



wwPDB EM Validation Summary Report ⓘ

Jul 16, 2026 – 04:26 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, 7JH7, 6SFA, 8DD0, 7KO5

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

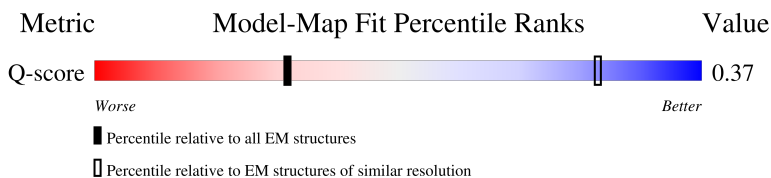
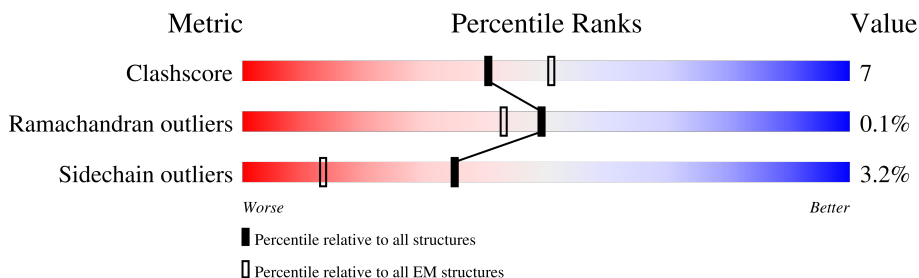
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 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.



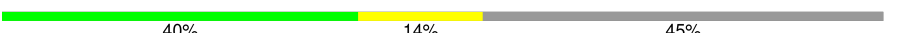
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2937 (4.00 - 5.00)

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 $\leq 5\%$. 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	 8% 88%
2	F	284	 7% 5% 88%
2	G	284	 38% 16% 45%
2	H	284	 40% 14% 45%
3	I	285	 14% 84%
4	J	1935	 35% 6% 58%
4	K	1935	 39% 58%
5	L	196	 63% 15% 22%
5	M	196	 61% 17% 22%

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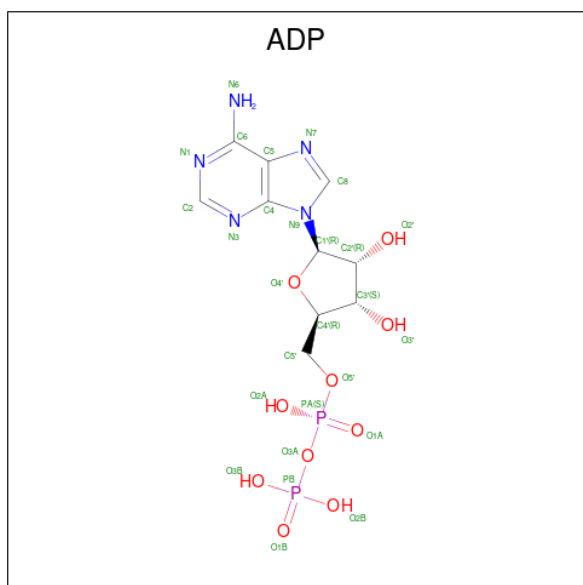
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Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	805	Total	C	N	O	S	0	0
			6475	4127	1114	1202	32		

- 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	

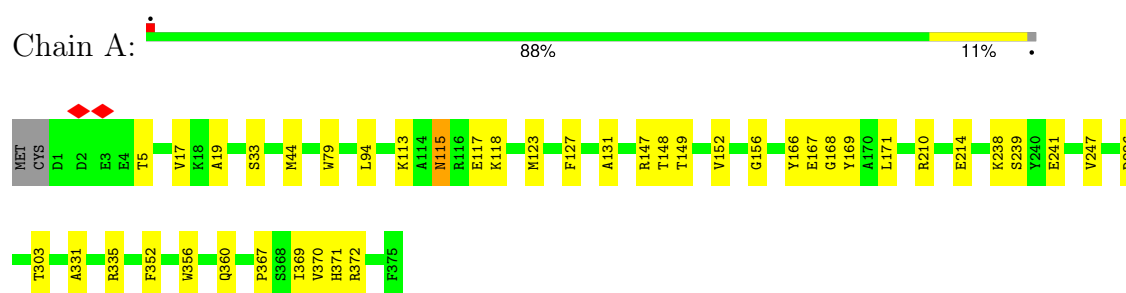
- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

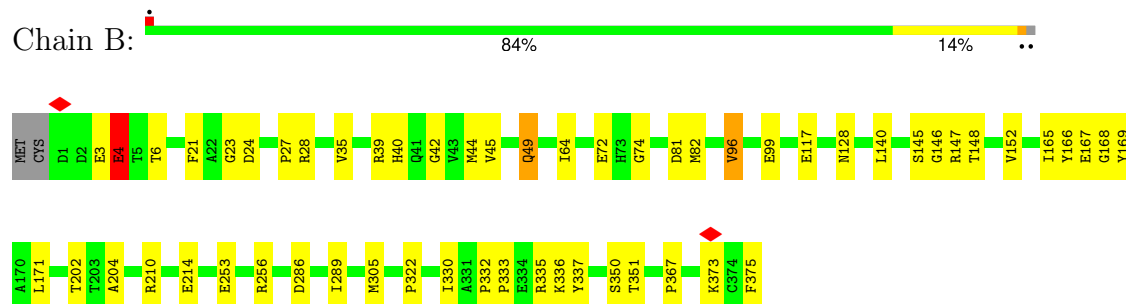
3 Residue-property plots

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.

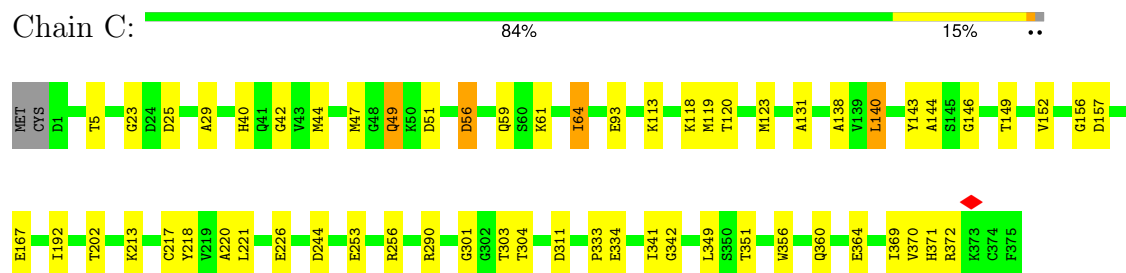
- Molecule 1: Actin, alpha cardiac muscle 1



- Molecule 1: Actin, alpha cardiac muscle 1



- Molecule 1: Actin, alpha cardiac muscle 1



- Molecule 1: Actin, alpha cardiac muscle 1





Chain E: 8% . 88%



Chain F: 7% 5% 88%



Chain G: 38% 16% 45%

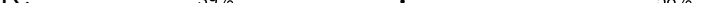






LYS ARG GLN ALA ALA GLU GLU ALA ALA GLN GLN ASN THR ASN LEU SER LYS PHE ARG ARG LYS VAL GLN HIS GLU GLU LEU ASP GLU GLU ALA ALA GLU GLU ARG ARG ALA ASP ASP LLE LLE ALA ALA GLU GLU SER SER LLE LLE THR LYS SER ARG ASP ASP LLE LLE GLY THR LYS GLY LEU LEU ASN ASN GLU GLU

- Molecule 4: Myosin-7

Chain K:  39% . 58%

NET	VAL	ASP	A4	R17	D32	V37	K43	E44	E62	E68	D89	N90	T116	S156	T201	G202	D203	R204	S205	K206	E208	Q209	T210	E217	N305	A326	L339	E344	K365	Q368	D376	H401	P402	R403	V404	K405	V406	T412	G413
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G414
Y422
L447
F470
N471
S472
E536
F540
P541
K551
D587
E603
V606
A627
V631
E632
K633
G634
K635
G636
K637
A638
K639
F644
E700
R703
R723
R787
I788
Q789
R793
G794
S797
R798
R808
ASP
SER
LEU
LEU
ILE

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

GLU	THR	LEU	THR	ALA	LYS	ARG	LYS	ASP	GLY	GLU	CYS	SER	GLU	LEU	LYS	ARG	ASP	ASP	ASP	LEU	GLU	GLU	VAL	GLY	LYS	GLU	HIS	ALA	THR	ASN	LYS	VAL	LYS	LYS	ASN	LEU	THR	GLU	MET	ALA	GLY	LEU	ASP	GLU	ILE	ILE	ALA	LYS	LEU	THR
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[illegible]

LEU
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GLN
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ASP
PHE
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GLU
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ASN
ALA
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ASN
ALA
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ALA
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[illegible]

ET	LU	LN	LE	LE	YS	LA	YS	SN	SN	SN	SN	SN	SN	SN	IS	RG	RG	RG	ER	ER	YS	YS	LU	LU	LU	LU	LU	HR	HR	AL	SN	SN	SP	SP	EU	EU	HR	HR	HR	HR	LN	LN	RG	RG	LA	LA	YS	YS	LN	LN	LN	LN	LN	LN	EU	EU	ER	ER	SP	SP	LU	LU	YS
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[illegible][illegible]

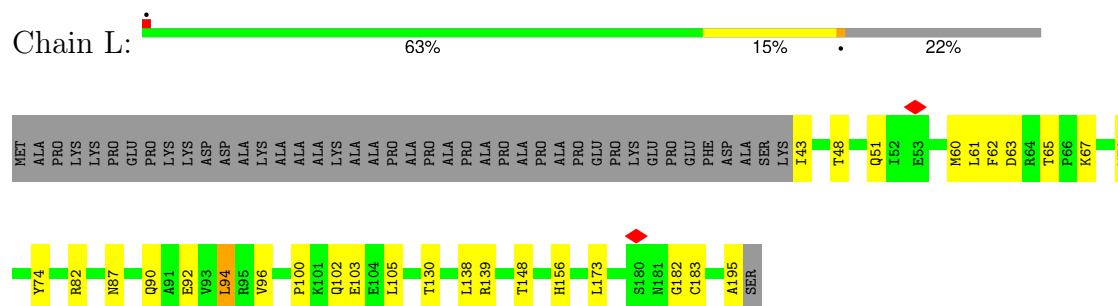
J U S S R R R S S S G G U U U U U E U E P P U U L L L U L G G R R R A A A A A A A U U S S S S S G G G E E P P S S S A A A U U U A A A P P S S S S S R R R U U U J U U N N N R R R U U U J U R R R R R S S S U

[illegible]

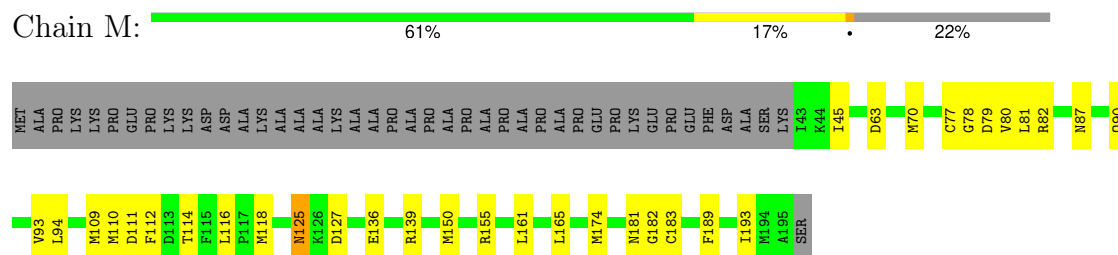
A U U S S S U U U N R R A A A U U U A A A A A U U U S S S E E G G G A A N N U U U E N N N N N E E S S A A U U T T T T T G G G S S U U U U U S S P P P U U U T T T U U N N U U A A S S C C G G S S S S S U U U G G G L L

[illegible]

- Molecule 5: Myosin light chain 3



- Molecule 5: Myosin light chain 3



4 Experimental information

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 ($e^-/\text{\AA}^2$)	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	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: ADP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.15	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(°)	Ideal(°)
5	M	182	GLY	CA-C-N	7.78	135.71	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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 ⓘ

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	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%)
6	ADP	C	401	7	28,29,29	1.38	4 (14%)	43,45,45	1.81	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	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
6	ADP	C	401	7	-	2/16/32/32	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(°)	Ideal(°)
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:

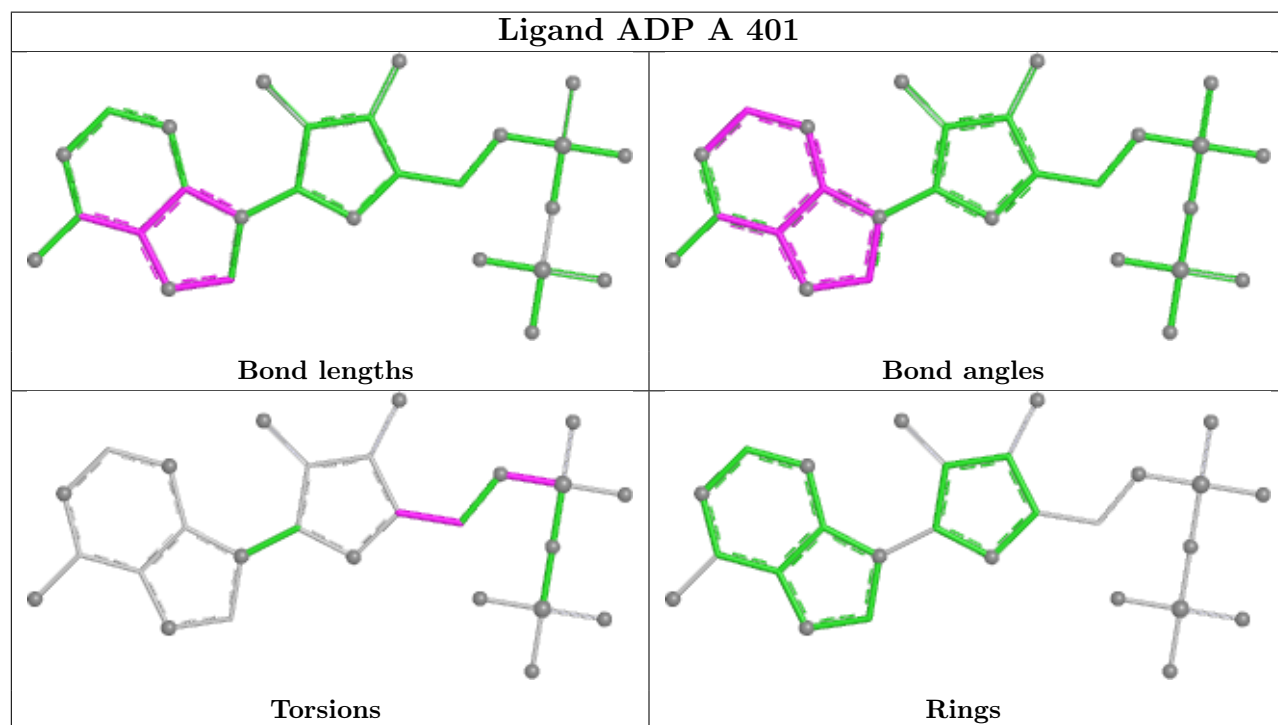
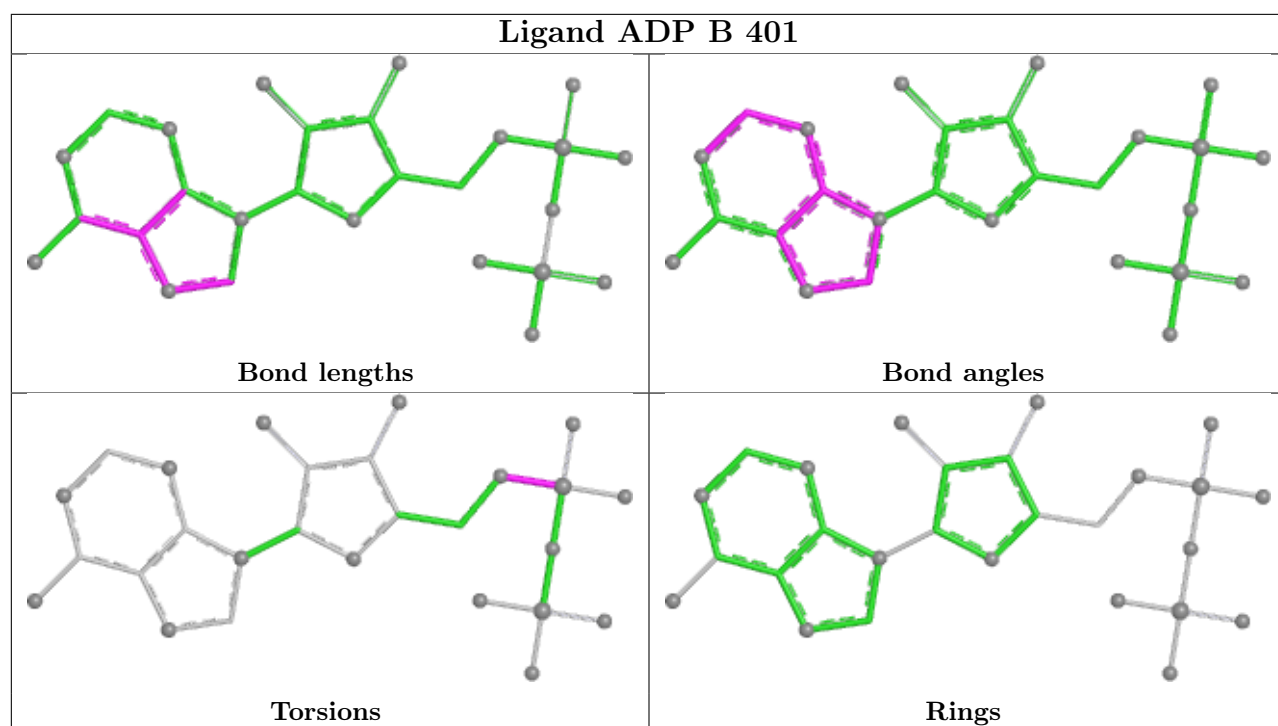
Mol	Chain	Res	Type	Atoms
6	A	401	ADP	C5'-O5'-PA-O1A
6	A	401	ADP	C5'-O5'-PA-O2A
6	A	401	ADP	C5'-O5'-PA-O3A
6	B	401	ADP	C5'-O5'-PA-O2A
6	B	401	ADP	C5'-O5'-PA-O3A

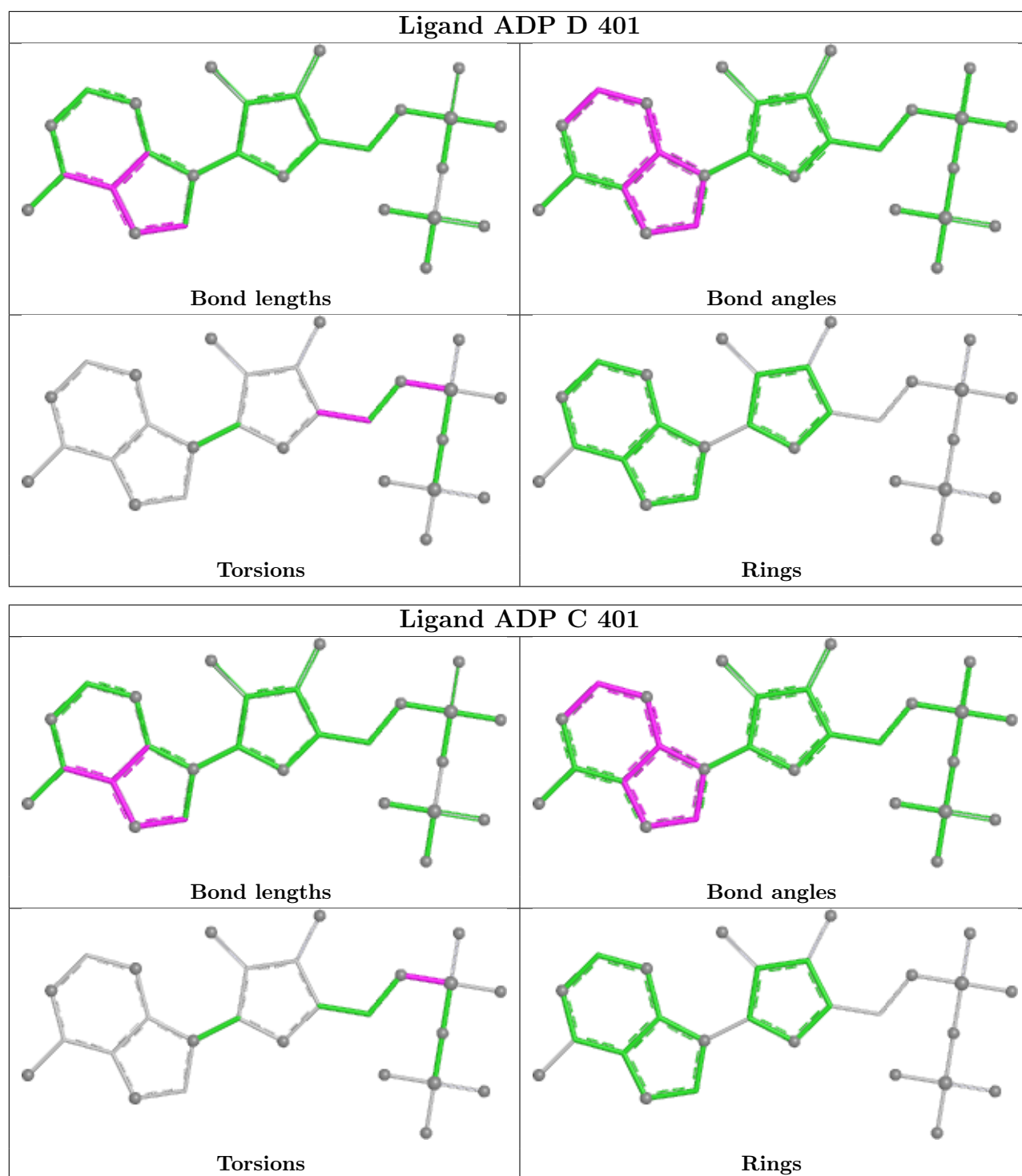
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	401	ADP	1	0
6	A	401	ADP	1	0
6	C	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-73042. These allow visual inspection of the internal detail of the map and identification of artifacts.

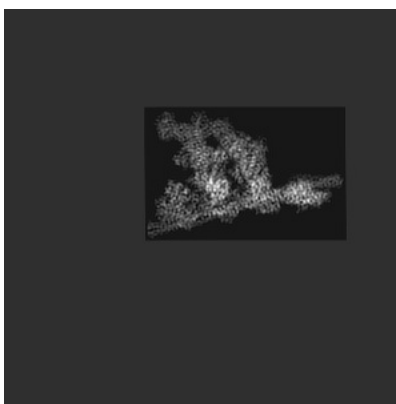
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

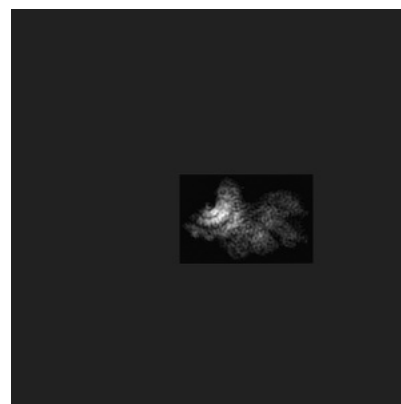
6.1.1 Primary map



X

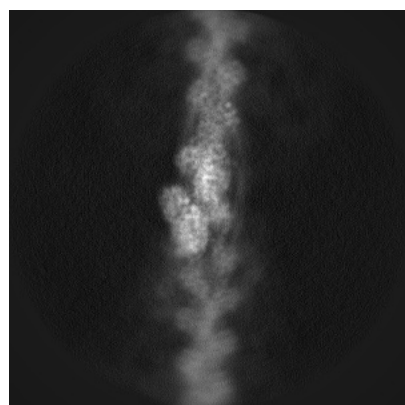


Y

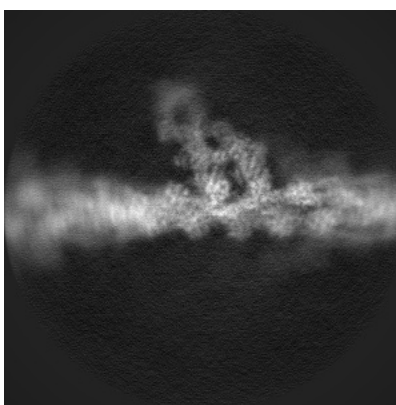


Z

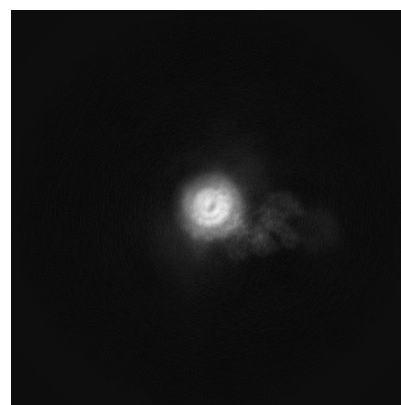
6.1.2 Raw map



X



Y



Z

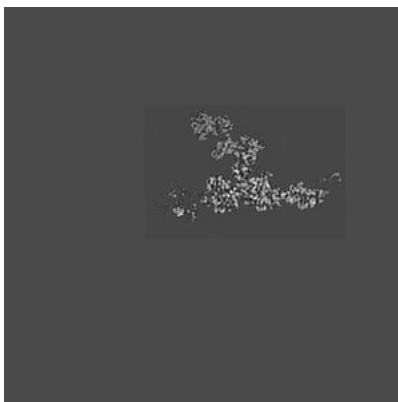
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 198

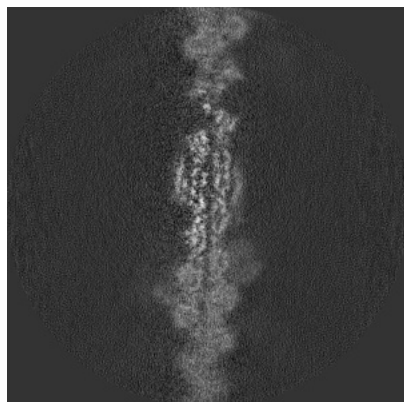


Y Index: 198

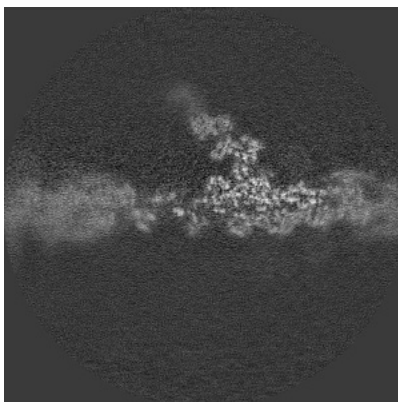


Z Index: 198

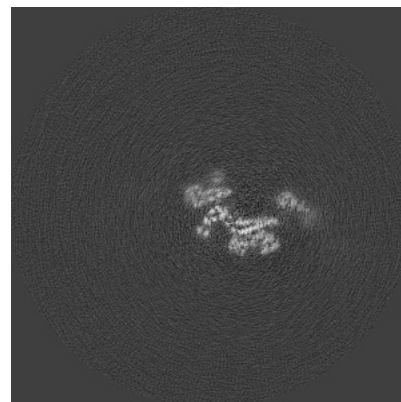
6.2.2 Raw map



X Index: 198



Y Index: 198

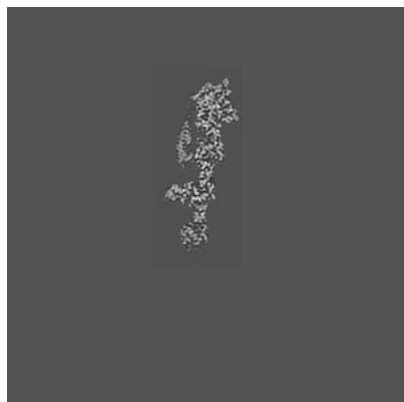


Z Index: 198

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: 211

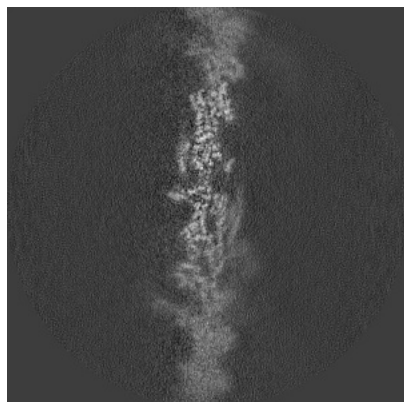


Y Index: 193

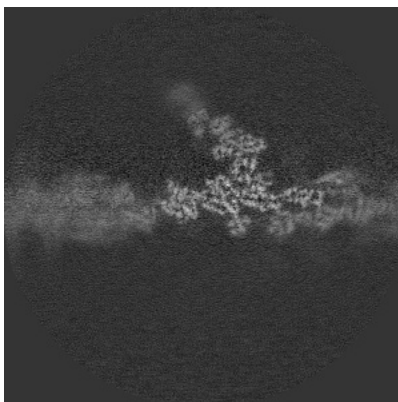


Z Index: 208

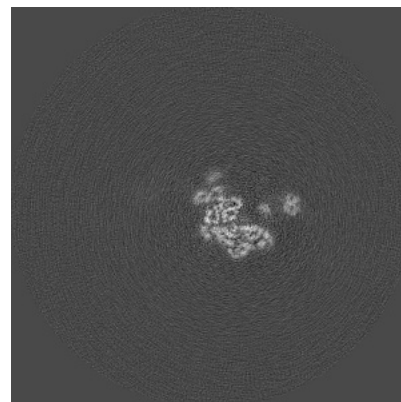
6.3.2 Raw map



X Index: 207



Y Index: 194

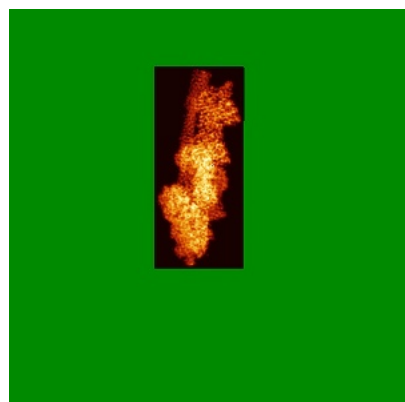


Z Index: 207

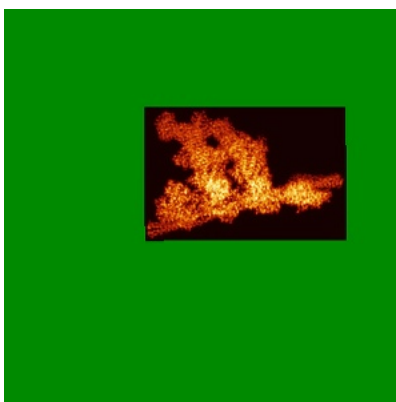
The images above show the largest variance slices of the map in three orthogonal directions.

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

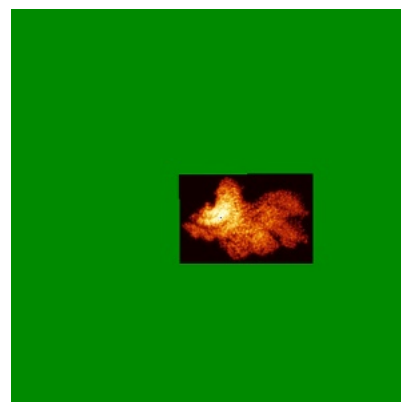
6.4.1 Primary map



X

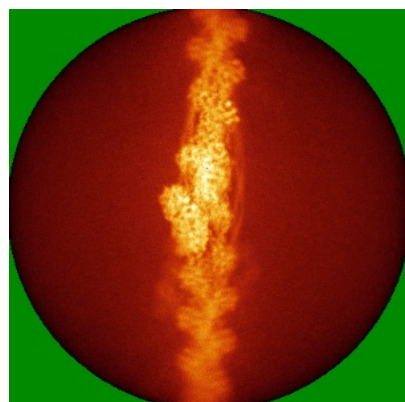


Y

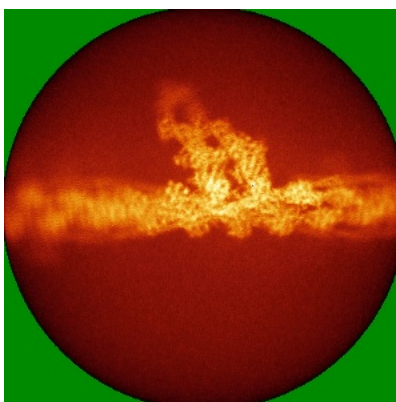


Z

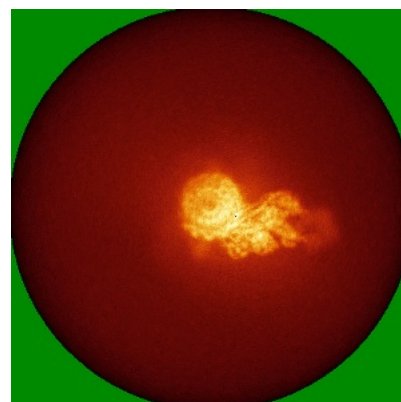
6.4.2 Raw map



X



Y

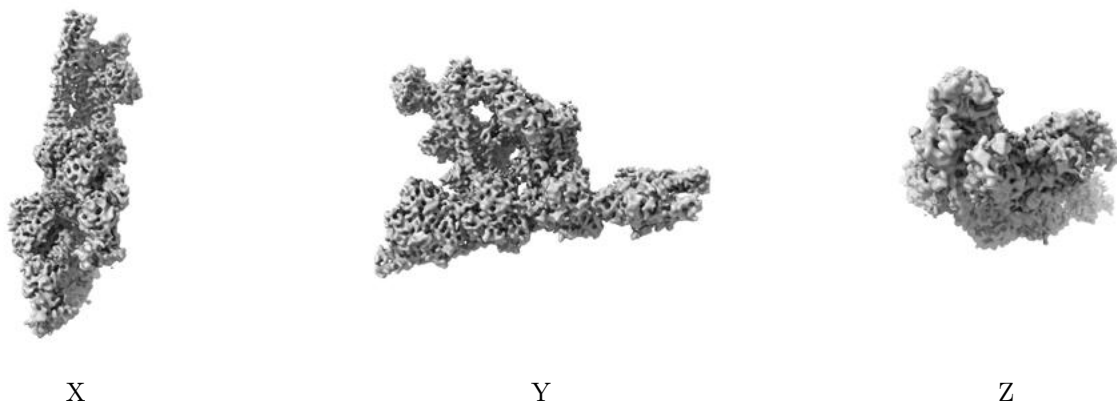


Z

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.

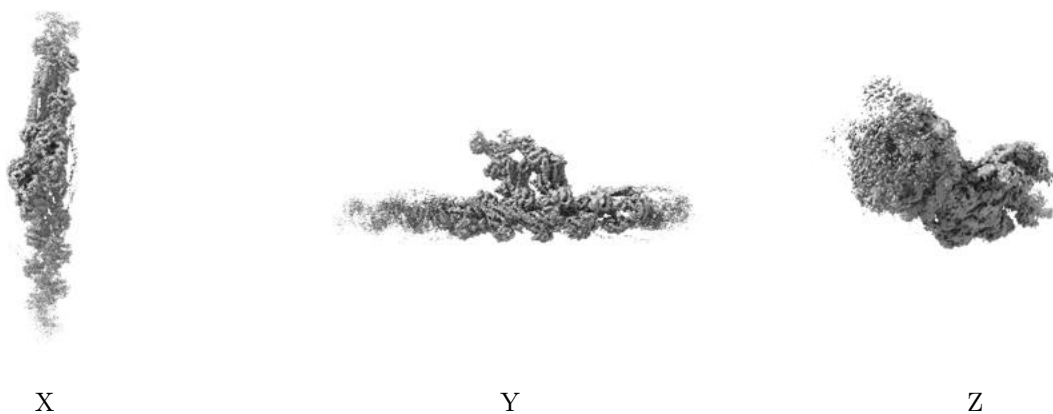
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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



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.

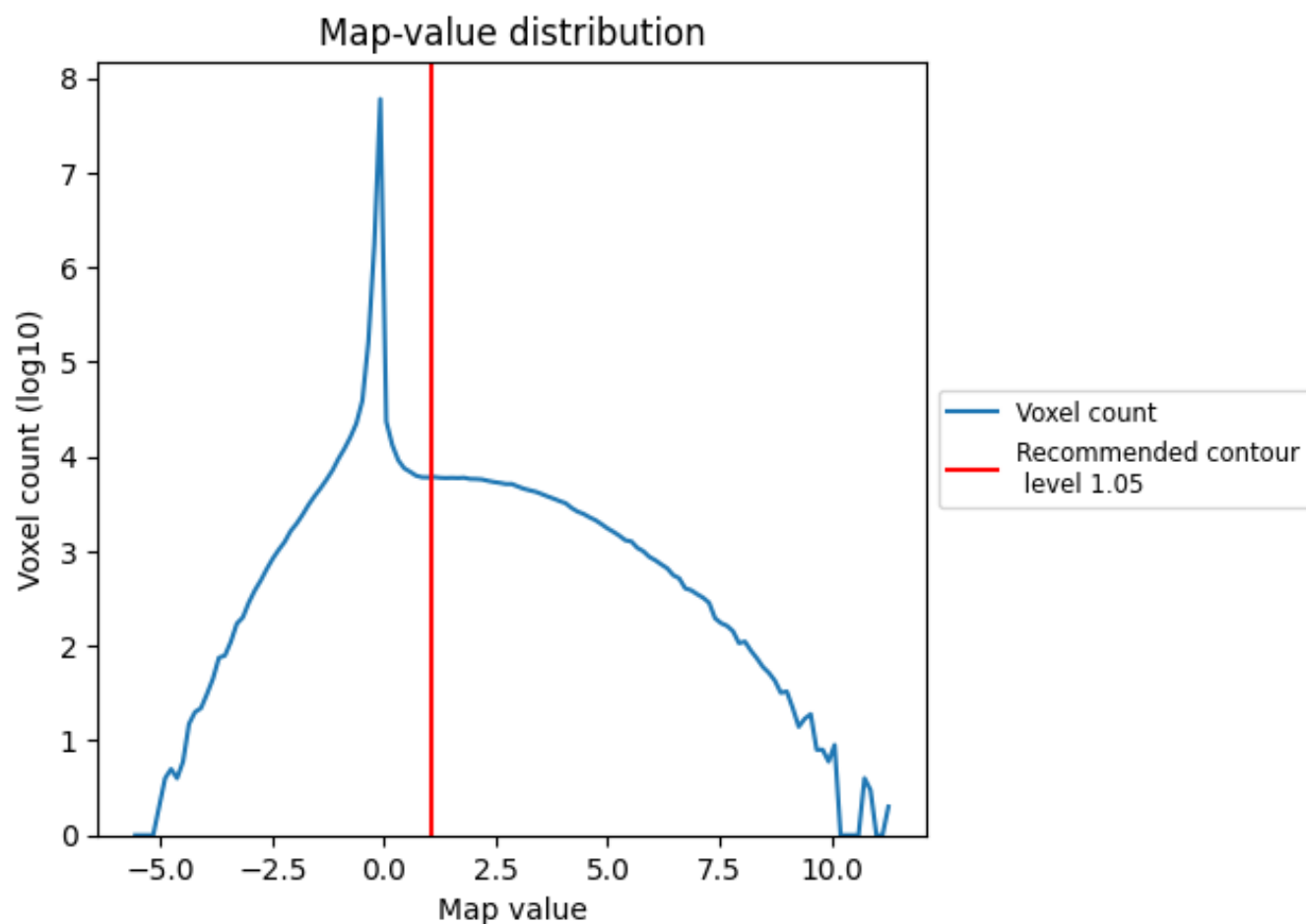
6.6 Mask visualisation [i](#)

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

7 Map analysis ⓘ

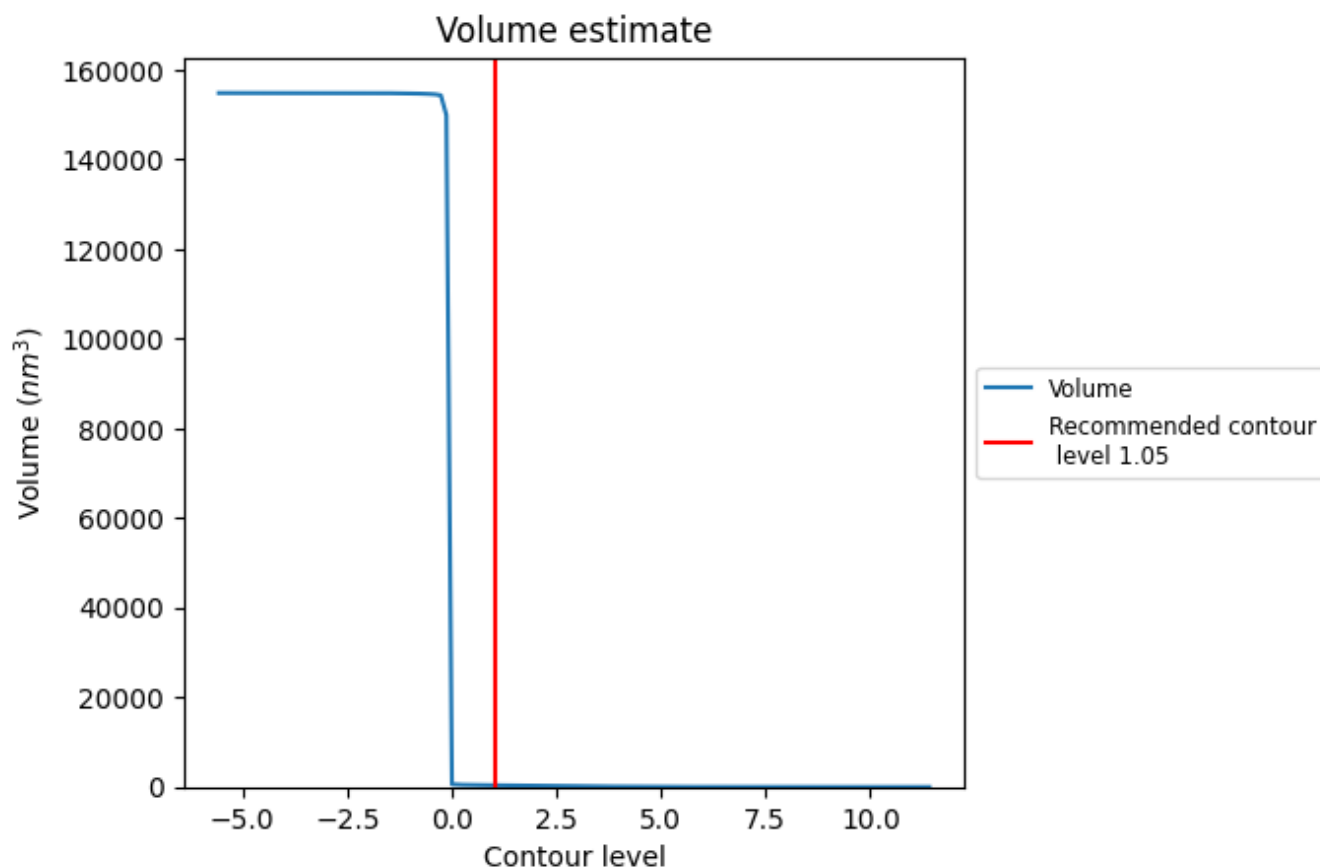
This section contains the results of statistical analysis of the map.

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.

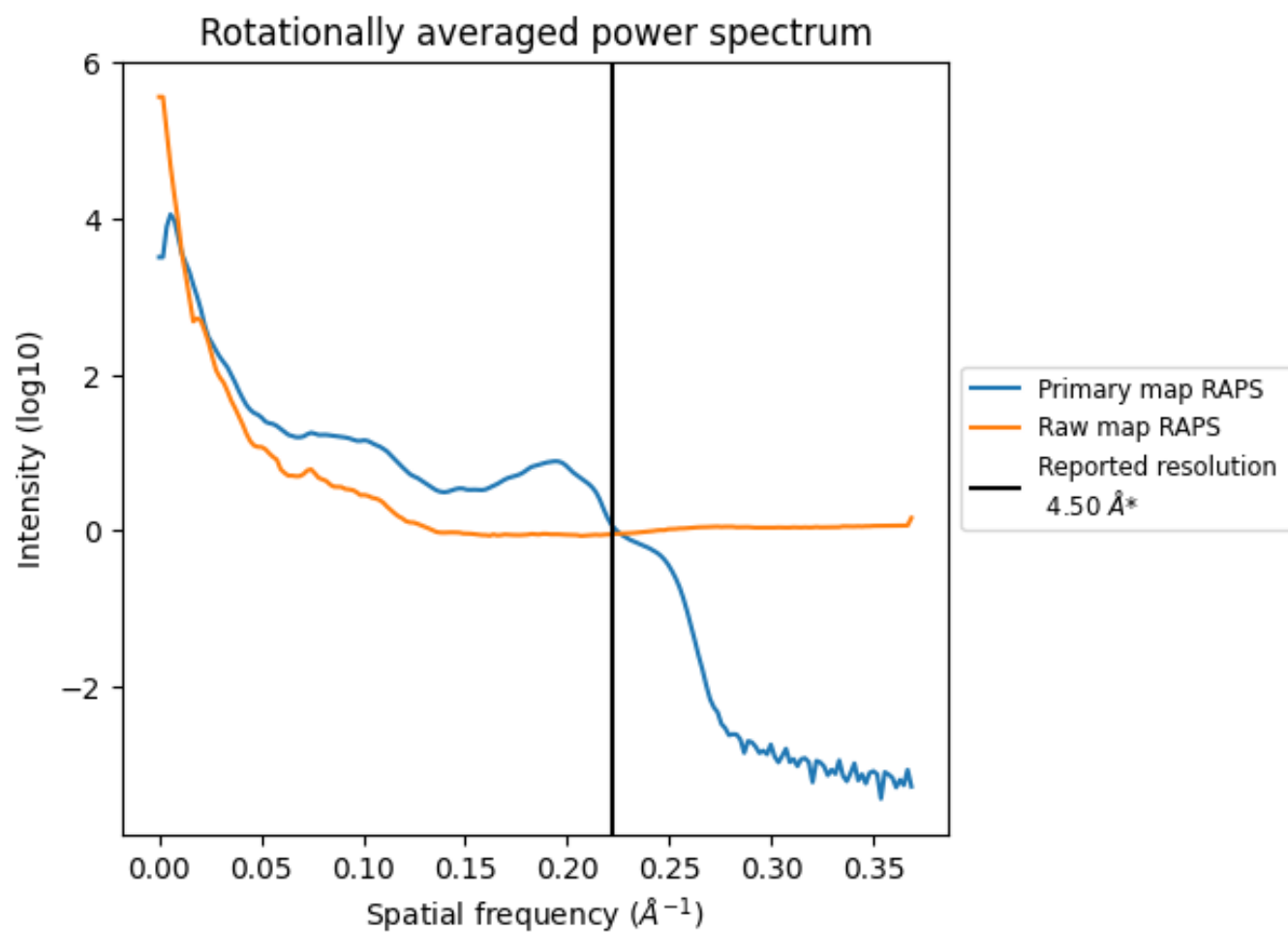
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 374 nm³; 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 ⓘ

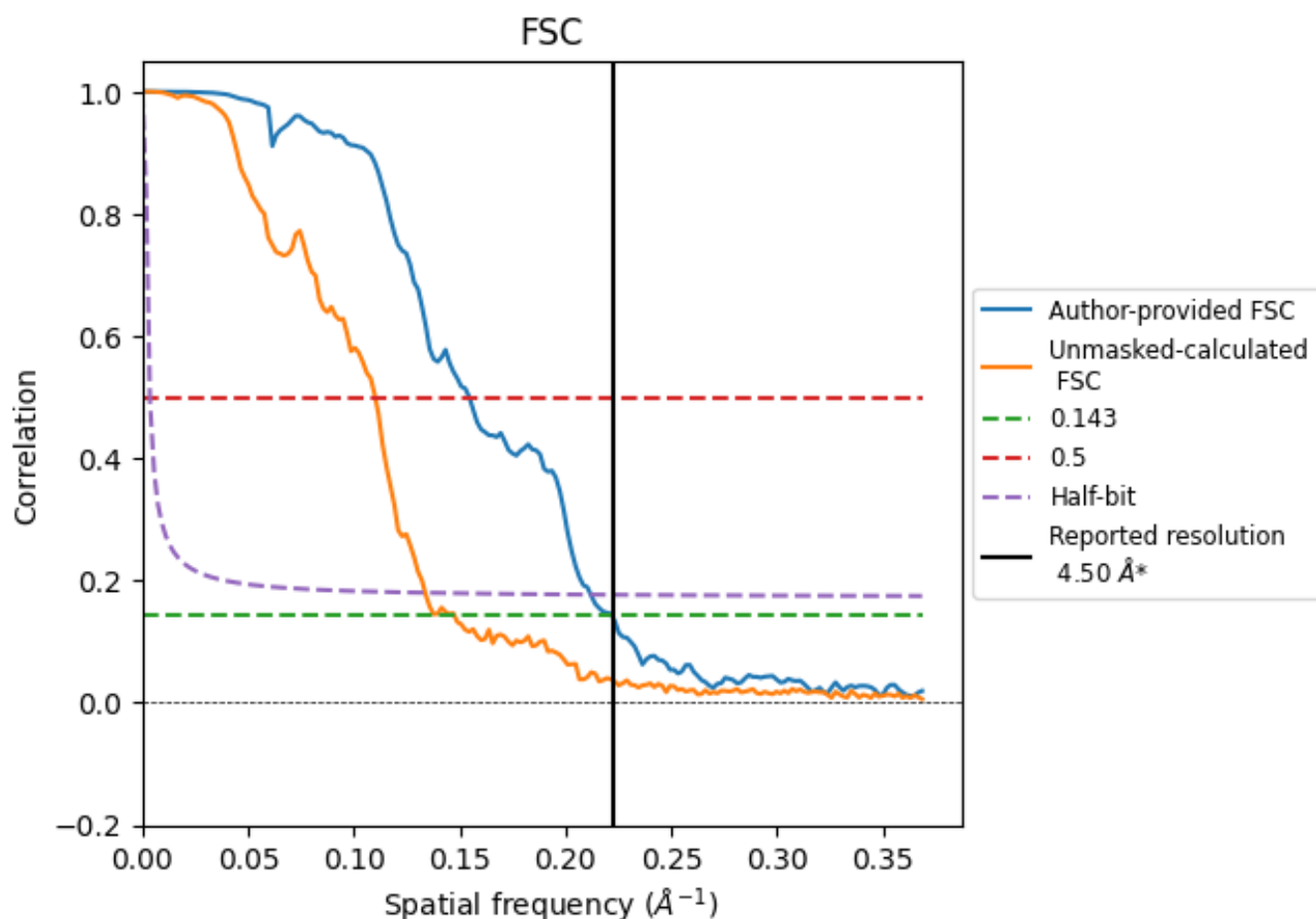


*Reported resolution corresponds to spatial frequency of 0.222 Å⁻¹

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 0.222 Å⁻¹

8.2 Resolution estimates [i](#)

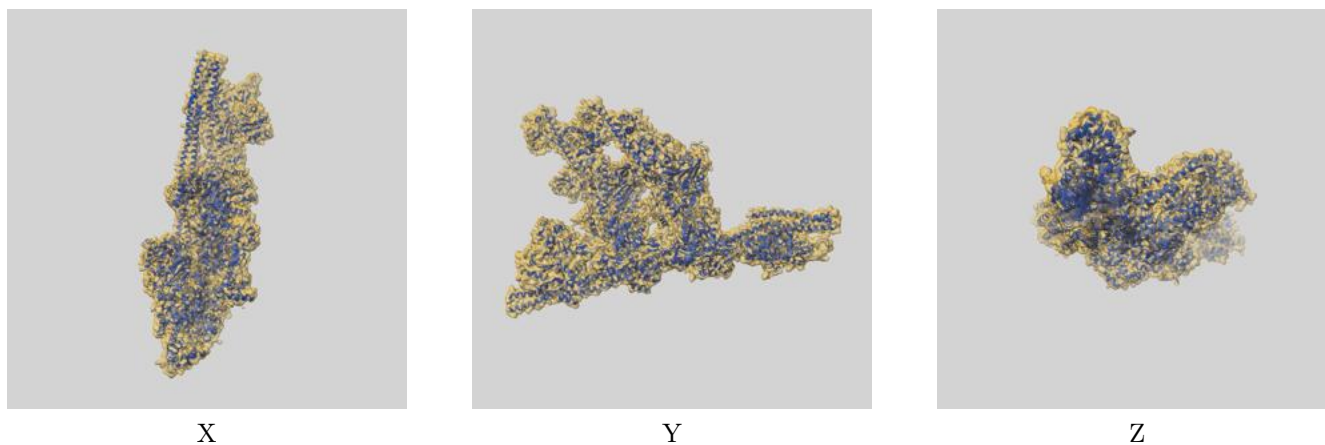
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	4.50	6.47	4.71
Unmasked-calculated*	6.78	9.08	7.47

*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 [i](#)

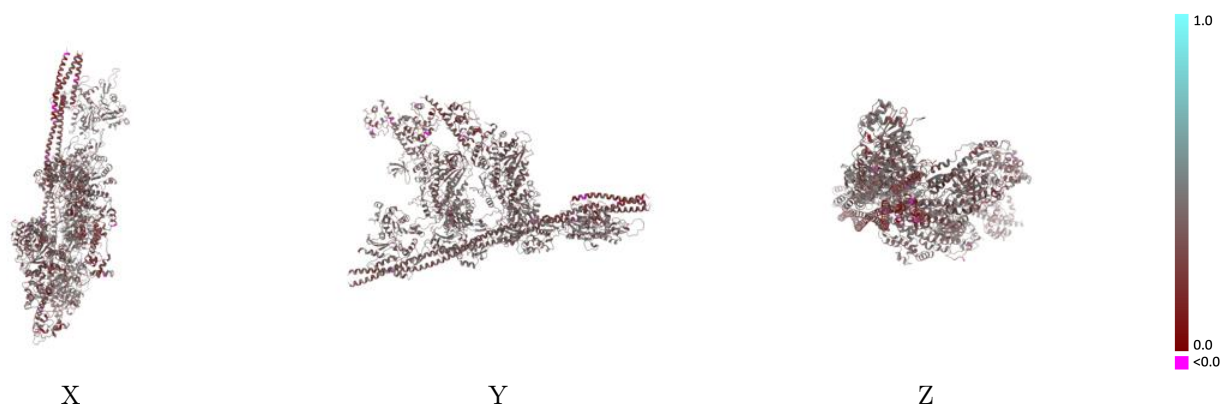
This section contains information regarding the fit between EMDB map EMD-73042 and PDB model 9YK9. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



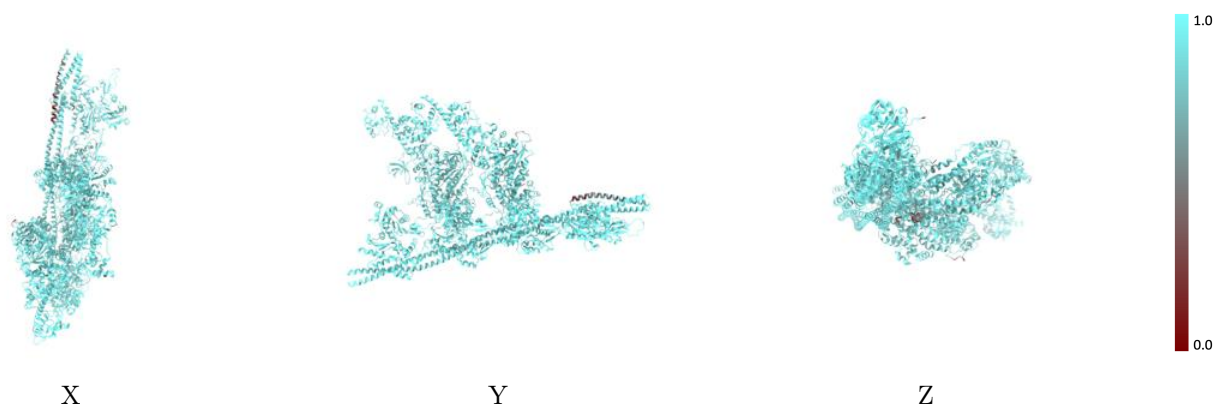
The images above show the 3D surface view of the map at the recommended contour level 1.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



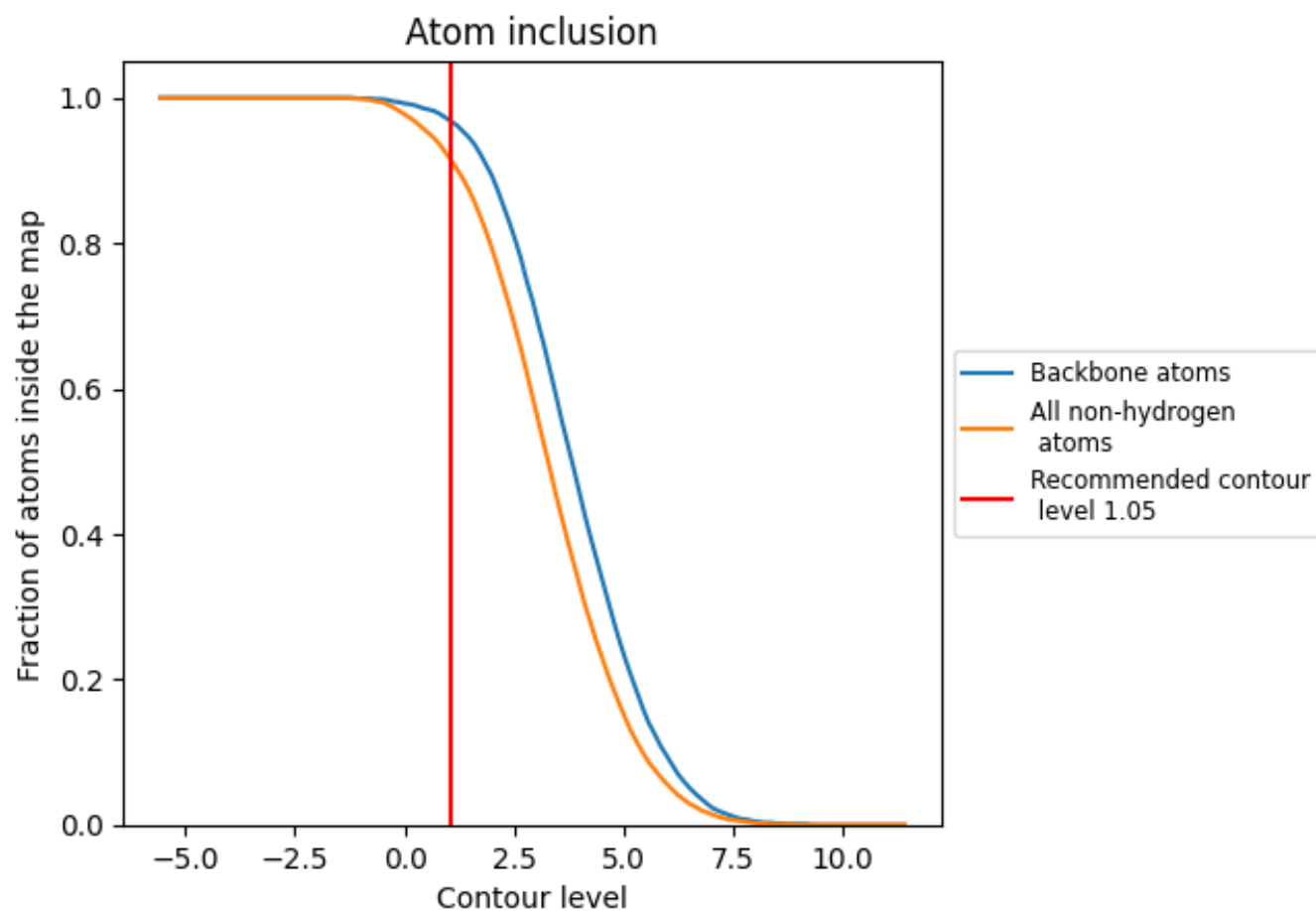
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

