



Full wwPDB EM Validation Report ⓘ

Apr 4, 2023 – 02:07 pm BST

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 : 6RWX, 6RWY, 6RWK

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:

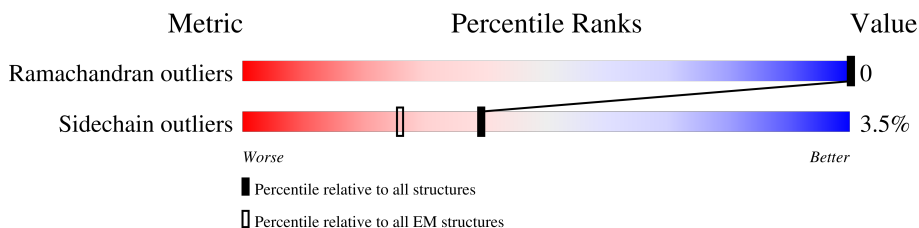
EMDB validation analysis : 0.0.1.dev50
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.32.2

1 Overall quality at a glance i

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

The reported resolution of this entry is 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	154571	4023
Sidechain outliers	154315	3826

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	 84% 13%
1	B	216	 83% 14%
1	C	216	 85% 13%
1	D	216	 83% 15%
1	E	216	 83% 14%
2	F	256	 95% 5%
3	G	86	 97%
3	H	86	 83% 5% 13%
3	I	86	 72% 27%

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Mol	Chain	Length	Quality of chain
3	J	86	9% 77% 22%
4	K	342	29% 67%
5	M	97	42% 57%
5	N	97	85% 12%
5	O	97	9% 94% 5% 2%
5	P	97	10% 91% 5% 2%
5	Q	97	7% 87% 12%
5	R	97	5% 88% 12%
6	S	98	60% 39%
6	T	98	59% 40%
6	U	98	60% 39%
6	V	98	60% 40%
6	W	98	60% 40%
6	a	98	7% 82% 16%
6	b	98	80% 17%
6	c	98	6% 83% 16%
6	d	98	6% 83% 16%
6	e	98	81% 17%
6	f	98	81% 17%
6	g	98	76% 22%
6	h	98	74% 23%
6	i	98	71% 5% 23%
6	j	98	74% 22%
6	k	98	72% 23%
6	l	98	77% 22%








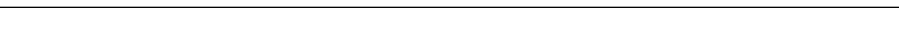
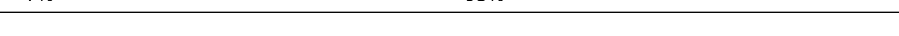
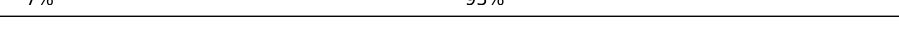
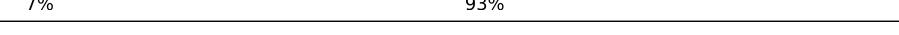
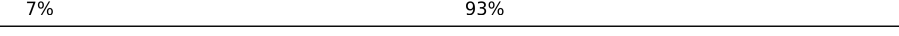












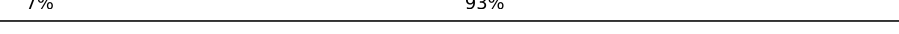
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Mol	Chain	Length	Quality of chain
6	m	98	6% 83% 16%
6	n	98	82% 16%
6	o	98	80% 17%
6	p	98	83% 16%
6	q	98	81% 16%
6	r	98	11% 82% 16%
6	s	98	8% 83% 17%
6	t	98	6% 77% 20%
6	u	98	5% 80% 17%
6	v	98	5% 81% 16%
6	w	98	5% 83% 16%
7	0	566	11% 89%
7	1	566	11% 89%
7	2	566	11% 89%
7	3	566	10% 89%
7	4	566	11% 89%
7	5	566	10% 89%
7	6	566	10% 89%
7	7	566	10% 89%
7	8	566	11% 89%
7	9	566	11% 89%
7	X	566	10% 89%
7	Y	566	11% 89%
7	Z	566	11% 89%
7	x	566	10% 89%


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Mol	Chain	Length	Quality of chain	
7	y	566		89%
7	z	566		89%
8	a0	241		93%
8	b0	241		93%
8	c0	241		93%
8	d0	241		93%
8	e0	241		93%
8	f0	241		93%
8	g0	241		93%
8	h0	241		93%
8	i0	241		93%
8	j0	241		93%
8	k0	241		93%
8	l0	241		93%
8	m0	241		93%
8	n0	241		93%
8	o0	241		93%
8	p0	241		93%
8	q0	241		93%
8	r0	241		93%
8	s0	241		93%
8	t0	241		93%
8	u0	241		93%
8	v0	241		93%
8	w0	241		93%

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Mol	Chain	Length	Quality of chain
8	x0	241	 7% 93%

2 Entry composition [i](#)

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

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

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

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

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

- 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 MxiI.

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

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
			Total	C	N	O		
7	X	62	497	325	80	92	0	0

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

- Molecule 8 is a protein called Lipoprotein MxiJ.

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

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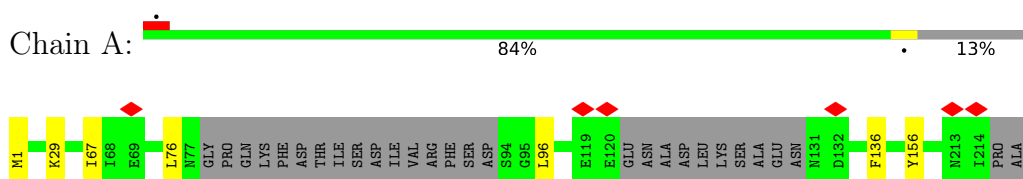
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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	e0	17	131	82	24	25	0	0
8	f0	17	131	82	24	25	0	0
8	g0	17	131	82	24	25	0	0
8	h0	17	131	82	24	25	0	0
8	i0	17	131	82	24	25	0	0
8	j0	17	131	82	24	25	0	0
8	k0	17	131	82	24	25	0	0
8	l0	17	131	82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

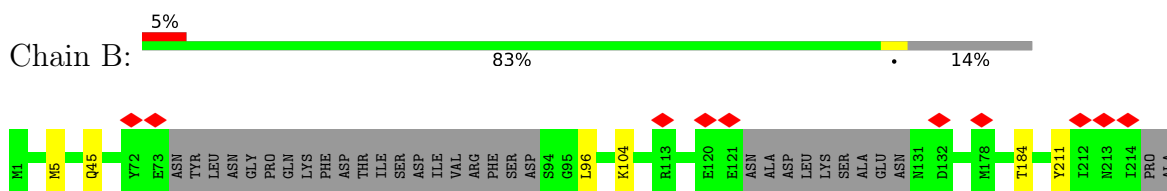
3 Residue-property plots [i](#)

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.

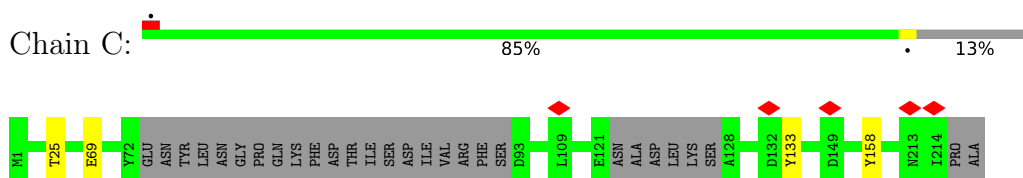
- Molecule 1: Surface presentation of antigens protein SpaP



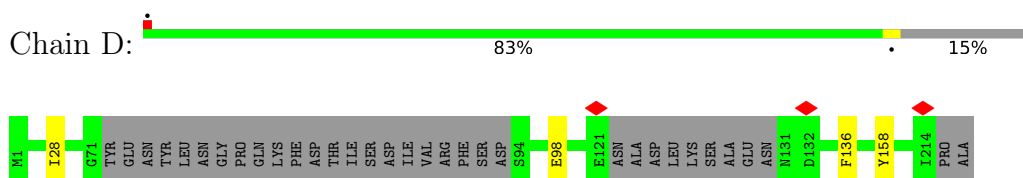
- Molecule 1: Surface presentation of antigens protein SpaP



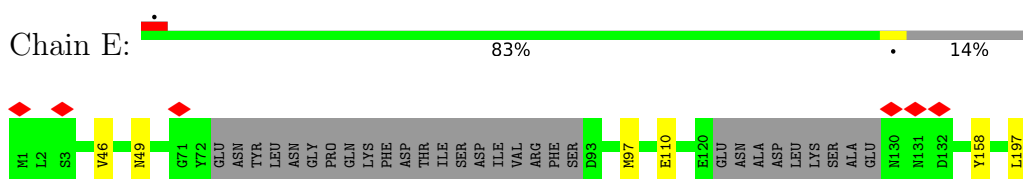
- Molecule 1: Surface presentation of antigens protein SpaP



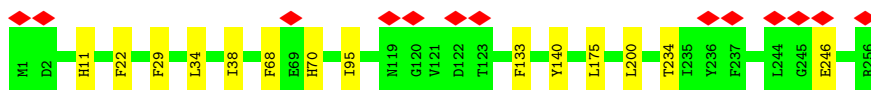
- Molecule 1: Surface presentation of antigens protein SpaP



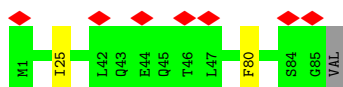
- Molecule 1: Surface presentation of antigens protein SpaP



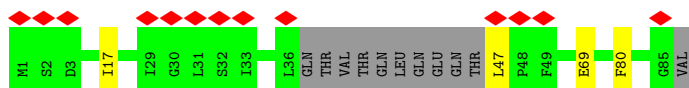
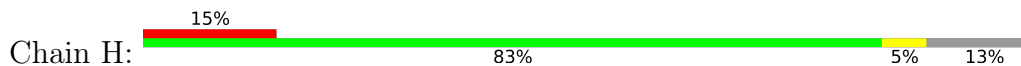
• Molecule 2: Surface presentation of antigens protein SpaR



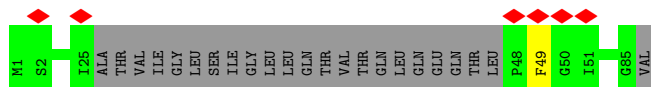
• Molecule 3: Surface presentation of antigens protein SpaQ



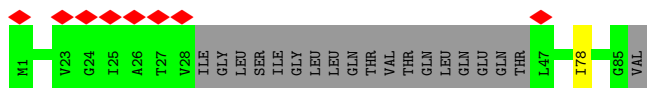
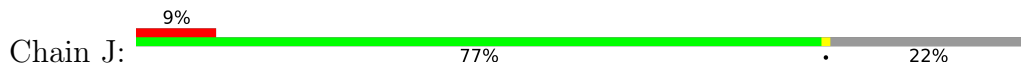
• Molecule 3: Surface presentation of antigens protein SpaQ



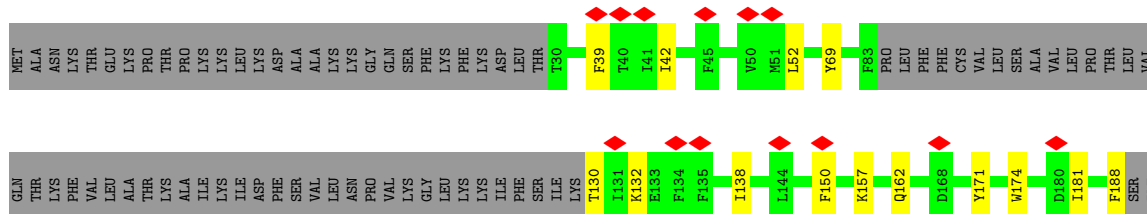
• Molecule 3: Surface presentation of antigens protein SpaQ

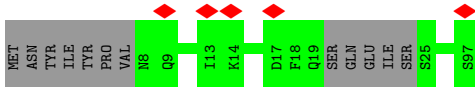


• Molecule 3: Surface presentation of antigens protein SpaQ

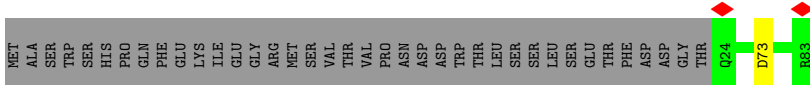


• Molecule 4: Surface presentation of antigens protein SpaS

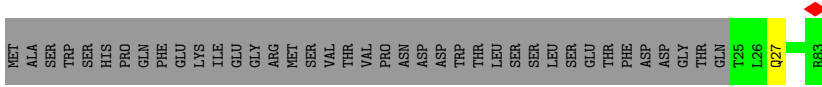




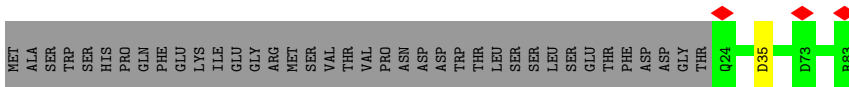
• Molecule 6: Protein MxiH



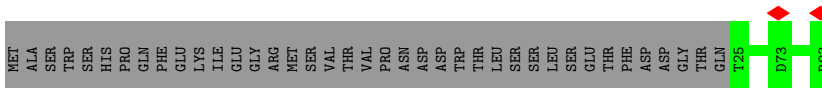
• Molecule 6: Protein MxiH



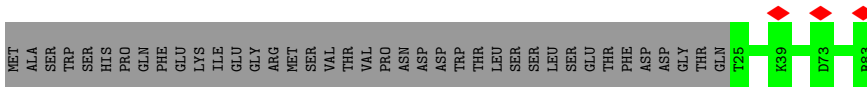
• Molecule 6: Protein MxiH



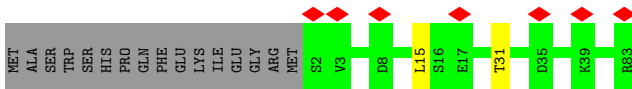
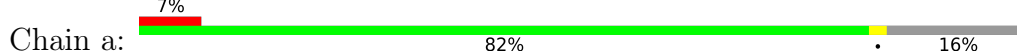
• Molecule 6: Protein MxiH



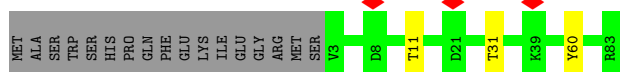
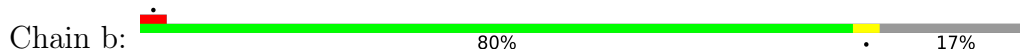
• Molecule 6: Protein MxiH



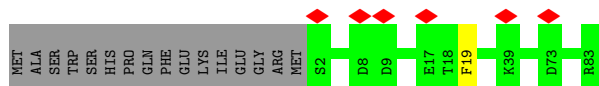
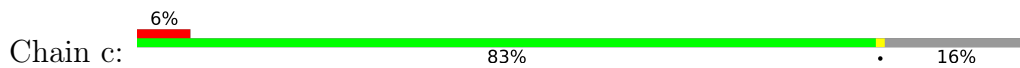
• Molecule 6: Protein MxiH



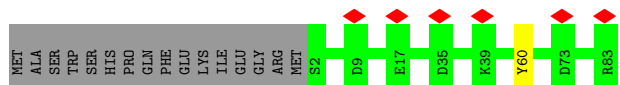
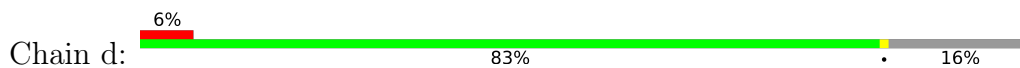
• Molecule 6: Protein MxiH



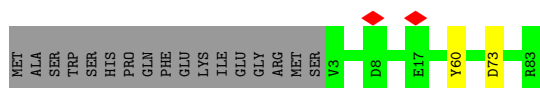
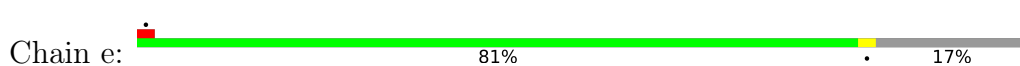
• Molecule 6: Protein MxiH



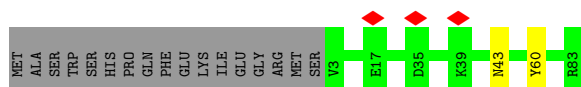
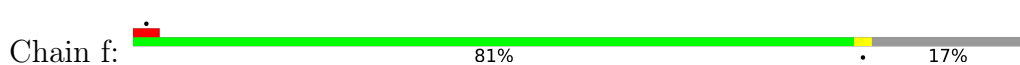
• Molecule 6: Protein MxiH



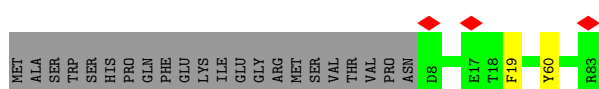
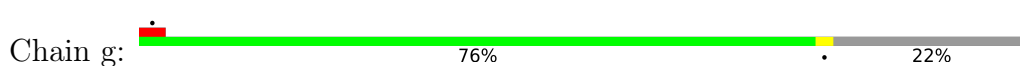
• Molecule 6: Protein MxiH



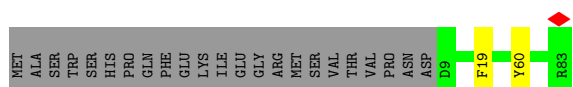
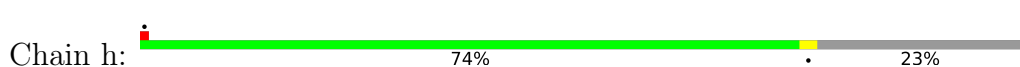
• Molecule 6: Protein MxiH



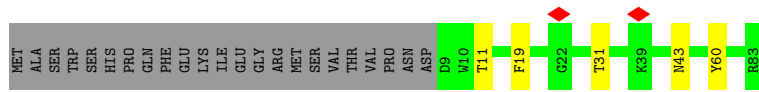
• Molecule 6: Protein MxiH



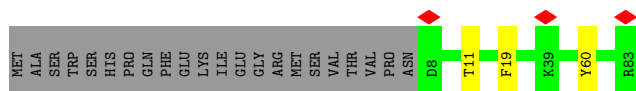
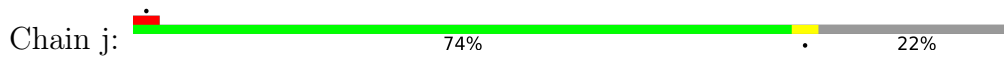
• Molecule 6: Protein MxiH



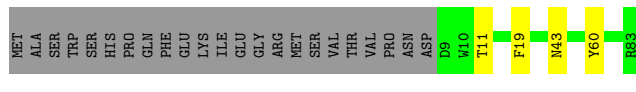
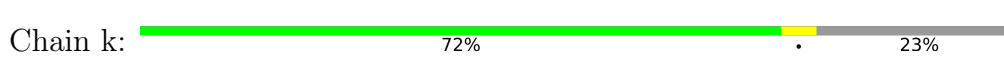
• Molecule 6: Protein MxiH



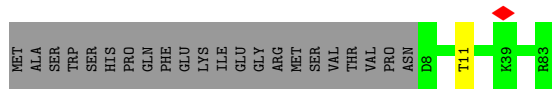
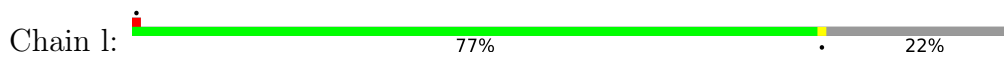
• Molecule 6: Protein MxiH



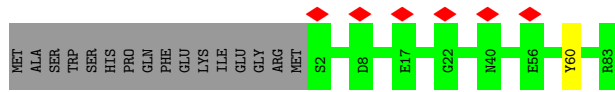
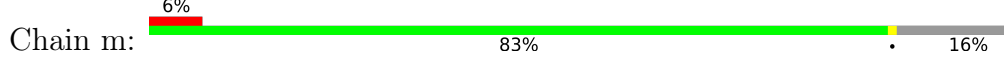
• Molecule 6: Protein MxiH



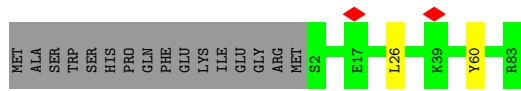
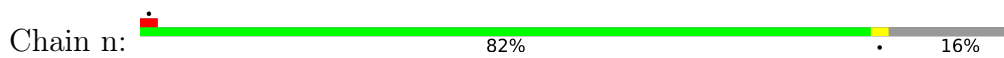
• Molecule 6: Protein MxiH



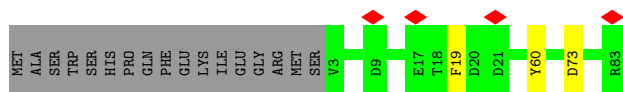
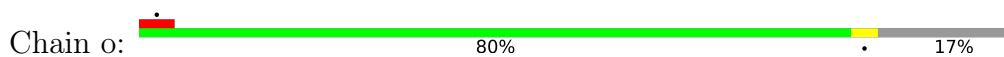
• Molecule 6: Protein MxiH




• Molecule 6: Protein MxiH

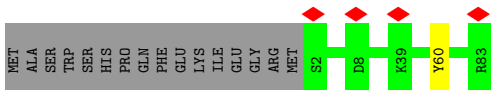


• Molecule 6: Protein MxiH




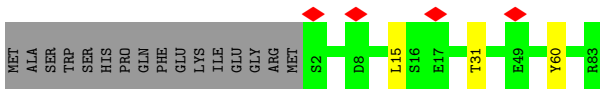
- Molecule 6: Protein MxiH

Chain p:  83% 16%




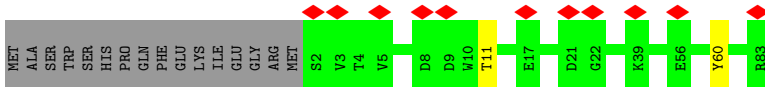
- Molecule 6: Protein MxiH

Chain q:  81% 16%




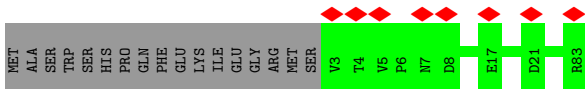
- Molecule 6: Protein MxiH

Chain r:  82% 16%




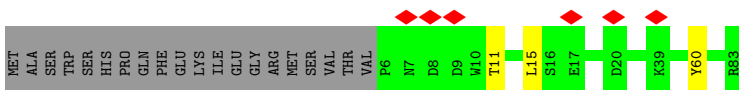
- Molecule 6: Protein MxiH

Chain s:  83% 17%




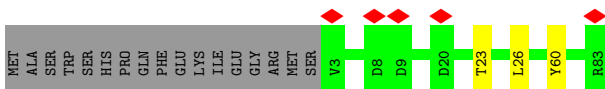
- Molecule 6: Protein MxiH

Chain t:  77% 20%




- Molecule 6: Protein MxiH

Chain u:  80% 17%



- Molecule 6: Protein MxiH

Chain v:  81% 16%

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 (\AA)	498.41714, 498.41714, 498.41714	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	165/189 (87%)	158 (96%)	7 (4%)	30	56
1	B	162/189 (86%)	156 (96%)	6 (4%)	34	59
1	C	164/189 (87%)	160 (98%)	4 (2%)	49	69
1	D	160/189 (85%)	156 (98%)	4 (2%)	47	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	163/189 (86%)	157 (96%)	6 (4%)	34	59
2	F	230/230 (100%)	216 (94%)	14 (6%)	18	47
3	G	74/75 (99%)	72 (97%)	2 (3%)	44	66
3	H	64/75 (85%)	60 (94%)	4 (6%)	18	45
3	I	55/75 (73%)	54 (98%)	1 (2%)	59	77
3	J	58/75 (77%)	57 (98%)	1 (2%)	60	78
4	K	105/316 (33%)	91 (87%)	14 (13%)	4	21
5	M	36/89 (40%)	35 (97%)	1 (3%)	43	65
5	N	78/89 (88%)	75 (96%)	3 (4%)	33	59
5	O	87/89 (98%)	83 (95%)	4 (5%)	27	54
5	P	85/89 (96%)	80 (94%)	5 (6%)	19	48
5	Q	77/89 (86%)	76 (99%)	1 (1%)	69	82
5	R	77/89 (86%)	77 (100%)	0	100	100
6	S	53/88 (60%)	52 (98%)	1 (2%)	57	75
6	T	52/88 (59%)	51 (98%)	1 (2%)	57	75
6	U	53/88 (60%)	52 (98%)	1 (2%)	57	75
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%)	44	66
6	b	73/88 (83%)	70 (96%)	3 (4%)	30	57
6	c	74/88 (84%)	73 (99%)	1 (1%)	67	80
6	d	74/88 (84%)	73 (99%)	1 (1%)	67	80
6	e	73/88 (83%)	71 (97%)	2 (3%)	44	66
6	f	73/88 (83%)	71 (97%)	2 (3%)	44	66
6	g	68/88 (77%)	66 (97%)	2 (3%)	42	64
6	h	67/88 (76%)	65 (97%)	2 (3%)	41	64
6	i	67/88 (76%)	62 (92%)	5 (8%)	13	40
6	j	68/88 (77%)	65 (96%)	3 (4%)	28	55
6	k	67/88 (76%)	63 (94%)	4 (6%)	19	47
6	l	68/88 (77%)	67 (98%)	1 (2%)	65	80
6	m	74/88 (84%)	73 (99%)	1 (1%)	67	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	n	74/88 (84%)	72 (97%)	2 (3%)	44	66
6	o	73/88 (83%)	70 (96%)	3 (4%)	30	57
6	p	74/88 (84%)	73 (99%)	1 (1%)	67	80
6	q	74/88 (84%)	71 (96%)	3 (4%)	30	57
6	r	74/88 (84%)	72 (97%)	2 (3%)	44	66
6	s	73/88 (83%)	73 (100%)	0	100	100
6	t	70/88 (80%)	67 (96%)	3 (4%)	29	56
6	u	73/88 (83%)	70 (96%)	3 (4%)	30	57
6	v	74/88 (84%)	71 (96%)	3 (4%)	30	57
6	w	74/88 (84%)	73 (99%)	1 (1%)	67	80
7	0	56/513 (11%)	54 (96%)	2 (4%)	35	60
7	1	56/513 (11%)	54 (96%)	2 (4%)	35	60
7	2	56/513 (11%)	56 (100%)	0	100	100
7	3	56/513 (11%)	53 (95%)	3 (5%)	22	50
7	4	56/513 (11%)	54 (96%)	2 (4%)	35	60
7	5	56/513 (11%)	53 (95%)	3 (5%)	22	50
7	6	56/513 (11%)	52 (93%)	4 (7%)	14	42
7	7	56/513 (11%)	53 (95%)	3 (5%)	22	50
7	8	56/513 (11%)	55 (98%)	1 (2%)	59	77
7	9	56/513 (11%)	54 (96%)	2 (4%)	35	60
7	X	56/513 (11%)	52 (93%)	4 (7%)	14	42
7	Y	56/513 (11%)	54 (96%)	2 (4%)	35	60
7	Z	56/513 (11%)	54 (96%)	2 (4%)	35	60
7	x	56/513 (11%)	53 (95%)	3 (5%)	22	50
7	y	56/513 (11%)	54 (96%)	2 (4%)	35	60
7	z	56/513 (11%)	53 (95%)	3 (5%)	22	50
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%)	16	44

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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%)	16	44
8	j0	15/220 (7%)	14 (93%)	1 (7%)	16	44
8	k0	15/220 (7%)	14 (93%)	1 (7%)	16	44
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%)	4	21
8	s0	15/220 (7%)	15 (100%)	0	100	100
8	t0	15/220 (7%)	14 (93%)	1 (7%)	16	44
8	u0	15/220 (7%)	15 (100%)	0	100	100
8	v0	15/220 (7%)	14 (93%)	1 (7%)	16	44
8	w0	15/220 (7%)	15 (100%)	0	100	100
8	x0	15/220 (7%)	14 (93%)	1 (7%)	16	44
All	All	5011/18277 (27%)	4834 (96%)	177 (4%)	39	61

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

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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 [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 monosaccharides 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.

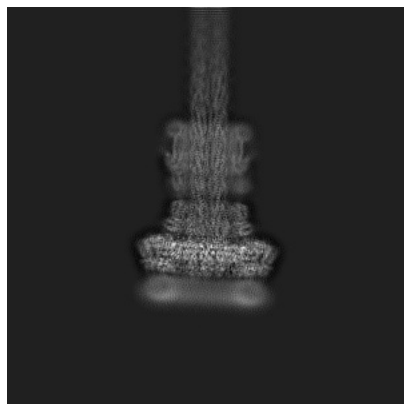
6 Map visualisation [i](#)

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

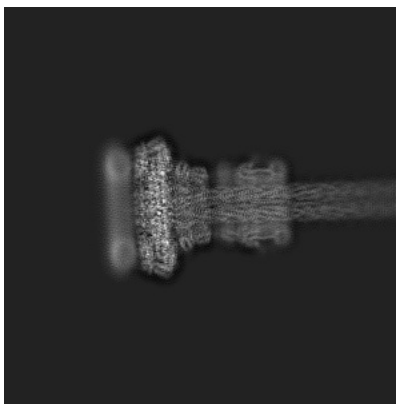
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

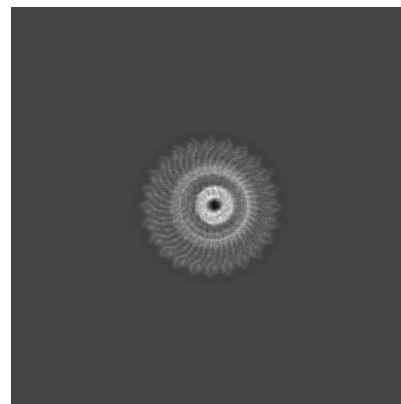
6.1.1 Primary map



X

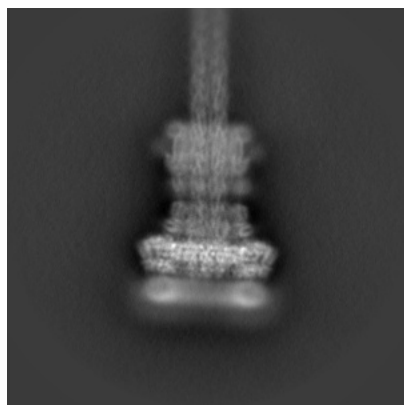


Y

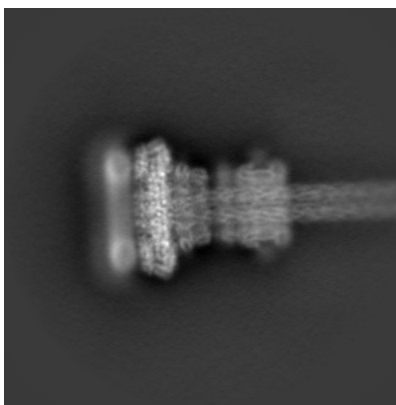


Z

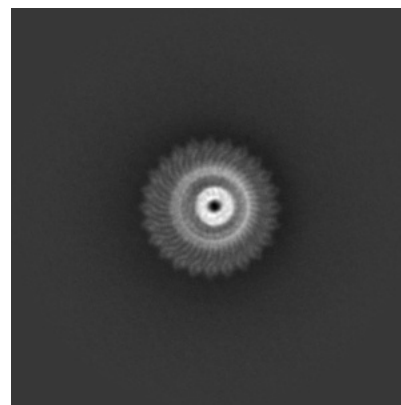
6.1.2 Raw map



X



Y

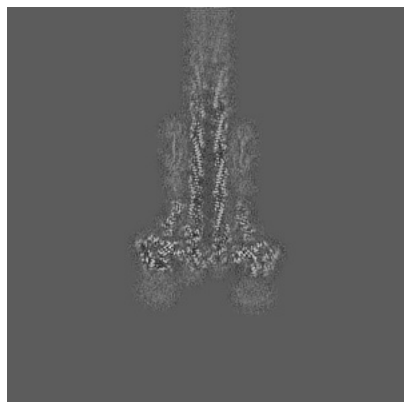


Z

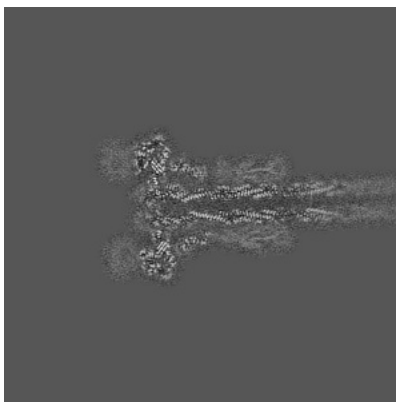
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

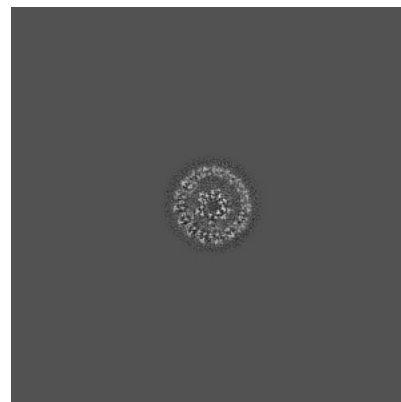
6.2.1 Primary map



X Index: 240

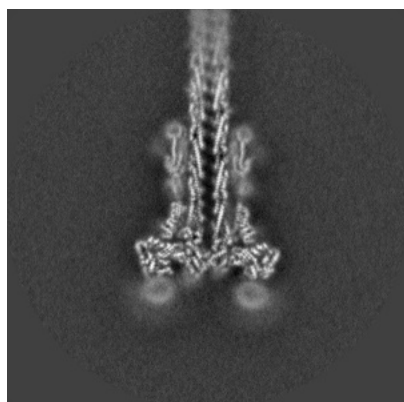


Y Index: 240

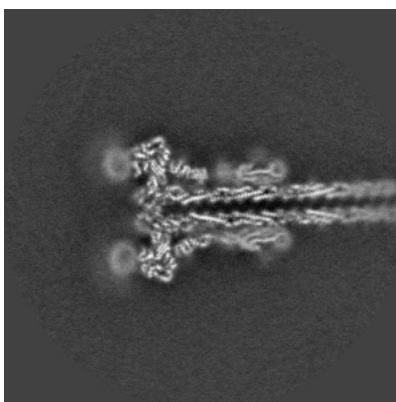


Z Index: 240

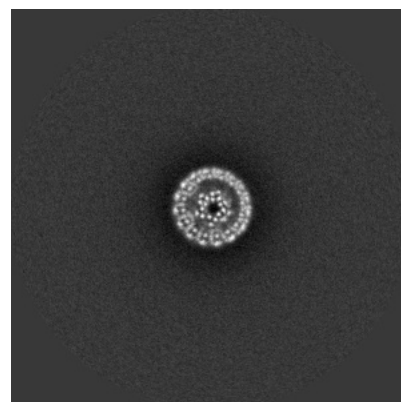
6.2.2 Raw map



X Index: 240



Y Index: 240

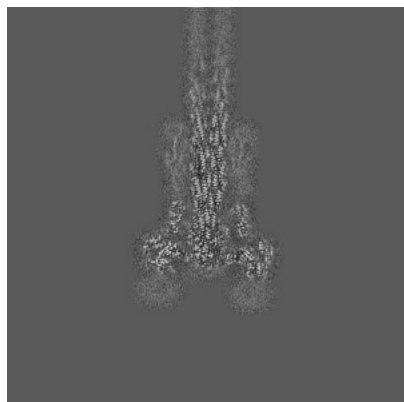


Z Index: 240

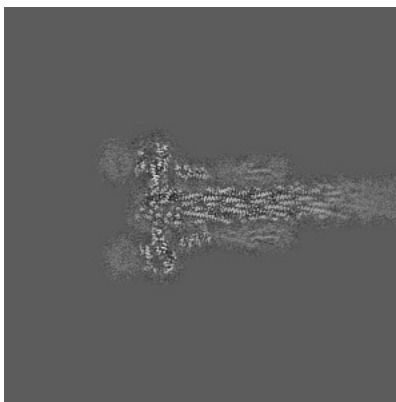
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

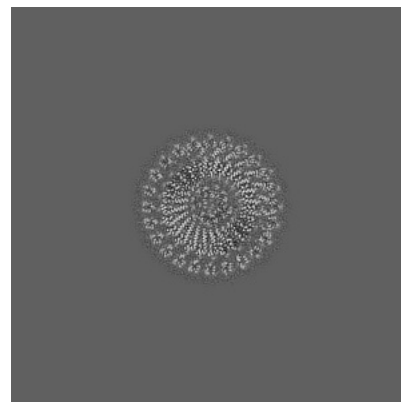
6.3.1 Primary map



X Index: 252

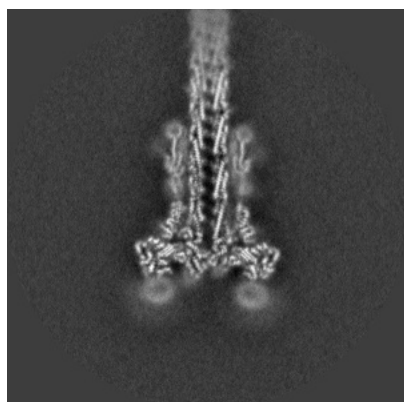


Y Index: 232

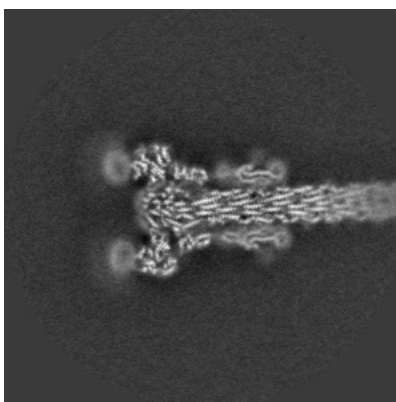


Z Index: 185

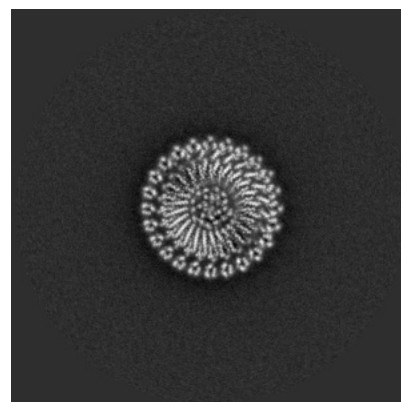
6.3.2 Raw map



X Index: 239



Y Index: 252

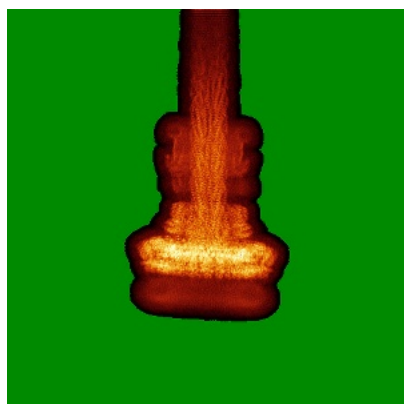


Z Index: 185

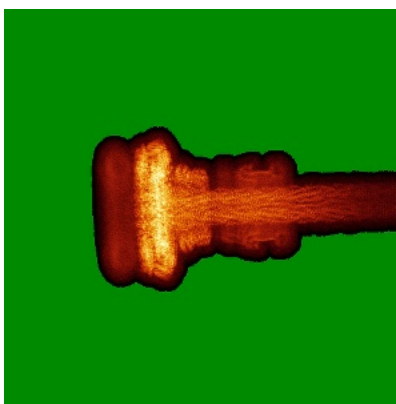
The images above show the largest variance slices of the map in three orthogonal directions.

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

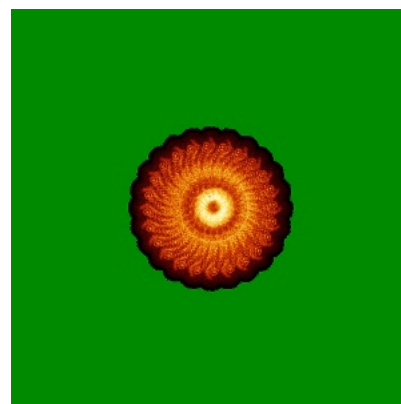
6.4.1 Primary map



X

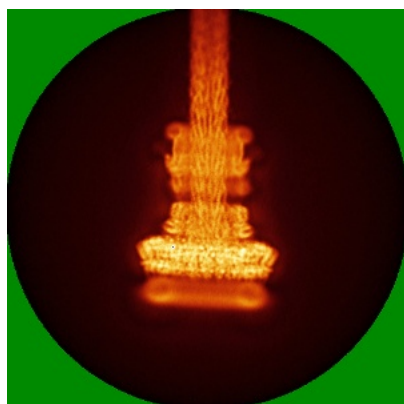


Y

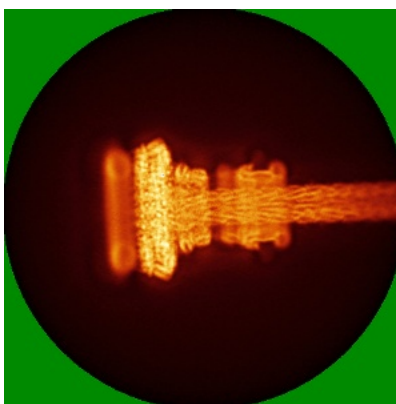


Z

6.4.2 Raw map



X



Y

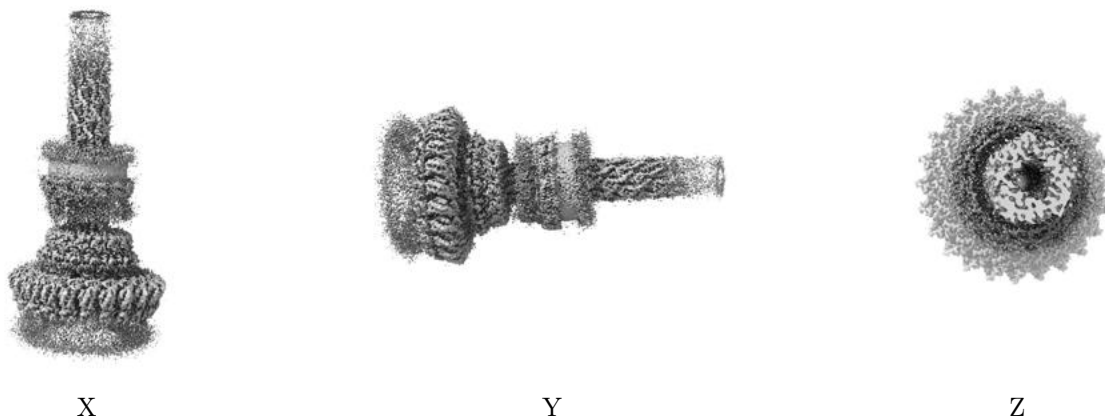


Z

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

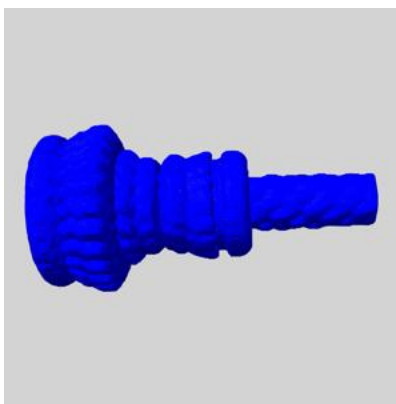
A mask typically either:

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

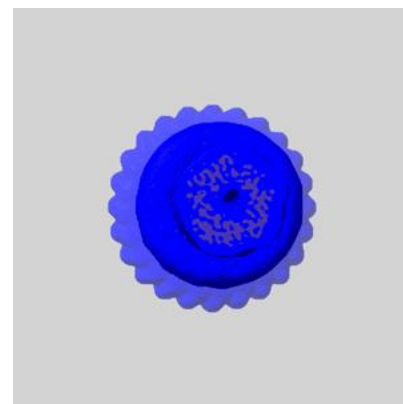
6.6.1 emd_15700_msk_1.map [i](#)



X



Y

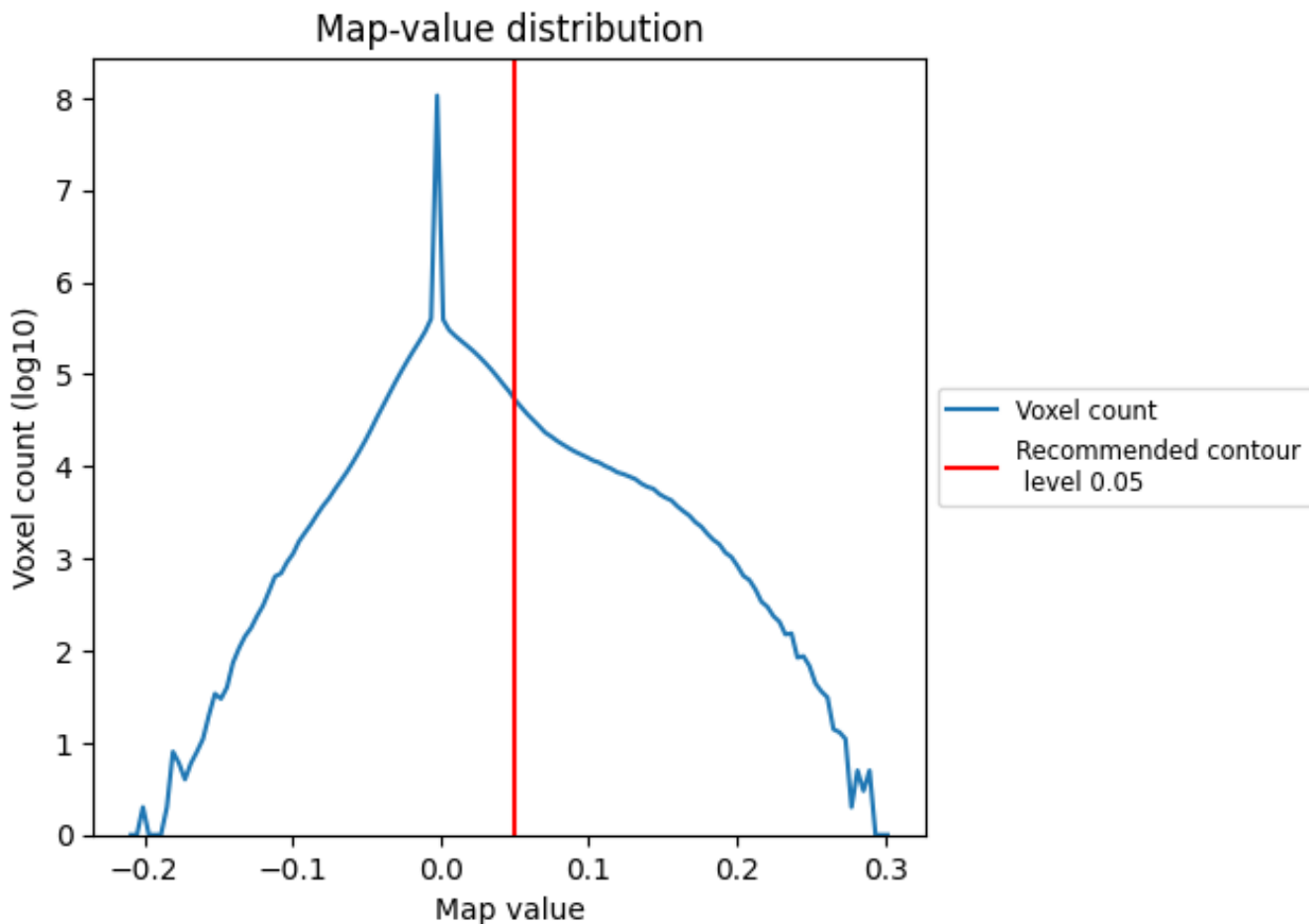


Z

7 Map analysis [i](#)

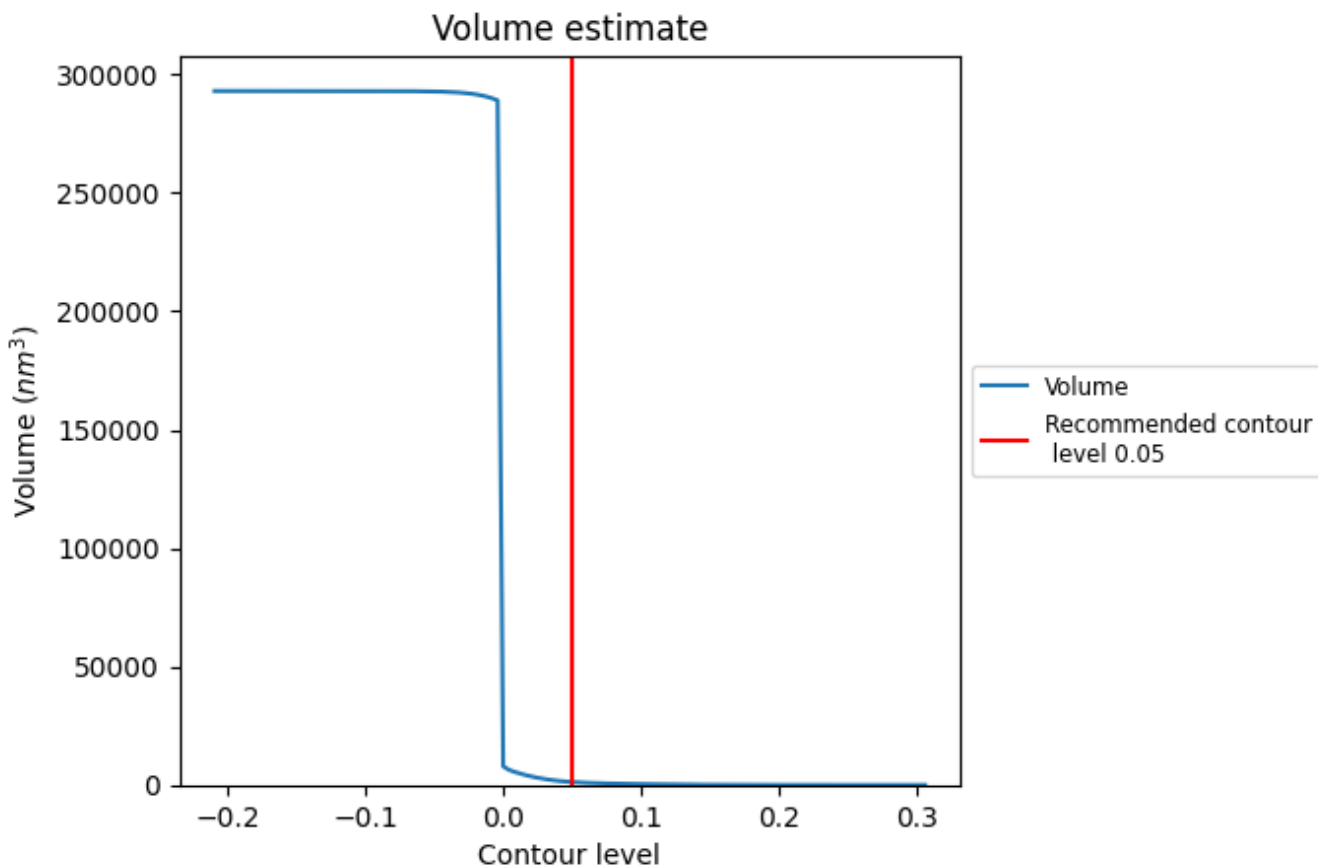
This section contains the results of statistical analysis of the map.

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.

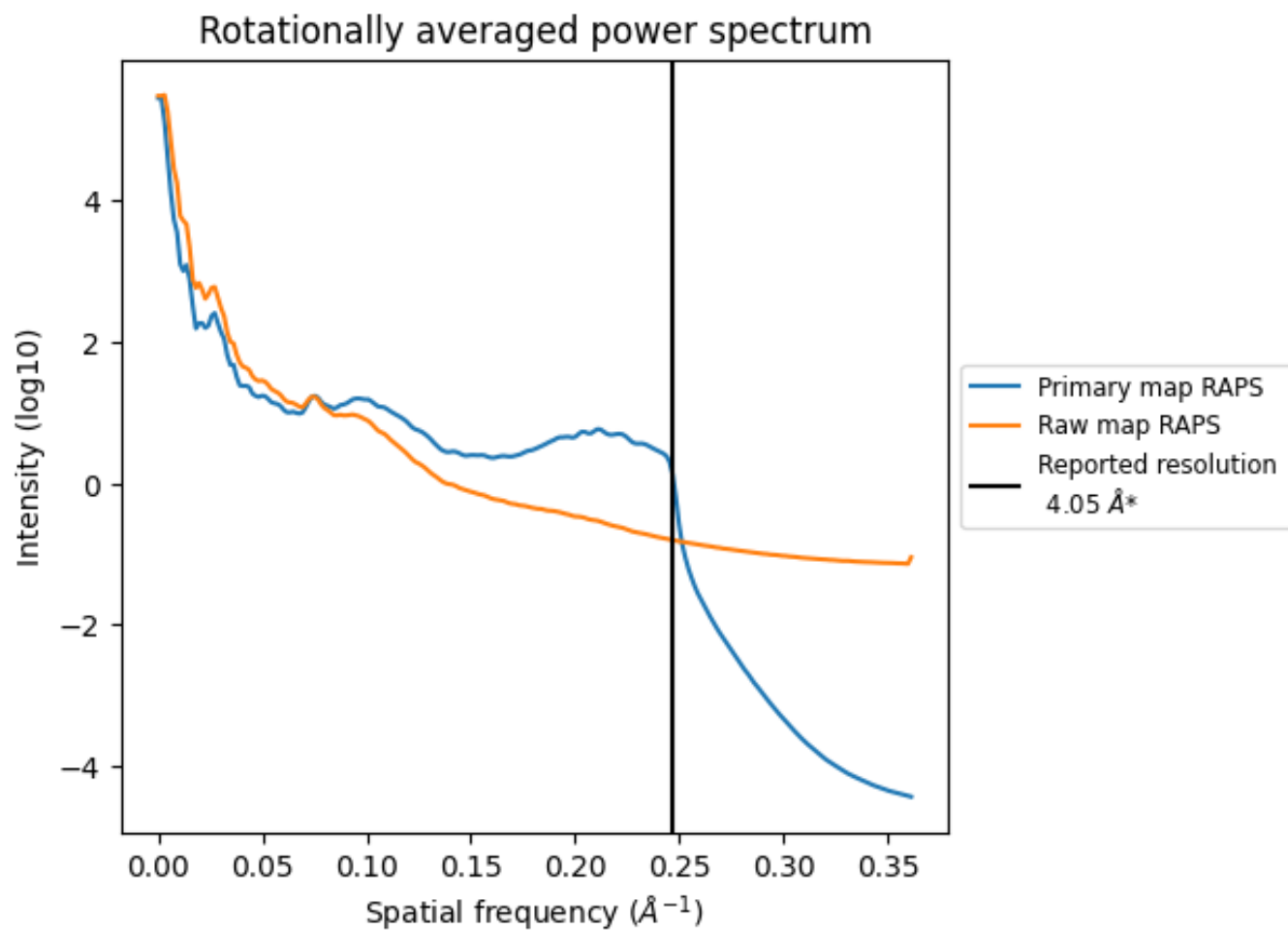
7.2 Volume estimate [\(i\)](#)



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

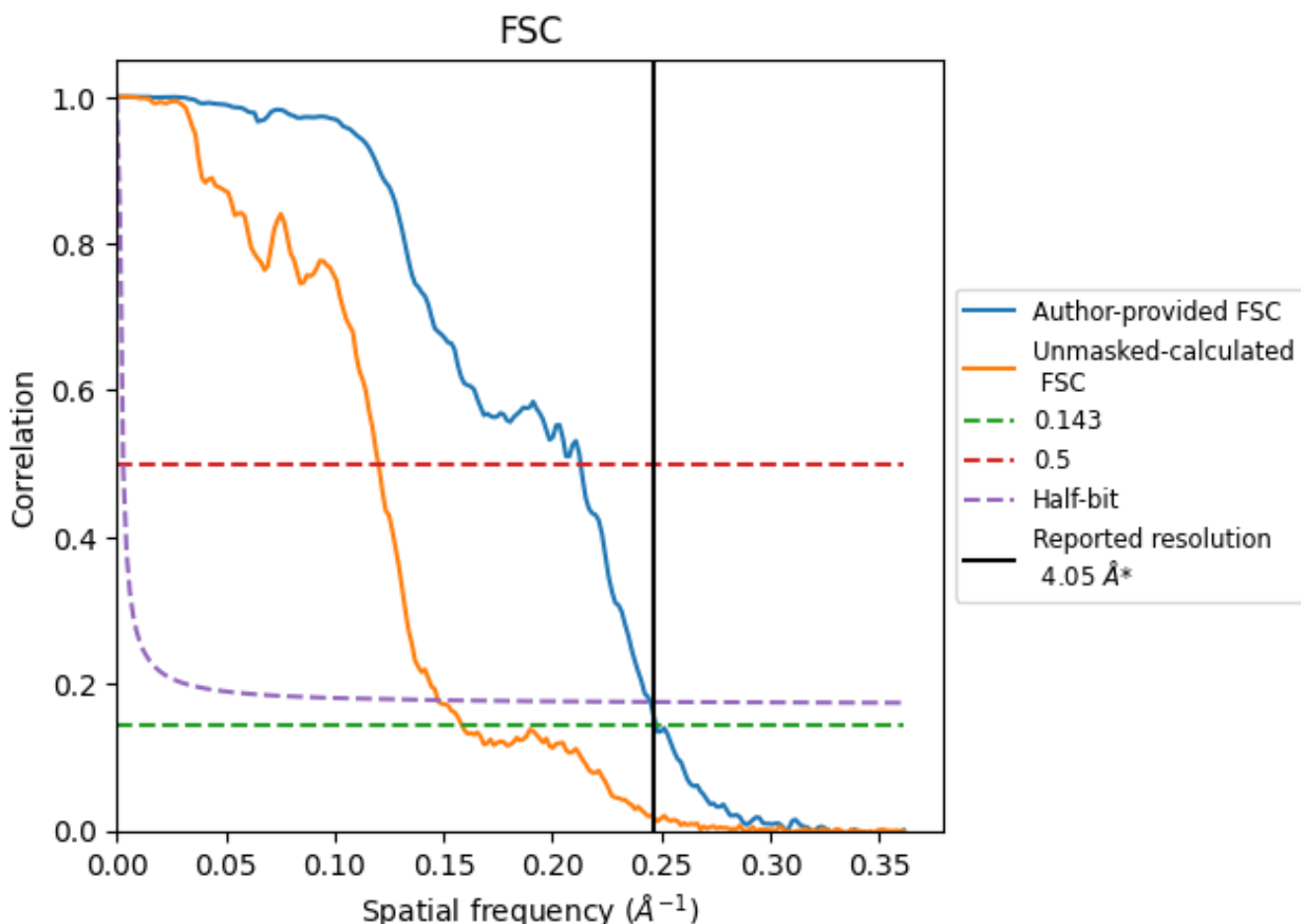


*Reported resolution corresponds to spatial frequency of 0.247 Å⁻¹

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 0.247 Å⁻¹

8.2 Resolution estimates [i](#)

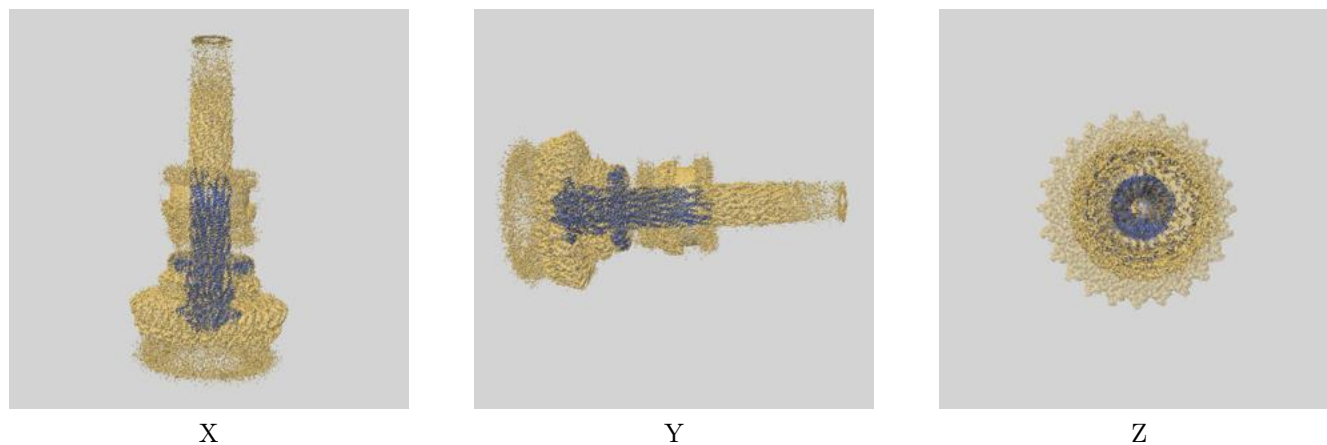
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.05	-	-
Author-provided FSC curve	4.04	4.69	4.08
Unmasked-calculated*	6.31	8.33	6.78

*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](#)

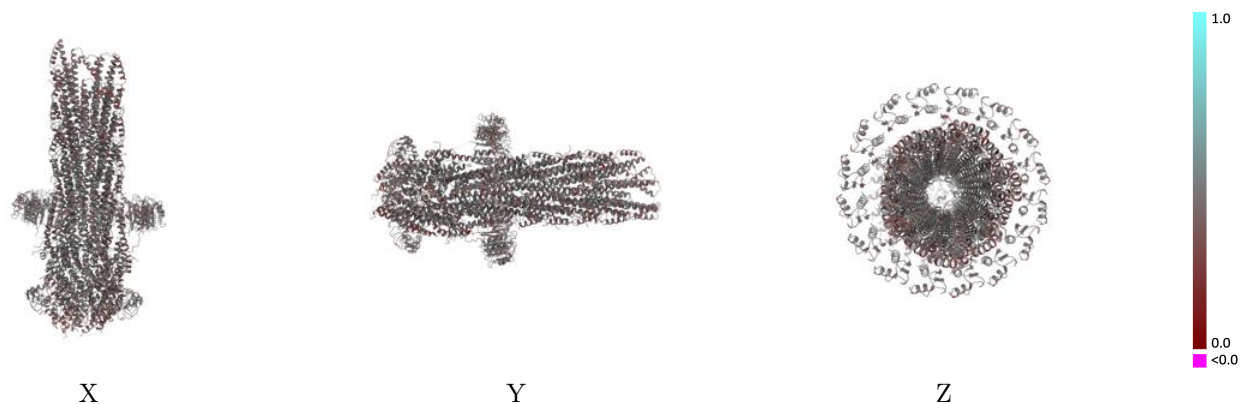
This section contains information regarding the fit between EMDB map EMD-15700 and PDB model 8AXK. Per-residue inclusion information can be found in section [3](#) on page [22](#).

9.1 Map-model overlay [i](#)



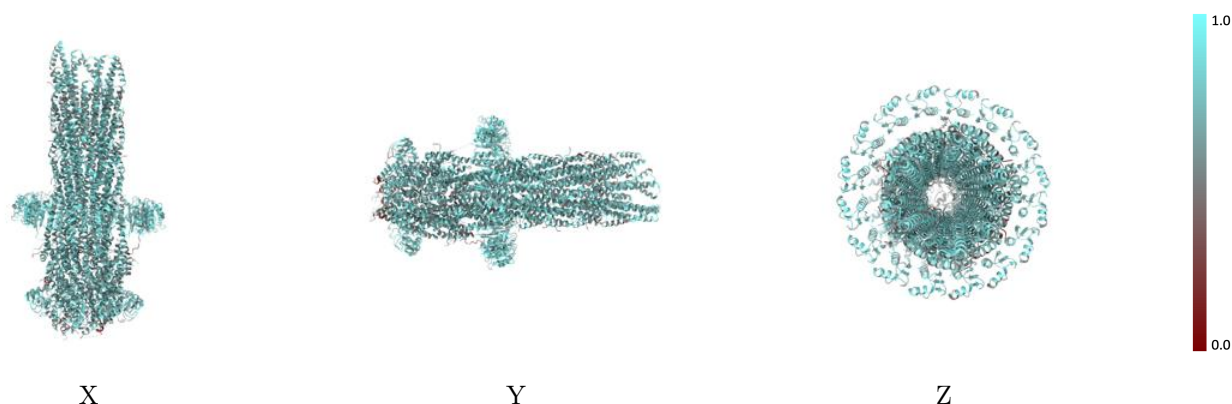
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



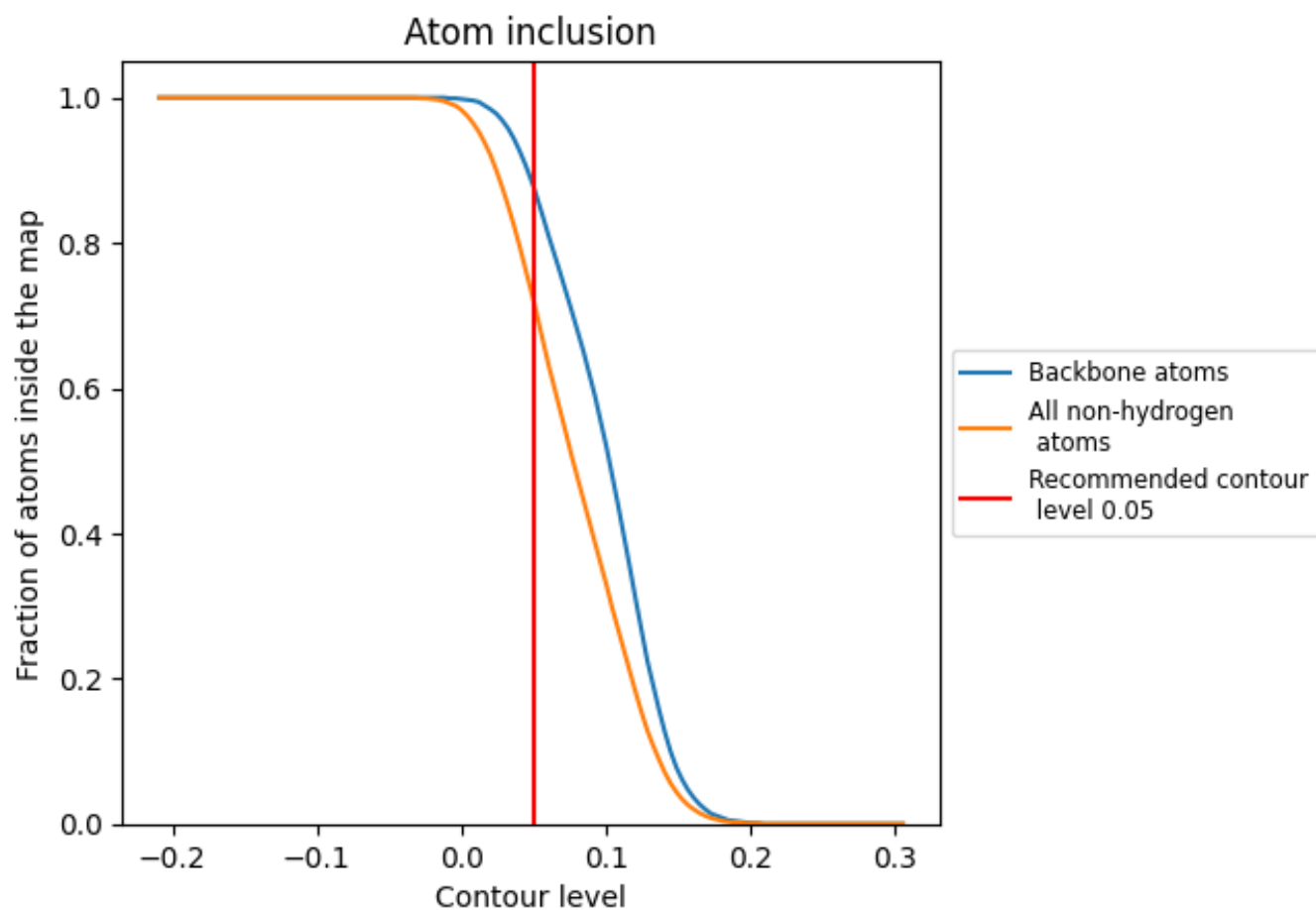
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.4240
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	 0.4300
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