Full wwPDB EM Validation 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 Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

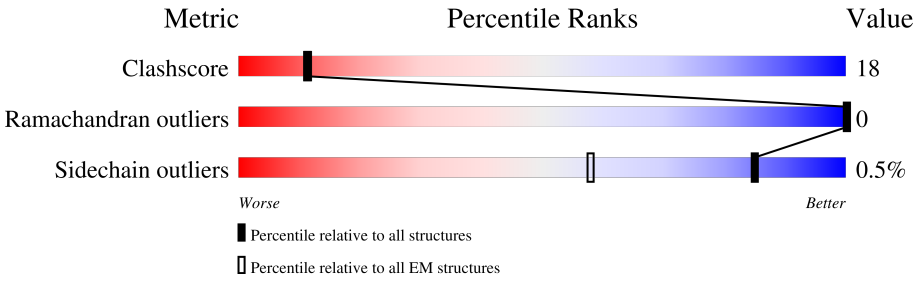
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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 <=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	13% · 83%
1	B	457	12% 5% 83%
1	E	457	10% 5% 85%
1	F	457	8% 5% 87%
1	G	457	13% · 83%
1	H	457	12% 5% 83%
1	K	457	9% 5% 85%
1	L	457	8% 5% 87%

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Mol	Chain	Length	Quality of chain
2	C	907	
2	D	907	
2	I	907	
2	J	907	

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.

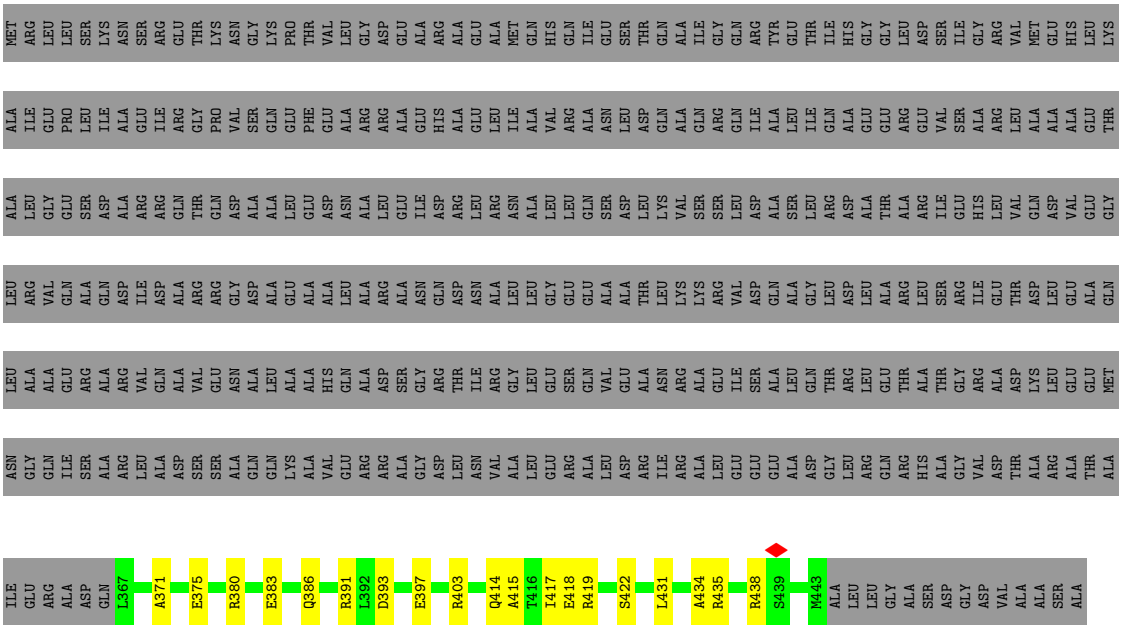
Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	112	Total	C	N	O	S	0	0
			869	539	155	170	5		
2	C	112	Total	C	N	O	S	0	0
			869	539	155	170	5		
2	J	112	Total	C	N	O	S	0	0
			869	539	155	170	5		
2	I	112	Total	C	N	O	S	0	0
			869	539	155	170	5		

3 Residue-property plots (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.

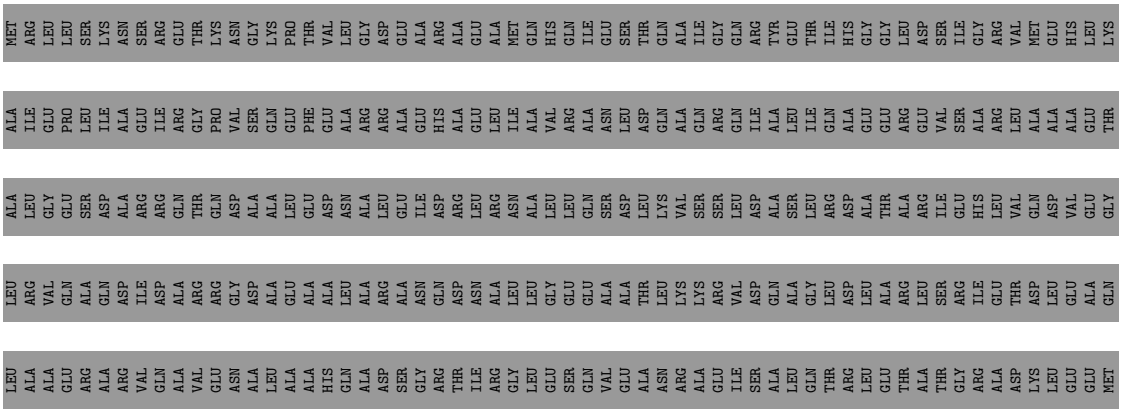
• Molecule 1: Crescentin

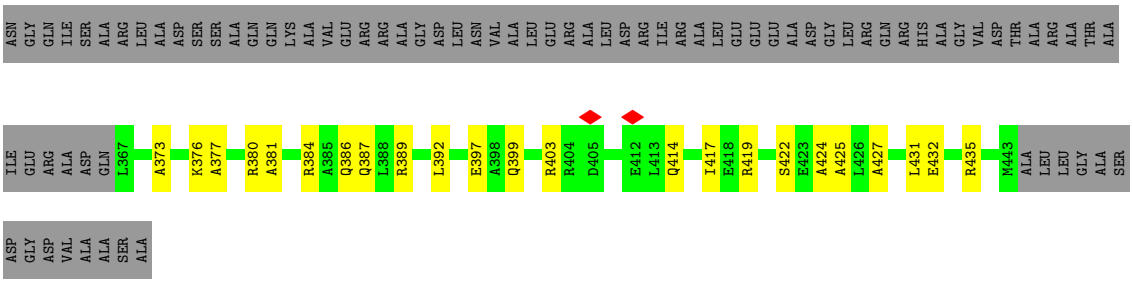
Chain A:



• Molecule 1: Crescentin

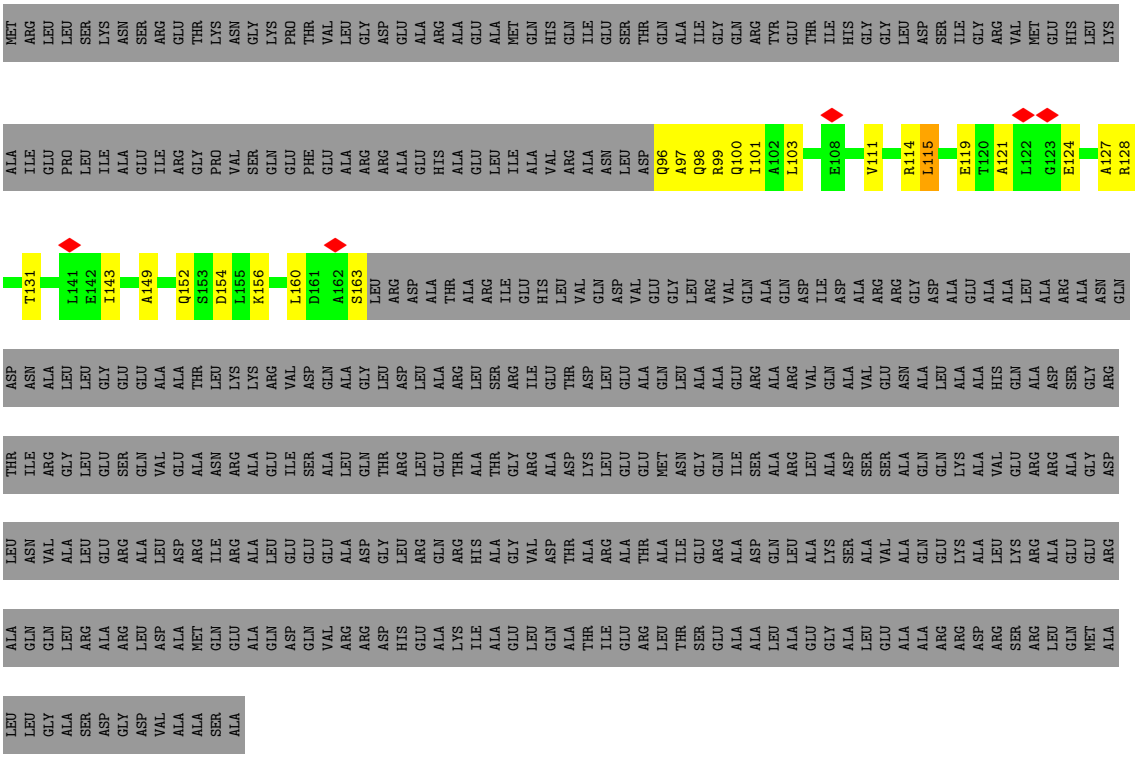
Chain B:





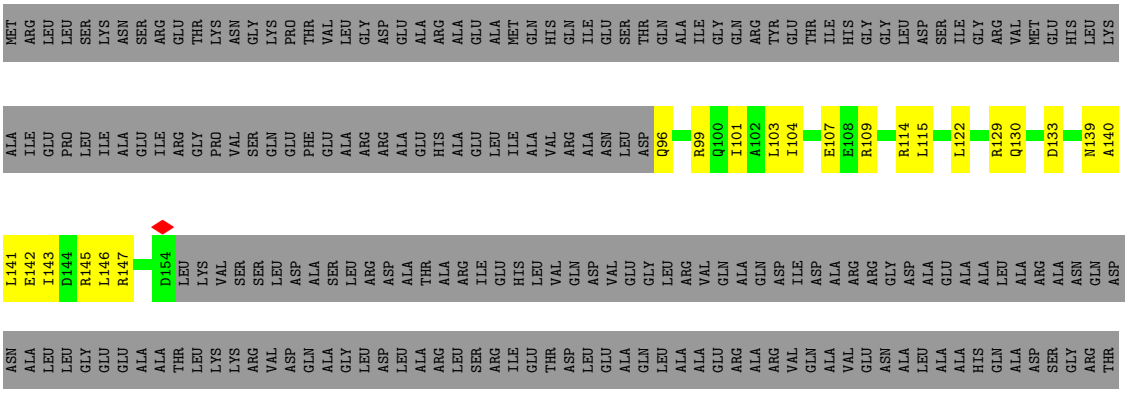
• Molecule 1: Crescentin

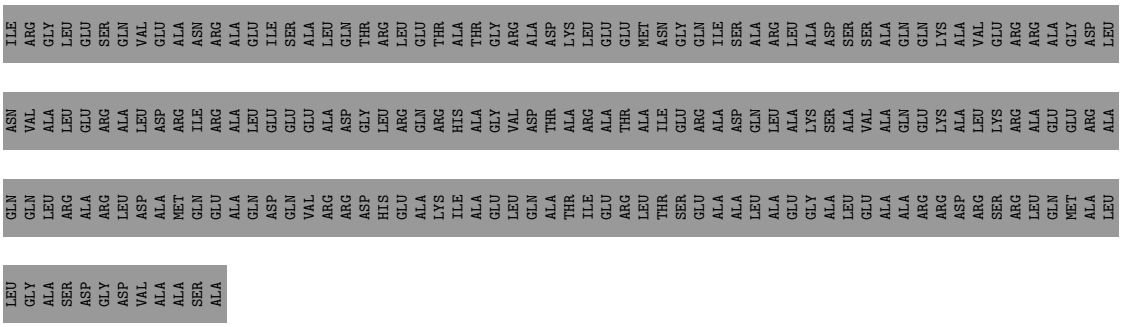
Chain E:



• Molecule 1: Crescentin

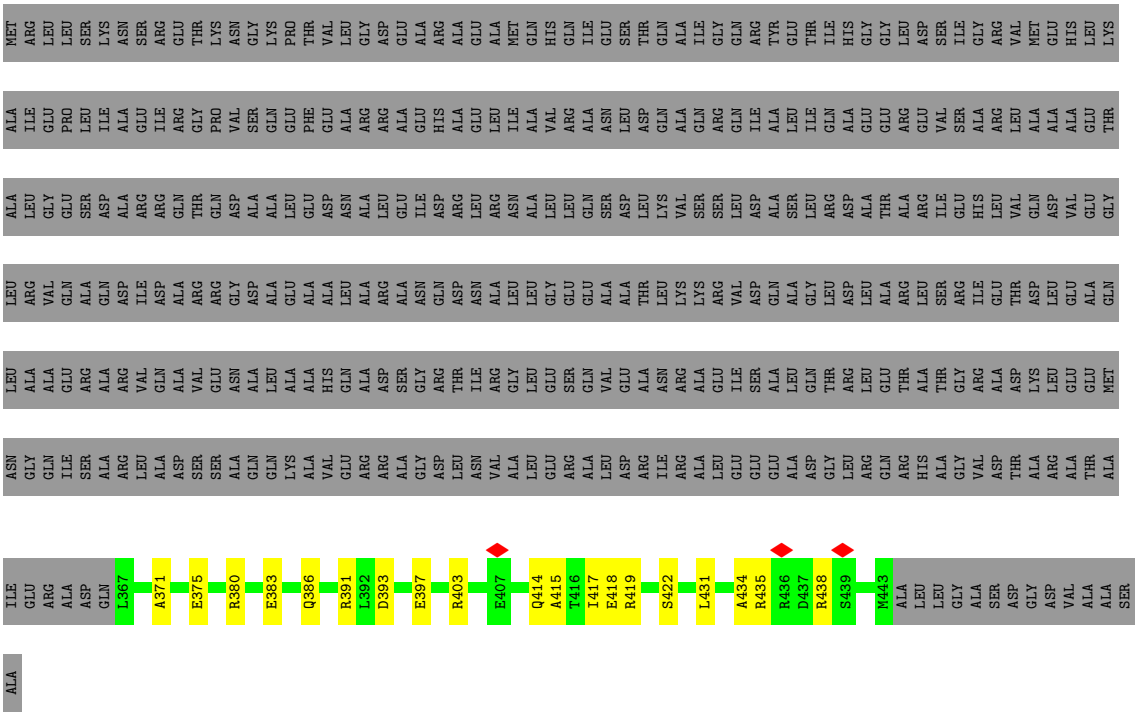
Chain F:





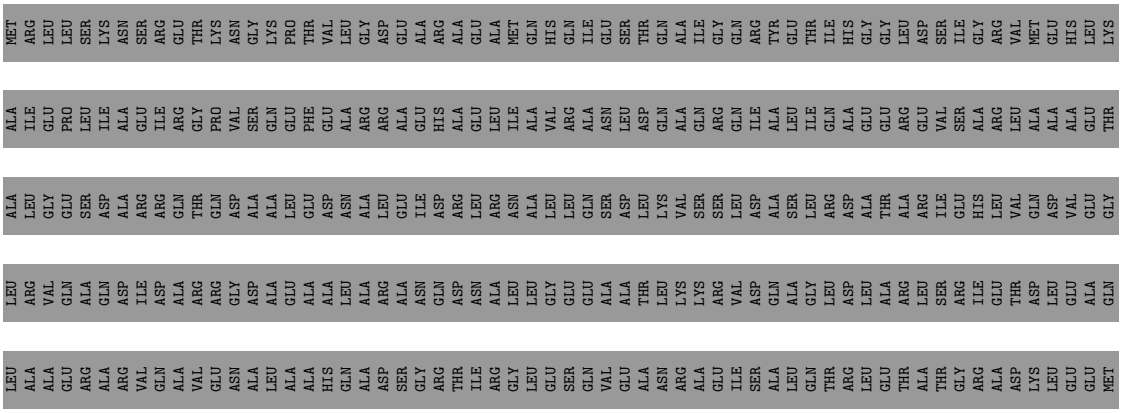
• Molecule 1: Crescentin

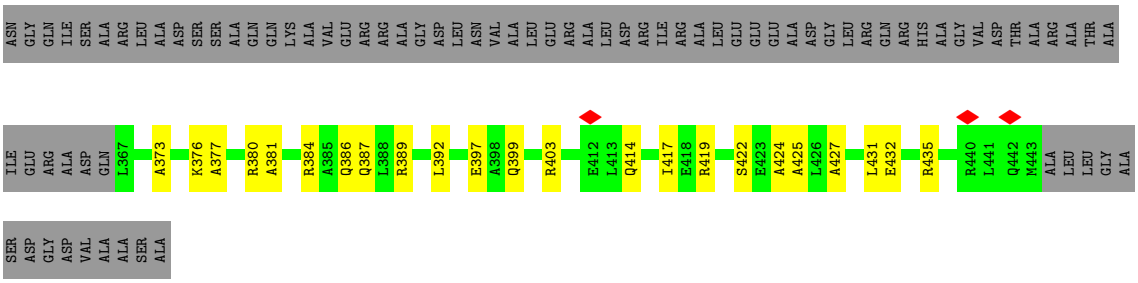
Chain G:



• Molecule 1: Crescentin

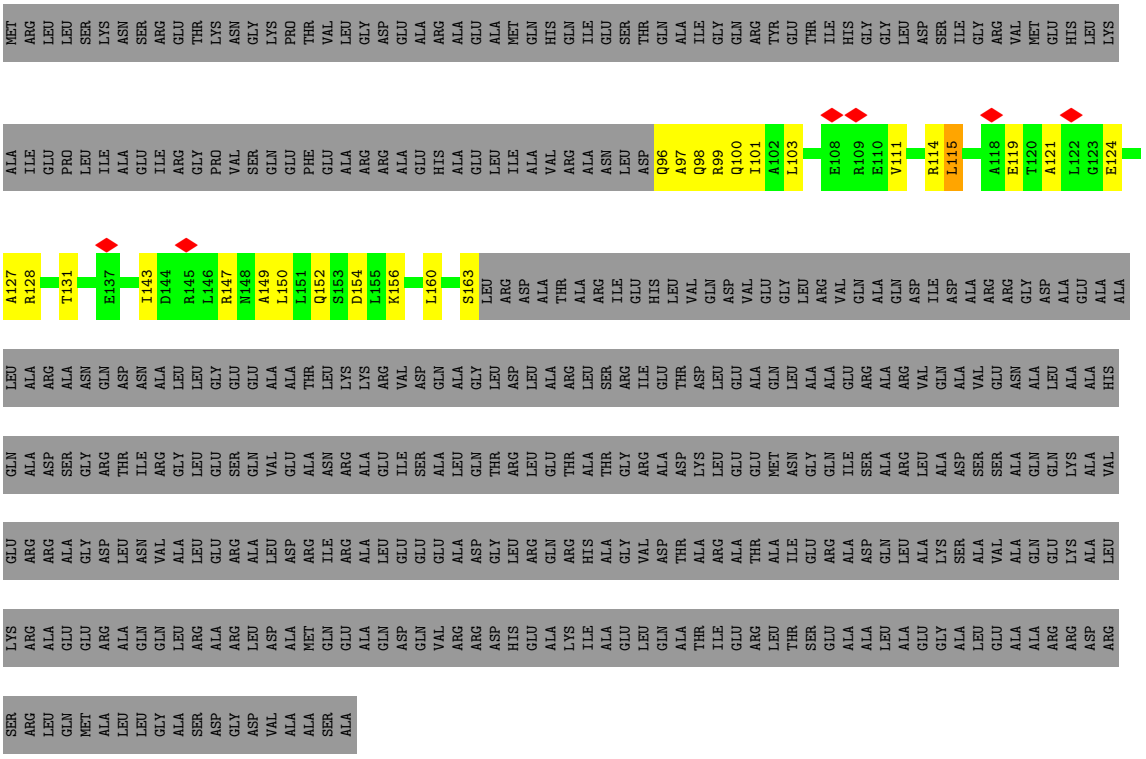
Chain H:





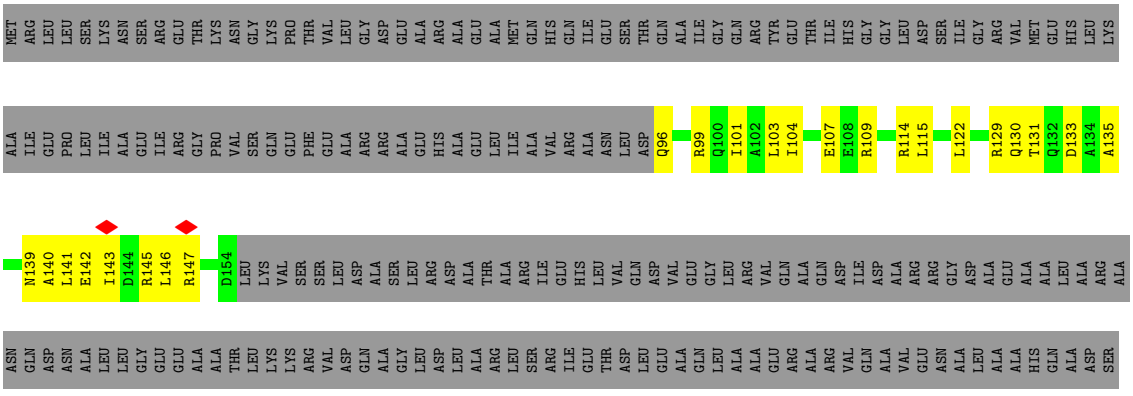
• Molecule 1: Crescentin

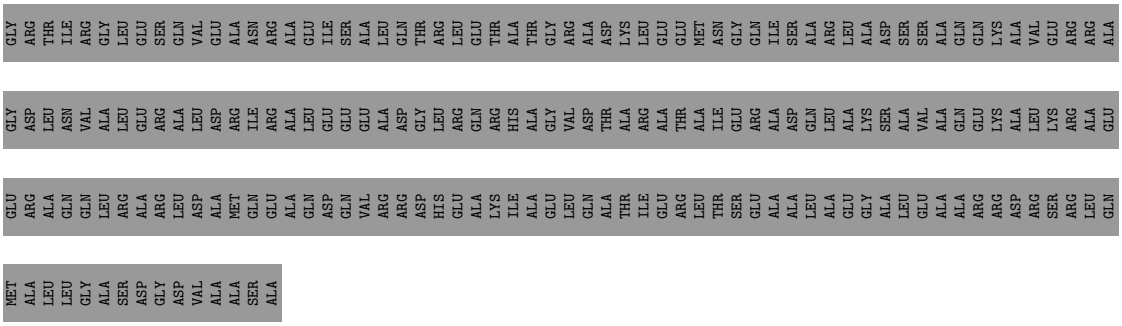
Chain K:



• Molecule 1: Crescentin

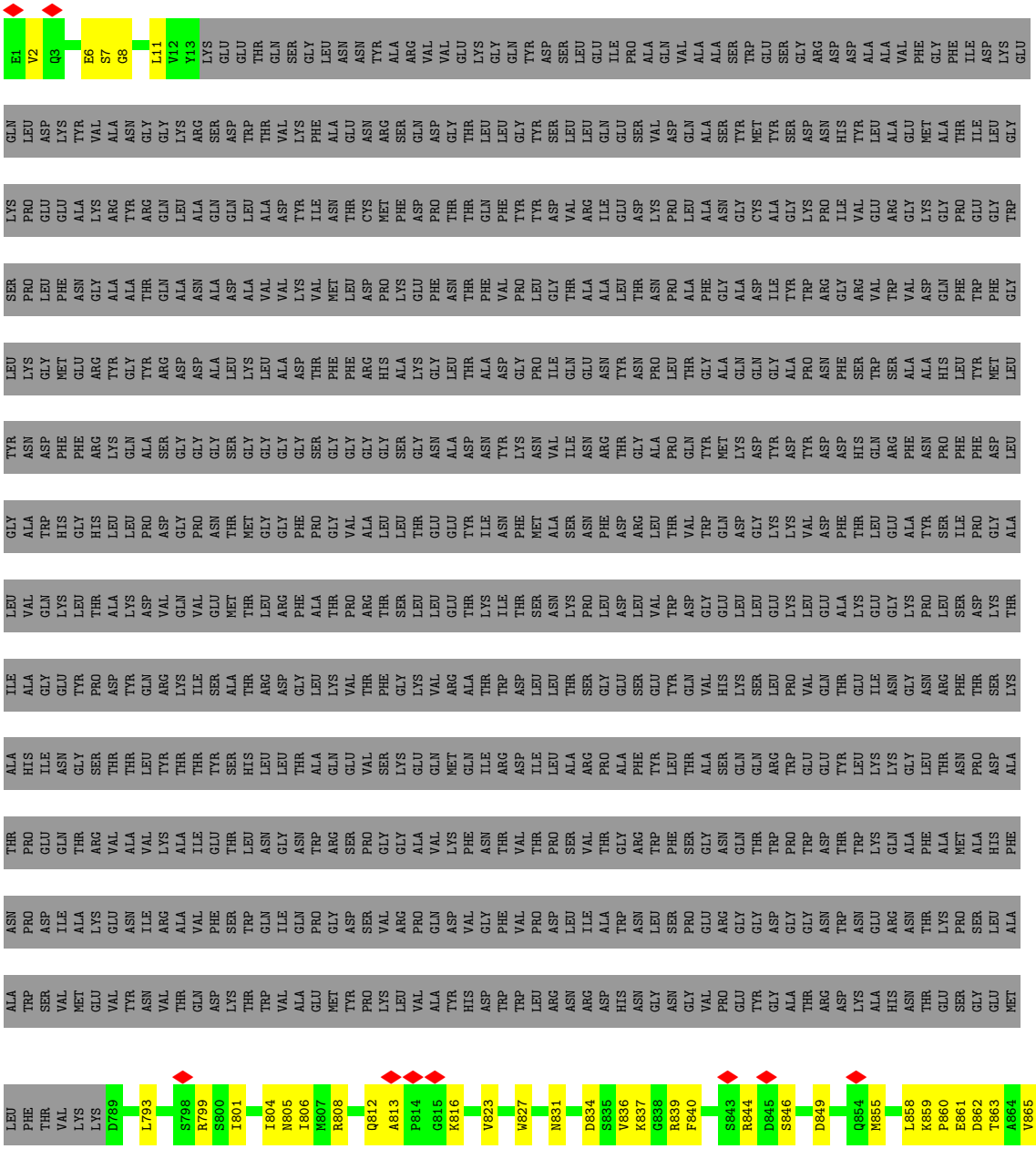
Chain L:

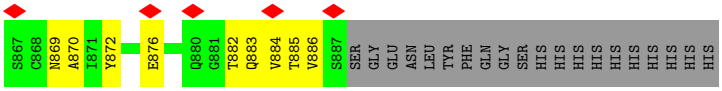




• Molecule 2: Crescentin-specific megabody MB13

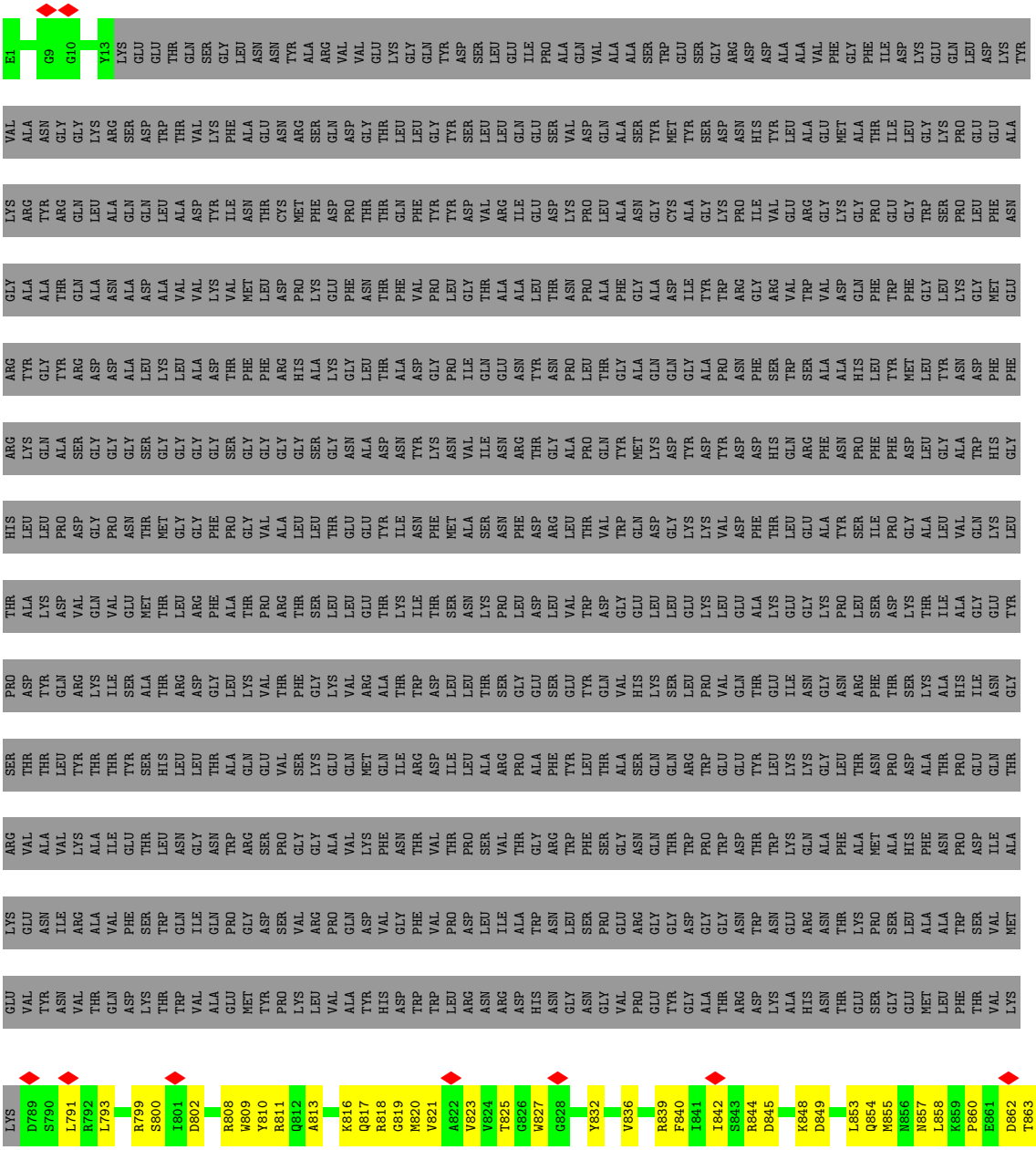
Chain D: 7% 5% 88%

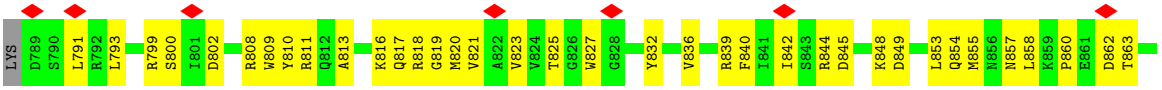




• Molecule 2: Crescentin-specific megabody MB13

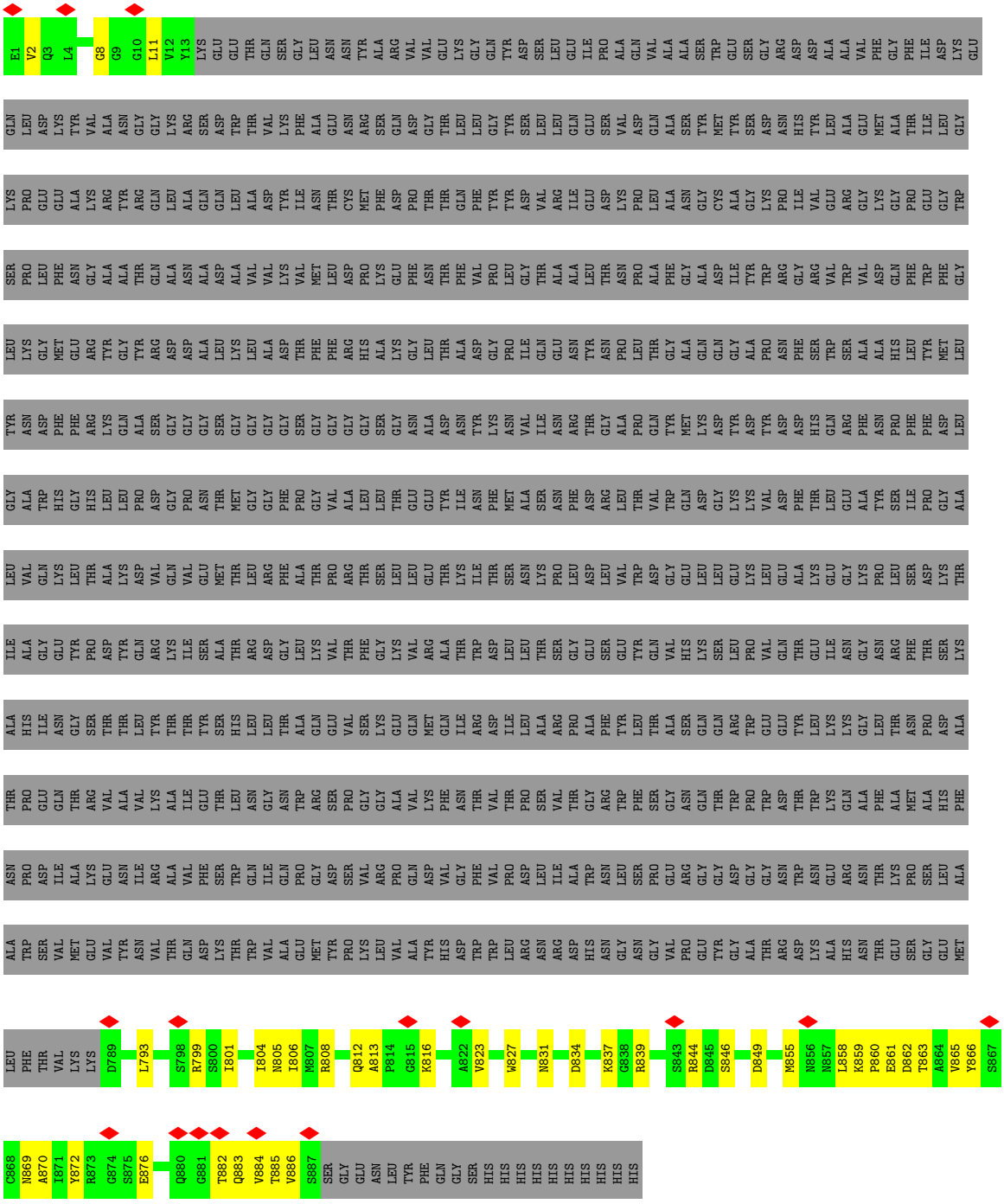
Chain C:





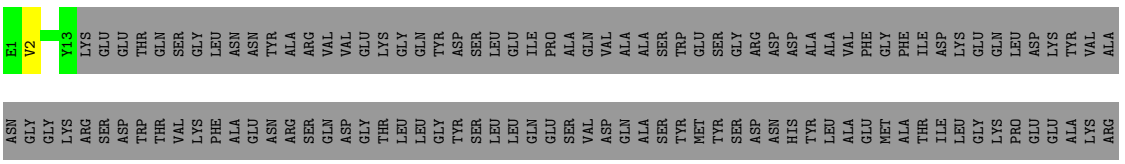
• Molecule 2: Crescentin-specific megabody MB13

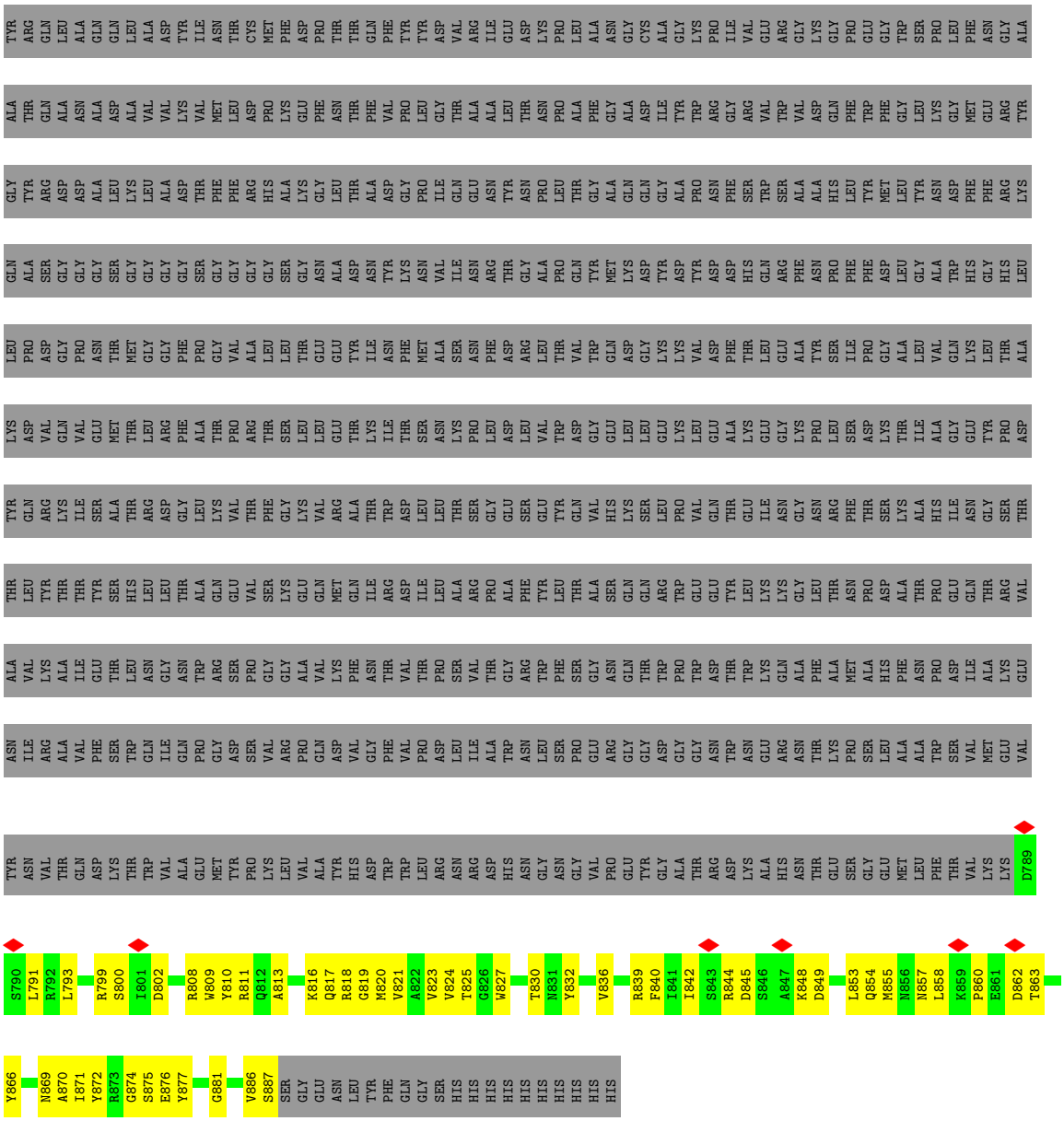
Chain J:



• Molecule 2: Crescentin-specific megabody MB13

Chain I:




TYR ARG GLN LEU ALA GLN GLN LEU ALA ASP TYR ILE ASN THR CYS MET PHE ASP PRO THR THR GLN PHE TYR TYR ASP VAL ARG ILE GLU ASP LYS PRO LEU ALA ASN GLY CYS ALA GLY LYS PRO ILE VAL GLU ARG GLY LYS GLY PRO GLU GLY TRP SER PRO LEU PHE ASN GLY ALA
ALA THR GLN ALA ASN ALA ASP ALA VAL VAL LYS VAL MET LEU ASP PRO LYS GLU PHE ASN THR PHE VAL PRO LEU GLY THR ALA ALA LEU THR ASN PRO ALA PHE GLY ALA ASP GLN GLY ILE TYR TRP ARG GLY ARG VAL TRP VAL ASP GLN PHE TRP PHE GLY LEU LYS GLY MET GLU ARG TYR
GLY TYR ARG ASP ASP ALA LEU LYS LEU ALA ASP THR PHE PHE ARG HIS ALA LYS GLY LEU THR ALA ASP GLY PRO ILE GLN GLU ASN TYR ASN PRO LEU THR GLY ALA GLN GLN GLY ALA PRO ASN PHE SER TRP SER ALA ALA HIS LEU TYR MET LEU GLY LEU TYR ASN ASP PHE GLY ARG
GLN ALA SER GLY GLY GLY SER GLY GLY SER GLY ASN ALA ASP ASN TYR LYS ASN VAL ILE ASN ARG THR GLY ALA PRO GLN TYR MET LYS ASP TYR ASP TYR ASP ASP HIS GLN ARG PHE ASN PRO PHE PHE ASP LEU GLY ALA TRP HIS GLY HIS LEU
LEU PRO ASP GLY PRO ASN THR MET GLY GLY PHE PRO GLY VAL ALA LEU LEU THR GLU GLU TYR ILE ASN PHE MET ALA SER ASN PHE ASP ARG LEU THR VAL TRP GLN ASP GLY LYS LYS VAL ASP PHE THR LEU GLU ALA TYR SER ILE PRO GLY ALA LEU VAL GLN LYS LEU THR ALA
LYS ASP VAL GLN VAL GLU MET THR LEU ARG PHE THR ARG THR LYS ILE THR SER ASN LYS PRO LEU ASP LEU VAL TRP ASP GLY GLU LEU LEU LEU GLU LYS LYS LEU GLU ALA LYS GLU TYR GLY LYS PRO LEU SER ASP LYS THR ILE ALA HIS ILE ASN GLY SER THR
TYR GLN ARG LYS ILE SER ALA THR ARG ASP GLY LEU LYS VAL ARG ALA THR TRP ASP LEU LEU LEU THR SER GLY GLU SER GLU TYR GLN VAL HIS LYS SER LEU PRO VAL GLN THR GLU ILE ASN GLY ARG PHE THR SER LYS ALA HIS ILE ASN GLY SER THR
THR LEU TYR THR THR TYR SER HIS LEU LEU THR ALA GLN GLU VAL SER LYS GLU GLN MET GLN ILE ARG ASP ILE LEU LEU ALA ARG PRO ALA PHE TYR LEU THR SER GLU GLN ILE GLN ARG TRP GLU GLU TYR LEU LYS LYS GLY LEU THR ASN PRO ASP ALA THR PRO GLU GLN THR ARG VAL
ALA VAL LYS ALA ILE GLU THR LEU ASN GLY ASN TRP ARG SER PRO GLY GLY ALA VAL LYS PHE ASN THR VAL THR PRO SER VAL THR GLY ARG TRP PHE SER GLY ASN GLN THR TRP PRO TRP GLU ASP THR TRP LYS GLN ALA PHE ALA MET ALA HIS PHE ASN PRO ASP ILE ALA LYS GLU
ASN ILE ARG ALA VAL PHE SER TRP GLN ILE GLN PRO GLY ASP SER VAL ARG PRO GLN ASP VAL GLY PHE VAL PRO ASP LEU ILE ALA TRP ASN LEU SER PRO GLU ARG GLY GLY ASP GLY GLY ASN TRP ASN GLU ARG ASN THR LYS PRO SER LEU ALA ALA TRP SER VAL MET GLU VAL
TYR ASN VAL THR GLN ASP LYS THR TRP VAL ALA GLU MET TYR PRO LYS LEU VAL ALA TYR HIS ASP TRP TRP LEU ARG ASN ARG ASP HIS ASN GLY ASN GLY VAL PRO GLU TYR GLY ALA THR ARG ASP LYS ALA HIS ASN THR GLU SER GLY GLU MET LEU PHE THR VAL LYS LYS D789
S790 L791 R792 L793 R799 S800 I801 D802 R808 W809 Y810 R811 Q812 A813 K816 Q817 R818 G819 M820 V821 A822 V823 V824 T825 G826 W827 T830 N831 Y832 V836 R839 F840 I841 I842 S843 R844 D845 S846 A847 K848 D849 L853 Q854 M855 N856 N857 L858 K859 P860 E861 D862 T863
Y866 N869 A870 I871 Y872 R873 G874 S875 E876 Y877 G881 V886 S887 SER GLY GLU ASN LEU TYR PHE GLN GLY SER HIS HIS HIS HIS HIS HIS HIS HIS HIS HIS

4 Experimental information (i)

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 ($e^-/Å^2$)	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

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	0.25	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

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.

All (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
1:E:111:VAL:CA	1:E:115:LEU:HB2	2.00	0.91
1:K:111:VAL:HA	1:K:115:LEU:CB	2.05	0.86
1:E:111:VAL:HA	1:E:115:LEU:CB	2.05	0.85
2:I:791:LEU:O	2:I:854:GLN:NE2	2.16	0.79
2:I:858:LEU:HB3	2:I:886:VAL:HG21	1.66	0.78
2:C:791:LEU:O	2:C:854:GLN:NE2	2.16	0.78
2:I:821:VAL:HG13	2:I:836:VAL:HG11	1.67	0.76
2:C:858:LEU:HB3	2:C:886:VAL:HG21	1.66	0.75
2:C:821:VAL:HG13	2:C:836:VAL:HG11	1.67	0.75
1:A:419:ARG:NH2	2:C:874:GLY:O	2.20	0.74
1:G:419:ARG:NH2	2:I:874:GLY:O	2.21	0.74
2:D:834:ASP:HA	2:D:837:LYS:HE3	1.69	0.73
2:C:871:ILE:HG12	2:C:876:GLU:HG3	1.72	0.72
1:K:111:VAL:O	1:K:115:LEU:HB2	1.89	0.72
1:E:111:VAL:O	1:E:115:LEU:HB2	1.89	0.72
2:J:834:ASP:HA	2:J:837:LYS:HE3	1.69	0.72
1:E:111:VAL:O	1:E:115:LEU:CB	2.38	0.71
2:D:860:PRO:HA	2:D:886:VAL:HG13	1.73	0.71
2:J:860:PRO:HA	2:J:886:VAL:HG13	1.73	0.71
2:I:858:LEU:HD13	2:I:886:VAL:HG11	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:377:ALA:HA	1:H:380:ARG:NH1	2.06	0.70
1:B:377:ALA:HA	1:B:380:ARG:NH1	2.06	0.70
2:C:858:LEU:HD13	2:C:886:VAL:HG11	1.73	0.70
1:K:111:VAL:O	1:K:115:LEU:CB	2.38	0.70
2:I:871:ILE:HG12	2:I:876:GLU:HG3	1.72	0.70
1:K:119:GLU:OE2	1:L:114:ARG:NH2	2.26	0.69
1:K:149:ALA:HA	1:K:152:GLN:HB2	1.74	0.69
1:E:149:ALA:HA	1:E:152:GLN:HB2	1.74	0.69
1:E:119:GLU:OE2	1:F:114:ARG:NH2	2.26	0.68
2:C:791:LEU:HB3	2:C:855:MET:HB2	1.75	0.68
2:I:791:LEU:HB3	2:I:855:MET:HB2	1.75	0.68
1:E:115:LEU:HD21	1:F:115:LEU:HD22	1.77	0.67
2:J:866:TYR:N	2:J:882:THR:O	2.28	0.67
2:D:812:GLN:HB3	2:D:865:VAL:HB	1.75	0.66
2:D:866:TYR:N	2:D:882:THR:O	2.28	0.66
2:J:812:GLN:HB3	2:J:865:VAL:HB	1.75	0.66
1:K:115:LEU:HD21	1:L:115:LEU:HD22	1.77	0.66
1:B:384:ARG:HA	1:B:387:GLN:HB3	1.78	0.66
1:A:434:ALA:O	1:B:435:ARG:NH2	2.28	0.65
1:H:384:ARG:HA	1:H:387:GLN:HB3	1.78	0.65
1:G:434:ALA:O	1:H:435:ARG:NH2	2.28	0.65
1:A:419:ARG:HH22	2:C:875:SER:HA	1.61	0.65
1:E:111:VAL:CB	1:E:115:LEU:HD12	2.25	0.65
1:G:419:ARG:HH22	2:I:875:SER:HA	1.61	0.65
2:D:812:GLN:N	2:D:865:VAL:O	2.30	0.65
2:D:869:ASN:ND2	2:D:876:GLU:OE2	2.28	0.64
1:L:96:GLN:HG3	1:L:99:ARG:HD2	1.79	0.64
2:C:813:ALA:HB3	2:C:816:LYS:HD3	1.80	0.64
2:J:812:GLN:N	2:J:865:VAL:O	2.30	0.64
1:K:96:GLN:HA	1:K:99:ARG:HG2	1.80	0.64
1:F:96:GLN:HG3	1:F:99:ARG:HD2	1.79	0.64
1:E:96:GLN:HA	1:E:99:ARG:HG2	1.79	0.64
1:E:111:VAL:C	1:E:115:LEU:HB2	2.19	0.64
1:K:111:VAL:CB	1:K:115:LEU:HD12	2.25	0.63
2:I:813:ALA:HB3	2:I:816:LYS:HD3	1.80	0.63
2:J:801:ILE:HG23	2:J:849:ASP:HB2	1.82	0.62
2:J:2:VAL:HA	2:J:799:ARG:HD2	1.82	0.62
2:D:2:VAL:HA	2:D:799:ARG:HD2	1.82	0.62
1:K:111:VAL:C	1:K:115:LEU:HB2	2.19	0.62
1:A:435:ARG:HH22	1:B:431:LEU:HD13	1.65	0.61
1:G:435:ARG:HH22	1:H:431:LEU:HD13	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:836:VAL:HB	2:I:840:PHE:HB2	1.82	0.61
2:D:801:ILE:HG23	2:D:849:ASP:HB2	1.82	0.61
2:C:810:TYR:HE1	2:C:869:ASN:HD22	1.49	0.61
2:D:806:ILE:HD12	2:D:806:ILE:H	1.66	0.61
1:H:377:ALA:HA	1:H:380:ARG:HH12	1.65	0.61
2:I:810:TYR:HE1	2:I:869:ASN:HD22	1.49	0.60
1:A:414:GLN:HG2	2:D:827:TRP:CE2	2.36	0.60
1:G:414:GLN:HG2	2:J:827:TRP:CE2	2.36	0.60
2:D:839:ARG:HH11	2:D:858:LEU:HA	1.67	0.60
2:J:844:ARG:HH21	2:J:846:SER:HA	1.66	0.60
1:L:129:ARG:NH2	1:L:130:GLN:OE1	2.34	0.60
2:I:842:ILE:HB	2:I:853:LEU:HD13	1.82	0.60
1:B:377:ALA:HA	1:B:380:ARG:HH12	1.65	0.60
1:F:129:ARG:NH2	1:F:130:GLN:OE1	2.34	0.60
2:J:839:ARG:HH11	2:J:858:LEU:HA	1.67	0.60
2:C:842:ILE:HB	2:C:853:LEU:HD13	1.82	0.60
2:J:806:ILE:HD12	2:J:806:ILE:H	1.66	0.59
2:C:836:VAL:HB	2:C:840:PHE:HB2	1.82	0.59
2:C:872:TYR:HB2	2:C:877:TYR:HE2	1.68	0.59
1:L:129:ARG:NH1	1:L:133:ASP:OD2	2.35	0.59
2:J:869:ASN:ND2	2:J:876:GLU:OE2	2.28	0.59
2:C:802:ASP:N	2:C:849:ASP:OD2	2.25	0.59
1:E:160:LEU:O	1:E:163:SER:OG	2.16	0.59
2:I:869:ASN:OD1	2:I:870:ALA:N	2.36	0.59
2:I:872:TYR:HB2	2:I:877:TYR:HE2	1.68	0.59
2:D:844:ARG:HH21	2:D:846:SER:HA	1.66	0.59
1:H:424:ALA:HA	1:H:427:ALA:HB3	1.84	0.58
2:I:808:ARG:HB3	2:I:823:VAL:HG23	1.85	0.58
2:C:808:ARG:HB3	2:C:823:VAL:HG23	1.85	0.58
2:C:869:ASN:OD1	2:C:870:ALA:N	2.36	0.58
1:F:129:ARG:NH1	1:F:133:ASP:OD2	2.35	0.57
1:B:424:ALA:HA	1:B:427:ALA:HB3	1.84	0.57
1:A:417:ILE:HG21	2:D:806:ILE:HD11	1.87	0.57
2:C:855:MET:HB3	2:C:858:LEU:HD21	1.86	0.57
2:I:802:ASP:N	2:I:849:ASP:OD2	2.25	0.57
1:G:417:ILE:HG21	2:J:806:ILE:HD11	1.87	0.56
2:I:855:MET:HB3	2:I:858:LEU:HD21	1.86	0.56
2:J:839:ARG:NH1	2:J:862:ASP:OD2	2.38	0.56
1:H:380:ARG:HG3	1:H:384:ARG:HH12	1.71	0.56
1:A:431:LEU:HD11	1:B:432:GLU:HG2	1.88	0.55
2:C:821:VAL:HG21	2:C:866:TYR:HE2	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:431:LEU:HD11	1:H:432:GLU:HG2	1.88	0.55
2:I:832:TYR:CZ	2:I:842:ILE:HG22	2.42	0.55
2:D:812:GLN:O	2:D:865:VAL:N	2.37	0.55
1:B:386:GLN:HA	1:B:389:ARG:HG2	1.87	0.55
2:C:832:TYR:CZ	2:C:842:ILE:HG22	2.42	0.55
2:I:802:ASP:CG	2:I:844:ARG:HH22	2.10	0.55
1:B:380:ARG:HG3	1:B:384:ARG:HH12	1.71	0.55
2:D:839:ARG:NH1	2:D:862:ASP:OD2	2.38	0.55
2:C:845:ASP:OD2	2:C:848:LYS:NZ	2.32	0.55
1:H:386:GLN:HA	1:H:389:ARG:HG2	1.88	0.55
1:K:143:ILE:HG12	1:L:143:ILE:HB	1.89	0.55
1:K:160:LEU:O	1:K:163:SER:OG	2.16	0.55
2:C:802:ASP:CG	2:C:844:ARG:HH22	2.10	0.54
2:C:817:GLN:OE1	2:C:817:GLN:N	2.38	0.54
2:J:813:ALA:HB3	2:J:816:LYS:HB2	1.90	0.54
1:B:414:GLN:O	1:B:417:ILE:HG22	2.07	0.54
1:E:143:ILE:HG12	1:F:143:ILE:HB	1.89	0.54
1:H:414:GLN:O	1:H:417:ILE:HG22	2.07	0.54
2:D:8:GLY:HA3	2:D:793:LEU:HA	1.90	0.54
2:C:818:ARG:HH11	2:C:818:ARG:HG2	1.72	0.54
2:I:860:PRO:HA	2:I:887:SER:HA	1.90	0.54
2:J:812:GLN:O	2:J:865:VAL:N	2.37	0.54
2:I:821:VAL:HG21	2:I:866:TYR:HE2	1.71	0.54
2:J:883:GLN:OE1	2:J:885:THR:OG1	2.15	0.53
2:I:845:ASP:OD2	2:I:848:LYS:NZ	2.32	0.53
1:K:111:VAL:HA	1:K:115:LEU:CG	2.39	0.53
2:C:860:PRO:HA	2:C:887:SER:HA	1.90	0.53
2:I:818:ARG:HG2	2:I:818:ARG:HH11	1.72	0.53
2:J:869:ASN:OD1	2:J:870:ALA:N	2.42	0.53
2:D:813:ALA:HB3	2:D:816:LYS:HB2	1.90	0.53
2:D:808:ARG:CB	2:D:823:VAL:HG12	2.39	0.53
2:J:8:GLY:HA3	2:J:793:LEU:HA	1.90	0.53
2:D:808:ARG:NH1	2:D:876:GLU:OE2	2.43	0.52
1:G:383:GLU:HA	1:G:386:GLN:HB2	1.91	0.52
2:J:808:ARG:NH1	2:J:876:GLU:OE2	2.43	0.52
2:D:804:ILE:HG23	2:D:872:TYR:HE1	1.75	0.52
2:D:808:ARG:HB3	2:D:823:VAL:HG12	1.92	0.52
2:D:869:ASN:OD1	2:D:870:ALA:N	2.42	0.52
1:E:111:VAL:HA	1:E:115:LEU:CG	2.39	0.52
2:J:804:ILE:HG23	2:J:872:TYR:HE1	1.75	0.52
2:J:808:ARG:CB	2:J:823:VAL:HG12	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:808:ARG:HB3	2:J:823:VAL:HG12	1.92	0.51
2:I:817:GLN:OE1	2:I:817:GLN:N	2.38	0.51
1:K:127:ALA:O	1:K:131:THR:HG23	2.10	0.51
1:L:143:ILE:HA	1:L:146:LEU:HG	1.93	0.51
1:E:127:ALA:O	1:E:131:THR:HG23	2.10	0.51
1:A:383:GLU:HA	1:A:386:GLN:HB2	1.91	0.51
1:F:143:ILE:HA	1:F:146:LEU:HG	1.93	0.51
2:I:799:ARG:NH1	2:I:800:SER:HB3	2.27	0.50
2:C:866:TYR:O	2:C:881:GLY:HA3	2.11	0.50
1:L:101:ILE:O	1:L:104:ILE:HG22	2.12	0.50
1:A:415:ALA:O	1:A:418:GLU:HG3	2.12	0.50
1:F:139:ASN:O	1:F:142:GLU:HB3	2.12	0.50
1:H:425:ALA:HA	2:I:820:MET:HE3	1.94	0.50
2:C:799:ARG:NH1	2:C:800:SER:HB3	2.27	0.49
1:F:101:ILE:O	1:F:104:ILE:HG22	2.12	0.49
2:I:810:TYR:HA	2:I:820:MET:HA	1.94	0.49
2:D:883:GLN:OE1	2:D:885:THR:OG1	2.15	0.49
2:J:865:VAL:HA	2:J:883:GLN:HA	1.95	0.49
2:I:866:TYR:O	2:I:881:GLY:HA3	2.11	0.49
1:G:415:ALA:O	1:G:418:GLU:HG3	2.12	0.49
2:I:839:ARG:NH2	2:I:862:ASP:OD2	2.45	0.49
2:C:810:TYR:HA	2:C:820:MET:HA	1.94	0.49
2:C:839:ARG:NH2	2:C:862:ASP:OD2	2.45	0.49
1:K:121:ALA:HB3	1:L:122:LEU:HD11	1.94	0.49
1:A:393:ASP:O	1:F:109:ARG:NH2	2.34	0.49
1:B:373:ALA:HA	1:B:376:LYS:NZ	2.28	0.49
1:F:103:LEU:O	1:F:107:GLU:N	2.34	0.49
1:K:111:VAL:CA	1:K:115:LEU:CB	2.80	0.49
1:B:419:ARG:HD3	1:B:422:SER:HB3	1.95	0.49
2:J:804:ILE:HG22	2:J:805:ASN:O	2.13	0.49
1:L:139:ASN:O	1:L:142:GLU:HB3	2.12	0.48
1:H:373:ALA:HA	1:H:376:LYS:NZ	2.28	0.48
2:D:865:VAL:HA	2:D:883:GLN:HA	1.95	0.48
1:H:419:ARG:HD3	1:H:422:SER:HB3	1.95	0.48
1:B:425:ALA:HA	2:C:820:MET:HE3	1.96	0.48
2:C:839:ARG:HG2	2:C:857:ASN:HB3	1.95	0.47
2:D:804:ILE:HG22	2:D:805:ASN:O	2.13	0.47
1:E:121:ALA:HB3	1:F:122:LEU:HD11	1.94	0.47
1:F:143:ILE:O	1:F:147:ARG:HG3	2.14	0.47
2:I:839:ARG:HG2	2:I:857:ASN:HB3	1.95	0.47
1:E:98:GLN:HA	1:E:101:ILE:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:99:ARG:O	1:E:103:LEU:HG	2.15	0.47
1:L:143:ILE:O	1:L:147:ARG:HG3	2.14	0.47
1:E:96:GLN:HG2	1:E:100:GLN:HE22	1.79	0.47
1:E:98:GLN:HG3	1:E:101:ILE:HD12	1.97	0.47
1:K:98:GLN:HA	1:K:101:ILE:HD12	1.96	0.47
2:I:818:ARG:HG2	2:I:818:ARG:NH1	2.29	0.47
1:K:111:VAL:O	1:K:115:LEU:HB3	2.14	0.47
1:L:103:LEU:O	1:L:107:GLU:N	2.34	0.46
1:L:131:THR:O	1:L:135:ALA:N	2.37	0.46
1:B:381:ALA:HA	1:B:384:ARG:HH11	1.81	0.46
2:D:6:GLU:O	2:D:7:SER:OG	2.30	0.46
1:E:111:VAL:O	1:E:115:LEU:HB3	2.14	0.46
1:K:98:GLN:HG3	1:K:101:ILE:HD12	1.97	0.46
2:C:818:ARG:HG2	2:C:818:ARG:NH1	2.29	0.46
1:K:96:GLN:HG2	1:K:100:GLN:HE22	1.79	0.46
1:K:99:ARG:O	1:K:103:LEU:HG	2.14	0.46
1:H:381:ALA:HA	1:H:384:ARG:HH11	1.81	0.45
1:A:397:GLU:OE1	1:A:397:GLU:N	2.50	0.45
1:H:399:GLN:O	1:H:403:ARG:HG3	2.17	0.45
2:I:793:LEU:HB3	2:I:809:TRP:CZ3	2.52	0.45
1:G:422:SER:HB2	2:J:831:ASN:HD22	1.82	0.45
2:I:811:ARG:N	2:I:819:GLY:O	2.40	0.45
2:J:863:THR:OG1	2:J:885:THR:HA	2.18	0.44
1:G:397:GLU:OE1	1:G:397:GLU:N	2.50	0.44
2:C:821:VAL:HG21	2:C:866:TYR:CE2	2.53	0.44
1:G:393:ASP:O	1:L:109:ARG:NH2	2.34	0.44
1:A:422:SER:HB2	2:D:831:ASN:HD22	1.82	0.44
1:B:399:GLN:O	1:B:403:ARG:HG3	2.17	0.44
2:J:866:TYR:CE1	2:J:884:VAL:HB	2.53	0.44
1:E:97:ALA:O	1:E:101:ILE:HG13	2.18	0.44
1:L:142:GLU:N	1:L:145:ARG:HH21	2.16	0.44
2:D:866:TYR:CE1	2:D:884:VAL:HB	2.53	0.44
2:C:793:LEU:HB3	2:C:809:TRP:CZ3	2.52	0.44
2:D:8:GLY:HA3	2:D:793:LEU:HD23	2.01	0.43
2:D:863:THR:OG1	2:D:885:THR:HA	2.18	0.43
1:L:141:LEU:O	1:L:145:ARG:N	2.44	0.43
2:I:821:VAL:HG21	2:I:866:TYR:CE2	2.53	0.43
1:L:140:ALA:O	1:L:143:ILE:HG22	2.19	0.43
1:F:142:GLU:N	1:F:145:ARG:HH21	2.16	0.43
1:K:97:ALA:O	1:K:101:ILE:HG13	2.18	0.43
1:K:111:VAL:HA	1:K:115:LEU:HG	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:8:GLY:HA3	2:J:793:LEU:HD23	2.01	0.43
2:J:11:LEU:HD13	2:J:885:THR:O	2.19	0.43
2:J:855:MET:SD	2:J:855:MET:N	2.92	0.43
2:D:11:LEU:HD13	2:D:885:THR:O	2.19	0.43
2:D:855:MET:SD	2:D:855:MET:N	2.92	0.43
1:L:141:LEU:C	1:L:145:ARG:HE	2.22	0.43
1:A:391:ARG:NE	1:B:392:LEU:HD21	2.34	0.43
1:B:397:GLU:HA	1:B:397:GLU:OE1	2.19	0.42
1:G:435:ARG:HD3	1:G:438:ARG:HH22	1.84	0.42
1:G:391:ARG:NE	1:H:392:LEU:HD21	2.34	0.42
1:F:140:ALA:O	1:F:143:ILE:HG22	2.19	0.42
2:C:825:THR:HG22	2:C:827:TRP:CE3	2.55	0.42
1:F:141:LEU:C	1:F:145:ARG:HE	2.22	0.42
1:K:154:ASP:O	1:K:156:LYS:N	2.53	0.42
1:A:435:ARG:HD3	1:A:438:ARG:HH22	1.85	0.42
1:E:124:GLU:HB3	1:E:128:ARG:CZ	2.50	0.42
1:E:154:ASP:O	1:E:156:LYS:N	2.53	0.42
1:A:419:ARG:O	1:A:419:ARG:HG2	2.20	0.42
2:C:863:THR:HG22	2:C:886:VAL:N	2.35	0.42
1:A:380:ARG:HA	1:A:383:GLU:CD	2.41	0.42
1:G:419:ARG:O	1:G:419:ARG:HG2	2.20	0.42
2:I:825:THR:HG22	2:I:827:TRP:CE3	2.55	0.42
1:K:124:GLU:HB3	1:K:128:ARG:CZ	2.50	0.42
2:C:799:ARG:CZ	2:C:800:SER:HB3	2.50	0.41
2:C:811:ARG:N	2:C:819:GLY:O	2.40	0.41
1:G:397:GLU:OE1	1:L:109:ARG:NH2	2.53	0.41
1:G:403:ARG:HD3	1:G:403:ARG:HA	1.61	0.41
1:A:397:GLU:OE1	1:F:109:ARG:NH2	2.53	0.41
1:H:397:GLU:OE1	1:H:397:GLU:HA	2.19	0.41
1:G:391:ARG:HE	1:H:392:LEU:HD21	1.85	0.41
1:G:380:ARG:HA	1:G:383:GLU:CD	2.41	0.41
1:K:147:ARG:O	1:K:150:LEU:HB3	2.21	0.41
1:A:403:ARG:HA	1:A:403:ARG:HD3	1.61	0.41
2:D:859:LYS:O	2:D:861:GLU:N	2.54	0.41
2:I:863:THR:HG22	2:I:886:VAL:N	2.35	0.41
1:A:391:ARG:HE	1:B:392:LEU:HD21	1.85	0.41
1:E:111:VAL:HA	1:E:115:LEU:HG	2.01	0.41
2:I:2:VAL:HG12	2:I:877:TYR:HB2	2.03	0.41
2:I:799:ARG:CZ	2:I:800:SER:HB3	2.50	0.41
1:G:371:ALA:O	1:G:375:GLU:N	2.54	0.40
2:J:859:LYS:O	2:J:861:GLU:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:824:VAL:HG12	2:I:830:THR:HG22	2.04	0.40
1:E:111:VAL:CA	1:E:115:LEU:CB	2.80	0.40
1:A:371:ALA:O	1:A:375:GLU:N	2.54	0.40
2:D:836:VAL:HG11	2:D:840:PHE:CE2	2.56	0.40
1:E:115:LEU:CD2	1:F:115:LEU:HD22	2.49	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	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
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 (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	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
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

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

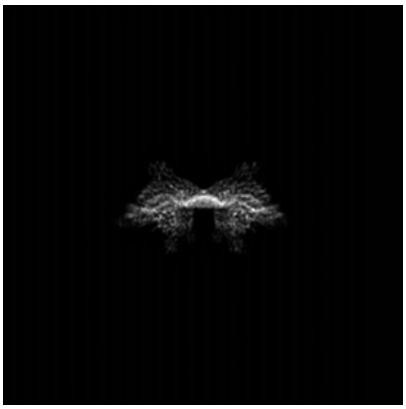
6 Map visualisation

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.

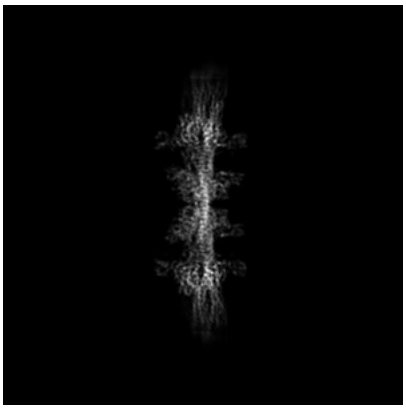
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

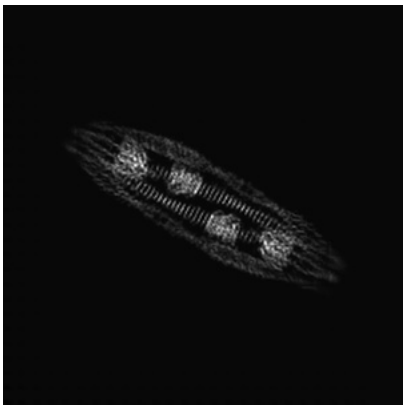
6.1.1 Primary map



X

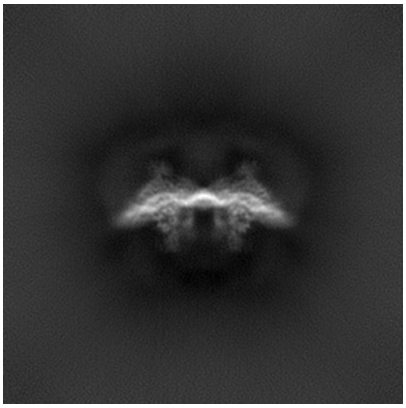


Y

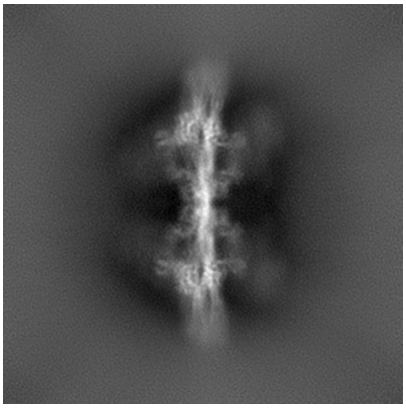


Z

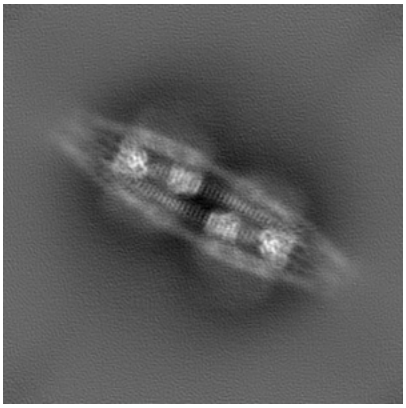
6.1.2 Raw map



X



Y

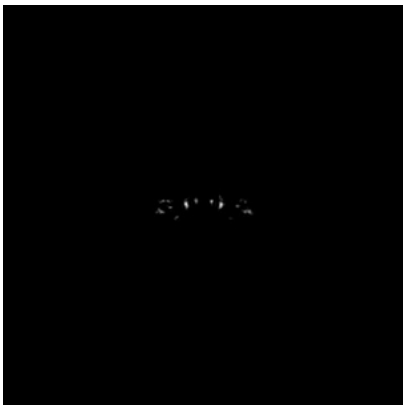


Z

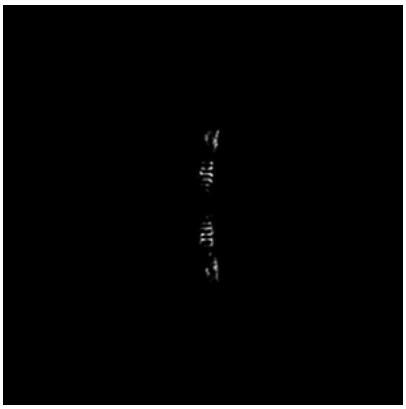
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



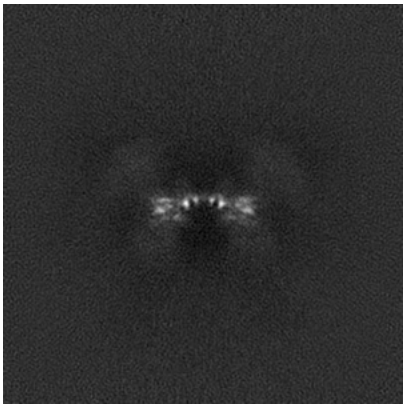
X Index: 125



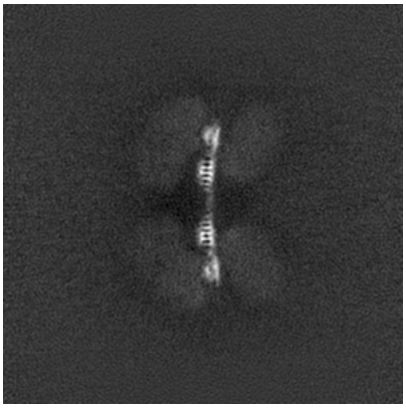
Y Index: 125

Z Index: 125

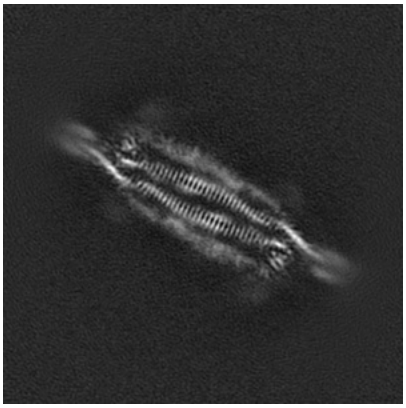
6.2.2 Raw map



X Index: 125



Y Index: 125

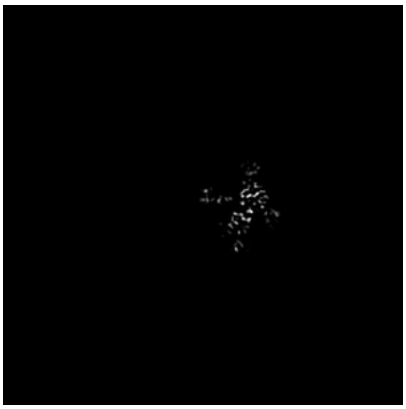


Z Index: 125

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

6.3 Largest variance slices (i)

6.3.1 Primary map

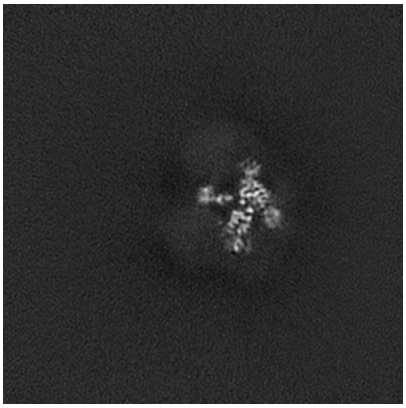


X Index: 82

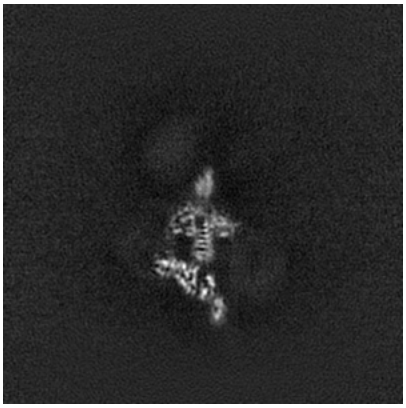
Y Index: 144

Z Index: 126

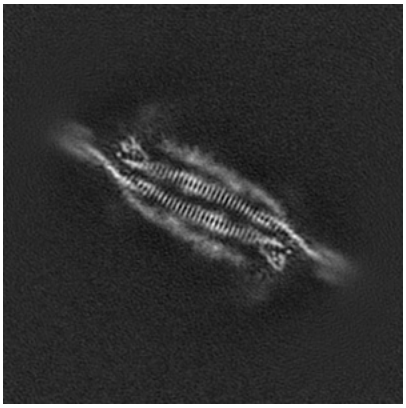
6.3.2 Raw map



X Index: 82



Y Index: 144

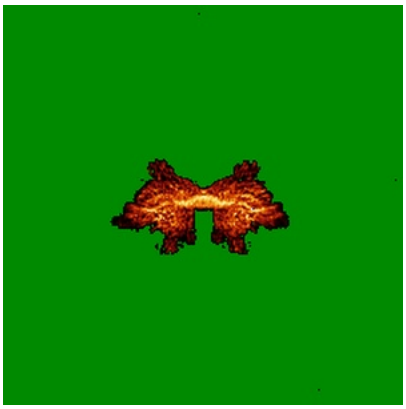


Z Index: 126

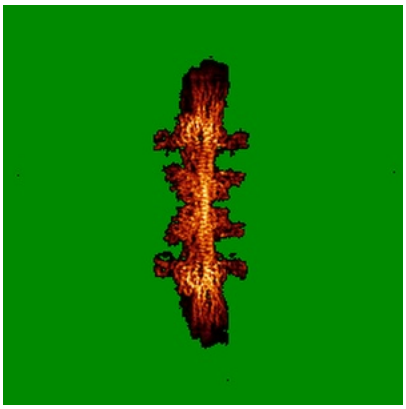
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

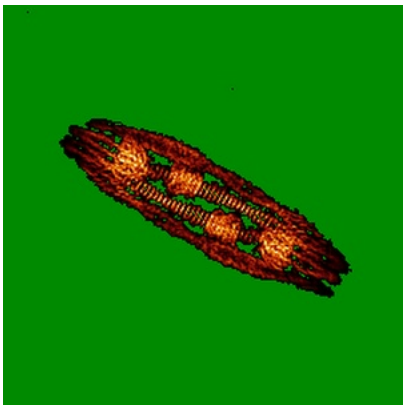
6.4.1 Primary map



X

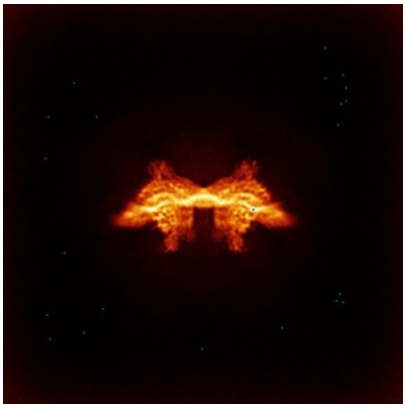


Y

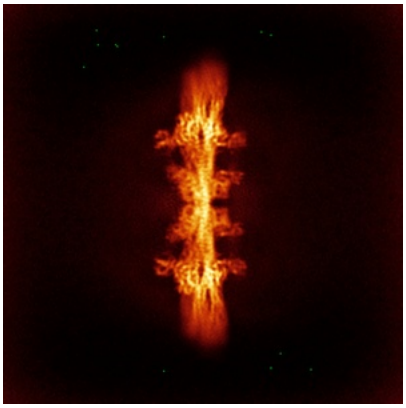


Z

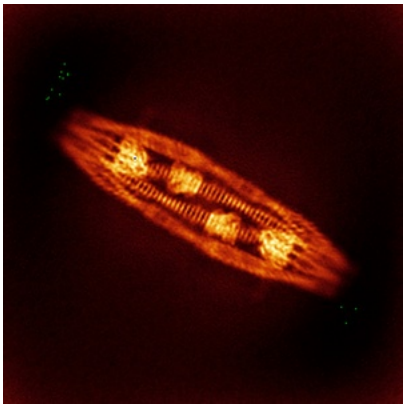
6.4.2 Raw map



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

X Y Z

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

X Y Z

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.

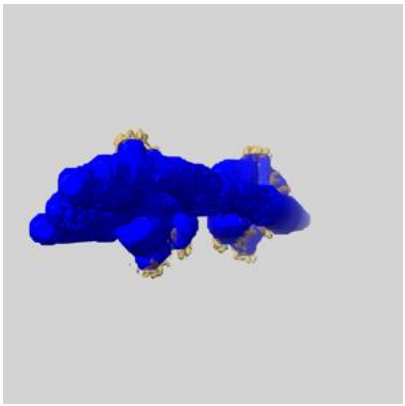
6.6 Mask visualisation (i)

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

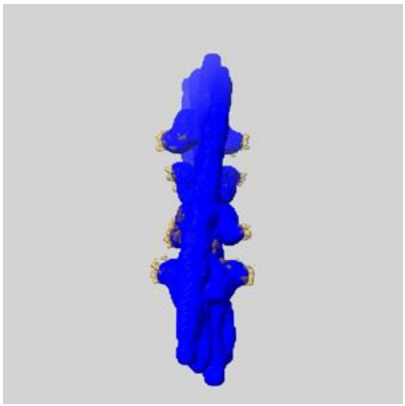
A mask typically either:

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

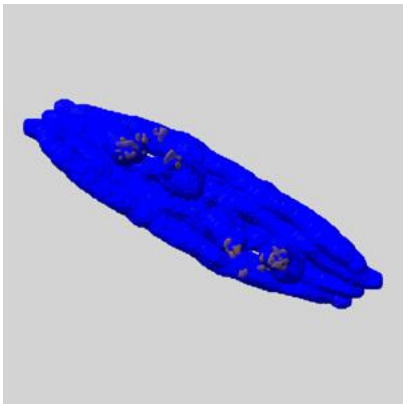
6.6.1 emd_15402_msk_1.map (i)



X



Y

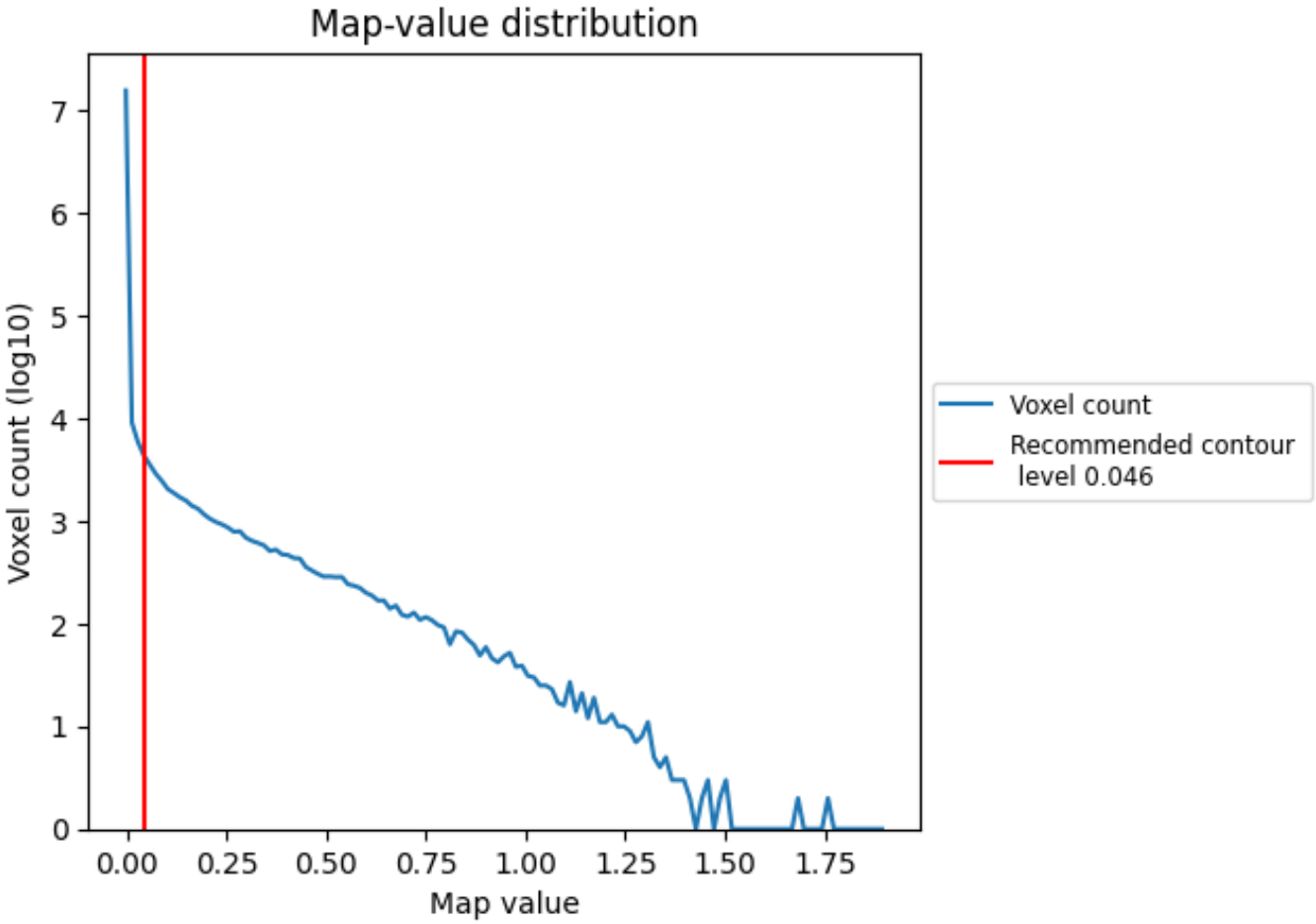


Z

7 Map analysis

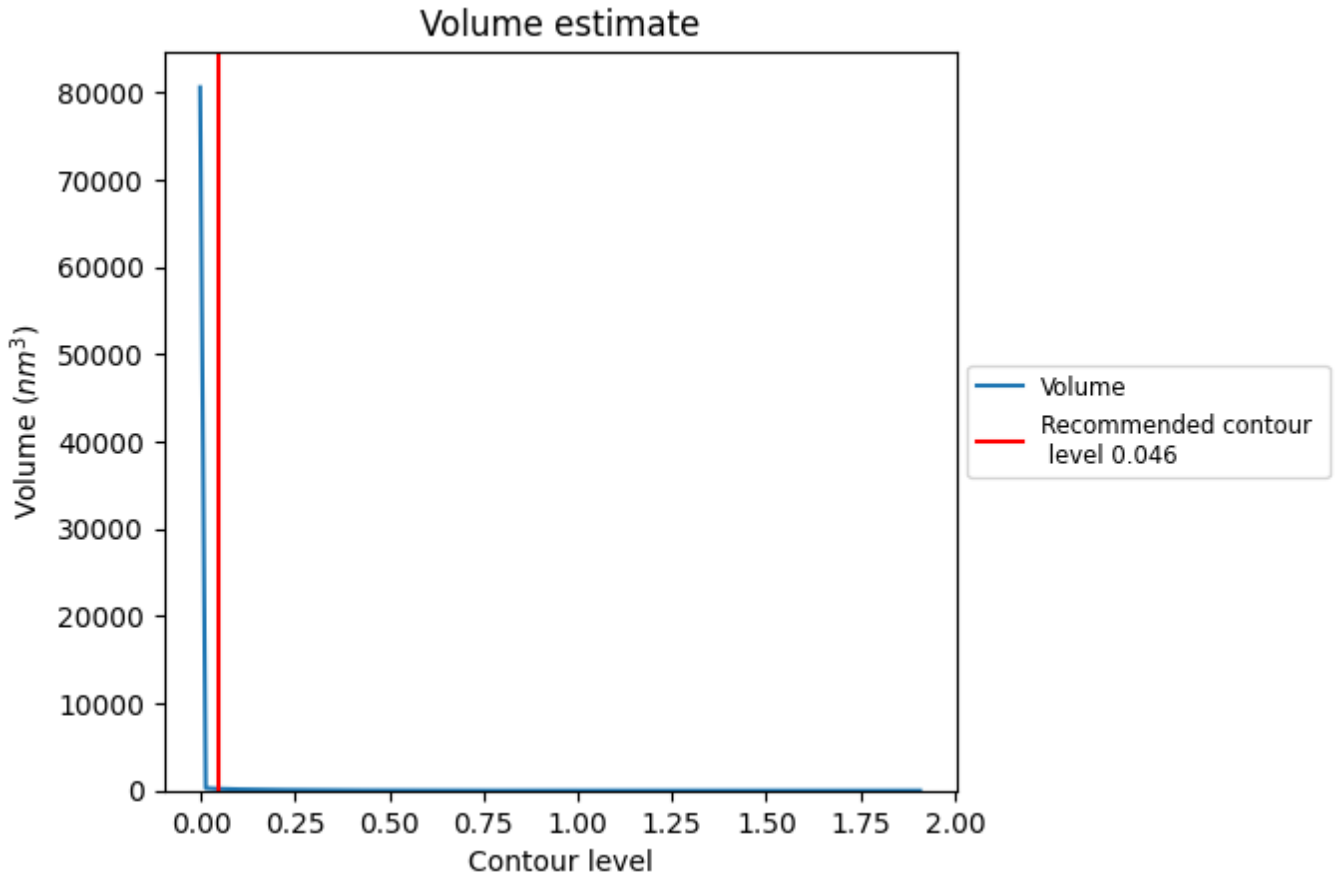
This section contains the results of statistical analysis of the map.

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.

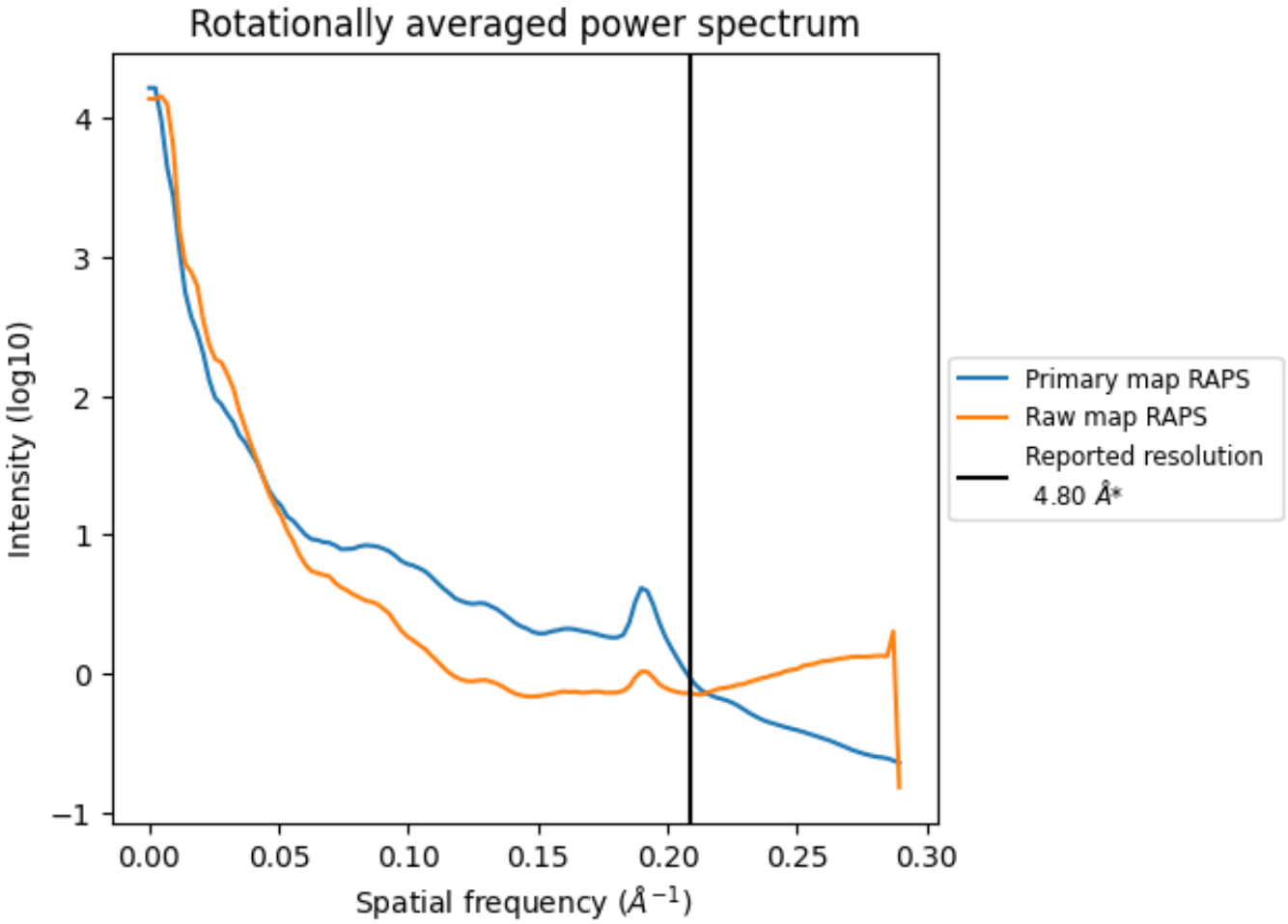
7.2 Volume estimate



The volume at the recommended contour level is 207 nm^3; 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 (i)

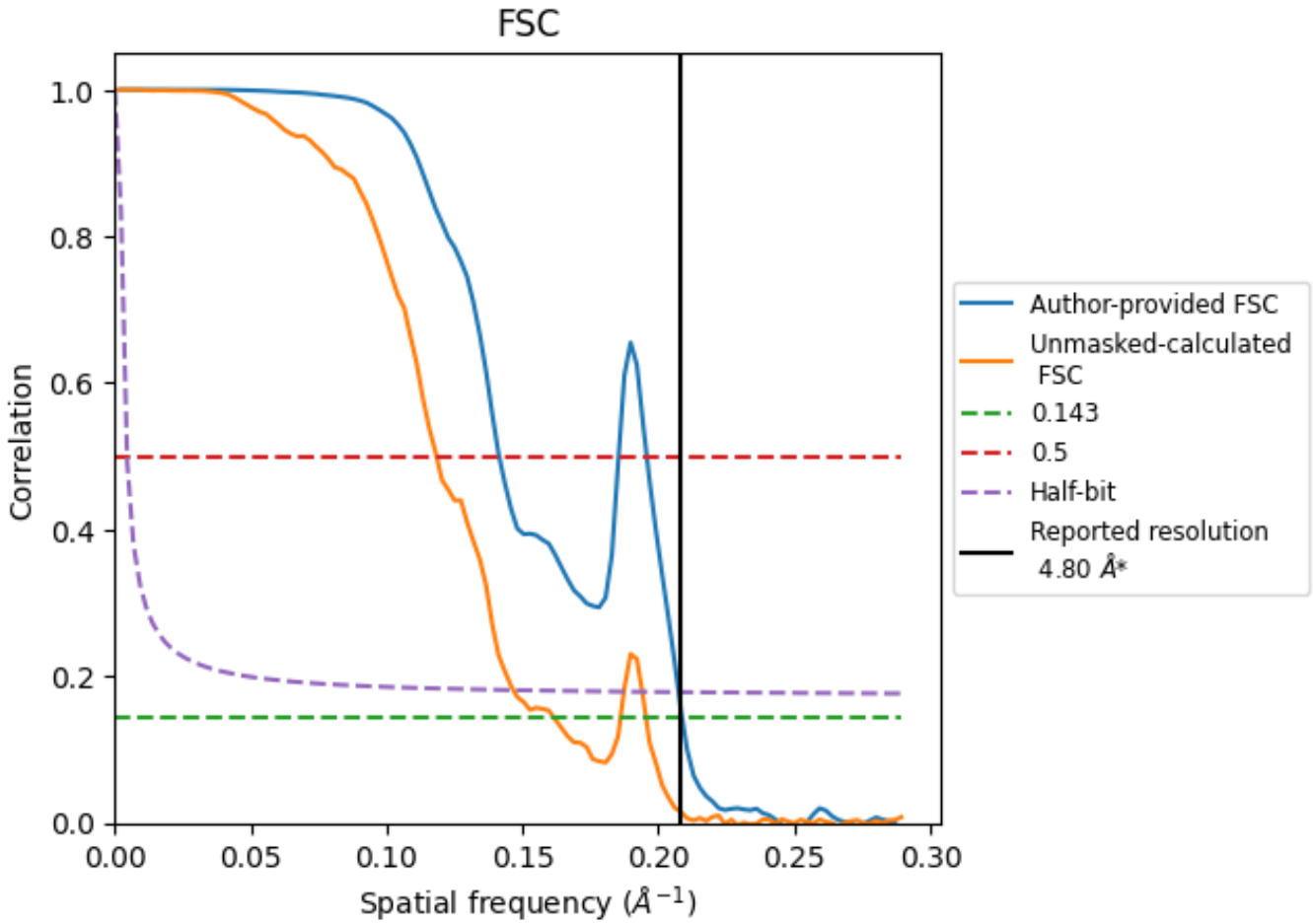


*Reported resolution corresponds to spatial frequency of 0.208 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.208 Å^{-1}

8.2 Resolution estimates (i)

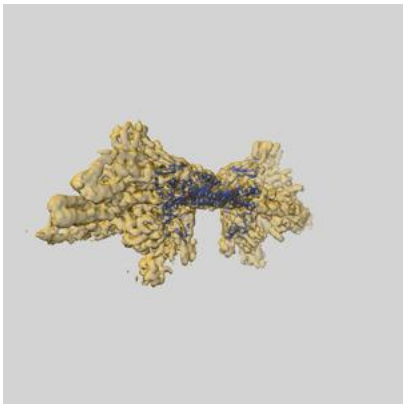
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.80	-	-
Author-provided FSC curve	4.79	7.07	4.82
Unmasked-calculated*	6.19	8.45	6.82

*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 %

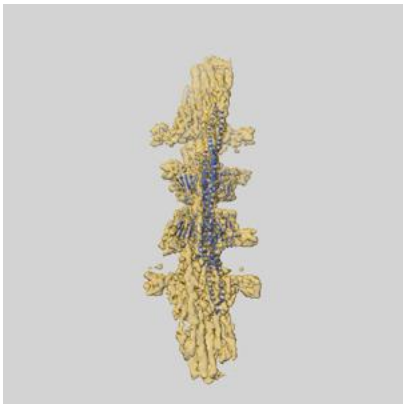
9 Map-model fit

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.

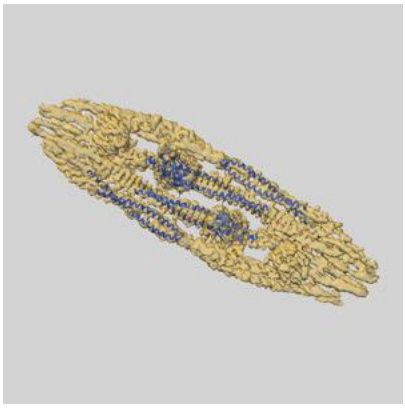
9.1 Map-model overlay



X



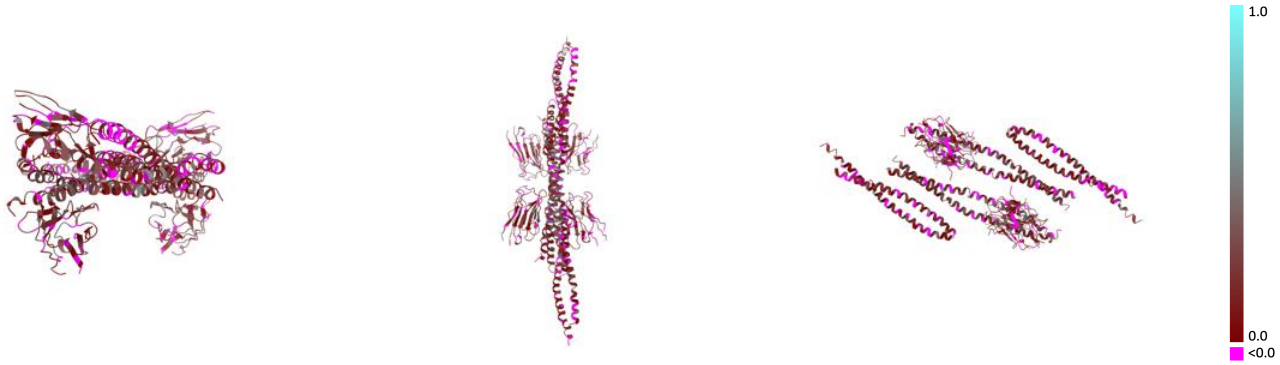
Y



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.

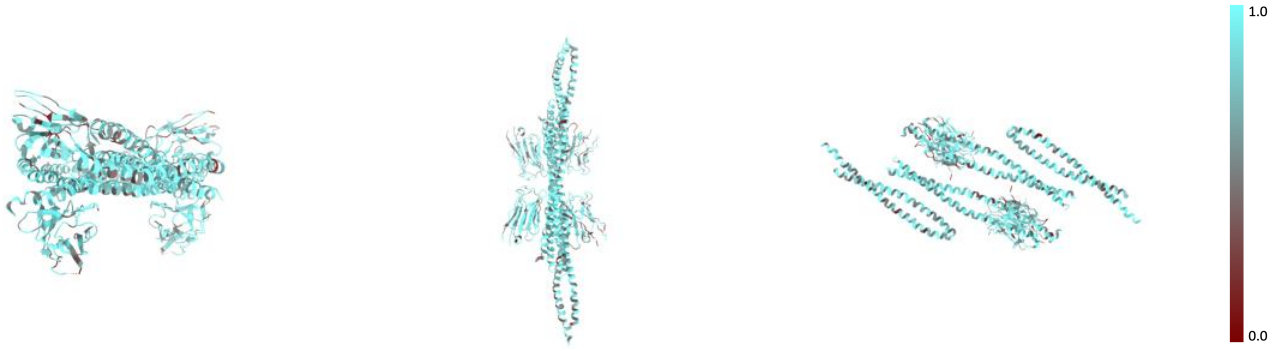
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

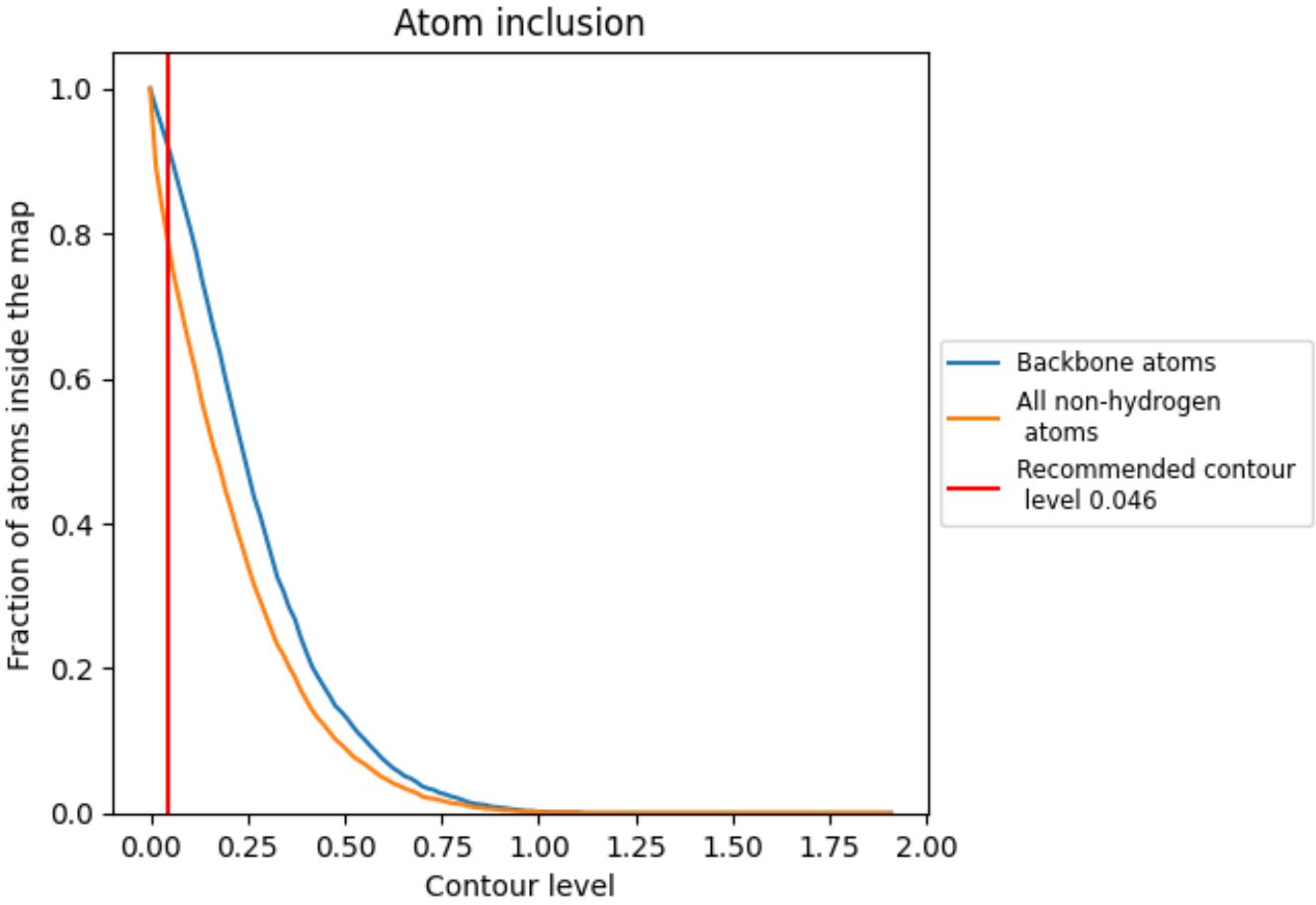
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (i)



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	0.7830	0.1640
A	0.8530	0.2180
B	0.8420	0.2100
C	0.7940	0.1780
D	0.7090	0.1390
E	0.7280	0.1050
F	0.7550	0.1120
G	0.8300	0.2160
H	0.8200	0.1810
I	0.8290	0.1930
J	0.7130	0.1470
K	0.7660	0.1190
L	0.7710	0.1110