



wwPDB EM Validation Summary Report ⓘ

Mar 27, 2026 – 01:57 PM UTC

PDB ID : 8PN8 / pdb_00008pn8
EMDB ID : EMD-17778
Title : Engineered glycolyl-CoA carboxylase (L100N variant) with bound CoA
Authors : Zarzycki, J.; Marchal, D.G.; Schulz, L.; Prinz, S.; Erb, T.J.
Deposited on : 2023-06-30
Resolution : 2.31 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:

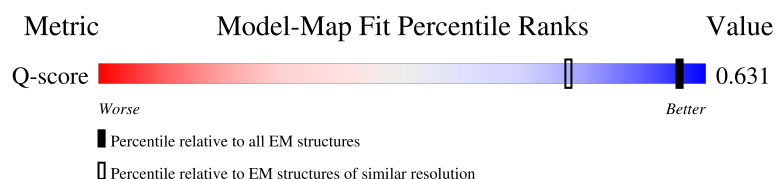
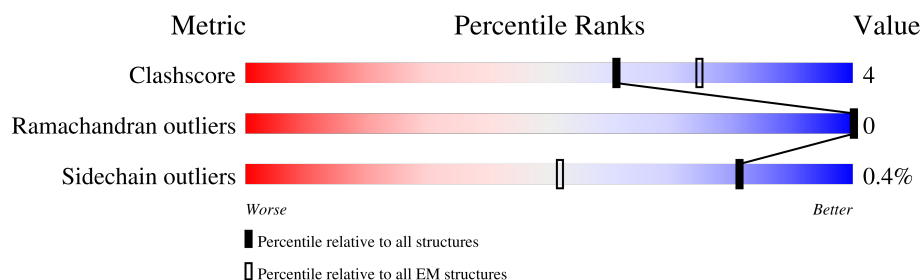
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.31 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	4306 (1.81 - 2.81)

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	510	
1	B	510	
1	C	510	
1	D	510	

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Mol	Chain	Length	Quality of chain
1	E	510	 85%14%
1	F	510	 85%15%
2	G	667	 30%68%
2	H	667	 28%68%
2	I	667	 30%68%
2	J	667	 30%68%
2	K	667	 29%68%
2	L	667	 30%68%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 34298 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 Propionyl-CoA carboxylase beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	506	Total	C	N	O	S	0	0
			3904	2474	689	725	16		
1	B	506	Total	C	N	O	S	0	0
			3904	2474	689	725	16		
1	C	506	Total	C	N	O	S	0	0
			3904	2474	689	725	16		
1	D	506	Total	C	N	O	S	0	0
			3904	2474	689	725	16		
1	E	506	Total	C	N	O	S	0	0
			3904	2474	689	725	16		
1	F	506	Total	C	N	O	S	0	0
			3904	2474	689	725	16		

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ASN	LEU	engineered mutation	UNP C5AP75
A	143	HIS	TYR	engineered mutation	UNP C5AP75
A	407	ILE	ASP	engineered mutation	UNP C5AP75
A	450	VAL	ILE	engineered mutation	UNP C5AP75
A	502	ARG	TRP	engineered mutation	UNP C5AP75
B	100	ASN	LEU	engineered mutation	UNP C5AP75
B	143	HIS	TYR	engineered mutation	UNP C5AP75
B	407	ILE	ASP	engineered mutation	UNP C5AP75
B	450	VAL	ILE	engineered mutation	UNP C5AP75
B	502	ARG	TRP	engineered mutation	UNP C5AP75
C	100	ASN	LEU	engineered mutation	UNP C5AP75
C	143	HIS	TYR	engineered mutation	UNP C5AP75
C	407	ILE	ASP	engineered mutation	UNP C5AP75
C	450	VAL	ILE	engineered mutation	UNP C5AP75
C	502	ARG	TRP	engineered mutation	UNP C5AP75
D	100	ASN	LEU	engineered mutation	UNP C5AP75
D	143	HIS	TYR	engineered mutation	UNP C5AP75
D	407	ILE	ASP	engineered mutation	UNP C5AP75

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Chain	Residue	Modelled	Actual	Comment	Reference
D	450	VAL	ILE	engineered mutation	UNP C5AP75
D	502	ARG	TRP	engineered mutation	UNP C5AP75
E	100	ASN	LEU	engineered mutation	UNP C5AP75
E	143	HIS	TYR	engineered mutation	UNP C5AP75
E	407	ILE	ASP	engineered mutation	UNP C5AP75
E	450	VAL	ILE	engineered mutation	UNP C5AP75
E	502	ARG	TRP	engineered mutation	UNP C5AP75
F	100	ASN	LEU	engineered mutation	UNP C5AP75
F	143	HIS	TYR	engineered mutation	UNP C5AP75
F	407	ILE	ASP	engineered mutation	UNP C5AP75
F	450	VAL	ILE	engineered mutation	UNP C5AP75
F	502	ARG	TRP	engineered mutation	UNP C5AP75

- Molecule 2 is a protein called Propionyl-CoA carboxylase alpha subunit.

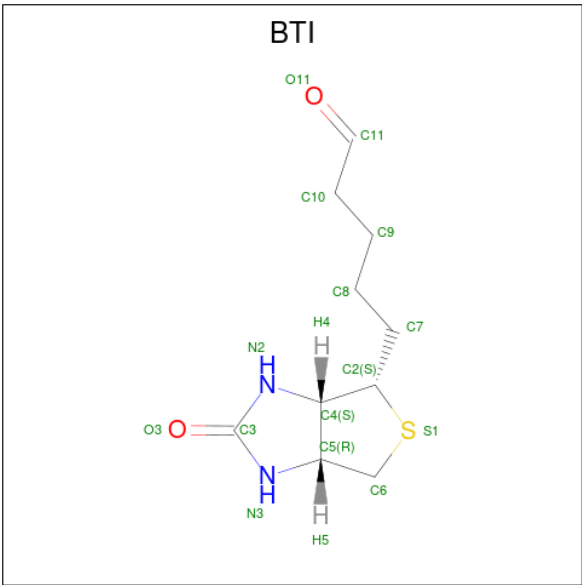
Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	213	Total	C	N	O	S	0	0
			1605	1006	290	302	7		
2	H	213	Total	C	N	O	S	0	0
			1605	1006	290	302	7		
2	I	213	Total	C	N	O	S	0	0
			1605	1006	290	302	7		
2	J	213	Total	C	N	O	S	0	0
			1605	1006	290	302	7		
2	K	213	Total	C	N	O	S	0	0
			1605	1006	290	302	7		
2	L	213	Total	C	N	O	S	0	0
			1605	1006	290	302	7		

- Molecule 3 is COENZYME A (CCD ID: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total	C	N	O	P	S	0
			48	21	7	16	3	1	
3	B	1	Total	C	N	O	P	S	0
			48	21	7	16	3	1	
3	C	1	Total	C	N	O	P	S	0
			48	21	7	16	3	1	
3	D	1	Total	C	N	O	P	S	0
			48	21	7	16	3	1	
3	E	1	Total	C	N	O	P	S	0
			48	21	7	16	3	1	
3	F	1	Total	C	N	O	P	S	0
			48	21	7	16	3	1	

- Molecule 4 is 5-(HEXAHYDRO-2-OXO-1H-THIENO[3,4-D]IMIDAZOL-6-YL)PENTANAL (CCD ID: BTI) (formula: C₁₀H₁₆N₂O₂S).



Mol	Chain	Residues	Atoms					AltConf
4	G	1	Total	C	N	O	S	0
			15	10	2	2	1	
4	H	1	Total	C	N	O	S	0
			15	10	2	2	1	
4	I	1	Total	C	N	O	S	0
			15	10	2	2	1	
4	J	1	Total	C	N	O	S	0
			15	10	2	2	1	
4	K	1	Total	C	N	O	S	0
			15	10	2	2	1	
4	L	1	Total	C	N	O	S	0
			15	10	2	2	1	

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		AltConf
5	A	131	Total	O	0
			131	131	
5	B	126	Total	O	0
			126	126	
5	C	138	Total	O	0
			138	138	
5	D	124	Total	O	0
			124	124	
5	E	122	Total	O	0
			122	122	
5	F	136	Total	O	0
			136	136	

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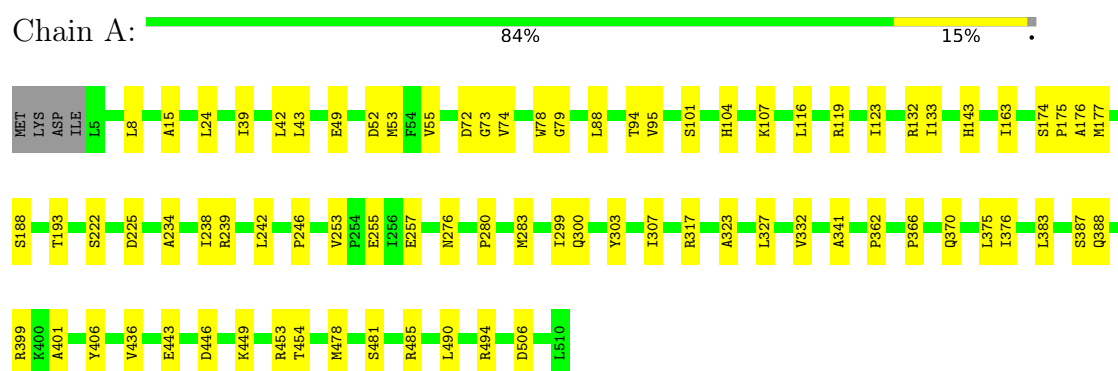
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Mol	Chain	Residues	Atoms		AltConf
5	G	15	Total 15	O 15	0
5	H	15	Total 15	O 15	0
5	I	14	Total 14	O 14	0
5	J	16	Total 16	O 16	0
5	K	16	Total 16	O 16	0
5	L	13	Total 13	O 13	0

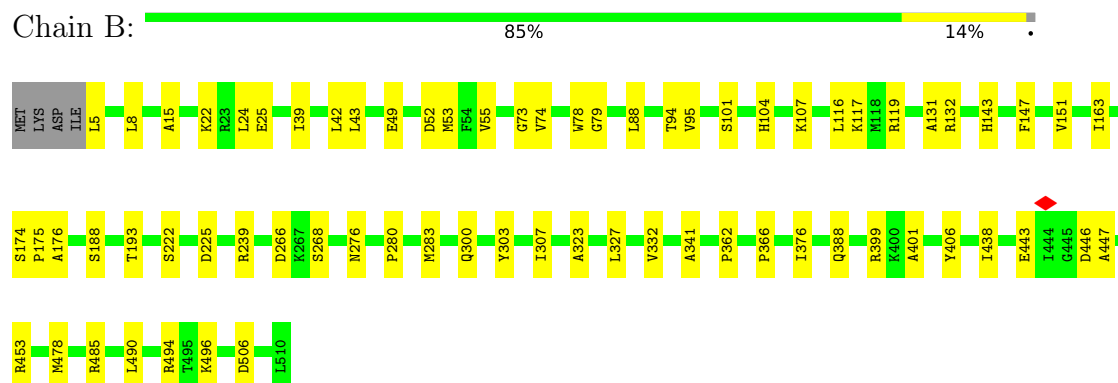
3 Residue-property plots [i](#)

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.

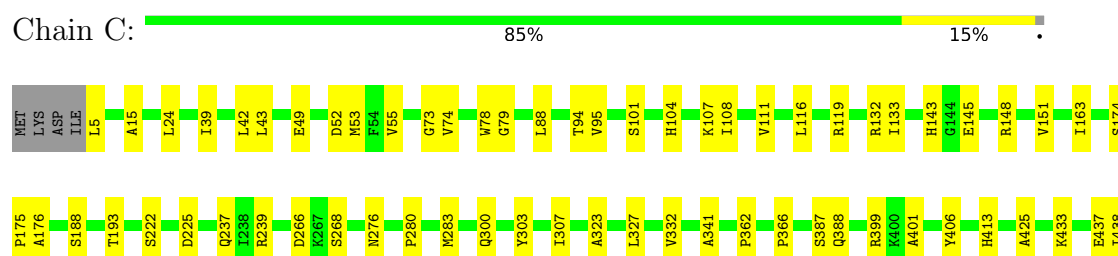
• Molecule 1: Propionyl-CoA carboxylase beta chain



• Molecule 1: Propionyl-CoA carboxylase beta chain



• Molecule 1: Propionyl-CoA carboxylase beta chain





- Molecule 1: Propionyl-CoA carboxylase beta chain

Chain D: 85% 14%



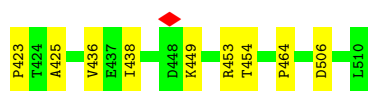
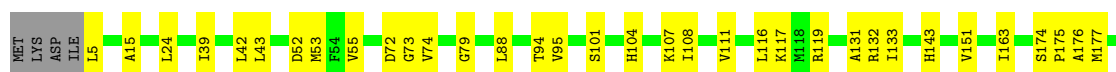
- Molecule 1: Propionyl-CoA carboxylase beta chain

Chain E: 85% 14%



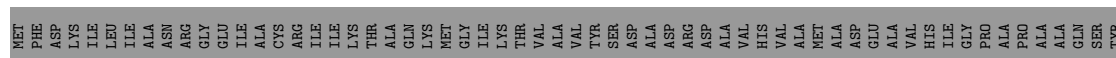
- Molecule 1: Propionyl-CoA carboxylase beta chain

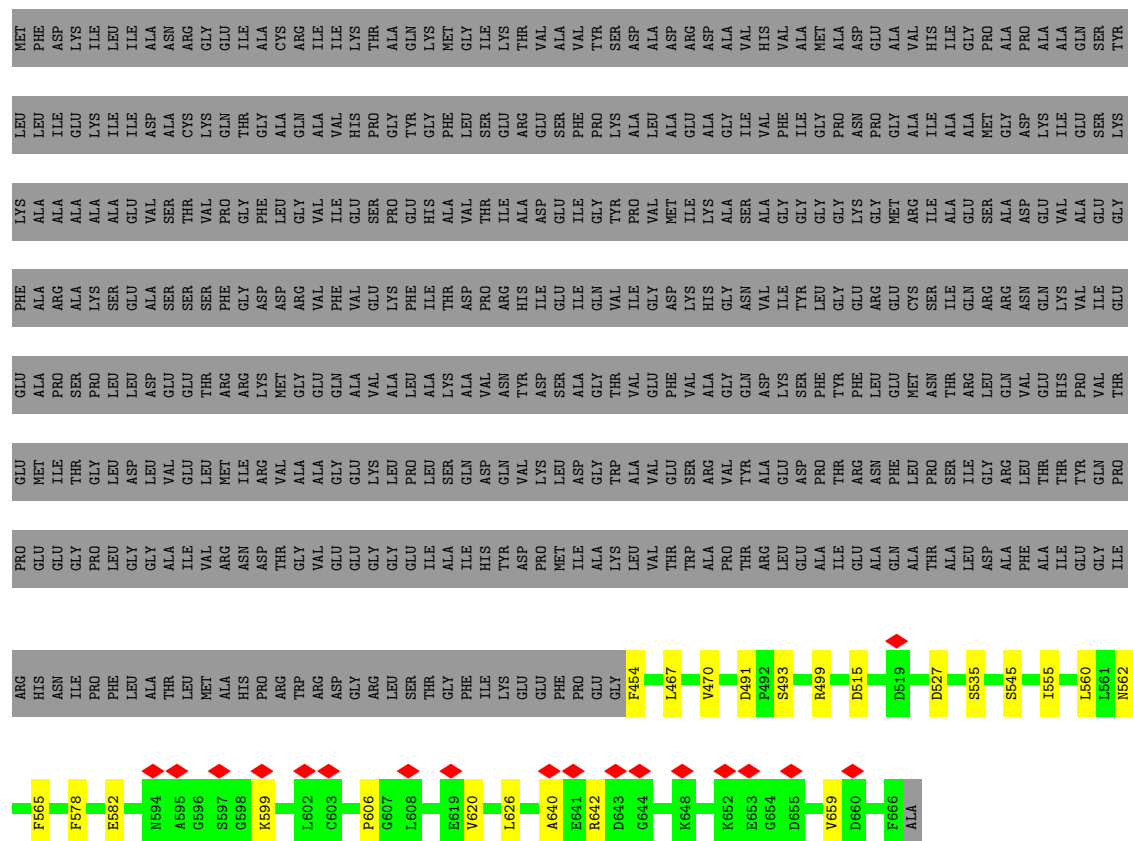
Chain F: 85% 15%



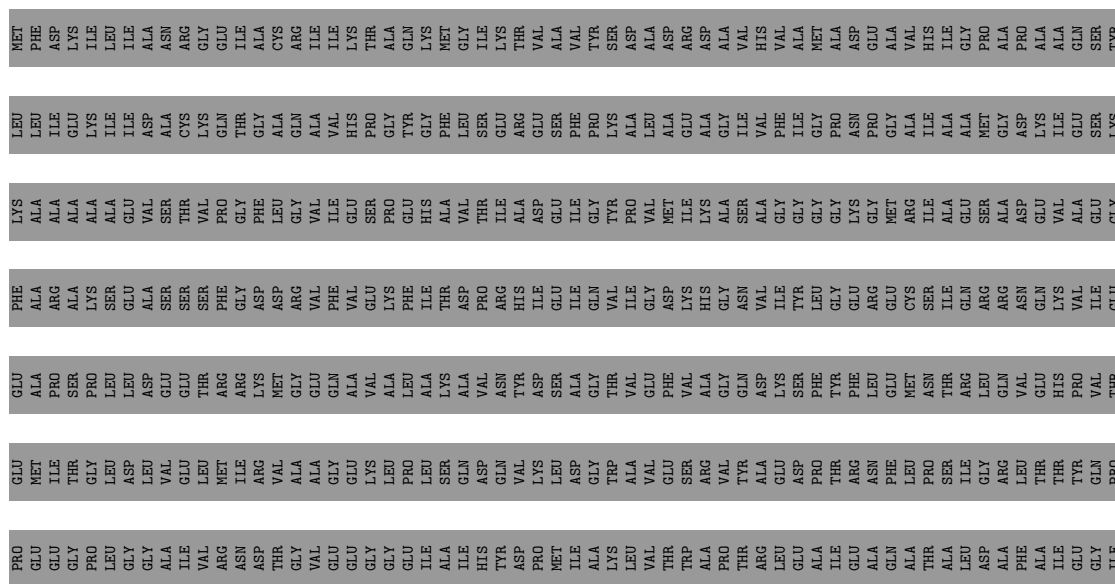
- Molecule 2: Propionyl-CoA carboxylase alpha subunit

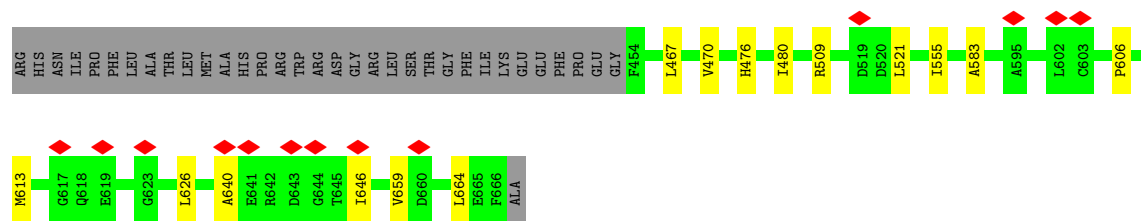
Chain G: 30% 68%



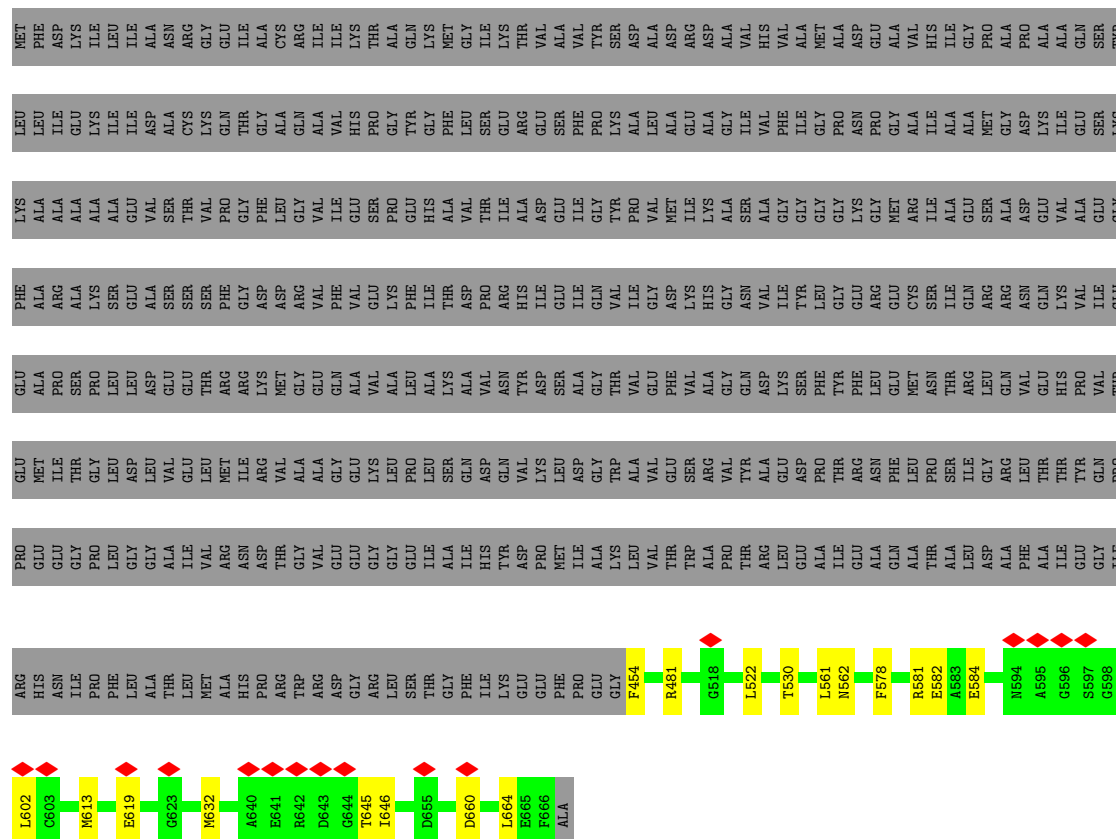


Chain I: 30% 68%

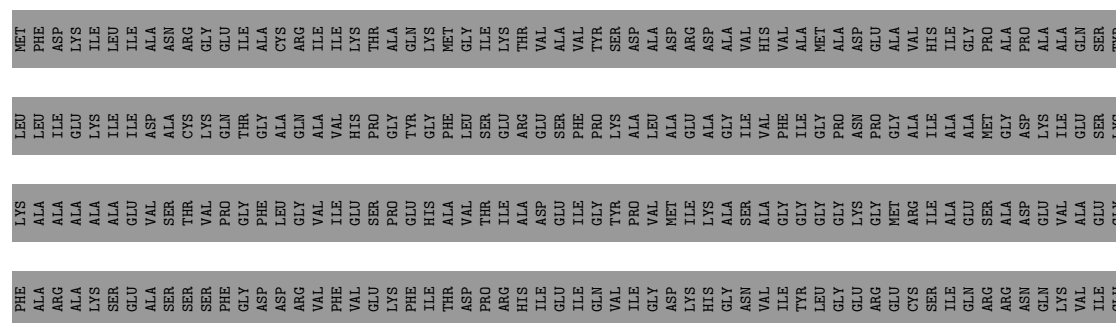




• Molecule 2: Propionyl-CoA carboxylase alpha subunit



• Molecule 2: Propionyl-CoA carboxylase alpha subunit



GLU	ALA	GLU	PRO	GLU	ARG
ILE	PRO	MET	GLU	HIS	ARG
SER	SER	ILE	GLU	ASN	GLU
PRO	GLY	THR	GLY	ILE	ASN
LEU	PRO	GLY	PRO	PRO	PHE
LEU	LEU	LEU	LEU	LEU	LEU
ASP	ASP	ASP	GLY	ALA	THR
LEU	LEU	LEU	GLY	LEU	LEU
GLU	VAL	GLU	ALA	THR	ALA
THR	GLU	LEU	ILE	MET	THR
ARG	THR	MET	VAL	ALA	GLN
ARG	ILE	ARG	ASN	HIS	VAL
LYS	ARG	ILE	ASP	PRO	GLU
MET	VAL	ARG	THR	ARG	THR
GLY	ALA	GLY	GLY	THR	GLY
GLU	ALA	GLY	GLU	ASP	GLY
ALA	GLY	GLN	GLY	GLY	ALA
VAL	VAL	VAL	GLY	ARG	LEU
ALA	PRO	VAL	GLU	SER	SER
LEU	LEU	VAL	GLU	THR	THR
ALA	LEU	VAL	ILE	GLY	GLN
LYS	SER	GLN	ALA	ILE	VAL
ALA	ASP	ALA	HIS	THR	GLU
VAL	ASP	VAL	TYR	ILE	HIS
TYR	VAL	GLN	ASP	GLY	PRO
ASP	LYS	LYS	PRO	GLU	VAL
SER	LEU	SER	MET	PHE	THR
ALA	ASP	ALA	ILE	PRO	THR
GLY	GLY	GLY	ALA	GLU	GLY
THR	THR	THR	LYS	GLY	THR
VAL	ALA	VAL	LEU	F454	ALA
PHE	GLU	PHE	VAL	L467	E653
VAL	SER	VAL	THR	V470	G654
ALA	ARG	ALA	ALA	R481	D655
GLN	VAL	THR	PRO	R499	D660
LYS	GLU	ARG	GLU	D515	L664
SER	PRO	GLU	ALA	D519	E665
PHE	THR	THR	ILE	D519	F666
TYR	ARG	ARG	GLU	I555	ALA
LEU	ASN	GLN	ALA	L560	
MET	LEU	THR	ALA	F565	
ASN	ILE	ASP	THR	F578	
THR	ARG	GLY	PHE	E582	
GLN	VAL	LEU	ALA	N594	
GLU	THR	THR	ILE	A595	
HIS	THR	TYR	GLY	G596	
PRO	VAL	GLN	VAL		
THR	THR	PRO	THR		

ARG	HIS	ASN	ILE	PRO	PHE	LEU	ALA	THR	LEU	MET	ALA	HIS	PRO	ARG	ASP	GLY	ARG	LEU	SER	THR	GLY	PHE	ILE	LYS	TYR	ASP	PRO	MET	ILE	ALA	LYS	GLY	F454	L467	V470	R481	R499	D515	D519	I555	L560	F565	F578	E582	N594	A595	G596
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S597	G598	K599	L602	C603	M613	G617	Q618	E619	V620	G623	E624	P625	L626	A640	E641	R642	D643	G644	T645	I646	S647	K648	I649	A650	E653	G654	D655	D660	L664	E665	F666	ALA
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ARG	HIS	ASN	ILE	PRO	PHE	LEU	ALA	THR	LEU	MET	ALA	HIS	PRO	ARG	ASP	GLY	ARG	LEU	SER	THR	GLY	PHE	ILE	LYS	TYR	ASP	PRO	MET	ILE	ALA	LYS	GLY	F454	L467	V470	R481	R499	D515	D519	I555	L560	F565	F578	E582	N594	A595	G596
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S597	G598	K599	L602	C603	M613	G617	Q618	E619	V620	G623	E624	P625	L626	A640	E641	R642	D643	G644	T645	I646	S647	K648	I649	A650	E653	G654	D655	D660	L664	E665	F666	ALA
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D3	Depositor
Number of particles used	113824	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 ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.405	Depositor
Minimum map value	-0.778	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.09	Depositor
Map size (Å)	418.5, 418.5, 418.5	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.837, 0.837, 0.837	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.11	0/3978	0.25	0/5368
1	B	0.11	0/3978	0.25	0/5368
1	C	0.11	0/3978	0.25	0/5368
1	D	0.11	0/3978	0.25	0/5368
1	E	0.11	0/3978	0.26	0/5368
1	F	0.11	0/3978	0.25	0/5368
2	G	0.07	0/1631	0.21	0/2211
2	H	0.07	0/1631	0.20	0/2211
2	I	0.08	0/1631	0.23	0/2211
2	J	0.08	0/1631	0.22	0/2211
2	K	0.07	0/1631	0.21	0/2211
2	L	0.08	0/1631	0.22	0/2211
All	All	0.10	0/33654	0.24	0/45474

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	A	3904	0	3914	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3904	0	3914	42	0
1	C	3904	0	3914	43	0
1	D	3904	0	3914	42	0
1	E	3904	0	3914	43	0
1	F	3904	0	3914	47	0
2	G	1605	0	1629	10	0
2	H	1605	0	1629	13	0
2	I	1605	0	1629	8	0
2	J	1605	0	1629	9	0
2	K	1605	0	1629	12	0
2	L	1605	0	1629	10	0
3	A	48	0	32	2	0
3	B	48	0	32	2	0
3	C	48	0	32	2	0
3	D	48	0	32	2	0
3	E	48	0	32	3	0
3	F	48	0	32	3	0
4	G	15	0	15	0	0
4	H	15	0	15	0	0
4	I	15	0	15	0	0
4	J	15	0	15	0	0
4	K	15	0	15	1	0
4	L	15	0	15	0	0
5	A	131	0	0	0	0
5	B	126	0	0	0	0
5	C	138	0	0	0	0
5	D	124	0	0	0	0
5	E	122	0	0	0	0
5	F	136	0	0	0	0
5	G	15	0	0	0	0
5	H	15	0	0	1	0
5	I	14	0	0	0	0
5	J	16	0	0	0	0
5	K	16	0	0	1	0
5	L	13	0	0	0	0
All	All	34298	0	33540	291	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 4.

The worst 5 of 291 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:E:276:ASN:O	1:E:399:ARG:NH2	2.30	0.64
1:A:388:GLN:NE2	1:A:506:ASP:OD2	2.31	0.64
1:F:388:GLN:NE2	1:F:506:ASP:OD2	2.30	0.64
1:C:413:HIS:O	1:D:148:ARG:NH1	2.30	0.63
1:F:276:ASN:O	1:F:399:ARG:NH2	2.32	0.62

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	504/510 (99%)	498 (99%)	6 (1%)	0	100	100
1	B	504/510 (99%)	500 (99%)	4 (1%)	0	100	100
1	C	504/510 (99%)	497 (99%)	7 (1%)	0	100	100
1	D	504/510 (99%)	499 (99%)	5 (1%)	0	100	100
1	E	504/510 (99%)	502 (100%)	2 (0%)	0	100	100
1	F	504/510 (99%)	497 (99%)	7 (1%)	0	100	100
2	G	211/667 (32%)	211 (100%)	0	0	100	100
2	H	211/667 (32%)	210 (100%)	1 (0%)	0	100	100
2	I	211/667 (32%)	208 (99%)	3 (1%)	0	100	100
2	J	211/667 (32%)	207 (98%)	4 (2%)	0	100	100
2	K	211/667 (32%)	208 (99%)	3 (1%)	0	100	100
2	L	211/667 (32%)	209 (99%)	2 (1%)	0	100	100
All	All	4290/7062 (61%)	4246 (99%)	44 (1%)	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	406/410 (99%)	404 (100%)	2 (0%)	81	89
1	B	406/410 (99%)	404 (100%)	2 (0%)	81	89
1	C	406/410 (99%)	404 (100%)	2 (0%)	81	89
1	D	406/410 (99%)	404 (100%)	2 (0%)	81	89
1	E	406/410 (99%)	404 (100%)	2 (0%)	81	89
1	F	406/410 (99%)	404 (100%)	2 (0%)	81	89
2	G	169/523 (32%)	168 (99%)	1 (1%)	78	88
2	H	169/523 (32%)	168 (99%)	1 (1%)	78	88
2	I	169/523 (32%)	169 (100%)	0	100	100
2	J	169/523 (32%)	168 (99%)	1 (1%)	78	88
2	K	169/523 (32%)	169 (100%)	0	100	100
2	L	169/523 (32%)	169 (100%)	0	100	100
All	All	3450/5598 (62%)	3435 (100%)	15 (0%)	81	91

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	143	HIS
2	H	527	ASP
1	E	55	VAL
2	J	480	ILE
1	F	143	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	278	ASN
2	J	636	ASN
1	E	230	ASN
1	F	378	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	159	GLN

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](#)

12 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	COA	C	601	-	47,50,50	0.94	1 (2%)	69,75,75	1.70	11 (15%)
4	BTI	L	701	2	15,16,16	1.48	2 (13%)	20,21,21	1.43	3 (15%)
4	BTI	H	701	2	15,16,16	1.46	2 (13%)	20,21,21	1.41	3 (15%)
3	COA	B	601	-	47,50,50	0.94	0	69,75,75	1.70	11 (15%)
4	BTI	I	701	2	15,16,16	1.48	2 (13%)	20,21,21	1.43	3 (15%)
3	COA	D	601	-	47,50,50	0.94	1 (2%)	69,75,75	1.70	11 (15%)
3	COA	A	601	-	47,50,50	0.95	2 (4%)	69,75,75	1.70	11 (15%)
3	COA	F	601	-	47,50,50	0.94	1 (2%)	69,75,75	1.70	10 (14%)
4	BTI	J	701	2	15,16,16	1.48	2 (13%)	20,21,21	1.42	3 (15%)
4	BTI	K	701	2	15,16,16	1.48	2 (13%)	20,21,21	1.43	3 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BTI	G	701	2	15,16,16	1.48	2 (13%)	20,21,21	1.42	3 (15%)
3	COA	E	601	-	47,50,50	0.93	0	69,75,75	1.70	11 (15%)

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	COA	C	601	-	-	10/48/64/64	0/3/3/3
4	BTI	L	701	2	-	2/6/27/27	0/2/2/2
4	BTI	H	701	2	-	2/6/27/27	0/2/2/2
3	COA	B	601	-	-	11/48/64/64	0/3/3/3
4	BTI	I	701	2	-	2/6/27/27	0/2/2/2
3	COA	D	601	-	-	12/48/64/64	0/3/3/3
3	COA	A	601	-	-	14/48/64/64	0/3/3/3
3	COA	F	601	-	-	13/48/64/64	0/3/3/3
4	BTI	J	701	2	-	2/6/27/27	0/2/2/2
4	BTI	K	701	2	-	2/6/27/27	0/2/2/2
4	BTI	G	701	2	-	2/6/27/27	0/2/2/2
3	COA	E	601	-	-	12/48/64/64	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)
4	J	701	BTI	C3-N3	3.86	1.42	1.35
4	G	701	BTI	C3-N3	3.84	1.42	1.35
4	L	701	BTI	C3-N3	3.84	1.42	1.35
4	I	701	BTI	C3-N3	3.83	1.42	1.35
4	H	701	BTI	C3-N3	3.81	1.42	1.35

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	COA	P3B-O3B-C3B	-5.74	108.09	123.43
3	B	601	COA	P3B-O3B-C3B	-5.74	108.10	123.43
3	F	601	COA	P3B-O3B-C3B	-5.72	108.14	123.43
3	C	601	COA	P3B-O3B-C3B	-5.70	108.21	123.43
3	E	601	COA	P3B-O3B-C3B	-5.67	108.30	123.43

There are no chirality outliers.

5 of 84 torsion outliers are listed below:

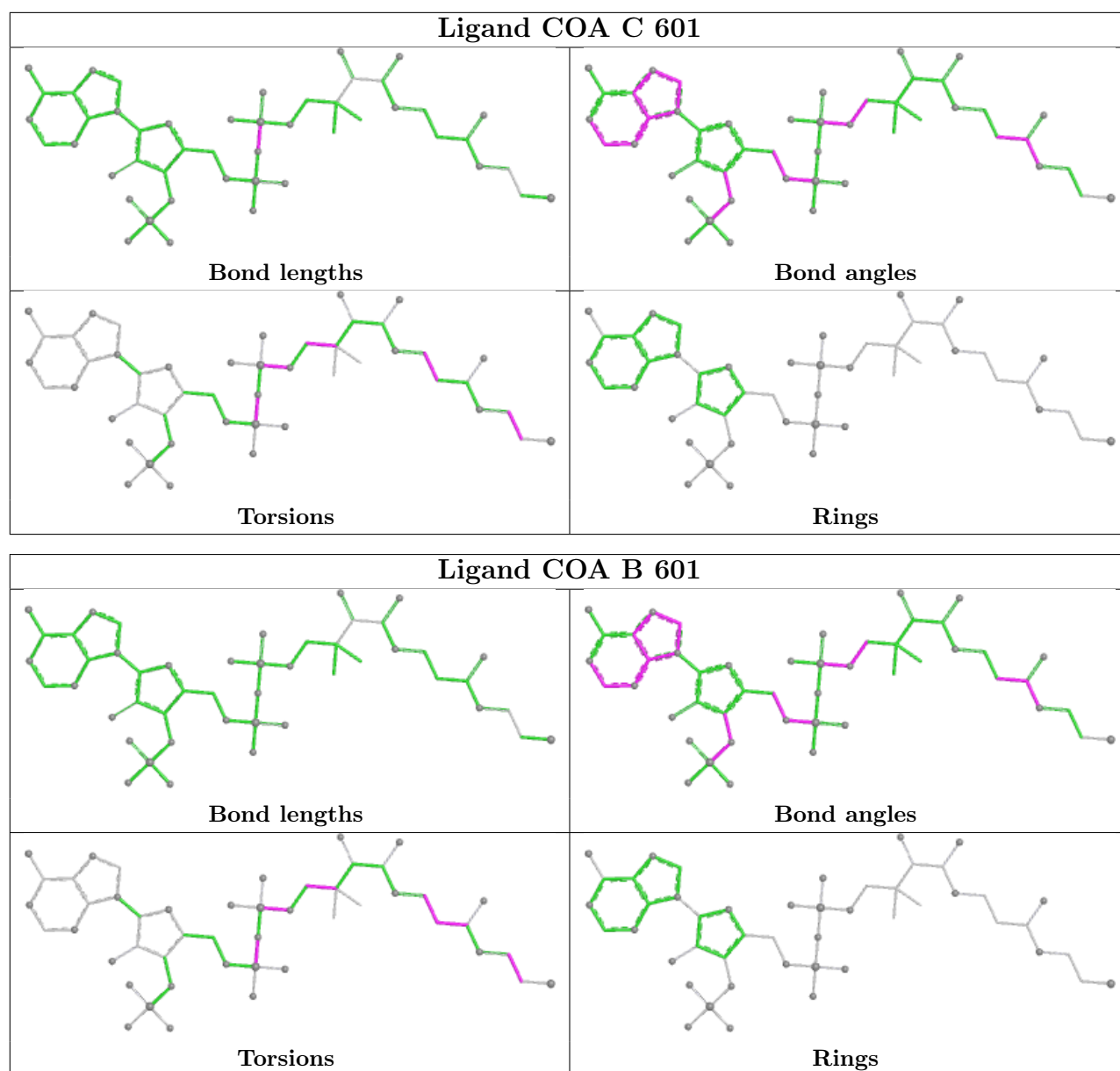
Mol	Chain	Res	Type	Atoms
3	A	601	COA	CCP-O6A-P2A-O3A
3	A	601	COA	CCP-O6A-P2A-O4A
3	A	601	COA	CCP-O6A-P2A-O5A
3	A	601	COA	CDP-CBP-CCP-O6A
3	A	601	COA	CEP-CBP-CCP-O6A

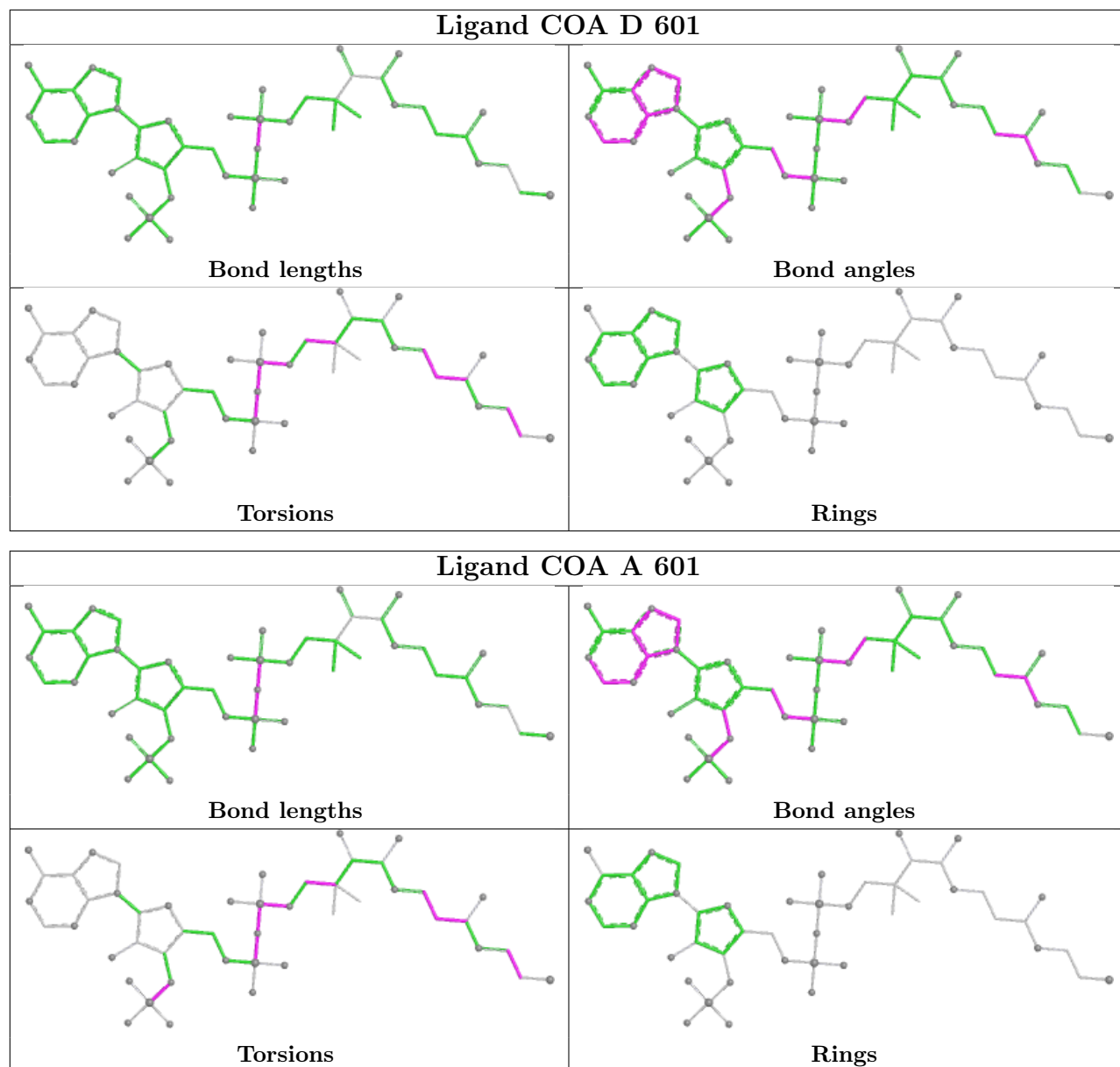
There are no ring outliers.

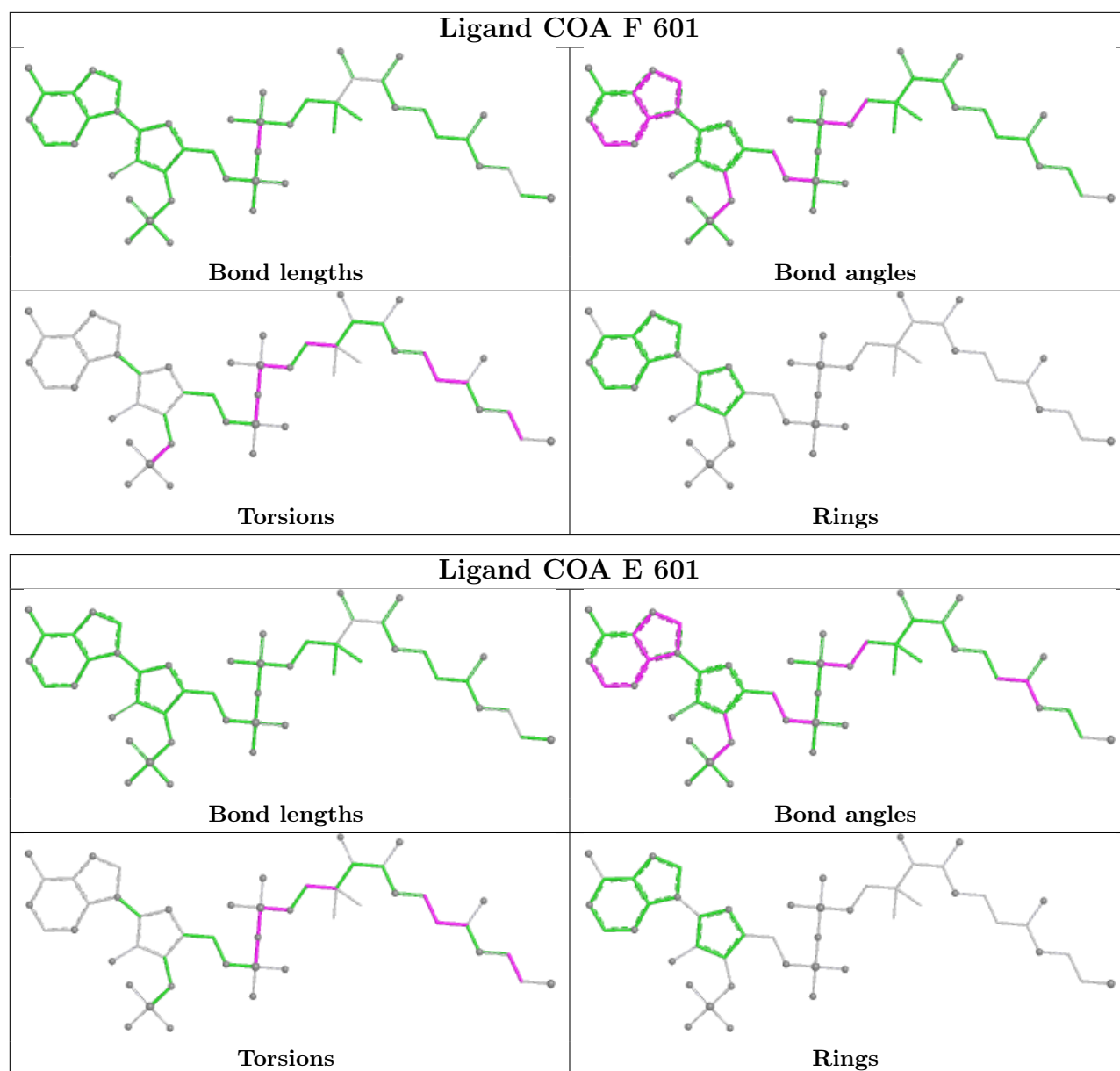
7 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	601	COA	2	0
3	B	601	COA	2	0
3	D	601	COA	2	0
3	A	601	COA	2	0
3	F	601	COA	3	0
4	K	701	BTI	1	0
3	E	601	COA	3	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.

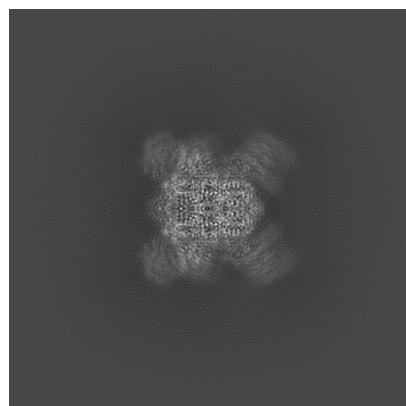
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17778. These allow visual inspection of the internal detail of the map and identification of artifacts.

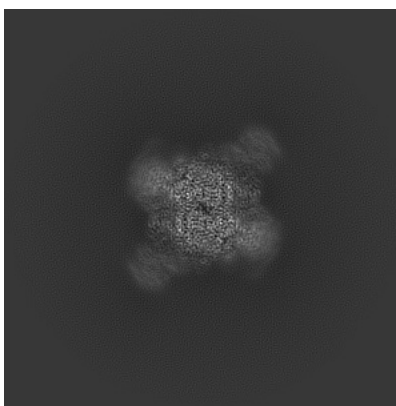
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

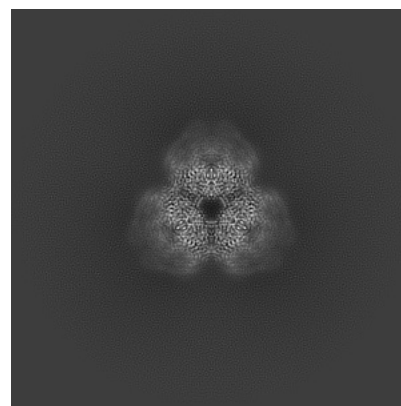
6.1.1 Primary map



X

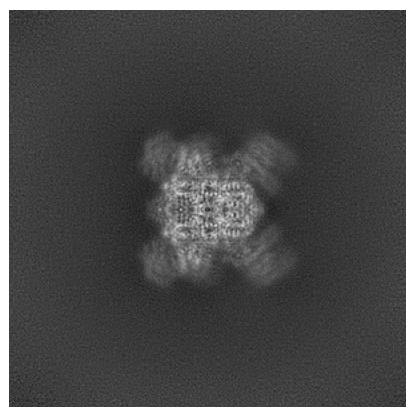


Y

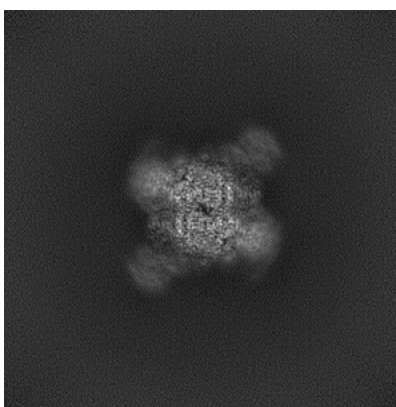


Z

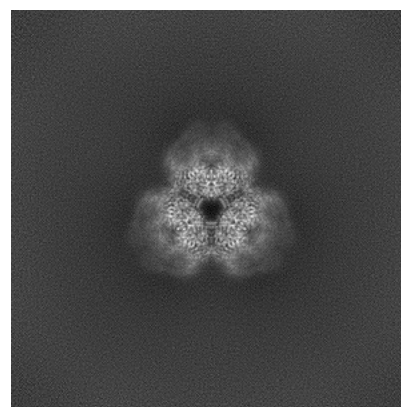
6.1.2 Raw map



X



Y

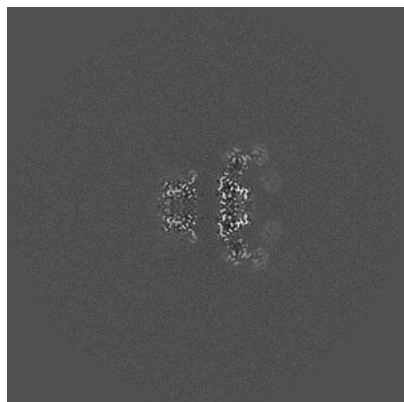


Z

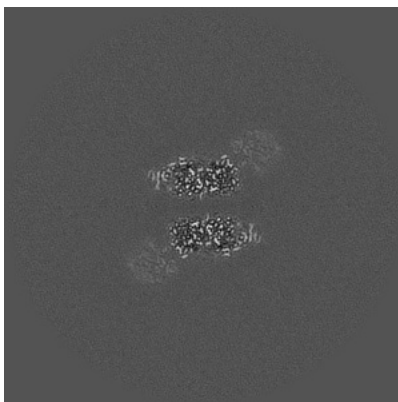
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

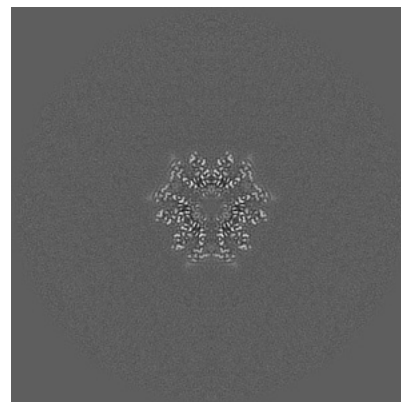
6.2.1 Primary map



X Index: 250

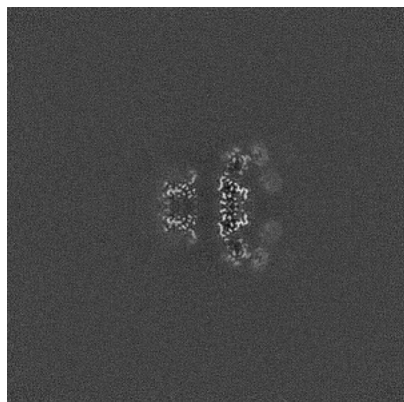


Y Index: 250

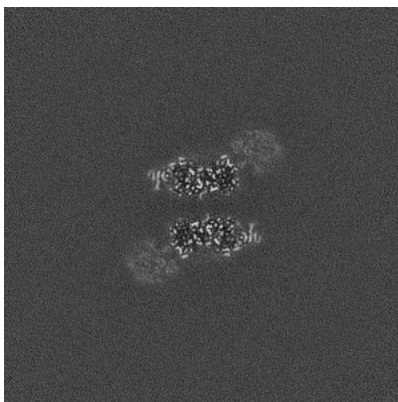


Z Index: 250

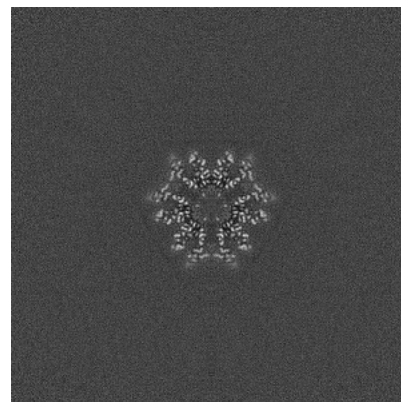
6.2.2 Raw map



X Index: 250



Y Index: 250

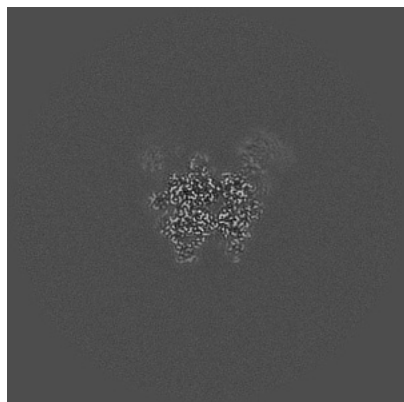


Z Index: 250

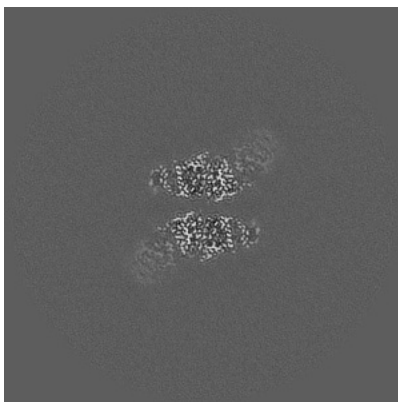
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

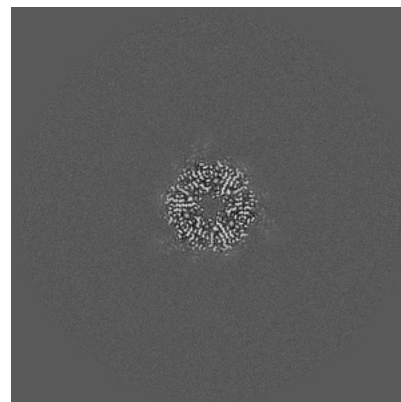
6.3.1 Primary map



X Index: 228

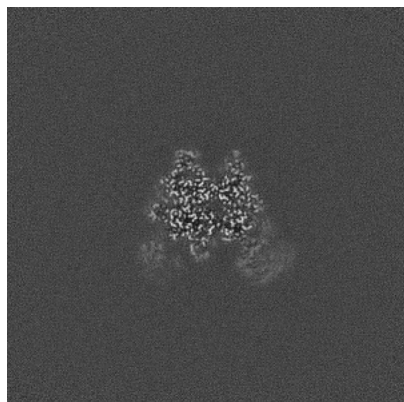


Y Index: 242

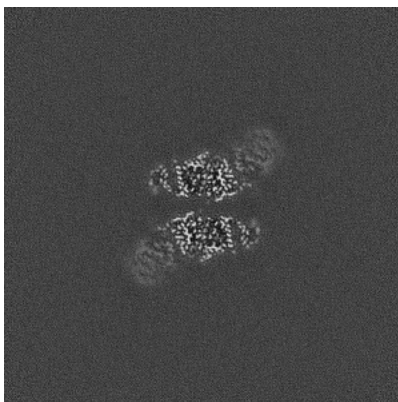


Z Index: 269

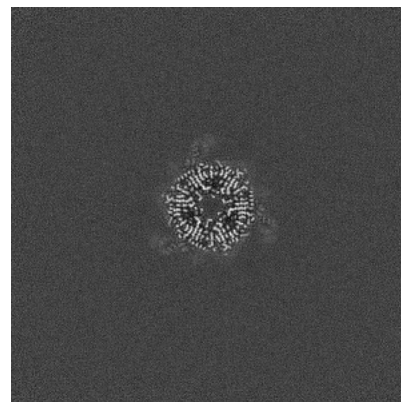
6.3.2 Raw map



X Index: 272



Y Index: 242

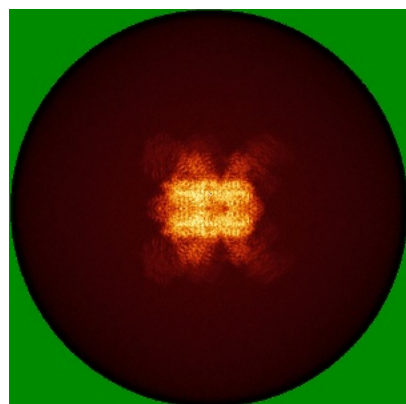


Z Index: 270

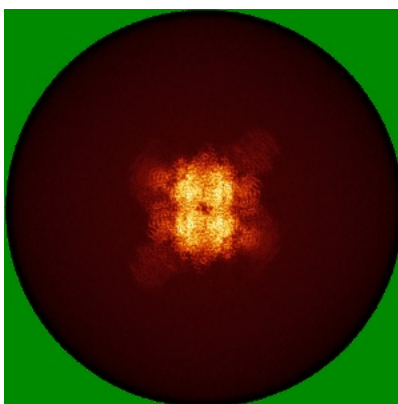
The images above show the largest variance slices of the map in three orthogonal directions.

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

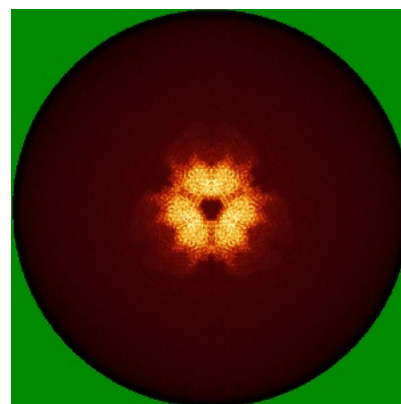
6.4.1 Primary map



X

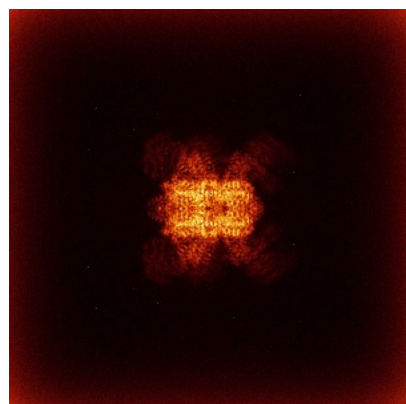


Y

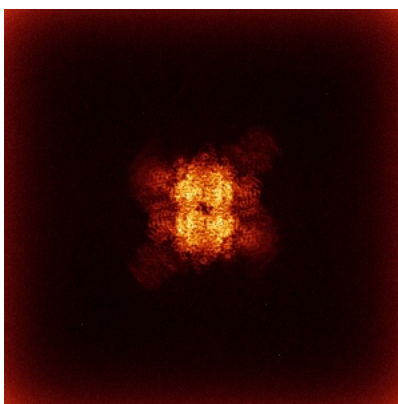


Z

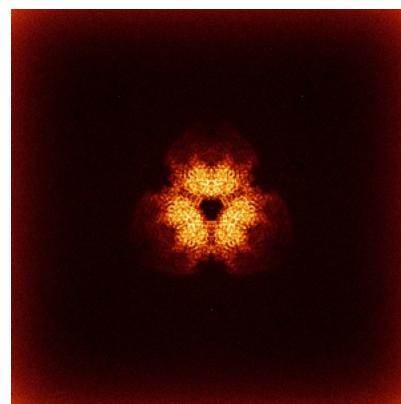
6.4.2 Raw map



X



Y

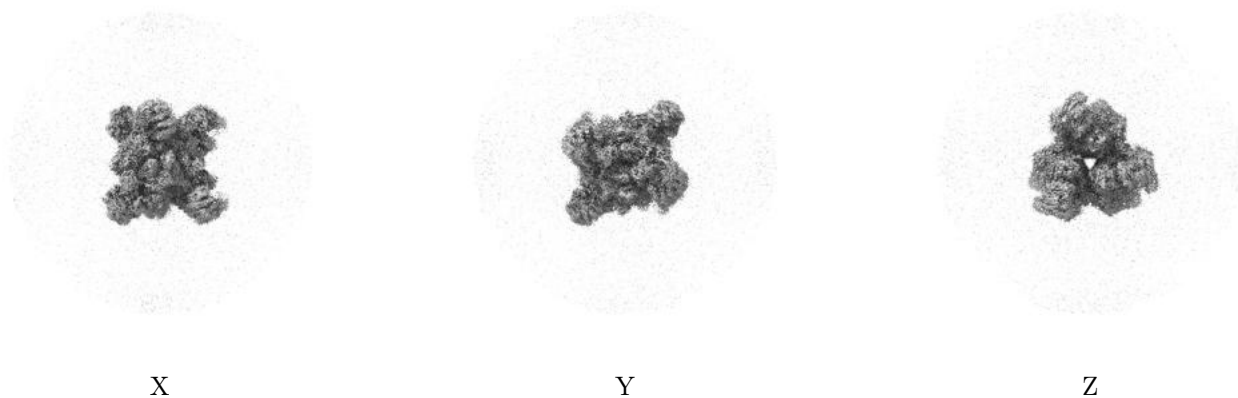


Z

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.

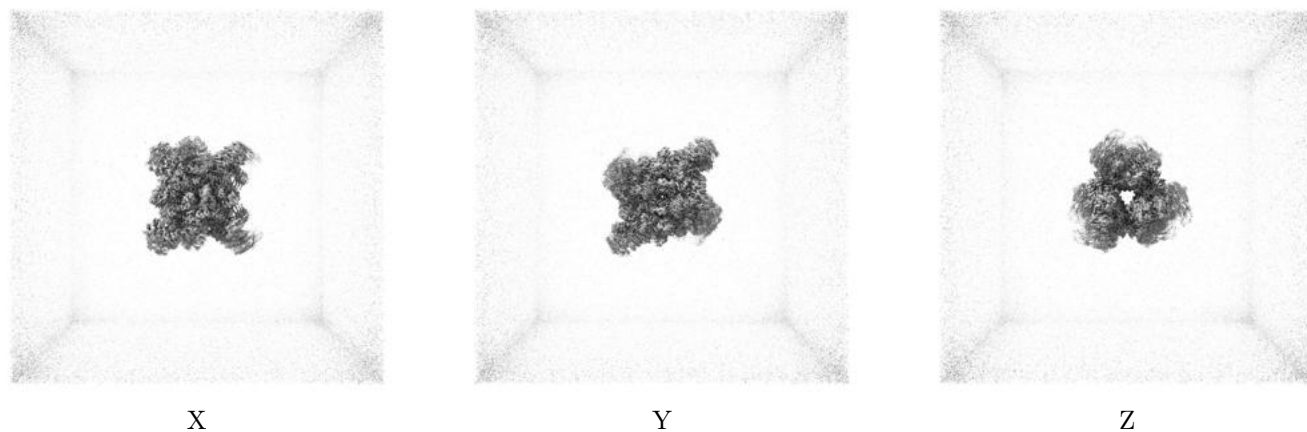
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.09. 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.

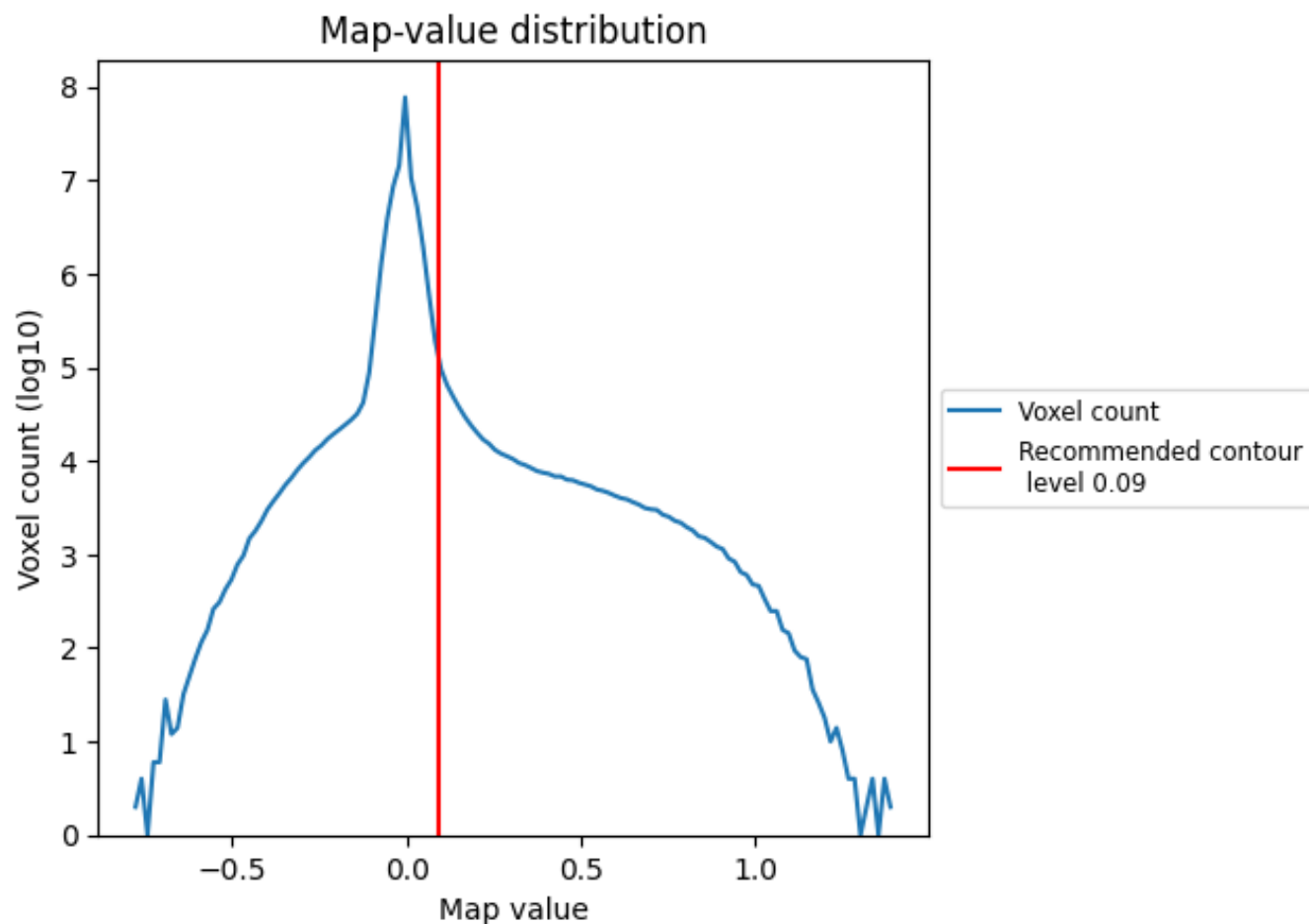
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

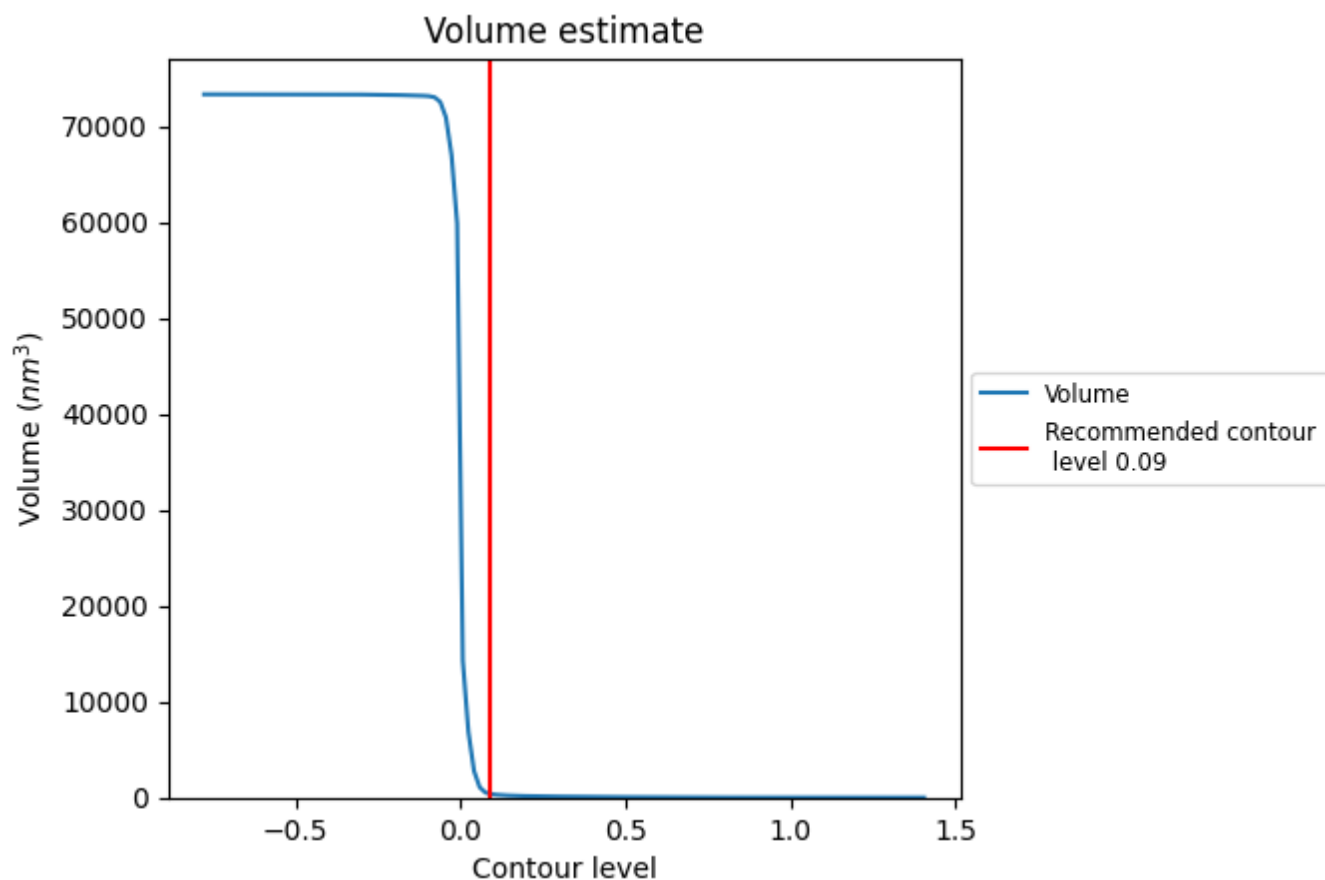
This section contains the results of statistical analysis of the map.

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.

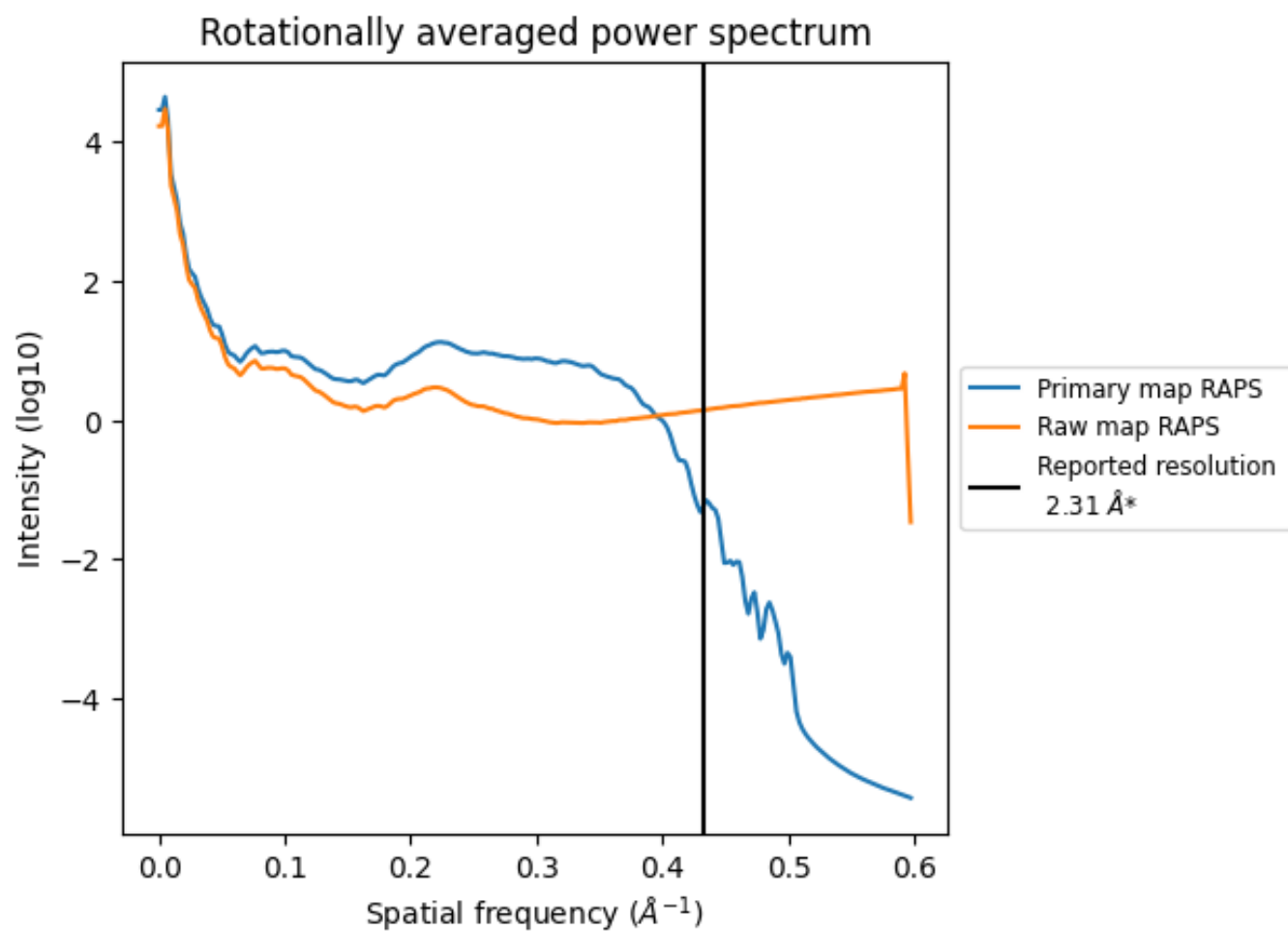
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 381 nm³; this corresponds to an approximate mass of 344 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 [i](#)

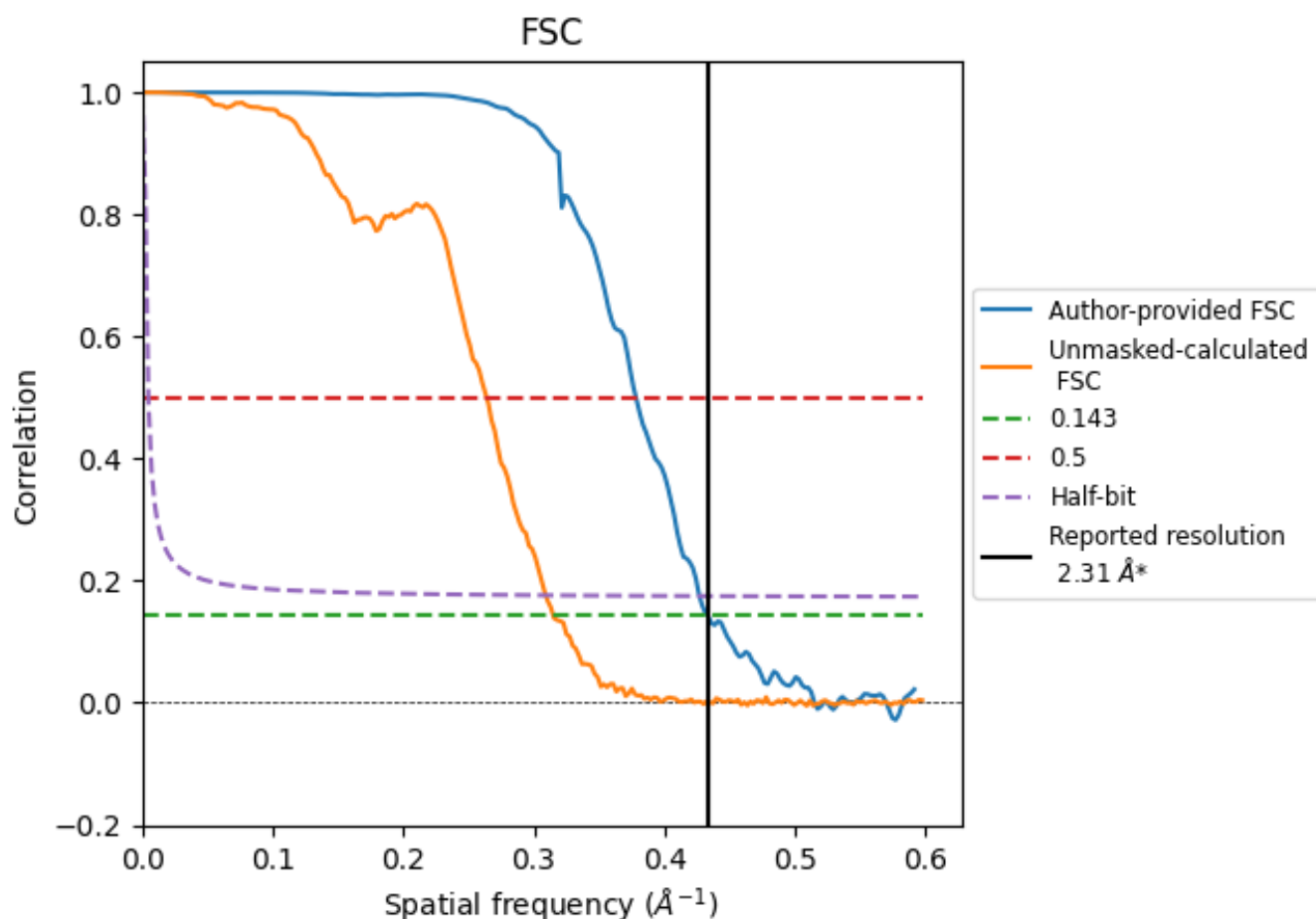


*Reported resolution corresponds to spatial frequency of 0.433 Å⁻¹

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 $0.433 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

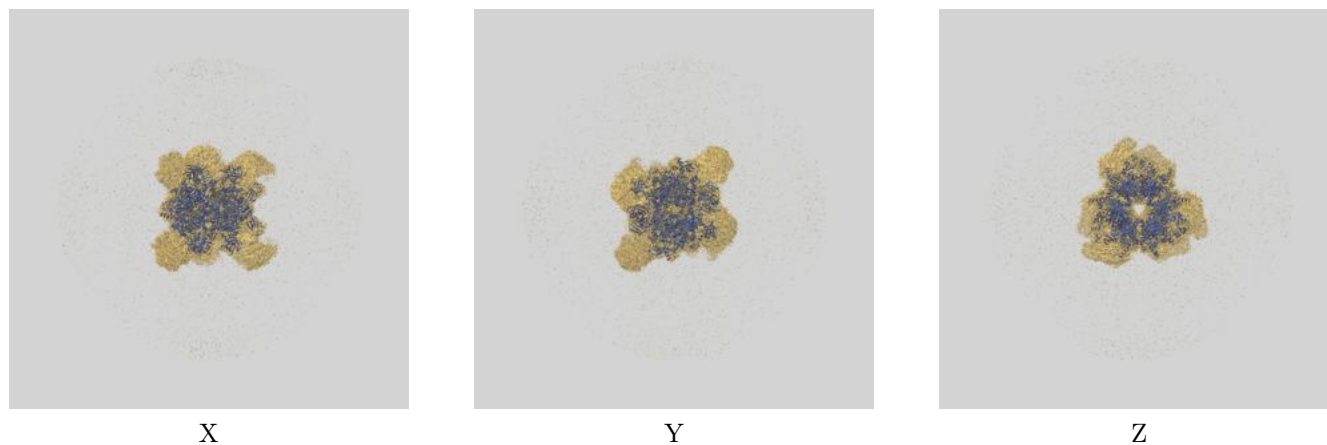
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.31	-	-
Author-provided FSC curve	2.31	2.64	2.34
Unmasked-calculated*	3.18	3.79	3.23

*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 3.18 differs from the reported value 2.31 by more than 10 %

9 Map-model fit [i](#)

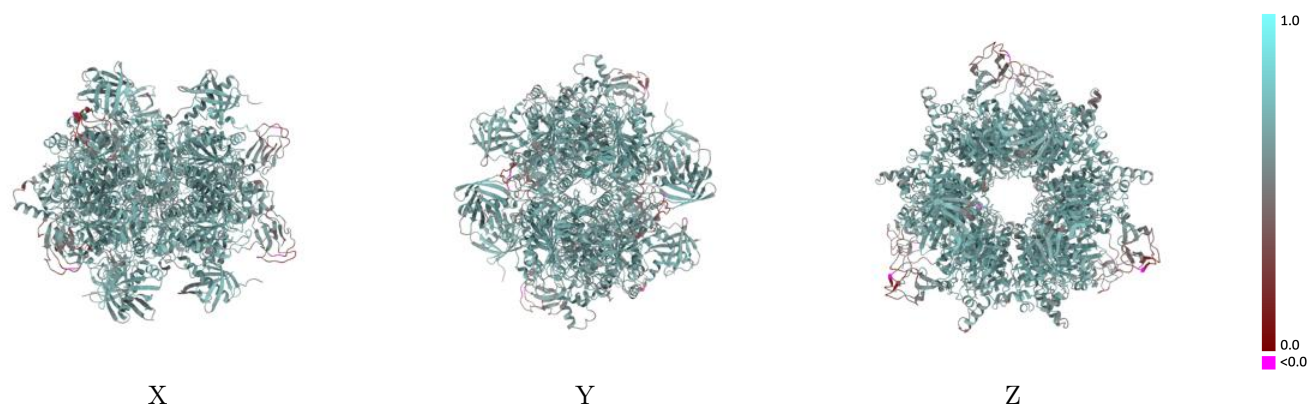
This section contains information regarding the fit between EMDB map EMD-17778 and PDB model 8PN8. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



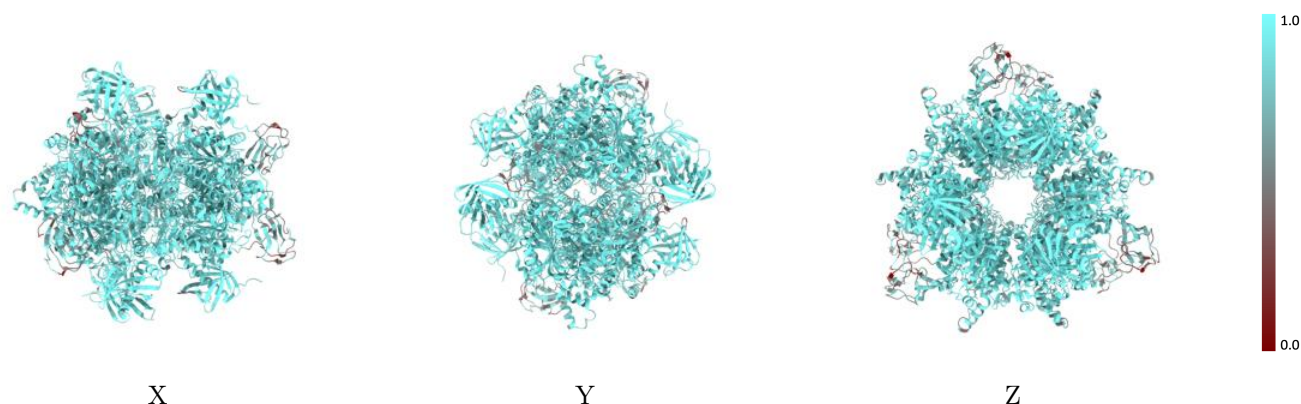
The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



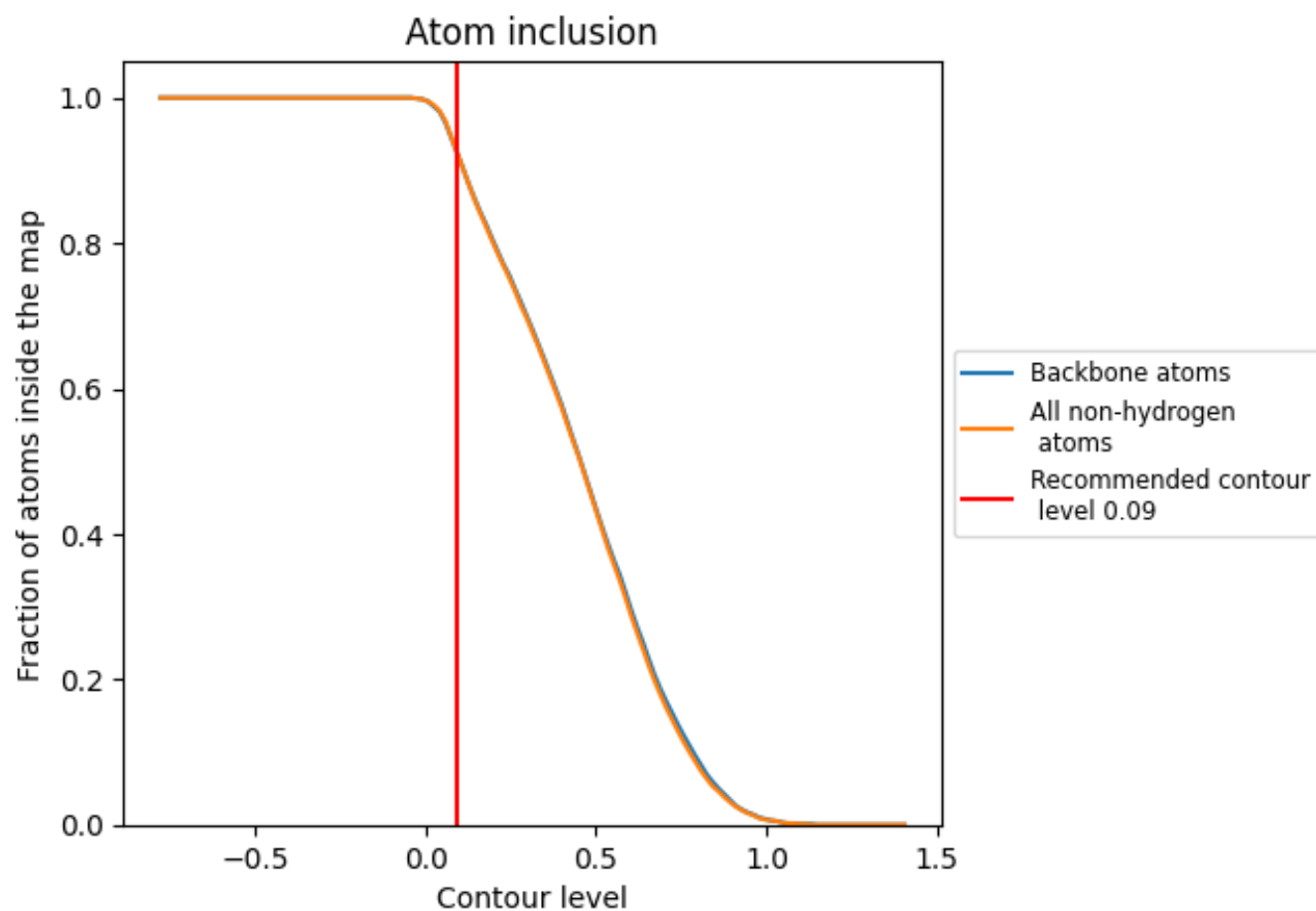
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.09).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 93% 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 (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9270	0.6310
A	0.9720	0.6640
B	0.9710	0.6640
C	0.9720	0.6640
D	0.9700	0.6630
E	0.9710	0.6620
F	0.9720	0.6630
G	0.8210	0.5510
H	0.8300	0.5560
I	0.8170	0.5460
J	0.8290	0.5530
K	0.8260	0.5510
L	0.8100	0.5440

1.0

0.0

<0.0