



wwPDB EM Validation Summary Report ⓘ

Nov 16, 2022 – 04:23 AM EST

PDB ID : 6WC7
EMDB ID : EMD-21602
Title : Acyl carrier protein (ACP) domain bound to dehydratase (DH) domain in fungal fatty acid synthase (FAS)
Authors : Lou, J.W.; Mazhab-Jafari, M.T.
Deposited on : 2020-03-29
Resolution : 5.80 Å(reported)
Based on initial model : 2UV8

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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

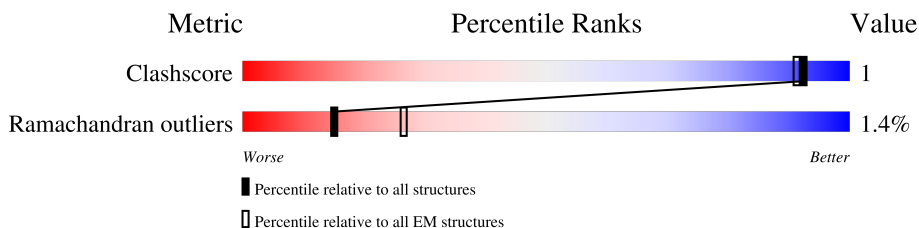
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY



The reported resolution of this entry is 5.80 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	158937	4297
Ramachandran outliers	154571	4023

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	G	2057	 20% 79%
2	A	1887	 8% 91%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2879 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 Fatty acid synthase subunit beta.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	G	422	Total	C	N	O	0	0
			2078	1234	422	422		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	2052	HIS	-	expression tag	UNP P07149
G	2053	HIS	-	expression tag	UNP P07149
G	2054	HIS	-	expression tag	UNP P07149
G	2055	HIS	-	expression tag	UNP P07149
G	2056	HIS	-	expression tag	UNP P07149
G	2057	HIS	-	expression tag	UNP P07149

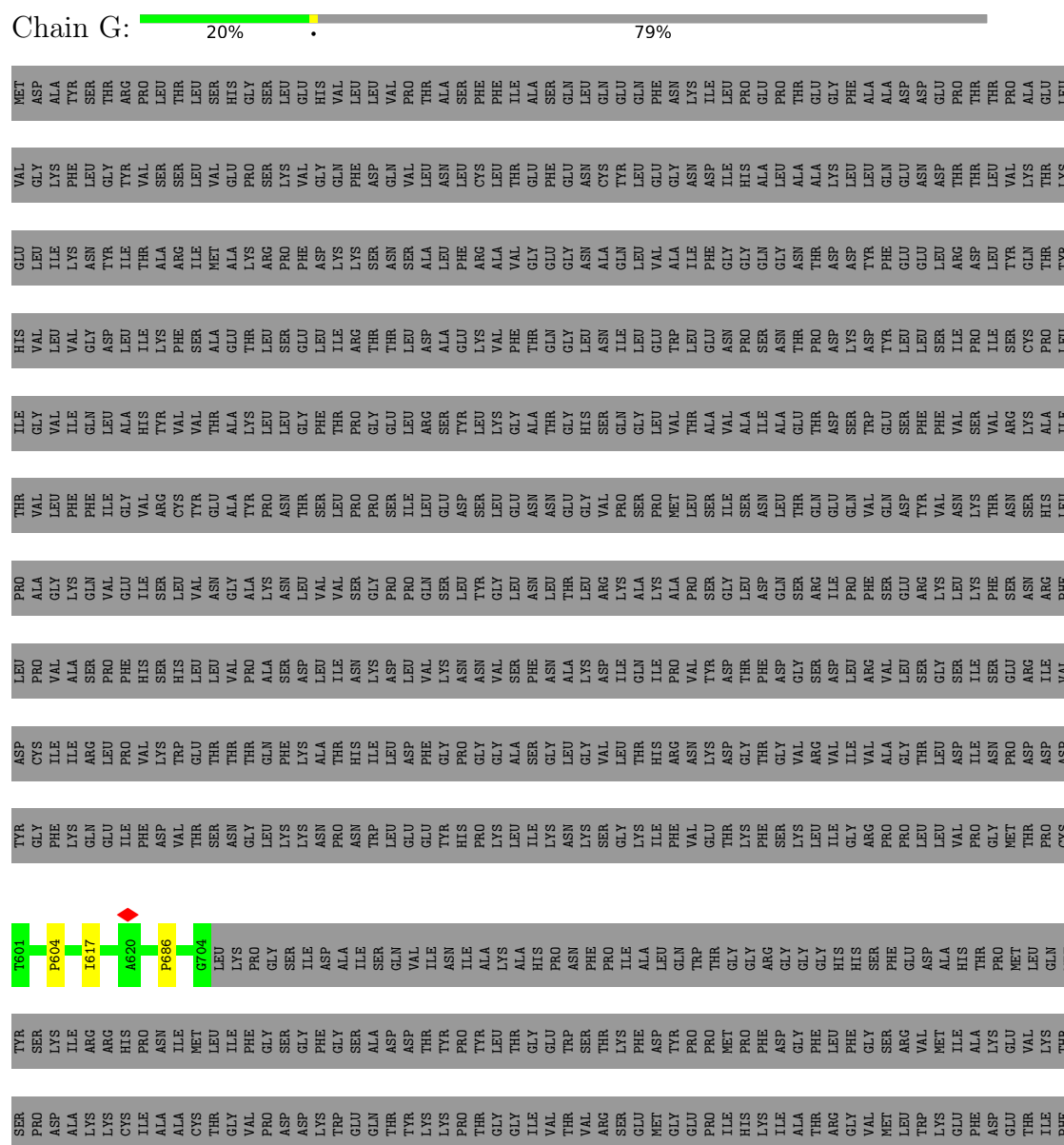
- Molecule 2 is a protein called Fatty acid synthase subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	A	163	Total	C	N	O	0	0
			801	475	163	163		

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: Fatty acid synthase subunit beta







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

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	15767	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	36	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.810	Depositor
Minimum map value	-1.451	Depositor
Average map value	-0.009	Depositor
Map value standard deviation	0.088	Depositor
Recommended contour level	0.6	Depositor
Map size (Å)	371.2, 371.2, 371.2	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.45, 1.45, 1.45	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	G	0.24	0/2075	0.44	0/2881
2	A	0.23	0/800	0.39	0/1110
All	All	0.24	0/2875	0.42	0/3991

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	G	2078	0	936	4	0
2	A	801	0	373	2	0
All	All	2879	0	1309	6	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 1.

The worst 5 of 6 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:A:171:THR:HA	2:A:205:PRO:HA	1.91	0.53
1:G:1395:THR:HA	1:G:1405:GLU:HA	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1357:TYR:HA	1:G:1406:VAL:HA	1.95	0.48
1:G:1356:GLY:HA2	1:G:1609:THR:HA	1.97	0.47
1:G:1605:VAL:HA	1:G:1657:ILE:HA	2.00	0.43

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	G	416/2057 (20%)	351 (84%)	58 (14%)	7 (2%)	9	42
2	A	161/1887 (8%)	149 (92%)	11 (7%)	1 (1%)	25	66
All	All	577/3944 (15%)	500 (87%)	69 (12%)	8 (1%)	15	46

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	604	PRO
2	A	257	PRO
1	G	1250	PRO
1	G	617	ILE
1	G	1369	GLY

5.3.2 Protein sidechains [i](#)

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

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

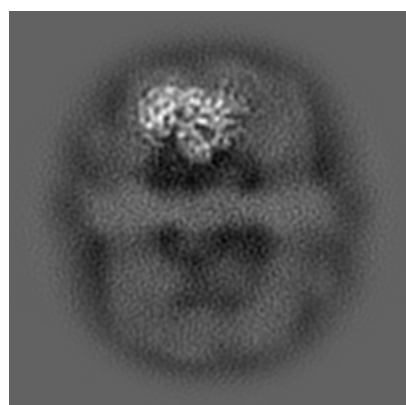
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21602. These allow visual inspection of the internal detail of the map and identification of artifacts.

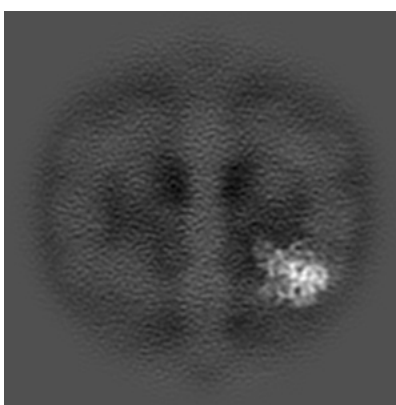
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

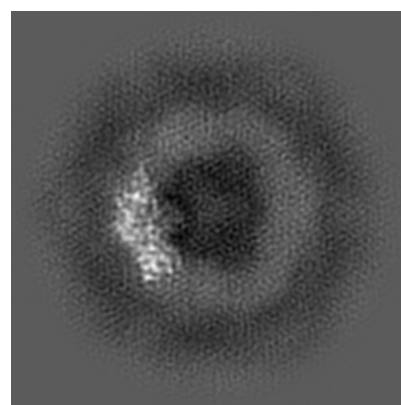
6.1.1 Primary map



X



Y

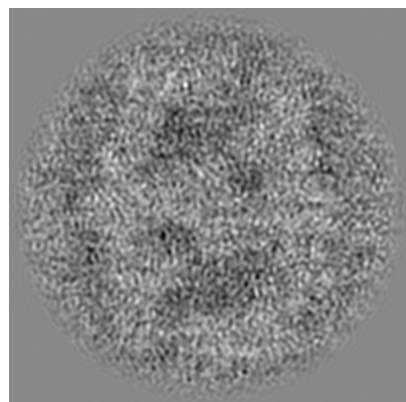


Z

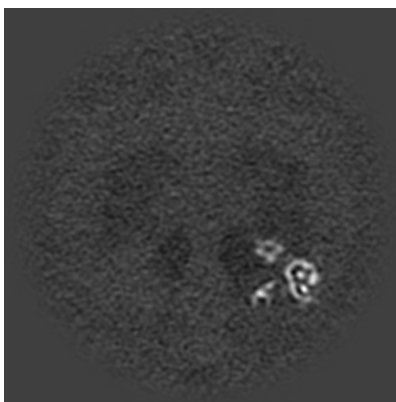
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

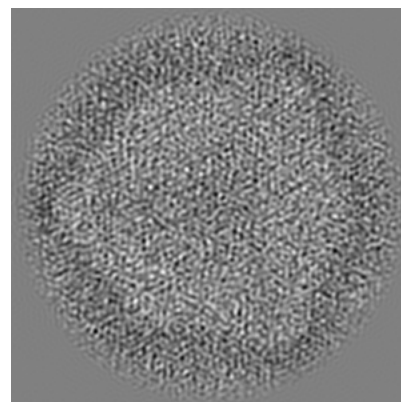
6.2.1 Primary map



X Index: 128



Y Index: 128

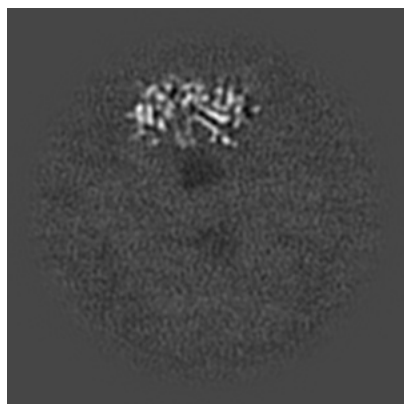


Z Index: 128

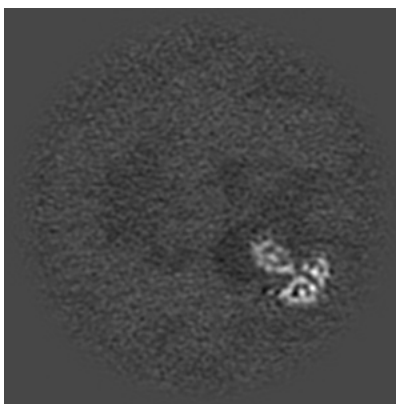
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

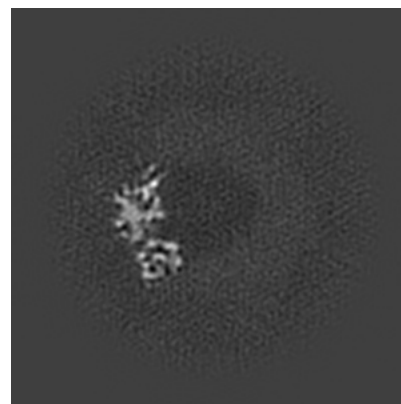
6.3.1 Primary map



X Index: 86



Y Index: 116

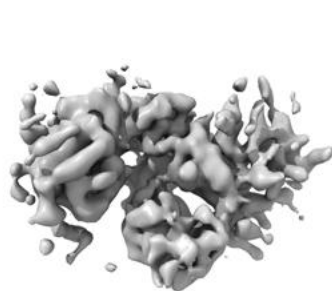


Z Index: 185

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

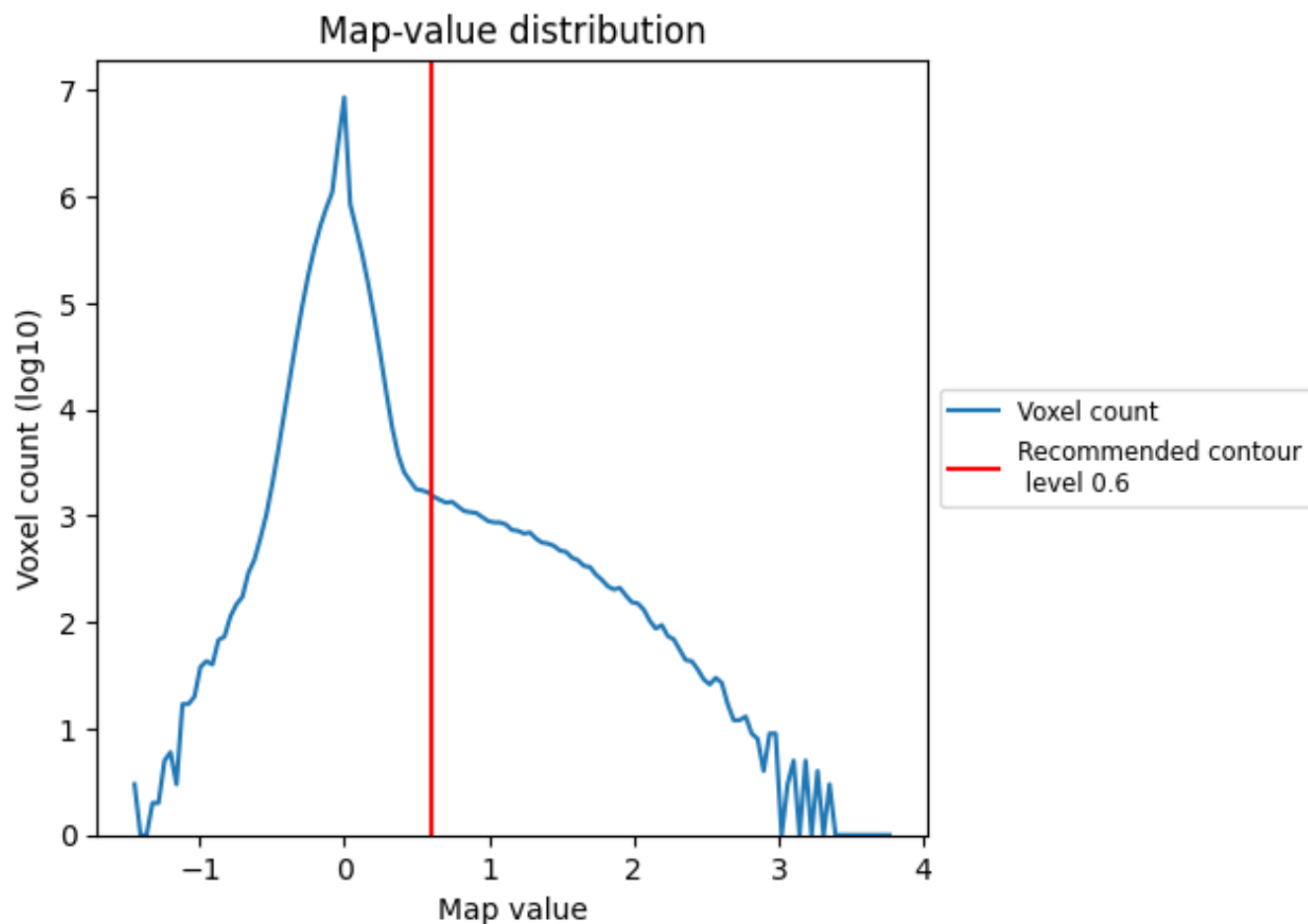
6.5 Mask visualisation

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

7 Map analysis ⓘ

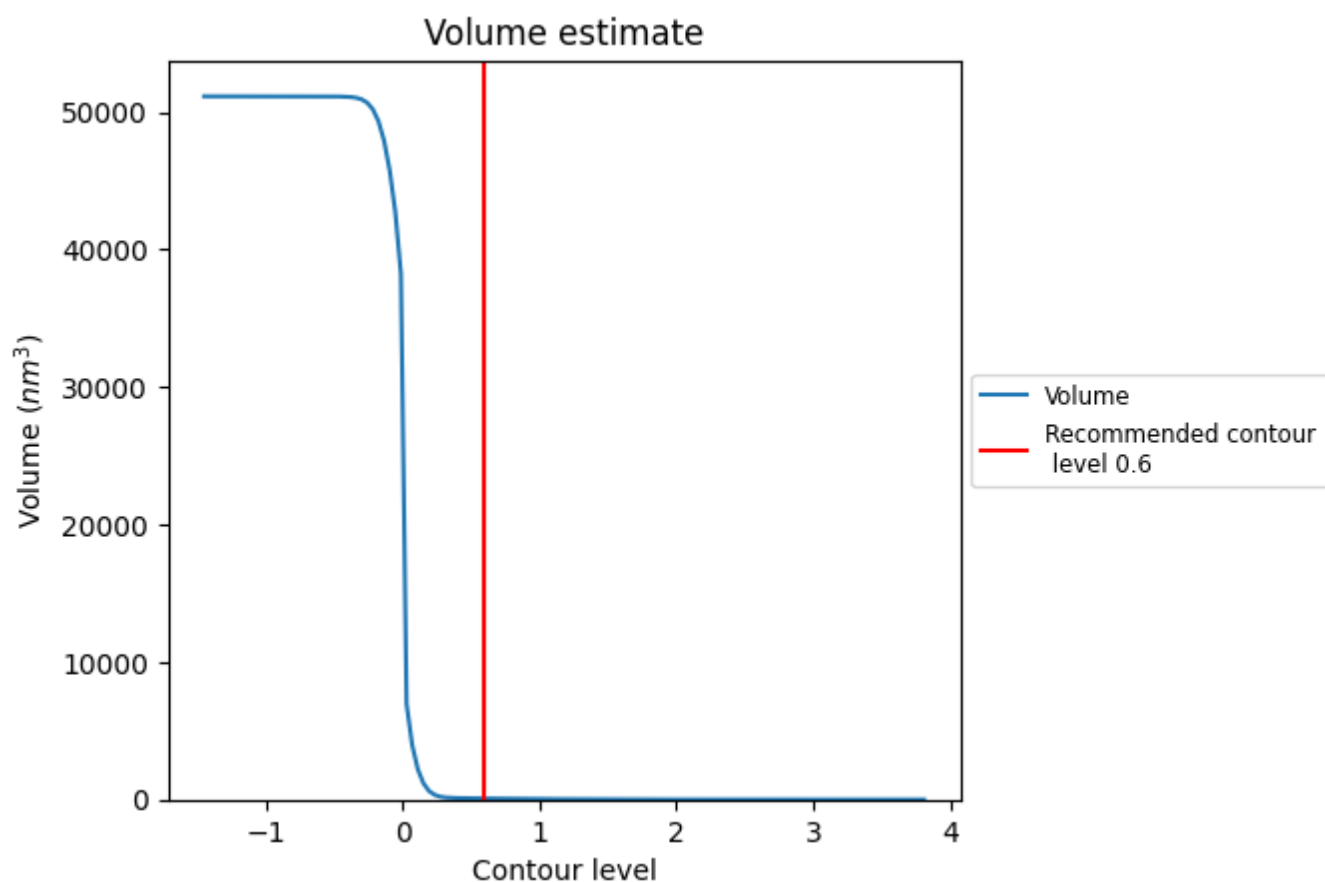
This section contains the results of statistical analysis of the map.

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.

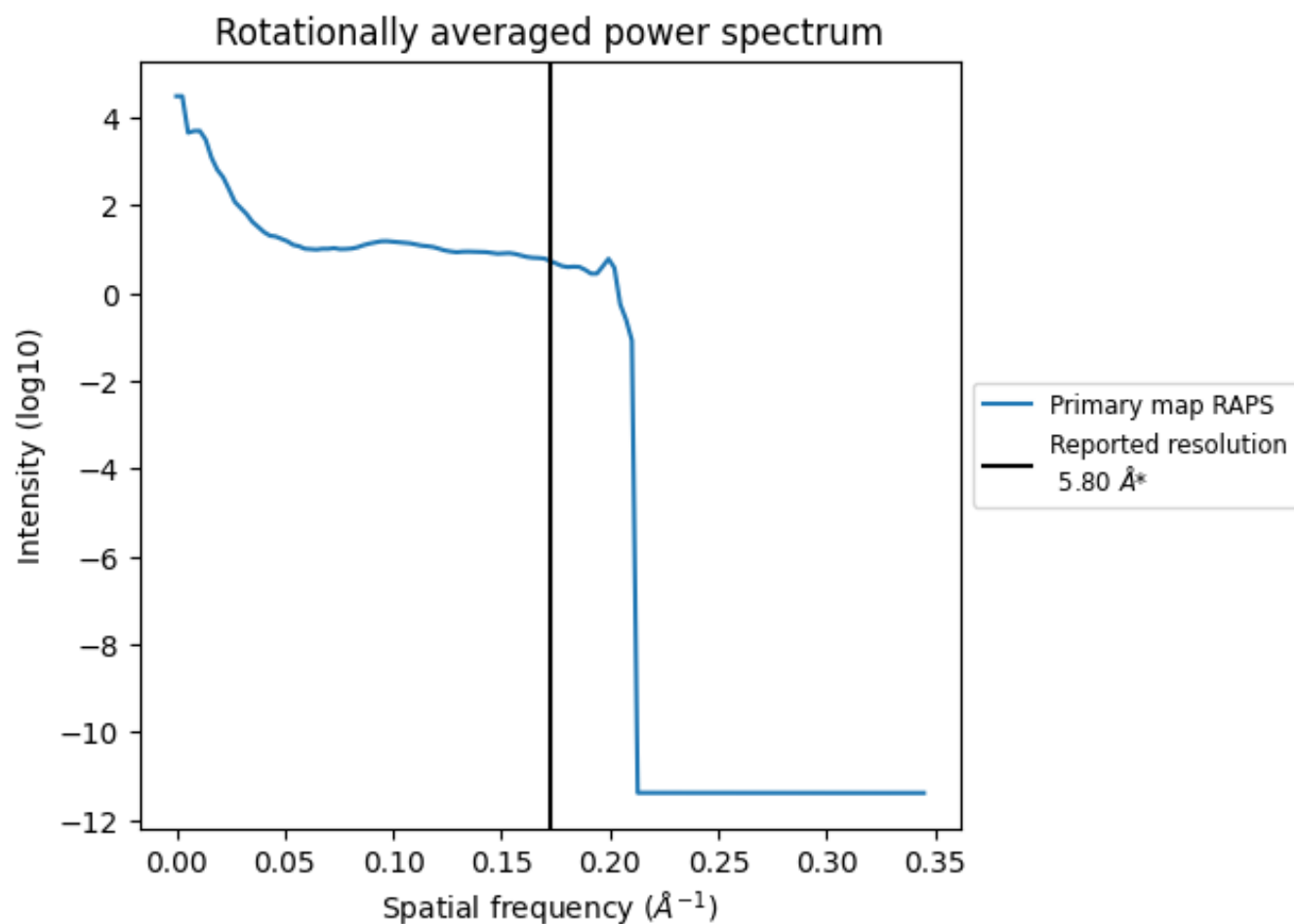
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 77 nm^3 ; this corresponds to an approximate mass of 70 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 0.172 Å⁻¹

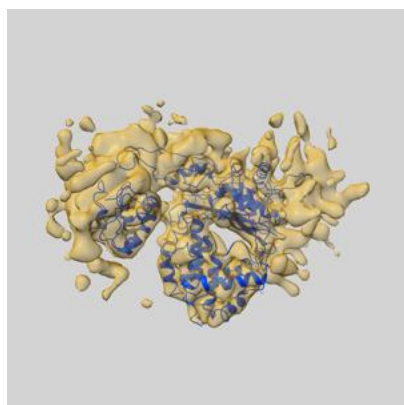
8 Fourier-Shell correlation

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

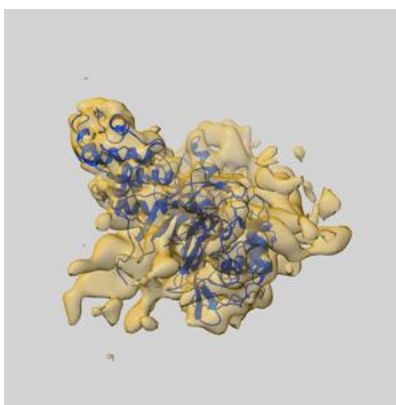
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21602 and PDB model 6WC7. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

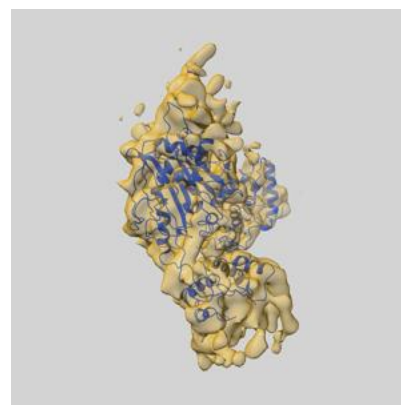
9.1 Map-model overlay [i](#)



X



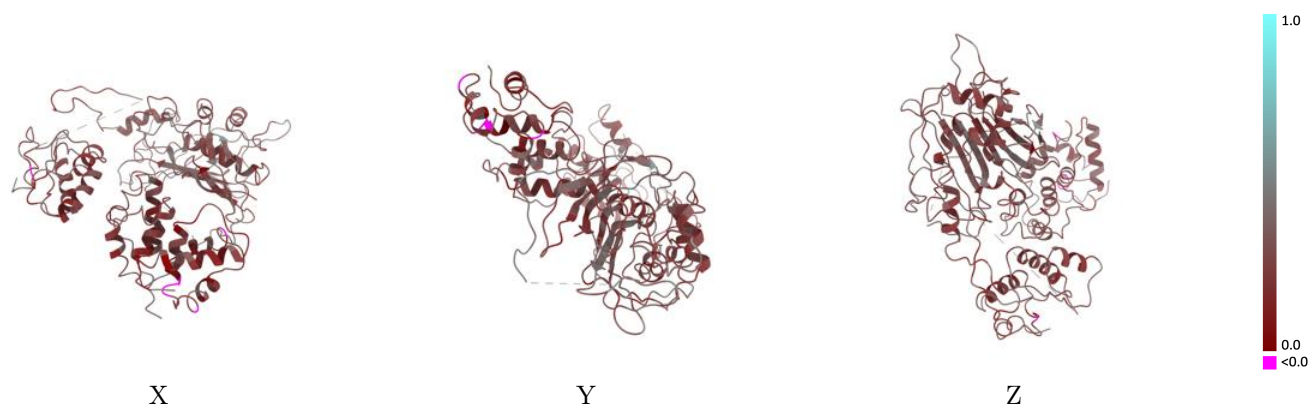
Y



Z

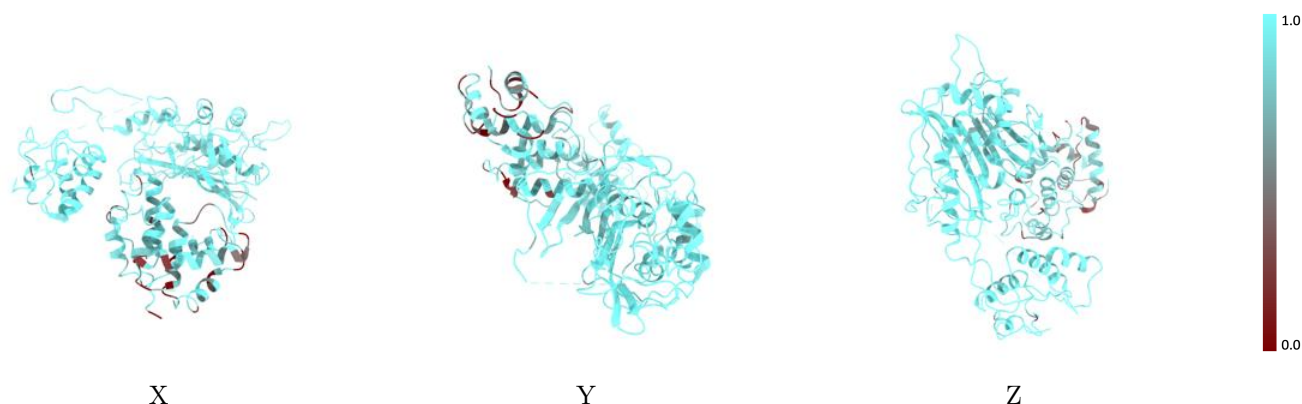
The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



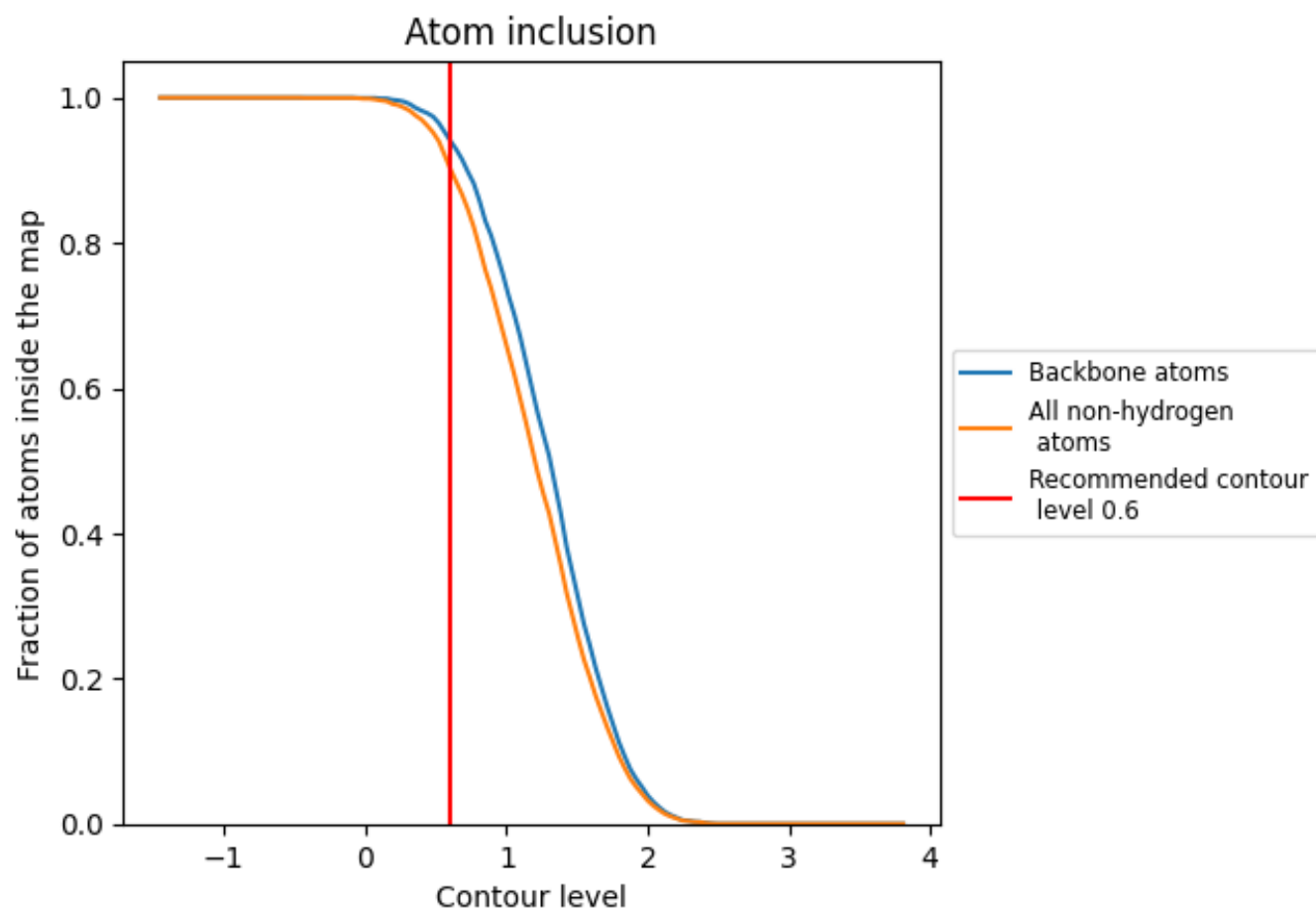
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.6).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 90% 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 (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9027	<div></div> 0.2830
A	<div></div> 0.7516	<div></div> 0.2400
G	<div></div> 0.9610	<div></div> 0.3000

