



wwPDB EM Validation Summary Report ⓘ

Mar 15, 2026 – 01:05 AM UTC

PDB ID : 7JTH / pdb_00007jth
EMDB ID : EMD-22473
Title : Cryo-EM structure of unliganded octameric prenyltransferase domain of Phomopsis amygdali fusicoccadiene synthase
Authors : Faylo, J.L.; van Eeuwen, T.; Murakami, K.; Christianson, D.W.
Deposited on : 2020-08-17
Resolution : 4.00 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:

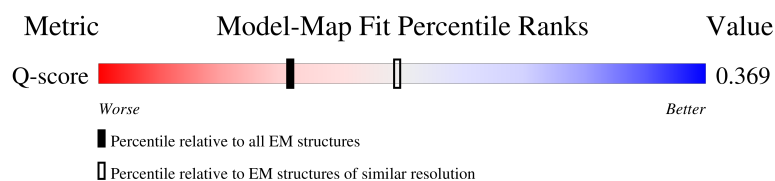
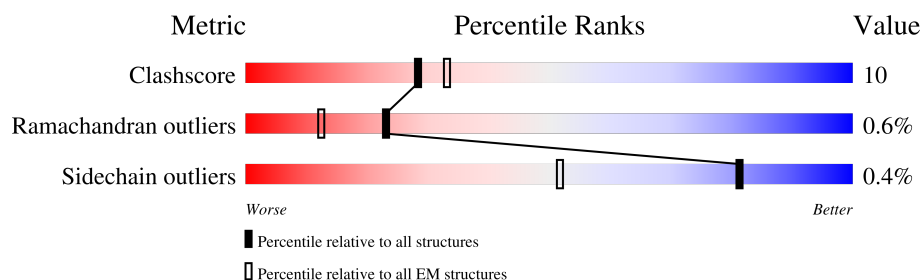
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 4.00 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	7587 (3.50 - 4.50)

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	739	33% 6% 60%
1	B	739	33% 6% 61%
1	C	739	34% 6% 60%
1	D	739	33% 6% 61%

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Mol	Chain	Length	Quality of chain
1	E	739	 34%6%60%
1	F	739	 33%6%61%
1	G	739	 35%5%60%
1	H	739	 33%6%61%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 14628 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 Fusicoccadiene synthase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	294	Total	C	N	O	S	0	0
			1823	1156	324	337	6		
1	B	289	Total	C	N	O	S	1	0
			1841	1170	334	333	4		
1	C	294	Total	C	N	O	S	0	0
			1830	1163	323	338	6		
1	D	289	Total	C	N	O	S	1	0
			1820	1154	329	331	6		
1	E	294	Total	C	N	O	S	0	0
			1823	1156	324	337	6		
1	F	289	Total	C	N	O	S	1	0
			1841	1170	334	333	4		
1	G	294	Total	C	N	O	S	0	0
			1830	1163	323	338	6		
1	H	289	Total	C	N	O	S	1	0
			1820	1154	329	331	6		

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP A2PZA5
A	-18	GLY	-	expression tag	UNP A2PZA5
A	-17	SER	-	expression tag	UNP A2PZA5
A	-16	SER	-	expression tag	UNP A2PZA5
A	-15	HIS	-	expression tag	UNP A2PZA5
A	-14	HIS	-	expression tag	UNP A2PZA5
A	-13	HIS	-	expression tag	UNP A2PZA5
A	-12	HIS	-	expression tag	UNP A2PZA5
A	-11	HIS	-	expression tag	UNP A2PZA5
A	-10	HIS	-	expression tag	UNP A2PZA5
A	-9	SER	-	expression tag	UNP A2PZA5
A	-8	SER	-	expression tag	UNP A2PZA5
A	-7	GLY	-	expression tag	UNP A2PZA5
A	-6	LEU	-	expression tag	UNP A2PZA5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	VAL	-	expression tag	UNP A2PZA5
A	-4	PRO	-	expression tag	UNP A2PZA5
A	-3	ARG	-	expression tag	UNP A2PZA5
A	-2	GLY	-	expression tag	UNP A2PZA5
A	-1	SER	-	expression tag	UNP A2PZA5
A	0	HIS	-	expression tag	UNP A2PZA5
B	-19	MET	-	expression tag	UNP A2PZA5
B	-18	GLY	-	expression tag	UNP A2PZA5
B	-17	SER	-	expression tag	UNP A2PZA5
B	-16	SER	-	expression tag	UNP A2PZA5
B	-15	HIS	-	expression tag	UNP A2PZA5
B	-14	HIS	-	expression tag	UNP A2PZA5
B	-13	HIS	-	expression tag	UNP A2PZA5
B	-12	HIS	-	expression tag	UNP A2PZA5
B	-11	HIS	-	expression tag	UNP A2PZA5
B	-10	HIS	-	expression tag	UNP A2PZA5
B	-9	SER	-	expression tag	UNP A2PZA5
B	-8	SER	-	expression tag	UNP A2PZA5
B	-7	GLY	-	expression tag	UNP A2PZA5
B	-6	LEU	-	expression tag	UNP A2PZA5
B	-5	VAL	-	expression tag	UNP A2PZA5
B	-4	PRO	-	expression tag	UNP A2PZA5
B	-3	ARG	-	expression tag	UNP A2PZA5
B	-2	GLY	-	expression tag	UNP A2PZA5
B	-1	SER	-	expression tag	UNP A2PZA5
B	0	HIS	-	expression tag	UNP A2PZA5
C	-19	MET	-	expression tag	UNP A2PZA5
C	-18	GLY	-	expression tag	UNP A2PZA5
C	-17	SER	-	expression tag	UNP A2PZA5
C	-16	SER	-	expression tag	UNP A2PZA5
C	-15	HIS	-	expression tag	UNP A2PZA5
C	-14	HIS	-	expression tag	UNP A2PZA5
C	-13	HIS	-	expression tag	UNP A2PZA5
C	-12	HIS	-	expression tag	UNP A2PZA5
C	-11	HIS	-	expression tag	UNP A2PZA5
C	-10	HIS	-	expression tag	UNP A2PZA5
C	-9	SER	-	expression tag	UNP A2PZA5
C	-8	SER	-	expression tag	UNP A2PZA5
C	-7	GLY	-	expression tag	UNP A2PZA5
C	-6	LEU	-	expression tag	UNP A2PZA5
C	-5	VAL	-	expression tag	UNP A2PZA5
C	-4	PRO	-	expression tag	UNP A2PZA5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	ARG	-	expression tag	UNP A2PZA5
C	-2	GLY	-	expression tag	UNP A2PZA5
C	-1	SER	-	expression tag	UNP A2PZA5
C	0	HIS	-	expression tag	UNP A2PZA5
D	-19	MET	-	expression tag	UNP A2PZA5
D	-18	GLY	-	expression tag	UNP A2PZA5
D	-17	SER	-	expression tag	UNP A2PZA5
D	-16	SER	-	expression tag	UNP A2PZA5
D	-15	HIS	-	expression tag	UNP A2PZA5
D	-14	HIS	-	expression tag	UNP A2PZA5
D	-13	HIS	-	expression tag	UNP A2PZA5
D	-12	HIS	-	expression tag	UNP A2PZA5
D	-11	HIS	-	expression tag	UNP A2PZA5
D	-10	HIS	-	expression tag	UNP A2PZA5
D	-9	SER	-	expression tag	UNP A2PZA5
D	-8	SER	-	expression tag	UNP A2PZA5
D	-7	GLY	-	expression tag	UNP A2PZA5
D	-6	LEU	-	expression tag	UNP A2PZA5
D	-5	VAL	-	expression tag	UNP A2PZA5
D	-4	PRO	-	expression tag	UNP A2PZA5
D	-3	ARG	-	expression tag	UNP A2PZA5
D	-2	GLY	-	expression tag	UNP A2PZA5
D	-1	SER	-	expression tag	UNP A2PZA5
D	0	HIS	-	expression tag	UNP A2PZA5
E	-19	MET	-	expression tag	UNP A2PZA5
E	-18	GLY	-	expression tag	UNP A2PZA5
E	-17	SER	-	expression tag	UNP A2PZA5
E	-16	SER	-	expression tag	UNP A2PZA5
E	-15	HIS	-	expression tag	UNP A2PZA5
E	-14	HIS	-	expression tag	UNP A2PZA5
E	-13	HIS	-	expression tag	UNP A2PZA5
E	-12	HIS	-	expression tag	UNP A2PZA5
E	-11	HIS	-	expression tag	UNP A2PZA5
E	-10	HIS	-	expression tag	UNP A2PZA5
E	-9	SER	-	expression tag	UNP A2PZA5
E	-8	SER	-	expression tag	UNP A2PZA5
E	-7	GLY	-	expression tag	UNP A2PZA5
E	-6	LEU	-	expression tag	UNP A2PZA5
E	-5	VAL	-	expression tag	UNP A2PZA5
E	-4	PRO	-	expression tag	UNP A2PZA5
E	-3	ARG	-	expression tag	UNP A2PZA5
E	-2	GLY	-	expression tag	UNP A2PZA5

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	SER	-	expression tag	UNP A2PZA5
E	0	HIS	-	expression tag	UNP A2PZA5
F	-19	MET	-	expression tag	UNP A2PZA5
F	-18	GLY	-	expression tag	UNP A2PZA5
F	-17	SER	-	expression tag	UNP A2PZA5
F	-16	SER	-	expression tag	UNP A2PZA5
F	-15	HIS	-	expression tag	UNP A2PZA5
F	-14	HIS	-	expression tag	UNP A2PZA5
F	-13	HIS	-	expression tag	UNP A2PZA5
F	-12	HIS	-	expression tag	UNP A2PZA5
F	-11	HIS	-	expression tag	UNP A2PZA5
F	-10	HIS	-	expression tag	UNP A2PZA5
F	-9	SER	-	expression tag	UNP A2PZA5
F	-8	SER	-	expression tag	UNP A2PZA5
F	-7	GLY	-	expression tag	UNP A2PZA5
F	-6	LEU	-	expression tag	UNP A2PZA5
F	-5	VAL	-	expression tag	UNP A2PZA5
F	-4	PRO	-	expression tag	UNP A2PZA5
F	-3	ARG	-	expression tag	UNP A2PZA5
F	-2	GLY	-	expression tag	UNP A2PZA5
F	-1	SER	-	expression tag	UNP A2PZA5
F	0	HIS	-	expression tag	UNP A2PZA5
G	-19	MET	-	expression tag	UNP A2PZA5
G	-18	GLY	-	expression tag	UNP A2PZA5
G	-17	SER	-	expression tag	UNP A2PZA5
G	-16	SER	-	expression tag	UNP A2PZA5
G	-15	HIS	-	expression tag	UNP A2PZA5
G	-14	HIS	-	expression tag	UNP A2PZA5
G	-13	HIS	-	expression tag	UNP A2PZA5
G	-12	HIS	-	expression tag	UNP A2PZA5
G	-11	HIS	-	expression tag	UNP A2PZA5
G	-10	HIS	-	expression tag	UNP A2PZA5
G	-9	SER	-	expression tag	UNP A2PZA5
G	-8	SER	-	expression tag	UNP A2PZA5
G	-7	GLY	-	expression tag	UNP A2PZA5
G	-6	LEU	-	expression tag	UNP A2PZA5
G	-5	VAL	-	expression tag	UNP A2PZA5
G	-4	PRO	-	expression tag	UNP A2PZA5
G	-3	ARG	-	expression tag	UNP A2PZA5
G	-2	GLY	-	expression tag	UNP A2PZA5
G	-1	SER	-	expression tag	UNP A2PZA5
G	0	HIS	-	expression tag	UNP A2PZA5

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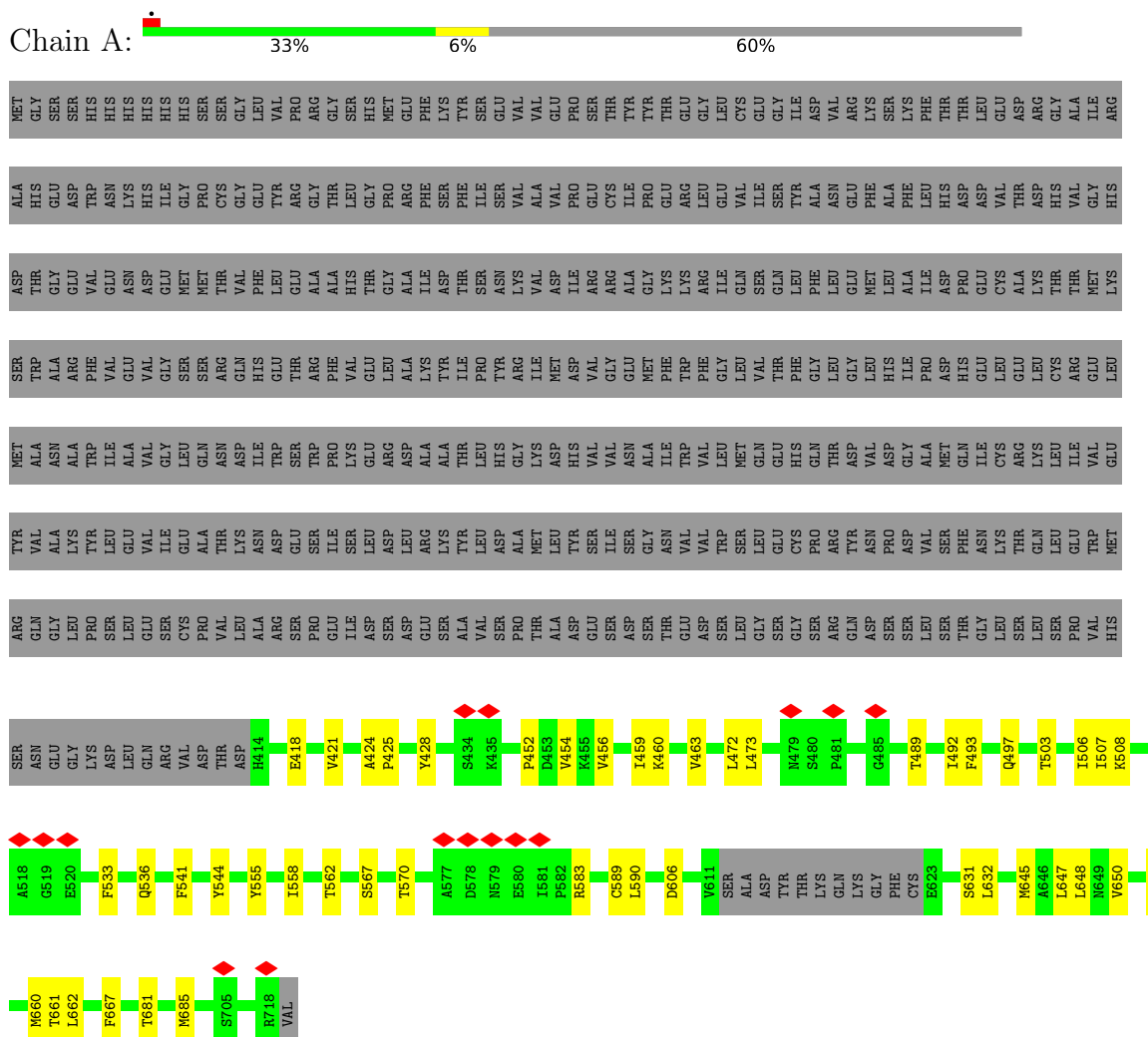
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Chain	Residue	Modelled	Actual	Comment	Reference
H	-19	MET	-	expression tag	UNP A2PZA5
H	-18	GLY	-	expression tag	UNP A2PZA5
H	-17	SER	-	expression tag	UNP A2PZA5
H	-16	SER	-	expression tag	UNP A2PZA5
H	-15	HIS	-	expression tag	UNP A2PZA5
H	-14	HIS	-	expression tag	UNP A2PZA5
H	-13	HIS	-	expression tag	UNP A2PZA5
H	-12	HIS	-	expression tag	UNP A2PZA5
H	-11	HIS	-	expression tag	UNP A2PZA5
H	-10	HIS	-	expression tag	UNP A2PZA5
H	-9	SER	-	expression tag	UNP A2PZA5
H	-8	SER	-	expression tag	UNP A2PZA5
H	-7	GLY	-	expression tag	UNP A2PZA5
H	-6	LEU	-	expression tag	UNP A2PZA5
H	-5	VAL	-	expression tag	UNP A2PZA5
H	-4	PRO	-	expression tag	UNP A2PZA5
H	-3	ARG	-	expression tag	UNP A2PZA5
H	-2	GLY	-	expression tag	UNP A2PZA5
H	-1	SER	-	expression tag	UNP A2PZA5
H	0	HIS	-	expression tag	UNP A2PZA5

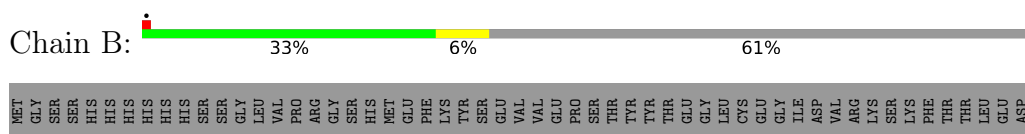
3 Residue-property plots

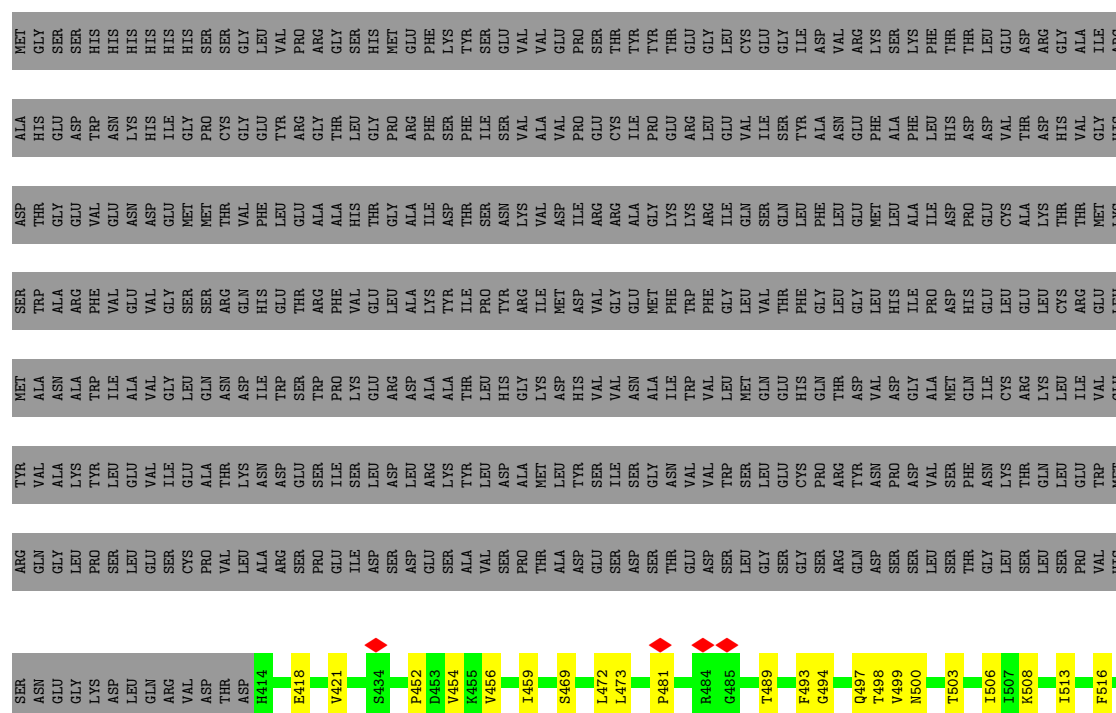
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

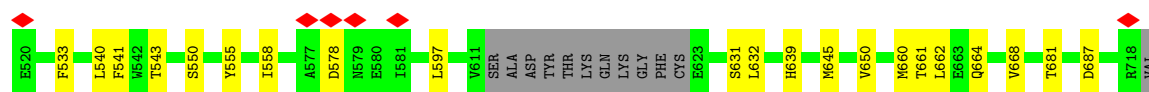
• Molecule 1: Fusicoccadiene synthase



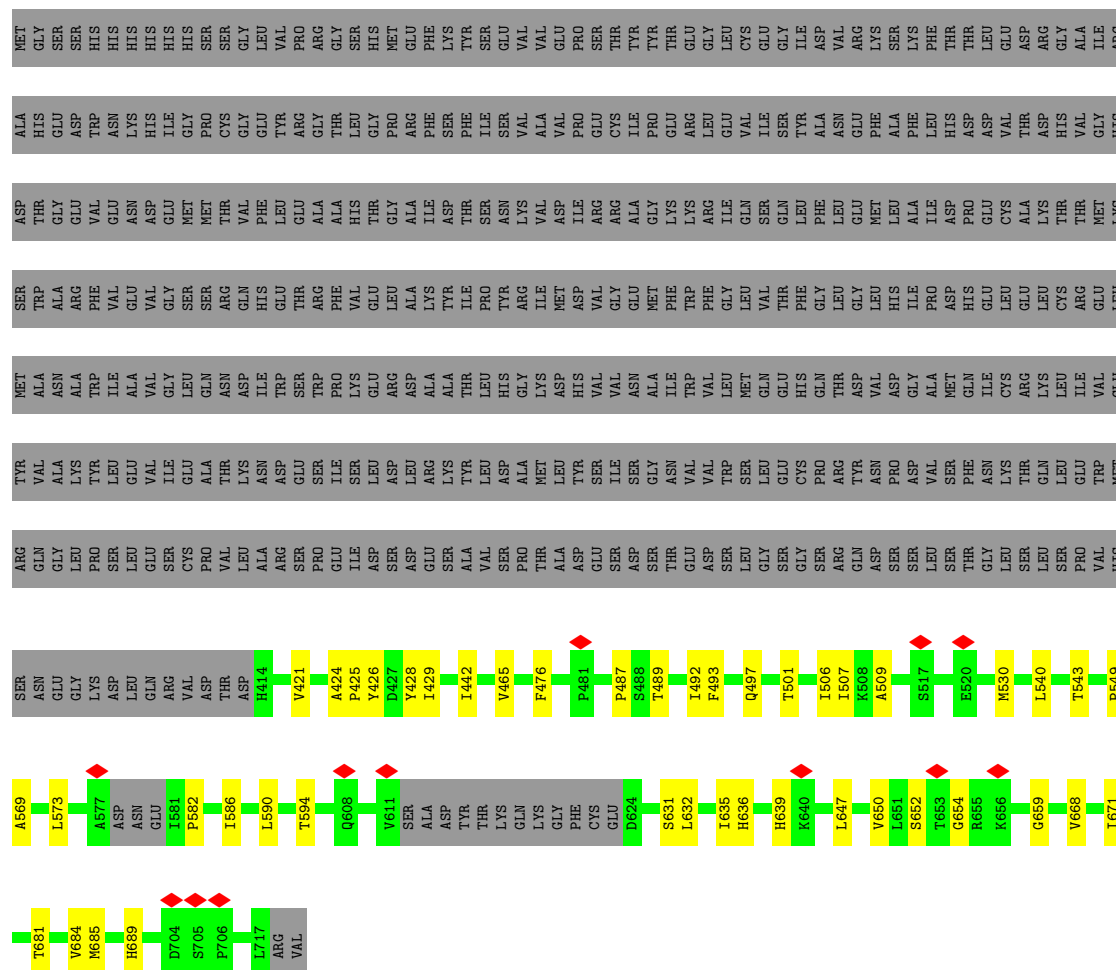
• Molecule 1: Fusicoccadiene synthase



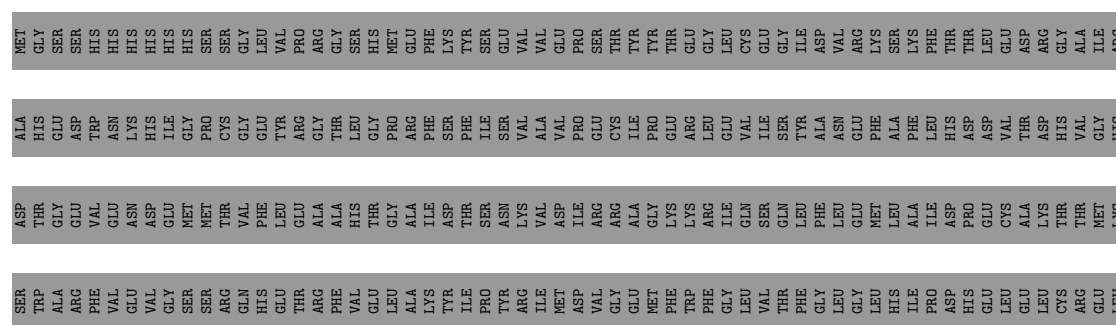


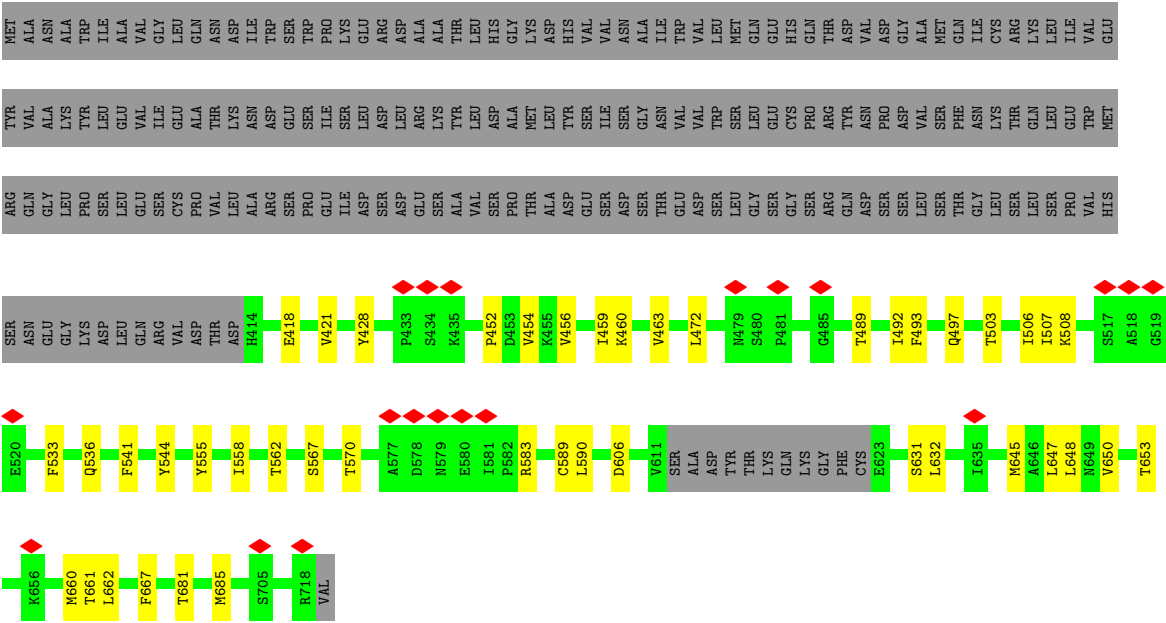


• Molecule 1: Fusicoccadiene synthase

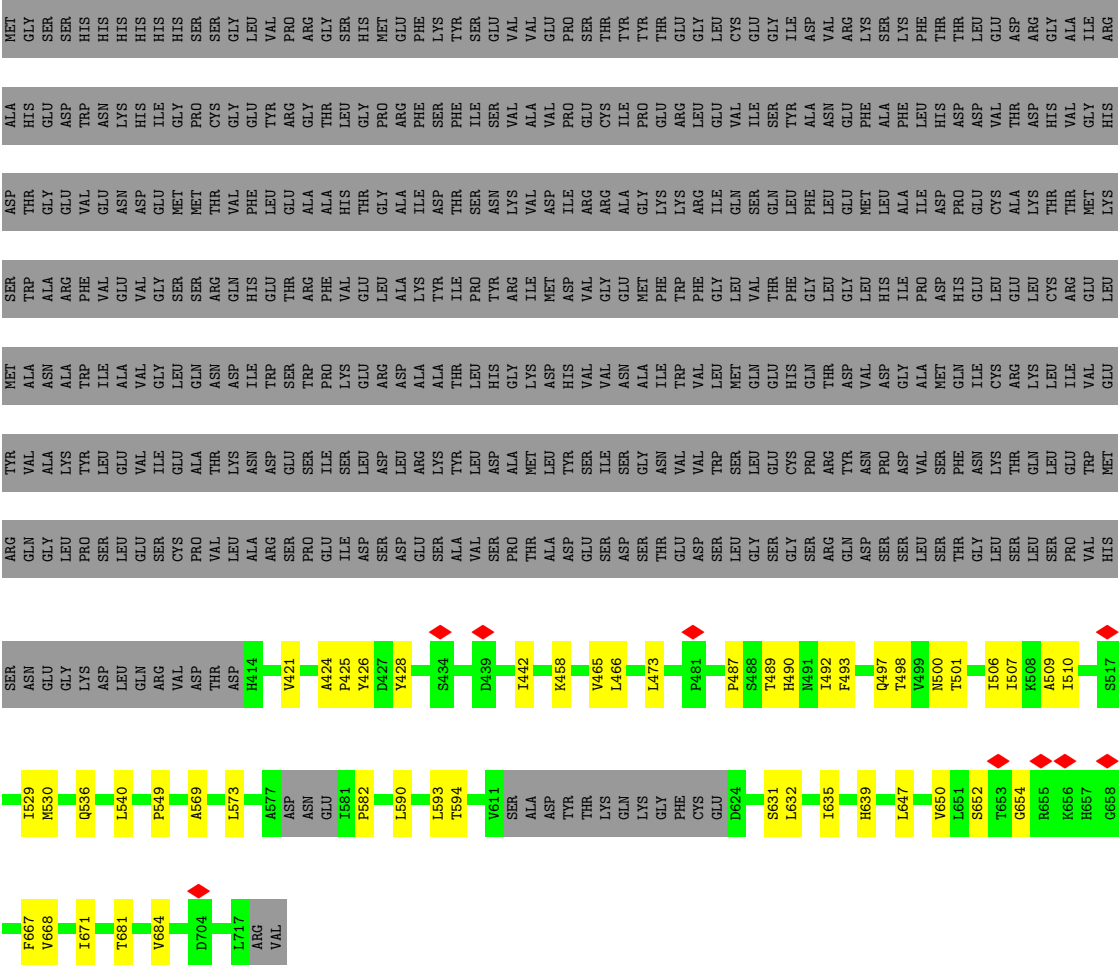


• Molecule 1: Fusicoccadiene synthase





● Molecule 1: Fusicoccadiene synthase



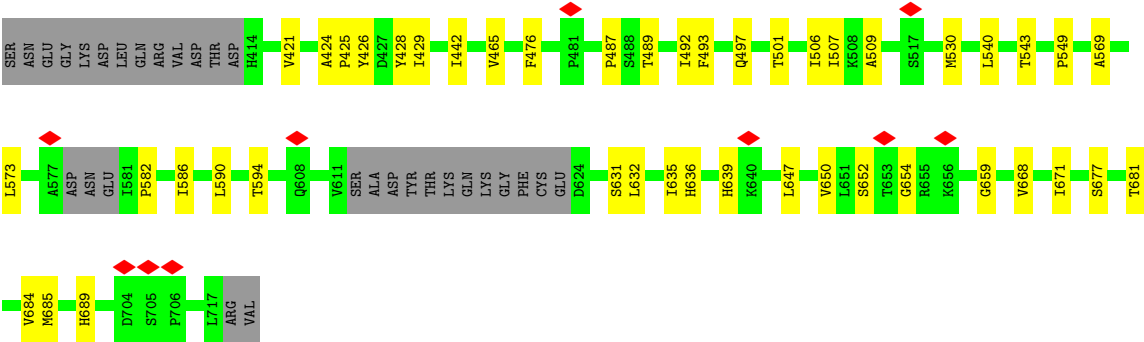
Chain G:



F533	F541	F542	F543	S550	F555	F558	A577	D578	M579	F580	F581	F611	SER	ASN	GLN	ARG	TTR	MET	SER	ALA	TRP	THR	ASP	ALA	MET
L540	F541	F542	F543	S550	F555	F558	A577	D578	M579	F580	F581	F611	GLU	GLU	GLY	GLY	ALA	ASN	GLY	HIS	TRP	GLU	THR	HIS	GLY
F541	F541	F542	F543	S550	F555	F558	A577	D578	M579	F580	F581	F611	LYS	PRO	LYS	PRO	TTR	TRP	TRP	ASP	PHE	VAL	GLU	ASP	GLY
F542	F541	F542	F543	S550	F555	F558	A577	D578	M579	F580	F581	F611	ASP	SER	LEU	SER	LEU	ILE	ILE	ASN	VAL	GLU	VAL	GLY	GLY
F543	F541	F542	F543	S550	F555	F558	A577	D578	M579	F580	F581	F611	LEU	LEU	GLU	GLY	VAL	ALA	ASN	HIS	GLU	ASN	LYS	HIS	HIS
S550	F541	F542	F543	S550	F555	F558	A577	D578	M579	F580	F581	F611	GLN	GLN	GLU	GLY	VAL	VAL	ASP	HIS	VAL	VAL	ASP	HIS	HIS
F555	F541	F542	F543	S550	F555	F558	A577	D578	M579	F580	F581	F611	VAL	ARG	SER	SER	GLU	GLY	MET	ILE	SER	GLU	GLY	ILE	GLY
F558	F541	F542	F543	S550	F555	F558	A577	D578	M579	F580	F581	F611	ASP	ASP	THR	PRO	ALA	GLN	THR	CYS	ARG	THR	VAL	SER	SER
A577	F541	F542	F543	S550	F555	F558	A577	D578	M579	F580	F581	F611	ASP	ASP	LEU	LEU	LYS	ASP	VAL	GLY	GLN	VAL	GLY	GLY	GLY
D578	F541	F542	F543	S550	F555	F558	A577	D578	M579	F580	F581	F611	H414	H414	ALA	ARG	ASN	TRP	ILE	ILE	HIS	PHE	GLU	THR	LEU
M579	F541	F542	F543	S550	F555	F558	A577	D578	M579	F580	F581	F611	E418	E418	SER	SER	GLU	SER	SER	THR	ARG	GLU	THR	GLU	GLY
F580	F541	F542	F543	S550	F555	F558	A577	D578	M579	F580	F581	F611	V421	V421	GLY	ILE	ILE	PRO	PRO	PHE	VAL	VAL	VAL	ALA	GLY
F581	F541	F542	F543	S550	F555	F558	A577	D578	M579	F580	F581	F611	S434	S434	ASP	ASP	LEU	SER	GLY	VAL	VAL	VAL	VAL	ALA	THR
F611	F541	F542	F543	S550	F555	F558	A577	D578	M579	F580	F581	F611	S434	S434	ASP	ASP	LEU	SER	GLY	VAL	VAL	VAL	VAL	ALA	THR
SER	F541	F542	F543	S550	F555	F558	A577	D578	M579	F580	F581	F611	P452	P452	SER	ASP	LEU	ASP	ALA	LYS	ILE	ASP	ASP	VAL	GLY
ALA	F541	F542	F543	S550	F555	F558	A577	D578	M579	F580	F581	F611	D453	D453	GLU	GLU	ARG	ASP	ALA	LYS	ILE	ASP	ASP	VAL	GLY
ASP	F541	F542	F543	S550	F555	F558	A577	D578	M579	F580	F581	F611	V454	V454	SER	ASP	LEU	ASP	ALA	LYS	ILE	ASP	ASP	VAL	GLY
TTR	F541	F542	F543	S550	F555	F558	A577	D578	M579	F580	F581	F611	F455	F455	ALA	ALA	TTR	THR	THR	ILE	THR	THR	THR	PHE	PHE
LYS	F541	F542	F543	S550	F555	F558	A577	D578	M579	F580	F581	F611	V456	V456	VAL	SER	LEU	ASP	ASP	PRO	THR	THR	THR	THR	TTR
GLN	F541	F542	F543	S550	F555	F558	A577	D578	M579	F580	F581	F611	V459	V459	PRO	ALA	MET	GLY	ARG	VAL	VAL	VAL	VAL	VAL	VAL
LYS	F541	F542	F543	S550	F555	F558	A577	D578	M579	F580	F581	F611	L459	L459	THR	THR	LEU	ASP	ILE	ILE	MET	ASP	ASP	VAL	GLY
GLY	F541	F542	F543	S550	F555	F558	A577	D578	M579	F580	F581	F611	S469	S469	ALA	ASP	LEU	ASP	HIS	MET	MET	ASP	ASP	VAL	GLY
PHE	F541	F542	F543	S550	F555	F558	A577	D578	M579	F580	F581	F611	P469	P469	ASP	ASP	TTR	SER	VAL	VAL	VAL	VAL	ILE	PRO	PRO
CYS	F541	F542	F543	S550	F555	F558	A577	D578	M579	F580	F581	F611	L472	L472	GLU	GLU	SER	ILE	VAL	VAL	GLY	ARG	ARG	GLU	GLY
E623	F541	F542	F543	S550	F555	F558	A577	D578	M579	F580	F581	F611	P481	P481	ASP	ASP	SER	ASN	ALA	GLU	MET	GLY	LYS	ILE	THR
L632	F541	F542	F543	S550	F555	F558	A577	D578	M579	F580	F581	F611	P481	P481	SER	SER	GLY	ALA	ALA	MET	PHE	GLY	LYS	GLU	THR
H639	F541	F542	F543	S550	F555	F558	A577	D578	M579	F580	F581	F611	S484	S484	THR	GLU	ASN	VAL	VAL	PHE	TRP	LYS	ARG	GLU	GLY
M645	F541	F542	F543	S550	F555	F558	A577	D578	M579	F580	F581	F611	G485	G485	GLU	ASP	VAL	VAL	PHE	PHE	GLY	ARG	LEU	LEU	GLY
V650	F541	F542	F543	S550	F555	F558	A577	D578	M579	F580	F581	F611	T489	T489	LEU	LEU	SER	GLN	LEU	VAL	VAL	SER	VAL	ILE	GLY
M660	F541	F542	F543	S550	F555	F558	A577	D578	M579	F580	F581	F611	F493	F493	SER	SER	GLU	GLU	THR	THR	THR	GLN	SER	ILE	GLY
T661	F541	F542	F543	S550	F555	F558	A577	D578	M579	F580	F581	F611	G497	G497	GLY	GLY	PRO	GLN	PHE	PHE	GLY	PHE	LEU	TYR	ILE
L662	F541	F542	F543	S550	F555	F558	A577	D578	M579	F580	F581	F611	T498	T498	SER	ARG	CYS	THR	THR	GLY	LEU	ASN	ALA	ALA	ASP
F663	F541	F542	F543	S550	F555	F558	A577	D578	M579	F580	F581	F611	V499	V499	GLN	GLN	TTR	ASP	ASP	GLY	GLY	GLU	GLU	VAL	ARG
Q654	F541	F542	F543	S550	F555	F558	A577	D578	M579	F580	F581	F611	M500	M500	ASP	ASP	ASN	VAL	VAL	LEU	LEU	MET	LYS	PHE	LYS
V668	F541	F542	F543	S550	F555	F558	A577	D578	M579	F580	F581	F611	T503	T503	SER	SER	PRO	ASP	ASP	HIS	HIS	LEU	ALA	ALA	SER
T661	F541	F542	F543	S550	F555	F558	A577	D578	M579	F580	F581	F611	L506	L506	LEU	LEU	VAL	ASP	VAL	PRO	PRO	ILE	ILE	LEU	PHE
D687	F541	F542	F543	S550	F555	F558	A577	D578	M579	F580	F581	F611	F507	F507	THR	THR	PHE	ASN	ASN	HIS	GLU	PRO	GLU	LEU	THR
L703	F541	F542	F543	S550	F555	F558	A577	D578	M579	F580	F581	F611	K508	K508	LEU	LEU	LYS	LYS	LEU	GLY	LEU	CYS	VAL	VAL	GLU
R718	F541	F542	F543	S550	F555	F558	A577	D578	M579	F580	F581	F611	T513	T513	SER	SER	THR	GLN	GLN	ARG	GLU	ALA	THR	THR	ASP
VAL	F541	F542	F543	S550	F555	F558	A577	D578	M579	F580	F581	F611	F516	F516	SER	PRO	GLU	LEU	LEU	CYS	ARG	LYS	ASP	GLY	GLY
	F541	F542	F543	S550	F555	F558	A577	D578	M579	F580	F581	F611	G519	G519	VAL	VAL	TTR	THR	THR	ILE	ARG	THR	THR	THR	THR
	F541	F542	F543	S550	F555	F558	A577	D578	M579	F580	F581	F611	G519	G519	VAL	VAL	TTR	THR	THR	ILE	ARG	THR	THR	THR	THR

Chain H:

[illegible]



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	94974	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	43	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.855	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.141	Depositor
Map size (Å)	438.52798, 438.52798, 438.52798	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.142, 1.142, 1.142	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.12	0/1860	0.38	0/2569
1	B	0.12	0/1881	0.36	0/2590
1	C	0.13	0/1866	0.43	0/2577
1	D	0.13	0/1860	0.36	0/2563
1	E	0.12	0/1860	0.38	0/2569
1	F	0.12	0/1881	0.36	0/2590
1	G	0.13	0/1866	0.43	0/2577
1	H	0.13	0/1860	0.36	0/2563
All	All	0.12	0/14934	0.38	0/20598

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	1823	0	1336	52	0
1	B	1841	0	1398	34	0
1	C	1830	0	1362	34	0
1	D	1820	0	1357	31	0
1	E	1823	0	1336	50	0
1	F	1841	0	1398	34	0
1	G	1830	0	1362	29	0
1	H	1820	0	1357	32	0

Continued on next page...

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	14628	0	10906	243	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.

The worst 5 of 243 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:C:645:MET:HE1	1:G:541:PHE:CE1	1.72	1.25
1:C:541:PHE:CE1	1:G:645:MET:HE1	1.72	1.24
1:A:541:PHE:CE1	1:E:645:MET:HE1	1.80	1.17
1:A:645:MET:HE1	1:E:541:PHE:CE1	1.80	1.15
1:C:541:PHE:CE1	1:G:645:MET:CE	2.51	0.93

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	290/739 (39%)	254 (88%)	35 (12%)	1 (0%)	36	70
1	B	284/739 (38%)	257 (90%)	25 (9%)	2 (1%)	18	54
1	C	290/739 (39%)	258 (89%)	30 (10%)	2 (1%)	18	54
1	D	284/739 (38%)	257 (90%)	25 (9%)	2 (1%)	18	54
1	E	290/739 (39%)	254 (88%)	35 (12%)	1 (0%)	36	70
1	F	284/739 (38%)	257 (90%)	25 (9%)	2 (1%)	18	54
1	G	290/739 (39%)	258 (89%)	30 (10%)	2 (1%)	18	54
1	H	284/739 (38%)	257 (90%)	25 (9%)	2 (1%)	18	54
All	All	2296/5912 (39%)	2052 (89%)	230 (10%)	14 (1%)	23	57

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	481	PRO
1	G	481	PRO
1	B	659	GLY
1	D	582	PRO
1	F	659	GLY

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	109/651 (17%)	109 (100%)	0	100	100
1	B	116/651 (18%)	115 (99%)	1 (1%)	70	76
1	C	112/651 (17%)	111 (99%)	1 (1%)	70	76
1	D	112/651 (17%)	112 (100%)	0	100	100
1	E	109/651 (17%)	109 (100%)	0	100	100
1	F	116/651 (18%)	115 (99%)	1 (1%)	70	76
1	G	112/651 (17%)	111 (99%)	1 (1%)	70	76
1	H	112/651 (17%)	112 (100%)	0	100	100
All	All	898/5208 (17%)	894 (100%)	4 (0%)	81	84

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	458	LYS
1	C	687	ASP
1	F	458	LYS
1	G	687	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	664	GLN

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Mol	Chain	Res	Type
1	H	636	HIS
1	G	414	HIS
1	G	560	GLN
1	H	689	HIS

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

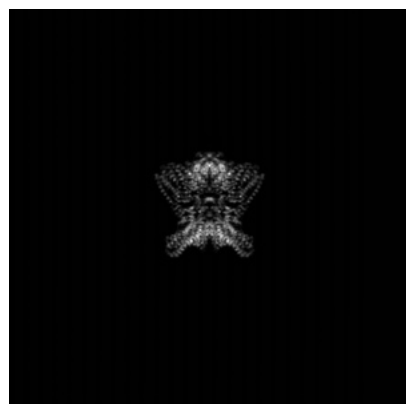
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22473. These allow visual inspection of the internal detail of the map and identification of artifacts.

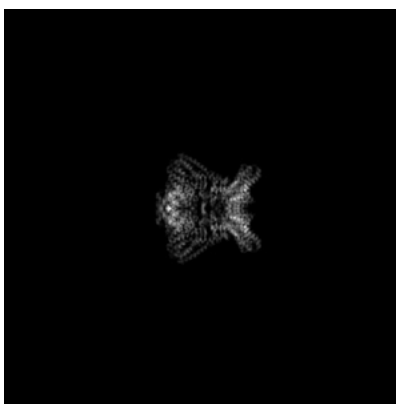
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

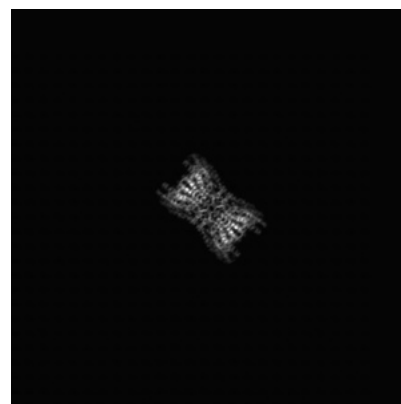
6.1.1 Primary map



X

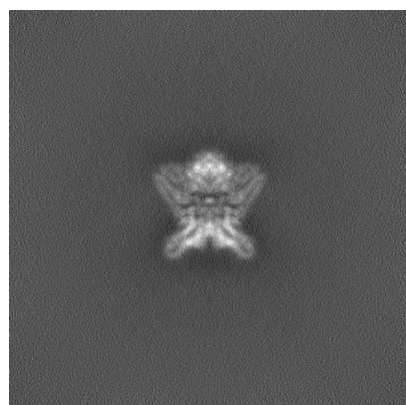


Y

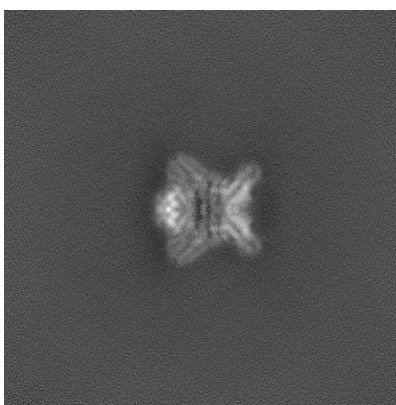


Z

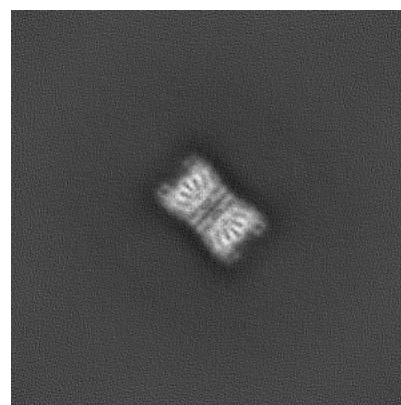
6.1.2 Raw map



X



Y

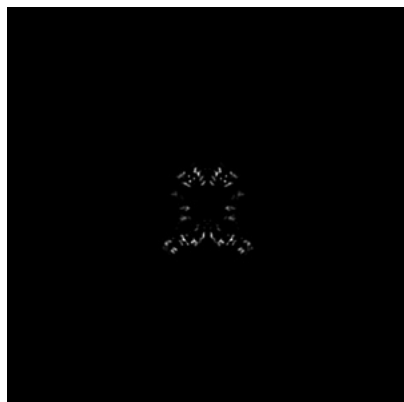


Z

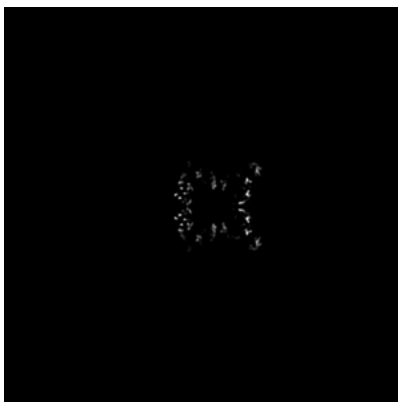
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

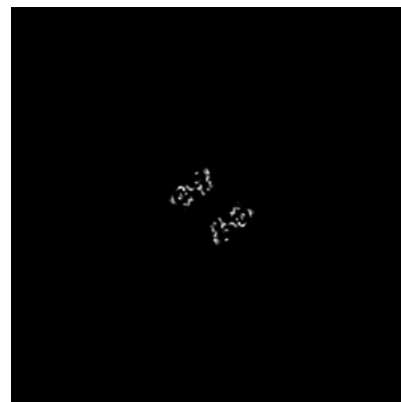
6.2.1 Primary map



X Index: 192

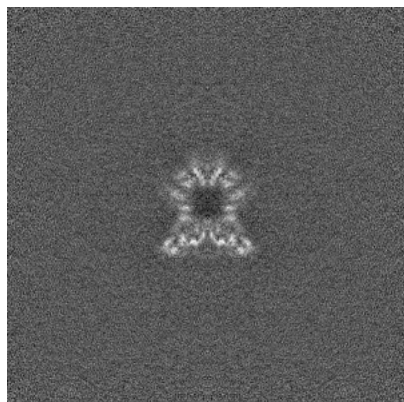


Y Index: 192

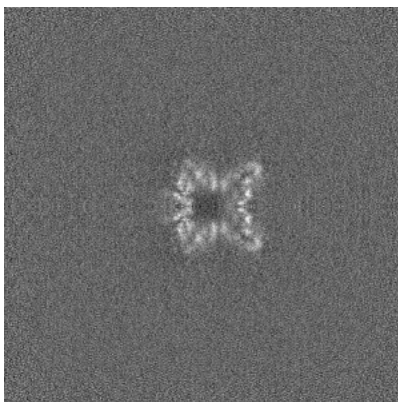


Z Index: 192

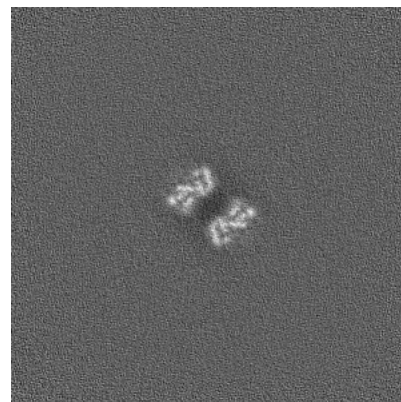
6.2.2 Raw map



X Index: 192



Y Index: 192

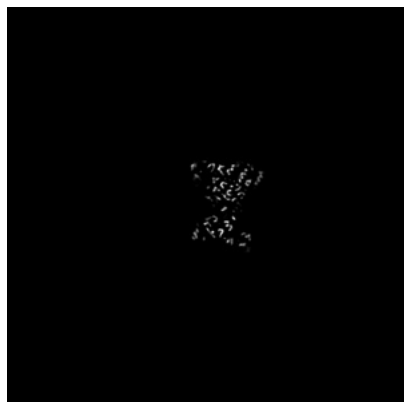


Z Index: 192

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

6.3 Largest variance slices [i](#)

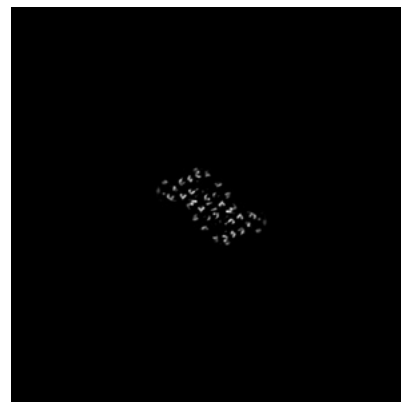
6.3.1 Primary map



X Index: 175

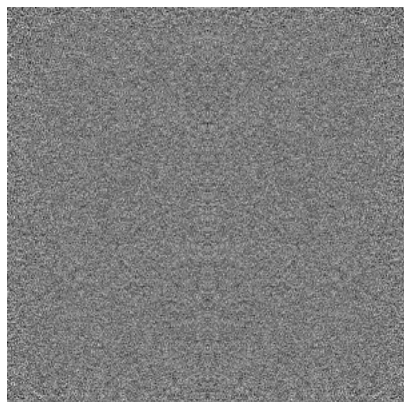


Y Index: 203

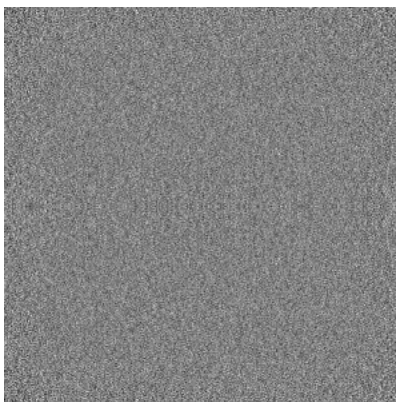


Z Index: 167

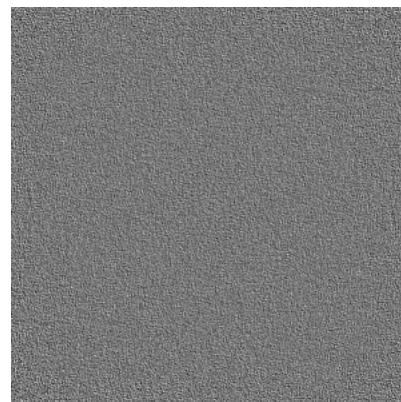
6.3.2 Raw map



X Index: 0



Y Index: 0

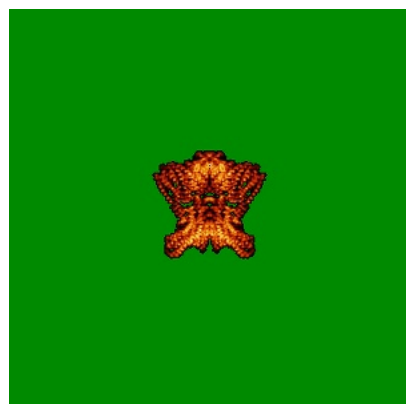


Z Index: 0

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

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

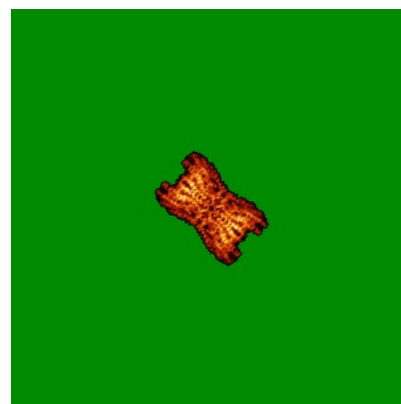
6.4.1 Primary map



X

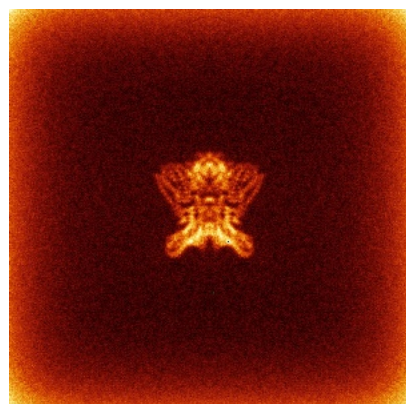


Y

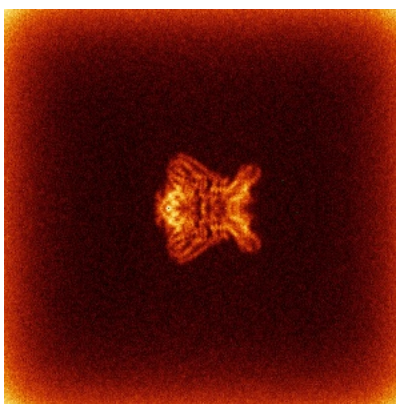


Z

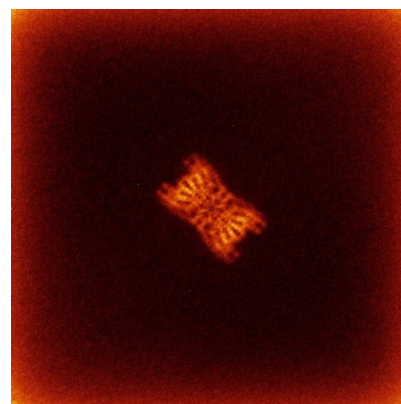
6.4.2 Raw map



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.

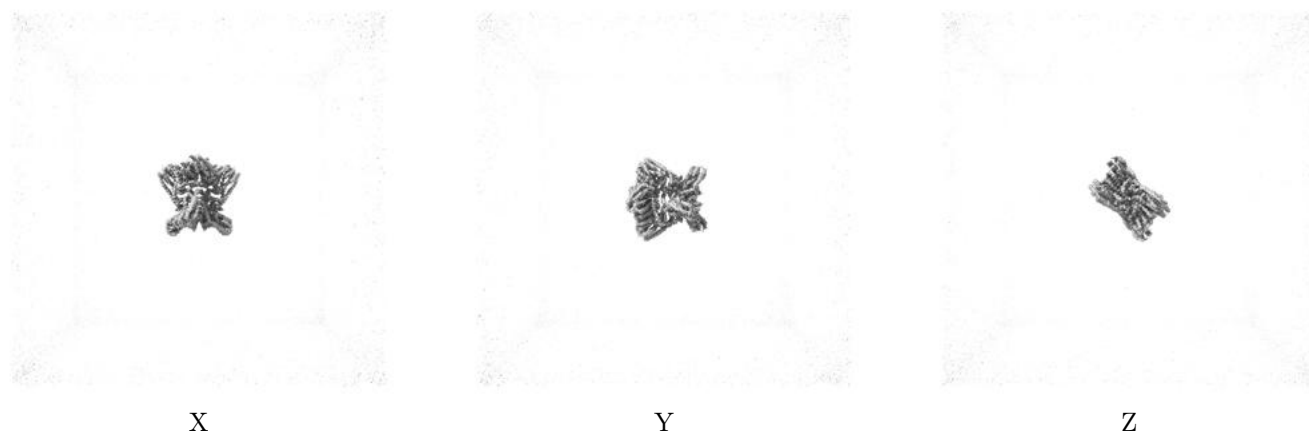
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.141. 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.

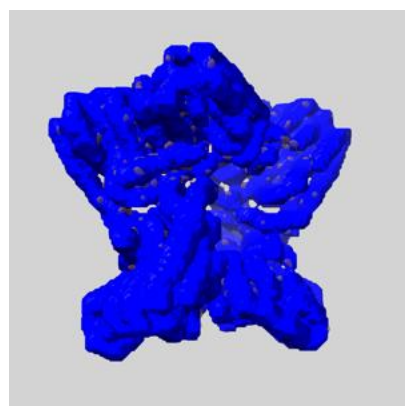
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

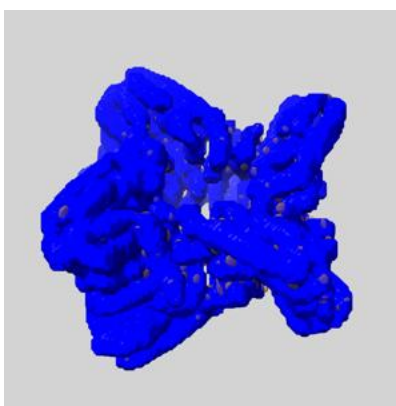
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

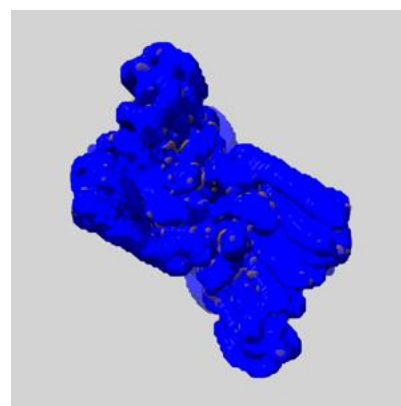
6.6.1 emd_22473_msk_1.map [i](#)



X



Y

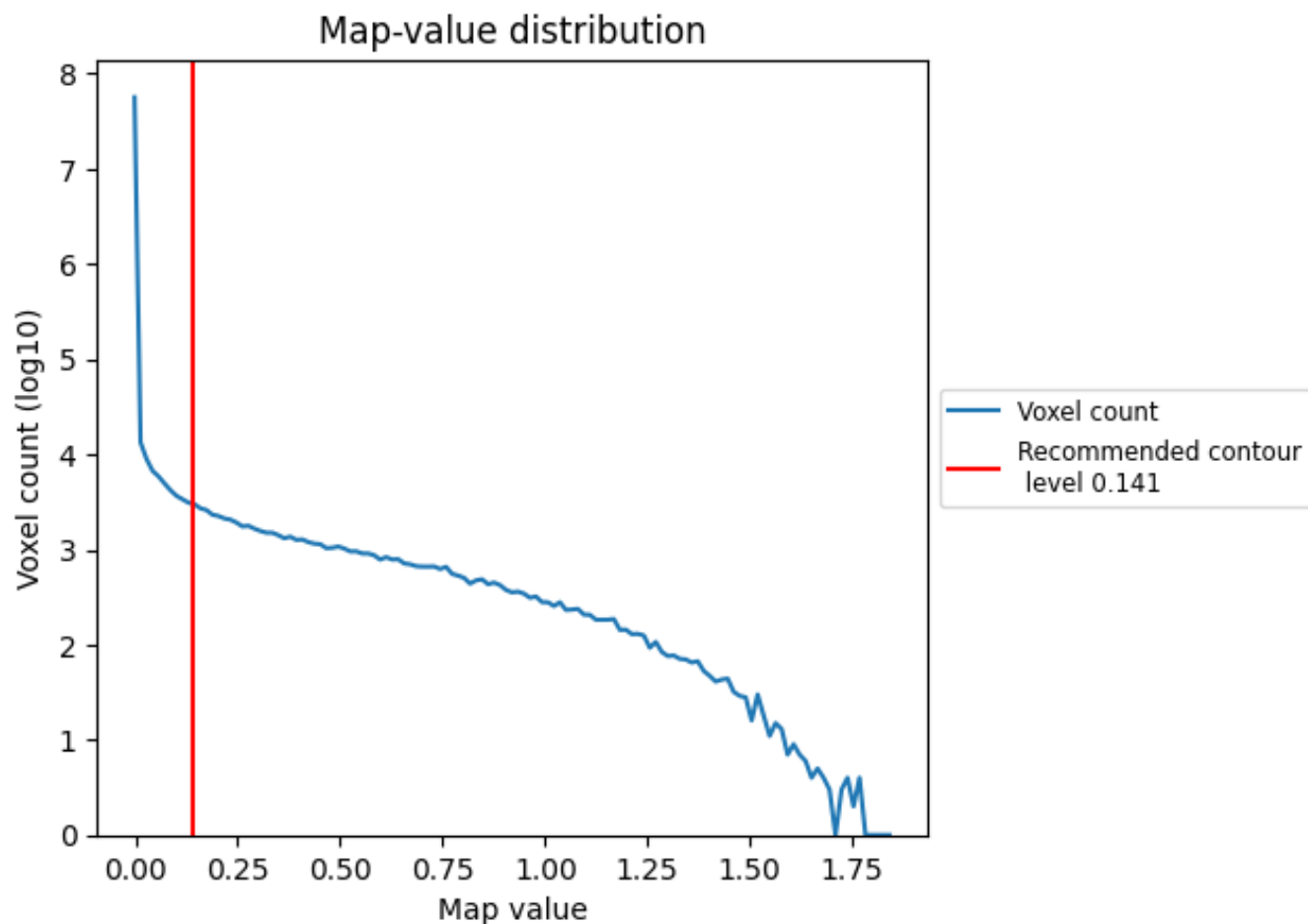


Z

7 Map analysis [i](#)

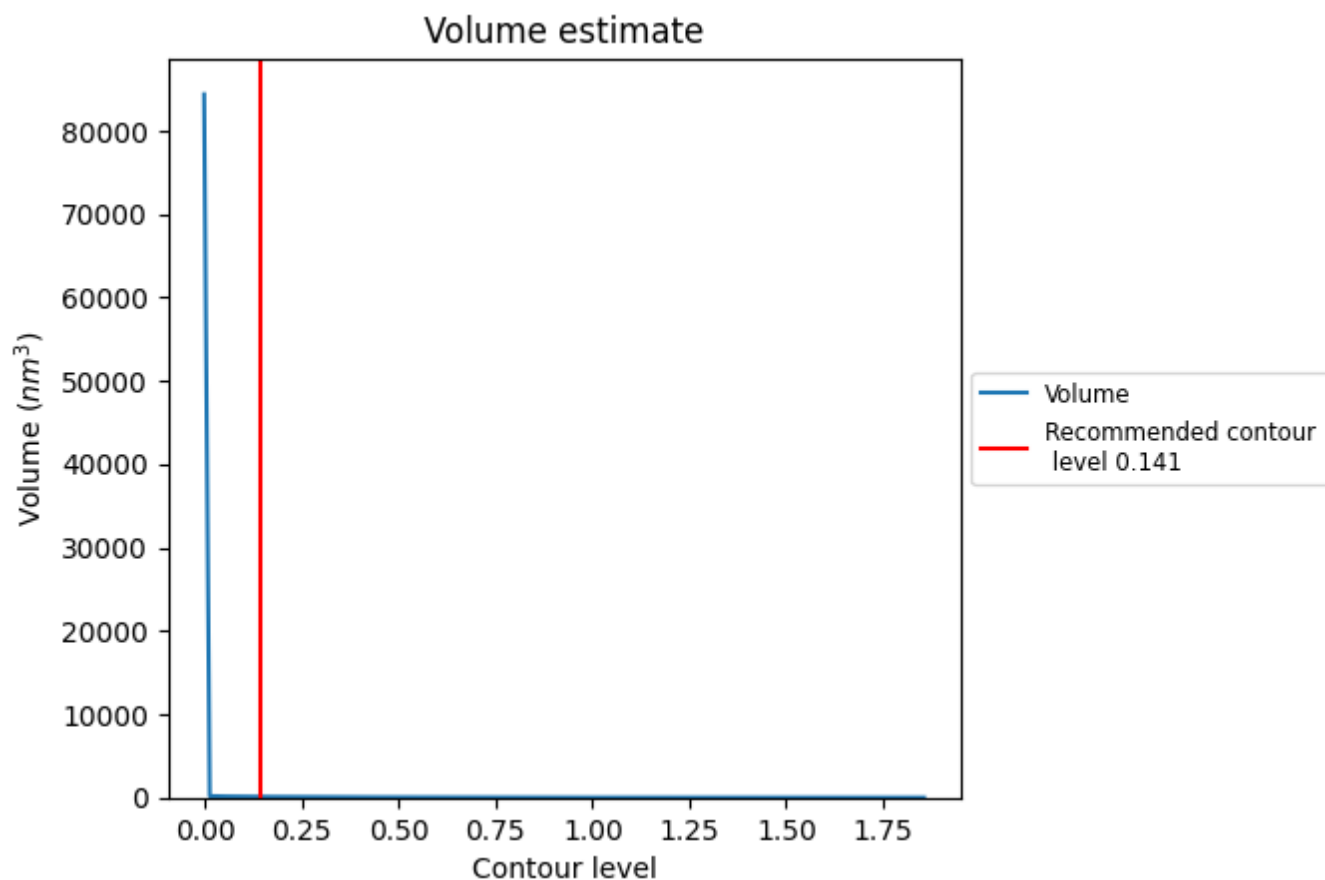
This section contains the results of statistical analysis of the map.

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.

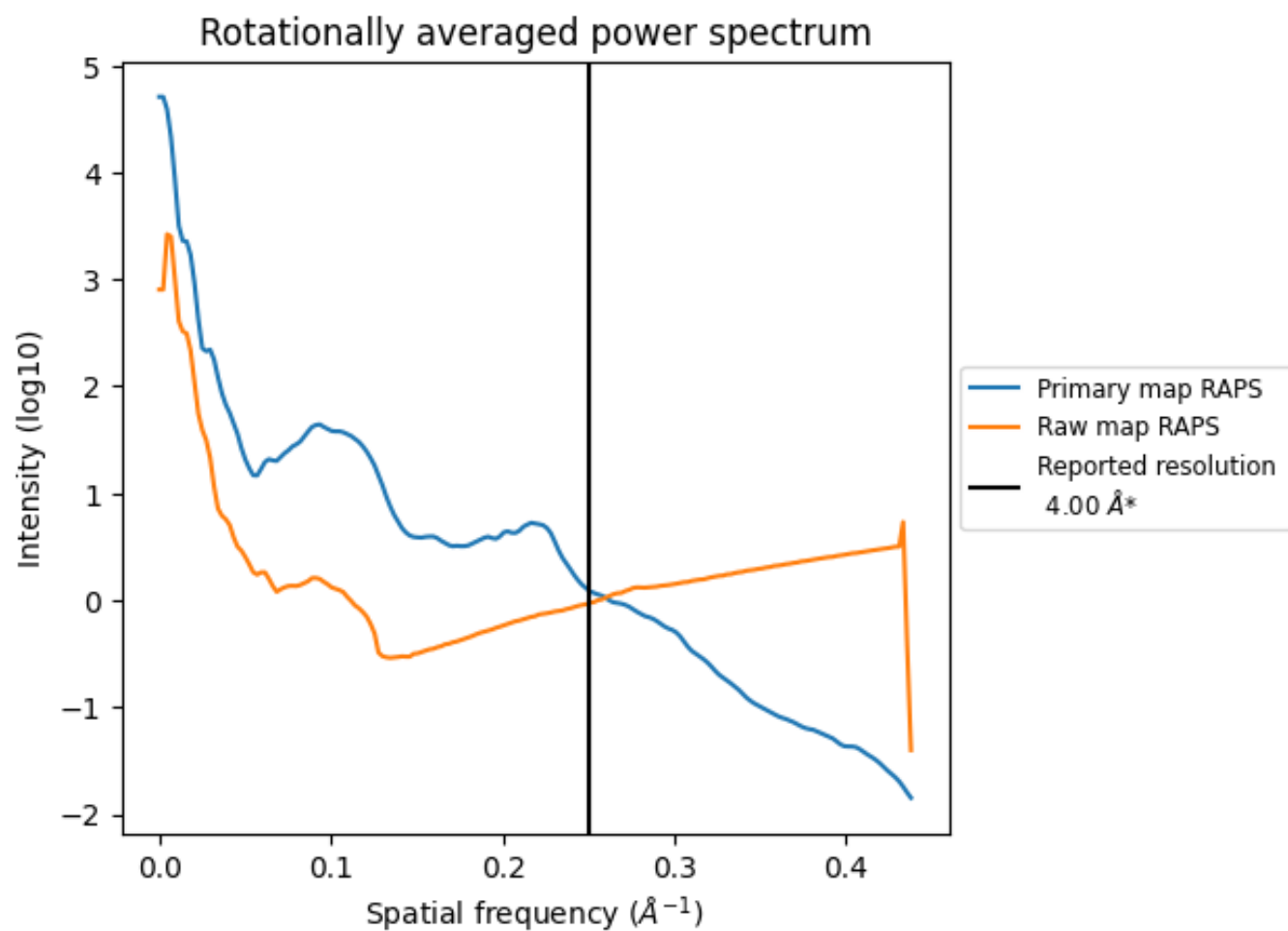
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 101 nm³; this corresponds to an approximate mass of 92 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 ⓘ

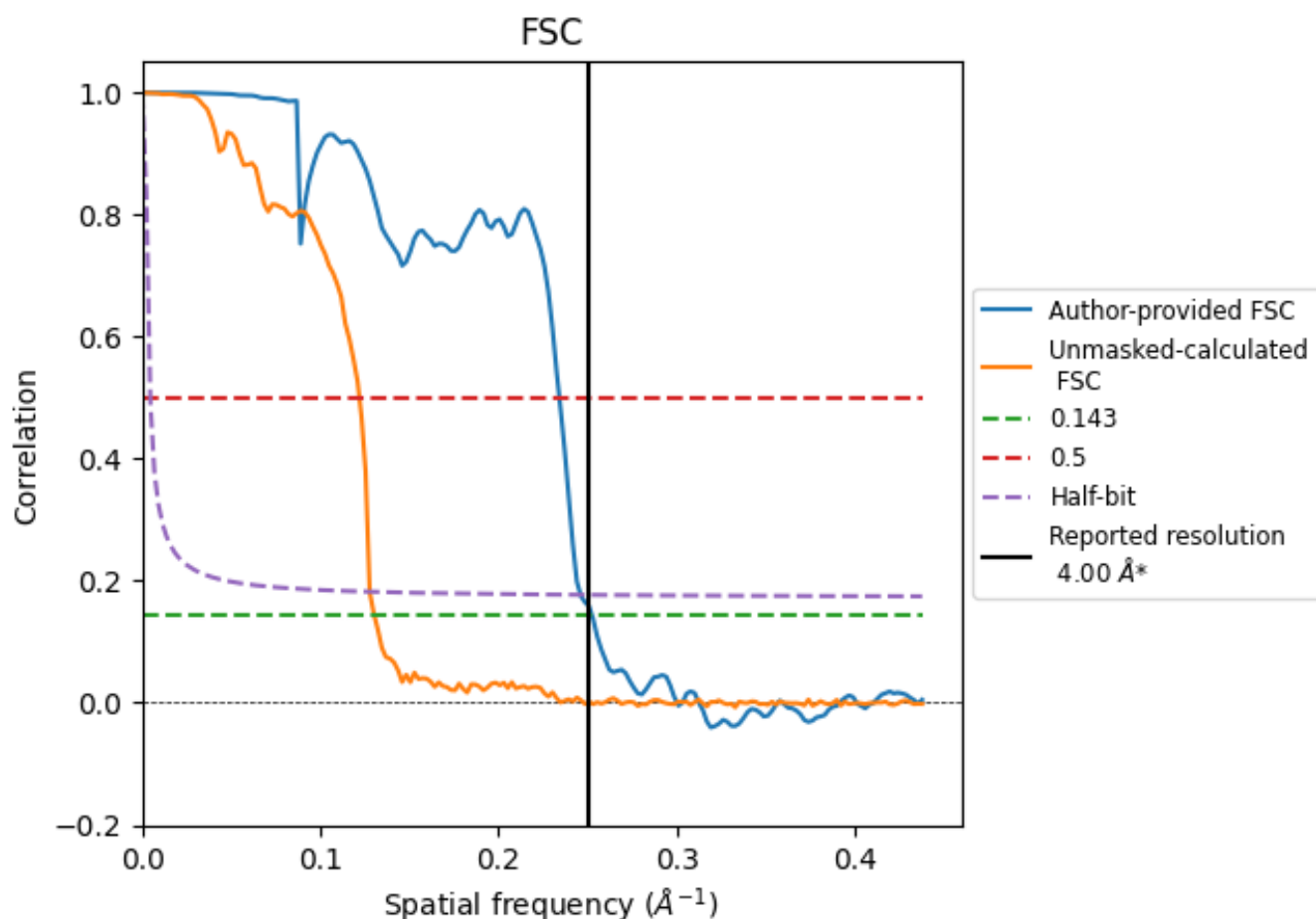


*Reported resolution corresponds to spatial frequency of $0.250 \text{ \AA}^{-1}$

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 0.250 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

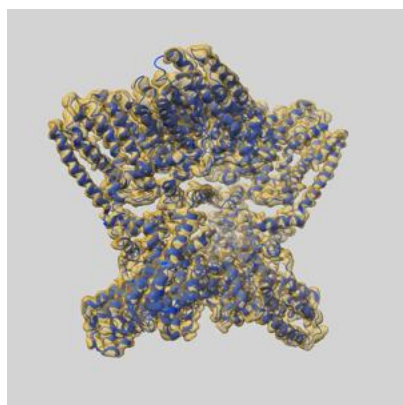
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	3.96	4.27	4.06
Unmasked-calculated*	7.67	8.20	7.83

*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 7.67 differs from the reported value 4.0 by more than 10 %

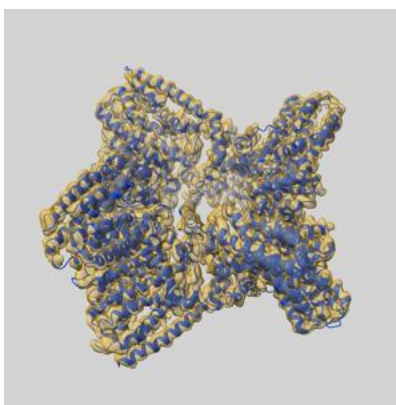
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22473 and PDB model 7JTH. Per-residue inclusion information can be found in section [3](#) on page [9](#).

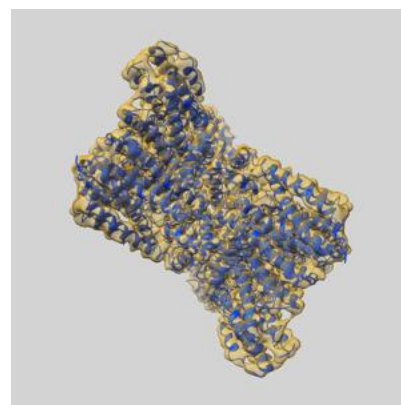
9.1 Map-model overlay [i](#)



X



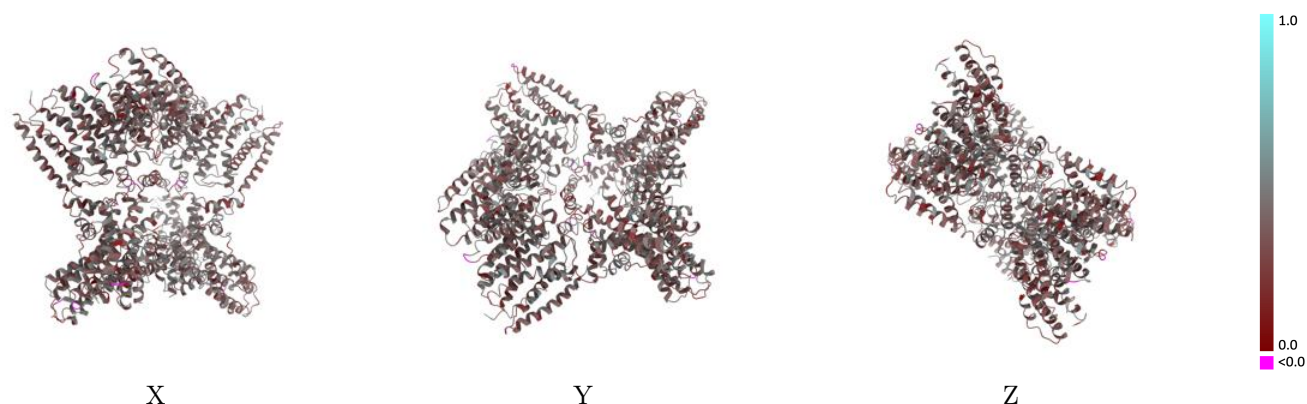
Y



Z

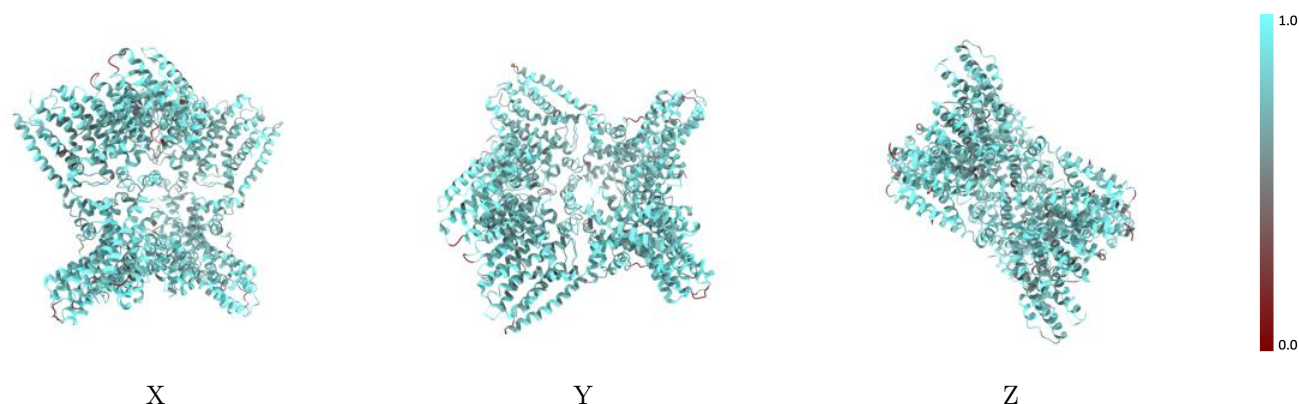
The images above show the 3D surface view of the map at the recommended contour level 0.141 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



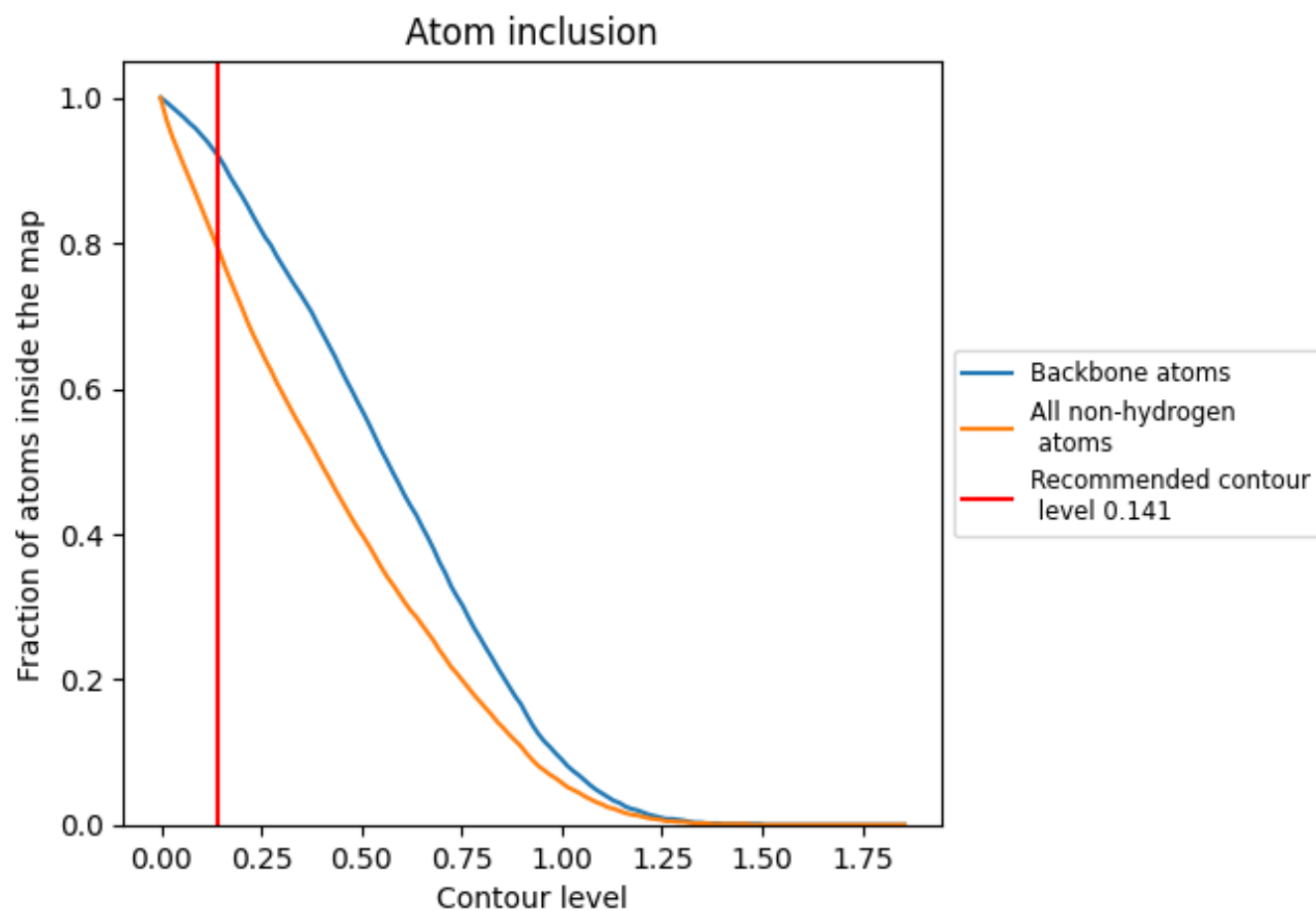
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.141).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 79% 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 (0.141) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7930	0.3690
A	0.7950	0.3640
B	0.7960	0.3680
C	0.8030	0.3830
D	0.7910	0.3690
E	0.7790	0.3630
F	0.7810	0.3620
G	0.8140	0.3800
H	0.7870	0.3620

1.0

0.0

<0.0