



wwPDB EM Validation Summary Report ⓘ

Aug 27, 2026 – 02:30 PM EDT

PDB ID : 9YAQ / pdb_00009yaq
EMDB ID : EMD-72734
Title : The structure of the cardiac native cross bridge in the rigor state, myosin heads bound to actin molecules 5 and 6.
Authors : Galkin, V.E.; Risi, C.M.
Deposited on : 2025-09-16
Resolution : 4.63 Å (reported)
Based on initial models : 5H53, 7JH7, 7KO5, 8DD0, 6SFA

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.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

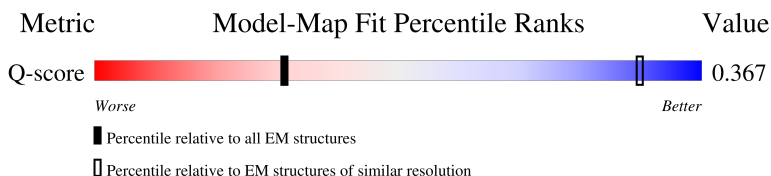
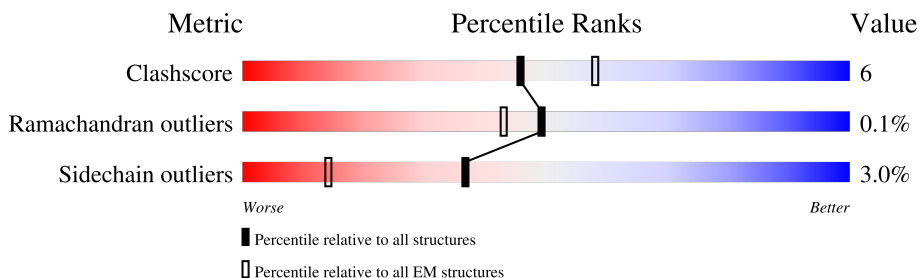
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.63 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.



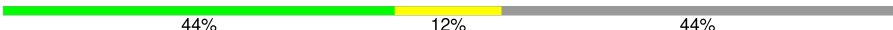
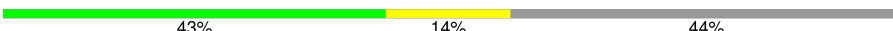
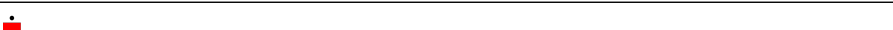
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2068 (4.13 - 5.13)

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	377	
1	B	377	
1	C	377	
1	D	377	

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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	
3	P	285	
4	J	1935	
4	K	1935	
5	L	196	
5	M	196	
6	N	161	
7	O	211	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 33966 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	160	Total	C	N	O	S	0	0
			1304	802	218	280	4		
2	F	160	Total	C	N	O	S	0	0
			1304	802	218	280	4		
2	G	35	Total	C	N	O	S	0	0
			278	168	51	56	3		
2	H	35	Total	C	N	O	S	0	0
			278	168	51	56	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	68	Total	C	N	O	S	0	0
			595	359	121	114	1		
3	P	74	Total	C	N	O		0	0
			643	401	123	119			

- Molecule 4 is a protein called Myosin-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	802	Total	C	N	O	S	0	0
			6461	4119	1111	1199	32		
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		

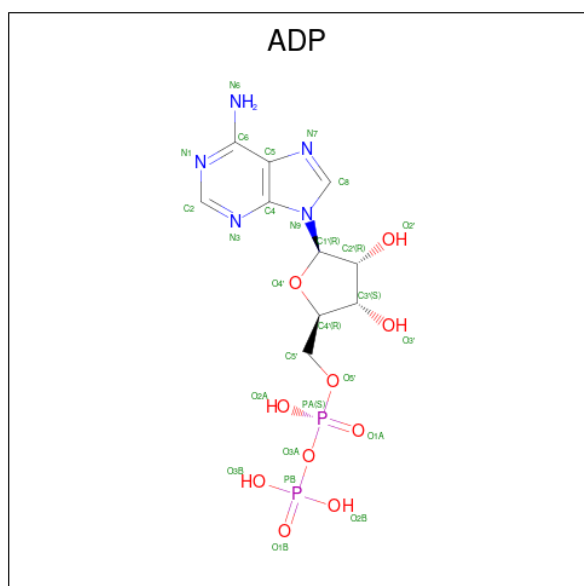
- Molecule 6 is a protein called Troponin C, slow skeletal and cardiac muscles.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	160	Total	C	N	O	S	0	0
			1274	789	195	278	12		

- Molecule 7 is a protein called Troponin I, cardiac muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	134	Total	C	N	O	S	0	0
			1077	667	208	197	5		

- 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	
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	

- 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	

- Molecule 10 is CALCIUM ION (CCD ID: CA) (formula: Ca).

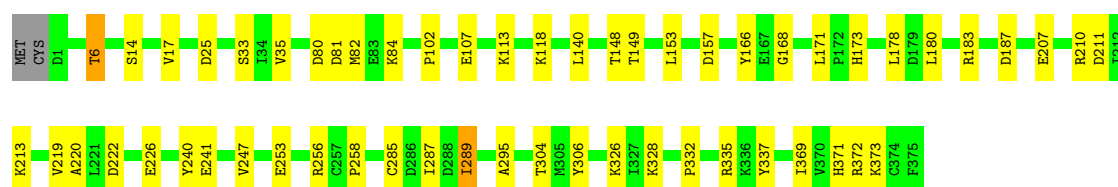
Mol	Chain	Residues	Atoms		AltConf
10	N	3	Total	Ca	0
			3	3	

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.

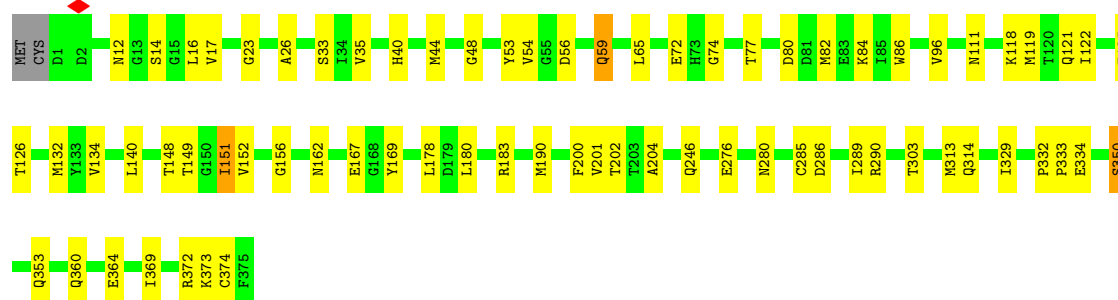
- Molecule 1: Actin, alpha cardiac muscle 1

Chain A: 



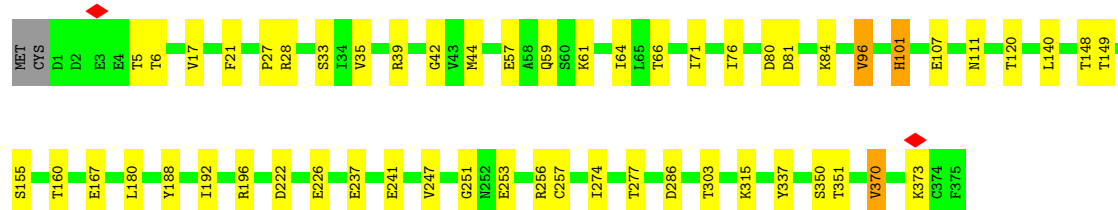
- Molecule 1: Actin, alpha cardiac muscle 1

Chain B: 

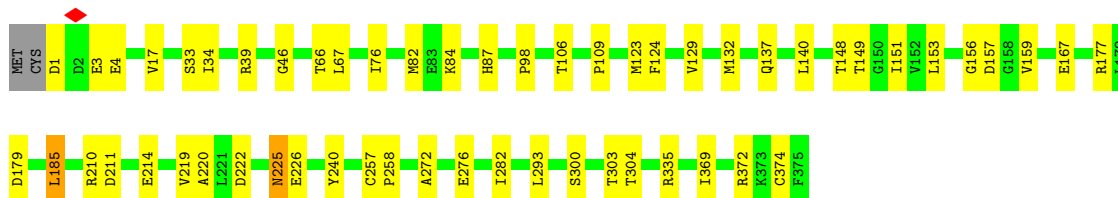


- Molecule 1: Actin, alpha cardiac muscle 1

Chain C: 



- Molecule 1: Actin, alpha cardiac muscle 1

[illegible]

K264	ASP	SER	MET
L265	GLU	GLU	ASP
K266	SER	ALA	ALA
Y267	PRO	LYS	ILE
K268	GLU	LYS	LYS
	R125	ASP	LYS
L274	T130	ALA	LYS
		GLN	MET
L278	R133	GLU	GLN
N279	A134	LYS	MET
D280	K135	LEU	LEU
K281	Q136	GLU	LYS
T282	D137	LEU	LEU
S283		ALA	ASP
I284	K140	GLU	LYS
		LYS	GLU
	K152	LYS	ASN
	E156	ALA	ALA
		THR	LEU
	K161	ASP	ASP
		ALA	ARG
	V165	GLU	ALA
		ALA	GLU
	S174	ASP	GLN
D175		VAL	ALA
L176	D175	ALA	GLU
E177	L176	SER	GLU
R178	E177	LEU	ALA
A179	R178	ASN	ASP
E180	A179	ASN	LYS
		ARG	LYS
	L204	ILE	ALA
		GLN	ALA
	E208	LEU	GLU
		VAL	ASP
	E212	GLU	ARG
Q216		GLU	SER
K217	Q216	LEU	LYS
E218	K217	LEU	ARG
		ASP	ARG
	K231	ALA	GLU
		GLN	GLU
	A242	GLU	LEU
E243		ARG	VAL
R244	E243	LEU	SER
S245	R244	ALA	LEU
V246	S245	GLN	GLN
T247	V246	THR	LYS
K248	T247	ALA	LYS
L249	K248	LEU	LYS
		GLN	LEU
	L253	LYS	ALA
		LEU	THR
	L256	GLU	GLU
		ALA	GLU
	L260	LYS	ASP
		LYS	LEU
	O263	ALA	TYR

GLU	THR	M1
LYS	ASP	D2
MET	ALA	A3
ILE	GLU	I4
GLN	ALA	K5
GLU	ASP	K6
ILE	VAL	K7
GLN	ALA	M8
LEU	SER	Q9
LYS	LEU	
ASN	ALA	R21
ARG	ARG	
ALA	ARG	E26
LYS	ILE	
HIS	GLN	K30
ILE	LEU	
ALA	VAL	R35
GLU	GLU	SER
ASP	GLU	LYS
ALA	GLU	ARG
ASP	LEU	LEU
ARG	ASP	GLU
TYR	ARG	ASP
LYS	ALA	GLU
GLU	GLN	LEU
GLU	GLU	VAL
VAL	ARG	SER
ALA	LEU	LEU
ARG	ALA	GLN
LYS	THR	LYS
LEU	ALA	LYS
VAL	LEU	LEU
ILE	GLN	LYS
ILE	LYS	ALA
SER	LEU	THR
GLU	GLU	GLU
ASP	GLU	ASP
LEU	ALA	GLU
GLU	GLU	LEU
ARG	LYS	ASP
ALA	ALA	LYS
GLU	ALA	TYR
ARG	ASP	SER
GLU	GLU	GLU
LYS	VAL	GLN
CYS	ILE	LYS
ALA	GLU	LEU
GLU	SER	GLU
LEU	ARG	LEU
GLY	MET	ALA
GLU	LYS	GLN
GLY	VAL	GLU
CYS	ILE	LYS
ALA	GLU	LEU
GLU	SER	GLU
LEU	ARG	LEU
GLU	ALA	ALA
GLU	GLN	GLU
LYS	LYS	LYS
LEU	ASP	LYS
LYS	GLU	ALA

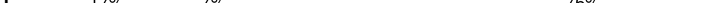
[illegible]

- Molecule 2: Tropomyosin alpha-1 chain

Chain H: 8% . 88%

[illegible]

- Molecule 3: Troponin T2, cardiac type

Chain I:  17% 7% 76%

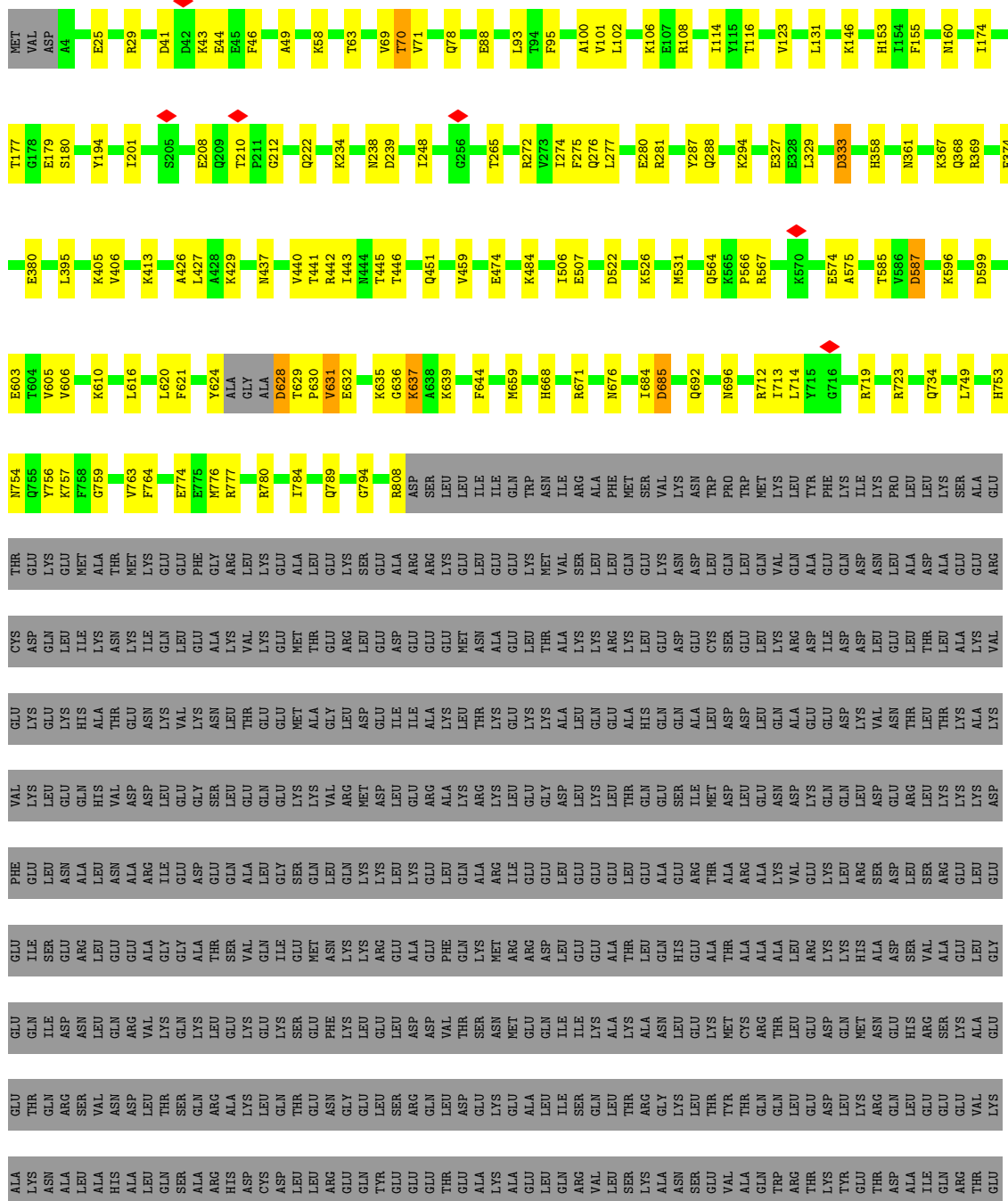
[illegible]

- Molecule 3: Troponin T2, cardiac type

Chain P: 18% 8% 74%

[illegible]

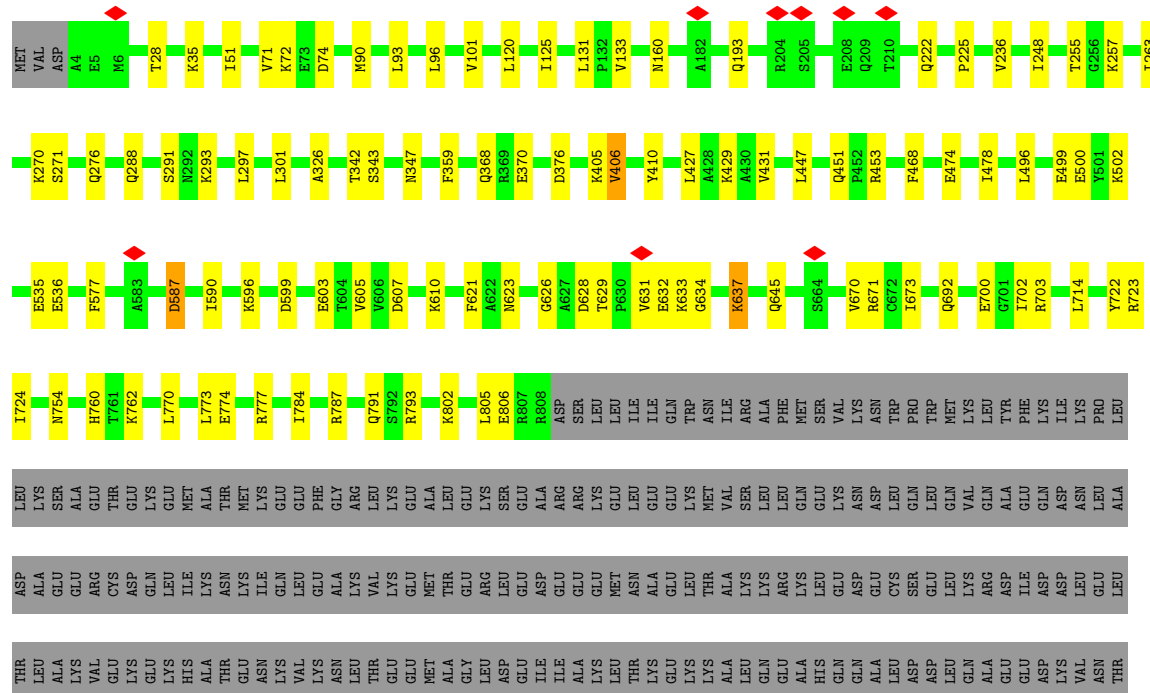
- Molecule 4: Myosin-7



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

- Molecule 4: Myosin-7

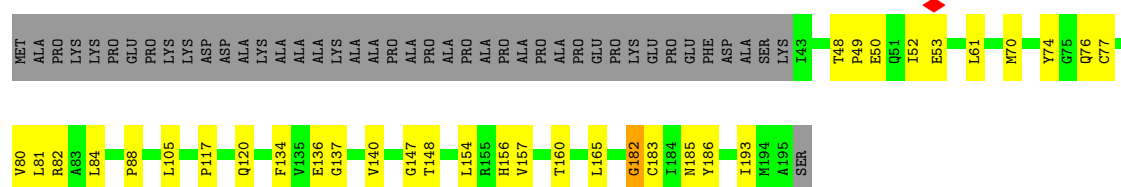
Chain K: 36% 5% 58%





- Molecule 5: Myosin light chain 3

Chain M: 



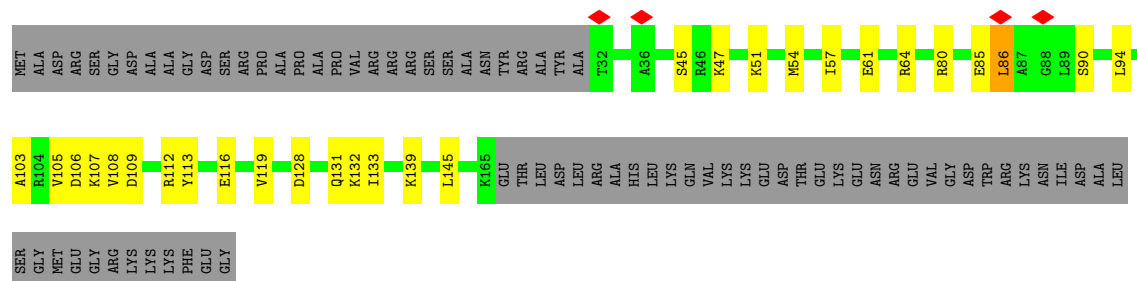
- Molecule 6: Troponin C, slow skeletal and cardiac muscles

Chain N: 



- Molecule 7: Troponin I, cardiac muscle

Chain O: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55229	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 ($e^-/\text{\AA}^2$)	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	13.125	Depositor
Minimum map value	-6.174	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.213	Depositor
Recommended contour level	1.35	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: ADP, CA, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.10	0/2995	0.30	0/4057
1	B	0.10	0/2995	0.29	0/4057
1	C	0.10	0/2995	0.31	0/4057
1	D	0.10	0/2995	0.29	0/4057
2	E	0.13	0/1311	0.27	0/1746
2	F	0.14	0/1311	0.26	0/1746
2	G	0.09	0/277	0.22	0/363
2	H	0.09	0/277	0.23	0/363
3	I	0.10	0/598	0.28	0/791
3	P	0.11	0/649	0.27	0/861
4	J	0.12	0/6594	0.33	0/8877
4	K	0.11	0/6609	0.32	0/8899
5	L	0.11	0/1236	0.40	2/1658 (0.1%)
5	M	0.11	0/1236	0.39	2/1658 (0.1%)
6	N	0.10	0/1287	0.29	0/1720
7	O	0.10	0/1085	0.25	0/1445
All	All	0.11	0/34450	0.31	4/46355 (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
4	J	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	182	GLY	CA-C-N	7.44	135.09	121.70
5	M	182	GLY	C-N-CA	7.44	135.09	121.70
5	L	182	GLY	CA-C-N	7.07	134.43	121.70
5	L	182	GLY	C-N-CA	7.07	134.43	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	J	628	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	2932	0	2894	32	0
1	B	2932	0	2894	48	0
1	C	2932	0	2894	31	0
1	D	2932	0	2894	29	0
2	E	1304	0	1301	32	0
2	F	1304	0	1301	39	0
2	G	278	0	291	11	0
2	H	278	0	291	10	0
3	I	595	0	603	16	0
3	P	643	0	663	24	0
4	J	6461	0	6461	101	0
4	K	6475	0	6475	55	0
5	L	1217	0	1199	19	0
5	M	1217	0	1199	19	0
6	N	1274	0	1203	16	0
7	O	1077	0	1143	23	0
8	A	27	0	12	1	0
8	B	27	0	12	1	0
8	C	27	0	12	0	0
8	D	27	0	12	2	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
9	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	D	1	0	0	0	0
10	N	3	0	0	0	0
All	All	33966	0	33754	420	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 6.

The worst 5 of 420 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:628:ASP:HB2	4:J:630:PRO:CD	1.71	1.19
4:J:603:GLU:HG2	4:J:628:ASP:CG	1.82	1.05
4:J:628:ASP:HB2	4:J:630:PRO:HD3	1.07	1.05
4:J:603:GLU:HB3	4:J:628:ASP:OD1	1.57	1.04
4:J:628:ASP:HB3	4:J:630:PRO:N	1.75	1.02

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%)	357 (96%)	16 (4%)	0	100	100
1	B	373/377 (99%)	359 (96%)	14 (4%)	0	100	100
1	C	373/377 (99%)	353 (95%)	20 (5%)	0	100	100
1	D	373/377 (99%)	359 (96%)	14 (4%)	0	100	100
2	E	158/284 (56%)	158 (100%)	0	0	100	100
2	F	158/284 (56%)	158 (100%)	0	0	100	100
2	G	33/284 (12%)	33 (100%)	0	0	100	100
2	H	33/284 (12%)	33 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	I	66/285 (23%)	66 (100%)	0	0	100	100
3	P	72/285 (25%)	70 (97%)	2 (3%)	0	100	100
4	J	798/1935 (41%)	762 (96%)	34 (4%)	2 (0%)	36	71
4	K	803/1935 (42%)	766 (95%)	37 (5%)	0	100	100
5	L	151/196 (77%)	143 (95%)	8 (5%)	0	100	100
5	M	151/196 (77%)	147 (97%)	4 (3%)	0	100	100
6	N	158/161 (98%)	148 (94%)	9 (6%)	1 (1%)	21	58
7	O	132/211 (63%)	131 (99%)	1 (1%)	0	100	100
All	All	4205/7848 (54%)	4043 (96%)	159 (4%)	3 (0%)	49	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	N	93	SER
4	J	46	PHE
4	J	180	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	318/320 (99%)	308 (97%)	10 (3%)	35	56
1	B	318/320 (99%)	308 (97%)	10 (3%)	35	56
1	C	318/320 (99%)	307 (96%)	11 (4%)	32	53
1	D	318/320 (99%)	308 (97%)	10 (3%)	35	56
2	E	142/245 (58%)	138 (97%)	4 (3%)	38	59
2	F	142/245 (58%)	141 (99%)	1 (1%)	76	79
2	G	28/245 (11%)	28 (100%)	0	100	100
2	H	28/245 (11%)	28 (100%)	0	100	100
3	I	64/249 (26%)	64 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	P	69/249 (28%)	67 (97%)	2 (3%)	37	57
4	J	695/1697 (41%)	668 (96%)	27 (4%)	28	49
4	K	695/1697 (41%)	676 (97%)	19 (3%)	39	59
5	L	133/163 (82%)	125 (94%)	8 (6%)	17	39
5	M	133/163 (82%)	129 (97%)	4 (3%)	36	56
6	N	141/142 (99%)	138 (98%)	3 (2%)	47	65
7	O	115/176 (65%)	113 (98%)	2 (2%)	53	67
All	All	3657/6796 (54%)	3546 (97%)	111 (3%)	37	56

5 of 111 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	J	177	THR
3	P	226	LEU
4	J	734	GLN
3	P	202	ARG
5	L	184	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
4	J	451	GLN
3	P	225	GLN
4	K	437	ASN
7	O	157	GLN
6	N	144	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 7 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
8	ADP	B	401	-	28,29,29	1.41	4 (14%)	43,45,45	1.81	9 (20%)
8	ADP	C	401	-	28,29,29	1.41	4 (14%)	43,45,45	1.84	10 (23%)
8	ADP	D	401	-	28,29,29	1.41	4 (14%)	43,45,45	1.83	9 (20%)
8	ADP	A	401	-	28,29,29	1.42	4 (14%)	43,45,45	1.81	9 (20%)

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	B	401	-	-	4/16/32/32	0/3/3/3
8	ADP	C	401	-	-	4/16/32/32	0/3/3/3
8	ADP	D	401	-	-	4/16/32/32	0/3/3/3
8	ADP	A	401	-	-	3/16/32/32	0/3/3/3

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	401	ADP	C5-C4	4.77	1.47	1.39
8	C	401	ADP	C5-C4	4.76	1.47	1.39
8	A	401	ADP	C5-C4	4.68	1.47	1.39
8	B	401	ADP	C5-C4	4.67	1.47	1.39
8	C	401	ADP	C5-C6	2.70	1.48	1.41

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	401	ADP	C5-C4-N3	-5.94	118.54	126.72
8	C	401	ADP	C5-C4-N3	-5.88	118.62	126.72
8	B	401	ADP	C5-C4-N3	-5.84	118.67	126.72
8	A	401	ADP	C5-C4-N3	-5.78	118.75	126.72
8	B	401	ADP	N3-C4-N9	4.72	135.19	127.17

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

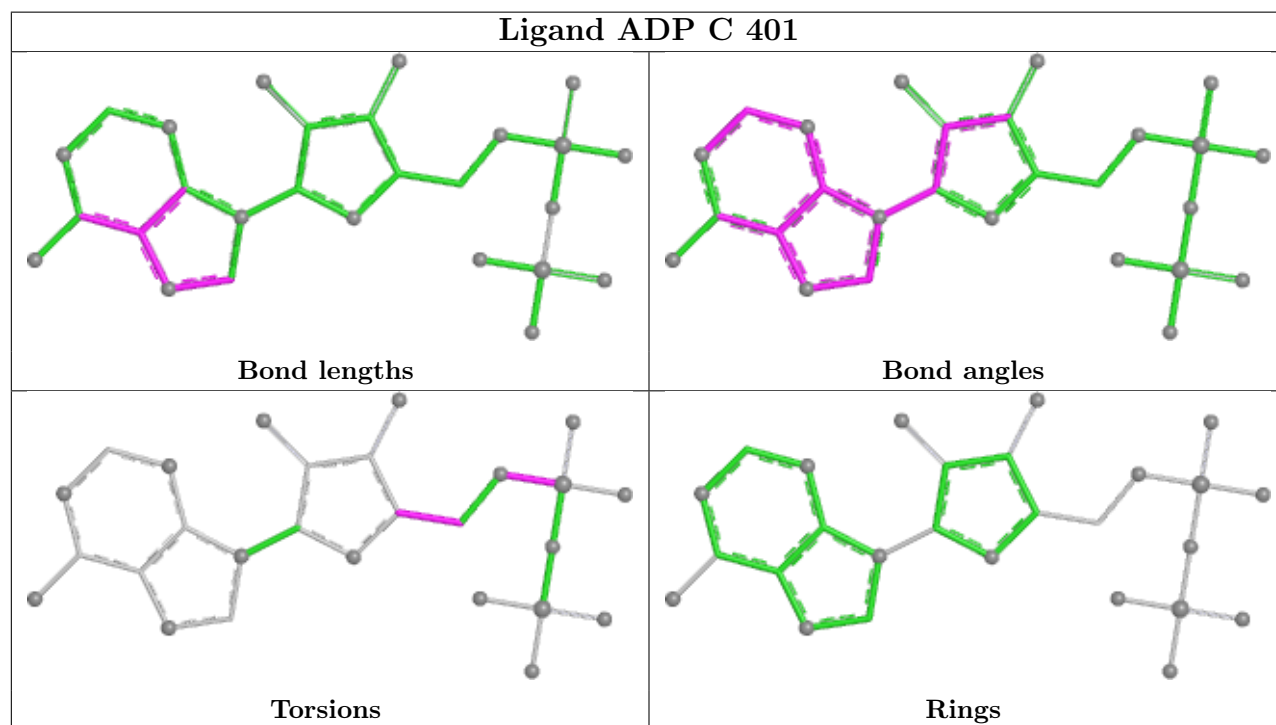
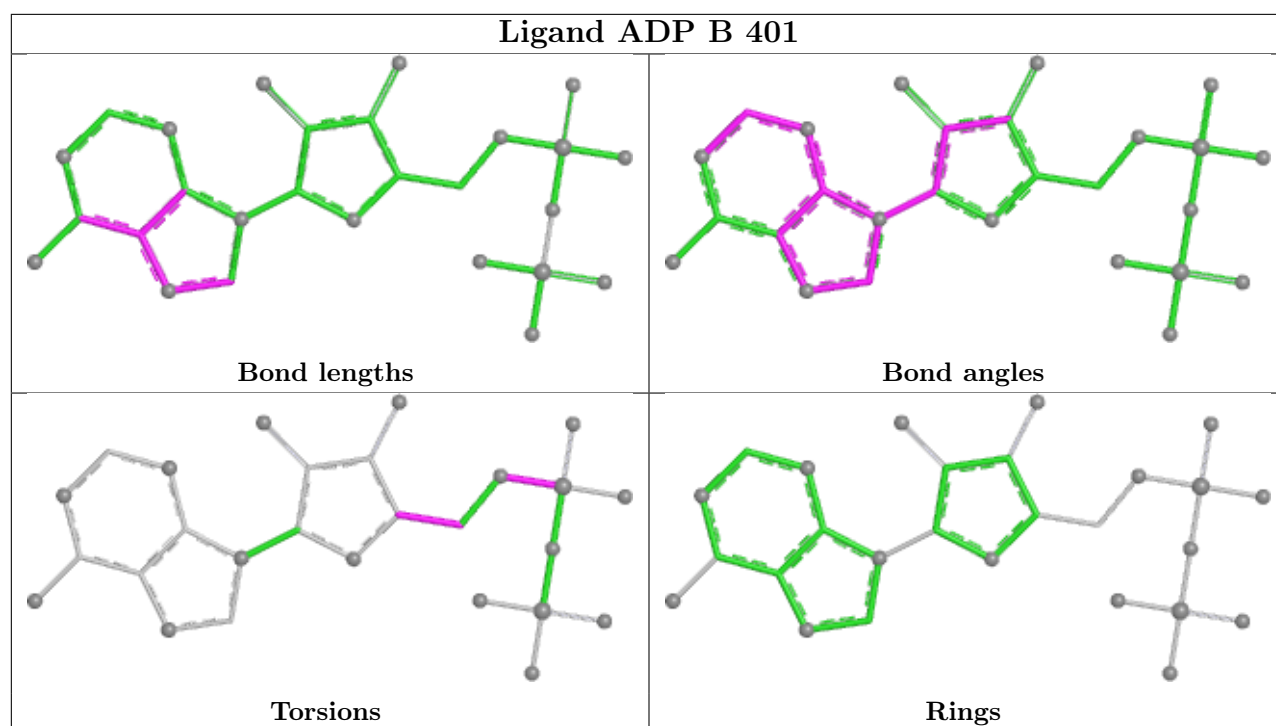
Mol	Chain	Res	Type	Atoms
8	A	401	ADP	C5'-O5'-PA-O1A
8	A	401	ADP	C5'-O5'-PA-O2A
8	A	401	ADP	C5'-O5'-PA-O3A
8	B	401	ADP	C5'-O5'-PA-O3A
8	C	401	ADP	C5'-O5'-PA-O3A

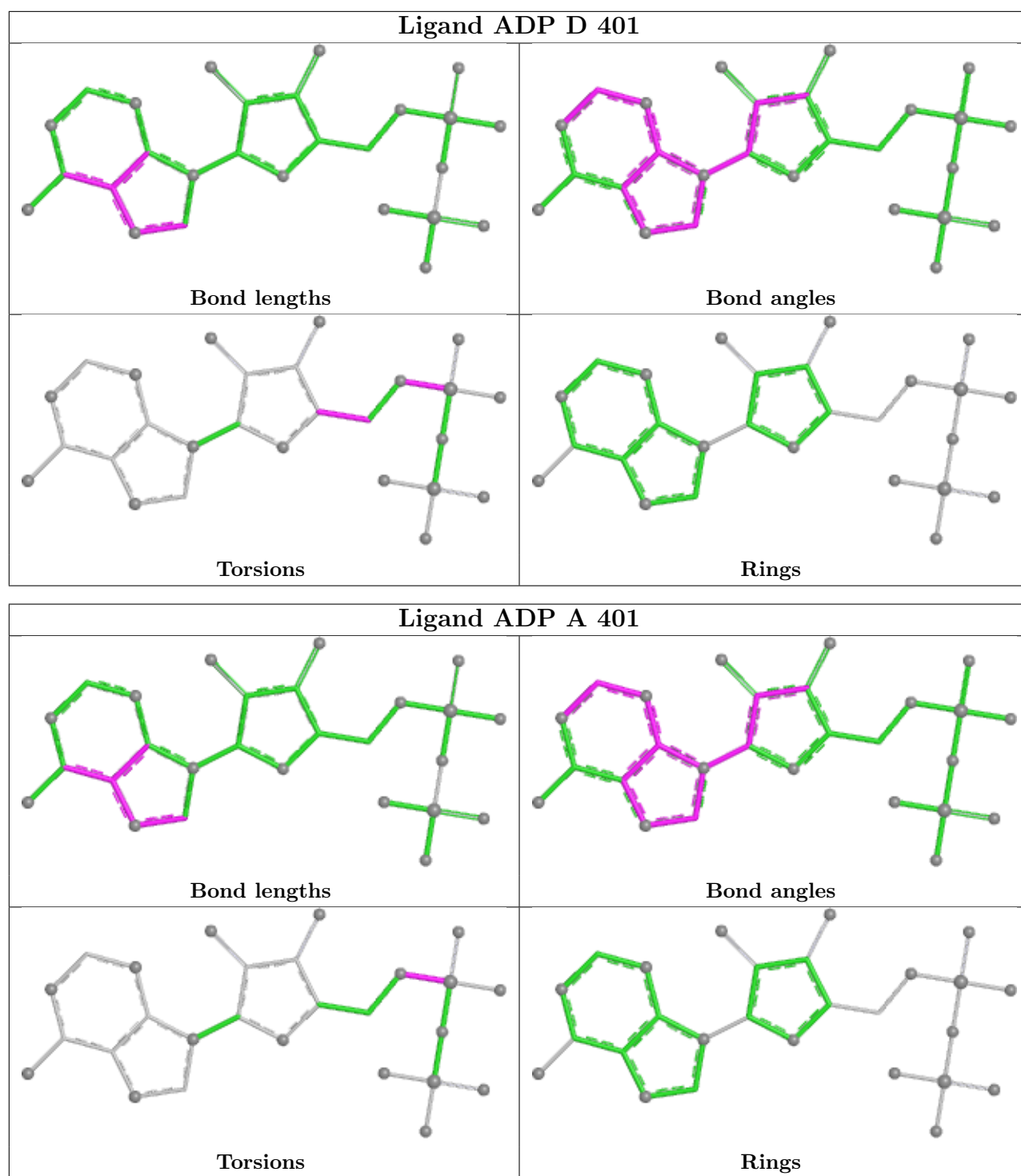
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	401	ADP	1	0
8	D	401	ADP	2	0
8	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 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72734. These allow visual inspection of the internal detail of the map and identification of artifacts.

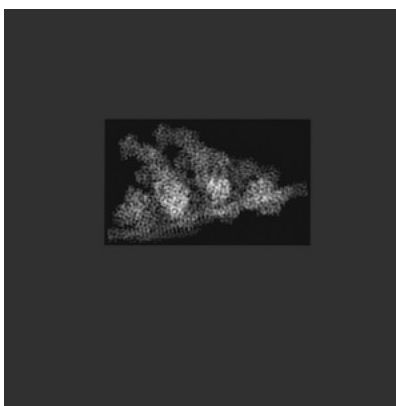
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

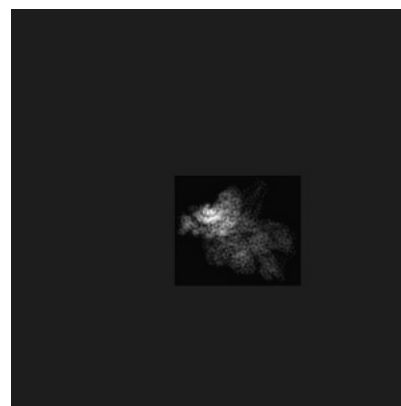
6.1.1 Primary map



X

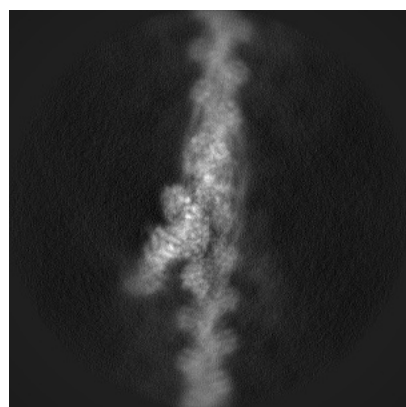


Y

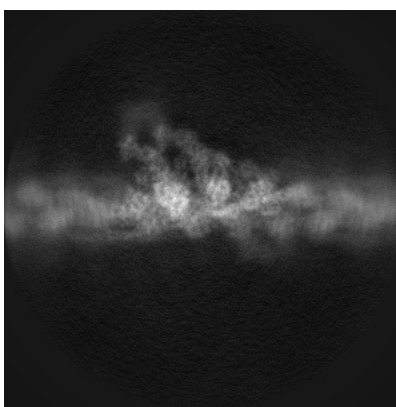


Z

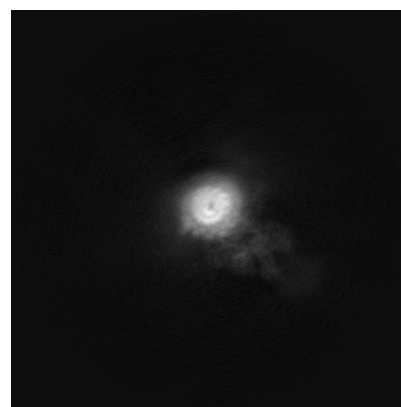
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

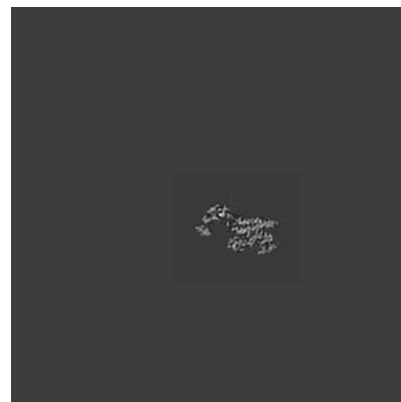
6.2.1 Primary map



X Index: 198

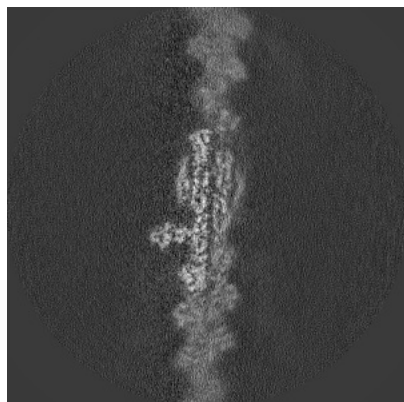


Y Index: 198

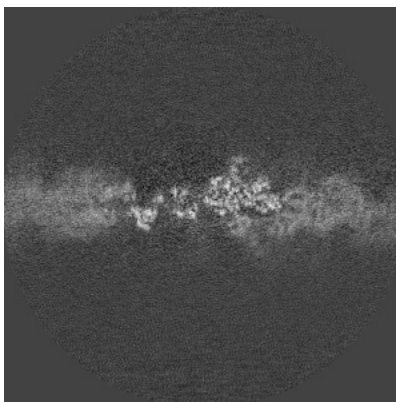


Z Index: 198

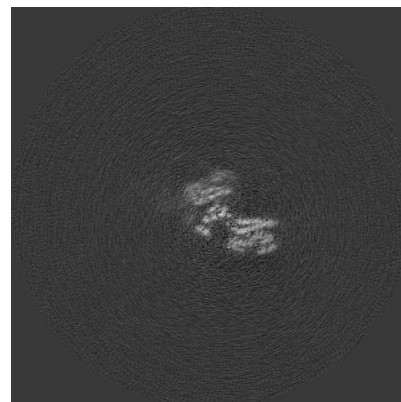
6.2.2 Raw map



X Index: 198



Y Index: 198



Z Index: 198

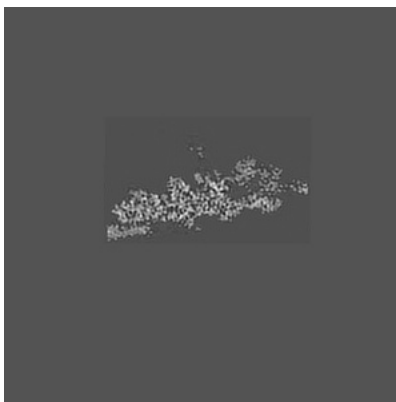
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 208

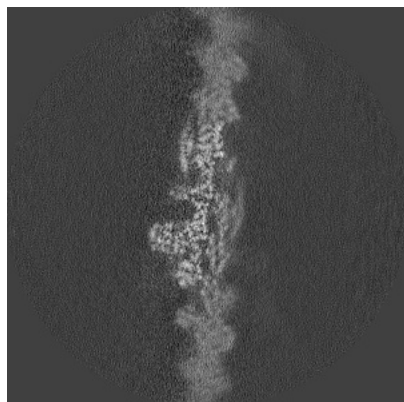


Y Index: 188

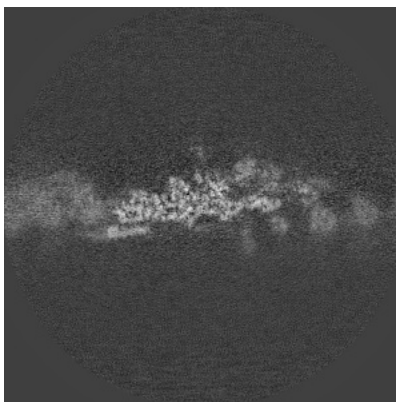


Z Index: 166

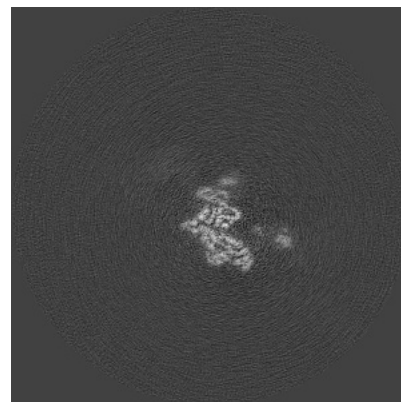
6.3.2 Raw map



X Index: 207



Y Index: 188

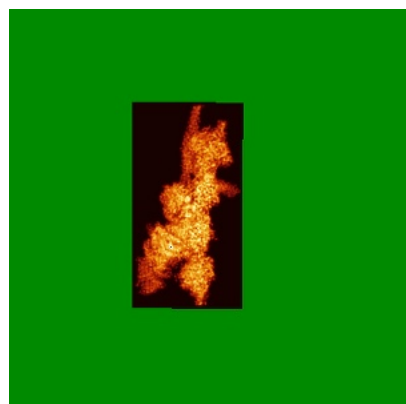


Z Index: 167

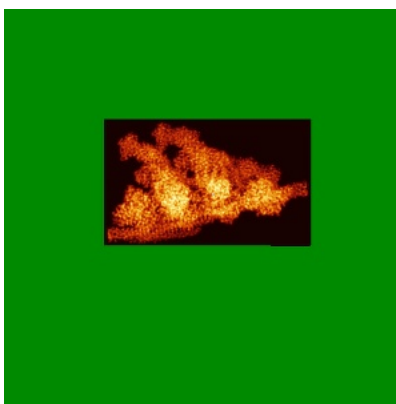
The images above show the largest variance slices of the map in three orthogonal directions.

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

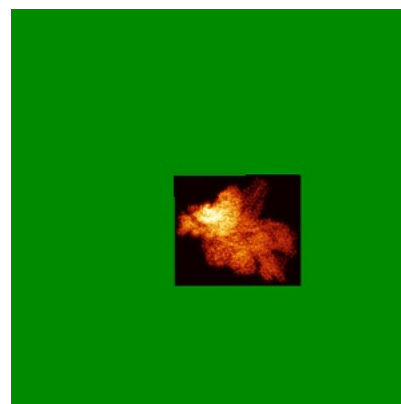
6.4.1 Primary map



X

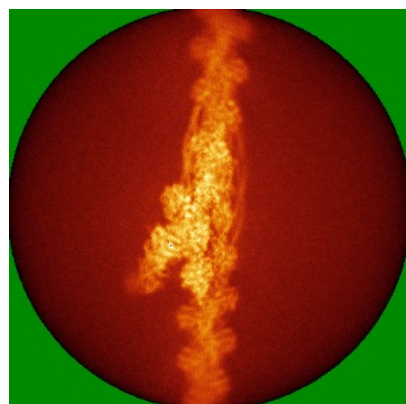


Y

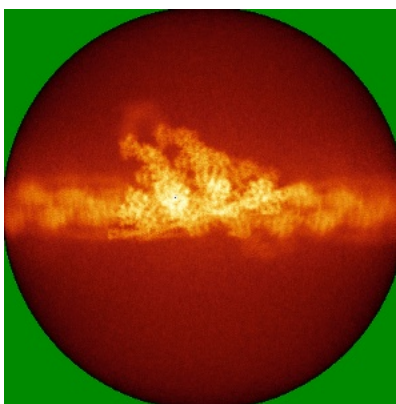


Z

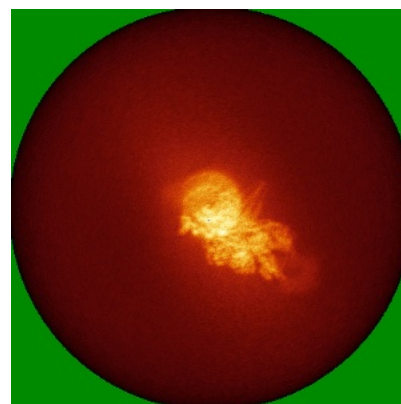
6.4.2 Raw map



X



Y

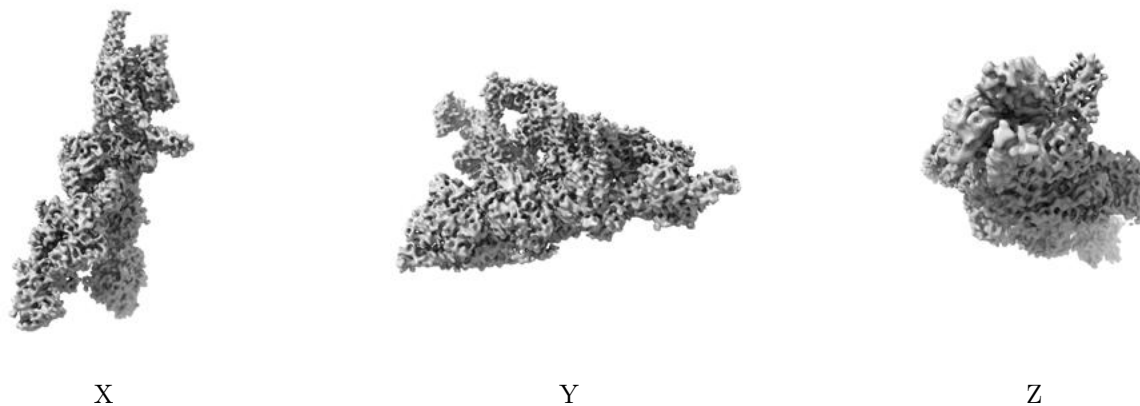


Z

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



The images above show the 3D surface view of the map at the recommended contour level 1.35. 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



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.

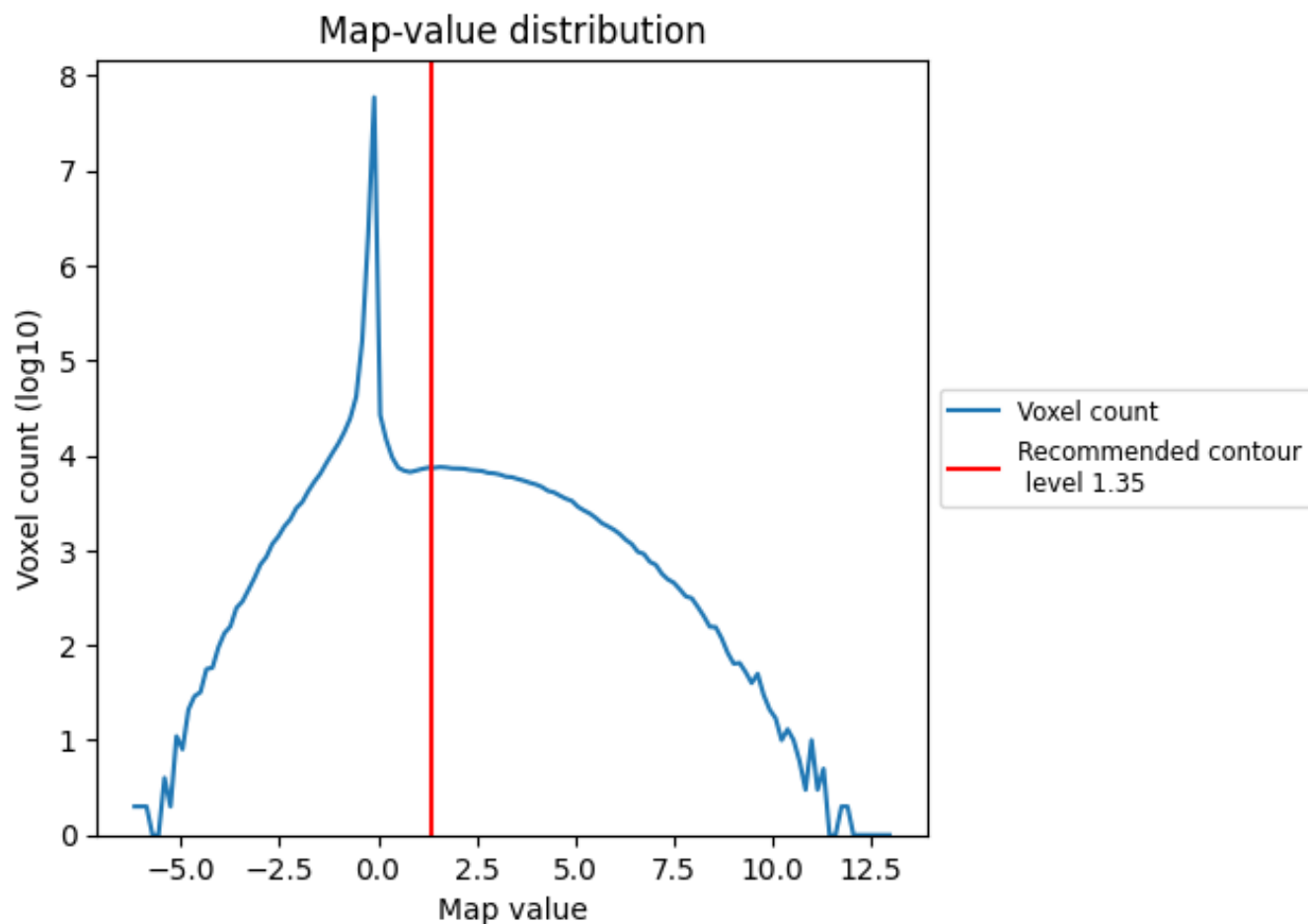
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

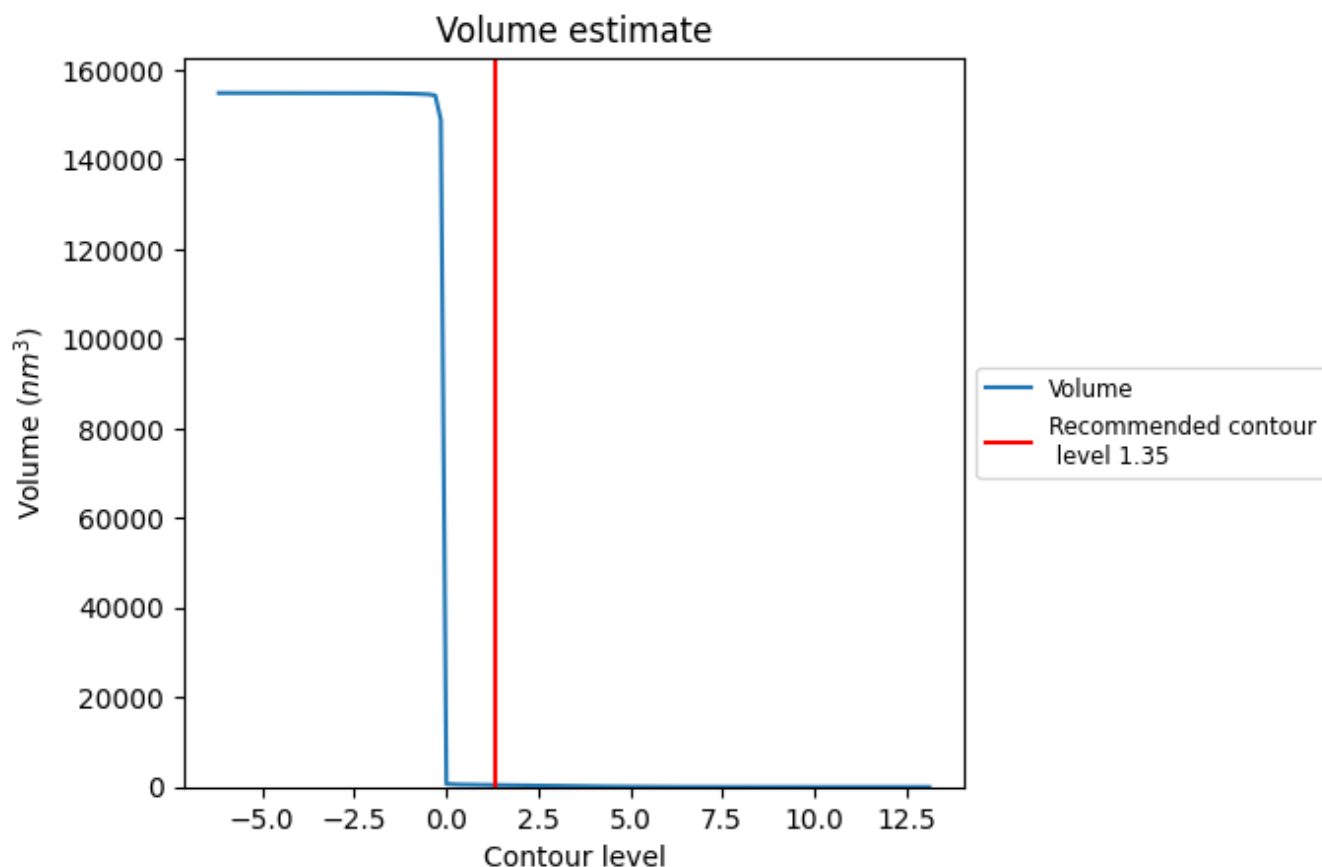
This section contains the results of statistical analysis of the map.

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.

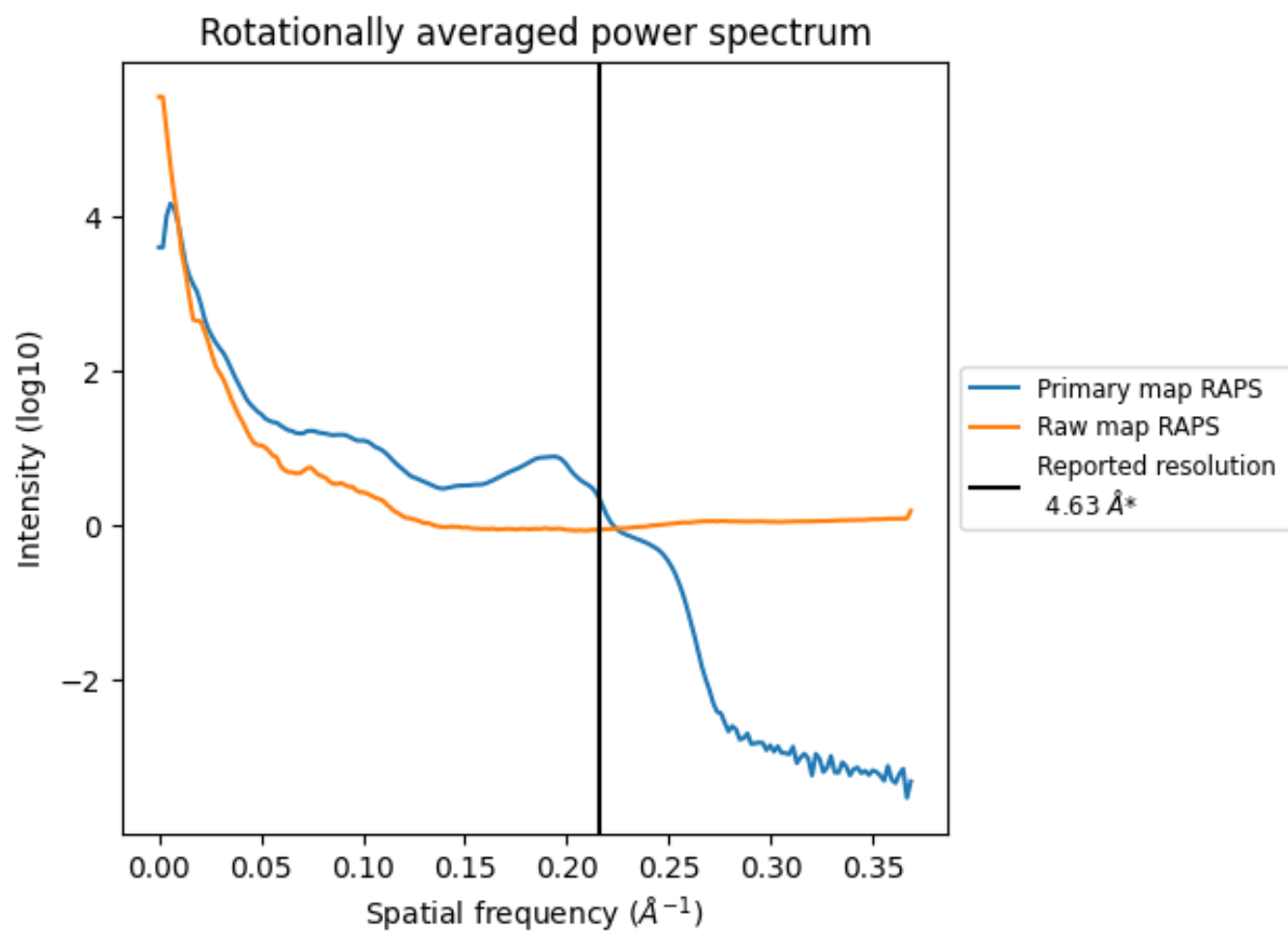
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 427 nm³; this corresponds to an approximate mass of 386 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 ⓘ

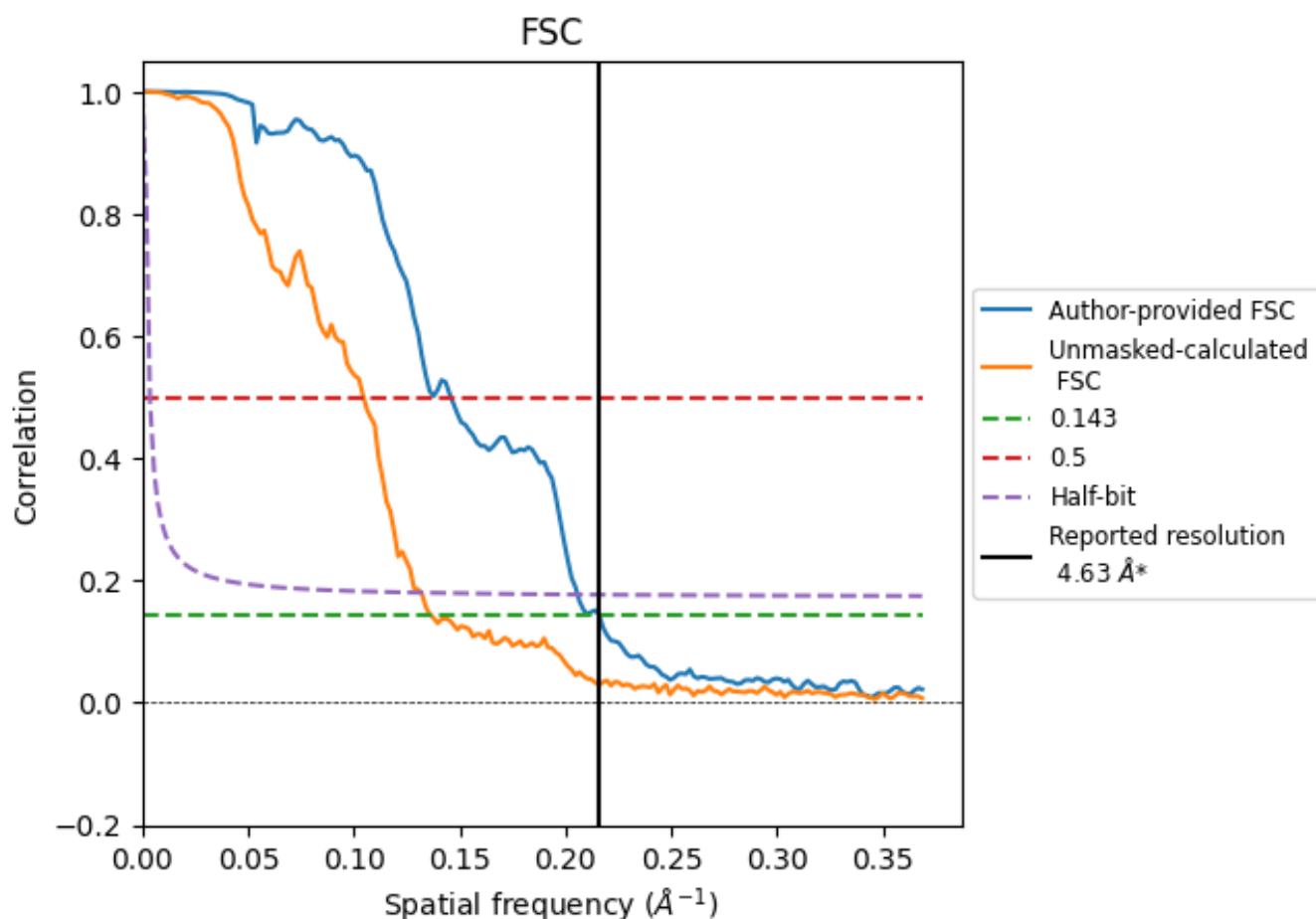


*Reported resolution corresponds to spatial frequency of 0.216 $\text{\AA}^{-1}$

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 0.216 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

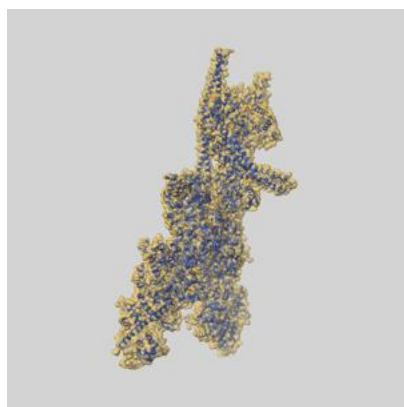
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.63	-	-
Author-provided FSC curve	4.63	6.85	4.86
Unmasked-calculated*	7.33	9.56	7.58

*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 7.33 differs from the reported value 4.63 by more than 10 %

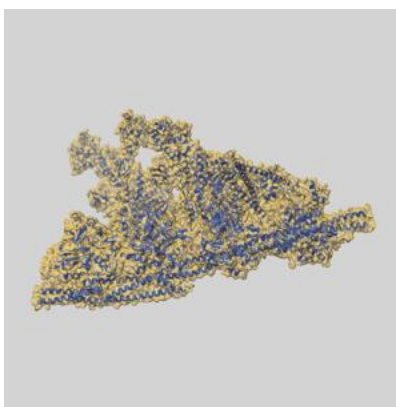
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-72734 and PDB model 9YAQ. Per-residue inclusion information can be found in section [3](#) on page [7](#).

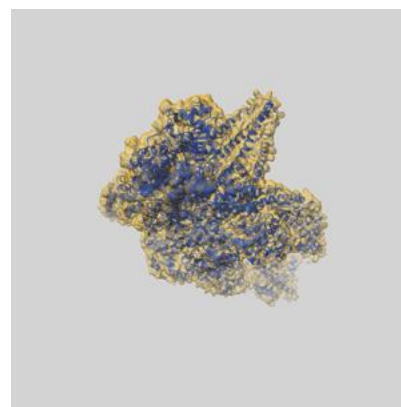
9.1 Map-model overlay [i](#)



X



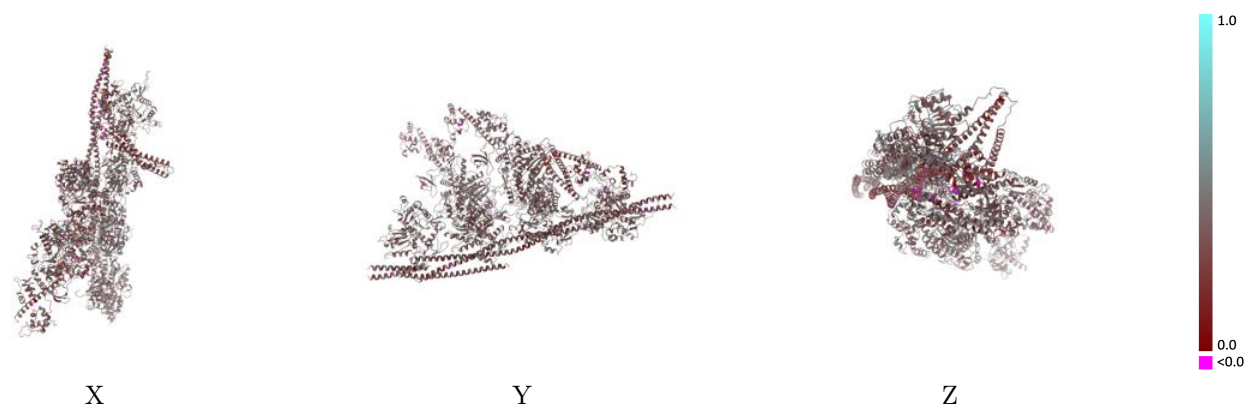
Y



Z

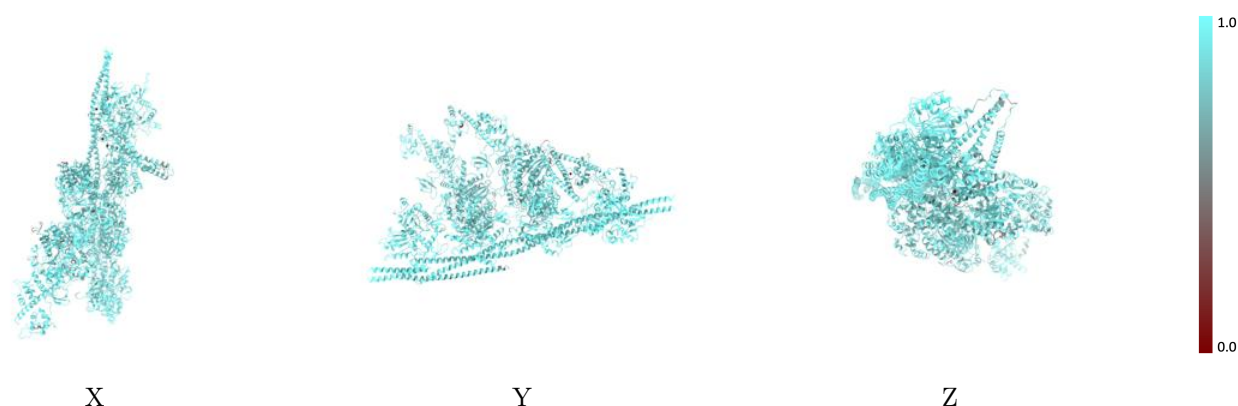
The images above show the 3D surface view of the map at the recommended contour level 1.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



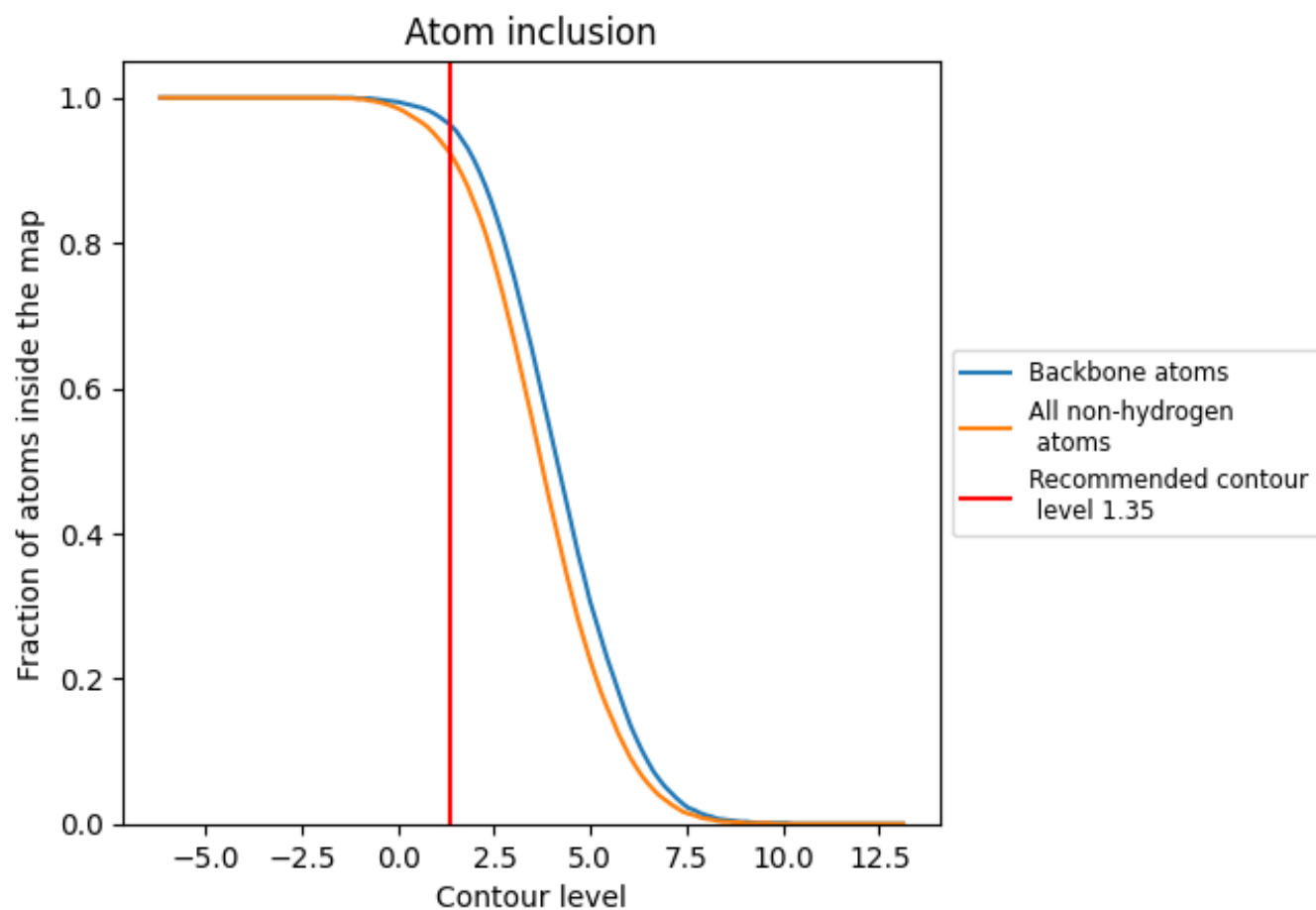
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.35).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% 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 (1.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9240	 0.3670
A	 0.9630	 0.4000
B	 0.9420	 0.4040
C	 0.9340	 0.3980
D	 0.9590	 0.3980
E	 0.9550	 0.2890
F	 0.9560	 0.3100
G	 0.9930	 0.3270
H	 0.9670	 0.3440
I	 0.8690	 0.3220
J	 0.9060	 0.3670
K	 0.9270	 0.3680
L	 0.8570	 0.3670
M	 0.9220	 0.3630
N	 0.8600	 0.2840
O	 0.8600	 0.3320
P	 0.8500	 0.3110

