wwPDB EM Validation Summary Report (i)

Aug 27, 2026 – 02:31 PM EDT

PDB ID	:	9YKN / pdb_00009ykn
EMDB ID	:	EMD-73055
Title	:	The structure of the cardiac native crossbridge in the rigor state, myosin heads with essential and regulatory light chains bound to actin molecules 6 and 7
Authors	:	Galkin, V.E.; Risi, C.M.
Deposited on	:	2025-10-07
Resolution	:	5.30 Å(reported)
Based on initial models	:	6SFA, 7JH7, 7KO5, 8DD0, 5H53

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 (i) 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 (i)) were used in the production of this report:

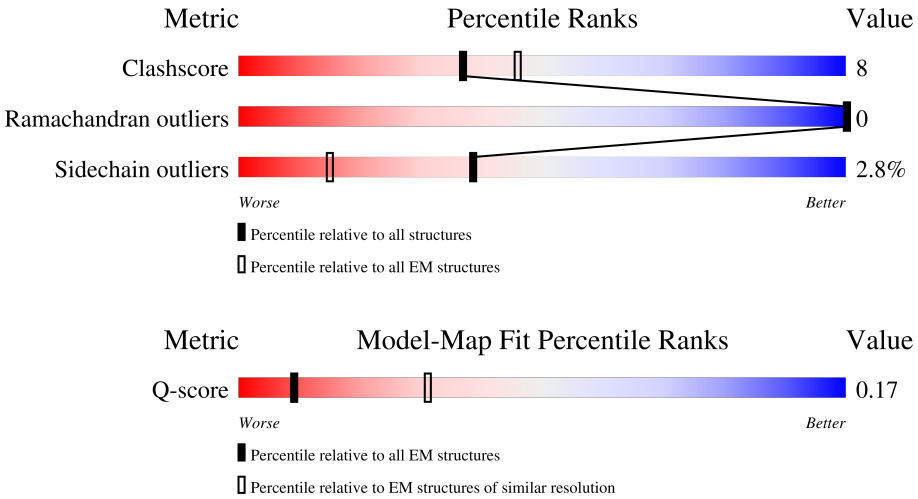
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 5.30 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.



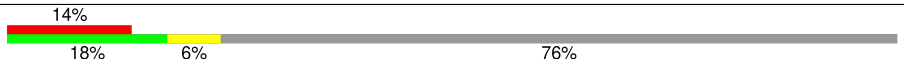
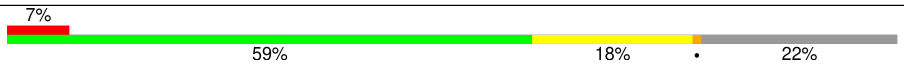
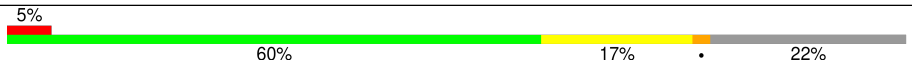
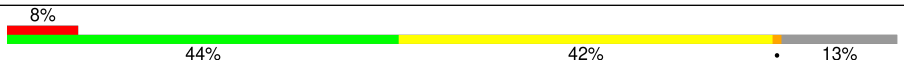
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	625 (4.80 - 5.80)

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	377	83% 15%
1	B	377	87% 12%
2	C	284	22% 74%
2	D	284	18% 8% 74%

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Mol	Chain	Length	Quality of chain
2	E	284	
2	F	284	
3	G	285	
4	H	1935	
4	I	1935	
5	J	196	
5	K	196	
6	L	166	
6	M	166	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 26677 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 Actin, alpha cardiac muscle 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	375	Total	C	N	O	S	0	0
			2932	1854	493	565	20		
1	B	375	Total	C	N	O	S	0	0
			2932	1854	493	565	20		

- Molecule 2 is a protein called Tropomyosin alpha-1 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	75	Total	C	N	O	S	0	0
			618	384	98	135	1		
2	D	75	Total	C	N	O	S	0	0
			618	384	98	135	1		
2	E	40	Total	C	N	O	S	0	0
			321	194	60	64	3		
2	F	40	Total	C	N	O	S	0	0
			321	194	60	64	3		

- Molecule 3 is a protein called Troponin T2, cardiac type.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	68	Total	C	N	O	S	0	0
			595	359	121	114	1		

- Molecule 4 is a protein called Myosin-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	837	Total	C	N	O	S	0	0
			6757	4322	1159	1242	34		
4	I	837	Total	C	N	O	S	0	0
			6757	4322	1159	1242	34		

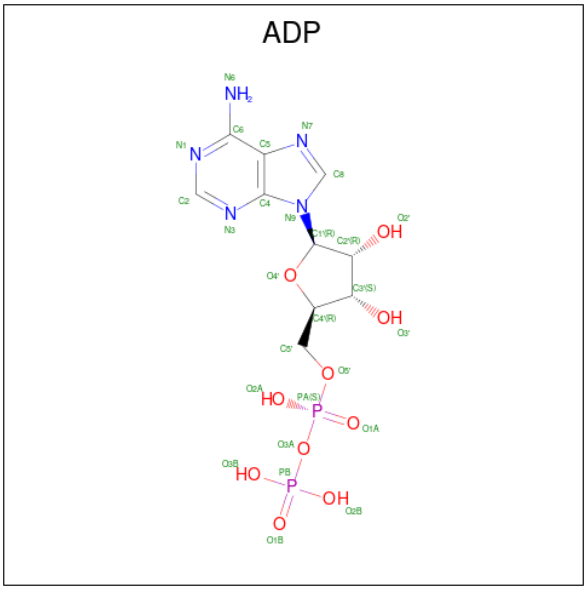
- Molecule 5 is a protein called Myosin light chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	J	153	Total	C	N	O	S	0	0
			1217	766	202	238	11		
5	K	153	Total	C	N	O	S	0	0
			1217	766	202	238	11		

- Molecule 6 is a protein called MYL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	145	Total	C	N	O	S	0	0
			1168	740	190	233	5		
6	M	145	Total	C	N	O	S	0	0
			1168	740	190	233	5		

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
7	B	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
8	A	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
8	B	1	1	1	0

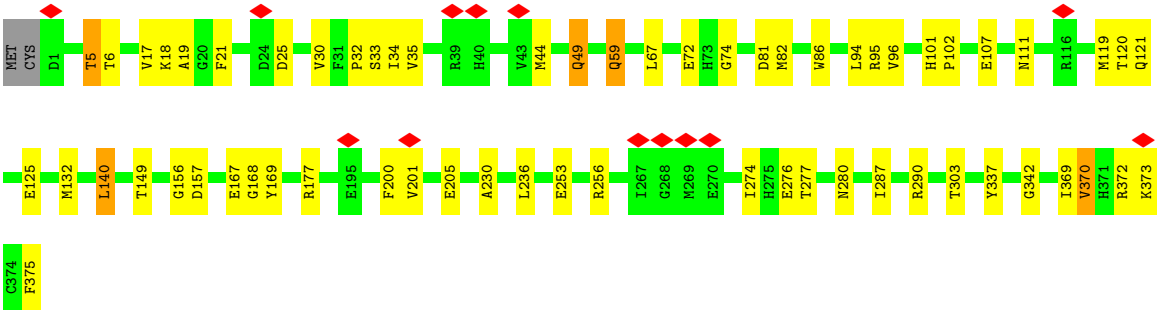
3 Residue-property plots (i)

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: Actin, alpha cardiac muscle 1

Chain A:

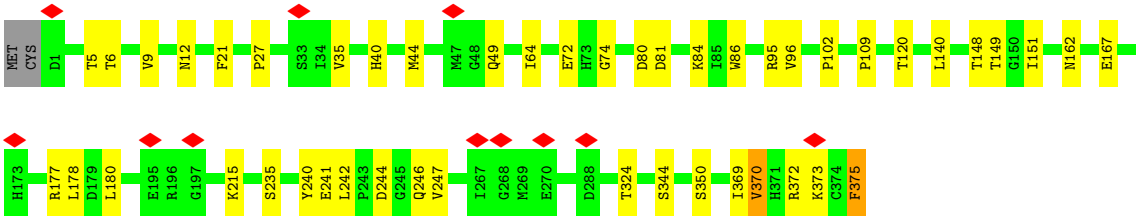




• Molecule 1: Actin, alpha cardiac muscle 1

Chain B:

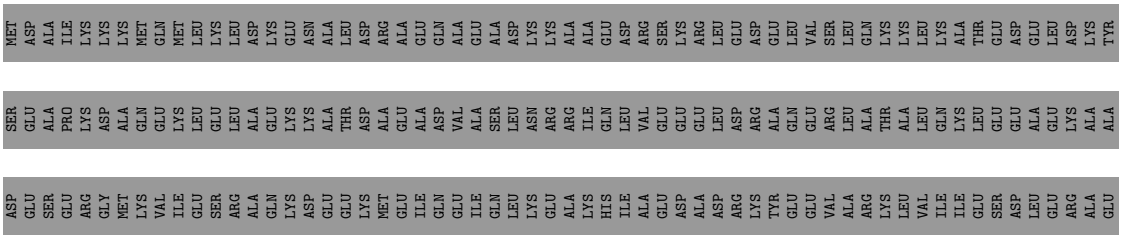


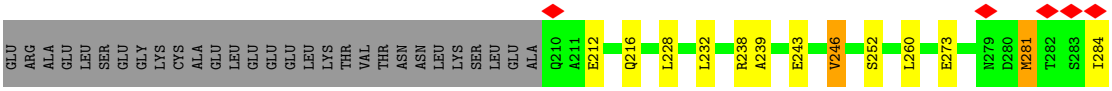


• Molecule 2: Tropomyosin alpha-1 chain

Chain C:

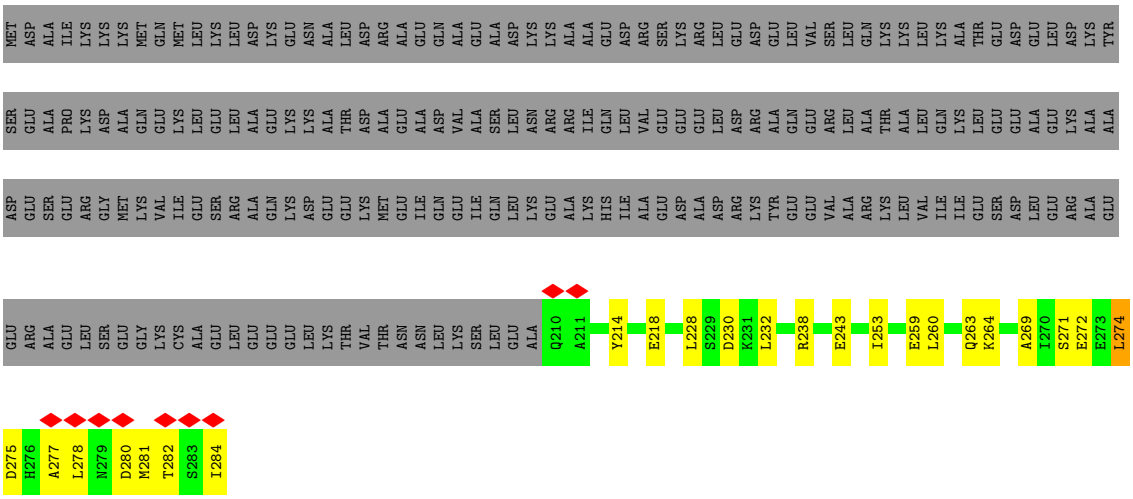






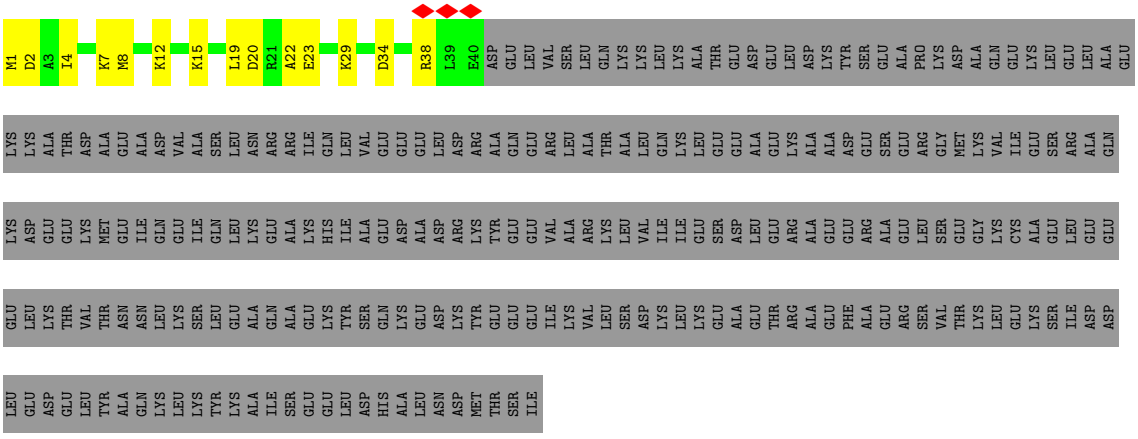
• Molecule 2: Tropomyosin alpha-1 chain





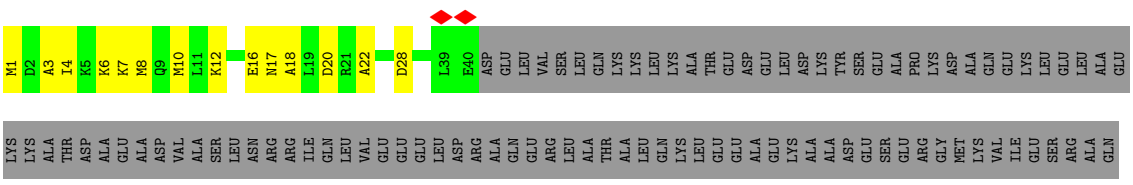
• Molecule 2: Tropomyosin alpha-1 chain

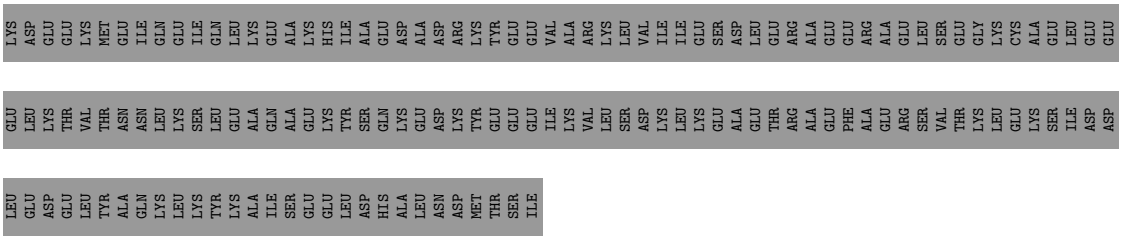




• Molecule 2: Tropomyosin alpha-1 chain



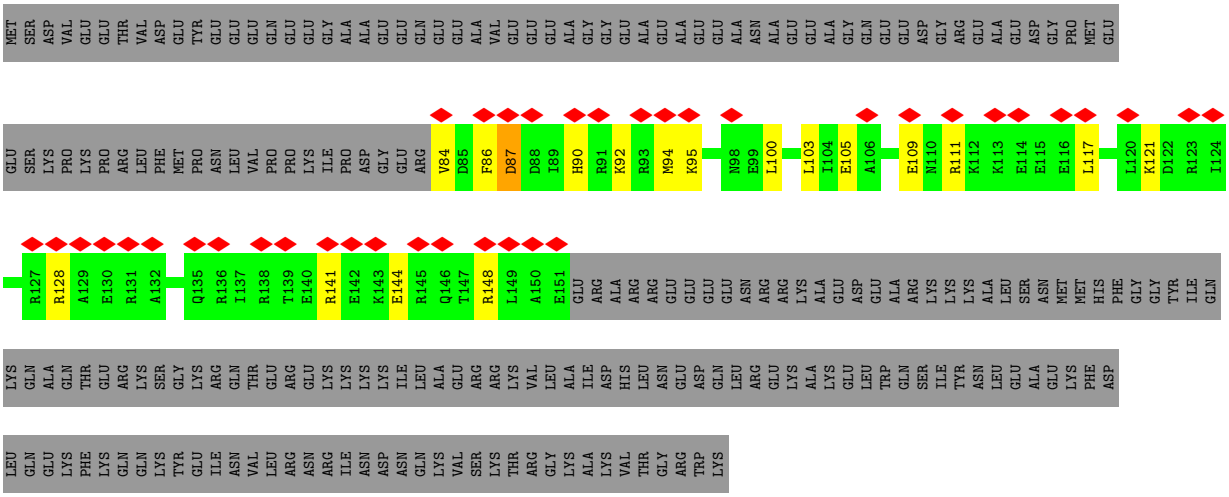




• Molecule 3: Troponin T2, cardiac type

Chain G:

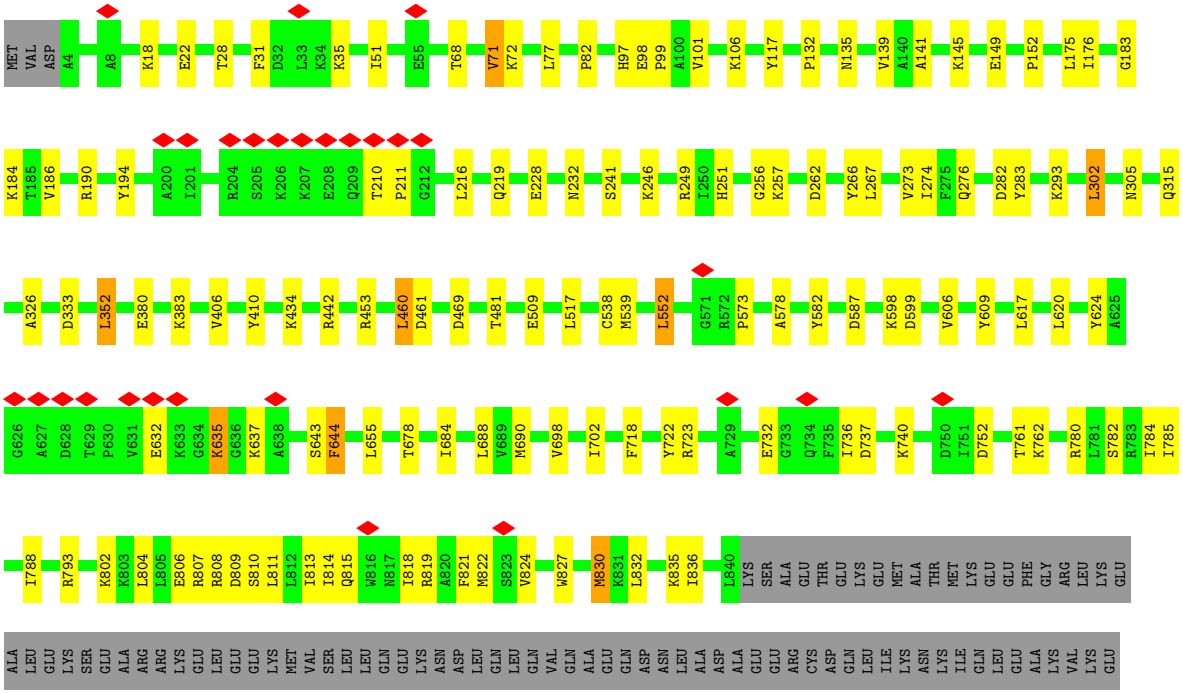


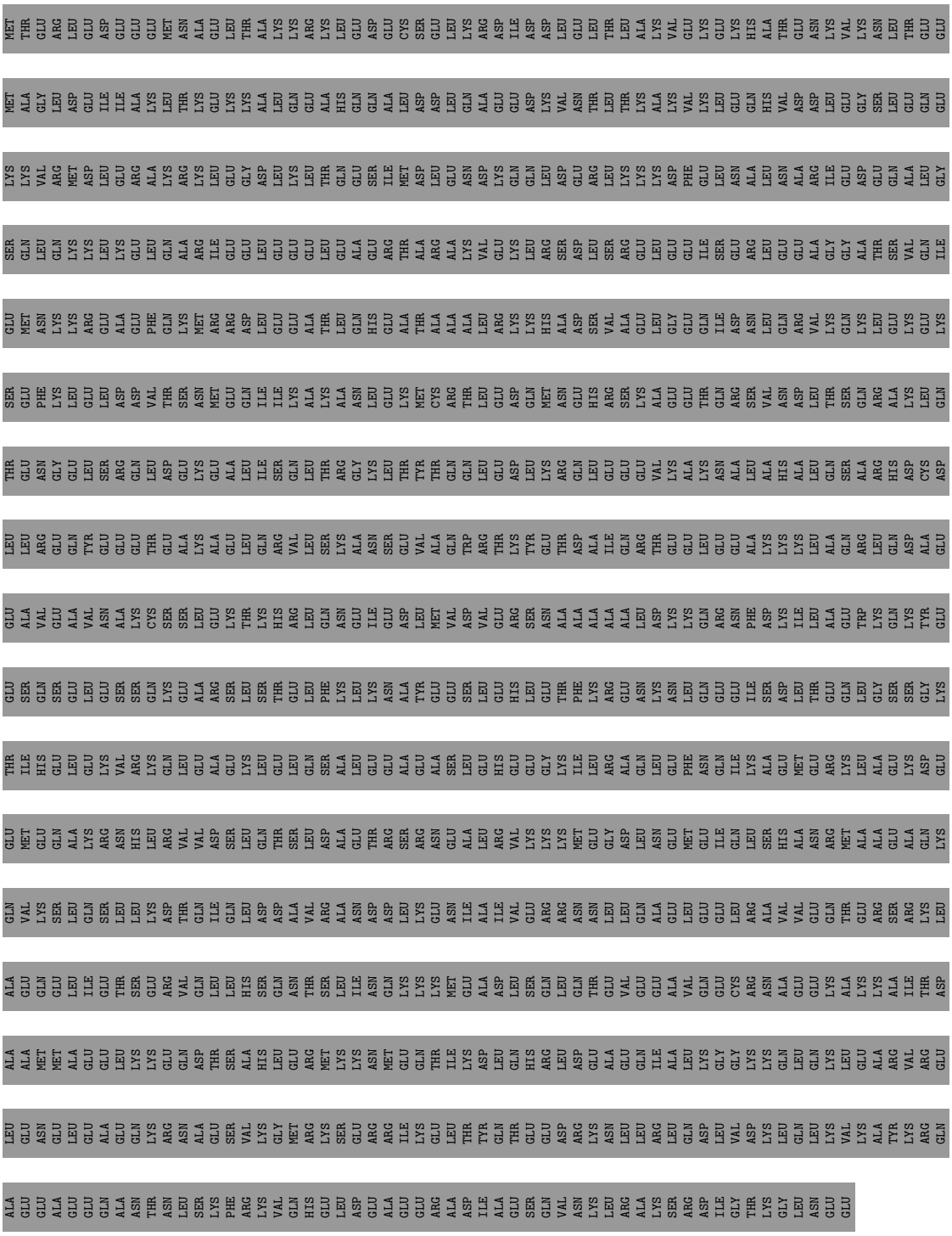


• Molecule 4: Myosin-7

Chain H:



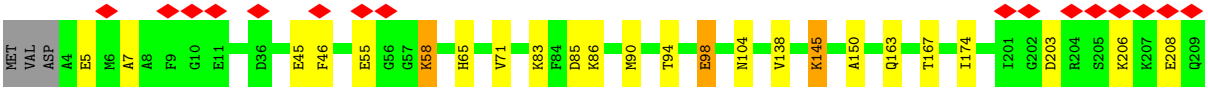


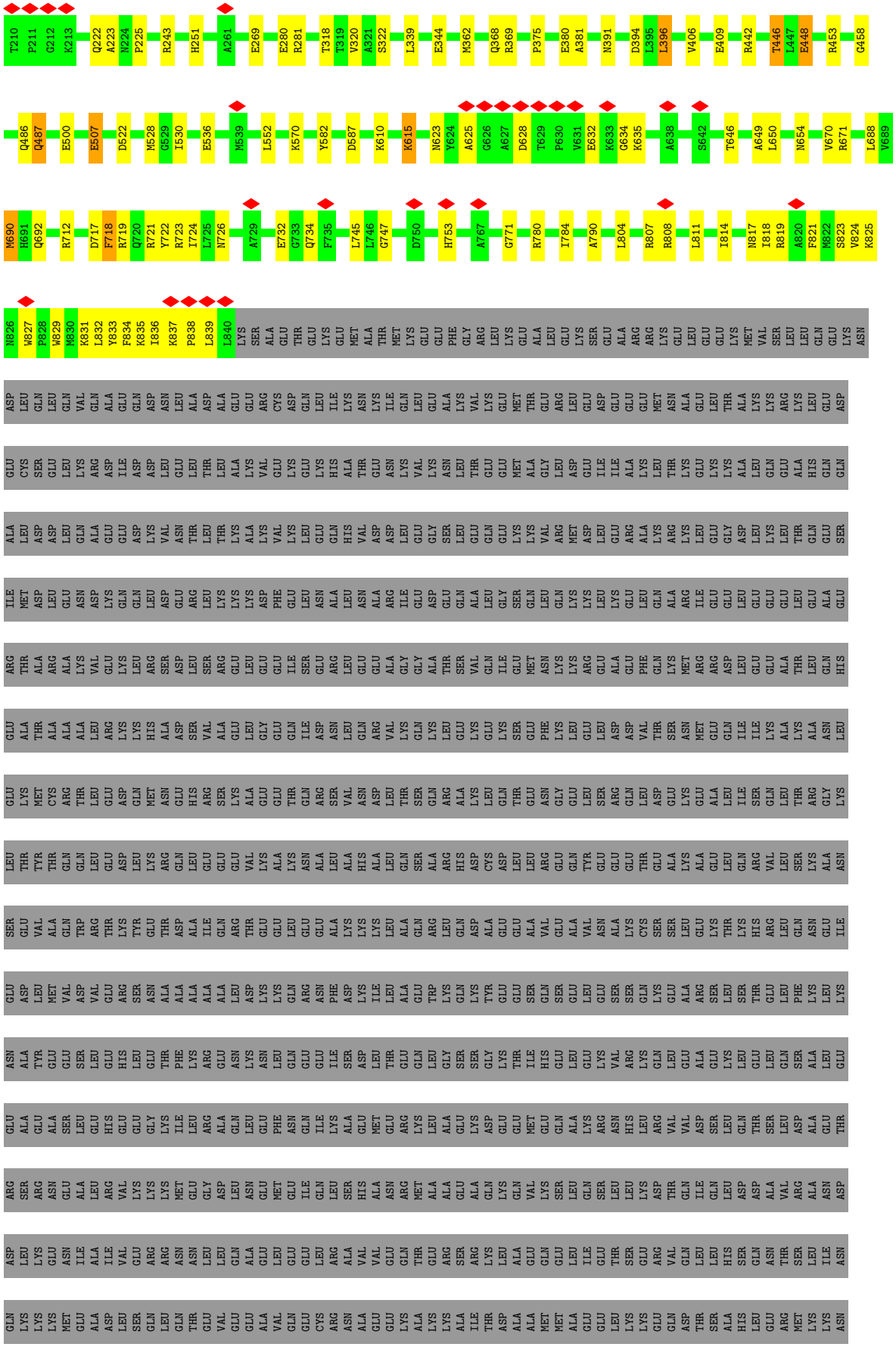


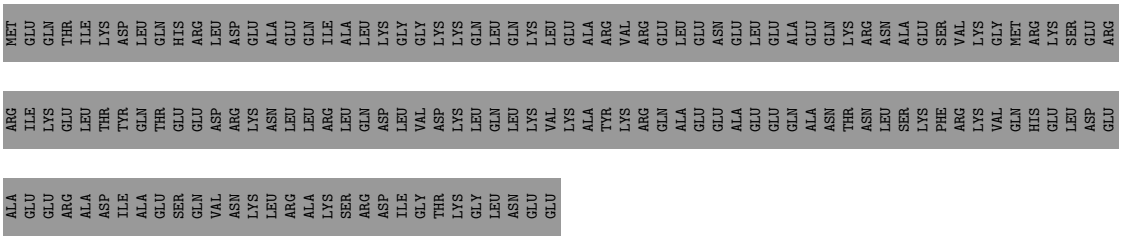
• Molecule 4: Myosin-7

Chain I:





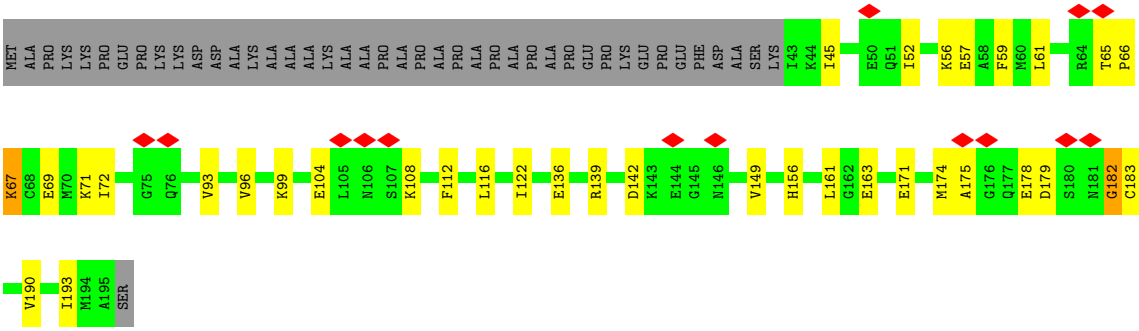

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Q486 Q487 E500 E507 D522 M528 Q529 I530 E536 M539 L552 K570 Y582 D587 K610 K615 N623 Y624 A625 G626 A627 D628 T629 P630 V631 E632 K633 G634 K635 A638 S642 T646 A649 L650 N654 V670 R671 L688 V689
N690 H691 Q692 R712 D717 F718 R719 Q720 R721 Y722 R723 I724 L725 N726 A729 E732 G733 Q734 F735 L745 L746 G747 D750 H753 A767 G771 R780 I784 A790 L804 R807 R808 L811 I814 N817 I818 R819 A820 F821 M822 S823 V824 K825
N826 W827 P828 W829 M830 K831 L832 Y833 F834 K835 I836 K837 P838 L839 L840 LYS SER ALA GLU THR GLU LYS GLU MET ALA THR MET LYS GLU GLU PHE GLY ARG LEU LYS GLU ALA LEU GLU LYS SER GLU ALA ARG ARG LYS GLU LEU GLU GLU LYS MET LYS ALA GLU GLN LEU GLU GLU LYS ASN
ASP LEU GLN LEU GLN VAL GLN ALA GLU GLN ASP ASN LEU ALA ASP ALA GLU GLU ARG CYS ASP GLN LEU ILE LYS ASN LYS ILE GLN LEU GLU ALA LYS VAL LYS GLU MET THR GLU ARG LEU GLU ASP GLU GLU LEU THR GLU ASN MET ALA GLU GLU LYS ARG LEU ASP
GLU CYS SER GLU LEU LYS ARG ASP ASP ILE ASP ASP LEU LEU THR LEU ALA LYS VAL GLU LYS GLU LYS HIS ALA THR GLU ASN LYS VAL LYS ASN LEU THR GLU GLU MET ALA GLY LEU ASP GLU ILE ILE ALA LYS LEU THR LYS GLU LYS LYS ALA LEU GLN GLU ALA HIS GLN GLN
ALA LEU ASP ASP LEU GLN ALA GLU GLU ASP LYS VAL ASN THR LEU THR LYS ALA LYS VAL LYS LEU GLU GLU GLN HIS VAL ASP ASP LEU GLU GLY SER LEU GLU GLN GLU LYS LYS VAL ARG MET ASP LEU GLU ALA LYS ARG LYS LEU GLU GLY ASP LEU LYS LEU THR GLN GLU SER
ILE MET ASP LEU GLU ASN ASP LYS GLN GLN LEU ASP GLU ARG LEU LYS LYS LYS ASP PHE GLU LEU ASN ALA LEU ASN ALA ARG ILE GLU ASP GLU GLN ALA LEU GLY SER GLN LEU GLN LYS LYS LEU LYS GLU GLU ARG LYS LEU GLU GLY GLN ILE GLU MET ASN LYS LYS ARG GLU ALA GLU PHE GLN LYS MET ARG ILE GLU GLU LEU GLU GLU GLU LEU GLU ALA
ARG THR ALA ARG ALA LYS VAL GLU LYS LEU ARG SER ASP LEU SER ARG GLU LEU GLU GLU ILE SER GLU ARG LEU GLU GLU ALA ALA GLY GLY ALA THR SER VAL GLN ILE GLU MET ASN LYS LYS ARG GLU ALA GLU PHE GLN LYS MET ARG ARG ASP LEU GLU GLU GLU ALA THR LEU GLN HIS
GLU ALA THR ALA ALA LEU ARG LYS LYS HIS ALA ASP SER VAL ALA GLU LEU GLY GLU GLN GLN ILE ASP ASN LEU GLN ARG VAL LYS LYS GLN LYS LEU GLN LEU GLU LYS GLU LYS SER GLU PHE LYS LEU GLU LEU ASP ASP VAL THR SER ASN MET GLU GLN ILE ILE LYS ALA LYS ALA ASN LEU
GLU LYS MET CYS ARG THR LEU GLU ASP GLN SER MET ASN GLU HIS ARG SER LYS ALA GLU GLU THR GLN ILE ASP SER VAL ASN ASP LEU THR SER GLN ARG ALA LYS LEU GLN LEU THR GLU GLN ILE ASN GLY GLU LEU SER ARG GLN LEU GLU ASP THR GLU LYS GLU ALA LEU ILE LEU SER GLN LEU THR ARG GLY LYS
LEU THR TYR THR GLN GLN LEU GLU GLU ASP LEU GLN LEU GLU GLU VAL LYS ALA LYS ASN ALA LEU ALA HIS ALA LEU GLN SER ALA ARG HIS ASP CYS ASP LEU LEU ARG GLU GLN TYR GLU GLU GLU THR GLU ALA LYS ALA GLU LEU GLN ARG VAL LEU SER GLU ALA ASN
SER GLU VAL ALA GLN TRP ARG THR LYS TYR GLU THR ASP ALA ILE GLN ARG THR GLU GLU LEU GLU GLU ALA LYS LYS LEU ALA GLN ARG LEU GLN LEU ASP ALA GLU GLU ALA VAL ASN ALA LYS CYS SER SER LEU GLU ALA GLU LYS THR LYS HIS ARG LEU GLN ARG GLU ILE
GLU ASP LEU MET VAL ASP VAL GLU ARG SER ASN ALA ALA ALA LEU ASP LYS LYS GLN ILE LEU ALA GLU TRP LYS GLN LEU LYS GLU GLU SER GLN SER GLU LEU GLU SER SER LEU GLN LYS GLU ALA ARG SER LEU SER THR GLU LEU LEU GLU LYS
ASN ALA TYR GLU GLU SER LEU GLU GLU HIS LEU GLU GLU THR GLU LYS ASN LEU GLY SER SER GLY LYS THR ILE HIS GLU LEU GLU LEU GLU LYS VAL ARG LYS GLN LEU GLU ALA GLU LEU GLN LEU GLN SER LEU LEU GLU
GLU ALA ALA SER LEU GLU HIS GLU GLY LYS ILE LEU GLU GLU PHE ASN MET GLU GLU ARG LYS ALA GLU LYS ASP GLU GLU MET GLU GLN ALA LYS ARG ASN HIS LEU GLN THR SER LEU GLN LEU
ARG SER ARG ASN GLU ALA LYS LYS LEU ARG VAL LYS LYS MET GLU GLY ASP LEU ASN GLU MET GLU ILE GLN LEU GLU SER HIS ALA ASN ARG MET ALA ALA GLU GLN LYS ALA GLN VAL LYS SER LEU GLN SER LEU LEU LYS ASP THR GLN ILE GLN LEU LEU ASP ASP ALA VAL ARG ALA ASN ASP
ASP LEU LYS GLU ASN ILE ALA ARG GLN GLU LEU ARG ALA VAL VAL GLU GLN THR GLU ARG GLY SER ARG LYS LEU ALA GLU GLN ILE GLU GLU THR SER GLU ARG VAL GLN LEU LEU HIS SER GLN ASN THR SER LEU ILE ASN
GLN LYS LYS MET GLU LYS ALA ASP LEU GLU LYS LYS ALA ILE THR ASP ALA ALA MET MET ALA GLU GLU LEU LYS LYS GLU GLN ASP THR SER ALA HIS LEU GLU ARG MET LYS LYS ASN



• Molecule 5: Myosin light chain 3

Chain J:

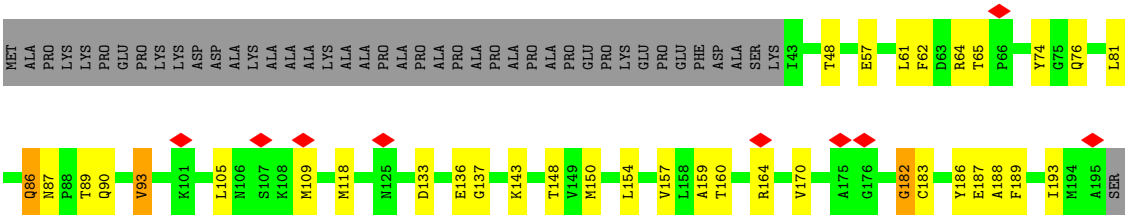




• Molecule 5: Myosin light chain 3

Chain K:

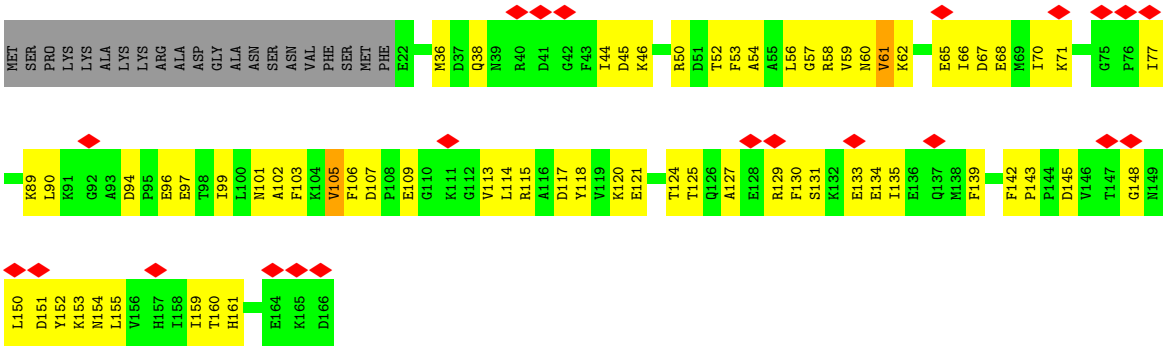




• Molecule 6: MYL2

Chain L:

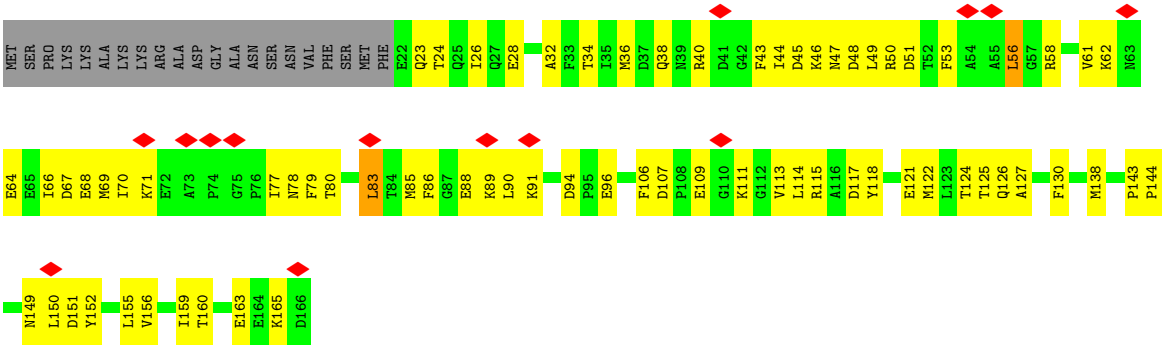




• Molecule 6: MYL2

Chain M:




MET SER PRO LYS LYS ALA LYS LYS ARG ALA ASP GLY ALA ASN SER ASN VAL PHE SER MET PHE E22 Q23 T24 Q25 I26 Q27 E28 A32 F33 T34 I35 M36 D37 Q38 N39 R40 D41 G42 F43 I44 D45 K46 N47 D48 L49 R50 D51 T52 F53 A54 A55 L56 G57 R58 V61 K62 N63
E64 E65 I66 D67 E68 M69 I70 K71 E72 A73 P74 G75 P76 I77 N78 F79 T80 L83 T84 M85 F86 G87 E88 K89 L90 K91 D94 P95 E96 F106 D107 P108 E109 G110 K111 G112 V113 L114 R115 A116 D117 Y118 E121 M122 L123 T124 T125 Q126 A127 F130 M138 P143 P144
N149 L150 D151 Y152 L155 V156 I159 T160 E163 E164 K165 D166

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	17875	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	34	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	10.200	Depositor
Minimum map value	-3.487	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.181	Depositor
Recommended contour level	1.8	Depositor
Map size (Å)	536.97595, 536.97595, 536.97595	wwPDB
Map dimensions	396, 396, 396	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3559998, 1.3559998, 1.3559998	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.10	0/2995	0.27	0/4057
1	B	0.09	0/2995	0.28	0/4057
2	C	0.18	0/623	0.23	0/830
2	D	0.17	0/623	0.26	0/830
2	E	0.11	0/320	0.20	0/419
2	F	0.13	0/320	0.24	0/419
3	G	0.11	0/598	0.24	0/791
4	H	0.12	0/6902	0.31	0/9297
4	I	0.12	0/6902	0.34	2/9297 (0.0%)
5	J	0.11	0/1236	0.36	2/1658 (0.1%)
5	K	0.11	0/1236	0.41	2/1658 (0.1%)
6	L	0.14	0/1189	0.31	0/1599
6	M	0.13	0/1189	0.29	0/1599
All	All	0.12	0/27128	0.31	6/36511 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
6	M	0	1

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	I	628	ASP	CA-C-N	7.91	135.94	121.70
4	I	628	ASP	C-N-CA	7.91	135.94	121.70
5	K	182	GLY	CA-C-N	7.26	134.78	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	K	182	GLY	C-N-CA	7.26	134.78	121.70
5	J	182	GLY	CA-C-N	6.49	133.38	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	M	127	ALA	Peptide

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	2932	0	2894	40	0
1	B	2932	0	2894	29	0
2	C	618	0	607	15	0
2	D	618	0	607	23	0
2	E	321	0	339	11	0
2	F	321	0	339	21	0
3	G	595	0	603	21	0
4	H	6757	0	6776	90	0
4	I	6757	0	6776	81	0
5	J	1217	0	1199	29	0
5	K	1217	0	1199	24	0
6	L	1168	0	1132	64	0
6	M	1168	0	1132	60	0
7	A	27	0	12	1	0
7	B	27	0	12	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
All	All	26677	0	26521	406	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 8.

The worst 5 of 406 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)
4:H:176:ILE:HG22	4:H:184:LYS:HZ2	1.40	0.86
6:M:86:PHE:O	6:M:90:LEU:HB2	1.78	0.82
6:L:58:ARG:HG2	6:L:61:VAL:HG13	1.63	0.78
1:B:149:THR:HG22	1:B:167:GLU:H	1.48	0.77
2:F:6:LYS:NZ	2:F:10:MET:SD	2.58	0.76

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	373/377 (99%)	354 (95%)	19 (5%)	0	100	100
1	B	373/377 (99%)	355 (95%)	18 (5%)	0	100	100
2	C	73/284 (26%)	73 (100%)	0	0	100	100
2	D	73/284 (26%)	73 (100%)	0	0	100	100
2	E	38/284 (13%)	38 (100%)	0	0	100	100
2	F	38/284 (13%)	38 (100%)	0	0	100	100
3	G	66/285 (23%)	66 (100%)	0	0	100	100
4	H	835/1935 (43%)	805 (96%)	30 (4%)	0	100	100
4	I	835/1935 (43%)	799 (96%)	36 (4%)	0	100	100
5	J	151/196 (77%)	145 (96%)	6 (4%)	0	100	100
5	K	151/196 (77%)	142 (94%)	9 (6%)	0	100	100
6	L	143/166 (86%)	133 (93%)	10 (7%)	0	100	100
6	M	143/166 (86%)	133 (93%)	10 (7%)	0	100	100
All	All	3292/6769 (49%)	3154 (96%)	138 (4%)	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	318/320 (99%)	309 (97%)	9 (3%)	38	59
1	B	318/320 (99%)	313 (98%)	5 (2%)	55	69
2	C	68/245 (28%)	66 (97%)	2 (3%)	37	57
2	D	68/245 (28%)	64 (94%)	4 (6%)	18	39
2	E	33/245 (14%)	32 (97%)	1 (3%)	36	56
2	F	33/245 (14%)	33 (100%)	0	100	100
3	G	64/249 (26%)	63 (98%)	1 (2%)	55	69
4	H	726/1697 (43%)	704 (97%)	22 (3%)	36	56
4	I	726/1697 (43%)	703 (97%)	23 (3%)	34	55
5	J	133/163 (82%)	132 (99%)	1 (1%)	73	78
5	K	133/163 (82%)	129 (97%)	4 (3%)	36	56
6	L	126/143 (88%)	122 (97%)	4 (3%)	34	55
6	M	126/143 (88%)	122 (97%)	4 (3%)	34	55
All	All	2872/5875 (49%)	2792 (97%)	80 (3%)	38	59

5 of 80 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	I	522	ASP
5	K	148	THR
4	I	570	LYS
4	I	745	LEU
6	L	155	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
4	I	187	ASN
4	I	437	ASN

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Mol	Chain	Res	Type
4	I	238	ASN
4	I	415	GLN
4	I	581	HIS

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)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	ADP	A	401	8	28,29,29	1.41	4 (14%)	43,45,45	1.82	9 (20%)
7	ADP	B	401	8	28,29,29	1.40	4 (14%)	43,45,45	1.84	10 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	ADP	A	401	8	-	4/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	ADP	B	401	8	-	4/16/32/32	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	401	ADP	C5-C4	4.68	1.47	1.39
7	B	401	ADP	C5-C4	4.65	1.47	1.39
7	A	401	ADP	C5-C6	2.71	1.48	1.41
7	B	401	ADP	C5-C6	2.65	1.48	1.41
7	A	401	ADP	C5-N7	-2.33	1.34	1.39

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	401	ADP	C5-C4-N3	-5.85	118.66	126.72
7	A	401	ADP	C5-C4-N3	-5.79	118.74	126.72
7	B	401	ADP	N3-C4-N9	4.71	135.17	127.17
7	A	401	ADP	N3-C4-N9	4.65	135.08	127.17
7	A	401	ADP	C2-N3-C4	3.68	120.83	111.83

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	401	ADP	C5'-O5'-PA-O1A
7	A	401	ADP	C5'-O5'-PA-O3A
7	B	401	ADP	C5'-O5'-PA-O3A
7	A	401	ADP	C3'-C4'-C5'-O5'
7	B	401	ADP	C3'-C4'-C5'-O5'

There are no ring outliers.

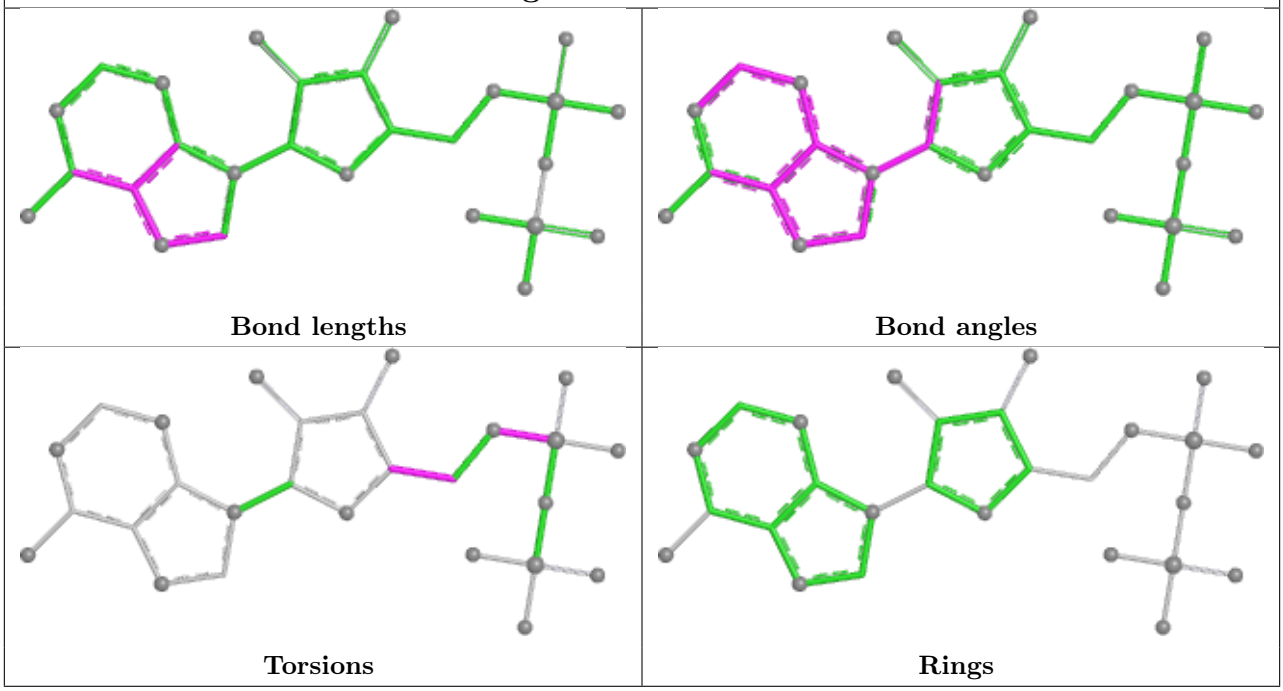
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	401	ADP	1	0

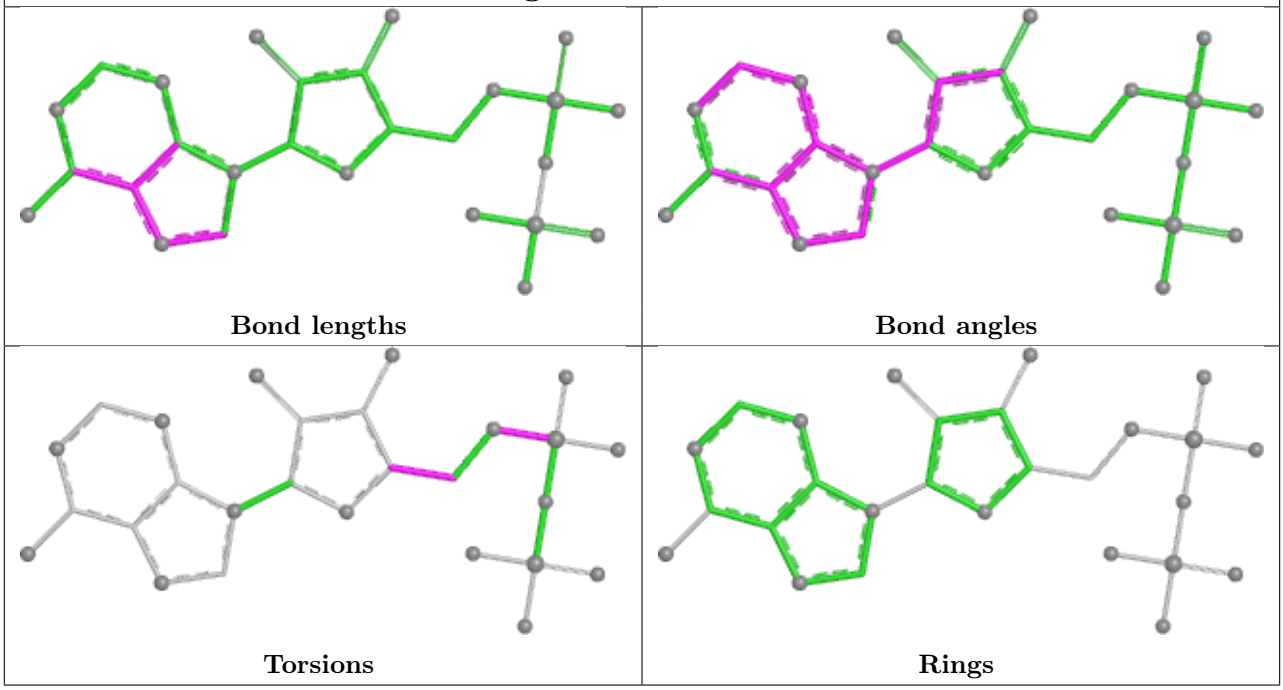
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ADP A 401



Ligand ADP B 401



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.

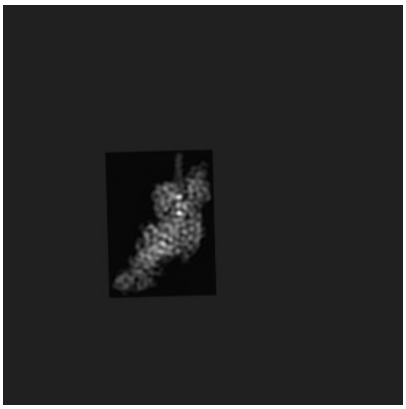
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-73055. These allow visual inspection of the internal detail of the map and identification of artifacts.

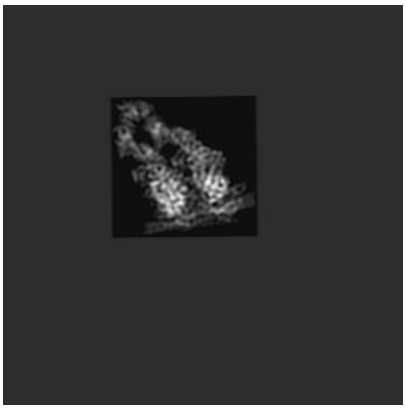
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

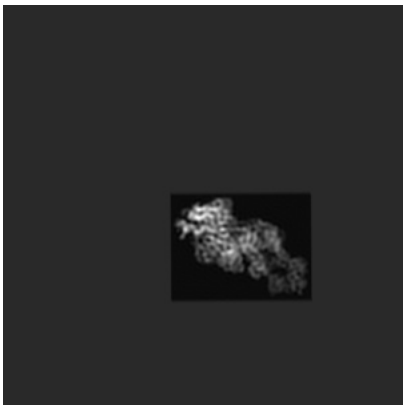
6.1.1 Primary map



X

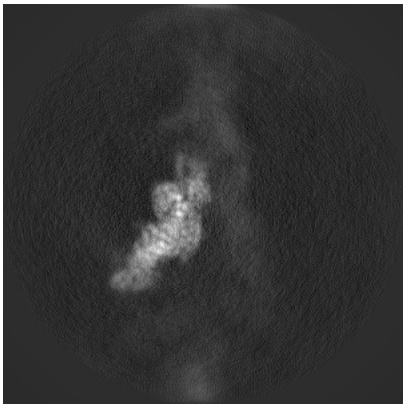


Y

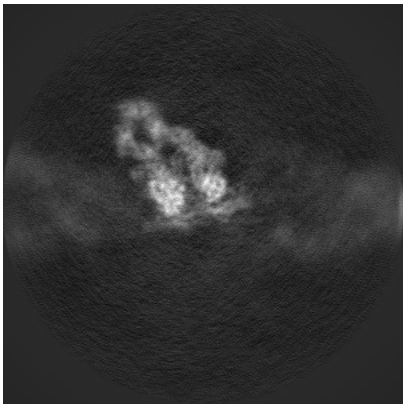


Z

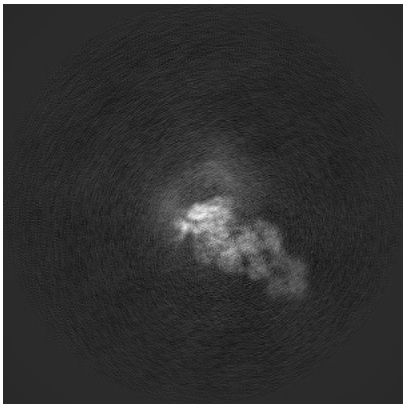
6.1.2 Raw map



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: 198

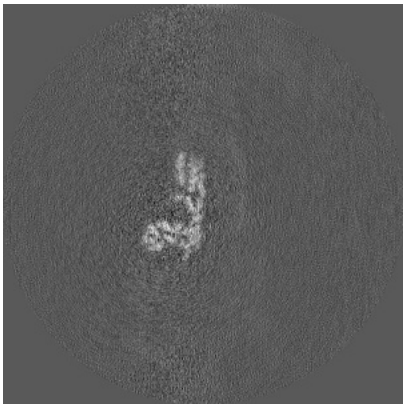


Y Index: 198

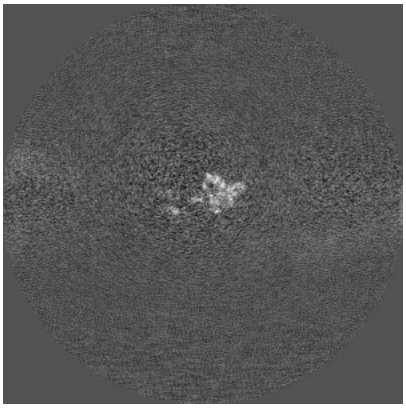


Z Index: 198

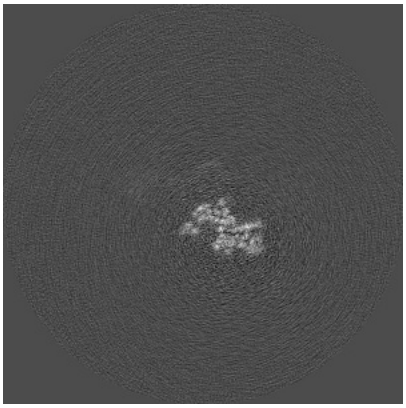
6.2.2 Raw map



X Index: 198



Y Index: 198



Z Index: 198

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: 219

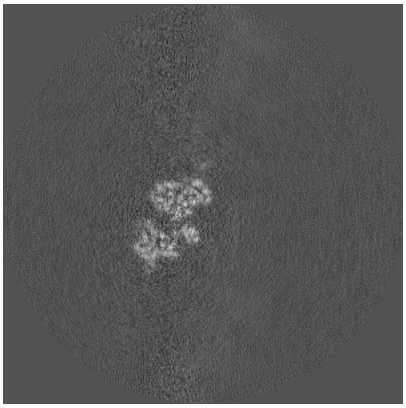


Y Index: 173

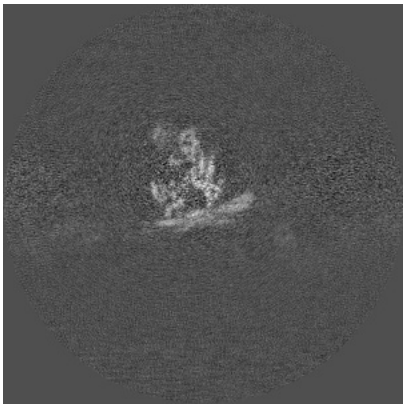


Z Index: 164

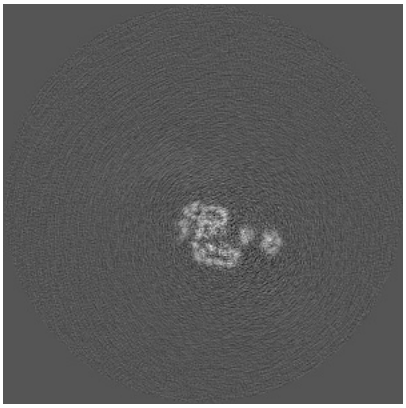
6.3.2 Raw map



X Index: 219



Y Index: 173

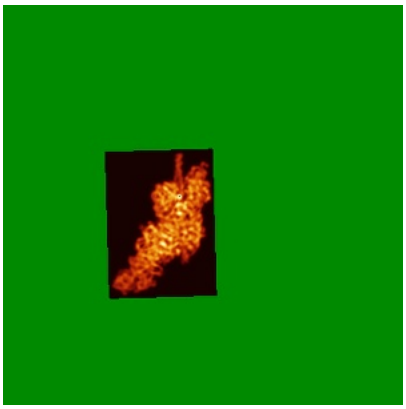


Z Index: 169

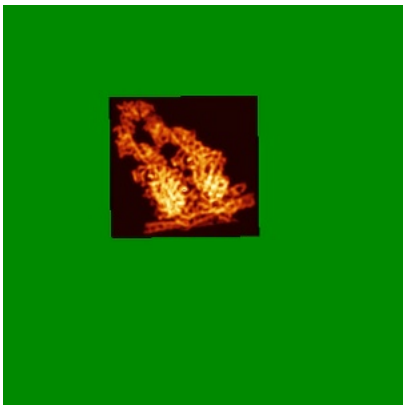
The images above show the largest variance slices of the map in three orthogonal directions.

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

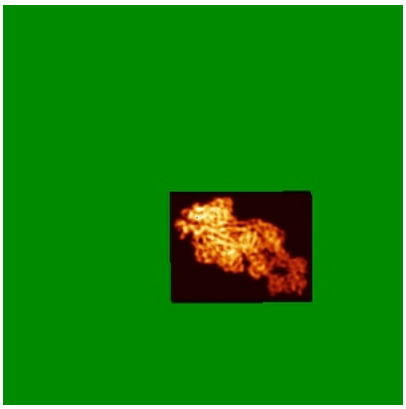
6.4.1 Primary map



X

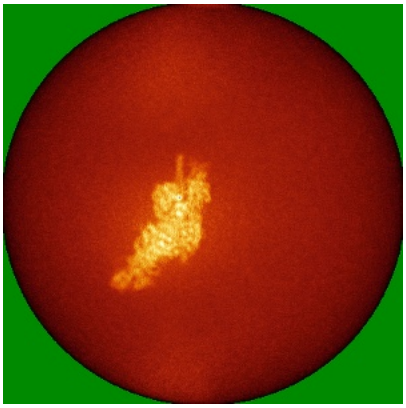


Y

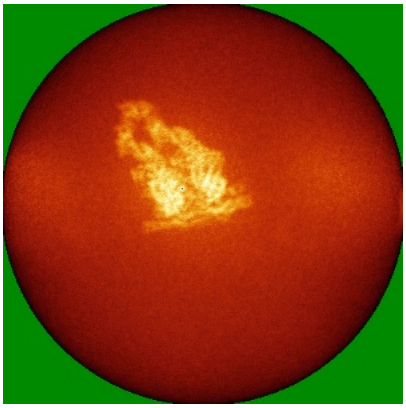


Z

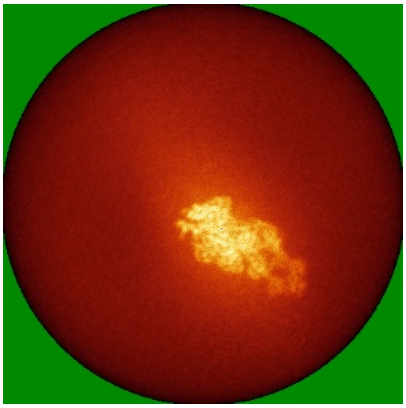
6.4.2 Raw map



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 1.8. 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.

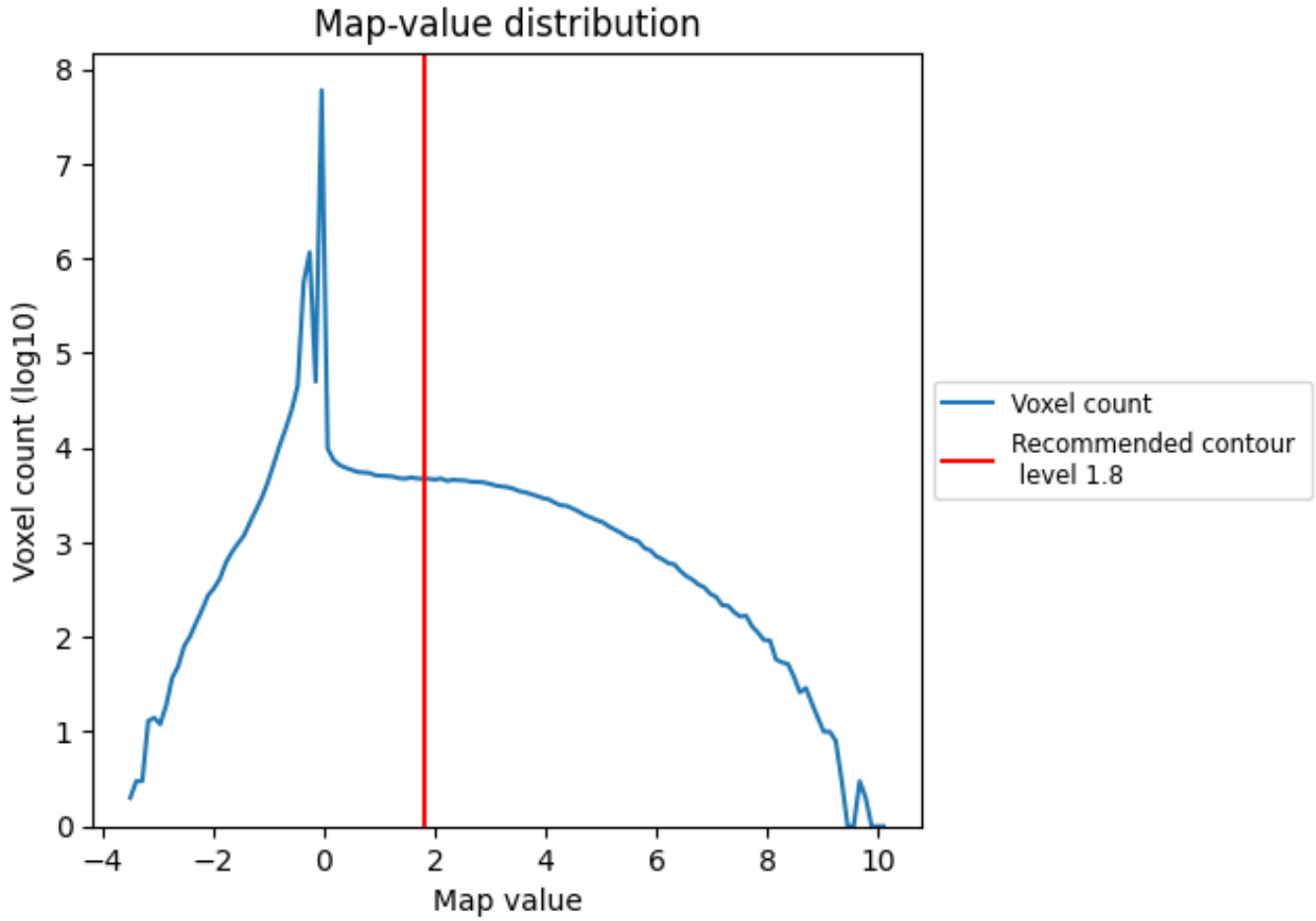
6.6 Mask visualisation (i)

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

7 Map analysis

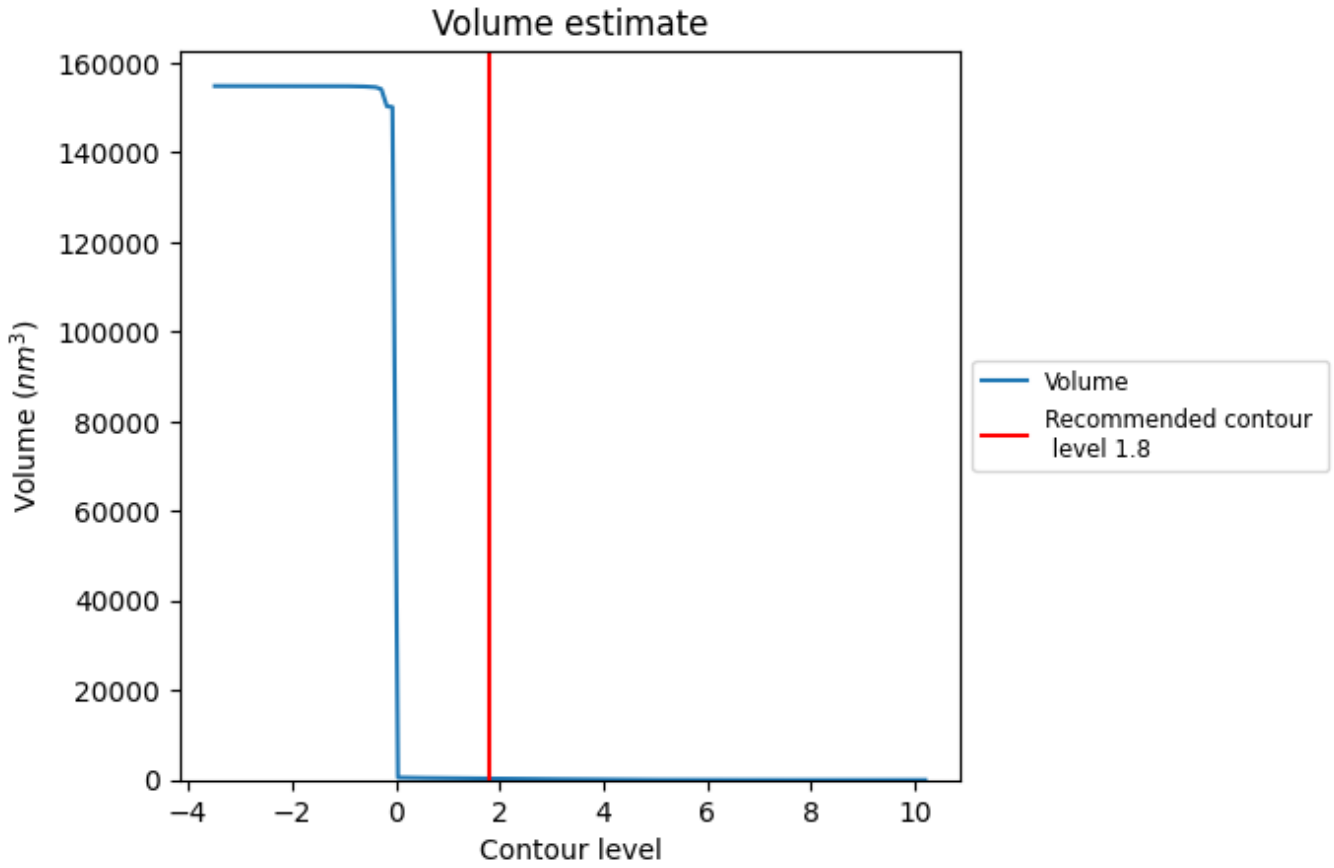
This section contains the results of statistical analysis of the map.

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.

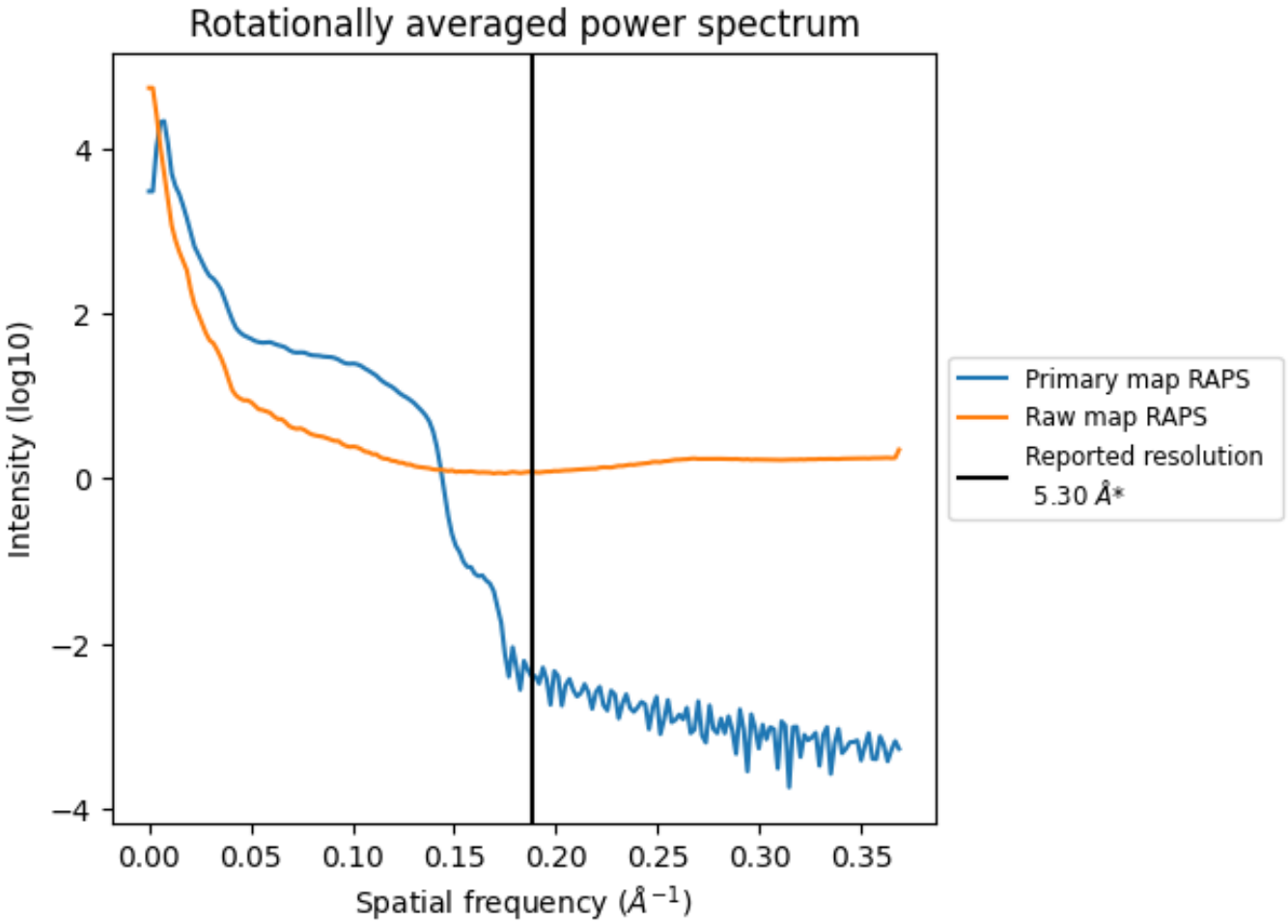
7.2 Volume estimate (i)



The volume at the recommended contour level is 307 nm^3; this corresponds to an approximate mass of 278 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)

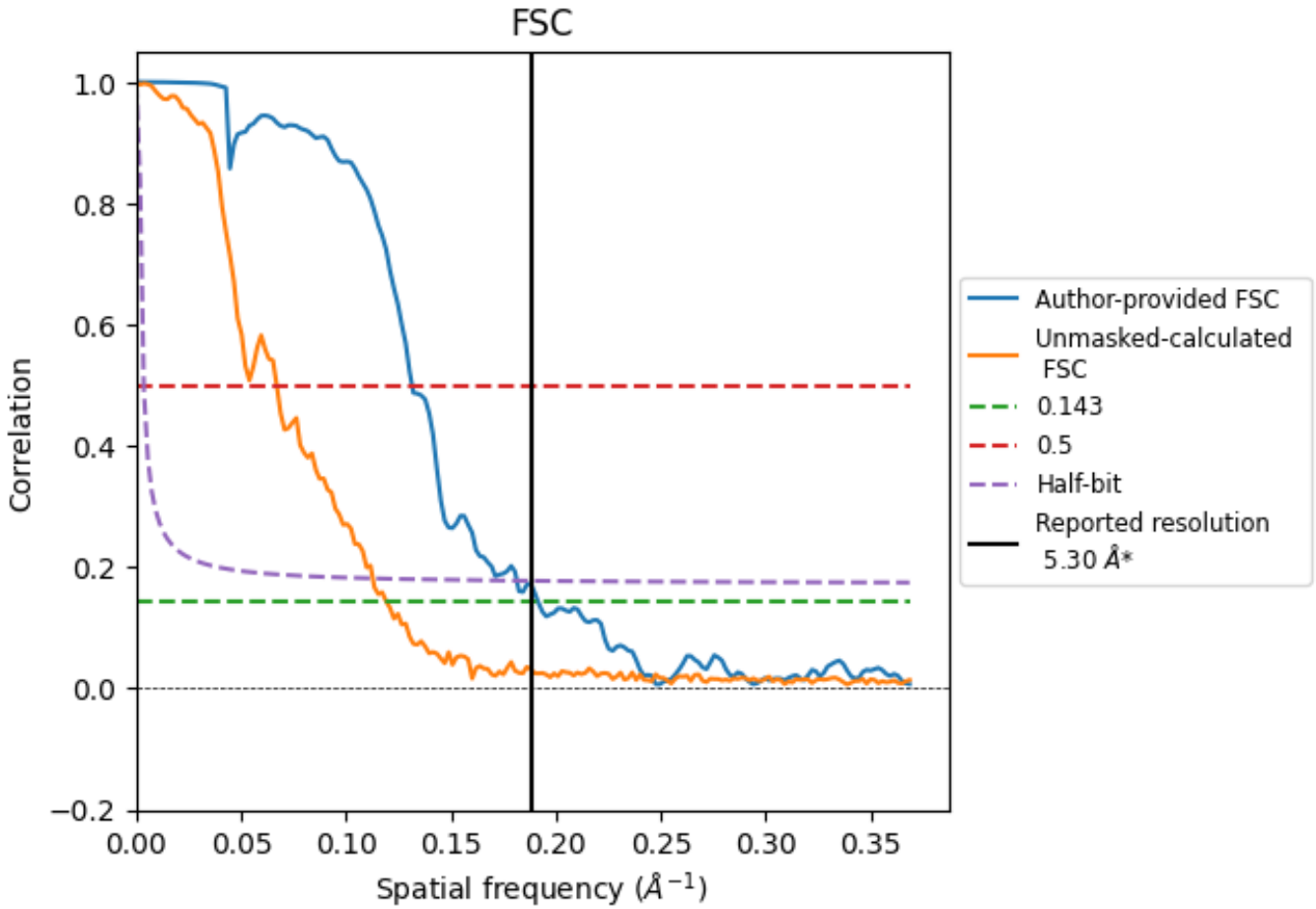


*Reported resolution corresponds to spatial frequency of 0.189 Å^{-1}

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 0.189 Å^{-1}

8.2 Resolution estimates (i)

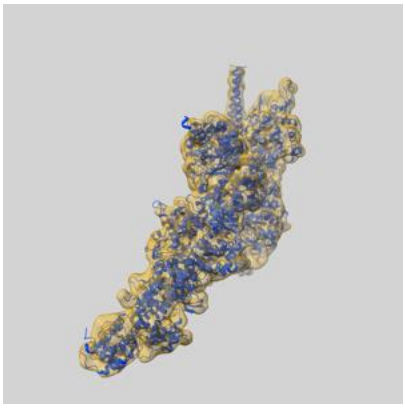
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.30	-	-
Author-provided FSC curve	5.22	7.60	5.51
Unmasked-calculated*	8.39	14.90	8.87

*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 8.39 differs from the reported value 5.3 by more than 10 %

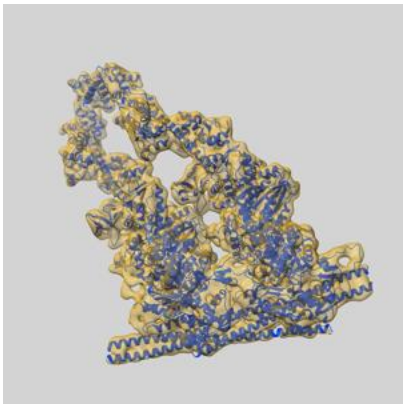
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-73055 and PDB model 9YKN. Per-residue inclusion information can be found in section 3 on page 7.

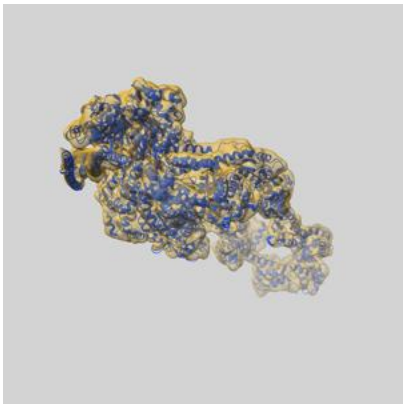
9.1 Map-model overlay



X



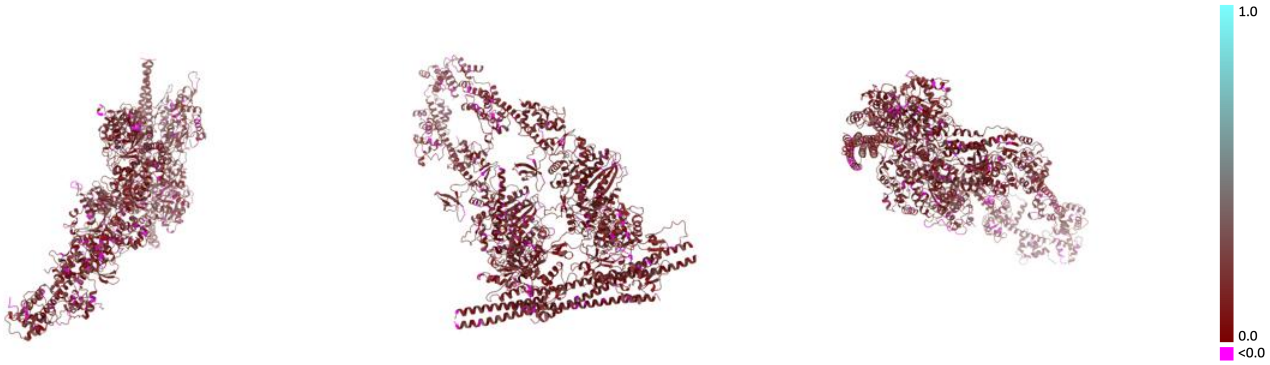
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.8 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.

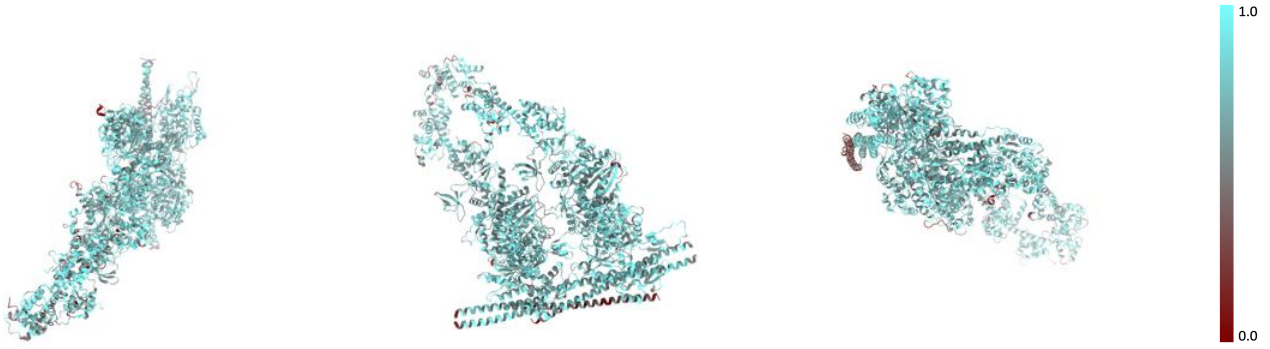
9.2 Q-score mapped to coordinate model



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.

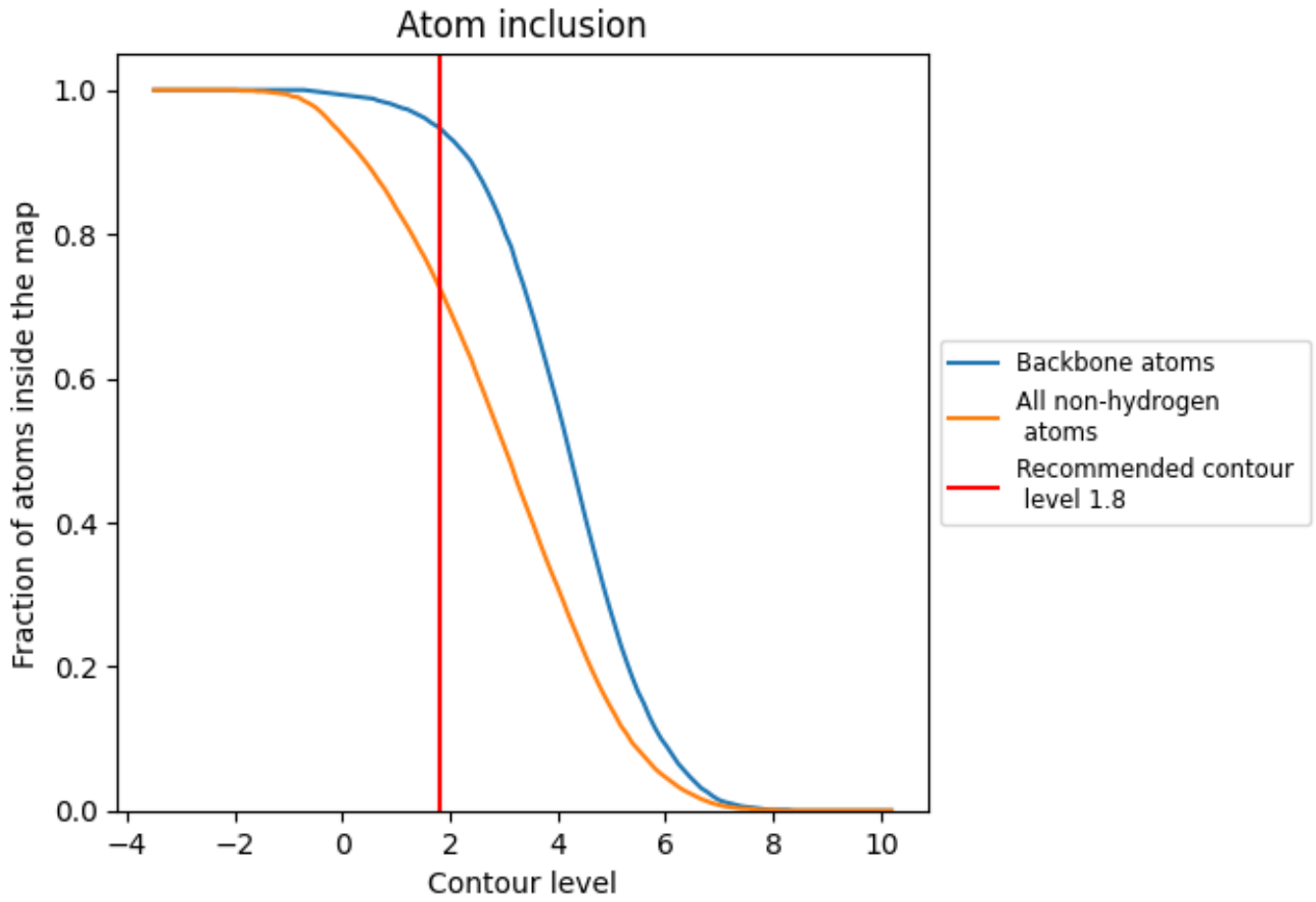
9.3 Atom inclusion mapped to coordinate model



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 (1.8).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (1.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7270	0.1700
A	0.7550	0.1690
B	0.7530	0.1700
C	0.7160	0.1820
D	0.6770	0.1640
E	0.6860	0.1810
F	0.6920	0.1620
G	0.3550	0.1200
H	0.7500	0.1740
I	0.7210	0.1580
J	0.7720	0.1810
K	0.7300	0.1670
L	0.6820	0.1860
M	0.7300	0.2120

