



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 08:35 AM UTC

PDB ID : 7QIN / pdb_00007qin
EMDB ID : EMD-13991
Title : In situ structure of actomyosin complex in skeletal sarcomere
Authors : Wang, Z.; Grange, M.; Pospich, S.; Wagner, T.; Kho, A.L.; Gautel, M.;
Raunser, S.
Deposited on : 2021-12-15
Resolution : 6.60 Å(reported)
Based on initial models : 3I5G, 5JLH

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
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) : 2.49

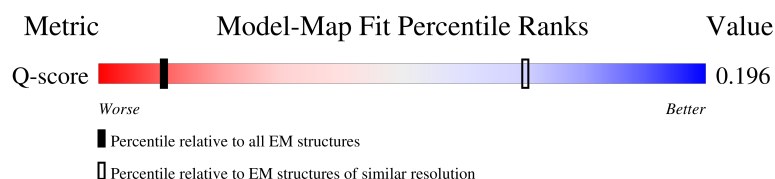
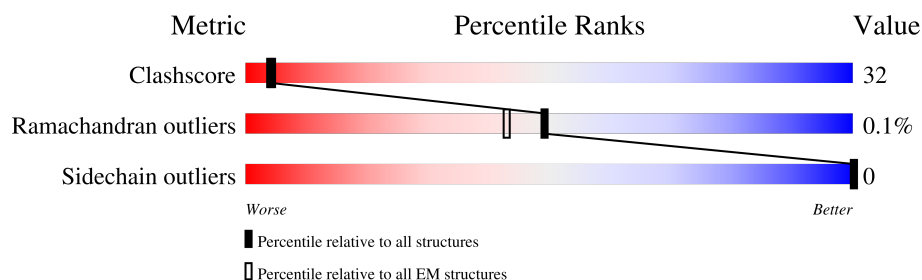
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.60 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.



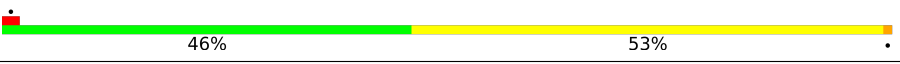
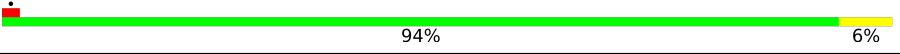
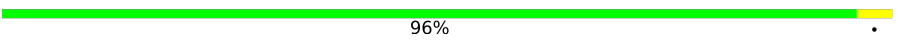
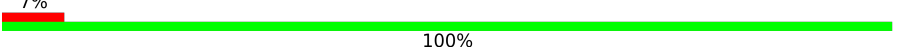
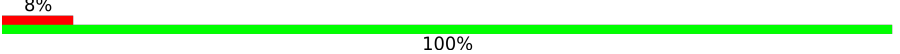
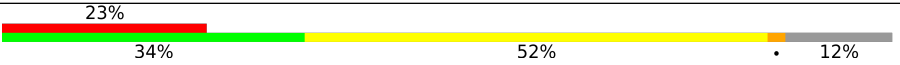
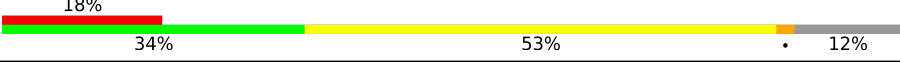
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	531 (6.10 - 7.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	371	
1	B	371	
1	C	371	
1	D	371	

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Mol	Chain	Length	Quality of chain
1	E	371	
2	F	105	
3	G	70	
4	H	117	
5	I	118	
6	J	88	
6	K	88	
7	L	848	
7	M	848	

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 29589 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 skeletal muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	371	Total	C	N	O	S	0	0
			2900	1837	489	553	21		
1	B	371	Total	C	N	O	S	0	0
			2900	1837	489	553	21		
1	C	371	Total	C	N	O	S	0	0
			2900	1837	489	553	21		
1	D	371	Total	C	N	O	S	0	0
			2900	1837	489	553	21		
1	E	371	Total	C	N	O	S	0	0
			2900	1837	489	553	21		

- Molecule 2 is a protein called nebulin (mouse).

Mol	Chain	Residues	Atoms				AltConf	Trace
2	F	105	Total	C	N	O	0	0
			546	333	105	108		

- Molecule 3 is a protein called nebulin (mouse).

Mol	Chain	Residues	Atoms				AltConf	Trace
3	G	70	Total	C	N	O	0	0
			364	222	70	72		

- Molecule 4 is a protein called tropomyosin, alpha-1 (mouse).

Mol	Chain	Residues	Atoms				AltConf	Trace
4	H	117	Total	C	N	O	0	0
			585	351	117	117		

- Molecule 5 is a protein called tropomyosin, alpha-1 (mouse).

Mol	Chain	Residues	Atoms				AltConf	Trace
5	I	118	Total	C	N	O	0	0
			590	354	118	118		

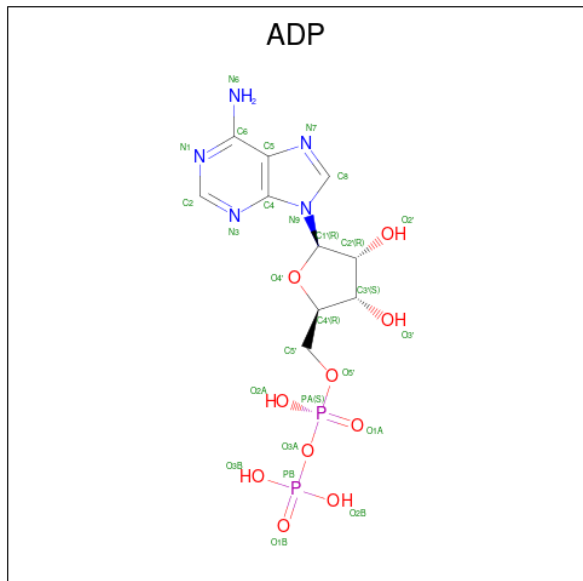
- Molecule 6 is a protein called tropomyosin, alpha-1 (mouse).

Mol	Chain	Residues	Atoms				AltConf	Trace
6	J	88	Total	C	N	O	0	0
			440	264	88	88		
6	K	88	Total	C	N	O	0	0
			440	264	88	88		

- Molecule 7 is a protein called Myosin-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L	749	Total	C	N	O	S	0	0
			5992	3836	1002	1125	29		
7	M	749	Total	C	N	O	S	0	0
			5992	3836	1002	1125	29		

- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

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Mol	Chain	Residues	Atoms					AltConf
8	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
8	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
8	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

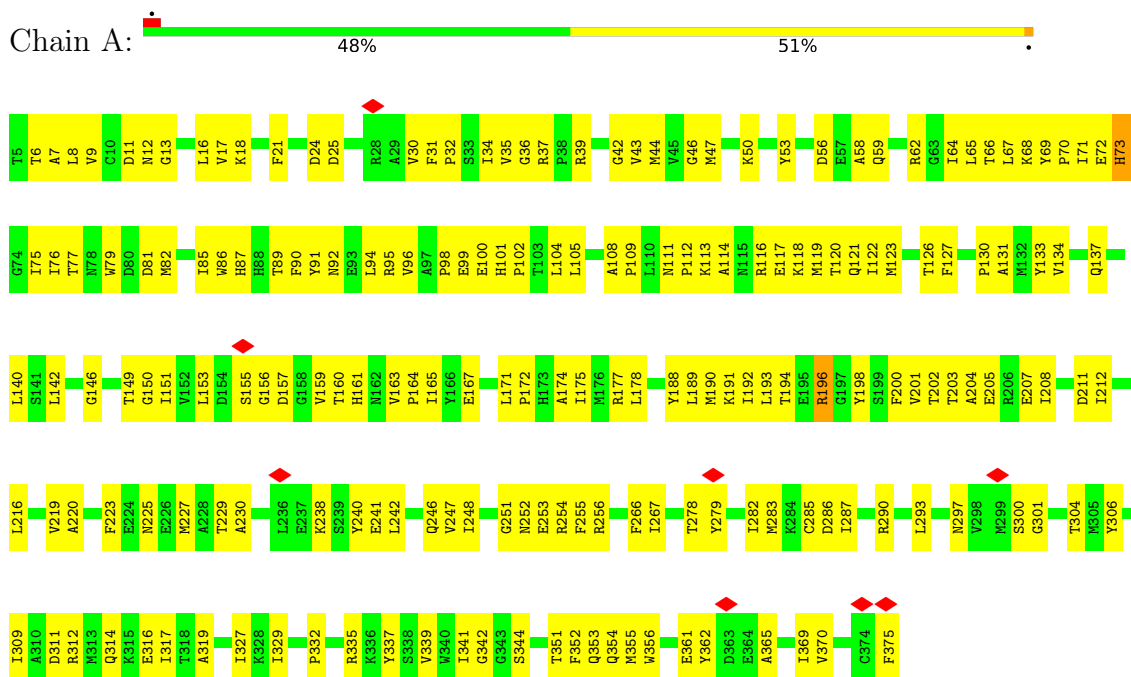
- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

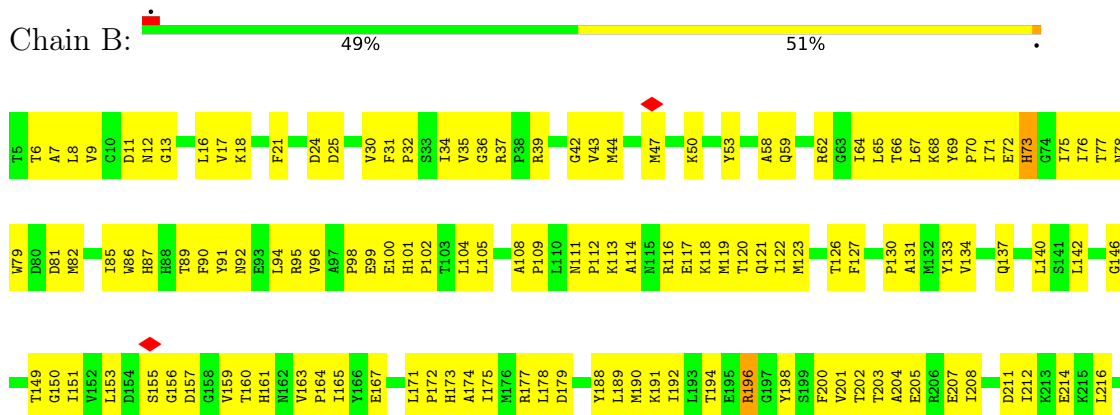
3 Residue-property plots

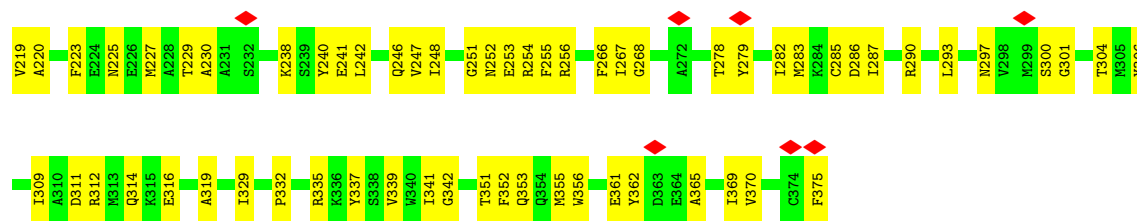
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

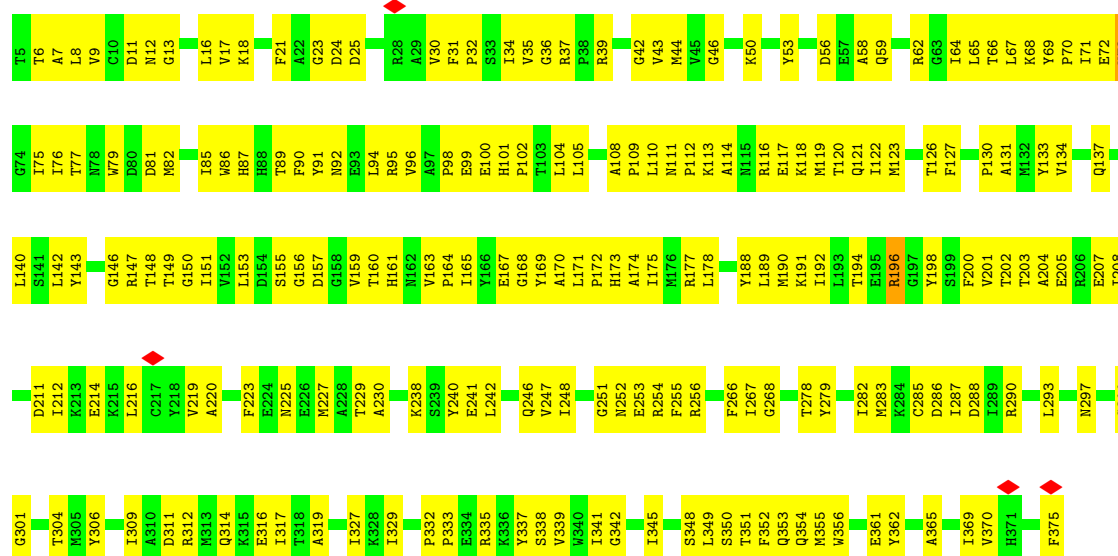


- Molecule 1: Actin, alpha skeletal muscle

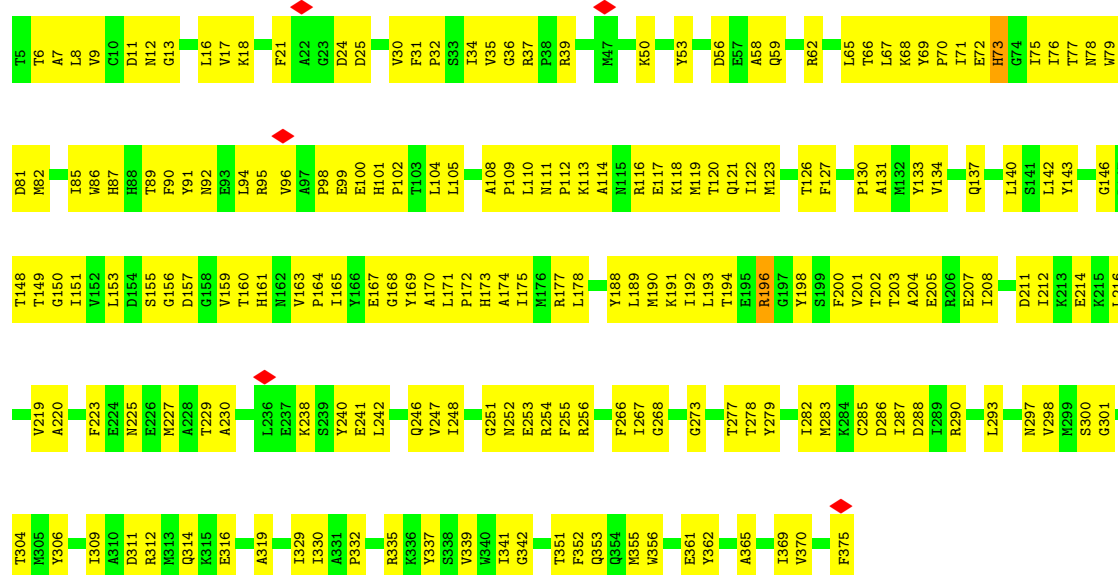




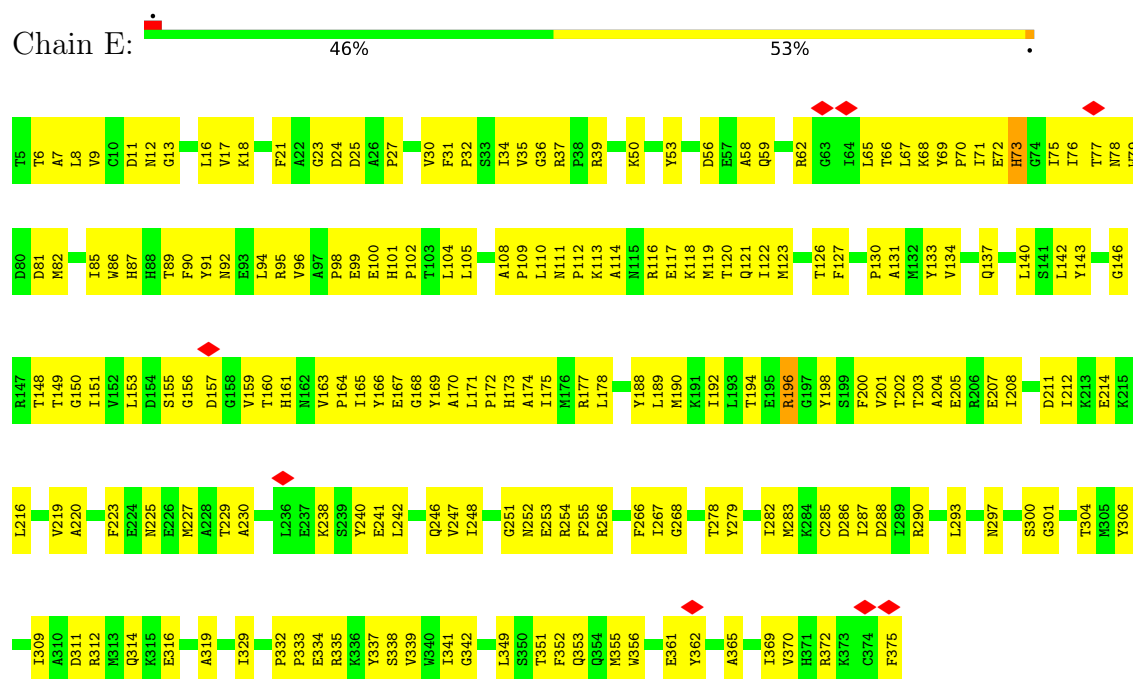
• Molecule 1: Actin, alpha skeletal muscle



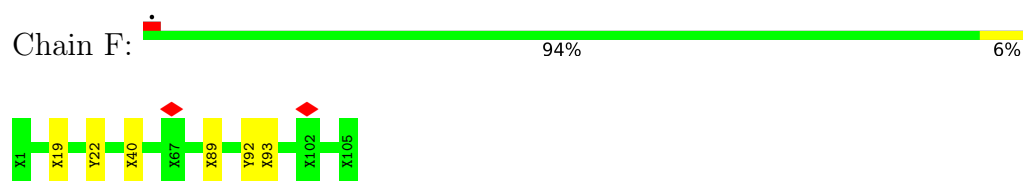
• Molecule 1: Actin, alpha skeletal muscle



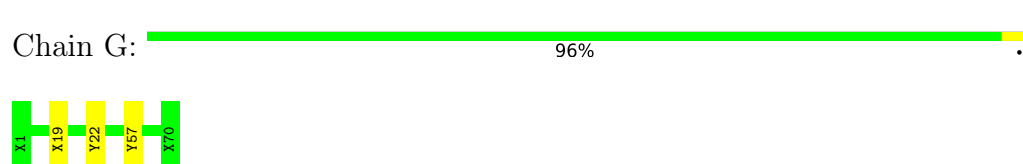
- Molecule 1: Actin, alpha skeletal muscle



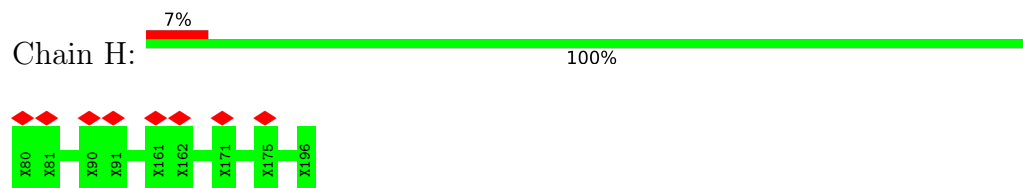
- Molecule 2: nebulin (mouse)



- Molecule 3: nebulin (mouse)

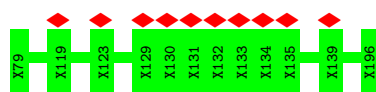


- Molecule 4: tropomyosin, alpha-1 (mouse)

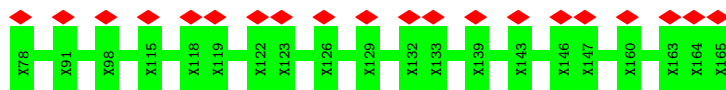


- Molecule 5: tropomyosin, alpha-1 (mouse)

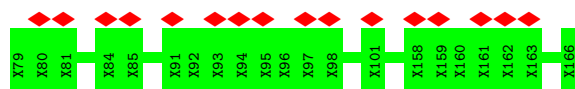




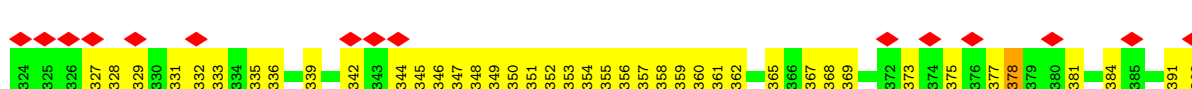
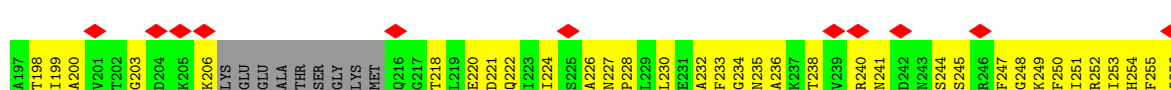
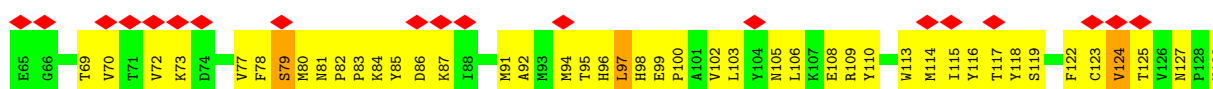
- Molecule 6: tropomyosin, alpha-1 (mouse)

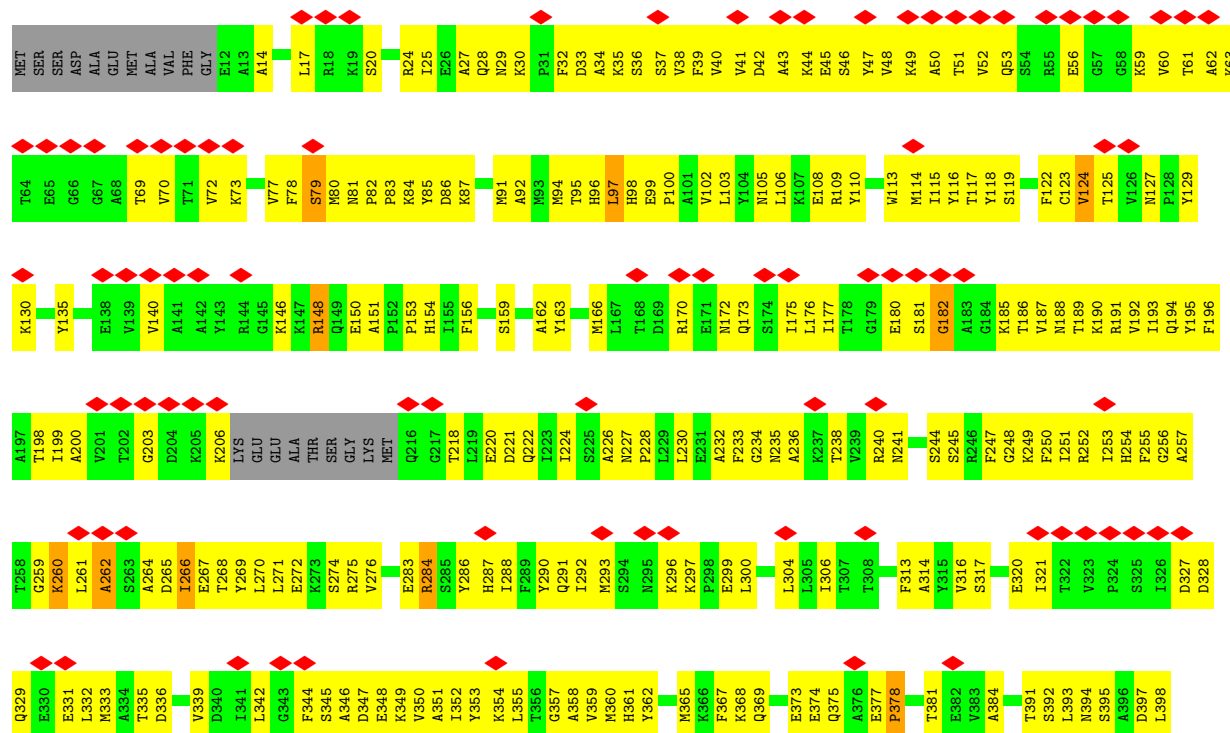


- Molecule 6: tropomyosin, alpha-1 (mouse)



- Molecule 7: Myosin-4





MET	L399	E469	FS34	P603	R675	G737
ARG	K400	I470	SS35	V608	C676	Q738
VAL	A401	F471	I536	V609	L677	F739
GLU	L402	D472	L537	Y612	I678	I740
PHE	C403	F473	E538	Q613	P679	D741
LYS	Y404	M474	E539	K614	M680	L744
LYS	P405	E477	E540	S615	E681	A745
MET	R406	Q478	C541	T619	T684	L749
MET	V407	L479	M542	L620	P685	L750
GLU	K408	C480	FS43	A621	G686	G751
ARG	G410	I481	T547	F622	T684	L750
ARG	M411	M482	D548	L623	P685	L750
ARG	E412	F483	T549	F624	G686	L750
GLU	Y413	T484	K552	S625	A687	L750
SER	V414	M485	K553	GLY	M688	L750
ILE	T415	E486	K554	GLY	E689	L750
LYS	K416	K487	L555	GLN	H690	L750
LYS	G417	Q490	Y556	ALA	E691	L750
LYS	M425	F491	E557	ALA	L692	L750
LYS	S426	F492	Q558	ALA	V693	L750
LYS	A429	M493	H559	ALA	L694	L750
LYS	L430	H494	L560	GLU	H695	L750
LYS	A431	H495	G561	GLU	Q696	L750
LYS	E436	M496	K562	GLY	L697	L750
LYS	K437	F497	SS63	GLY	R698	L750
LYS	M438	V498	N564	GLY	C699	L750
LYS	F439	L499	GLY	GLY	G701	L750
LYS	L440	E502	K570	GLY	V702	L750
LYS	M441	E503	K573	LYS	L703	L750
LYS	M442	Y504	G574	K644	E704	L750
LYS	V443	K505	G575	S647	G705	L750
LYS	T444	E507	A576	F648	I706	L750
LYS	R445	I509	E577	Q649	R707	L750
LYS	I446	D510	A578	T650	I708	L750
LYS	M447	M511	H579	V651	C709	L750
LYS	Q448	E512	FS80	S652	R710	L750
LYS	L450	F513	S881	A653	K711	L750
LYS	D451	I514	L582	L654	G712	L750
LYS	T452	D515	V583	F655	F713	L750
LYS	K453	F516	T588	L659	R716	L750
LYS	Q454	G517	V589	L662	I717	L750
LYS	P455	M518	D590	M663	L718	L750
LYS	R456	A521	N592	K667	Y719	L750
LYS	Q457	I524	Y593	S668	A720	L750
LYS	Y458	E525	I594	T669	K723	L750
LYS	I460	L526	G595	H670	Q724	L750
LYS	V462	I527	M596	P671	Y726	L750
LYS	L463	E528	L597	H672	K727	L750
LYS	D464	K529	D598	F673	V728	L750
LYS	I465	P530	K601	V674	L729	L750
LYS	A466	M531	D602		N730	L750
LYS	G467	G532			A731	L750
LYS	F468	I533			S732	L750
					A733	L750
					I734	L750
					P735	L750
					E736	L750
						L777
						E778
						E779
						M780
						R781
						D782
						E783
						K784
						L785
						A786
						Q787
						LEU
						ILE
						THR
						ARG
						THR
						GLN
						ALA
						VAL
						CYS
						I734
						ARG
						GLY
						TYR
						LEU

4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	104302	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	3.4	Depositor
Minimum defocus (nm)	2400	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.033	Depositor
Minimum map value	-0.012	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	346.0, 346.0, 346.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.73, 1.73, 1.73	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, HIC

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	0.39	0/2950	0.77	0/3994
1	B	0.39	0/2950	0.77	0/3994
1	C	0.39	0/2950	0.77	0/3994
1	D	0.39	0/2950	0.77	0/3994
1	E	0.39	0/2950	0.77	0/3994
2	F	0.24	0/36	0.39	0/45
3	G	0.22	0/24	0.41	0/30
7	L	0.37	0/6119	0.86	7/8251 (0.1%)
7	M	0.37	0/6119	0.86	7/8251 (0.1%)
All	All	0.38	0/27048	0.81	14/36547 (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	A	0	3
1	B	0	3
1	C	0	3
1	D	0	3
1	E	0	3
7	L	0	11
7	M	0	11
All	All	0	37

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	182	GLY	N-CA-C	6.93	129.61	113.18
7	L	182	GLY	N-CA-C	6.92	129.57	113.18
7	L	529	LYS	N-CA-C	-6.06	98.28	109.06
7	M	529	LYS	N-CA-C	-6.06	98.28	109.06
7	M	284	ARG	CA-C-N	6.03	134.15	122.03

There are no chirality outliers.

5 of 37 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	196	ARG	Sidechain
1	A	267	ILE	Peptide
1	A	301	GLY	Peptide
1	B	196	ARG	Sidechain
1	B	267	ILE	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2900	0	2873	180	0
1	B	2900	0	2873	181	0
1	C	2900	0	2873	211	0
1	D	2900	0	2873	186	0
1	E	2900	0	2873	200	0
2	F	546	0	139	6	0
3	G	364	0	93	2	0
4	H	585	0	119	0	0
5	I	590	0	120	0	0
6	J	440	0	90	0	0
6	K	440	0	90	0	0
7	L	5992	0	5971	457	0
7	M	5992	0	5971	448	0
8	A	27	0	12	5	0
8	B	27	0	12	6	0
8	C	27	0	12	6	0
8	D	27	0	12	6	0
8	E	27	0	12	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	1	0	0	0	0
9	B	1	0	0	0	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0
9	E	1	0	0	0	0
All	All	29589	0	27018	1792	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 32.

The worst 5 of 1792 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)
7:M:235:ASN:HD22	7:M:245:SER:HB3	1.29	0.96
1:E:333:PRO:HG3	7:L:416:LYS:H	1.28	0.96
7:M:196:PHE:HA	7:M:199:ILE:HD12	1.49	0.94
7:L:196:PHE:HA	7:L:199:ILE:HD12	1.50	0.94
7:M:359:VAL:HG13	7:M:431:ALA:HB1	1.50	0.94

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	368/371 (99%)	367 (100%)	1 (0%)	0	100	100
1	B	368/371 (99%)	367 (100%)	1 (0%)	0	100	100
1	C	368/371 (99%)	367 (100%)	1 (0%)	0	100	100
1	D	368/371 (99%)	367 (100%)	1 (0%)	0	100	100
1	E	368/371 (99%)	367 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	3/105 (3%)	3 (100%)	0	0	100	100
3	G	2/70 (3%)	2 (100%)	0	0	100	100
7	L	743/848 (88%)	740 (100%)	2 (0%)	1 (0%)	48	83
7	M	743/848 (88%)	740 (100%)	2 (0%)	1 (0%)	48	83
All	All	3331/3726 (89%)	3320 (100%)	9 (0%)	2 (0%)	49	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	L	181	SER
7	M	181	SER

5.3.2 Protein sidechains ⓘ

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	313/313 (100%)	313 (100%)	0	100	100
1	B	313/313 (100%)	313 (100%)	0	100	100
1	C	313/313 (100%)	313 (100%)	0	100	100
1	D	313/313 (100%)	313 (100%)	0	100	100
1	E	313/313 (100%)	313 (100%)	0	100	100
2	F	3/3 (100%)	3 (100%)	0	100	100
3	G	2/2 (100%)	2 (100%)	0	100	100
7	L	648/727 (89%)	648 (100%)	0	100	100
7	M	648/727 (89%)	648 (100%)	0	100	100
All	All	2866/3024 (95%)	2866 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

Mol	Chain	Res	Type
7	L	696	GLN
7	M	243	ASN
7	M	482	ASN
1	C	162	ASN
1	C	161	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

5 non-standard protein/DNA/RNA residues are modelled in this entry.

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
1	HIC	B	73	1	10,11,12	1.45	1 (10%)	9,14,16	1.46	2 (22%)
1	HIC	D	73	1	10,11,12	1.44	1 (10%)	9,14,16	1.49	2 (22%)
1	HIC	E	73	1	10,11,12	1.45	1 (10%)	9,14,16	1.45	2 (22%)
1	HIC	C	73	1	10,11,12	1.46	1 (10%)	9,14,16	1.48	2 (22%)
1	HIC	A	73	1	10,11,12	1.46	1 (10%)	9,14,16	1.49	2 (22%)

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
1	HIC	B	73	1	-	3/5/6/8	0/1/1/1
1	HIC	D	73	1	-	3/5/6/8	0/1/1/1
1	HIC	E	73	1	-	3/5/6/8	0/1/1/1
1	HIC	C	73	1	-	3/5/6/8	0/1/1/1
1	HIC	A	73	1	-	3/5/6/8	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	73	HIC	CD2-CG	2.77	1.41	1.36
1	A	73	HIC	CD2-CG	2.75	1.41	1.36
1	E	73	HIC	CD2-CG	2.70	1.41	1.36
1	D	73	HIC	CD2-CG	2.69	1.41	1.36
1	B	73	HIC	CD2-CG	2.69	1.41	1.36

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	73	HIC	NE2-CE1-ND1	-3.58	111.29	112.66
1	A	73	HIC	NE2-CE1-ND1	-3.58	111.29	112.66
1	C	73	HIC	NE2-CE1-ND1	-3.55	111.31	112.66
1	B	73	HIC	NE2-CE1-ND1	-3.49	111.33	112.66
1	E	73	HIC	NE2-CE1-ND1	-3.46	111.34	112.66

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	73	HIC	N-CA-CB-CG
1	B	73	HIC	N-CA-CB-CG
1	C	73	HIC	N-CA-CB-CG
1	D	73	HIC	N-CA-CB-CG
1	E	73	HIC	N-CA-CB-CG

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	73	HIC	2	0
1	D	73	HIC	2	0
1	E	73	HIC	2	0
1	C	73	HIC	2	0
1	A	73	HIC	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 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
8	ADP	A	401	9	28,29,29	1.39	5 (17%)	43,45,45	1.69	8 (18%)
8	ADP	C	401	9	28,29,29	1.40	5 (17%)	43,45,45	1.70	8 (18%)
8	ADP	B	401	9	28,29,29	1.39	5 (17%)	43,45,45	1.69	8 (18%)
8	ADP	E	401	9	28,29,29	1.39	5 (17%)	43,45,45	1.70	8 (18%)
8	ADP	D	401	9	28,29,29	1.39	5 (17%)	43,45,45	1.70	8 (18%)

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
8	ADP	A	401	9	-	5/16/32/32	0/3/3/3
8	ADP	C	401	9	-	5/16/32/32	0/3/3/3
8	ADP	B	401	9	-	5/16/32/32	0/3/3/3
8	ADP	E	401	9	-	5/16/32/32	0/3/3/3
8	ADP	D	401	9	-	5/16/32/32	0/3/3/3

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	401	ADP	C5-C4	4.42	1.47	1.39
8	C	401	ADP	C5-C4	4.41	1.47	1.39
8	A	401	ADP	C5-C4	4.40	1.46	1.39
8	E	401	ADP	C5-C4	4.38	1.46	1.39
8	B	401	ADP	C5-C4	4.37	1.46	1.39

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	401	ADP	C5-C4-N3	-5.38	119.31	126.72
8	C	401	ADP	C5-C4-N3	-5.34	119.36	126.72
8	A	401	ADP	C5-C4-N3	-5.34	119.37	126.72
8	E	401	ADP	C5-C4-N3	-5.32	119.39	126.72
8	B	401	ADP	C5-C4-N3	-5.31	119.40	126.72

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

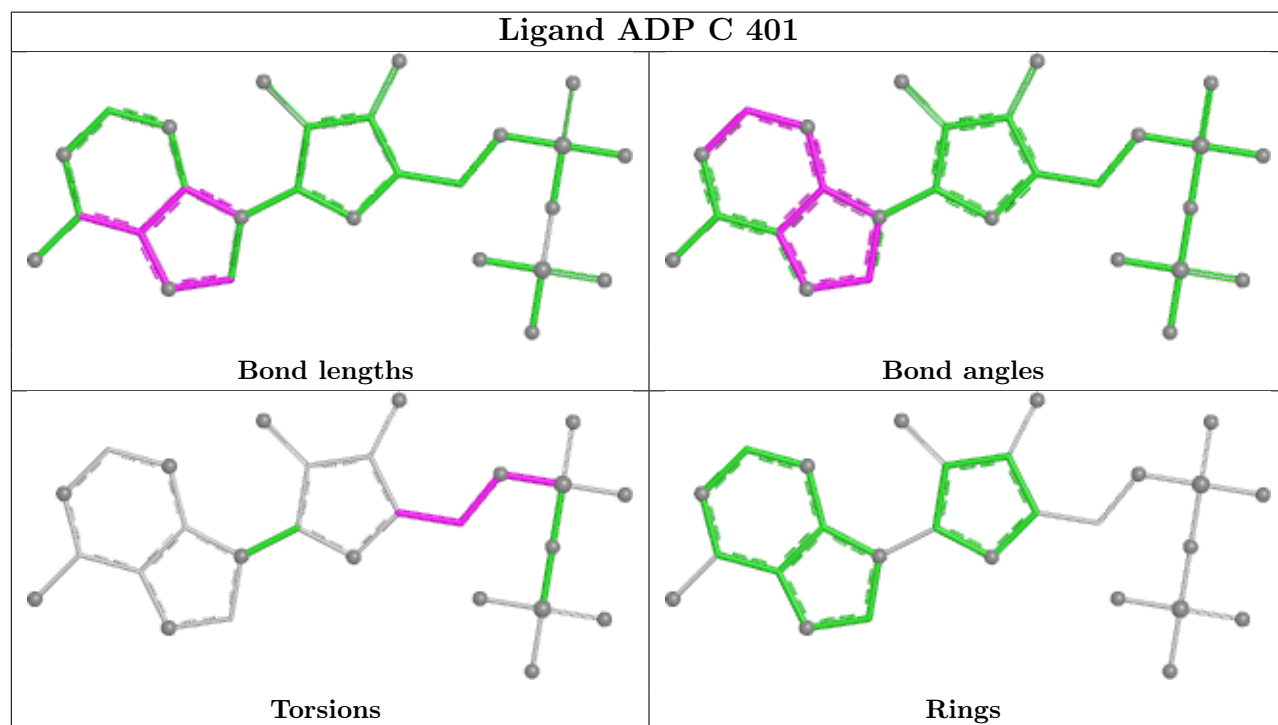
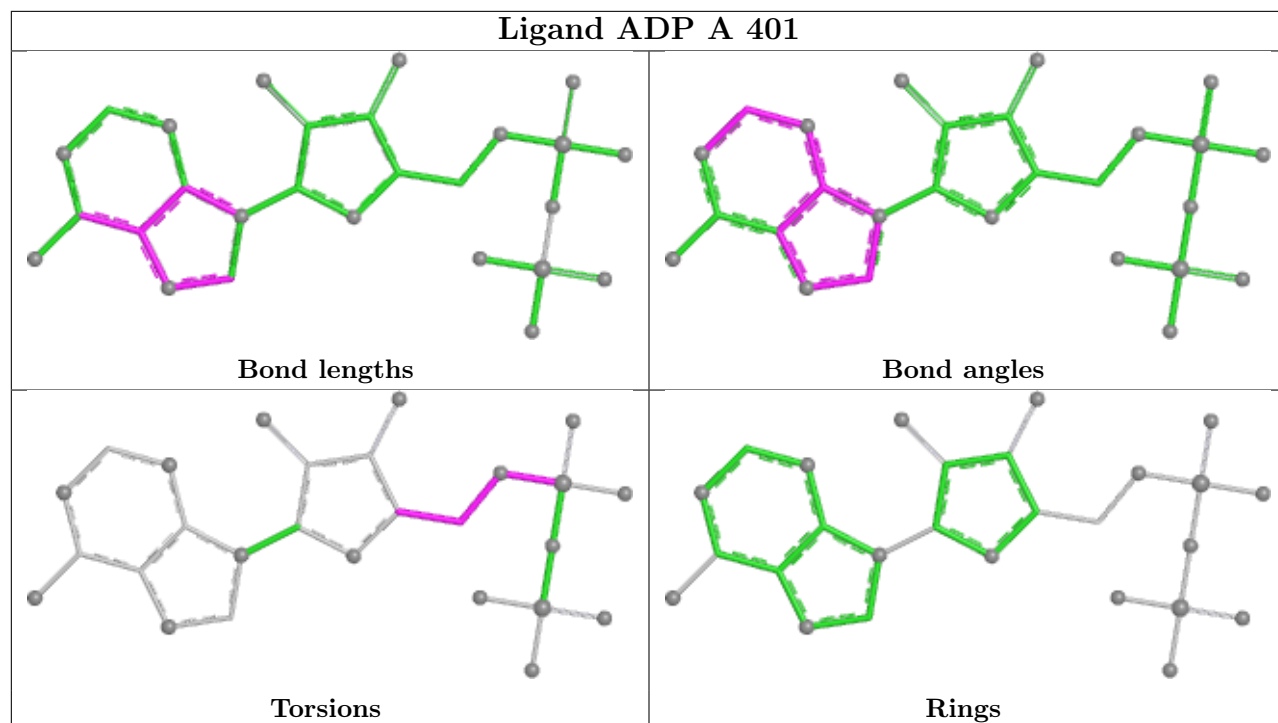
Mol	Chain	Res	Type	Atoms
8	A	401	ADP	C5'-O5'-PA-O2A
8	A	401	ADP	C5'-O5'-PA-O3A
8	B	401	ADP	C5'-O5'-PA-O2A
8	B	401	ADP	C5'-O5'-PA-O3A
8	C	401	ADP	C5'-O5'-PA-O2A

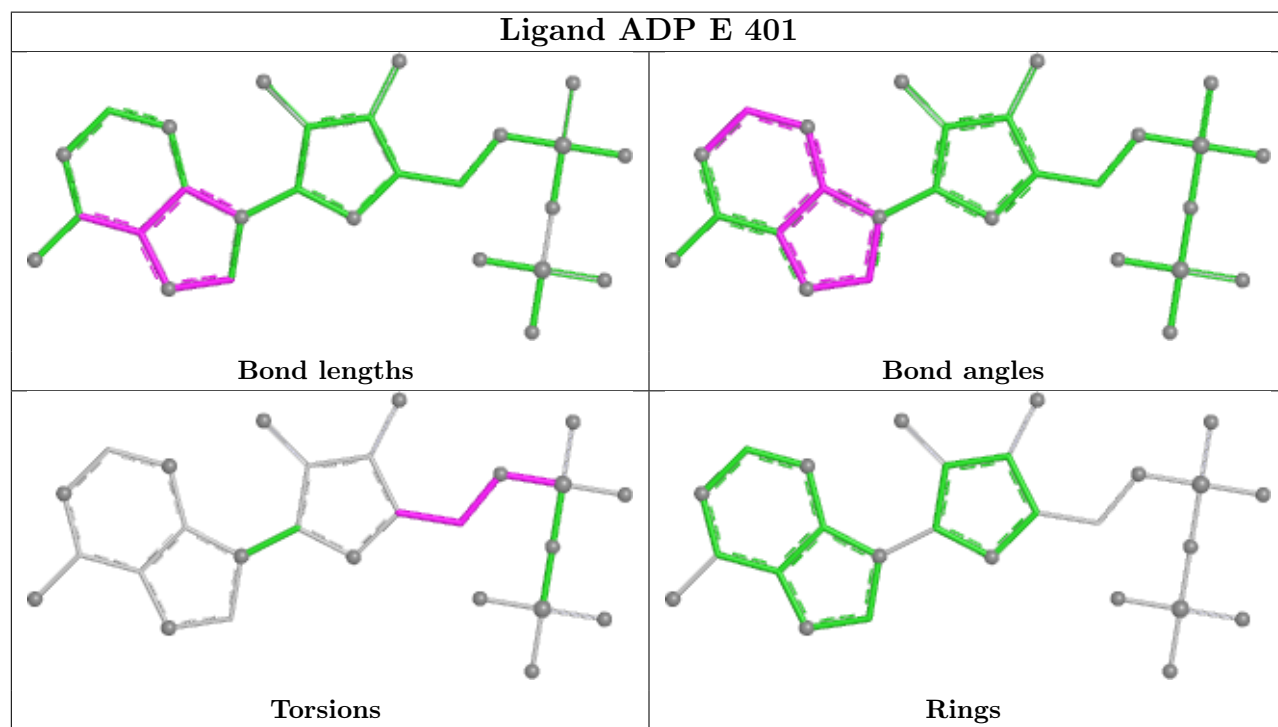
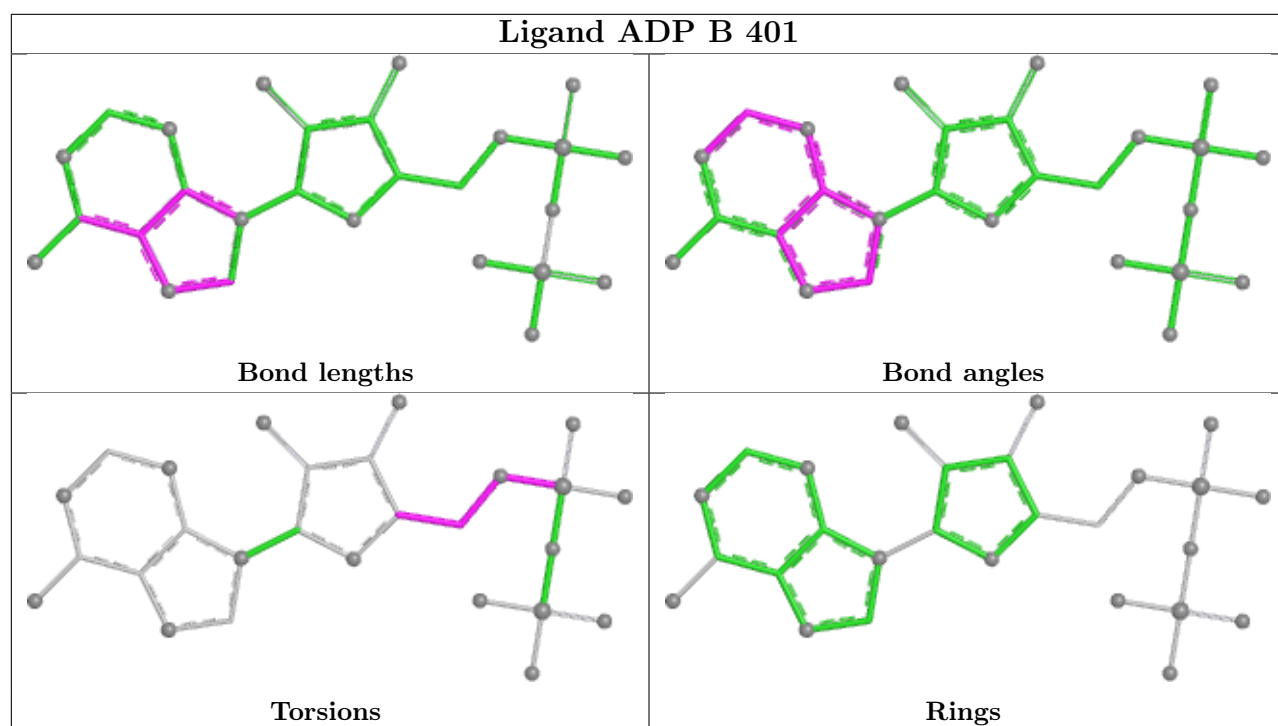
There are no ring outliers.

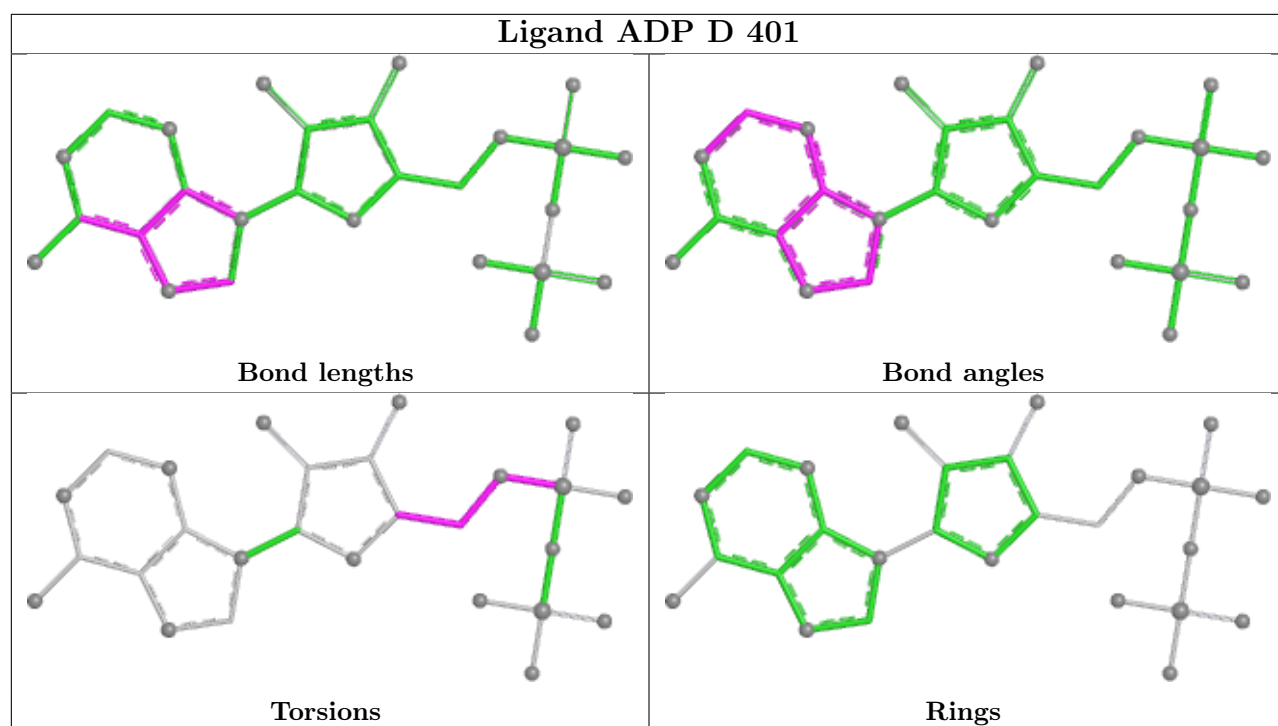
5 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	401	ADP	5	0
8	C	401	ADP	6	0
8	B	401	ADP	6	0
8	E	401	ADP	6	0
8	D	401	ADP	6	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 than 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.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

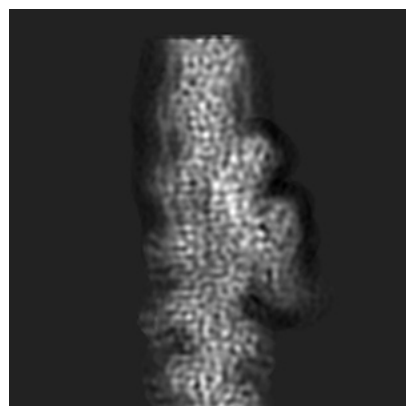
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13991. These allow visual inspection of the internal detail of the map and identification of artifacts.

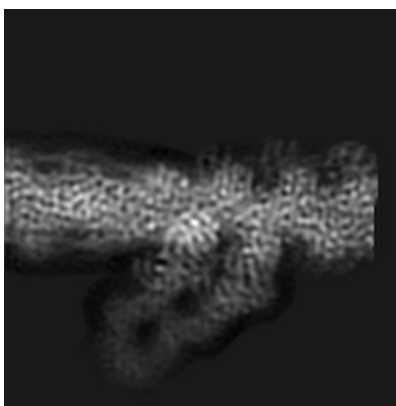
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

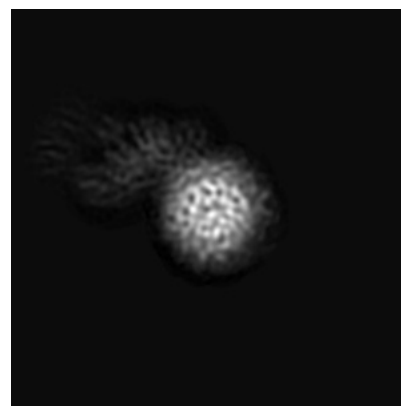
6.1.1 Primary map



X

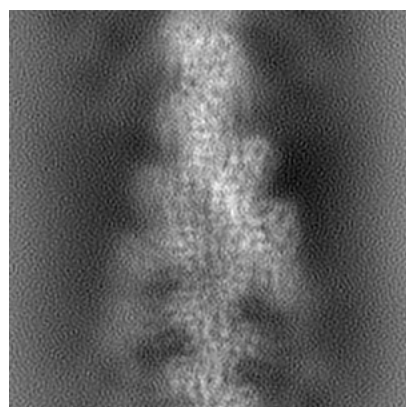


Y

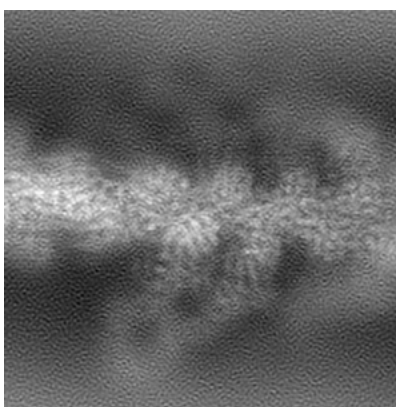


Z

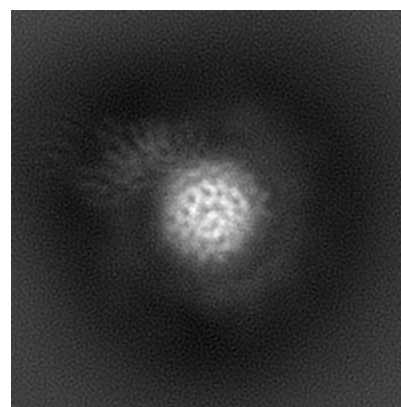
6.1.2 Raw map



X



Y

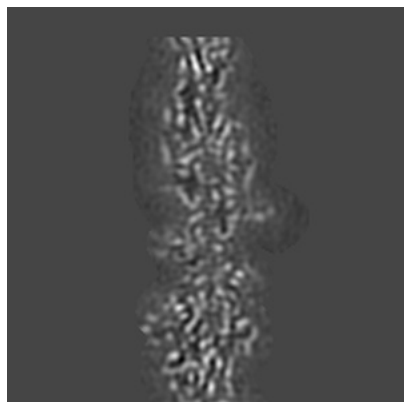


Z

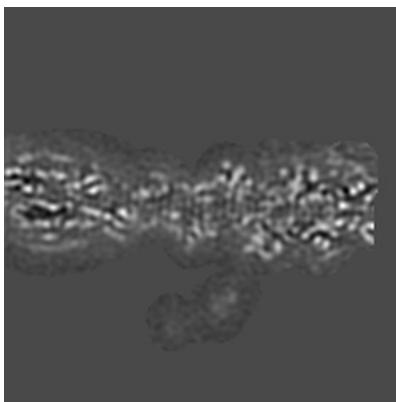
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

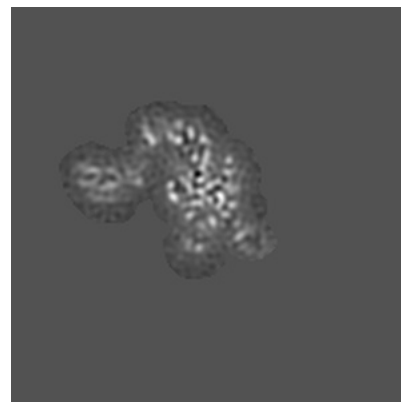
6.2.1 Primary map



X Index: 100

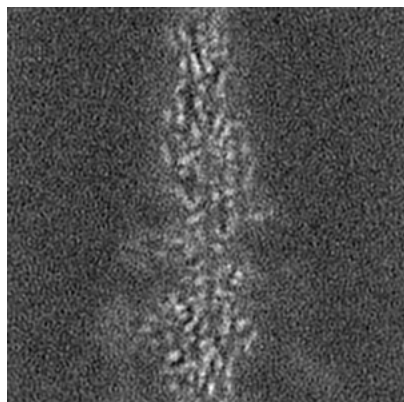


Y Index: 100

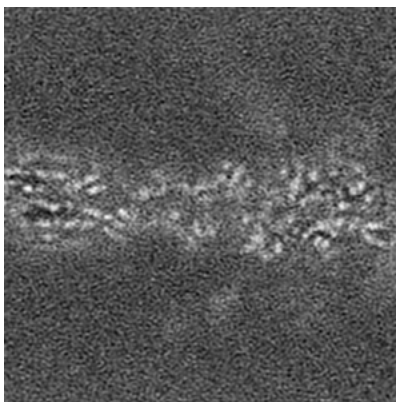


Z Index: 100

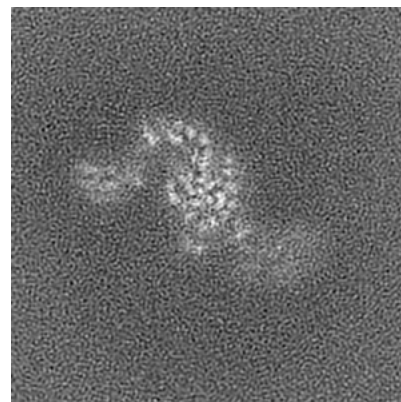
6.2.2 Raw map



X Index: 100



Y Index: 100

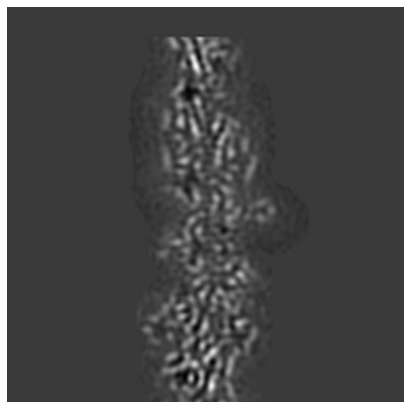


Z Index: 100

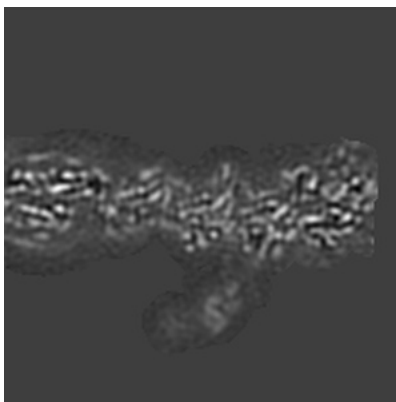
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

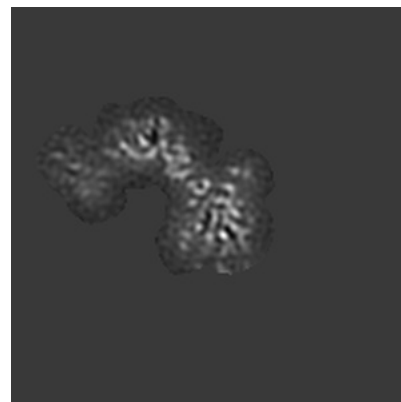
6.3.1 Primary map



X Index: 99

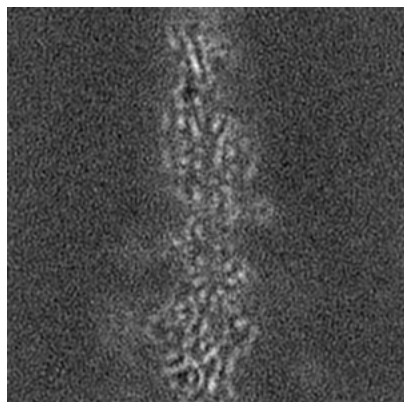


Y Index: 103

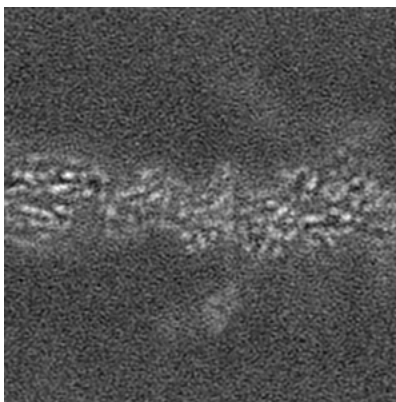


Z Index: 81

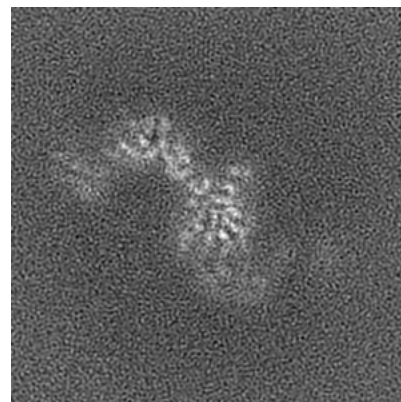
6.3.2 Raw map



X Index: 99



Y Index: 103

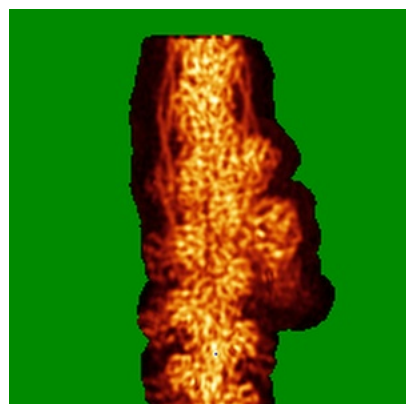


Z Index: 81

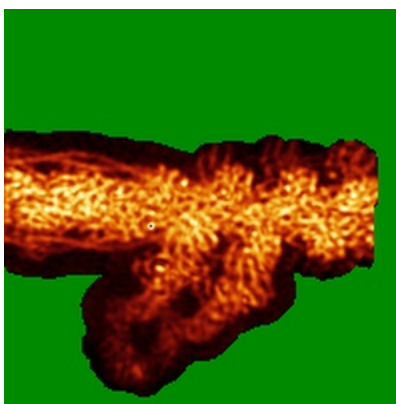
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

6.4.1 Primary map



X

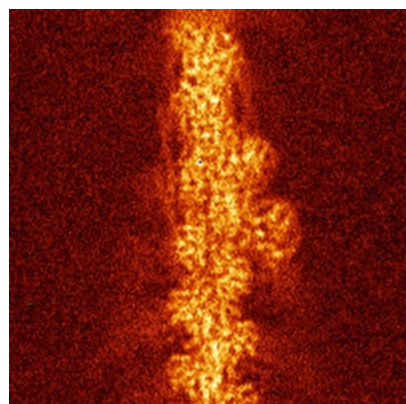


Y

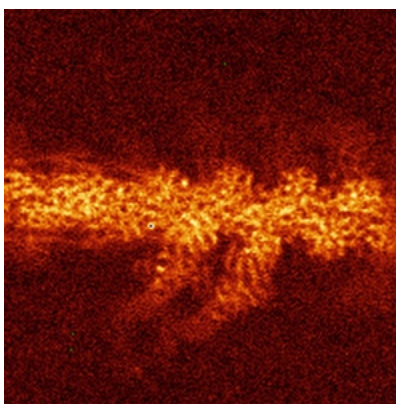


Z

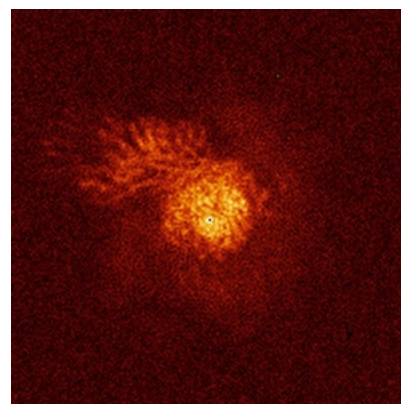
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

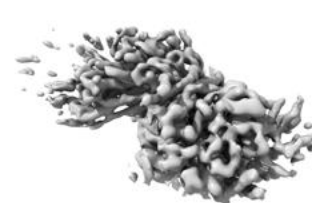
6.5.1 Primary map



X



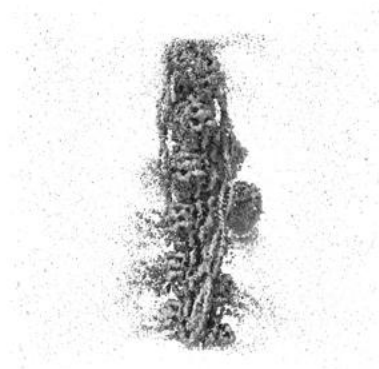
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

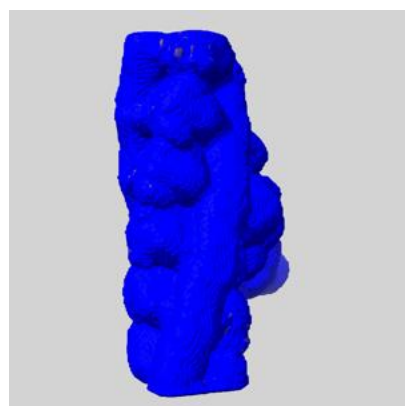
6.6 Mask visualisation [i](#)

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

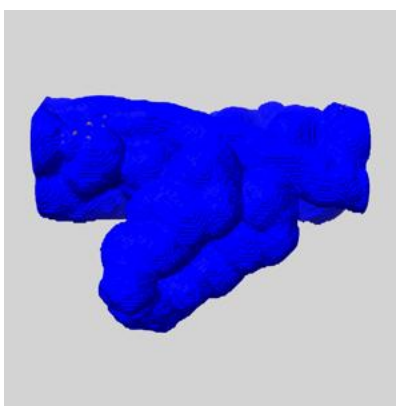
A mask typically either:

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

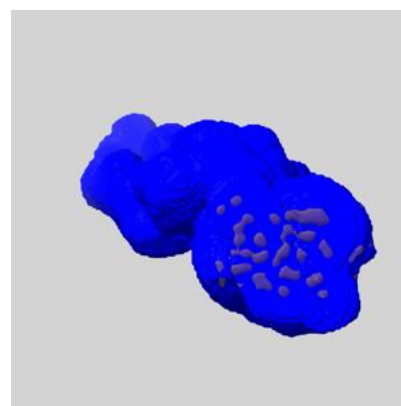
6.6.1 emd_13991_msk_1.map [i](#)



X



Y

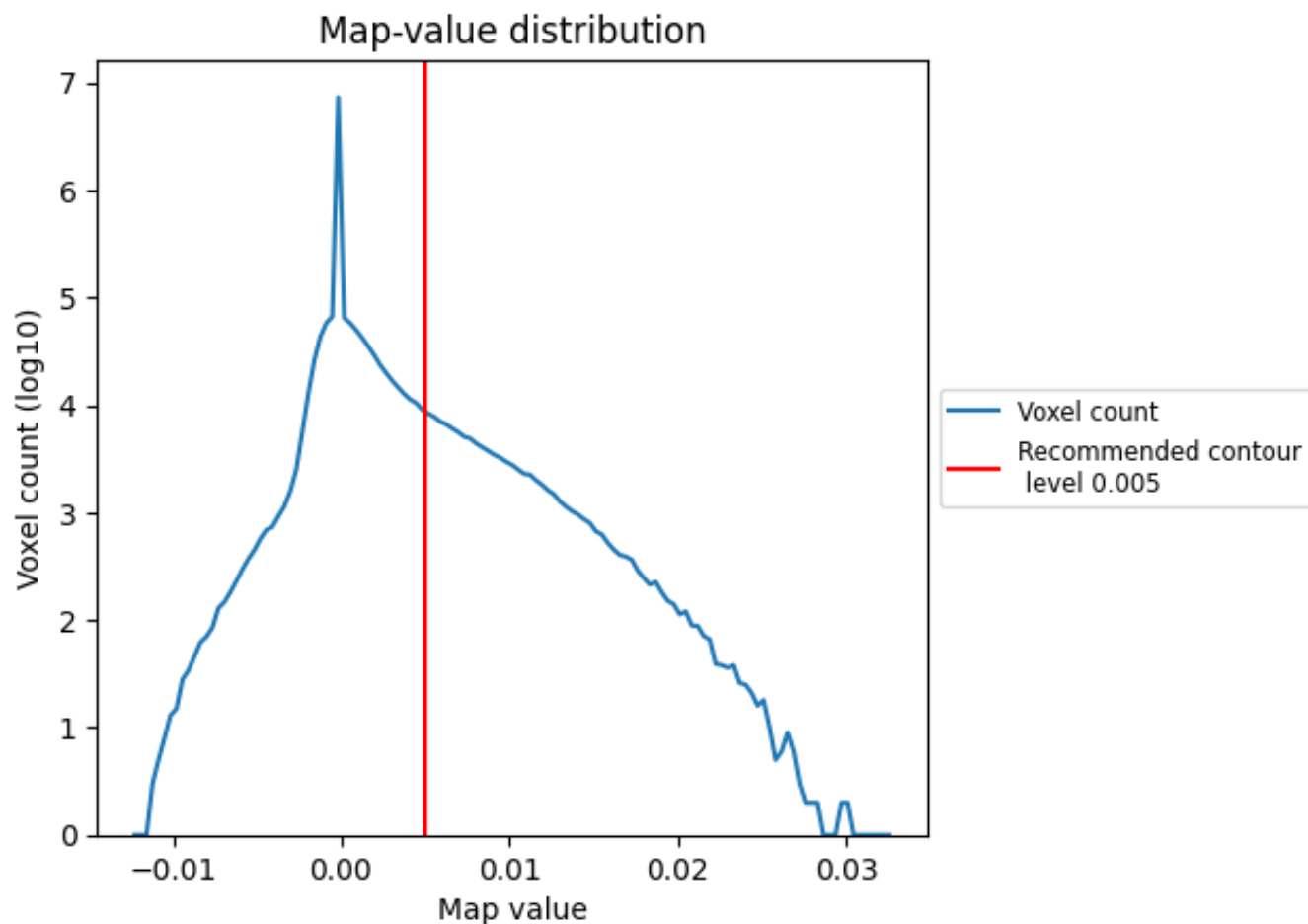


Z

7 Map analysis [i](#)

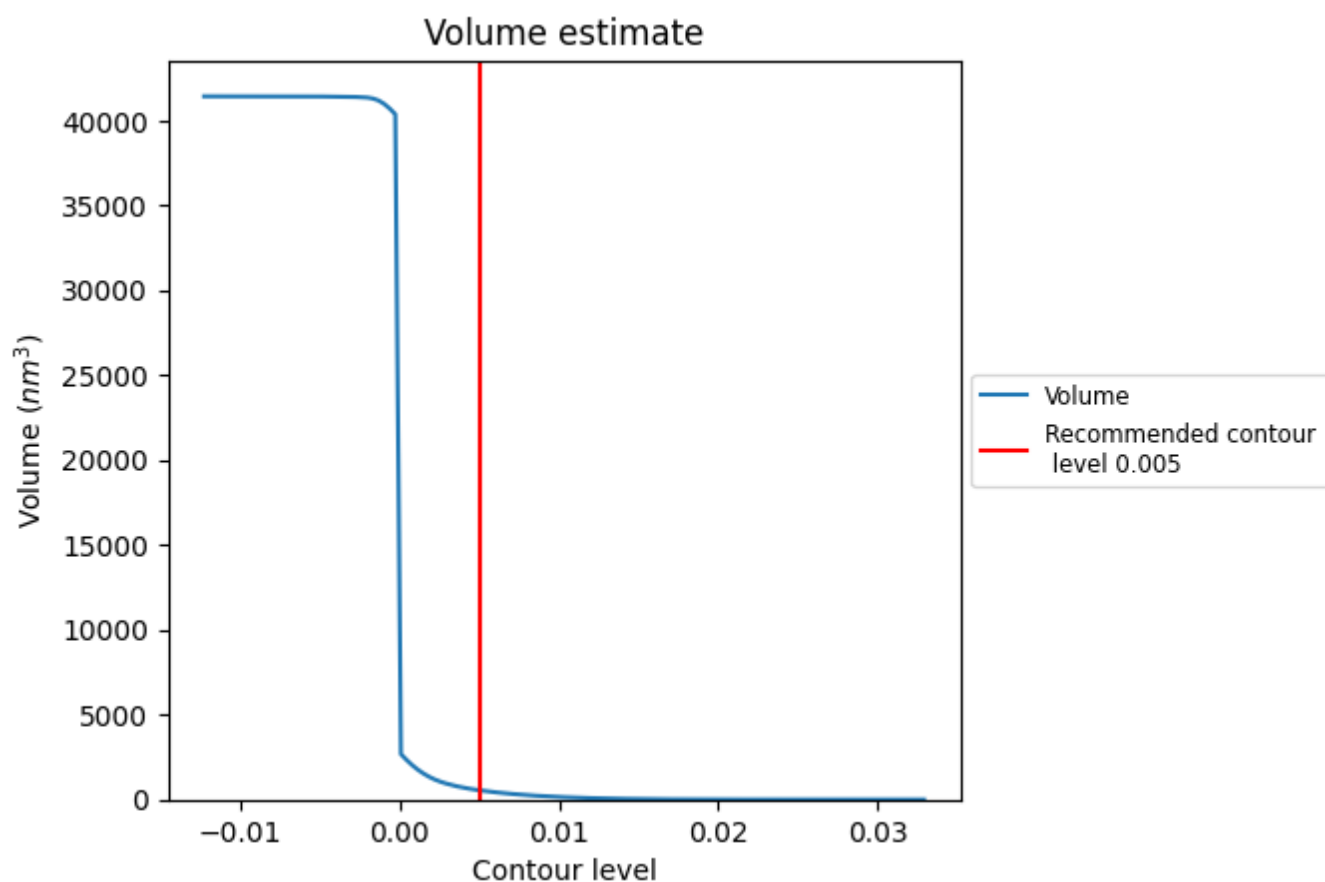
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

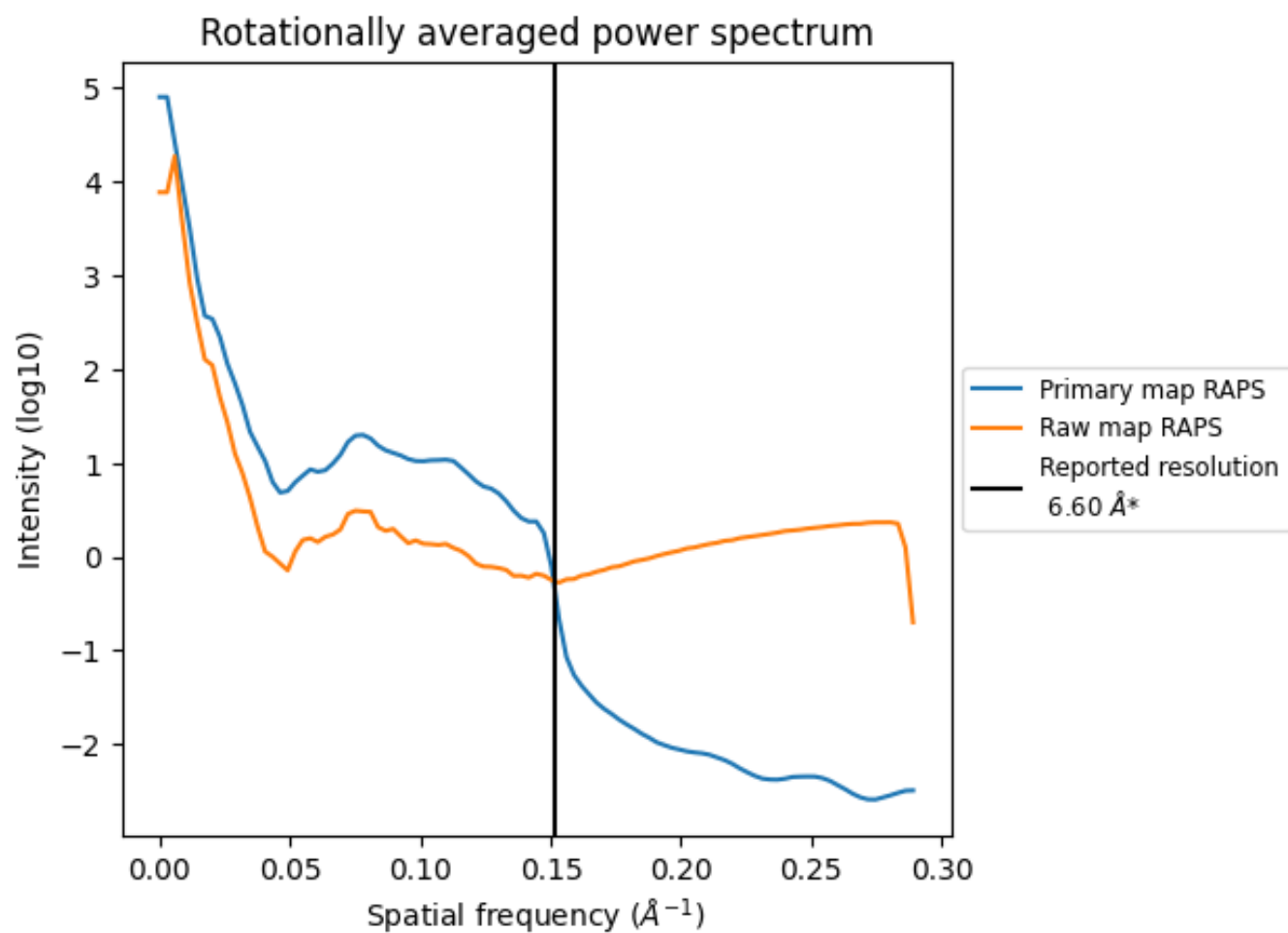
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 549 nm³; this corresponds to an approximate mass of 496 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 ⓘ

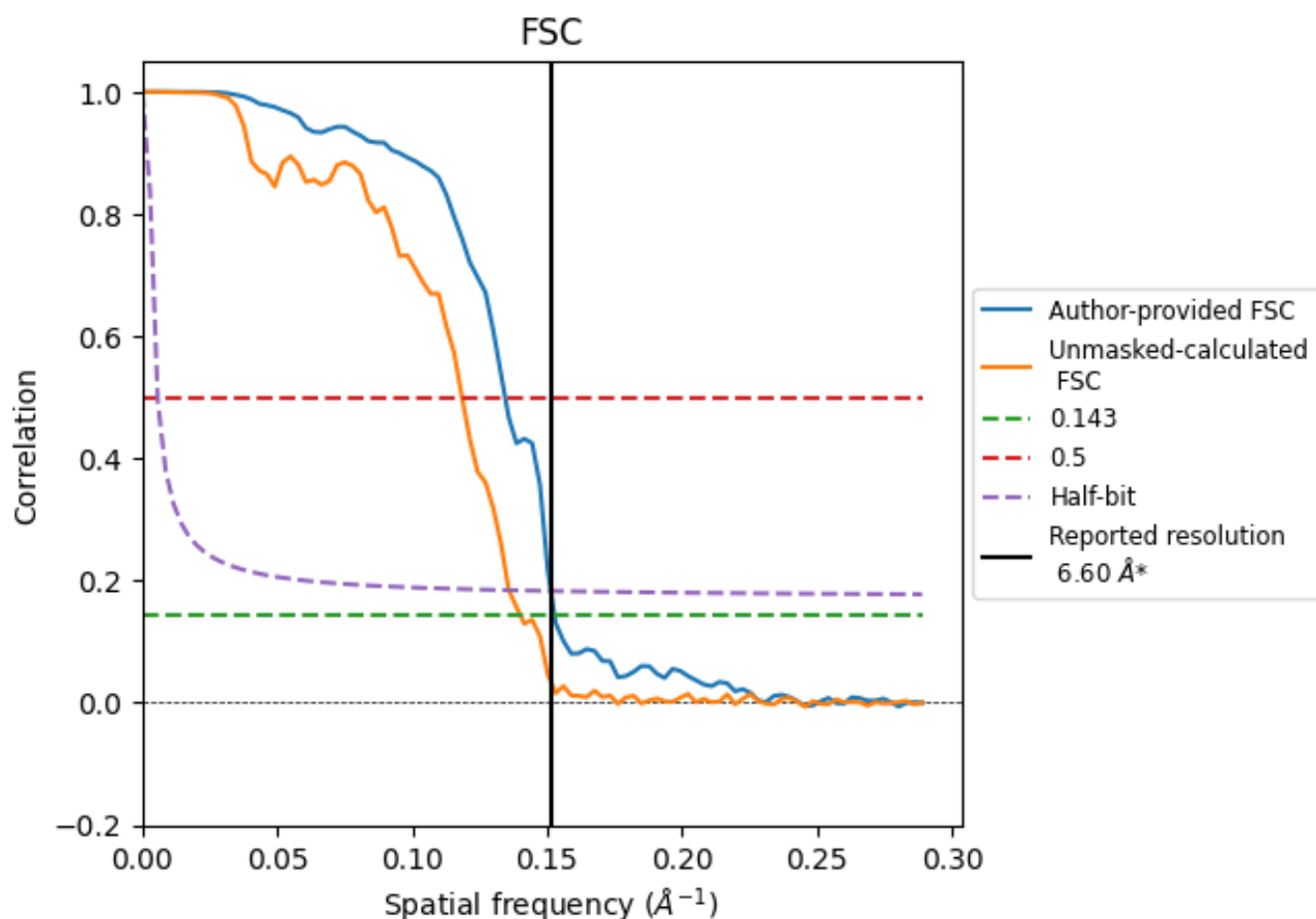


*Reported resolution corresponds to spatial frequency of 0.152 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.152 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

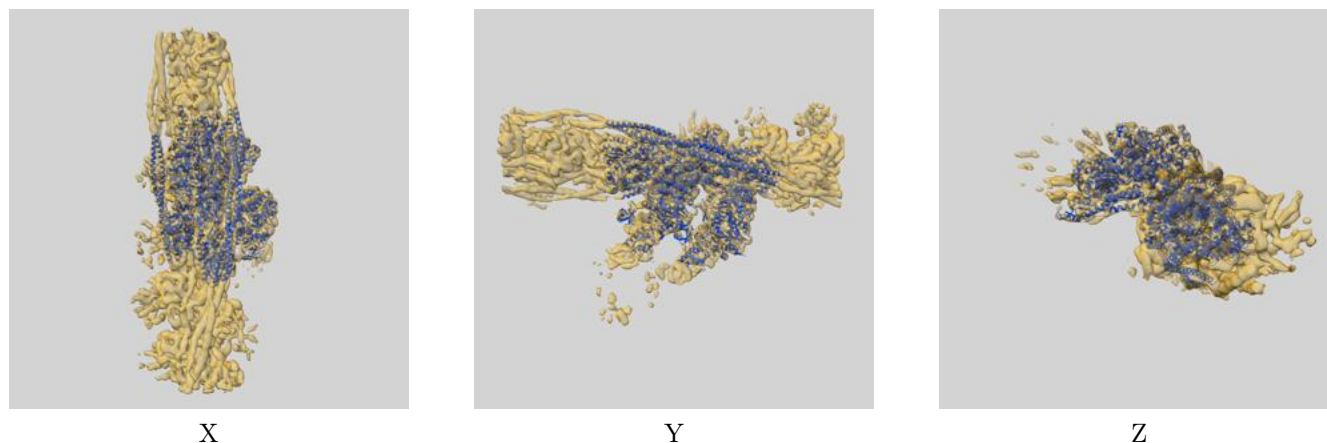
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.60	-	-
Author-provided FSC curve	6.55	7.43	6.61
Unmasked-calculated*	7.14	8.44	7.36

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

9 Map-model fit [i](#)

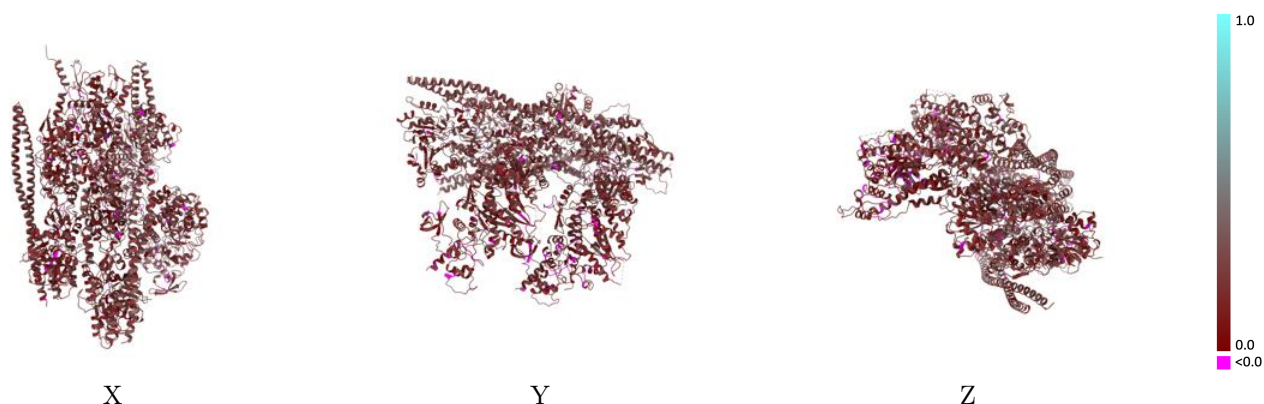
This section contains information regarding the fit between EMDB map EMD-13991 and PDB model 7QIN. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



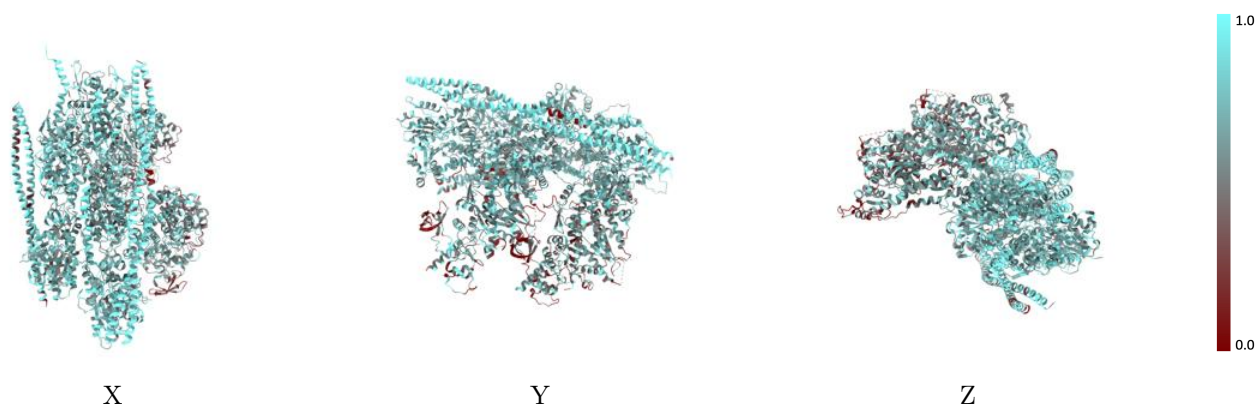
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



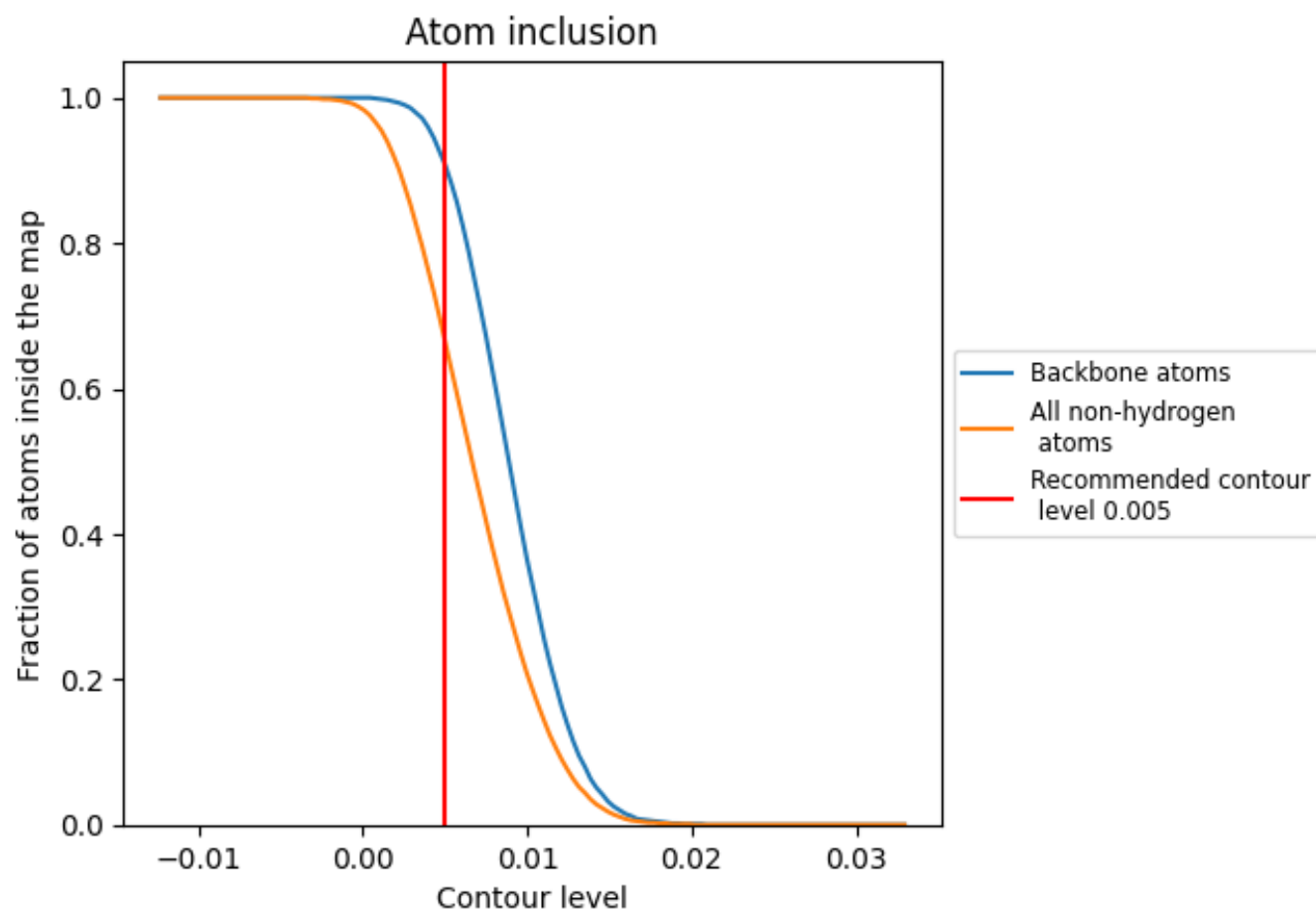
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.005).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 67% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6670	 0.1960
A	 0.7110	 0.1900
B	 0.7140	 0.1940
C	 0.7190	 0.1950
D	 0.7130	 0.1900
E	 0.7120	 0.1930
F	 0.9130	 0.2850
G	 0.9170	 0.2730
H	 0.8580	 0.2730
I	 0.8750	 0.2770
J	 0.7300	 0.2360
K	 0.7730	 0.2560
L	 0.5400	 0.1690
M	 0.5880	 0.1960

