



wwPDB EM Validation Summary Report ⓘ

Aug 13, 2024 – 02:13 AM JST

PDB ID : 8KF1
EMDB ID : EMD-37195
Title : The cryo-EM structure of AV-45 bound type1 amyloid beta 42 fibril.
Authors : Zhao, Q.Y.; Tao, Y.Q.; Liu, C.; Li, D.
Deposited on : 2023-08-15
Resolution : 3.30 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.dev92
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

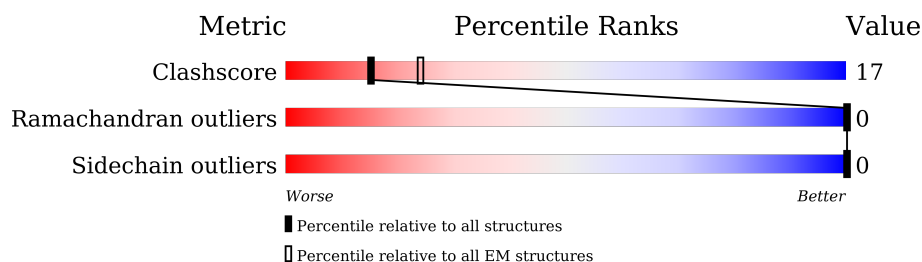
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

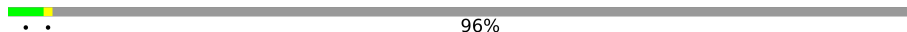
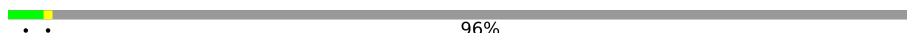
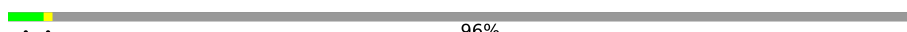
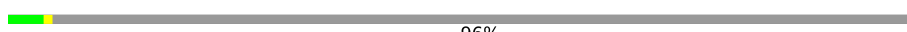
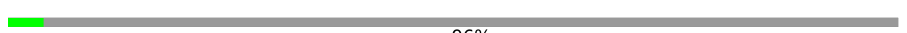



The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



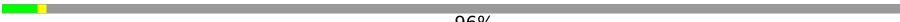

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	770	 96%
1	B	770	 96%
1	C	770	 96%
1	D	770	 96%
1	E	770	 96%
1	F	770	 96%
1	G	770	 96%
1	H	770	 96%

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Mol	Chain	Length	Quality of chain
1	I	770	 96%
1	J	770	 96%
1	K	770	 96%
1	L	770	 96%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3052 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 P3(40).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	34	Total	C	N	O	S	0	0
			250	163	42	44	1		
1	F	34	Total	C	N	O	S	0	0
			250	163	42	44	1		
1	H	34	Total	C	N	O	S	0	0
			250	163	42	44	1		
1	A	34	Total	C	N	O	S	0	0
			250	163	42	44	1		
1	I	34	Total	C	N	O	S	0	0
			250	163	42	44	1		
1	B	34	Total	C	N	O	S	0	0
			250	163	42	44	1		
1	J	34	Total	C	N	O	S	0	0
			250	163	42	44	1		
1	C	34	Total	C	N	O	S	0	0
			250	163	42	44	1		
1	K	34	Total	C	N	O	S	0	0
			250	163	42	44	1		
1	D	34	Total	C	N	O	S	0	0
			250	163	42	44	1		
1	L	34	Total	C	N	O	S	0	0
			250	163	42	44	1		
1	E	34	Total	C	N	O	S	0	0
			250	163	42	44	1		

- Molecule 2 is 4-[2-[6-[2-[2-(2-fluoranyloxy)ethoxy]ethoxy]pyridin-3-yl]ethyl]- {N}-methyl-aniline (three-letter code: VW6) (formula: C₂₀H₂₇FN₂O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	F	1	Total 26	C 20	F 1	N 2	O 3	0
2	J	1	Total 26	C 20	F 1	N 2	O 3	0

96%

- Molecule 1: P3(40)

96%

[illegible]

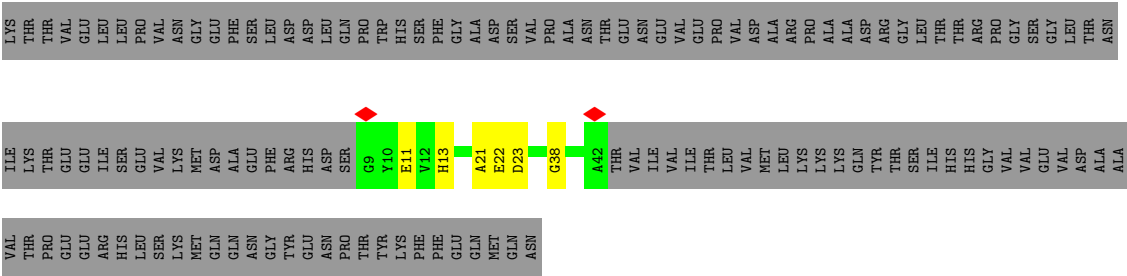
[illegible]

Chain A: 96%

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

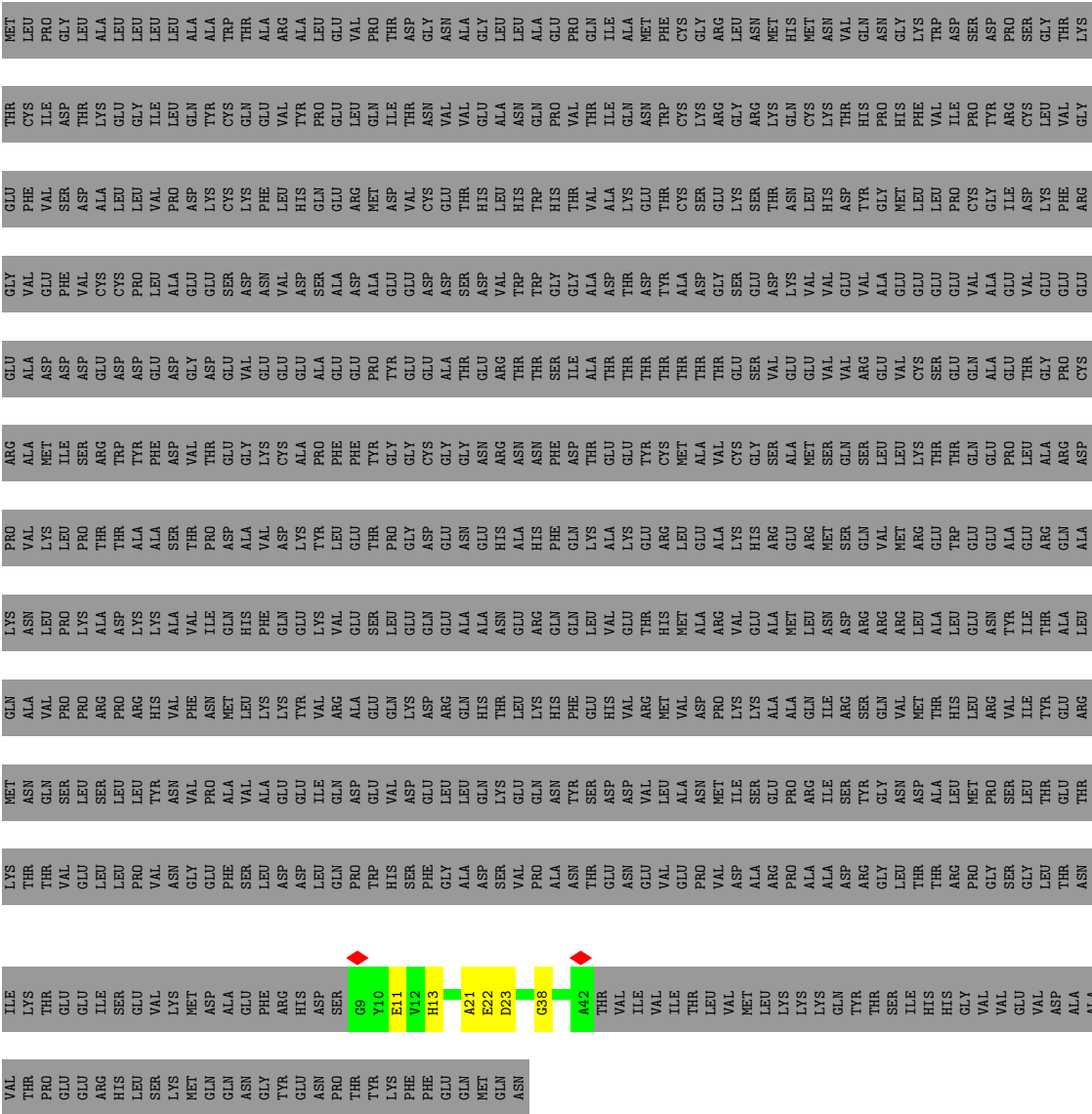






● Molecule 1: P3(40)

Chain K: 96%



● Molecule 1: P3(40)

Chain D: 96%

VAL	THR	PRO	GLU	GLU	ARG	HIS	LEU	SER	VAL	LYS	MET	GLN	ASN	GLY	THR	GLU	ASN	PRO	THR	TYR	LYS	PHE	PHE	GLU	GLN	MET	GLN	ASN																										
ILE	LYS	THR	GLU	GLU	ILE	SER	GLU	VAL	LYS	MET	ASP	ALA	GLU	PHE	ARG	HIS	ASP	SER	G9	Y10	E11	V12	H13	A21	E22	D23	G38	A42	THR	VAL	ILE	VAL	ILE	THR	LEU	VAL	MET	LYS	LYS	GLN	TYR	THR	SER	ILE	HIS	HIS	GLY	VAL	VAL	GLU	VAL	ASP	ALA	ALA

Chain L: 1% 96%

[illegible]

● Molecule 1: P3(40)

Chain E: ● ■

Chain E: 96%

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



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=178.54°, rise=2.396 Å, axial sym=C1	Depositor
Number of segments used	11034	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	55	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.033	Depositor
Minimum map value	-0.020	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0054	Depositor
Map size (Å)	239.04, 239.04, 239.04	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	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: VW6

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	0.39	0/254	0.48	0/341
1	B	0.39	0/254	0.48	0/341
1	C	0.39	0/254	0.48	0/341
1	D	0.39	0/254	0.47	0/341
1	E	0.39	0/254	0.47	0/341
1	F	0.39	0/254	0.47	0/341
1	G	0.39	0/254	0.48	0/341
1	H	0.39	0/254	0.47	0/341
1	I	0.39	0/254	0.47	0/341
1	J	0.39	0/254	0.47	0/341
1	K	0.39	0/254	0.48	0/341
1	L	0.39	0/254	0.48	0/341
All	All	0.39	0/3048	0.48	0/4092

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	250	0	252	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	250	0	252	19	0
1	C	250	0	252	18	0
1	D	250	0	252	10	0
1	E	250	0	252	11	0
1	F	250	0	252	18	0
1	G	250	0	252	17	0
1	H	250	0	252	17	0
1	I	250	0	252	19	0
1	J	250	0	252	18	0
1	K	250	0	252	10	0
1	L	250	0	252	11	0
2	F	26	0	0	3	0
2	J	26	0	0	2	0
All	All	3052	0	3024	101	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 17.

The worst 5 of 101 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:21:ALA:O	1:E:22:GLU:HG2	1.37	1.25
1:I:21:ALA:O	1:L:22:GLU:HG2	1.33	1.24
1:G:21:ALA:O	1:H:22:GLU:HG2	1.40	1.21
1:F:22:GLU:HG2	1:C:21:ALA:O	1.38	1.20
1:H:21:ALA:O	1:I:22:GLU:HG2	1.39	1.20

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	32/770 (4%)	31 (97%)	1 (3%)	0	100	100
1	B	32/770 (4%)	31 (97%)	1 (3%)	0	100	100
1	C	32/770 (4%)	31 (97%)	1 (3%)	0	100	100
1	D	32/770 (4%)	31 (97%)	1 (3%)	0	100	100
1	E	32/770 (4%)	31 (97%)	1 (3%)	0	100	100
1	F	32/770 (4%)	31 (97%)	1 (3%)	0	100	100
1	G	32/770 (4%)	31 (97%)	1 (3%)	0	100	100
1	H	32/770 (4%)	31 (97%)	1 (3%)	0	100	100
1	I	32/770 (4%)	31 (97%)	1 (3%)	0	100	100
1	J	32/770 (4%)	31 (97%)	1 (3%)	0	100	100
1	K	32/770 (4%)	31 (97%)	1 (3%)	0	100	100
1	L	32/770 (4%)	31 (97%)	1 (3%)	0	100	100
All	All	384/9240 (4%)	372 (97%)	12 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	25/669 (4%)	25 (100%)	0	100	100
1	B	25/669 (4%)	25 (100%)	0	100	100
1	C	25/669 (4%)	25 (100%)	0	100	100
1	D	25/669 (4%)	25 (100%)	0	100	100
1	E	25/669 (4%)	25 (100%)	0	100	100
1	F	25/669 (4%)	25 (100%)	0	100	100
1	G	25/669 (4%)	25 (100%)	0	100	100
1	H	25/669 (4%)	25 (100%)	0	100	100
1	I	25/669 (4%)	25 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	25/669 (4%)	25 (100%)	0	100	100
1	K	25/669 (4%)	25 (100%)	0	100	100
1	L	25/669 (4%)	25 (100%)	0	100	100
All	All	300/8028 (4%)	300 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 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
2	VW6	J	101	-	27,27,27	1.65	4 (14%)	32,32,32	1.64	4 (12%)
2	VW6	F	101	-	27,27,27	1.64	4 (14%)	32,32,32	1.64	4 (12%)

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	VW6	J	101	-	-	9/17/17/17	0/2/2/2
2	VW6	F	101	-	-	9/17/17/17	0/2/2/2

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	101	VW6	C03-N02	5.18	1.47	1.37
2	F	101	VW6	C03-N02	5.13	1.46	1.37
2	J	101	VW6	C21-C20	3.90	1.54	1.49
2	F	101	VW6	C21-C20	3.86	1.54	1.49
2	J	101	VW6	O13-C12	2.98	1.42	1.36

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	101	VW6	C24-N23-C12	7.06	122.83	116.63
2	J	101	VW6	C24-N23-C12	7.05	122.83	116.63
2	F	101	VW6	C11-C12-N23	-3.16	120.15	124.87
2	J	101	VW6	C11-C12-N23	-3.16	120.15	124.87
2	F	101	VW6	C09-C24-N23	-2.62	119.83	123.95

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

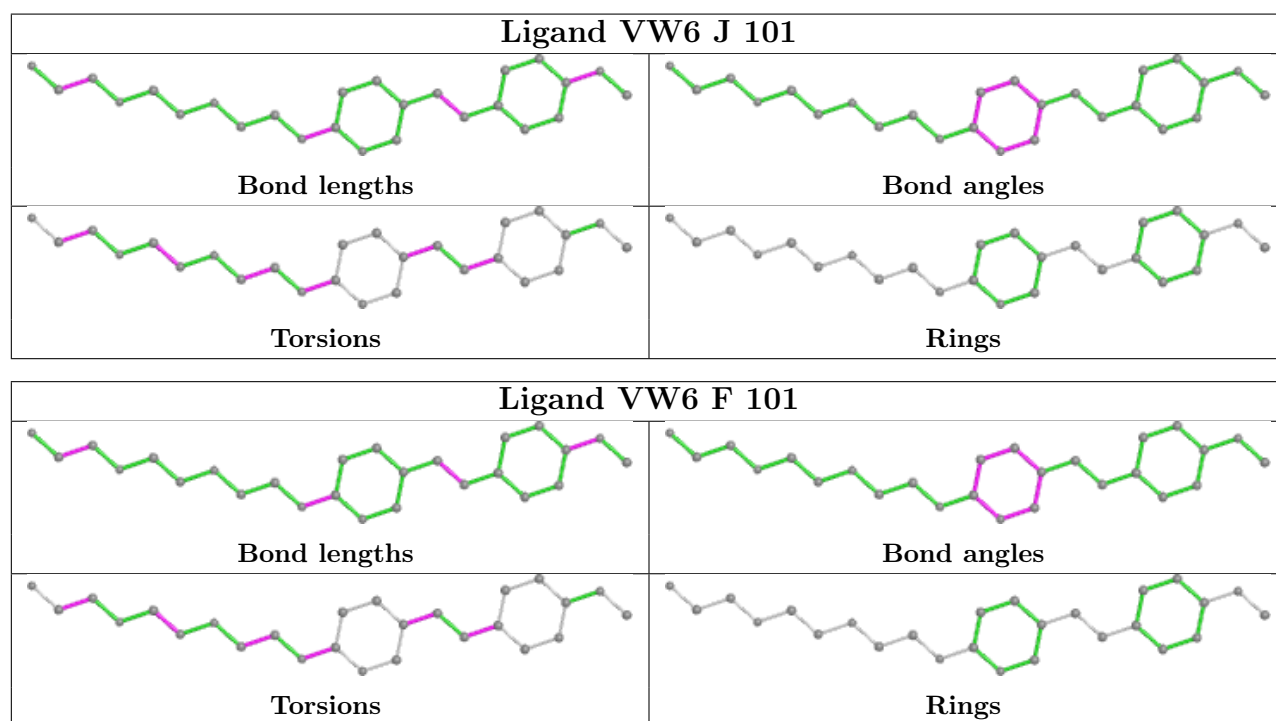
Mol	Chain	Res	Type	Atoms
2	F	101	VW6	O13-C14-C15-O16
2	J	101	VW6	O13-C14-C15-O16
2	J	101	VW6	O16-C17-C18-O19
2	F	101	VW6	O16-C17-C18-O19
2	F	101	VW6	O19-C20-C21-F22

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	101	VW6	2	0
2	F	101	VW6	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.

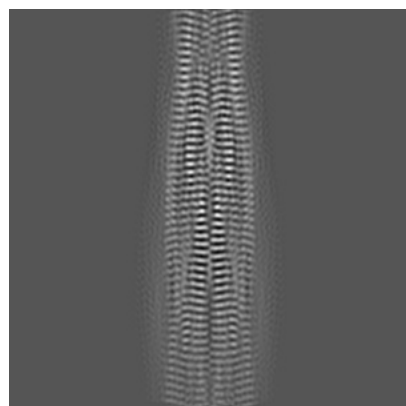
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37195. These allow visual inspection of the internal detail of the map and identification of artifacts.

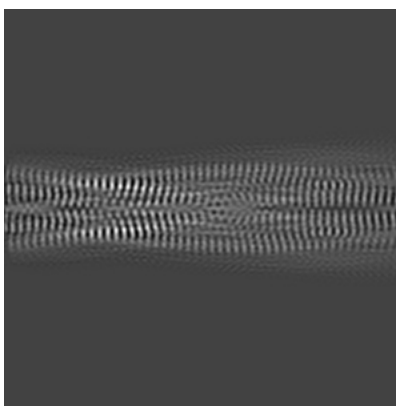
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

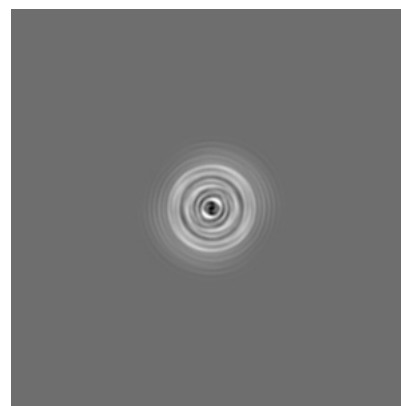
6.1.1 Primary map



X

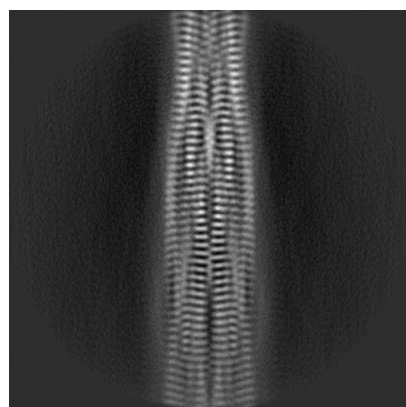


Y

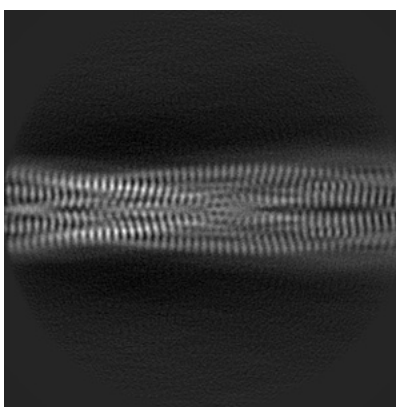


Z

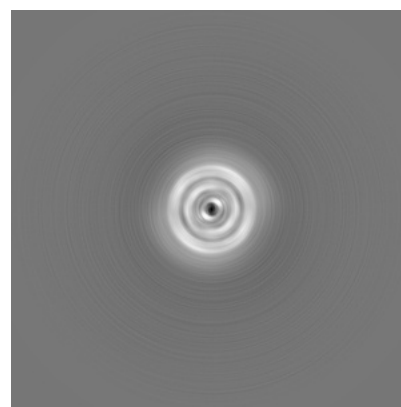
6.1.2 Raw map



X



Y

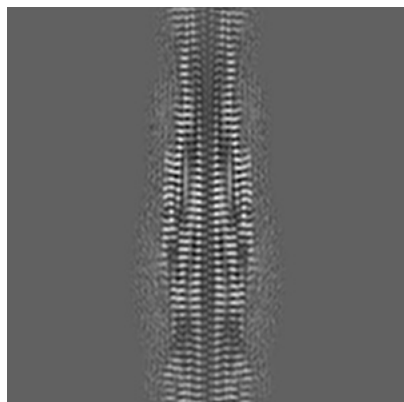


Z

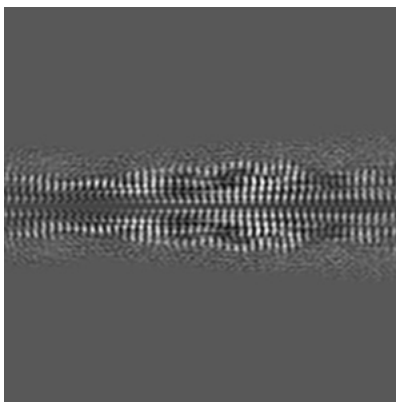
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

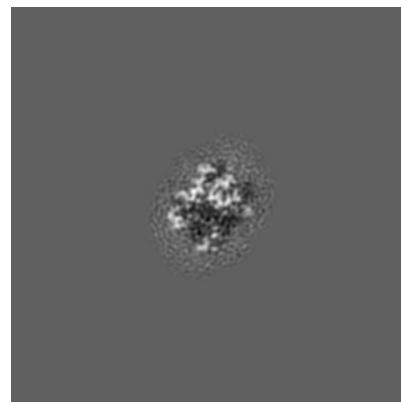
6.2.1 Primary map



X Index: 144

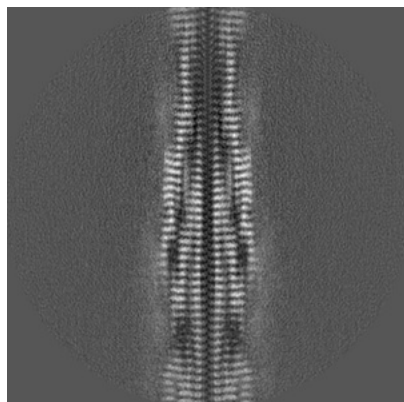


Y Index: 144

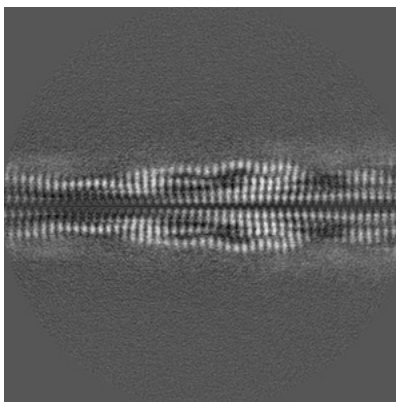


Z Index: 144

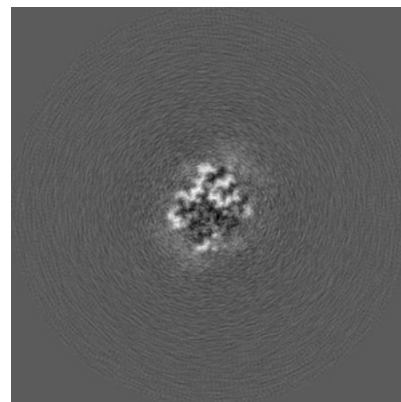
6.2.2 Raw map



X Index: 144



Y Index: 144

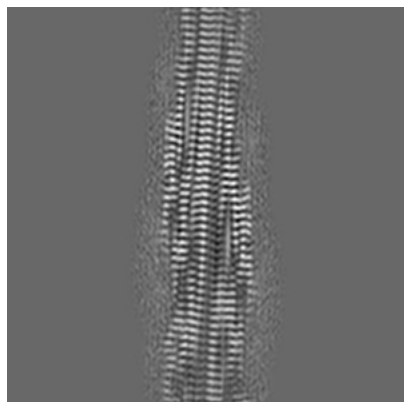


Z Index: 144

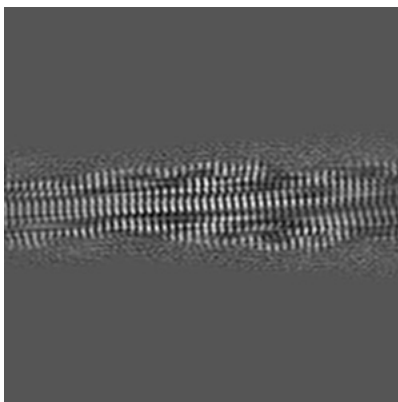
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

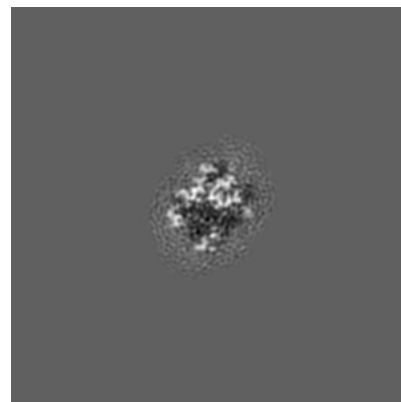
6.3.1 Primary map



X Index: 138

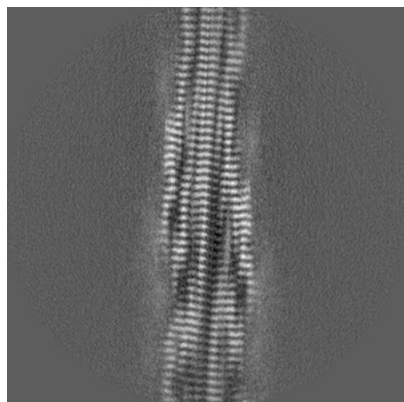


Y Index: 150

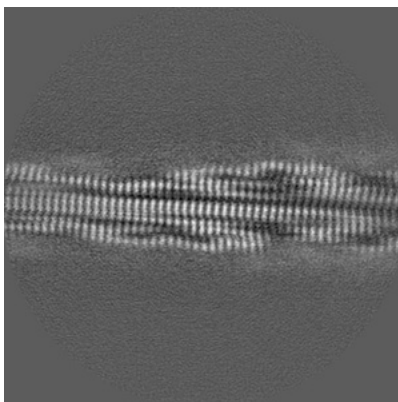


Z Index: 150

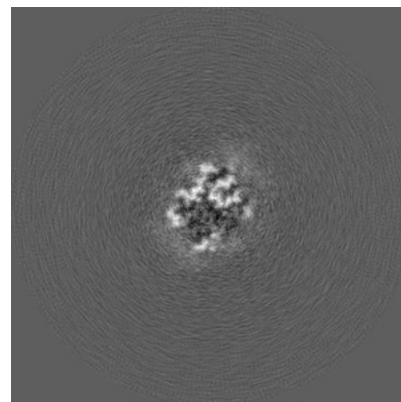
6.3.2 Raw map



X Index: 138



Y Index: 138

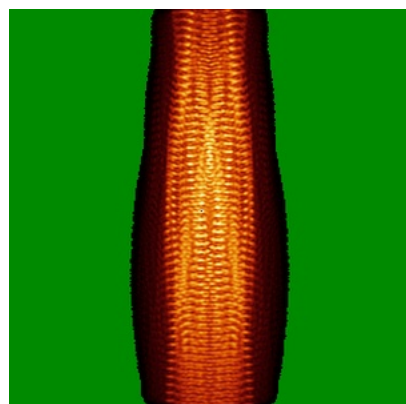


Z Index: 150

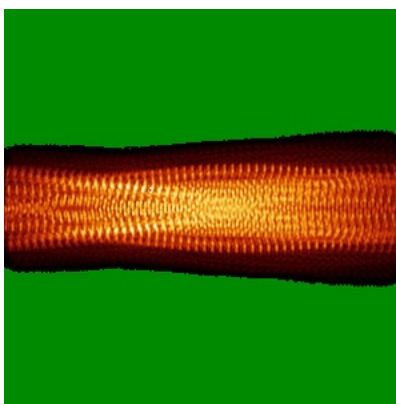
The images above show the largest variance slices of the map in three orthogonal directions.

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

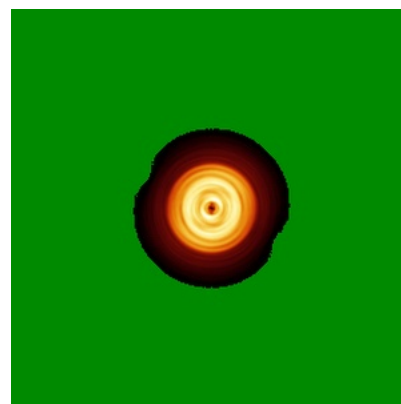
6.4.1 Primary map



X

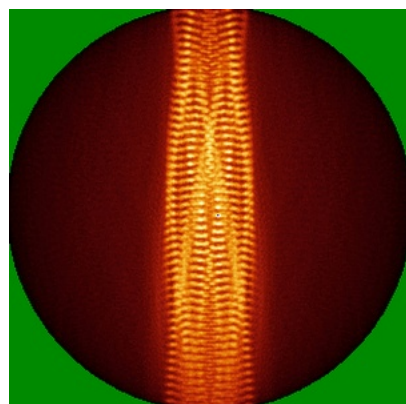


Y

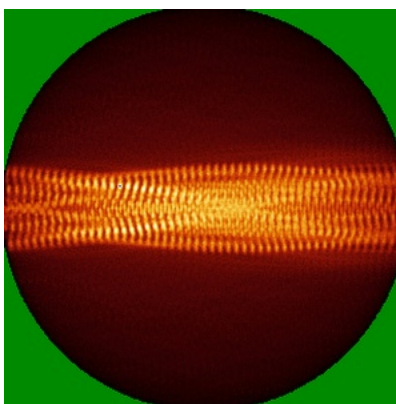


Z

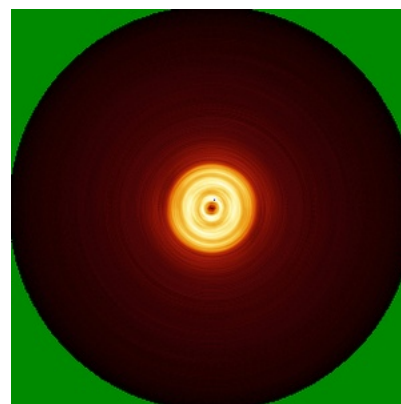
6.4.2 Raw map



X



Y

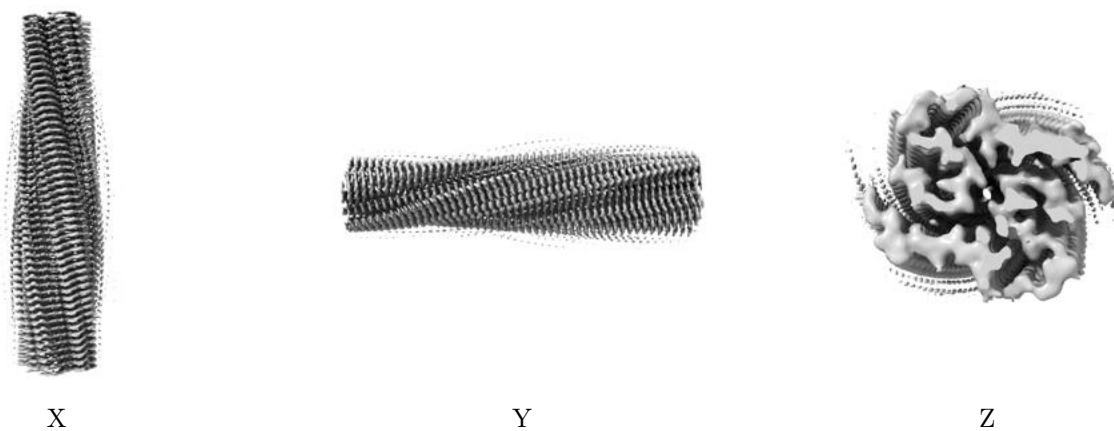


Z

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.

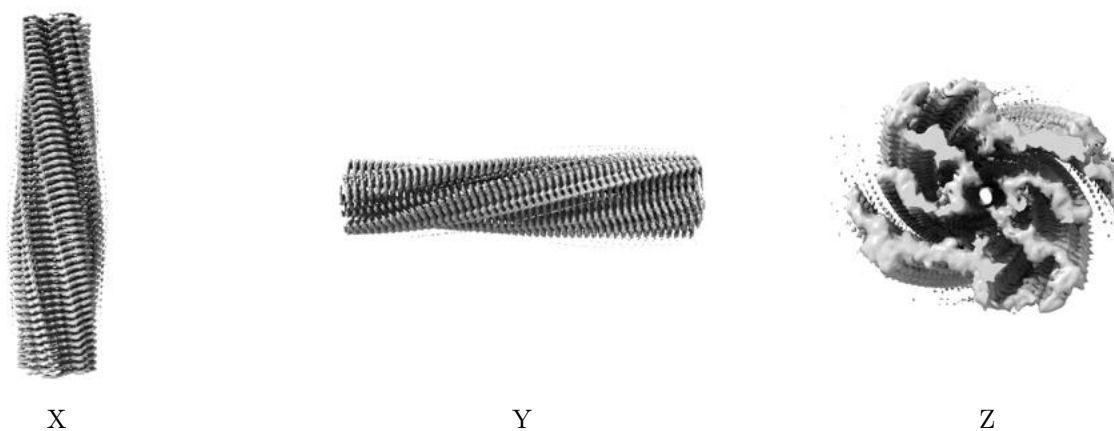
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0054. 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.

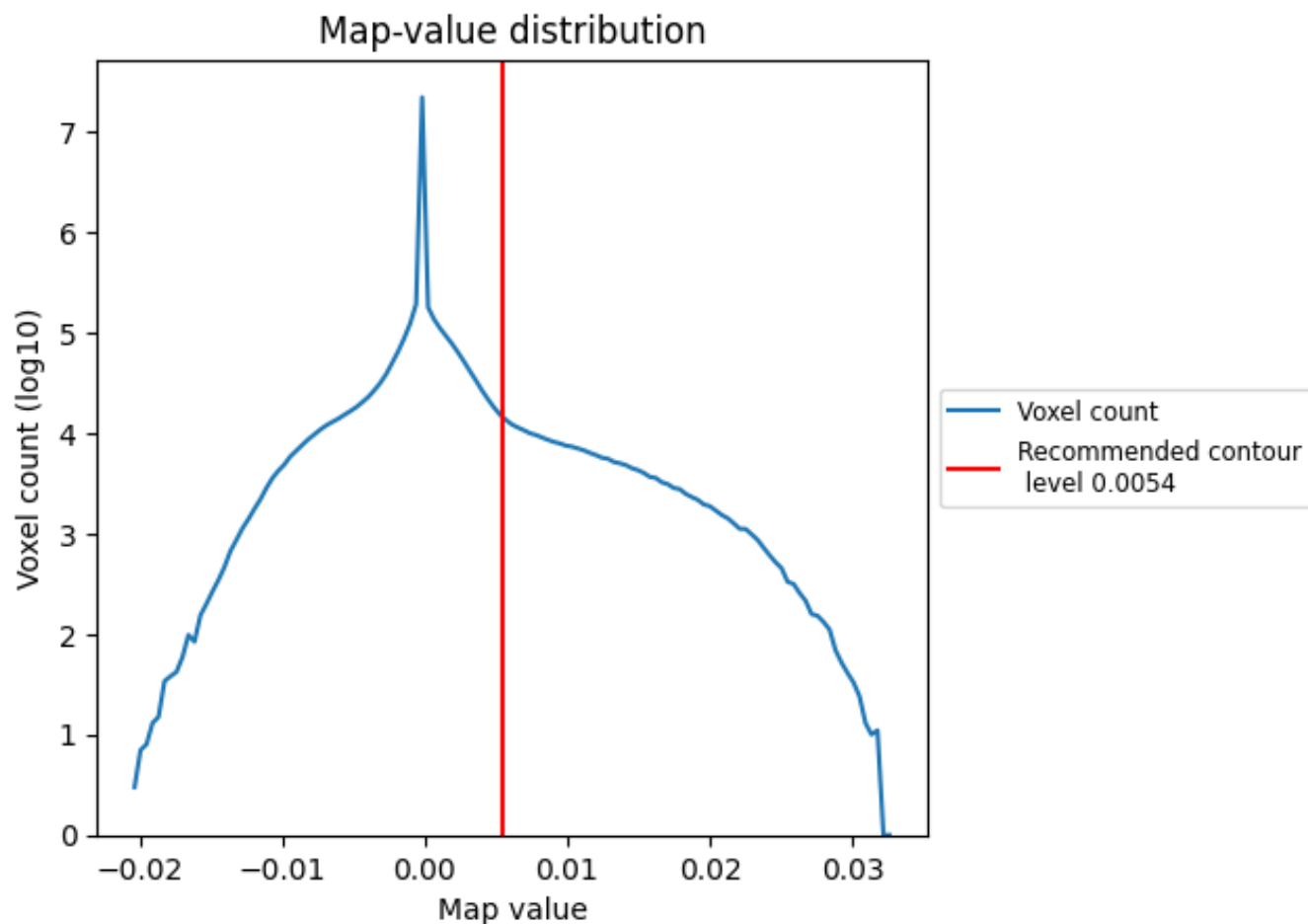
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

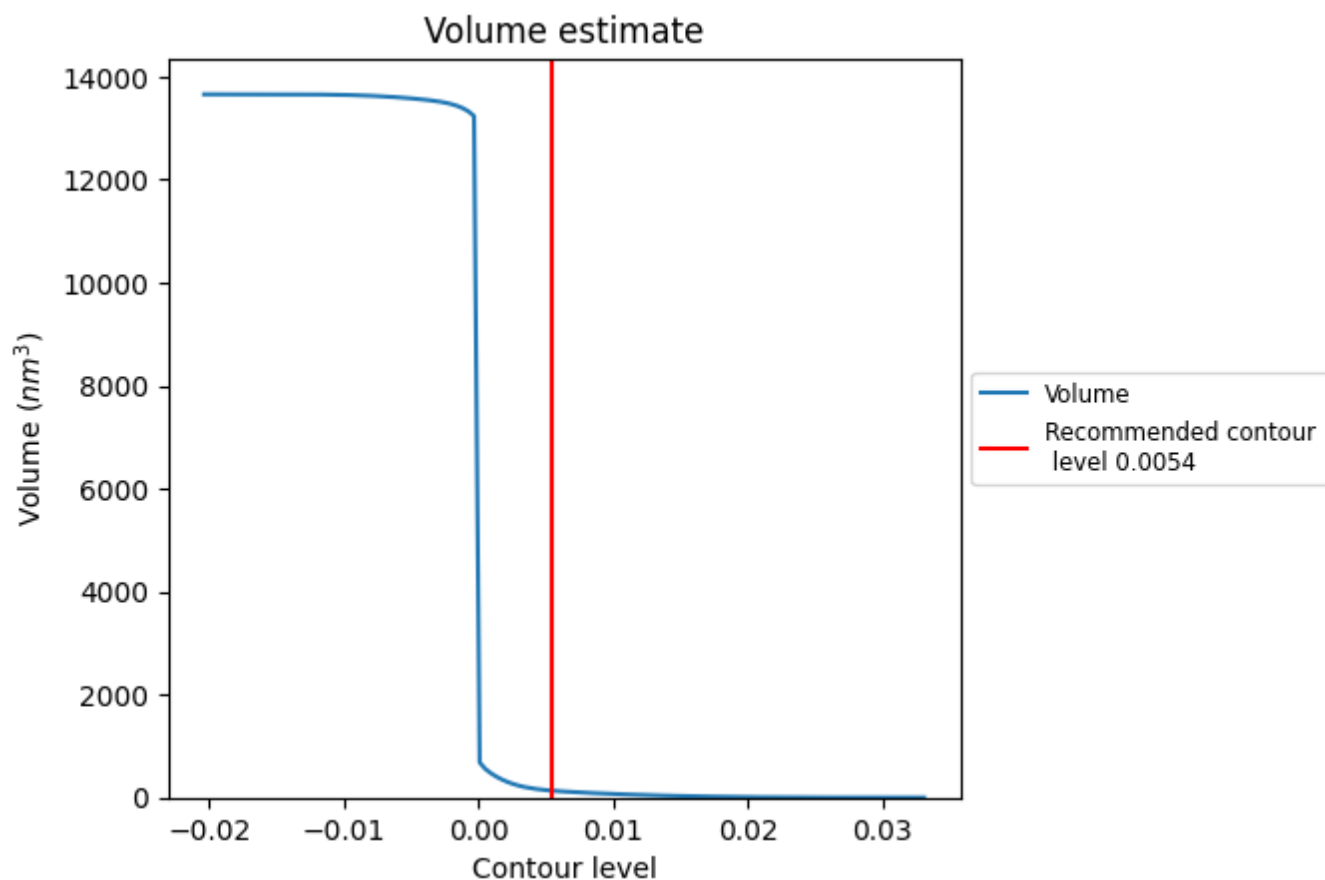
This section contains the results of statistical analysis of the map.

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.

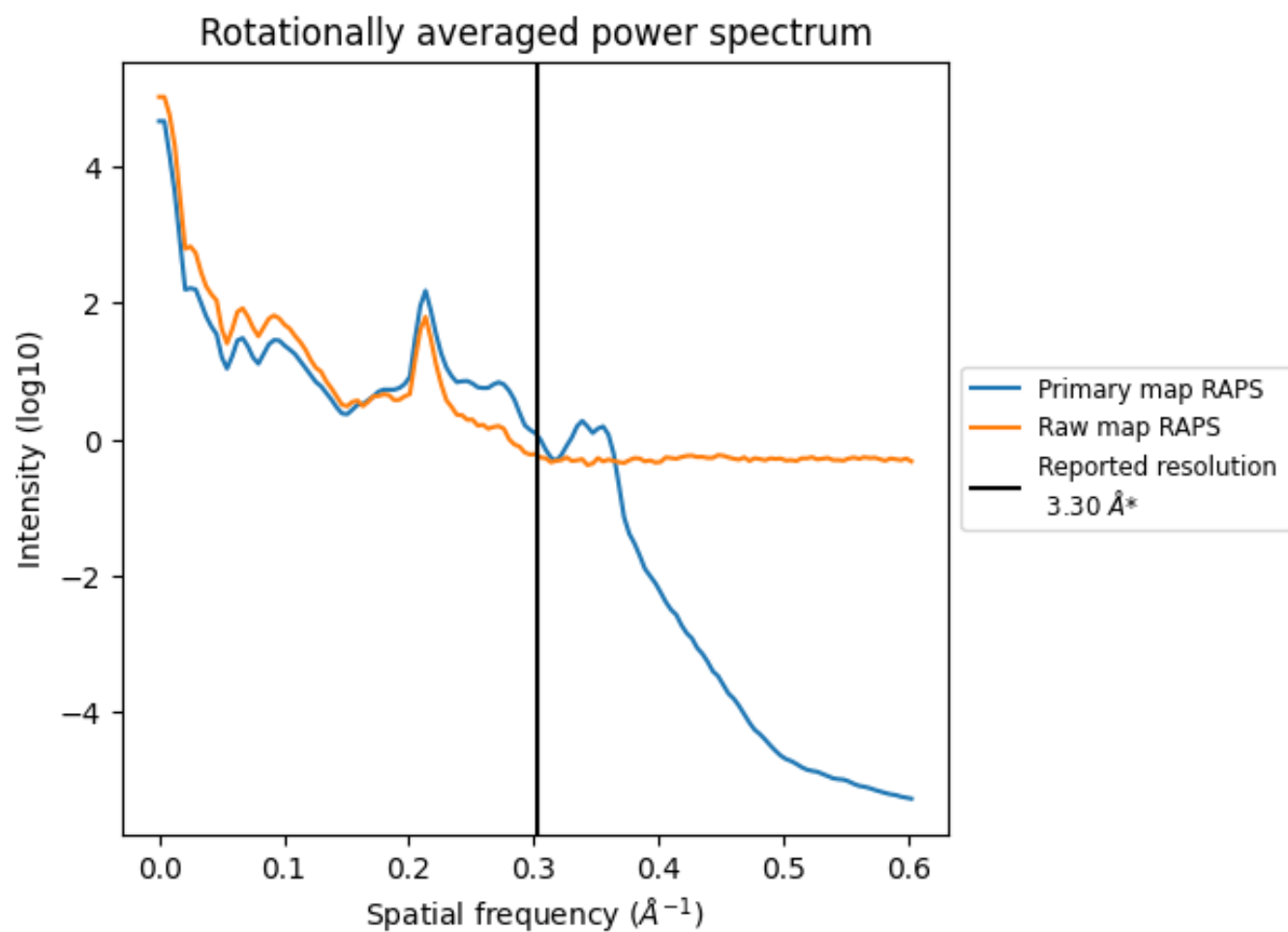
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 135 nm³; this corresponds to an approximate mass of 122 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 ⓘ

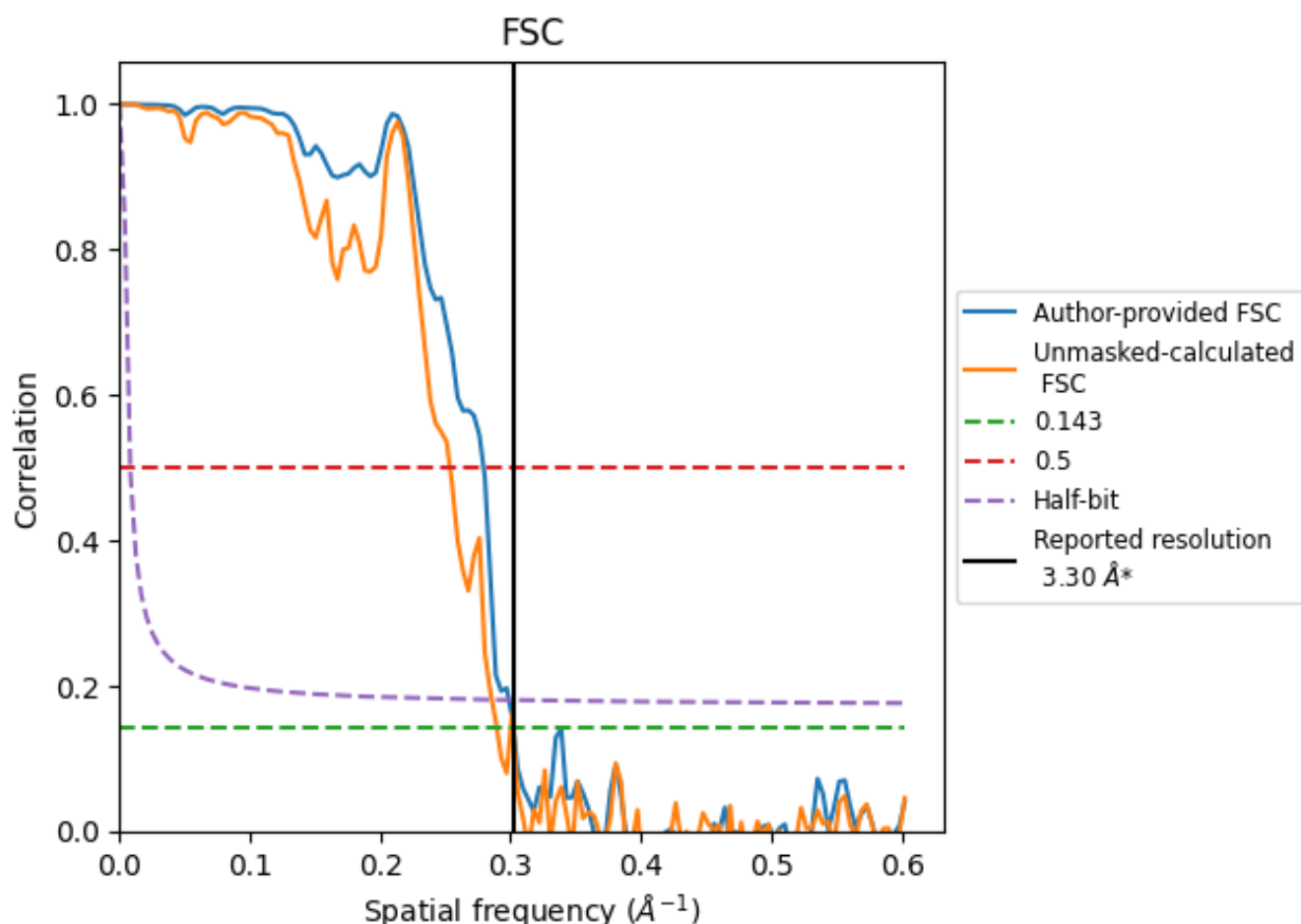


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

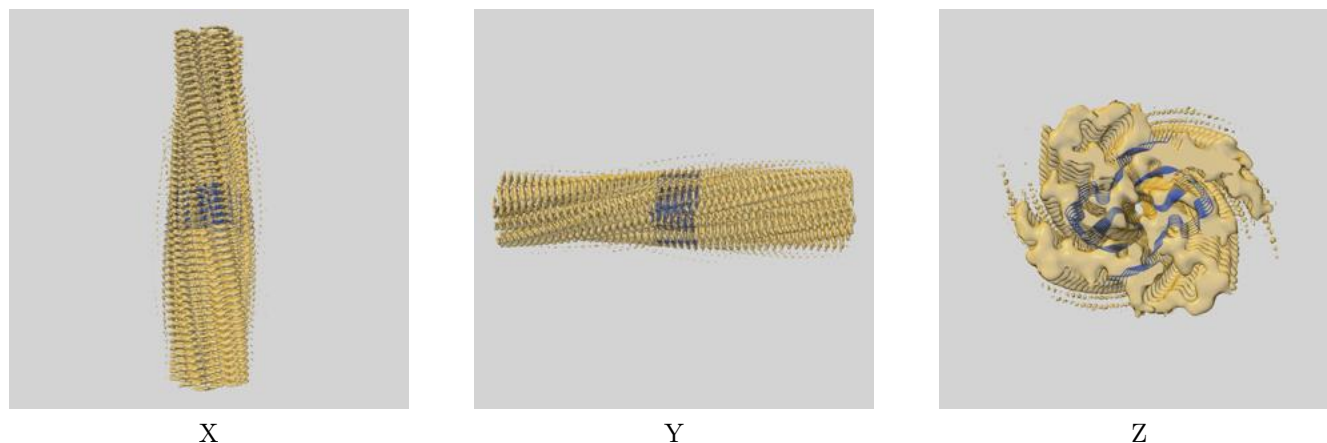
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.31	3.58	3.35
Unmasked-calculated*	3.46	3.94	3.50

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

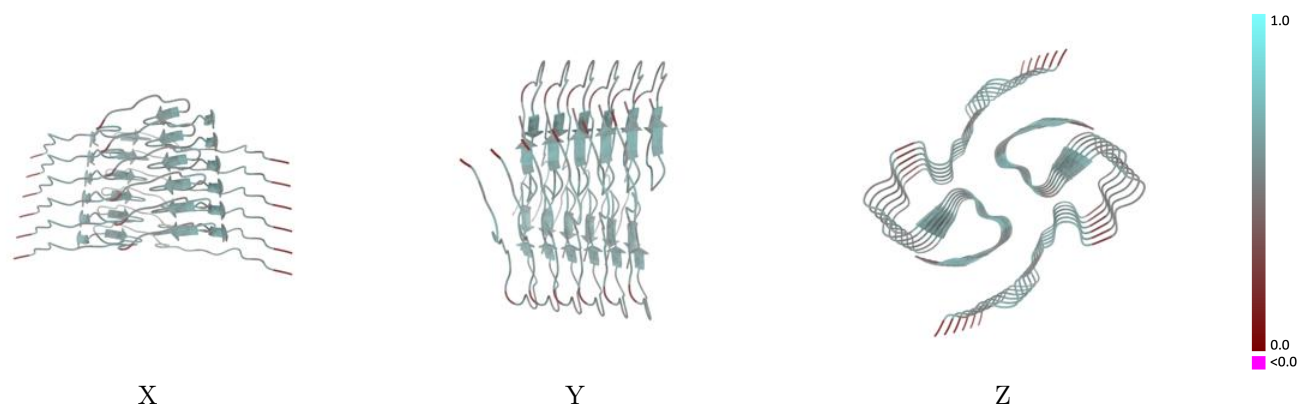
This section contains information regarding the fit between EMDB map EMD-37195 and PDB model 8KF1. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



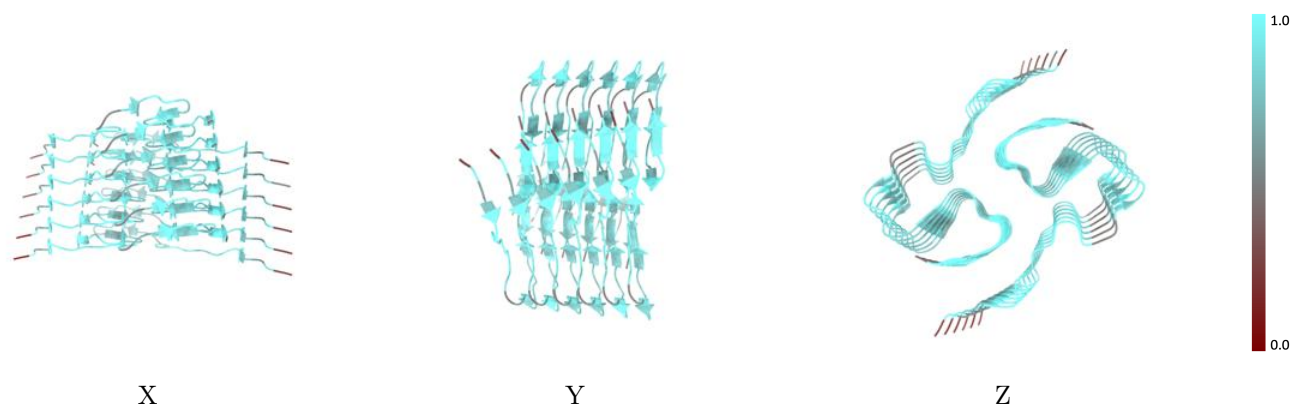
The images above show the 3D surface view of the map at the recommended contour level 0.0054 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



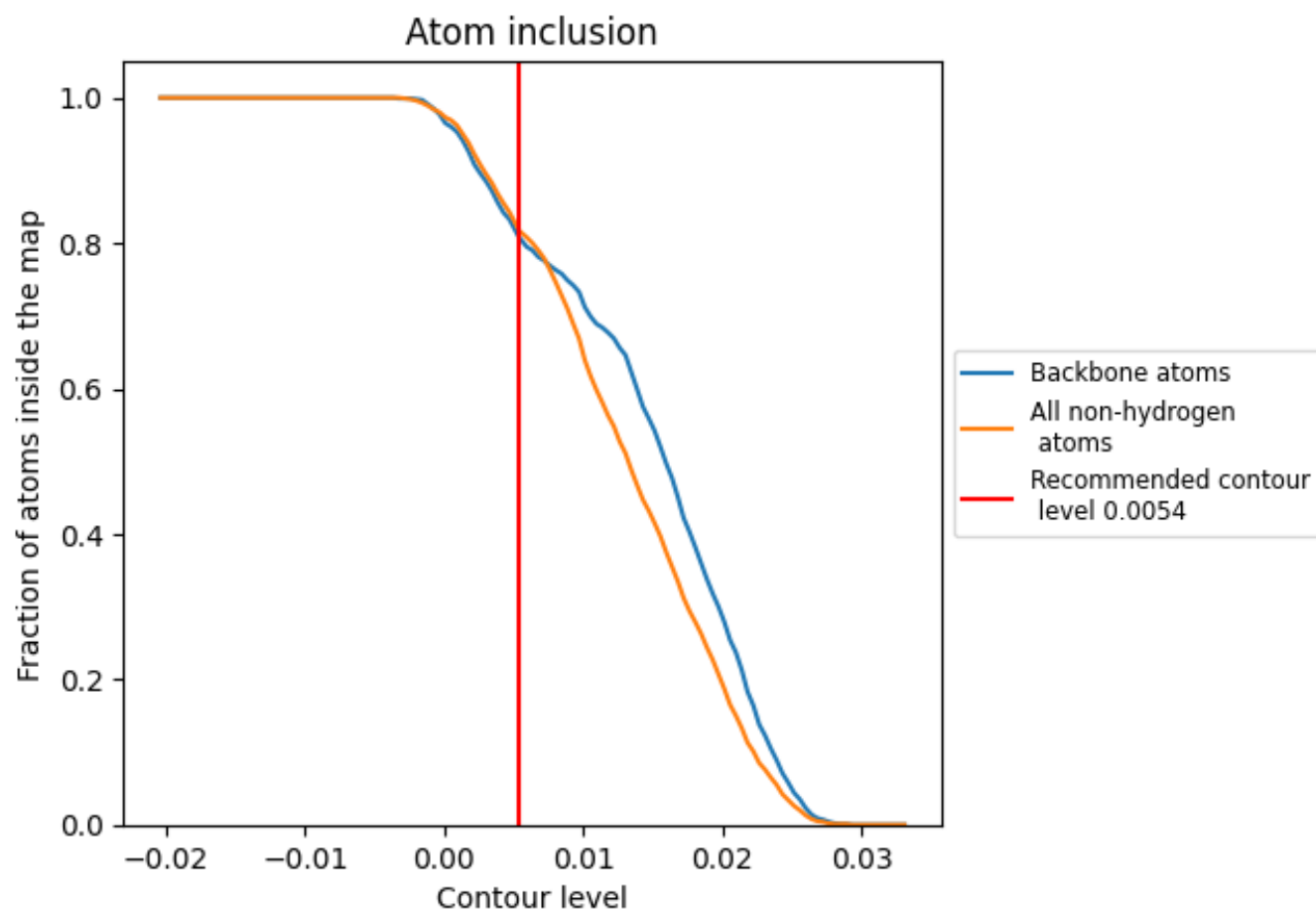
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0054).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 82% 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 (0.0054) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8170	<div><div></div></div> 0.5340
A	<div><div></div></div> 0.8110	<div><div></div></div> 0.5350
B	<div><div></div></div> 0.8150	<div><div></div></div> 0.5360
C	<div><div></div></div> 0.8230	<div><div></div></div> 0.5360
D	<div><div></div></div> 0.8110	<div><div></div></div> 0.5330
E	<div><div></div></div> 0.8110	<div><div></div></div> 0.5310
F	<div><div></div></div> 0.8290	<div><div></div></div> 0.5430
G	<div><div></div></div> 0.8150	<div><div></div></div> 0.5340
H	<div><div></div></div> 0.8110	<div><div></div></div> 0.5340
I	<div><div></div></div> 0.8150	<div><div></div></div> 0.5340
J	<div><div></div></div> 0.8290	<div><div></div></div> 0.5400
K	<div><div></div></div> 0.8190	<div><div></div></div> 0.5290
L	<div><div></div></div> 0.8150	<div><div></div></div> 0.5260

1.0

0.0

<0.0