



Full wwPDB EM Validation Report ⓘ

Sep 24, 2026 – 11:07 am BST

PDB ID : 28XH / pdb_000028xh
EMDB ID : EMD-56939
Title : DIT2 nanofibril
Authors : Stoyanov, N.; Schmidt, M.; Faendrich, M.
Deposited on : 2026-02-26
Resolution : 1.91 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.dev133
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) : 2.50

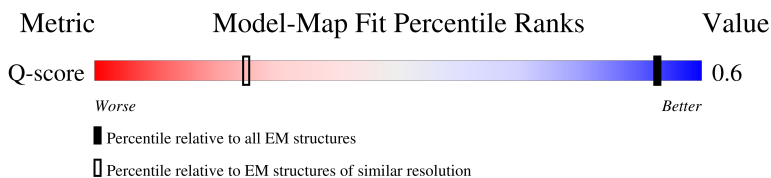
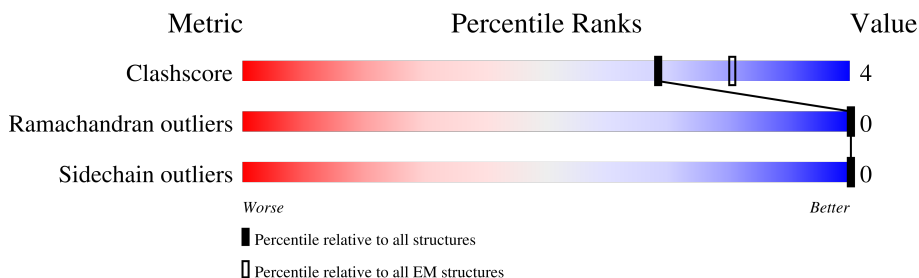
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 1.91 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	1204 (1.42 - 2.41)

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	9	11% 100%
1	A1	9	11% 100%
1	A2	9	11% 100%
1	AA	9	100%

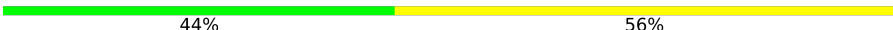
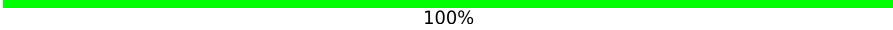
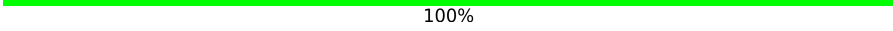
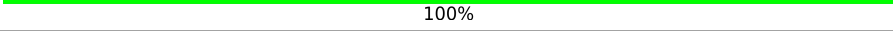
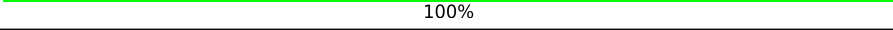
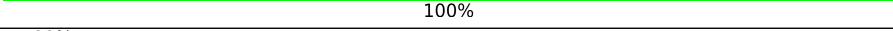
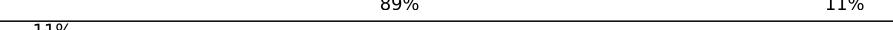
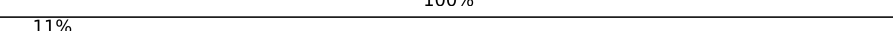
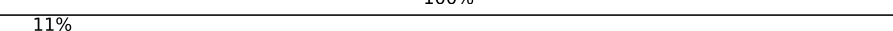
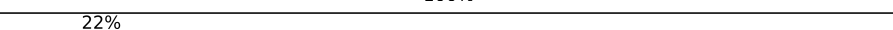
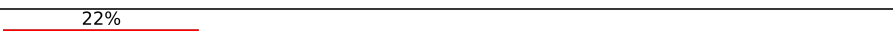
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Mol	Chain	Length	Quality of chain
1	AA1	9	100%
1	AA2	9	100%
1	AB	9	100%
1	AB1	9	100%
1	AB2	9	100%
1	AC	9	11% 100%
1	AC1	9	11% 100%
1	AC2	9	11% 100%
1	AD	9	89% 11%
1	AD1	9	89% 11%
1	AD2	9	89% 11%
1	AE	9	11% 100%
1	AE1	9	11% 100%
1	AE2	9	11% 89% 11%
1	AF	9	100%
1	AG	9	11% 100%
1	AG1	9	11% 100%
1	AG2	9	100%
1	AH	9	100%
1	AI	9	100%
1	B	9	89% 11%
1	B1	9	89% 11%
1	B2	9	89% 11%
1	C	9	44% 56%
1	C1	9	44% 56%

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Mol	Chain	Length	Quality of chain
1	C2	9	 44%56%
1	D	9	 78%22%
1	D1	9	 78%22%
1	D2	9	 78%22%
1	E	9	 100%
1	E1	9	 100%
1	E2	9	 100%
1	F	9	 100%
1	F1	9	 100%
1	F2	9	 100%
1	G	9	 11%78%22%
1	G1	9	 11%78%22%
1	G2	9	 11%78%22%
1	H	9	 11%89%11%
1	H1	9	 11%78%22%
1	H2	9	 89%11%
1	I	9	 11%100%
1	I1	9	 11%100%
1	I2	9	 11%100%
1	K	9	 22%100%
1	K1	9	 22%100%
1	K2	9	 11%100%
1	L	9	 22%89%11%
1	L1	9	 11%89%11%
1	L3	9	 11%100%

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Mol	Chain	Length	Quality of chain
1	M	9	100%
1	M1	9	89% 11%
1	M2	9	89% 11%
1	N	9	89% 11%
1	N1	9	89% 11%
1	N2	9	11% 100%
1	O	9	89% 11%
1	O1	9	78% 22%
1	O2	9	78% 22%
1	P	9	100%
1	P1	9	100%
1	P2	9	100%
1	Q	9	100%
1	Q1	9	100%
1	Q2	9	100%
1	R	9	89% 11%
1	R1	9	89% 11%
1	R2	9	89% 11%
1	S	9	11% 67% 33%
1	S1	9	67% 33%
1	S2	9	67% 33%
1	T	9	100%
1	T1	9	100%
1	T2	9	100%
1	U	9	11% 100%

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Mol	Chain	Length	Quality of chain
1	U1	9	100%
1	U2	9	100%
1	V	9	11% 89% 11%
1	V1	9	11% 89% 11%
1	V2	9	11% 100%
1	W	9	100%
1	W1	9	100%
1	W2	9	100%
1	X	9	100%
1	X1	9	100%
1	X2	9	11% 100%
1	Y	9	100%
1	Y1	9	89% 11%
1	Y2	9	100%
1	Z	9	100%
1	Z1	9	100%
1	Z2	9	100%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 7104 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 nanofibril peptide (RVKVSQINM).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	9	Total	C	N	O	S	0	0
			74	45	15	13	1		
1	A1	9	Total	C	N	O	S	0	0
			74	45	15	13	1		
1	A2	9	Total	C	N	O	S	0	0
			74	45	15	13	1		
1	AA	9	Total	C	N	O	S	0	0
			74	45	15	13	1		
1	AA1	9	Total	C	N	O	S	0	0
			74	45	15	13	1		
1	AA2	9	Total	C	N	O	S	0	0
			74	45	15	13	1		
1	AB	9	Total	C	N	O	S	0	0
			74	45	15	13	1		
1	AB1	9	Total	C	N	O	S	0	0
			74	45	15	13	1		
1	AB2	9	Total	C	N	O	S	0	0
			74	45	15	13	1		
1	AC	9	Total	C	N	O	S	0	0
			74	45	15	13	1		
1	AC1	9	Total	C	N	O	S	0	0
			74	45	15	13	1		
1	AC2	9	Total	C	N	O	S	0	0
			74	45	15	13	1		
1	AD	9	Total	C	N	O	S	0	0
			74	45	15	13	1		
1	AD1	9	Total	C	N	O	S	0	0
			74	45	15	13	1		
1	AD2	9	Total	C	N	O	S	0	0
			74	45	15	13	1		
1	AE	9	Total	C	N	O	S	0	0
			74	45	15	13	1		
1	AE1	9	Total	C	N	O	S	0	0
			74	45	15	13	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	AE2	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	AG	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	AG1	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	AG2	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	B	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	B1	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	B2	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	C	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	C1	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	C2	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	D	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	D1	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	D2	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	E	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	E1	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	E2	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	F	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	F1	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	F2	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	G	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	G1	9	Total 74	C 45	N 15	O 13	S 1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	G2	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	H	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	H1	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	H2	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	I	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	I1	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	I2	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	K	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	K1	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	K2	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	L	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	L1	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	L3	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	M	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	M1	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	M2	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	N	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	N1	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	N2	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	O	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	O1	9	Total 74	C 45	N 15	O 13	S 1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	O2	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	P	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	P1	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	P2	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	Q	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	Q1	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	Q2	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	R	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	R1	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	R2	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	S	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	S1	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	S2	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	T	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	T1	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	T2	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	U	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	U1	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	U2	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	V	9	Total 74	C 45	N 15	O 13	S 1	0	0
1	V1	9	Total 74	C 45	N 15	O 13	S 1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	V2	9	Total	C	N	O	S	0	0
			74	45	15	13	1		
1	W	9	Total	C	N	O	S	0	0
			74	45	15	13	1		
1	W1	9	Total	C	N	O	S	0	0
			74	45	15	13	1		
1	W2	9	Total	C	N	O	S	0	0
			74	45	15	13	1		
1	X	9	Total	C	N	O	S	0	0
			74	45	15	13	1		
1	X1	9	Total	C	N	O	S	0	0
			74	45	15	13	1		
1	X2	9	Total	C	N	O	S	0	0
			74	45	15	13	1		
1	Y	9	Total	C	N	O	S	0	0
			74	45	15	13	1		
1	Y1	9	Total	C	N	O	S	0	0
			74	45	15	13	1		
1	Y2	9	Total	C	N	O	S	0	0
			74	45	15	13	1		
1	Z	9	Total	C	N	O	S	0	0
			74	45	15	13	1		
1	Z1	9	Total	C	N	O	S	0	0
			74	45	15	13	1		
1	Z2	9	Total	C	N	O	S	0	0
			74	45	15	13	1		
1	AF	9	Total	C	N	O	S	0	0
			74	45	15	13	1		
1	AH	9	Total	C	N	O	S	0	0
			74	45	15	13	1		
1	AI	9	Total	C	N	O	S	0	0
			74	45	15	13	1		

3 Residue-property plots

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

- Molecule 1: nanofibril peptide (RVKVSQINM)



- Molecule 1: nanofibril peptide (RVKVSQINM)



- Molecule 1: nanofibril peptide (RVKVSQINM)



- Molecule 1: nanofibril peptide (RVKVSQINM)



There are no outlier residues recorded for this chain.

- Molecule 1: nanofibril peptide (RVKVSQINM)



There are no outlier residues recorded for this chain.

- Molecule 1: nanofibril peptide (RVKVSQINM)



There are no outlier residues recorded for this chain.

- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain AB:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain AB1:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain AB2:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain AC:  100%



- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain AC1:  100%



- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain AC2:  100%



- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain AD:  89% 11%



- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain AD1:  89% 11%



- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain AD2:  89% 11%



- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain AE:  11% 100%



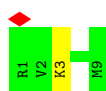
- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain AE1:  11% 100%



- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain AE2:  11% 89% 11%



- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain AG:  11% 100%



- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain AG1:  11% 100%



- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain AG2:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain B:  89% 11%



- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain B1:  89% 11%

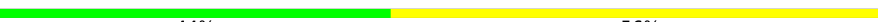


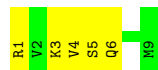
- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain B2:  89% 11%

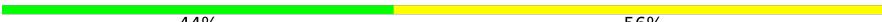


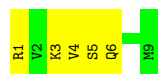
- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain C:  44% 56%



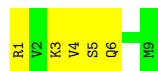
- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain C1:  44% 56%



- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain C2:  44% 56%



- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain D:  78% 22%



- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain D1:  78% 22%



- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain D2:  78% 22%



- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain E:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain E1:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain E2:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain F:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain F1:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain F2:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain G:  11% 78% 22%



- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain G1:  11% 78% 22%



- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain G2:  11% 78% 22%



- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain H:  11% 89% 11%



- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain H1:  11% 78% 22%



- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain H2:  89% 11%



- Molecule 1: nanofibril peptide (RVKVSQINM)



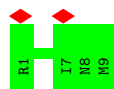
- Molecule 1: nanofibril peptide (RVKVSQINM)



- Molecule 1: nanofibril peptide (RVKVSQINM)



- Molecule 1: nanofibril peptide (RVKVSQINM)



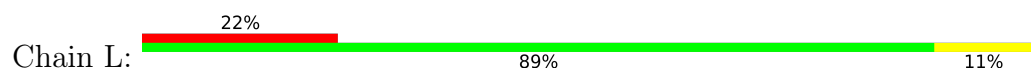
- Molecule 1: nanofibril peptide (RVKVSQINM)



- Molecule 1: nanofibril peptide (RVKVSQINM)

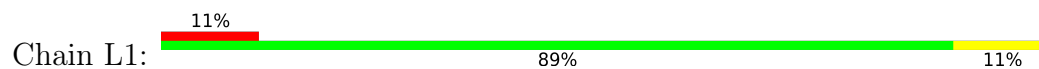


- Molecule 1: nanofibril peptide (RVKVSQINM)





- Molecule 1: nanofibril peptide (RVKVSQINM)



- Molecule 1: nanofibril peptide (RVKVSQINM)



- Molecule 1: nanofibril peptide (RVKVSQINM)



There are no outlier residues recorded for this chain.

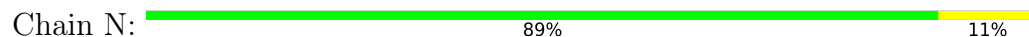
- Molecule 1: nanofibril peptide (RVKVSQINM)



- Molecule 1: nanofibril peptide (RVKVSQINM)



- Molecule 1: nanofibril peptide (RVKVSQINM)



- Molecule 1: nanofibril peptide (RVKVSQINM)

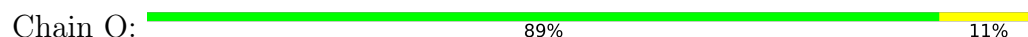




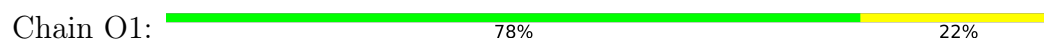
- Molecule 1: nanofibril peptide (RVKVSQINM)



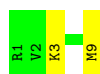
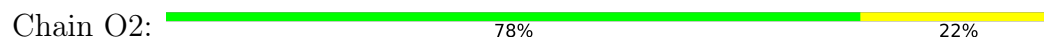
- Molecule 1: nanofibril peptide (RVKVSQINM)



- Molecule 1: nanofibril peptide (RVKVSQINM)



- Molecule 1: nanofibril peptide (RVKVSQINM)



- Molecule 1: nanofibril peptide (RVKVSQINM)



There are no outlier residues recorded for this chain.

- Molecule 1: nanofibril peptide (RVKVSQINM)



There are no outlier residues recorded for this chain.

- Molecule 1: nanofibril peptide (RVKVSQINM)



There are no outlier residues recorded for this chain.

- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain Q:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain Q1:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain Q2:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain R:  89% 11%



- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain R1:  89% 11%



- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain R2:  89% 11%



- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain S:  11% 67% 33%



- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain S1:  67% 33%

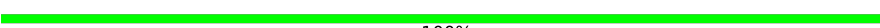


- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain S2:  67% 33%

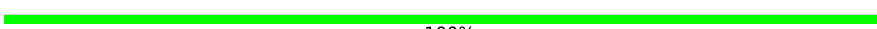


- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain T:  100%

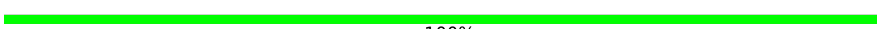
There are no outlier residues recorded for this chain.

- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain T1:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain T2:  100%

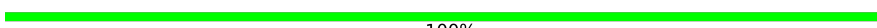
There are no outlier residues recorded for this chain.

- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain U:  11% 100%

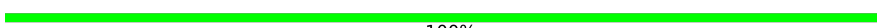


- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain U1:  100%

There are no outlier residues recorded for this chain.

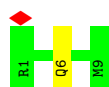
- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain U2:  100%

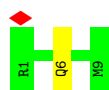
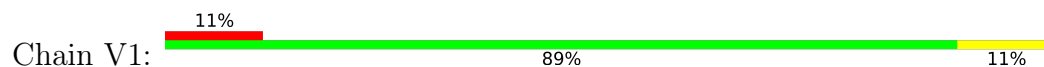
There are no outlier residues recorded for this chain.

- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain V:  11% 89% 11%



- Molecule 1: nanofibril peptide (RVKVSQINM)



- Molecule 1: nanofibril peptide (RVKVSQINM)



- Molecule 1: nanofibril peptide (RVKVSQINM)



There are no outlier residues recorded for this chain.

- Molecule 1: nanofibril peptide (RVKVSQINM)



There are no outlier residues recorded for this chain.

- Molecule 1: nanofibril peptide (RVKVSQINM)



There are no outlier residues recorded for this chain.

- Molecule 1: nanofibril peptide (RVKVSQINM)



There are no outlier residues recorded for this chain.

- Molecule 1: nanofibril peptide (RVKVSQINM)



There are no outlier residues recorded for this chain.

- Molecule 1: nanofibril peptide (RVKVSQINM)



- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain Y:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain Y1:  89% 11%



- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain Y2:  100%

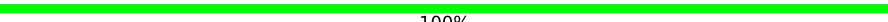
There are no outlier residues recorded for this chain.

- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain Z:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain Z1:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain Z2:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain AF:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain AH:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: nanofibril peptide (RVKVSQINM)

Chain AI:  100%

There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-0.409°, rise=4.781 Å, axial sym=C3	Depositor
Number of segments used	38411	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 ($e^-/\text{Å}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.109	Depositor
Minimum map value	-0.057	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.011	Depositor
Map size (Å)	560.4, 560.4, 560.4	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.934, 0.934, 0.934	Depositor

5 Model quality

5.1 Standard geometry

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	0.90	0/73	1.34	0/94
1	A1	0.90	0/73	1.34	0/94
1	A2	0.89	0/73	1.34	0/94
1	AA	0.74	0/73	1.19	0/94
1	AA1	0.75	0/73	1.19	0/94
1	AA2	0.75	0/73	1.18	0/94
1	AB	0.71	0/73	1.31	0/94
1	AB1	0.70	0/73	1.32	0/94
1	AB2	0.71	0/73	1.31	0/94
1	AC	0.78	0/73	1.30	0/94
1	AC1	0.77	0/73	1.30	0/94
1	AC2	0.77	0/73	1.30	0/94
1	AD	0.74	0/73	1.40	0/94
1	AD1	0.74	0/73	1.39	0/94
1	AD2	0.75	0/73	1.39	0/94
1	AE	0.71	0/73	1.31	0/94
1	AE1	0.72	0/73	1.32	0/94
1	AE2	0.71	0/73	1.32	0/94
1	AF	0.72	0/73	1.25	0/94
1	AG	0.72	0/73	1.34	0/94
1	AG1	0.73	0/73	1.33	0/94
1	AG2	0.73	0/73	1.34	0/94
1	AH	0.71	0/73	1.25	0/94
1	AI	0.72	0/73	1.25	0/94
1	B	1.05	0/73	1.53	0/94
1	B1	1.05	0/73	1.54	0/94
1	B2	1.04	0/73	1.53	0/94
1	C	0.80	0/73	1.44	0/94
1	C1	0.80	0/73	1.45	0/94
1	C2	0.80	0/73	1.45	0/94
1	D	0.83	0/73	1.38	0/94
1	D1	0.83	0/73	1.38	0/94
1	D2	0.84	0/73	1.38	0/94
1	E	0.85	0/73	1.07	0/94

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	E1	0.85	0/73	1.07	0/94
1	E2	0.85	0/73	1.07	0/94
1	F	0.72	0/73	1.35	0/94
1	F1	0.71	0/73	1.34	0/94
1	F2	0.72	0/73	1.34	0/94
1	G	0.81	0/73	1.29	0/94
1	G1	0.82	0/73	1.29	0/94
1	G2	0.82	0/73	1.29	0/94
1	H	0.76	0/73	1.23	0/94
1	H1	0.76	0/73	1.24	0/94
1	H2	0.76	0/73	1.23	0/94
1	I	0.74	0/73	1.29	0/94
1	I1	0.75	0/73	1.28	0/94
1	I2	0.75	0/73	1.28	0/94
1	K	0.74	0/73	1.37	0/94
1	K1	0.74	0/73	1.37	0/94
1	K2	0.74	0/73	1.37	0/94
1	L	0.73	0/73	1.14	0/94
1	L1	0.72	0/73	1.13	0/94
1	L3	0.72	0/73	1.15	0/94
1	M	0.74	0/73	1.25	0/94
1	M1	0.73	0/73	1.25	0/94
1	M2	0.72	0/73	1.24	0/94
1	N	0.74	0/73	1.22	0/94
1	N1	0.74	0/73	1.21	0/94
1	N2	0.75	0/73	1.22	0/94
1	O	0.72	0/73	1.28	0/94
1	O1	0.73	0/73	1.28	0/94
1	O2	0.73	0/73	1.28	0/94
1	P	0.74	0/73	1.24	0/94
1	P1	0.74	0/73	1.23	0/94
1	P2	0.75	0/73	1.23	0/94
1	Q	0.79	0/73	1.42	0/94
1	Q1	0.79	0/73	1.43	0/94
1	Q2	0.79	0/73	1.43	0/94
1	R	0.79	0/73	1.39	0/94
1	R1	0.79	0/73	1.38	0/94
1	R2	0.78	0/73	1.39	0/94
1	S	0.79	0/73	1.12	0/94
1	S1	0.81	0/73	1.12	0/94
1	S2	0.79	0/73	1.12	0/94
1	T	0.73	0/73	1.18	0/94
1	T1	0.73	0/73	1.19	0/94

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	T2	0.73	0/73	1.19	0/94
1	U	0.70	0/73	1.34	0/94
1	U1	0.69	0/73	1.34	0/94
1	U2	0.69	0/73	1.35	0/94
1	V	0.77	0/73	1.06	0/94
1	V1	0.77	0/73	1.06	0/94
1	V2	0.76	0/73	1.06	0/94
1	W	0.75	0/73	1.43	0/94
1	W1	0.74	0/73	1.43	0/94
1	W2	0.75	0/73	1.43	0/94
1	X	0.72	0/73	1.27	0/94
1	X1	0.72	0/73	1.27	0/94
1	X2	0.71	0/73	1.27	0/94
1	Y	0.73	0/73	1.22	0/94
1	Y1	0.74	0/73	1.22	0/94
1	Y2	0.74	0/73	1.23	0/94
1	Z	0.76	0/73	1.26	0/94
1	Z1	0.77	0/73	1.25	0/94
1	Z2	0.76	0/73	1.25	0/94
All	All	0.77	0/7008	1.29	0/9024

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	74	0	85	0	0
1	A1	74	0	85	0	0
1	A2	74	0	85	0	0
1	AA	74	0	85	0	0
1	AA1	74	0	85	0	0
1	AA2	74	0	85	0	0

Continued on next page...

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AB	74	0	85	0	0
1	AB1	74	0	85	0	0
1	AB2	74	0	85	0	0
1	AC	74	0	85	0	0
1	AC1	74	0	85	0	0
1	AC2	74	0	85	0	0
1	AD	74	0	85	2	0
1	AD1	74	0	85	4	0
1	AD2	74	0	85	2	0
1	AE	74	0	85	0	0
1	AE1	74	0	85	0	0
1	AE2	74	0	85	1	0
1	AF	74	0	85	0	0
1	AG	74	0	85	0	0
1	AG1	74	0	85	0	0
1	AG2	74	0	85	0	0
1	AH	74	0	85	0	0
1	AI	74	0	85	0	0
1	B	74	0	85	1	0
1	B1	74	0	85	2	0
1	B2	74	0	85	1	0
1	C	74	0	85	14	0
1	C1	74	0	85	28	0
1	C2	74	0	85	14	0
1	D	74	0	85	2	0
1	D1	74	0	85	3	0
1	D2	74	0	85	2	0
1	E	74	0	85	0	0
1	E1	74	0	85	0	0
1	E2	74	0	85	0	0
1	F	74	0	85	0	0
1	F1	74	0	85	0	0
1	F2	74	0	85	0	0
1	G	74	0	85	2	0
1	G1	74	0	85	4	0
1	G2	74	0	85	2	0
1	H	74	0	85	1	0
1	H1	74	0	85	2	0
1	H2	74	0	85	1	0
1	I	74	0	85	0	0
1	I1	74	0	85	0	0
1	I2	74	0	85	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	74	0	85	0	0
1	K1	74	0	85	0	0
1	K2	74	0	85	0	0
1	L	74	0	85	1	0
1	L1	74	0	85	1	0
1	L3	74	0	85	0	0
1	M	74	0	85	0	0
1	M1	74	0	85	1	0
1	M2	74	0	85	1	0
1	N	74	0	85	1	0
1	N1	74	0	85	1	0
1	N2	74	0	85	0	0
1	O	74	0	85	1	0
1	O1	74	0	85	2	0
1	O2	74	0	85	2	0
1	P	74	0	85	0	0
1	P1	74	0	85	0	0
1	P2	74	0	85	0	0
1	Q	74	0	85	0	0
1	Q1	74	0	85	0	0
1	Q2	74	0	85	0	0
1	R	74	0	85	1	0
1	R1	74	0	85	1	0
1	R2	74	0	85	1	0
1	S	74	0	85	2	0
1	S1	74	0	85	2	0
1	S2	74	0	85	2	0
1	T	74	0	85	0	0
1	T1	74	0	85	0	0
1	T2	74	0	85	0	0
1	U	74	0	85	0	0
1	U1	74	0	85	0	0
1	U2	74	0	85	0	0
1	V	74	0	85	1	0
1	V1	74	0	85	1	0
1	V2	74	0	85	0	0
1	W	74	0	85	0	0
1	W1	74	0	85	0	0
1	W2	74	0	85	0	0
1	X	74	0	85	0	0
1	X1	74	0	85	0	0
1	X2	74	0	85	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Y	74	0	85	0	0
1	Y1	74	0	85	1	0
1	Y2	74	0	85	0	0
1	Z	74	0	85	0	0
1	Z1	74	0	85	0	0
1	Z2	74	0	85	0	0
All	All	7104	0	8160	57	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (57) 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:C1:3:LYS:HA	1:C2:3:LYS:O	1.84	0.78
1:C:3:LYS:HA	1:C1:3:LYS:O	1.84	0.78
1:D1:3:LYS:HA	1:D2:3:LYS:O	1.85	0.77
1:D:3:LYS:HA	1:D1:3:LYS:O	1.85	0.77
1:AD1:3:LYS:HG3	1:AD2:3:LYS:HE3	1.72	0.71
1:AD:3:LYS:HG3	1:AD1:3:LYS:HE3	1.72	0.70
1:C1:4:VAL:CG2	1:C2:4:VAL:HG12	2.21	0.70
1:C:4:VAL:CG2	1:C1:4:VAL:HG12	2.21	0.70
1:C:4:VAL:CG2	1:C1:4:VAL:CG1	2.73	0.67
1:C1:4:VAL:CG2	1:C2:4:VAL:CG1	2.73	0.67
1:C:4:VAL:HG22	1:C1:4:VAL:CG1	2.24	0.67
1:C1:4:VAL:HG22	1:C2:4:VAL:CG1	2.24	0.67
1:C:1:ARG:HA	1:C1:1:ARG:O	1.94	0.67
1:C1:1:ARG:HA	1:C2:1:ARG:O	1.94	0.66
1:C:4:VAL:HG22	1:C1:4:VAL:HG12	1.78	0.65
1:C1:4:VAL:HG22	1:C2:4:VAL:HG12	1.78	0.65
1:C:6:GLN:HB2	1:C1:6:GLN:OE1	1.98	0.63
1:C1:6:GLN:HB2	1:C2:6:GLN:OE1	1.98	0.63
1:C:6:GLN:O	1:C1:6:GLN:HA	2.01	0.61
1:C1:6:GLN:O	1:C2:6:GLN:HA	2.01	0.61
1:C:4:VAL:H	1:C1:4:VAL:HG12	1.67	0.60
1:C1:4:VAL:H	1:C2:4:VAL:HG12	1.67	0.60
1:N:9:MET:OXT	1:O1:3:LYS:NZ	2.33	0.59
1:N1:9:MET:OXT	1:O2:3:LYS:NZ	2.33	0.59
1:D:9:MET:O	1:R:3:LYS:NZ	2.40	0.54
1:O2:9:MET:O	1:S2:3:LYS:HE2	2.07	0.54
1:C:4:VAL:HG23	1:C1:4:VAL:CG1	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:4:VAL:HG23	1:C2:4:VAL:CG1	2.37	0.54
1:D1:9:MET:O	1:R1:3:LYS:NZ	2.40	0.54
1:D2:9:MET:O	1:R2:3:LYS:NZ	2.40	0.54
1:O1:9:MET:O	1:S1:3:LYS:HE2	2.07	0.54
1:O:9:MET:O	1:S:3:LYS:HE2	2.08	0.53
1:H:8:ASN:O	1:H1:9:MET:HG2	2.10	0.52
1:H1:8:ASN:O	1:H2:9:MET:HG2	2.10	0.52
1:C:4:VAL:CG2	1:C1:4:VAL:HG11	2.41	0.50
1:C1:4:VAL:CG2	1:C2:4:VAL:HG11	2.41	0.50
1:S2:6:GLN:NE2	1:S2:8:ASN:OD1	2.45	0.50
1:S:6:GLN:NE2	1:S:8:ASN:OD1	2.44	0.50
1:S1:6:GLN:NE2	1:S1:8:ASN:OD1	2.45	0.50
1:C:5:SER:HA	1:C1:5:SER:O	2.12	0.48
1:C1:5:SER:HA	1:C2:5:SER:O	2.12	0.48
1:G1:5:SER:HA	1:G2:5:SER:O	2.14	0.47
1:G:5:SER:HA	1:G1:5:SER:O	2.14	0.47
1:AD1:3:LYS:HG3	1:AD2:3:LYS:CE	2.44	0.47
1:AD:3:LYS:HG3	1:AD1:3:LYS:CE	2.44	0.47
1:V:6:GLN:NE2	1:V1:6:GLN:OE1	2.47	0.47
1:L1:9:MET:OXT	1:M2:3:LYS:NZ	2.46	0.46
1:L:9:MET:OXT	1:M1:3:LYS:NZ	2.46	0.46
1:G:3:LYS:HA	1:G1:3:LYS:O	2.15	0.45
1:G1:3:LYS:HA	1:G2:3:LYS:O	2.15	0.45
1:AE2:3:LYS:NZ	1:Y1:9:MET:OXT	2.47	0.45
1:C:4:VAL:HG23	1:C1:4:VAL:HG12	1.94	0.44
1:C:4:VAL:HG22	1:C1:4:VAL:HG11	1.99	0.43
1:C1:4:VAL:HG22	1:C2:4:VAL:HG11	1.99	0.43
1:C1:4:VAL:HG23	1:C2:4:VAL:HG12	1.94	0.42
1:B:3:LYS:HG3	1:B1:3:LYS:O	2.21	0.40
1:B1:3:LYS:HG3	1:B2:3:LYS:O	2.21	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	7/9 (78%)	7 (100%)	0	0	100	100
1	A1	7/9 (78%)	7 (100%)	0	0	100	100
1	A2	7/9 (78%)	7 (100%)	0	0	100	100
1	AA	7/9 (78%)	7 (100%)	0	0	100	100
1	AA1	7/9 (78%)	7 (100%)	0	0	100	100
1	AA2	7/9 (78%)	7 (100%)	0	0	100	100
1	AB	7/9 (78%)	7 (100%)	0	0	100	100
1	AB1	7/9 (78%)	7 (100%)	0	0	100	100
1	AB2	7/9 (78%)	7 (100%)	0	0	100	100
1	AC	7/9 (78%)	7 (100%)	0	0	100	100
1	AC1	7/9 (78%)	7 (100%)	0	0	100	100
1	AC2	7/9 (78%)	7 (100%)	0	0	100	100
1	AD	7/9 (78%)	7 (100%)	0	0	100	100
1	AD1	7/9 (78%)	7 (100%)	0	0	100	100
1	AD2	7/9 (78%)	7 (100%)	0	0	100	100
1	AE	7/9 (78%)	7 (100%)	0	0	100	100
1	AE1	7/9 (78%)	7 (100%)	0	0	100	100
1	AE2	7/9 (78%)	7 (100%)	0	0	100	100
1	AF	7/9 (78%)	7 (100%)	0	0	100	100
1	AG	7/9 (78%)	7 (100%)	0	0	100	100
1	AG1	7/9 (78%)	7 (100%)	0	0	100	100
1	AG2	7/9 (78%)	7 (100%)	0	0	100	100
1	AH	7/9 (78%)	7 (100%)	0	0	100	100
1	AI	7/9 (78%)	7 (100%)	0	0	100	100
1	B	7/9 (78%)	7 (100%)	0	0	100	100
1	B1	7/9 (78%)	7 (100%)	0	0	100	100
1	B2	7/9 (78%)	7 (100%)	0	0	100	100
1	C	7/9 (78%)	7 (100%)	0	0	100	100
1	C1	7/9 (78%)	7 (100%)	0	0	100	100
1	C2	7/9 (78%)	7 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	7/9 (78%)	7 (100%)	0	0	100	100
1	D1	7/9 (78%)	7 (100%)	0	0	100	100
1	D2	7/9 (78%)	7 (100%)	0	0	100	100
1	E	7/9 (78%)	7 (100%)	0	0	100	100
1	E1	7/9 (78%)	7 (100%)	0	0	100	100
1	E2	7/9 (78%)	7 (100%)	0	0	100	100
1	F	7/9 (78%)	7 (100%)	0	0	100	100
1	F1	7/9 (78%)	7 (100%)	0	0	100	100
1	F2	7/9 (78%)	7 (100%)	0	0	100	100
1	G	7/9 (78%)	7 (100%)	0	0	100	100
1	G1	7/9 (78%)	7 (100%)	0	0	100	100
1	G2	7/9 (78%)	7 (100%)	0	0	100	100
1	H	7/9 (78%)	7 (100%)	0	0	100	100
1	H1	7/9 (78%)	7 (100%)	0	0	100	100
1	H2	7/9 (78%)	7 (100%)	0	0	100	100
1	I	7/9 (78%)	7 (100%)	0	0	100	100
1	I1	7/9 (78%)	7 (100%)	0	0	100	100
1	I2	7/9 (78%)	7 (100%)	0	0	100	100
1	K	7/9 (78%)	7 (100%)	0	0	100	100
1	K1	7/9 (78%)	7 (100%)	0	0	100	100
1	K2	7/9 (78%)	7 (100%)	0	0	100	100
1	L	7/9 (78%)	7 (100%)	0	0	100	100
1	L1	7/9 (78%)	7 (100%)	0	0	100	100
1	L3	7/9 (78%)	7 (100%)	0	0	100	100
1	M	7/9 (78%)	7 (100%)	0	0	100	100
1	M1	7/9 (78%)	7 (100%)	0	0	100	100
1	M2	7/9 (78%)	7 (100%)	0	0	100	100
1	N	7/9 (78%)	7 (100%)	0	0	100	100
1	N1	7/9 (78%)	7 (100%)	0	0	100	100
1	N2	7/9 (78%)	7 (100%)	0	0	100	100
1	O	7/9 (78%)	7 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O1	7/9 (78%)	7 (100%)	0	0	100	100
1	O2	7/9 (78%)	7 (100%)	0	0	100	100
1	P	7/9 (78%)	7 (100%)	0	0	100	100
1	P1	7/9 (78%)	7 (100%)	0	0	100	100
1	P2	7/9 (78%)	7 (100%)	0	0	100	100
1	Q	7/9 (78%)	7 (100%)	0	0	100	100
1	Q1	7/9 (78%)	7 (100%)	0	0	100	100
1	Q2	7/9 (78%)	7 (100%)	0	0	100	100
1	R	7/9 (78%)	7 (100%)	0	0	100	100
1	R1	7/9 (78%)	7 (100%)	0	0	100	100
1	R2	7/9 (78%)	7 (100%)	0	0	100	100
1	S	7/9 (78%)	7 (100%)	0	0	100	100
1	S1	7/9 (78%)	7 (100%)	0	0	100	100
1	S2	7/9 (78%)	7 (100%)	0	0	100	100
1	T	7/9 (78%)	7 (100%)	0	0	100	100
1	T1	7/9 (78%)	7 (100%)	0	0	100	100
1	T2	7/9 (78%)	7 (100%)	0	0	100	100
1	U	7/9 (78%)	7 (100%)	0	0	100	100
1	U1	7/9 (78%)	7 (100%)	0	0	100	100
1	U2	7/9 (78%)	7 (100%)	0	0	100	100
1	V	7/9 (78%)	7 (100%)	0	0	100	100
1	V1	7/9 (78%)	7 (100%)	0	0	100	100
1	V2	7/9 (78%)	7 (100%)	0	0	100	100
1	W	7/9 (78%)	7 (100%)	0	0	100	100
1	W1	7/9 (78%)	7 (100%)	0	0	100	100
1	W2	7/9 (78%)	7 (100%)	0	0	100	100
1	X	7/9 (78%)	7 (100%)	0	0	100	100
1	X1	7/9 (78%)	7 (100%)	0	0	100	100
1	X2	7/9 (78%)	7 (100%)	0	0	100	100
1	Y	7/9 (78%)	7 (100%)	0	0	100	100
1	Y1	7/9 (78%)	7 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Y2	7/9 (78%)	7 (100%)	0	0	100	100
1	Z	7/9 (78%)	7 (100%)	0	0	100	100
1	Z1	7/9 (78%)	7 (100%)	0	0	100	100
1	Z2	7/9 (78%)	7 (100%)	0	0	100	100
All	All	672/864 (78%)	672 (100%)	0	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	9/9 (100%)	9 (100%)	0	100	100
1	A1	9/9 (100%)	9 (100%)	0	100	100
1	A2	9/9 (100%)	9 (100%)	0	100	100
1	AA	9/9 (100%)	9 (100%)	0	100	100
1	AA1	9/9 (100%)	9 (100%)	0	100	100
1	AA2	9/9 (100%)	9 (100%)	0	100	100
1	AB	9/9 (100%)	9 (100%)	0	100	100
1	AB1	9/9 (100%)	9 (100%)	0	100	100
1	AB2	9/9 (100%)	9 (100%)	0	100	100
1	AC	9/9 (100%)	9 (100%)	0	100	100
1	AC1	9/9 (100%)	9 (100%)	0	100	100
1	AC2	9/9 (100%)	9 (100%)	0	100	100
1	AD	9/9 (100%)	9 (100%)	0	100	100
1	AD1	9/9 (100%)	9 (100%)	0	100	100
1	AD2	9/9 (100%)	9 (100%)	0	100	100
1	AE	9/9 (100%)	9 (100%)	0	100	100
1	AE1	9/9 (100%)	9 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AE2	9/9 (100%)	9 (100%)	0	100	100
1	AF	9/9 (100%)	9 (100%)	0	100	100
1	AG	9/9 (100%)	9 (100%)	0	100	100
1	AG1	9/9 (100%)	9 (100%)	0	100	100
1	AG2	9/9 (100%)	9 (100%)	0	100	100
1	AH	9/9 (100%)	9 (100%)	0	100	100
1	AI	9/9 (100%)	9 (100%)	0	100	100
1	B	9/9 (100%)	9 (100%)	0	100	100
1	B1	9/9 (100%)	9 (100%)	0	100	100
1	B2	9/9 (100%)	9 (100%)	0	100	100
1	C	9/9 (100%)	9 (100%)	0	100	100
1	C1	9/9 (100%)	9 (100%)	0	100	100
1	C2	9/9 (100%)	9 (100%)	0	100	100
1	D	9/9 (100%)	9 (100%)	0	100	100
1	D1	9/9 (100%)	9 (100%)	0	100	100
1	D2	9/9 (100%)	9 (100%)	0	100	100
1	E	9/9 (100%)	9 (100%)	0	100	100
1	E1	9/9 (100%)	9 (100%)	0	100	100
1	E2	9/9 (100%)	9 (100%)	0	100	100
1	F	9/9 (100%)	9 (100%)	0	100	100
1	F1	9/9 (100%)	9 (100%)	0	100	100
1	F2	9/9 (100%)	9 (100%)	0	100	100
1	G	9/9 (100%)	9 (100%)	0	100	100
1	G1	9/9 (100%)	9 (100%)	0	100	100
1	G2	9/9 (100%)	9 (100%)	0	100	100
1	H	9/9 (100%)	9 (100%)	0	100	100
1	H1	9/9 (100%)	9 (100%)	0	100	100
1	H2	9/9 (100%)	9 (100%)	0	100	100
1	I	9/9 (100%)	9 (100%)	0	100	100
1	I1	9/9 (100%)	9 (100%)	0	100	100
1	I2	9/9 (100%)	9 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	9/9 (100%)	9 (100%)	0	100	100
1	K1	9/9 (100%)	9 (100%)	0	100	100
1	K2	9/9 (100%)	9 (100%)	0	100	100
1	L	9/9 (100%)	9 (100%)	0	100	100
1	L1	9/9 (100%)	9 (100%)	0	100	100
1	L3	9/9 (100%)	9 (100%)	0	100	100
1	M	9/9 (100%)	9 (100%)	0	100	100
1	M1	9/9 (100%)	9 (100%)	0	100	100
1	M2	9/9 (100%)	9 (100%)	0	100	100
1	N	9/9 (100%)	9 (100%)	0	100	100
1	N1	9/9 (100%)	9 (100%)	0	100	100
1	N2	9/9 (100%)	9 (100%)	0	100	100
1	O	9/9 (100%)	9 (100%)	0	100	100
1	O1	9/9 (100%)	9 (100%)	0	100	100
1	O2	9/9 (100%)	9 (100%)	0	100	100
1	P	9/9 (100%)	9 (100%)	0	100	100
1	P1	9/9 (100%)	9 (100%)	0	100	100
1	P2	9/9 (100%)	9 (100%)	0	100	100
1	Q	9/9 (100%)	9 (100%)	0	100	100
1	Q1	9/9 (100%)	9 (100%)	0	100	100
1	Q2	9/9 (100%)	9 (100%)	0	100	100
1	R	9/9 (100%)	9 (100%)	0	100	100
1	R1	9/9 (100%)	9 (100%)	0	100	100
1	R2	9/9 (100%)	9 (100%)	0	100	100
1	S	9/9 (100%)	9 (100%)	0	100	100
1	S1	9/9 (100%)	9 (100%)	0	100	100
1	S2	9/9 (100%)	9 (100%)	0	100	100
1	T	9/9 (100%)	9 (100%)	0	100	100
1	T1	9/9 (100%)	9 (100%)	0	100	100
1	T2	9/9 (100%)	9 (100%)	0	100	100
1	U	9/9 (100%)	9 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	U1	9/9 (100%)	9 (100%)	0	100	100
1	U2	9/9 (100%)	9 (100%)	0	100	100
1	V	9/9 (100%)	9 (100%)	0	100	100
1	V1	9/9 (100%)	9 (100%)	0	100	100
1	V2	9/9 (100%)	9 (100%)	0	100	100
1	W	9/9 (100%)	9 (100%)	0	100	100
1	W1	9/9 (100%)	9 (100%)	0	100	100
1	W2	9/9 (100%)	9 (100%)	0	100	100
1	X	9/9 (100%)	9 (100%)	0	100	100
1	X1	9/9 (100%)	9 (100%)	0	100	100
1	X2	9/9 (100%)	9 (100%)	0	100	100
1	Y	9/9 (100%)	9 (100%)	0	100	100
1	Y1	9/9 (100%)	9 (100%)	0	100	100
1	Y2	9/9 (100%)	9 (100%)	0	100	100
1	Z	9/9 (100%)	9 (100%)	0	100	100
1	Z1	9/9 (100%)	9 (100%)	0	100	100
1	Z2	9/9 (100%)	9 (100%)	0	100	100
All	All	864/864 (100%)	864 (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. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A1	8	ASN
1	A2	8	ASN
1	AD	8	ASN
1	AG	6	GLN
1	C	8	ASN
1	C1	8	ASN
1	C2	8	ASN
1	D	6	GLN
1	D	8	ASN
1	D1	6	GLN
1	D1	8	ASN

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Mol	Chain	Res	Type
1	D2	6	GLN
1	D2	8	ASN
1	E	6	GLN
1	E	8	ASN
1	E1	6	GLN
1	E1	8	ASN
1	E2	6	GLN
1	E2	8	ASN
1	G	6	GLN
1	G1	6	GLN
1	G2	6	GLN
1	I	6	GLN
1	I	8	ASN
1	I1	6	GLN
1	I1	8	ASN
1	I2	6	GLN
1	I2	8	ASN
1	K1	6	GLN
1	K2	6	GLN
1	N	8	ASN
1	N1	8	ASN
1	O	8	ASN
1	O1	8	ASN
1	O2	6	GLN
1	P	8	ASN
1	P1	8	ASN
1	P2	8	ASN
1	Q	8	ASN
1	Q1	6	GLN
1	Q1	8	ASN
1	Q2	6	GLN
1	Q2	8	ASN
1	R2	6	GLN
1	S	6	GLN
1	S	8	ASN
1	S1	6	GLN
1	S1	8	ASN
1	S2	6	GLN
1	S2	8	ASN
1	U2	6	GLN
1	V	6	GLN
1	V	8	ASN

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Mol	Chain	Res	Type
1	V1	6	GLN
1	V1	8	ASN
1	V2	8	ASN
1	W	8	ASN
1	W1	6	GLN
1	W2	6	GLN
1	Y	8	ASN
1	Y1	6	GLN
1	Y1	8	ASN
1	Y2	6	GLN
1	Y2	8	ASN

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.

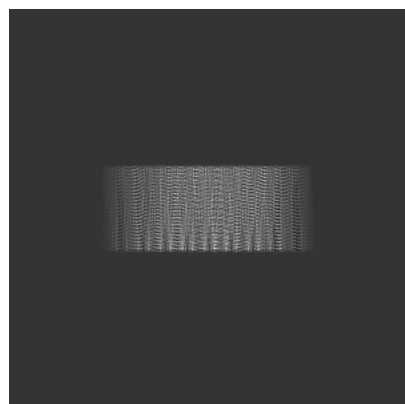
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-56939. These allow visual inspection of the internal detail of the map and identification of artifacts.

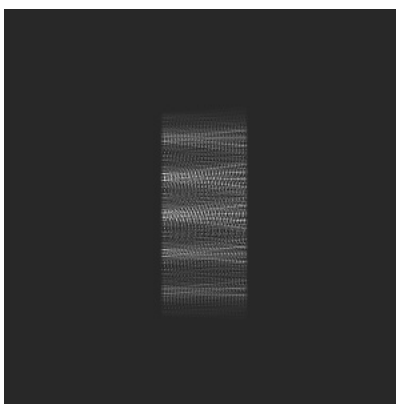
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

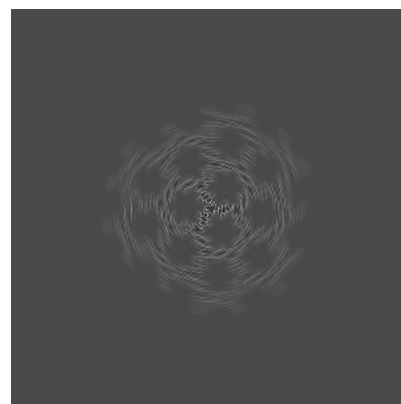
6.1.1 Primary map



X

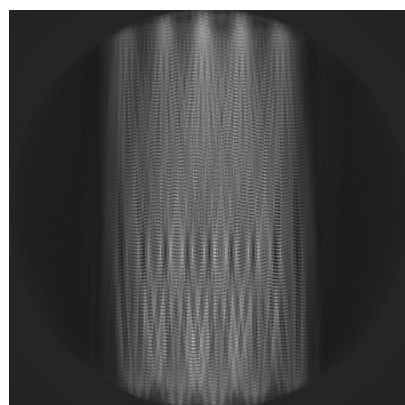


Y

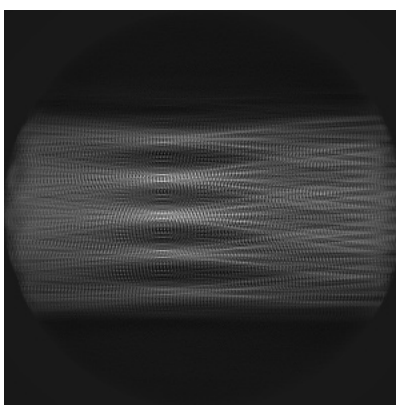


Z

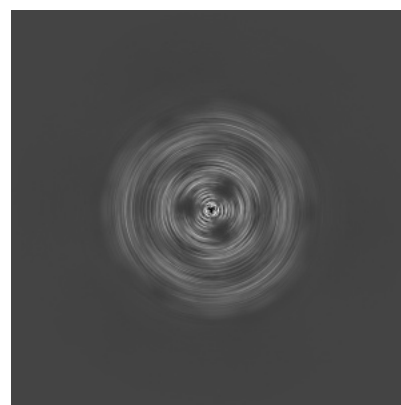
6.1.2 Raw map



X



Y



Z

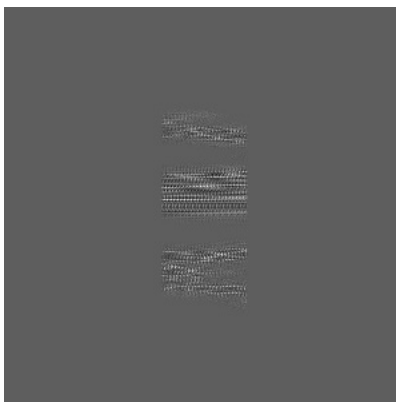
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

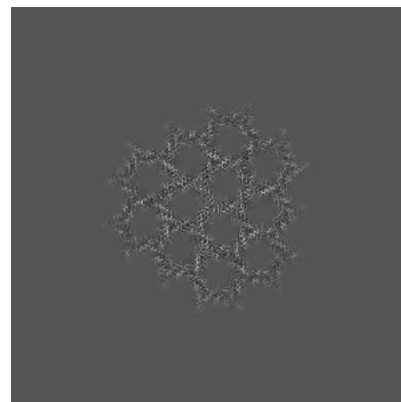
6.2.1 Primary map



X Index: 300

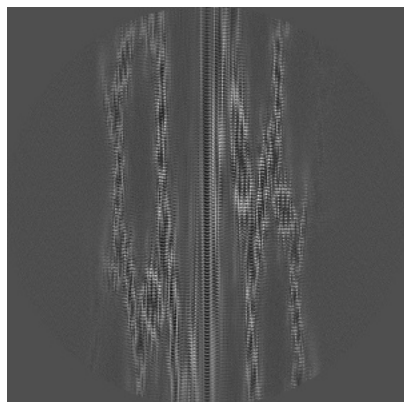


Y Index: 300

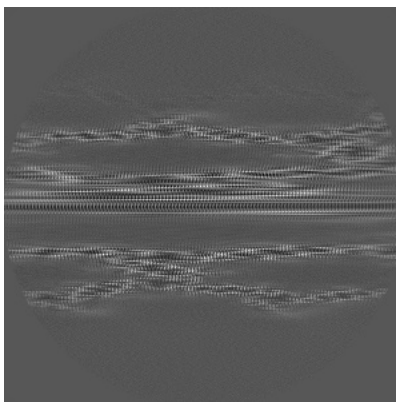


Z Index: 300

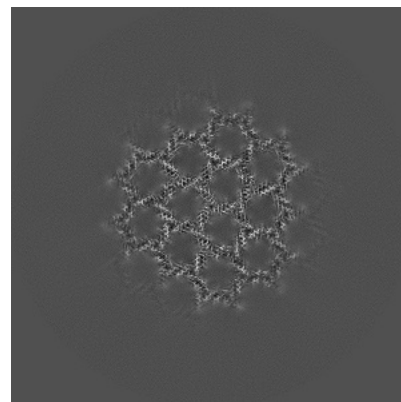
6.2.2 Raw map



X Index: 300



Y Index: 300

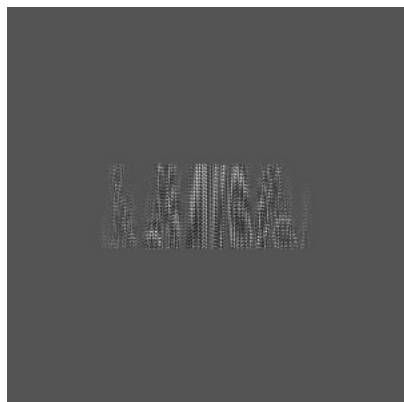


Z Index: 300

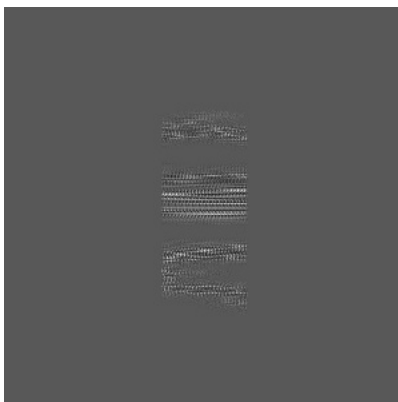
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

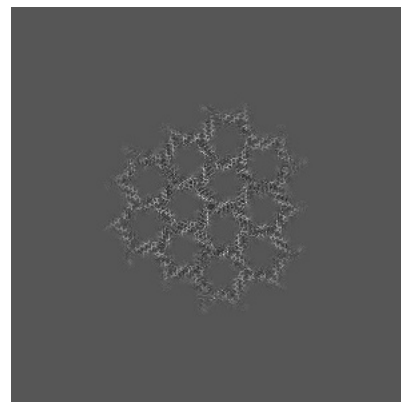
6.3.1 Primary map



X Index: 293

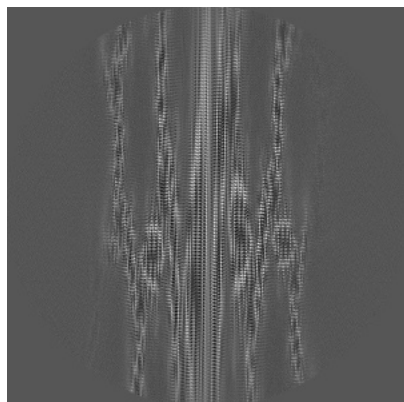


Y Index: 294

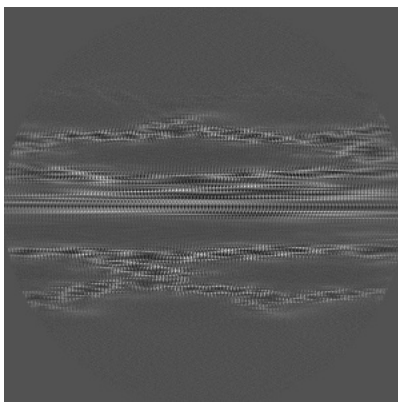


Z Index: 271

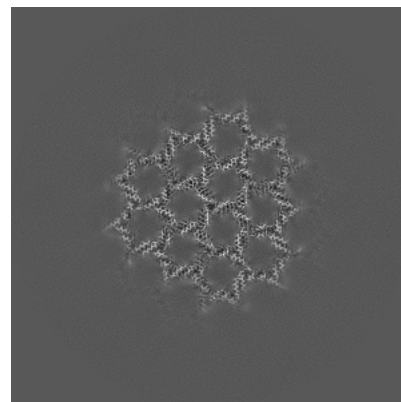
6.3.2 Raw map



X Index: 292



Y Index: 297

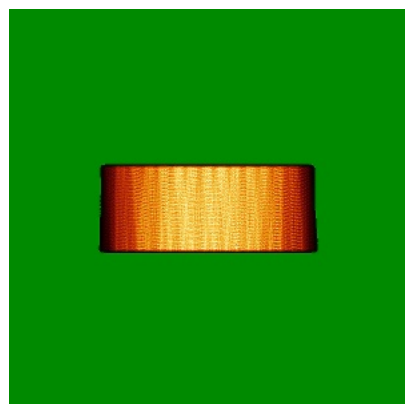


Z Index: 271

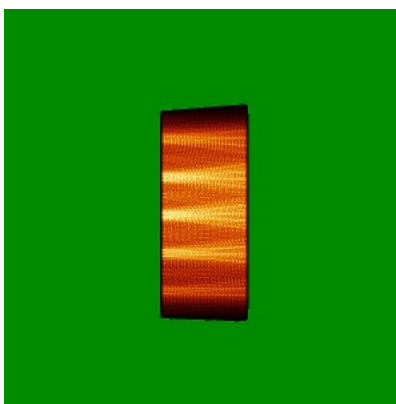
The images above show the largest variance slices of the map in three orthogonal directions.

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

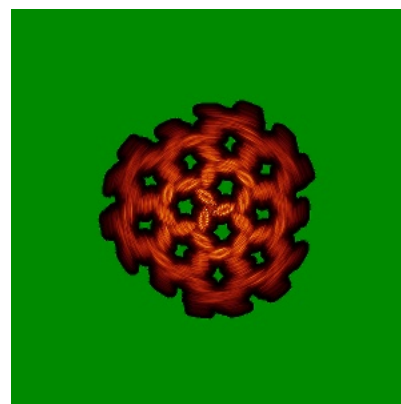
6.4.1 Primary map



X

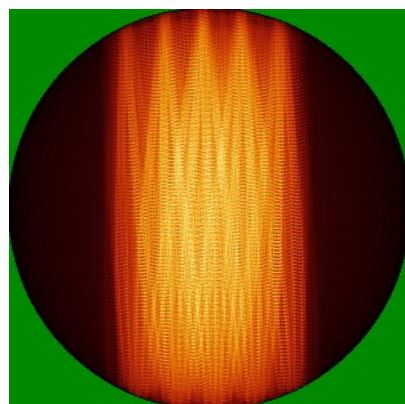


Y

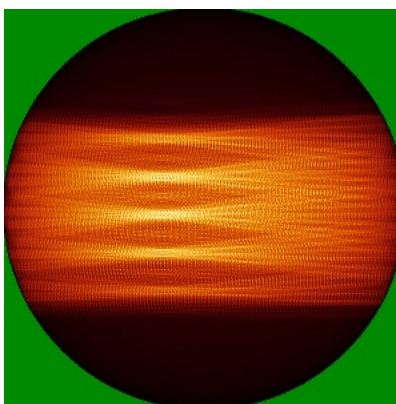


Z

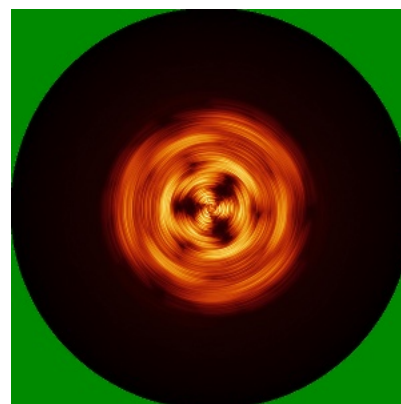
6.4.2 Raw map



X



Y

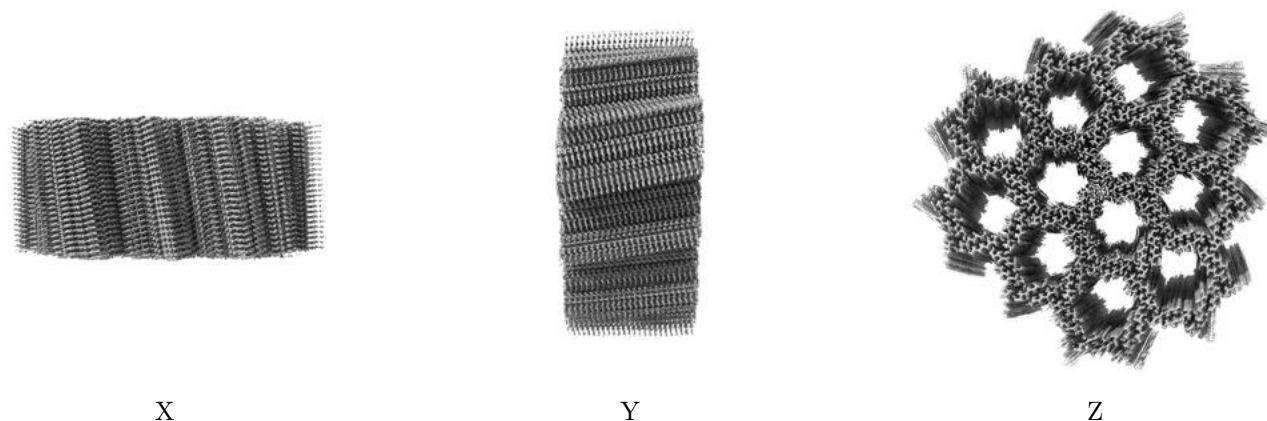


Z

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.

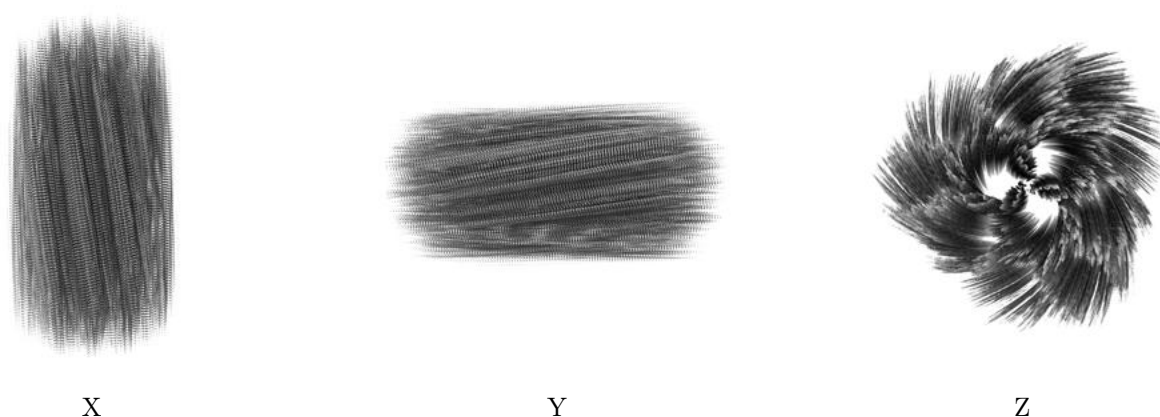
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.011. 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.

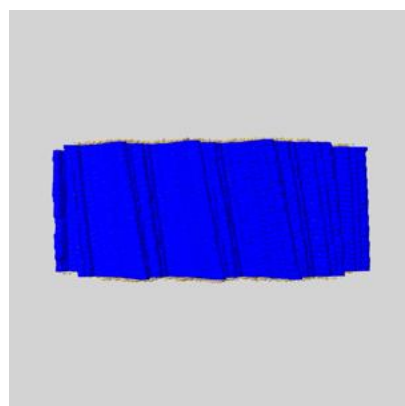
6.6 Mask visualisation [i](#)

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

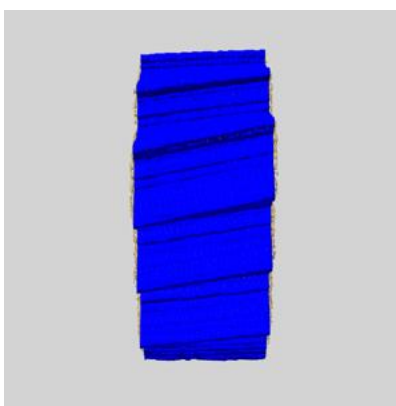
A mask typically either:

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

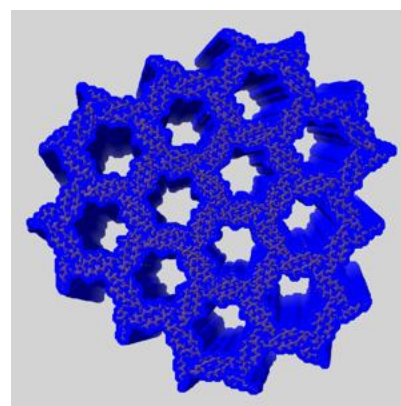
6.6.1 emd_56939_msk_1.map [i](#)



X



Y

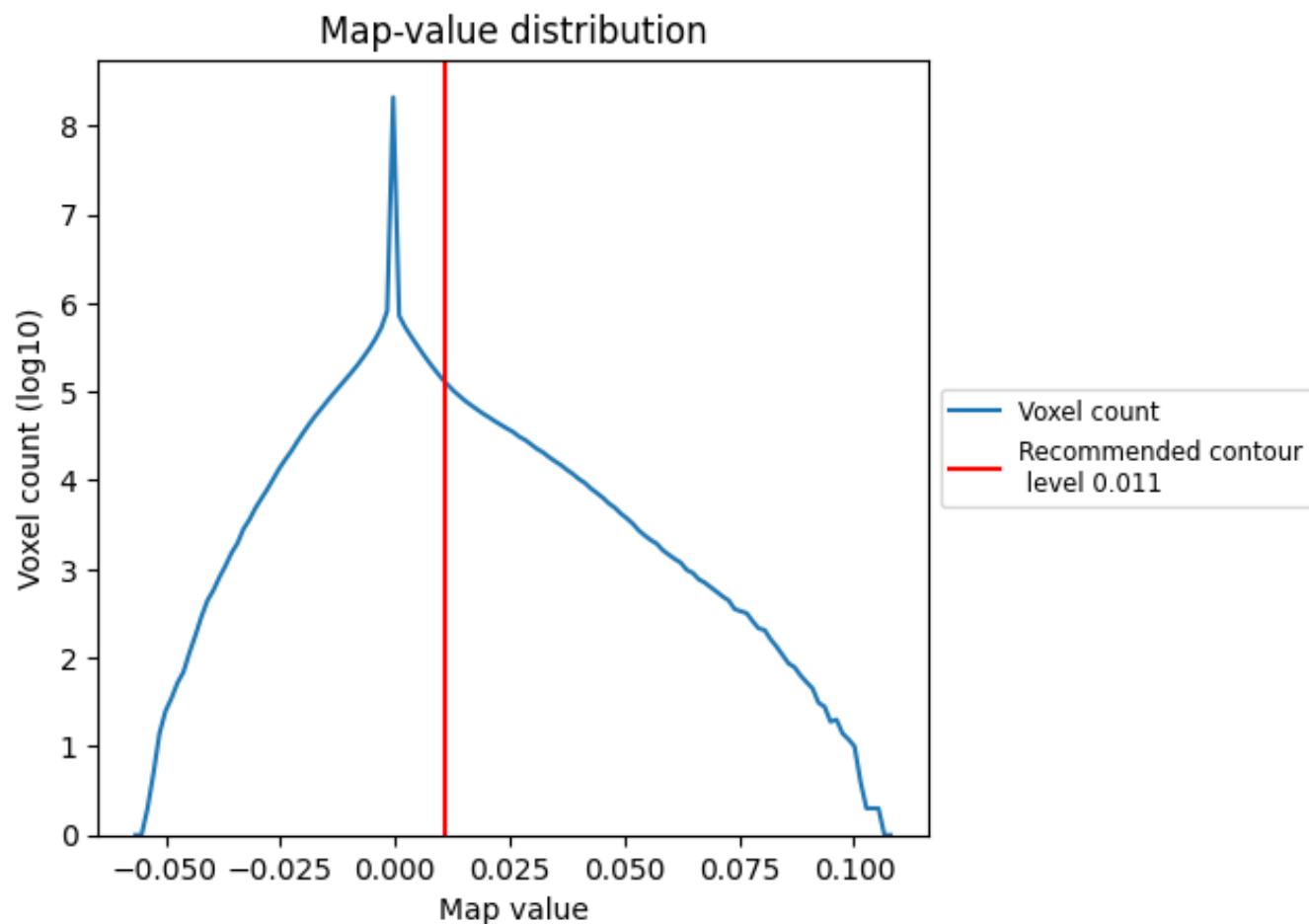


Z

7 Map analysis [i](#)

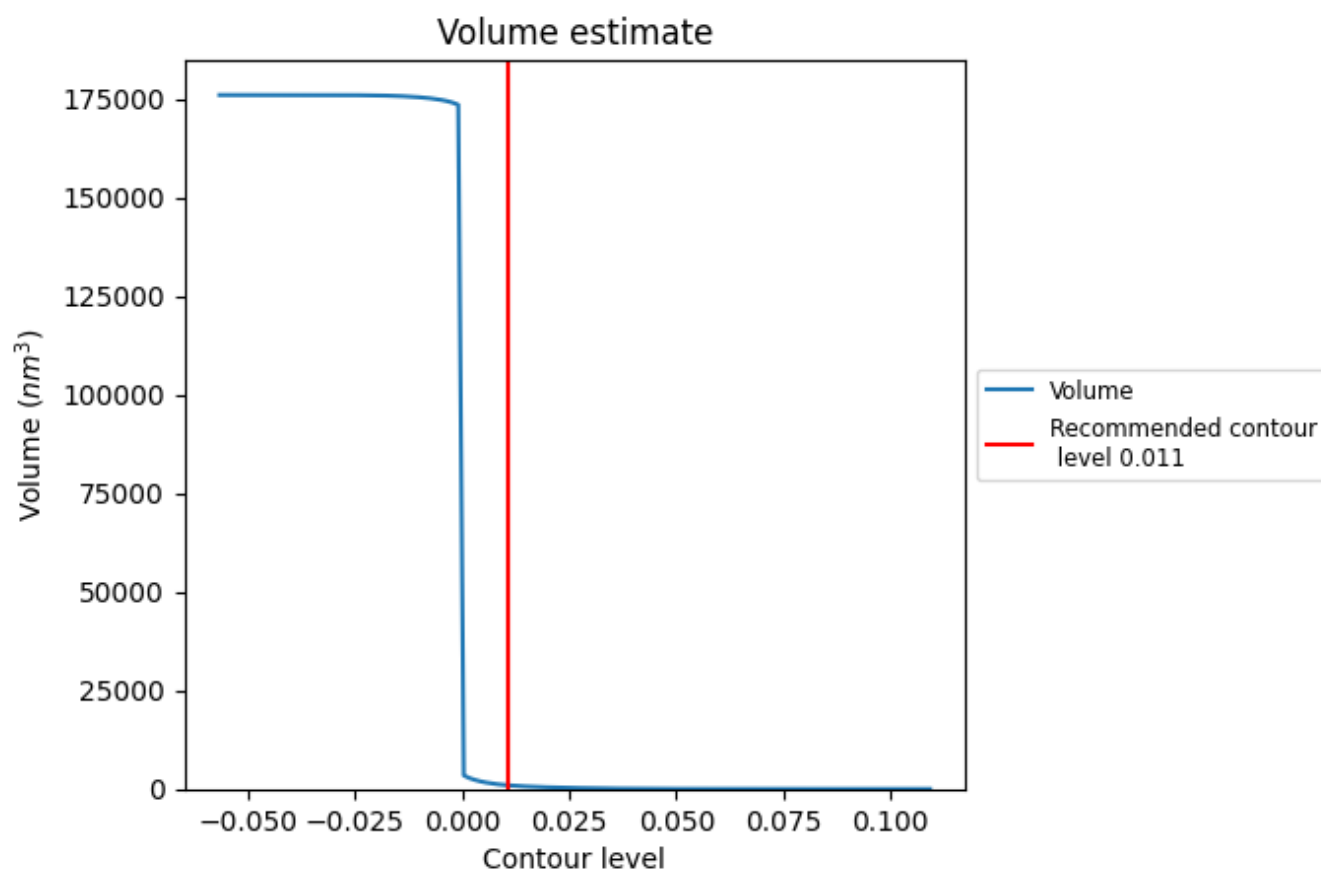
This section contains the results of statistical analysis of the map.

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.

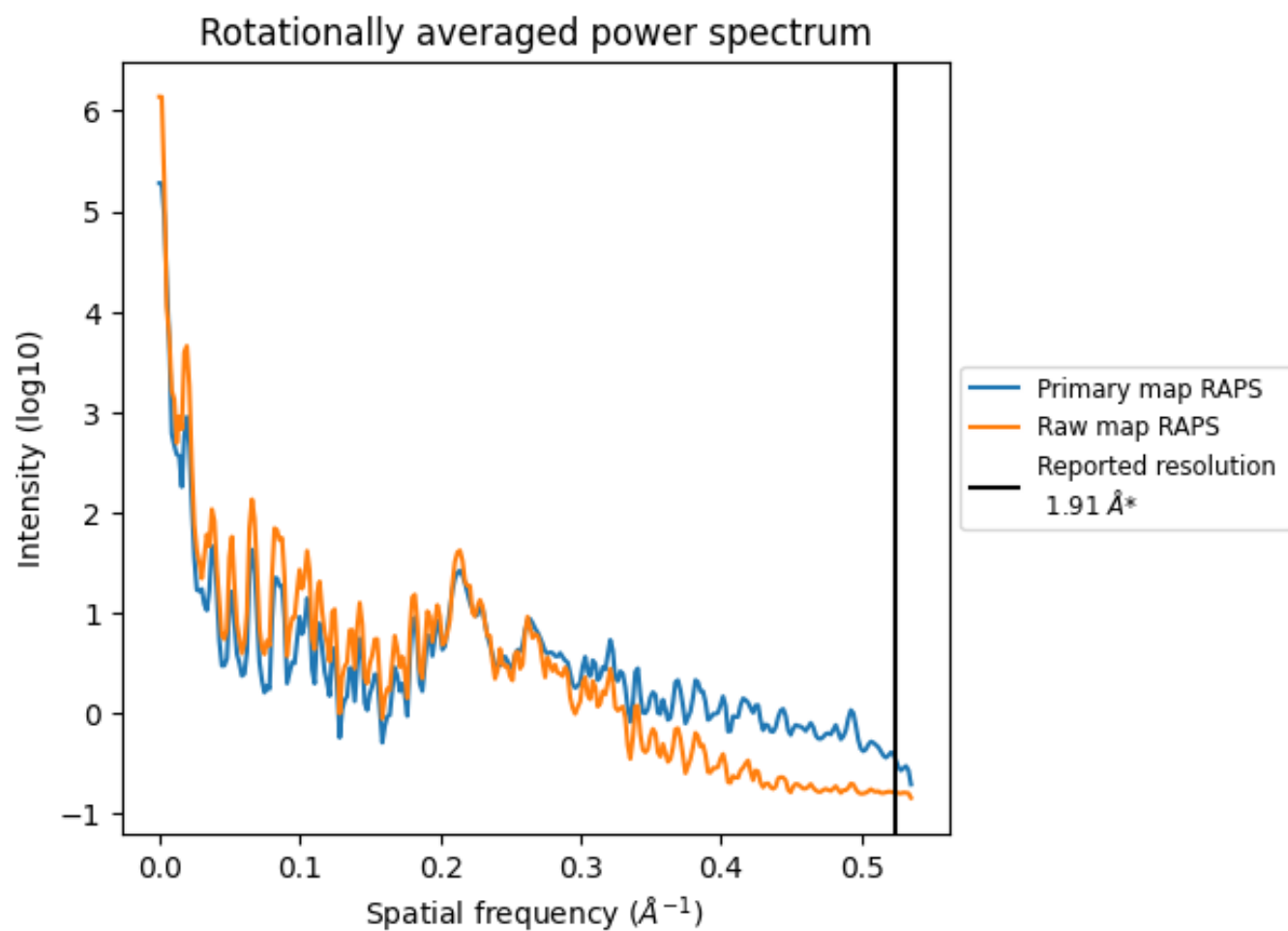
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 916 nm^3 ; this corresponds to an approximate mass of 827 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 ⓘ

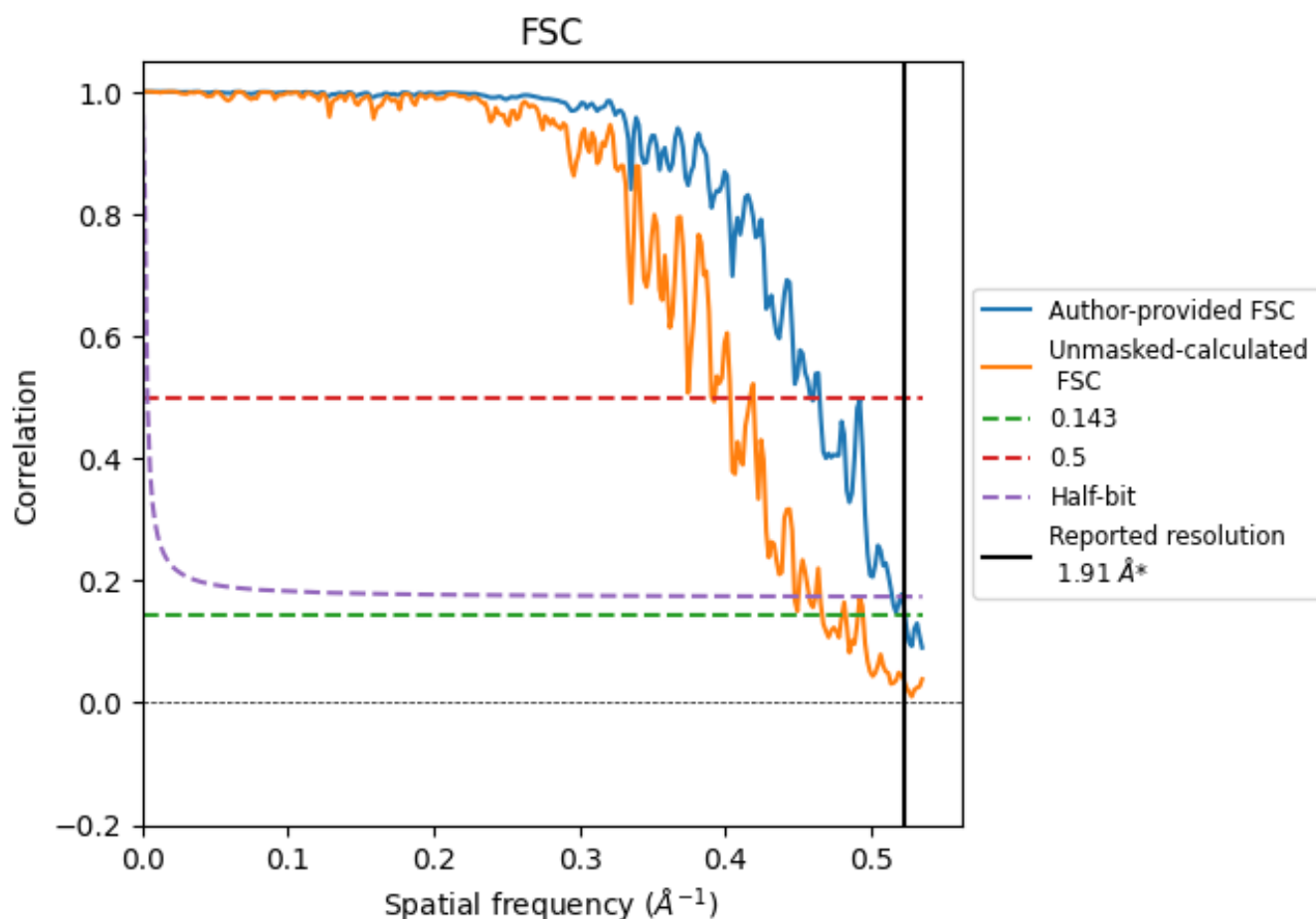


*Reported resolution corresponds to spatial frequency of 0.524 Å⁻¹

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 0.524 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.91	-	-
Author-provided FSC curve	1.91	2.18	1.94
Unmasked-calculated*	2.14	2.56	2.23

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.14 differs from the reported value 1.91 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-56939 and PDB model 28XH. Per-residue inclusion information can be found in section 3 on page 12.

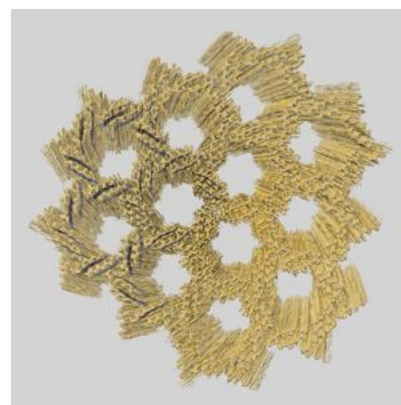
9.1 Map-model overlay [i](#)



X



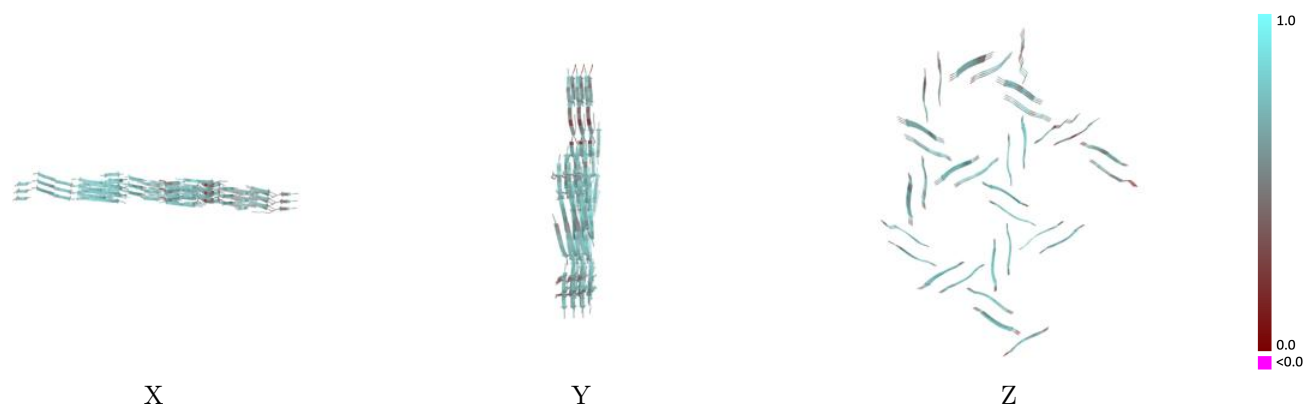
Y



Z

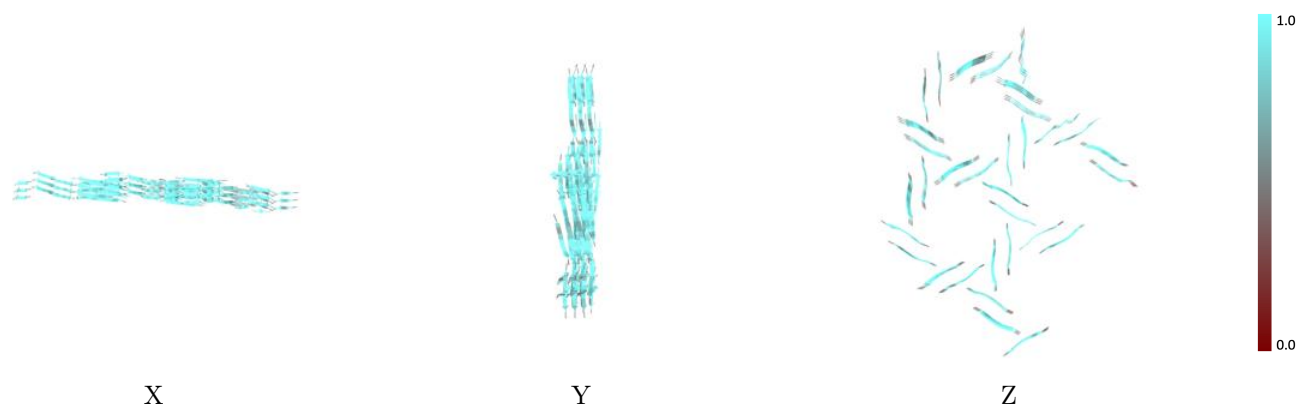
The images above show the 3D surface view of the map at the recommended contour level 0.011 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



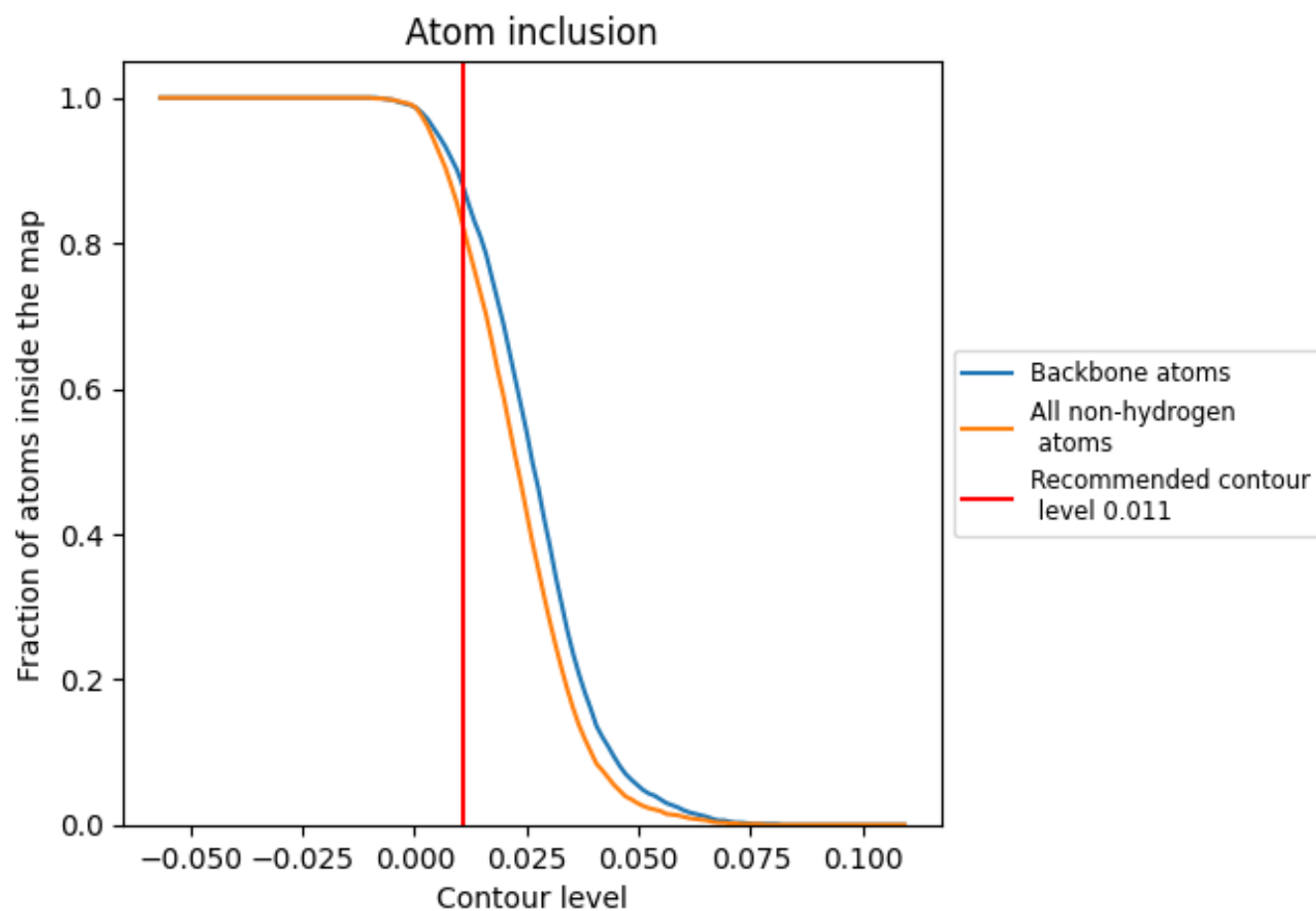
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.011).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% 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 (0.011) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8200	 0.6000
A	 0.7500	 0.4650
A1	 0.7080	 0.4590
A2	 0.7220	 0.4520
AA	 0.9030	 0.6630
AA1	 0.8890	 0.6630
AA2	 0.9030	 0.6580
AB	 0.8750	 0.6630
AB1	 0.8330	 0.6610
AB2	 0.8610	 0.6590
AC	 0.8750	 0.6230
AC1	 0.8750	 0.6320
AC2	 0.8610	 0.6280
AD	 0.8750	 0.6290
AD1	 0.8750	 0.6280
AD2	 0.8750	 0.6210
AE	 0.8330	 0.6460
AE1	 0.8470	 0.6590
AE2	 0.8470	 0.6430
AF	 0.8610	 0.5970
AG	 0.7640	 0.5550
AG1	 0.7780	 0.5620
AG2	 0.7920	 0.5730
AH	 0.8470	 0.6100
AI	 0.8470	 0.5960
B	 0.8470	 0.5480
B1	 0.8610	 0.5530
B2	 0.8610	 0.5560
C	 0.8060	 0.4930
C1	 0.8190	 0.5030
C2	 0.8190	 0.4960
D	 0.8470	 0.5440
D1	 0.8610	 0.5580
D2	 0.8890	 0.5410
E	 0.8190	 0.6030



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Chain	Atom inclusion	Q-score
E1	 0.8470	 0.6110
E2	 0.8190	 0.6000
F	 0.8060	 0.6060
F1	 0.8330	 0.6120
F2	 0.8330	 0.6060
G	 0.7920	 0.5140
G1	 0.7640	 0.5170
G2	 0.8190	 0.5240
H	 0.8190	 0.5760
H1	 0.8190	 0.5690
H2	 0.8610	 0.5740
I	 0.7360	 0.5320
I1	 0.7220	 0.5380
I2	 0.7080	 0.5340
K	 0.6390	 0.4910
K1	 0.6110	 0.4930
K2	 0.6250	 0.4920
L	 0.6810	 0.5180
L1	 0.6940	 0.5200
L3	 0.6390	 0.5100
M	 0.7640	 0.6000
M1	 0.7220	 0.6050
M2	 0.7220	 0.5980
N	 0.8470	 0.6010
N1	 0.8330	 0.6190
N2	 0.8060	 0.6070
O	 0.8470	 0.6480
O1	 0.8610	 0.6610
O2	 0.8610	 0.6590
P	 0.8750	 0.6730
P1	 0.8610	 0.6790
P2	 0.8610	 0.6710
Q	 0.9170	 0.6670
Q1	 0.9310	 0.6780
Q2	 0.9170	 0.6660
R	 0.9310	 0.6610
R1	 0.9170	 0.6700
R2	 0.9170	 0.6690
S	 0.7640	 0.5860
S1	 0.7920	 0.5880
S2	 0.7920	 0.5880
T	 0.7920	 0.5770

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Chain	Atom inclusion	Q-score
T1	 0.7920	 0.5760
T2	 0.7920	 0.5910
U	 0.7780	 0.6170
U1	 0.7920	 0.6110
U2	 0.8060	 0.6150
V	 0.8470	 0.6220
V1	 0.7640	 0.6110
V2	 0.7640	 0.5900
W	 0.8190	 0.6530
W1	 0.8330	 0.6550
W2	 0.8330	 0.6500
X	 0.8190	 0.6530
X1	 0.8060	 0.6550
X2	 0.8330	 0.6660
Y	 0.9170	 0.6710
Y1	 0.9170	 0.6660
Y2	 0.9170	 0.6580
Z	 0.8470	 0.6660
Z1	 0.8750	 0.6520
Z2	 0.8610	 0.6680