



wwPDB EM Validation Summary Report ⓘ

Nov 9, 2024 – 11:12 am GMT

PDB ID : 6GYU
EMDB ID : EMD-0097
Title : Cryo-EM structure of the CBF3-msk complex of the budding yeast kinetochore
Authors : Yan, K.; Zhang, Z.; Yang, J.; McLaughlin, S.H.; Barford, D.
Deposited on : 2018-07-02
Resolution : 3.00 Å(reported)
Based on initial model : 6GYP

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.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

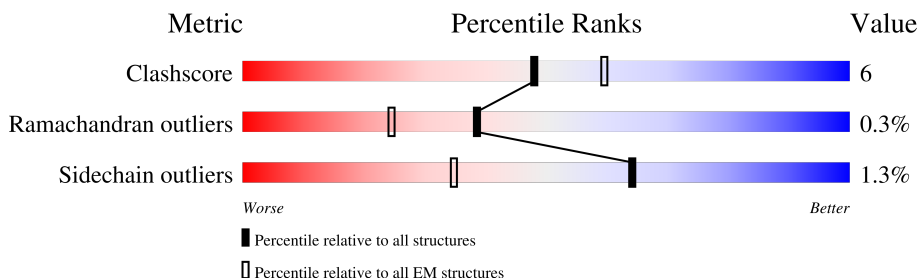
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	B	608	<div> <div>5%</div> <div>79%</div> <div>15%</div> <div>• 5%</div> </div>
2	A	478	<div> <div>•</div> <div>69%</div> <div>19%</div> <div>• 12%</div> </div>
3	C	564	<div> <div>5%</div> <div>83%</div> <div>10%</div> <div>6%</div> </div>
4	D	194	<div> <div>•</div> <div>67%</div> <div>10%</div> <div>• 22%</div> </div>
5	E	956	<div> <div>20%</div> <div>44%</div> <div>9%</div> <div>46%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18159 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 Centromere DNA-binding protein complex CBF3 subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	579	Total	C	N	O	S	0	0
			4778	3085	787	877	29		

- Molecule 2 is a protein called Centromere DNA-binding protein complex CBF3 subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	423	Total	C	N	O	S	0	0
			3526	2299	594	621	12		

- Molecule 3 is a protein called Centromere DNA-binding protein complex CBF3 subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	528	Total	C	N	O	S	0	1
			4362	2839	702	800	21		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MET	-	initiating methionine	UNP P40969
C	2	PHE	-	expression tag	UNP P40969
C	3	ASN	-	expression tag	UNP P40969
C	4	ARG	-	expression tag	UNP P40969

- Molecule 4 is a protein called Suppressor of kinetochore protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	151	Total	C	N	O	S	0	0
			1226	767	214	241	4		

- Molecule 5 is a protein called Centromere DNA-binding protein complex CBF3 subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	512	Total	C	N	O	S	0	0
			4265	2755	706	794	10		

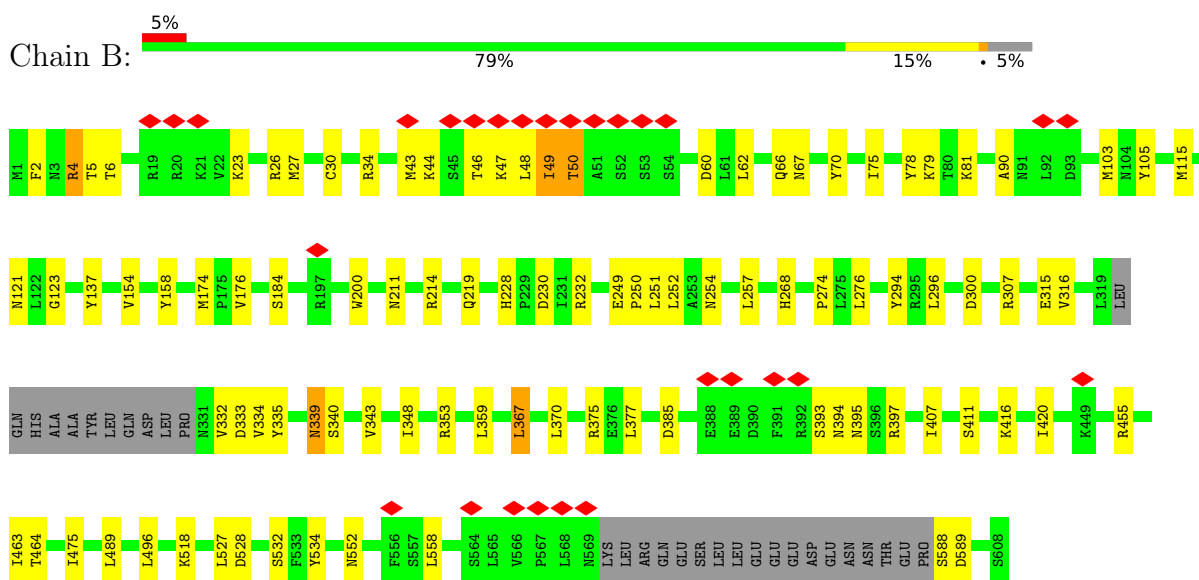
- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
6	B	2	Total	Zn	0
			2	2	

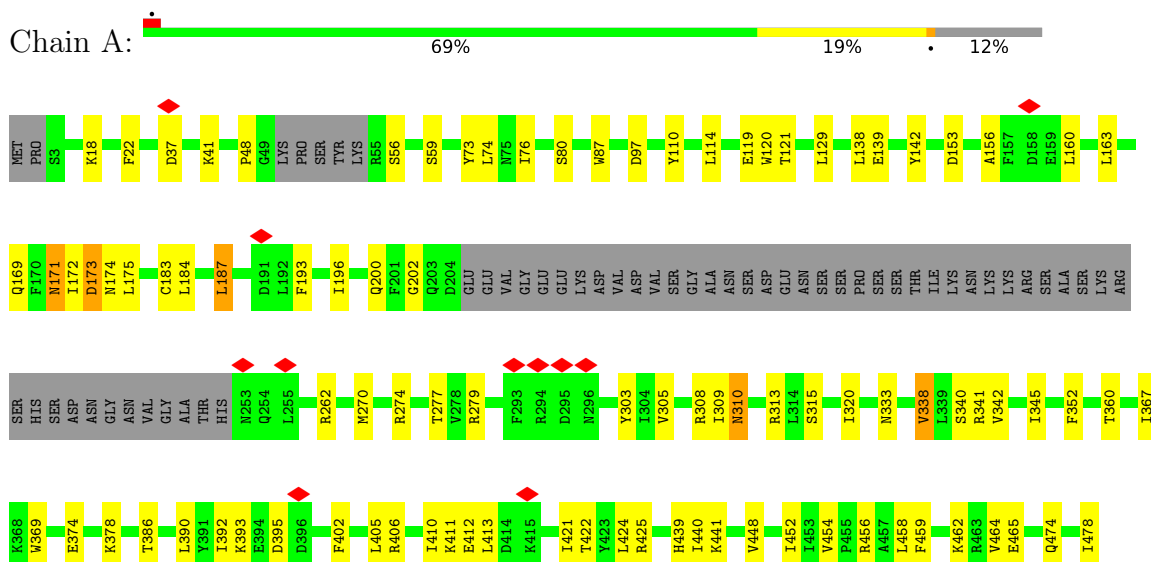
3 Residue-property plots [i](#)

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.

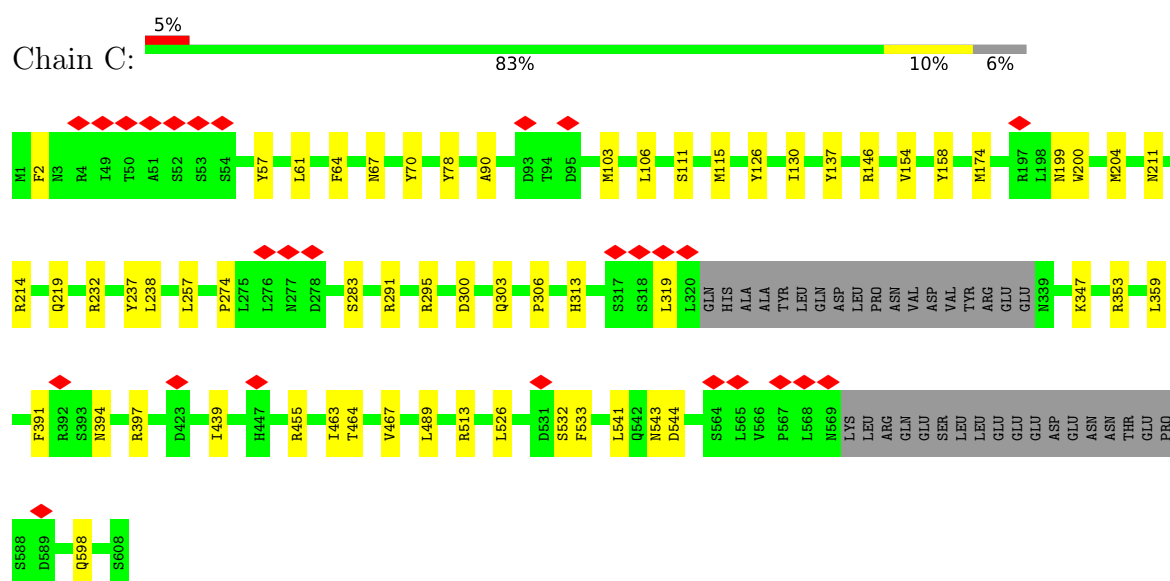
- Molecule 1: Centromere DNA-binding protein complex CBF3 subunit B



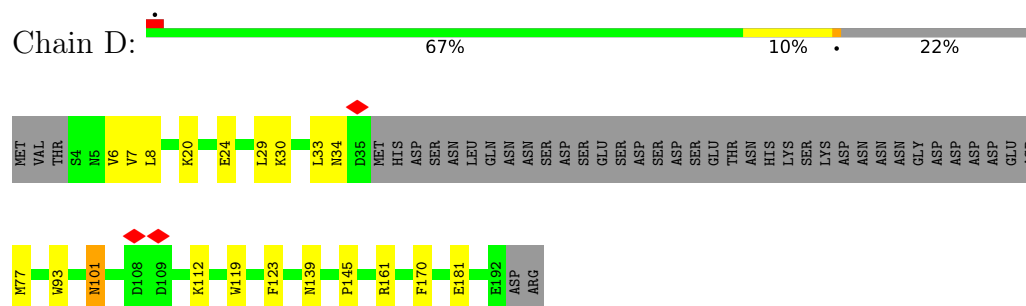
- Molecule 2: Centromere DNA-binding protein complex CBF3 subunit C



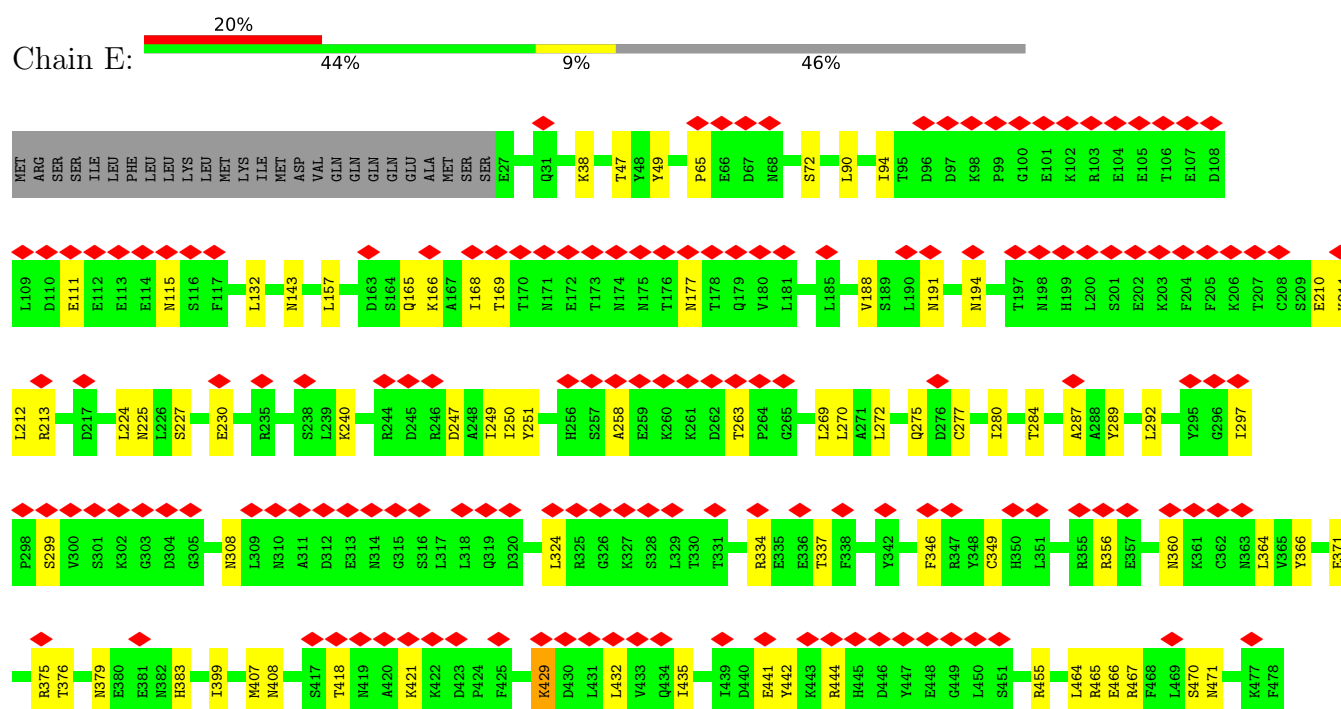
- Molecule 3: Centromere DNA-binding protein complex CBF3 subunit B



- Molecule 4: Suppressor of kinetochore protein 1



- Molecule 5: Centromere DNA-binding protein complex CBF3 subunit A



ASN	GLU	MET	ILE	SER	GLU	SER	GLU	SER	F479
HIS	ASP	THR	ASN	ARG	LYS	SER	LEU	SER	P480
GLU	LYS	GLU	GLU	ARG	LEU	ARG	LEU	HIS	N481
SER	SER	GLU	LEU	THR	THR	LYS	MET	ASN	H482
LEU	ILE	HIS	ILE	LYS	ILE	ARG	LYS	PRO	D483
ASP	ASP	ASN	ASN	ARG	LYS	PRO	LYS	ASP	I484
ASP	SER	VAL	SER	PRO	LYS	LYS	THR	HIS	T484
TYR	ILE	GLY	LYS	LYS	LYS	LYS	THR	PRO	F485
LYS	GLU	PHE	ILE	GLN	SER	GLN	SER	THR	Q486
ALA	GLY	ASP	SER	ILE	ARG	GLY	GLN	GLN	D487
VAL	ILE	MET	THR	ARG	TYR	TYR	LYS	LYS	F488
ASP	ILE	GLU	PHE	LEU	GLY	LEU	GLN	GLN	I489
ILE	LEU	VAL	ARG	LEU	ILE	LEU	GLU	GLU	T489
CYS	GLU	PRO	ASP	SER	LEU	LEU	GLU	SER	F490
GLU	THR	LYS	GLN	ILE	HIS	GLN	GLY	GLY	G491
LYS	PHE	LYS	MET	ALA	GLN	ASP	LEU	GLY	N492
LEU	THR	ARG	ASP	SER	LEU	ASN	PRO	PRO	F493
ARG	PRO	ASN	ASP	SER	GLN	SER	LEU	LEU	D494
GLN	ALA	SER	PHE	ASP	PHE	ASP	PHE	GLN	D494
ASN	LYS	GLY	GLU	GLU	LYS	GLU	LYS	MET	S497
GLU	TYR	LYS	LEU	SER	ILE	SER	ILE	GLN	Y498
GLY	ALA	TYR	THR	LYS	THR	THR	LEU	GLN	F499
ALA	ASN	ALA	ILE	THR	LEU	THR	LEU	LEU	N500
SER	GLN	GLU	ASN	GLU	ASP	GLU	ASP	ASP	D501
PHE	VAL	THR	ALA	ASP	GLY	GLY	ARG	THR	K502
ARG	VAL	VAL	LEU	SER	ILE	ASP	ILE	THR	T503
LEU	HIS	LYS	LEU	ASN	ILE	ASN	ILE	GLN	I504
ALA	SER	ASP	ASP	VAL	ASP	VAL	LYS	LEU	H505
ALA	SER	ASP	ASN	PHE	LYS	PHE	LYS	LEU	S506
LYS	MET	ASN	ILE	LYS	ASP	ILE	ASP	LYS	K507
PHE	ASN	ASP	ILE	LYS	GLY	GLY	ASP	GLN	F510
LEU	LYS	GLN	GLY	GLU	GLU	GLU	ASP	GLN	I511
ARG	ASN	ALA	LYS	SER	VAL	ILE	ALA	GLN	L512
HIS	SER	SER	THR	THR	THR	ARG	LYS	SER	S513
HIS	ASP	THR	THR	GLU	THR	ILE	THR	PHE	F514
GLN	ALA	ALA	ILE	ALA	ILE	GLY	ILE	TYR	D515
ASN	ASN	SER	GLU	ALA	GLN	TYR	ARG	VAL	L516
SER	CYS	PRO	GLN	GLN	LYS	GLY	ASN	GLN	L517
PHE	GLU	SER	LEU	GLY	GLU	GLY	PRO	THR	LYS
GLY	ALA	GLU	GLY	ASN	GLU	ASN	PRO	THR	LEU
ASP	LEU	TYR	TYR	SER	SER	HIS	ILE	LEU	LEU
LEU	VAL	GLY	VAL	ASP	ASP	ASP	VAL	SER	N521
VAL	GLU	GLN	THR	GLN	GLN	GLU	GLN	ASN	K522
ARG	ARG	GLU	GLY	GLU	GLY	GLU	GLY	PHE	F525
LEU	LYS	ALA	LYS	ASP	ASP	ASP	GLU	GLN	K526
TYR	SER	LYS	PHE	SER	LYS	SER	ILE	ILE	N526
ASN	ASN	ILE	SER	GLU	THR	GLU	VAL	LEU	K527
	VAL	TYR	THR	MET	VAL	ASN	ASN	SER	T528
	GLU	THR	LEU	GLN	GLY	GLN	GLY	VAL	N529
	PHE	ASP	LYS	GLU	ARG	GLN	GLU	PHE	F532
	TYR	GLU	ARG	GLN	THR	LEU	GLY	ASN	L533
	ILE	GLN	PRO	LEU	PRO	LEU	GLY	LYS	L534
	TYR	PHE	GLN	SER	GLN	LYS	PRO	ILE	I535
	LEU	PHE	LEU	SER	THR	SER	ASN	ILE	E536
	VAL	MET	TYR	MET	THR	MET	THR	PHE	R537
									F538
									SER
									GLN
									LEU
									THR
									PHE

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	198010	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 ($e^-/\text{\AA}^2$)	27	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.442	Depositor
Minimum map value	-0.224	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.064	Depositor
Map size (Å)	254.4, 254.4, 254.4	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

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	B	0.31	0/4888	0.53	1/6610 (0.0%)
2	A	0.34	0/3604	0.66	5/4869 (0.1%)
3	C	0.29	0/4467	0.48	0/6050
4	D	0.30	0/1247	0.51	0/1687
5	E	0.27	0/4391	0.49	0/5960
All	All	0.30	0/18597	0.54	6/25176 (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
5	E	0	2
All	All	0	3

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	173	ASP	CB-CG-OD1	7.94	125.45	118.30
2	A	74	LEU	CA-CB-CG	6.88	131.12	115.30
2	A	138	LEU	CA-CB-CG	5.98	129.06	115.30
2	A	172	ILE	C-N-CA	5.67	135.88	121.70
1	B	558	LEU	CA-CB-CG	5.12	127.07	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	333	ASP	Peptide
5	E	258	ALA	Peptide
5	E	263	THR	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	B	4778	0	4755	69	0
2	A	3526	0	3558	58	0
3	C	4362	0	4332	30	0
4	D	1226	0	1194	14	0
5	E	4265	0	4150	47	0
6	B	2	0	0	0	0
All	All	18159	0	17989	205	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 205 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)
1:B:44:LYS:CA	1:B:48:LEU:HD21	1.51	1.40
1:B:44:LYS:HA	1:B:48:LEU:CD2	1.49	1.38
1:B:43:MET:O	1:B:48:LEU:HD23	1.30	1.24
1:B:46:THR:O	1:B:48:LEU:N	1.90	1.03
1:B:43:MET:O	1:B:48:LEU:CD2	2.09	1.00

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	B	573/608 (94%)	539 (94%)	31 (5%)	3 (0%)	25	61
2	A	417/478 (87%)	363 (87%)	51 (12%)	3 (1%)	19	54
3	C	520/564 (92%)	509 (98%)	11 (2%)	0	100	100
4	D	147/194 (76%)	140 (95%)	7 (5%)	0	100	100
5	E	510/956 (53%)	472 (92%)	38 (8%)	0	100	100
All	All	2167/2800 (77%)	2023 (93%)	138 (6%)	6 (0%)	38	70

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	47	LYS
1	B	49	ILE
1	B	50	THR
2	A	303	TYR
2	A	369	TRP

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	B	540/569 (95%)	534 (99%)	6 (1%)	70	87
2	A	388/449 (86%)	381 (98%)	7 (2%)	54	80
3	C	490/527 (93%)	483 (99%)	7 (1%)	62	83
4	D	136/179 (76%)	134 (98%)	2 (2%)	60	83
5	E	481/897 (54%)	476 (99%)	5 (1%)	73	88
All	All	2035/2621 (78%)	2008 (99%)	27 (1%)	64	85

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	146	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	232	ARG
5	E	379	ASN
3	C	199	ASN
3	C	291	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	394	ASN
5	E	143	ASN
4	D	174	ASN
5	E	191	ASN
2	A	171	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

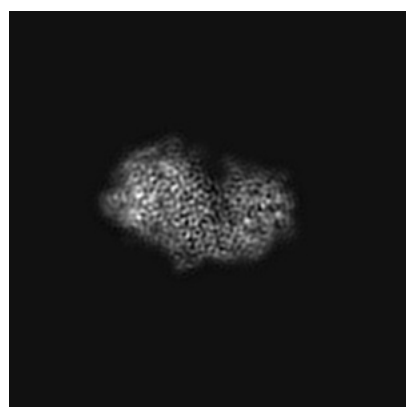
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0097. These allow visual inspection of the internal detail of the map and identification of artifacts.

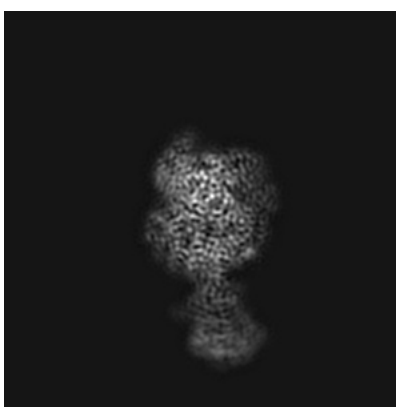
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

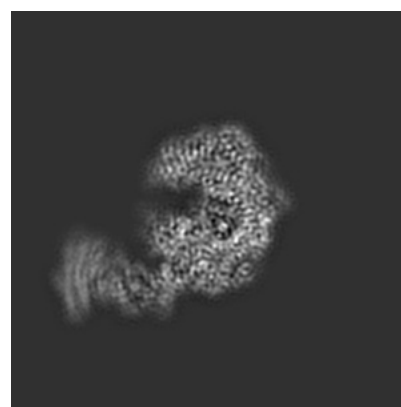
6.1.1 Primary map



X



Y



Z

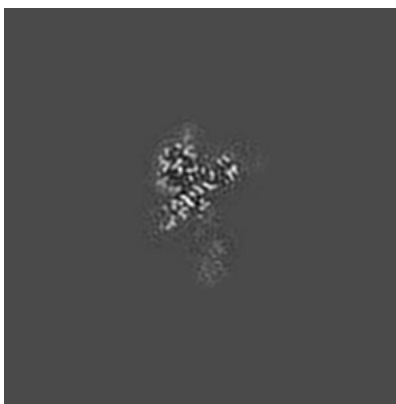
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

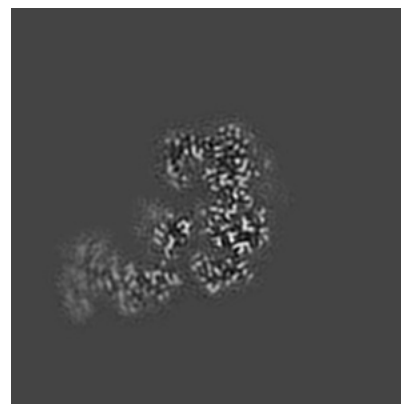
6.2.1 Primary map



X Index: 120



Y Index: 120

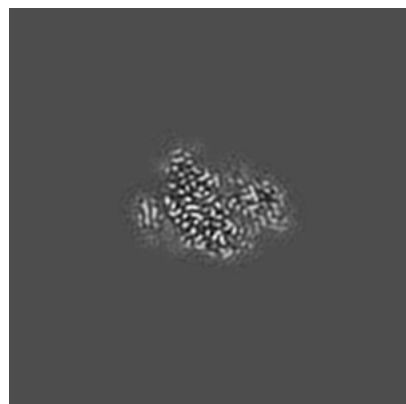


Z Index: 120

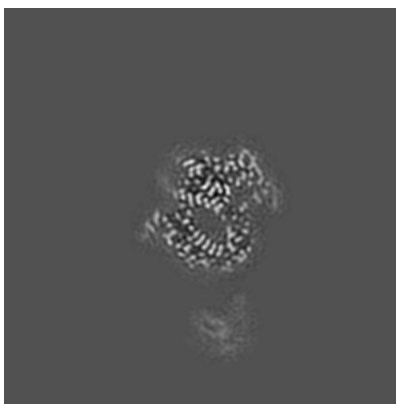
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

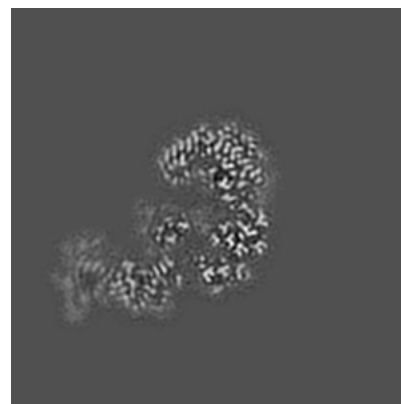
6.3.1 Primary map



X Index: 140



Y Index: 100

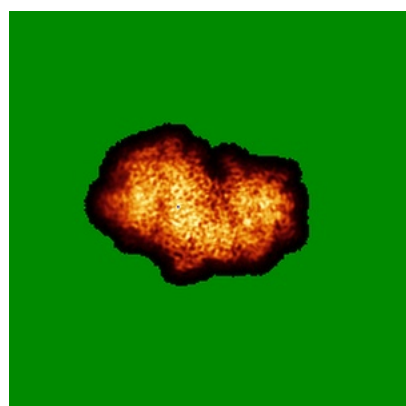


Z Index: 125

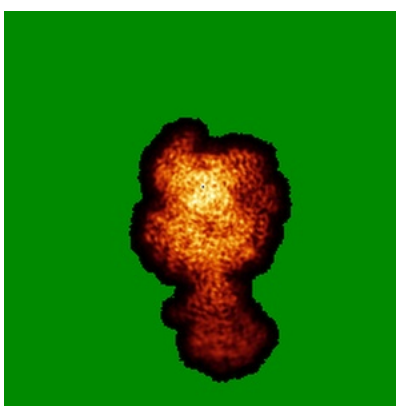
The images above show the largest variance slices of the map in three orthogonal directions.

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

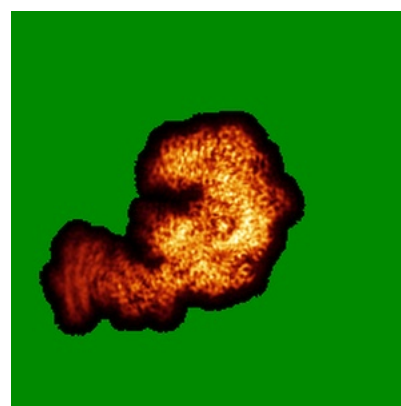
6.4.1 Primary map



X



Y

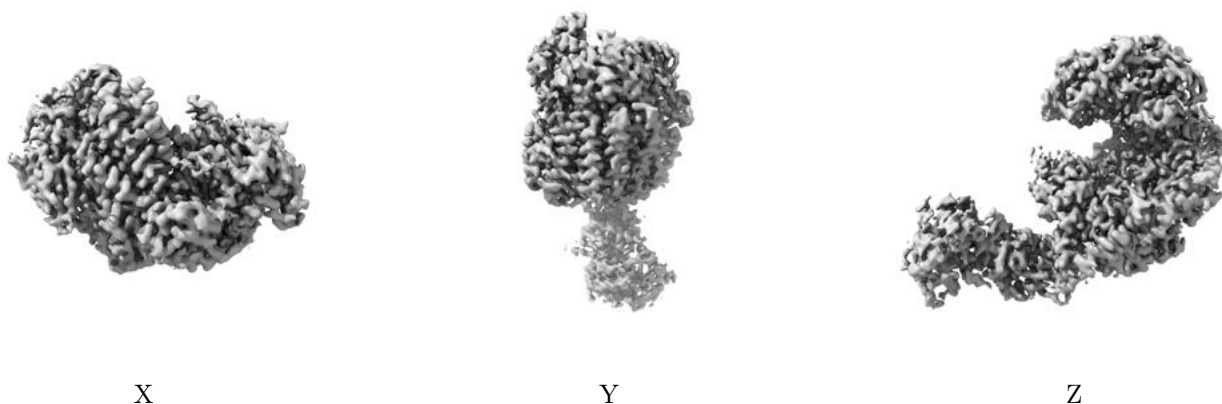


Z

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 0.064. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

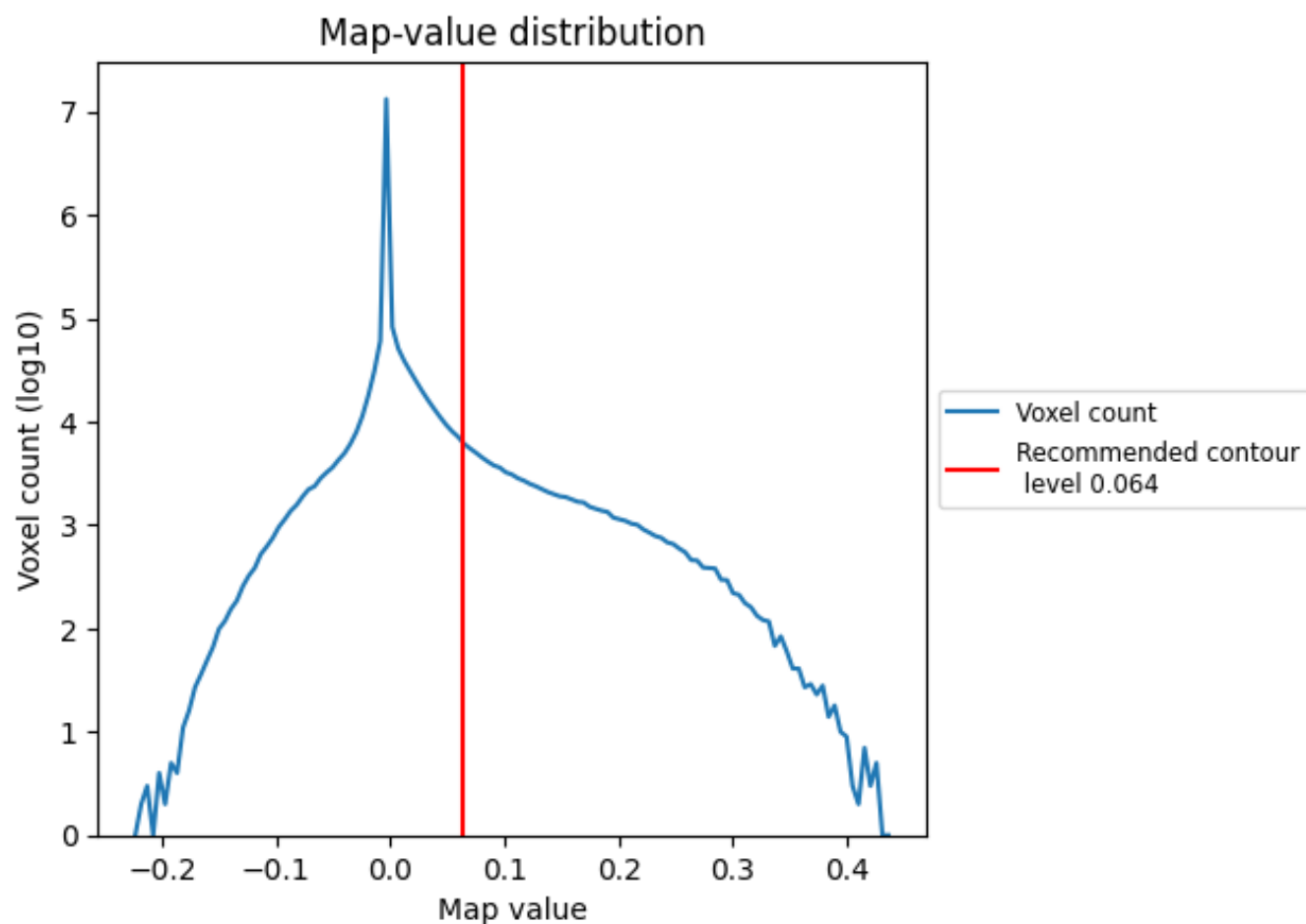
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

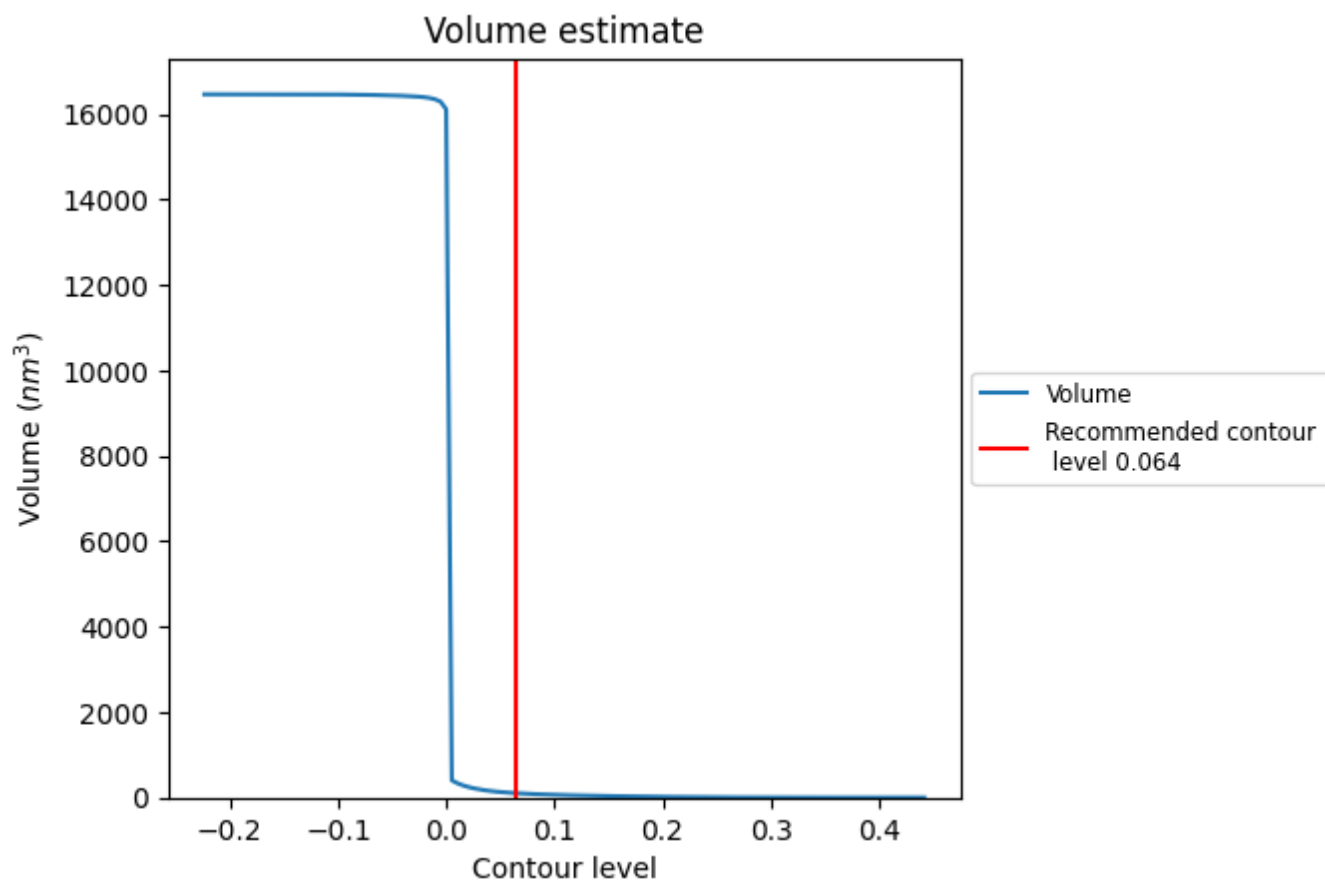
This section contains the results of statistical analysis of the map.

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.

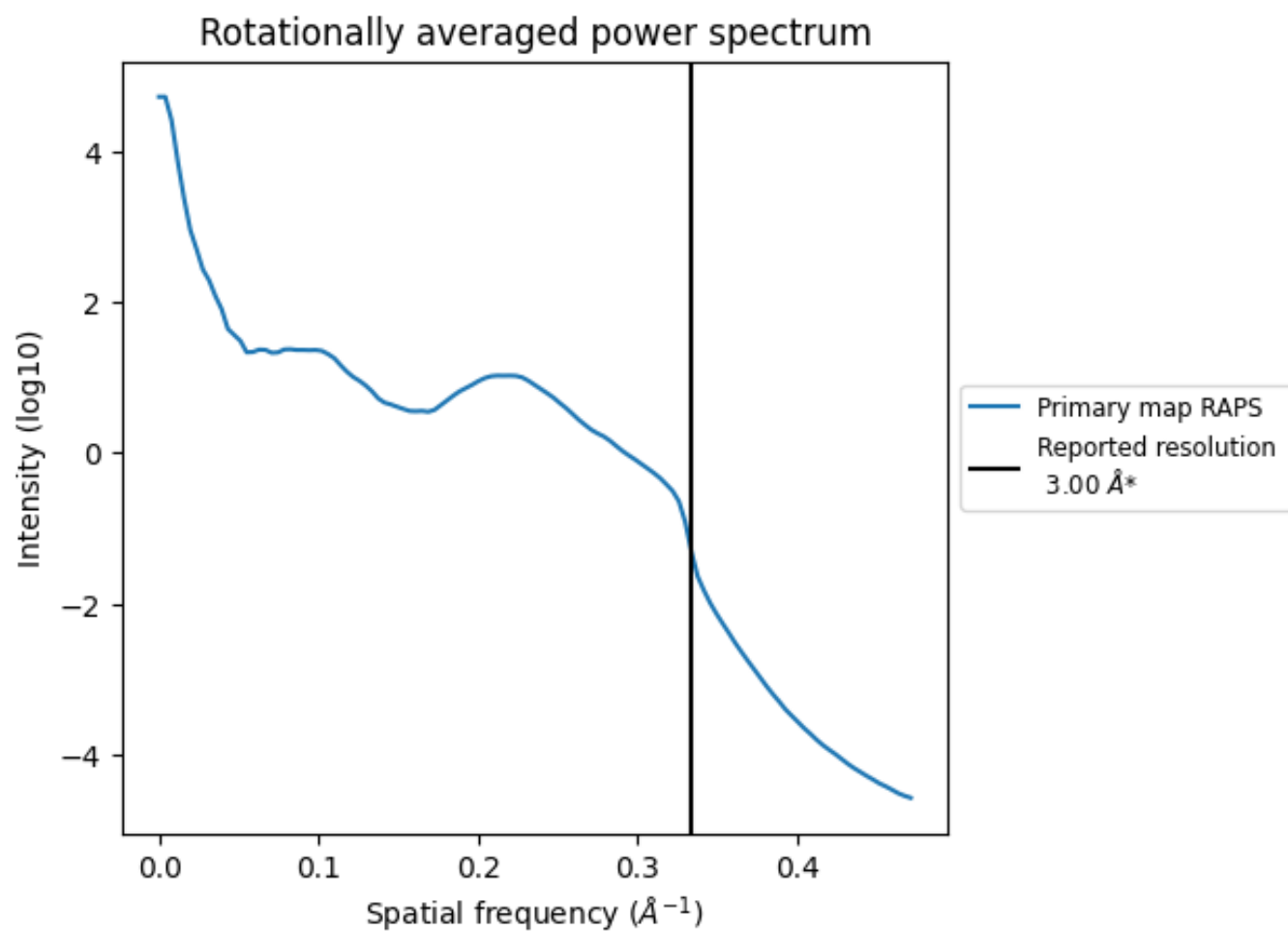
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 103 nm^3 ; this corresponds to an approximate mass of 93 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 0.333 Å⁻¹

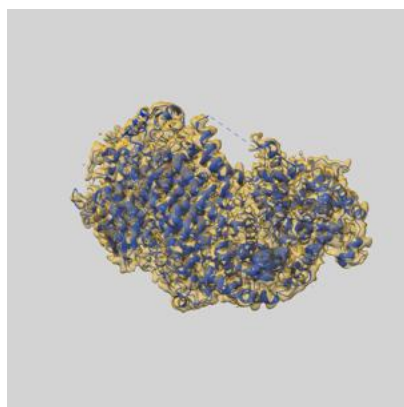
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

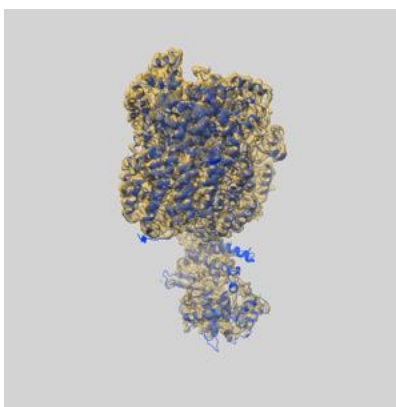
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0097 and PDB model 6GYU. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

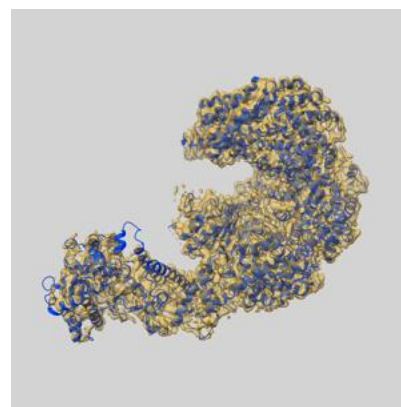
9.1 Map-model overlay [i](#)



X



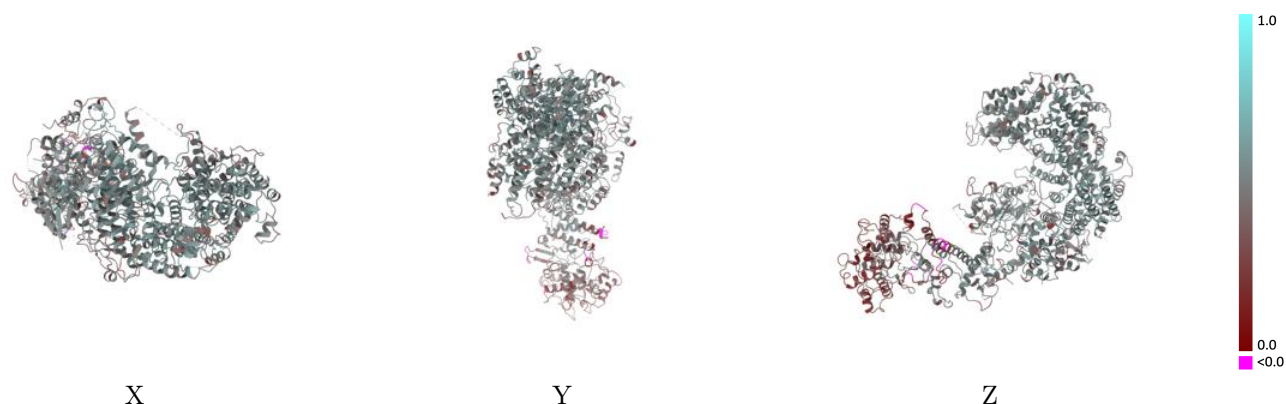
Y



Z

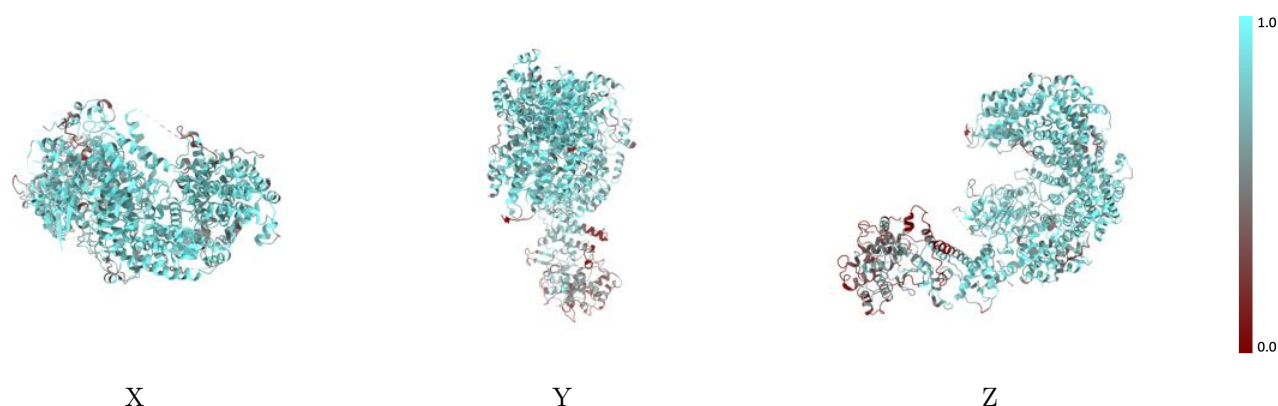
The images above show the 3D surface view of the map at the recommended contour level 0.064 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



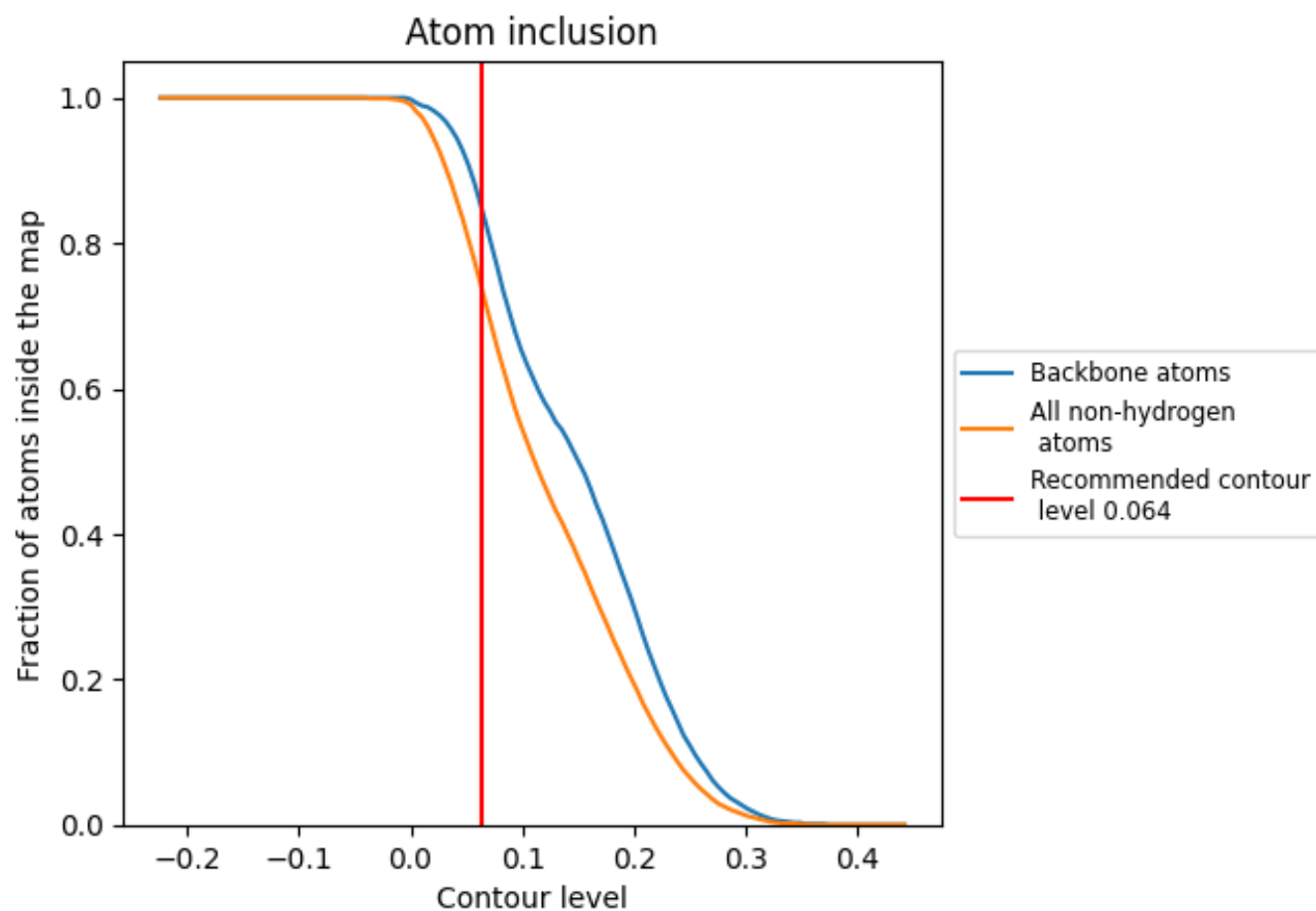
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.064).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 74% 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 (0.064) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7360	<div></div> 0.4700
A	<div></div> 0.8030	<div></div> 0.4900
B	<div></div> 0.8200	<div></div> 0.5200
C	<div></div> 0.8030	<div></div> 0.5080
D	<div></div> 0.8190	<div></div> 0.4980
E	<div></div> 0.4960	<div></div> 0.3490

