wwPDB EM Validation Summary Report (i)

Aug 27, 2026 – 02:32 PM EDT

PDB ID	:	9YK9 / pdb_00009yk9
EMDB ID	:	EMD-73042
Title	:	The structure of the cardiac native crossbridge in the rigor state, myosin heads bound to actin molecules 1 and 2
Authors	:	Galkin, V.E.; Risi, C.M.
Deposited on	:	2025-10-06
Resolution	:	4.50 Å(reported)
Based on initial models	:	5H53, 7KO5, 6SFA, 8DD0, 7JH7

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:

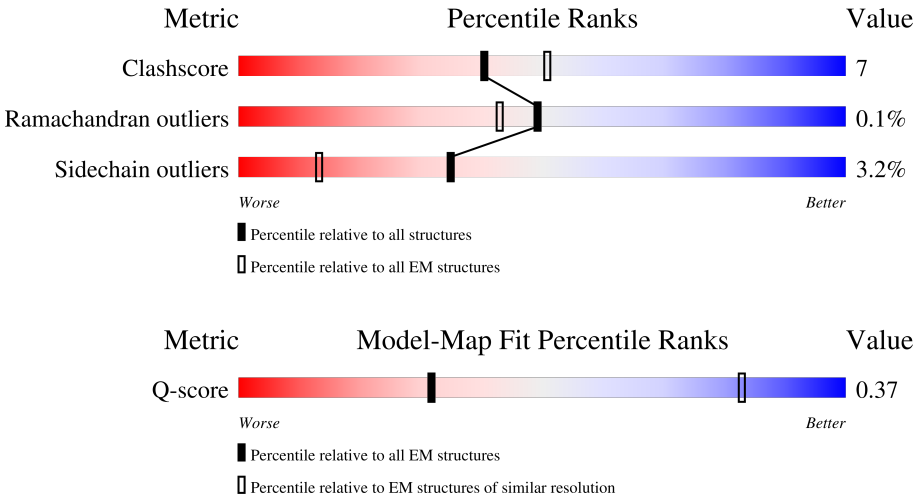
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 4.50 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.



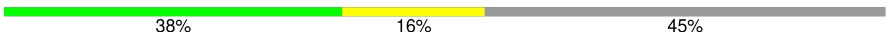
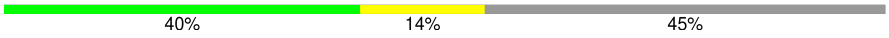
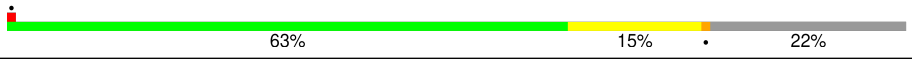
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2937 (4.00 - 5.00)

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	88% 11%
1	B	377	84% 14%
1	C	377	84% 15%
1	D	377	90% 8%

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

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 30678 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		
1	C	375	Total	C	N	O	S	0	0
			2932	1854	493	565	20		
1	D	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	E	35	Total	C	N	O	S	0	0
			285	177	43	64	1		
2	F	35	Total	C	N	O	S	0	0
			285	177	43	64	1		
2	G	155	Total	C	N	O	S	0	0
			1238	753	219	261	5		
2	H	155	Total	C	N	O	S	0	0
			1238	753	219	261	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	47	Total	C	N	O	S	0	0
			408	251	78	78	1		

- Molecule 4 is a protein called Myosin-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	805	Total	C	N	O	S	0	0
			6475	4127	1114	1202	32		

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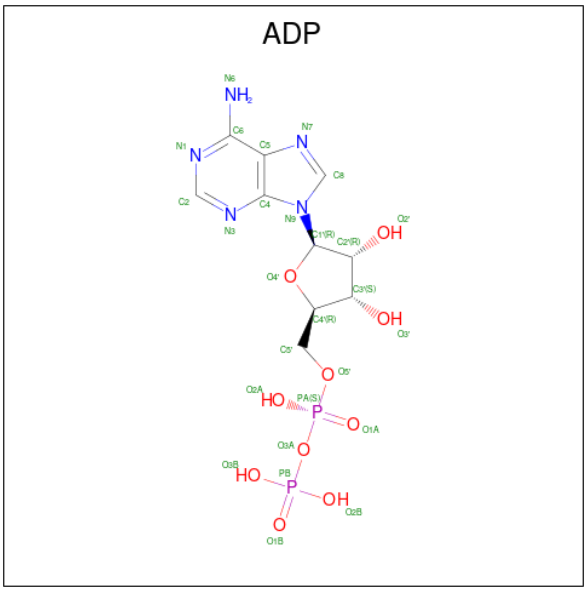
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	805	Total	C	N	O	S	0	0
			6475	4127	1114	1202	32		

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

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

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
7	A	1	Total Mg 1 1	0
7	B	1	Total Mg 1 1	0
7	C	1	Total Mg 1 1	0
7	D	1	Total Mg 1 1	0

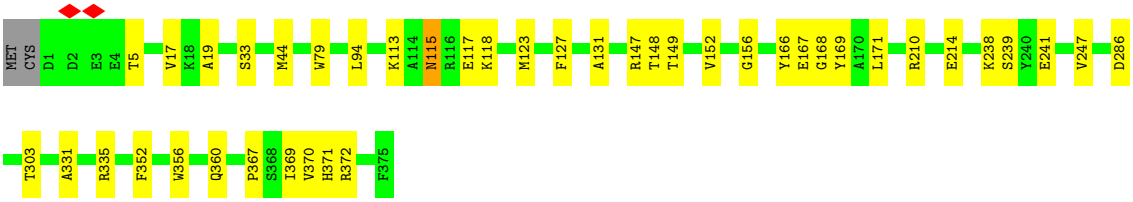
3 Residue-property plots (i)

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:

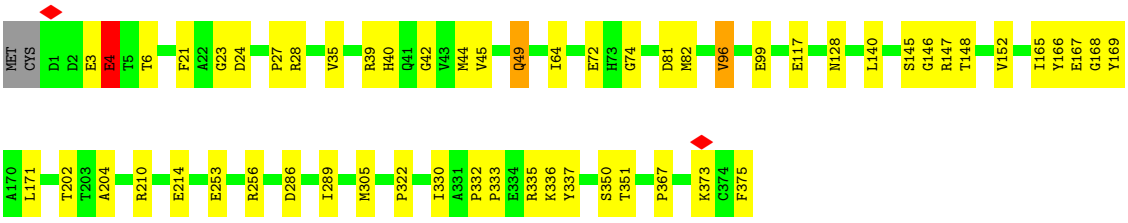




• Molecule 1: Actin, alpha cardiac muscle 1

Chain B:

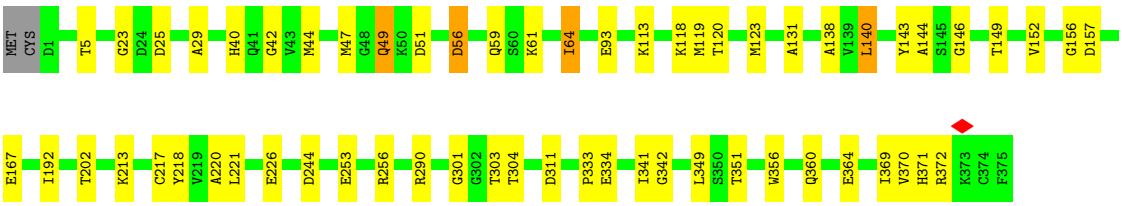




• Molecule 1: Actin, alpha cardiac muscle 1

Chain C:

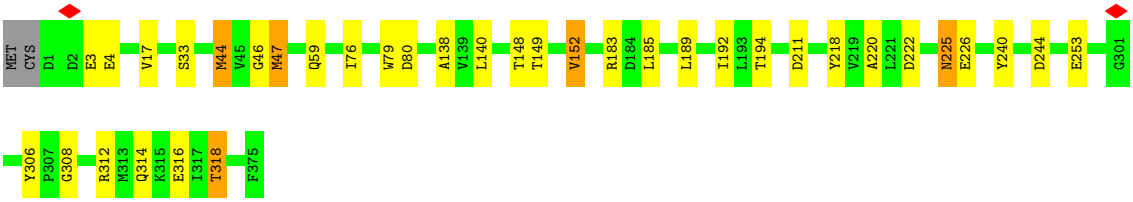




• Molecule 1: Actin, alpha cardiac muscle 1

Chain D:

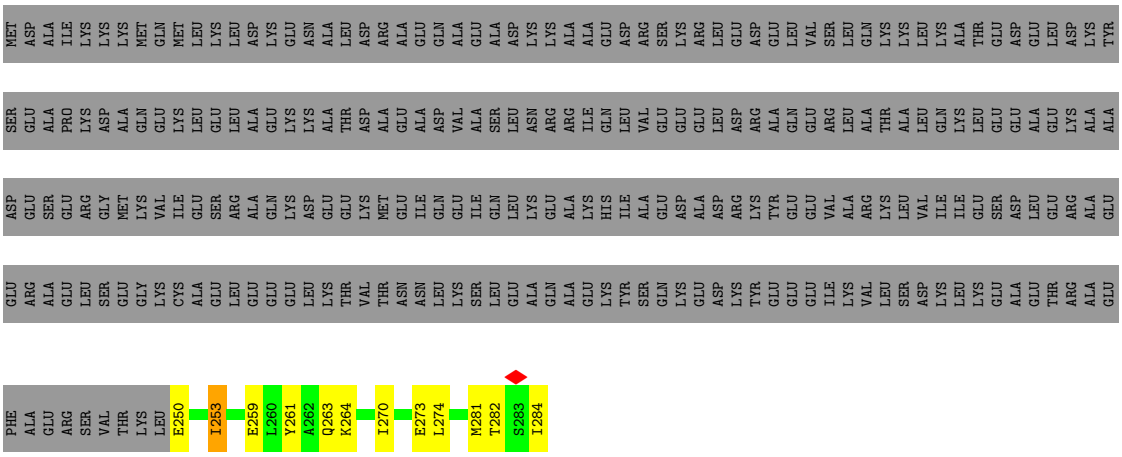




• Molecule 2: Tropomyosin alpha-1 chain

Chain E:

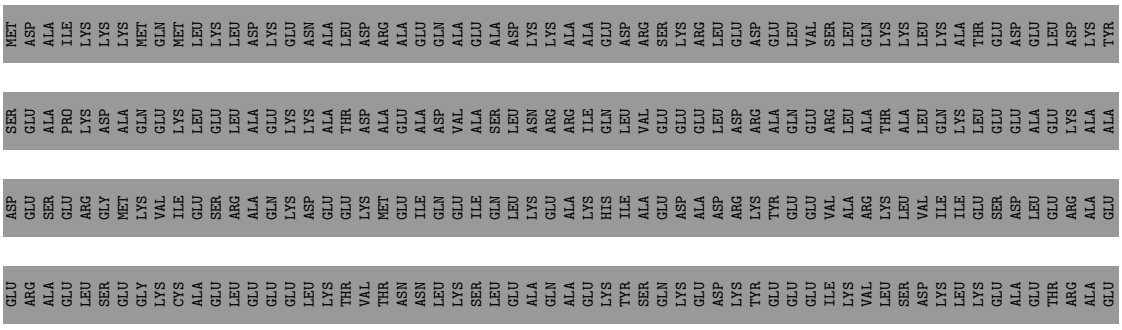


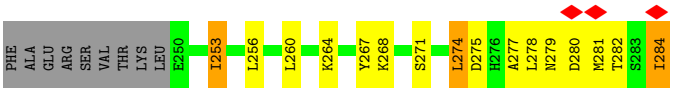


• Molecule 2: Tropomyosin alpha-1 chain

Chain F:



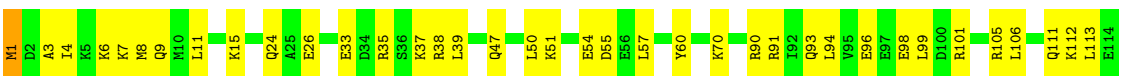


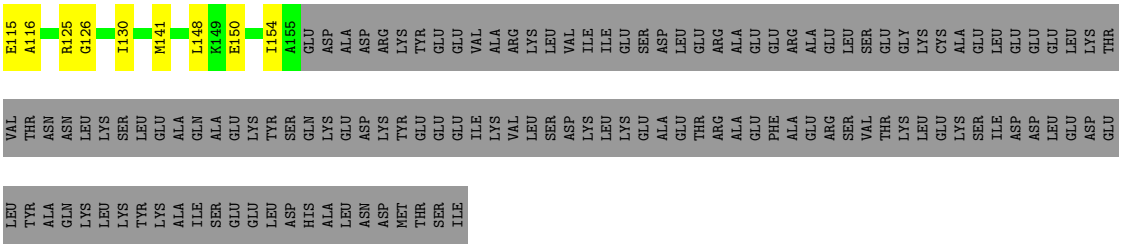


• Molecule 2: Tropomyosin alpha-1 chain

Chain G:

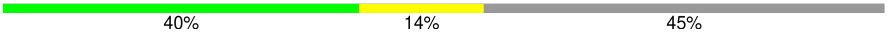


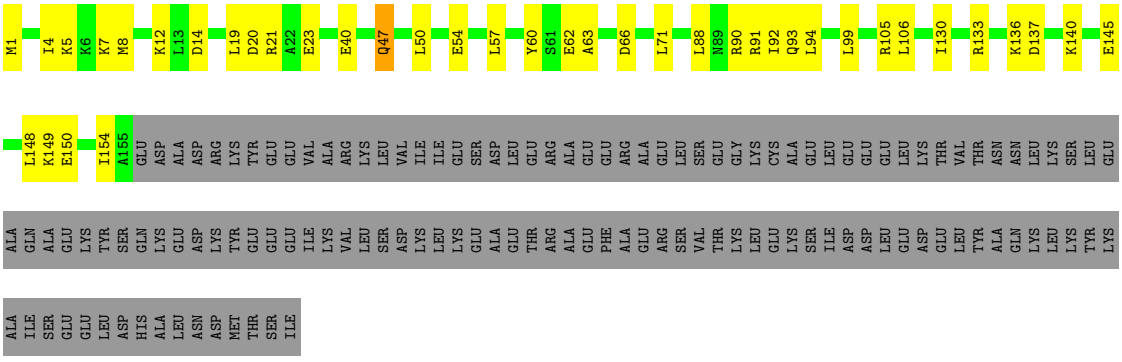




• Molecule 2: Tropomyosin alpha-1 chain

Chain H:

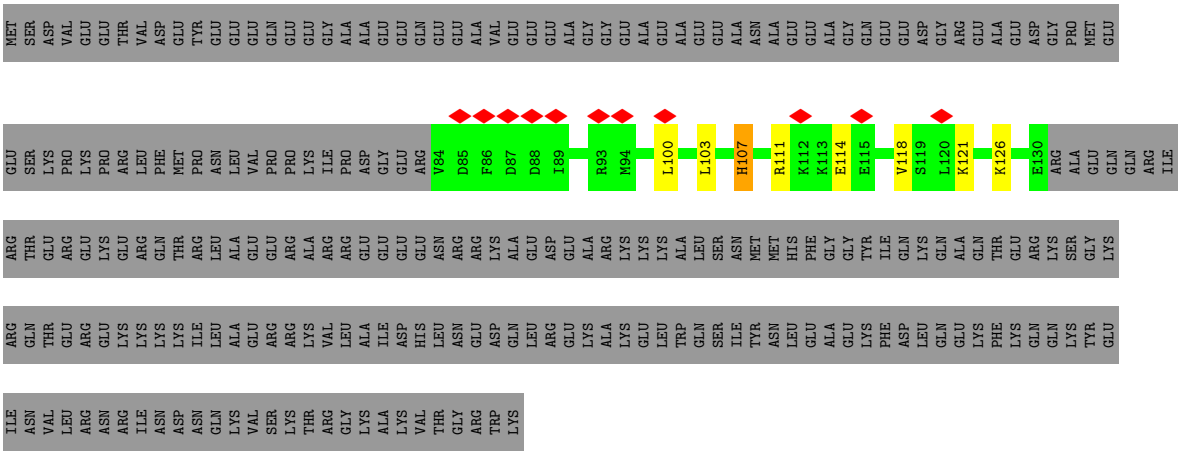




• Molecule 3: Troponin T2, cardiac type

Chain I:

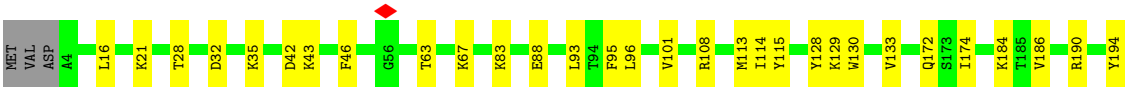


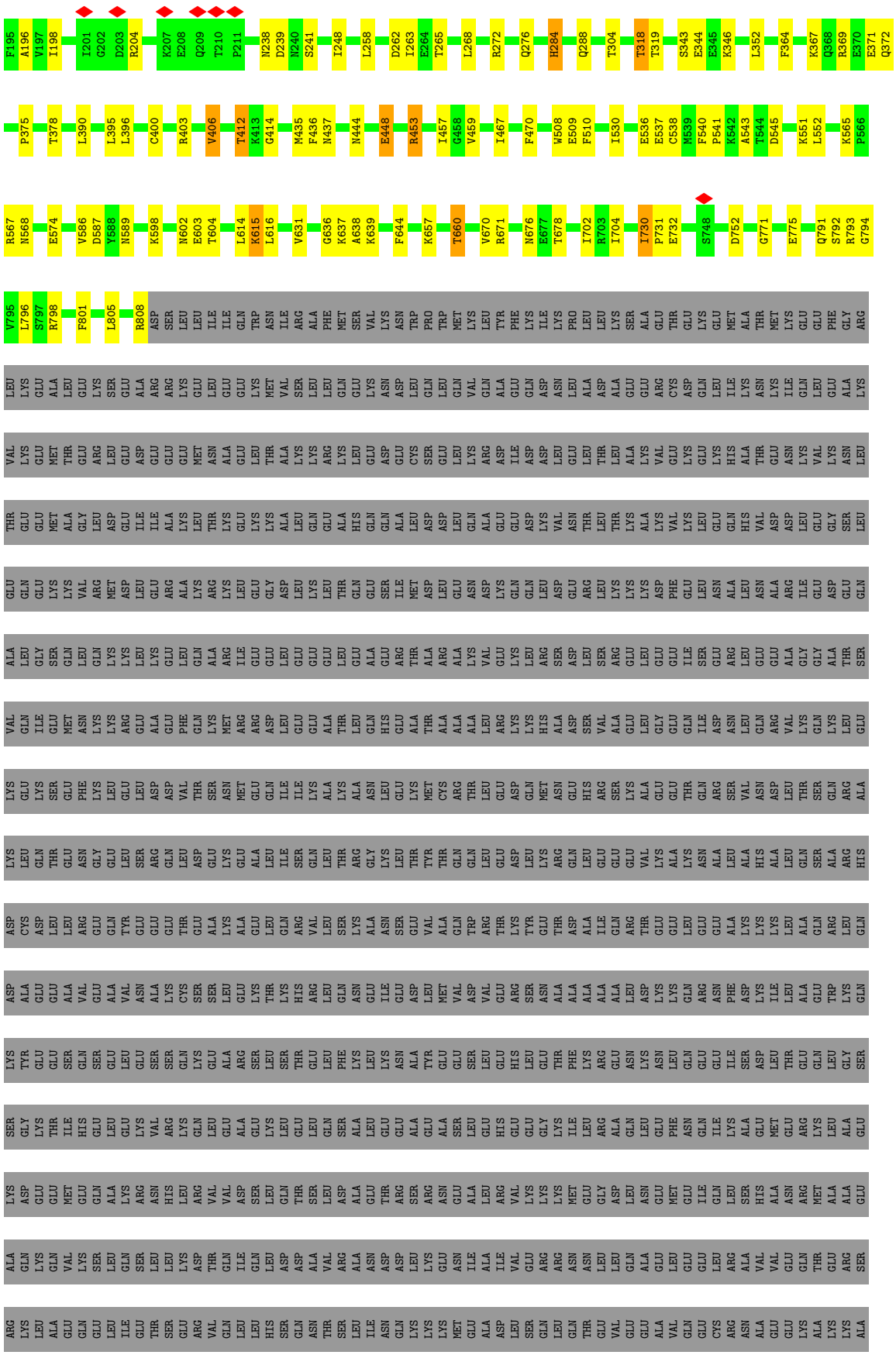


• Molecule 4: Myosin-7

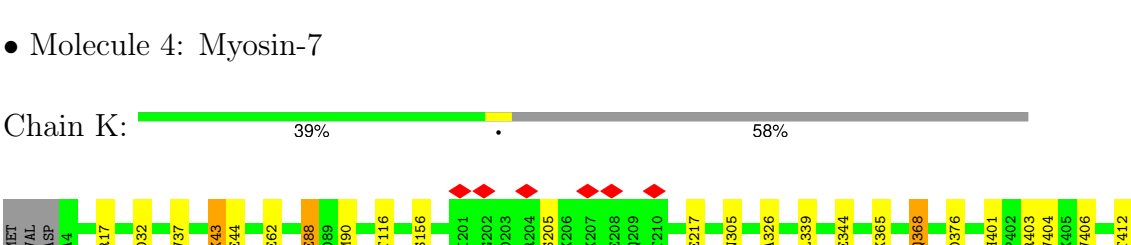
Chain J:

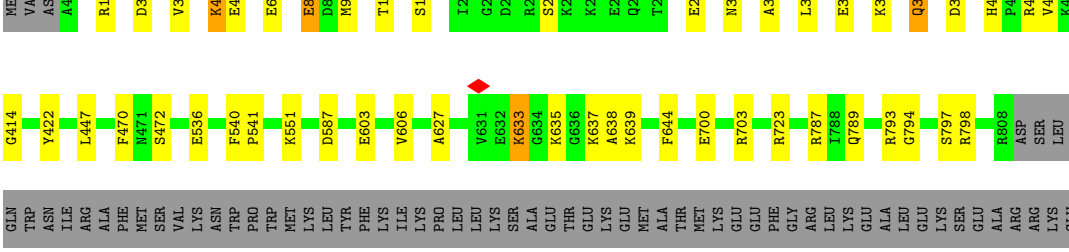





F195 A196 V197 I198 I201 G202 D203 R204 K207 E208 Q209 T210 P211 N238 D239 N240 S241 I248 L258 D262 I263 E264 T265 L268 R272 Q276 H284 Q288 T304 T318 T319 S343 E344 E345 K346 L352 F364 K367 Q368 R369 E370 E371 Q372
P375 T378 L390 L395 L396 C400 R403 V406 T412 K413 G414 M435 F436 N437 N444 E448 R453 I457 G458 V459 I467 F470 W508 E509 F510 I530 E536 E537 C538 M539 F540 P541 K542 A543 T544 D545 K551 L552 K565 P566
R567 N568 E574 V586 D587 V588 N589 K598 N602 E603 T604 L614 K615 L616 V631 G636 K637 A638 K639 F644 K657 T660 V670 R671 N676 E677 T678 I702 R703 I704 I730 P731 E732 S748 D752 G771 E775 Q791 S792 R793 G794
V795 L796 S797 R798 F801 L805 R808 ASP SER LEU LEU ILE ILE GLU GLN TRP ASN ILE ARG ALA PHE MET SER VAL LYS ASN TRP PRO TRP MET LYS LEU TYR PHE LYS ILE LYS PRO LEU LEU LEU 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 VAL SER LEU LEU GLN GLU LYS ASN ASP LEU GLN LEU GLN VAL GLN ALA GLU GLN ASP ASN LEU GLU ALA ASP ALA GLU GLU ARG CYS ASP GLN LEU ILE LYS ASN LYS ILE GLN LEU GLU ILE
VAL LYS GLU MET THR GLU ARG LEU GLU GLU GLU MET ASN ALA GLU LEU THR ALA LYS LYS ARG CYS SER GLU LEU LYS ARG ASP ILE ASP ASP LEU GLU LEU THR LEU ALA LYS VAL GLU LYS GLU LYS HIS ALA THR GLU ASN LYS ILE GLU GLU ASN LEU
THR GLU GLU MET ALA GLY LEU ASP GLU ILE ILE ALA LYS LEU THR LYS GLU LYS ALA LEU GLN GLU ALA HIS GLN GLN GLN ASP ASP LEU GLN ALA GLU GLU ASP LYS VAL ASN THR LEU THR LYS ALA LYS VAL LYS LEU GLU GLN HIS VAL ASP ASP LEU GLU GLY SER LEU
GLU GLN GLU LYS LYS VAL ARG MET ASP LEU GLU ARG ALA LYS LYS ARG LYS GLU MET ASP LYS GLN GLN LEU ASP GLU ARG LEU LYS LYS ASP PHE GLU LEU GLU ASN ALA LEU GLU ASN ALA ARG ILE GLU ASP GLU GLN
ALA LEU GLY SER GLN LEU GLN LYS LYS LEU GLU GLU ALA ARG ILE GLU GLU LEU GLU LEU LYS LEU GLU GLU GLU LEU GLU ALA GLU 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 GLY GLY ALA THR SER
VAL GLN ILE GLU MET ASN LYS LYS ARG GLU ALA ALA GLU PHE GLN LYS MET ARG ARG ASP LEU GLU GLU ALA THR LEU GLN HIS GLU ALA ALA ALA LEU GLU ALA ALA THR ALA ALA ALA LEU GLU GLN LYS LYS HIS ALA ASP SER VAL ALA GLU LEU GLY GLU GLN ILE ASP ASN LEU GLN VAL LYS GLN THR LYS SER
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 GLU ASP GLN MET ASN GLU HIS ARG SER LYS ALA GLU GLU THR GLN ARG GLU VAL LYS ARG GLN LEU GLU GLU ASP ASN ALA LEU GLN ARG SER VAL ASN ASP LEU THR SER GLN ARG ALA
LYS LEU GLN THR GLU ASN GLY GLU GLU LEU SER ARG GLN LEU ASP GLU LYS GLU GLU ALA LEU ILE SER GLN LEU GLU THR TYR THR GLN GLN LEU GLU GLU ASP LEU LYS ARG GLN LEU GLU GLU THR ARG GLY LYS ALA ASN SER LEU THR GLN GLN LEU GLU GLU VAL LYS ALA LYS ASN ALA LEU ALA HIS ALA LEU GLN SER ALA HIS
ASP CYS ASP LEU LEU ARG GLU GLN TYR GLU GLU GLU GLN THR GLU ALA LYS GLU LEU GLN GLU ALA ASN SER GLU VAL ALA GLN THR GLU SER LEU ARG VAL LEU GLN LEU GLU GLU ALA ALA LYS ALA ILE GLN ARG THR GLU GLU LEU GLU GLU GLU ALA LYS LYS LEU ALA GLN ARG LEU GLN
ASP ALA GLU GLU ALA VAL GLU ALA VAL ASN ALA LYS CYS SER SER LEU GLU ALA GLU LYS THR LYS HIS ARG LEU GLN GLN ASN GLU ILE GLU ASP LEU MET VAL ASP VAL GLU GLU ARG SER ASN ALA ALA ALA ALA LEU GLU ASP LEU GLN LYS LYS GLN ARG GLU ASN PHE ASP LYS ILE LEU ALA GLU TRP LYS GLN
LYS TYR GLU GLU SER GLN LYS GLU ALA ARG SER LEU SER THR GLU LEU PHE LYS LEU LYS ASN ALA TYR GLU GLU SER LEU GLU GLU HIS LEU GLU THR PHE LYS ARG GLU ASN LYS ASN LEU GLN GLU GLU ILE LEU ASP GLN LEU GLY SER
SER GLY LYS THR ILE HIS GLU LEU GLU LYS VAL ARG LYS GLN LEU GLU ALA GLU LYS LEU GLU GLN ALA SER LEU GLU GLU ALA GLU GLU HIS GLU GLU LYS ILE LEU ARG GLU ALA ASN LEU GLU GLU PHE ASN GLN ILE LYS ALA GLU MET GLU ARG LYS LEU LEU ALA GLU
LYS ASP GLU GLU MET GLU ASN HIS LEU ARG VAL VAL ASP SER LEU GLN THR ARG SER LEU ASP ALA LYS ARG ASN GLU ALA LEU ARG VAL LYS LYS LYS MET GLU GLY ASP LEU ASN GLU GLU ILE GLN LEU SER ALA GLU HIS ALA ASN ARG MET ALA ALA GLU
ALA GLN LYS GLN VAL SER LEU GLN ILE LEU GLN LEU ASP ASP THR ASP ASP ASP LEU ASP ASP LEU LYS ILE ASN ASP ASN VAL ASN ARG VAL ARG ARG ASP ASN ALA LEU GLU GLU LEU GLU GLN LEU GLN GLN GLU LEU GLN ALA GLU LEU GLU GLU GLN GLN THR GLU ARG SER
ARG LYS LEU ALA GLU ILE HIS SER GLN ASN THR SER LEU ILE ASN GLN LYS LYS LYS MET GLU ALA ASP LEU SER GLN LEU GLN THR GLU VAL GLU GLU ALA VAL GLN GLU CYS ARG ASN ALA GLU GLU LYS ALA LYS LYS ALA
WORLDWIDE PDB PROTEIN DATA BANK







• Molecule 4: Myosin-7

Chain K:

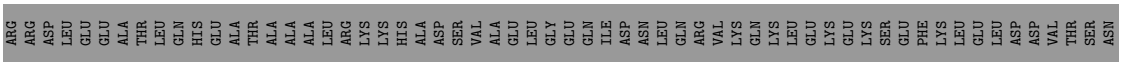
















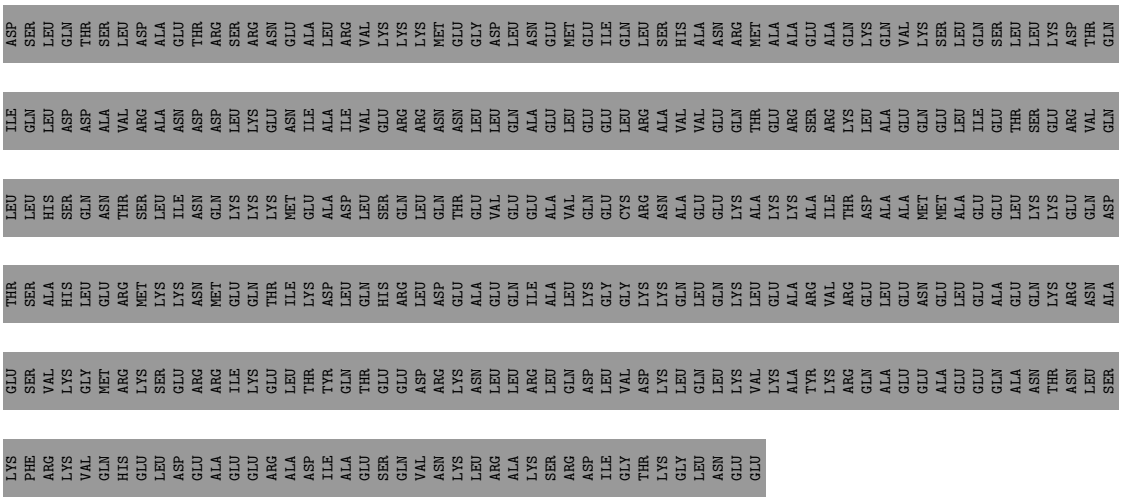






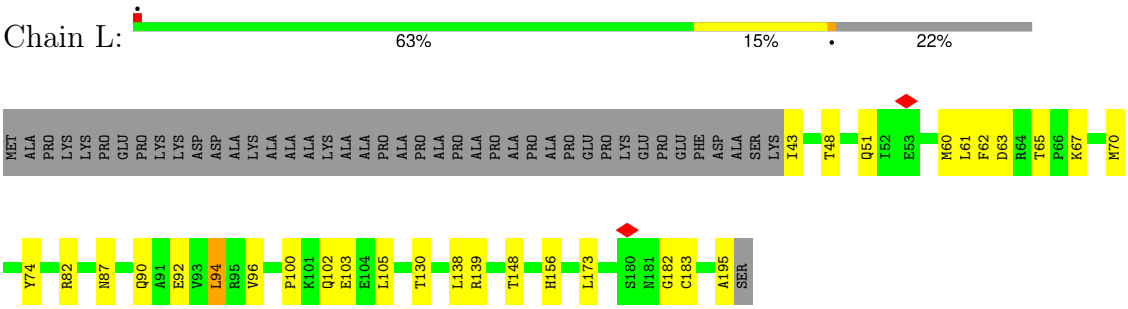






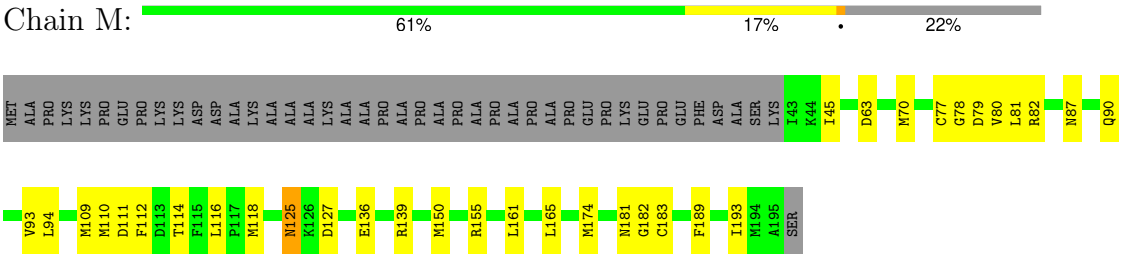
• Molecule 5: Myosin light chain 3

Chain L:



• Molecule 5: Myosin light chain 3

Chain M:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	54451	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	11.410	Depositor
Minimum map value	-5.567	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.178	Depositor
Recommended contour level	1.05	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

5.1 Standard geometry

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

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	0.15	0/2995	0.34	0/4057
1	B	0.17	0/2995	0.39	0/4057
1	C	0.17	0/2995	0.37	0/4057
1	D	0.15	0/2995	0.33	0/4057
2	E	0.16	0/287	0.29	0/383
2	F	0.18	0/287	0.28	0/383
2	G	0.26	0/1240	0.43	0/1647
2	H	0.24	0/1240	0.39	0/1647
3	I	0.16	0/411	0.23	0/544
4	J	0.12	0/6609	0.33	0/8899
4	K	0.82	0/6609	1.33	8/8899 (0.1%)
5	L	0.16	0/1236	0.43	2/1658 (0.1%)
5	M	0.15	0/1236	0.44	2/1658 (0.1%)
All	All	0.41	0/31135	0.69	12/41946 (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
1	B	0	1
4	K	0	1
All	All	0	2

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	182	GLY	CA-C-N	7.78	135.71	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	182	GLY	C-N-CA	7.78	135.71	121.70
5	L	182	GLY	CA-C-N	7.29	134.82	121.70
5	L	182	GLY	C-N-CA	7.29	134.82	121.70
4	K	401	HIS	CA-C-N	6.18	127.04	120.11

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	4	GLU	Peptide
4	K	422	TYR	Sidechain

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	25	0
1	B	2932	0	2894	71	0
1	C	2932	0	2894	81	0
1	D	2932	0	2894	23	0
2	E	285	0	274	13	0
2	F	285	0	274	31	0
2	G	1238	0	1265	78	0
2	H	1238	0	1265	66	0
3	I	408	0	412	13	0
4	J	6475	0	6475	99	0
4	K	6475	0	6475	67	0
5	L	1217	0	1199	25	0
5	M	1217	0	1199	22	0
6	A	27	0	12	1	0
6	B	27	0	12	1	0
6	C	27	0	12	1	0
6	D	27	0	12	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	30678	0	30462	425	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 7.

The worst 5 of 425 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:91:ARG:HH21	2:H:92:ILE:CD1	1.22	1.52
2:G:91:ARG:NH2	2:H:92:ILE:HD13	1.39	1.38
1:C:334:GLU:CB	4:K:413:LYS:HE2	1.54	1.36
1:C:341:ILE:HD11	4:K:413:LYS:NZ	1.56	1.20
2:G:105:ARG:HH21	2:H:106:LEU:CD2	1.58	1.14

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%)	352 (94%)	21 (6%)	0	100	100
1	B	373/377 (99%)	357 (96%)	15 (4%)	1 (0%)	36	71
1	C	373/377 (99%)	348 (93%)	25 (7%)	0	100	100
1	D	373/377 (99%)	355 (95%)	18 (5%)	0	100	100
2	E	33/284 (12%)	33 (100%)	0	0	100	100
2	F	33/284 (12%)	33 (100%)	0	0	100	100
2	G	153/284 (54%)	153 (100%)	0	0	100	100
2	H	153/284 (54%)	153 (100%)	0	0	100	100
3	I	45/285 (16%)	45 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	J	803/1935 (42%)	763 (95%)	38 (5%)	2 (0%)	43 77
4	K	803/1935 (42%)	747 (93%)	55 (7%)	1 (0%)	48 83
5	L	151/196 (77%)	141 (93%)	9 (6%)	1 (1%)	18 55
5	M	151/196 (77%)	145 (96%)	6 (4%)	0	100 100
All	All	3817/7191 (53%)	3625 (95%)	187 (5%)	5 (0%)	49 83

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	4	GLU
4	J	615	LYS
5	L	102	GLN
4	K	638	ALA
4	J	46	PHE

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%)	311 (98%)	7 (2%)	45 64
1	B	318/320 (99%)	310 (98%)	8 (2%)	42 62
1	C	318/320 (99%)	308 (97%)	10 (3%)	35 56
1	D	318/320 (99%)	305 (96%)	13 (4%)	27 49
2	E	32/245 (13%)	30 (94%)	2 (6%)	16 38
2	F	32/245 (13%)	29 (91%)	3 (9%)	8 26
2	G	130/245 (53%)	124 (95%)	6 (5%)	24 46
2	H	130/245 (53%)	127 (98%)	3 (2%)	44 63
3	I	45/249 (18%)	44 (98%)	1 (2%)	45 64
4	J	695/1697 (41%)	667 (96%)	28 (4%)	28 49
4	K	695/1697 (41%)	680 (98%)	15 (2%)	45 64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	L	133/163 (82%)	127 (96%)	6 (4%)	24 46
5	M	133/163 (82%)	129 (97%)	4 (3%)	36 57
All	All	3297/6229 (53%)	3191 (97%)	106 (3%)	35 55

5 of 106 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	J	184	LYS
4	J	587	ASP
5	L	130	THR
4	J	284	HIS
4	J	406	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
4	J	238	ASN
4	J	791	GLN
5	L	156	HIS
4	J	288	GLN
4	J	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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
6	ADP	C	401	7	28,29,29	1.38	4 (14%)	43,45,45	1.81	7 (16%)
6	ADP	B	401	7	28,29,29	1.38	4 (14%)	43,45,45	1.81	7 (16%)
6	ADP	A	401	7	28,29,29	1.39	5 (17%)	43,45,45	1.78	9 (20%)
6	ADP	D	401	7	28,29,29	1.37	4 (14%)	43,45,45	1.75	7 (16%)

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
6	ADP	C	401	7	-	2/16/32/32	0/3/3/3
6	ADP	B	401	7	-	3/16/32/32	0/3/3/3
6	ADP	A	401	7	-	4/16/32/32	0/3/3/3
6	ADP	D	401	7	-	3/16/32/32	0/3/3/3

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	401	ADP	C5-C4	4.59	1.47	1.39
6	B	401	ADP	C5-C4	4.53	1.47	1.39
6	D	401	ADP	C5-C4	4.46	1.47	1.39
6	A	401	ADP	C5-C4	4.35	1.46	1.39
6	A	401	ADP	C5-C6	2.69	1.48	1.41

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	401	ADP	C5-C4-N3	-6.04	118.40	126.72
6	C	401	ADP	C5-C4-N3	-6.01	118.44	126.72
6	D	401	ADP	C5-C4-N3	-5.89	118.61	126.72
6	A	401	ADP	C5-C4-N3	-5.55	119.07	126.72
6	C	401	ADP	N3-C4-N9	4.75	135.24	127.17

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	401	ADP	C5'-O5'-PA-O1A
6	A	401	ADP	C5'-O5'-PA-O2A
6	A	401	ADP	C5'-O5'-PA-O3A
6	B	401	ADP	C5'-O5'-PA-O2A
6	B	401	ADP	C5'-O5'-PA-O3A

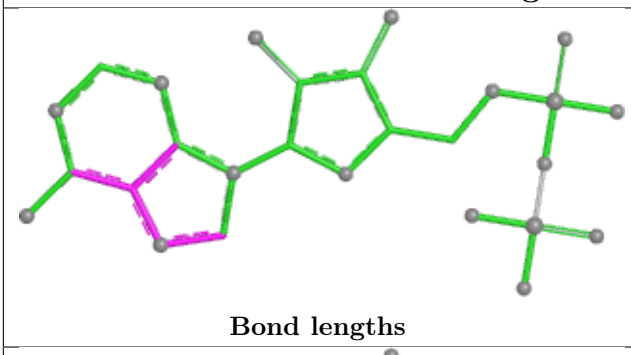
There are no ring outliers.

3 monomers are involved in 3 short contacts:

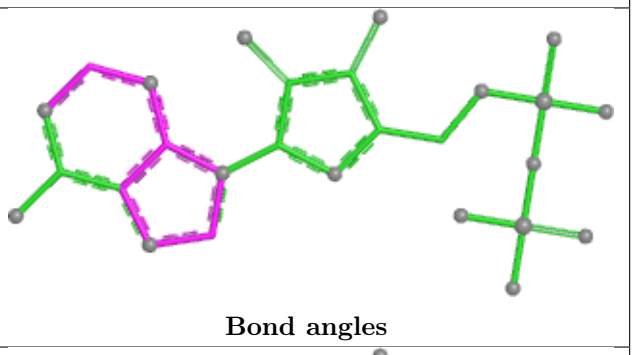
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	401	ADP	1	0
6	B	401	ADP	1	0
6	A	401	ADP	1	0

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.

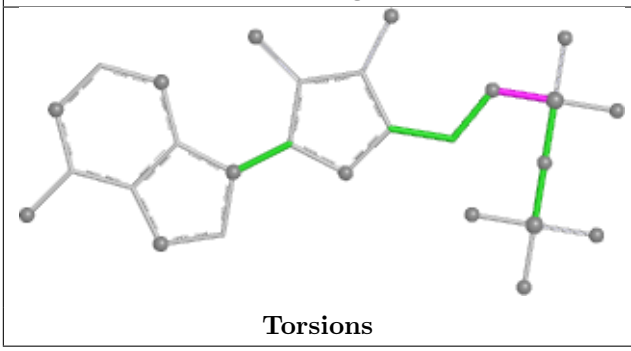
Ligand ADP C 401



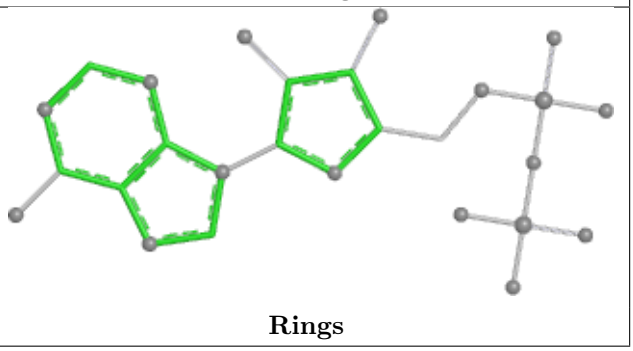
Bond lengths



Bond angles

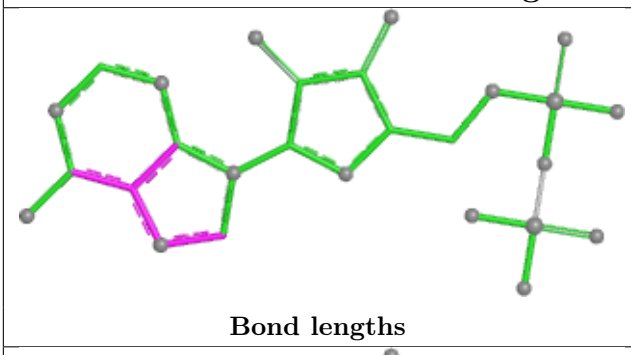


Torsions

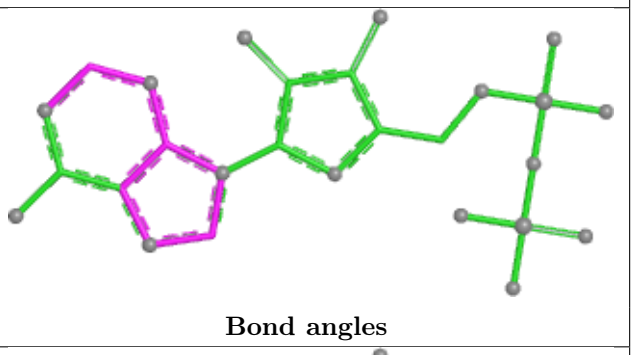


Rings

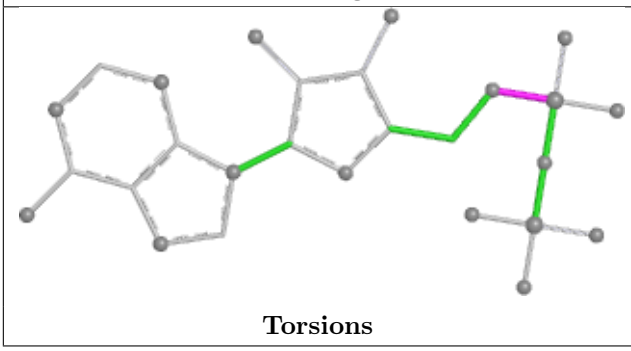
Ligand ADP B 401



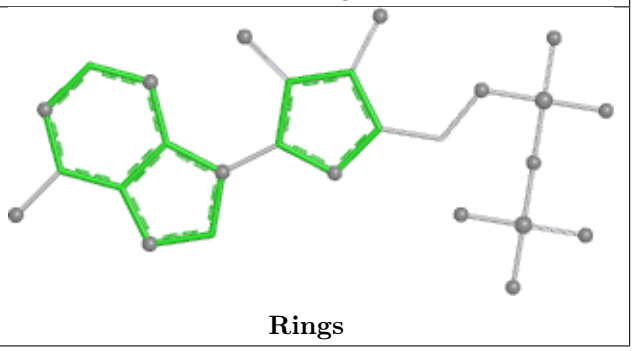
Bond lengths



Bond angles

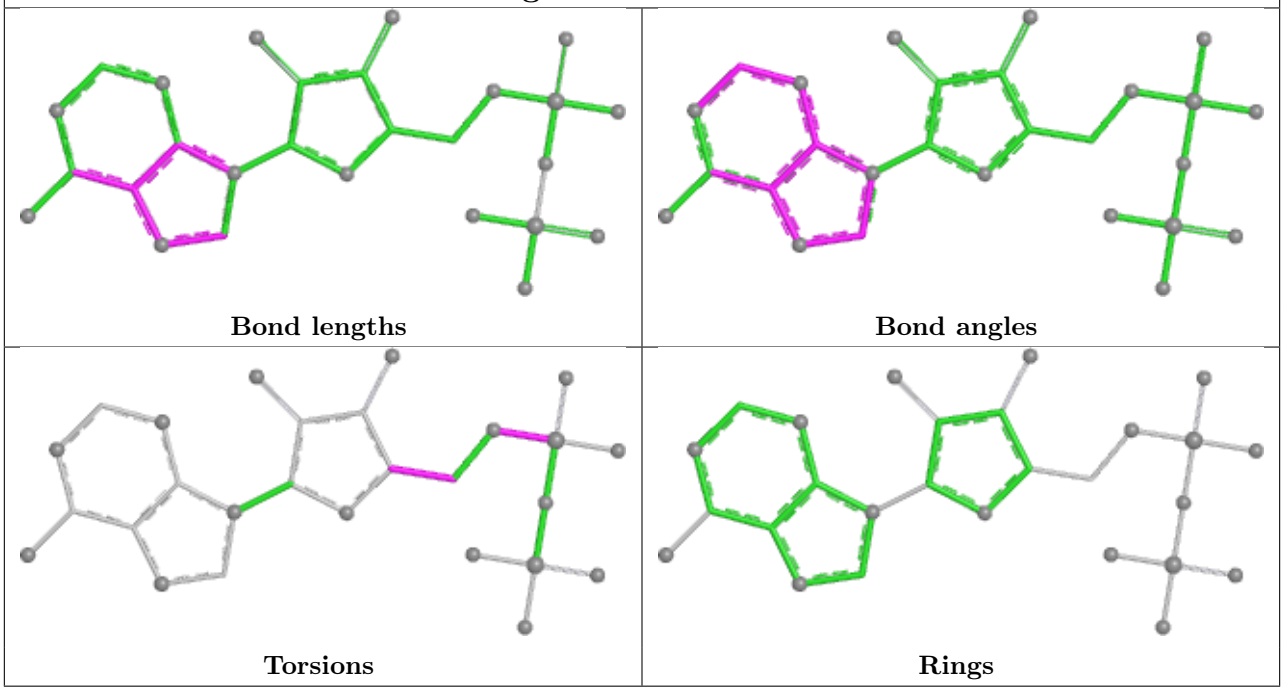


Torsions

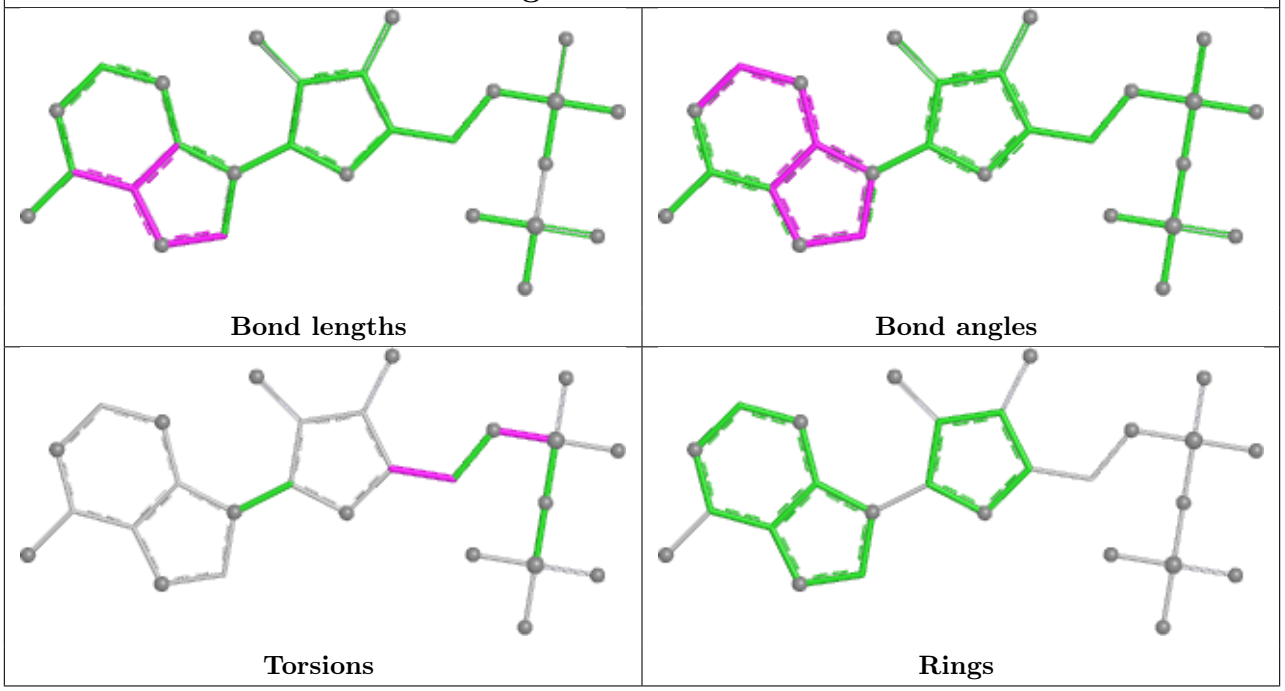


Rings

Ligand ADP A 401



Ligand ADP D 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.

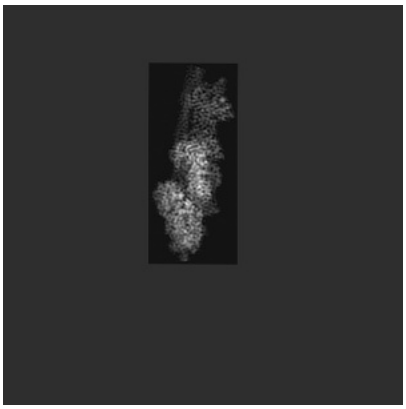
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-73042. These allow visual inspection of the internal detail of the map and identification of artifacts.

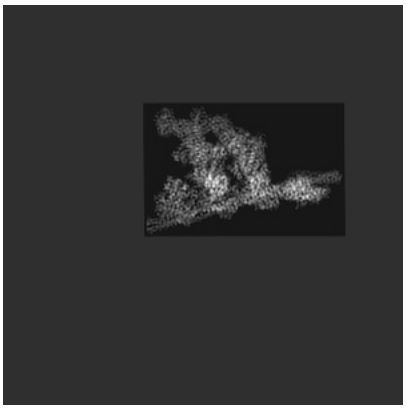
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

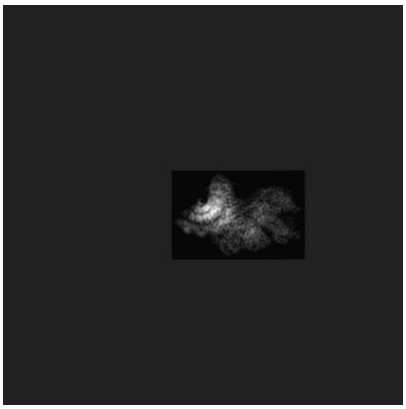
6.1.1 Primary map



X

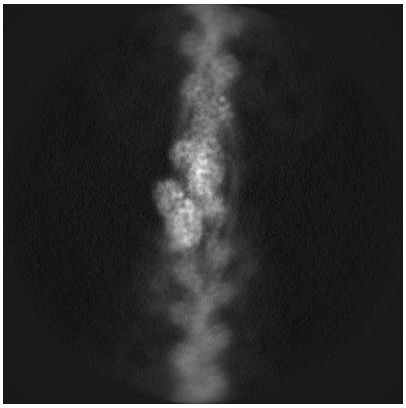


Y

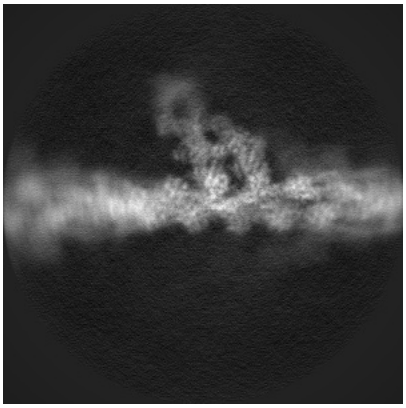


Z

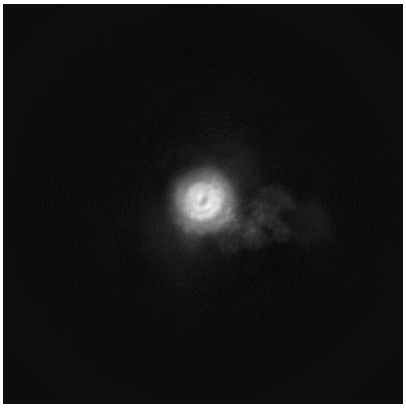
6.1.2 Raw map



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

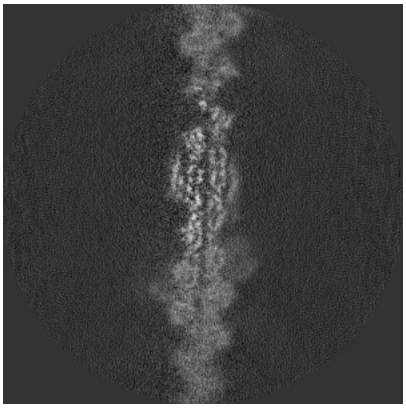


Y Index: 198

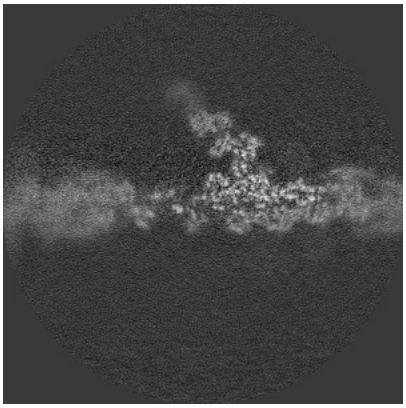


Z Index: 198

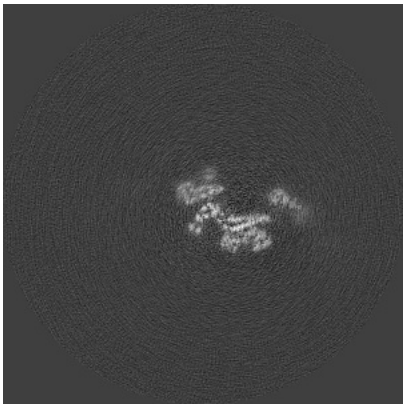
6.2.2 Raw map



X Index: 198



Y Index: 198

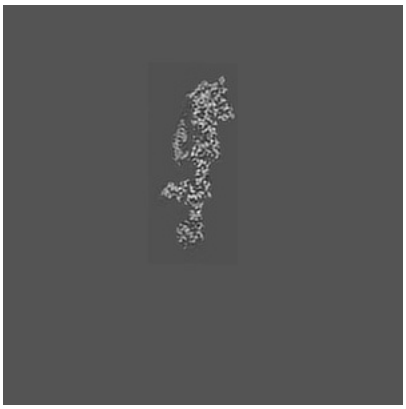


Z Index: 198

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

6.3 Largest variance slices (i)

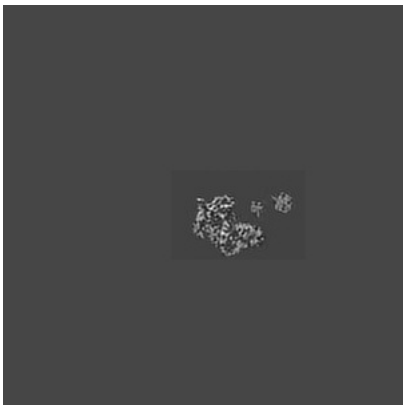
6.3.1 Primary map



X Index: 211

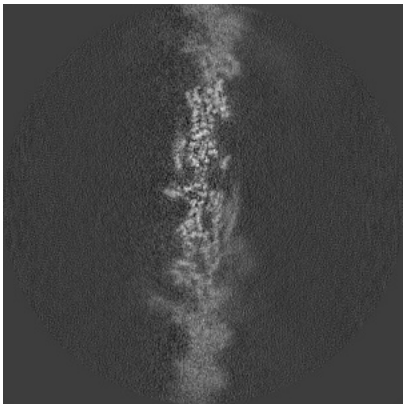


Y Index: 193

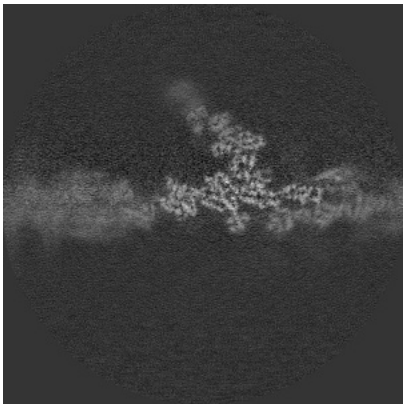


Z Index: 208

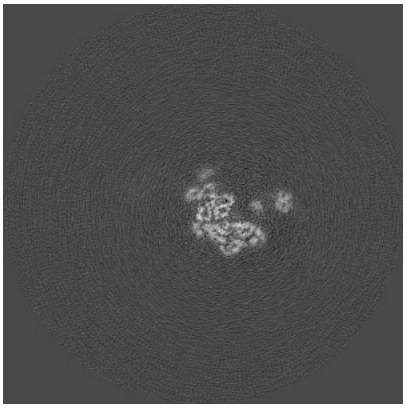
6.3.2 Raw map



X Index: 207



Y Index: 194

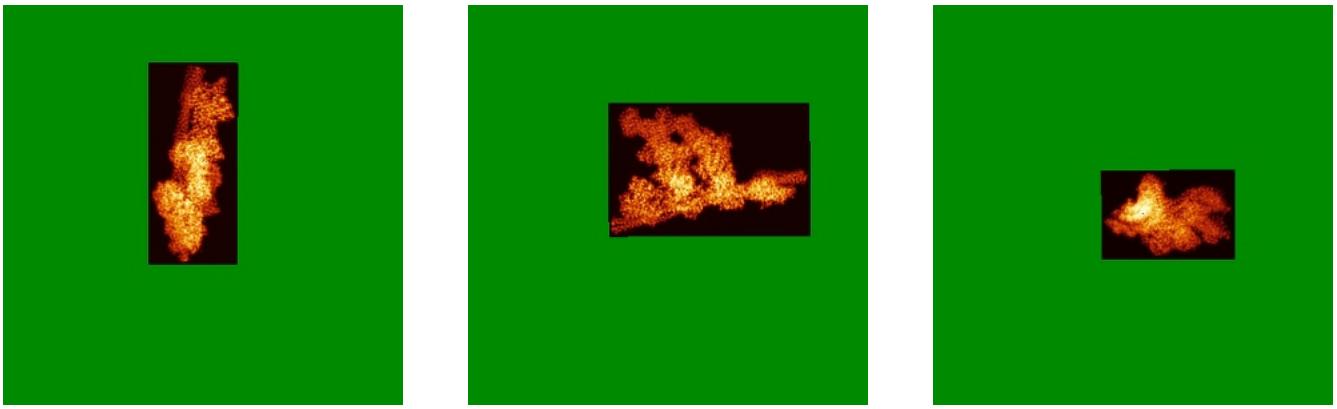


Z Index: 207

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

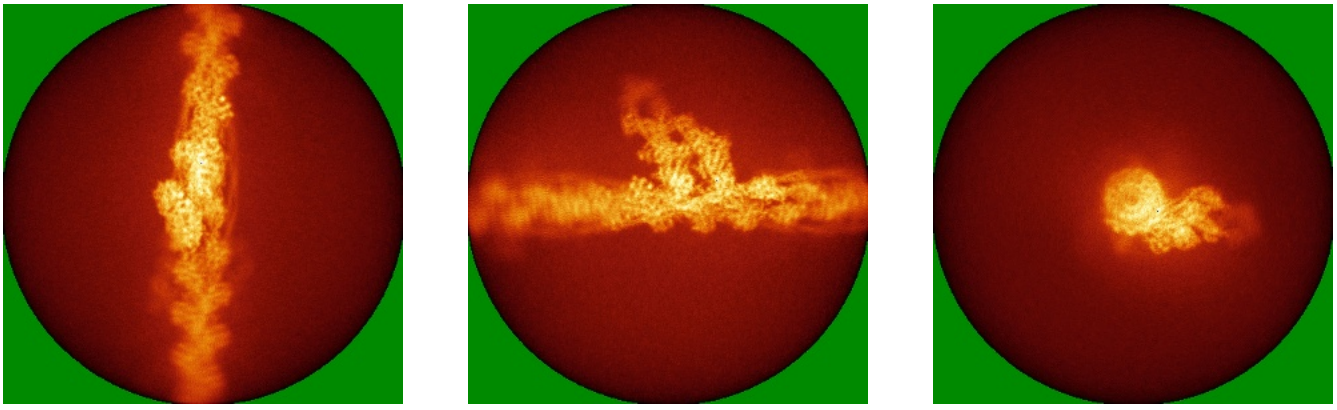
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



X Y Z

6.4.2 Raw map

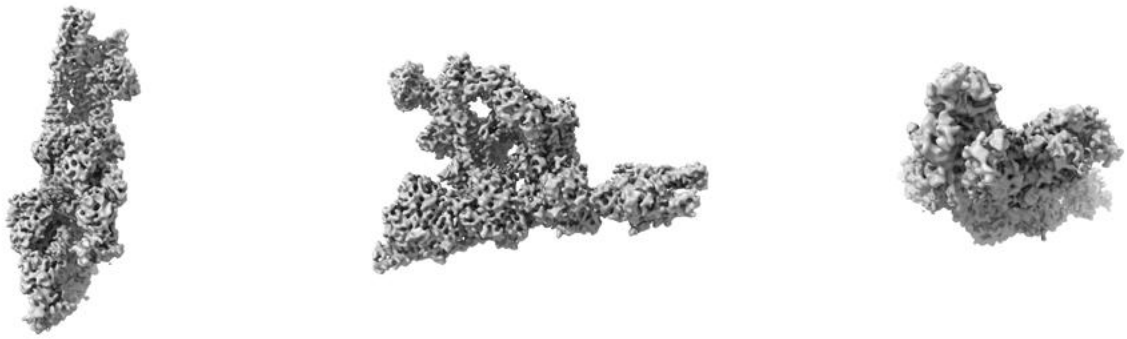


X Y Z

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 1.05. 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.

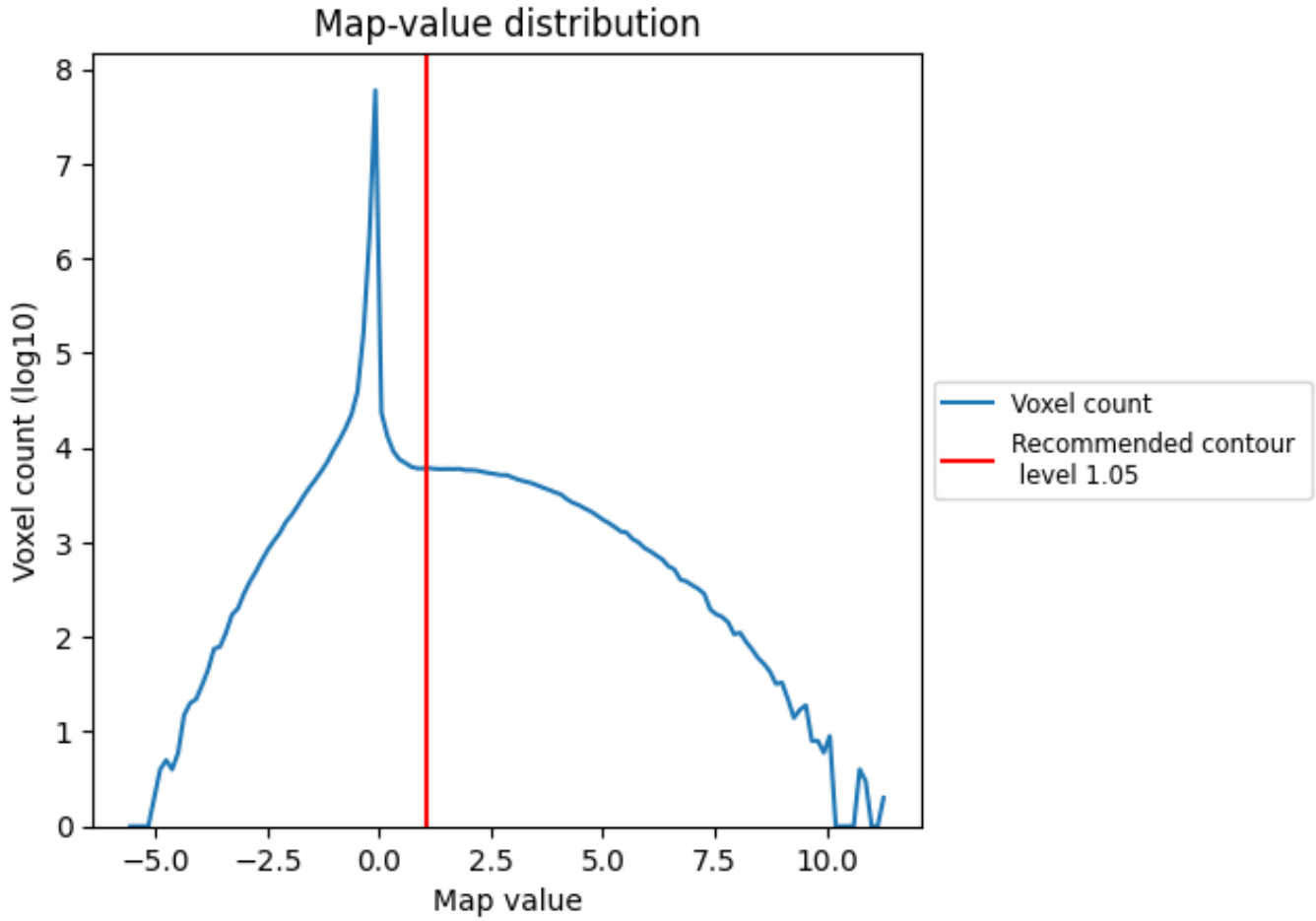
6.6 Mask visualisation (i)

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

7 Map analysis

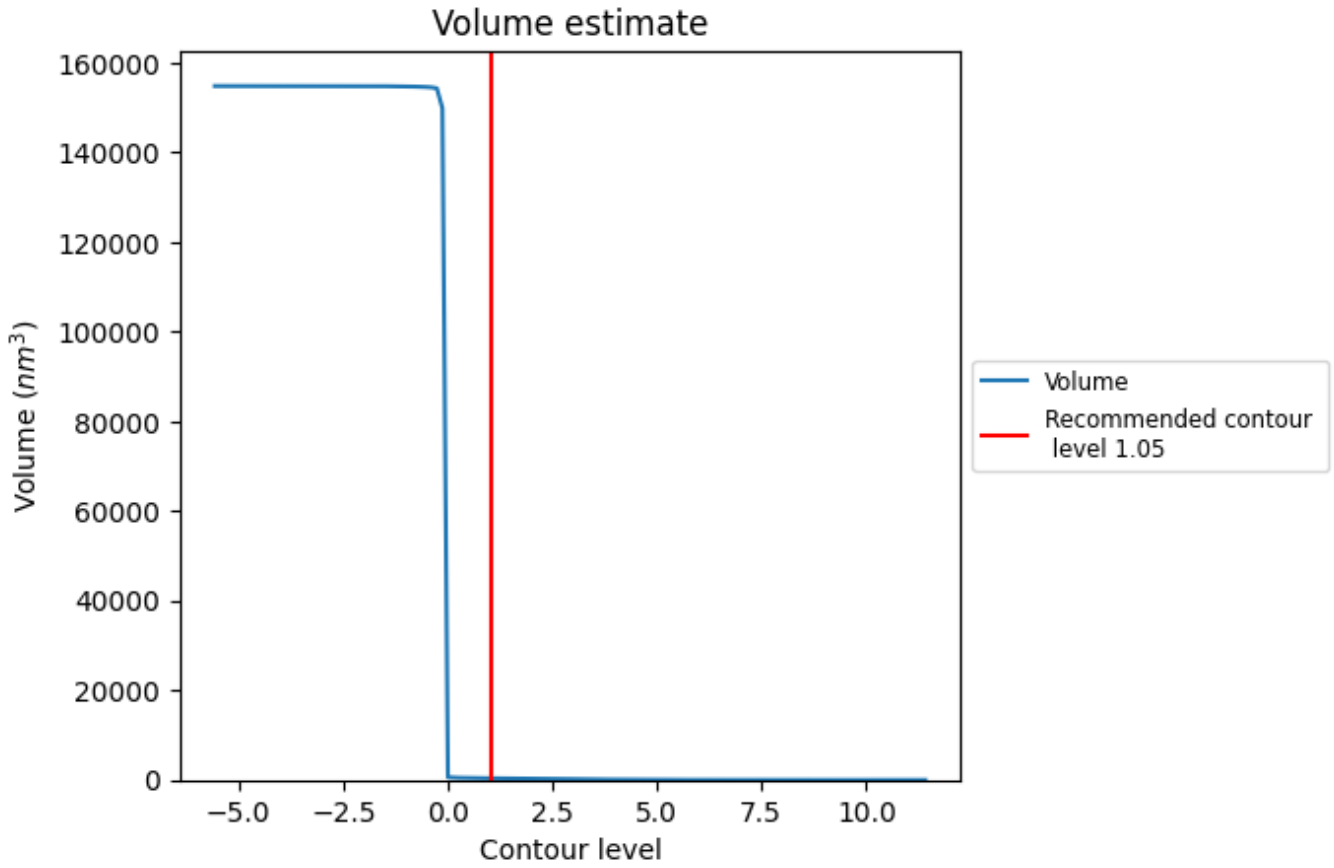
This section contains the results of statistical analysis of the map.

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.

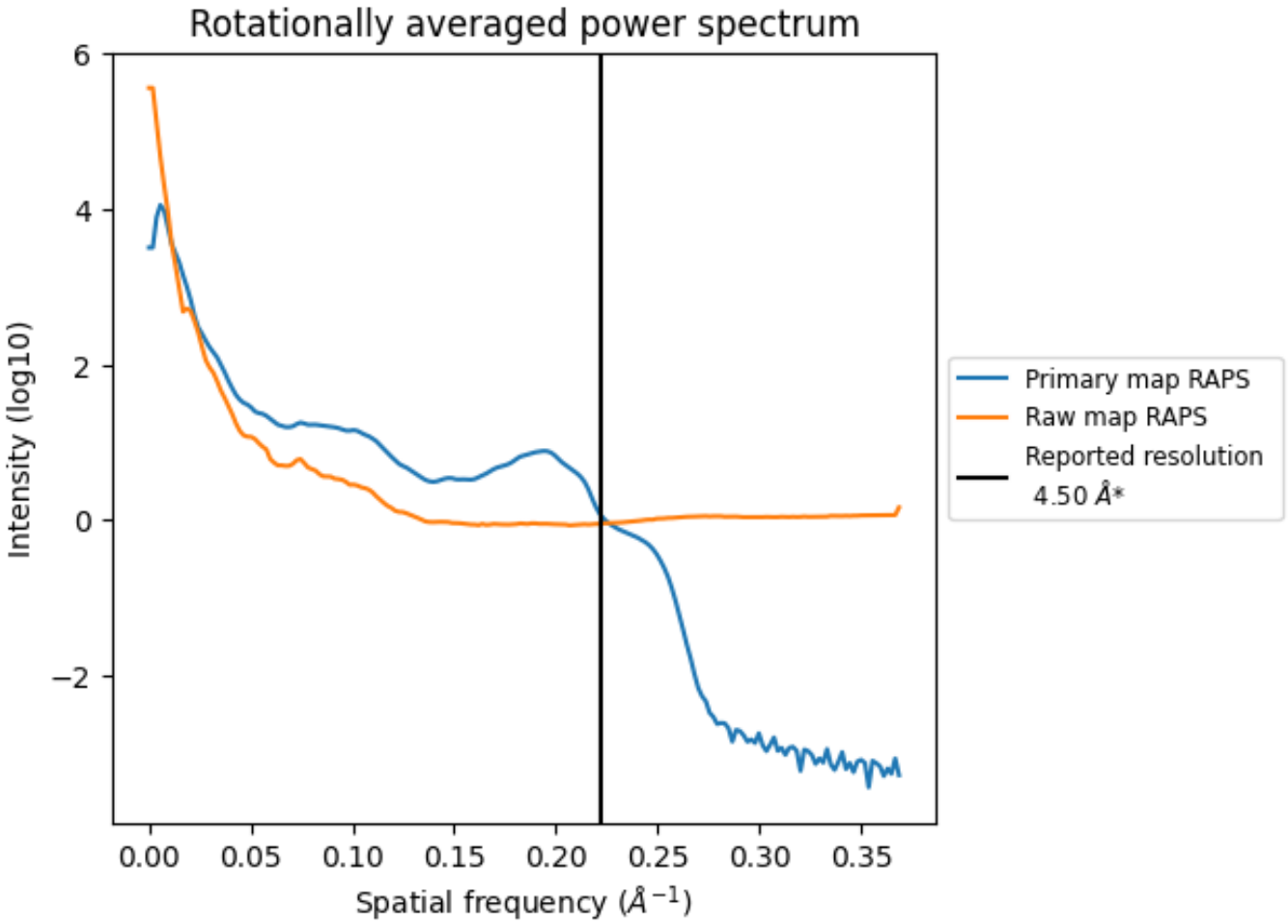
7.2 Volume estimate (i)



The volume at the recommended contour level is 374 nm^3; this corresponds to an approximate mass of 337 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)

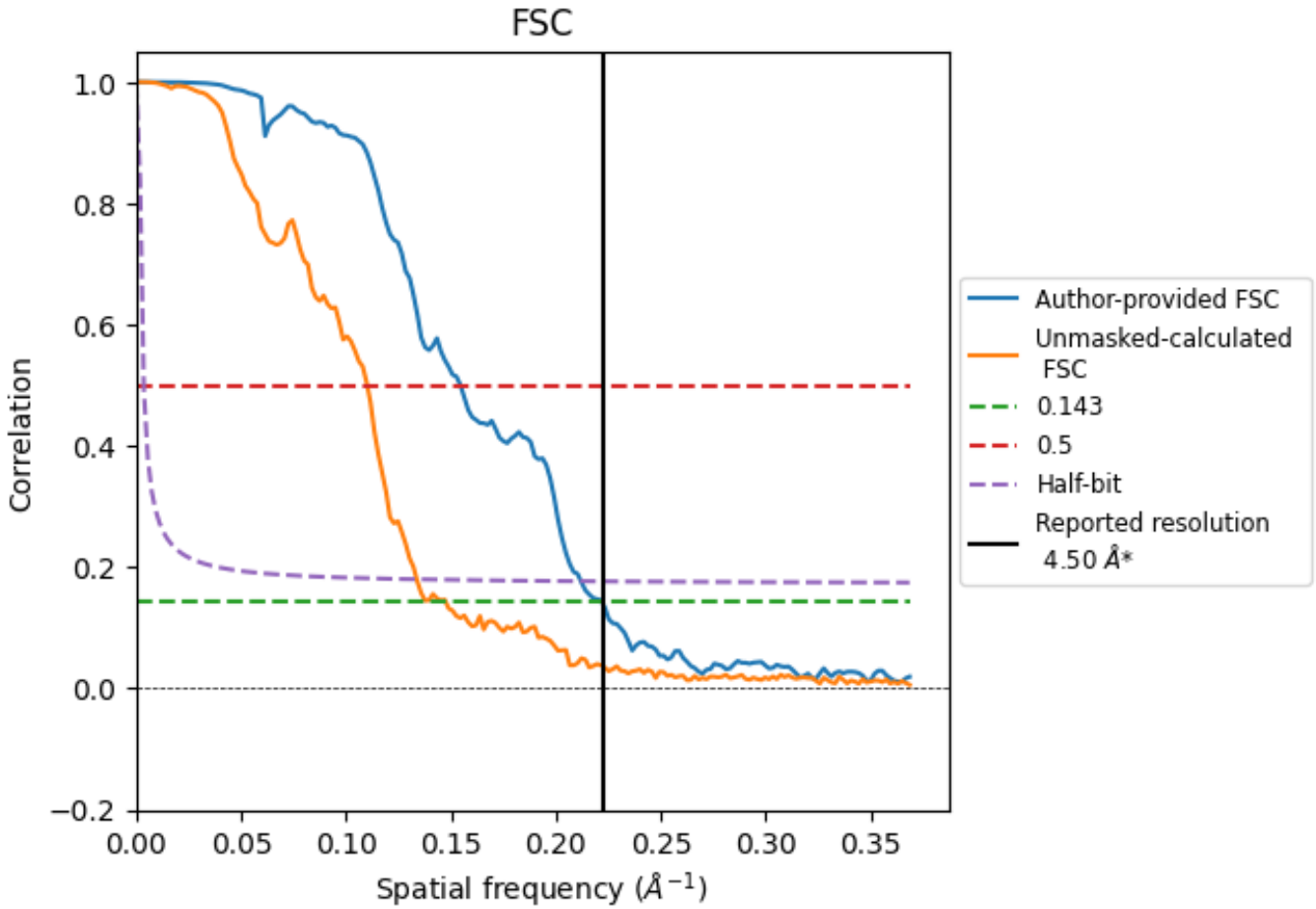


*Reported resolution corresponds to spatial frequency of 0.222 Å^{-1}

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 0.222 Å^{-1}

8.2 Resolution estimates (i)

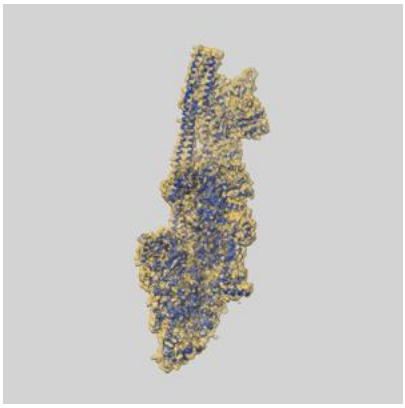
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	4.50	6.47	4.71
Unmasked-calculated*	6.78	9.08	7.47

*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 6.78 differs from the reported value 4.5 by more than 10 %

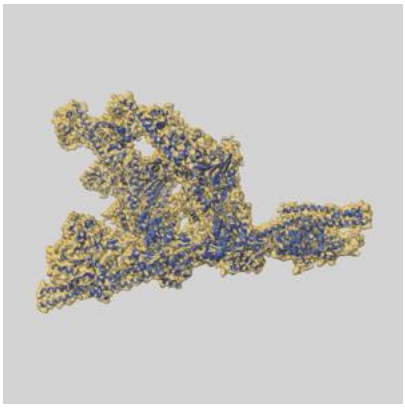
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-73042 and PDB model 9YK9. Per-residue inclusion information can be found in section 3 on page 7.

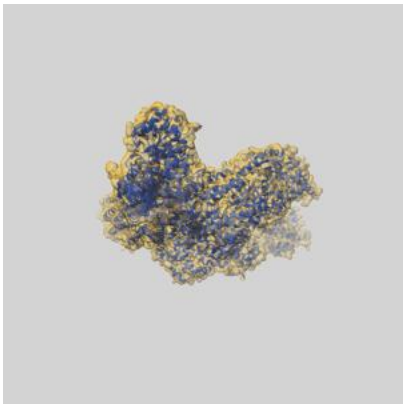
9.1 Map-model overlay



X



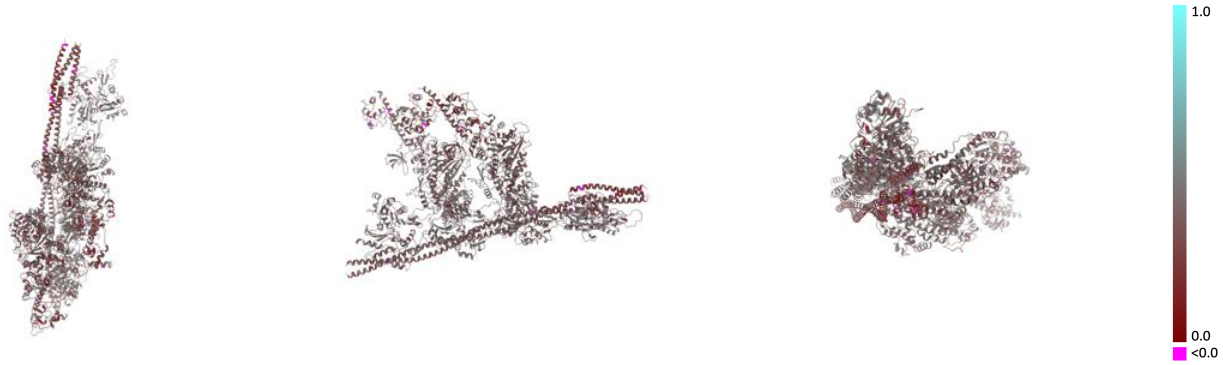
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.05 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.

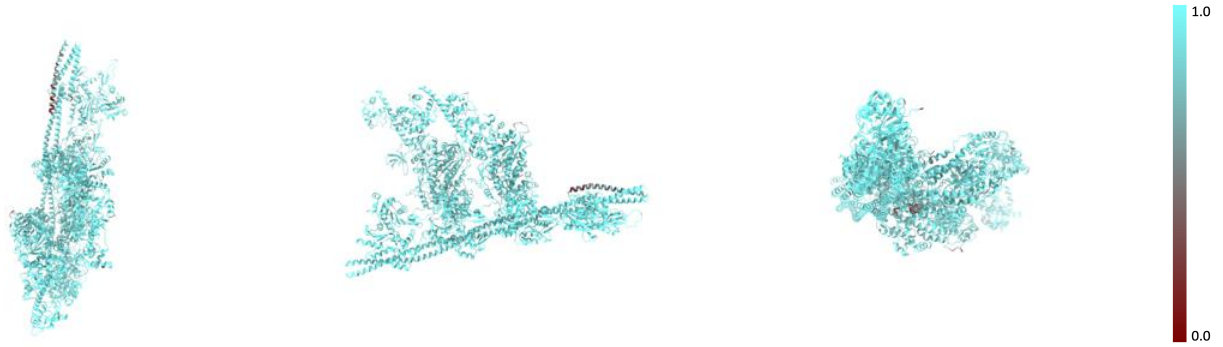
9.2 Q-score mapped to coordinate model



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.

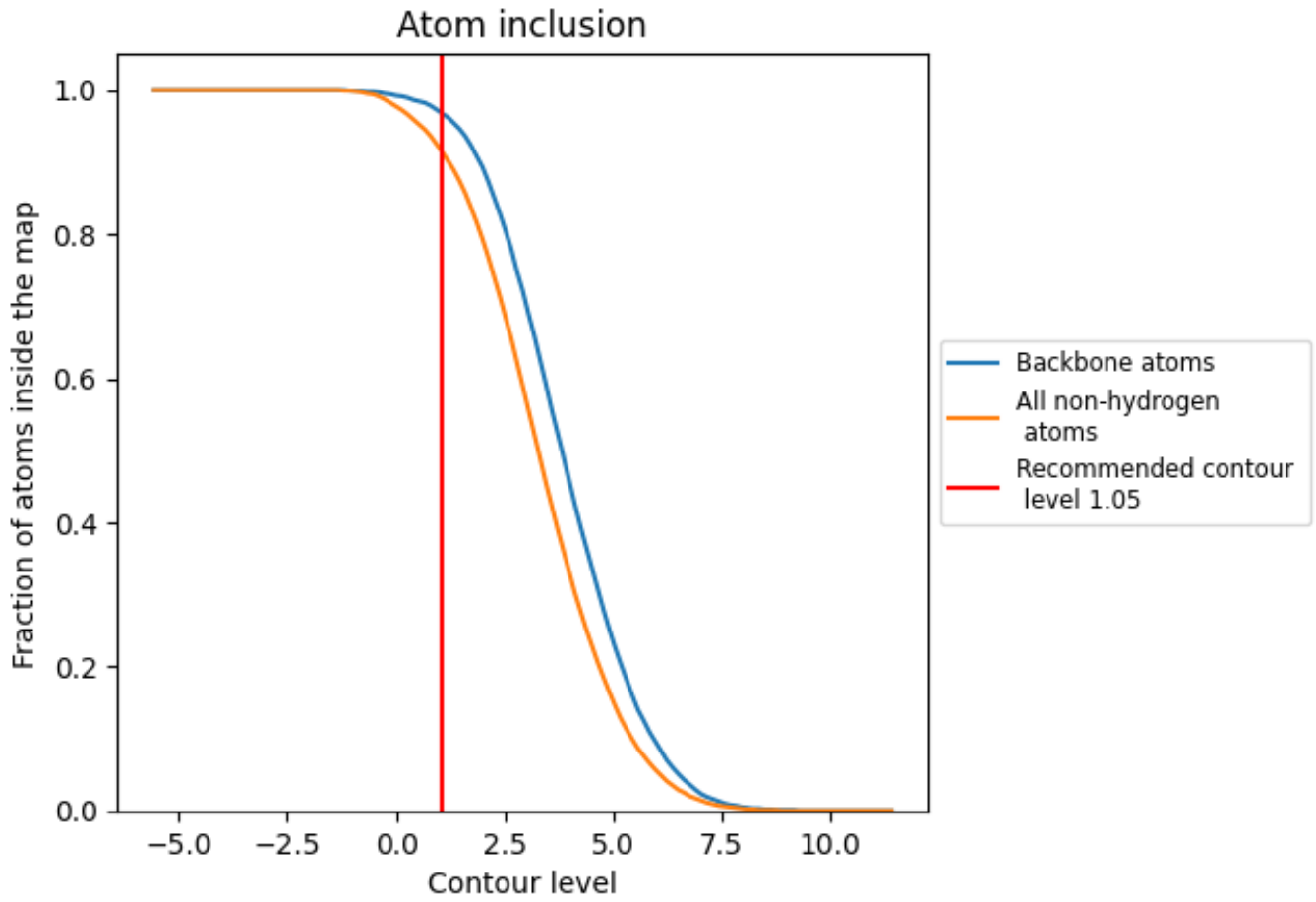
9.3 Atom inclusion mapped to coordinate model



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 (1.05).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 92% 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 (1.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9150	0.3700
A	0.9460	0.4050
B	0.9240	0.3970
C	0.9270	0.4130
D	0.9390	0.4020
E	0.9120	0.2370
F	0.8300	0.2590
G	0.9230	0.3120
H	0.8880	0.2720
I	0.5580	0.1870
J	0.9090	0.3680
K	0.9190	0.3730
L	0.8990	0.3290
M	0.9220	0.3440

