



wwPDB EM Validation Summary Report ⓘ

Mar 10, 2026 – 07:19 PM UTC

PDB ID : 9COD / pdb_00009cod
EMDB ID : EMD-45776
Title : C15 symmetrized DEV collar
Authors : Iglesias, S.M.; Hou, C.F.D.; Li, F.; Cingolani, G.
Deposited on : 2024-07-16
Resolution : 4.70 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

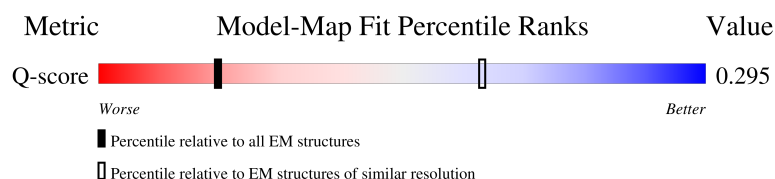
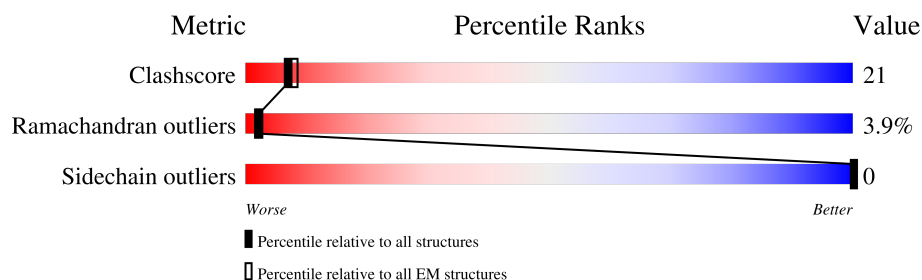
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.70 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	217187	24013	-
Ramachandran outliers	211220	23611	-
Sidechain outliers	210688	23127	-
Q-score	-	25397	1989 (4.20 - 5.20)

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	1090	
1	B	1090	
1	C	1090	
1	D	1090	

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Mol	Chain	Length	Quality of chain
1	E	1090	 6% . 90%
1	F	1090	 6% . 90%
1	G	1090	 6% . 90%
1	H	1090	 6% . 90%
1	I	1090	 6% . 90%
1	J	1090	 6% . 90%
1	K	1090	 6% . 90%
1	L	1090	 6% . 90%
1	M	1090	 6% . 90%
1	N	1090	 6% . 90%
1	O	1090	 6% . 90%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12405 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 SGNH hydrolase-type esterase domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	105	Total	C	N	O	S	0	0
			827	520	126	175	6		
1	B	105	Total	C	N	O	S	0	0
			827	520	126	175	6		
1	C	105	Total	C	N	O	S	0	0
			827	520	126	175	6		
1	D	105	Total	C	N	O	S	0	0
			827	520	126	175	6		
1	E	105	Total	C	N	O	S	0	0
			827	520	126	175	6		
1	F	105	Total	C	N	O	S	0	0
			827	520	126	175	6		
1	G	105	Total	C	N	O	S	0	0
			827	520	126	175	6		
1	H	105	Total	C	N	O	S	0	0
			827	520	126	175	6		
1	I	105	Total	C	N	O	S	0	0
			827	520	126	175	6		
1	J	105	Total	C	N	O	S	0	0
			827	520	126	175	6		
1	K	105	Total	C	N	O	S	0	0
			827	520	126	175	6		
1	L	105	Total	C	N	O	S	0	0
			827	520	126	175	6		
1	M	105	Total	C	N	O	S	0	0
			827	520	126	175	6		
1	N	105	Total	C	N	O	S	0	0
			827	520	126	175	6		
1	O	105	Total	C	N	O	S	0	0
			827	520	126	175	6		

3 Residue-property plots

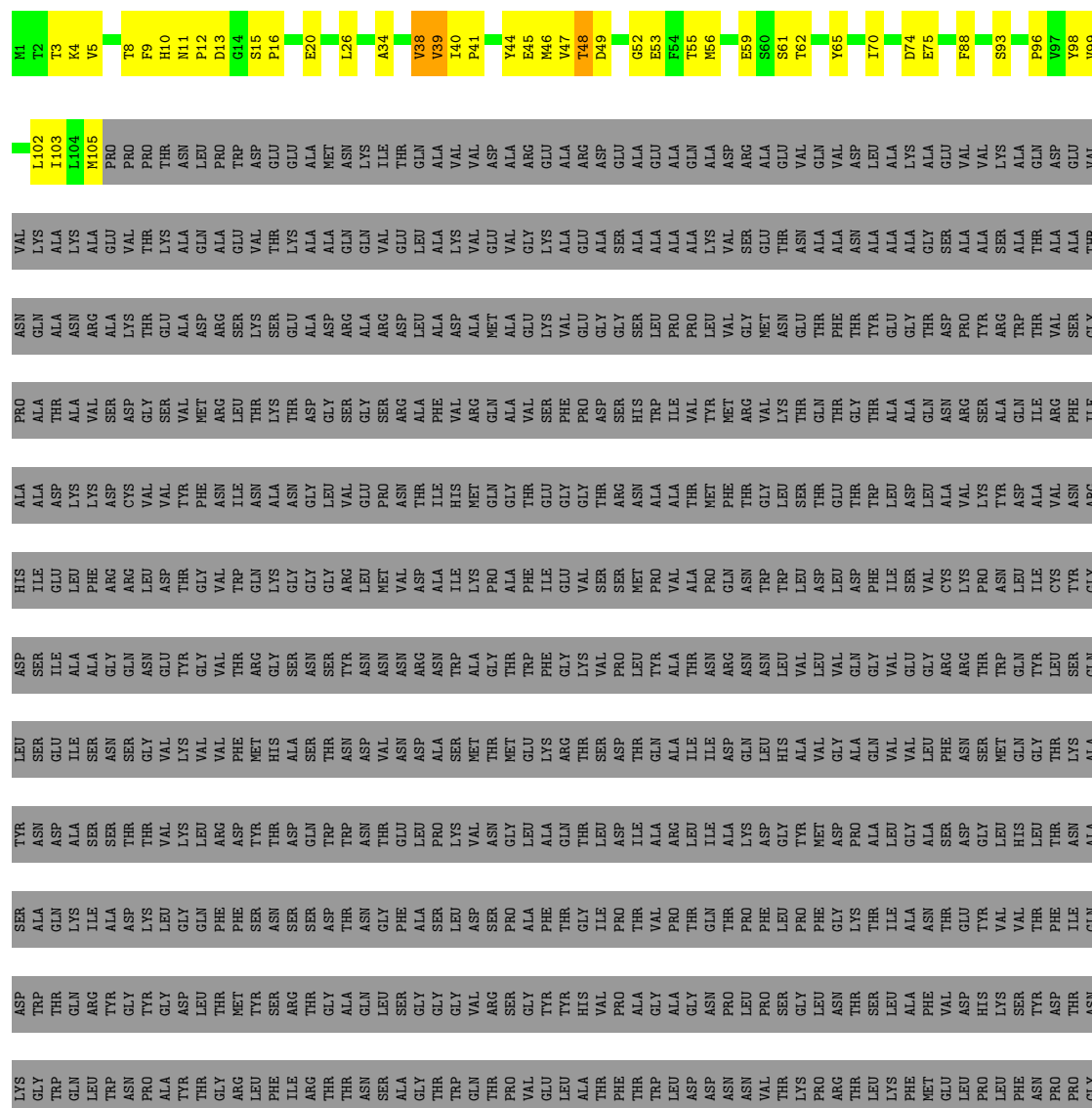
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



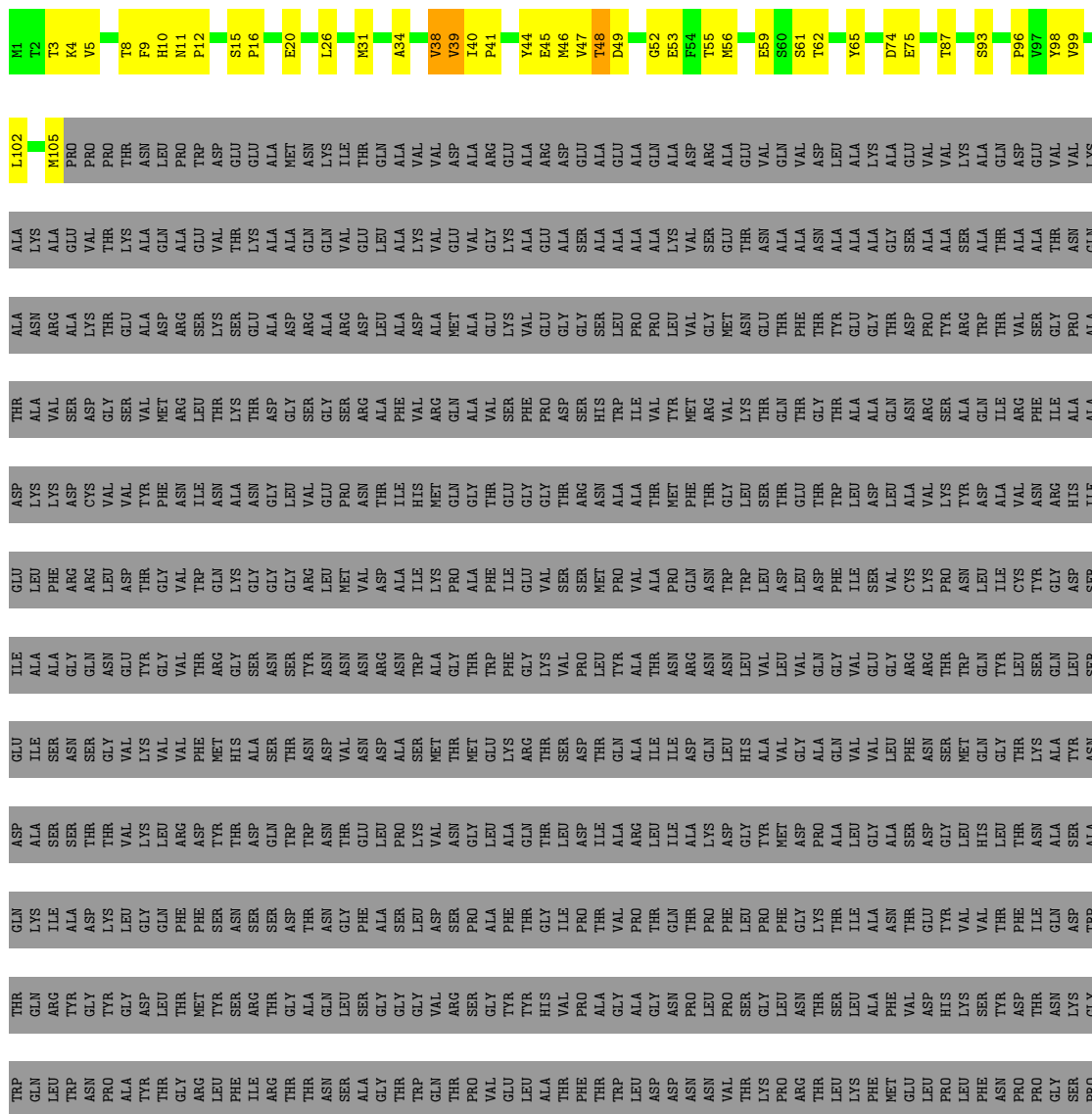
- Molecule 1: SGNH hydrolase-type esterase domain-containing protein

Chain C:  6% 1% 93%



- Molecule 1: SGNH hydrolase-type esterase domain-containing protein

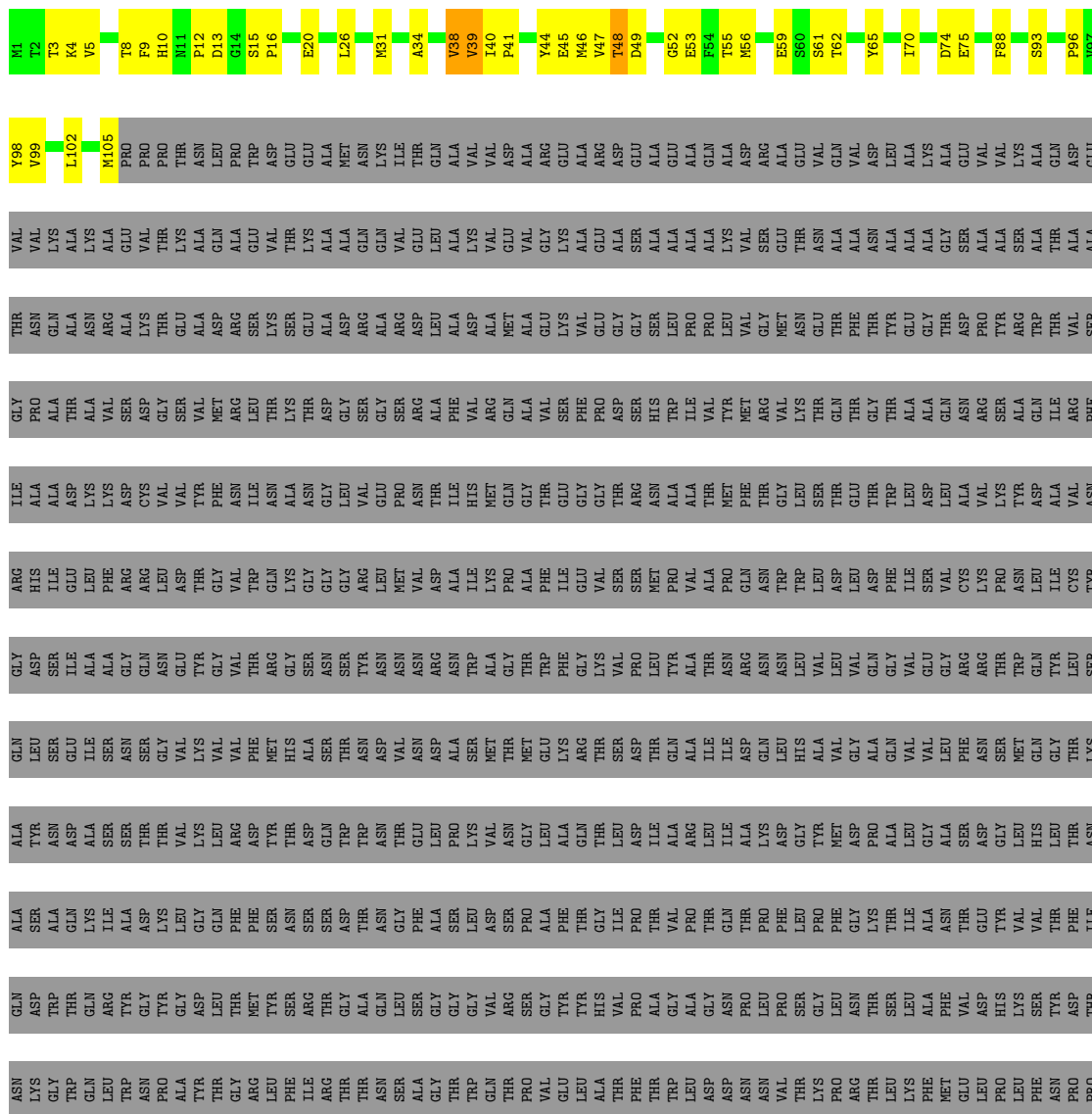
Chain D: 6% 90%





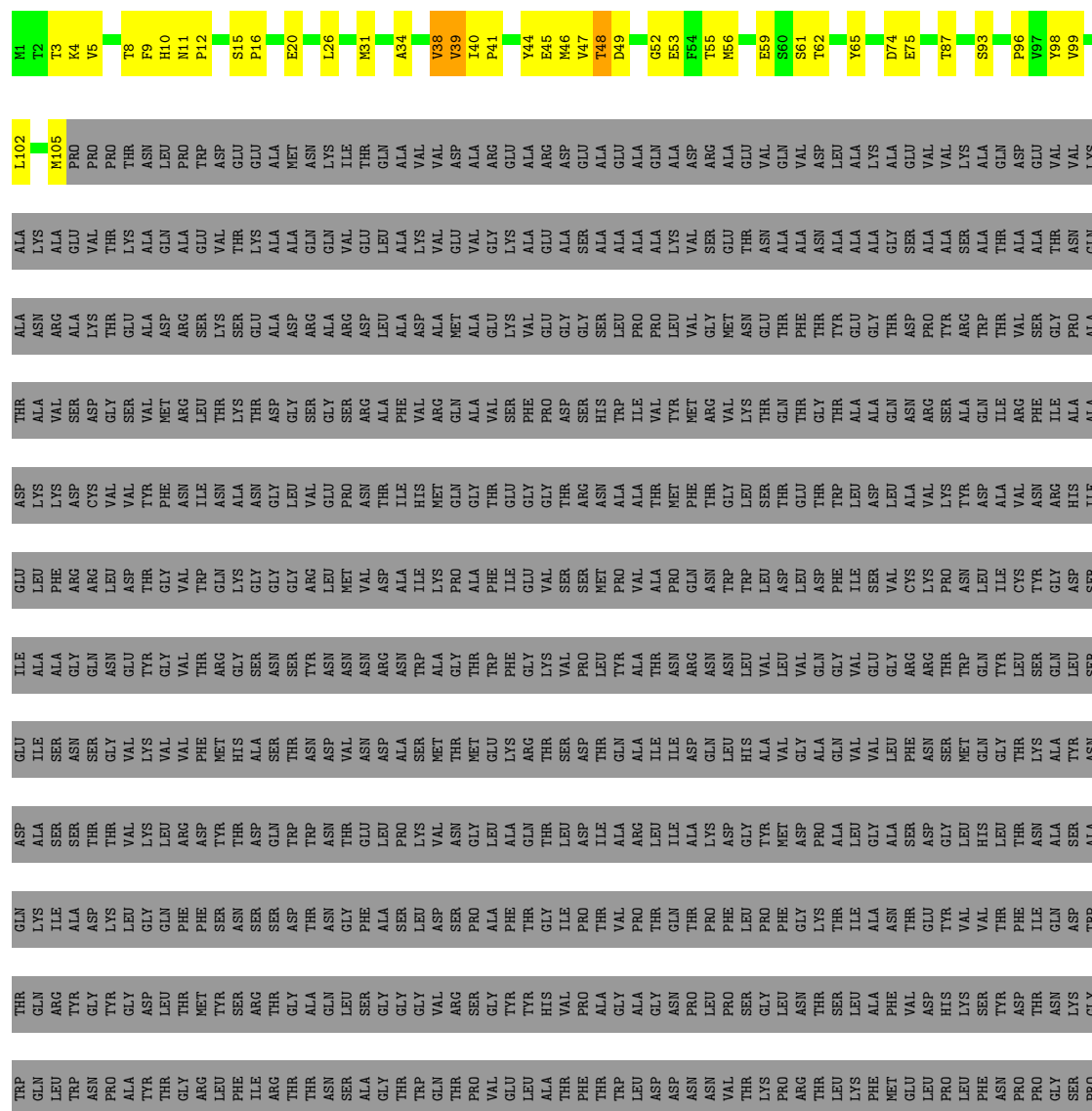
- Molecule 1: SGNH hydrolase-type esterase domain-containing protein

Chain F: 6% 90%



- Molecule 1: SGNH hydrolase-type esterase domain-containing protein

Chain G: 6% . 90%

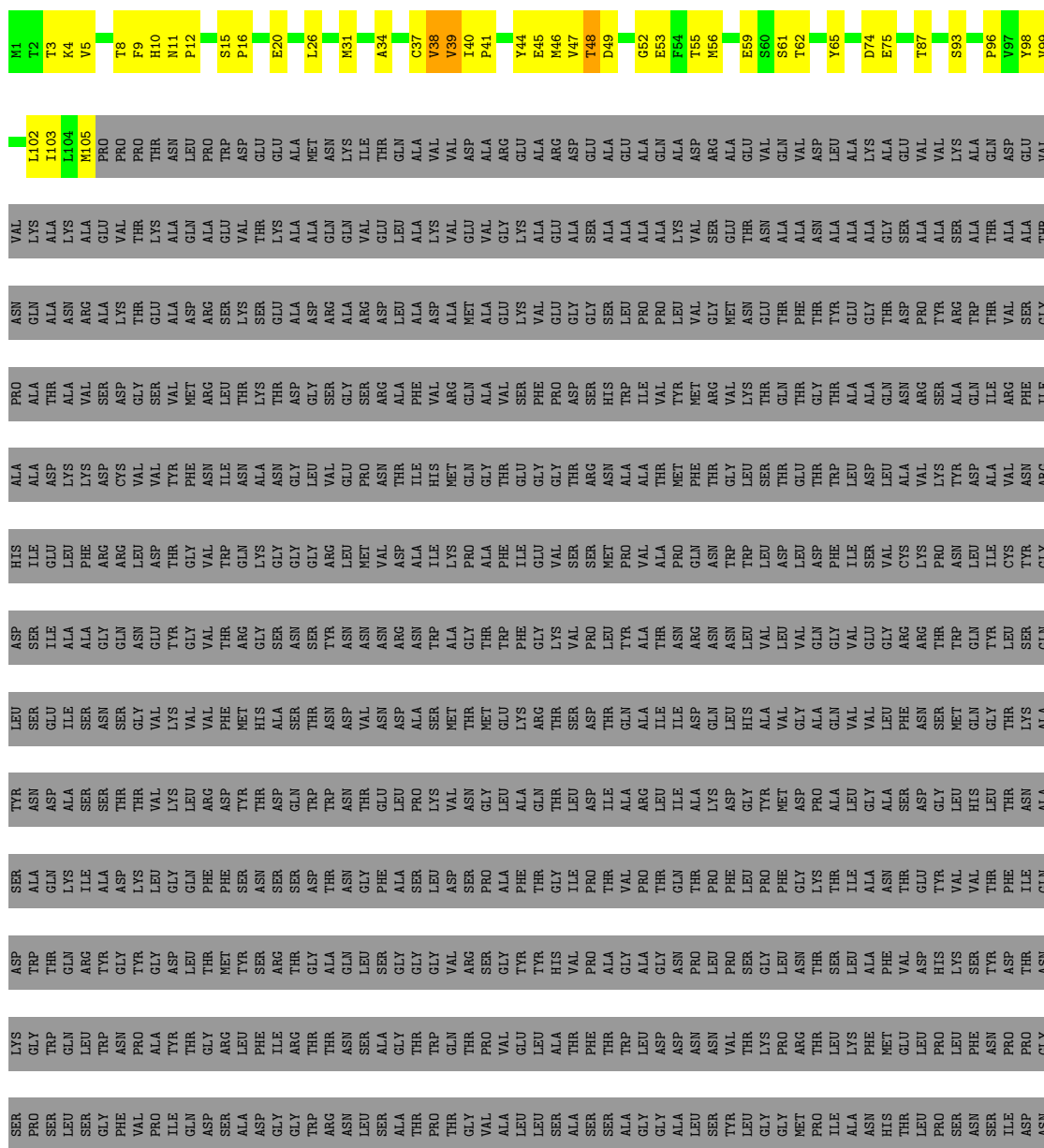




ILE	TYR	THR	SER	ALA
ARG	SER	TYR	ASN	LEU
VAL	ALA	VAL	GLY	ASN
ALA	VAL	ASP	GLU	PHE
GLY	TYR	VAL	SER	TYR
THR	THR	VAL	TRP	SER
ALA	ALA	GLN	VAL	VAL
HIS	TYR	THR	ARG	PRO
SER	THR	THR	LEU	GLY
PHE	THR	THR	LEU	THR
ALA	THR	THR	ALA	ALA
SER	SER	TYR	SER	GLY
THR	THR	PRO	ASN	LEU
SER	SER	MET	GLN	PRO
PHE	PHE	GLY	LEU	LEU
ILE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

- Molecule 1: SGNH hydrolase-type esterase domain-containing protein

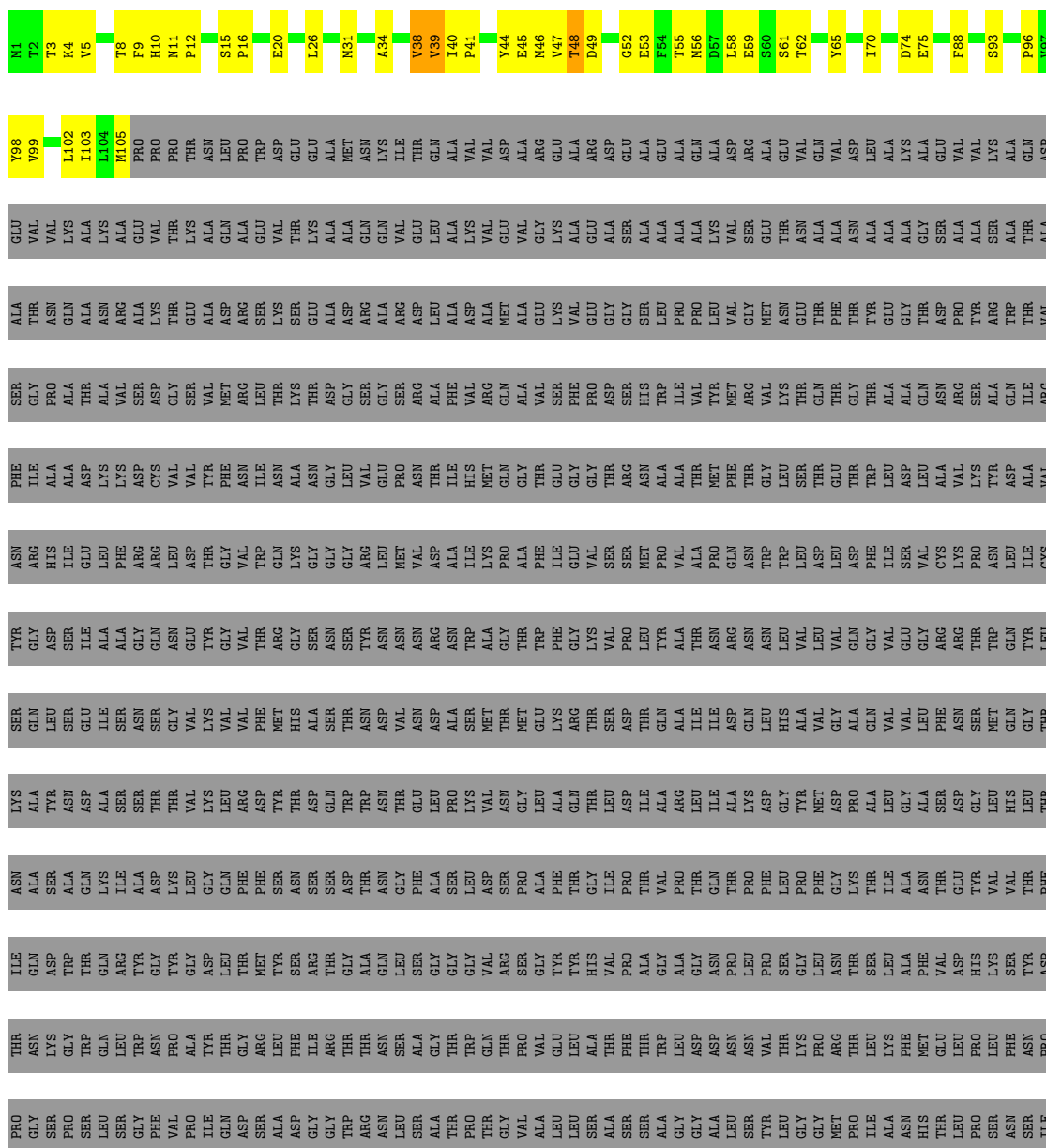
Chain I: 6% . 90%



[illegible]

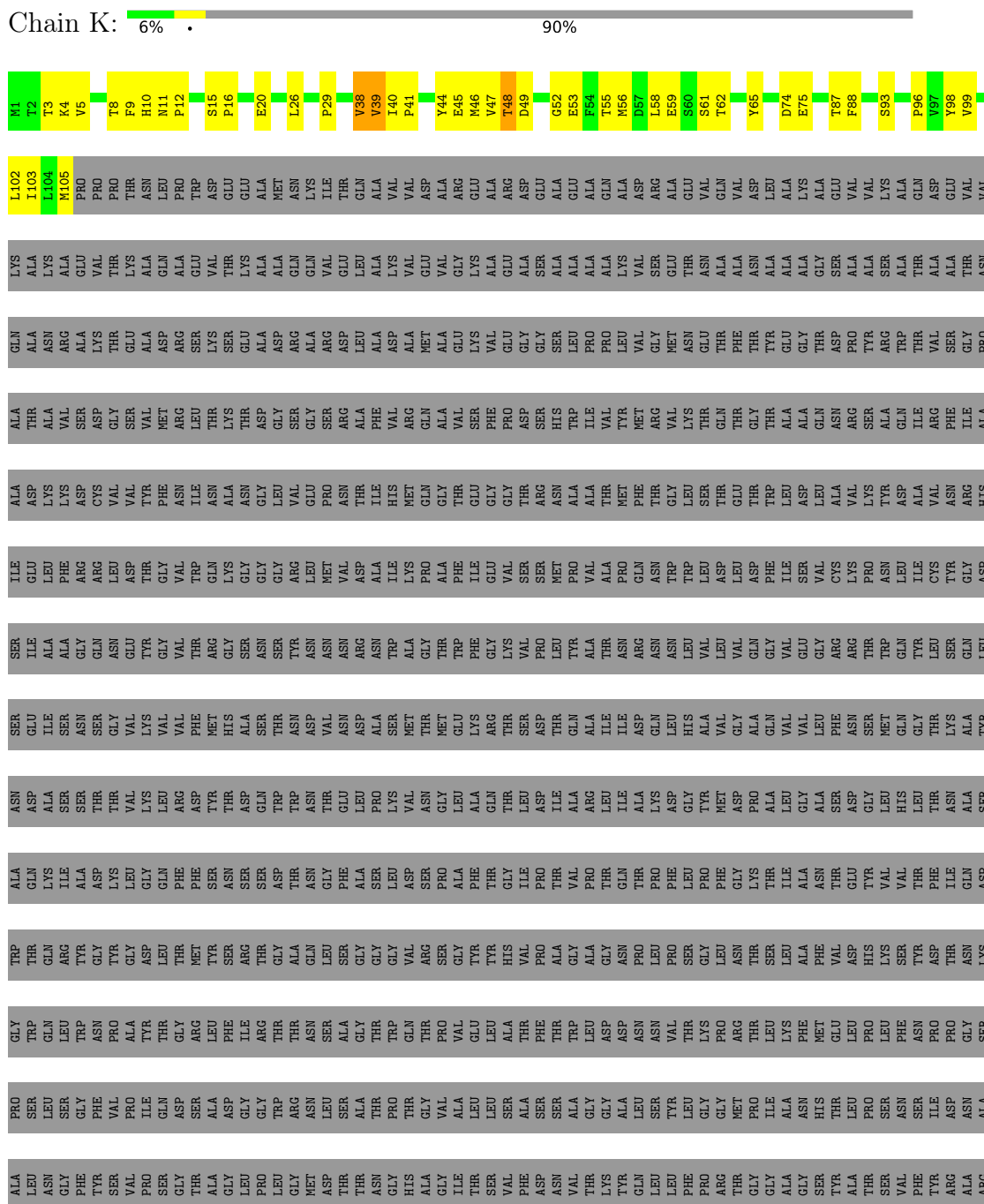
- Molecule 1: SGNH hydrolase-type esterase domain-containing protein

Chain J: 6% 1% 90%



[illegible]

- Molecule 1: SGNH hydrolase-type esterase domain-containing protein



- Molecule 1: SGNH hydrolase-type esterase domain-containing protein

[illegible]

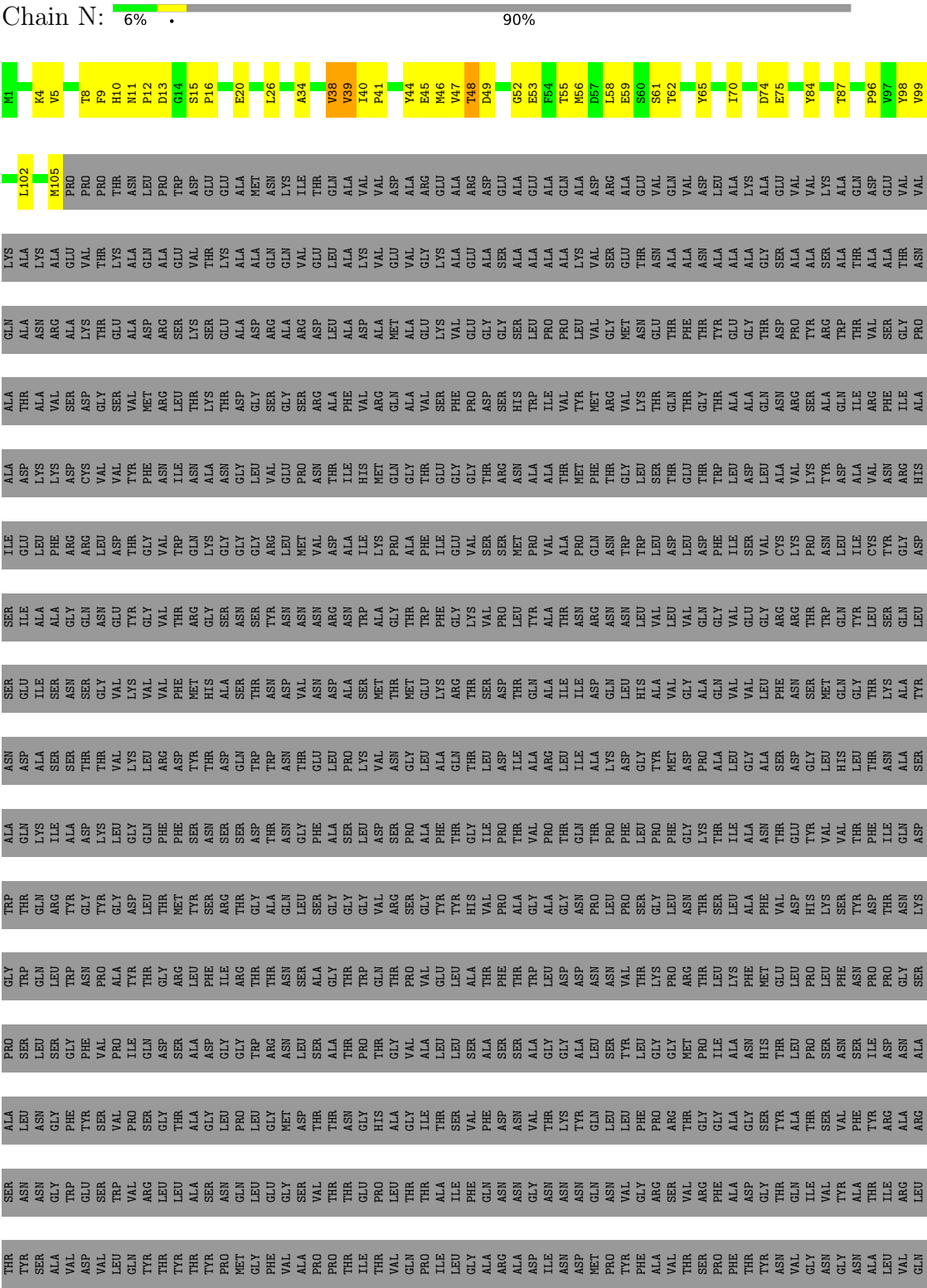
- Molecule 1: SGNH hydrolase-type esterase domain-containing protein

Chain M:  6% 90%

[illegible]

VAL
ALA
GLY
TYR
THR
ALA
HIS
SER
PHE
PHE
ALA
SER
THR
SER
PHE
PHE
ILE
ASN
CYS
VAL
ALA
VAL
VAL
ALA
VAL
GLY
GLY
ARG
TRP
TRP
LYS

● Molecule 1: SGNH hydrolase-type esterase domain-containing protein



ILE
TYR
ARG
VAL
ALA
GLY
TYR
THR
ALA
HIS
SER
PHE
ALA
SER
THR
SER
PHE
ILE
ASN
CYS
ALA
VAL
VAL
ALA
VAL
GLY
ARG
TRP
LYS

● Molecule 1: SGNH hydrolase-type esterase domain-containing protein



M1	K4	V5	T8	F9	H10	N11	P12	S15	P16	E20	L26	V38	V39	T40	P41	Y44	E45	M46	V47	T48	D49	G52	E53	F54	T55	M56	E59	S60	S61	T62	Y65	I70	D74	E75	T87	F88	P96	Y97	Y98	V99	L102	I103	L104	M105		
PRO	PRO	PRO	THR	LEU	PRO	TRP	GLU	GLU	ALA	ASN	ILE	GLN	VAL	VAL	ASP	ALA	GLU	GLU	ALA	ARG	ASP	GLU	ALA	GLN	ALA	ASP	ASP	GLY	ALA	VAL	GLN	ALA	LYS	ALA	GLU	VAL	VAL	GLN	ASP	GLU	GLU	VAL	LYS	ALA	LYS	ALA
GLU	VAL	THR	LYS	ALA	GLN	VAL	THR	LYS	ALA	GLN	VAL	ARG	LYS	VAL	VAL	VAL	LYS	VAL	ALA	GLU	ALA	SER	ALA	PRO	LEU	LYS	VAL	SER	THR	ASN	VAL	ALA	ALA	GLY	THR	GLY	ASP	VAL	VAL	THR	ALA	ASN	ARG	VAL	ALA	
ALA	LYS	THR	GLY	ASP	ARG	SER	LYS	GLU	ASP	ARG	ASP	LEU	ALA	ASP	MET	GLU	VAL	VAL	GLY	GLY	GLY	SER	PRO	PRO	GLY	LEU	GLN	MET	VAL	ASN	THR	PHE	GLU	THR	GLY	TYR	ARG	TRP	THR	VAL	GLN	THR	VAL	VAL		
SER	ASP	GLY	SER	VAL	PHE	ASN	ILE	GLY	ARG	VAL	PRO	ASN	HIS	VAL	GLN	THR	GLY	GLY	GLY	PRO	ASP	THR	ALA	THR	MET	THR	MET	PHE	GLY	LEU	GLN	THR	ALA	GLY	LEU	ASP	VAL	VAL	ASN	VAL	ARG	PHE	SER	GLY		
ASP	CYS	VAL	VAL	THR	THR	ASN	GLN	GLY	ASN	GLU	MET	VAL	ILE	LYS	GLN	GLY	GLY	GLY	GLY	SER	THR	ASN	VAL	PRO	THR	MET	PHE	THR	GLY	LEU	THR	ILE	ALA	LEU	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	PHE		
ARG	ARG	LEU	ASP	THR	THR	GLY	LYS	GLY	GLY	ARG	MET	VAL	ILE	PRO	GLN	PHE	THR	THR	VAL	SER	THR	ASN	PRO	THR	ALA	THR	GLN	GLN	THR	LEU	ASP	THR	ILE	SER	VAL	CYS	THR	VAL	THR	ASN	THR	GLY	ALA			
GLY	GLN	ASN	GLY	TYR	GLY	VAL	THR	ASN	THR	ASN	ASN	ASN	ASN	THR	GLY	THR	THR	GLY	LYS	VAL	SER	PRO	ASN	THR	ALA	ASN	ARG	ASN	LEU	VAL	GLY	VAL	GLY	VAL	GLY	ARG	GLY	THR	THR	GLN	GLY	GLY	THR	ALA		
ASN	SER	GLY	VAL	LYS	VAL	PHE	THR	THR	THR	ASN	ASN	ASN	ALA	MET	THR	GLY	GLY	LYS	VAL	SER	ASP	PRO	THR	ASN	ILE	ASN	ARG	GLN	LEU	VAL	VAL	GLY	VAL	VAL	VAL	PHE	THR	LYS	THR	ALA	ALA	SER	ALA			
SER	THR	THR	VAL	VAL	ARG	MET	THR	ASN	THR	ASN	VAL	ASN	SER	MET	THR	THR	GLY	ARG	THR	THR	ASN	THR	GLN	ILE	ILE	ASN	GLN	LEU	HIS	ALA	VAL	VAL	GLY	VAL	LEU	PHE	THR	THR	LYS	ALA	ALA	SER	ALA			
THR	THR	THR	THR	THR	THR	HIS	THR	THR	THR	THR	THR	GLU	LYS	VAL	ASN	GLY	GLY	GLY	THR	SER	ASP	THR	ILE	THR	ILE	ALA	GLN	THR	GLY	ALA	GLY	THR	ALA	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR		
ALA	ASP	LYS	GLY	GLN	PHE	SER	ASN	GLY	ASP	GLY	PHE	THR	LEU	ASP	SER	PRO	THR	THR	GLY	LEU	ASP	PRO	GLN	THR	THR	THR	ALA	ASP	PRO	PHE	THR	GLY	LYS	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR		
TYR	GLY	TYR	GLY	ASP	LEU	THR	MET	THR	GLY	GLN	SER	PHE	GLY	GLY	VAL	ANG	SER	VAL	HIS	GLY	ILE	VAL	ASN	GLY	THR	GLY	ASN	PRO	GLY	LEU	PHE	ALA	ALA	ASN	PHE	LYS	THR	THR	THR	THR	THR	THR	THR			
TRP	ASN	PRO	THR	THR	GLY	ARG	THR	THR	THR	ASN	SER	THR	GLN	THR	THR	PRO	GLY	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR		
GLY	PHE	VAL	PRO	ILE	GLN	SER	MET	ASN	LEU	THR	ALA	GLY	THR	PRO	GLY	VAL	VAL	LEU	SER	ALA	THR	PRO	ALA	GLY	GLY	ALA	LEU	THR	GLY	GLY	GLY	THR	MET	ALA	ASN	GLY	THR	GLY	THR	THR	THR	THR	THR			
PHE	THR	SER	VAL	PRO	SER	GLY	GLY	THR	GLY	THR	SER	THR	GLY	HIS	ALA	GLY	VAL	THR	PHE	ALA	THR	ASN	GLN	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR			
TRP	GLU	SER	VAL	ARG	LEU	SER	ALA	GLU	GLY	GLY	VAL	GLU	GLY	PRO	GLY	VAL	GLY	LEU	GLY	GLN	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY			
VAL	ASP	VAL	GLN	TYR	THR	THR	THR	PRO	THR	ALA	PRO	PRO	ILE	THR	THR	GLN	GLN	ILE	GLY	ALA	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR		
ALA	GLY	TYR	ALA	HIS	SER	PHE	ALA	THR	THR	CYS	ALA	VAL	ALA	VAL	GLY	ARG	THR	GLY	GLY	ALA	ARG	ILE	ASN	ASN	ASP	MET	THR	THR	PHE	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	3200	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.035	Depositor
Minimum map value	-0.017	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0018	Depositor
Map size (Å)	573.44, 573.44, 573.44	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.12, 1.12, 1.12	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	0.21	0/847	0.67	2/1156 (0.2%)
1	B	0.21	0/847	0.67	2/1156 (0.2%)
1	C	0.21	0/847	0.67	2/1156 (0.2%)
1	D	0.21	0/847	0.67	2/1156 (0.2%)
1	E	0.21	0/847	0.67	2/1156 (0.2%)
1	F	0.21	0/847	0.67	2/1156 (0.2%)
1	G	0.21	0/847	0.68	2/1156 (0.2%)
1	H	0.21	0/847	0.68	2/1156 (0.2%)
1	I	0.21	0/847	0.67	2/1156 (0.2%)
1	J	0.21	0/847	0.67	2/1156 (0.2%)
1	K	0.21	0/847	0.67	2/1156 (0.2%)
1	L	0.21	0/847	0.67	2/1156 (0.2%)
1	M	0.21	0/847	0.67	2/1156 (0.2%)
1	N	0.21	0/847	0.67	2/1156 (0.2%)
1	O	0.21	0/847	0.68	2/1156 (0.2%)
All	All	0.21	0/12705	0.67	30/17340 (0.2%)

There are no bond length outliers.

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	48	THR	CA-C-N	6.15	133.28	121.54
1	C	48	THR	C-N-CA	6.15	133.28	121.54
1	M	48	THR	CA-C-N	6.15	133.28	121.54
1	M	48	THR	C-N-CA	6.15	133.28	121.54
1	F	48	THR	CA-C-N	6.14	133.28	121.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	827	0	763	40	0
1	B	827	0	763	45	0
1	C	827	0	763	40	0
1	D	827	0	763	36	0
1	E	827	0	763	39	0
1	F	827	0	763	37	0
1	G	827	0	763	38	0
1	H	827	0	763	39	0
1	I	827	0	763	40	0
1	J	827	0	763	43	0
1	K	827	0	763	47	0
1	L	827	0	763	39	0
1	M	827	0	763	37	0
1	N	827	0	763	42	0
1	O	827	0	763	38	0
All	All	12405	0	11445	506	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 21.

The worst 5 of 506 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:A:38:VAL:HG13	1:A:39:VAL:H	1.34	0.93
1:F:38:VAL:HG13	1:F:39:VAL:H	1.34	0.93
1:D:38:VAL:HG13	1:D:39:VAL:H	1.34	0.93
1:K:38:VAL:HG13	1:K:39:VAL:H	1.34	0.92
1:J:38:VAL:HG13	1:J:39:VAL:H	1.34	0.92

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	103/1090 (9%)	74 (72%)	25 (24%)	4 (4%)	2	18
1	B	103/1090 (9%)	74 (72%)	25 (24%)	4 (4%)	2	18
1	C	103/1090 (9%)	74 (72%)	25 (24%)	4 (4%)	2	18
1	D	103/1090 (9%)	74 (72%)	25 (24%)	4 (4%)	2	18
1	E	103/1090 (9%)	74 (72%)	25 (24%)	4 (4%)	2	18
1	F	103/1090 (9%)	74 (72%)	25 (24%)	4 (4%)	2	18
1	G	103/1090 (9%)	74 (72%)	25 (24%)	4 (4%)	2	18
1	H	103/1090 (9%)	74 (72%)	25 (24%)	4 (4%)	2	18
1	I	103/1090 (9%)	74 (72%)	25 (24%)	4 (4%)	2	18
1	J	103/1090 (9%)	74 (72%)	25 (24%)	4 (4%)	2	18
1	K	103/1090 (9%)	74 (72%)	25 (24%)	4 (4%)	2	18
1	L	103/1090 (9%)	74 (72%)	25 (24%)	4 (4%)	2	18
1	M	103/1090 (9%)	74 (72%)	25 (24%)	4 (4%)	2	18
1	N	103/1090 (9%)	74 (72%)	25 (24%)	4 (4%)	2	18
1	O	103/1090 (9%)	74 (72%)	25 (24%)	4 (4%)	2	18
All	All	1545/16350 (9%)	1110 (72%)	375 (24%)	60 (4%)	2	18

5 of 60 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	VAL
1	A	47	VAL
1	B	38	VAL
1	B	47	VAL
1	C	38	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	94/882 (11%)	94 (100%)	0	100	100
1	B	94/882 (11%)	94 (100%)	0	100	100
1	C	94/882 (11%)	94 (100%)	0	100	100
1	D	94/882 (11%)	94 (100%)	0	100	100
1	E	94/882 (11%)	94 (100%)	0	100	100
1	F	94/882 (11%)	94 (100%)	0	100	100
1	G	94/882 (11%)	94 (100%)	0	100	100
1	H	94/882 (11%)	94 (100%)	0	100	100
1	I	94/882 (11%)	94 (100%)	0	100	100
1	J	94/882 (11%)	94 (100%)	0	100	100
1	K	94/882 (11%)	94 (100%)	0	100	100
1	L	94/882 (11%)	94 (100%)	0	100	100
1	M	94/882 (11%)	94 (100%)	0	100	100
1	N	94/882 (11%)	94 (100%)	0	100	100
1	O	94/882 (11%)	94 (100%)	0	100	100
All	All	1410/13230 (11%)	1410 (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. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	10	HIS
1	K	11	ASN
1	N	17	GLN
1	K	10	HIS
1	L	11	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.

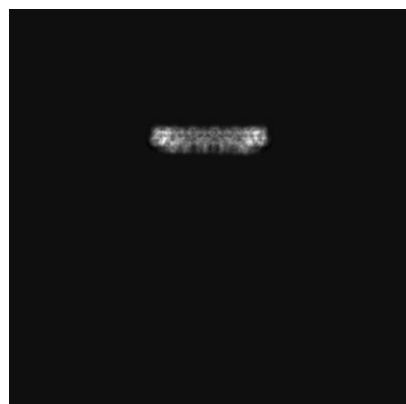
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45776. These allow visual inspection of the internal detail of the map and identification of artifacts.

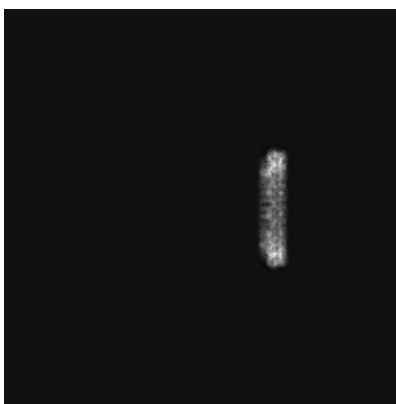
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

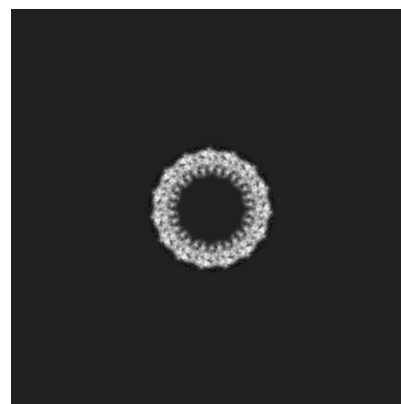
6.1.1 Primary map



X

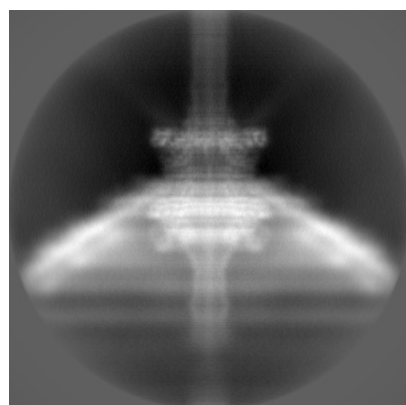


Y

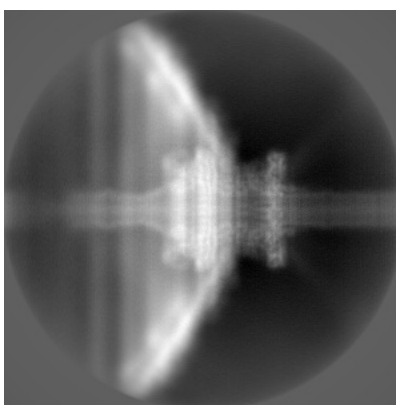


Z

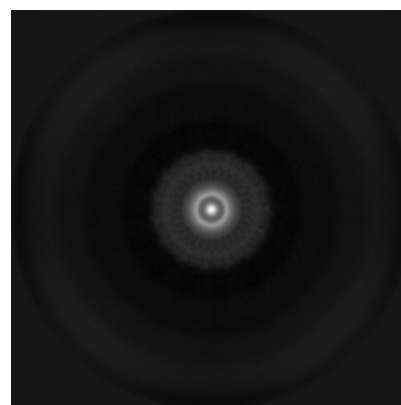
6.1.2 Raw map



X



Y



Z

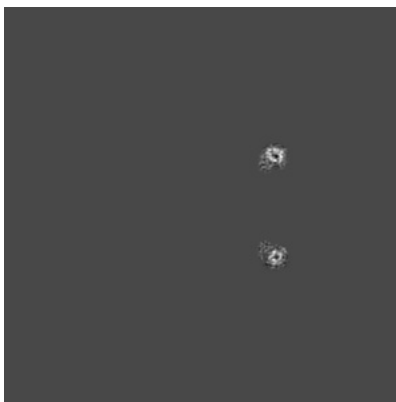
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

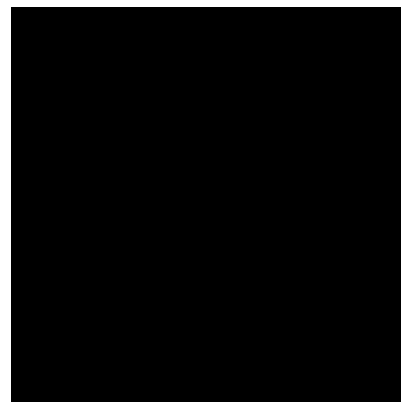
6.2.1 Primary map



X Index: 256

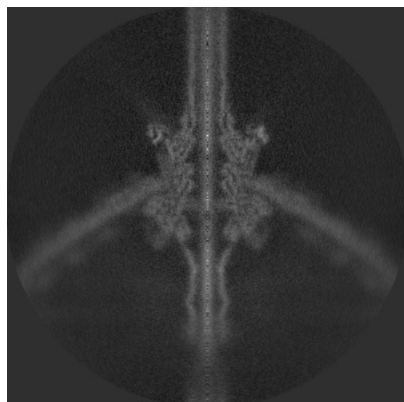


Y Index: 256

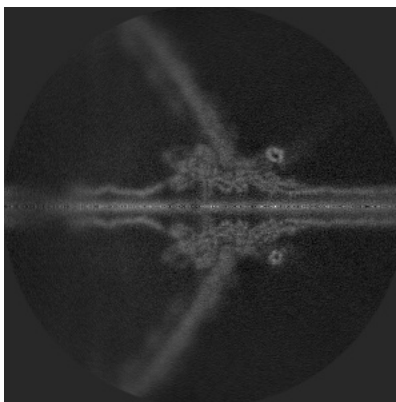


Z Index: 256

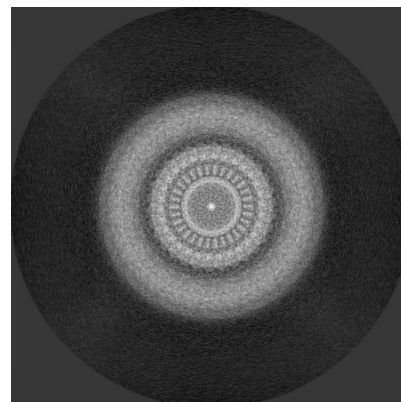
6.2.2 Raw map



X Index: 256



Y Index: 256

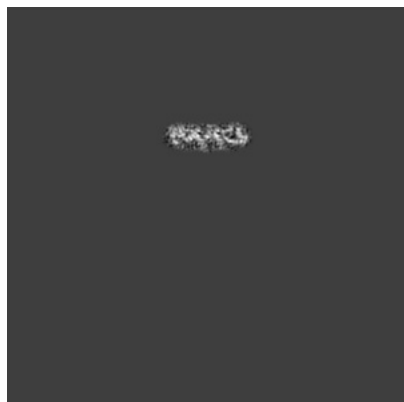


Z Index: 256

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

6.3 Largest variance slices [i](#)

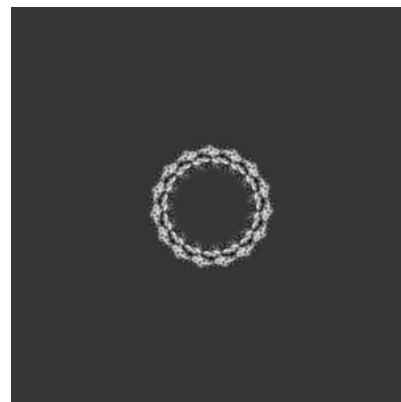
6.3.1 Primary map



X Index: 198

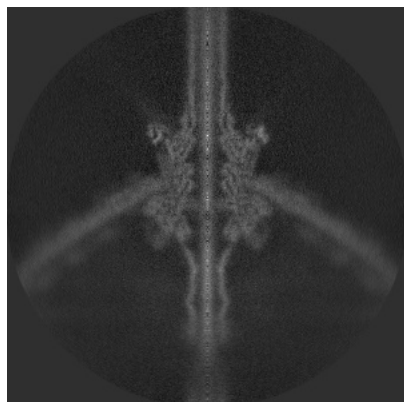


Y Index: 197

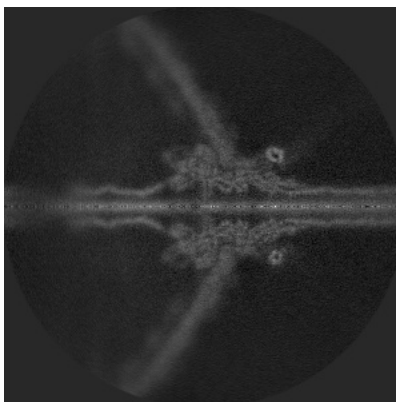


Z Index: 346

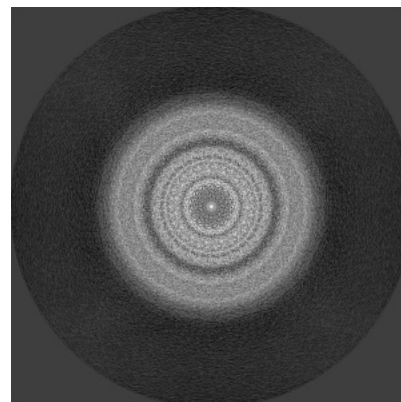
6.3.2 Raw map



X Index: 256



Y Index: 256

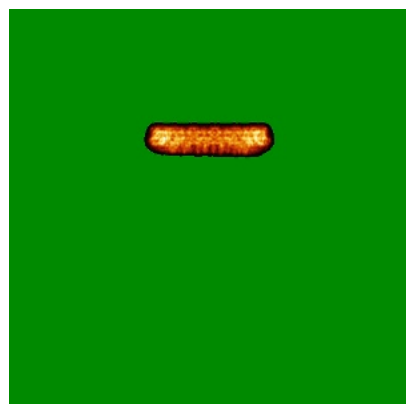


Z Index: 262

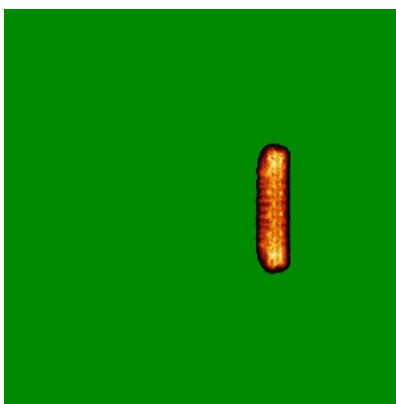
The images above show the largest variance slices of the map in three orthogonal directions.

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

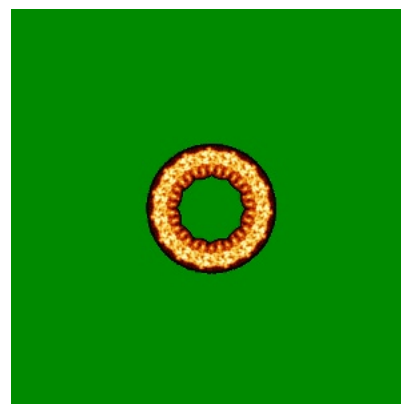
6.4.1 Primary map



X

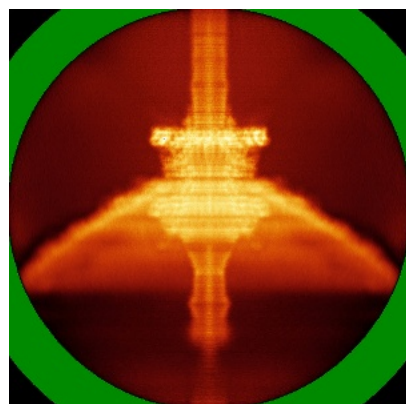


Y

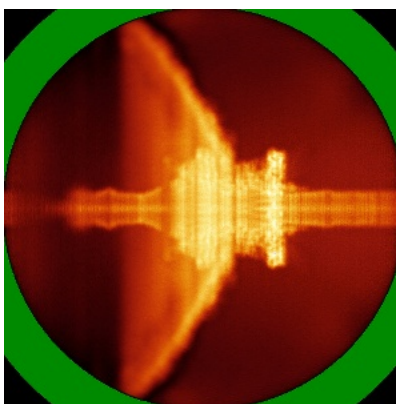


Z

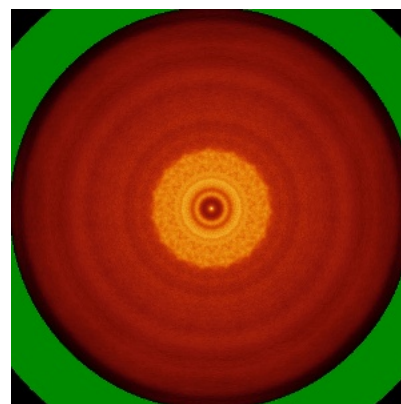
6.4.2 Raw map



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.

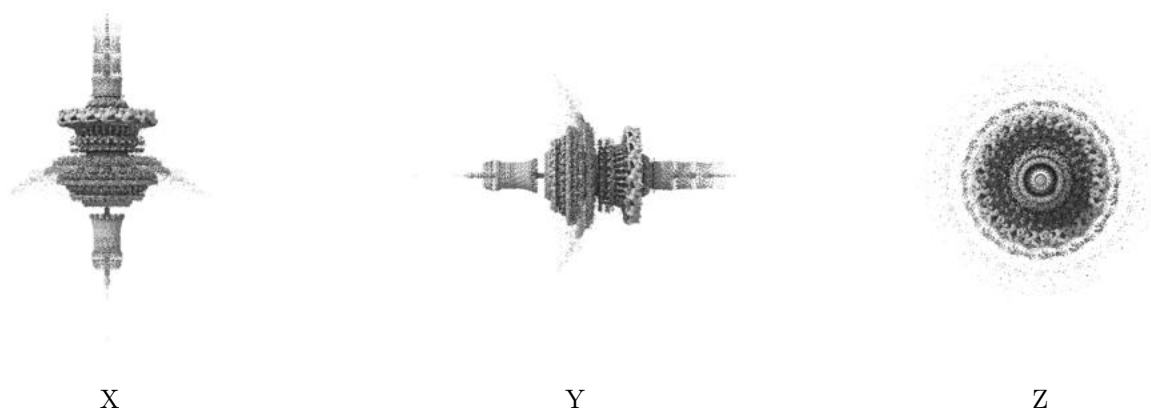
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0018. 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.

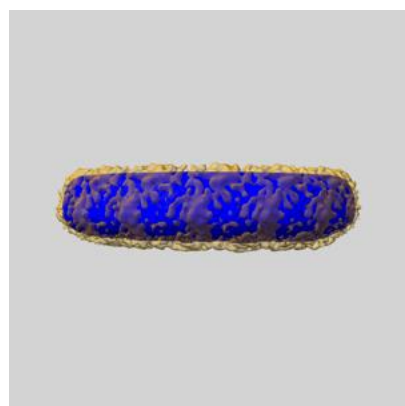
6.6 Mask visualisation [i](#)

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

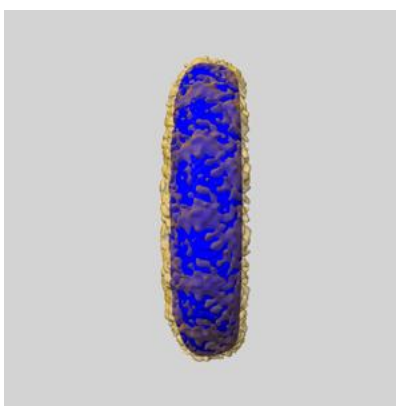
A mask typically either:

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

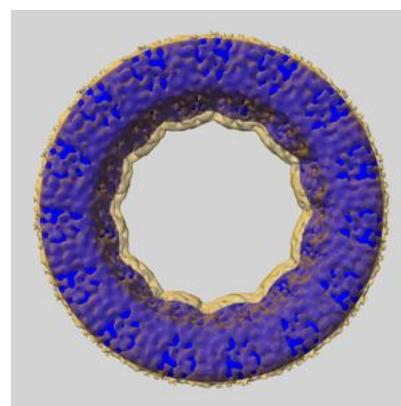
6.6.1 emd_45776_msk_1.map [i](#)



X



Y

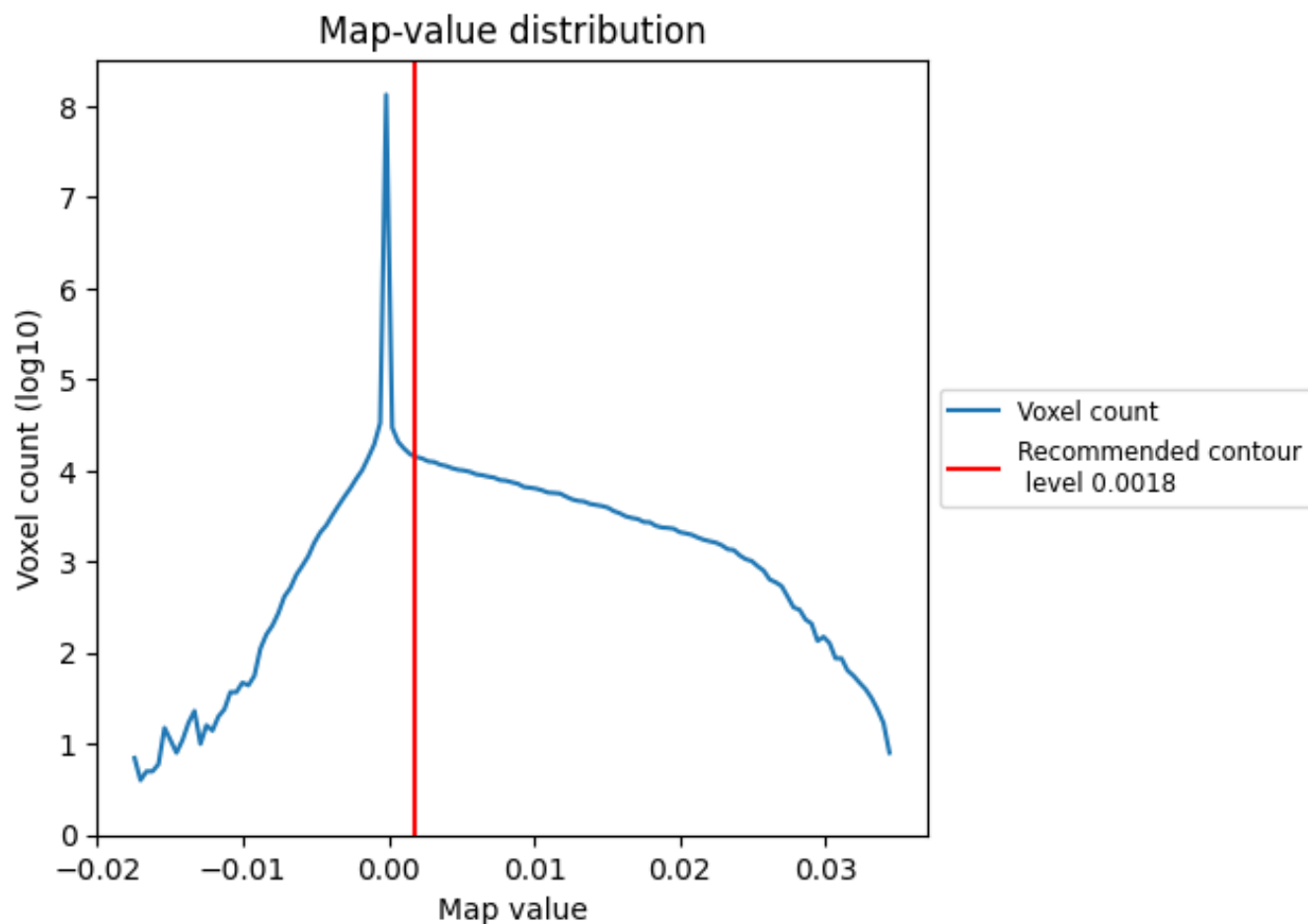


Z

7 Map analysis [i](#)

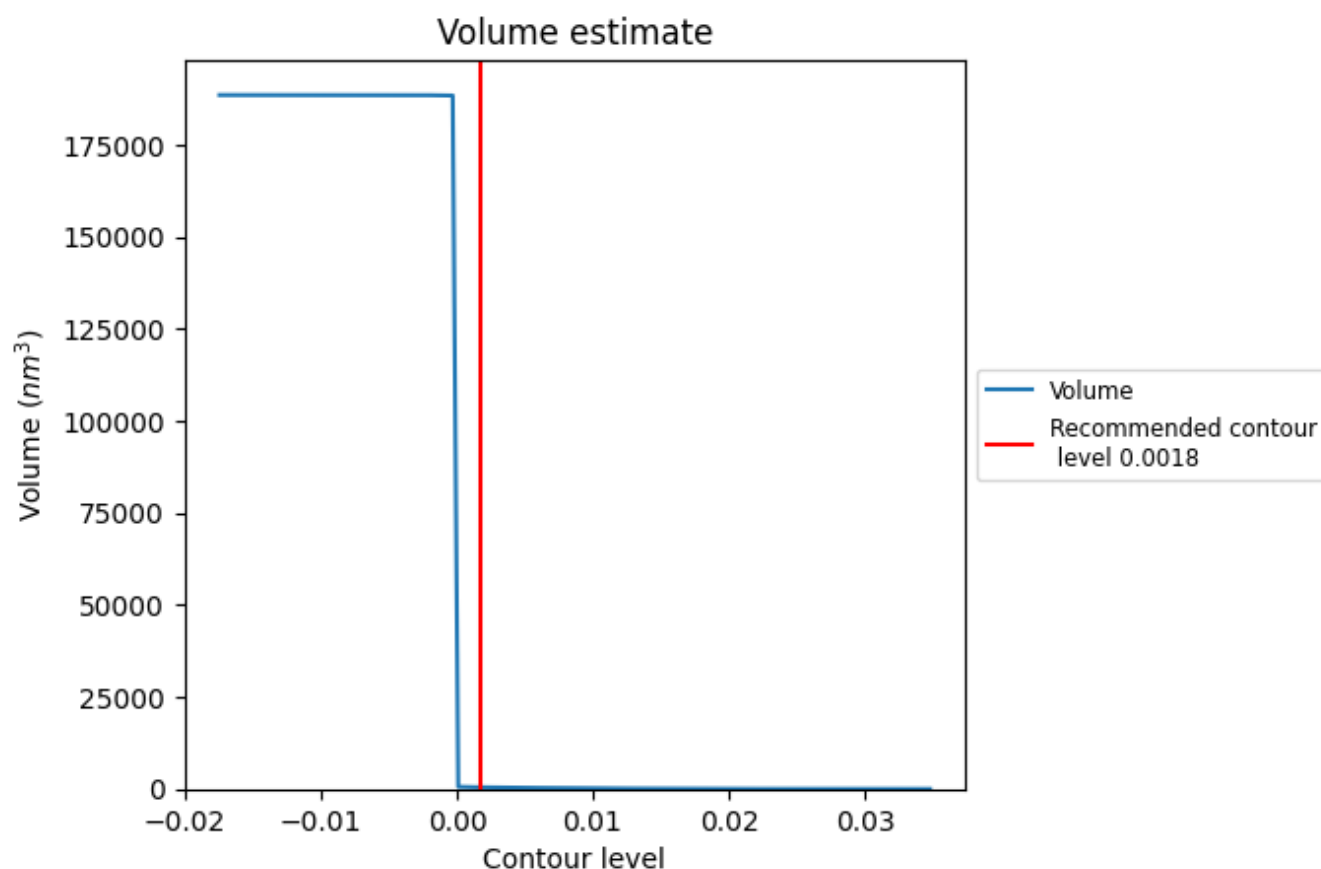
This section contains the results of statistical analysis of the map.

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.

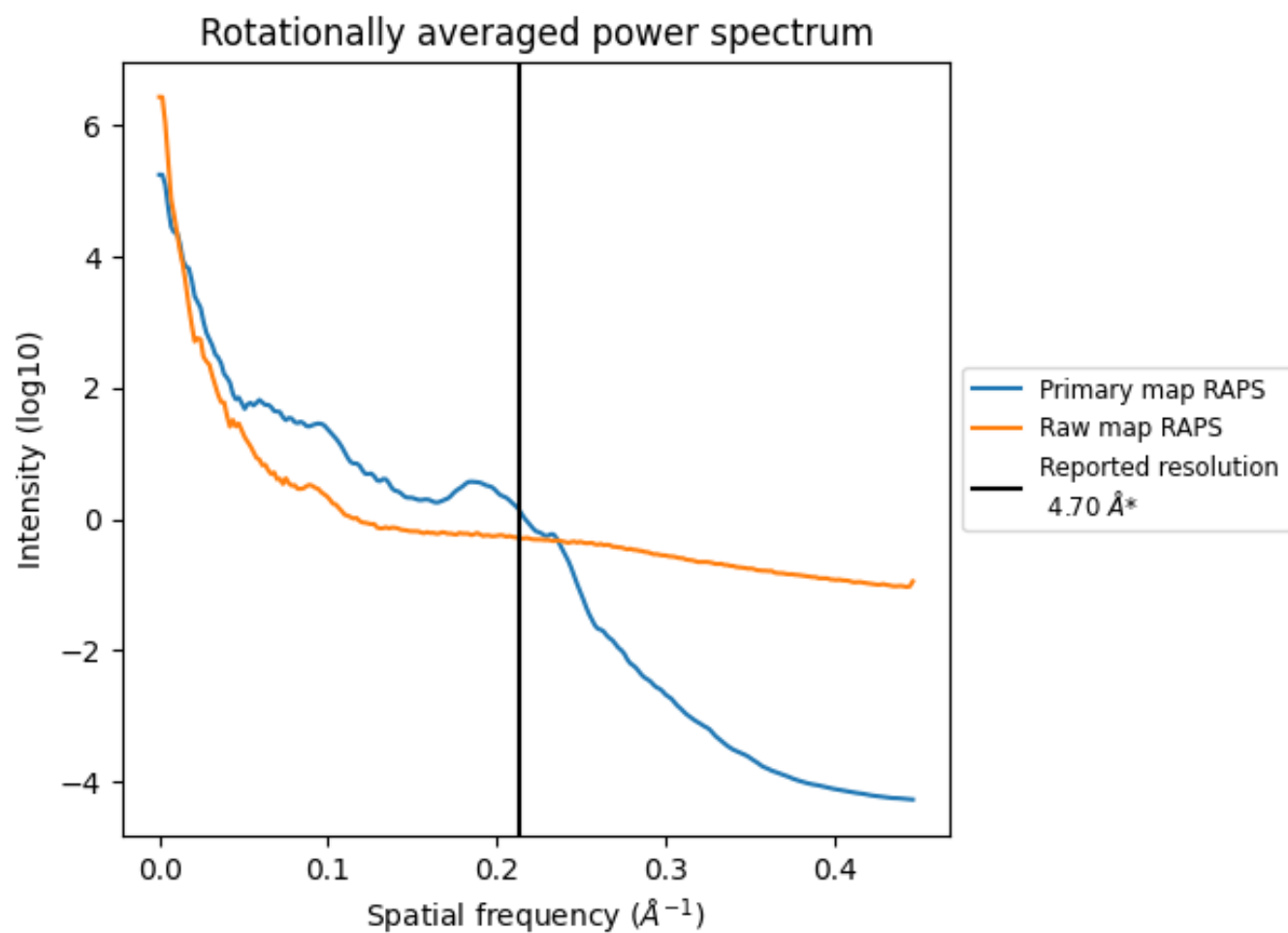
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 451 nm³; this corresponds to an approximate mass of 407 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 ⓘ

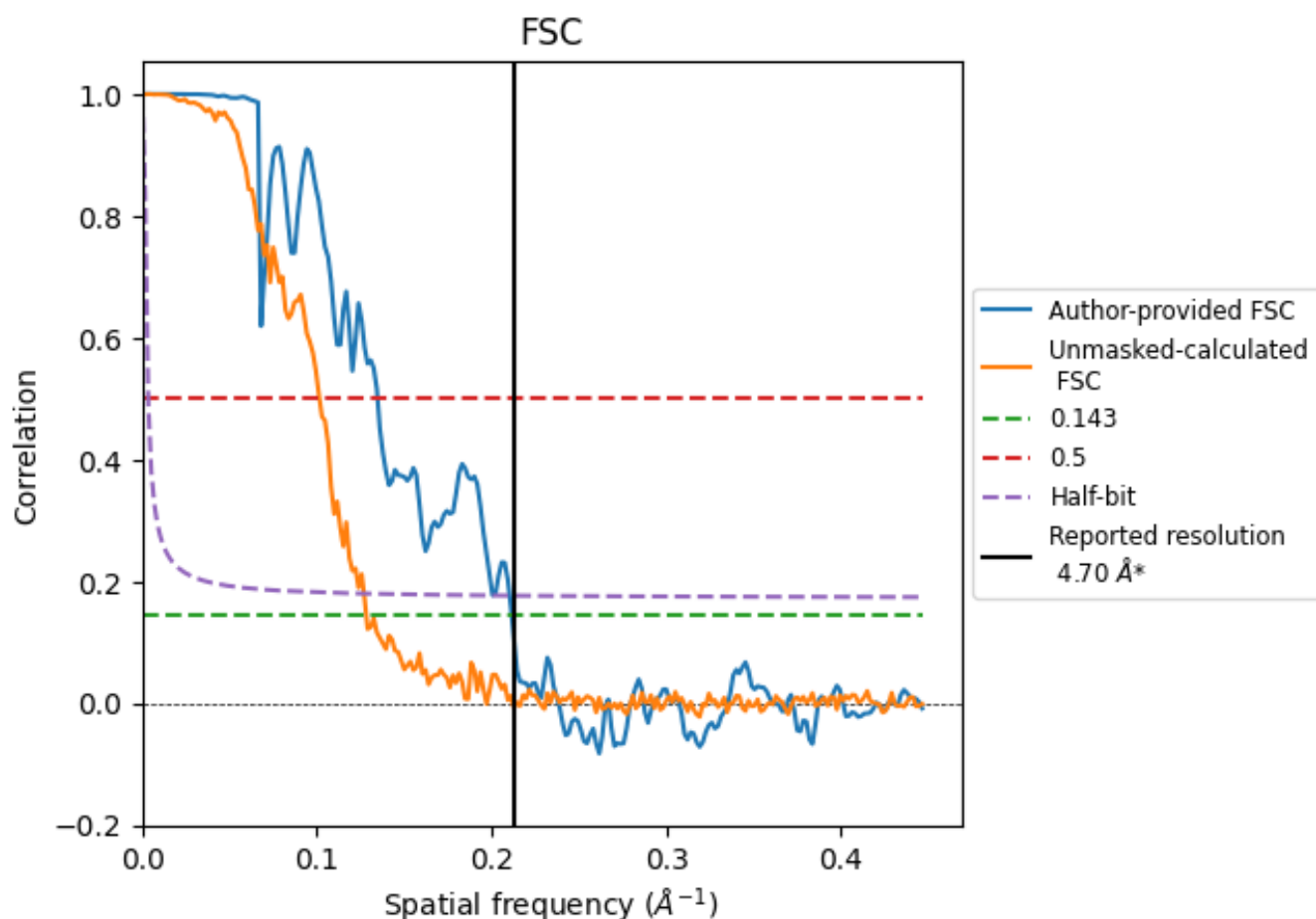


*Reported resolution corresponds to spatial frequency of 0.213 Å⁻¹

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 0.213 \AA^{-1}

8.2 Resolution estimates [i](#)

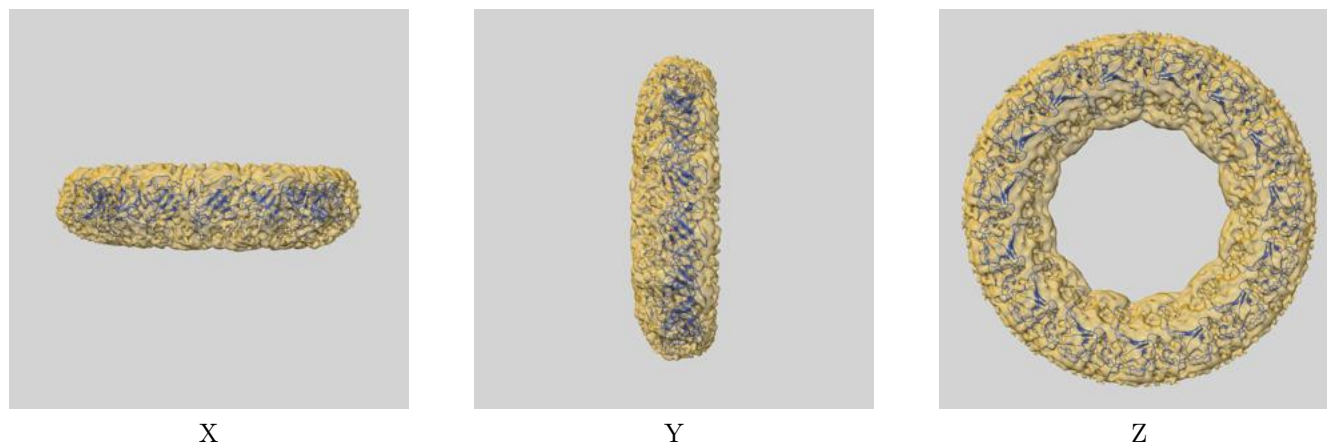
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.70	-	-
Author-provided FSC curve	4.73	7.42	4.76
Unmasked-calculated*	7.79	9.85	7.88

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.79 differs from the reported value 4.7 by more than 10 %

9 Map-model fit [i](#)

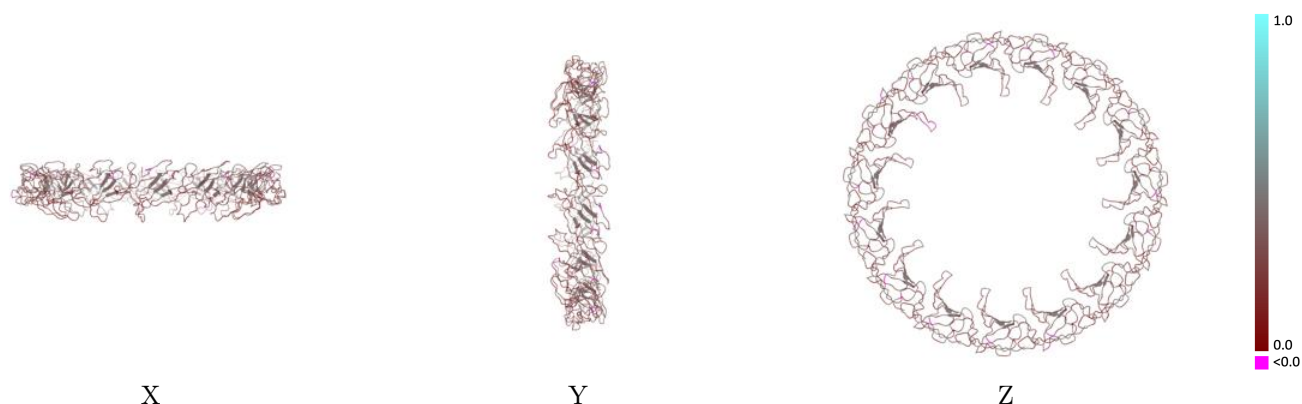
This section contains information regarding the fit between EMDB map EMD-45776 and PDB model 9COD. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



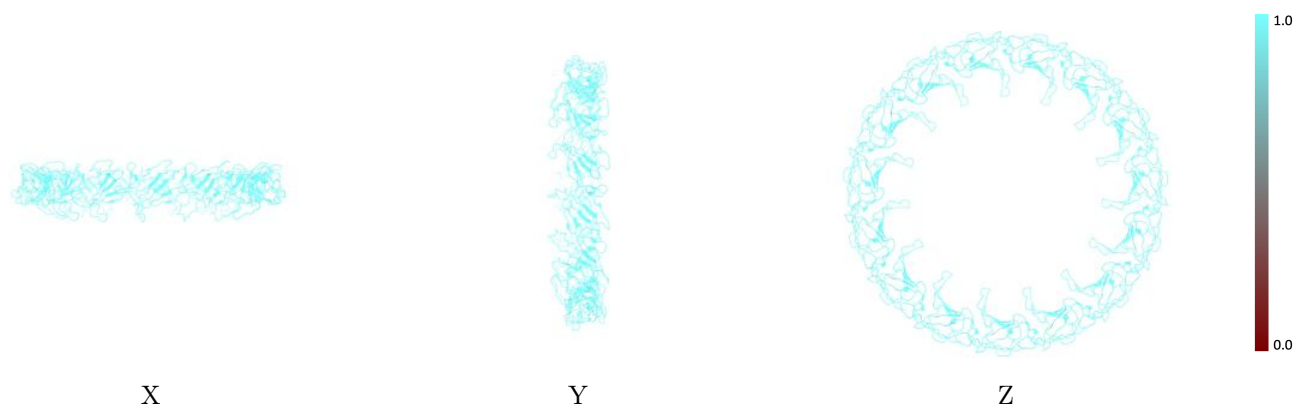
The images above show the 3D surface view of the map at the recommended contour level 0.0018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



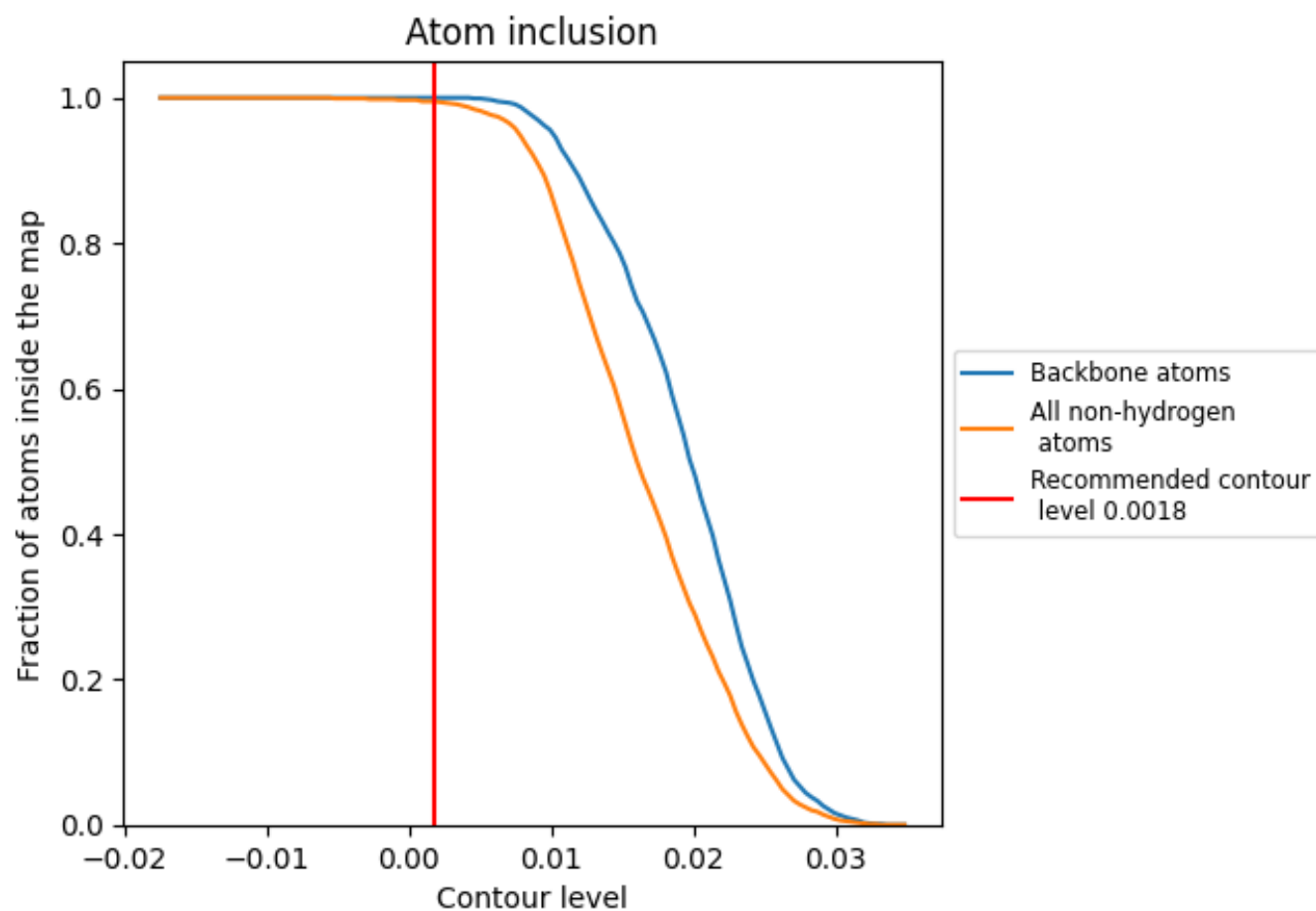
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0018).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 100% 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 (0.0018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9950	<div></div> 0.2950
A	<div></div> 0.9950	<div></div> 0.2960
B	<div></div> 0.9950	<div></div> 0.2960
C	<div></div> 0.9950	<div></div> 0.2980
D	<div></div> 0.9950	<div></div> 0.2940
E	<div></div> 0.9950	<div></div> 0.2960
F	<div></div> 0.9950	<div></div> 0.2960
G	<div></div> 0.9950	<div></div> 0.3000
H	<div></div> 0.9950	<div></div> 0.2970
I	<div></div> 0.9950	<div></div> 0.2960
J	<div></div> 0.9950	<div></div> 0.2970
K	<div></div> 0.9940	<div></div> 0.2950
L	<div></div> 0.9950	<div></div> 0.2960
M	<div></div> 0.9950	<div></div> 0.2940
N	<div></div> 0.9940	<div></div> 0.2710
O	<div></div> 0.9950	<div></div> 0.2990

1.0

0.0

<0.0