



Full wwPDB EM Validation Report ⓘ

Nov 6, 2024 – 04:03 pm GMT

PDB ID : 8AXK
EMDB ID : EMD-15700
Title : Type 3 secretion system export apparatus core, inner rod and needle of *Shigella flexneri*
Authors : Lunelli, M.
Deposited on : 2022-08-31
Resolution : 4.05 Å (reported)
Based on initial models : 6RWK, 6RWY, 6RWX

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

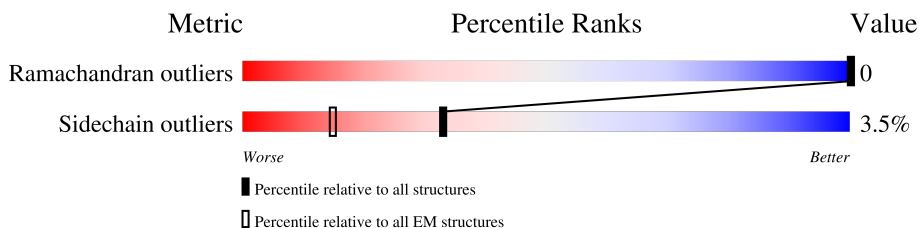
EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

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 4.05 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	216	
1	B	216	
1	C	216	
1	D	216	
1	E	216	
2	F	256	
3	G	86	
3	H	86	
3	I	86	






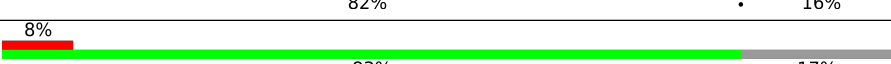
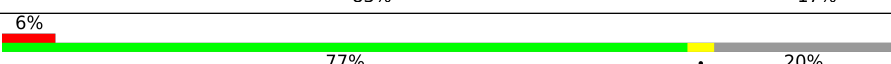
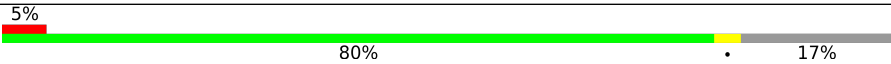


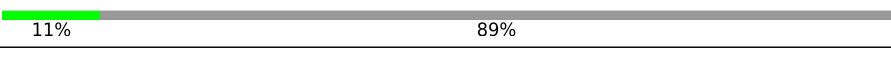




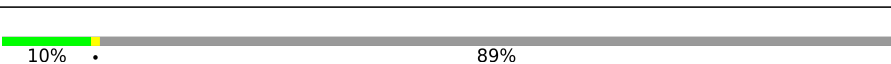









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Mol	Chain	Length	Quality of chain
3	J	86	
4	K	342	
5	M	97	
5	N	97	
5	O	97	
5	P	97	
5	Q	97	
5	R	97	
6	S	98	
6	T	98	
6	U	98	
6	V	98	
6	W	98	
6	a	98	
6	b	98	
6	c	98	
6	d	98	
6	e	98	
6	f	98	
6	g	98	
6	h	98	
6	i	98	
6	j	98	
6	k	98	
6	l	98	
















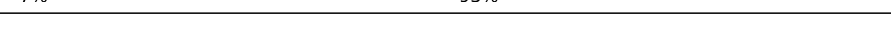
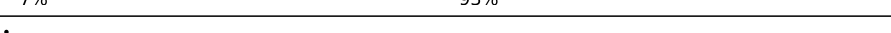
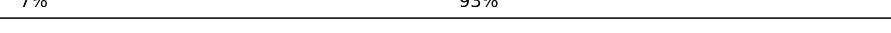
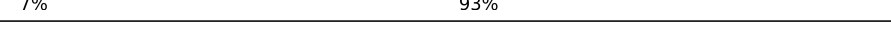
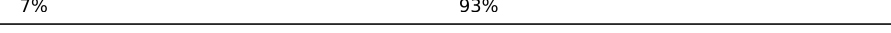
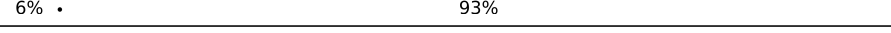
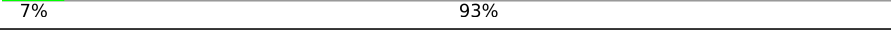

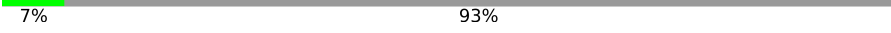

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Mol	Chain	Length	Quality of chain
6	m	98	
6	n	98	
6	o	98	
6	p	98	
6	q	98	
6	r	98	
6	s	98	
6	t	98	
6	u	98	
6	v	98	
6	w	98	
7	0	566	
7	1	566	
7	2	566	
7	3	566	
7	4	566	
7	5	566	
7	6	566	
7	7	566	
7	8	566	
7	9	566	
7	X	566	
7	Y	566	
7	Z	566	
7	x	566	

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Mol	Chain	Length	Quality of chain	
7	y	566		
7	z	566		
8	a0	241		
8	b0	241		
8	c0	241		
8	d0	241		
8	e0	241		
8	f0	241		
8	g0	241		
8	h0	241		
8	i0	241		
8	j0	241		
8	k0	241		
8	l0	241		
8	m0	241		
8	n0	241		
8	o0	241		
8	p0	241		
8	q0	241		
8	r0	241		
8	s0	241		
8	t0	241		
8	u0	241		
8	v0	241		
8	w0	241		

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Mol	Chain	Length	Quality of chain
8	x0	241	<div><div></div><div>7%</div><div>93%</div></div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 44141 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 Surface presentation of antigens protein SpaP.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	188	Total	C	N	O	S	0	0
			1486	994	221	259	12		
1	B	185	Total	C	N	O	S	0	0
			1459	976	216	255	12		
1	C	188	Total	C	N	O	S	0	0
			1480	987	220	261	12		
1	D	183	Total	C	N	O	S	0	0
			1438	962	214	250	12		
1	E	186	Total	C	N	O	S	0	0
			1464	979	218	255	12		

- Molecule 2 is a protein called Surface presentation of antigens protein SpaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	256	Total	C	N	O	S	0	0
			2018	1361	306	342	9		

- Molecule 3 is a protein called Surface presentation of antigens protein SpaQ.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	85	Total	C	N	O	S	0	0
			656	442	97	113	4		
3	H	75	Total	C	N	O	S	0	0
			575	394	83	94	4		
3	I	63	Total	C	N	O	S	0	0
			494	339	71	80	4		
3	J	67	Total	C	N	O	S	0	0
			521	357	75	85	4		

- Molecule 4 is a protein called Surface presentation of antigens protein SpaS.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	113	Total	C	N	O	S	0	0
			953	667	134	151	1		

- Molecule 5 is a protein called Protein MxiL.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	42	Total	C	N	O		0	0
			308	192	51	65			
5	N	85	Total	C	N	O	S	0	0
			644	403	102	136	3		
5	O	95	Total	C	N	O	S	0	0
			727	455	114	155	3		
5	P	93	Total	C	N	O	S	0	0
			707	440	112	152	3		
5	Q	85	Total	C	N	O	S	0	0
			641	400	102	136	3		
5	R	85	Total	C	N	O	S	0	0
			643	399	103	138	3		

- Molecule 6 is a protein called Protein MxiH.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	S	60	Total	C	N	O	0	0
			477	300	82	95		
6	T	59	Total	C	N	O	0	0
			468	295	80	93		
6	U	60	Total	C	N	O	0	0
			477	300	82	95		
6	V	59	Total	C	N	O	0	0
			468	295	80	93		
6	W	59	Total	C	N	O	0	0
			468	295	80	93		
6	a	82	Total	C	N	O	0	0
			644	402	106	136		
6	b	81	Total	C	N	O	0	0
			638	399	105	134		
6	c	82	Total	C	N	O	0	0
			644	402	106	136		
6	d	82	Total	C	N	O	0	0
			644	402	106	136		
6	e	81	Total	C	N	O	0	0
			638	399	105	134		
6	f	81	Total	C	N	O	0	0
			638	399	105	134		

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Mol	Chain	Residues	Atoms				AltConf	Trace
6	g	76	Total	C	N	O	0	0
			602	376	99	127		
6	h	75	Total	C	N	O	0	0
			594	372	98	124		
6	i	75	Total	C	N	O	0	0
			594	372	98	124		
6	j	76	Total	C	N	O	0	0
			602	376	99	127		
6	k	75	Total	C	N	O	0	0
			594	372	98	124		
6	l	76	Total	C	N	O	0	0
			602	376	99	127		
6	m	82	Total	C	N	O	0	0
			644	402	106	136		
6	n	82	Total	C	N	O	0	0
			644	402	106	136		
6	o	81	Total	C	N	O	0	0
			638	399	105	134		
6	p	82	Total	C	N	O	0	0
			644	402	106	136		
6	q	82	Total	C	N	O	0	0
			644	402	106	136		
6	r	82	Total	C	N	O	0	0
			644	402	106	136		
6	s	81	Total	C	N	O	0	0
			638	399	105	134		
6	t	78	Total	C	N	O	0	0
			617	385	102	130		
6	u	81	Total	C	N	O	0	0
			638	399	105	134		
6	v	82	Total	C	N	O	0	0
			644	402	106	136		
6	w	82	Total	C	N	O	0	0
			644	402	106	136		

There are 420 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	-14	MET	-	initiating methionine	UNP P0A223
S	-13	ALA	-	expression tag	UNP P0A223
S	-12	SER	-	expression tag	UNP P0A223
S	-11	TRP	-	expression tag	UNP P0A223
S	-10	SER	-	expression tag	UNP P0A223

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Chain	Residue	Modelled	Actual	Comment	Reference
S	-9	HIS	-	expression tag	UNP P0A223
S	-8	PRO	-	expression tag	UNP P0A223
S	-7	GLN	-	expression tag	UNP P0A223
S	-6	PHE	-	expression tag	UNP P0A223
S	-5	GLU	-	expression tag	UNP P0A223
S	-4	LYS	-	expression tag	UNP P0A223
S	-3	ILE	-	expression tag	UNP P0A223
S	-2	GLU	-	expression tag	UNP P0A223
S	-1	GLY	-	expression tag	UNP P0A223
S	0	ARG	-	expression tag	UNP P0A223
T	-14	MET	-	initiating methionine	UNP P0A223
T	-13	ALA	-	expression tag	UNP P0A223
T	-12	SER	-	expression tag	UNP P0A223
T	-11	TRP	-	expression tag	UNP P0A223
T	-10	SER	-	expression tag	UNP P0A223
T	-9	HIS	-	expression tag	UNP P0A223
T	-8	PRO	-	expression tag	UNP P0A223
T	-7	GLN	-	expression tag	UNP P0A223
T	-6	PHE	-	expression tag	UNP P0A223
T	-5	GLU	-	expression tag	UNP P0A223
T	-4	LYS	-	expression tag	UNP P0A223
T	-3	ILE	-	expression tag	UNP P0A223
T	-2	GLU	-	expression tag	UNP P0A223
T	-1	GLY	-	expression tag	UNP P0A223
T	0	ARG	-	expression tag	UNP P0A223
U	-14	MET	-	initiating methionine	UNP P0A223
U	-13	ALA	-	expression tag	UNP P0A223
U	-12	SER	-	expression tag	UNP P0A223
U	-11	TRP	-	expression tag	UNP P0A223
U	-10	SER	-	expression tag	UNP P0A223
U	-9	HIS	-	expression tag	UNP P0A223
U	-8	PRO	-	expression tag	UNP P0A223
U	-7	GLN	-	expression tag	UNP P0A223
U	-6	PHE	-	expression tag	UNP P0A223
U	-5	GLU	-	expression tag	UNP P0A223
U	-4	LYS	-	expression tag	UNP P0A223
U	-3	ILE	-	expression tag	UNP P0A223
U	-2	GLU	-	expression tag	UNP P0A223
U	-1	GLY	-	expression tag	UNP P0A223
U	0	ARG	-	expression tag	UNP P0A223
V	-14	MET	-	initiating methionine	UNP P0A223
V	-13	ALA	-	expression tag	UNP P0A223

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Chain	Residue	Modelled	Actual	Comment	Reference
V	-12	SER	-	expression tag	UNP P0A223
V	-11	TRP	-	expression tag	UNP P0A223
V	-10	SER	-	expression tag	UNP P0A223
V	-9	HIS	-	expression tag	UNP P0A223
V	-8	PRO	-	expression tag	UNP P0A223
V	-7	GLN	-	expression tag	UNP P0A223
V	-6	PHE	-	expression tag	UNP P0A223
V	-5	GLU	-	expression tag	UNP P0A223
V	-4	LYS	-	expression tag	UNP P0A223
V	-3	ILE	-	expression tag	UNP P0A223
V	-2	GLU	-	expression tag	UNP P0A223
V	-1	GLY	-	expression tag	UNP P0A223
V	0	ARG	-	expression tag	UNP P0A223
W	-14	MET	-	initiating methionine	UNP P0A223
W	-13	ALA	-	expression tag	UNP P0A223
W	-12	SER	-	expression tag	UNP P0A223
W	-11	TRP	-	expression tag	UNP P0A223
W	-10	SER	-	expression tag	UNP P0A223
W	-9	HIS	-	expression tag	UNP P0A223
W	-8	PRO	-	expression tag	UNP P0A223
W	-7	GLN	-	expression tag	UNP P0A223
W	-6	PHE	-	expression tag	UNP P0A223
W	-5	GLU	-	expression tag	UNP P0A223
W	-4	LYS	-	expression tag	UNP P0A223
W	-3	ILE	-	expression tag	UNP P0A223
W	-2	GLU	-	expression tag	UNP P0A223
W	-1	GLY	-	expression tag	UNP P0A223
W	0	ARG	-	expression tag	UNP P0A223
a	-14	MET	-	initiating methionine	UNP P0A223
a	-13	ALA	-	expression tag	UNP P0A223
a	-12	SER	-	expression tag	UNP P0A223
a	-11	TRP	-	expression tag	UNP P0A223
a	-10	SER	-	expression tag	UNP P0A223
a	-9	HIS	-	expression tag	UNP P0A223
a	-8	PRO	-	expression tag	UNP P0A223
a	-7	GLN	-	expression tag	UNP P0A223
a	-6	PHE	-	expression tag	UNP P0A223
a	-5	GLU	-	expression tag	UNP P0A223
a	-4	LYS	-	expression tag	UNP P0A223
a	-3	ILE	-	expression tag	UNP P0A223
a	-2	GLU	-	expression tag	UNP P0A223
a	-1	GLY	-	expression tag	UNP P0A223

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Chain	Residue	Modelled	Actual	Comment	Reference
a	0	ARG	-	expression tag	UNP P0A223
b	-14	MET	-	initiating methionine	UNP P0A223
b	-13	ALA	-	expression tag	UNP P0A223
b	-12	SER	-	expression tag	UNP P0A223
b	-11	TRP	-	expression tag	UNP P0A223
b	-10	SER	-	expression tag	UNP P0A223
b	-9	HIS	-	expression tag	UNP P0A223
b	-8	PRO	-	expression tag	UNP P0A223
b	-7	GLN	-	expression tag	UNP P0A223
b	-6	PHE	-	expression tag	UNP P0A223
b	-5	GLU	-	expression tag	UNP P0A223
b	-4	LYS	-	expression tag	UNP P0A223
b	-3	ILE	-	expression tag	UNP P0A223
b	-2	GLU	-	expression tag	UNP P0A223
b	-1	GLY	-	expression tag	UNP P0A223
b	0	ARG	-	expression tag	UNP P0A223
c	-14	MET	-	initiating methionine	UNP P0A223
c	-13	ALA	-	expression tag	UNP P0A223
c	-12	SER	-	expression tag	UNP P0A223
c	-11	TRP	-	expression tag	UNP P0A223
c	-10	SER	-	expression tag	UNP P0A223
c	-9	HIS	-	expression tag	UNP P0A223
c	-8	PRO	-	expression tag	UNP P0A223
c	-7	GLN	-	expression tag	UNP P0A223
c	-6	PHE	-	expression tag	UNP P0A223
c	-5	GLU	-	expression tag	UNP P0A223
c	-4	LYS	-	expression tag	UNP P0A223
c	-3	ILE	-	expression tag	UNP P0A223
c	-2	GLU	-	expression tag	UNP P0A223
c	-1	GLY	-	expression tag	UNP P0A223
c	0	ARG	-	expression tag	UNP P0A223
d	-14	MET	-	initiating methionine	UNP P0A223
d	-13	ALA	-	expression tag	UNP P0A223
d	-12	SER	-	expression tag	UNP P0A223
d	-11	TRP	-	expression tag	UNP P0A223
d	-10	SER	-	expression tag	UNP P0A223
d	-9	HIS	-	expression tag	UNP P0A223
d	-8	PRO	-	expression tag	UNP P0A223
d	-7	GLN	-	expression tag	UNP P0A223
d	-6	PHE	-	expression tag	UNP P0A223
d	-5	GLU	-	expression tag	UNP P0A223
d	-4	LYS	-	expression tag	UNP P0A223

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Chain	Residue	Modelled	Actual	Comment	Reference
d	-3	ILE	-	expression tag	UNP P0A223
d	-2	GLU	-	expression tag	UNP P0A223
d	-1	GLY	-	expression tag	UNP P0A223
d	0	ARG	-	expression tag	UNP P0A223
e	-14	MET	-	initiating methionine	UNP P0A223
e	-13	ALA	-	expression tag	UNP P0A223
e	-12	SER	-	expression tag	UNP P0A223
e	-11	TRP	-	expression tag	UNP P0A223
e	-10	SER	-	expression tag	UNP P0A223
e	-9	HIS	-	expression tag	UNP P0A223
e	-8	PRO	-	expression tag	UNP P0A223
e	-7	GLN	-	expression tag	UNP P0A223
e	-6	PHE	-	expression tag	UNP P0A223
e	-5	GLU	-	expression tag	UNP P0A223
e	-4	LYS	-	expression tag	UNP P0A223
e	-3	ILE	-	expression tag	UNP P0A223
e	-2	GLU	-	expression tag	UNP P0A223
e	-1	GLY	-	expression tag	UNP P0A223
e	0	ARG	-	expression tag	UNP P0A223
f	-14	MET	-	initiating methionine	UNP P0A223
f	-13	ALA	-	expression tag	UNP P0A223
f	-12	SER	-	expression tag	UNP P0A223
f	-11	TRP	-	expression tag	UNP P0A223
f	-10	SER	-	expression tag	UNP P0A223
f	-9	HIS	-	expression tag	UNP P0A223
f	-8	PRO	-	expression tag	UNP P0A223
f	-7	GLN	-	expression tag	UNP P0A223
f	-6	PHE	-	expression tag	UNP P0A223
f	-5	GLU	-	expression tag	UNP P0A223
f	-4	LYS	-	expression tag	UNP P0A223
f	-3	ILE	-	expression tag	UNP P0A223
f	-2	GLU	-	expression tag	UNP P0A223
f	-1	GLY	-	expression tag	UNP P0A223
f	0	ARG	-	expression tag	UNP P0A223
g	-14	MET	-	initiating methionine	UNP P0A223
g	-13	ALA	-	expression tag	UNP P0A223
g	-12	SER	-	expression tag	UNP P0A223
g	-11	TRP	-	expression tag	UNP P0A223
g	-10	SER	-	expression tag	UNP P0A223
g	-9	HIS	-	expression tag	UNP P0A223
g	-8	PRO	-	expression tag	UNP P0A223
g	-7	GLN	-	expression tag	UNP P0A223

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Chain	Residue	Modelled	Actual	Comment	Reference
g	-6	PHE	-	expression tag	UNP P0A223
g	-5	GLU	-	expression tag	UNP P0A223
g	-4	LYS	-	expression tag	UNP P0A223
g	-3	ILE	-	expression tag	UNP P0A223
g	-2	GLU	-	expression tag	UNP P0A223
g	-1	GLY	-	expression tag	UNP P0A223
g	0	ARG	-	expression tag	UNP P0A223
h	-14	MET	-	initiating methionine	UNP P0A223
h	-13	ALA	-	expression tag	UNP P0A223
h	-12	SER	-	expression tag	UNP P0A223
h	-11	TRP	-	expression tag	UNP P0A223
h	-10	SER	-	expression tag	UNP P0A223
h	-9	HIS	-	expression tag	UNP P0A223
h	-8	PRO	-	expression tag	UNP P0A223
h	-7	GLN	-	expression tag	UNP P0A223
h	-6	PHE	-	expression tag	UNP P0A223
h	-5	GLU	-	expression tag	UNP P0A223
h	-4	LYS	-	expression tag	UNP P0A223
h	-3	ILE	-	expression tag	UNP P0A223
h	-2	GLU	-	expression tag	UNP P0A223
h	-1	GLY	-	expression tag	UNP P0A223
h	0	ARG	-	expression tag	UNP P0A223
i	-14	MET	-	initiating methionine	UNP P0A223
i	-13	ALA	-	expression tag	UNP P0A223
i	-12	SER	-	expression tag	UNP P0A223
i	-11	TRP	-	expression tag	UNP P0A223
i	-10	SER	-	expression tag	UNP P0A223
i	-9	HIS	-	expression tag	UNP P0A223
i	-8	PRO	-	expression tag	UNP P0A223
i	-7	GLN	-	expression tag	UNP P0A223
i	-6	PHE	-	expression tag	UNP P0A223
i	-5	GLU	-	expression tag	UNP P0A223
i	-4	LYS	-	expression tag	UNP P0A223
i	-3	ILE	-	expression tag	UNP P0A223
i	-2	GLU	-	expression tag	UNP P0A223
i	-1	GLY	-	expression tag	UNP P0A223
i	0	ARG	-	expression tag	UNP P0A223
j	-14	MET	-	initiating methionine	UNP P0A223
j	-13	ALA	-	expression tag	UNP P0A223
j	-12	SER	-	expression tag	UNP P0A223
j	-11	TRP	-	expression tag	UNP P0A223
j	-10	SER	-	expression tag	UNP P0A223

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Chain	Residue	Modelled	Actual	Comment	Reference
j	-9	HIS	-	expression tag	UNP P0A223
j	-8	PRO	-	expression tag	UNP P0A223
j	-7	GLN	-	expression tag	UNP P0A223
j	-6	PHE	-	expression tag	UNP P0A223
j	-5	GLU	-	expression tag	UNP P0A223
j	-4	LYS	-	expression tag	UNP P0A223
j	-3	ILE	-	expression tag	UNP P0A223
j	-2	GLU	-	expression tag	UNP P0A223
j	-1	GLY	-	expression tag	UNP P0A223
j	0	ARG	-	expression tag	UNP P0A223
k	-14	MET	-	initiating methionine	UNP P0A223
k	-13	ALA	-	expression tag	UNP P0A223
k	-12	SER	-	expression tag	UNP P0A223
k	-11	TRP	-	expression tag	UNP P0A223
k	-10	SER	-	expression tag	UNP P0A223
k	-9	HIS	-	expression tag	UNP P0A223
k	-8	PRO	-	expression tag	UNP P0A223
k	-7	GLN	-	expression tag	UNP P0A223
k	-6	PHE	-	expression tag	UNP P0A223
k	-5	GLU	-	expression tag	UNP P0A223
k	-4	LYS	-	expression tag	UNP P0A223
k	-3	ILE	-	expression tag	UNP P0A223
k	-2	GLU	-	expression tag	UNP P0A223
k	-1	GLY	-	expression tag	UNP P0A223
k	0	ARG	-	expression tag	UNP P0A223
l	-14	MET	-	initiating methionine	UNP P0A223
l	-13	ALA	-	expression tag	UNP P0A223
l	-12	SER	-	expression tag	UNP P0A223
l	-11	TRP	-	expression tag	UNP P0A223
l	-10	SER	-	expression tag	UNP P0A223
l	-9	HIS	-	expression tag	UNP P0A223
l	-8	PRO	-	expression tag	UNP P0A223
l	-7	GLN	-	expression tag	UNP P0A223
l	-6	PHE	-	expression tag	UNP P0A223
l	-5	GLU	-	expression tag	UNP P0A223
l	-4	LYS	-	expression tag	UNP P0A223
l	-3	ILE	-	expression tag	UNP P0A223
l	-2	GLU	-	expression tag	UNP P0A223
l	-1	GLY	-	expression tag	UNP P0A223
l	0	ARG	-	expression tag	UNP P0A223
m	-14	MET	-	initiating methionine	UNP P0A223
m	-13	ALA	-	expression tag	UNP P0A223

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Chain	Residue	Modelled	Actual	Comment	Reference
m	-12	SER	-	expression tag	UNP P0A223
m	-11	TRP	-	expression tag	UNP P0A223
m	-10	SER	-	expression tag	UNP P0A223
m	-9	HIS	-	expression tag	UNP P0A223
m	-8	PRO	-	expression tag	UNP P0A223
m	-7	GLN	-	expression tag	UNP P0A223
m	-6	PHE	-	expression tag	UNP P0A223
m	-5	GLU	-	expression tag	UNP P0A223
m	-4	LYS	-	expression tag	UNP P0A223
m	-3	ILE	-	expression tag	UNP P0A223
m	-2	GLU	-	expression tag	UNP P0A223
m	-1	GLY	-	expression tag	UNP P0A223
m	0	ARG	-	expression tag	UNP P0A223
n	-14	MET	-	initiating methionine	UNP P0A223
n	-13	ALA	-	expression tag	UNP P0A223
n	-12	SER	-	expression tag	UNP P0A223
n	-11	TRP	-	expression tag	UNP P0A223
n	-10	SER	-	expression tag	UNP P0A223
n	-9	HIS	-	expression tag	UNP P0A223
n	-8	PRO	-	expression tag	UNP P0A223
n	-7	GLN	-	expression tag	UNP P0A223
n	-6	PHE	-	expression tag	UNP P0A223
n	-5	GLU	-	expression tag	UNP P0A223
n	-4	LYS	-	expression tag	UNP P0A223
n	-3	ILE	-	expression tag	UNP P0A223
n	-2	GLU	-	expression tag	UNP P0A223
n	-1	GLY	-	expression tag	UNP P0A223
n	0	ARG	-	expression tag	UNP P0A223
o	-14	MET	-	initiating methionine	UNP P0A223
o	-13	ALA	-	expression tag	UNP P0A223
o	-12	SER	-	expression tag	UNP P0A223
o	-11	TRP	-	expression tag	UNP P0A223
o	-10	SER	-	expression tag	UNP P0A223
o	-9	HIS	-	expression tag	UNP P0A223
o	-8	PRO	-	expression tag	UNP P0A223
o	-7	GLN	-	expression tag	UNP P0A223
o	-6	PHE	-	expression tag	UNP P0A223
o	-5	GLU	-	expression tag	UNP P0A223
o	-4	LYS	-	expression tag	UNP P0A223
o	-3	ILE	-	expression tag	UNP P0A223
o	-2	GLU	-	expression tag	UNP P0A223
o	-1	GLY	-	expression tag	UNP P0A223

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Chain	Residue	Modelled	Actual	Comment	Reference
o	0	ARG	-	expression tag	UNP P0A223
p	-14	MET	-	initiating methionine	UNP P0A223
p	-13	ALA	-	expression tag	UNP P0A223
p	-12	SER	-	expression tag	UNP P0A223
p	-11	TRP	-	expression tag	UNP P0A223
p	-10	SER	-	expression tag	UNP P0A223
p	-9	HIS	-	expression tag	UNP P0A223
p	-8	PRO	-	expression tag	UNP P0A223
p	-7	GLN	-	expression tag	UNP P0A223
p	-6	PHE	-	expression tag	UNP P0A223
p	-5	GLU	-	expression tag	UNP P0A223
p	-4	LYS	-	expression tag	UNP P0A223
p	-3	ILE	-	expression tag	UNP P0A223
p	-2	GLU	-	expression tag	UNP P0A223
p	-1	GLY	-	expression tag	UNP P0A223
p	0	ARG	-	expression tag	UNP P0A223
q	-14	MET	-	initiating methionine	UNP P0A223
q	-13	ALA	-	expression tag	UNP P0A223
q	-12	SER	-	expression tag	UNP P0A223
q	-11	TRP	-	expression tag	UNP P0A223
q	-10	SER	-	expression tag	UNP P0A223
q	-9	HIS	-	expression tag	UNP P0A223
q	-8	PRO	-	expression tag	UNP P0A223
q	-7	GLN	-	expression tag	UNP P0A223
q	-6	PHE	-	expression tag	UNP P0A223
q	-5	GLU	-	expression tag	UNP P0A223
q	-4	LYS	-	expression tag	UNP P0A223
q	-3	ILE	-	expression tag	UNP P0A223
q	-2	GLU	-	expression tag	UNP P0A223
q	-1	GLY	-	expression tag	UNP P0A223
q	0	ARG	-	expression tag	UNP P0A223
r	-14	MET	-	initiating methionine	UNP P0A223
r	-13	ALA	-	expression tag	UNP P0A223
r	-12	SER	-	expression tag	UNP P0A223
r	-11	TRP	-	expression tag	UNP P0A223
r	-10	SER	-	expression tag	UNP P0A223
r	-9	HIS	-	expression tag	UNP P0A223
r	-8	PRO	-	expression tag	UNP P0A223
r	-7	GLN	-	expression tag	UNP P0A223
r	-6	PHE	-	expression tag	UNP P0A223
r	-5	GLU	-	expression tag	UNP P0A223
r	-4	LYS	-	expression tag	UNP P0A223

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Chain	Residue	Modelled	Actual	Comment	Reference
r	-3	ILE	-	expression tag	UNP P0A223
r	-2	GLU	-	expression tag	UNP P0A223
r	-1	GLY	-	expression tag	UNP P0A223
r	0	ARG	-	expression tag	UNP P0A223
s	-14	MET	-	initiating methionine	UNP P0A223
s	-13	ALA	-	expression tag	UNP P0A223
s	-12	SER	-	expression tag	UNP P0A223
s	-11	TRP	-	expression tag	UNP P0A223
s	-10	SER	-	expression tag	UNP P0A223
s	-9	HIS	-	expression tag	UNP P0A223
s	-8	PRO	-	expression tag	UNP P0A223
s	-7	GLN	-	expression tag	UNP P0A223
s	-6	PHE	-	expression tag	UNP P0A223
s	-5	GLU	-	expression tag	UNP P0A223
s	-4	LYS	-	expression tag	UNP P0A223
s	-3	ILE	-	expression tag	UNP P0A223
s	-2	GLU	-	expression tag	UNP P0A223
s	-1	GLY	-	expression tag	UNP P0A223
s	0	ARG	-	expression tag	UNP P0A223
t	-14	MET	-	initiating methionine	UNP P0A223
t	-13	ALA	-	expression tag	UNP P0A223
t	-12	SER	-	expression tag	UNP P0A223
t	-11	TRP	-	expression tag	UNP P0A223
t	-10	SER	-	expression tag	UNP P0A223
t	-9	HIS	-	expression tag	UNP P0A223
t	-8	PRO	-	expression tag	UNP P0A223
t	-7	GLN	-	expression tag	UNP P0A223
t	-6	PHE	-	expression tag	UNP P0A223
t	-5	GLU	-	expression tag	UNP P0A223
t	-4	LYS	-	expression tag	UNP P0A223
t	-3	ILE	-	expression tag	UNP P0A223
t	-2	GLU	-	expression tag	UNP P0A223
t	-1	GLY	-	expression tag	UNP P0A223
t	0	ARG	-	expression tag	UNP P0A223
u	-14	MET	-	initiating methionine	UNP P0A223
u	-13	ALA	-	expression tag	UNP P0A223
u	-12	SER	-	expression tag	UNP P0A223
u	-11	TRP	-	expression tag	UNP P0A223
u	-10	SER	-	expression tag	UNP P0A223
u	-9	HIS	-	expression tag	UNP P0A223
u	-8	PRO	-	expression tag	UNP P0A223
u	-7	GLN	-	expression tag	UNP P0A223

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Chain	Residue	Modelled	Actual	Comment	Reference
u	-6	PHE	-	expression tag	UNP P0A223
u	-5	GLU	-	expression tag	UNP P0A223
u	-4	LYS	-	expression tag	UNP P0A223
u	-3	ILE	-	expression tag	UNP P0A223
u	-2	GLU	-	expression tag	UNP P0A223
u	-1	GLY	-	expression tag	UNP P0A223
u	0	ARG	-	expression tag	UNP P0A223
v	-14	MET	-	initiating methionine	UNP P0A223
v	-13	ALA	-	expression tag	UNP P0A223
v	-12	SER	-	expression tag	UNP P0A223
v	-11	TRP	-	expression tag	UNP P0A223
v	-10	SER	-	expression tag	UNP P0A223
v	-9	HIS	-	expression tag	UNP P0A223
v	-8	PRO	-	expression tag	UNP P0A223
v	-7	GLN	-	expression tag	UNP P0A223
v	-6	PHE	-	expression tag	UNP P0A223
v	-5	GLU	-	expression tag	UNP P0A223
v	-4	LYS	-	expression tag	UNP P0A223
v	-3	ILE	-	expression tag	UNP P0A223
v	-2	GLU	-	expression tag	UNP P0A223
v	-1	GLY	-	expression tag	UNP P0A223
v	0	ARG	-	expression tag	UNP P0A223
w	-14	MET	-	initiating methionine	UNP P0A223
w	-13	ALA	-	expression tag	UNP P0A223
w	-12	SER	-	expression tag	UNP P0A223
w	-11	TRP	-	expression tag	UNP P0A223
w	-10	SER	-	expression tag	UNP P0A223
w	-9	HIS	-	expression tag	UNP P0A223
w	-8	PRO	-	expression tag	UNP P0A223
w	-7	GLN	-	expression tag	UNP P0A223
w	-6	PHE	-	expression tag	UNP P0A223
w	-5	GLU	-	expression tag	UNP P0A223
w	-4	LYS	-	expression tag	UNP P0A223
w	-3	ILE	-	expression tag	UNP P0A223
w	-2	GLU	-	expression tag	UNP P0A223
w	-1	GLY	-	expression tag	UNP P0A223
w	0	ARG	-	expression tag	UNP P0A223

- Molecule 7 is a protein called Outer membrane protein MxiD.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	X	62	Total	C	N	O	0	0
			497	325	80	92		

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Mol	Chain	Residues	Atoms				AltConf	Trace
7	Y	62	Total 497	C 325	N 80	O 92	0	0
7	Z	62	Total 497	C 325	N 80	O 92	0	0
7	0	62	Total 497	C 325	N 80	O 92	0	0
7	2	62	Total 497	C 325	N 80	O 92	0	0
7	4	62	Total 497	C 325	N 80	O 92	0	0
7	6	62	Total 497	C 325	N 80	O 92	0	0
7	8	62	Total 497	C 325	N 80	O 92	0	0
7	x	62	Total 497	C 325	N 80	O 92	0	0
7	y	62	Total 497	C 325	N 80	O 92	0	0
7	z	62	Total 497	C 325	N 80	O 92	0	0
7	1	62	Total 497	C 325	N 80	O 92	0	0
7	3	62	Total 497	C 325	N 80	O 92	0	0
7	5	62	Total 497	C 325	N 80	O 92	0	0
7	7	62	Total 497	C 325	N 80	O 92	0	0
7	9	62	Total 497	C 325	N 80	O 92	0	0

- Molecule 8 is a protein called Lipoprotein MxiJ.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	a0	17	Total 131	C 82	N 24	O 25	0	0
8	b0	17	Total 131	C 82	N 24	O 25	0	0
8	c0	17	Total 131	C 82	N 24	O 25	0	0
8	d0	17	Total 131	C 82	N 24	O 25	0	0

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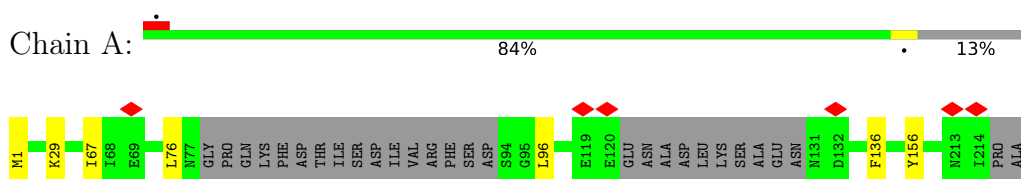
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Mol	Chain	Residues	Atoms				AltConf	Trace
8	e0	17	Total 131	C 82	N 24	O 25	0	0
8	f0	17	Total 131	C 82	N 24	O 25	0	0
8	g0	17	Total 131	C 82	N 24	O 25	0	0
8	h0	17	Total 131	C 82	N 24	O 25	0	0
8	i0	17	Total 131	C 82	N 24	O 25	0	0
8	j0	17	Total 131	C 82	N 24	O 25	0	0
8	k0	17	Total 131	C 82	N 24	O 25	0	0
8	l0	17	Total 131	C 82	N 24	O 25	0	0
8	m0	17	Total 131	C 82	N 24	O 25	0	0
8	n0	17	Total 131	C 82	N 24	O 25	0	0
8	o0	17	Total 131	C 82	N 24	O 25	0	0
8	p0	17	Total 131	C 82	N 24	O 25	0	0
8	q0	17	Total 131	C 82	N 24	O 25	0	0
8	r0	17	Total 131	C 82	N 24	O 25	0	0
8	s0	17	Total 131	C 82	N 24	O 25	0	0
8	t0	17	Total 131	C 82	N 24	O 25	0	0
8	u0	17	Total 131	C 82	N 24	O 25	0	0
8	v0	17	Total 131	C 82	N 24	O 25	0	0
8	w0	17	Total 131	C 82	N 24	O 25	0	0
8	x0	17	Total 131	C 82	N 24	O 25	0	0

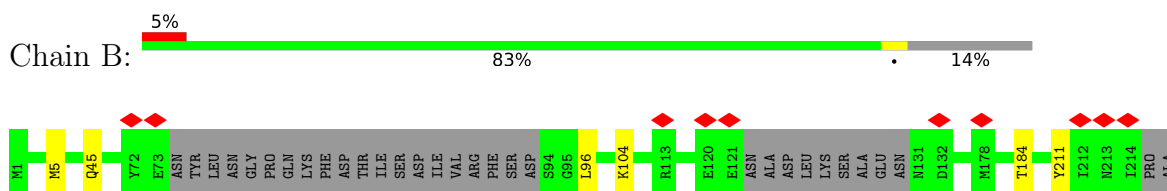
3 Residue-property plots [i](#)

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.

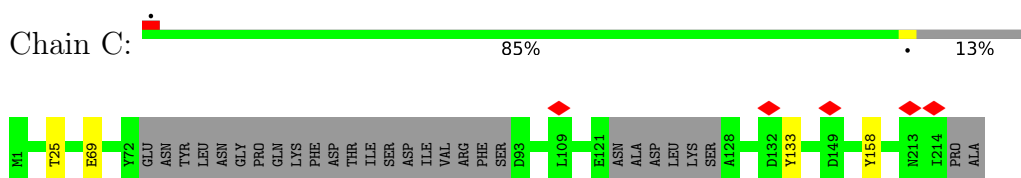
- Molecule 1: Surface presentation of antigens protein SpaP



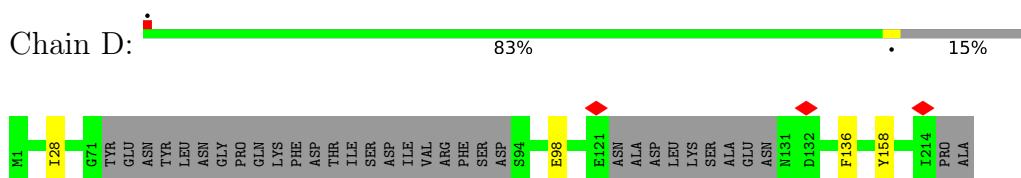
- Molecule 1: Surface presentation of antigens protein SpaP



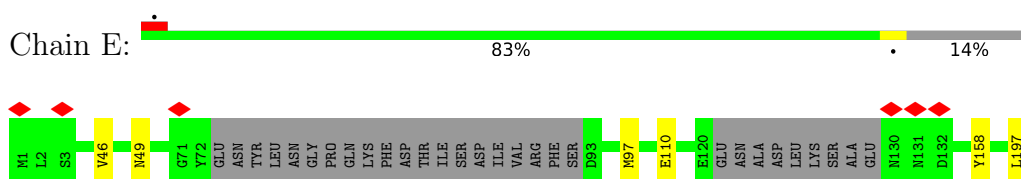
- Molecule 1: Surface presentation of antigens protein SpaP



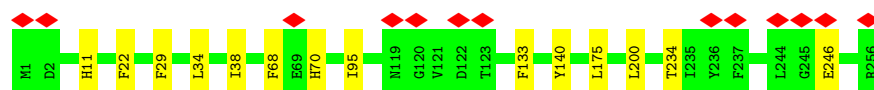
- Molecule 1: Surface presentation of antigens protein SpaP



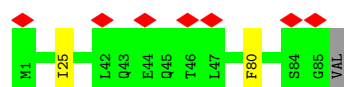
- Molecule 1: Surface presentation of antigens protein SpaP




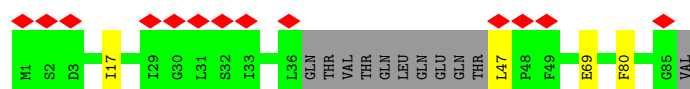
- Chain F:  5% 95% 5%



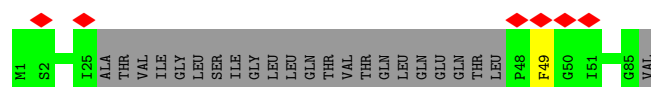
- Chain G:  8% 97%



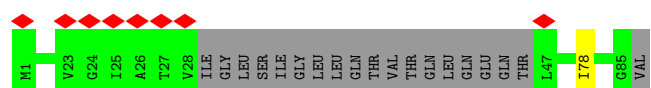
- Chain H: 



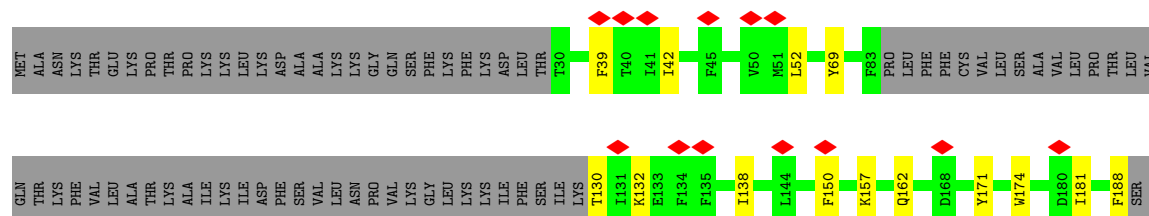
- Chain I:  7% 72% 27%

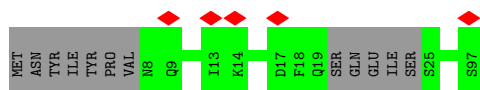


- Chain J: 9% 77% 22%

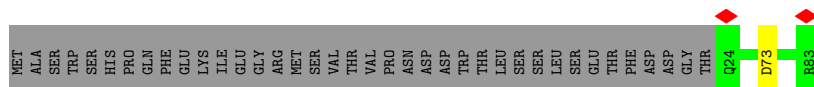


- Chain K:  29% 67%

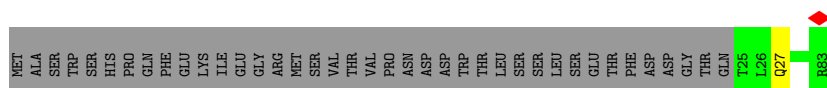




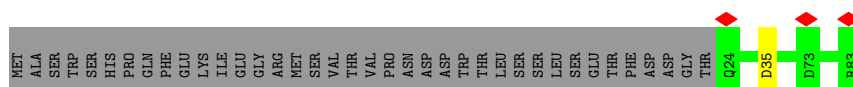
• Molecule 6: Protein MxiH



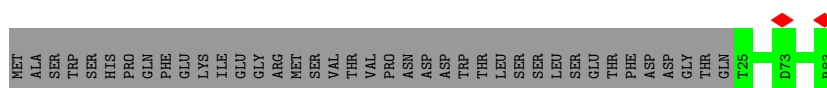
• Molecule 6: Protein MxiH



• Molecule 6: Protein MxiH



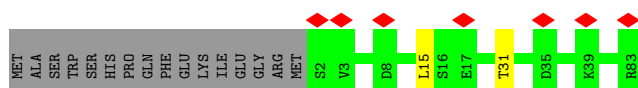
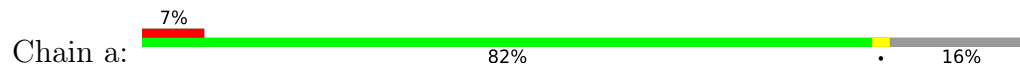
• Molecule 6: Protein MxiH




• Molecule 6: Protein MxiH

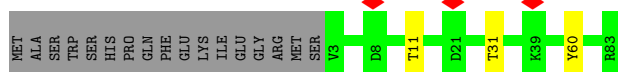


• Molecule 6: Protein MxiH




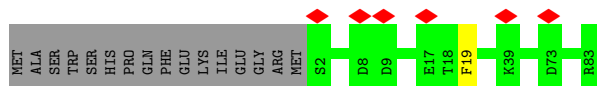
• Molecule 6: Protein MxiH

Chain b:  80% 17%




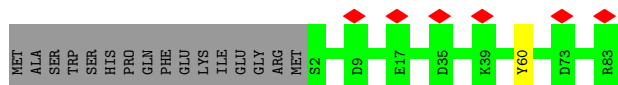
• Molecule 6: Protein MxiH

Chain c:  83% 16%




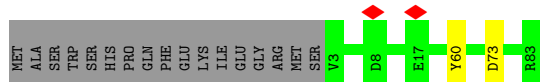
• Molecule 6: Protein MxiH

Chain d:  83% 16%




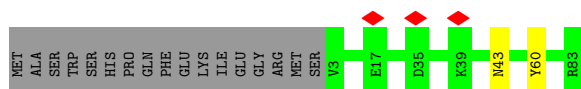
• Molecule 6: Protein MxiH

Chain e:  81% 17%




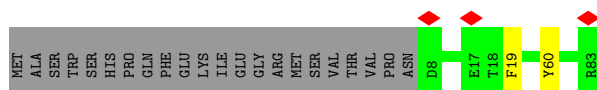
• Molecule 6: Protein MxiH

Chain f:  81% 17%



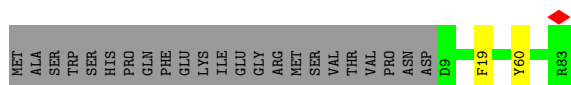
• Molecule 6: Protein MxiH

Chain g:  76% 22%



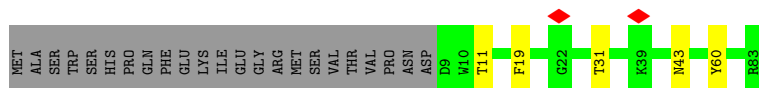
• Molecule 6: Protein MxiH

Chain h:  74% 23%




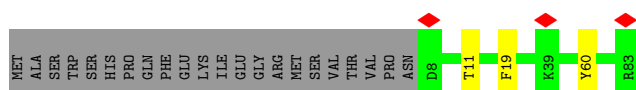
• Molecule 6: Protein MxiH

Chain i:  71% 5% 23%




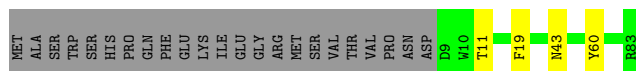
• Molecule 6: Protein MxiH

Chain j:  74% 0% 22%




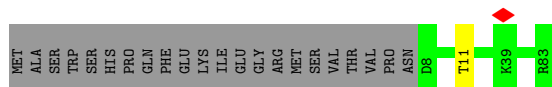
• Molecule 6: Protein MxiH

Chain k:  72% 0% 23%




• Molecule 6: Protein MxiH

Chain l:  77% 0% 22%




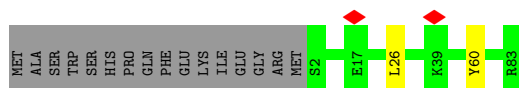
• Molecule 6: Protein MxiH

Chain m:  6% 83% 0% 16%




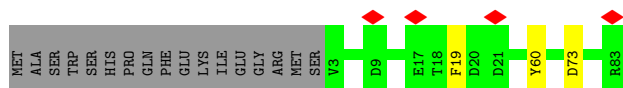
• Molecule 6: Protein MxiH

Chain n:  0% 82% 0% 16%




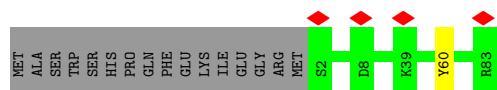
• Molecule 6: Protein MxiH

Chain o:  0% 80% 0% 17%




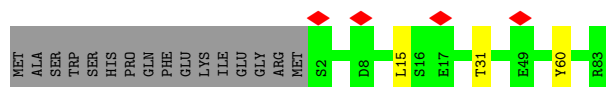
• Molecule 6: Protein MxiH

Chain p:  83% 16%




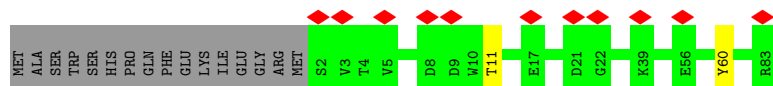
• Molecule 6: Protein MxiH

Chain q:  81% 16%




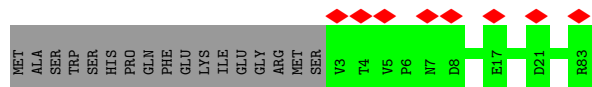
• Molecule 6: Protein MxiH

Chain r:  82% 16%




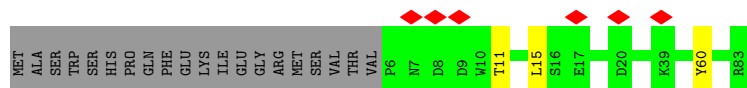
• Molecule 6: Protein MxiH

Chain s:  83% 17%




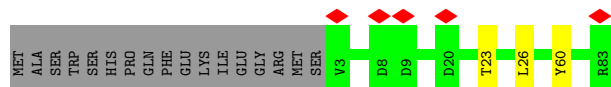
• Molecule 6: Protein MxiH

Chain t:  77% 20%




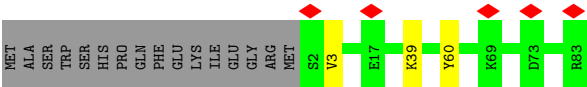
• Molecule 6: Protein MxiH

Chain u:  80% 17%

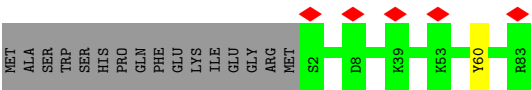
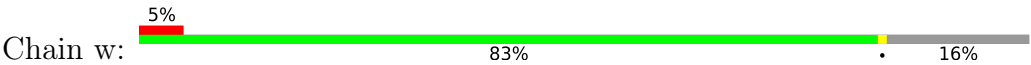


• Molecule 6: Protein MxiH

Chain v:  81% 16%



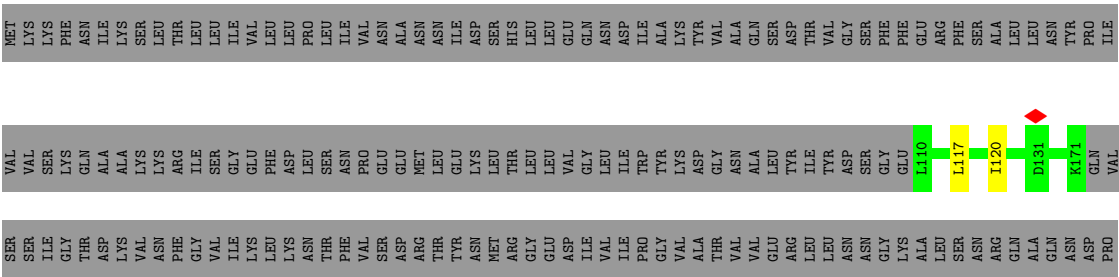
• Molecule 6: Protein MxiH



• Molecule 7: Outer membrane protein MxiD



• Molecule 7: Outer membrane protein MxiD





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

- Molecule 7: Outer membrane protein MxiD

Chain 2:  11% 89%

[illegible]

- Molecule 7: Outer membrane protein MxiD

Chain 4: 11% 89%

MET	LYS	LYS	LYS	ASP	PHE	ASN	ILE	LYS	SER	LEU	THR	LEU	LEU	LEU	ILE	VAL	ASN	ALA	ASN	ASN	ASN	ILE	GLY	GLN	GLN	GLY	LEU	LEU	LEU	LEU	LEU	PRO	TYR	ILE
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

Chain 8:  11% 89%

[illegible]

- Molecule 7: Outer membrane protein MxiD

Chain x: 10% . 89%

[illegible]

[illegible]

- Molecule 7: Outer membrane protein MxiD

Chain 1: 11% 89%

ARG	GLU	ASN	THR	SER	ALA	LYS	ASN	THR	VAL	MET
ILE	ILE	ASN	ASN	GLY	LEU	ARG	ILE	THR	VAL	LYS
GLN	GLN	ASN	GLU	GLN	GLN	HIS	THR	ASP	VAL	LYS
LYS	LYS	ILE	GLU	ILE	LYS	ILE	VAL	VAL	GLN	ASN
THR	THR	ILE	ILE	MET	LYS	LEU	SER	GLY	ALA	ILE
ILE	GLN	ILE	ILE	THR	ALA	LEU	GLU	VAL	ALA	LYS
PRO	ILE	PRO	THR	LEU	VAL	ASP	ASP	LYS	LYS	SER
SER	GLU	LEU	PHE	ILE	VAL	ILE	ASN	LYS	ILE	THR
GLU	THR	SER	SER	ASP	ARG	ILE	PHE	ASN	GLY	LEU
THR	THR	ILE	THR	GLY	PRO	ASP	SER	THR	GLU	ILE
LEU	LEU	PRO	GLY	GLY	ILE	SER	VAL	VAL	ASP	VAL
LEU	LEU	VAL	ASN	ASN	THR	SER	SER	SER	LEU	PRO
GLU	ILE	ILE	SER	SER	THR	LEU	VAL	ASP	SER	LEU
ASP	GLY	ASN	GLN	GLN	GLN	ASN	THR	ARG	ASN	ILE
GLU	ASN	SER	ASN	SER	GLU	ASN	THR	THR	PRO	VAL
LYS	VAL	ASN	VAL	ASN	ASN	ASN	THR	TYR	GLU	ASN
SER	PHE	THR	THR	TYR	ILE	GLY	SER	ASN	GLU	ALA
LEU	VAL	LYS	LYS	ASN	PRO	VAL	ILE	MET	MET	ASN
VAL	VAL	TYR	TYR	TYR	ALA	ALA	LEU	ARG	LEU	ASN
SER	SER	LYS	LYS	ASN	ILE	TRP	GLU	GLY	GLU	ILE
TYR	LEU	THR	THR	ASN	PHE	SER	VAL	ASP	VAL	GLN
					GLN	ASP	GLY	GLY	LYS	LYS
					THR	THR	THR	THR	TRP	ILE
					LEU	ALA	ASN	VAL	TYR	ALA
					VAL	GLY	ILE	VAL	LYS	LYS
					THR	THR	ILE	GLU	ASP	TYR
					GLY	GLY	LEU	ARG	GLY	VAL
					ASN	ASN	VAL	ARG	ASN	ALA
					ASN	ASN	ASN	ASN	ALA	GLN
					SER	SER	LYS	LEU	LEU	SER
					THR	THR	GLY	ASN	TYR	ASN
					ILE	ASN	ASN	ASN	ILE	THR
					ALA	LEU	ASN	GLY	VAL	GLY
					PHE	THR	ALA	VAL	ASP	THR
					THR	THR	THR	THR	GLY	ASN
					ARG	THR	THR	THR	GLY	ASN
					THR	THR	THR	THR	GLY	ASN
					ILE	ILE	LYS	ASN	TYR	ASN
					LYS	ALA	ALA	GLN	TYR	ASN
					ARG	GLU	GLU	GLN	ASP	ALA
					PRO	VAL	VAL	ILE	LEU	THR
					ASN	THR	THR	GLN	SER	THR
					GLY	THR	THR	ASN	GLY	PHE
					THR	THR	THR	ASN	GLY	THR
					ASN	ASN	LEU	ARG	GLU	ARG
					THR	THR	ILE	GLN	LYS	PHE
					LEU	LEU	GLY	ASP	ALA	SER
					ILE	THR	THR	GLN	GLN	THR
					THR	THR	ILE	ASN	GLN	SER
					ILE	ASN	ILE	ILE	ASN	ALA
					LYS	VAL	PHE	ASP	K171	ALA
					GLY	ILE	THR	GLN	GLN	LEU
					THR	THR	THR	PRO	VAL	LEU
					LEU	TYR	TYR	MET	SER	ASN
					ILE	THR	THR	PRO	SER	TYR
					SER	THR	THR	VAL	ILE	PRO
					ASN	THR	ALA	THR	THR	THR

- Molecule 7: Outer membrane protein MxiD

Chain 3: 10% . 89%

[illegible]

[illegible]

- Molecule 7: Outer membrane protein MxiD

Chain 5:  10% . 89%

[illegible]

- Molecule 7: Outer membrane protein MxiD

Chain 7: 10% . 89%

[illegible]

[illegible]

- Molecule 7: Outer membrane protein MxiD

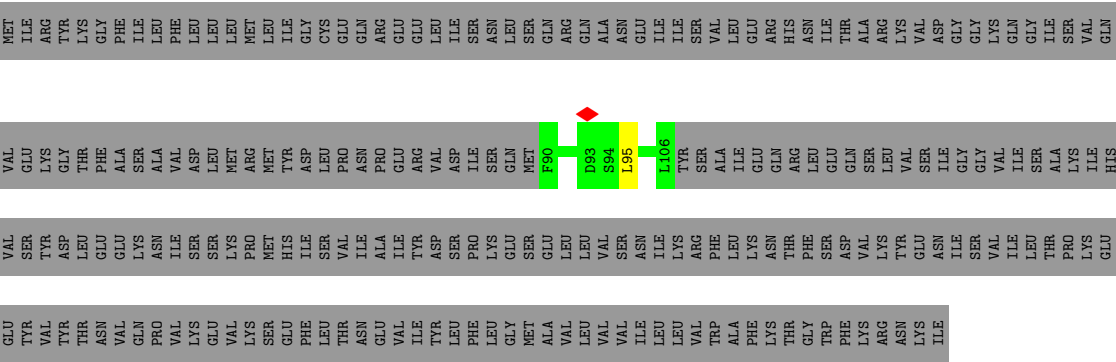
Chain 9: 11% 89%

[illegible]

- Molecule 8: Lipoprotein MxiJ

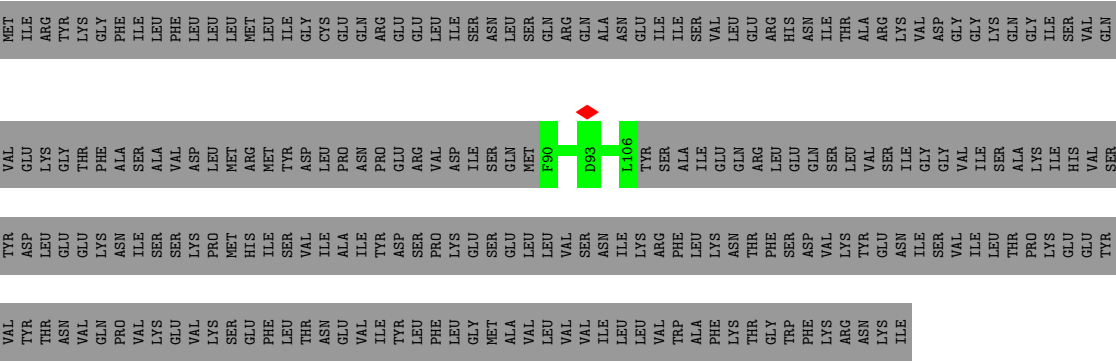
Chain a0: 7% 93%

[illegible]



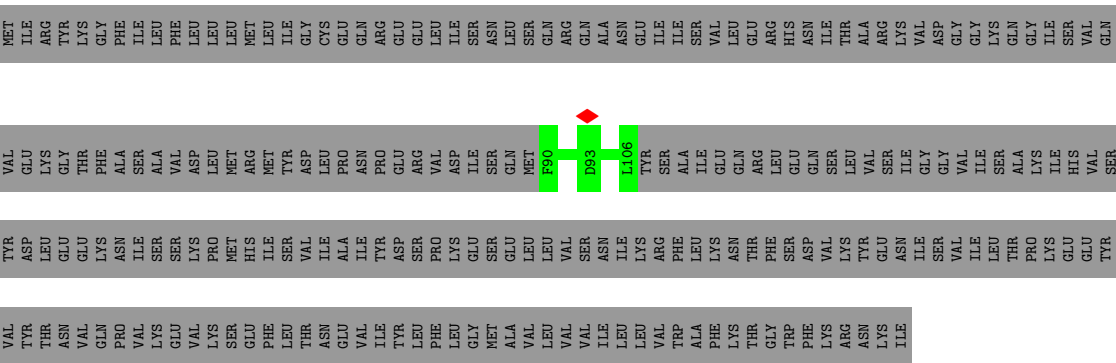
● Molecule 8: Lipoprotein MxiJ

Chain f0: 7% 93%



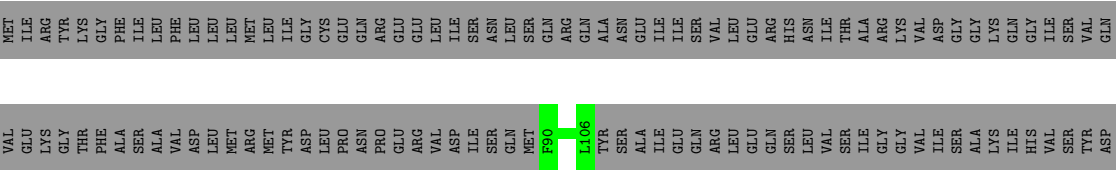
● Molecule 8: Lipoprotein MxiJ

Chain g0: 7% 93%



● Molecule 8: Lipoprotein MxiJ

Chain h0: 7% 93%



[illegible]

- Molecule 8: Lipoprotein MxiJ

Chain i0:  7% 93%

[illegible]

- Molecule 8: Lipoprotein MxiJ

Chain j0:  7% 93%

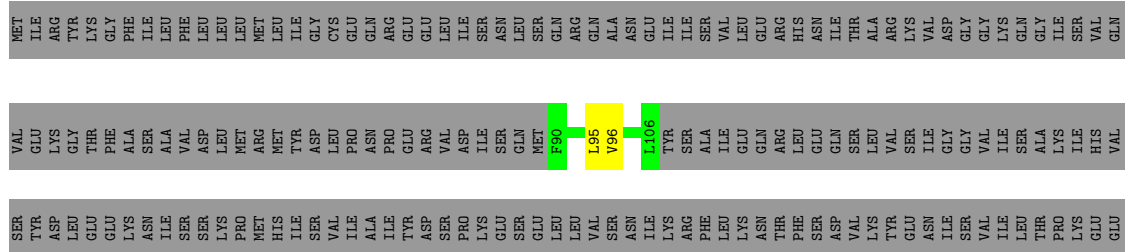
[illegible]

- Molecule 8: Lipoprotein MxiJ

Chain k0: 7% 93%

TRP	VAL	TYR	SER	VAL	MET
VAL	TRP	ASP	ASP	GLU	ILE
TRP	VAL	LEU	GLY	LYS	ARG
ASN	ASN	GLU	THR	THR	TYR
VAL	VAL	GLU	GLU	PHE	GLY
GLN	GLN	LYS	LYS	ALA	PHE
PRO	PRO	ASN	ASN	SER	ILE
VAL	VAL	ILE	ILE	ALA	LEU
LYS	LYS	SER	SER	VAL	PHE
GLU	GLU	GLY	GLY	ASP	LEU
VAL	VAL	LYS	LYS	LEU	LEU
LYS	LYS	PRO	PRO	MET	LEU
SER	SER	MET	MET	ARG	MET
GLU	GLU	HIS	HIS	MET	LEU
PHE	PHE	ILE	ILE	TYR	ILE
LEU	LEU	SER	SER	ASP	GLY
THR	THR	VAL	VAL	LEU	ILE
ASN	ASN	ILE	ILE	PRO	CYS
GLU	GLU	ALA	ALA	ASN	GLN
VAL	VAL	ILE	ILE	PRO	GLU
ILE	ILE	TYR	TYR	GLU	ARG
TYR	TYR	ASP	ASP	ARG	GLU
LEU	LEU	SER	SER	VAL	LEU
PHE	PHE	PRO	PRO	ASP	ILE
LEU	LEU	LYS	LYS	ILE	SER
GLY	GLY	GLU	GLU	ILE	ASN
MET	MET	SER	SER	GLN	LEU
ALA	ALA	GLU	GLU	MET	SER
VAL	VAL	LEU	LEU	F90	GLN
LEU	LEU	LEU	LEU	F91	ARG
VAL	VAL	VAL	VAL	T92	GLN
ILE	ILE	SER	SER	D93	ALA
LEU	LEU	ASN	ASN	D93	ASN
LEU	LEU	ILE	ILE	L106	GLU
LEU	LEU	LYS	LYS	TYR	ILE
VAL	VAL	ARG	ARG	SER	ILE
TRP	TRP	PHE	PHE	SER	SER
ALA	ALA	LEU	LEU	ALA	VAL
PHE	PHE	LYS	LYS	GLU	LEU
LYS	LYS	ASN	ASN	GLN	GLU
THR	THR	THR	THR	ARG	ARG
GLY	GLY	PHE	PHE	GLN	HIS
TRP	TRP	SER	SER	LEU	LYS
PHE	PHE	ASP	ASP	GLU	ASN
ARG	ARG	LYS	LYS	SER	THR
ASN	ASN	LYS	LYS	LEU	ALA
LYS	LYS	GLU	GLU	VAL	ARG
ILE	ILE	ASN	ASN	SER	LYS
		ILE	ILE	VAL	ASP
		ILE	ILE	GLY	GLY
		VAL	VAL	GLY	GLY
		ILE	ILE	VAL	LYS
		LEU	LEU	ILE	GLN
		THR	THR	SER	GLY
		PRO	PRO	ALA	ILE
		LYS	LYS	ILE	TYR
		GLU	GLU	HIS	GLN

- Molecule 8: Lipoprotein MxiJ

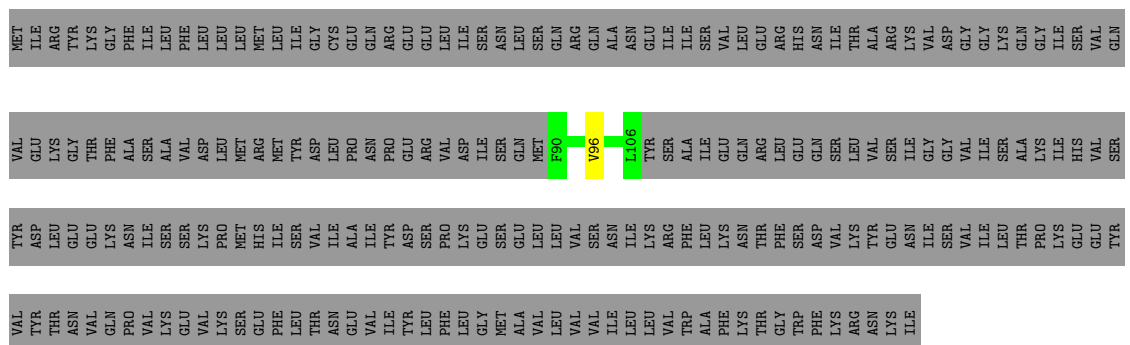


Chain v0:  7% 93%

- Molecule 8: Lipoprotein MxiJ



- Molecule 8: Lipoprotein MxiJ



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	90547	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 ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	101179	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.306	Depositor
Minimum map value	-0.209	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	498.41714, 498.41714, 498.41714	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.038369, 1.038369, 1.038369	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	0.26	0/1516	0.38	0/2051
1	B	0.25	0/1488	0.39	0/2012
1	C	0.26	0/1509	0.39	0/2041
1	D	0.26	0/1466	0.39	0/1982
1	E	0.26	0/1494	0.39	0/2022
2	F	0.27	0/2071	0.38	0/2811
3	G	0.25	0/669	0.39	0/908
3	H	0.24	0/587	0.36	0/794
3	I	0.25	0/506	0.34	0/682
3	J	0.24	0/533	0.35	0/721
4	K	0.27	0/979	0.38	0/1324
5	M	0.23	0/309	0.39	0/417
5	N	0.24	0/648	0.38	0/876
5	O	0.24	0/734	0.40	0/994
5	P	0.24	0/713	0.39	0/965
5	Q	0.23	0/645	0.38	0/872
5	R	0.24	0/646	0.38	0/871
6	S	0.25	0/482	0.36	0/651
6	T	0.25	0/473	0.35	0/639
6	U	0.25	0/482	0.35	0/651
6	V	0.24	0/473	0.34	0/639
6	W	0.24	0/473	0.35	0/639
6	a	0.25	0/653	0.38	0/888
6	b	0.24	0/647	0.38	0/880
6	c	0.24	0/653	0.37	0/888
6	d	0.24	0/653	0.38	0/888
6	e	0.24	0/647	0.37	0/880
6	f	0.24	0/647	0.37	0/880
6	g	0.24	0/610	0.36	0/827
6	h	0.24	0/602	0.36	0/816
6	i	0.24	0/602	0.37	0/816
6	j	0.24	0/610	0.36	0/827
6	k	0.24	0/602	0.36	0/816
6	l	0.25	0/610	0.36	0/827

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	m	0.24	0/653	0.38	0/888
6	n	0.24	0/653	0.39	0/888
6	o	0.24	0/647	0.39	0/880
6	p	0.24	0/653	0.39	0/888
6	q	0.24	0/653	0.38	0/888
6	r	0.24	0/653	0.38	0/888
6	s	0.24	0/647	0.38	0/880
6	t	0.24	0/626	0.36	0/849
6	u	0.24	0/647	0.37	0/880
6	v	0.24	0/653	0.39	0/888
6	w	0.24	0/653	0.38	0/888
7	0	0.24	0/506	0.38	0/689
7	1	0.24	0/506	0.40	0/689
7	2	0.24	0/506	0.38	0/689
7	3	0.24	0/506	0.39	0/689
7	4	0.24	0/506	0.39	0/689
7	5	0.24	0/506	0.38	0/689
7	6	0.24	0/506	0.41	0/689
7	7	0.24	0/506	0.39	0/689
7	8	0.25	0/506	0.38	0/689
7	9	0.24	0/506	0.41	0/689
7	X	0.25	0/506	0.38	0/689
7	Y	0.25	0/506	0.38	0/689
7	Z	0.24	0/506	0.39	0/689
7	x	0.25	0/506	0.39	0/689
7	y	0.25	0/506	0.38	0/689
7	z	0.24	0/506	0.38	0/689
8	a0	0.26	0/133	0.41	0/179
8	b0	0.24	0/133	0.44	0/179
8	c0	0.24	0/133	0.39	0/179
8	d0	0.24	0/133	0.38	0/179
8	e0	0.23	0/133	0.41	0/179
8	f0	0.24	0/133	0.39	0/179
8	g0	0.23	0/133	0.36	0/179
8	h0	0.22	0/133	0.37	0/179
8	i0	0.23	0/133	0.39	0/179
8	j0	0.25	0/133	0.41	0/179
8	k0	0.25	0/133	0.38	0/179
8	l0	0.24	0/133	0.33	0/179
8	m0	0.23	0/133	0.35	0/179
8	n0	0.23	0/133	0.39	0/179
8	o0	0.23	0/133	0.40	0/179
8	p0	0.23	0/133	0.42	0/179

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
8	q0	0.25	0/133	0.39	0/179
8	r0	0.24	0/133	0.39	0/179
8	s0	0.24	0/133	0.38	0/179
8	t0	0.23	0/133	0.50	0/179
8	u0	0.24	0/133	0.39	0/179
8	v0	0.23	0/133	0.41	0/179
8	w0	0.23	0/133	0.40	0/179
8	x0	0.24	0/133	0.36	0/179
All	All	0.25	0/44858	0.38	0/60820

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	182/216 (84%)	171 (94%)	11 (6%)	0	100	100
1	B	179/216 (83%)	168 (94%)	11 (6%)	0	100	100
1	C	182/216 (84%)	172 (94%)	10 (6%)	0	100	100
1	D	177/216 (82%)	164 (93%)	13 (7%)	0	100	100
1	E	180/216 (83%)	170 (94%)	10 (6%)	0	100	100
2	F	254/256 (99%)	243 (96%)	11 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	G	83/86 (96%)	79 (95%)	4 (5%)	0	100	100
3	H	71/86 (83%)	71 (100%)	0	0	100	100
3	I	59/86 (69%)	58 (98%)	1 (2%)	0	100	100
3	J	63/86 (73%)	63 (100%)	0	0	100	100
4	K	109/342 (32%)	102 (94%)	7 (6%)	0	100	100
5	M	40/97 (41%)	39 (98%)	1 (2%)	0	100	100
5	N	81/97 (84%)	78 (96%)	3 (4%)	0	100	100
5	O	93/97 (96%)	84 (90%)	9 (10%)	0	100	100
5	P	91/97 (94%)	84 (92%)	7 (8%)	0	100	100
5	Q	81/97 (84%)	79 (98%)	2 (2%)	0	100	100
5	R	81/97 (84%)	77 (95%)	4 (5%)	0	100	100
6	S	58/98 (59%)	58 (100%)	0	0	100	100
6	T	57/98 (58%)	57 (100%)	0	0	100	100
6	U	58/98 (59%)	56 (97%)	2 (3%)	0	100	100
6	V	57/98 (58%)	55 (96%)	2 (4%)	0	100	100
6	W	57/98 (58%)	57 (100%)	0	0	100	100
6	a	80/98 (82%)	75 (94%)	5 (6%)	0	100	100
6	b	79/98 (81%)	75 (95%)	4 (5%)	0	100	100
6	c	80/98 (82%)	76 (95%)	4 (5%)	0	100	100
6	d	80/98 (82%)	76 (95%)	4 (5%)	0	100	100
6	e	79/98 (81%)	75 (95%)	4 (5%)	0	100	100
6	f	79/98 (81%)	75 (95%)	4 (5%)	0	100	100
6	g	74/98 (76%)	73 (99%)	1 (1%)	0	100	100
6	h	73/98 (74%)	70 (96%)	3 (4%)	0	100	100
6	i	73/98 (74%)	70 (96%)	3 (4%)	0	100	100
6	j	74/98 (76%)	72 (97%)	2 (3%)	0	100	100
6	k	73/98 (74%)	71 (97%)	2 (3%)	0	100	100
6	l	74/98 (76%)	72 (97%)	2 (3%)	0	100	100
6	m	80/98 (82%)	75 (94%)	5 (6%)	0	100	100
6	n	80/98 (82%)	75 (94%)	5 (6%)	0	100	100
6	o	79/98 (81%)	75 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	p	80/98 (82%)	76 (95%)	4 (5%)	0	100	100
6	q	80/98 (82%)	75 (94%)	5 (6%)	0	100	100
6	r	80/98 (82%)	76 (95%)	4 (5%)	0	100	100
6	s	79/98 (81%)	74 (94%)	5 (6%)	0	100	100
6	t	76/98 (78%)	74 (97%)	2 (3%)	0	100	100
6	u	79/98 (81%)	74 (94%)	5 (6%)	0	100	100
6	v	80/98 (82%)	75 (94%)	5 (6%)	0	100	100
6	w	80/98 (82%)	78 (98%)	2 (2%)	0	100	100
7	0	60/566 (11%)	59 (98%)	1 (2%)	0	100	100
7	1	60/566 (11%)	59 (98%)	1 (2%)	0	100	100
7	2	60/566 (11%)	58 (97%)	2 (3%)	0	100	100
7	3	60/566 (11%)	58 (97%)	2 (3%)	0	100	100
7	4	60/566 (11%)	59 (98%)	1 (2%)	0	100	100
7	5	60/566 (11%)	59 (98%)	1 (2%)	0	100	100
7	6	60/566 (11%)	56 (93%)	4 (7%)	0	100	100
7	7	60/566 (11%)	59 (98%)	1 (2%)	0	100	100
7	8	60/566 (11%)	58 (97%)	2 (3%)	0	100	100
7	9	60/566 (11%)	58 (97%)	2 (3%)	0	100	100
7	X	60/566 (11%)	57 (95%)	3 (5%)	0	100	100
7	Y	60/566 (11%)	54 (90%)	6 (10%)	0	100	100
7	Z	60/566 (11%)	57 (95%)	3 (5%)	0	100	100
7	x	60/566 (11%)	60 (100%)	0	0	100	100
7	y	60/566 (11%)	55 (92%)	5 (8%)	0	100	100
7	z	60/566 (11%)	58 (97%)	2 (3%)	0	100	100
8	a0	15/241 (6%)	14 (93%)	1 (7%)	0	100	100
8	b0	15/241 (6%)	14 (93%)	1 (7%)	0	100	100
8	c0	15/241 (6%)	14 (93%)	1 (7%)	0	100	100
8	d0	15/241 (6%)	13 (87%)	2 (13%)	0	100	100
8	e0	15/241 (6%)	13 (87%)	2 (13%)	0	100	100
8	f0	15/241 (6%)	14 (93%)	1 (7%)	0	100	100
8	g0	15/241 (6%)	14 (93%)	1 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	h0	15/241 (6%)	15 (100%)	0	0	100	100
8	i0	15/241 (6%)	15 (100%)	0	0	100	100
8	j0	15/241 (6%)	14 (93%)	1 (7%)	0	100	100
8	k0	15/241 (6%)	13 (87%)	2 (13%)	0	100	100
8	l0	15/241 (6%)	15 (100%)	0	0	100	100
8	m0	15/241 (6%)	13 (87%)	2 (13%)	0	100	100
8	n0	15/241 (6%)	15 (100%)	0	0	100	100
8	o0	15/241 (6%)	8 (53%)	7 (47%)	0	100	100
8	p0	15/241 (6%)	10 (67%)	5 (33%)	0	100	100
8	q0	15/241 (6%)	14 (93%)	1 (7%)	0	100	100
8	r0	15/241 (6%)	13 (87%)	2 (13%)	0	100	100
8	s0	15/241 (6%)	14 (93%)	1 (7%)	0	100	100
8	t0	15/241 (6%)	9 (60%)	6 (40%)	0	100	100
8	u0	15/241 (6%)	13 (87%)	2 (13%)	0	100	100
8	v0	15/241 (6%)	12 (80%)	3 (20%)	0	100	100
8	w0	15/241 (6%)	15 (100%)	0	0	100	100
8	x0	15/241 (6%)	15 (100%)	0	0	100	100
All	All	5404/20188 (27%)	5135 (95%)	269 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	165/189 (87%)	158 (96%)	7 (4%)	25	49
1	B	162/189 (86%)	156 (96%)	6 (4%)	29	52
1	C	164/189 (87%)	160 (98%)	4 (2%)	44	63
1	D	160/189 (85%)	156 (98%)	4 (2%)	42	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	163/189 (86%)	157 (96%)	6 (4%)	29	52
2	F	230/230 (100%)	216 (94%)	14 (6%)	15	39
3	G	74/75 (99%)	72 (97%)	2 (3%)	40	61
3	H	64/75 (85%)	60 (94%)	4 (6%)	15	38
3	I	55/75 (73%)	54 (98%)	1 (2%)	54	72
3	J	58/75 (77%)	57 (98%)	1 (2%)	56	73
4	K	105/316 (33%)	91 (87%)	14 (13%)	3	17
5	M	36/89 (40%)	35 (97%)	1 (3%)	38	60
5	N	78/89 (88%)	75 (96%)	3 (4%)	28	51
5	O	87/89 (98%)	83 (95%)	4 (5%)	23	46
5	P	85/89 (96%)	80 (94%)	5 (6%)	16	40
5	Q	77/89 (86%)	76 (99%)	1 (1%)	65	77
5	R	77/89 (86%)	77 (100%)	0	100	100
6	S	53/88 (60%)	52 (98%)	1 (2%)	52	70
6	T	52/88 (59%)	51 (98%)	1 (2%)	52	70
6	U	53/88 (60%)	52 (98%)	1 (2%)	52	70
6	V	52/88 (59%)	52 (100%)	0	100	100
6	W	52/88 (59%)	52 (100%)	0	100	100
6	a	74/88 (84%)	72 (97%)	2 (3%)	40	61
6	b	73/88 (83%)	70 (96%)	3 (4%)	26	49
6	c	74/88 (84%)	73 (99%)	1 (1%)	62	76
6	d	74/88 (84%)	73 (99%)	1 (1%)	62	76
6	e	73/88 (83%)	71 (97%)	2 (3%)	40	61
6	f	73/88 (83%)	71 (97%)	2 (3%)	40	61
6	g	68/88 (77%)	66 (97%)	2 (3%)	37	59
6	h	67/88 (76%)	65 (97%)	2 (3%)	36	58
6	i	67/88 (76%)	62 (92%)	5 (8%)	11	33
6	j	68/88 (77%)	65 (96%)	3 (4%)	24	47
6	k	67/88 (76%)	63 (94%)	4 (6%)	16	39
6	l	68/88 (77%)	67 (98%)	1 (2%)	60	75
6	m	74/88 (84%)	73 (99%)	1 (1%)	62	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	n	74/88 (84%)	72 (97%)	2 (3%)	40	61
6	o	73/88 (83%)	70 (96%)	3 (4%)	26	49
6	p	74/88 (84%)	73 (99%)	1 (1%)	62	76
6	q	74/88 (84%)	71 (96%)	3 (4%)	26	49
6	r	74/88 (84%)	72 (97%)	2 (3%)	40	61
6	s	73/88 (83%)	73 (100%)	0	100	100
6	t	70/88 (80%)	67 (96%)	3 (4%)	25	48
6	u	73/88 (83%)	70 (96%)	3 (4%)	26	49
6	v	74/88 (84%)	71 (96%)	3 (4%)	26	49
6	w	74/88 (84%)	73 (99%)	1 (1%)	62	76
7	0	56/513 (11%)	54 (96%)	2 (4%)	30	53
7	1	56/513 (11%)	54 (96%)	2 (4%)	30	53
7	2	56/513 (11%)	56 (100%)	0	100	100
7	3	56/513 (11%)	53 (95%)	3 (5%)	18	42
7	4	56/513 (11%)	54 (96%)	2 (4%)	30	53
7	5	56/513 (11%)	53 (95%)	3 (5%)	18	42
7	6	56/513 (11%)	52 (93%)	4 (7%)	12	35
7	7	56/513 (11%)	53 (95%)	3 (5%)	18	42
7	8	56/513 (11%)	55 (98%)	1 (2%)	54	72
7	9	56/513 (11%)	54 (96%)	2 (4%)	30	53
7	X	56/513 (11%)	52 (93%)	4 (7%)	12	35
7	Y	56/513 (11%)	54 (96%)	2 (4%)	30	53
7	Z	56/513 (11%)	54 (96%)	2 (4%)	30	53
7	x	56/513 (11%)	53 (95%)	3 (5%)	18	42
7	y	56/513 (11%)	54 (96%)	2 (4%)	30	53
7	z	56/513 (11%)	53 (95%)	3 (5%)	18	42
8	a0	15/220 (7%)	15 (100%)	0	100	100
8	b0	15/220 (7%)	15 (100%)	0	100	100
8	c0	15/220 (7%)	15 (100%)	0	100	100
8	d0	15/220 (7%)	15 (100%)	0	100	100
8	e0	15/220 (7%)	14 (93%)	1 (7%)	13	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	f0	15/220 (7%)	15 (100%)	0	100	100
8	g0	15/220 (7%)	15 (100%)	0	100	100
8	h0	15/220 (7%)	15 (100%)	0	100	100
8	i0	15/220 (7%)	14 (93%)	1 (7%)	13	36
8	j0	15/220 (7%)	14 (93%)	1 (7%)	13	36
8	k0	15/220 (7%)	14 (93%)	1 (7%)	13	36
8	l0	15/220 (7%)	15 (100%)	0	100	100
8	m0	15/220 (7%)	15 (100%)	0	100	100
8	n0	15/220 (7%)	15 (100%)	0	100	100
8	o0	15/220 (7%)	15 (100%)	0	100	100
8	p0	15/220 (7%)	15 (100%)	0	100	100
8	q0	15/220 (7%)	15 (100%)	0	100	100
8	r0	15/220 (7%)	13 (87%)	2 (13%)	3	17
8	s0	15/220 (7%)	15 (100%)	0	100	100
8	t0	15/220 (7%)	14 (93%)	1 (7%)	13	36
8	u0	15/220 (7%)	15 (100%)	0	100	100
8	v0	15/220 (7%)	14 (93%)	1 (7%)	13	36
8	w0	15/220 (7%)	15 (100%)	0	100	100
8	x0	15/220 (7%)	14 (93%)	1 (7%)	13	36
All	All	5011/18277 (27%)	4834 (96%)	177 (4%)	33	53

All (177) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	29	LYS
1	A	67	ILE
1	A	76	LEU
1	A	96	LEU
1	A	136	PHE
1	A	156	TYR
1	B	5	MET
1	B	45	GLN
1	B	96	LEU
1	B	104	LYS

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Mol	Chain	Res	Type
1	B	184	THR
1	B	211	TYR
1	C	25	THR
1	C	69	GLU
1	C	133	TYR
1	C	158	TYR
1	D	28	ILE
1	D	98	GLU
1	D	136	PHE
1	D	158	TYR
1	E	46	VAL
1	E	49	ASN
1	E	97	MET
1	E	110	GLU
1	E	158	TYR
1	E	197	LEU
2	F	11	HIS
2	F	22	PHE
2	F	29	PHE
2	F	34	LEU
2	F	38	ILE
2	F	68	PHE
2	F	70	HIS
2	F	95	ILE
2	F	133	PHE
2	F	140	TYR
2	F	175	LEU
2	F	200	LEU
2	F	234	THR
2	F	246	GLU
3	G	25	ILE
3	G	80	PHE
3	H	17	ILE
3	H	47	LEU
3	H	69	GLU
3	H	80	PHE
3	I	49	PHE
3	J	78	ILE
4	K	39	PHE
4	K	42	ILE
4	K	52	LEU
4	K	69	TYR

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Mol	Chain	Res	Type
4	K	130	THR
4	K	132	LYS
4	K	138	ILE
4	K	150	PHE
4	K	157	LYS
4	K	162	GLN
4	K	171	TYR
4	K	174	TRP
4	K	181	ILE
4	K	188	PHE
5	M	56	GLU
5	N	8	ASN
5	N	10	VAL
5	N	14	LYS
5	O	5	TYR
5	O	7	VAL
5	O	10	VAL
5	O	36	ASP
5	P	10	VAL
5	P	14	LYS
5	P	18	PHE
5	P	40	ASP
5	P	59	ASN
5	Q	11	ASP
6	S	73	ASP
6	T	27	GLN
6	U	35	ASP
7	X	117	LEU
7	X	120	ILE
7	X	131	ASP
7	X	169	LEU
7	Y	117	LEU
7	Y	120	ILE
7	Z	117	LEU
7	Z	169	LEU
7	0	123	ASN
7	0	131	ASP
7	4	117	LEU
7	4	131	ASP
7	6	111	ILE
7	6	117	LEU
7	6	131	ASP

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Mol	Chain	Res	Type
7	6	147	ASP
7	8	131	ASP
7	x	117	LEU
7	x	137	HIS
7	x	171	LYS
7	y	117	LEU
7	y	171	LYS
7	z	117	LEU
7	z	131	ASP
7	z	171	LYS
7	1	117	LEU
7	1	171	LYS
7	3	117	LEU
7	3	136	ASP
7	3	171	LYS
7	5	117	LEU
7	5	131	ASP
7	5	171	LYS
7	7	117	LEU
7	7	125	LEU
7	7	171	LYS
7	9	117	LEU
7	9	171	LYS
6	a	15	LEU
6	a	31	THR
6	b	11	THR
6	b	31	THR
6	b	60	TYR
6	c	19	PHE
6	d	60	TYR
6	e	60	TYR
6	e	73	ASP
6	f	43	ASN
6	f	60	TYR
6	g	19	PHE
6	g	60	TYR
6	h	19	PHE
6	h	60	TYR
6	i	11	THR
6	i	19	PHE
6	i	31	THR
6	i	43	ASN

Continued on next page...

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Mol	Chain	Res	Type
6	i	60	TYR
6	j	11	THR
6	j	19	PHE
6	j	60	TYR
6	k	11	THR
6	k	19	PHE
6	k	43	ASN
6	k	60	TYR
6	l	11	THR
6	m	60	TYR
6	n	26	LEU
6	n	60	TYR
6	o	19	PHE
6	o	60	TYR
6	o	73	ASP
6	p	60	TYR
6	q	15	LEU
6	q	31	THR
6	q	60	TYR
6	r	11	THR
6	r	60	TYR
6	t	11	THR
6	t	15	LEU
6	t	60	TYR
6	u	23	THR
6	u	26	LEU
6	u	60	TYR
6	v	3	VAL
6	v	39	LYS
6	v	60	TYR
6	w	60	TYR
8	e0	95	LEU
8	i0	90	PHE
8	j0	95	LEU
8	k0	92	THR
8	r0	95	LEU
8	r0	96	VAL
8	t0	93	ASP
8	v0	95	LEU
8	x0	96	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	ASN
1	A	116	GLN
1	B	45	GLN
1	B	210	GLN
1	E	44	GLN
2	F	11	HIS
2	F	163	GLN
4	K	60	ASN
5	P	67	GLN
6	T	27	GLN
7	1	164	ASN
6	f	40	ASN
6	f	43	ASN
6	h	43	ASN
6	i	43	ASN
6	j	43	ASN
6	l	43	ASN
6	m	64	GLN
6	n	40	ASN
6	o	27	GLN
6	v	81	ASN
6	w	40	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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.

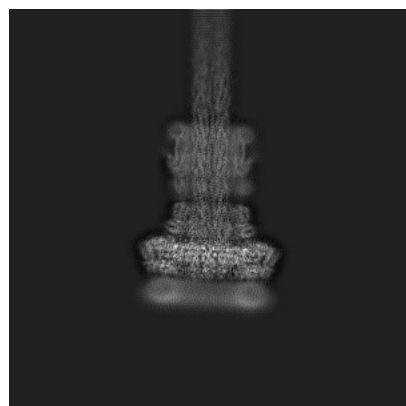
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15700. These allow visual inspection of the internal detail of the map and identification of artifacts.

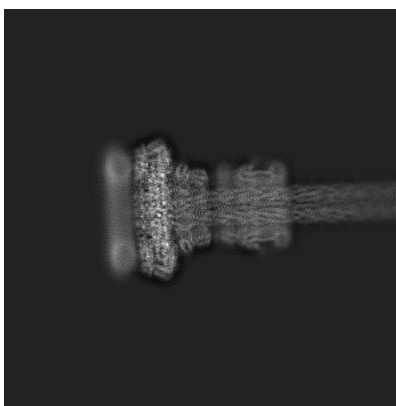
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

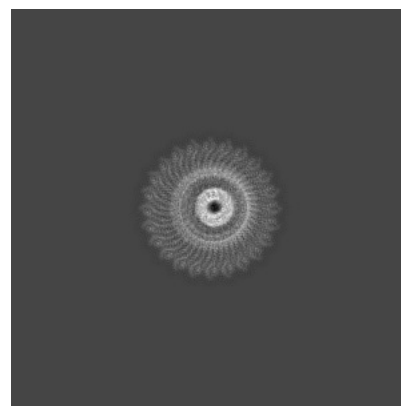
6.1.1 Primary map



X

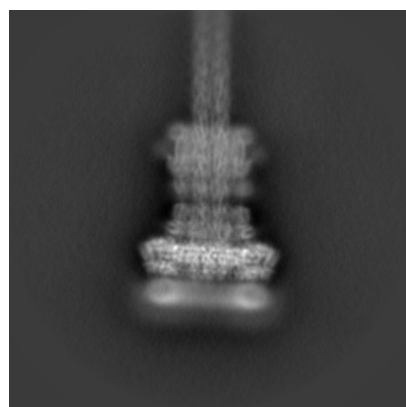


Y

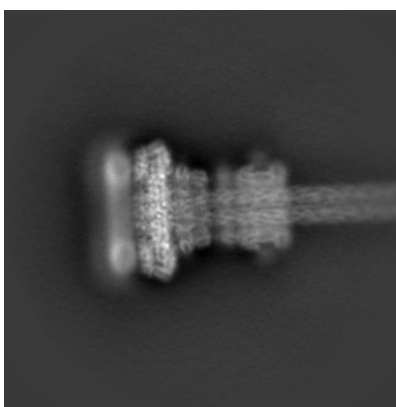


Z

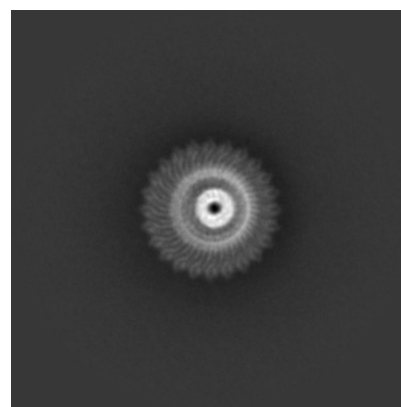
6.1.2 Raw map



X



Y

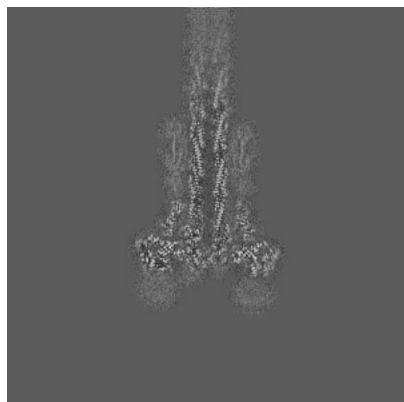


Z

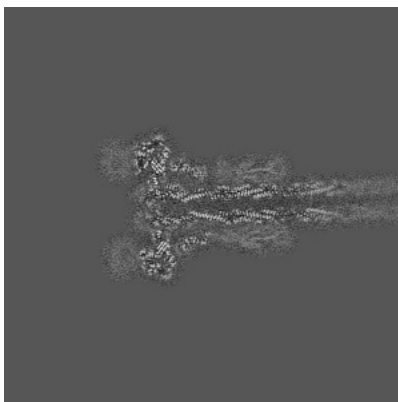
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

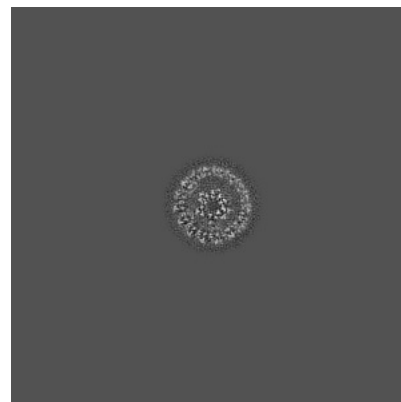
6.2.1 Primary map



X Index: 240

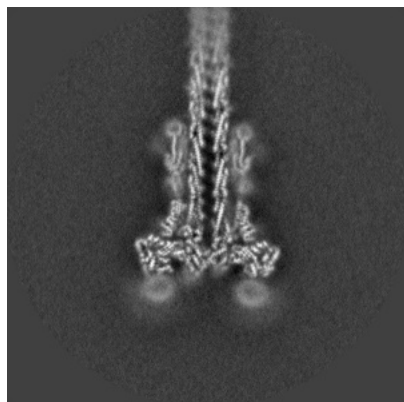


Y Index: 240

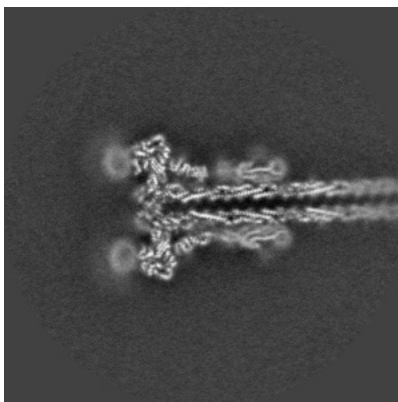


Z Index: 240

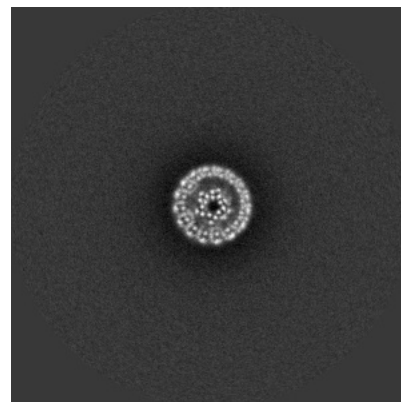
6.2.2 Raw map



X Index: 240



Y Index: 240

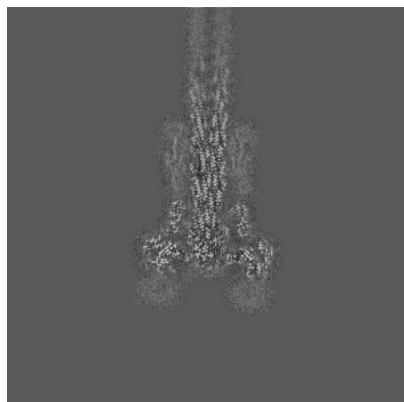


Z Index: 240

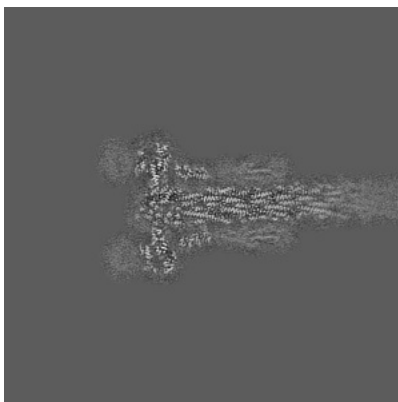
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

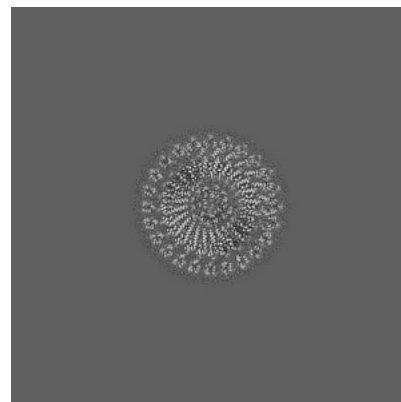
6.3.1 Primary map



X Index: 252

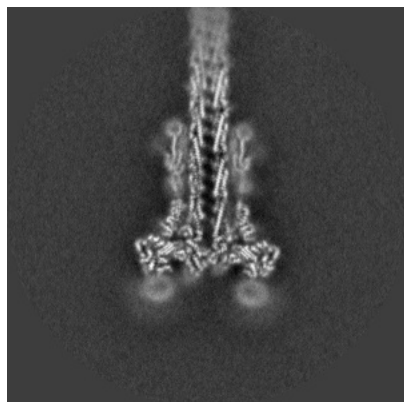


Y Index: 232

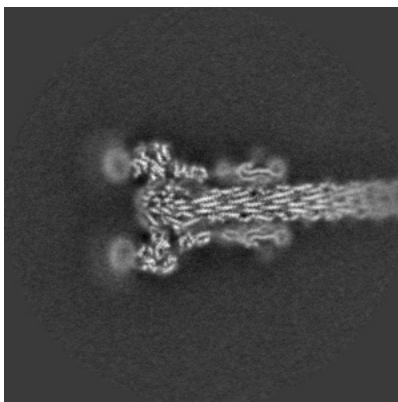


Z Index: 185

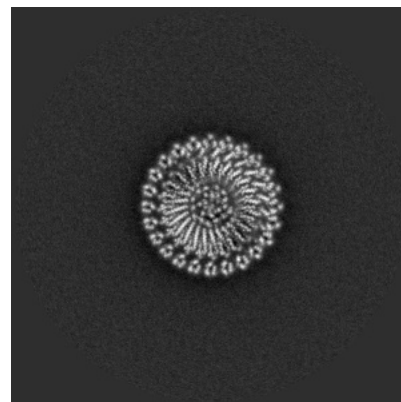
6.3.2 Raw map



X Index: 239



Y Index: 252

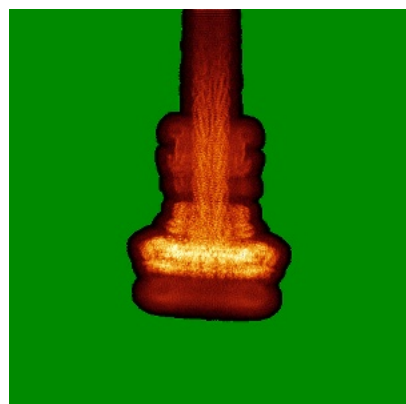


Z Index: 185

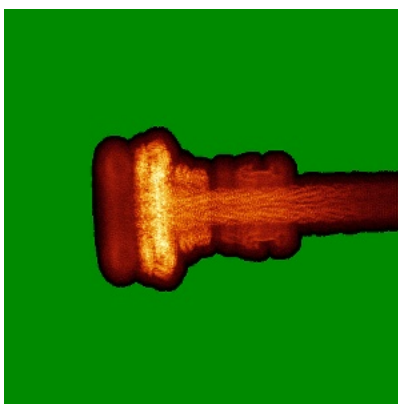
The images above show the largest variance slices of the map in three orthogonal directions.

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

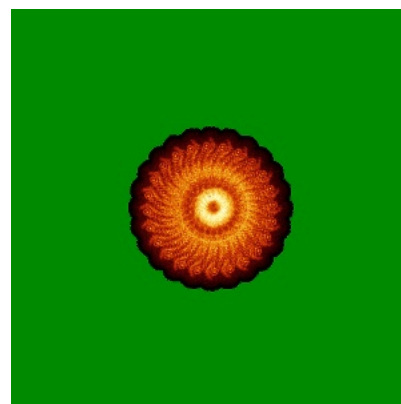
6.4.1 Primary map



X

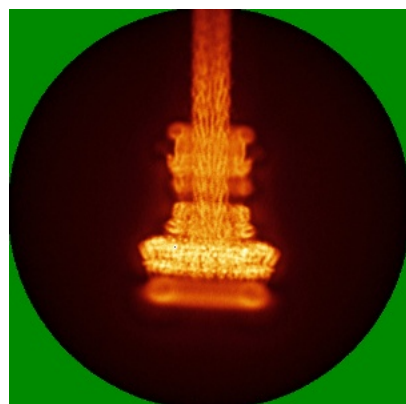


Y

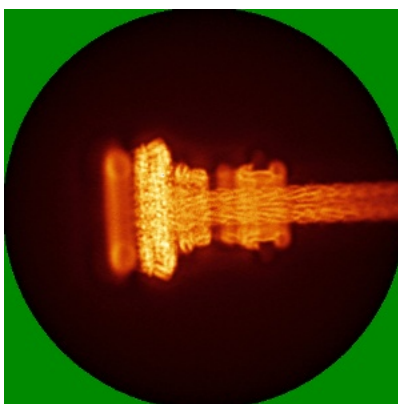


Z

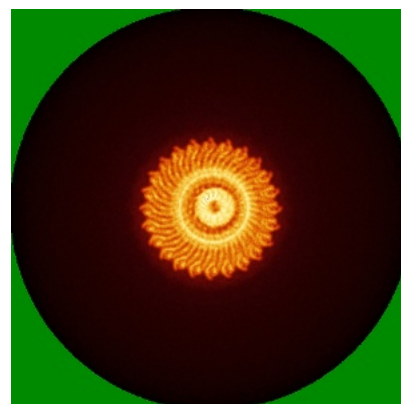
6.4.2 Raw map



X



Y

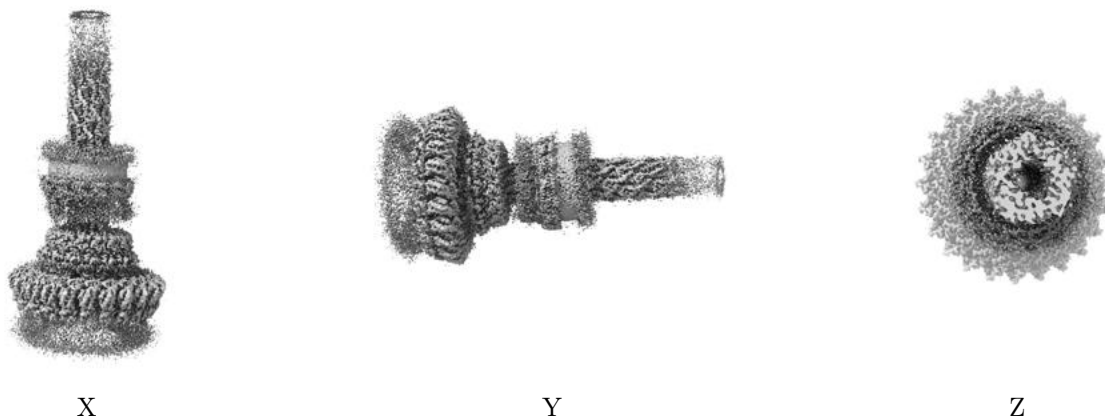


Z

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 0.05. 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

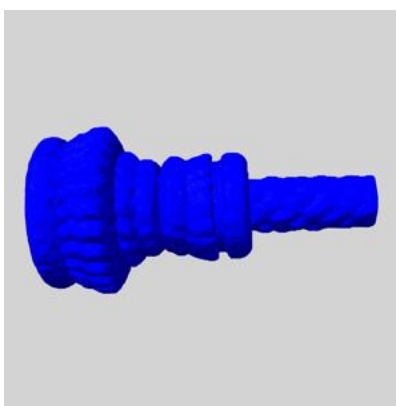
A mask typically either:

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

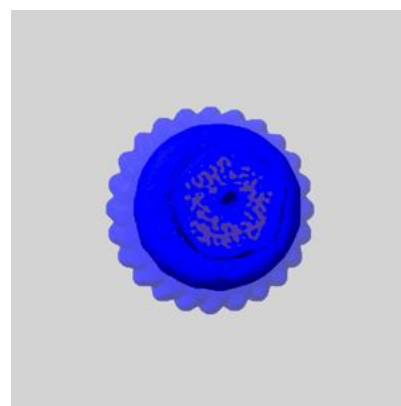
6.6.1 emd_15700_msk_1.map [i](#)



X



Y

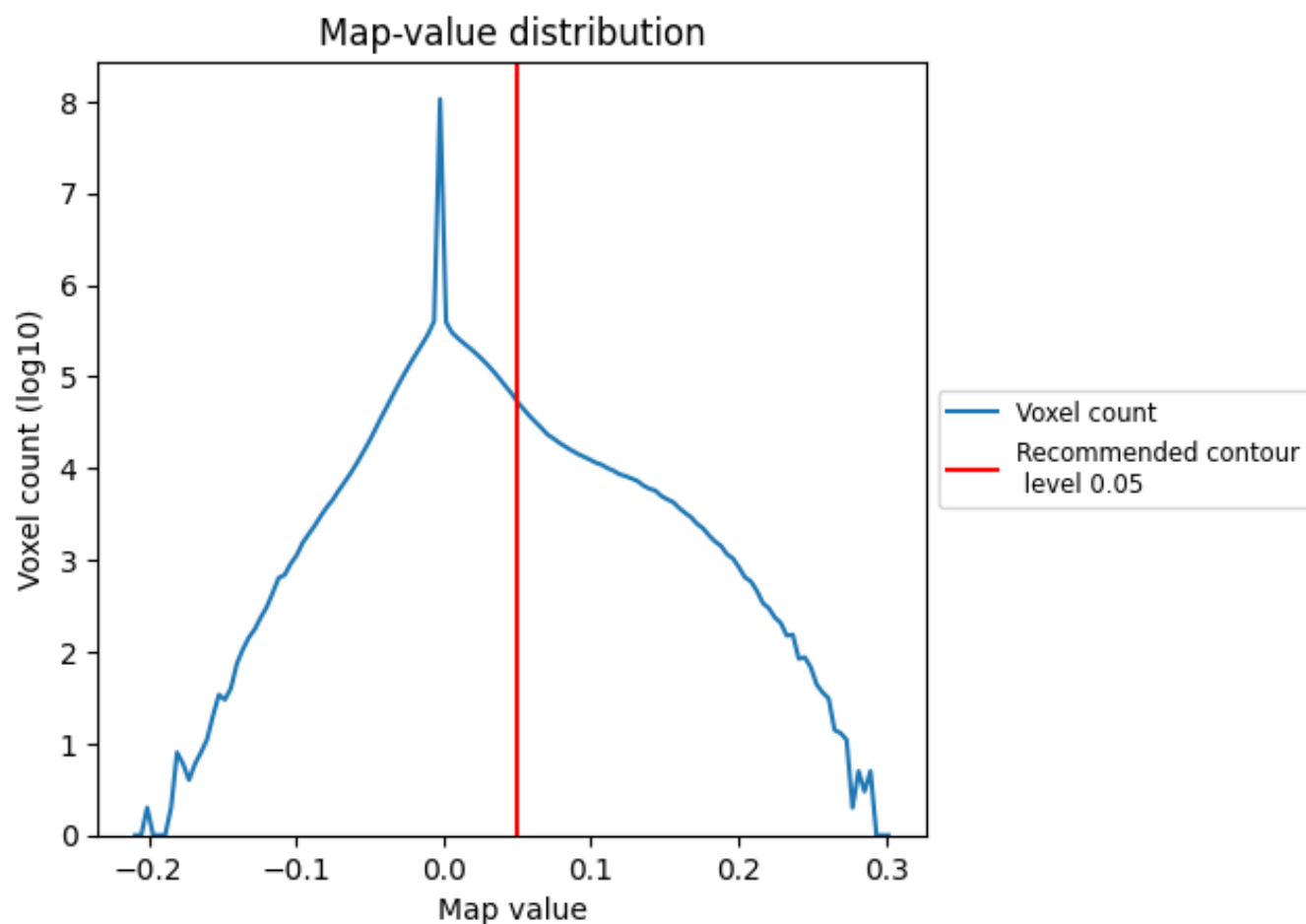


Z

7 Map analysis [i](#)

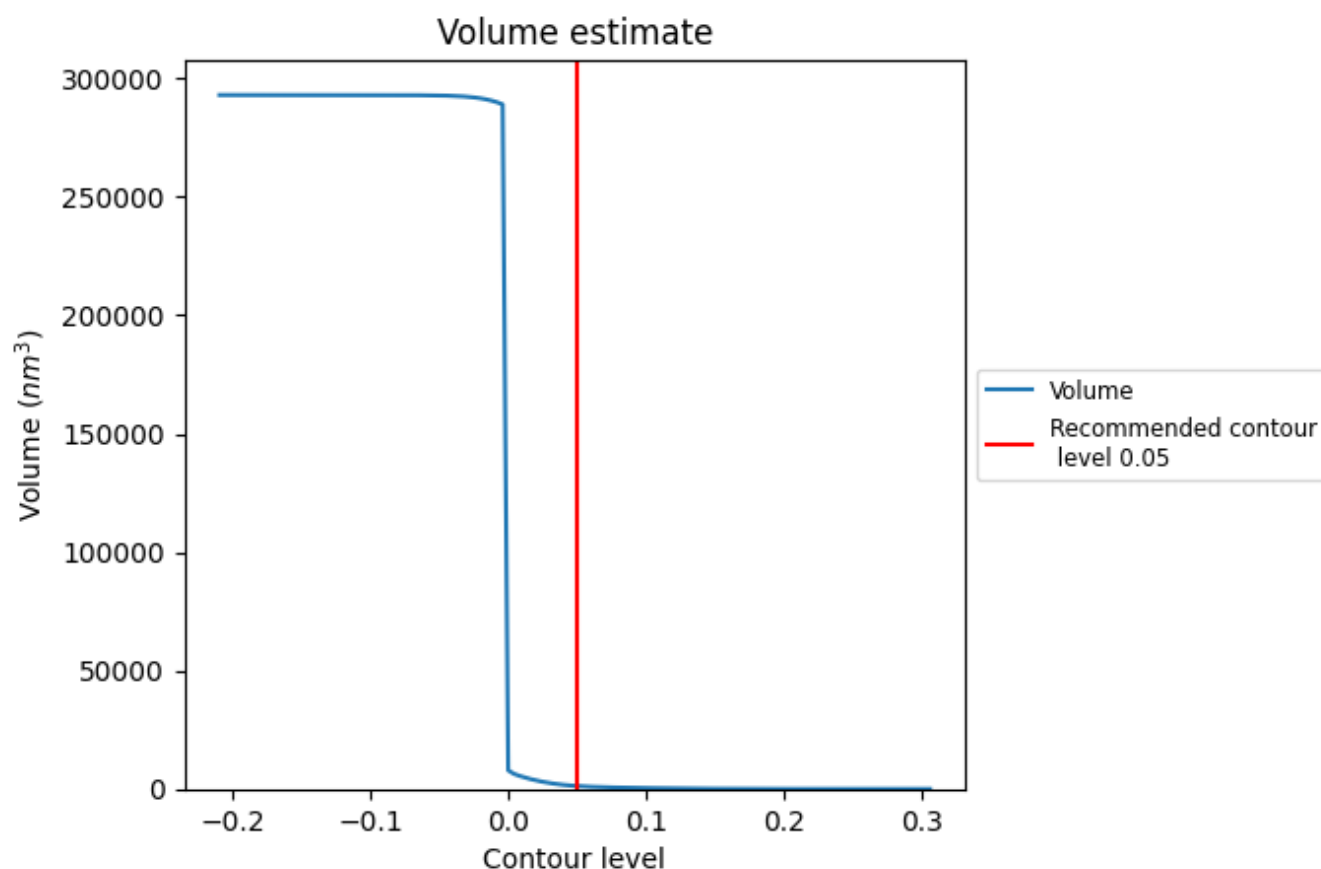
This section contains the results of statistical analysis of the map.

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.

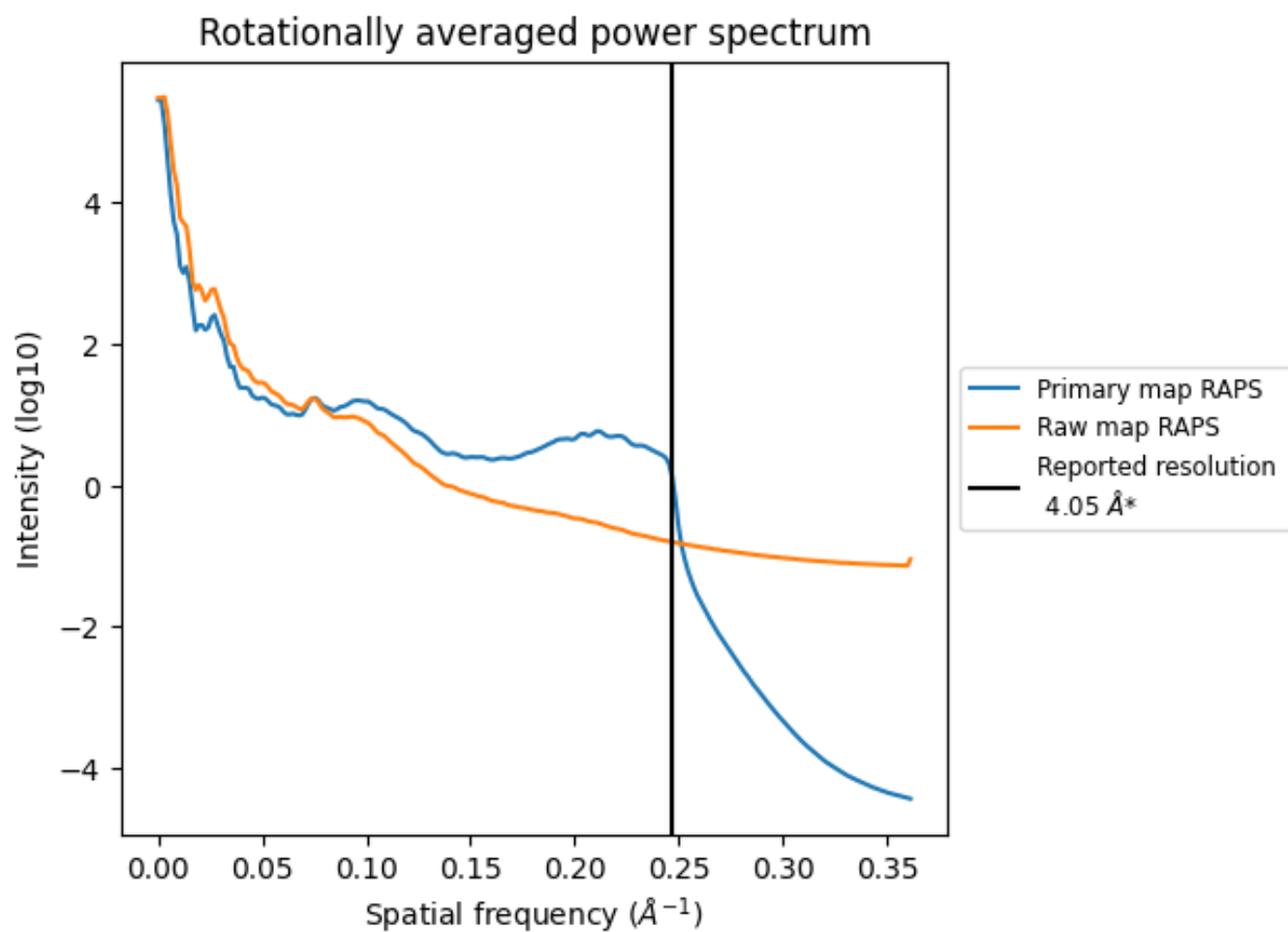
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1241 nm³; this corresponds to an approximate mass of 1121 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](#)

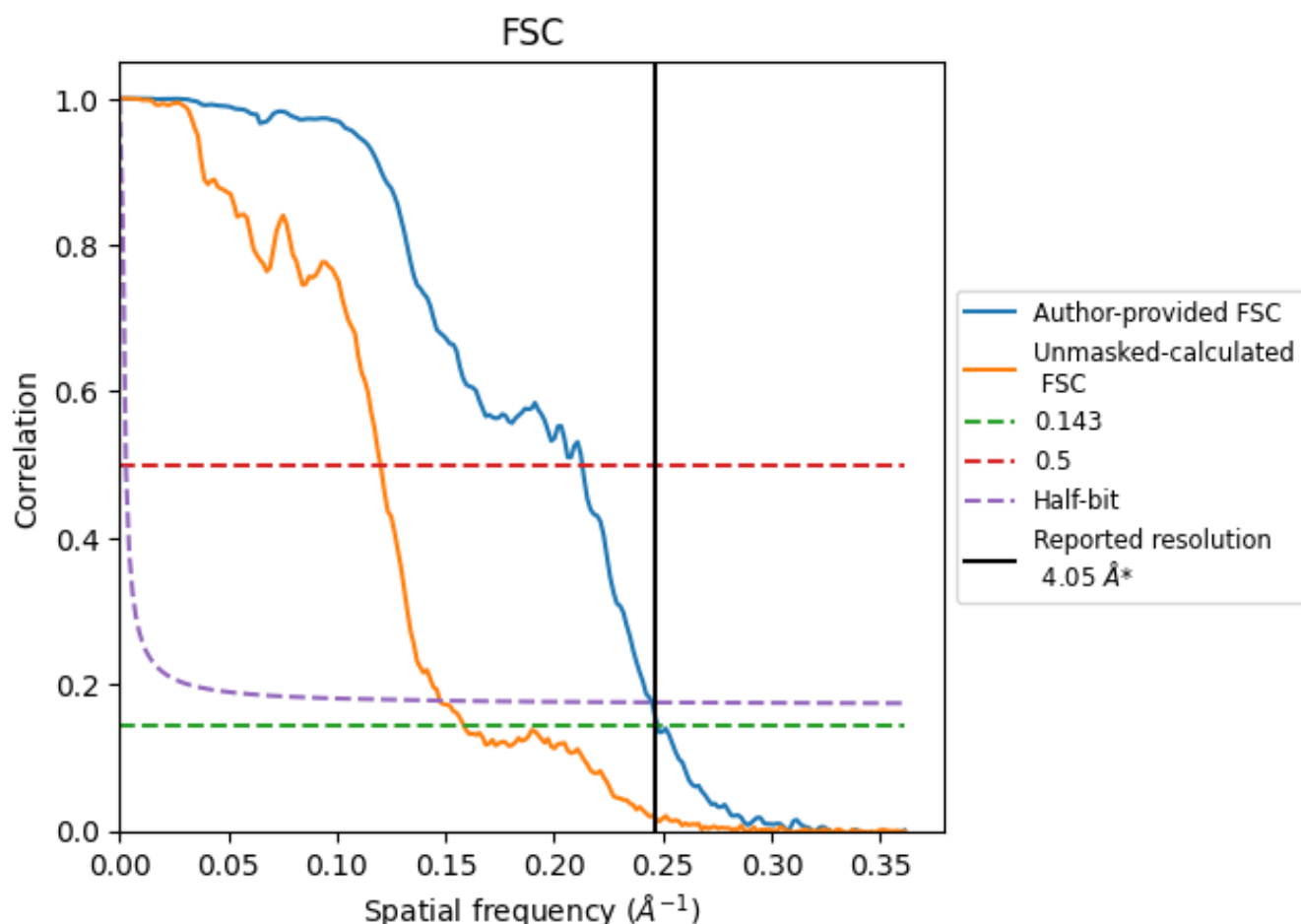


*Reported resolution corresponds to spatial frequency of 0.247 \AA^{-1}

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 0.247 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.05	-	-
Author-provided FSC curve	4.04	4.69	4.08
Unmasked-calculated*	6.31	8.33	6.78

*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 6.31 differs from the reported value 4.05 by more than 10 %

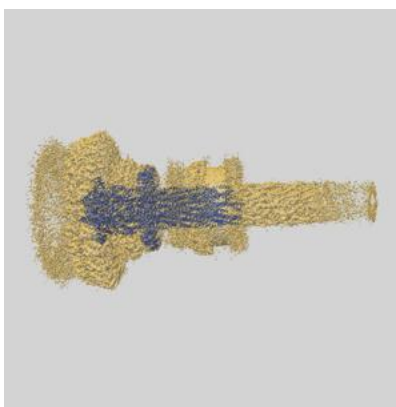
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15700 and PDB model 8AXK. Per-residue inclusion information can be found in section [3](#) on page [22](#).

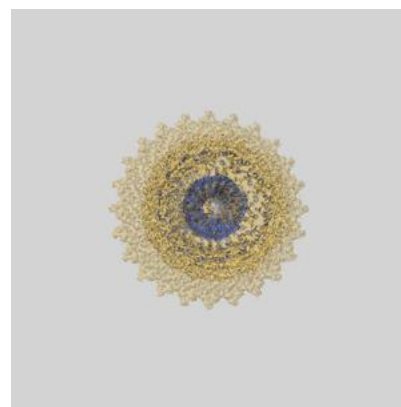
9.1 Map-model overlay [i](#)



X



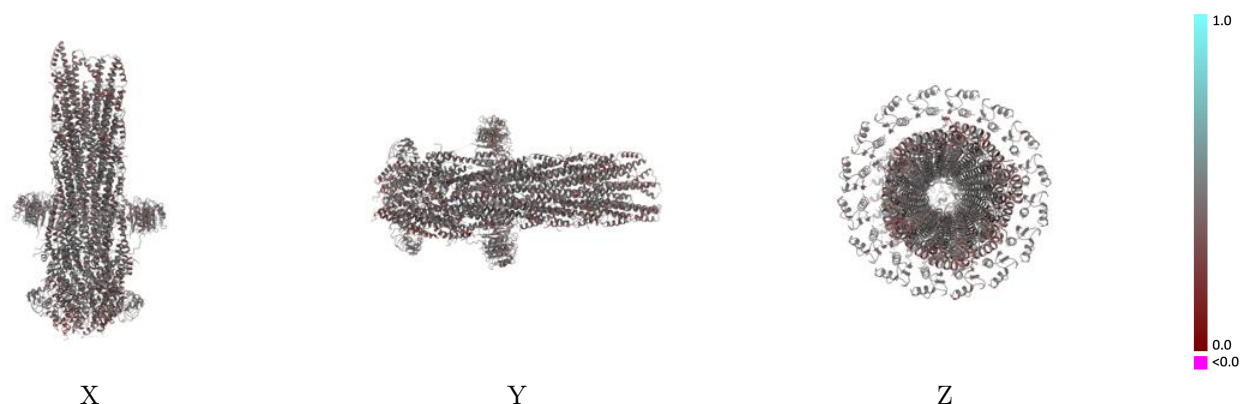
Y



Z

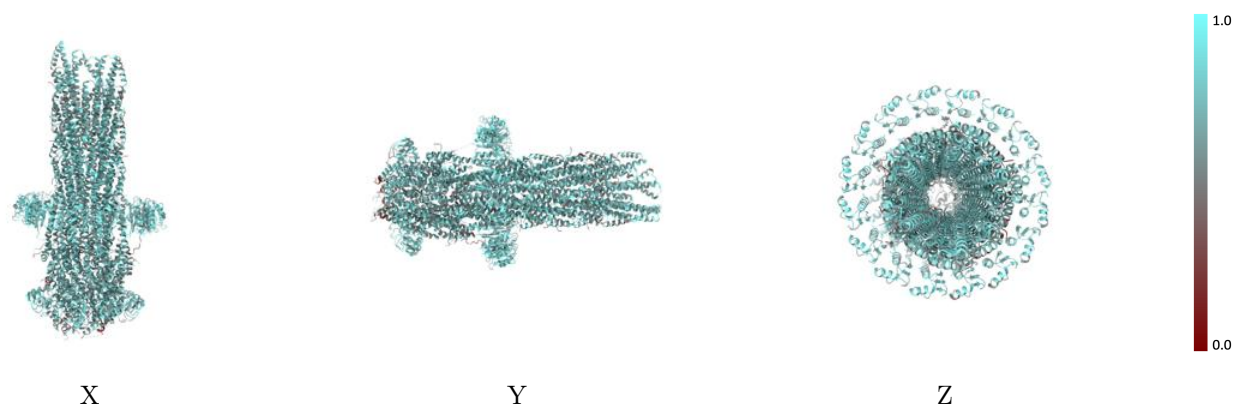
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



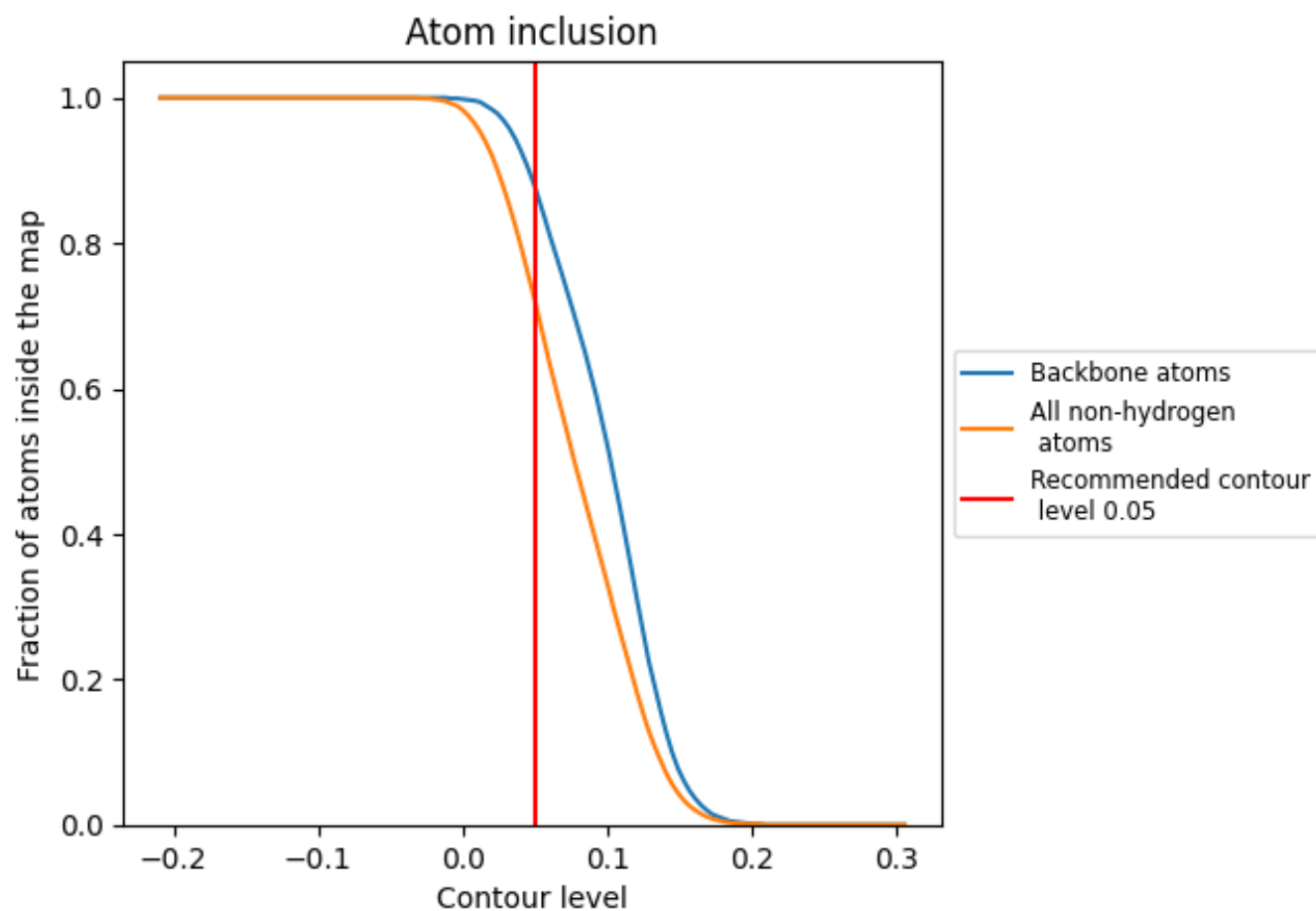
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 72% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7210	 0.4310
0	 0.7970	 0.4480
1	 0.7540	 0.4280
2	 0.7850	 0.4370
3	 0.7890	 0.4470
4	 0.7540	 0.4480
5	 0.7680	 0.4390
6	 0.7580	 0.4310
7	 0.7890	 0.4440
8	 0.7770	 0.4480
9	 0.7810	 0.4420
A	 0.7300	 0.4460
B	 0.6960	 0.4320
C	 0.6910	 0.4300
D	 0.7220	 0.4370
E	 0.7450	 0.4540
F	 0.6990	 0.4350
G	 0.6760	 0.3910
H	 0.5970	 0.3670
I	 0.6440	 0.3930
J	 0.6390	 0.4120
K	 0.6220	 0.3810
M	 0.7440	 0.4350
N	 0.6960	 0.4290
O	 0.6490	 0.4150
P	 0.6670	 0.4240
Q	 0.6870	 0.4160
R	 0.6850	 0.4250
S	 0.7530	 0.4400
T	 0.7530	 0.4460
U	 0.7280	 0.4360
V	 0.7290	 0.4330
W	 0.7440	 0.4310
X	 0.7640	 0.4500
Y	 0.7750	 0.4410





















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Chain	Atom inclusion	Q-score
Z	 0.7830	 0.4400
a	 0.7190	 0.4340
a0	 0.7950	 0.4550
b	 0.7320	 0.4230
b0	 0.7320	 0.4130
c	 0.6930	 0.4250
c0	 0.7790	 0.4540
d	 0.7260	 0.4280
d0	 0.7320	 0.4370
e	 0.7440	 0.4370
e0	 0.7010	 0.4530
f	 0.7380	 0.4310
f0	 0.7320	 0.4370
g	 0.7390	 0.4380
g0	 0.7400	 0.4320
h	 0.7320	 0.4390
h0	 0.7870	 0.4740
i	 0.7510	 0.4320
i0	 0.8030	 0.4510
j	 0.7660	 0.4450
j0	 0.7170	 0.4390
k	 0.7730	 0.4480
k0	 0.7240	 0.4300
l	 0.7560	 0.4550
l0	 0.7790	 0.4570
m	 0.6930	 0.4300
m0	 0.7790	 0.4640
n	 0.7200	 0.4320
n0	 0.7790	 0.4630
o	 0.7220	 0.4290
o0	 0.6690	 0.4110
p	 0.6790	 0.4250
p0	 0.7320	 0.4340
q	 0.6950	 0.4220
q0	 0.7870	 0.4310
r	 0.6650	 0.4190
r0	 0.7400	 0.4520
s	 0.6650	 0.4160
s0	 0.8270	 0.4770
t	 0.6900	 0.4210
t0	 0.7320	 0.4440
u	 0.7100	 0.4170

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Chain	Atom inclusion	Q-score
u0	 0.7560	 0.4570
v	 0.6840	 0.4120
v0	 0.6850	 0.3980
w	 0.6930	 0.4150
w0	 0.6610	 0.4040
x	 0.7990	 0.4550
x0	 0.7170	 0.4480
y	 0.7640	 0.4410
z	 0.7620	 0.4270