Full wwPDB EM Validation Report (i)

Sep 7, 2026 – 04:15 PM JST

PDB ID	:	9XDB / pdb_00009xdb
EMDB ID	:	EMD-66761
Title	:	Structure of Plasmodium vivax Perforin-like protein2 pore in acr form
Authors	:	Zhang, Y.; Zhong, L.J.; Song, Y.; Gilbert, R.J.C.; Ni, T.; Yu, X.L.
Deposited on	:	2025-10-27
Resolution	:	3.90 Å(reported)
Based on initial model	:	.

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 (i) 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 (i)) were used in the production of this report:

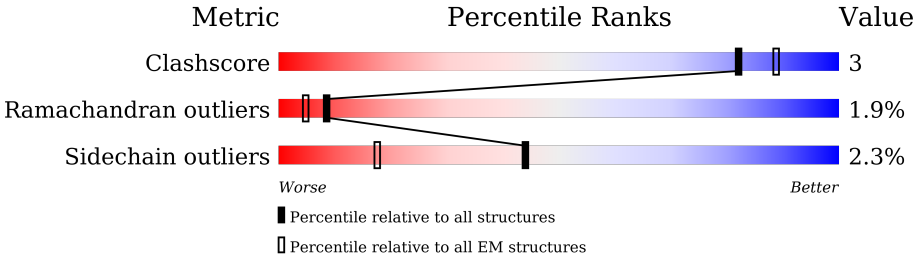
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

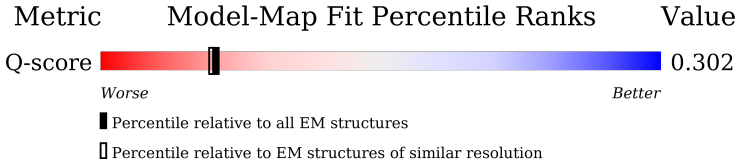
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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	8855 (3.40 - 4.40)

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 <=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	1120	11% 47% • • 48%
1	B	1120	12% 46% • • 48%
1	C	1120	14% 47% • • 48%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 13698 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 MAC/Perforin domain containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	578	4566	2917	754	859	36	0	0
1	B	578	4566	2917	754	859	36	0	0
1	C	578	4566	2917	754	859	36	0	0

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP A5JZX6
A	-5	GLY	-	expression tag	UNP A5JZX6
A	-4	ILE	-	expression tag	UNP A5JZX6
A	-3	LEU	-	expression tag	UNP A5JZX6
A	-2	PRO	-	expression tag	UNP A5JZX6
A	-1	SER	-	expression tag	UNP A5JZX6
A	0	PRO	-	expression tag	UNP A5JZX6
A	1	GLY	-	expression tag	UNP A5JZX6
A	2	MET	-	expression tag	UNP A5JZX6
A	3	PRO	-	expression tag	UNP A5JZX6
A	4	ALA	-	expression tag	UNP A5JZX6
A	5	LEU	-	expression tag	UNP A5JZX6
A	6	LEU	-	expression tag	UNP A5JZX6
A	7	SER	-	expression tag	UNP A5JZX6
A	8	LEU	-	expression tag	UNP A5JZX6
A	9	VAL	-	expression tag	UNP A5JZX6
A	10	SER	-	expression tag	UNP A5JZX6
A	11	LEU	-	expression tag	UNP A5JZX6
A	12	LEU	-	expression tag	UNP A5JZX6
A	13	SER	-	expression tag	UNP A5JZX6
A	14	VAL	-	expression tag	UNP A5JZX6
A	15	LEU	-	expression tag	UNP A5JZX6
A	16	LEU	-	expression tag	UNP A5JZX6
A	17	MET	-	expression tag	UNP A5JZX6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	18	GLY	-	expression tag	UNP A5JZX6
A	19	CYS	-	expression tag	UNP A5JZX6
A	20	VAL	-	expression tag	UNP A5JZX6
A	21	ALA	-	expression tag	UNP A5JZX6
A	22	GLU	-	expression tag	UNP A5JZX6
A	23	THR	-	expression tag	UNP A5JZX6
A	24	GLY	-	expression tag	UNP A5JZX6
A	1105	GLY	-	expression tag	UNP A5JZX6
A	1106	THR	-	expression tag	UNP A5JZX6
A	1107	LYS	-	expression tag	UNP A5JZX6
A	1108	HIS	-	expression tag	UNP A5JZX6
A	1109	HIS	-	expression tag	UNP A5JZX6
A	1110	HIS	-	expression tag	UNP A5JZX6
A	1111	HIS	-	expression tag	UNP A5JZX6
A	1112	HIS	-	expression tag	UNP A5JZX6
A	1113	HIS	-	expression tag	UNP A5JZX6
B	-6	MET	-	initiating methionine	UNP A5JZX6
B	-5	GLY	-	expression tag	UNP A5JZX6
B	-4	ILE	-	expression tag	UNP A5JZX6
B	-3	LEU	-	expression tag	UNP A5JZX6
B	-2	PRO	-	expression tag	UNP A5JZX6
B	-1	SER	-	expression tag	UNP A5JZX6
B	0	PRO	-	expression tag	UNP A5JZX6
B	1	GLY	-	expression tag	UNP A5JZX6
B	2	MET	-	expression tag	UNP A5JZX6
B	3	PRO	-	expression tag	UNP A5JZX6
B	4	ALA	-	expression tag	UNP A5JZX6
B	5	LEU	-	expression tag	UNP A5JZX6
B	6	LEU	-	expression tag	UNP A5JZX6
B	7	SER	-	expression tag	UNP A5JZX6
B	8	LEU	-	expression tag	UNP A5JZX6
B	9	VAL	-	expression tag	UNP A5JZX6
B	10	SER	-	expression tag	UNP A5JZX6
B	11	LEU	-	expression tag	UNP A5JZX6
B	12	LEU	-	expression tag	UNP A5JZX6
B	13	SER	-	expression tag	UNP A5JZX6
B	14	VAL	-	expression tag	UNP A5JZX6
B	15	LEU	-	expression tag	UNP A5JZX6
B	16	LEU	-	expression tag	UNP A5JZX6
B	17	MET	-	expression tag	UNP A5JZX6
B	18	GLY	-	expression tag	UNP A5JZX6
B	19	CYS	-	expression tag	UNP A5JZX6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	20	VAL	-	expression tag	UNP A5JZX6
B	21	ALA	-	expression tag	UNP A5JZX6
B	22	GLU	-	expression tag	UNP A5JZX6
B	23	THR	-	expression tag	UNP A5JZX6
B	24	GLY	-	expression tag	UNP A5JZX6
B	1105	GLY	-	expression tag	UNP A5JZX6
B	1106	THR	-	expression tag	UNP A5JZX6
B	1107	LYS	-	expression tag	UNP A5JZX6
B	1108	HIS	-	expression tag	UNP A5JZX6
B	1109	HIS	-	expression tag	UNP A5JZX6
B	1110	HIS	-	expression tag	UNP A5JZX6
B	1111	HIS	-	expression tag	UNP A5JZX6
B	1112	HIS	-	expression tag	UNP A5JZX6
B	1113	HIS	-	expression tag	UNP A5JZX6
C	-6	MET	-	initiating methionine	UNP A5JZX6
C	-5	GLY	-	expression tag	UNP A5JZX6
C	-4	ILE	-	expression tag	UNP A5JZX6
C	-3	LEU	-	expression tag	UNP A5JZX6
C	-2	PRO	-	expression tag	UNP A5JZX6
C	-1	SER	-	expression tag	UNP A5JZX6
C	0	PRO	-	expression tag	UNP A5JZX6
C	1	GLY	-	expression tag	UNP A5JZX6
C	2	MET	-	expression tag	UNP A5JZX6
C	3	PRO	-	expression tag	UNP A5JZX6
C	4	ALA	-	expression tag	UNP A5JZX6
C	5	LEU	-	expression tag	UNP A5JZX6
C	6	LEU	-	expression tag	UNP A5JZX6
C	7	SER	-	expression tag	UNP A5JZX6
C	8	LEU	-	expression tag	UNP A5JZX6
C	9	VAL	-	expression tag	UNP A5JZX6
C	10	SER	-	expression tag	UNP A5JZX6
C	11	LEU	-	expression tag	UNP A5JZX6
C	12	LEU	-	expression tag	UNP A5JZX6
C	13	SER	-	expression tag	UNP A5JZX6
C	14	VAL	-	expression tag	UNP A5JZX6
C	15	LEU	-	expression tag	UNP A5JZX6
C	16	LEU	-	expression tag	UNP A5JZX6
C	17	MET	-	expression tag	UNP A5JZX6
C	18	GLY	-	expression tag	UNP A5JZX6
C	19	CYS	-	expression tag	UNP A5JZX6
C	20	VAL	-	expression tag	UNP A5JZX6
C	21	ALA	-	expression tag	UNP A5JZX6

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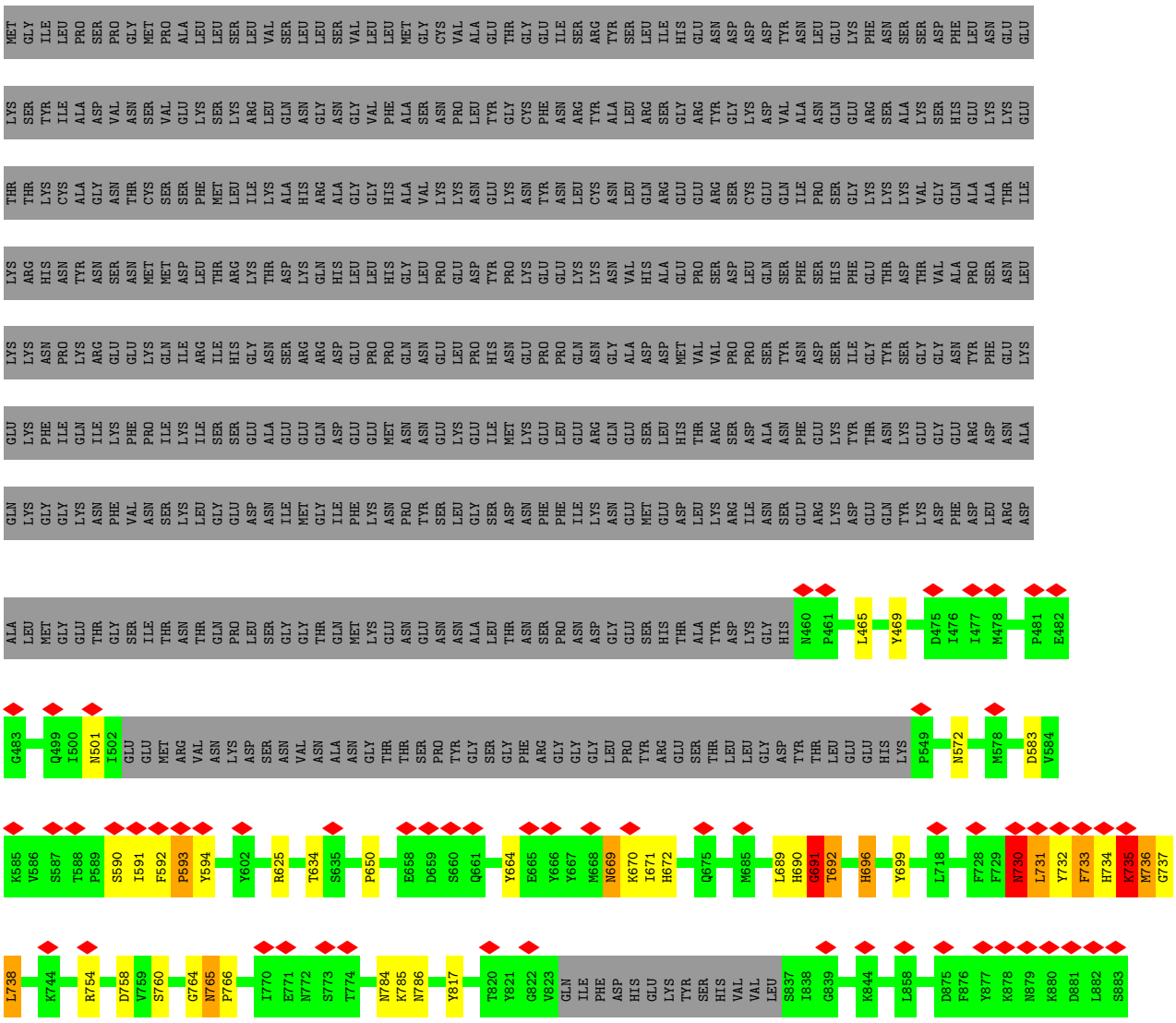
Chain	Residue	Modelled	Actual	Comment	Reference
C	22	GLU	-	expression tag	UNP A5JZX6
C	23	THR	-	expression tag	UNP A5JZX6
C	24	GLY	-	expression tag	UNP A5JZX6
C	1105	GLY	-	expression tag	UNP A5JZX6
C	1106	THR	-	expression tag	UNP A5JZX6
C	1107	LYS	-	expression tag	UNP A5JZX6
C	1108	HIS	-	expression tag	UNP A5JZX6
C	1109	HIS	-	expression tag	UNP A5JZX6
C	1110	HIS	-	expression tag	UNP A5JZX6
C	1111	HIS	-	expression tag	UNP A5JZX6
C	1112	HIS	-	expression tag	UNP A5JZX6
C	1113	HIS	-	expression tag	UNP A5JZX6

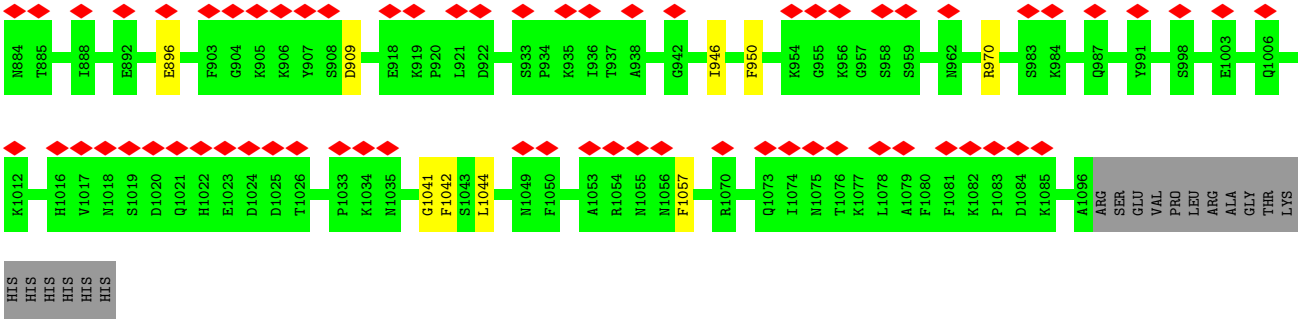
3 Residue-property plots (i)

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: MAC/Perforin domain containing protein

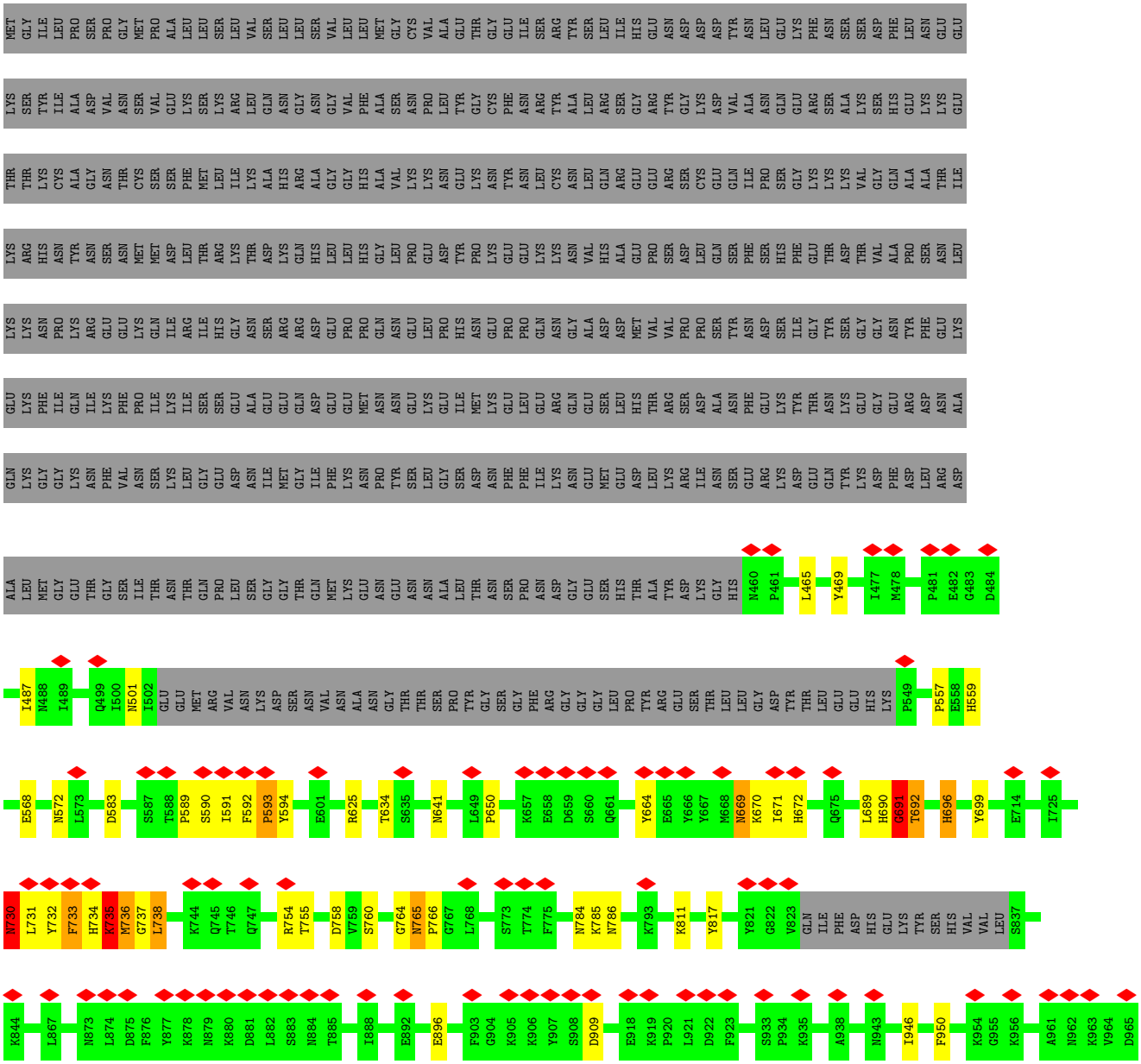
Chain A: 11% 47% 48%

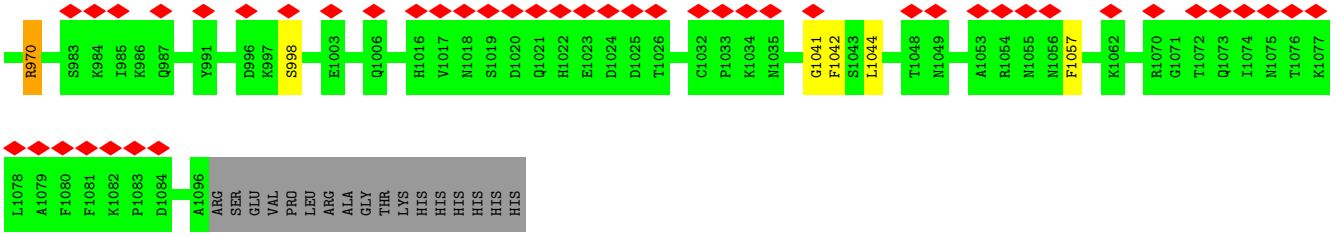




- Molecule 1: MAC/Perforin domain containing protein

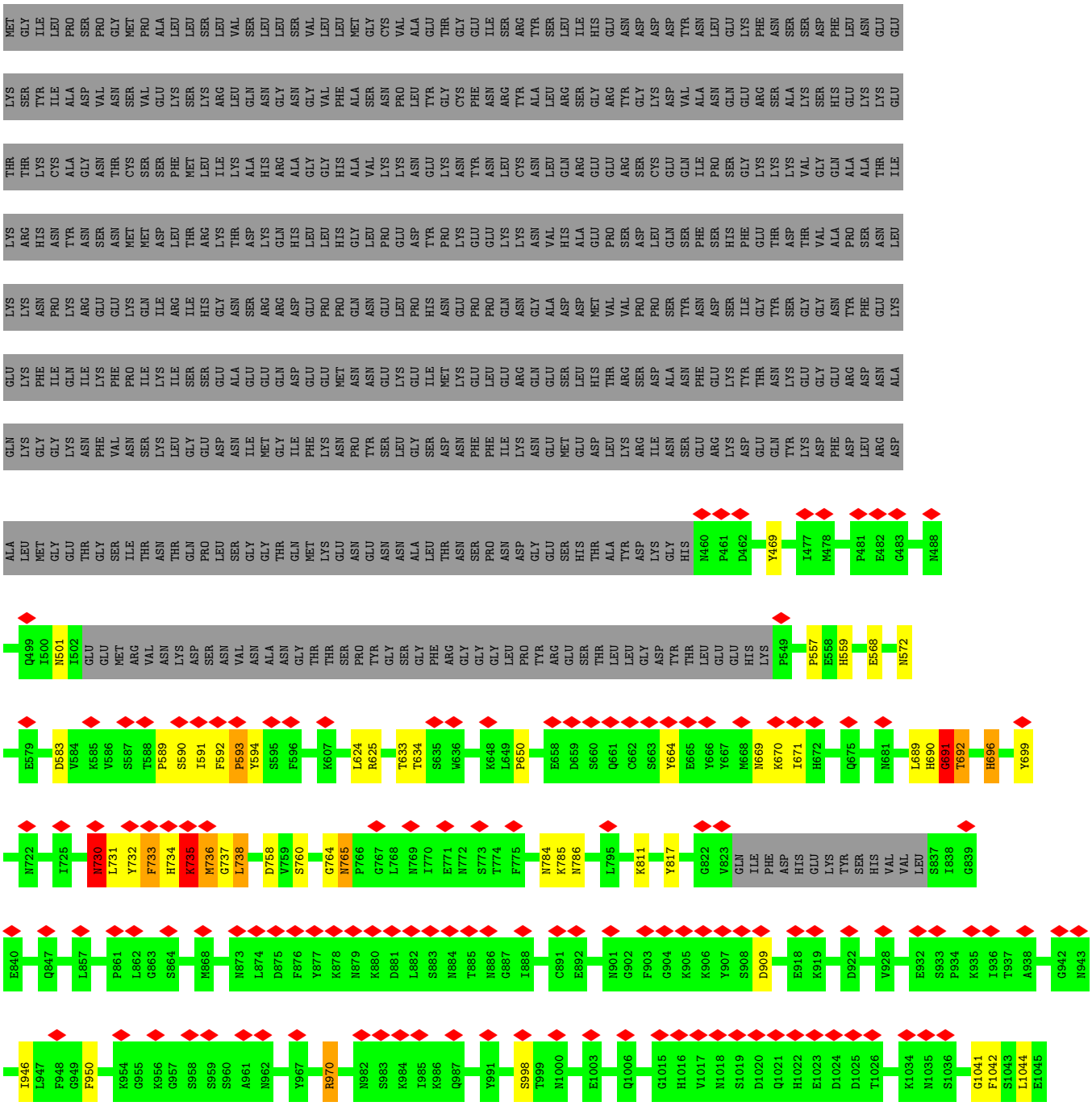
Chain B:

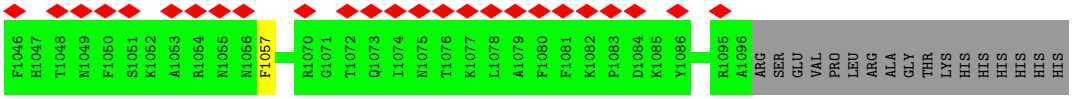




- Molecule 1: MAC/Perforin domain containing protein

Chain C:




F1046
H1047
T1048
N1049
F1050
S1051
K1052
A1053
R1054
N1055
N1056
F1057
R1070
G1071
T1072
Q1073
I1074
N1075
T1076
K1077
L1078
A1079
F1080
F1081
K1082
P1083
D1084
K1085
Y1086
R1095
A1096
ARG
SER
GLU
VAL
PRO
LEU
ARG
ALA
GLY
THR
LYS
HIS
HIS
HIS
HIS
HIS
HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	68218	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	130000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.523	Depositor
Minimum map value	-0.351	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	344.052, 344.052, 344.052	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9557, 0.9557, 0.9557	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.82	4/4669 (0.1%)	1.41	25/6297 (0.4%)
1	B	0.82	4/4669 (0.1%)	1.41	25/6297 (0.4%)
1	C	0.82	4/4669 (0.1%)	1.41	25/6297 (0.4%)
All	All	0.82	12/14007 (0.1%)	1.41	75/18891 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	5
1	C	0	5
All	All	0	15

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	592	PHE	C-O	-9.34	1.12	1.24
1	B	592	PHE	C-O	-9.33	1.12	1.24
1	A	592	PHE	C-O	-9.33	1.12	1.24
1	C	592	PHE	CG-CD2	-6.73	1.24	1.38
1	B	592	PHE	CG-CD2	-6.73	1.24	1.38
1	A	592	PHE	CG-CD2	-6.72	1.24	1.38
1	B	765	ASN	CA-C	5.92	1.57	1.52
1	A	765	ASN	CA-C	5.89	1.57	1.52
1	C	765	ASN	CA-C	5.86	1.57	1.52
1	C	592	PHE	CE1-CZ	-5.41	1.22	1.38
1	A	592	PHE	CE1-CZ	-5.39	1.22	1.38
1	B	592	PHE	CE1-CZ	-5.39	1.22	1.38

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	786	ASN	N-CA-C	8.22	122.59	112.23
1	A	786	ASN	N-CA-C	8.19	122.55	112.23
1	B	786	ASN	N-CA-C	8.19	122.55	112.23
1	A	946	ILE	CA-C-N	7.69	136.73	122.74
1	A	946	ILE	C-N-CA	7.69	136.73	122.74
1	C	946	ILE	CA-C-N	7.67	136.71	122.74
1	C	946	ILE	C-N-CA	7.67	136.71	122.74
1	B	946	ILE	CA-C-N	7.66	136.67	122.74
1	B	946	ILE	C-N-CA	7.66	136.67	122.74
1	B	590	SER	N-CA-C	6.80	118.12	108.74
1	A	590	SER	N-CA-C	6.77	118.09	108.74
1	C	590	SER	N-CA-C	6.77	118.08	108.74
1	A	572	ASN	CA-CB-CG	6.67	119.27	112.60
1	C	572	ASN	CA-CB-CG	6.66	119.26	112.60
1	B	572	ASN	CA-CB-CG	6.65	119.25	112.60
1	B	583	ASP	CA-CB-CG	6.46	119.06	112.60
1	A	583	ASP	CA-CB-CG	6.46	119.06	112.60
1	C	583	ASP	CA-CB-CG	6.45	119.05	112.60
1	A	696	HIS	O-C-N	-6.20	114.35	122.59
1	B	696	HIS	O-C-N	-6.20	114.35	122.59
1	C	696	HIS	O-C-N	-6.17	114.39	122.59
1	B	909	ASP	CA-CB-CG	6.10	118.70	112.60
1	C	909	ASP	CA-CB-CG	6.10	118.70	112.60
1	A	909	ASP	CA-CB-CG	6.07	118.67	112.60
1	B	784	ASN	CA-CB-CG	5.76	118.36	112.60
1	A	690	HIS	CA-C-N	5.76	132.69	121.41
1	A	690	HIS	C-N-CA	5.76	132.69	121.41
1	B	690	HIS	CA-C-N	5.75	132.68	121.41
1	B	690	HIS	C-N-CA	5.75	132.68	121.41
1	A	784	ASN	CA-CB-CG	5.74	118.34	112.60
1	C	690	HIS	CA-C-N	5.74	132.66	121.41
1	C	690	HIS	C-N-CA	5.74	132.66	121.41
1	C	784	ASN	CA-CB-CG	5.74	118.34	112.60
1	B	625	ARG	N-CA-CB	-5.72	102.08	111.74
1	A	625	ARG	N-CA-CB	-5.71	102.09	111.74
1	C	625	ARG	N-CA-CB	-5.70	102.11	111.74
1	B	670	LYS	N-CA-C	5.68	118.41	111.82
1	A	670	LYS	N-CA-C	5.66	118.39	111.82
1	C	670	LYS	N-CA-C	5.62	118.34	111.82
1	C	691	GLY	N-CA-C	5.60	126.44	113.18
1	B	691	GLY	N-CA-C	5.59	126.44	113.18
1	A	691	GLY	N-CA-C	5.58	126.41	113.18
1	C	758	ASP	CA-CB-CG	5.50	118.10	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	765	ASN	CB-CA-C	5.49	117.90	110.37
1	A	765	ASN	CB-CA-C	5.48	117.88	110.37
1	A	758	ASP	CA-CB-CG	5.47	118.07	112.60
1	B	758	ASP	CA-CB-CG	5.46	118.06	112.60
1	C	765	ASN	CB-CA-C	5.46	117.85	110.37
1	C	699	TYR	CA-C-N	5.43	130.80	122.93
1	C	699	TYR	C-N-CA	5.43	130.80	122.93
1	A	699	TYR	CA-C-N	5.41	130.78	122.93
1	A	699	TYR	C-N-CA	5.41	130.78	122.93
1	B	699	TYR	CA-C-N	5.38	130.74	122.93
1	B	699	TYR	C-N-CA	5.38	130.74	122.93
1	A	593	PRO	CA-N-CD	-5.37	104.48	112.00
1	C	593	PRO	CA-N-CD	-5.37	104.48	112.00
1	B	593	PRO	CA-N-CD	-5.37	104.49	112.00
1	B	785	LYS	CA-C-N	5.36	129.79	120.68
1	B	785	LYS	C-N-CA	5.36	129.79	120.68
1	A	785	LYS	CA-C-N	5.35	129.77	120.68
1	A	785	LYS	C-N-CA	5.35	129.77	120.68
1	C	785	LYS	CA-C-N	5.34	129.77	120.68
1	C	785	LYS	C-N-CA	5.34	129.77	120.68
1	C	669	ASN	CA-C-N	5.25	128.29	120.31
1	C	669	ASN	C-N-CA	5.25	128.29	120.31
1	A	669	ASN	CA-C-N	5.25	128.28	120.31
1	A	669	ASN	C-N-CA	5.25	128.28	120.31
1	B	669	ASN	CA-C-N	5.24	128.28	120.31
1	B	669	ASN	C-N-CA	5.24	128.28	120.31
1	B	689	LEU	CA-C-N	5.08	132.86	122.55
1	B	689	LEU	C-N-CA	5.08	132.86	122.55
1	C	689	LEU	CA-C-N	5.06	132.83	122.55
1	C	689	LEU	C-N-CA	5.06	132.83	122.55
1	A	689	LEU	CA-C-N	5.06	132.82	122.55
1	A	689	LEU	C-N-CA	5.06	132.82	122.55

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	469	TYR	Sidechain
1	A	594	TYR	Sidechain
1	A	664	TYR	Sidechain
1	A	696	HIS	Mainchain
1	A	817	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	B	469	TYR	Sidechain
1	B	594	TYR	Sidechain
1	B	664	TYR	Sidechain
1	B	696	HIS	Mainchain
1	B	817	TYR	Sidechain
1	C	469	TYR	Sidechain
1	C	594	TYR	Sidechain
1	C	664	TYR	Sidechain
1	C	696	HIS	Mainchain
1	C	817	TYR	Sidechain

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	4566	0	4543	26	0
1	B	4566	0	4543	47	0
1	C	4566	0	4543	33	0
All	All	13698	0	13629	69	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 3.

All (69) 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:754:ARG:NH1	1:B:568:GLU:OE2	1.74	1.19
1:B:754:ARG:NH1	1:C:568:GLU:OE2	1.81	1.10
1:C:730:ASN:CA	1:C:737:GLY:HA3	1.82	1.10
1:A:730:ASN:CA	1:A:737:GLY:HA3	1.82	1.09
1:A:730:ASN:HA	1:A:737:GLY:CA	1.83	1.08
1:C:730:ASN:HA	1:C:737:GLY:CA	1.83	1.08
1:B:730:ASN:CA	1:B:737:GLY:HA3	1.82	1.08
1:B:730:ASN:HA	1:B:737:GLY:CA	1.83	1.08
1:B:735:LYS:HE3	1:C:589:PRO:O	1.67	0.94
1:A:896:GLU:OE2	1:B:970:ARG:NH2	2.01	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:735:LYS:HE3	1:B:589:PRO:O	1.78	0.84
1:B:754:ARG:HH11	1:C:568:GLU:CD	1.88	0.81
1:B:896:GLU:OE2	1:C:970:ARG:NH2	2.15	0.80
1:B:641:ASN:OD1	1:C:633:THR:OG1	2.07	0.72
1:A:735:LYS:CE	1:B:589:PRO:O	2.39	0.71
1:B:735:LYS:CE	1:C:589:PRO:O	2.38	0.69
1:A:465:LEU:HB3	1:B:557:PRO:HG3	1.79	0.64
1:B:766:PRO:HG3	1:C:559:HIS:CD2	2.33	0.64
1:B:735:LYS:HZ1	1:C:589:PRO:HB3	1.64	0.63
1:A:754:ARG:HH11	1:B:568:GLU:CD	1.95	0.63
1:A:669:ASN:HA	1:B:998:SER:HA	1.81	0.61
1:B:735:LYS:NZ	1:C:589:PRO:HB3	2.16	0.61
1:B:465:LEU:HB3	1:C:557:PRO:HG3	1.83	0.60
1:B:766:PRO:HD3	1:C:559:HIS:CD2	2.38	0.58
1:A:754:ARG:NH1	1:B:568:GLU:CD	2.57	0.57
1:B:754:ARG:NH1	1:C:568:GLU:CD	2.54	0.55
1:B:766:PRO:HG3	1:C:559:HIS:HD2	1.74	0.50
1:B:766:PRO:CG	1:C:559:HIS:CD2	2.95	0.50
1:A:736:MET:HB3	1:B:589:PRO:HA	1.94	0.50
1:C:1044:LEU:HD22	1:C:1057:PHE:CE2	2.47	0.49
1:A:672:HIS:CG	1:B:811:LYS:HE3	2.48	0.49
1:A:1044:LEU:HD22	1:A:1057:PHE:CE2	2.47	0.49
1:B:672:HIS:CG	1:C:811:LYS:HE3	2.48	0.49
1:B:1044:LEU:HD22	1:B:1057:PHE:CE2	2.47	0.48
1:A:766:PRO:HG3	1:B:559:HIS:CD2	2.49	0.48
1:B:730:ASN:HA	1:B:737:GLY:HA3	0.86	0.48
1:C:691:GLY:O	1:C:692:THR:HG23	2.14	0.48
1:B:691:GLY:O	1:B:692:THR:HG23	2.14	0.47
1:A:730:ASN:HA	1:A:737:GLY:HA3	0.86	0.47
1:A:735:LYS:NZ	1:B:589:PRO:HB3	2.30	0.47
1:A:691:GLY:O	1:A:692:THR:HG23	2.14	0.46
1:A:735:LYS:HD2	1:A:735:LYS:HA	1.47	0.46
1:A:735:LYS:HZ1	1:B:589:PRO:HB3	1.81	0.46
1:B:735:LYS:HD2	1:B:735:LYS:HA	1.47	0.46
1:B:487:ILE:HB	1:C:624:LEU:CD1	2.46	0.46
1:C:735:LYS:HA	1:C:735:LYS:HD2	1.47	0.45
1:B:669:ASN:HA	1:C:998:SER:HA	2.00	0.43
1:B:766:PRO:CG	1:C:559:HIS:HD2	2.30	0.42
1:B:672:HIS:CD2	1:C:811:LYS:HE3	2.54	0.42
1:B:736:MET:HB3	1:C:589:PRO:HA	2.01	0.42
1:B:755:THR:O	1:C:568:GLU:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:732:TYR:O	1:A:733:PHE:C	2.63	0.42
1:C:1041:GLY:O	1:C:1042:PHE:CD1	2.73	0.42
1:B:732:TYR:O	1:B:733:PHE:C	2.63	0.42
1:B:732:TYR:HA	1:B:735:LYS:O	2.20	0.42
1:B:1041:GLY:O	1:B:1042:PHE:CD1	2.73	0.42
1:C:732:TYR:O	1:C:733:PHE:C	2.63	0.42
1:C:732:TYR:HA	1:C:735:LYS:O	2.20	0.42
1:A:732:TYR:HA	1:A:735:LYS:O	2.20	0.41
1:B:735:LYS:HZ2	1:B:735:LYS:HG3	1.67	0.41
1:B:487:ILE:HB	1:C:624:LEU:HD11	2.01	0.41
1:A:735:LYS:HB3	1:A:736:MET:H	1.54	0.41
1:A:766:PRO:HG3	1:B:559:HIS:HD2	1.86	0.41
1:A:1041:GLY:O	1:A:1042:PHE:CD1	2.73	0.41
1:C:730:ASN:HA	1:C:737:GLY:HA3	0.86	0.41
1:C:735:LYS:HB3	1:C:736:MET:H	1.54	0.41
1:B:766:PRO:HD3	1:C:559:HIS:CG	2.56	0.41
1:A:731:LEU:HD12	1:A:731:LEU:HA	1.93	0.41
1:A:735:LYS:HZ2	1:A:735:LYS:HG3	1.72	0.41

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	572/1120 (51%)	518 (91%)	43 (8%)	11 (2%)	6 33
1	B	572/1120 (51%)	518 (91%)	43 (8%)	11 (2%)	6 33
1	C	572/1120 (51%)	518 (91%)	43 (8%)	11 (2%)	6 33
All	All	1716/3360 (51%)	1554 (91%)	129 (8%)	33 (2%)	8 33

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	650	PRO
1	A	671	ILE
1	A	691	GLY
1	B	650	PRO
1	B	671	ILE
1	B	691	GLY
1	C	650	PRO
1	C	671	ILE
1	C	691	GLY
1	A	593	PRO
1	A	692	THR
1	A	735	LYS
1	A	970	ARG
1	B	593	PRO
1	B	692	THR
1	B	735	LYS
1	B	970	ARG
1	C	593	PRO
1	C	692	THR
1	C	735	LYS
1	C	970	ARG
1	A	730	ASN
1	A	738	LEU
1	B	730	ASN
1	B	738	LEU
1	C	730	ASN
1	C	738	LEU
1	A	764	GLY
1	B	764	GLY
1	C	764	GLY
1	A	591	ILE
1	B	591	ILE
1	C	591	ILE

5.3.2 Protein sidechains (i)

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	518/996 (52%)	506 (98%)	12 (2%)	44	63
1	B	518/996 (52%)	506 (98%)	12 (2%)	44	63
1	C	518/996 (52%)	506 (98%)	12 (2%)	44	63
All	All	1554/2988 (52%)	1518 (98%)	36 (2%)	44	63

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	501	ASN
1	A	634	THR
1	A	730	ASN
1	A	731	LEU
1	A	733	PHE
1	A	734	HIS
1	A	735	LYS
1	A	736	MET
1	A	738	LEU
1	A	760	SER
1	A	765	ASN
1	A	950	PHE
1	B	501	ASN
1	B	634	THR
1	B	730	ASN
1	B	731	LEU
1	B	733	PHE
1	B	734	HIS
1	B	735	LYS
1	B	736	MET
1	B	738	LEU
1	B	760	SER
1	B	765	ASN
1	B	950	PHE
1	C	501	ASN
1	C	634	THR
1	C	730	ASN
1	C	731	LEU
1	C	733	PHE
1	C	734	HIS
1	C	735	LYS
1	C	736	MET
1	C	738	LEU
1	C	760	SER

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Mol	Chain	Res	Type
1	C	765	ASN
1	C	950	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	612	GLN
1	A	613	ASN
1	A	614	ASN
1	A	661	GLN
1	A	669	ASN
1	A	696	HIS
1	A	722	ASN
1	A	747	GLN
1	A	784	ASN
1	A	873	ASN
1	A	1035	ASN
1	B	559	HIS
1	B	612	GLN
1	B	613	ASN
1	B	614	ASN
1	B	669	ASN
1	B	696	HIS
1	B	722	ASN
1	B	784	ASN
1	B	873	ASN
1	B	1035	ASN
1	C	559	HIS
1	C	613	ASN
1	C	696	HIS
1	C	722	ASN
1	C	784	ASN
1	C	873	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.

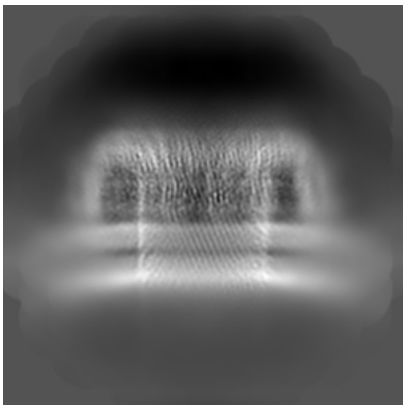
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-66761. These allow visual inspection of the internal detail of the map and identification of artifacts.

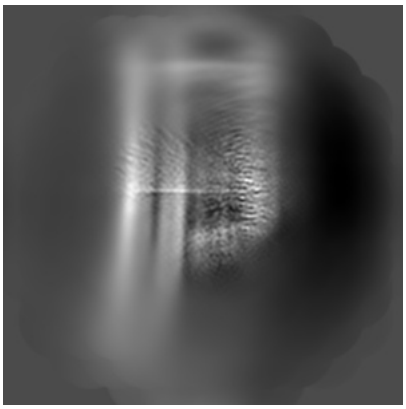
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

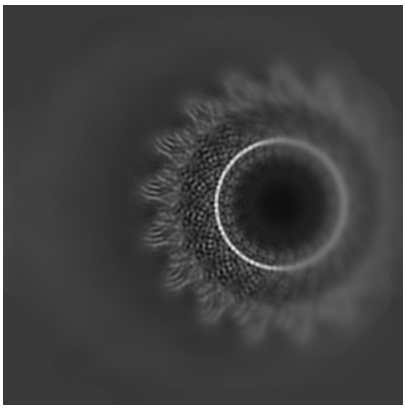
6.1.1 Primary map



X

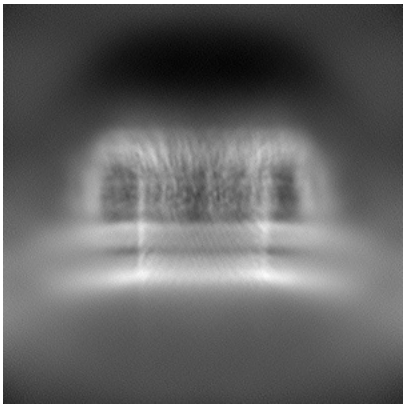


Y



Z

6.1.2 Raw map



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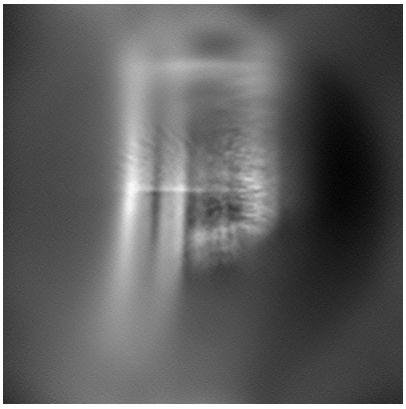
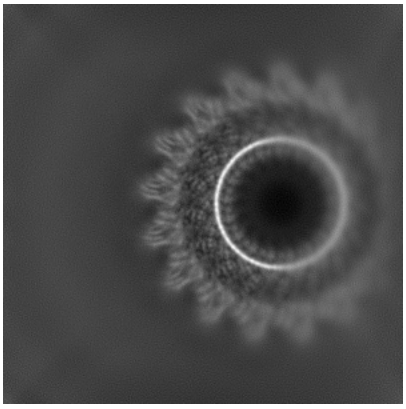


Y

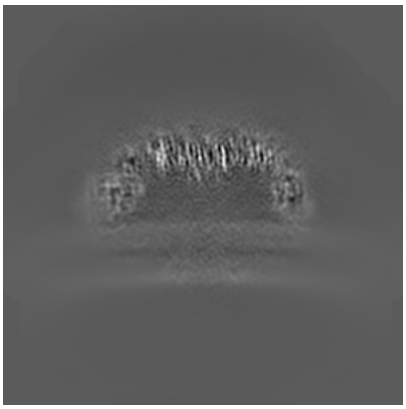


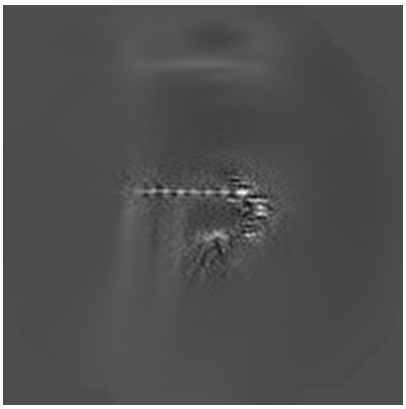
Z

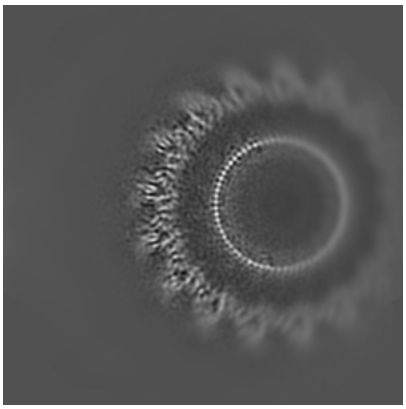
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

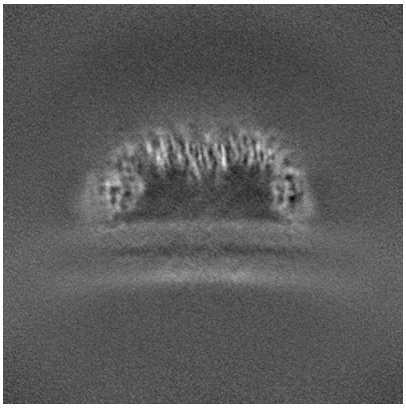
6.2.1 Primary map

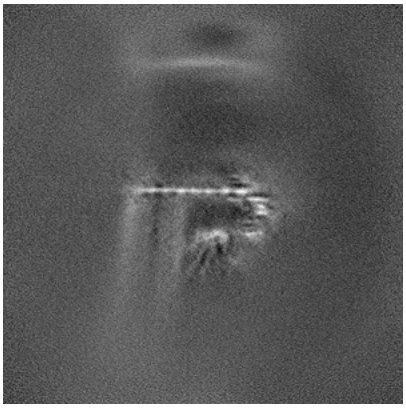

X Index: 180

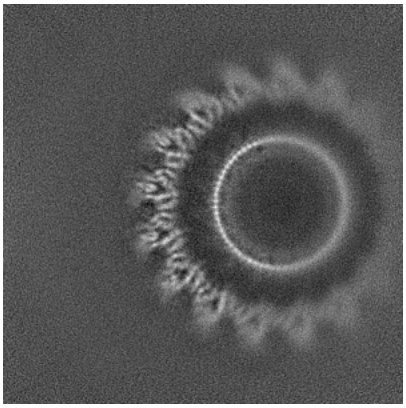

Y Index: 180


Z Index: 180

6.2.2 Raw map


X Index: 180

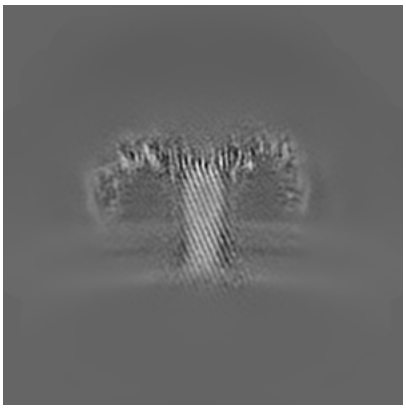

Y Index: 180

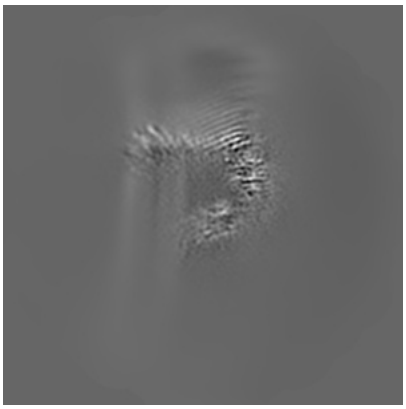

Z Index: 180

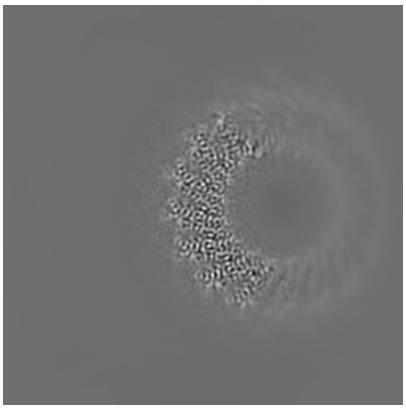
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

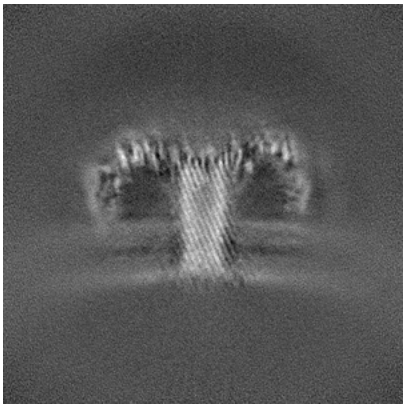
6.3.1 Primary map

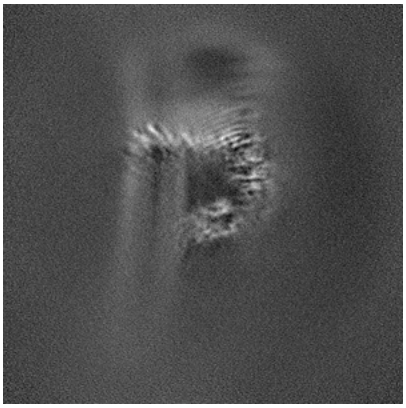

X Index: 192

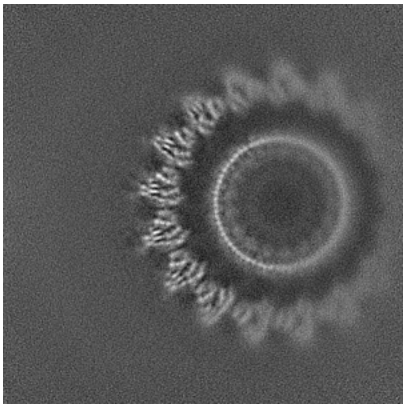

Y Index: 123


Z Index: 221

6.3.2 Raw map


X Index: 193

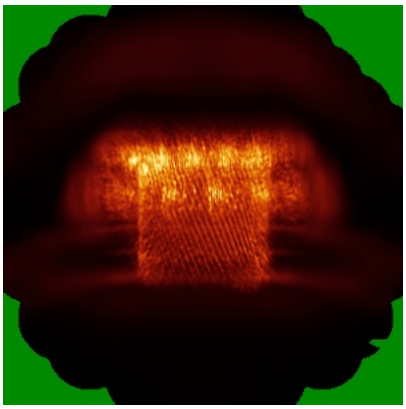

Y Index: 123

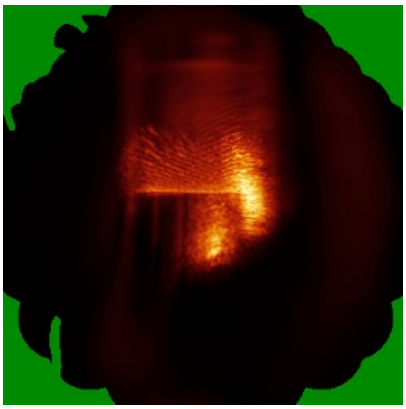

Z Index: 189

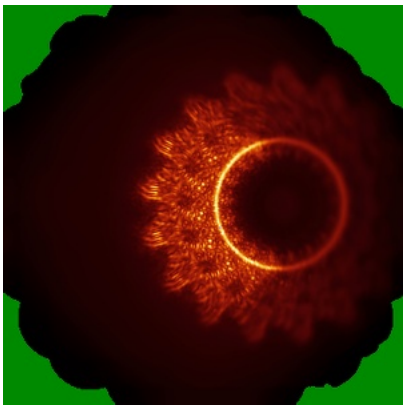
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

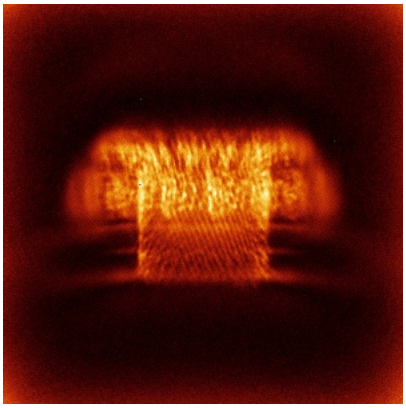
6.4.1 Primary map

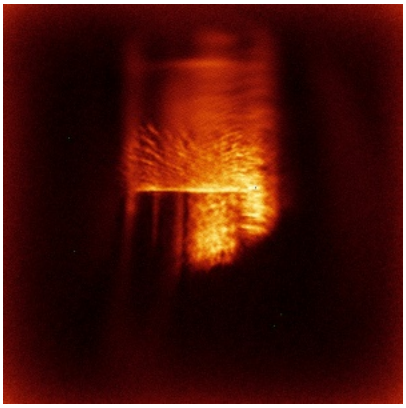

X

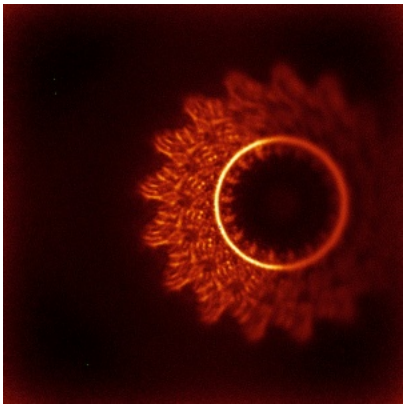

Y


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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.06. 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

X Y Z

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.

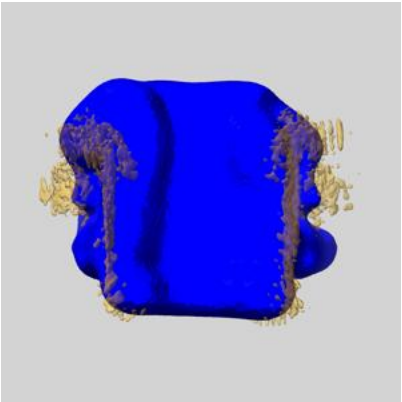
6.6 Mask visualisation (i)

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

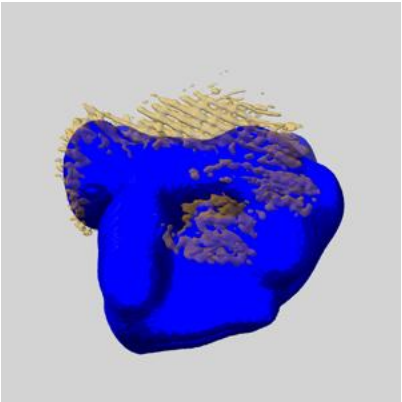
A mask typically either:

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

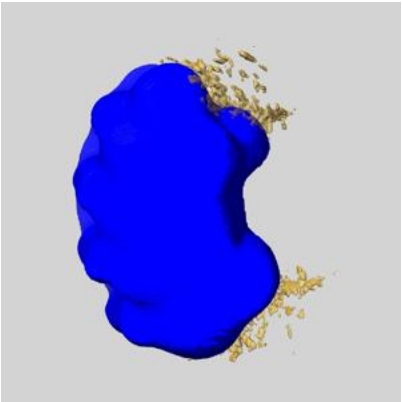
6.6.1 emd_66761_msk_1.map (i)



X



Y

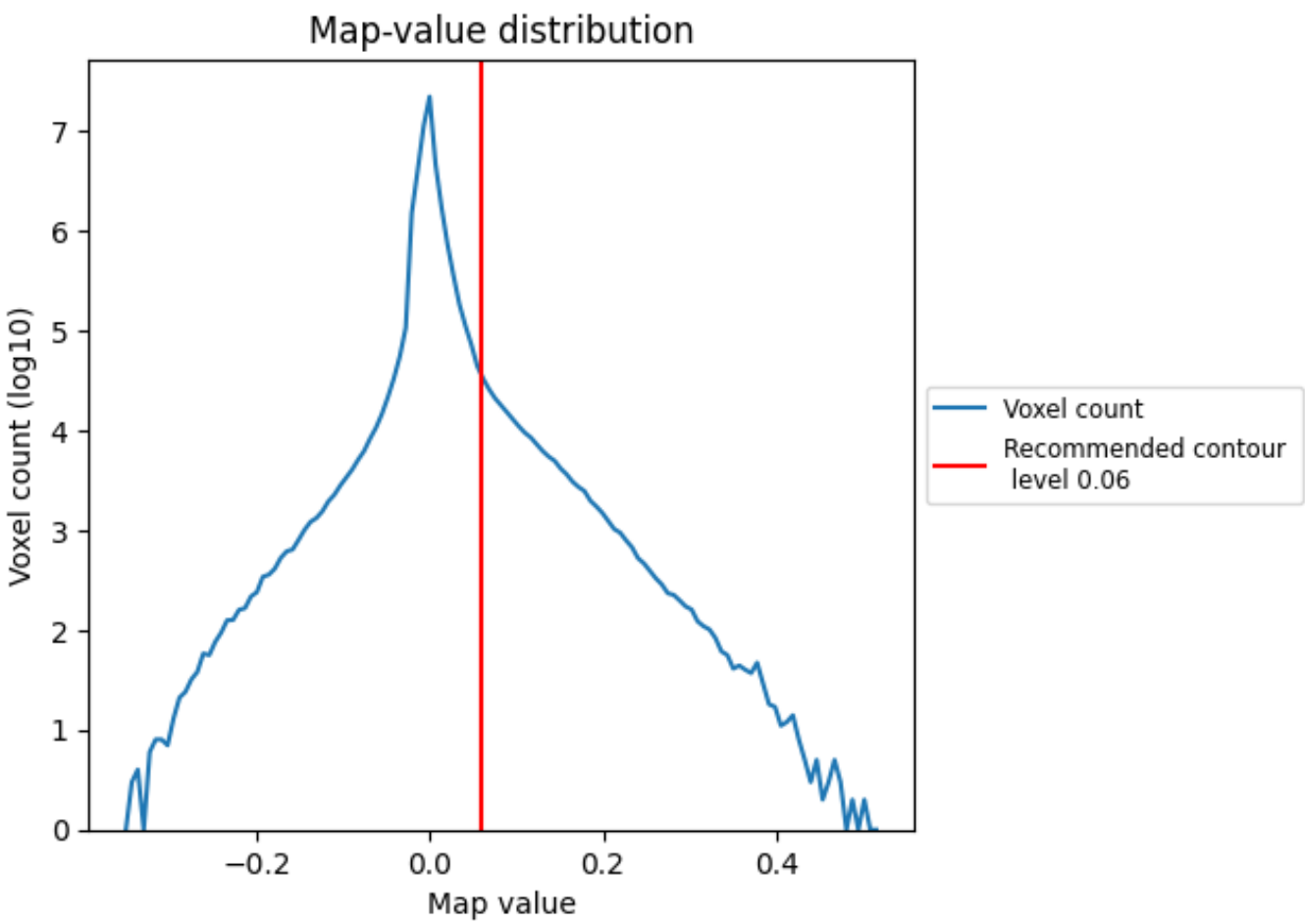


Z

7 Map analysis (i)

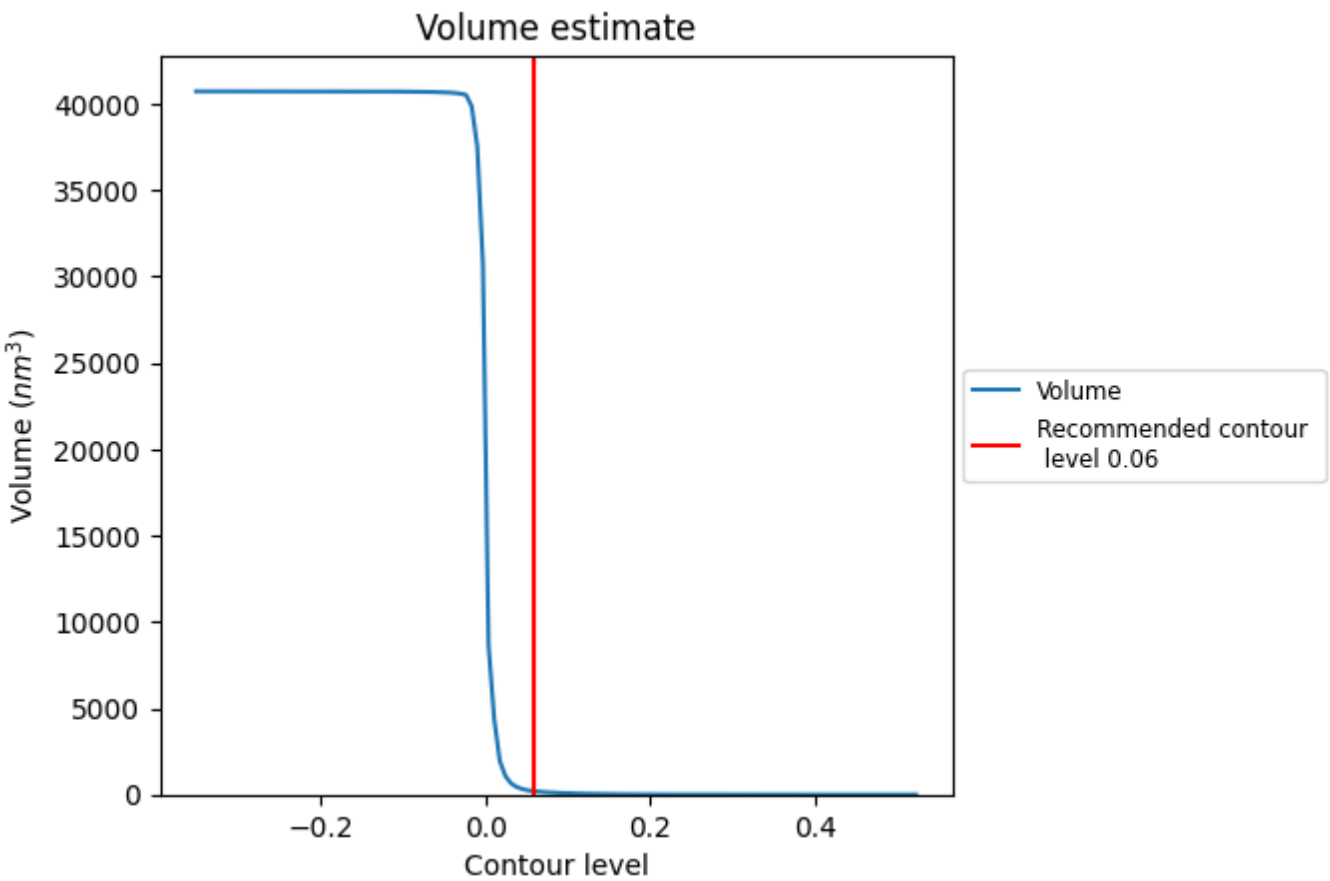
This section contains the results of statistical analysis of the map.

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.

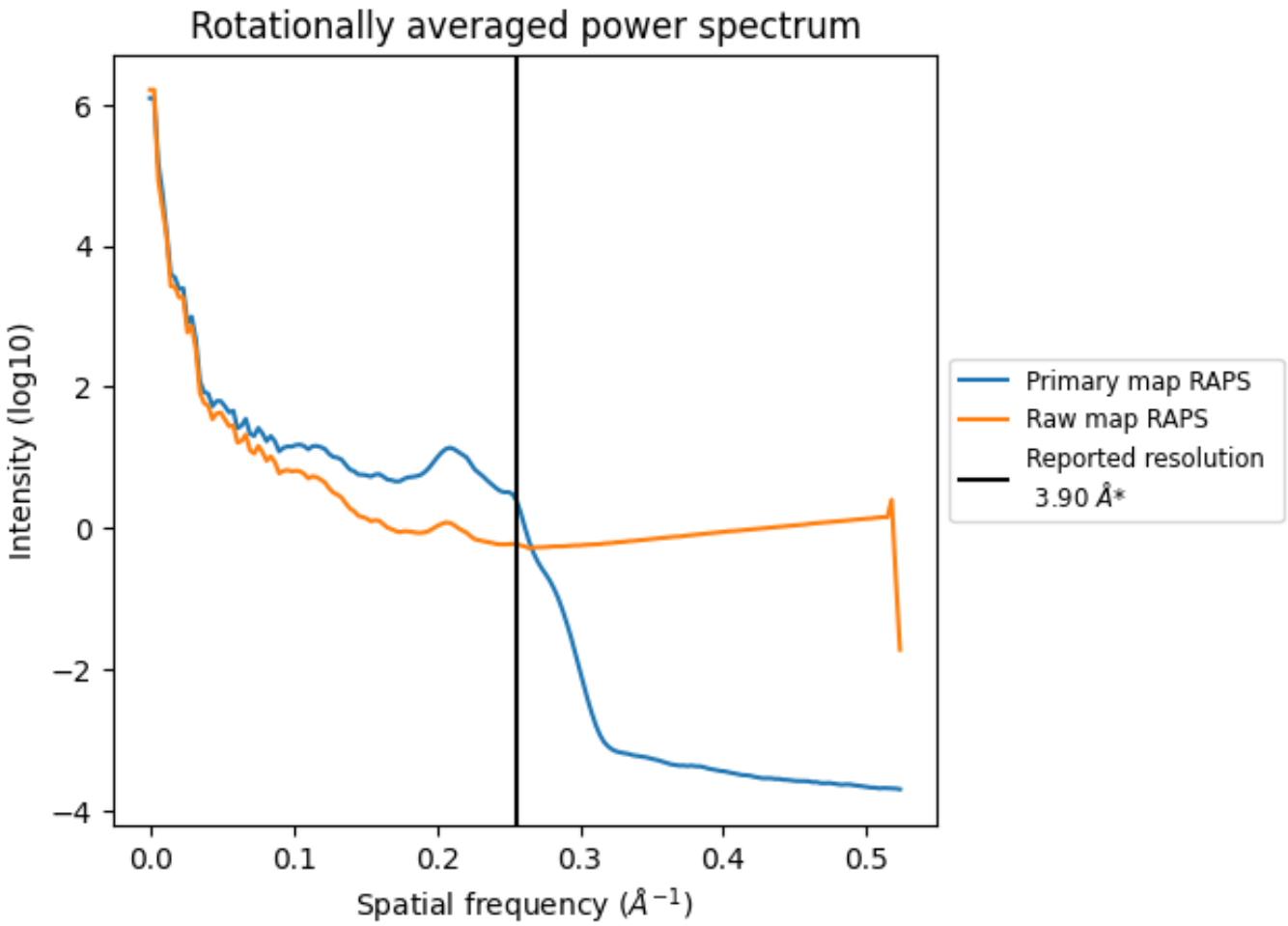
7.2 Volume estimate (i)



The volume at the recommended contour level is 190 nm^3; this corresponds to an approximate mass of 172 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 (i)

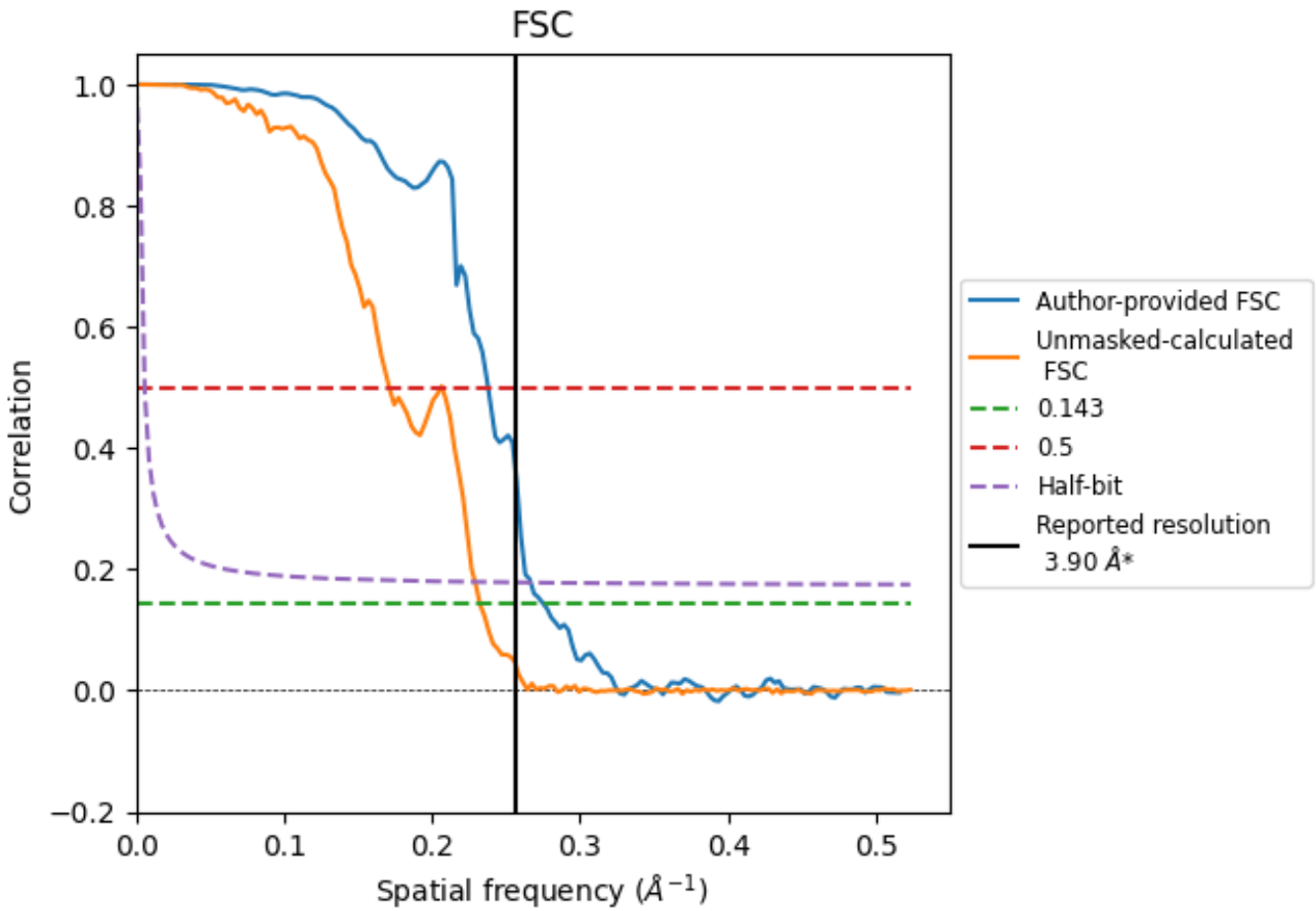


*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

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 0.256 Å^{-1}

8.2 Resolution estimates (i)

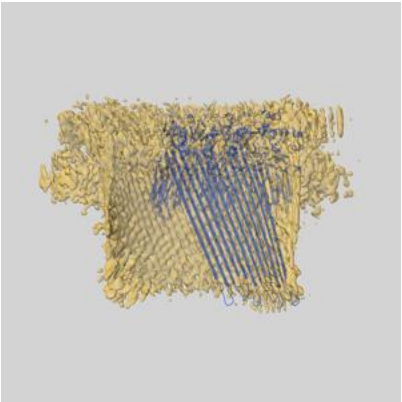
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.64	4.21	3.75
Unmasked-calculated*	4.30	5.85	4.37

*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 4.30 differs from the reported value 3.9 by more than 10 %

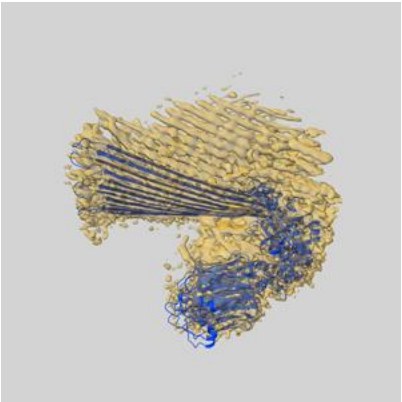
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-66761 and PDB model 9XDB. Per-residue inclusion information can be found in section 3 on page 7.

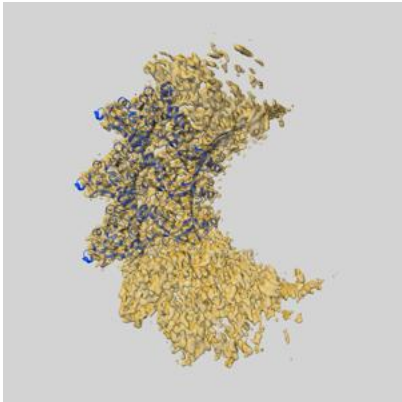
9.1 Map-model overlay (i)



X



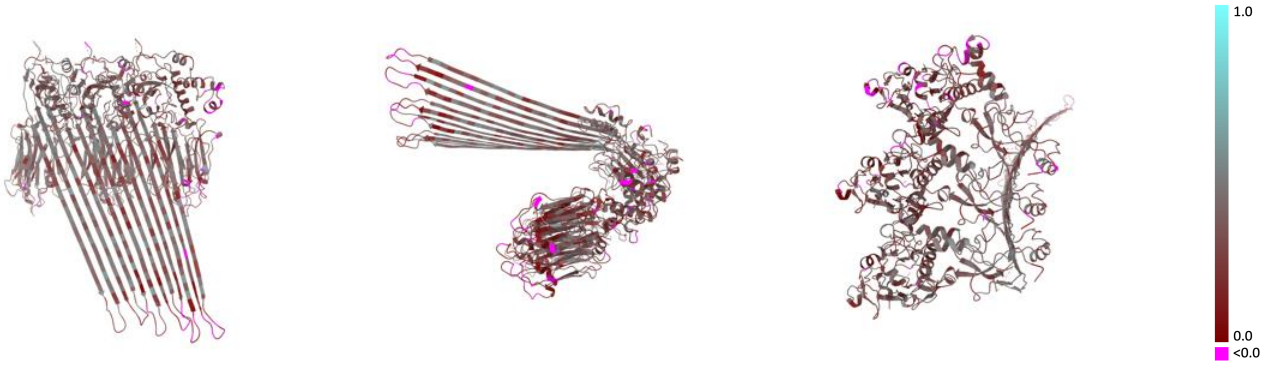
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06 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.

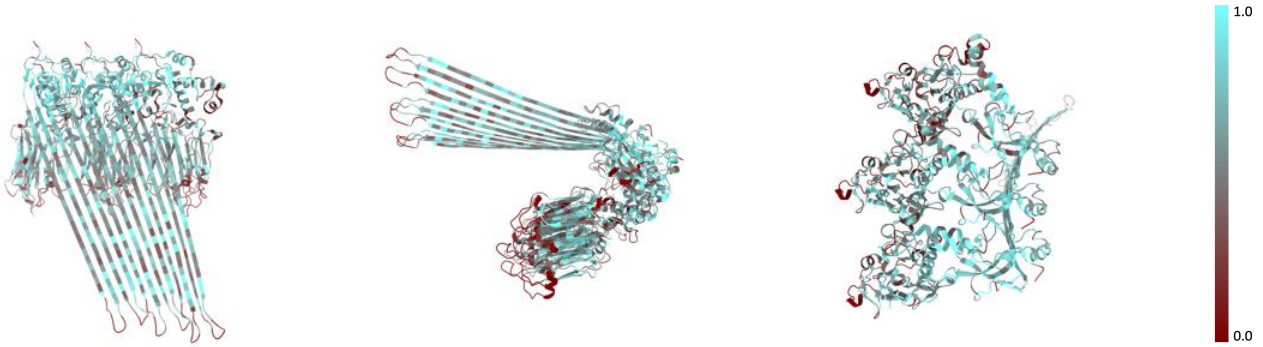
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

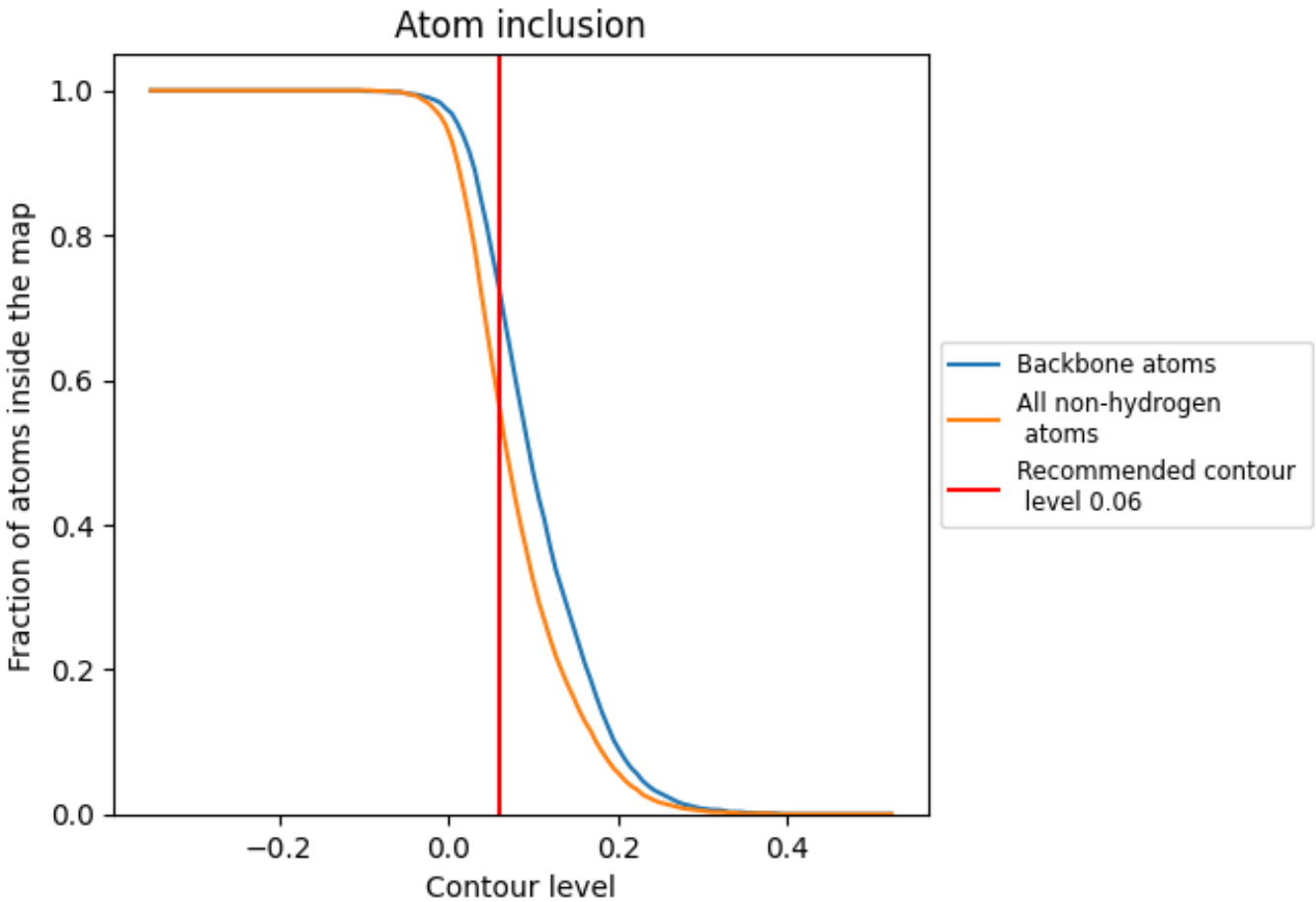
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.06).

9.4 Atom inclusion (i)



At the recommended contour level, 72% of all backbone atoms, 56% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5630	0.3020
A	0.5880	0.3430
B	0.5690	0.2960
C	0.5330	0.2680