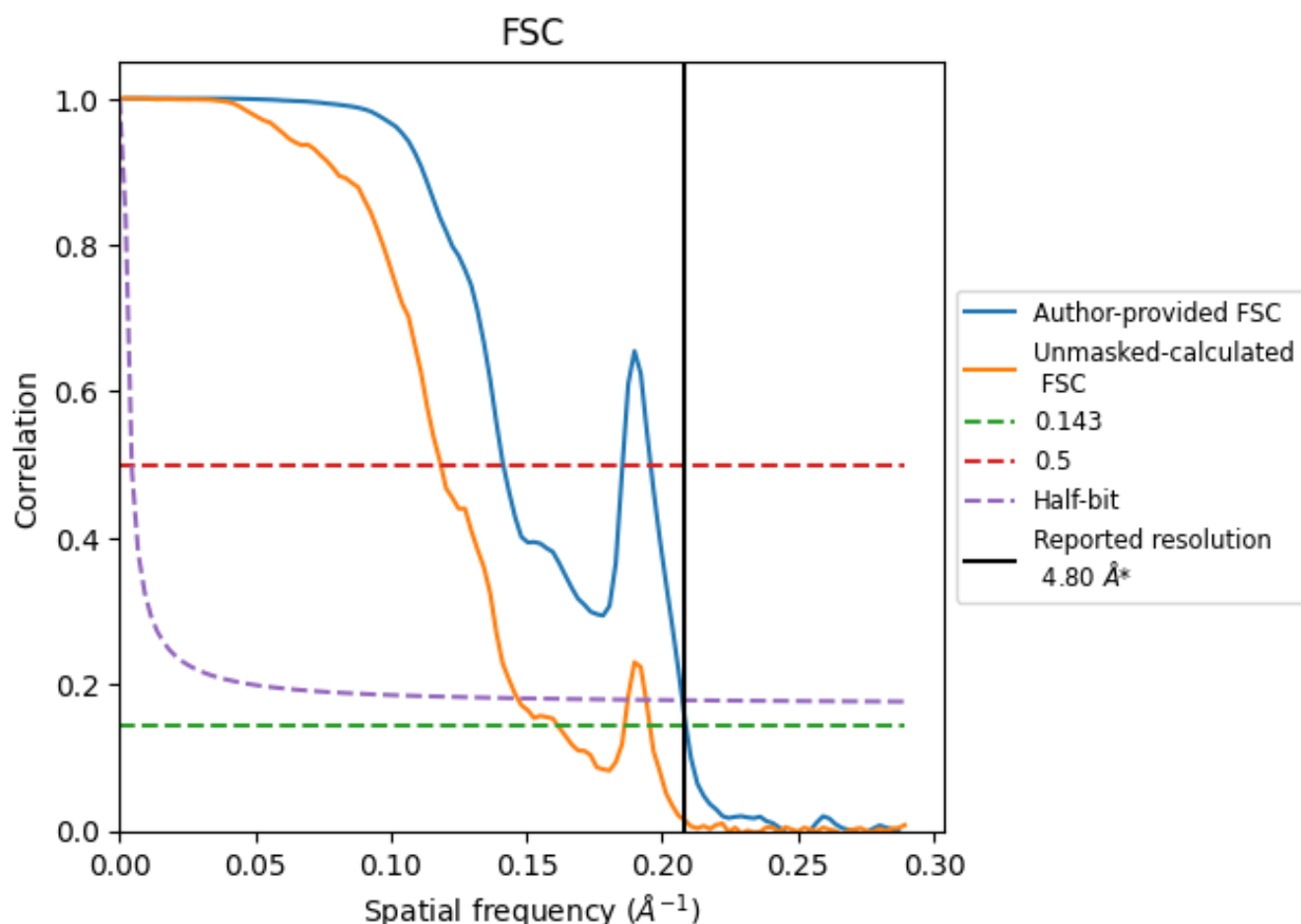


*Reported resolution corresponds to spatial frequency of 0.208 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.208 Å⁻¹

8.2 Resolution estimates [i](#)

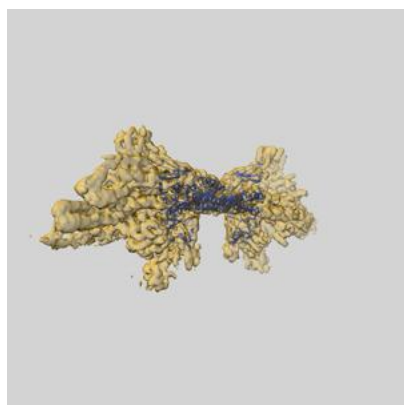
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.80	-	-
Author-provided FSC curve	4.79	7.07	4.82
Unmasked-calculated*	6.19	8.45	6.82

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.19 differs from the reported value 4.8 by more than 10 %

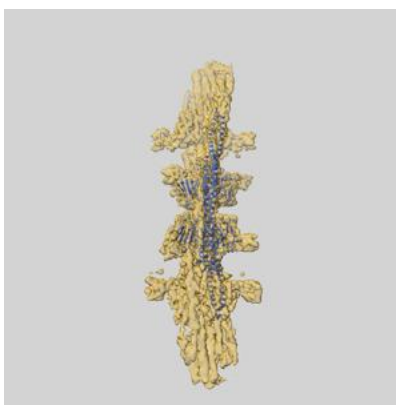
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15402 and PDB model 8AFM. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

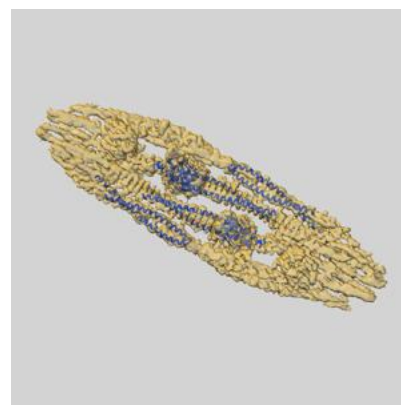
9.1 Map-model overlay [i](#)



X



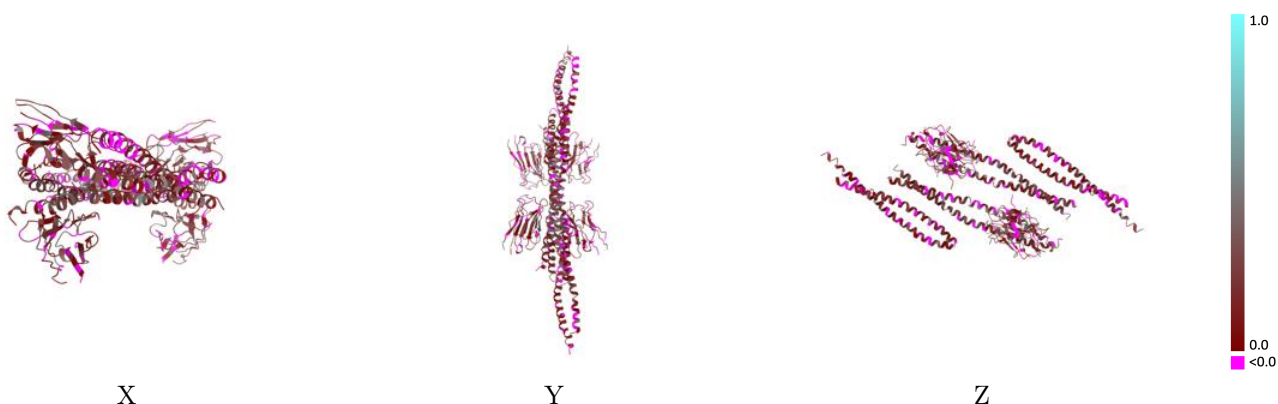
Y



Z

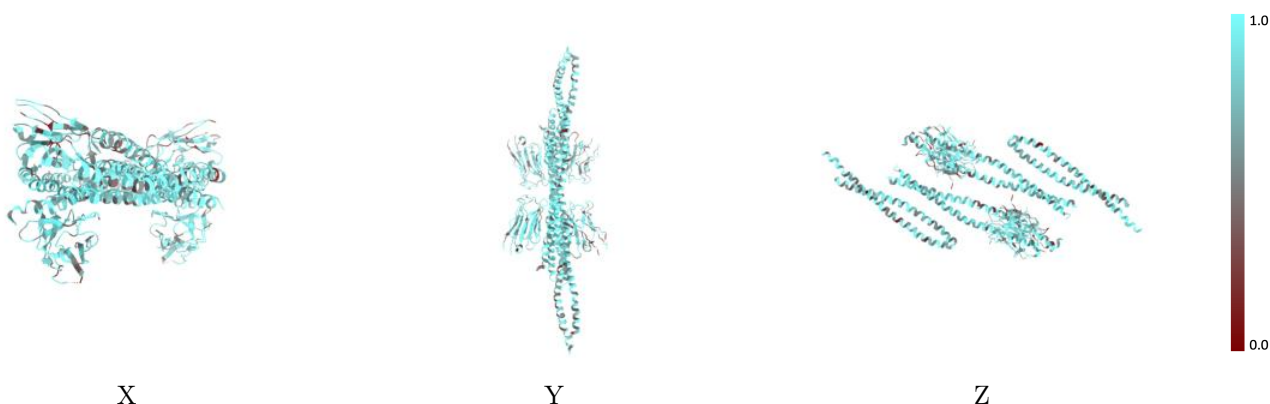
The images above show the 3D surface view of the map at the recommended contour level 0.046 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



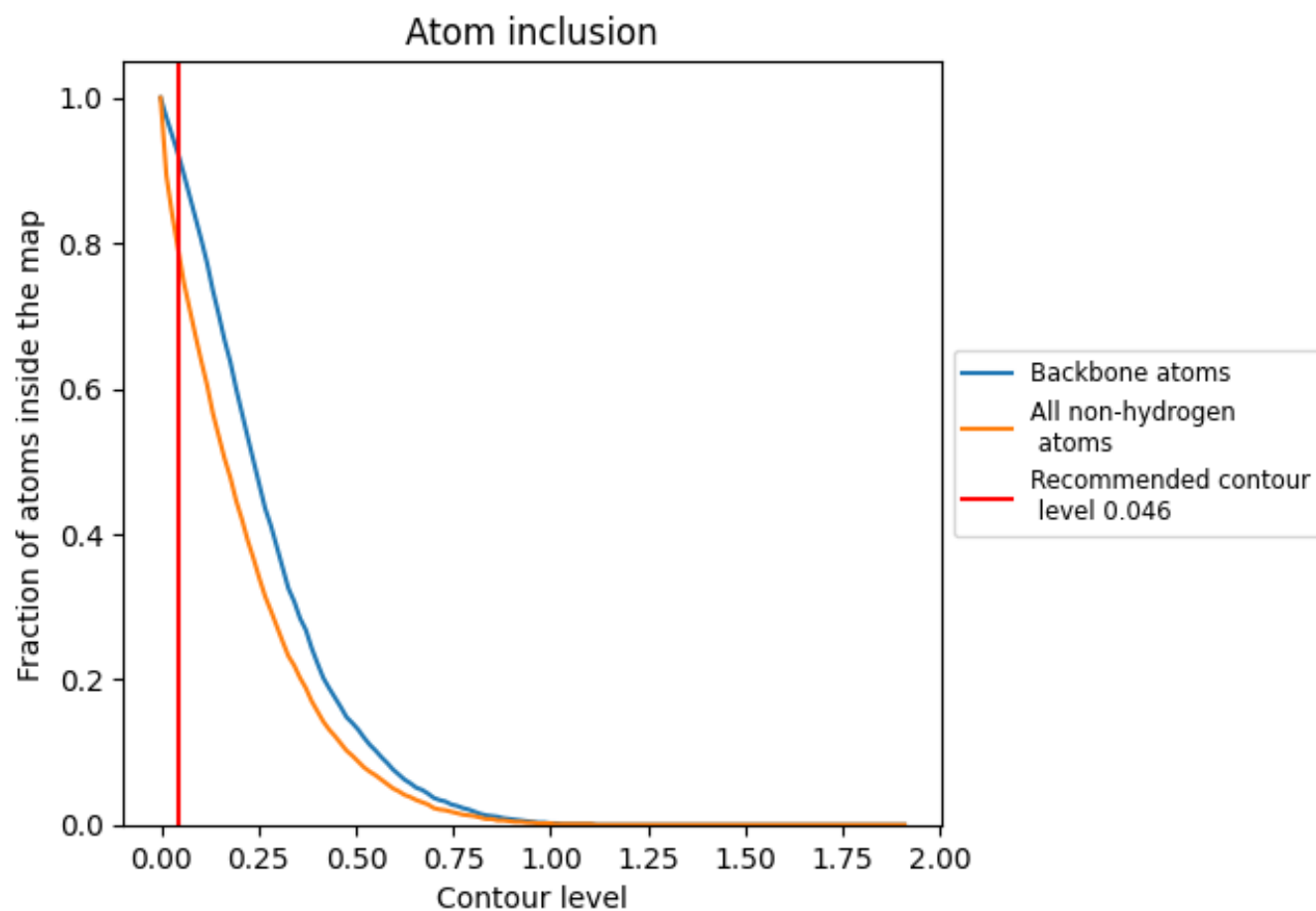
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.046).

9.4 Atom inclusion ⓘ



At the recommended contour level, 92% of all backbone atoms, 78% 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 (0.046) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.7830</div>	<div><div></div>0.1640</div>
A	<div><div></div>0.8530</div>	<div><div></div>0.2180</div>
B	<div><div></div>0.8420</div>	<div><div></div>0.2100</div>
C	<div><div></div>0.7940</div>	<div><div></div>0.1780</div>
D	<div><div></div>0.7090</div>	<div><div></div>0.1390</div>
E	<div><div></div>0.7280</div>	<div><div></div>0.1050</div>
F	<div><div></div>0.7550</div>	<div><div></div>0.1120</div>
G	<div><div></div>0.8300</div>	<div><div></div>0.2160</div>
H	<div><div></div>0.8200</div>	<div><div></div>0.1810</div>
I	<div><div></div>0.8290</div>	<div><div></div>0.1930</div>
J	<div><div></div>0.7130</div>	<div><div></div>0.1470</div>
K	<div><div></div>0.7660</div>	<div><div></div>0.1190</div>
L	<div><div></div>0.7710</div>	<div><div></div>0.1110</div>

1.0

0.0

<0.0