



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 10:50 AM UTC

PDB ID : 8J99 / pdb_00008j99
EMDB ID : EMD-36092
Title : Human 3-methylcrotonyl-CoA carboxylase in BCS-mcoa state
Authors : Liu, D.S.; Su, J.Y.
Deposited on : 2023-05-02
Resolution : 2.87 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

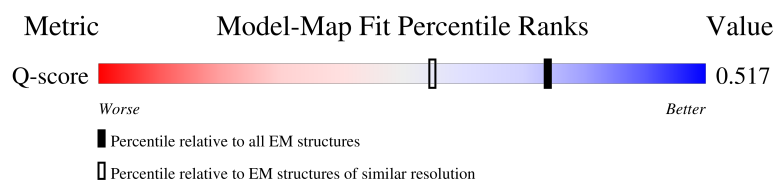
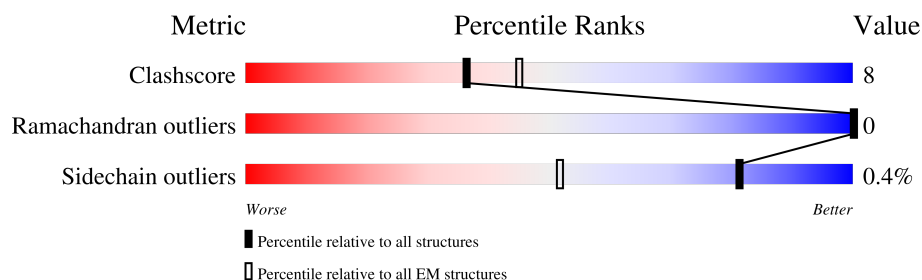
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.87 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.



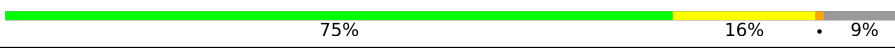
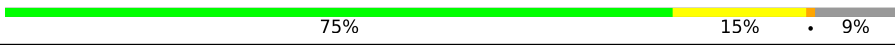
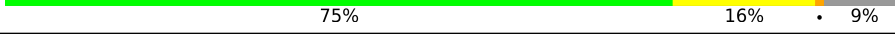
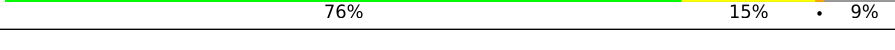
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12062 (2.37 - 3.37)

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	725	 15% 14% 5% 81%
1	C	725	 14% 14% 5% 81%
1	E	725	 14% 14% 5% 81%
1	F	725	 15% 14% 5% 81%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	I	725	 14% 5% 81%
1	K	725	 14% 5% 81%
2	B	563	 75% 16% 9%
2	D	563	 75% 15% 9%
2	G	563	 76% 15% 9%
2	H	563	 75% 16% 9%
2	J	563	 75% 16% 9%
2	L	563	 76% 15% 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 30533 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.

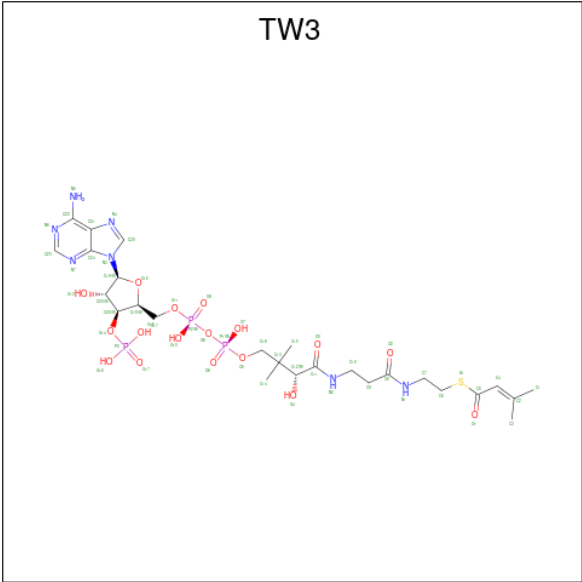
- Molecule 1 is a protein called Methylocrotonoyl-CoA carboxylase subunit alpha, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	138	Total	C	N	O	S	0	0
			1065	673	176	210	6		
1	C	138	Total	C	N	O	S	0	0
			1065	673	176	210	6		
1	E	138	Total	C	N	O	S	0	0
			1064	673	176	209	6		
1	F	138	Total	C	N	O	S	0	0
			1065	673	176	210	6		
1	I	138	Total	C	N	O	S	0	0
			1065	673	176	210	6		
1	K	138	Total	C	N	O	S	0	0
			1065	673	176	210	6		

- Molecule 2 is a protein called Methylocrotonoyl-CoA carboxylase beta chain, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	514	Total	C	N	O	S	0	0
			3970	2517	697	737	19		
2	D	514	Total	C	N	O	S	0	0
			3970	2517	697	737	19		
2	G	514	Total	C	N	O	S	0	0
			3970	2517	697	737	19		
2	H	514	Total	C	N	O	S	0	0
			3970	2517	697	737	19		
2	J	514	Total	C	N	O	S	0	0
			3970	2517	697	737	19		
2	L	514	Total	C	N	O	S	0	0
			3970	2517	697	737	19		

- Molecule 3 is {S}-[2-[3-[(2 {R})-4-[[[(2 {S}),3 {S}),4 {S}),5 {S}]-5-(6-aminopurin-9-yl)-4-oxidanyl-3-phosphonooxy-oxolan-2-yl]methoxy-oxidanyl-phosphoryl]oxy-oxidanyl-phosphoryl]oxy-3,3-dimethyl-2-oxidanyl-butanoyl]amino]propanoylamino]ethyl] 3-methylbut-2-enethioate (CCD ID: TW3) (formula: C₂₆H₄₂N₇O₁₇P₃S).

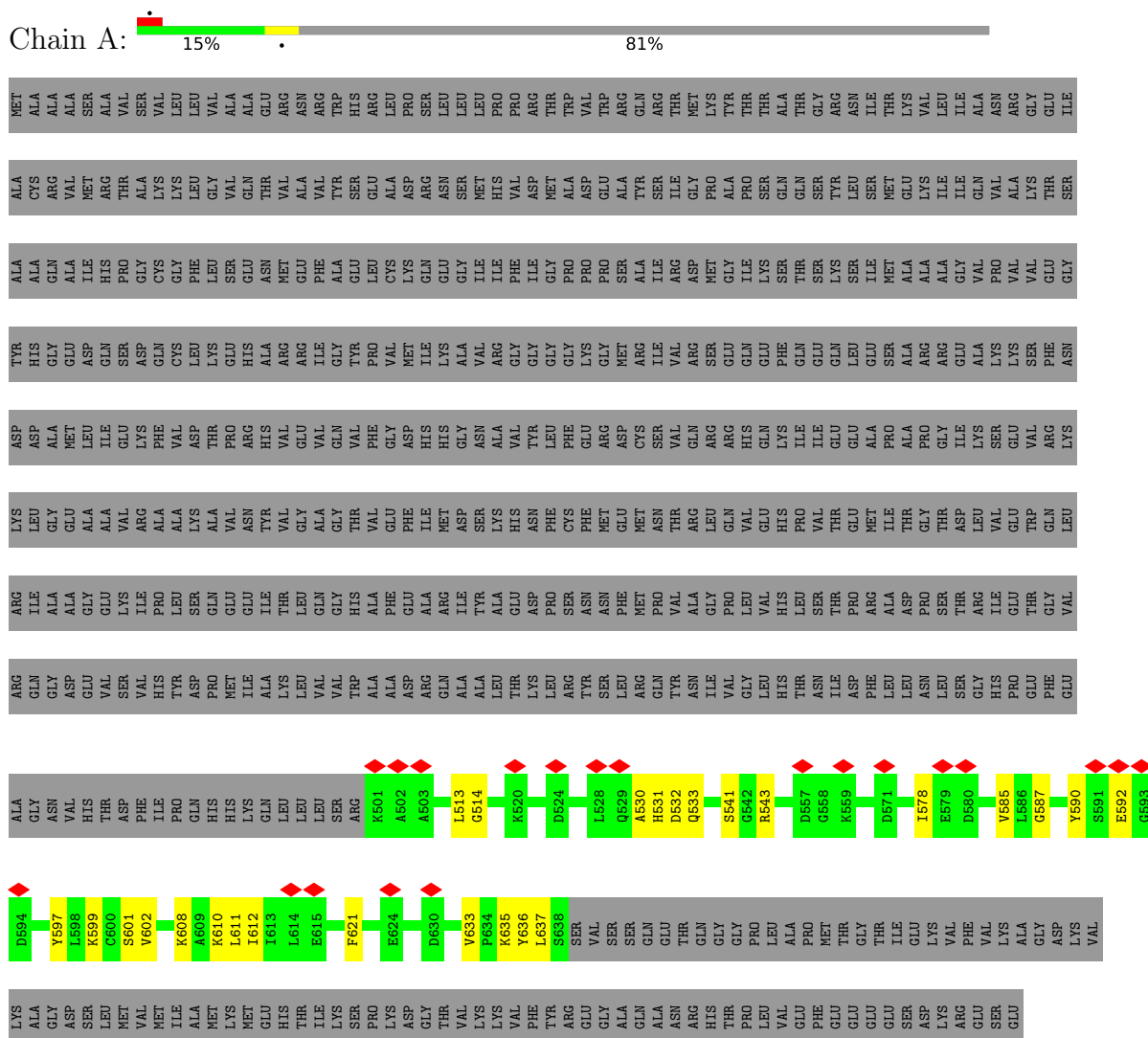


Mol	Chain	Residues	Atoms						AltConf
3	B	1	Total	C	N	O	P	S	0
			54	26	7	17	3	1	
3	D	1	Total	C	N	O	P	S	0
			54	26	7	17	3	1	
3	G	1	Total	C	N	O	P	S	0
			54	26	7	17	3	1	
3	H	1	Total	C	N	O	P	S	0
			54	26	7	17	3	1	
3	J	1	Total	C	N	O	P	S	0
			54	26	7	17	3	1	
3	L	1	Total	C	N	O	P	S	0
			54	26	7	17	3	1	

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Methylcrotonoyl-CoA carboxylase subunit alpha, mitochondrial

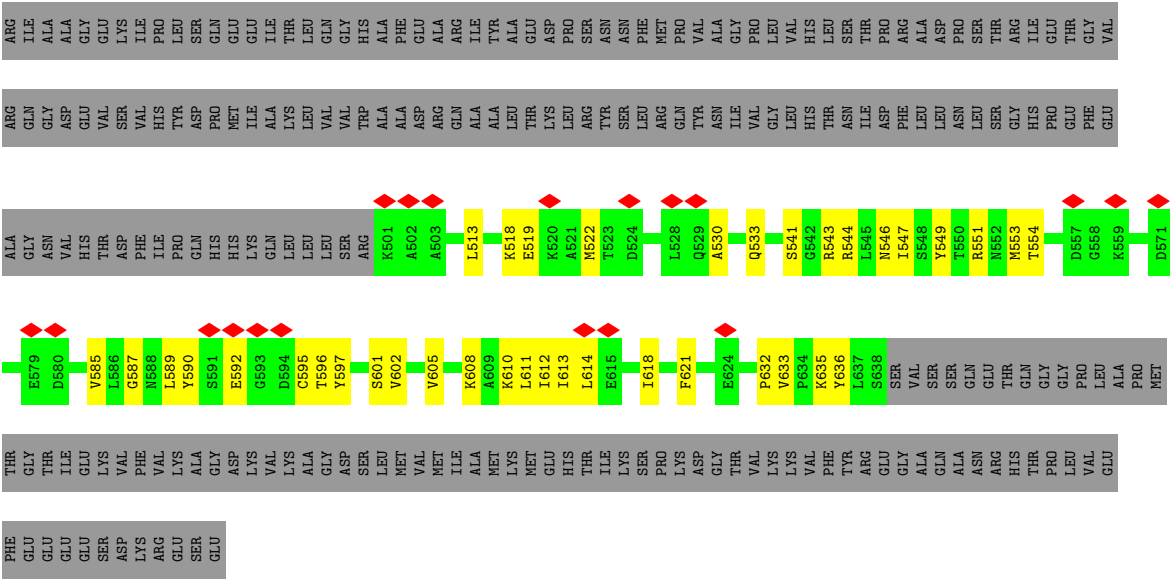


- Molecule 1: Methylcrotonoyl-CoA carboxylase subunit alpha, mitochondrial

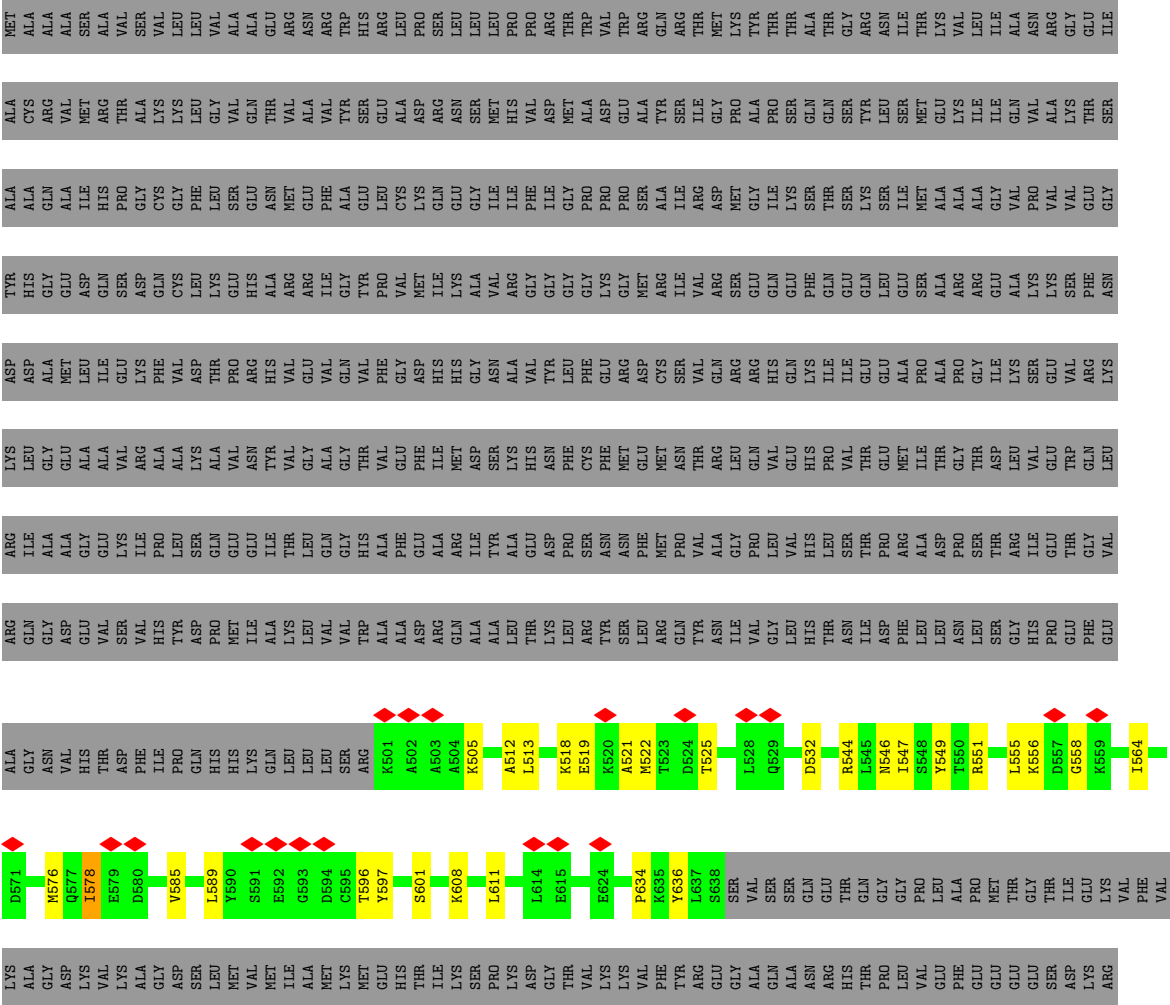




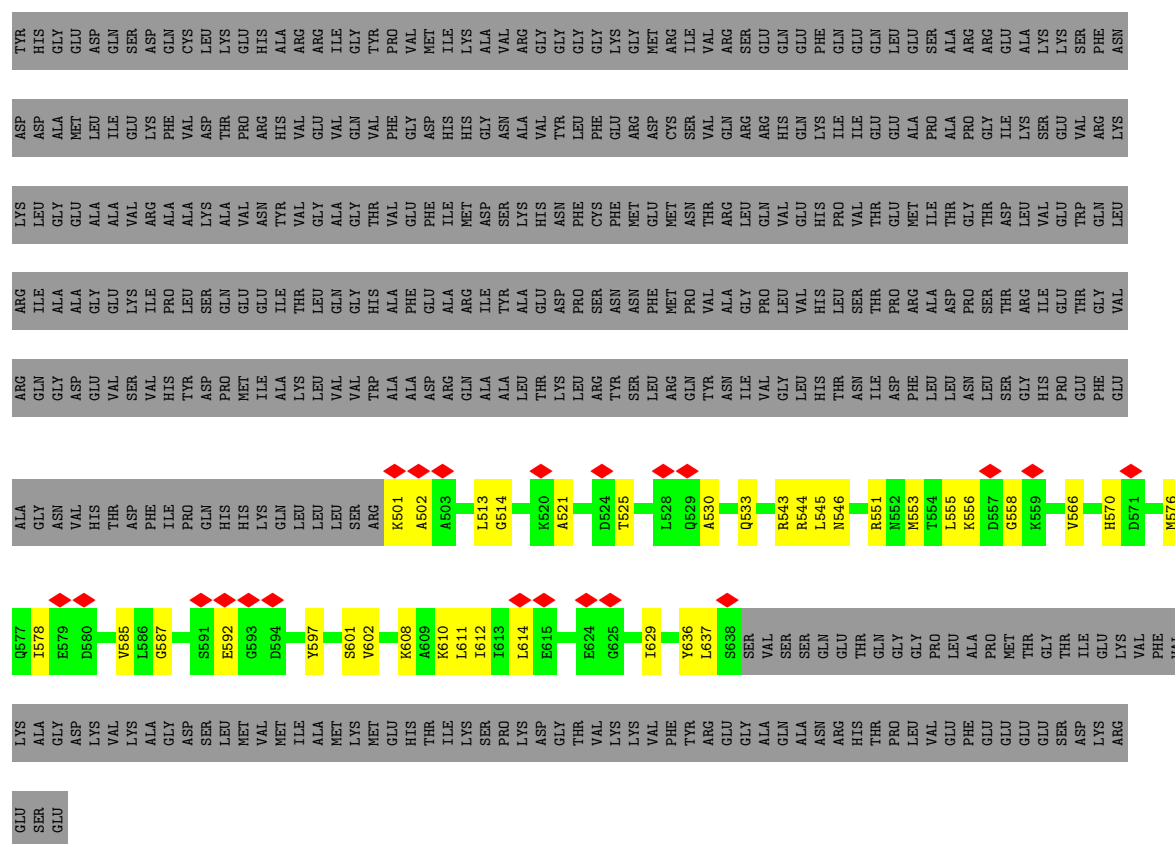
LYS	ASP	TYR	ALA	ALA	MET
LEU	ASP	HIS	ALA	CYS	ALA
GLY	ALA	GLY	GLN	ARG	ALA
GLU	MET	GLU	ALA	VAL	ALA
ALA	LEU	ASP	ILE	MET	ALA
VAL	ILE	GLN	PRO	ARG	ALA
ARG	GLY	SER	SER	THR	VAL
ALA	LYS	ASP	GLY	ALA	SER
ALA	PHE	GLN	CYS	LYS	VAL
ALA	VAL	CYS	ALA	LEU	LEU
LYS	VAL	LEU	PHE	LEU	VAL
ALA	THR	LYS	SER	GLY	VAL
VAL	PRO	GLU	SER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



● Molecule 1: Methylcrotonoyl-CoA carboxylase subunit alpha, mitochondrial

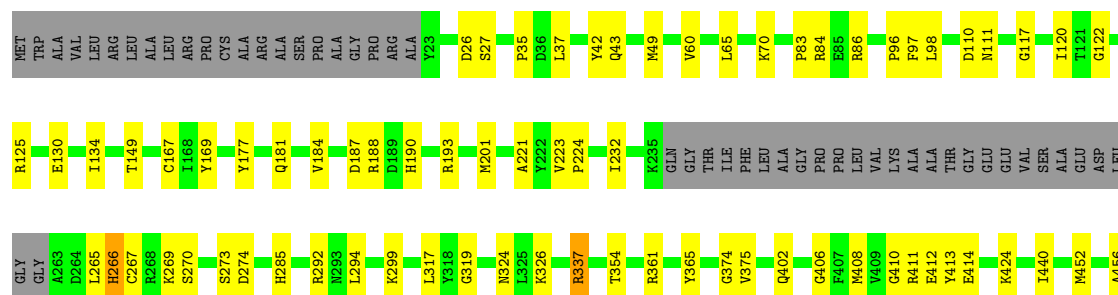


[illegible]



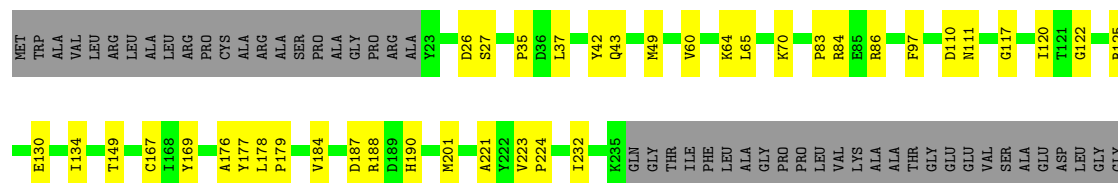
• Molecule 2: Methylcrotonoyl-CoA carboxylase beta chain, mitochondrial

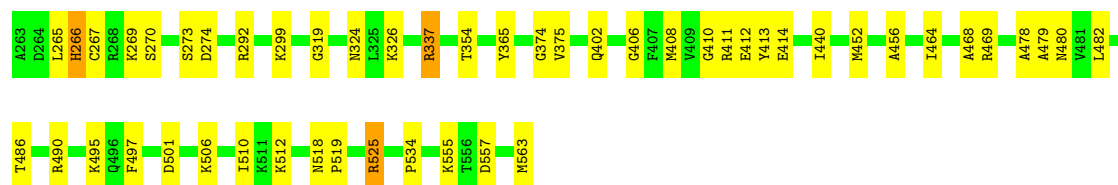
Chain B: 75% 16% 9%



• Molecule 2: Methylcrotonoyl-CoA carboxylase beta chain, mitochondrial

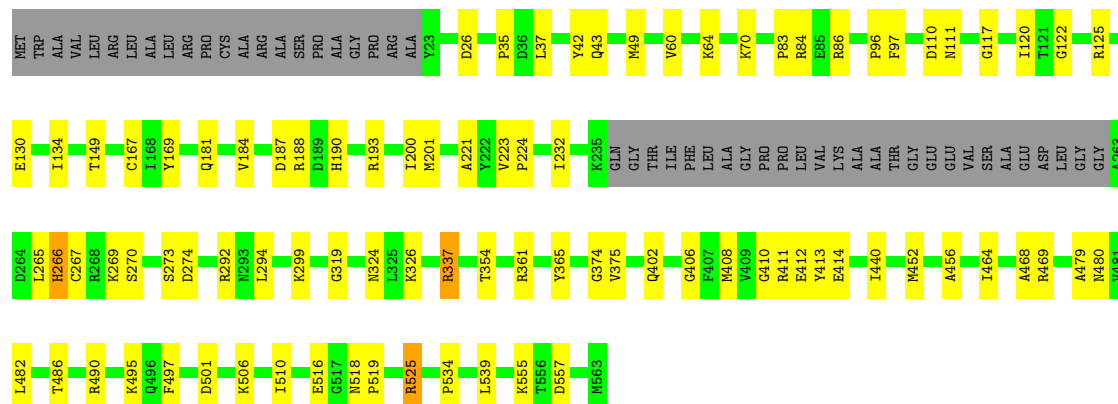
Chain D: 75% 15% 9%





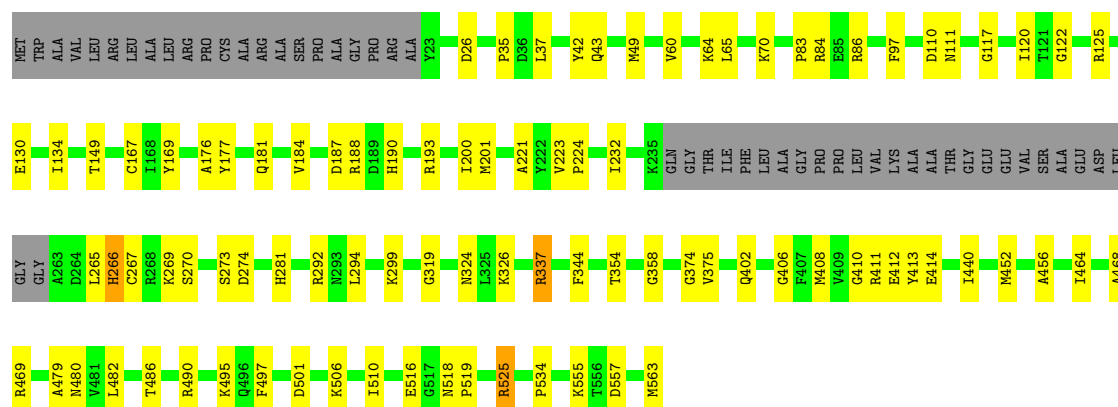
- Molecule 2: Methylcrotonoyl-CoA carboxylase beta chain, mitochondrial

Chain G: 76% 15% 9%



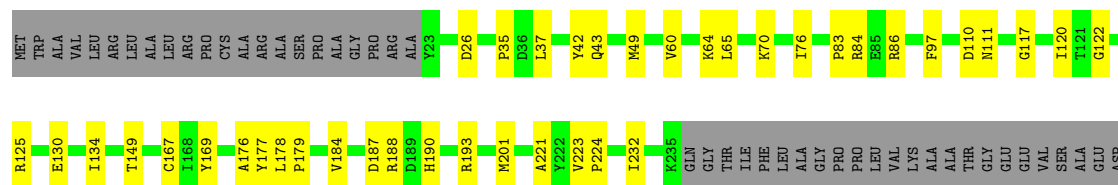
- Molecule 2: Methylcrotonoyl-CoA carboxylase beta chain, mitochondrial

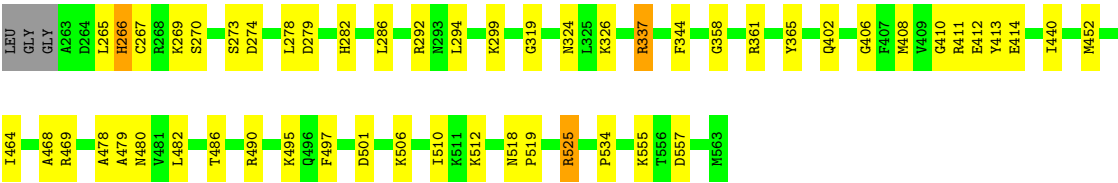
Chain H: 75% 16% 9%



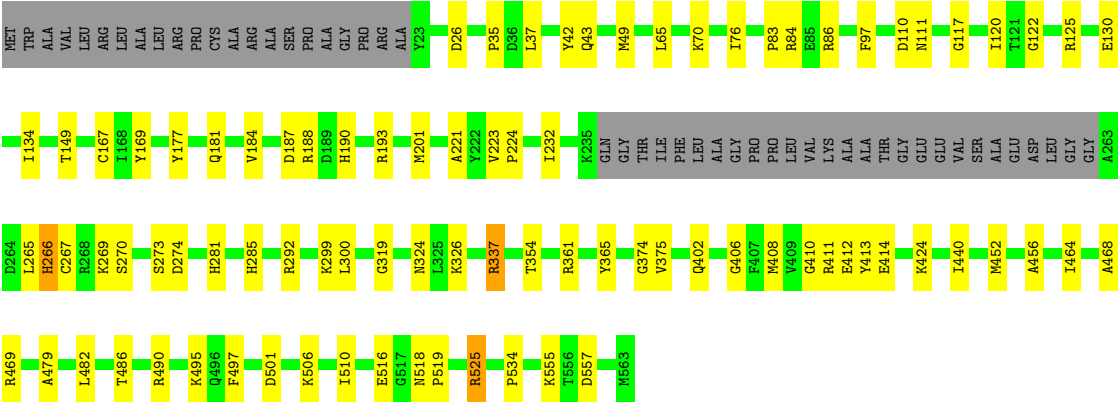
- Molecule 2: Methylcrotonoyl-CoA carboxylase beta chain, mitochondrial

Chain J: 75% 16% 9%





• Molecule 2: Methylcrotonoyl-CoA carboxylase beta chain, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	152533	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.896	Depositor
Minimum map value	-0.294	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.108	Depositor
Map size ($\text{\AA}$)	349.2, 349.2, 349.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.97, 0.97, 0.97	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TW3

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	0.36	0/1081	0.60	0/1457
1	C	0.38	0/1081	0.63	0/1457
1	E	0.38	0/1080	0.64	0/1456
1	F	0.37	0/1081	0.57	0/1457
1	I	0.38	0/1081	0.64	0/1457
1	K	0.36	0/1081	0.58	0/1457
2	B	0.40	0/4051	0.52	6/5473 (0.1%)
2	D	0.40	0/4051	0.52	6/5473 (0.1%)
2	G	0.40	0/4051	0.52	6/5473 (0.1%)
2	H	0.40	0/4051	0.52	6/5473 (0.1%)
2	J	0.40	0/4051	0.52	6/5473 (0.1%)
2	L	0.40	0/4051	0.52	6/5473 (0.1%)
All	All	0.39	0/30791	0.54	36/41579 (0.1%)

There are no bond length outliers.

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	274	ASP	N-CA-C	-6.39	105.61	113.41
2	B	274	ASP	N-CA-C	-6.36	105.65	113.41
2	H	274	ASP	N-CA-C	-6.35	105.66	113.41
2	J	274	ASP	N-CA-C	-6.35	105.67	113.41
2	L	274	ASP	N-CA-C	-6.34	105.67	113.41

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1065	0	1072	21	0
1	C	1065	0	1072	24	0
1	E	1064	0	1069	28	0
1	F	1065	0	1072	21	0
1	I	1065	0	1072	34	0
1	K	1065	0	1072	27	0
2	B	3970	0	3947	67	0
2	D	3970	0	3947	62	0
2	G	3970	0	3947	60	0
2	H	3970	0	3947	61	0
2	J	3970	0	3947	61	0
2	L	3970	0	3947	61	0
3	B	54	0	0	1	0
3	D	54	0	0	2	0
3	G	54	0	0	0	0
3	H	54	0	0	2	0
3	J	54	0	0	2	0
3	L	54	0	0	1	0
All	All	30533	0	30111	469	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 8.

The worst 5 of 469 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:B:354:THR:HG21	2:B:375:VAL:O	1.57	1.03
2:L:354:THR:HG21	2:L:375:VAL:O	1.70	0.91
2:G:354:THR:HG21	2:G:375:VAL:O	1.71	0.89
2:H:354:THR:HG21	2:H:375:VAL:O	1.73	0.89
2:D:354:THR:HG21	2:D:375:VAL:O	1.73	0.87

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	A	136/725 (19%)	132 (97%)	4 (3%)	0	100	100
1	C	136/725 (19%)	132 (97%)	4 (3%)	0	100	100
1	E	136/725 (19%)	132 (97%)	4 (3%)	0	100	100
1	F	136/725 (19%)	133 (98%)	3 (2%)	0	100	100
1	I	136/725 (19%)	134 (98%)	2 (2%)	0	100	100
1	K	136/725 (19%)	133 (98%)	3 (2%)	0	100	100
2	B	510/563 (91%)	494 (97%)	16 (3%)	0	100	100
2	D	510/563 (91%)	494 (97%)	16 (3%)	0	100	100
2	G	510/563 (91%)	495 (97%)	15 (3%)	0	100	100
2	H	510/563 (91%)	495 (97%)	15 (3%)	0	100	100
2	J	510/563 (91%)	495 (97%)	15 (3%)	0	100	100
2	L	510/563 (91%)	494 (97%)	16 (3%)	0	100	100
All	All	3876/7728 (50%)	3763 (97%)	113 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	119/609 (20%)	118 (99%)	1 (1%)	73	89
1	C	119/609 (20%)	119 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	118/609 (19%)	117 (99%)	1 (1%)	73	89
1	F	119/609 (20%)	118 (99%)	1 (1%)	73	89
1	I	119/609 (20%)	118 (99%)	1 (1%)	73	89
1	K	119/609 (20%)	117 (98%)	2 (2%)	53	80
2	B	412/445 (93%)	411 (100%)	1 (0%)	87	96
2	D	412/445 (93%)	411 (100%)	1 (0%)	87	96
2	G	412/445 (93%)	411 (100%)	1 (0%)	87	96
2	H	412/445 (93%)	411 (100%)	1 (0%)	87	96
2	J	412/445 (93%)	411 (100%)	1 (0%)	87	96
2	L	412/445 (93%)	411 (100%)	1 (0%)	87	96
All	All	3185/6324 (50%)	3173 (100%)	12 (0%)	81	94

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	614	LEU
2	J	266	HIS
2	L	266	HIS
1	K	578	ILE
1	E	614	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
2	G	386	HIS
2	L	266	HIS
2	H	386	HIS
2	L	386	HIS
1	K	531	HIS

5.3.3 RNA ⓘ

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](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	TW3	H	801	-	53,56,56	0.42	0	77,83,83	1.22	5 (6%)
3	TW3	B	801	-	53,56,56	0.41	0	77,83,83	1.22	5 (6%)
3	TW3	D	801	-	53,56,56	0.42	0	77,83,83	1.22	5 (6%)
3	TW3	L	801	-	53,56,56	0.42	0	77,83,83	1.22	5 (6%)
3	TW3	J	801	-	53,56,56	0.42	0	77,83,83	1.22	5 (6%)
3	TW3	G	801	-	53,56,56	0.42	0	77,83,83	1.22	5 (6%)

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
3	TW3	H	801	-	-	14/54/71/71	0/3/3/3
3	TW3	B	801	-	-	14/54/71/71	0/3/3/3
3	TW3	D	801	-	-	14/54/71/71	0/3/3/3
3	TW3	L	801	-	-	14/54/71/71	0/3/3/3
3	TW3	J	801	-	-	14/54/71/71	0/3/3/3
3	TW3	G	801	-	-	14/54/71/71	0/3/3/3

There are no bond length outliers.

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	801	TW3	C4-C5-S1	7.83	121.27	111.32
3	B	801	TW3	C4-C5-S1	7.82	121.26	111.32
3	H	801	TW3	C4-C5-S1	7.82	121.25	111.32
3	G	801	TW3	C4-C5-S1	7.82	121.25	111.32
3	L	801	TW3	C4-C5-S1	7.79	121.22	111.32

There are no chirality outliers.

5 of 84 torsion outliers are listed below:

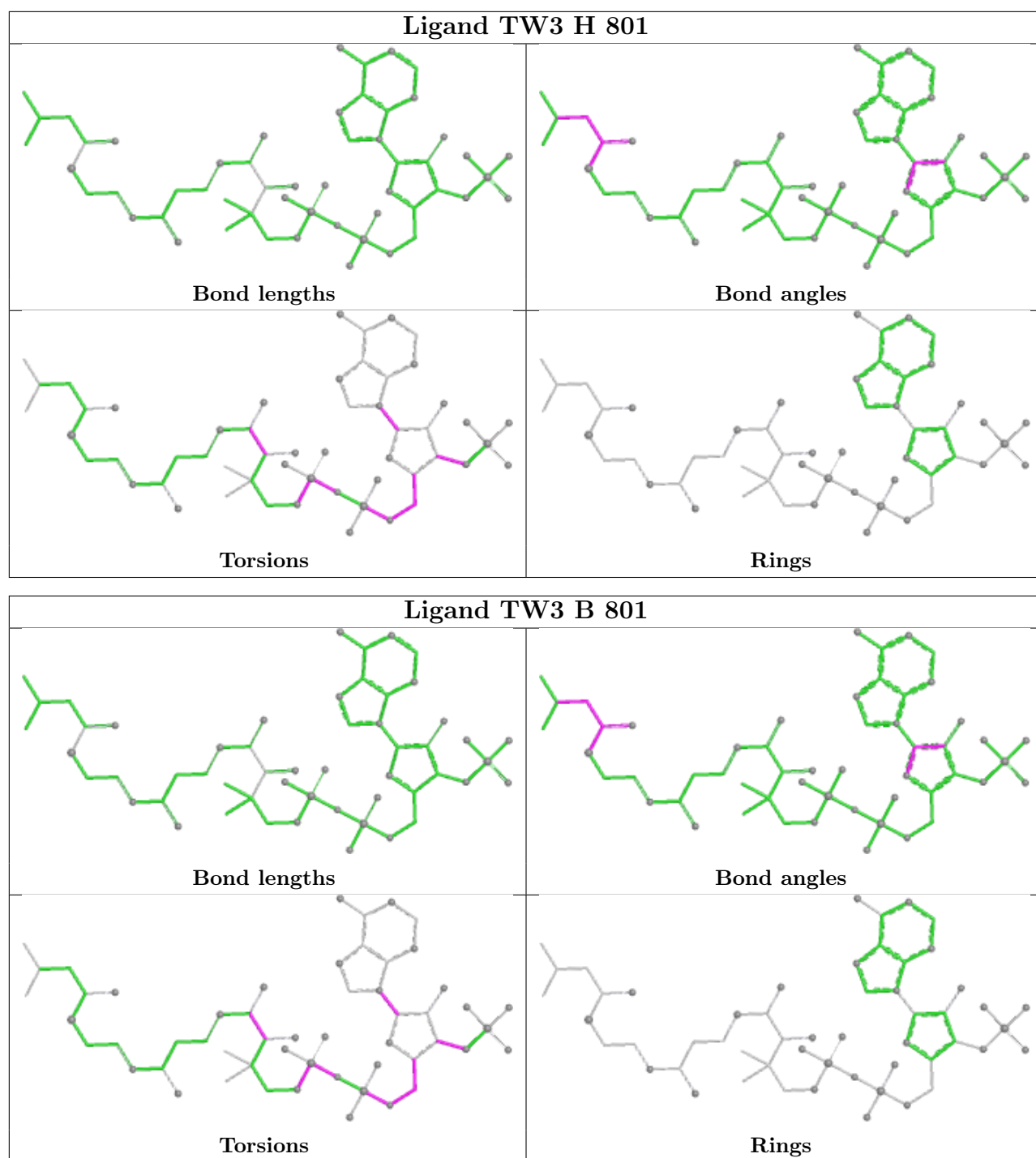
Mol	Chain	Res	Type	Atoms
3	B	801	TW3	N2-C11-C12-C13
3	B	801	TW3	N2-C11-C12-O4
3	B	801	TW3	O3-C11-C12-C13
3	B	801	TW3	O3-C11-C12-O4
3	B	801	TW3	C18-C17-O11-P2

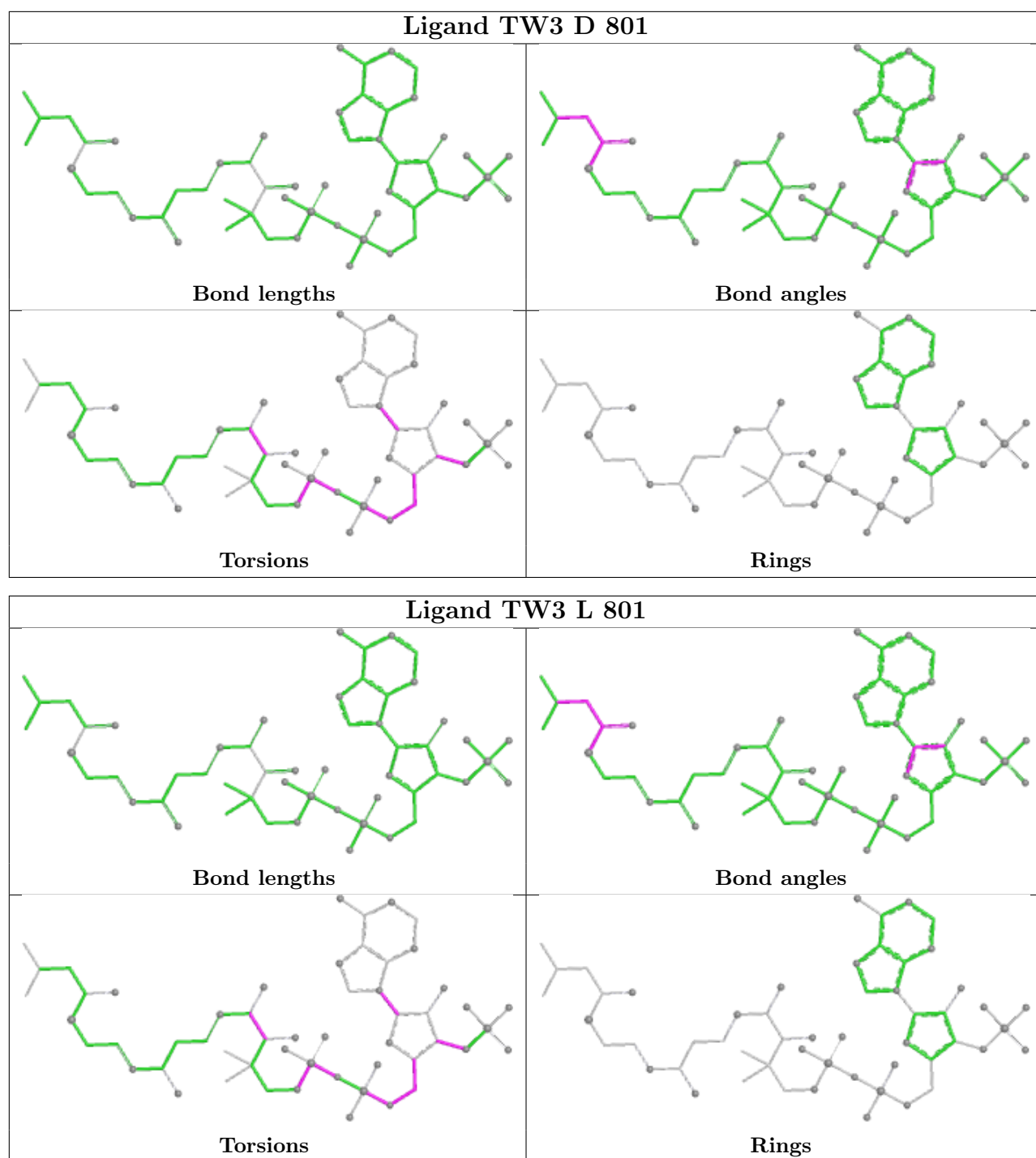
There are no ring outliers.

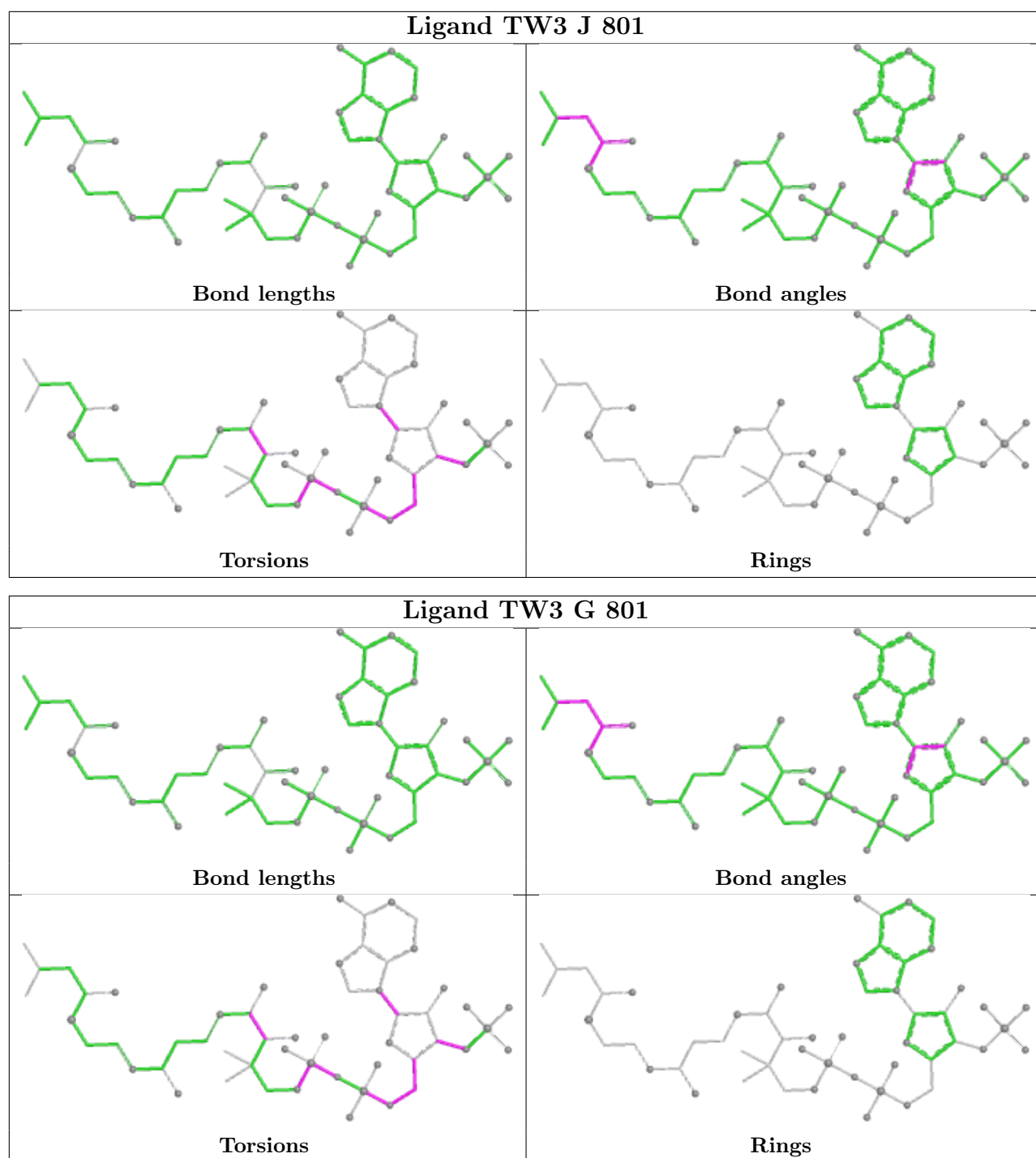
5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	801	TW3	2	0
3	B	801	TW3	1	0
3	D	801	TW3	2	0
3	L	801	TW3	1	0
3	J	801	TW3	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

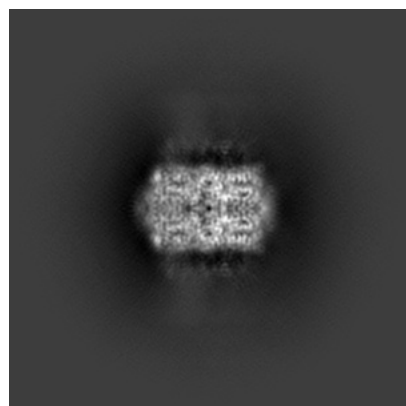
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36092. These allow visual inspection of the internal detail of the map and identification of artifacts.

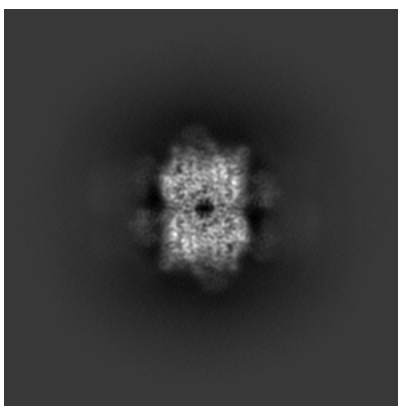
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

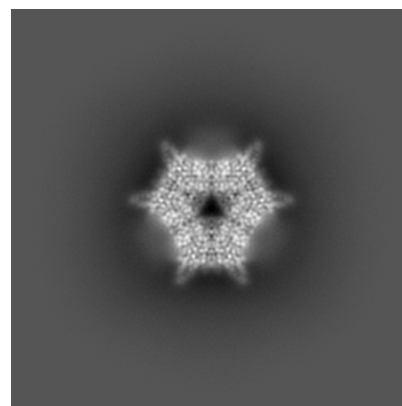
6.1.1 Primary map



X

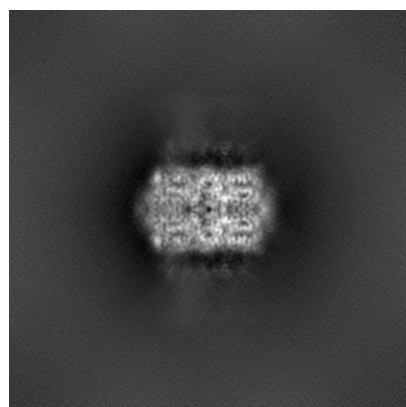


Y

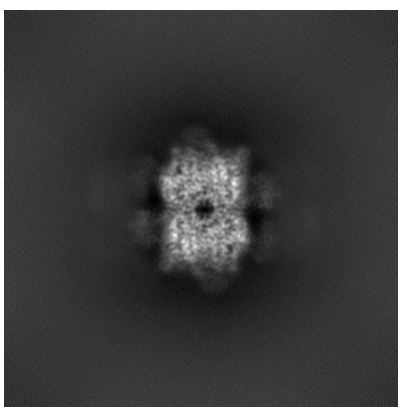


Z

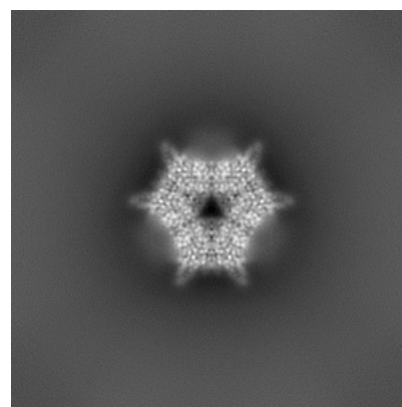
6.1.2 Raw map



X



Y

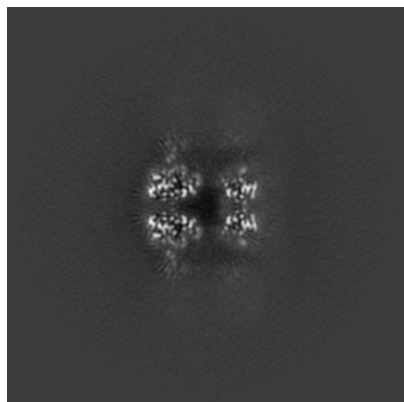


Z

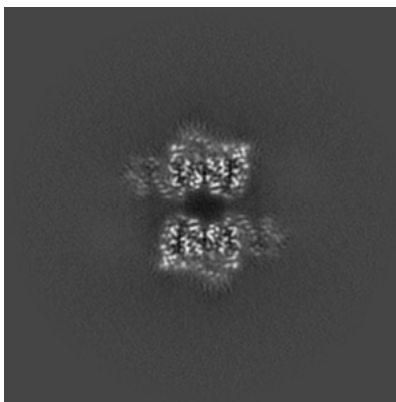
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

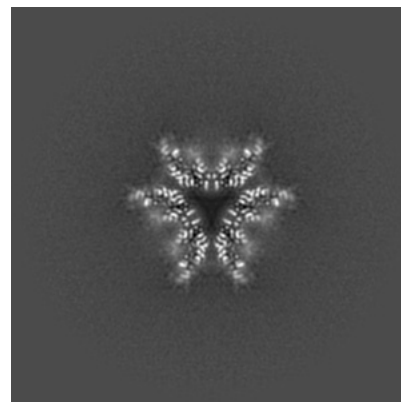
6.2.1 Primary map



X Index: 180

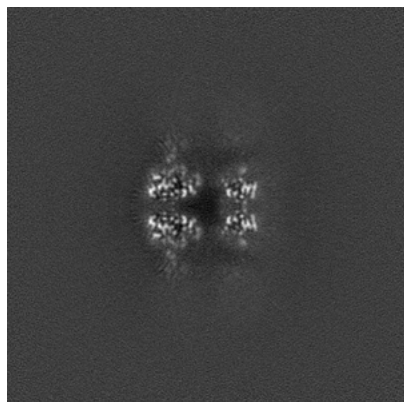


Y Index: 180

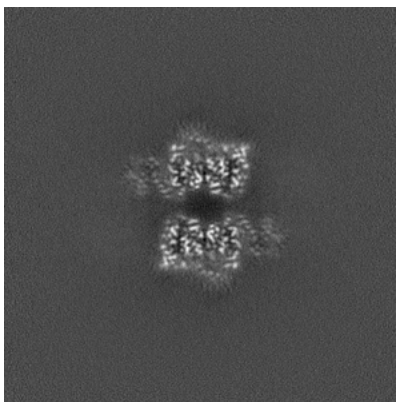


Z Index: 180

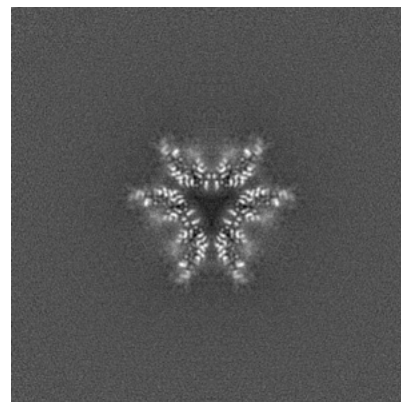
6.2.2 Raw map



X Index: 180



Y Index: 180

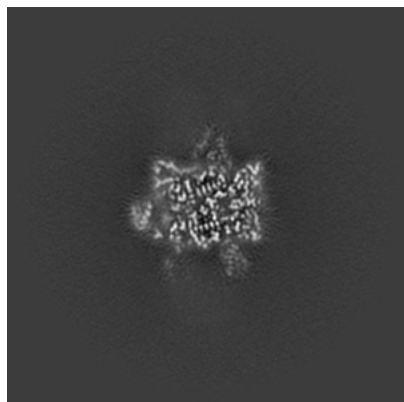


Z Index: 180

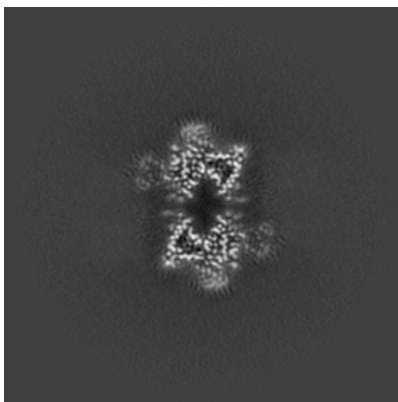
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

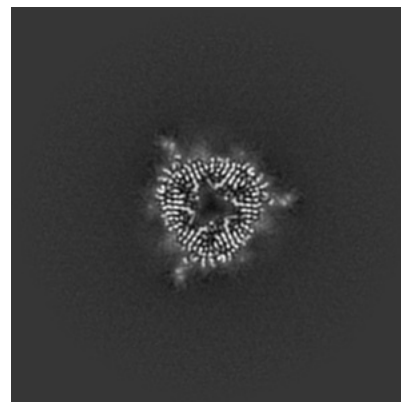
6.3.1 Primary map



X Index: 152

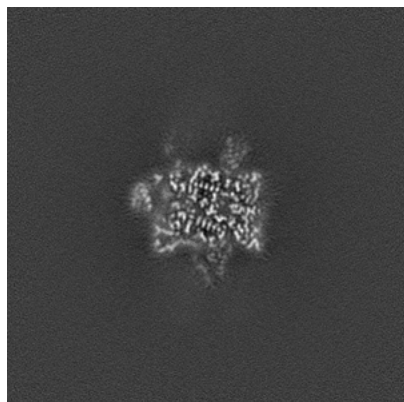


Y Index: 187

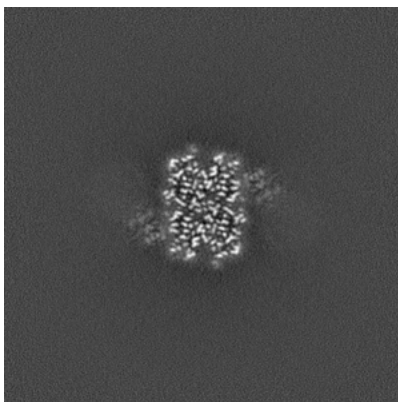


Z Index: 164

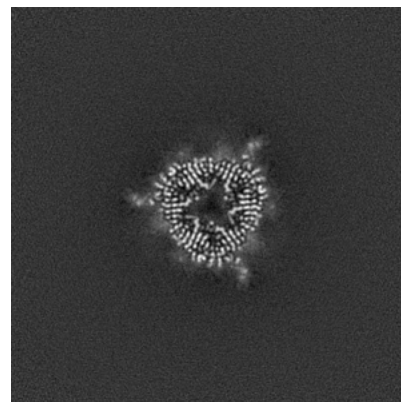
6.3.2 Raw map



X Index: 208



Y Index: 206

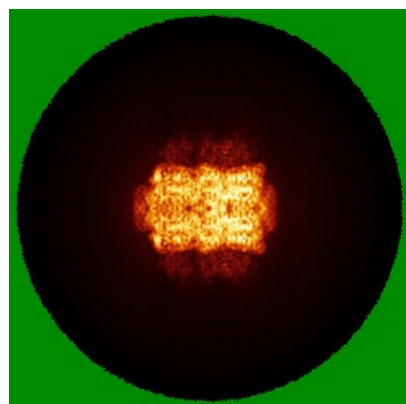


Z Index: 196

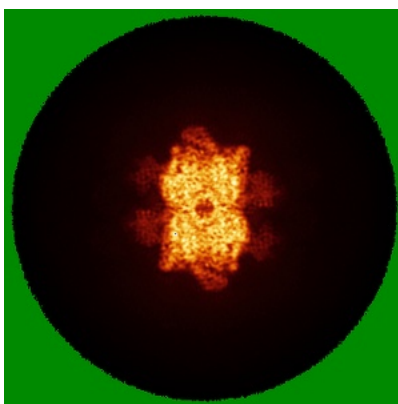
The images above show the largest variance slices of the map in three orthogonal directions.

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

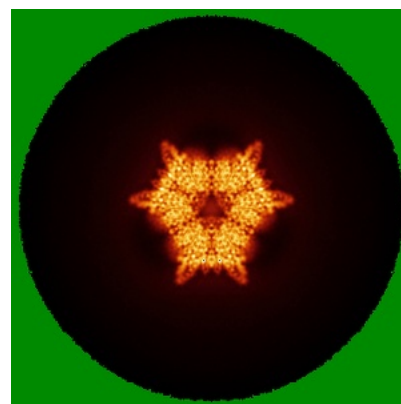
6.4.1 Primary map



X

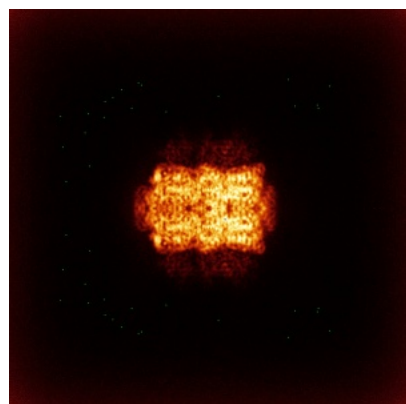


Y

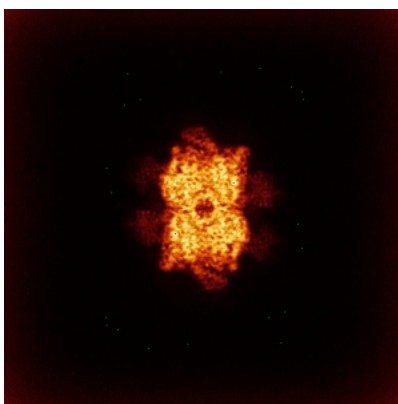


Z

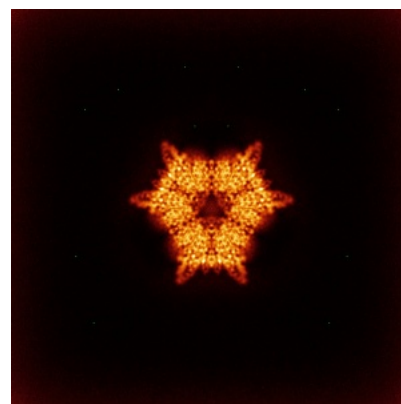
6.4.2 Raw map



X



Y

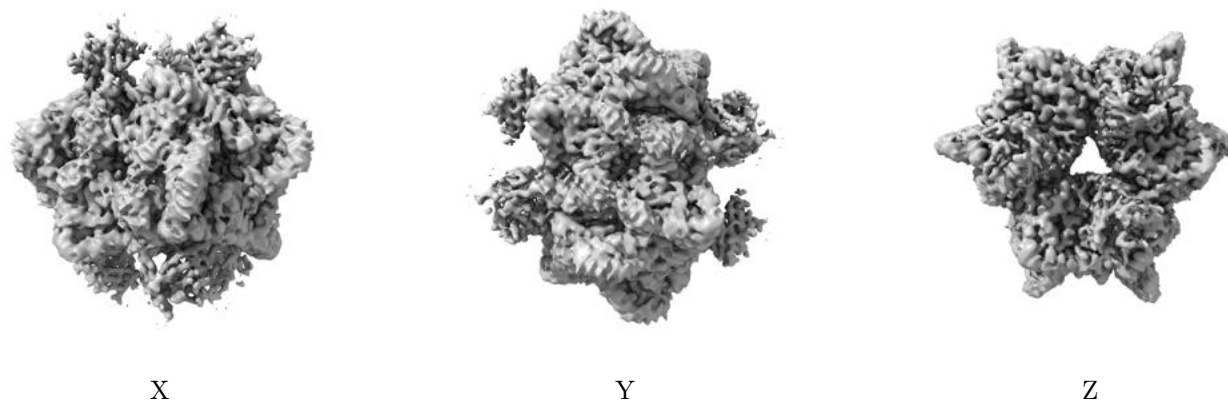


Z

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.

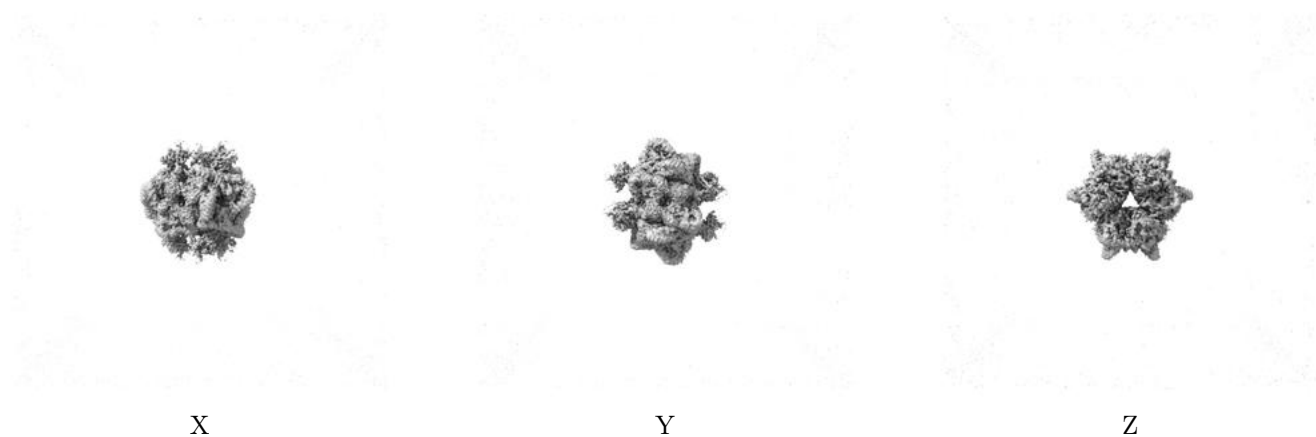
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.108. 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.

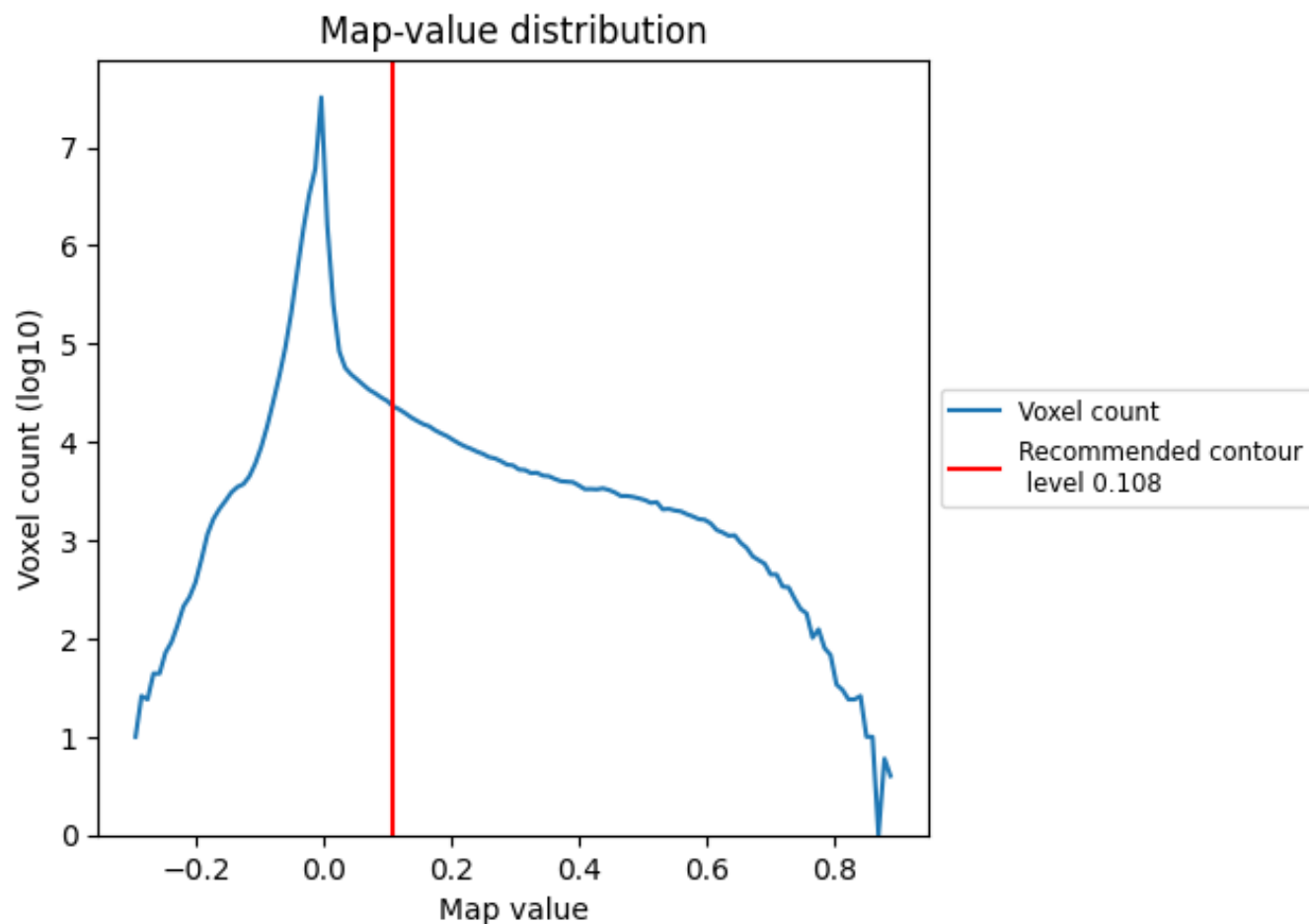
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

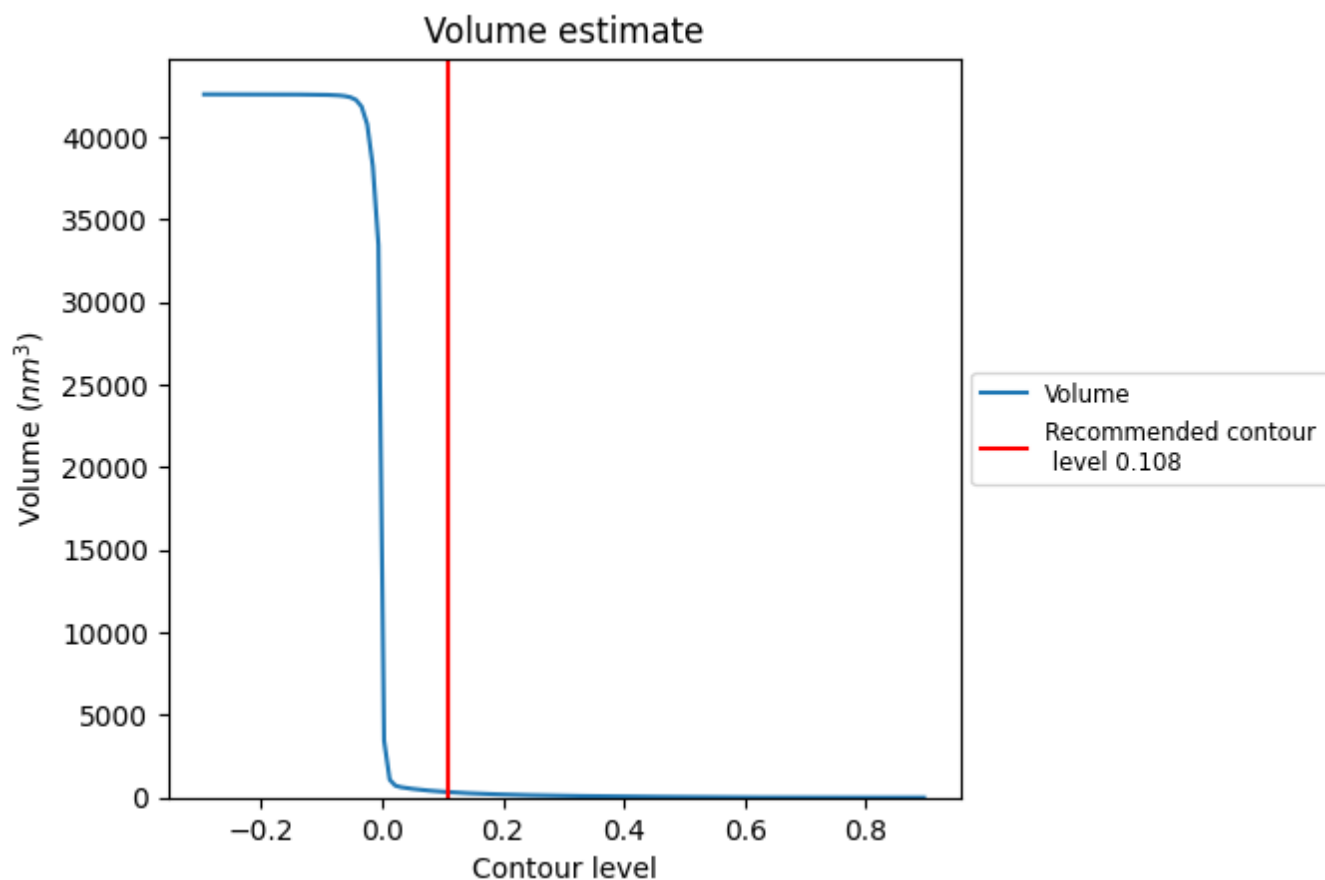
This section contains the results of statistical analysis of the map.

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.

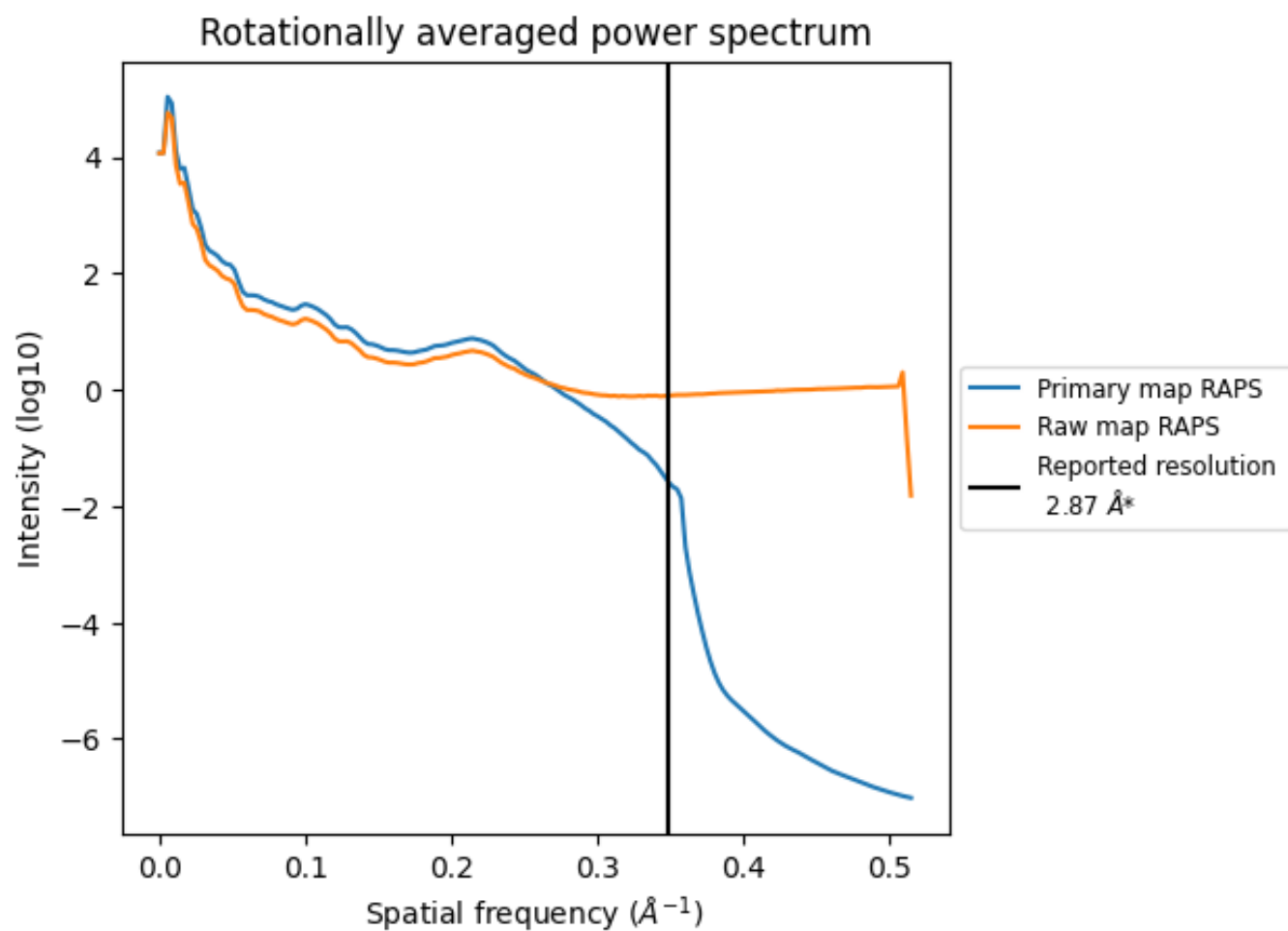
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 336 nm³; this corresponds to an approximate mass of 303 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 ⓘ

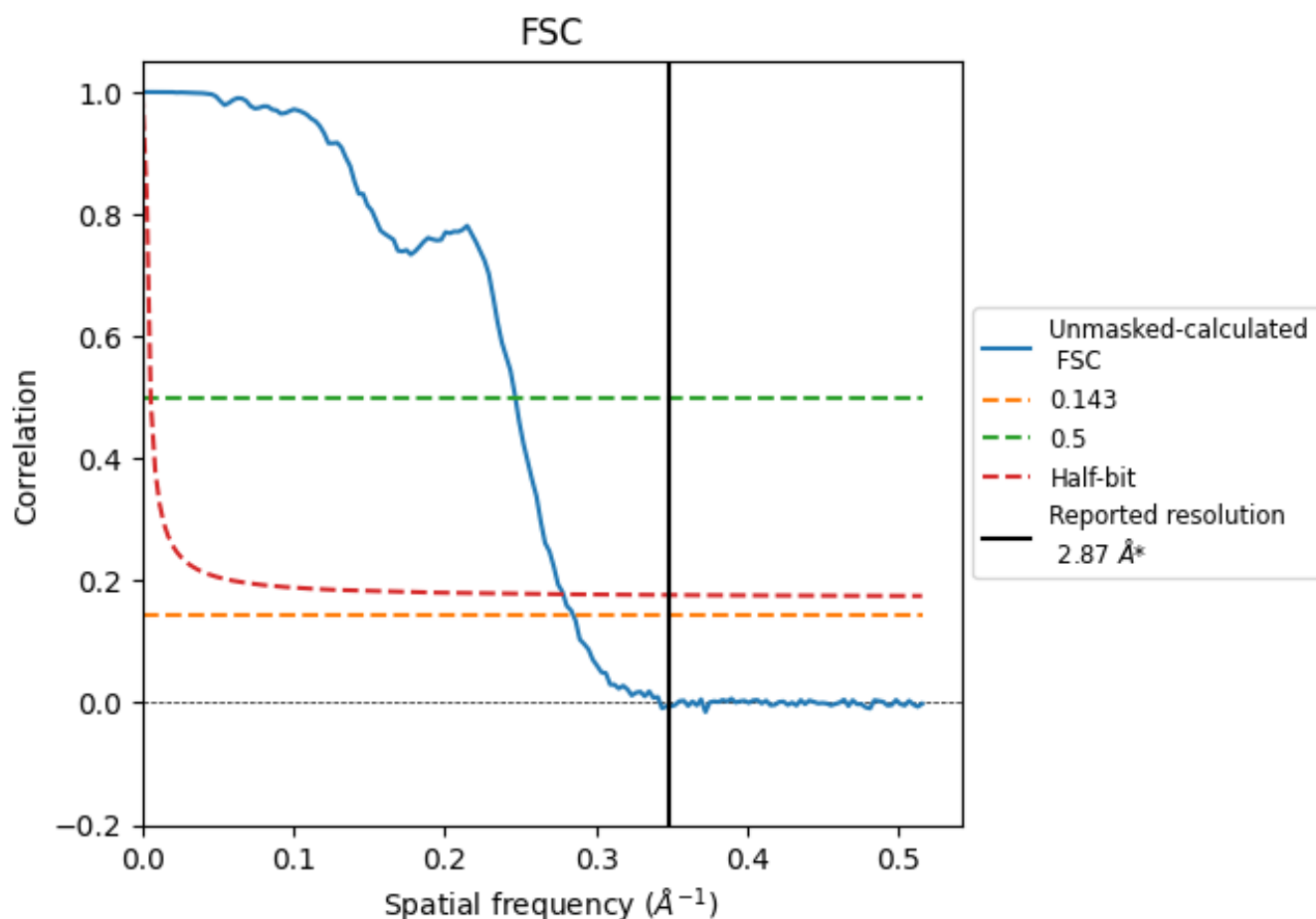


*Reported resolution corresponds to spatial frequency of 0.348 Å⁻¹

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 0.348 Å⁻¹

8.2 Resolution estimates [i](#)

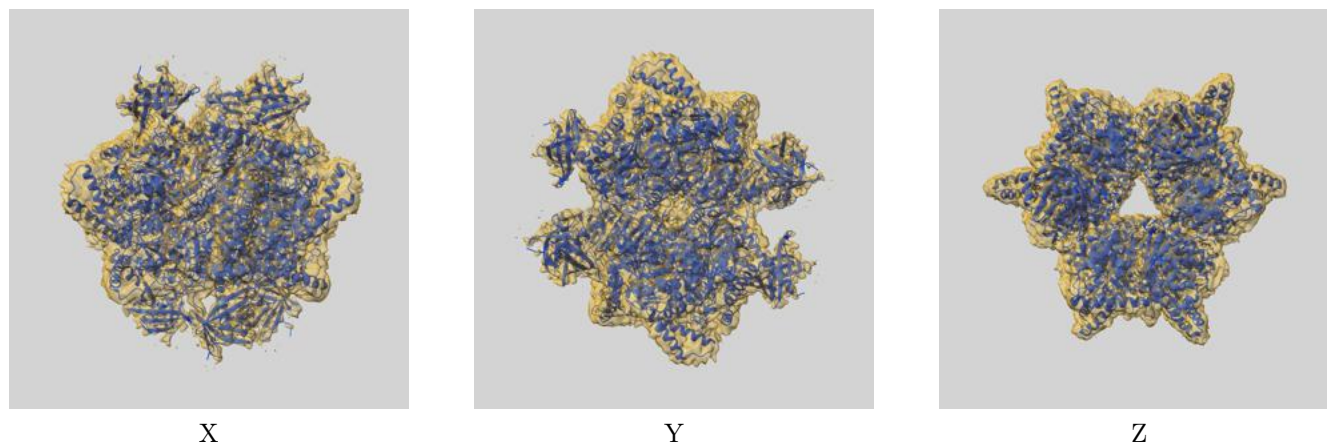
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.87	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.51	4.06	3.59

*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 3.51 differs from the reported value 2.87 by more than 10 %

9 Map-model fit [i](#)

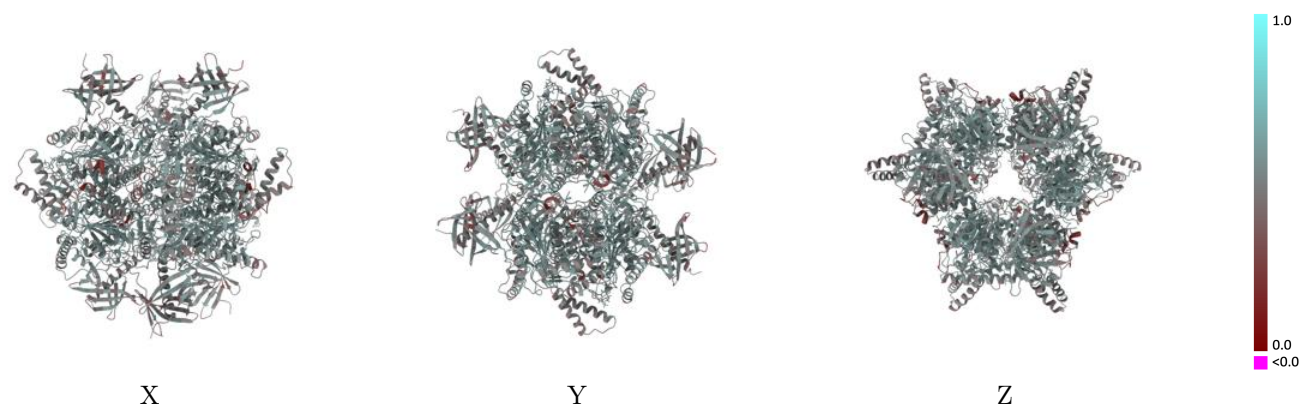
This section contains information regarding the fit between EMDB map EMD-36092 and PDB model 8J99. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



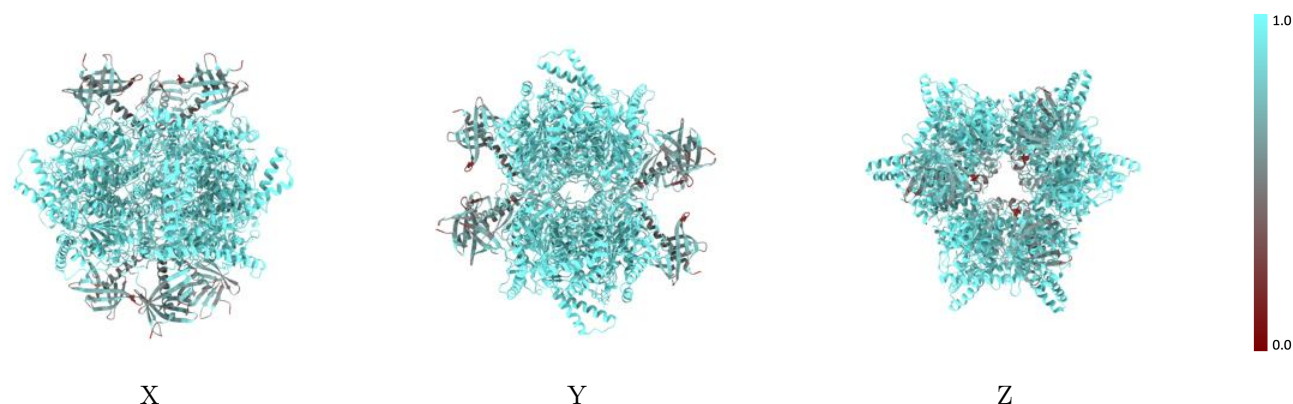
The images above show the 3D surface view of the map at the recommended contour level 0.108 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



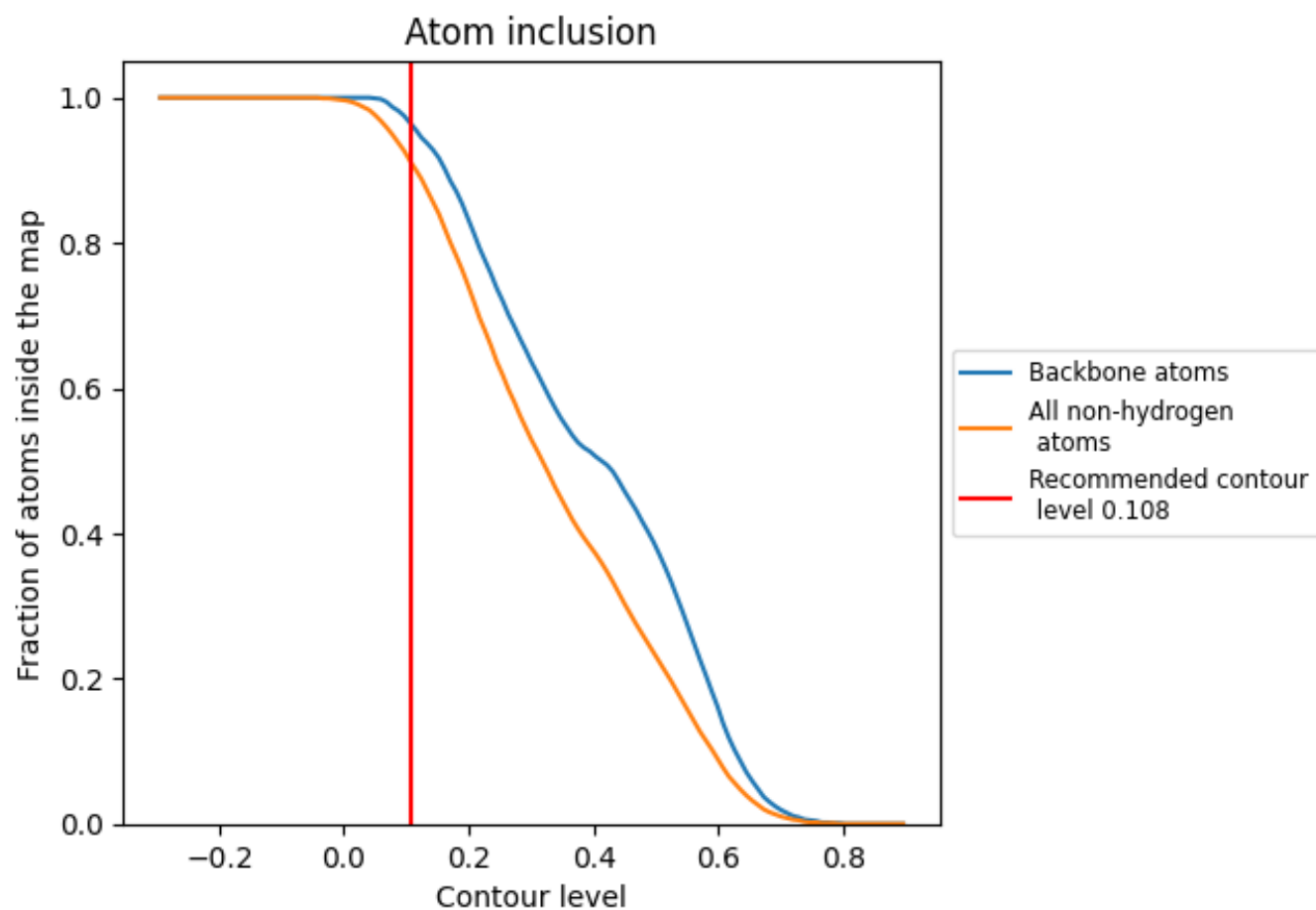
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.108).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 91% 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 (0.108) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9100	0.5170
A	0.6480	0.4760
B	0.9800	0.5270
C	0.6470	0.4790
D	0.9810	0.5280
E	0.6460	0.4720
F	0.6470	0.4780
G	0.9810	0.5290
H	0.9810	0.5270
I	0.6460	0.4750
J	0.9800	0.5290
K	0.6440	0.4720
L	0.9810	0.5280

1.0

0.0

<0.0