



wwPDB EM Validation Summary Report ⓘ

Feb 19, 2025 – 07:09 PM JST

PDB ID : 9JG6
EMDB ID : EMD-61457
Title : The tail-complex structure of phage P22
Authors : Liu, H.R.; Xiao, H.
Deposited on : 2024-09-06
Resolution : 3.21 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:

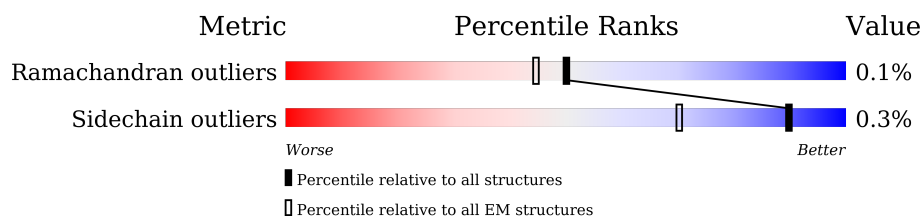
EMDB validation analysis : 0.0.1.dev117
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.2

1 Overall quality at a glance

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







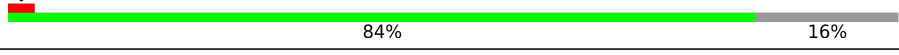
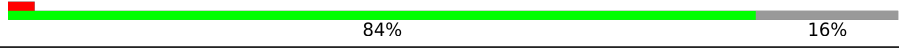
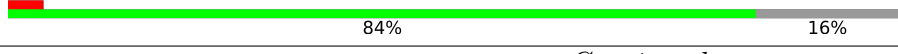
The reported resolution of this entry is 3.21 Å.

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.








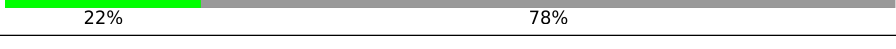

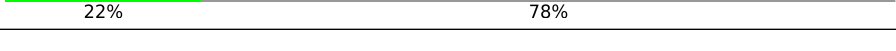
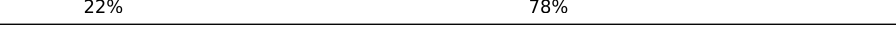
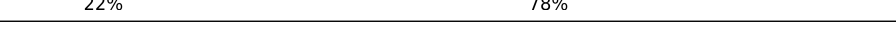










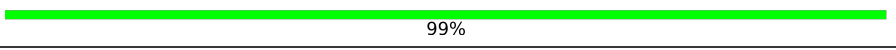
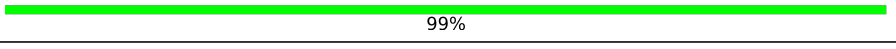
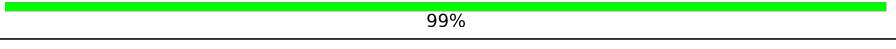
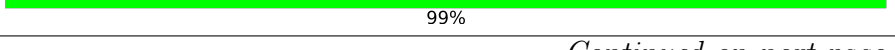

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	725	 84% 16%
1	B	725	 84% 16%
1	C	725	 84% 16%
1	D	725	 84% 16%
1	E	725	 84% 16%
1	F	725	 83% 16%
1	G	725	 84% 16%
1	H	725	 84% 16%
1	I	725	 84% 16%

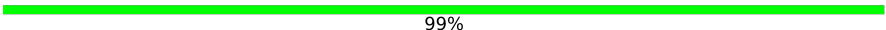













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Mol	Chain	Length	Quality of chain
1	J	725	 84%16%
1	K	725	 83%16%
1	L	725	 83%16%
2	M	667	 22%78%
2	N	667	 22%78%
2	O	667	 22%78%
2	P	667	 22%78%
2	Q	667	 22%78%
2	R	667	 22%78%
2	S	667	 22%78%
2	T	667	 22%78%
2	U	667	 22%78%
2	V	667	 22%78%
2	W	667	 22%78%
2	X	667	 22%78%
2	Y	667	 22%78%
2	Z	667	 22%78%
2	s	667	 22%78%
2	v	667	 22%78%
2	w	667	 22%78%
2	x	667	 22%78%
3	a	472	 99%
3	b	472	 99%
3	c	472	 99%
3	d	472	 99%

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Mol	Chain	Length	Quality of chain
3	e	472	 99%
3	f	472	 99%
4	g	166	 92% 8%
4	h	166	 92% 8%
4	i	166	 92% 8%
4	j	166	 92% 8%
4	k	166	 92% 8%
4	l	166	 92% 8%
4	m	166	 92% 8%
4	n	166	 92% 8%
4	o	166	 92% 8%
4	p	166	 92% 8%
4	q	166	 92% 8%
4	r	166	 92% 8%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 115680 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 Portal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	608	Total	C	N	O	S	0	0
			4908	3090	840	957	21		
1	B	608	Total	C	N	O	S	0	0
			4908	3090	840	957	21		
1	C	608	Total	C	N	O	S	0	0
			4908	3090	840	957	21		
1	D	608	Total	C	N	O	S	0	0
			4908	3090	840	957	21		
1	E	608	Total	C	N	O	S	0	0
			4908	3090	840	957	21		
1	F	608	Total	C	N	O	S	0	0
			4908	3090	840	957	21		
1	G	608	Total	C	N	O	S	0	0
			4908	3090	840	957	21		
1	H	608	Total	C	N	O	S	0	0
			4908	3090	840	957	21		
1	I	608	Total	C	N	O	S	0	0
			4908	3090	840	957	21		
1	J	608	Total	C	N	O	S	0	0
			4908	3090	840	957	21		
1	K	608	Total	C	N	O	S	0	0
			4908	3090	840	957	21		
1	L	608	Total	C	N	O	S	0	0
			4908	3090	840	957	21		

- Molecule 2 is a protein called Endorhamnosidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	147	Total	C	N	O	S	0	0
			1129	717	185	226	1		
2	N	147	Total	C	N	O	S	0	0
			1129	717	185	226	1		
2	O	147	Total	C	N	O	S	0	0
			1129	717	185	226	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	149	Total	C	N	O	S	0	0
			1161	740	191	229	1		
2	Q	149	Total	C	N	O	S	0	0
			1161	740	191	229	1		
2	R	149	Total	C	N	O	S	0	0
			1161	740	191	229	1		
2	S	149	Total	C	N	O	S	0	0
			1161	740	191	229	1		
2	T	149	Total	C	N	O	S	0	0
			1161	740	191	229	1		
2	U	149	Total	C	N	O	S	0	0
			1148	727	190	230	1		
2	V	149	Total	C	N	O	S	0	0
			1148	727	190	230	1		
2	W	149	Total	C	N	O	S	0	0
			1148	727	190	230	1		
2	X	149	Total	C	N	O	S	0	0
			1148	727	190	230	1		
2	Y	149	Total	C	N	O	S	0	0
			1148	727	190	230	1		
2	Z	147	Total	C	N	O	S	0	0
			1129	717	185	226	1		
2	s	147	Total	C	N	O	S	0	0
			1129	717	185	226	1		
2	v	149	Total	C	N	O	S	0	0
			1161	740	191	229	1		
2	w	149	Total	C	N	O	S	0	0
			1148	727	190	230	1		
2	x	147	Total	C	N	O	S	0	0
			1129	717	185	226	1		

- Molecule 3 is a protein called Phage stabilisation protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	a	470	Total	C	N	O	S	0	0
			3676	2320	630	708	18		
3	b	470	Total	C	N	O	S	0	0
			3676	2320	630	708	18		
3	c	470	Total	C	N	O	S	0	0
			3676	2320	630	708	18		
3	d	470	Total	C	N	O	S	0	0
			3676	2320	630	708	18		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	e	470	Total	C	N	O	S	0	0
			3676	2320	630	708	18		
3	f	470	Total	C	N	O	S	0	0
			3676	2320	630	708	18		

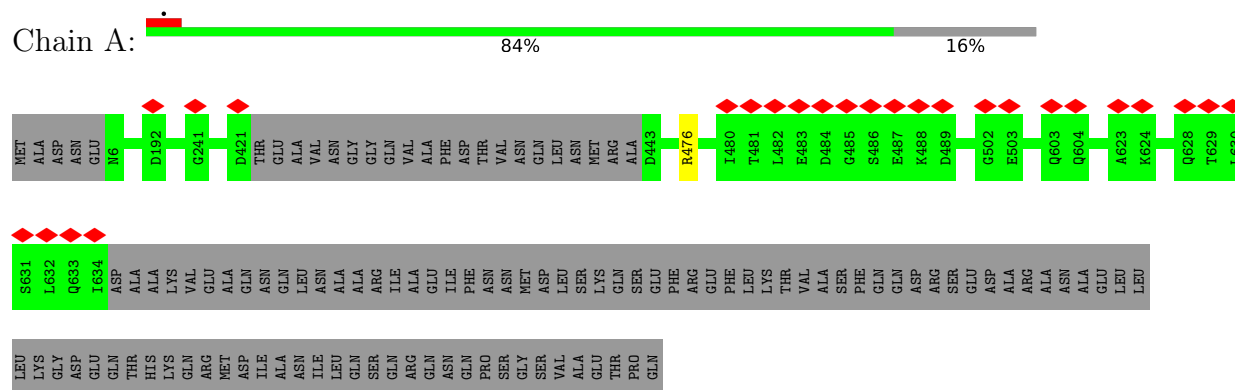
- Molecule 4 is a protein called P22 tail accessory factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	g	153	Total	C	N	O	S	0	0
			1175	736	202	231	6		
4	h	153	Total	C	N	O	S	0	0
			1175	736	202	231	6		
4	i	153	Total	C	N	O	S	0	0
			1175	736	202	231	6		
4	j	153	Total	C	N	O	S	0	0
			1175	736	202	231	6		
4	k	153	Total	C	N	O	S	0	0
			1175	736	202	231	6		
4	l	153	Total	C	N	O	S	0	0
			1175	736	202	231	6		
4	m	153	Total	C	N	O	S	0	0
			1175	736	202	231	6		
4	n	153	Total	C	N	O	S	0	0
			1175	736	202	231	6		
4	o	153	Total	C	N	O	S	0	0
			1175	736	202	231	6		
4	p	153	Total	C	N	O	S	0	0
			1175	736	202	231	6		
4	q	153	Total	C	N	O	S	0	0
			1175	736	202	231	6		
4	r	153	Total	C	N	O	S	0	0
			1175	736	202	231	6		

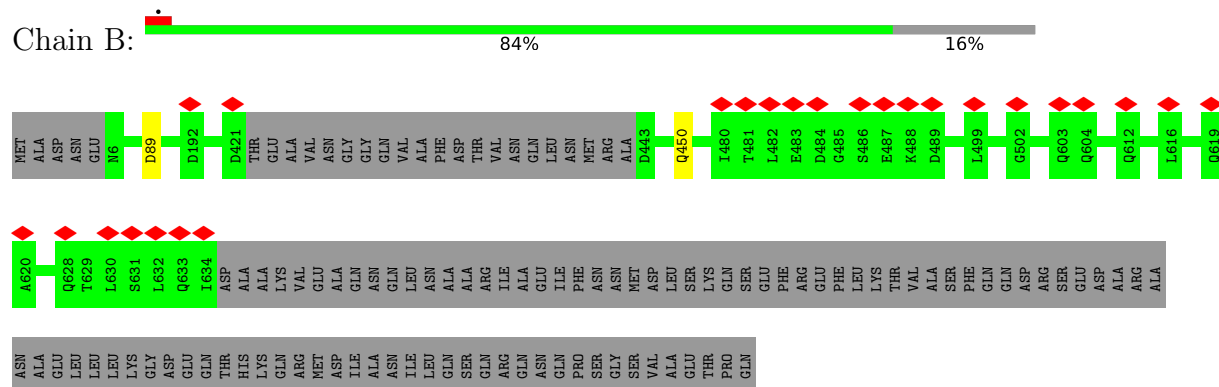
3 Residue-property plots

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.

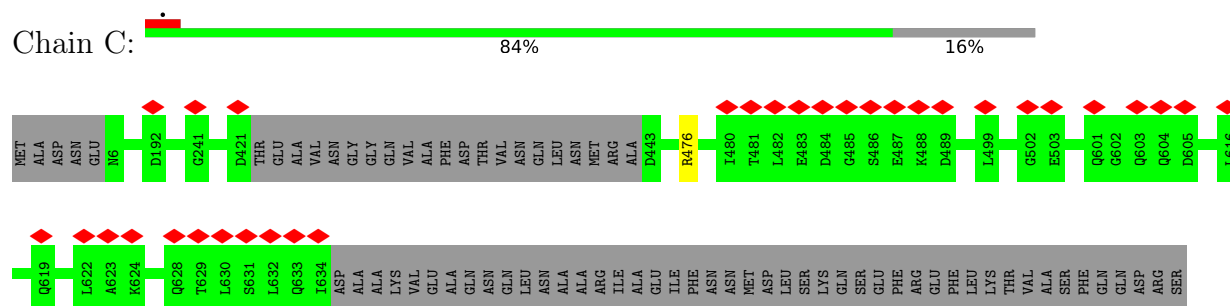
• Molecule 1: Portal protein

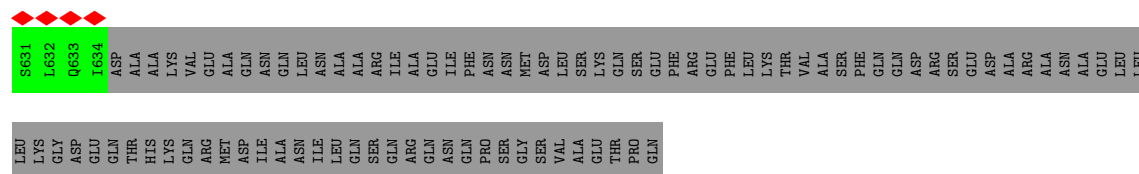


• Molecule 1: Portal protein



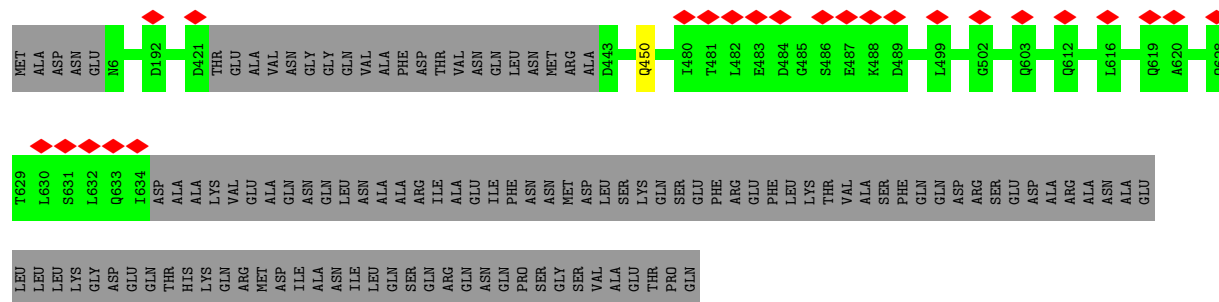
• Molecule 1: Portal protein





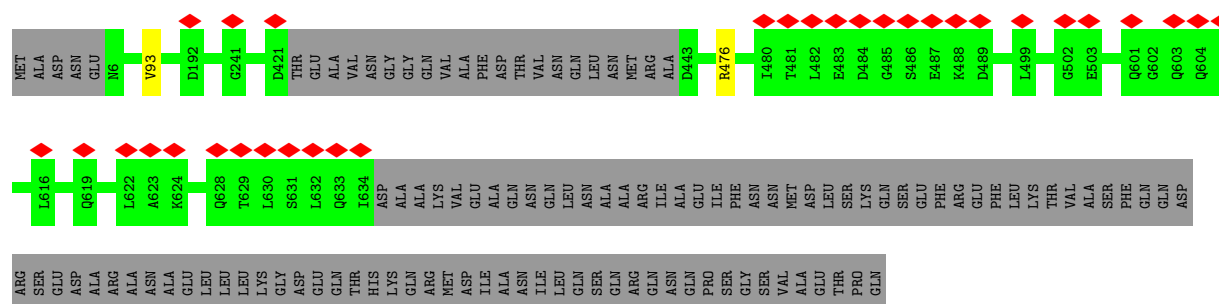
• Molecule 1: Portal protein

Chain H: 84% 16%



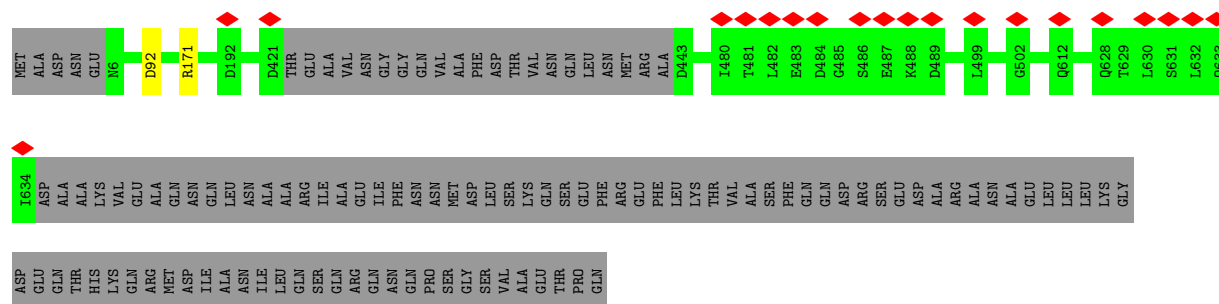
• Molecule 1: Portal protein

Chain I: 84% 16%



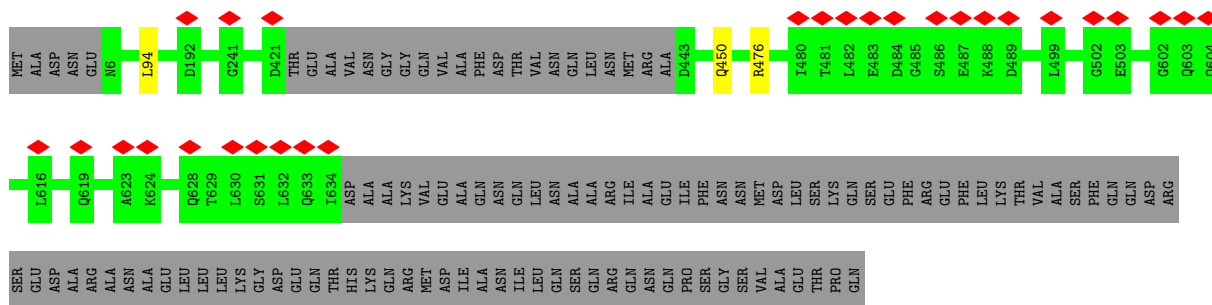
• Molecule 1: Portal protein

Chain J: 84% 16%

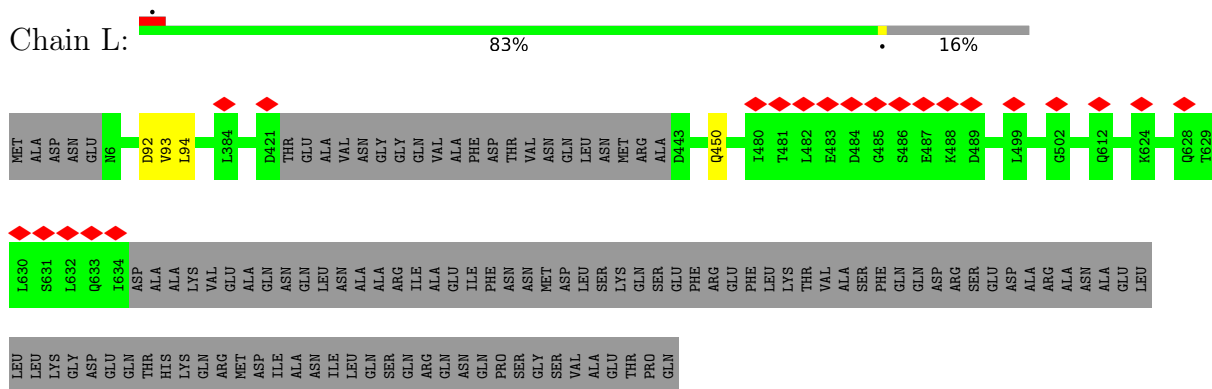


• Molecule 1: Portal protein

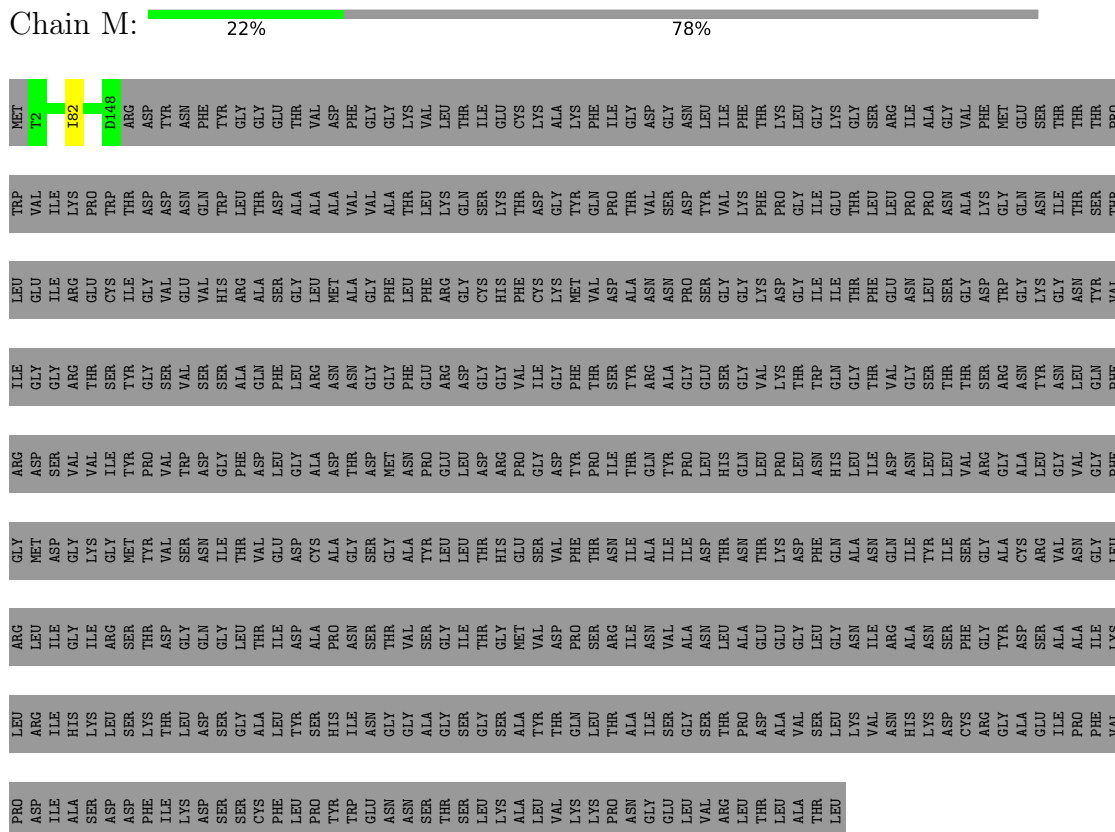
Chain K: 83% 16%



- Molecule 1: Portal protein



- Molecule 2: Endorhamnosidase



[illegible]

- Molecule 2: Endorhamnosidase

Chain R:  22% 78%

[illegible]

- Molecule 2: Endorhamnosidase

Chain S:  22% 78%

[illegible]



[illegible]

- Molecule 2: Endorhamnosidase

Chain V:  22% 78%

[illegible]

- Molecule 2: Endorhamnosidase

Chain W:  22% 78%

[illegible]

- Molecule 2: Endorhamnosidase

Chain w: 22% 78%

[illegible]

- Molecule 2: Endorhamnosidase

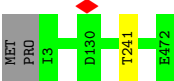
Chain x:  22% 78%

GLY	ARG	ILE	LEU	TRP	MET
MET	ASP	GLY	GLU	VAL	I2
ASP	SER	GLY	ILE	ILE	I82
GLY	VAL	THR	ARG	LYS	I82
GLY	ILE	SER	GLU	PRO	DI48
MET	TYR	TYR	CYS	TRP	DI48
TYR	PRO	GLY	ILE	THR	ASP
VAL	VAL	SER	VAL	ASP	ASP
SER	TRP	VAL	GLU	ASN	ASN
ASN	ASP	SER	VAL	GLN	PHE
ILE	GLY	SER	HIS	TRP	TYR
THR	PHE	ALA	ARG	LEU	GLY
VAL	ASP	GLN	ALA	THR	GLY
GLU	LEU	PHE	SER	ALA	THR
ASP	GLY	LEU	LEU	ALA	VAL
ALA	ASP	ARG	LEU	ALA	VAL
GLY	THR	ASN	MET	ALA	ASP
SER	ASP	GLY	ALA	VAL	PHE
GLY	MET	GLY	GLY	VAL	GLY
ALA	ASN	PHE	PHE	ALA	GLY
TYR	PRO	GLU	LEU	THR	LYS
LEU	GLU	ARG	PHE	LEU	VAL
LEU	LEU	ASP	GLY	LYS	LEU
HIS	ASP	GLY	CYS	GLN	THR
GLU	ARG	GLY	HIS	LYS	ILE
VAL	PRO	VAL	PHE	THR	GLU
SER	GLY	ILE	CYS	ASP	CYS
VAL	ASP	GLY	LYS	GLY	LYS
PHE	TYR	PHE	MET	TYR	ALA
ASN	ILE	SER	VAL	GLN	LYS
ILE	GLN	ARG	ASN	VAL	ASP
ILE	TYR	ALA	ASN	SER	GLY
ILE	PRO	GLY	PRO	ASP	ASN
ASP	LEU	GLU	SER	TYR	LEU
THR	HIS	THR	GLY	VAL	ILE
ASN	GLN	GLY	GLY	LYS	PHE
THR	LEU	VAL	LYS	PHE	THR
LYS	PRO	LYS	ASP	PRO	LYS
ASP	LEU	THR	GLY	PRO	LEU
PHE	ASN	TRP	ILE	ILE	GLY
GLN	HIS	GLN	ILE	GLY	LYS
ALA	LEU	GLY	THR	THR	GLY
ASN	ILE	THR	PHE	LEU	SER
GLN	ASP	VAL	GLU	LEU	ARG
ILE	ASN	GLY	VAL	PRO	ILE
TYR	LEU	SER	LEU	PRO	GLY
ILE	LEU	THR	SER	ASN	ALA
SER	ARG	THR	GLY	LYS	PHE
ALA	GLY	ARG	TRP	GLY	MET
CYS	ALA	ASN	GLY	GLN	GLU
ARG	LEU	TYR	LYS	ASN	THR
VAL	GLY	ASN	ASN	ILE	THR
ASN	VAL	ASN	GLY	THR	THR
GLY	PHE	GLN	TYR	THR	PRO

LEU	ARG	ILE	HIS	LYS	LEU	SER	LYS	THR	ASP	LEU	SER	ASP	GLY	ALA	LEU	TYR	THR	HIS	ILE	ASN	SER	THR	THR	VAL	SER	GLY	THR	GLY	MET	VAL	VAL	ASP	PRO	PRO	SER	THR	THR	GLY	GLY	ILE	ILE	ASN	ASN	ARG	ILE	ASN	VAL	GLY	GLY	GLY	GLY	ASN	ASN	LEU	ALA	ALA	GLU	GLU	GLY	GLY	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	
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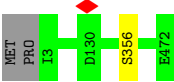
• Molecule 3: Phage stabilisation protein

Chain a: 99%



• Molecule 3: Phage stabilisation protein

Chain b: 99%



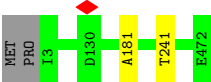
• Molecule 3: Phage stabilisation protein

Chain c: 99%



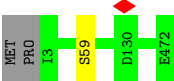
• Molecule 3: Phage stabilisation protein

Chain d: 99%



• Molecule 3: Phage stabilisation protein

Chain e: 99%

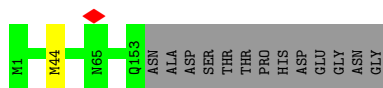
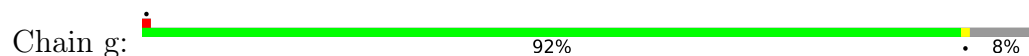


• Molecule 3: Phage stabilisation protein

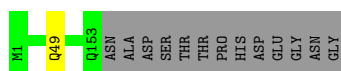
Chain f: 99%



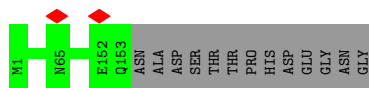
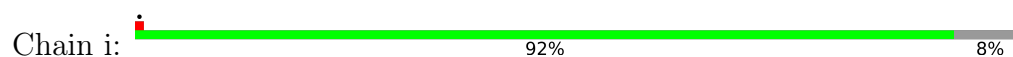
- Molecule 4: P22 tail accessory factor



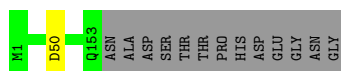
- Molecule 4: P22 tail accessory factor



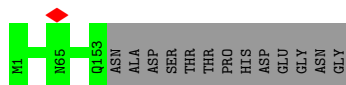
- Molecule 4: P22 tail accessory factor



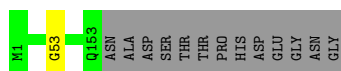
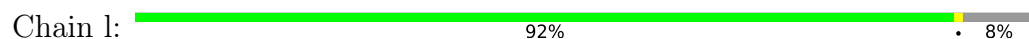
- Molecule 4: P22 tail accessory factor



- Molecule 4: P22 tail accessory factor



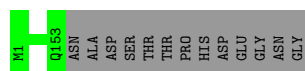
- Molecule 4: P22 tail accessory factor



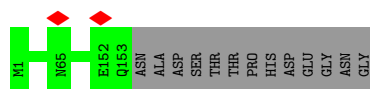
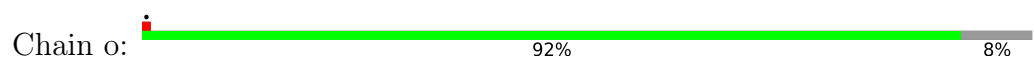
- Molecule 4: P22 tail accessory factor



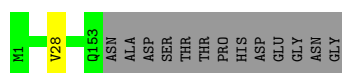
- Molecule 4: P22 tail accessory factor



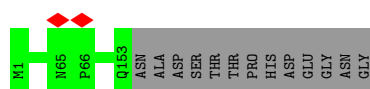
- Molecule 4: P22 tail accessory factor



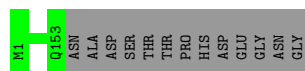
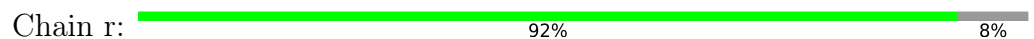
- Molecule 4: P22 tail accessory factor



- Molecule 4: P22 tail accessory factor



- Molecule 4: P22 tail accessory factor



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	82501	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	32	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	30.704	Depositor
Minimum map value	-16.371	Depositor
Average map value	0.005	Depositor
Map value standard deviation	1.237	Depositor
Recommended contour level	3	Depositor
Map size (\AA)	544.0, 544.0, 544.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.36, 1.36, 1.36	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	0.25	0/5009	0.48	0/6794
1	B	0.26	0/5009	0.48	0/6794
1	C	0.25	0/5009	0.48	0/6794
1	D	0.25	0/5009	0.48	0/6794
1	E	0.25	0/5009	0.49	0/6794
1	F	0.26	0/5009	0.48	0/6794
1	G	0.25	0/5009	0.49	0/6794
1	H	0.26	0/5009	0.49	0/6794
1	I	0.26	0/5009	0.48	0/6794
1	J	0.25	0/5009	0.48	0/6794
1	K	0.26	0/5009	0.49	0/6794
1	L	0.26	0/5009	0.48	0/6794
2	M	0.28	0/1150	0.49	0/1570
2	N	0.28	0/1150	0.50	0/1570
2	O	0.28	0/1150	0.51	0/1570
2	P	0.25	0/1185	0.48	0/1616
2	Q	0.25	0/1185	0.48	0/1616
2	R	0.25	0/1185	0.47	0/1616
2	S	0.25	0/1185	0.47	0/1616
2	T	0.25	0/1185	0.48	0/1616
2	U	0.26	0/1169	0.45	0/1595
2	V	0.26	0/1169	0.46	0/1595
2	W	0.26	0/1169	0.44	0/1595
2	X	0.28	0/1169	0.47	0/1595
2	Y	0.26	0/1169	0.46	0/1595
2	Z	0.30	0/1150	0.49	0/1570
2	s	0.29	0/1150	0.51	0/1570
2	v	0.25	0/1185	0.47	0/1616
2	w	0.26	0/1169	0.45	0/1595
2	x	0.28	0/1150	0.50	0/1570
3	a	0.27	0/3756	0.54	0/5086
3	b	0.27	0/3756	0.54	0/5086
3	c	0.28	0/3756	0.53	0/5086
3	d	0.27	0/3756	0.54	0/5086

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	e	0.28	0/3756	0.54	0/5086
3	f	0.28	0/3756	0.53	0/5086
4	g	0.44	0/1200	0.56	0/1626
4	h	0.29	0/1200	0.50	0/1626
4	i	0.29	0/1200	0.50	0/1626
4	j	0.29	0/1200	0.52	0/1626
4	k	0.30	0/1200	0.50	0/1626
4	l	0.30	0/1200	0.51	0/1626
4	m	0.29	0/1200	0.51	0/1626
4	n	0.31	0/1200	0.50	0/1626
4	o	0.29	0/1200	0.51	0/1626
4	p	0.32	0/1200	0.51	0/1626
4	q	0.30	0/1200	0.51	0/1626
4	r	0.32	0/1200	0.52	0/1626
All	All	0.27	0/118068	0.50	0/160242

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](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	604/725 (83%)	569 (94%)	35 (6%)	0	100	100
1	B	604/725 (83%)	567 (94%)	37 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	604/725 (83%)	572 (95%)	32 (5%)	0	100	100
1	D	604/725 (83%)	568 (94%)	36 (6%)	0	100	100
1	E	604/725 (83%)	569 (94%)	35 (6%)	0	100	100
1	F	604/725 (83%)	567 (94%)	37 (6%)	0	100	100
1	G	604/725 (83%)	568 (94%)	36 (6%)	0	100	100
1	H	604/725 (83%)	568 (94%)	36 (6%)	0	100	100
1	I	604/725 (83%)	565 (94%)	39 (6%)	0	100	100
1	J	604/725 (83%)	567 (94%)	37 (6%)	0	100	100
1	K	604/725 (83%)	569 (94%)	35 (6%)	0	100	100
1	L	604/725 (83%)	567 (94%)	37 (6%)	0	100	100
2	M	145/667 (22%)	133 (92%)	11 (8%)	1 (1%)	19	53
2	N	145/667 (22%)	134 (92%)	11 (8%)	0	100	100
2	O	145/667 (22%)	135 (93%)	9 (6%)	1 (1%)	19	53
2	P	147/667 (22%)	140 (95%)	6 (4%)	1 (1%)	19	53
2	Q	147/667 (22%)	138 (94%)	8 (5%)	1 (1%)	19	53
2	R	147/667 (22%)	139 (95%)	8 (5%)	0	100	100
2	S	147/667 (22%)	140 (95%)	7 (5%)	0	100	100
2	T	147/667 (22%)	139 (95%)	8 (5%)	0	100	100
2	U	147/667 (22%)	142 (97%)	5 (3%)	0	100	100
2	V	147/667 (22%)	141 (96%)	6 (4%)	0	100	100
2	W	147/667 (22%)	144 (98%)	3 (2%)	0	100	100
2	X	147/667 (22%)	143 (97%)	4 (3%)	0	100	100
2	Y	147/667 (22%)	141 (96%)	6 (4%)	0	100	100
2	Z	145/667 (22%)	134 (92%)	11 (8%)	0	100	100
2	s	145/667 (22%)	135 (93%)	9 (6%)	1 (1%)	19	53
2	v	147/667 (22%)	140 (95%)	7 (5%)	0	100	100
2	w	147/667 (22%)	143 (97%)	4 (3%)	0	100	100
2	x	145/667 (22%)	135 (93%)	9 (6%)	1 (1%)	19	53
3	a	468/472 (99%)	430 (92%)	38 (8%)	0	100	100
3	b	468/472 (99%)	432 (92%)	35 (8%)	1 (0%)	44	74
3	c	468/472 (99%)	432 (92%)	35 (8%)	1 (0%)	44	74

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	d	468/472 (99%)	431 (92%)	36 (8%)	1 (0%)	44	74
3	e	468/472 (99%)	432 (92%)	36 (8%)	0	100	100
3	f	468/472 (99%)	432 (92%)	35 (8%)	1 (0%)	44	74
4	g	151/166 (91%)	142 (94%)	9 (6%)	0	100	100
4	h	151/166 (91%)	138 (91%)	13 (9%)	0	100	100
4	i	151/166 (91%)	141 (93%)	10 (7%)	0	100	100
4	j	151/166 (91%)	138 (91%)	13 (9%)	0	100	100
4	k	151/166 (91%)	143 (95%)	8 (5%)	0	100	100
4	l	151/166 (91%)	137 (91%)	13 (9%)	1 (1%)	19	53
4	m	151/166 (91%)	143 (95%)	8 (5%)	0	100	100
4	n	151/166 (91%)	139 (92%)	12 (8%)	0	100	100
4	o	151/166 (91%)	140 (93%)	11 (7%)	0	100	100
4	p	151/166 (91%)	138 (91%)	13 (9%)	0	100	100
4	q	151/166 (91%)	142 (94%)	9 (6%)	0	100	100
4	r	151/166 (91%)	138 (91%)	13 (9%)	0	100	100
All	All	14502/25530 (57%)	13580 (94%)	911 (6%)	11 (0%)	50	79

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	b	356	SER
3	d	181	ALA
4	l	53	GLY
3	c	105	ALA
3	f	105	ALA

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	533/630 (85%)	532 (100%)	1 (0%)	92	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	533/630 (85%)	531 (100%)	2 (0%)	89	93
1	C	533/630 (85%)	532 (100%)	1 (0%)	92	96
1	D	533/630 (85%)	533 (100%)	0	100	100
1	E	533/630 (85%)	531 (100%)	2 (0%)	89	93
1	F	533/630 (85%)	530 (99%)	3 (1%)	84	91
1	G	533/630 (85%)	532 (100%)	1 (0%)	92	96
1	H	533/630 (85%)	532 (100%)	1 (0%)	92	96
1	I	533/630 (85%)	531 (100%)	2 (0%)	89	93
1	J	533/630 (85%)	531 (100%)	2 (0%)	89	93
1	K	533/630 (85%)	530 (99%)	3 (1%)	84	91
1	L	533/630 (85%)	529 (99%)	4 (1%)	79	89
2	M	125/548 (23%)	125 (100%)	0	100	100
2	N	125/548 (23%)	125 (100%)	0	100	100
2	O	125/548 (23%)	125 (100%)	0	100	100
2	P	127/548 (23%)	127 (100%)	0	100	100
2	Q	127/548 (23%)	127 (100%)	0	100	100
2	R	127/548 (23%)	127 (100%)	0	100	100
2	S	127/548 (23%)	127 (100%)	0	100	100
2	T	127/548 (23%)	125 (98%)	2 (2%)	58	78
2	U	127/548 (23%)	127 (100%)	0	100	100
2	V	127/548 (23%)	127 (100%)	0	100	100
2	W	127/548 (23%)	127 (100%)	0	100	100
2	X	127/548 (23%)	126 (99%)	1 (1%)	79	89
2	Y	127/548 (23%)	127 (100%)	0	100	100
2	Z	125/548 (23%)	125 (100%)	0	100	100
2	s	125/548 (23%)	125 (100%)	0	100	100
2	v	127/548 (23%)	127 (100%)	0	100	100
2	w	127/548 (23%)	127 (100%)	0	100	100
2	x	125/548 (23%)	125 (100%)	0	100	100
3	a	393/395 (100%)	392 (100%)	1 (0%)	91	95
3	b	393/395 (100%)	393 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	c	393/395 (100%)	392 (100%)	1 (0%)	91	95
3	d	393/395 (100%)	392 (100%)	1 (0%)	91	95
3	e	393/395 (100%)	392 (100%)	1 (0%)	91	95
3	f	393/395 (100%)	392 (100%)	1 (0%)	91	95
4	g	121/131 (92%)	120 (99%)	1 (1%)	79	89
4	h	121/131 (92%)	120 (99%)	1 (1%)	79	89
4	i	121/131 (92%)	121 (100%)	0	100	100
4	j	121/131 (92%)	120 (99%)	1 (1%)	79	89
4	k	121/131 (92%)	121 (100%)	0	100	100
4	l	121/131 (92%)	121 (100%)	0	100	100
4	m	121/131 (92%)	121 (100%)	0	100	100
4	n	121/131 (92%)	121 (100%)	0	100	100
4	o	121/131 (92%)	121 (100%)	0	100	100
4	p	121/131 (92%)	120 (99%)	1 (1%)	79	89
4	q	121/131 (92%)	121 (100%)	0	100	100
4	r	121/131 (92%)	121 (100%)	0	100	100
All	All	12480/21366 (58%)	12446 (100%)	34 (0%)	90	95

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	e	59	SER
3	f	102	THR
4	j	50	ASP
1	I	476	ARG
1	I	93	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
4	h	49	GLN
4	o	49	GLN
2	x	78	GLN
2	x	28	ASN
2	M	78	GLN

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.

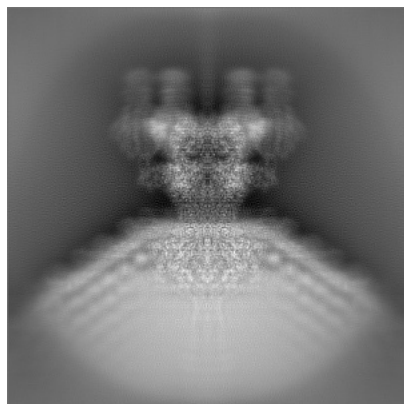
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61457. These allow visual inspection of the internal detail of the map and identification of artifacts.

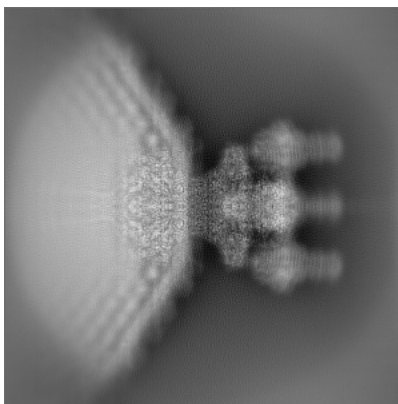
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

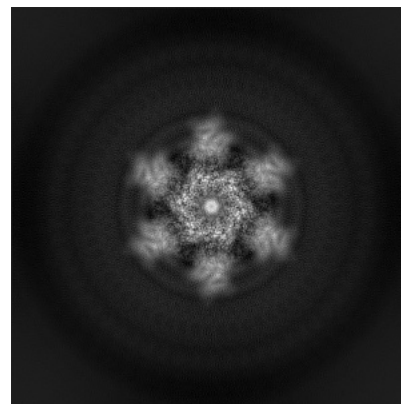
6.1.1 Primary map



X

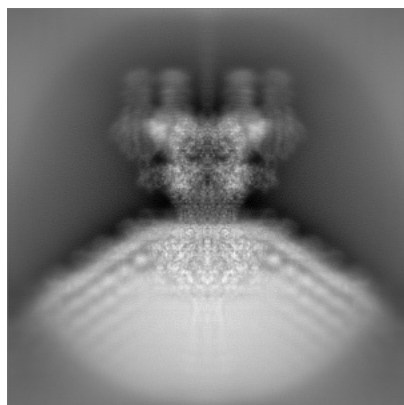


Y

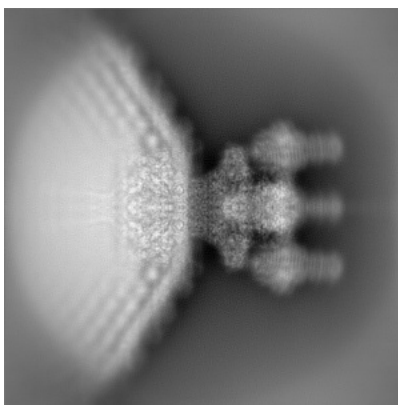


Z

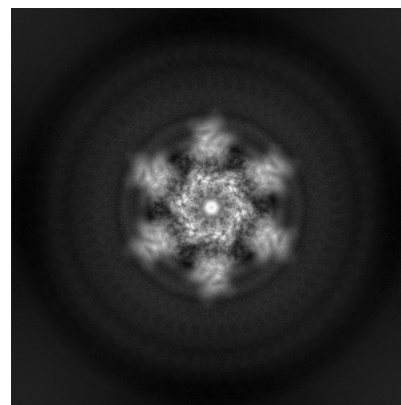
6.1.2 Raw map



X



Y

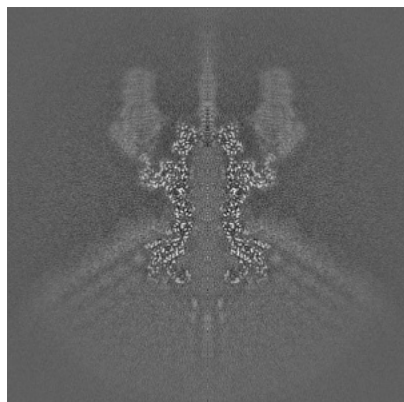


Z

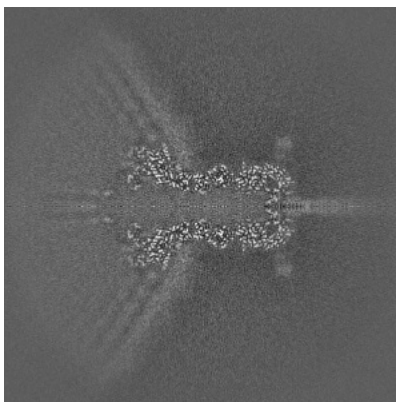
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

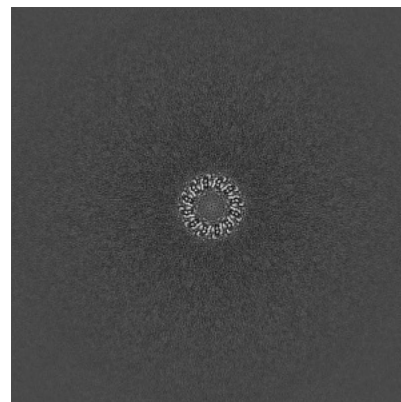
6.2.1 Primary map



X Index: 200

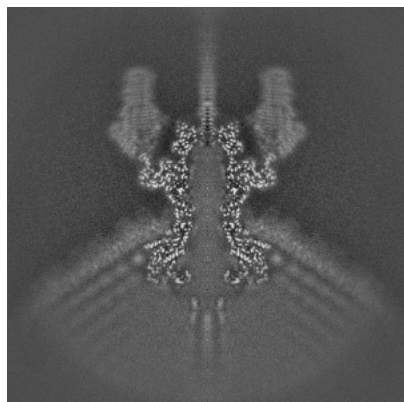


Y Index: 200

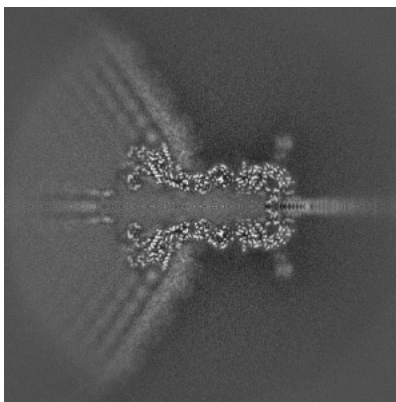


Z Index: 200

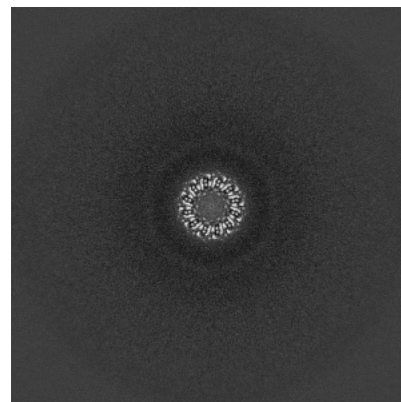
6.2.2 Raw map



X Index: 200



Y Index: 200

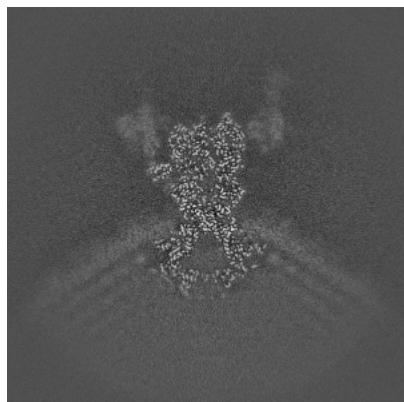


Z Index: 200

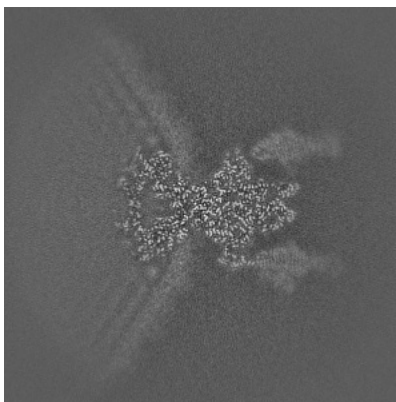
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

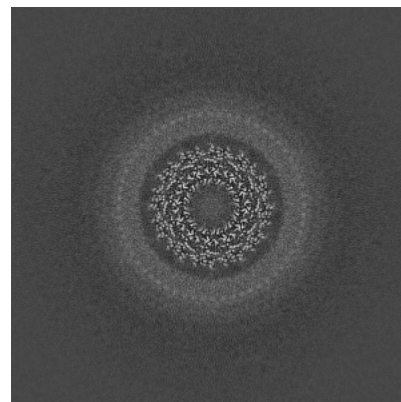
6.3.1 Primary map



X Index: 218

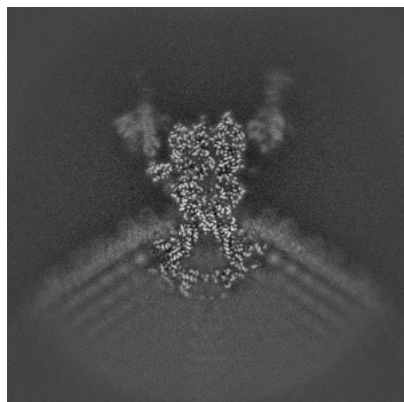


Y Index: 221

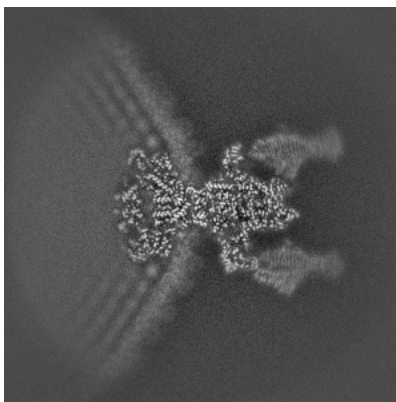


Z Index: 159

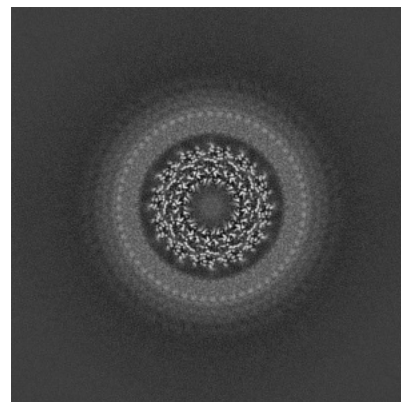
6.3.2 Raw map



X Index: 218



Y Index: 226

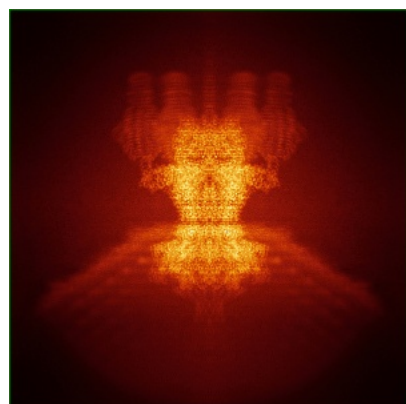


Z Index: 159

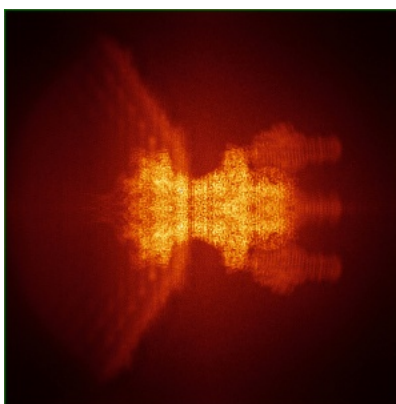
The images above show the largest variance slices of the map in three orthogonal directions.

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

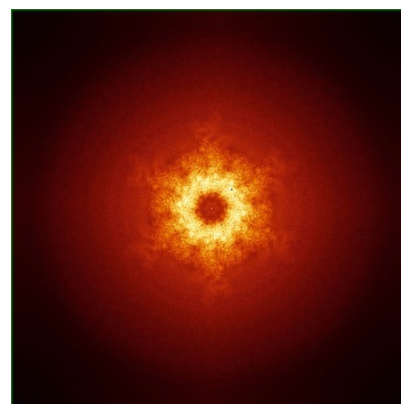
6.4.1 Primary map



X

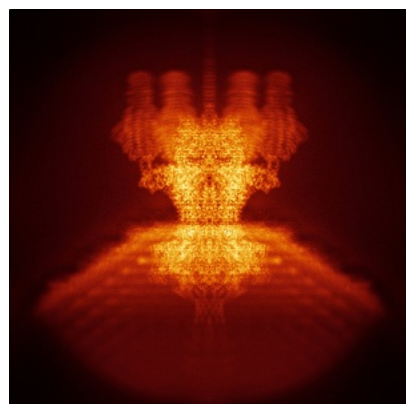


Y

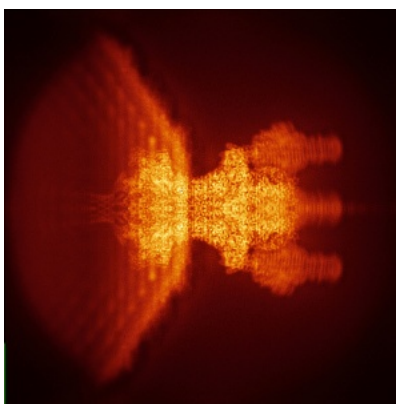


Z

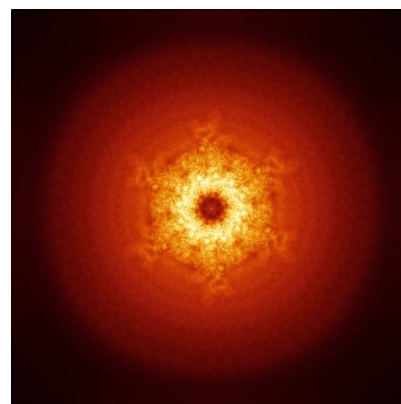
6.4.2 Raw map



X



Y

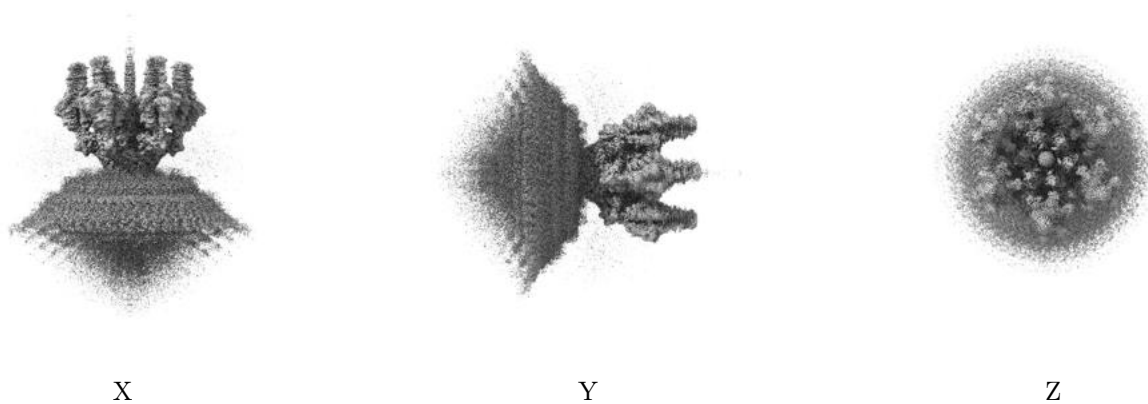


Z

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.

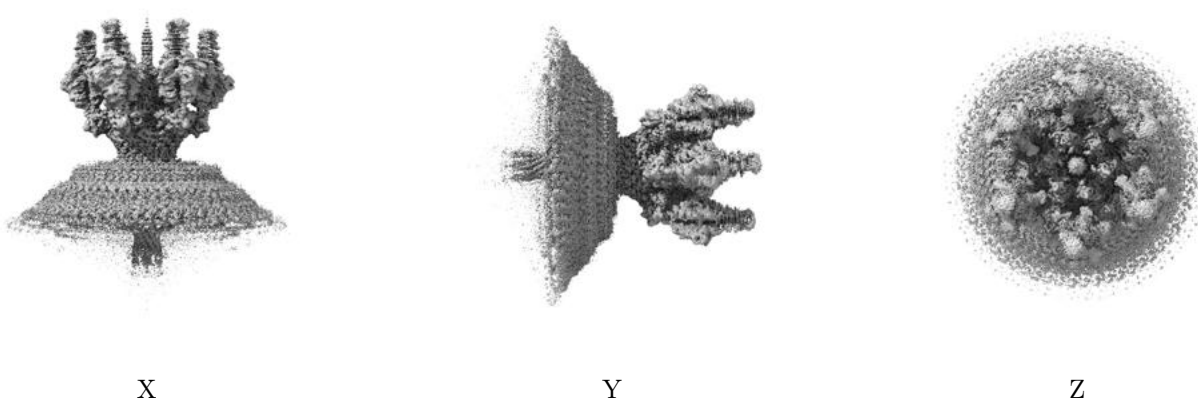
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

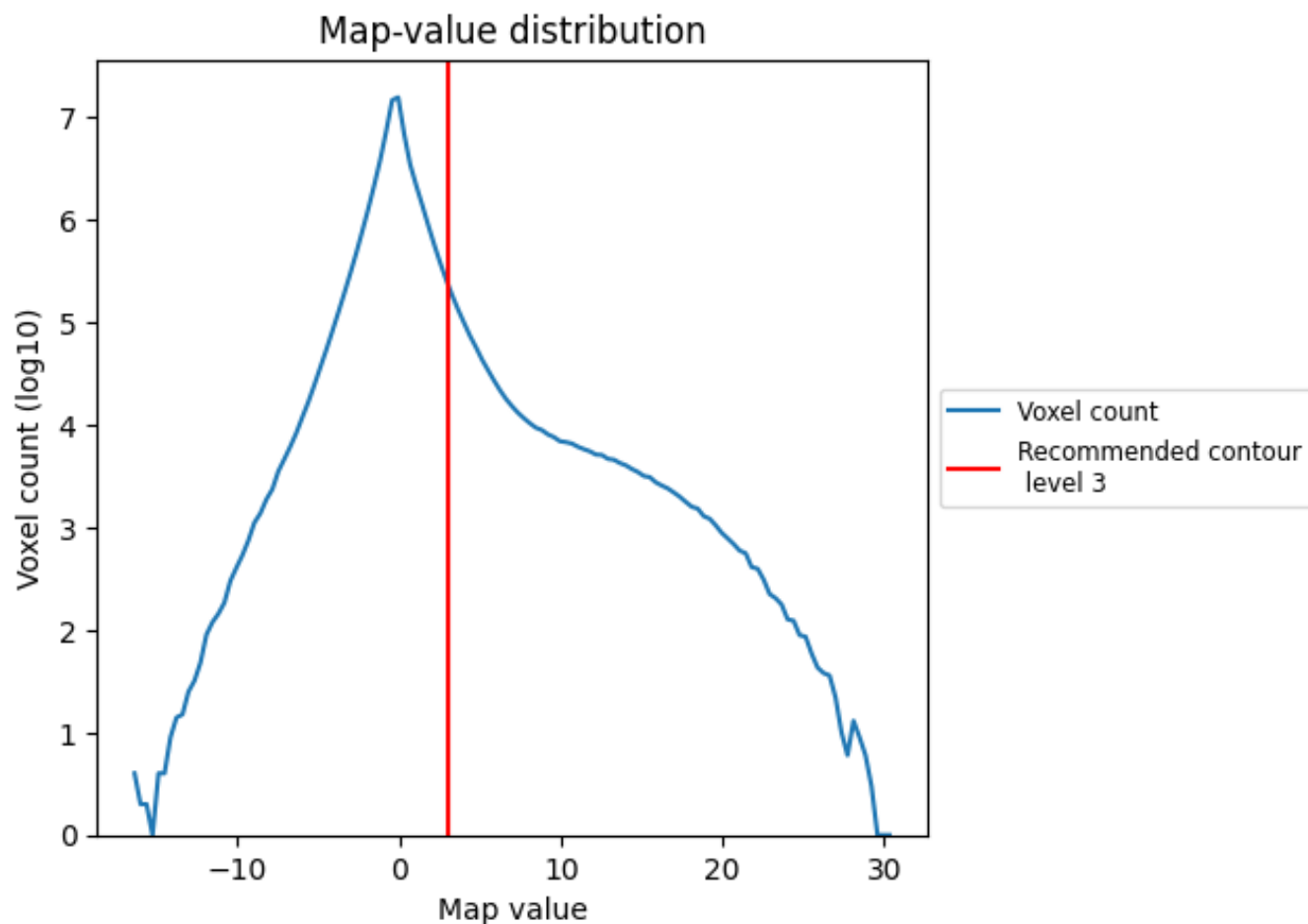
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

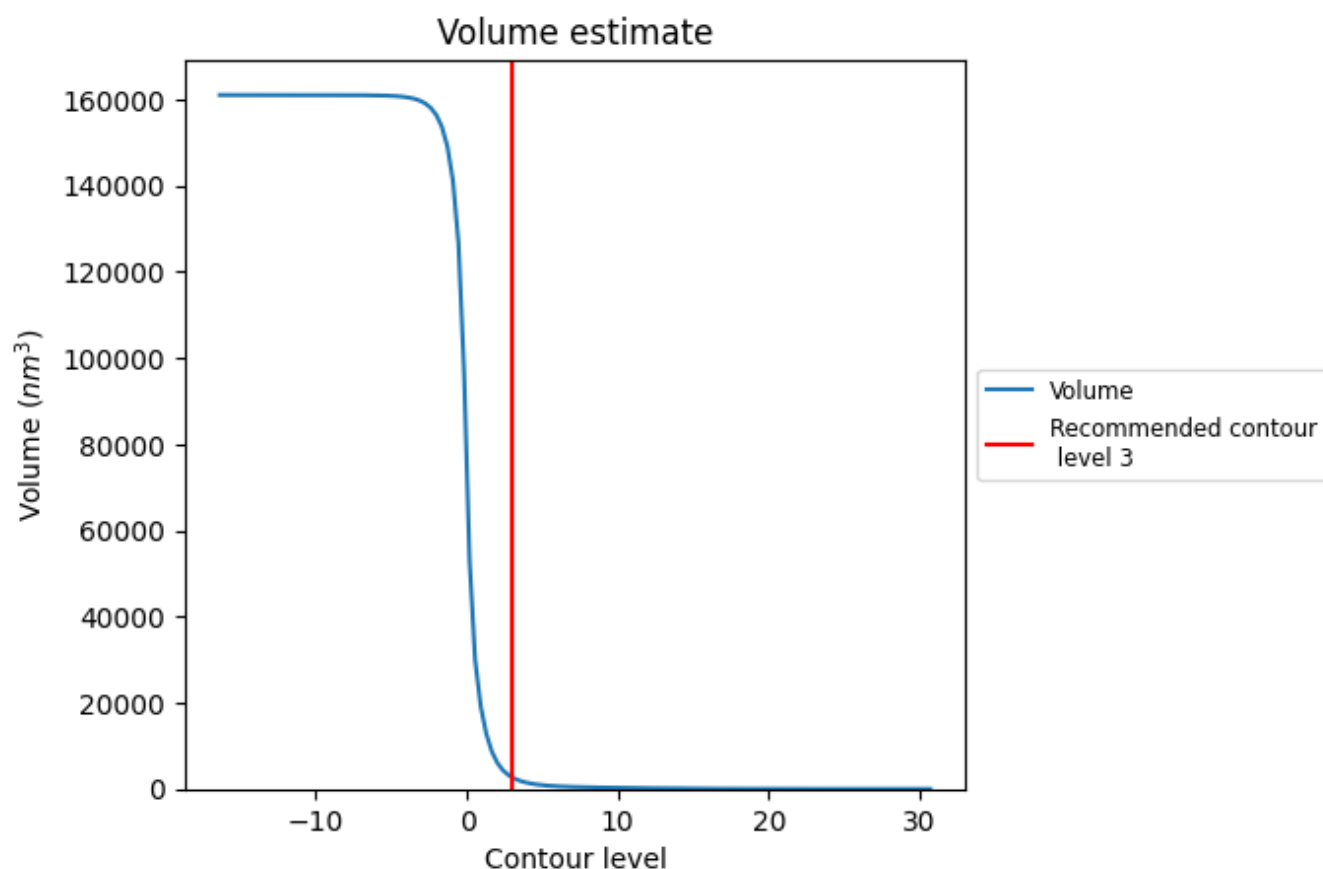
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

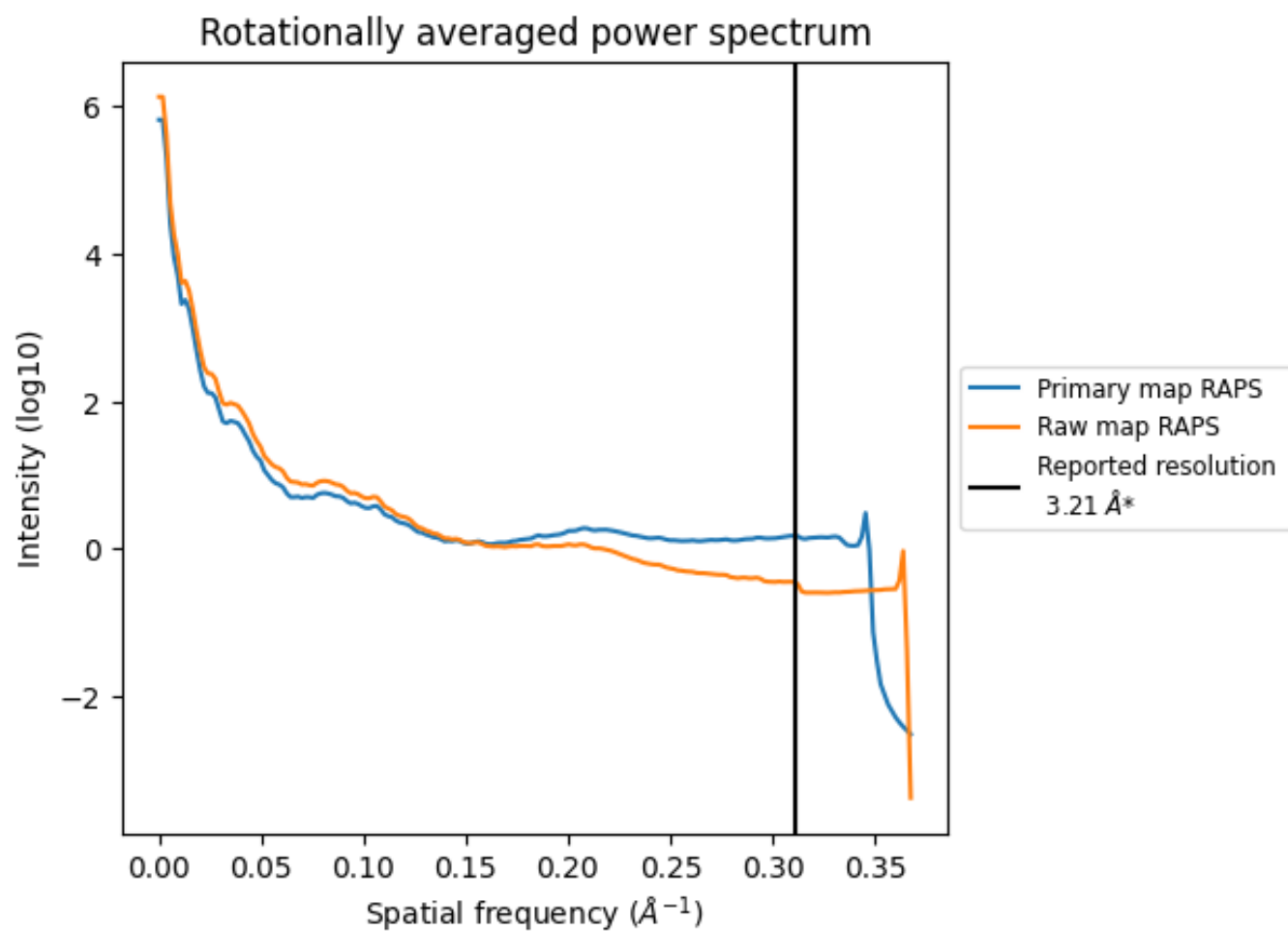
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2711 nm³; this corresponds to an approximate mass of 2449 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 ⓘ

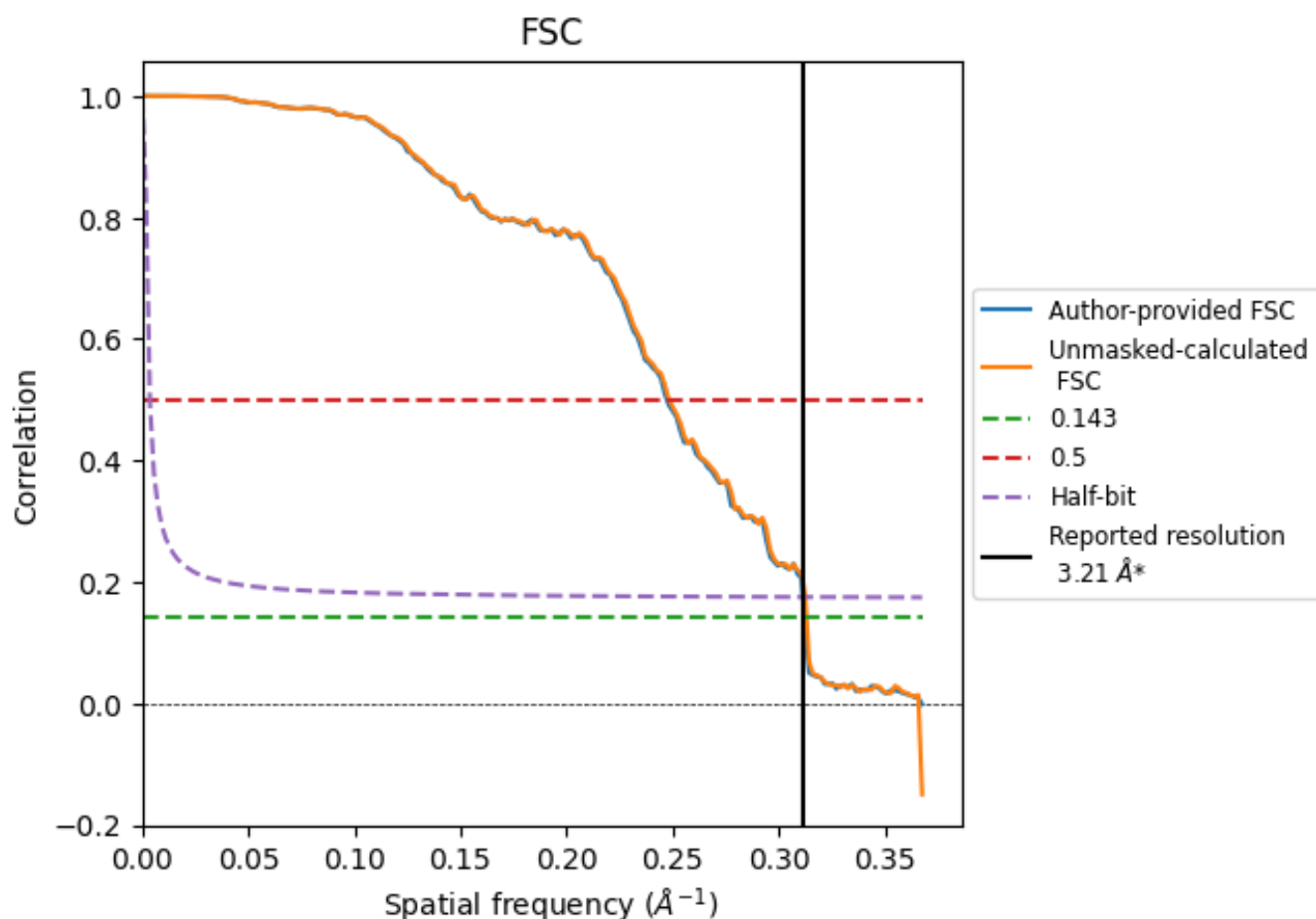


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312 \AA^{-1}

8.2 Resolution estimates [i](#)

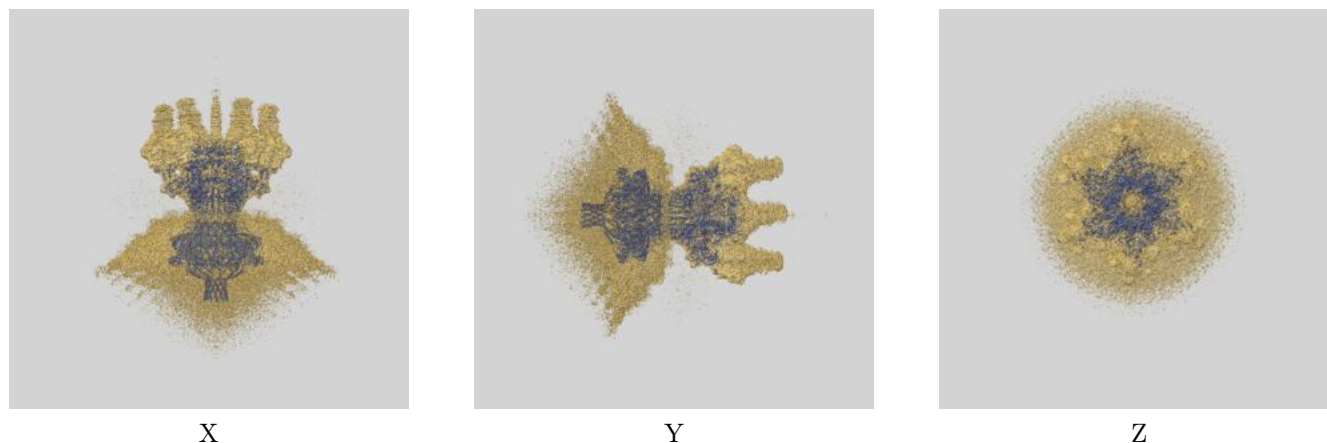
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.21	-	-
Author-provided FSC curve	3.21	4.04	3.21
Unmasked-calculated*	3.19	4.03	3.20

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

9 Map-model fit [i](#)

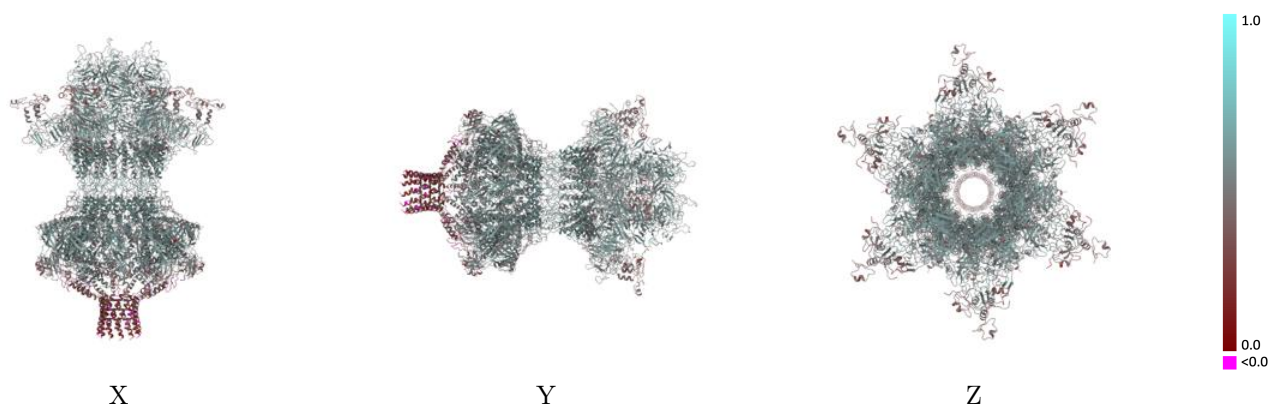
This section contains information regarding the fit between EMDB map EMD-61457 and PDB model 9JG6. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



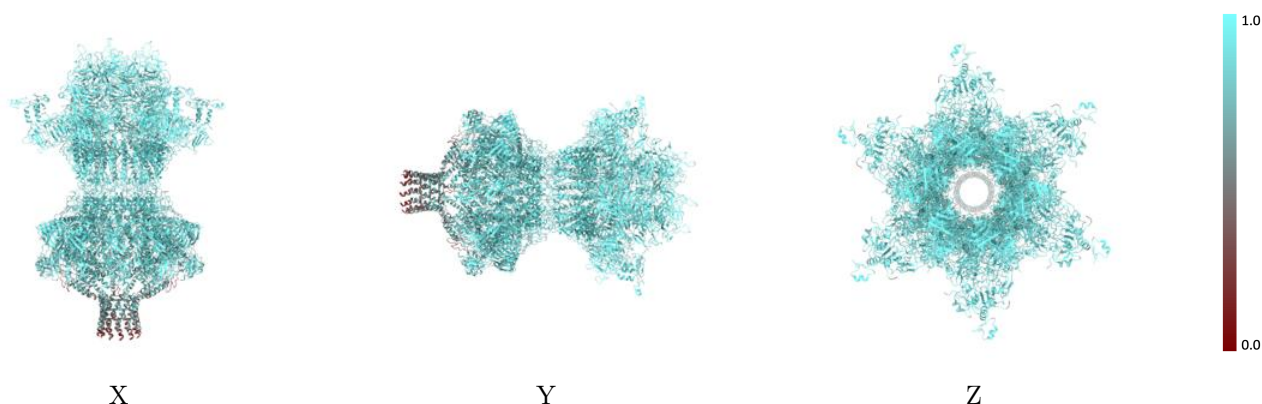
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



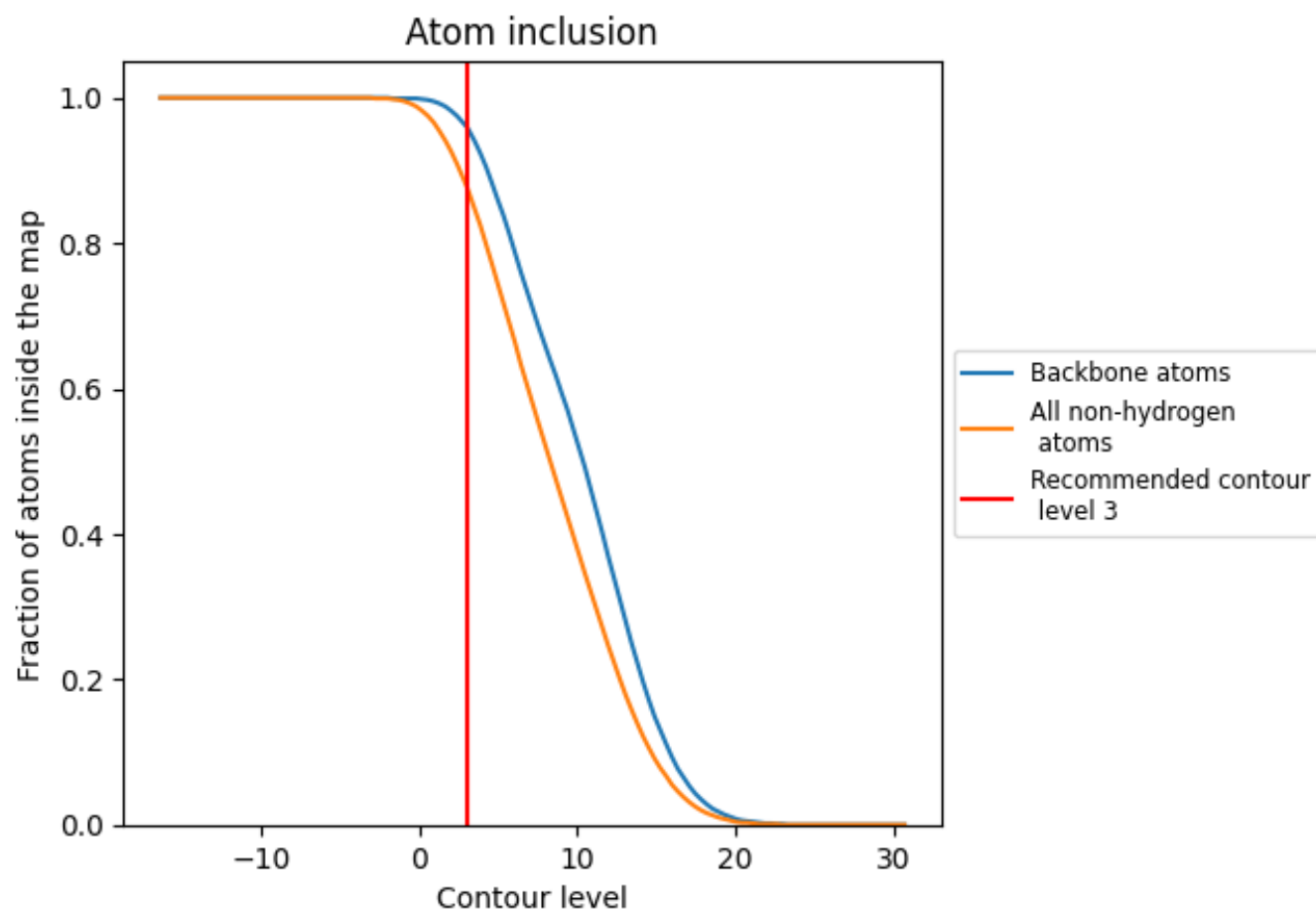
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 88% 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 (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8780	 0.5000
A	 0.8420	 0.4860
B	 0.8400	 0.4910
C	 0.8400	 0.4850
D	 0.8440	 0.4880
E	 0.8420	 0.4870
F	 0.8380	 0.4870
G	 0.8440	 0.4850
H	 0.8410	 0.4910
I	 0.8420	 0.4850
J	 0.8460	 0.4910
K	 0.8450	 0.4880
L	 0.8410	 0.4870
M	 0.9190	 0.4780
N	 0.9180	 0.4780
O	 0.9180	 0.4810
P	 0.8950	 0.4530
Q	 0.8950	 0.4510
R	 0.8970	 0.4490
S	 0.8970	 0.4530
T	 0.8990	 0.4550
U	 0.9060	 0.4950
V	 0.9040	 0.4920
W	 0.9070	 0.4920
X	 0.9070	 0.4960
Y	 0.9000	 0.4970
Z	 0.9180	 0.4830
a	 0.9240	 0.5420
b	 0.9250	 0.5420
c	 0.9240	 0.5420
d	 0.9250	 0.5420
e	 0.9240	 0.5410
f	 0.9220	 0.5430
g	 0.9130	 0.5140
h	 0.9150	 0.5240



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Chain	Atom inclusion	Q-score
i	 0.9080	 0.5170
j	 0.9140	 0.5250
k	 0.9070	 0.5160
l	 0.9210	 0.5260
m	 0.9130	 0.5130
n	 0.9160	 0.5210
o	 0.9070	 0.5160
p	 0.9170	 0.5270
q	 0.9080	 0.5110
r	 0.9180	 0.5230
s	 0.9180	 0.4840
v	 0.9010	 0.4540
w	 0.9070	 0.4940
x	 0.9180	 0.4790