



wwPDB EM Validation Summary Report ⓘ

Feb 13, 2024 – 08:58 pm GMT

PDB ID : 8AJB
EMDB ID : EMD-15476
Title : Cryo-EM structure of crescentin filaments (stutter mutant, C2 symmetry and large box)
Authors : Liu, Y.; Lowe, J.
Deposited on : 2022-07-28
Resolution : 4.30 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.dev70
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

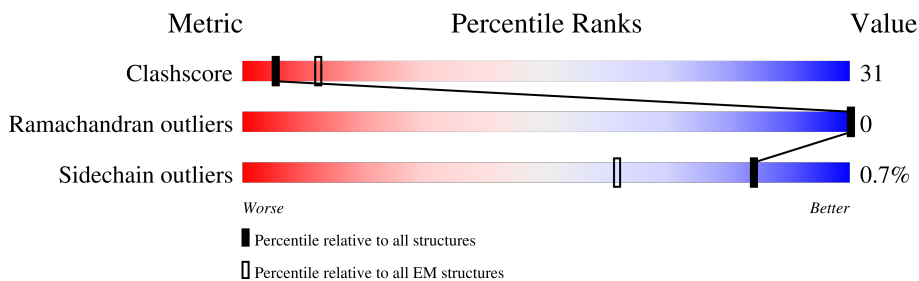
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 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	460	
1	B	460	
1	C	460	
1	D	460	
1	G	460	
1	H	460	
1	I	460	
1	J	460	

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Mol	Chain	Length	Quality of chain
1	M	460	30% 23% 47%
1	N	460	33% 19% 48%
1	O	460	30% 20% 49%
1	P	460	31% 19% 49%
1	S	460	17% 17% 66%
1	T	460	18% 17% 65%
1	U	460	12% 13% 74%
1	V	460	16% 10% 74%
2	E	907	5% 8% 88%
2	F	907	5% 7% 88%
2	K	907	5% 8% 88%
2	L	907	5% 7% 88%
2	Q	907	5% 8% 88%
2	R	907	5% 7% 88%
2	W	907	5% 8% 88%
2	X	907	5% 7% 88%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 30088 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
			Total	C	N	O	S		
1	A	245	Total 1876	C 1127	N 366	O 382	S 1	0	0
1	B	238	Total 1828	C 1099	N 358	O 370	S 1	0	0
1	C	234	Total 1793	C 1065	N 364	O 361	S 3	0	0
1	D	234	Total 1793	C 1065	N 364	O 361	S 3	0	0
1	G	155	Total 1203	C 727	N 234	O 241	S 1	0	0
1	H	163	Total 1264	C 764	N 244	O 255	S 1	0	0
1	I	120	Total 934	C 555	N 192	O 185	S 2	0	0
1	J	120	Total 934	C 555	N 192	O 185	S 2	0	0
1	M	245	Total 1876	C 1127	N 366	O 382	S 1	0	0
1	N	238	Total 1828	C 1099	N 358	O 370	S 1	0	0
1	O	234	Total 1793	C 1065	N 364	O 361	S 3	0	0
1	P	234	Total 1793	C 1065	N 364	O 361	S 3	0	0
1	S	155	Total 1203	C 727	N 234	O 241	S 1	0	0
1	T	163	Total 1264	C 764	N 244	O 255	S 1	0	0
1	U	120	Total 934	C 555	N 192	O 185	S 2	0	0
1	V	120	Total 934	C 555	N 192	O 185	S 2	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	406	SER	-	insertion	UNP A0A8F8EC09
A	407	ALA	-	insertion	UNP A0A8F8EC09
A	408	THR	-	insertion	UNP A0A8F8EC09
B	406	SER	-	insertion	UNP A0A8F8EC09
B	407	ALA	-	insertion	UNP A0A8F8EC09
B	408	THR	-	insertion	UNP A0A8F8EC09
C	406	SER	-	insertion	UNP A0A8F8EC09
C	407	ALA	-	insertion	UNP A0A8F8EC09
C	408	THR	-	insertion	UNP A0A8F8EC09
D	406	SER	-	insertion	UNP A0A8F8EC09
D	407	ALA	-	insertion	UNP A0A8F8EC09
D	408	THR	-	insertion	UNP A0A8F8EC09
G	406	SER	-	insertion	UNP A0A8F8EC09
G	407	ALA	-	insertion	UNP A0A8F8EC09
G	408	THR	-	insertion	UNP A0A8F8EC09
H	406	SER	-	insertion	UNP A0A8F8EC09
H	407	ALA	-	insertion	UNP A0A8F8EC09
H	408	THR	-	insertion	UNP A0A8F8EC09
I	406	SER	-	insertion	UNP A0A8F8EC09
I	407	ALA	-	insertion	UNP A0A8F8EC09
I	408	THR	-	insertion	UNP A0A8F8EC09
J	406	SER	-	insertion	UNP A0A8F8EC09
J	407	ALA	-	insertion	UNP A0A8F8EC09
J	408	THR	-	insertion	UNP A0A8F8EC09
M	406	SER	-	insertion	UNP A0A8F8EC09
M	407	ALA	-	insertion	UNP A0A8F8EC09
M	408	THR	-	insertion	UNP A0A8F8EC09
N	406	SER	-	insertion	UNP A0A8F8EC09
N	407	ALA	-	insertion	UNP A0A8F8EC09
N	408	THR	-	insertion	UNP A0A8F8EC09
O	406	SER	-	insertion	UNP A0A8F8EC09
O	407	ALA	-	insertion	UNP A0A8F8EC09
O	408	THR	-	insertion	UNP A0A8F8EC09
P	406	SER	-	insertion	UNP A0A8F8EC09
P	407	ALA	-	insertion	UNP A0A8F8EC09
P	408	THR	-	insertion	UNP A0A8F8EC09
S	406	SER	-	insertion	UNP A0A8F8EC09
S	407	ALA	-	insertion	UNP A0A8F8EC09
S	408	THR	-	insertion	UNP A0A8F8EC09
T	406	SER	-	insertion	UNP A0A8F8EC09
T	407	ALA	-	insertion	UNP A0A8F8EC09
T	408	THR	-	insertion	UNP A0A8F8EC09
U	406	SER	-	insertion	UNP A0A8F8EC09

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Chain	Residue	Modelled	Actual	Comment	Reference
U	407	ALA	-	insertion	UNP A0A8F8EC09
U	408	THR	-	insertion	UNP A0A8F8EC09
V	406	SER	-	insertion	UNP A0A8F8EC09
V	407	ALA	-	insertion	UNP A0A8F8EC09
V	408	THR	-	insertion	UNP A0A8F8EC09

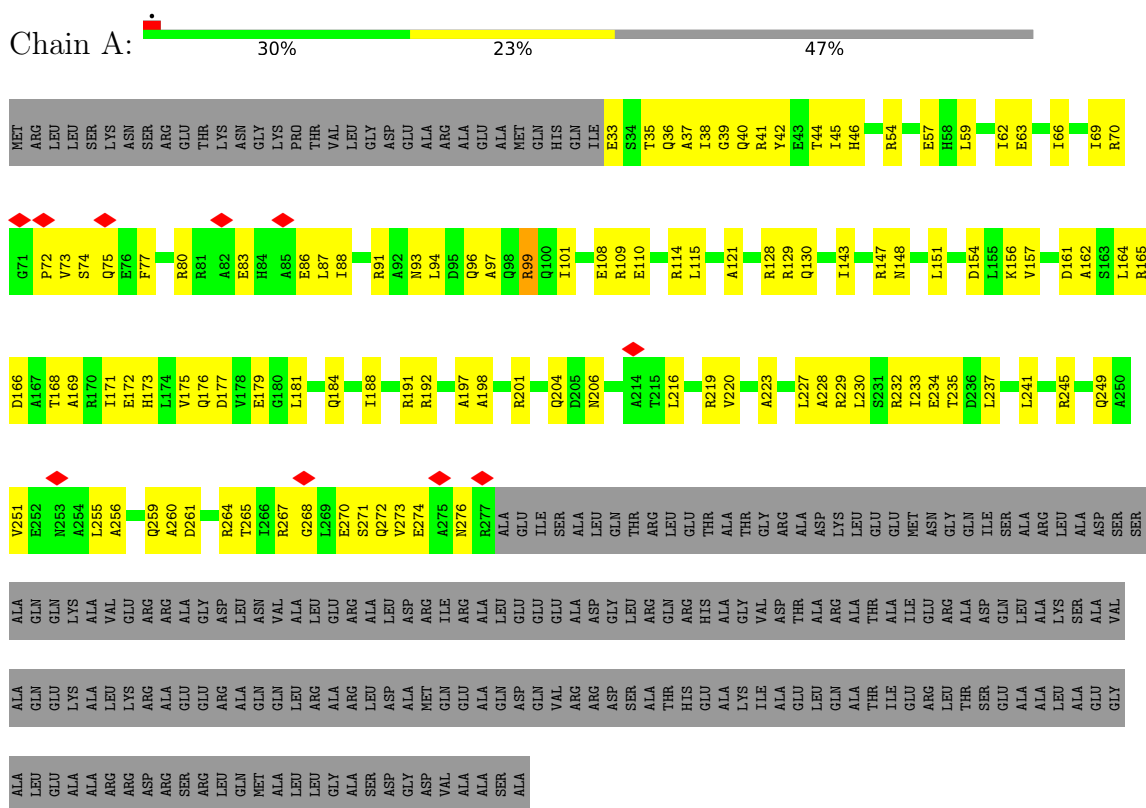
- Molecule 2 is a protein called Crescentin-specific megabody MB13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	E	112	869	539	155	170	5	0	0
2	F	111	861	535	154	167	5	0	0
2	K	112	869	539	155	170	5	0	0
2	L	105	820	508	148	159	5	0	0
2	Q	112	869	539	155	170	5	0	0
2	R	111	861	535	154	167	5	0	0
2	W	112	869	539	155	170	5	0	0
2	X	105	820	508	148	159	5	0	0

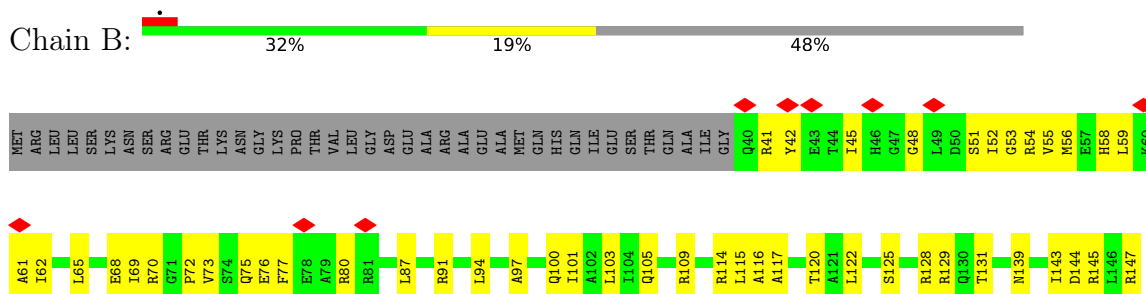
3 Residue-property plots [i](#)

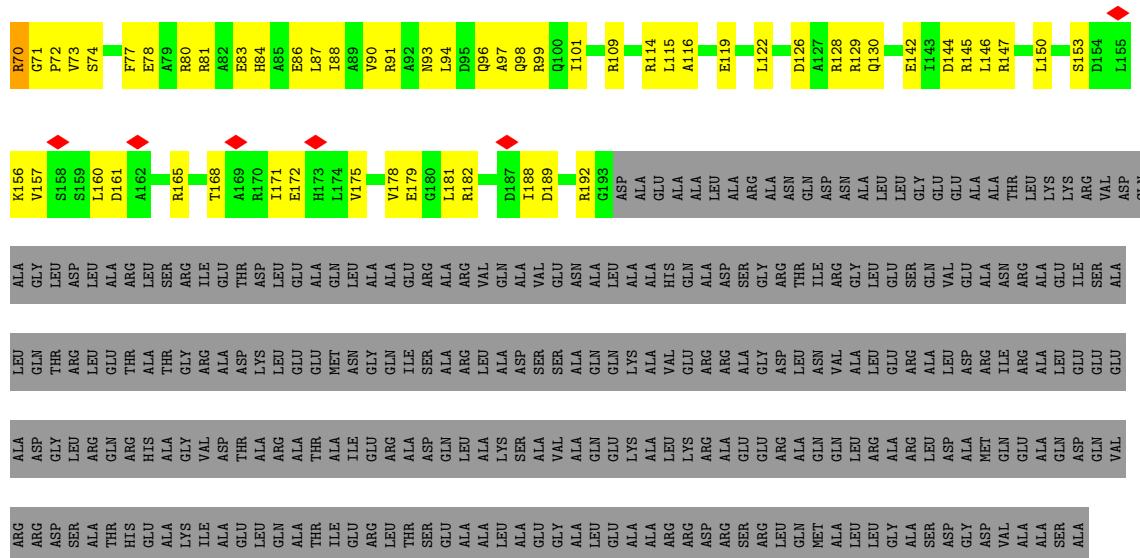
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



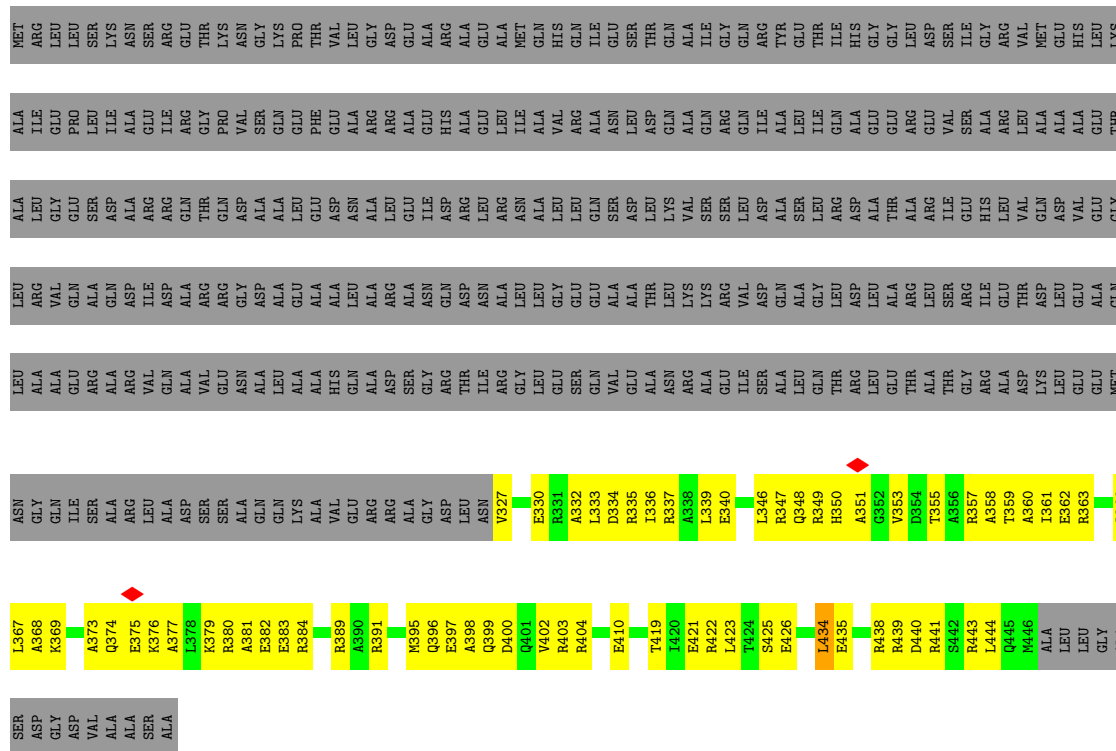
- Molecule 1: Crescentin





- Molecule 1: Crescentin

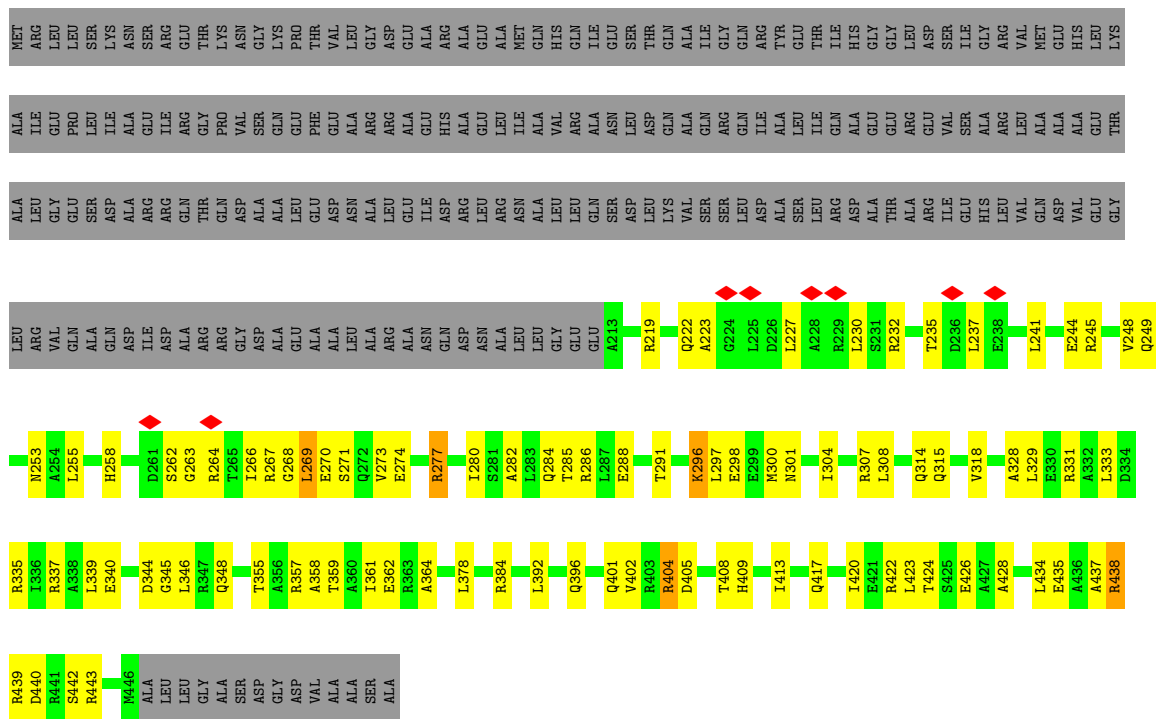
Chain I: 12% 14% 74%



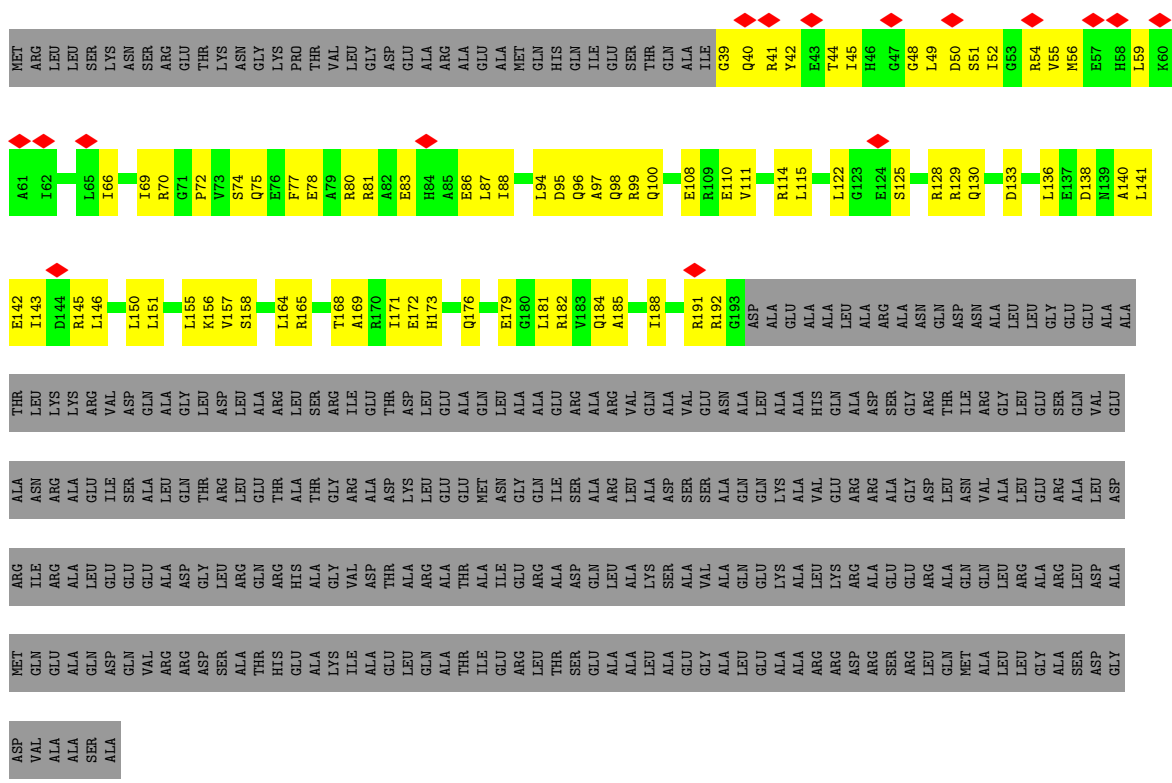
- Molecule 1: Crescentin

Chain J: 15% 10% 74%



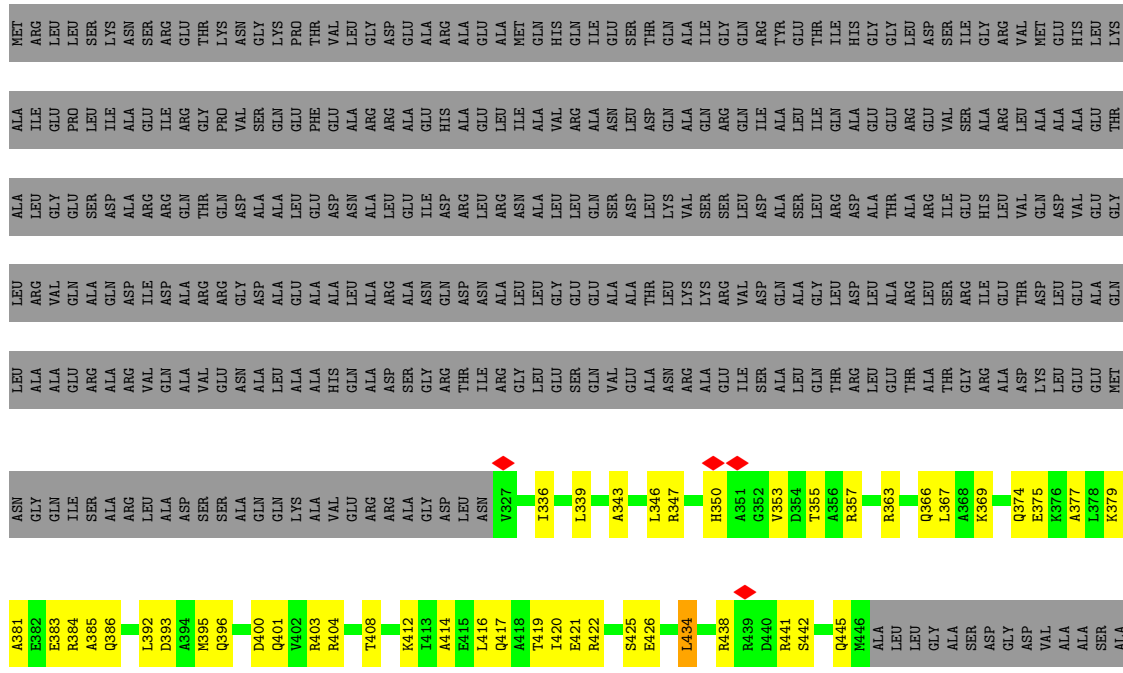


• Molecule 1: Crescentin



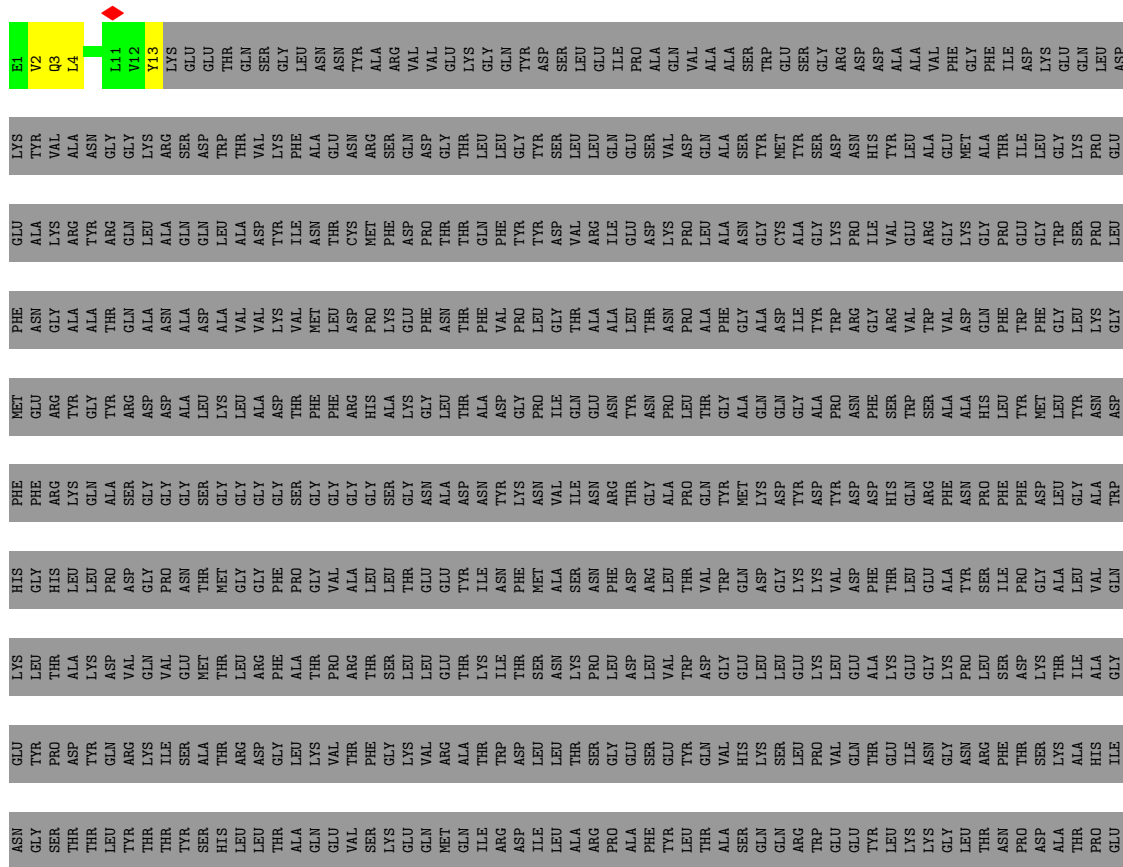
• Molecule 1: Crescentin

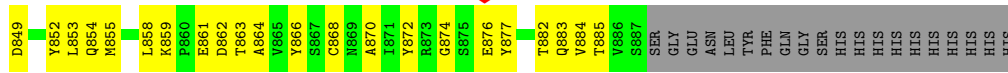
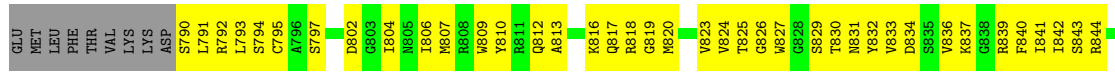




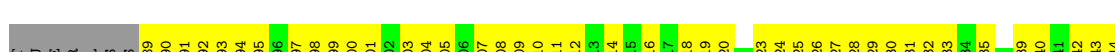
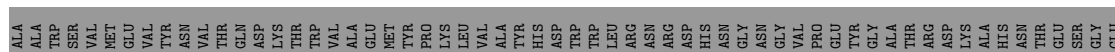
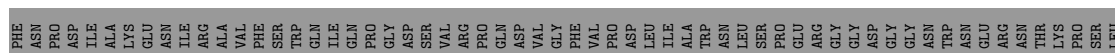
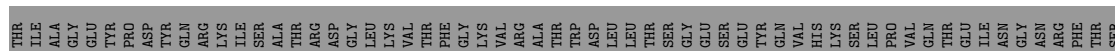
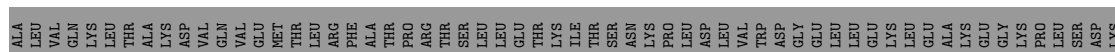
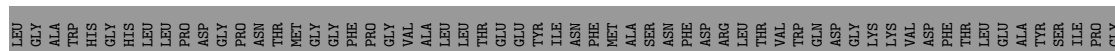
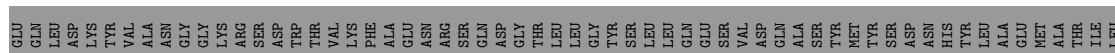
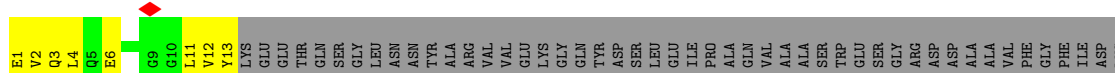
● Molecule 2: Crescentin-specific megabody MB13

Chain E: 5% 8% 88%



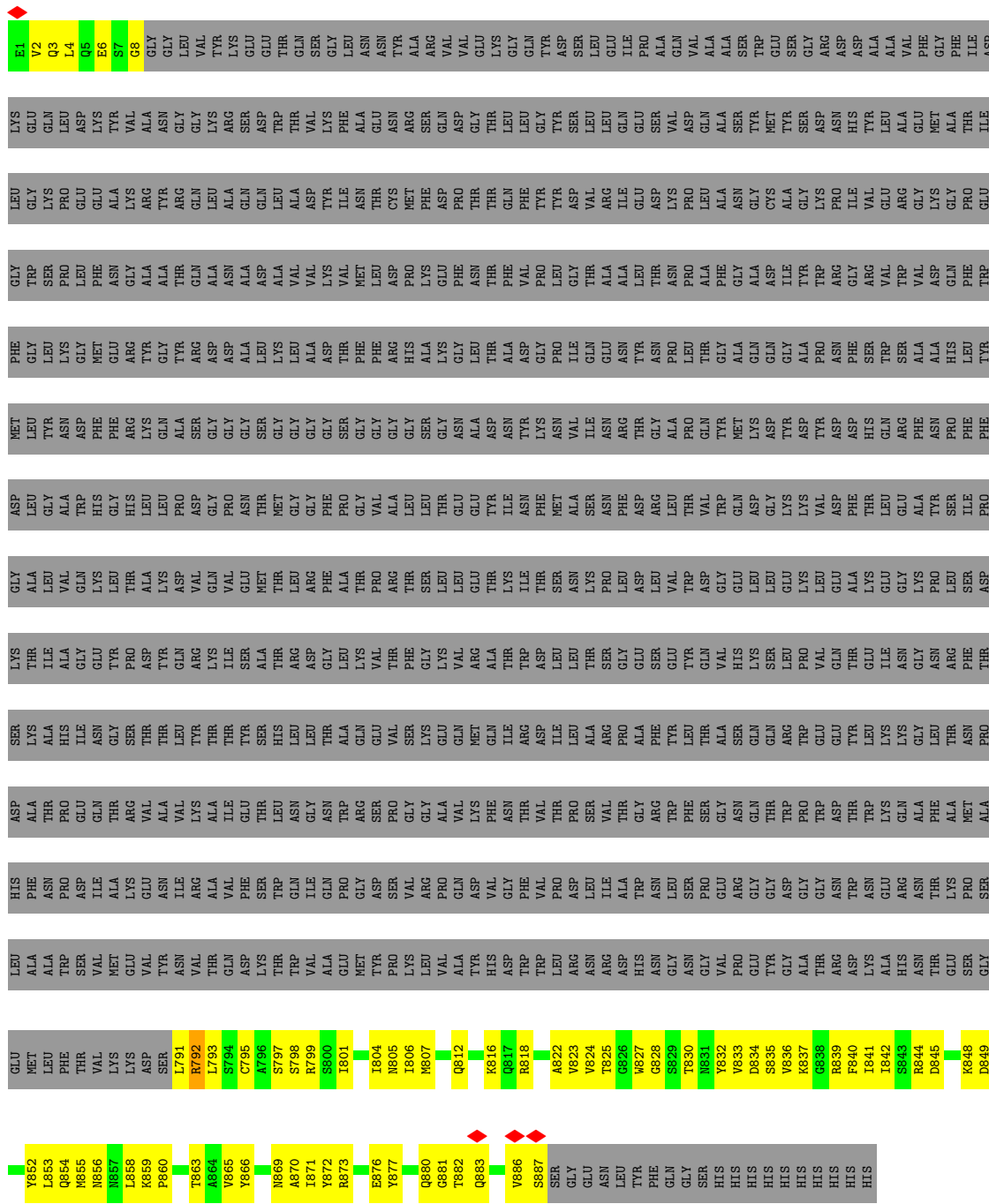


● Molecule 2: Crescentin-specific megabody MB13



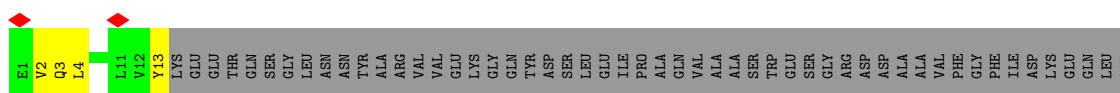
● Molecule 2: Crescentin-specific megabody MB13

Chain L: 7% 88%



● Molecule 2: Crescentin-specific megabody MB13

Chain Q: 5% 8%



ASP
ALA
THR
PRO
GLU
SER
GLN
THR
ARG
VAL
ASN
ALA
VAL
LYS
ALA
ILE
GLU
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LEU
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ASN
TRP
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GLY
ARG
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THR
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S797
S798
R799
S800
I801
I804
N805
I806
M807
Q812
K816
Q817
R818
A822
V823
V824
T825
G826
W827
S829
T830
N831
Y832
V833
D834
S835
V836
K837
G838
R839
F840
I841
I842
S843
R844
D845
K848
D849

Y852
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M855
N856
M857
L858
K859
P860
T863
A864
V865
Y866
N869
A870
I871
Y872
R873
E876
Y877
Q880
G881
T882
Q883
V886
S887
SER
GLY
GLU
ASN
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	585252	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 ($e^-/\text{\AA}^2$)	53	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.736	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.022	Depositor
Map size (\AA)	954.0, 954.0, 954.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.59, 1.59, 1.59	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	0.35	0/1884	0.57	0/2540
1	B	0.34	0/1836	0.61	1/2475 (0.0%)
1	C	0.31	0/1795	0.60	2/2407 (0.1%)
1	D	0.31	0/1795	0.57	1/2407 (0.0%)
1	G	0.34	0/1210	0.60	0/1630
1	H	0.36	0/1271	0.61	0/1713
1	I	0.33	0/935	0.57	1/1251 (0.1%)
1	J	0.32	0/935	0.56	1/1251 (0.1%)
1	M	0.35	0/1884	0.57	0/2540
1	N	0.34	0/1836	0.61	1/2475 (0.0%)
1	O	0.31	0/1795	0.60	2/2407 (0.1%)
1	P	0.31	0/1795	0.57	1/2407 (0.0%)
1	S	0.34	0/1210	0.60	0/1630
1	T	0.35	0/1271	0.61	0/1713
1	U	0.33	0/935	0.57	1/1251 (0.1%)
1	V	0.32	0/935	0.56	1/1251 (0.1%)
2	E	0.52	0/883	0.64	0/1192
2	F	0.47	0/875	0.68	0/1181
2	K	0.44	0/883	0.58	0/1192
2	L	0.43	0/833	0.61	0/1124
2	Q	0.52	0/883	0.64	0/1192
2	R	0.46	0/875	0.68	0/1181
2	W	0.44	0/883	0.58	0/1192
2	X	0.43	0/833	0.61	0/1124
All	All	0.37	0/30270	0.60	12/40726 (0.0%)

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	434	LEU	CA-CB-CG	-6.42	100.54	115.30
1	J	434	LEU	CA-CB-CG	-6.41	100.56	115.30
1	O	308	LEU	CA-CB-CG	-6.15	101.15	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	308	LEU	CA-CB-CG	-6.14	101.17	115.30
1	N	208	LEU	CA-CB-CG	5.83	128.71	115.30

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	1876	0	1869	136	0
1	B	1828	0	1824	128	0
1	C	1793	0	1815	111	0
1	D	1793	0	1813	99	0
1	G	1203	0	1200	103	0
1	H	1264	0	1261	104	0
1	I	934	0	946	84	0
1	J	934	0	946	72	0
1	M	1876	0	1869	138	0
1	N	1828	0	1824	124	0
1	O	1793	0	1815	110	0
1	P	1793	0	1813	102	0
1	S	1203	0	1200	102	0
1	T	1264	0	1261	103	0
1	U	934	0	946	82	0
1	V	934	0	946	72	0
2	E	869	0	846	83	0
2	F	861	0	842	71	0
2	K	869	0	846	119	0
2	L	820	0	802	77	0
2	Q	869	0	846	81	0
2	R	861	0	842	72	0
2	W	869	0	846	117	0
2	X	820	0	802	76	0
All	All	30088	0	30020	1875	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 31.

The worst 5 of 1875 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:K:804:ILE:HB	2:K:872:TYR:CZ	1.30	1.66
2:K:804:ILE:HD13	2:K:872:TYR:CD2	1.28	1.64
2:W:804:ILE:HD13	2:W:872:TYR:CD2	1.28	1.63
2:W:804:ILE:HB	2:W:872:TYR:CZ	1.29	1.62
2:W:804:ILE:CB	2:W:872:TYR:CE1	1.85	1.60

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	243/460 (53%)	239 (98%)	4 (2%)	0	100	100
1	B	236/460 (51%)	231 (98%)	5 (2%)	0	100	100
1	C	232/460 (50%)	230 (99%)	2 (1%)	0	100	100
1	D	232/460 (50%)	229 (99%)	3 (1%)	0	100	100
1	G	153/460 (33%)	152 (99%)	1 (1%)	0	100	100
1	H	161/460 (35%)	159 (99%)	2 (1%)	0	100	100
1	I	118/460 (26%)	117 (99%)	1 (1%)	0	100	100
1	J	118/460 (26%)	116 (98%)	2 (2%)	0	100	100
1	M	243/460 (53%)	239 (98%)	4 (2%)	0	100	100
1	N	236/460 (51%)	231 (98%)	5 (2%)	0	100	100
1	O	232/460 (50%)	230 (99%)	2 (1%)	0	100	100
1	P	232/460 (50%)	229 (99%)	3 (1%)	0	100	100
1	S	153/460 (33%)	152 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	T	161/460 (35%)	159 (99%)	2 (1%)	0	100	100
1	U	118/460 (26%)	117 (99%)	1 (1%)	0	100	100
1	V	118/460 (26%)	116 (98%)	2 (2%)	0	100	100
2	E	108/907 (12%)	90 (83%)	18 (17%)	0	100	100
2	F	107/907 (12%)	81 (76%)	26 (24%)	0	100	100
2	K	108/907 (12%)	92 (85%)	16 (15%)	0	100	100
2	L	101/907 (11%)	89 (88%)	12 (12%)	0	100	100
2	Q	108/907 (12%)	90 (83%)	18 (17%)	0	100	100
2	R	107/907 (12%)	81 (76%)	26 (24%)	0	100	100
2	W	108/907 (12%)	92 (85%)	16 (15%)	0	100	100
2	X	101/907 (11%)	90 (89%)	11 (11%)	0	100	100
All	All	3834/14616 (26%)	3651 (95%)	183 (5%)	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	A	187/347 (54%)	186 (100%)	1 (0%)	88	93
1	B	182/347 (52%)	182 (100%)	0	100	100
1	C	174/347 (50%)	174 (100%)	0	100	100
1	D	174/347 (50%)	170 (98%)	4 (2%)	50	70
1	G	122/347 (35%)	121 (99%)	1 (1%)	81	89
1	H	129/347 (37%)	127 (98%)	2 (2%)	62	79
1	I	89/347 (26%)	89 (100%)	0	100	100
1	J	89/347 (26%)	89 (100%)	0	100	100
1	M	187/347 (54%)	186 (100%)	1 (0%)	88	93
1	N	182/347 (52%)	182 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	174/347 (50%)	174 (100%)	0	100	100
1	P	174/347 (50%)	170 (98%)	4 (2%)	50	70
1	S	122/347 (35%)	121 (99%)	1 (1%)	81	89
1	T	129/347 (37%)	127 (98%)	2 (2%)	62	79
1	U	89/347 (26%)	89 (100%)	0	100	100
1	V	89/347 (26%)	89 (100%)	0	100	100
2	E	94/749 (13%)	94 (100%)	0	100	100
2	F	93/749 (12%)	93 (100%)	0	100	100
2	K	94/749 (13%)	94 (100%)	0	100	100
2	L	89/749 (12%)	87 (98%)	2 (2%)	52	71
2	Q	94/749 (13%)	94 (100%)	0	100	100
2	R	93/749 (12%)	93 (100%)	0	100	100
2	W	94/749 (13%)	94 (100%)	0	100	100
2	X	89/749 (12%)	87 (98%)	2 (2%)	52	71
All	All	3032/11544 (26%)	3012 (99%)	20 (1%)	84	90

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	438	ARG
1	T	93	ASN
2	X	799	ARG
2	X	792	ARG
1	H	70	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	249	GLN
1	O	301	ASN
1	V	374	GLN
1	M	276	ASN
1	N	259	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 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.

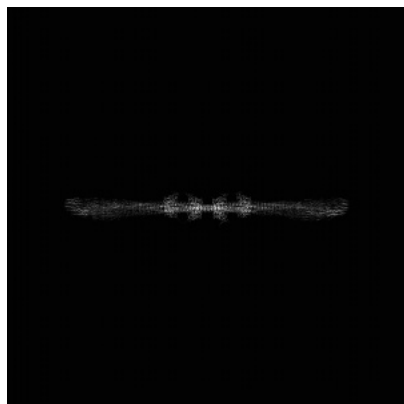
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15476. These allow visual inspection of the internal detail of the map and identification of artifacts.

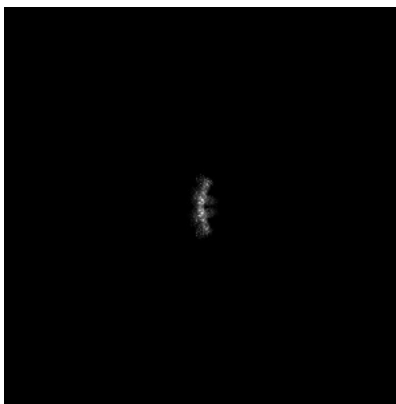
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X

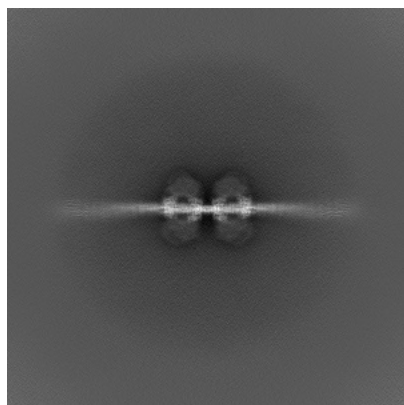


Y

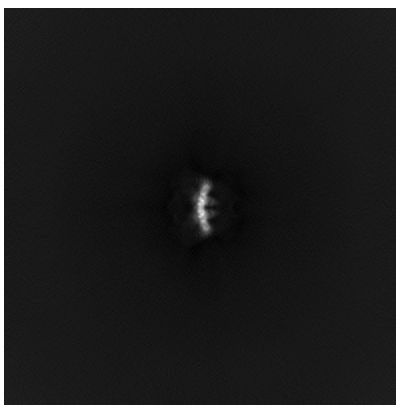


Z

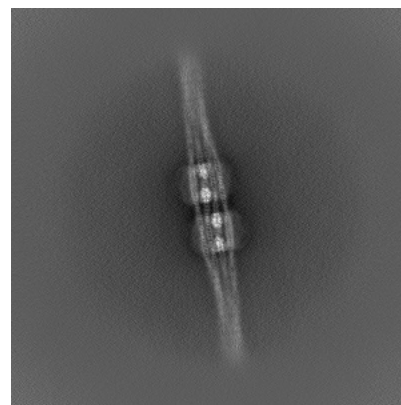
6.1.2 Raw map



X



Y

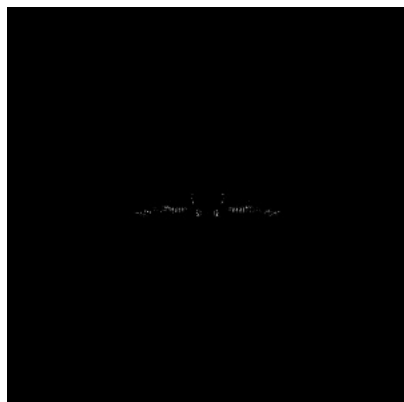


Z

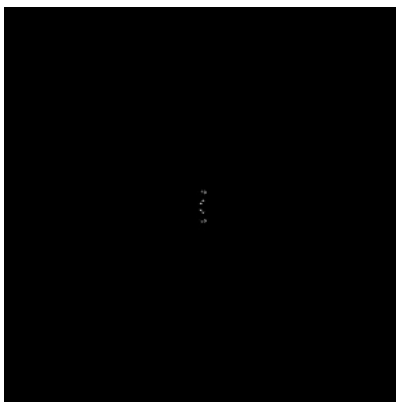
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 300

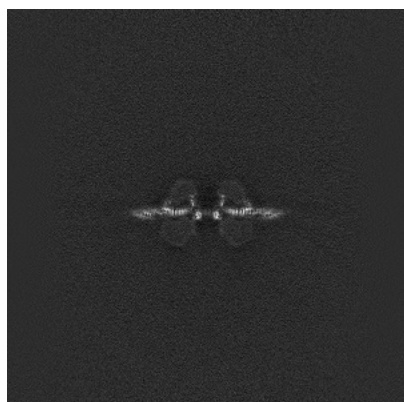


Y Index: 300

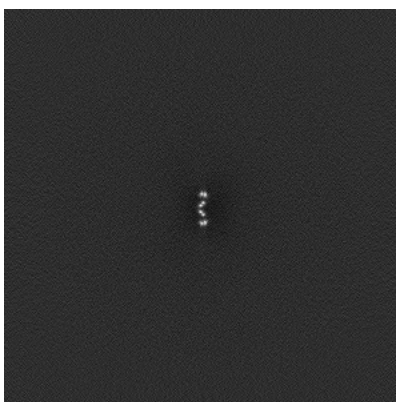


Z Index: 300

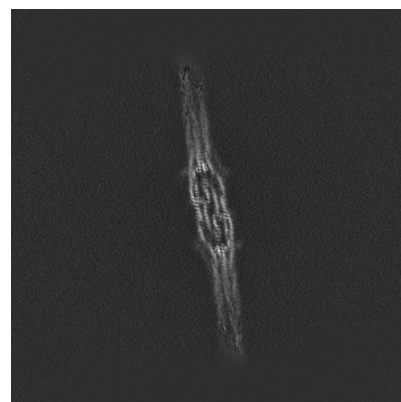
6.2.2 Raw map



X Index: 300



Y Index: 300



Z Index: 300

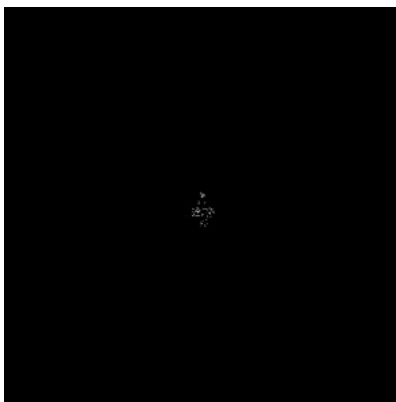
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

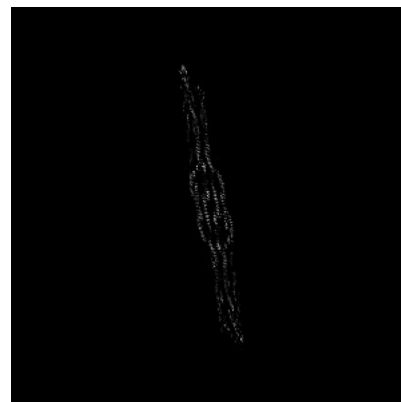
6.3.1 Primary map



X Index: 310



Y Index: 318

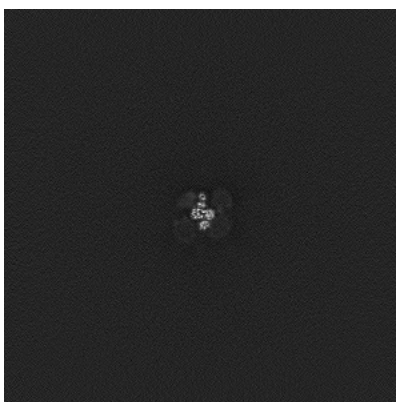


Z Index: 299

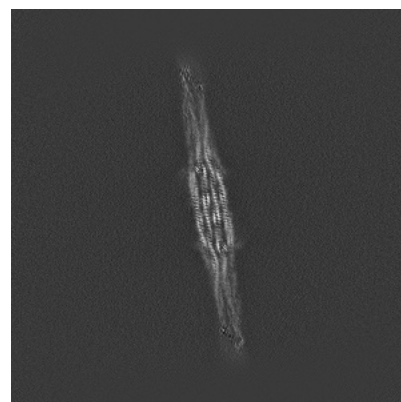
6.3.2 Raw map



X Index: 310



Y Index: 317

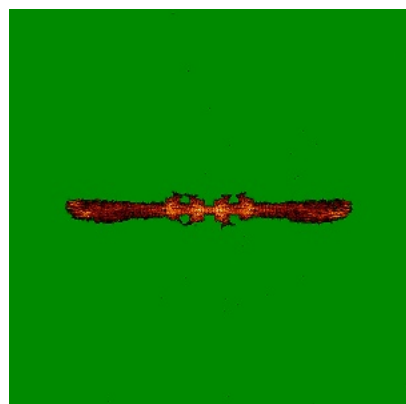


Z Index: 298

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

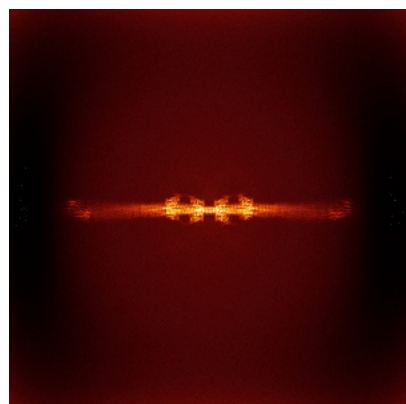


Y

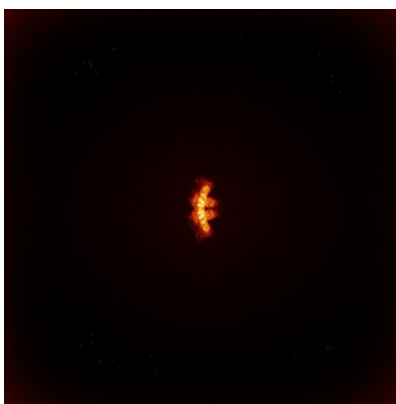


Z

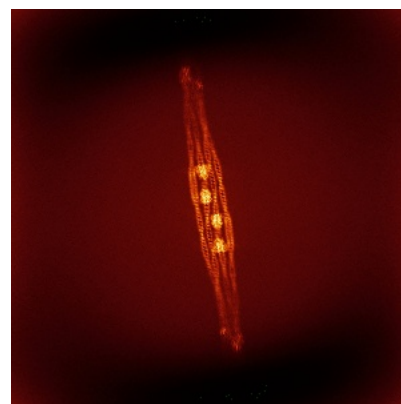
6.4.2 Raw map



X



Y

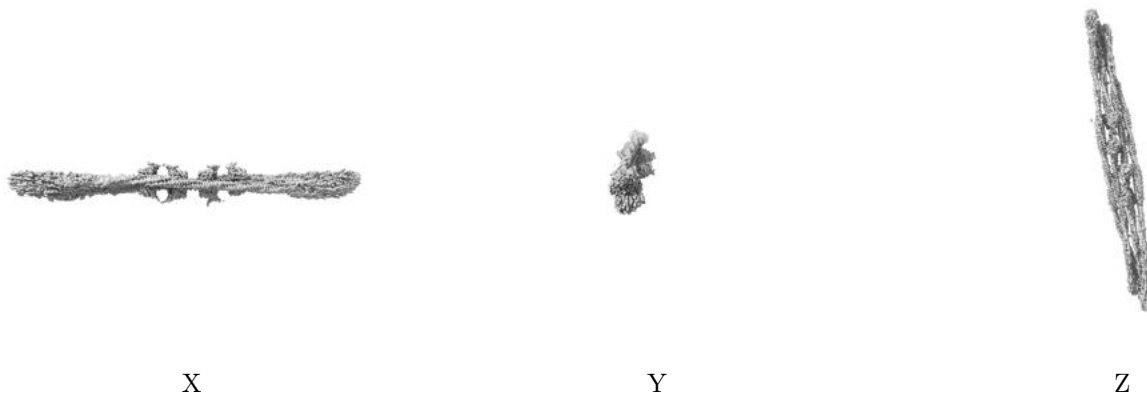


Z

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.

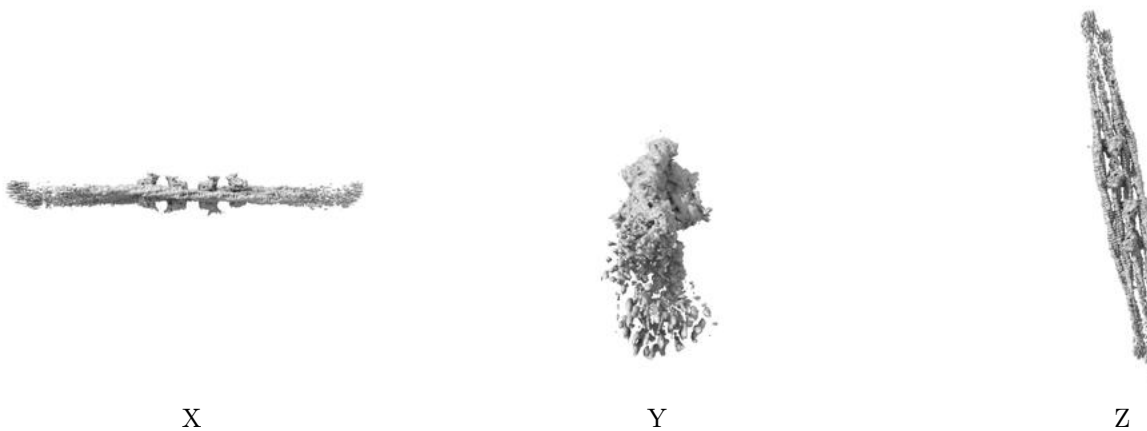
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.022. 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.

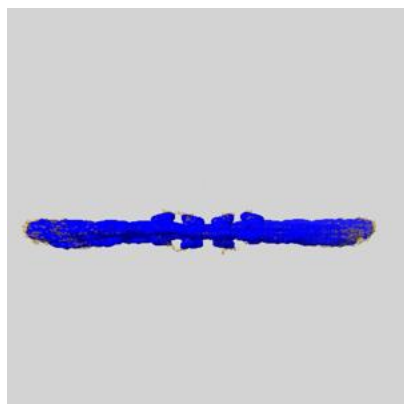
6.6 Mask visualisation [i](#)

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

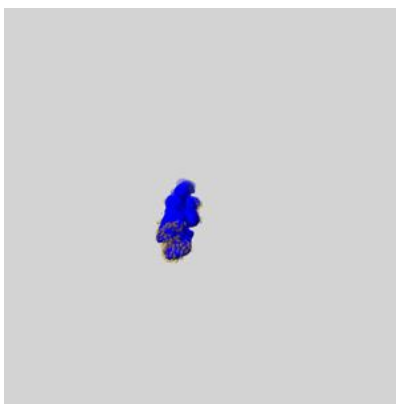
A mask typically either:

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

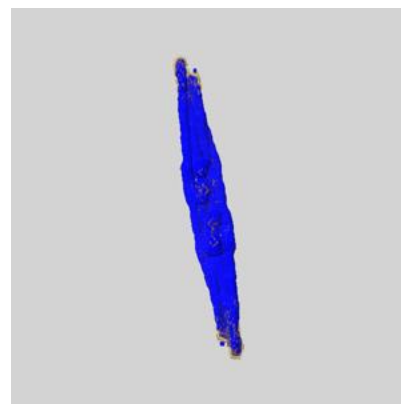
6.6.1 emd_15476_msk_1.map [i](#)



X



Y

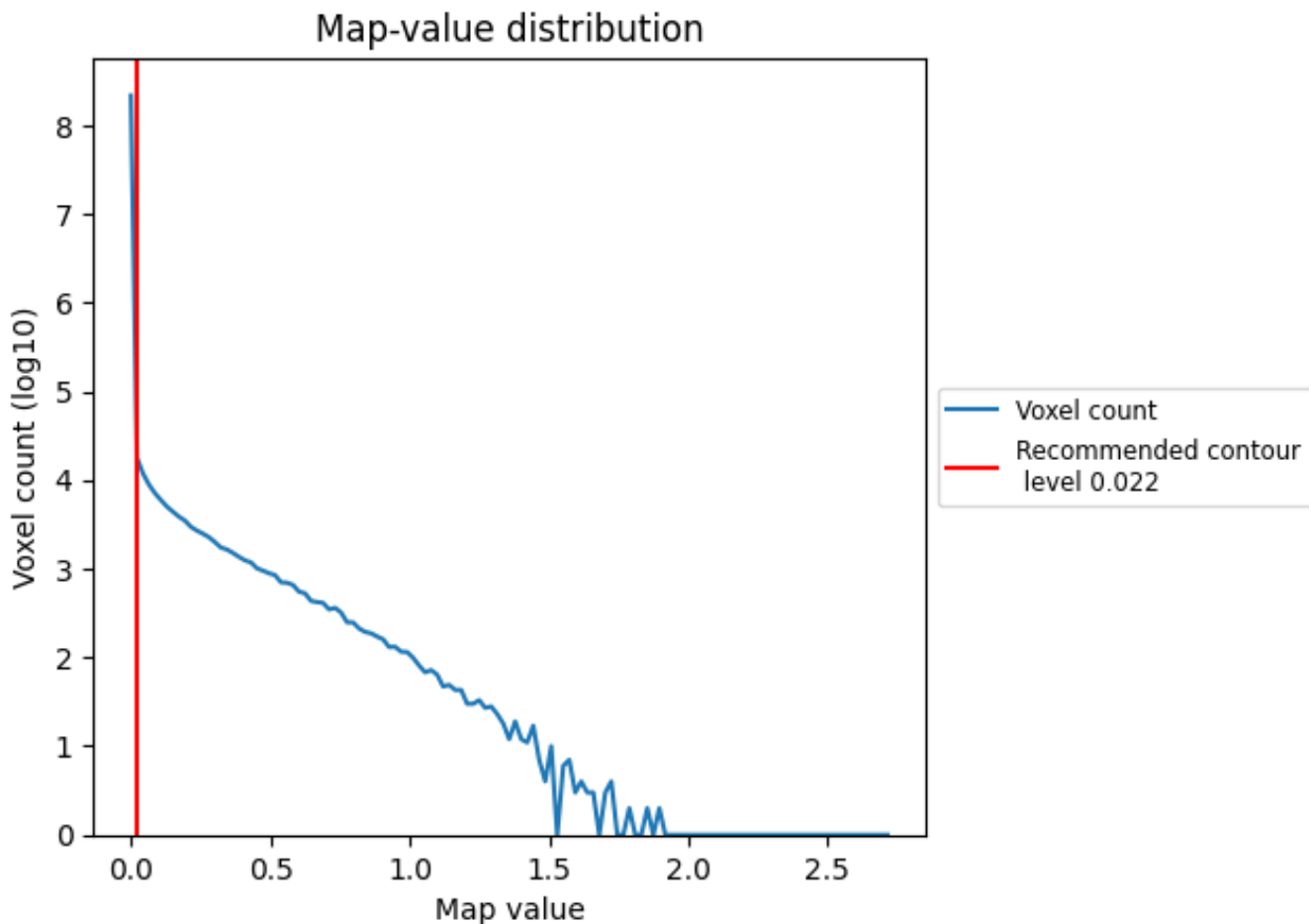


Z

7 Map analysis [i](#)

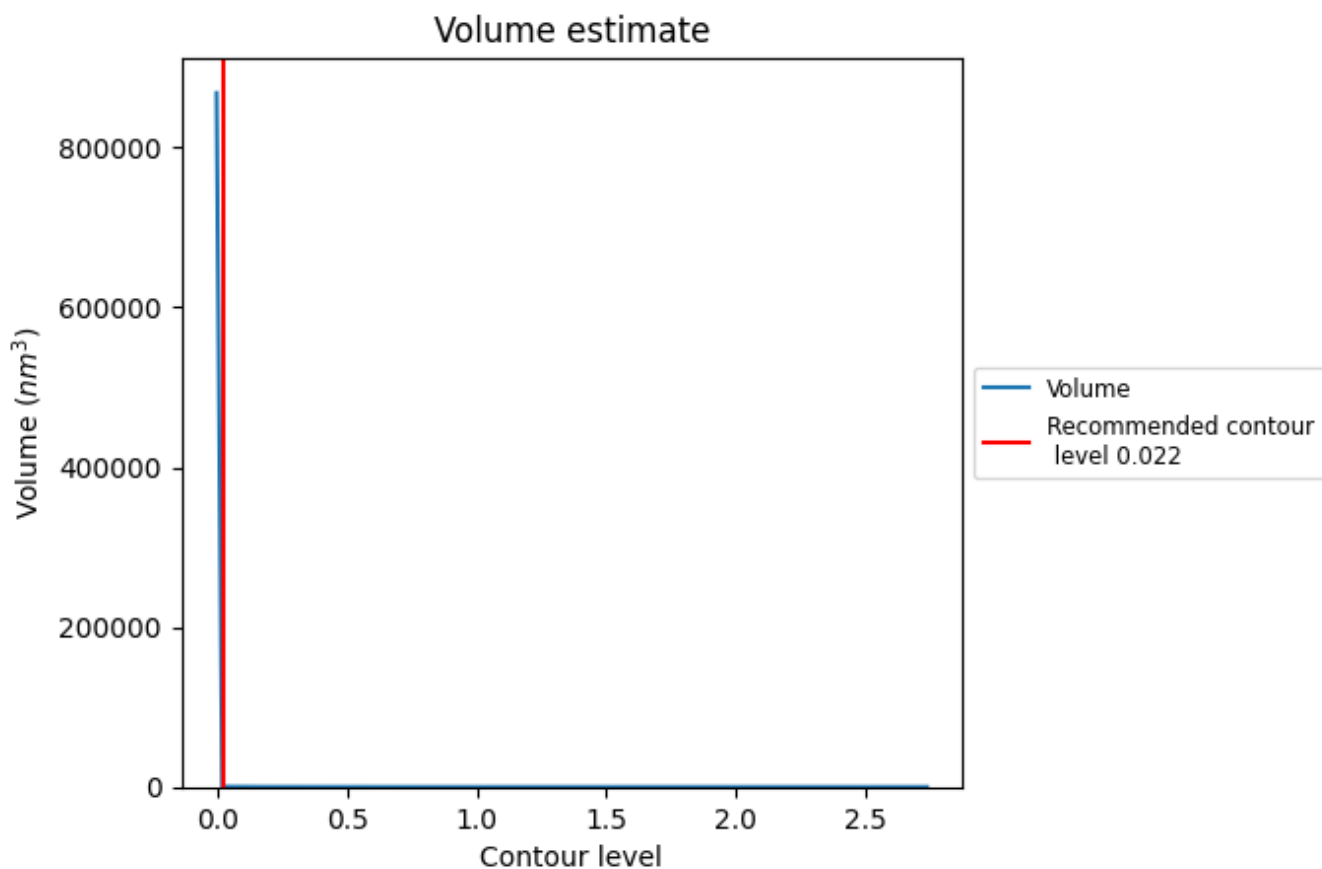
This section contains the results of statistical analysis of the map.

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.

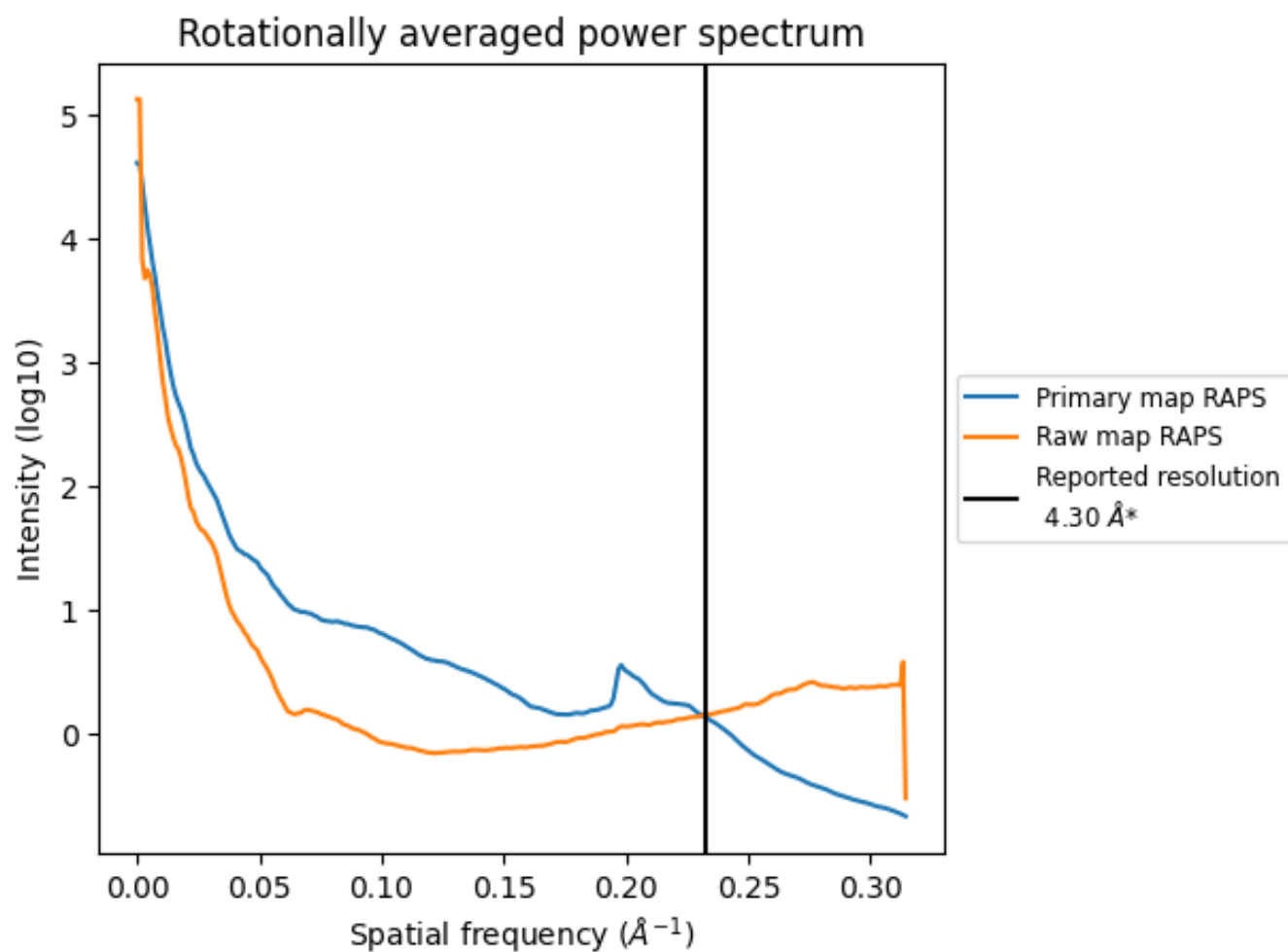
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 401 nm^3 ; this corresponds to an approximate mass of 362 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 i

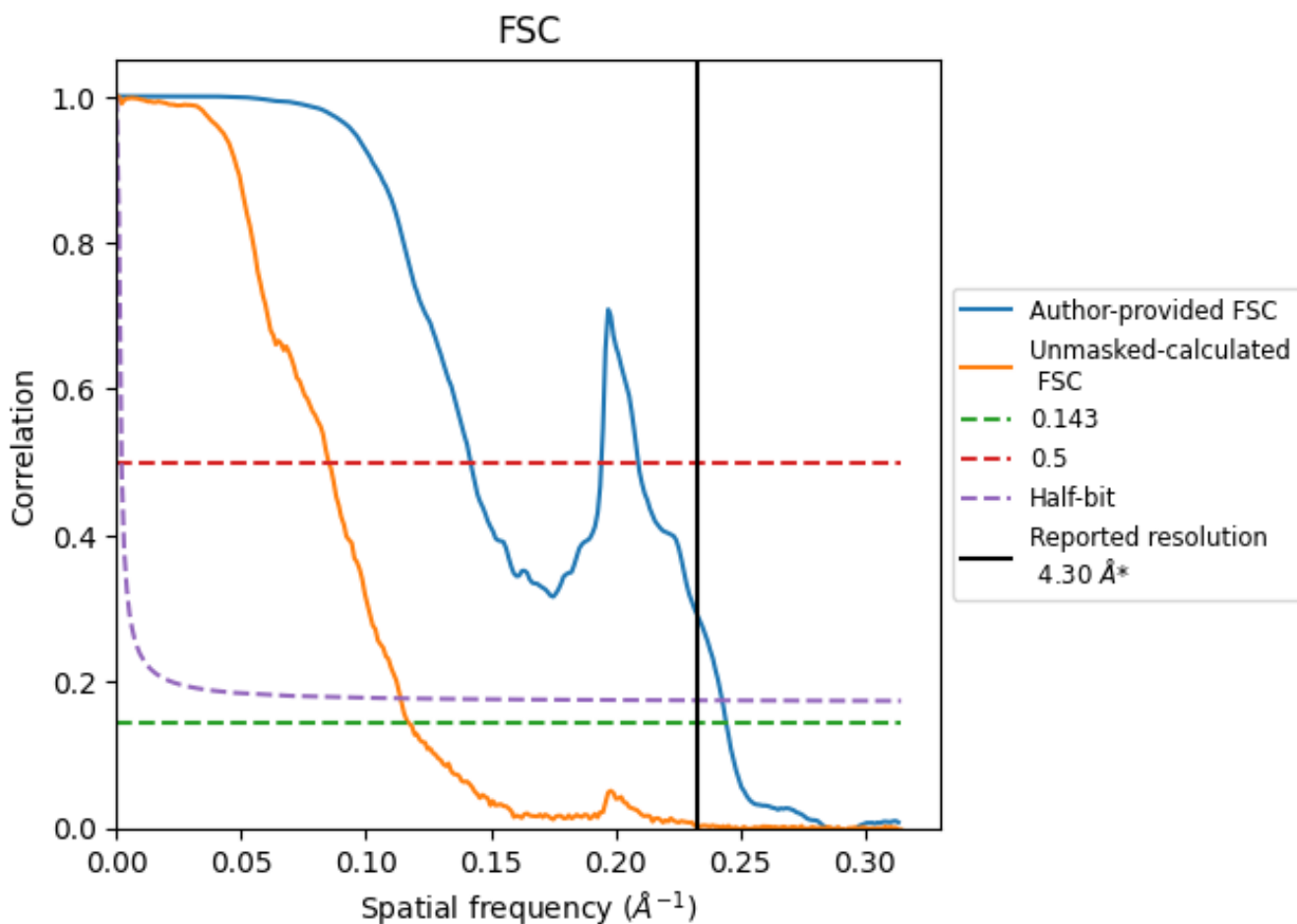


*Reported resolution corresponds to spatial frequency of 0.233 Å⁻¹

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 0.233 \AA^{-1}

8.2 Resolution estimates [i](#)

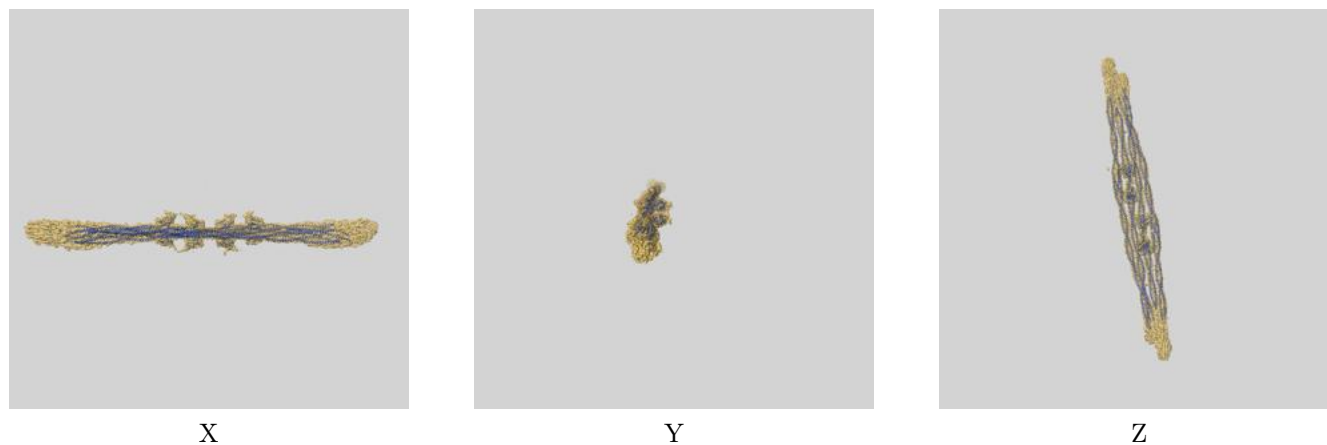
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.09	7.05	4.12
Unmasked-calculated*	8.53	11.75	8.78

*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 8.53 differs from the reported value 4.3 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15476 and PDB model 8AJB. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



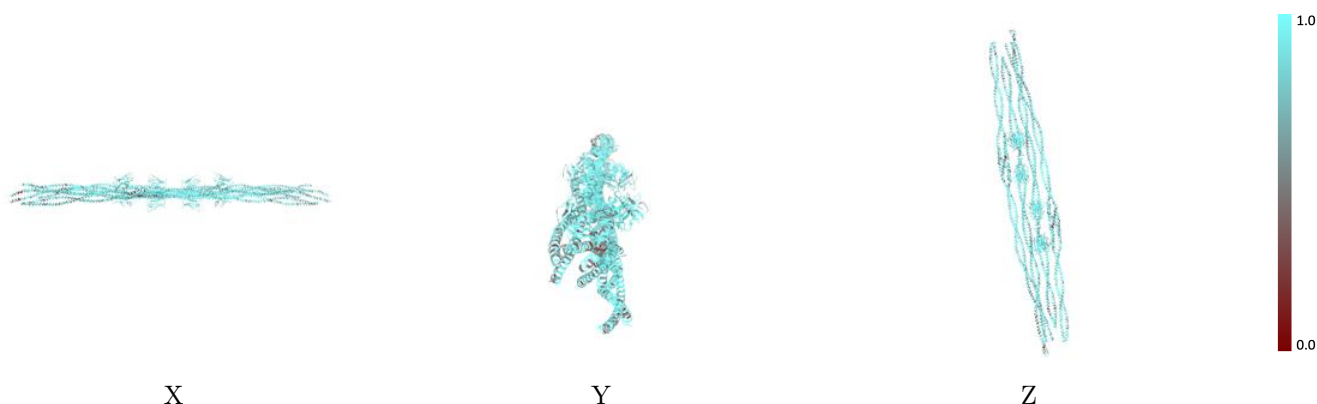
The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



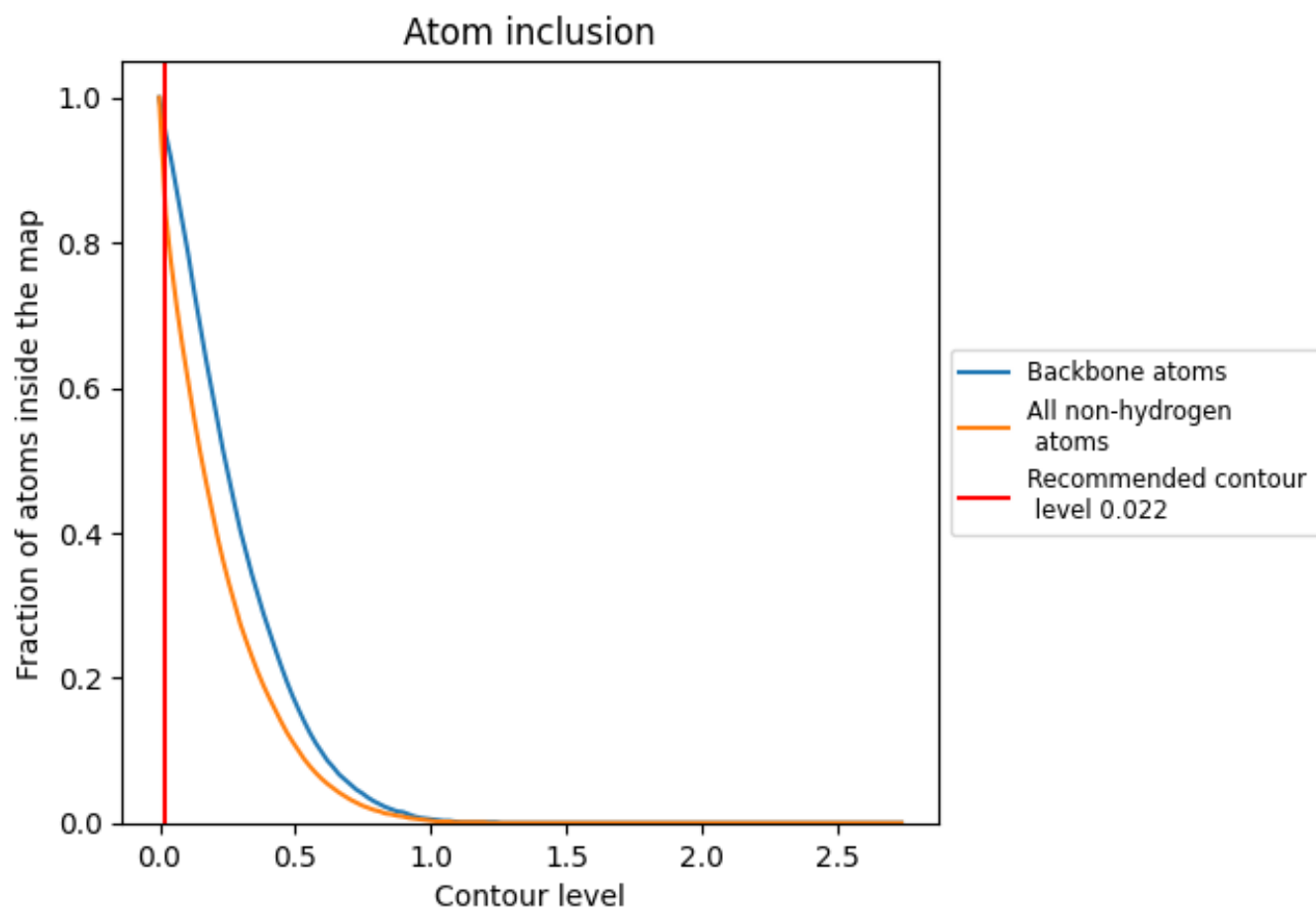
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.022).



















































9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 84% 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 (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8400	 0.1860
A	 0.8330	 0.1630
B	 0.8260	 0.1630
C	 0.8050	 0.1570
D	 0.8420	 0.1700
E	 0.9230	 0.3140
F	 0.9030	 0.2830
G	 0.7630	 0.0640
H	 0.8310	 0.0980
I	 0.8450	 0.1850
J	 0.8430	 0.1680
K	 0.9000	 0.2960
L	 0.8880	 0.3160
M	 0.8200	 0.1590
N	 0.8150	 0.1620
O	 0.8080	 0.1660
P	 0.8600	 0.1950
Q	 0.9050	 0.2970
R	 0.8990	 0.2710
S	 0.7620	 0.0650
T	 0.8280	 0.1230
U	 0.8440	 0.1940
V	 0.8330	 0.1830
W	 0.8920	 0.2850
X	 0.8960	 0.3280

