



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 01:58 PM UTC

PDB ID : 9E2K / pdb_00009e2k
EMDB ID : EMD-47455
Title : Variediene synthase with one cyclase (conformation 1)
Authors : Wenger, E.S.; Christianson, D.W.
Deposited on : 2024-10-22
Resolution : 3.00 Å(reported)

This is a Full wwPDB EM Validation 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:

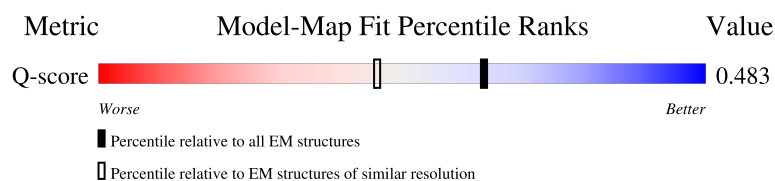
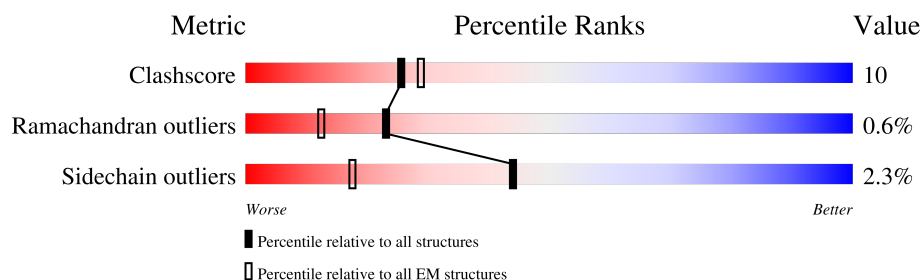
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	
1	B	725	
1	C	725	
1	D	725	

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Mol	Chain	Length	Quality of chain
1	E	725	29%8%62%
1	F	725	30%8%62%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15520 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 Variediene synthase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	289	Total	C	N	O	S	0	0
			2301	1450	400	438	13		
1	B	568	Total	C	N	O	S	0	0
			4600	2919	793	859	29		
1	C	274	Total	C	N	O	S	0	0
			2180	1371	375	421	13		
1	D	260	Total	C	N	O	S	0	0
			2074	1304	359	398	13		
1	E	273	Total	C	N	O	S	0	0
			2172	1365	374	420	13		
1	F	275	Total	C	N	O	S	0	0
			2184	1373	376	422	13		

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A0P0ZD79
A	2	GLY	-	expression tag	UNP A0A0P0ZD79
A	3	SER	-	expression tag	UNP A0A0P0ZD79
A	4	SER	-	expression tag	UNP A0A0P0ZD79
A	5	HIS	-	expression tag	UNP A0A0P0ZD79
A	6	HIS	-	expression tag	UNP A0A0P0ZD79
A	7	HIS	-	expression tag	UNP A0A0P0ZD79
A	8	HIS	-	expression tag	UNP A0A0P0ZD79
A	9	HIS	-	expression tag	UNP A0A0P0ZD79
A	10	HIS	-	expression tag	UNP A0A0P0ZD79
A	11	SER	-	expression tag	UNP A0A0P0ZD79
A	12	SER	-	expression tag	UNP A0A0P0ZD79
A	13	GLY	-	expression tag	UNP A0A0P0ZD79
A	14	LEU	-	expression tag	UNP A0A0P0ZD79
A	15	VAL	-	expression tag	UNP A0A0P0ZD79
A	16	PRO	-	expression tag	UNP A0A0P0ZD79
A	17	ARG	-	expression tag	UNP A0A0P0ZD79
A	18	GLY	-	expression tag	UNP A0A0P0ZD79

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Chain	Residue	Modelled	Actual	Comment	Reference
A	19	SER	-	expression tag	UNP A0A0P0ZD79
A	20	HIS	-	expression tag	UNP A0A0P0ZD79
B	1	MET	-	initiating methionine	UNP A0A0P0ZD79
B	2	GLY	-	expression tag	UNP A0A0P0ZD79
B	3	SER	-	expression tag	UNP A0A0P0ZD79
B	4	SER	-	expression tag	UNP A0A0P0ZD79
B	5	HIS	-	expression tag	UNP A0A0P0ZD79
B	6	HIS	-	expression tag	UNP A0A0P0ZD79
B	7	HIS	-	expression tag	UNP A0A0P0ZD79
B	8	HIS	-	expression tag	UNP A0A0P0ZD79
B	9	HIS	-	expression tag	UNP A0A0P0ZD79
B	10	HIS	-	expression tag	UNP A0A0P0ZD79
B	11	SER	-	expression tag	UNP A0A0P0ZD79
B	12	SER	-	expression tag	UNP A0A0P0ZD79
B	13	GLY	-	expression tag	UNP A0A0P0ZD79
B	14	LEU	-	expression tag	UNP A0A0P0ZD79
B	15	VAL	-	expression tag	UNP A0A0P0ZD79
B	16	PRO	-	expression tag	UNP A0A0P0ZD79
B	17	ARG	-	expression tag	UNP A0A0P0ZD79
B	18	GLY	-	expression tag	UNP A0A0P0ZD79
B	19	SER	-	expression tag	UNP A0A0P0ZD79
B	20	HIS	-	expression tag	UNP A0A0P0ZD79
C	1	MET	-	initiating methionine	UNP A0A0P0ZD79
C	2	GLY	-	expression tag	UNP A0A0P0ZD79
C	3	SER	-	expression tag	UNP A0A0P0ZD79
C	4	SER	-	expression tag	UNP A0A0P0ZD79
C	5	HIS	-	expression tag	UNP A0A0P0ZD79
C	6	HIS	-	expression tag	UNP A0A0P0ZD79
C	7	HIS	-	expression tag	UNP A0A0P0ZD79
C	8	HIS	-	expression tag	UNP A0A0P0ZD79
C	9	HIS	-	expression tag	UNP A0A0P0ZD79
C	10	HIS	-	expression tag	UNP A0A0P0ZD79
C	11	SER	-	expression tag	UNP A0A0P0ZD79
C	12	SER	-	expression tag	UNP A0A0P0ZD79
C	13	GLY	-	expression tag	UNP A0A0P0ZD79
C	14	LEU	-	expression tag	UNP A0A0P0ZD79
C	15	VAL	-	expression tag	UNP A0A0P0ZD79
C	16	PRO	-	expression tag	UNP A0A0P0ZD79
C	17	ARG	-	expression tag	UNP A0A0P0ZD79
C	18	GLY	-	expression tag	UNP A0A0P0ZD79
C	19	SER	-	expression tag	UNP A0A0P0ZD79
C	20	HIS	-	expression tag	UNP A0A0P0ZD79

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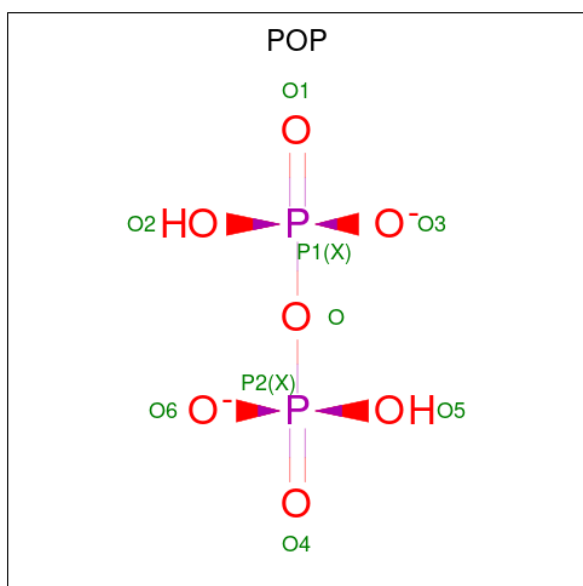
Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MET	-	initiating methionine	UNP A0A0P0ZD79
D	2	GLY	-	expression tag	UNP A0A0P0ZD79
D	3	SER	-	expression tag	UNP A0A0P0ZD79
D	4	SER	-	expression tag	UNP A0A0P0ZD79
D	5	HIS	-	expression tag	UNP A0A0P0ZD79
D	6	HIS	-	expression tag	UNP A0A0P0ZD79
D	7	HIS	-	expression tag	UNP A0A0P0ZD79
D	8	HIS	-	expression tag	UNP A0A0P0ZD79
D	9	HIS	-	expression tag	UNP A0A0P0ZD79
D	10	HIS	-	expression tag	UNP A0A0P0ZD79
D	11	SER	-	expression tag	UNP A0A0P0ZD79
D	12	SER	-	expression tag	UNP A0A0P0ZD79
D	13	GLY	-	expression tag	UNP A0A0P0ZD79
D	14	LEU	-	expression tag	UNP A0A0P0ZD79
D	15	VAL	-	expression tag	UNP A0A0P0ZD79
D	16	PRO	-	expression tag	UNP A0A0P0ZD79
D	17	ARG	-	expression tag	UNP A0A0P0ZD79
D	18	GLY	-	expression tag	UNP A0A0P0ZD79
D	19	SER	-	expression tag	UNP A0A0P0ZD79
D	20	HIS	-	expression tag	UNP A0A0P0ZD79
E	1	MET	-	initiating methionine	UNP A0A0P0ZD79
E	2	GLY	-	expression tag	UNP A0A0P0ZD79
E	3	SER	-	expression tag	UNP A0A0P0ZD79
E	4	SER	-	expression tag	UNP A0A0P0ZD79
E	5	HIS	-	expression tag	UNP A0A0P0ZD79
E	6	HIS	-	expression tag	UNP A0A0P0ZD79
E	7	HIS	-	expression tag	UNP A0A0P0ZD79
E	8	HIS	-	expression tag	UNP A0A0P0ZD79
E	9	HIS	-	expression tag	UNP A0A0P0ZD79
E	10	HIS	-	expression tag	UNP A0A0P0ZD79
E	11	SER	-	expression tag	UNP A0A0P0ZD79
E	12	SER	-	expression tag	UNP A0A0P0ZD79
E	13	GLY	-	expression tag	UNP A0A0P0ZD79
E	14	LEU	-	expression tag	UNP A0A0P0ZD79
E	15	VAL	-	expression tag	UNP A0A0P0ZD79
E	16	PRO	-	expression tag	UNP A0A0P0ZD79
E	17	ARG	-	expression tag	UNP A0A0P0ZD79
E	18	GLY	-	expression tag	UNP A0A0P0ZD79
E	19	SER	-	expression tag	UNP A0A0P0ZD79
E	20	HIS	-	expression tag	UNP A0A0P0ZD79
F	1	MET	-	initiating methionine	UNP A0A0P0ZD79
F	2	GLY	-	expression tag	UNP A0A0P0ZD79

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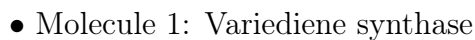
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Chain	Residue	Modelled	Actual	Comment	Reference
F	3	SER	-	expression tag	UNP A0A0P0ZD79
F	4	SER	-	expression tag	UNP A0A0P0ZD79
F	5	HIS	-	expression tag	UNP A0A0P0ZD79
F	6	HIS	-	expression tag	UNP A0A0P0ZD79
F	7	HIS	-	expression tag	UNP A0A0P0ZD79
F	8	HIS	-	expression tag	UNP A0A0P0ZD79
F	9	HIS	-	expression tag	UNP A0A0P0ZD79
F	10	HIS	-	expression tag	UNP A0A0P0ZD79
F	11	SER	-	expression tag	UNP A0A0P0ZD79
F	12	SER	-	expression tag	UNP A0A0P0ZD79
F	13	GLY	-	expression tag	UNP A0A0P0ZD79
F	14	LEU	-	expression tag	UNP A0A0P0ZD79
F	15	VAL	-	expression tag	UNP A0A0P0ZD79
F	16	PRO	-	expression tag	UNP A0A0P0ZD79
F	17	ARG	-	expression tag	UNP A0A0P0ZD79
F	18	GLY	-	expression tag	UNP A0A0P0ZD79
F	19	SER	-	expression tag	UNP A0A0P0ZD79
F	20	HIS	-	expression tag	UNP A0A0P0ZD79

- Molecule 2 is PYROPHOSPHATE 2- (CCD ID: POP) (formula: $\text{H}_2\text{O}_7\text{P}_2$) (labeled as "Ligand of Interest" by depositor).

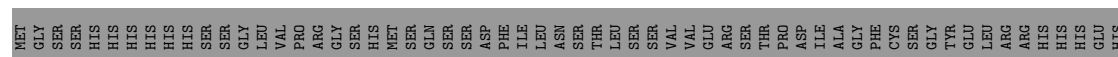


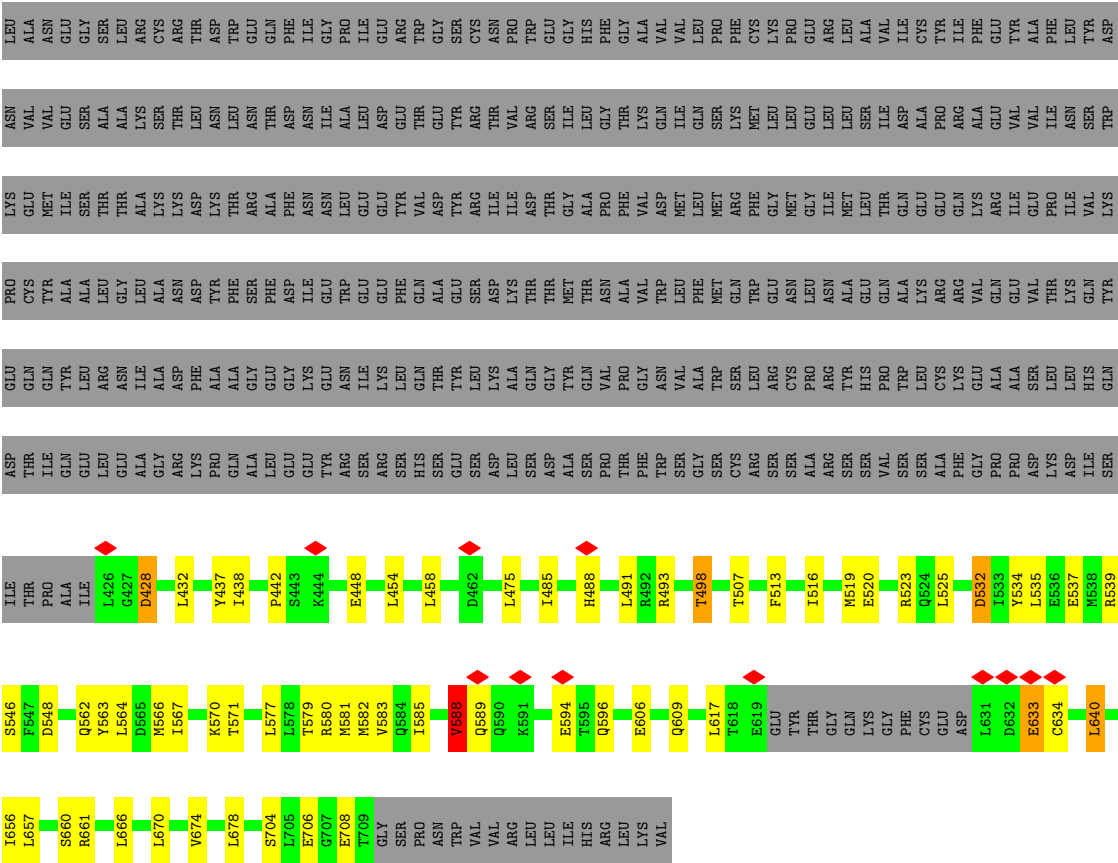
Mol	Chain	Residues	Atoms			AltConf
2	B	1	Total	O	P	0
			9	7	2	



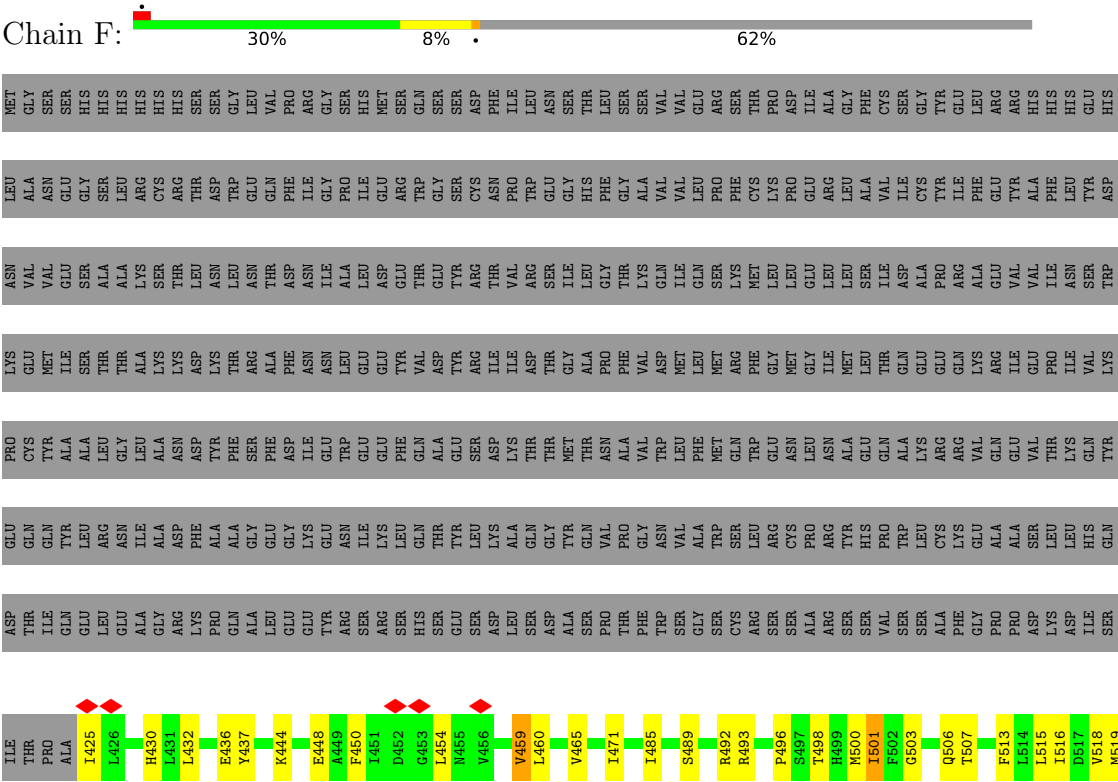
Frequency	Percentage
Daily	31%
Weekly	7%
Not at all	62%

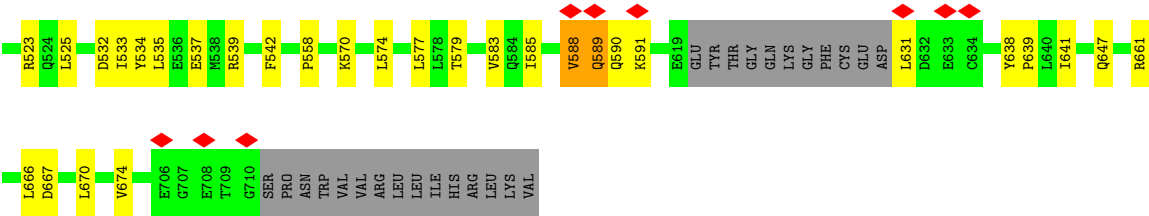
GLU	GLN	PRO	LYS	ASN	LEU	MET
GLN	GLN	CYS	GLU	VAL	ASN	GLY
TYR	TYR	TYR	MET	VAL	ASN	GLY
LEU	ALA	ALA	ILE	GLU	GLY	GLY
ARG	ALA	LEU	THR	ALA	SER	HIS
ASN	ASN	GLY	THR	ALA	LEU	HIS
ILE	LEU	LEU	ALA	LYS	ARG	HIS
ALA	ALA	ALA	LYS	SER	CYS	HIS
ASP	ASN	ASN	LYS	THR	ARG	HIS
PHE	ASP	ASP	ASP	LEU	THR	SER
ALA	TYR	TYR	LYS	ASN	ASP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





● Molecule 1: Variadiene synthase





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	298050	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	43	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.733	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.12	Depositor
Map size ($\text{\AA}$)	414.72003, 414.72003, 414.72003	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.08, 1.08, 1.08	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: POP

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	0.18	0/2341	0.43	0/3164
1	B	0.21	0/4697	0.57	3/6345 (0.0%)
1	C	0.18	0/2216	0.41	0/2992
1	D	0.19	0/2107	0.43	0/2840
1	E	0.18	0/2208	0.41	0/2981
1	F	0.19	0/2220	0.46	1/2997 (0.0%)
All	All	0.19	0/15789	0.47	4/21319 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	210	THR	N-CA-C	-6.12	103.94	111.40
1	B	530	CYS	N-CA-C	-5.60	106.12	114.64
1	B	501	ILE	N-CA-C	-5.55	108.09	113.53
1	F	501	ILE	N-CA-C	-5.26	108.37	113.53

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	2301	0	2300	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4600	0	4531	137	0
1	C	2180	0	2174	33	0
1	D	2074	0	2074	41	0
1	E	2172	0	2163	50	0
1	F	2184	0	2177	46	0
2	B	9	0	0	1	0
All	All	15520	0	15419	318	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 10.

All (318) 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:210:THR:HB	2:B:801:POP:O4	1.69	0.91
1:E:535:LEU:HD13	1:F:520:GLU:HG2	1.62	0.81
1:B:70:ARG:HH22	1:B:84:GLY:HA3	1.46	0.78
1:E:548:ASP:HB2	1:E:566:MET:HE3	1.67	0.76
1:A:634:CYS:SG	1:A:661:ARG:NH1	2.60	0.75
1:F:589:GLN:OE1	1:F:590:GLN:NE2	2.20	0.74
1:F:537:GLU:HB2	1:F:577:LEU:HD12	1.72	0.72
1:B:495:ARG:HG3	1:B:496:PRO:HD2	1.72	0.70
1:E:448:GLU:N	1:E:448:GLU:OE2	2.24	0.70
1:E:520:GLU:HG2	1:F:535:LEU:HD13	1.74	0.70
1:E:537:GLU:HB2	1:E:577:LEU:HD13	1.72	0.69
1:B:288:GLN:HG3	1:B:291:ARG:HH21	1.57	0.69
1:B:213:PRO:HA	1:B:216:ASP:HB3	1.76	0.67
1:B:475:LEU:HD13	1:B:518:VAL:HG21	1.76	0.67
1:C:523:ARG:NH2	1:D:532:ASP:OD1	2.27	0.67
1:B:263:GLN:N	1:B:263:GLN:OE1	2.28	0.67
1:B:206:ARG:HD2	1:B:210:THR:HG23	1.77	0.66
1:F:589:GLN:HB2	1:F:590:GLN:HE21	1.59	0.66
1:B:53:LEU:HB2	1:B:334:PRO:HB2	1.77	0.65
1:B:70:ARG:NH1	1:B:83:TRP:O	2.30	0.65
1:B:206:ARG:HA	1:B:209:ASP:HB3	1.80	0.64
1:A:464:ARG:HD2	1:A:585:ILE:HG21	1.79	0.64
1:B:217:MET:HE3	1:B:217:MET:HA	1.79	0.64
1:B:634:CYS:SG	1:B:661:ARG:NH2	2.71	0.64
1:A:505:GLU:HG2	1:B:486:GLU:HB3	1.79	0.63
1:E:534:TYR:HA	1:E:577:LEU:HD11	1.78	0.63
1:E:567:ILE:HG21	1:E:609:GLN:HG2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:VAL:HG12	1:B:152:LEU:HD22	1.82	0.62
1:A:462:ASP:OD2	1:A:462:ASP:N	2.32	0.62
1:D:442:PRO:O	1:D:493:ARG:NH1	2.31	0.62
1:B:168:ILE:HD11	1:B:221:PHE:HZ	1.63	0.62
1:C:660:SER:HB2	1:C:666:LEU:HG	1.80	0.62
1:E:660:SER:HB2	1:E:666:LEU:HG	1.82	0.62
1:E:562:GLN:HG2	1:F:425:ILE:HD13	1.81	0.61
1:B:360:GLN:H	1:B:360:GLN:CD	2.08	0.61
1:F:525:LEU:HD13	1:F:585:ILE:HD11	1.82	0.61
1:A:495:ARG:HB3	1:A:495:ARG:NH1	2.16	0.61
1:B:104:GLU:OE2	1:B:104:GLU:N	2.26	0.60
1:B:36:VAL:HG22	1:B:54:ARG:HD2	1.84	0.59
1:C:565:ASP:OD1	1:C:568:ARG:NH2	2.35	0.59
1:A:519:MET:SD	1:B:519:MET:HG3	2.43	0.59
1:E:596:GLN:NE2	1:E:708:GLU:OE2	2.32	0.59
1:E:519:MET:HG3	1:E:534:TYR:CE2	2.38	0.58
1:E:579:THR:O	1:E:583:VAL:HG23	2.03	0.58
1:E:539:ARG:HG2	1:F:513:PHE:HE2	1.68	0.58
1:A:532:ASP:OD2	1:B:523:ARG:NH2	2.37	0.58
1:D:604:LEU:HG	1:D:698:ILE:HD11	1.86	0.58
1:E:577:LEU:HG	1:E:581:MET:HE3	1.84	0.58
1:B:267:ASP:OD2	1:B:267:ASP:N	2.36	0.58
1:E:532:ASP:OD1	1:F:523:ARG:NH2	2.37	0.58
1:B:461:PRO:HB2	1:B:463:HIS:CE1	2.39	0.57
1:C:537:GLU:HB2	1:C:577:LEU:HD13	1.85	0.57
1:D:669:PRO:O	1:D:673:THR:HG23	2.04	0.57
1:D:656:ILE:HG23	1:D:670:LEU:HD22	1.85	0.57
1:C:462:ASP:OD1	1:C:462:ASP:N	2.37	0.57
1:C:684:ILE:O	1:C:688:GLU:HG2	2.04	0.57
1:F:588:VAL:HA	1:F:591:LYS:HE2	1.87	0.57
1:F:666:LEU:HD22	1:F:670:LEU:HB3	1.87	0.57
1:B:97:VAL:HA	1:B:335:GLY:HA3	1.84	0.57
1:B:430:HIS:HB3	1:B:506:GLN:HE21	1.68	0.57
1:D:588:VAL:O	1:D:590:GLN:N	2.38	0.57
1:E:525:LEU:HD13	1:E:585:ILE:HD11	1.85	0.57
1:A:520:GLU:HG3	1:B:535:LEU:HD13	1.87	0.56
1:B:93:PHE:HB2	1:B:339:TRP:CD2	2.40	0.56
1:B:177:ILE:HD12	1:B:177:ILE:H	1.70	0.56
1:B:197:ASN:ND2	1:B:201:GLU:OE1	2.38	0.56
1:C:448:GLU:OE1	1:C:448:GLU:N	2.34	0.56
1:B:70:ARG:NH2	1:B:84:GLY:HA3	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:566:MET:HE2	1:E:570:LYS:HD3	1.87	0.56
1:F:492:ARG:HG3	1:F:493:ARG:HD2	1.87	0.56
1:B:56:HIS:NE2	1:B:58:HIS:HB2	2.20	0.56
1:F:485:ILE:HD11	1:F:507:THR:HB	1.88	0.56
1:F:631:LEU:HD21	1:F:674:VAL:HG11	1.87	0.55
1:B:192:LYS:NZ	1:B:205:TYR:OH	2.39	0.55
1:E:670:LEU:O	1:E:674:VAL:HG23	2.05	0.55
1:B:656:ILE:HG13	1:F:501:ILE:HG23	1.89	0.55
1:B:39:ARG:O	1:B:39:ARG:NH1	2.37	0.55
1:B:206:ARG:NH1	1:B:210:THR:OG1	2.39	0.55
1:A:579:THR:O	1:A:583:VAL:HG23	2.07	0.55
1:D:634:CYS:SG	1:D:661:ARG:NH1	2.79	0.54
1:E:656:ILE:HG23	1:E:670:LEU:HD23	1.89	0.54
1:B:519:MET:HE1	1:B:531:MET:SD	2.47	0.54
1:E:640:LEU:HD21	1:E:657:LEU:HD11	1.89	0.54
1:B:34:SER:O	1:B:54:ARG:NH2	2.40	0.54
1:C:614:TYR:O	1:C:618:THR:OG1	2.22	0.54
1:B:260:GLU:OE2	1:B:260:GLU:N	2.31	0.54
1:A:547:PHE:HE2	1:B:427:GLY:HA2	1.72	0.54
1:E:516:ILE:HG13	1:F:542:PHE:HE2	1.72	0.54
1:B:70:ARG:NH2	1:B:114:GLU:OE2	2.29	0.53
1:F:534:TYR:HD1	1:F:577:LEU:HD11	1.72	0.53
1:B:36:VAL:HA	1:B:54:ARG:HA	1.90	0.53
1:B:60:HIS:CE1	1:B:61:LEU:HG	2.44	0.53
1:B:352:LYS:O	1:B:352:LYS:HD3	2.08	0.53
1:B:298:LYS:HD3	1:B:301:GLU:OE2	2.08	0.53
1:B:317:LYS:O	1:B:323:GLN:NE2	2.40	0.53
1:B:88:PRO:HB3	1:B:357:LEU:HD12	1.89	0.53
1:E:564:LEU:HD23	1:E:567:ILE:HD11	1.90	0.53
1:B:490:PRO:HB2	1:B:491:LEU:HD12	1.91	0.52
1:B:276:TRP:HA	1:B:279:MET:HG2	1.92	0.52
1:F:534:TYR:CD1	1:F:577:LEU:HD11	2.44	0.52
1:C:687:THR:HG22	1:C:691:MET:HE2	1.91	0.52
1:B:287:GLU:OE1	1:B:291:ARG:NH2	2.43	0.52
1:A:523:ARG:HD3	1:B:531:MET:HE3	1.91	0.52
1:A:537:GLU:OE2	1:A:580:ARG:HD3	2.10	0.52
1:B:246:LEU:HD21	1:B:333:VAL:HA	1.92	0.52
1:B:661:ARG:NH1	1:B:661:ARG:HB2	2.25	0.52
1:D:609:GLN:OE1	1:D:609:GLN:HA	2.10	0.52
1:B:279:MET:HE1	1:B:286:ALA:HA	1.90	0.51
1:C:460:LEU:HD21	1:C:585:ILE:HG13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:ARG:O	1:A:576:ARG:NH2	2.43	0.51
1:A:515:LEU:HD22	1:A:538:MET:HE1	1.93	0.51
1:B:43:ASP:N	1:B:43:ASP:OD1	2.42	0.51
1:D:432:LEU:O	1:D:436:GLU:HG3	2.10	0.51
1:A:713:ASN:O	1:A:717:ARG:HG3	2.09	0.51
1:C:486:GLU:HB3	1:D:505:GLU:HG2	1.92	0.51
1:B:102:LYS:HB3	1:B:104:GLU:OE2	2.10	0.51
1:B:593:LEU:O	1:B:595:THR:N	2.43	0.51
1:E:653:LEU:HD11	1:E:674:VAL:HG13	1.93	0.51
1:A:441:LEU:HD22	1:A:495:ARG:HD3	1.92	0.51
1:E:442:PRO:O	1:E:493:ARG:NH1	2.44	0.51
1:A:428:ASP:O	1:A:429:GLU:HG2	2.11	0.51
1:B:204:ASP:HA	1:B:207:ILE:HG22	1.93	0.51
1:B:233:LYS:HE3	1:B:233:LYS:HA	1.92	0.51
1:E:537:GLU:OE1	1:E:580:ARG:NH1	2.44	0.51
1:B:82:ARG:HD2	1:B:83:TRP:N	2.25	0.50
1:B:106:LEU:HD23	1:B:107:ALA:H	1.75	0.50
1:B:226:MET:SD	1:B:226:MET:N	2.85	0.50
1:B:350:LEU:HD12	1:B:350:LEU:H	1.76	0.50
1:B:670:LEU:O	1:B:673:THR:HG22	2.12	0.50
1:C:652:GLN:O	1:C:656:ILE:HG13	2.12	0.50
1:E:661:ARG:HG3	1:E:661:ARG:HH11	1.77	0.50
1:F:471:ILE:HG23	1:F:518:VAL:HG13	1.94	0.50
1:A:660:SER:HB2	1:A:666:LEU:HG	1.94	0.50
1:E:437:TYR:HD2	1:E:498:THR:HG23	1.77	0.50
1:D:471:ILE:HG23	1:D:518:VAL:HG13	1.93	0.49
1:C:534:TYR:HA	1:C:577:LEU:HD11	1.93	0.49
1:C:548:ASP:HB2	1:C:566:MET:SD	2.51	0.49
1:B:293:VAL:HA	1:B:296:VAL:HB	1.94	0.49
1:D:548:ASP:HB2	1:D:566:MET:SD	2.53	0.49
1:F:533:ILE:O	1:F:537:GLU:HG2	2.12	0.49
1:A:647:GLN:O	1:A:654:ARG:NH2	2.41	0.49
1:D:618:THR:HG22	1:D:618:THR:O	2.13	0.49
1:B:106:LEU:HD23	1:B:107:ALA:N	2.28	0.48
1:B:339:TRP:O	1:B:343:CYS:HB3	2.13	0.48
1:B:340:SER:HB3	1:B:346:TYR:CE2	2.47	0.48
1:D:505:GLU:OE1	1:D:505:GLU:N	2.28	0.48
1:E:488:HIS:ND1	1:E:633:GLU:OE2	2.35	0.48
1:C:458:LEU:HA	1:C:590:GLN:NE2	2.28	0.48
1:E:428:ASP:HB2	1:E:432:LEU:HD12	1.95	0.48
1:B:671:LYS:O	1:B:675:LEU:HD12	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:519:MET:HG3	1:A:531:MET:HE1	1.95	0.48
1:F:437:TYR:OH	1:F:496:PRO:O	2.21	0.48
1:D:490:PRO:HB2	1:D:491:LEU:HD12	1.96	0.48
1:D:519:MET:HA	1:D:519:MET:HE2	1.96	0.48
1:B:599:SER:O	1:B:603:VAL:HG23	2.14	0.47
1:C:611:ARG:NH1	1:C:615:LYS:HD2	2.29	0.47
1:B:240:LYS:HA	1:B:243:TYR:HB2	1.95	0.47
1:C:532:ASP:N	1:C:532:ASP:OD1	2.48	0.47
1:A:706:GLU:OE1	1:A:717:ARG:NH1	2.47	0.47
1:B:430:HIS:HB3	1:B:506:GLN:NE2	2.28	0.47
1:B:61:LEU:HD13	1:B:106:LEU:HD21	1.95	0.47
1:D:505:GLU:H	1:D:505:GLU:CD	2.21	0.47
1:B:203:VAL:O	1:B:207:ILE:N	2.44	0.47
1:B:206:ARG:NH2	1:B:207:ILE:HA	2.29	0.47
1:A:495:ARG:HB3	1:A:495:ARG:HH11	1.80	0.47
1:B:53:LEU:HD13	1:B:335:GLY:HA2	1.95	0.47
1:B:206:ARG:HH22	1:B:247:GLY:HA3	1.79	0.47
1:D:503:GLY:O	1:D:507:THR:OG1	2.29	0.46
1:F:570:LYS:HB3	1:F:570:LYS:HE3	1.68	0.46
1:A:547:PHE:CD2	1:B:425:ILE:HD11	2.50	0.46
1:C:438:ILE:HD13	1:C:481:MET:HG3	1.97	0.46
1:A:512:ASN:ND2	1:B:512:ASN:OD1	2.47	0.46
1:B:357:LEU:O	1:B:360:GLN:NE2	2.43	0.46
1:B:536:GLU:OE2	1:B:540:ASN:ND2	2.48	0.46
1:E:617:LEU:HD21	1:E:678:LEU:HD13	1.98	0.46
1:D:534:TYR:HD1	1:D:577:LEU:HD11	1.81	0.46
1:E:523:ARG:NH2	1:F:532:ASP:OD1	2.48	0.46
1:F:661:ARG:HB2	1:F:661:ARG:NH1	2.31	0.46
1:A:582:MET:HE2	1:A:582:MET:HB3	1.78	0.46
1:C:535:LEU:HD11	1:D:519:MET:HG3	1.97	0.46
1:D:468:LEU:HA	1:D:471:ILE:HD12	1.98	0.46
1:F:459:VAL:HG13	1:F:459:VAL:O	2.16	0.46
1:F:515:LEU:HB3	1:F:519:MET:HE3	1.97	0.46
1:B:251:ASP:O	1:B:255:PHE:N	2.50	0.45
1:A:588:VAL:O	1:A:591:LYS:HD2	2.16	0.45
1:B:72:ASP:OD1	1:B:111:TYR:OH	2.34	0.45
1:B:284:LEU:HD22	1:B:288:GLN:HB3	1.97	0.45
1:E:588:VAL:HG12	1:E:589:GLN:H	1.82	0.45
1:B:617:LEU:O	1:B:675:LEU:HD21	2.16	0.45
1:E:546:SER:OG	1:F:430:HIS:HB2	2.17	0.45
1:F:631:LEU:HD13	1:F:666:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:519:MET:HE1	1:F:519:MET:HB3	1.98	0.45
1:B:204:ASP:OD2	1:B:204:ASP:N	2.49	0.45
1:E:583:VAL:HG11	1:E:594:GLU:HG2	1.98	0.45
1:B:340:SER:HB3	1:B:346:TYR:CD2	2.51	0.45
1:E:513:PHE:HE1	1:F:539:ARG:HG3	1.81	0.45
1:C:611:ARG:HH12	1:C:615:LYS:HD2	1.82	0.45
1:B:98:LEU:HD11	1:B:219:MET:HB2	1.99	0.45
1:B:168:ILE:HD11	1:B:221:PHE:CZ	2.49	0.45
1:B:560:GLU:OE2	1:B:638:TYR:OH	2.26	0.45
1:C:468:LEU:HD11	1:C:585:ILE:HD11	1.97	0.45
1:D:662:SER:O	1:D:662:SER:OG	2.30	0.45
1:E:563:TYR:O	1:E:567:ILE:HG12	2.16	0.45
1:E:564:LEU:HD22	1:E:606:GLU:OE2	2.17	0.45
1:B:525:LEU:HD22	1:B:585:ILE:HD11	1.99	0.44
1:F:503:GLY:O	1:F:507:THR:OG1	2.27	0.44
1:A:541:LEU:HD21	1:A:573:GLY:HA3	1.99	0.44
1:B:228:THR:OG1	1:B:231:GLU:HB3	2.17	0.44
1:F:579:THR:O	1:F:583:VAL:HG13	2.18	0.44
1:D:574:LEU:HD12	1:D:574:LEU:HA	1.80	0.44
1:A:576:ARG:O	1:A:580:ARG:HG3	2.18	0.44
1:E:438:ILE:HD13	1:E:498:THR:OG1	2.18	0.44
1:A:532:ASP:OD2	1:A:532:ASP:N	2.50	0.44
1:B:475:LEU:HD12	1:B:475:LEU:HA	1.83	0.44
1:E:571:THR:HG21	1:E:609:GLN:HB2	1.99	0.44
1:B:697:LYS:HE3	1:B:697:LYS:HB2	1.80	0.44
1:A:429:GLU:C	1:A:431:LEU:H	2.25	0.44
1:B:105:ARG:NH1	1:B:168:ILE:HD12	2.33	0.44
1:F:450:PHE:CZ	1:F:454:LEU:HD11	2.52	0.44
1:B:170:ALA:HB3	1:B:171:PRO:HD3	1.99	0.43
1:B:207:ILE:HD11	1:B:243:TYR:HB3	2.00	0.43
1:B:679:ARG:HB2	1:B:679:ARG:CZ	2.47	0.43
1:D:461:PRO:O	1:D:465:VAL:HG23	2.18	0.43
1:F:432:LEU:O	1:F:436:GLU:HG3	2.18	0.43
1:B:514:LEU:O	1:B:518:VAL:HG23	2.19	0.43
1:E:532:ASP:OD1	1:E:532:ASP:N	2.51	0.43
1:B:668:VAL:O	1:B:672:GLU:HG2	2.18	0.43
1:A:519:MET:CG	1:A:531:MET:HE1	2.49	0.43
1:B:295:GLU:OE1	1:B:298:LYS:HG2	2.19	0.43
1:B:667:ASP:OD2	1:B:669:PRO:HD2	2.18	0.43
1:A:525:LEU:HD13	1:A:585:ILE:HD11	2.01	0.43
1:A:578:LEU:O	1:A:582:MET:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:ARG:HE	1:B:54:ARG:HB3	1.57	0.43
1:B:240:LYS:N	1:B:241:PRO:HD2	2.34	0.43
1:B:579:THR:HG21	1:B:597:LEU:HB3	1.99	0.43
1:B:655:GLY:HA3	1:F:501:ILE:O	2.18	0.43
1:C:614:TYR:HB2	1:C:687:THR:HG21	2.01	0.43
1:B:567:ILE:HD11	1:B:606:GLU:HG3	2.00	0.43
1:F:667:ASP:OD1	1:F:670:LEU:HD22	2.19	0.43
1:A:593:LEU:HD23	1:A:593:LEU:H	1.84	0.43
1:F:558:PRO:HG2	1:F:641:ILE:HD11	2.00	0.43
1:A:721:HIS:HE2	1:B:167:SER:HA	1.82	0.42
1:B:169:ASP:OD1	1:B:171:PRO:HD2	2.19	0.42
1:B:248:LEU:HD23	1:B:248:LEU:HA	1.87	0.42
1:F:574:LEU:HD12	1:F:574:LEU:HA	1.82	0.42
1:A:656:ILE:HG23	1:A:670:LEU:HD22	2.01	0.42
1:D:430:HIS:HB3	1:D:506:GLN:HE21	1.85	0.42
1:D:695:MET:HA	1:D:698:ILE:HG22	2.01	0.42
1:B:285:ASN:ND2	1:B:287:GLU:OE1	2.50	0.42
1:E:519:MET:SD	1:F:519:MET:SD	3.18	0.42
1:E:704:SER:O	1:E:708:GLU:HG3	2.19	0.42
1:A:460:LEU:HD22	1:A:582:MET:HE3	2.01	0.42
1:B:56:HIS:HB2	1:B:99:PRO:HB2	2.01	0.42
1:B:285:ASN:OD1	1:B:285:ASN:N	2.51	0.42
1:C:481:MET:HE2	1:C:511:ALA:HB2	2.01	0.42
1:C:700:ASP:O	1:C:703:VAL:HG12	2.19	0.42
1:D:679:ARG:CZ	1:D:679:ARG:HB2	2.49	0.42
1:F:437:TYR:HD2	1:F:498:THR:HG23	1.84	0.42
1:F:519:MET:HG2	1:F:534:TYR:CE2	2.54	0.42
1:D:579:THR:O	1:D:583:VAL:HG23	2.19	0.42
1:B:432:LEU:O	1:B:436:GLU:HG3	2.20	0.42
1:F:638:TYR:HB3	1:F:639:PRO:HD3	2.01	0.42
1:B:165:LEU:HD11	1:B:176:VAL:HG21	2.02	0.42
1:B:468:LEU:HD13	1:B:582:MET:HG2	2.02	0.42
1:B:518:VAL:O	1:B:522:VAL:HG23	2.19	0.42
1:C:670:LEU:O	1:C:674:VAL:HG23	2.20	0.42
1:C:695:MET:O	1:C:699:THR:HG23	2.19	0.42
1:B:661:ARG:HB2	1:B:661:ARG:CZ	2.50	0.42
1:C:426:LEU:HD21	1:D:569:GLN:HE22	1.84	0.42
1:B:471:ILE:HG23	1:B:518:VAL:HG13	2.02	0.42
1:E:519:MET:HG3	1:E:534:TYR:HE2	1.81	0.42
1:A:454:LEU:HD11	1:A:597:LEU:HD22	2.02	0.41
1:B:232:GLN:NE2	1:B:235:ILE:HD11	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:ASP:OD2	1:B:257:ILE:N	2.53	0.41
1:B:182:GLU:O	1:B:186:THR:HG23	2.20	0.41
1:A:543:ILE:HG13	1:B:431:LEU:HD22	2.02	0.41
1:C:487:ASP:O	1:C:633:GLU:HG3	2.20	0.41
1:D:537:GLU:HB2	1:D:577:LEU:HD12	2.02	0.41
1:E:458:LEU:HD13	1:E:582:MET:HB3	2.02	0.41
1:A:426:LEU:HD13	1:B:547:PHE:CD2	2.55	0.41
1:B:516:ILE:O	1:B:519:MET:HB2	2.20	0.41
1:E:485:ILE:HD11	1:E:507:THR:HB	2.03	0.41
1:A:485:ILE:HD11	1:A:507:THR:HB	2.02	0.41
1:A:539:ARG:HG3	1:B:513:PHE:HE2	1.85	0.41
1:D:514:LEU:O	1:D:518:VAL:HG23	2.20	0.41
1:E:454:LEU:HD21	1:E:579:THR:HG23	2.03	0.41
1:B:75:GLN:OE1	1:B:75:GLN:HA	2.20	0.41
1:B:485:ILE:HD11	1:B:507:THR:HB	2.03	0.41
1:B:501:ILE:HG23	1:D:656:ILE:HG13	2.02	0.41
1:C:482:LEU:O	1:C:486:GLU:HG3	2.21	0.41
1:D:430:HIS:HB3	1:D:506:GLN:NE2	2.36	0.41
1:D:485:ILE:HD11	1:D:507:THR:HB	2.03	0.41
1:D:566:MET:HE3	1:D:566:MET:HB3	1.89	0.41
1:E:617:LEU:HD12	1:E:617:LEU:HA	1.80	0.41
1:F:516:ILE:O	1:F:520:GLU:HG3	2.21	0.41
1:C:514:LEU:HD23	1:C:514:LEU:HA	1.87	0.41
1:C:640:LEU:O	1:C:640:LEU:HD23	2.21	0.41
1:D:474:THR:OG1	1:D:521:LYS:NZ	2.54	0.41
1:D:516:ILE:O	1:D:519:MET:HB3	2.21	0.41
1:B:59:GLU:CD	1:B:63:ASN:HD21	2.29	0.40
1:B:249:ALA:O	1:B:253:PHE:HD1	2.04	0.40
1:B:69:CYS:HB2	1:B:111:TYR:CD1	2.56	0.40
1:D:578:LEU:O	1:D:582:MET:HG3	2.21	0.40
1:E:513:PHE:CE1	1:F:539:ARG:HG3	2.57	0.40
1:F:500:MET:HE3	1:F:500:MET:HB3	1.89	0.40
1:F:589:GLN:HB2	1:F:590:GLN:H	1.78	0.40
1:B:501:ILE:O	1:D:655:GLY:HA3	2.20	0.40
1:D:448:GLU:N	1:D:448:GLU:OE2	2.55	0.40
1:E:567:ILE:CG2	1:E:609:GLN:HG2	2.49	0.40
1:B:251:ASP:HA	1:B:254:SER:OG	2.21	0.40
1:D:468:LEU:HD13	1:D:582:MET:HG2	2.04	0.40
1:A:704:SER:O	1:A:708:GLU:HG3	2.22	0.40
1:B:171:PRO:HA	1:B:174:GLU:HG3	2.04	0.40
1:B:255:PHE:CD1	1:B:275:VAL:HB	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:GLN:HA	1:B:305:LEU:HD23	2.02	0.40
1:B:668:VAL:HB	1:B:669:PRO:HD3	2.02	0.40
1:C:487:ASP:OD2	1:C:489:SER:OG	2.39	0.40
1:C:668:VAL:N	1:C:669:PRO:HD2	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	285/725 (39%)	270 (95%)	13 (5%)	2 (1%)	18	53
1	B	558/725 (77%)	522 (94%)	34 (6%)	2 (0%)	30	65
1	C	270/725 (37%)	262 (97%)	6 (2%)	2 (1%)	18	53
1	D	254/725 (35%)	243 (96%)	9 (4%)	2 (1%)	16	50
1	E	269/725 (37%)	263 (98%)	5 (2%)	1 (0%)	30	65
1	F	271/725 (37%)	264 (97%)	4 (2%)	3 (1%)	11	43
All	All	1907/4350 (44%)	1824 (96%)	71 (4%)	12 (1%)	23	56

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	588	VAL
1	B	594	GLU
1	C	589	GLN
1	D	589	GLN
1	F	589	GLN
1	B	286	ALA
1	C	588	VAL
1	D	588	VAL

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Mol	Chain	Res	Type
1	E	588	VAL
1	F	588	VAL
1	A	459	VAL
1	F	459	VAL

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	258/638 (40%)	249 (96%)	9 (4%)	32	65
1	B	501/638 (78%)	491 (98%)	10 (2%)	48	76
1	C	245/638 (38%)	242 (99%)	3 (1%)	63	82
1	D	233/638 (36%)	232 (100%)	1 (0%)	84	90
1	E	244/638 (38%)	234 (96%)	10 (4%)	27	61
1	F	245/638 (38%)	238 (97%)	7 (3%)	37	70
All	All	1726/3828 (45%)	1686 (98%)	40 (2%)	44	74

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	432	LEU
1	A	462	ASP
1	A	487	ASP
1	A	506	GLN
1	A	532	ASP
1	A	571	THR
1	A	574	LEU
1	A	593	LEU
1	A	718	LEU
1	B	117	PHE
1	B	157	ILE
1	B	320	ILE
1	B	340	SER
1	B	475	LEU

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Mol	Chain	Res	Type
1	B	506	GLN
1	B	516	ILE
1	B	565	ASP
1	B	604	LEU
1	B	675	LEU
1	C	475	LEU
1	C	480	LEU
1	C	566	MET
1	D	577	LEU
1	E	428	ASP
1	E	475	LEU
1	E	491	LEU
1	E	498	THR
1	E	532	ASP
1	E	588	VAL
1	E	633	GLU
1	E	634	CYS
1	E	640	LEU
1	E	706	GLU
1	F	444	LYS
1	F	448	GLU
1	F	460	LEU
1	F	465	VAL
1	F	489	SER
1	F	506	GLN
1	F	647	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	430	HIS
1	A	473	GLN
1	A	499	HIS
1	A	616	ASN
1	B	63	ASN
1	B	197	ASN
1	B	250	ASN
1	B	288	GLN
1	B	329	GLN
1	B	562	GLN
1	B	609	GLN
1	B	680	GLN

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Mol	Chain	Res	Type
1	C	467	GLN
1	C	509	ASN
1	C	680	GLN
1	D	430	HIS
1	D	509	ASN
1	D	647	GLN
1	E	466	ASN
1	F	455	ASN
1	F	466	ASN
1	F	589	GLN
1	F	590	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](#)

1 ligand is 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	$\# Z > 2$
2	POP	B	801	-	6,8,8	0.79	0	12,13,13	0.77	0

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
2	POP	B	801	-	-	0/6/6/6	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

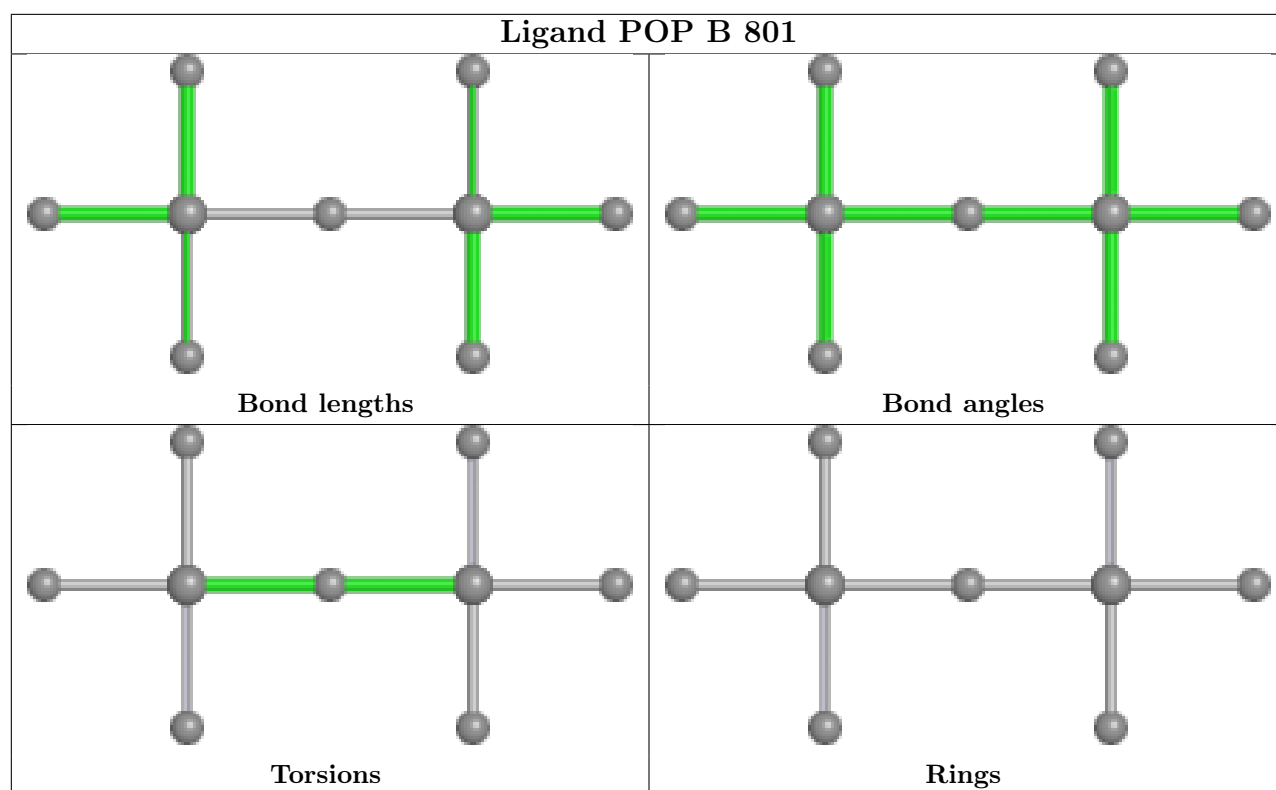
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	POP	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

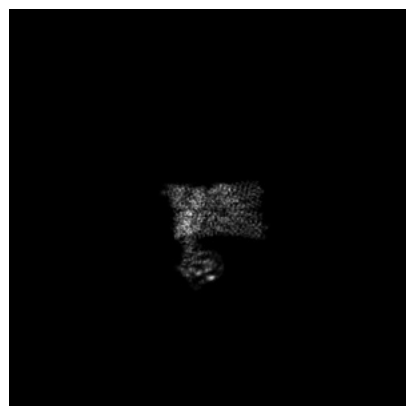
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47455. These allow visual inspection of the internal detail of the map and identification of artifacts.

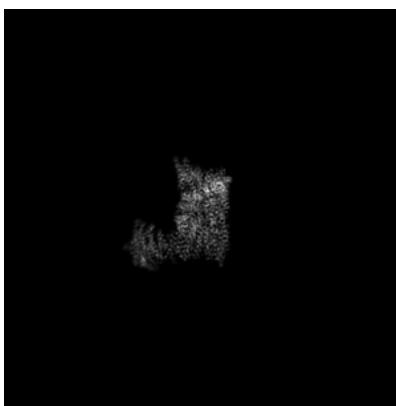
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X

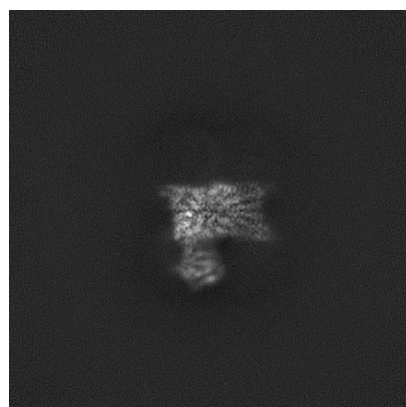


Y

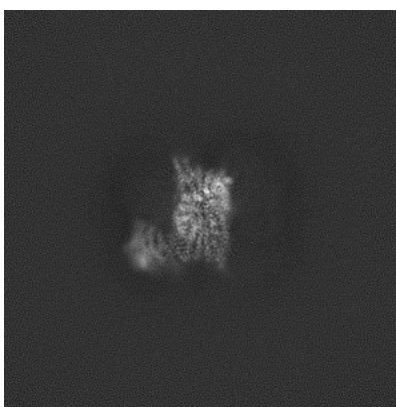


Z

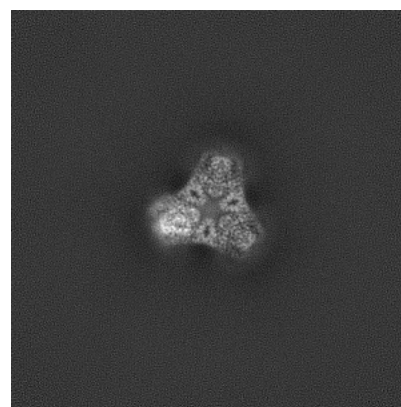
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

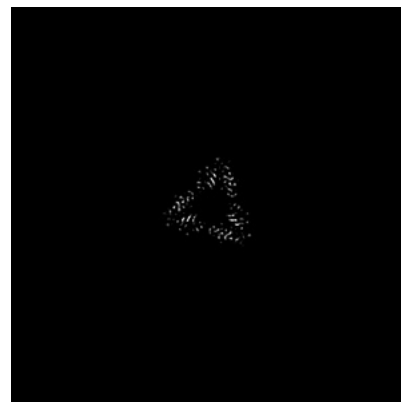
6.2.1 Primary map



X Index: 192



Y Index: 192



Z Index: 192

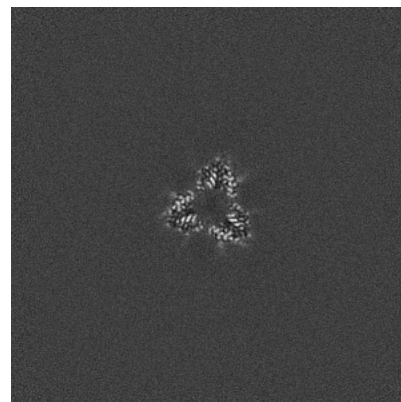
6.2.2 Raw map



X Index: 192



Y Index: 192

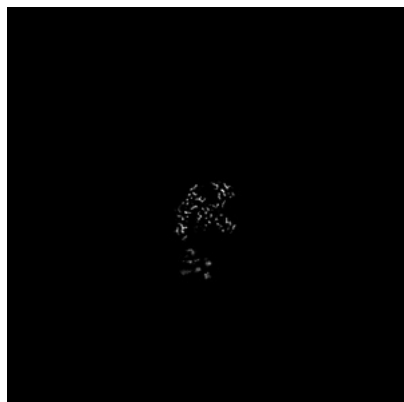


Z Index: 192

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

6.3 Largest variance slices [i](#)

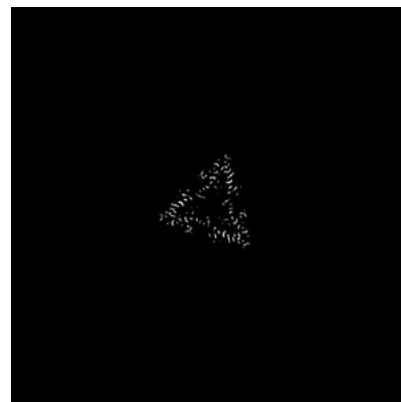
6.3.1 Primary map



X Index: 170

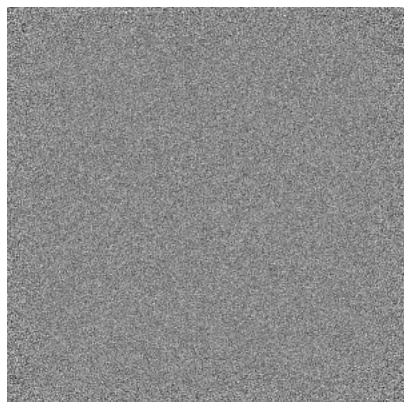


Y Index: 172

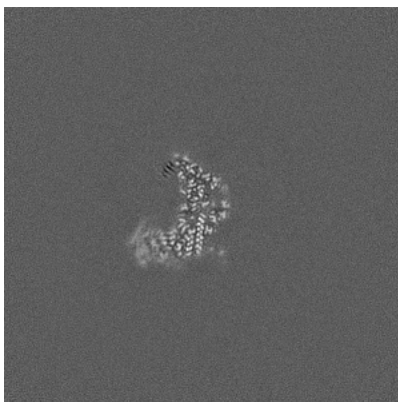


Z Index: 195

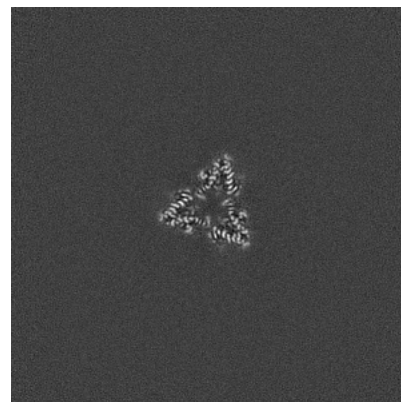
6.3.2 Raw map



X Index: 0



Y Index: 172

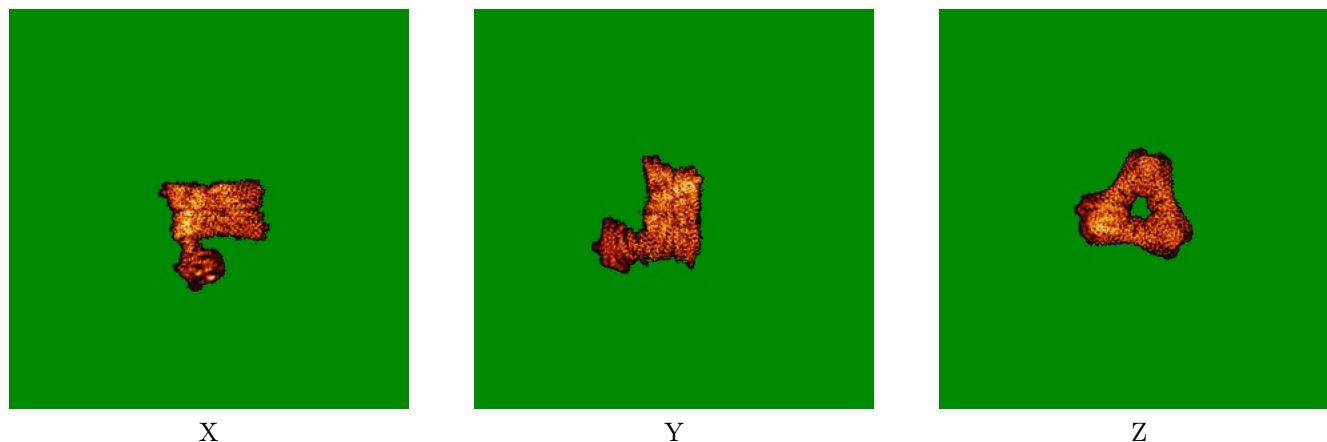


Z Index: 195

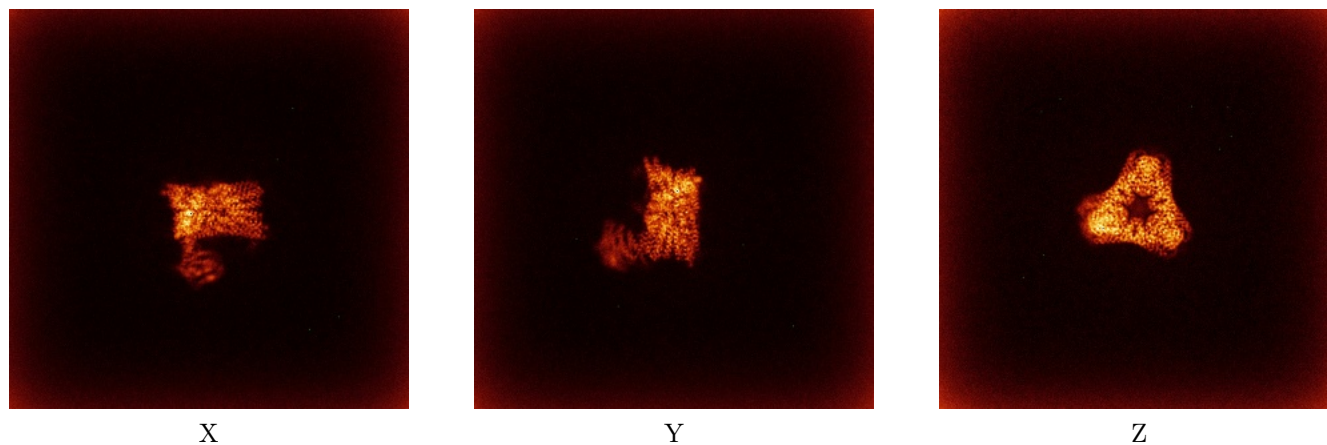
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



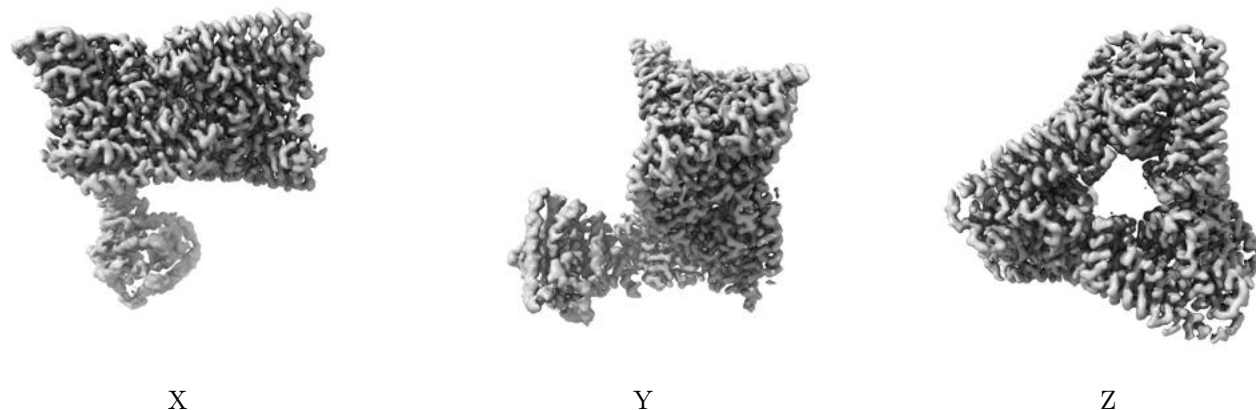
6.4.2 Raw map



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

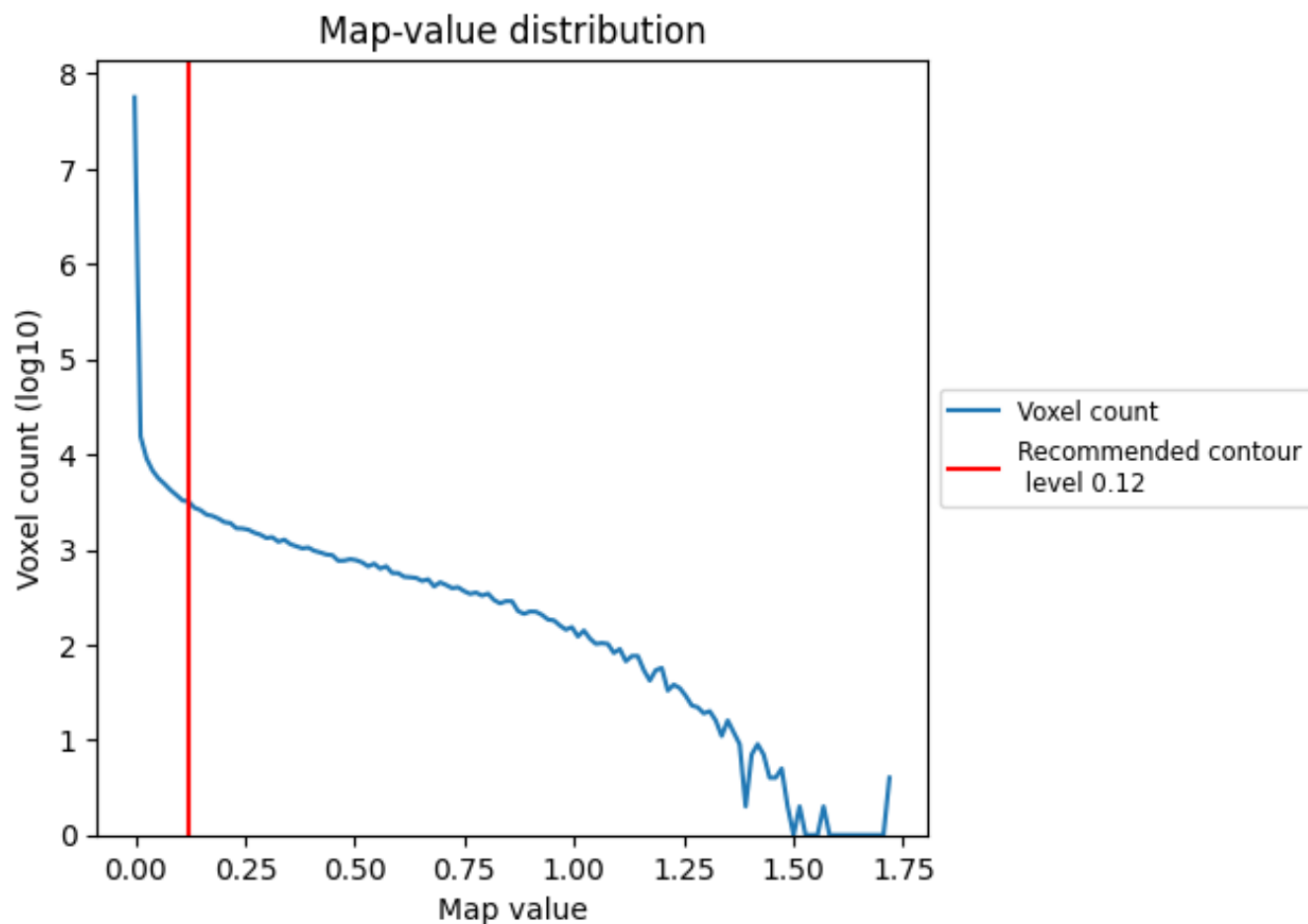
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

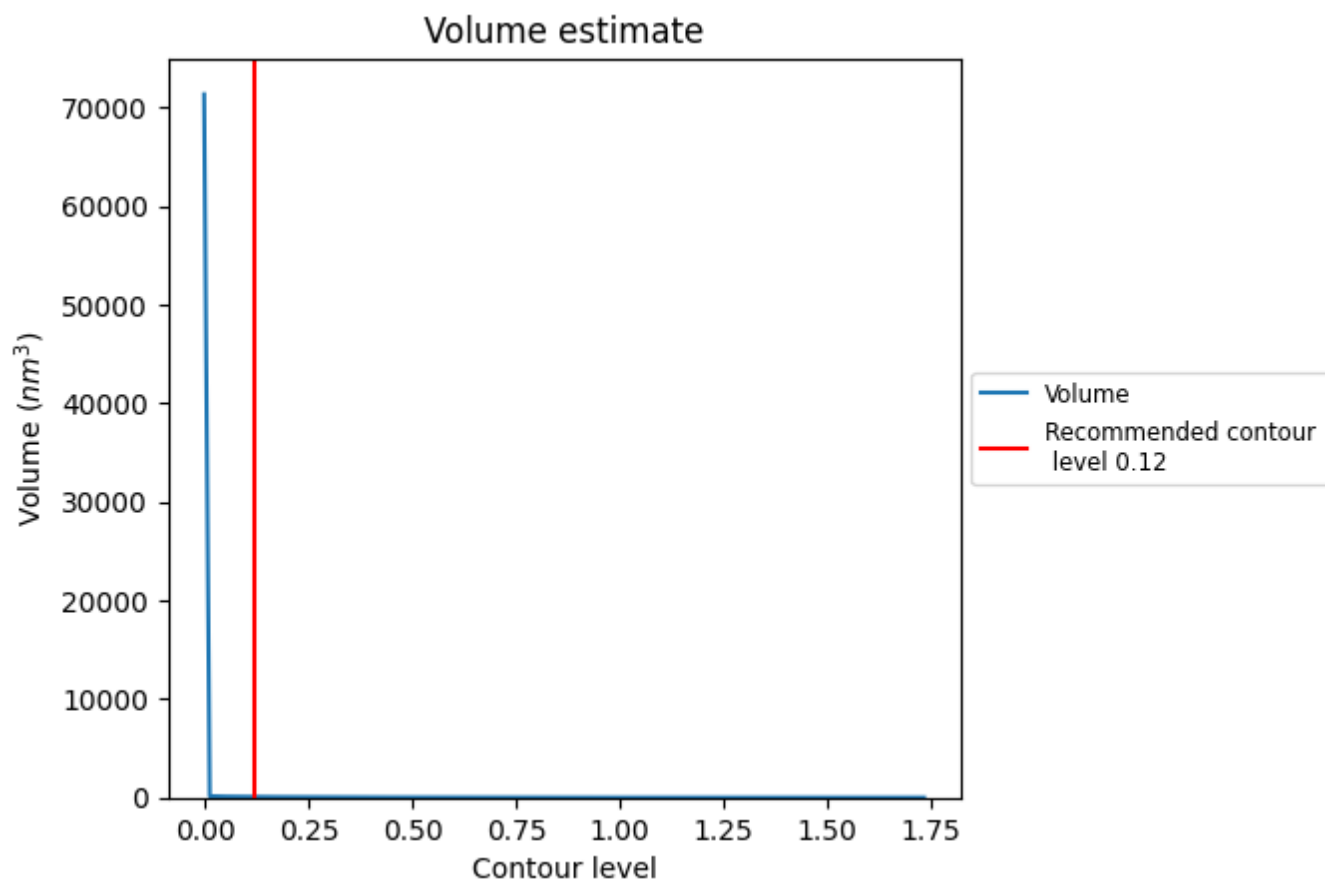
This section contains the results of statistical analysis of the map.

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.

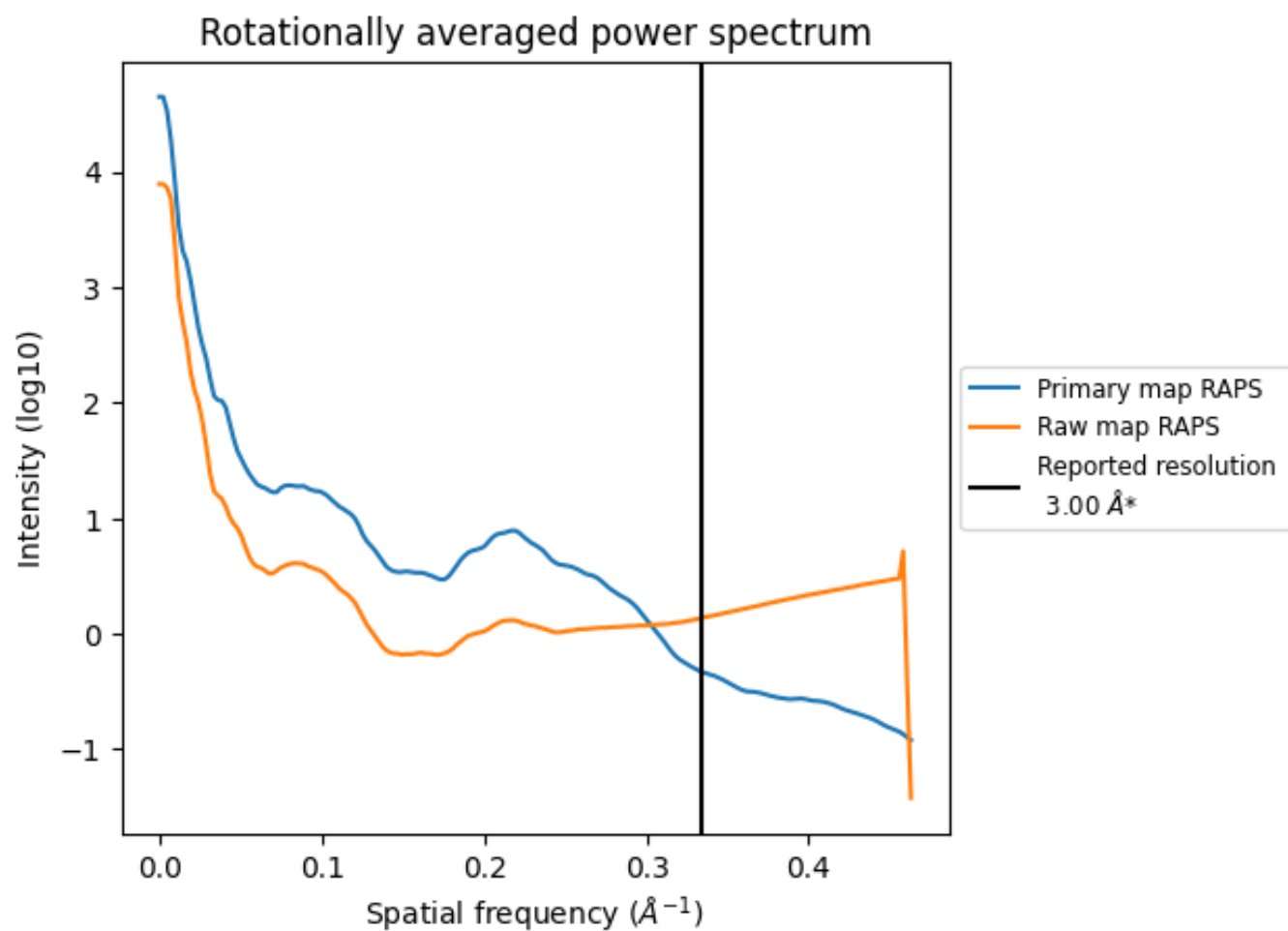
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 74 nm³; this corresponds to an approximate mass of 67 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 ⓘ

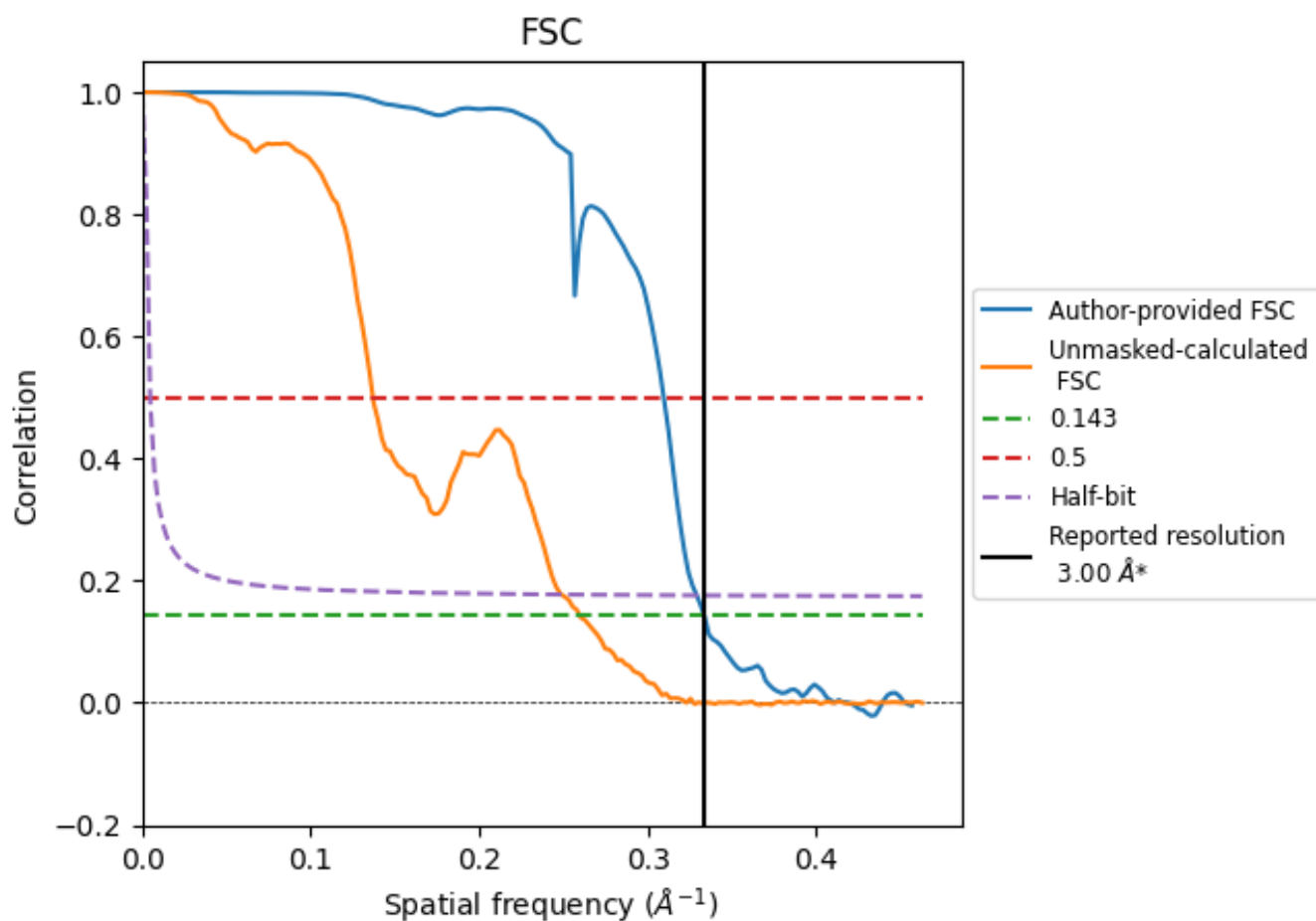


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8 Fourier-Shell correlation [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 0.333 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

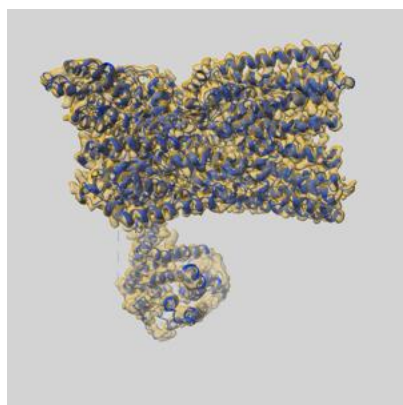
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.00	3.23	3.04
Unmasked-calculated*	3.85	7.30	4.02

*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 3.85 differs from the reported value 3.0 by more than 10 %

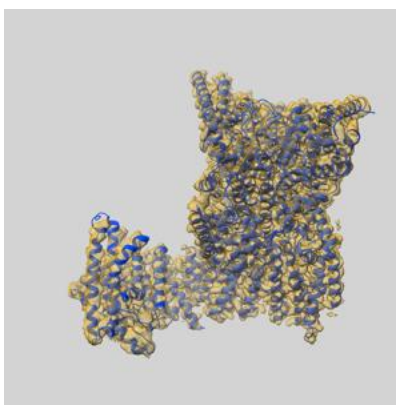
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-47455 and PDB model 9E2K. Per-residue inclusion information can be found in section [3](#) on page [8](#).

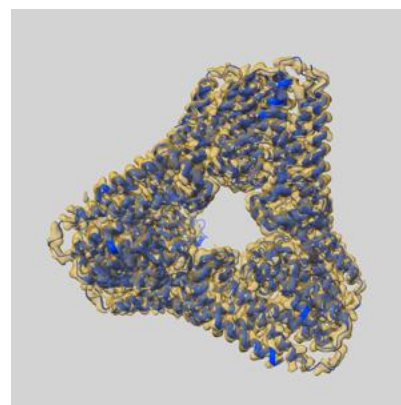
9.1 Map-model overlay [i](#)



X



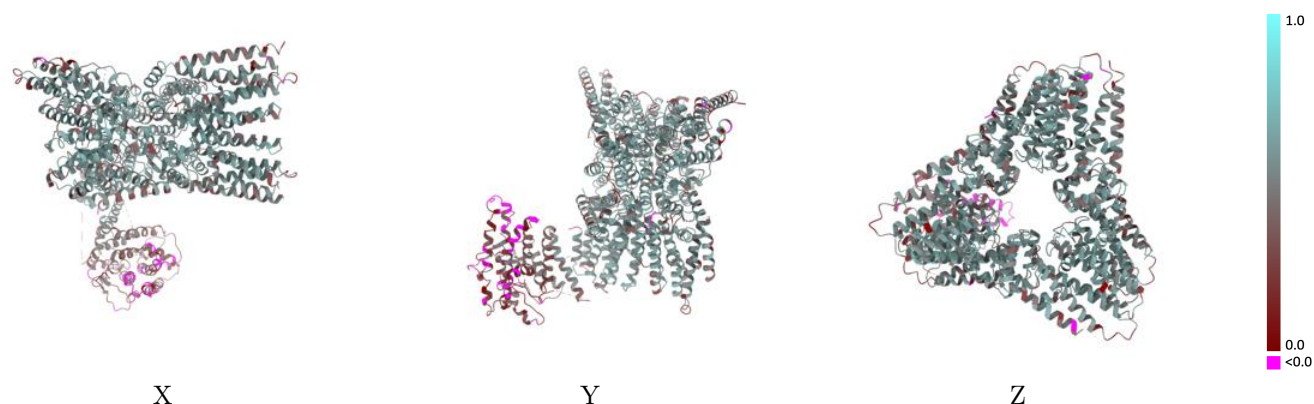
Y



Z

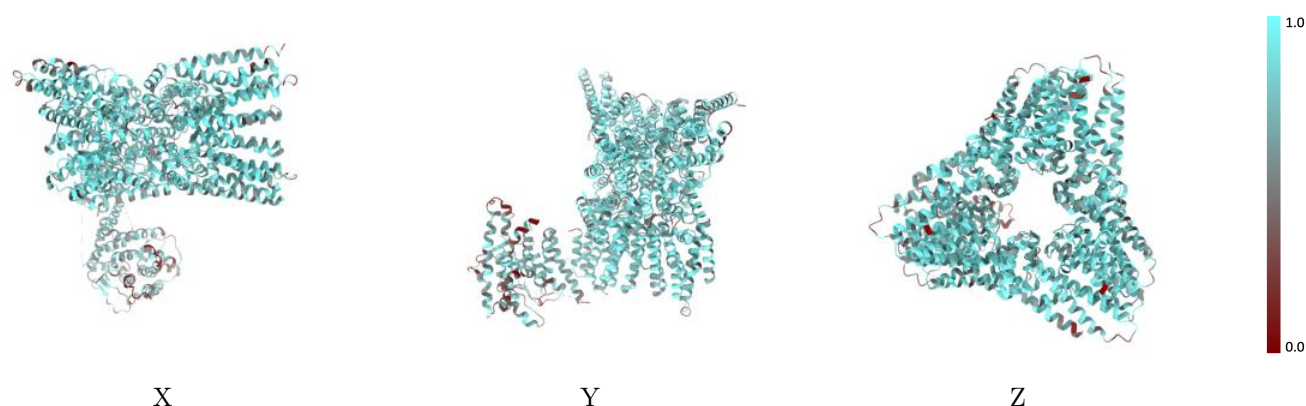
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



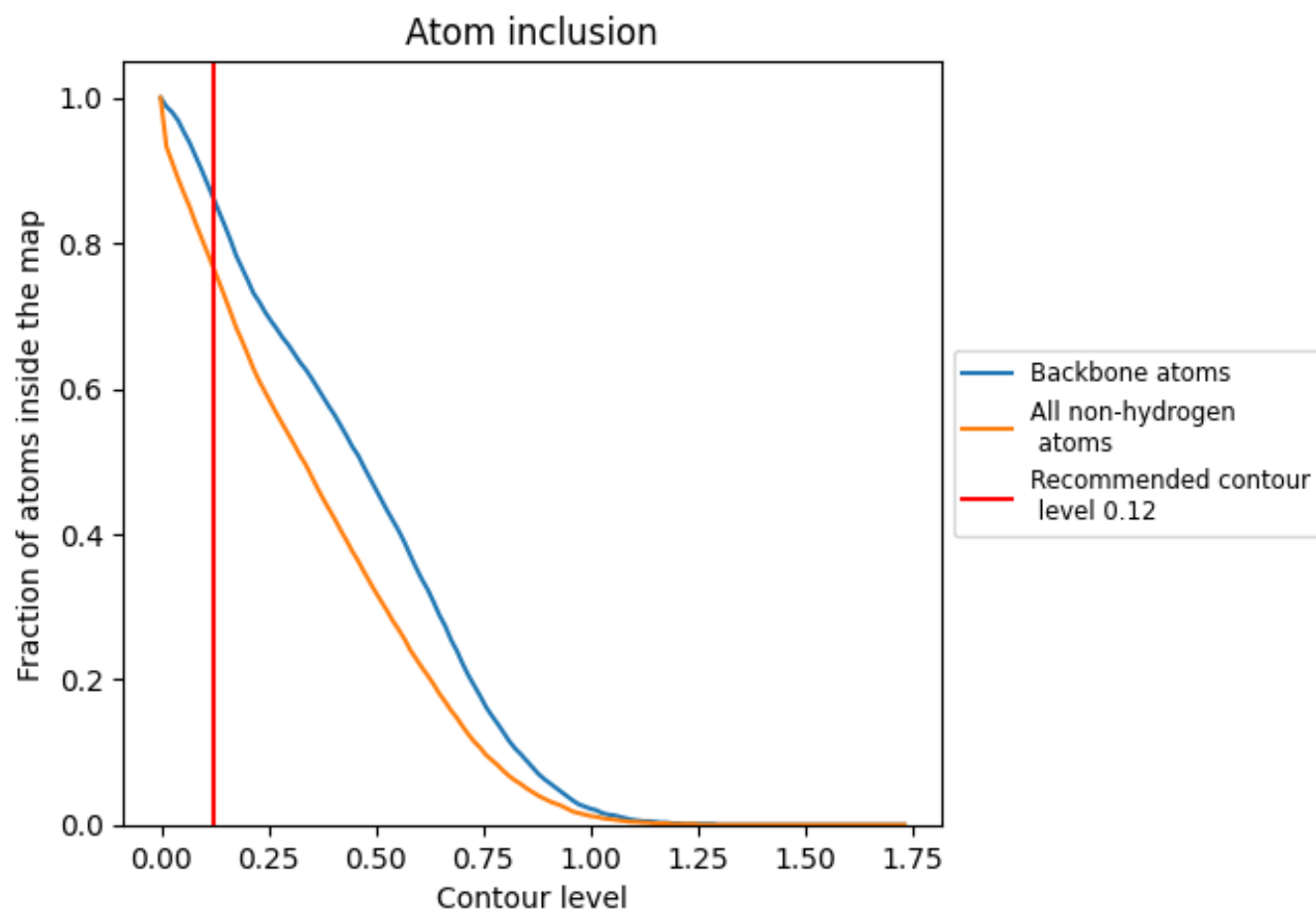
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).

9.4 Atom inclusion ⓘ



At the recommended contour level, 86% of all backbone atoms, 77% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7680	0.4830
A	0.8270	0.5470
B	0.6800	0.3640
C	0.8050	0.5360
D	0.7970	0.5260
E	0.8030	0.5360
F	0.7930	0.5230

1.0

0.0

<0.0