wwPDB EM Validation Summary Report (i)

Dec 11, 2022 – 03:48 pm GMT

PDB ID	:	6SO3
EMDB ID	:	EMD-7029
Title	:	The interacting head motif in insect flight muscle myosin thick filaments
Authors	:	Morris, E.P.; Knupp, C.; Squire, J.M.
Deposited on	:	2019-08-28
Resolution	:	6.20 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 (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:

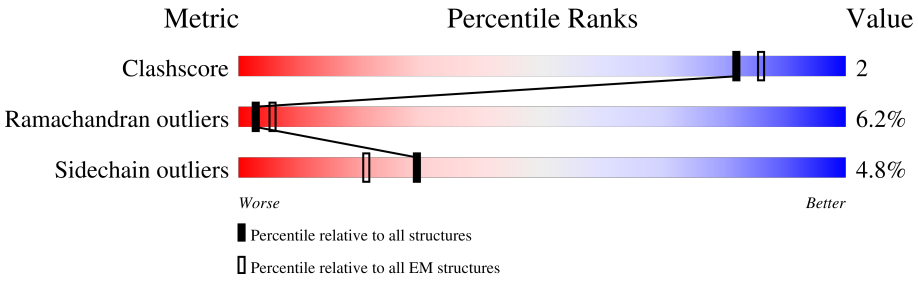
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 6.20 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 <=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	1953	43% 29% 12% 57%
1	B	1953	43% 30% 10% 57%
2	C	156	100% 71% 26%
2	D	156	100% 69% 25% 6%
3	E	196	100% 68% 23% 8%
3	F	196	100% 69% 24% 7%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 37957 atoms, of which 18956 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 Myosin 2 heavy chain striated muscle.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	B	840	Total	C	H	N	O	S	0	0
			13499	4302	6760	1164	1245	28		
1	A	840	Total	C	H	N	O	S	0	0
			13498	4302	6760	1164	1244	28		

- Molecule 2 is a protein called Myosin 2 essential light chain striated muscle.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	D	156	Total	C	H	N	O	S	0	0
			2460	779	1227	199	247	8		
2	C	156	Total	C	H	N	O	S	0	0
			2460	779	1227	199	247	8		

- Molecule 3 is a protein called Myosin 2 regulatory light chain striated muscle.

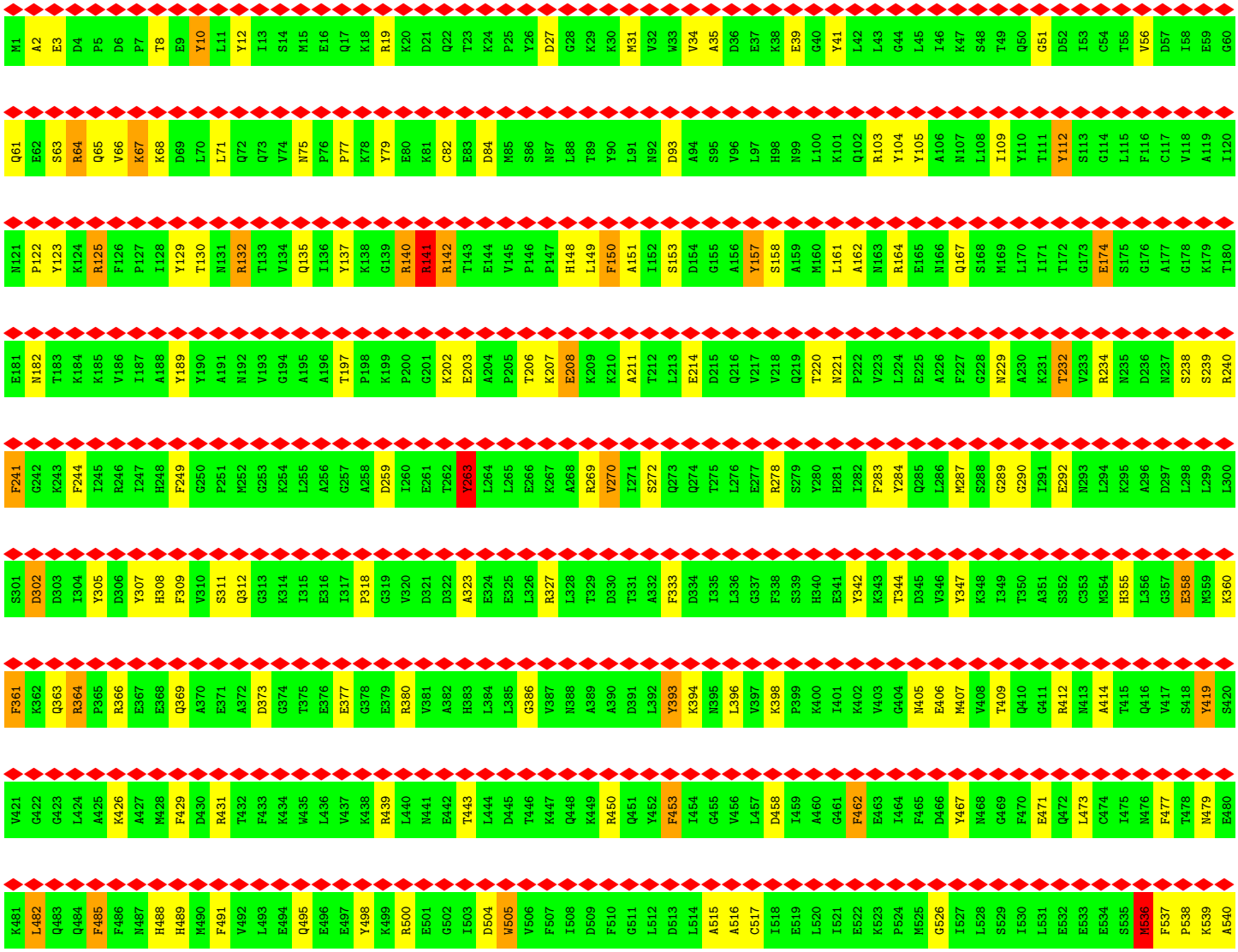
Mol	Chain	Residues	Atoms						AltConf	Trace
3	F	196	Total	C	H	N	O	S	0	0
			3020	952	1491	257	314	6		
3	E	196	Total	C	H	N	O	S	0	0
			3020	952	1491	257	314	6		

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: Myosin 2 heavy chain striated muscle

Chain B:



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D601 T602 V603 V604 D605 Q606 F607 K608 K609 G610 S611 N612 K613 L614 V615 Q616 E617 I618 F619 E620 D621 H622 P623 G624 L625 G626 A627 E628 E629 K630 G631 G632 G633 G634 K635 G636 G637 G638 G639 R640 K641 K642 G643 A644 S645 F646 Q647 T648 V649 S650 A651 L652 Y653 R654 E655 Q656 L657 N658 R659 L660

M661 A662 S663 L664 H665 S666 T667 Q668 P669 H670 F671 V672 R673 C674 I675 I676 P677 N678 E679 L680 K681 Q682 P683 G684 V685 I686 D687 S688 G689 L690 V691 M692 H693 Q694 L695 T696 C697 N698 G699 V700 L701 E702 G703 I704 R705 I706 C707 R708 K709 G710 F711 P712 N713 R714 M715 V716 Y717 P718 D719 F720

K721 Q722 R723 Y724 T725 I726 L727 A728 A729 S730 A731 V732 P733 K734 G735 F736 V737 D738 A739 K740 K741 V742 T743 E744 A745 V746 L747 G748 A749 I750 Q751 L752 D753 A754 N755 D756 Y757 R758 L759 G760 N761 T762 K763 V764 F765 F766 R767 A768 G769 V770 L771 G772 R773 L774 E775 E776 M777 R778 D779 D780

R781 L782 G783 K784 I785 V786 T787 W788 L789 Q790 A791 W792 I793 R794 W795 Y796 L797 S798 K799 K800 E801 F802 K803 K804 L805 Q806 E807 Q808 R809 V810 A811 L812 L813 V814 I815 Q816 R817 N818 L819 R820 K821 F822 L823 T824 L825 R826 N827 W828 L829 W830 Y831 K832 L833 Y834 I835 K836 V837 K838 P839 L840

LEU THR MET ALA LYS VAL GLU ASP GLU LEU LYS ALA LEU GLU GLU LYS LEU LYS LYS ALA LEU GLU SER LEU GLU LYS GLU GLU LYS VAL ARG LYS ASP ILE GLU VAL GLN ASN VAL LYS LEU LEU GLN GLU LYS ASN ASP LEU PHE LEU GLN LEU GLU SER GLU ARG SER GLY ALA GLY

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

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

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

LEU GLN ARG LYS GLU LYS GLU MET ALA SER LEU SER ALA LYS LEU GLU ASP GLU GLN GLY LEU VAL ALA LYS LEU GLN LYS GLN ILE LYS GLU LEU GLN ALA ARG ILE GLU GLU LEU GLU GLU GLU LEU GLU ALA GLU ARG GLN ALA ARG ALA LYS ALA GLU LYS GLN ARG ALA ASP LEU

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

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

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

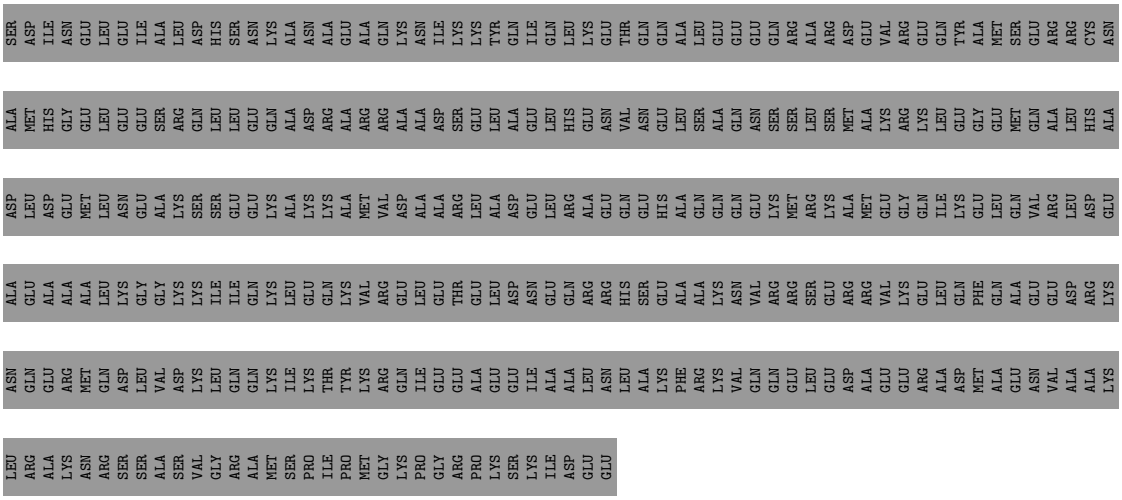
ASP GLU GLU SER ARG GLU ARG ALA THR ALA MET GLY LYS PHE ARG SER VAL GLU HIS ASP LEU ASP SER LEU ARG GLU GLN ILE ASP GLU GLU GLN GLU GLY LYS ALA ASP LEU GLN ARG GLN LEU SER LYS ALA ASN ALA GLU VAL GLN LEU TRP ARG SER LYS TYR GLU SER GLU GLY

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

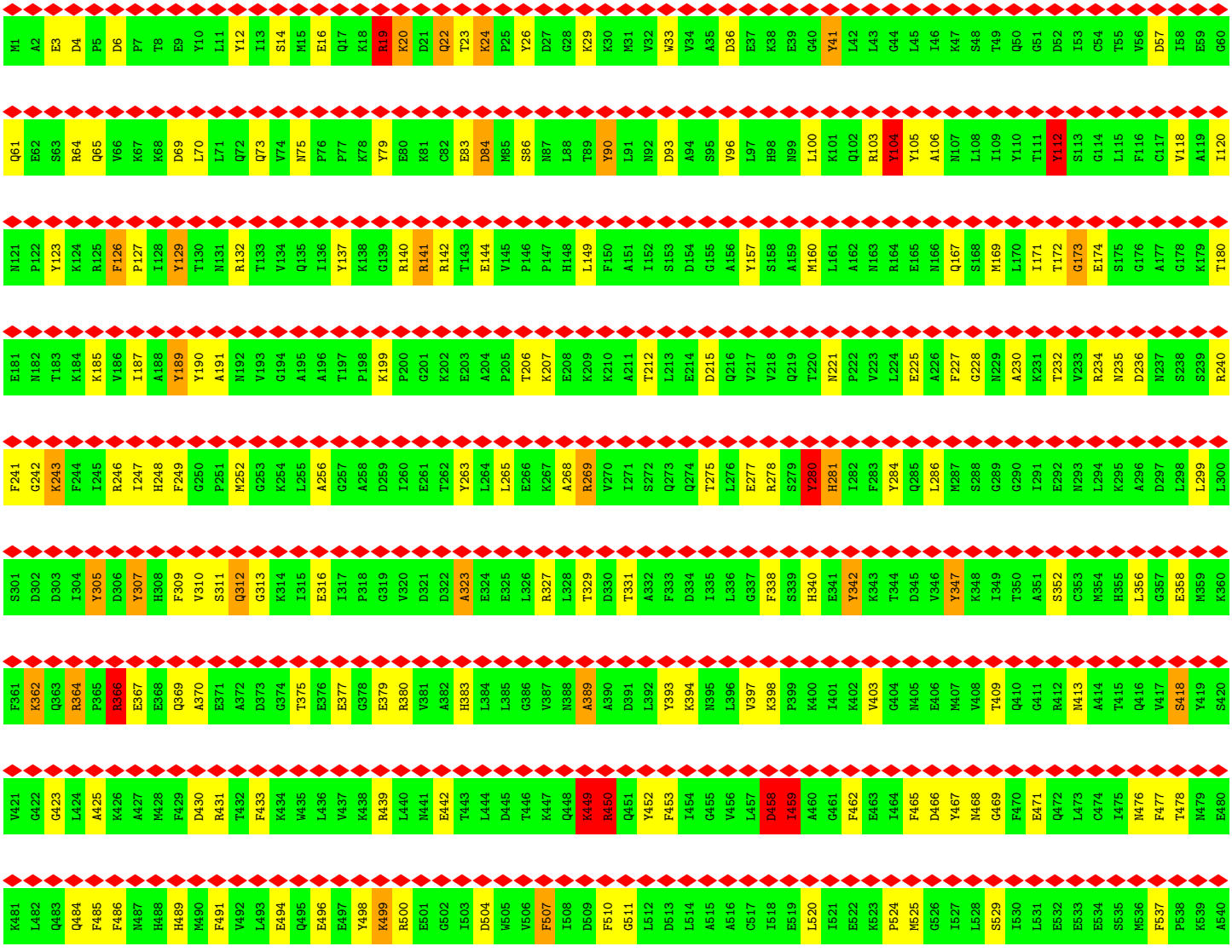
SER ALA MET GLU LYS LYS GLN LYS SER PHE ASP ARG ILE ILE SER GLU TRP LYS GLN LYS VAL ASP ASP LEU ALA LEU GLU LEU ASP ALA SER GLN LYS GLU CYS ARG ASN TYR SER THR GLU VAL PHE LYS LEU ARG SER GLN TYR GLU GLU SER GLN GLU HIS TYR GLU SER VAL LYS

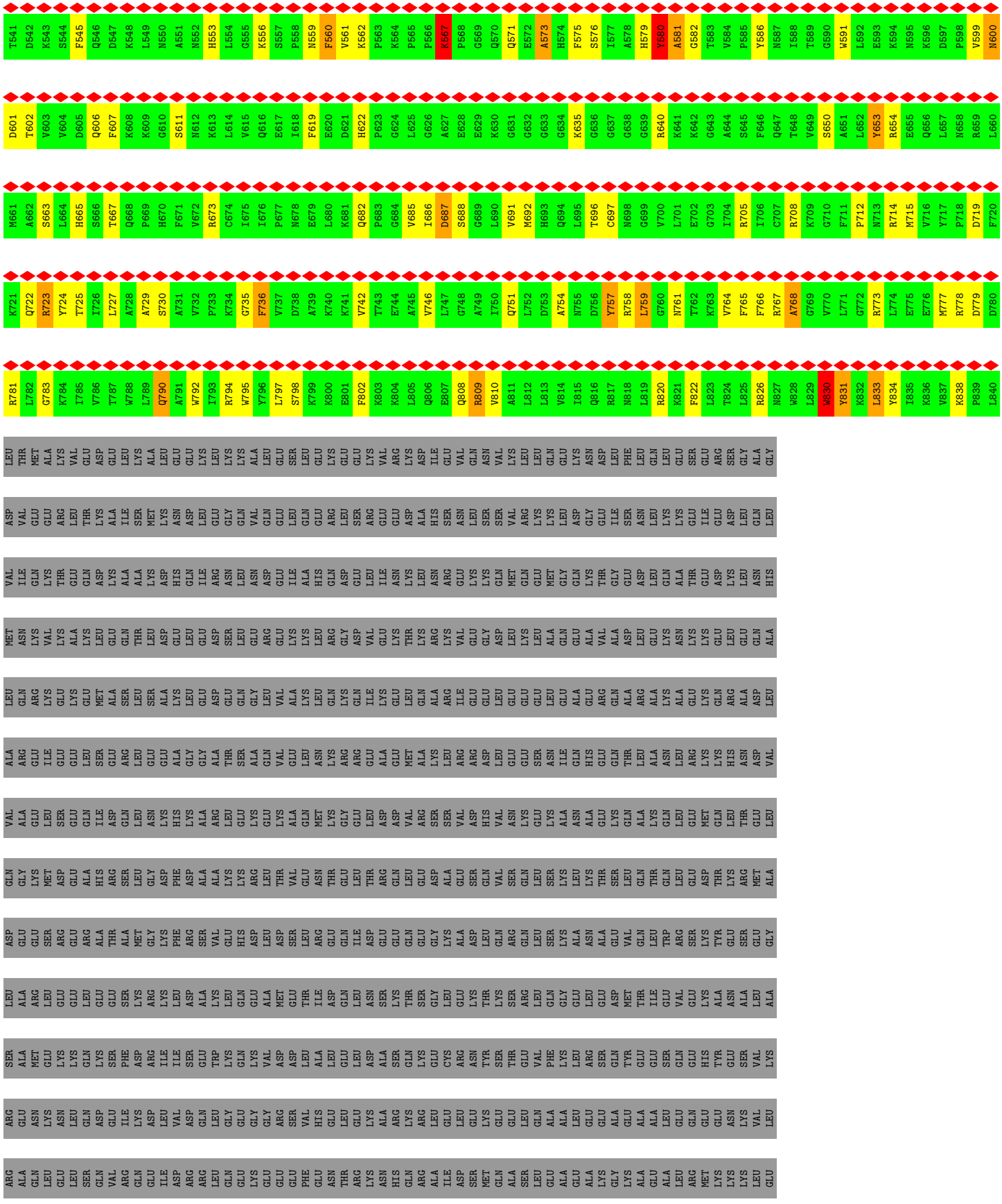
ARG GLU ASN LYS ASN LEU GLN ASP GLU ILE LYS ASP LEU VAL ASP GLN LEU GLY GLU GLY GLY ARG SER VAL HIS GLU LEU GLU LYS ALA ARG LYS ARG LEU GLU LEU GLU LYS GLU GLU LEU GLN ALA ALA LEU GLU GLU ALA GLU ALA ALA LEU GLU GLN GLU GLU ASN LYS VAL LEU

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



• Molecule 1: Myosin 2 heavy chain striated muscle

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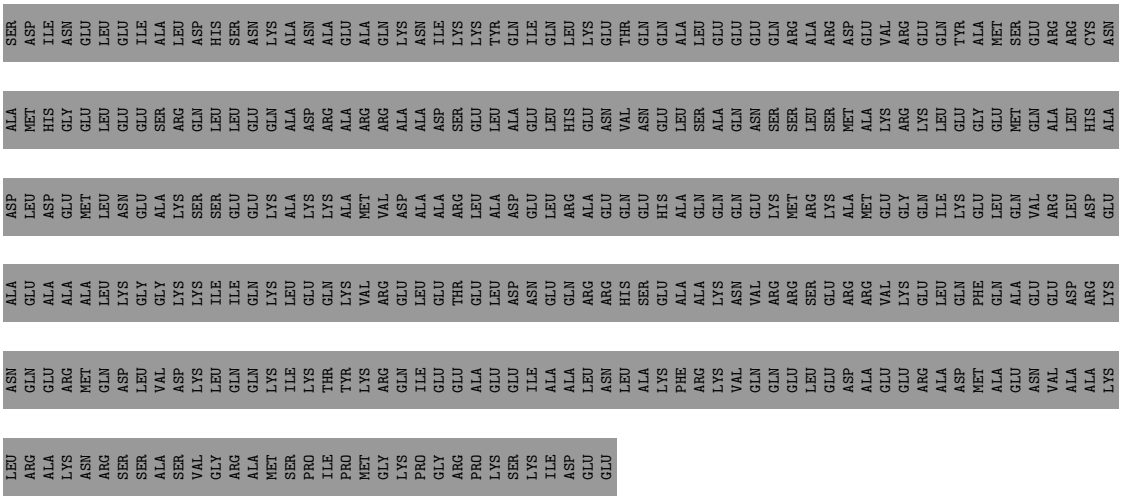
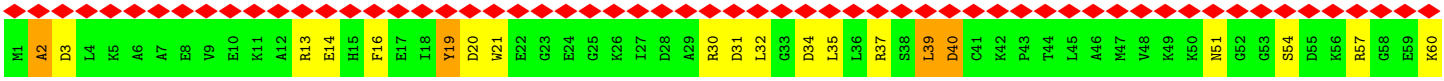
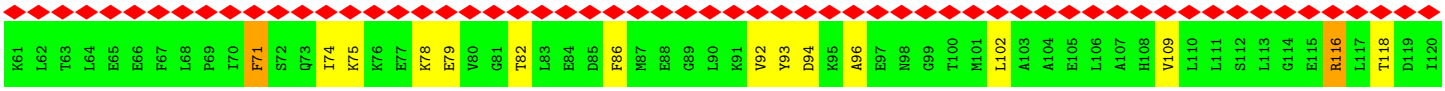
D601 T602 V603 V604 D605 Q606 F607 K608 K609 G610 S611 N612 K613 L614 V615 Q616 E617 I618 F619 E620 D621 H622 P623 G624 L625 G626 A627 E628 E629 K630 G631 G632 G633 G634 K635 G636 G637 G638 G639 R640 K641 K642 G643 A644 S645 F646 Q647 T648 V649 S650 A651 L652 Y653 R654 E655 Q656 L657 N658 R659 L660
M661 A662 S663 L664 H665 S666 T667 Q668 P669 H670 F671 V672 R673 C674 I675 I676 P677 N678 E679 L680 K681 Q682 P683 G684 V685 I686 D687 S688 G689 L690 V691 M692 H693 Q694 L695 T696 C697 N698 G699 V700 L701 E702 G703 I704 R705 I706 C707 R708 K709 G710 F711 P712 N713 R714 M715 V716 Y717 P718 D719 F720
K721 Q722 R723 Y724 T725 I726 L727 A728 A729 S730 A731 V732 P733 K734 G735 F736 V737 D738 A739 K740 K741 V742 T743 E744 A745 V746 L747 G748 A749 I750 Q751 L752 D753 A754 N755 D756 Y757 R758 L759 G760 N761 T762 K763 V764 F765 F766 R767 A768 G769 V770 L771 G772 R773 L774 E775 E776 M777 R778 D779 D780
R781 L782 G783 K784 I785 V786 T787 W788 L789 Q790 A791 W792 I793 R794 W795 Y796 L797 S798 K799 K800 E801 F802 K803 K804 L805 Q806 E807 Q808 R809 V810 A811 L812 L813 V814 I815 Q816 R817 N818 L819 R820 K821 F822 L823 T824 L825 R826 N827 W828 L829 W830 Y831 K832 L833 Y834 I835 K836 V837 K838 P839 L840

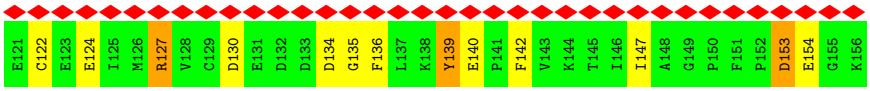


• Molecule 2: Myosin 2 essential light chain striated muscle

Chain D:

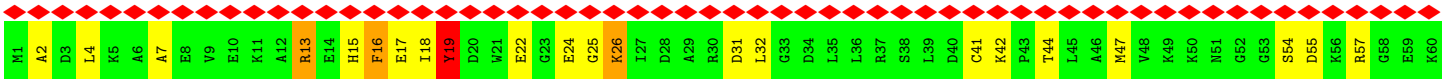


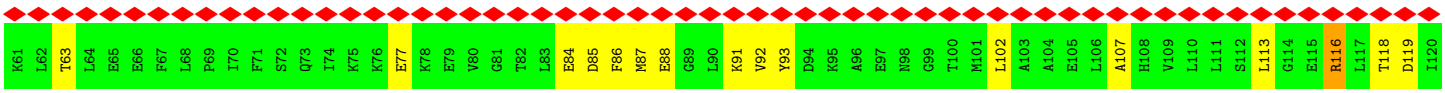


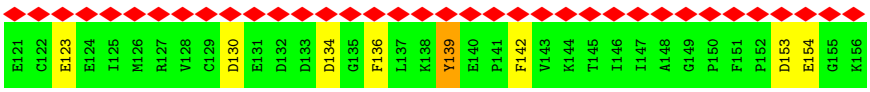


• Molecule 2: Myosin 2 essential light chain striated muscle

Chain C:

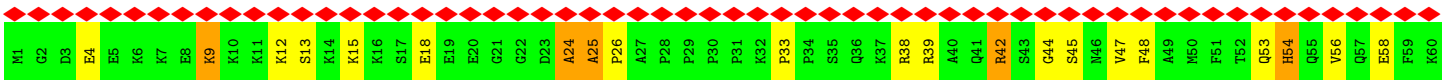






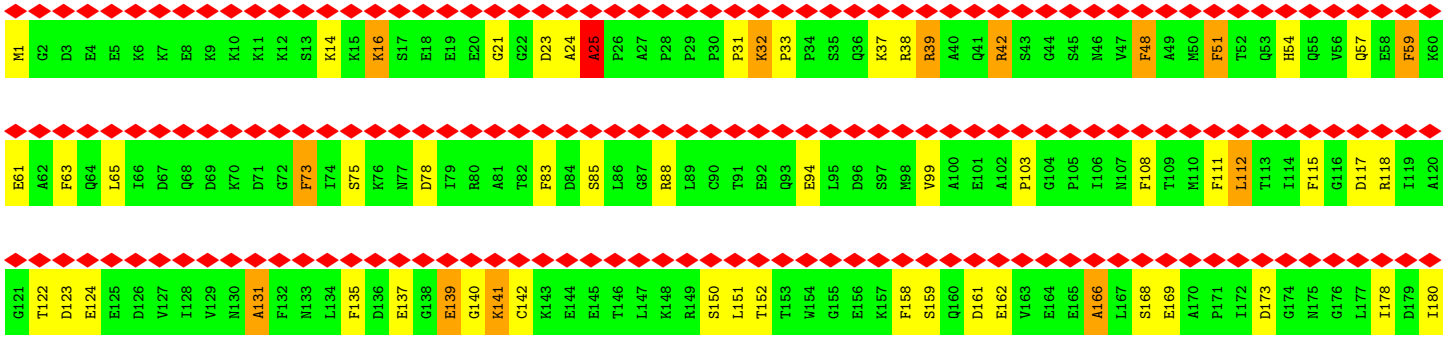
• Molecule 3: Myosin 2 regulatory light chain striated muscle

Chain F:



• Molecule 3: Myosin 2 regulatory light chain striated muscle

Chain E:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=33.98°, rise=145 Å, axial sym=C4	Depositor
Number of segments used	24000	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 ($e^-/Å^2$)	65	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	DIRECT ELECTRON DE-20 (5k x 3k)	Depositor
Maximum map value	0.181	Depositor
Minimum map value	-0.056	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.032	Depositor
Map size (Å)	528.336, 528.336, 528.336	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.223, 1.223, 1.223	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	1.70	50/6882 (0.7%)	2.01	194/9279 (2.1%)
1	B	1.70	56/6883 (0.8%)	1.98	158/9280 (1.7%)
2	C	1.70	9/1251 (0.7%)	1.94	26/1674 (1.6%)
2	D	1.65	6/1251 (0.5%)	1.99	43/1674 (2.6%)
3	E	1.66	8/1554 (0.5%)	1.94	38/2081 (1.8%)
3	F	1.68	8/1554 (0.5%)	1.98	33/2081 (1.6%)
All	All	1.69	137/19375 (0.7%)	1.99	492/26069 (1.9%)

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
1	A	0	18
1	B	0	31
2	C	0	6
2	D	0	1
3	E	0	3
3	F	0	3
All	All	0	62

The worst 5 of 137 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	42	ARG	CZ-NH2	8.38	1.44	1.33
1	B	796	TYR	CE2-CZ	8.13	1.49	1.38
1	A	342	TYR	CG-CD1	7.94	1.49	1.39
1	B	834	TYR	CE2-CZ	7.80	1.48	1.38
3	F	13	SER	CA-CB	7.50	1.64	1.52

The worst 5 of 492 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	809	ARG	NE-CZ-NH1	17.57	129.08	120.30
3	F	38	ARG	NE-CZ-NH2	17.39	128.99	120.30
3	F	149	ARG	NE-CZ-NH2	16.97	128.78	120.30
1	A	767	ARG	NE-CZ-NH2	16.62	128.61	120.30
1	B	809	ARG	NE-CZ-NH2	-16.00	112.30	120.30

There are no chirality outliers.

5 of 62 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	10	TYR	Sidechain
1	B	112	TYR	Sidechain
1	B	125	ARG	Sidechain
1	B	64	ARG	Sidechain
1	B	84	ASP	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	6738	6760	6760	41	0
1	B	6739	6760	6760	36	0
2	C	1233	1227	1227	4	0
2	D	1233	1227	1227	5	0
3	E	1529	1491	1491	10	0
3	F	1529	1491	1491	13	0
All	All	19001	18956	18956	94	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 2.

The worst 5 of 94 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)
3:E:32:LYS:H	3:E:33:PRO:HD2	1.44	0.81
1:A:20:LYS:HG2	1:A:22:GLN:H	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:LYS:HD2	1:B:67:LYS:H	1.62	0.65
1:B:815:ILE:HG23	3:F:147:LEU:HD22	1.81	0.63
1:A:729:ALA:HB1	2:C:88:GLU:HG3	1.85	0.58

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	838/1953 (43%)	675 (80%)	106 (13%)	57 (7%)	1	15
1	B	838/1953 (43%)	705 (84%)	89 (11%)	44 (5%)	2	19
2	C	154/156 (99%)	130 (84%)	16 (10%)	8 (5%)	2	19
2	D	154/156 (99%)	132 (86%)	15 (10%)	7 (4%)	2	21
3	E	194/196 (99%)	148 (76%)	31 (16%)	15 (8%)	1	13
3	F	194/196 (99%)	149 (77%)	28 (14%)	17 (9%)	1	11
All	All	2372/4610 (52%)	1939 (82%)	285 (12%)	148 (6%)	3	16

5 of 148 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	149	LEU
1	B	206	THR
1	B	208	GLU
1	B	270	VAL
1	B	358	GLU

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	721/1689 (43%)	686 (95%)	35 (5%)	25 50
1	B	721/1689 (43%)	686 (95%)	35 (5%)	25 50
2	C	132/132 (100%)	129 (98%)	3 (2%)	50 70
2	D	132/132 (100%)	125 (95%)	7 (5%)	22 47
3	E	164/164 (100%)	153 (93%)	11 (7%)	16 41
3	F	164/164 (100%)	157 (96%)	7 (4%)	29 53
All	All	2034/3970 (51%)	1936 (95%)	98 (5%)	29 51

5 of 98 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	185	LYS
1	A	459	ILE
1	A	252	MET
1	A	329	THR
1	A	600	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	722	GLN
1	A	698	ASN
1	B	827	ASN
1	A	808	GLN
1	A	552	ASN

5.3.3 RNA (i)

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 monosaccharides 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.

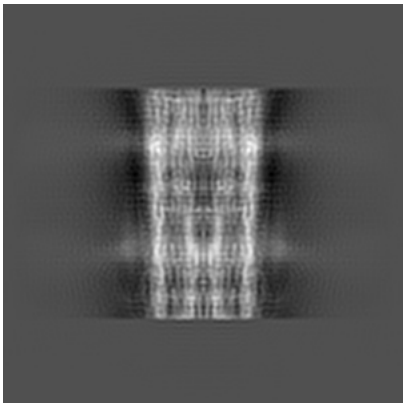
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-7029. These allow visual inspection of the internal detail of the map and identification of artifacts.

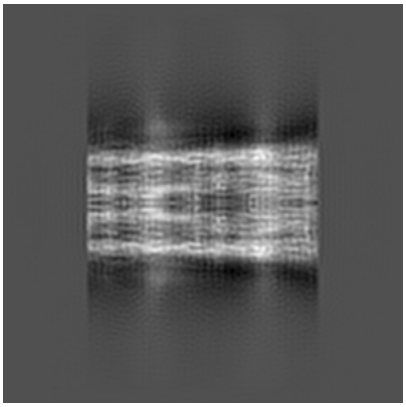
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

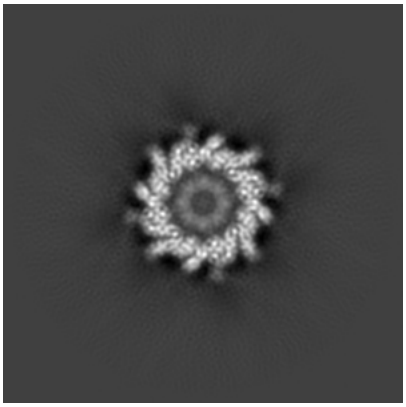
6.1.1 Primary map



X



Y

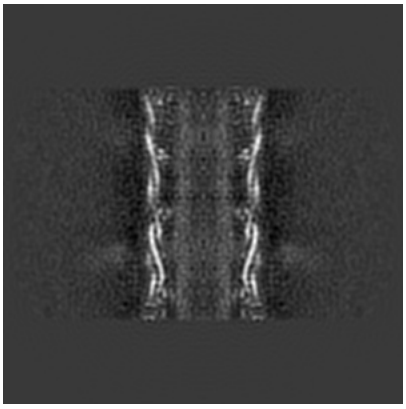


Z

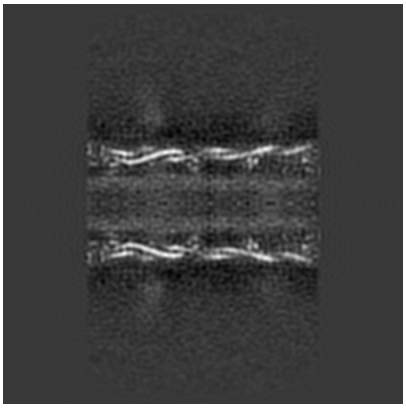
The images above show the map projected in three orthogonal directions.

6.2 Central slices

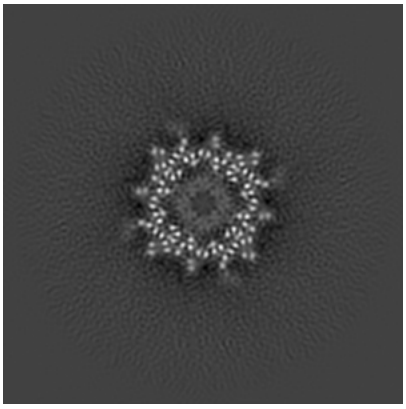
6.2.1 Primary map



X Index: 216



Y Index: 216

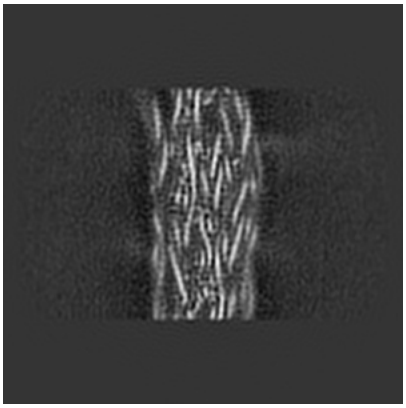


Z Index: 216

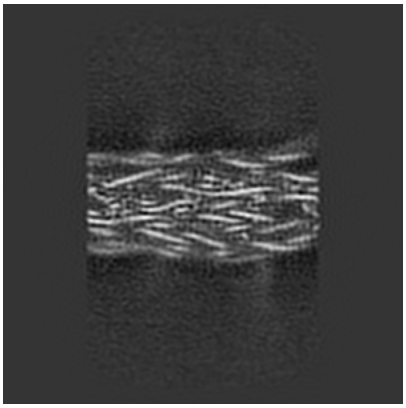
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

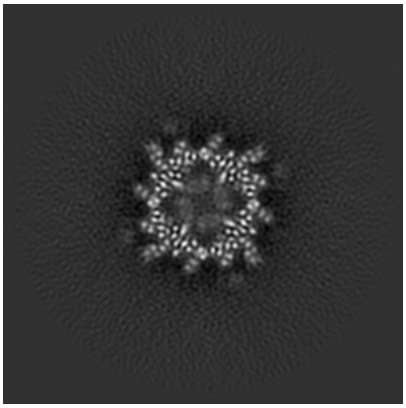
6.3.1 Primary map



X Index: 167



Y Index: 167



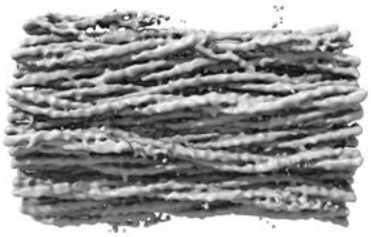
Z Index: 232

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

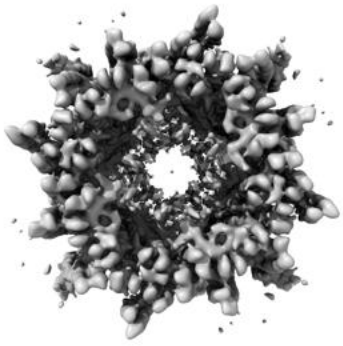
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.032. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

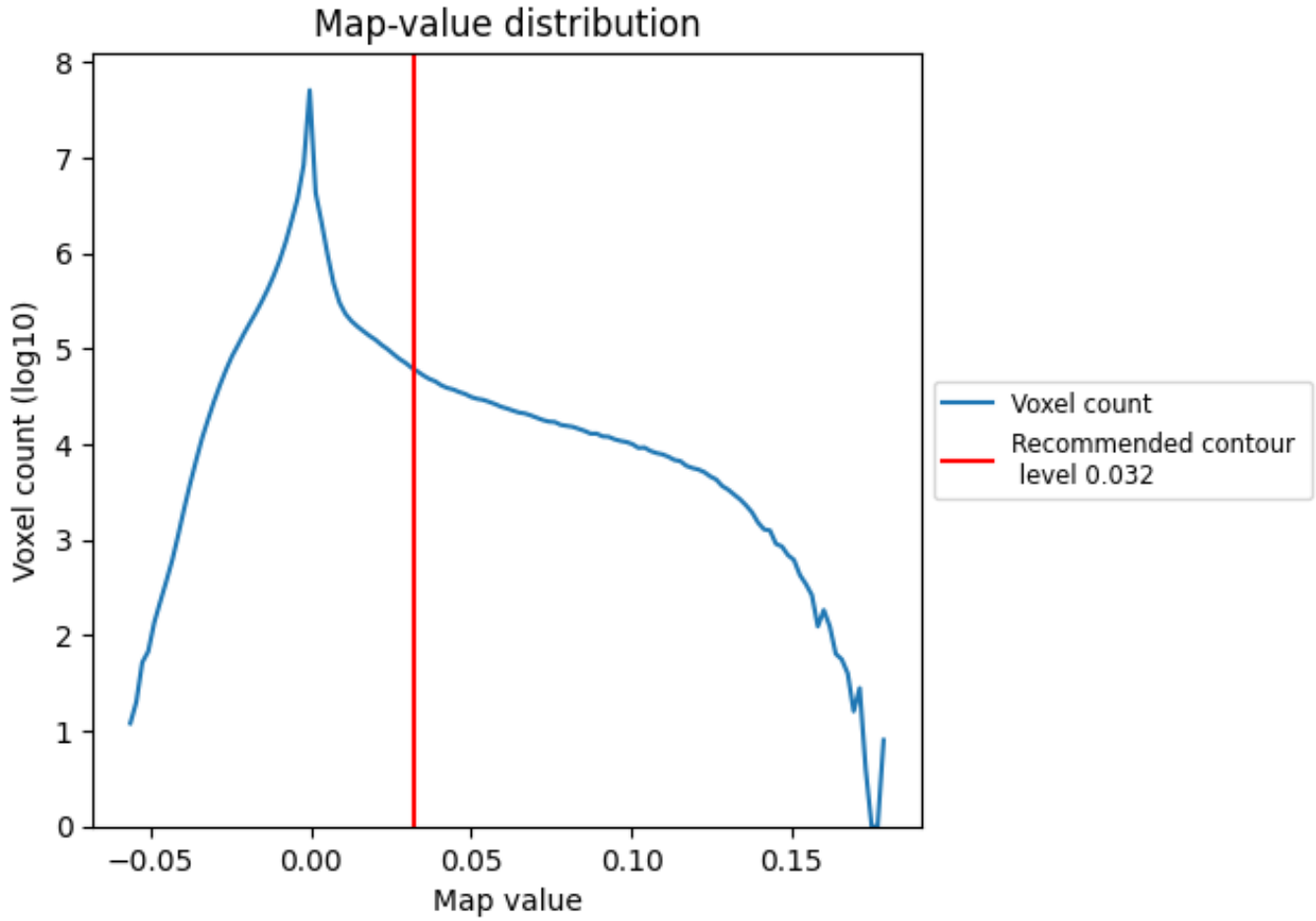
6.5 Mask visualisation (i)

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

7 Map analysis

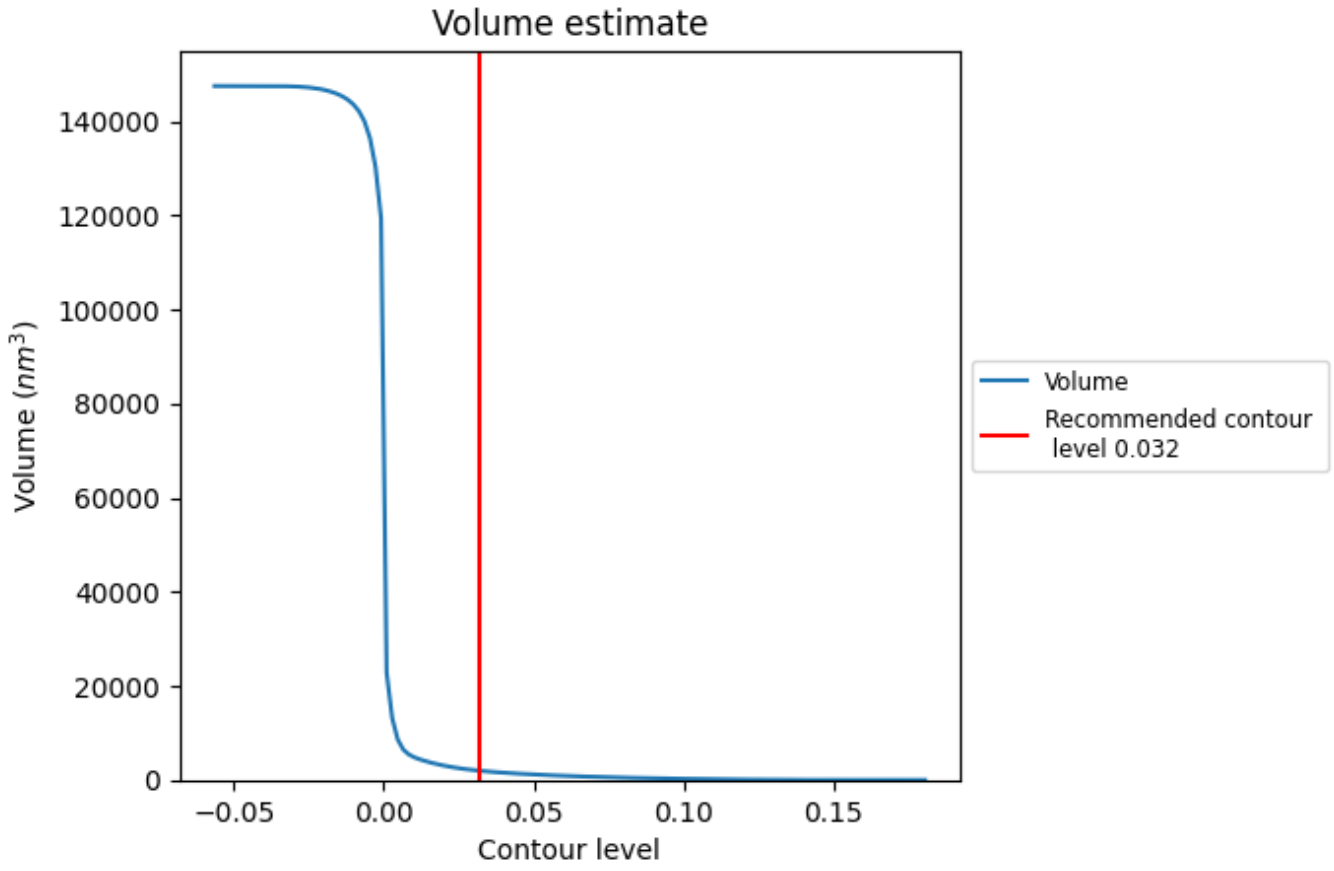
This section contains the results of statistical analysis of the map.

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.

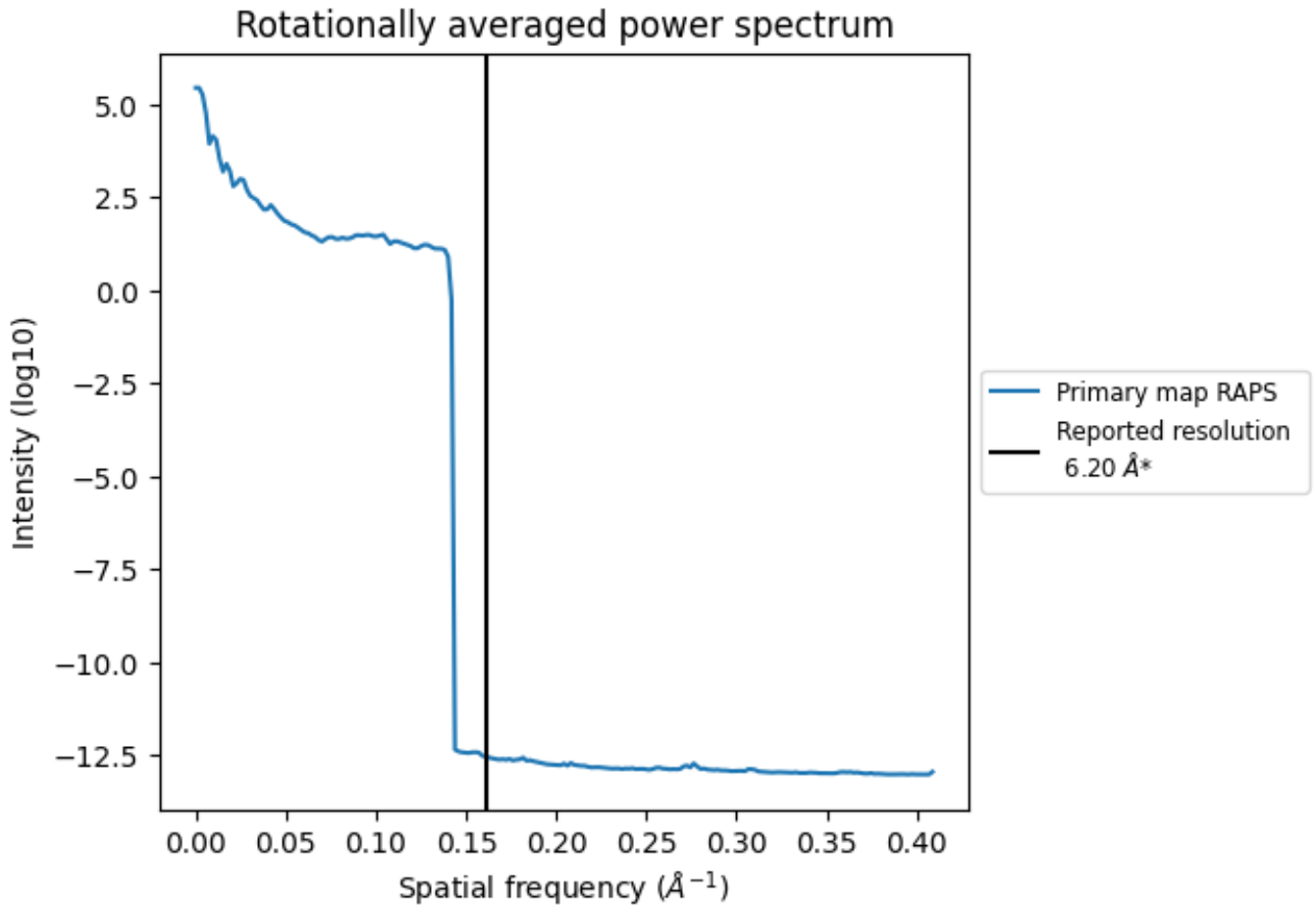
7.2 Volume estimate (i)



The volume at the recommended contour level is 1954 nm^3; this corresponds to an approximate mass of 1765 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)

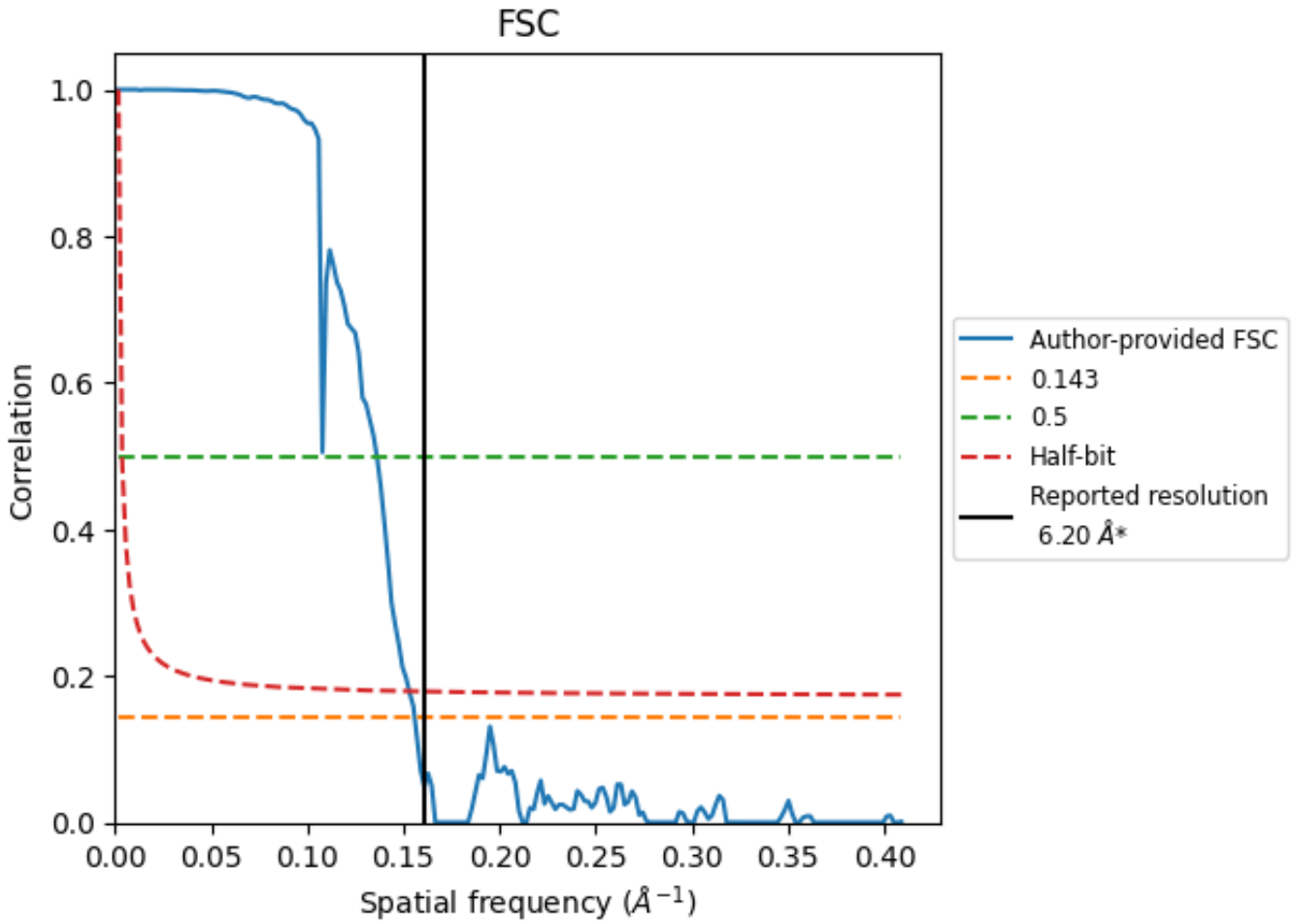


*Reported resolution corresponds to spatial frequency of 0.161 $Å^{-1}$

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 0.161 Å^{-1}

8.2 Resolution estimates (i)

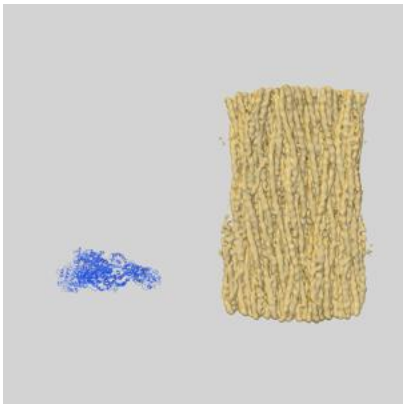
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.20	-	-
Author-provided FSC curve	6.41	7.35	6.53
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

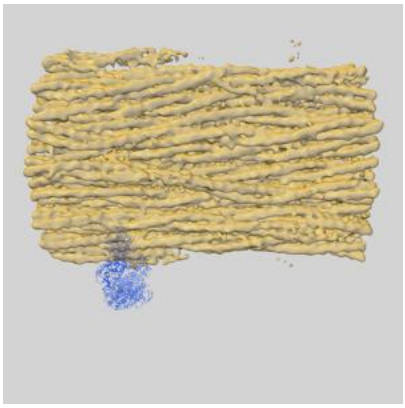
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-7029 and PDB model 6SO3. Per-residue inclusion information can be found in section 3 on page 4.

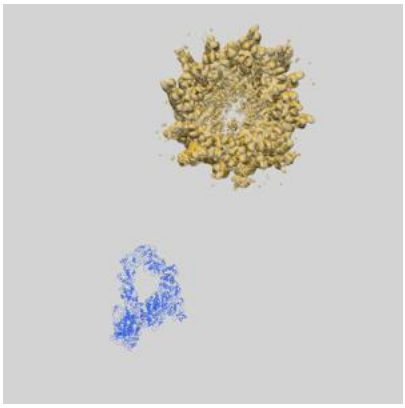
9.1 Map-model overlay



X



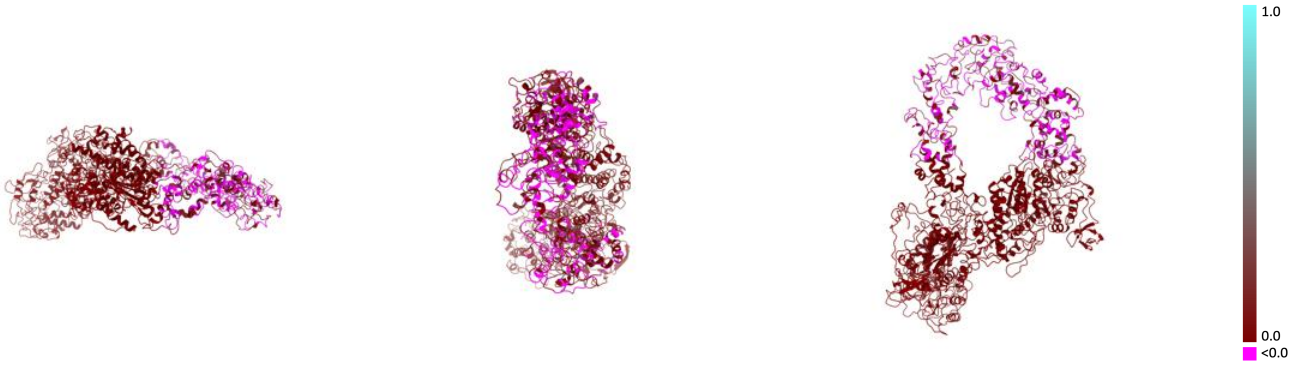
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.032 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.

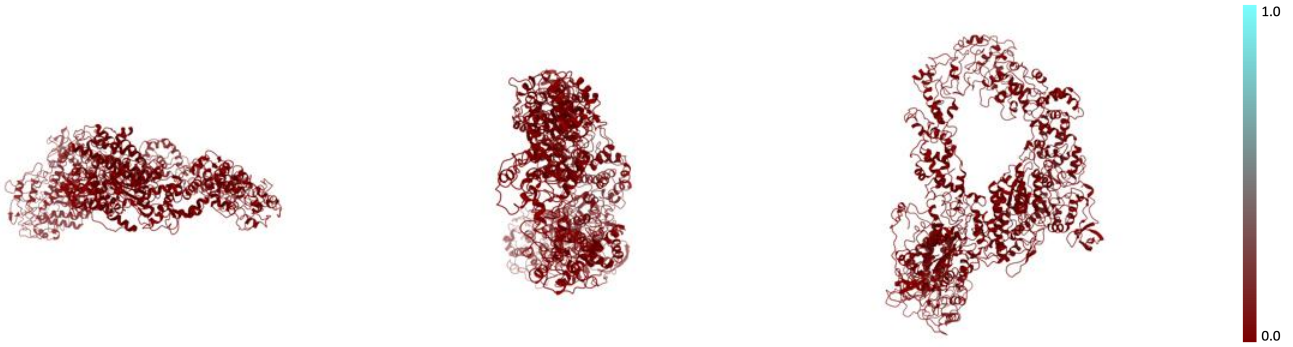
9.2 Q-score mapped to coordinate model (i)



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.

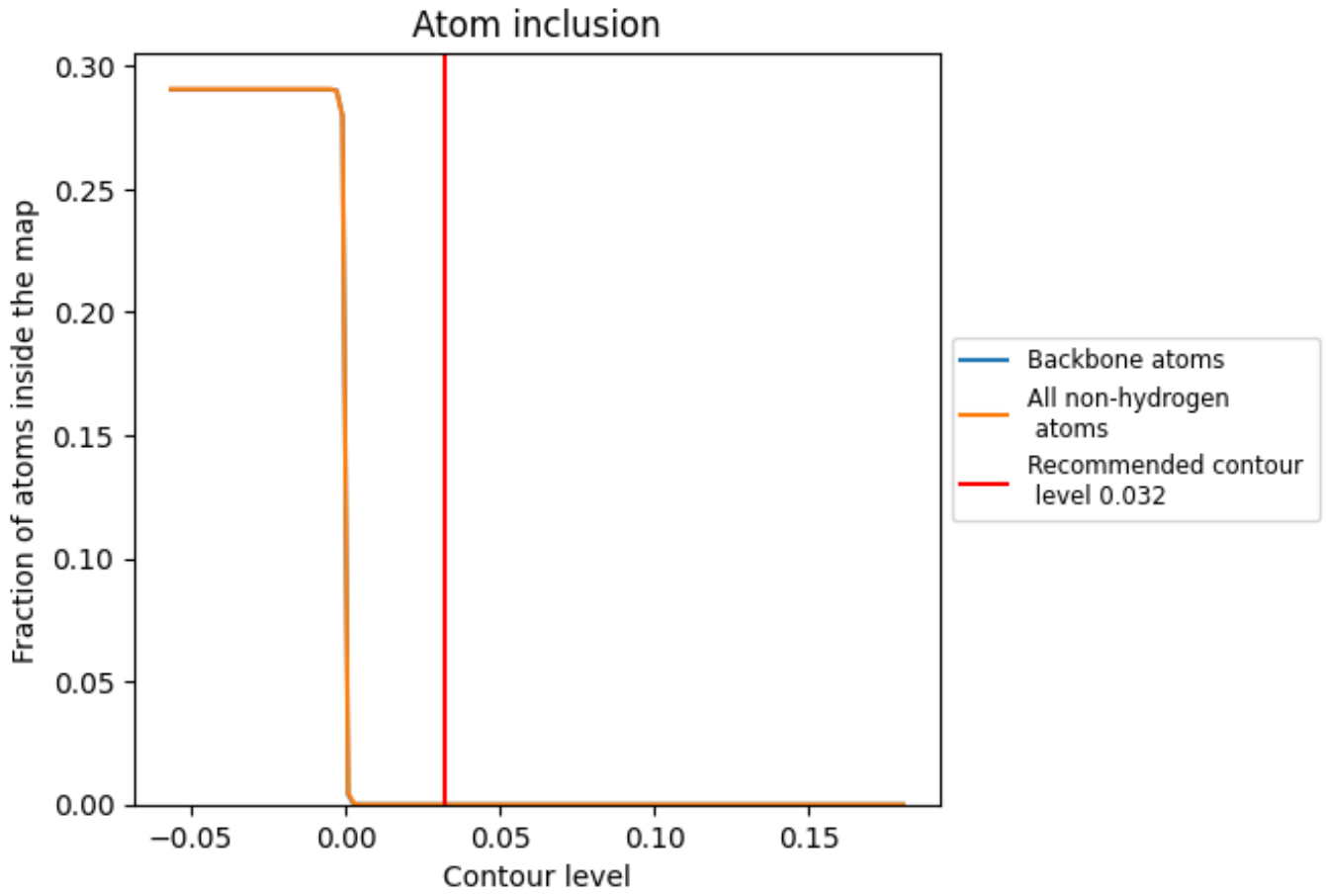
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.032).

9.4 Atom inclusion (i)



At the recommended contour level, 0% of all backbone atoms, 0% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.032) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.0000	0.0000
A	0.0000	0.0010
B	0.0000	0.0010
C	0.0000	-0.0010
D	0.0000	-0.0070
E	0.0000	0.0250
F	0.0000	-0.0260