



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

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

A user guide is available at

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

The types of validation reports are described at

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

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

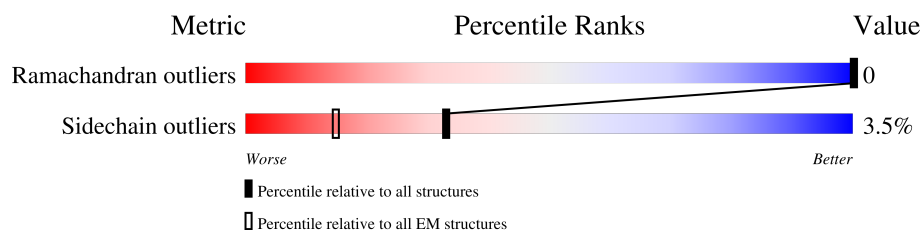
EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) :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



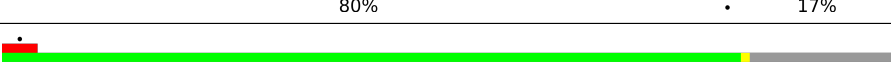
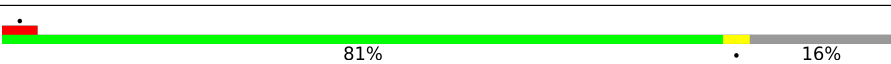


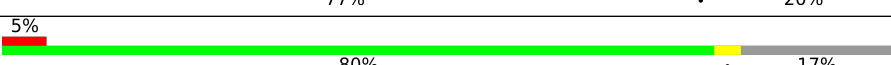

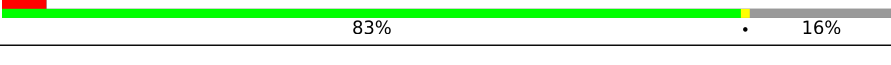


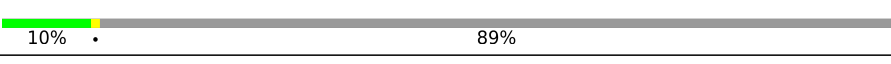

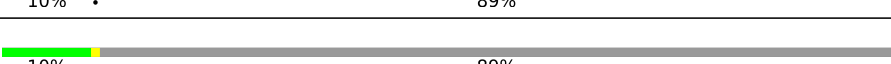









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Mol	Chain	Length	Quality of chain
3	J	86	
4	K	342	
5	M	97	
5	N	97	
5	O	97	
5	P	97	
5	Q	97	
5	R	97	
6	S	98	
6	T	98	
6	U	98	
6	V	98	
6	W	98	
6	a	98	
6	b	98	
6	c	98	
6	d	98	
6	e	98	
6	f	98	
6	g	98	
6	h	98	
6	i	98	
6	j	98	
6	k	98	
6	l	98	
















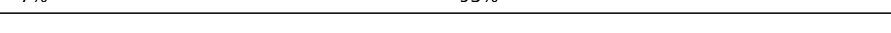
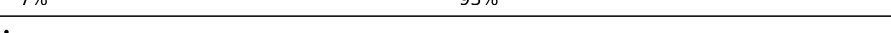
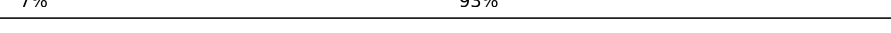
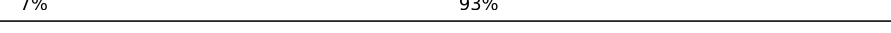
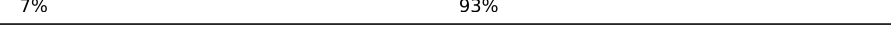
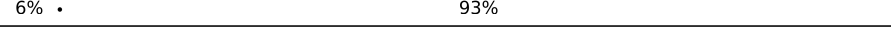
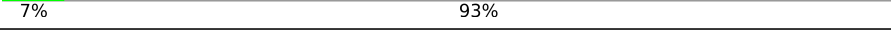

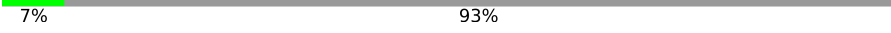

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Mol	Chain	Length	Quality of chain
6	m	98	
6	n	98	
6	o	98	
6	p	98	
6	q	98	
6	r	98	
6	s	98	
6	t	98	
6	u	98	
6	v	98	
6	w	98	
7	0	566	
7	1	566	
7	2	566	
7	3	566	
7	4	566	
7	5	566	
7	6	566	
7	7	566	
7	8	566	
7	9	566	
7	X	566	
7	Y	566	
7	Z	566	
7	x	566	


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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	 7% 93%

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 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
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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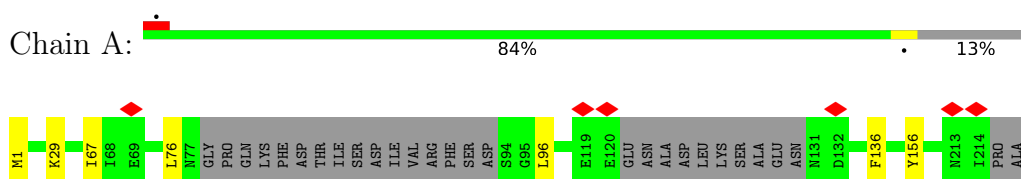
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Mol	Chain	Residues	Atoms				AltConf	Trace
8	e0	17	Total 131	C 82	N 24	O 25	0	0
8	f0	17	Total 131	C 82	N 24	O 25	0	0
8	g0	17	Total 131	C 82	N 24	O 25	0	0
8	h0	17	Total 131	C 82	N 24	O 25	0	0
8	i0	17	Total 131	C 82	N 24	O 25	0	0
8	j0	17	Total 131	C 82	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

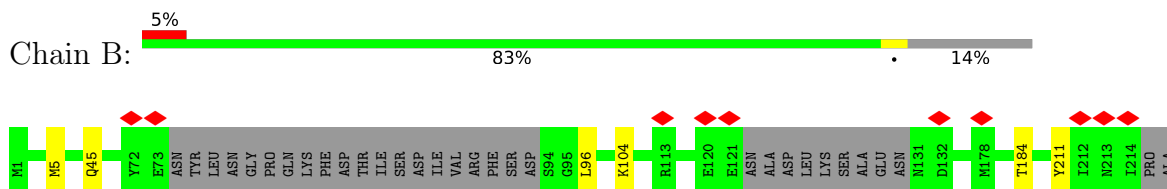
3 Residue-property plots [i](#)

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.

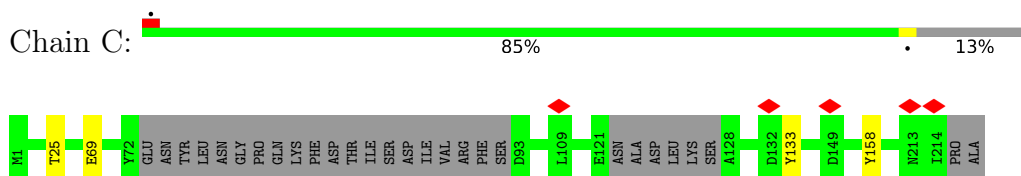
- Molecule 1: Surface presentation of antigens protein SpaP



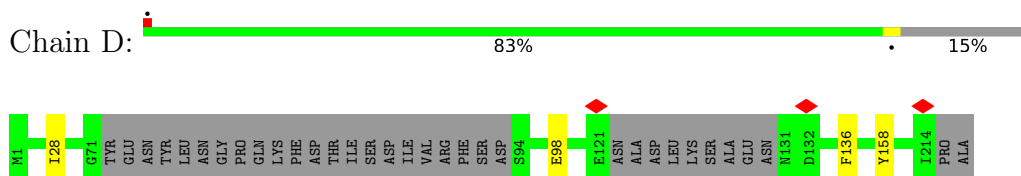
- Molecule 1: Surface presentation of antigens protein SpaP



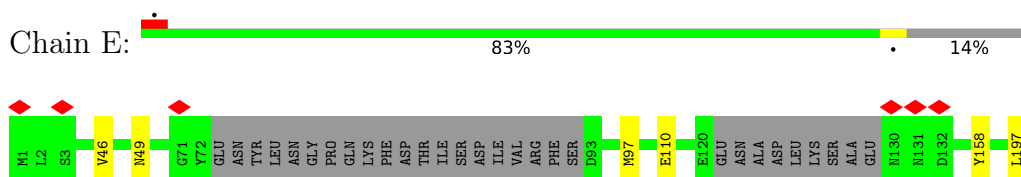
- Molecule 1: Surface presentation of antigens protein SpaP



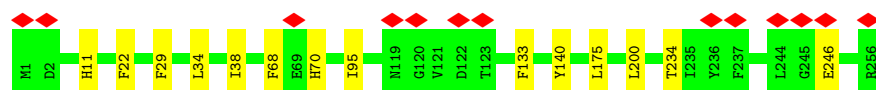
- Molecule 1: Surface presentation of antigens protein SpaP



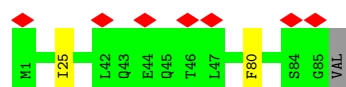
- Molecule 1: Surface presentation of antigens protein SpaP



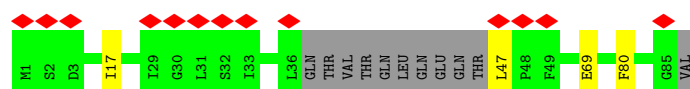
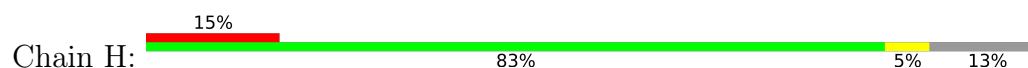
- Molecule 2: Surface presentation of antigens protein SpaR



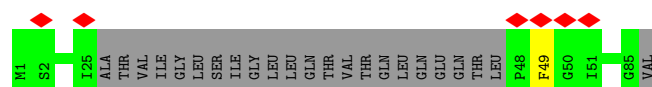
- Molecule 3: Surface presentation of antigens protein SpaQ



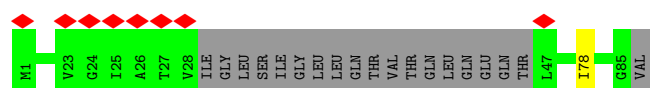
- Molecule 3: Surface presentation of antigens protein SpaQ



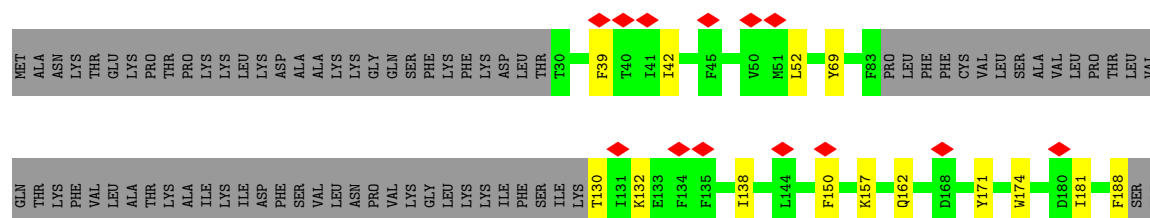
- Molecule 3: Surface presentation of antigens protein SpaQ

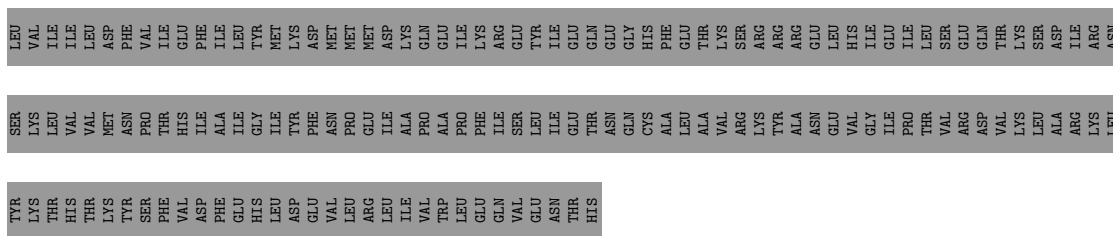


- Molecule 3: Surface presentation of antigens protein SpaQ

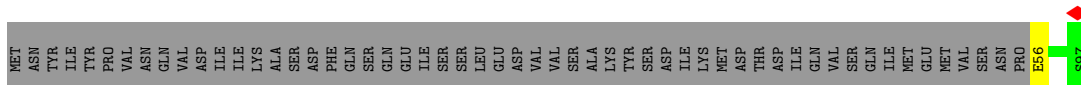


- Molecule 4: Surface presentation of antigens protein SpaS

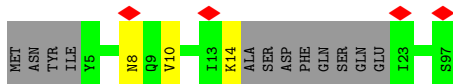
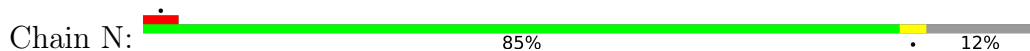




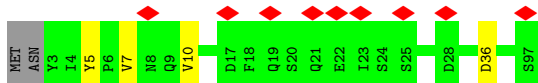
- Molecule 5: Protein MxiI



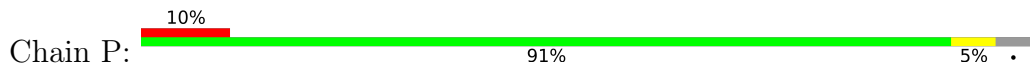
- Molecule 5: Protein MxiI



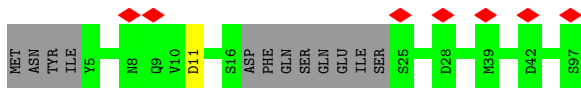
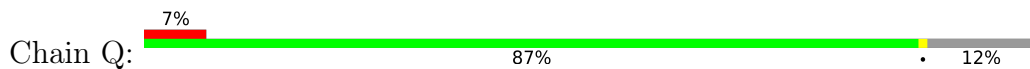
- Molecule 5: Protein MxiI



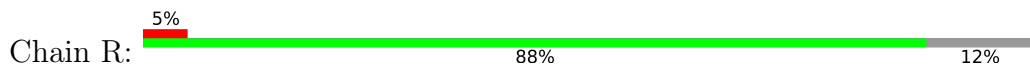
- Molecule 5: Protein MxiI

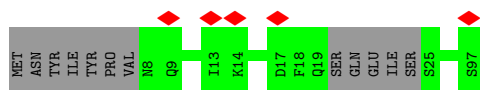


- Molecule 5: Protein MxiI

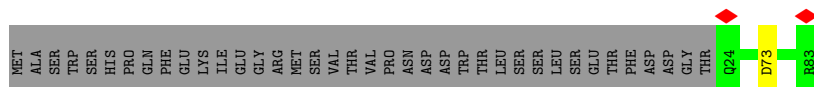


- Molecule 5: Protein MxiI

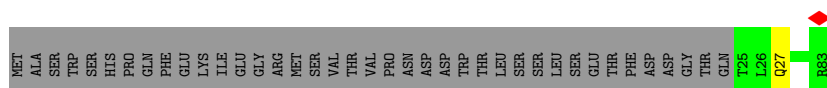




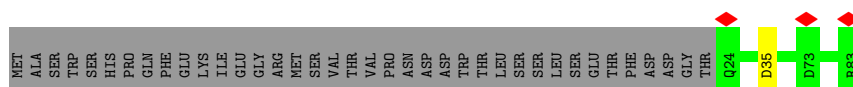
• Molecule 6: Protein MxiH



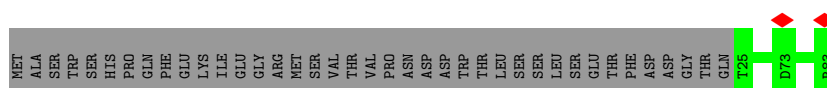
• Molecule 6: Protein MxiH



• Molecule 6: Protein MxiH



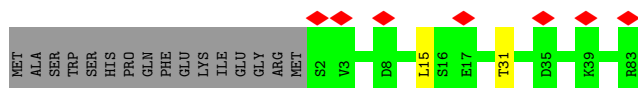
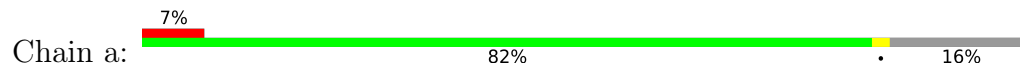
• Molecule 6: Protein MxiH




• Molecule 6: Protein MxiH

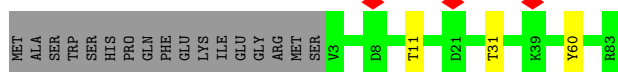


• Molecule 6: Protein MxiH




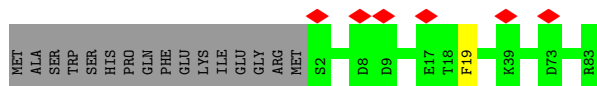
• Molecule 6: Protein MxiH

Chain b:  80% 17%




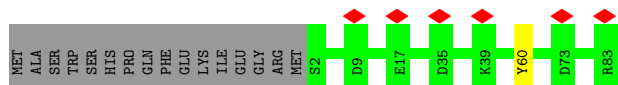
• Molecule 6: Protein MxiH

Chain c:  83% 16%




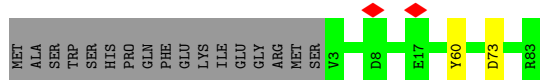
• Molecule 6: Protein MxiH

Chain d:  83% 16%




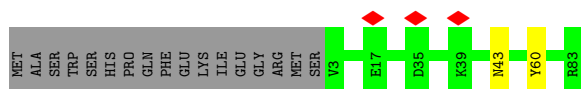
• Molecule 6: Protein MxiH

Chain e:  81% 17%




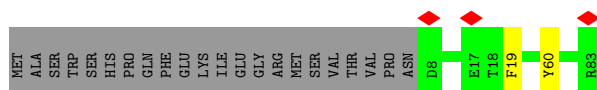
• Molecule 6: Protein MxiH

Chain f:  81% 17%



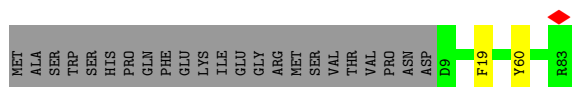
• Molecule 6: Protein MxiH

Chain g:  76% 22%



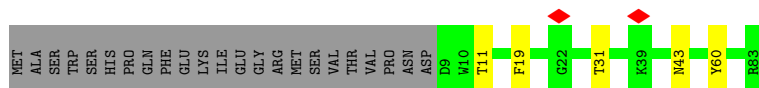
• Molecule 6: Protein MxiH

Chain h:  74% 23%




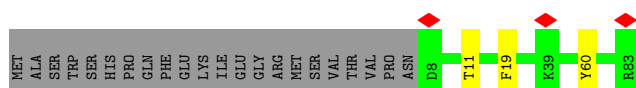
• Molecule 6: Protein MxiH

Chain i:  71% 5% 23%



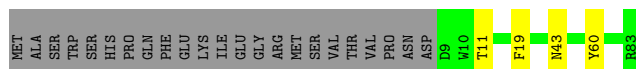
• Molecule 6: Protein MxiH

Chain j:  74% 0% 22%




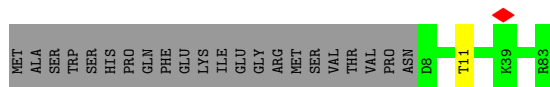
• Molecule 6: Protein MxiH

Chain k:  72% 0% 23%




• Molecule 6: Protein MxiH

Chain l:  77% 0% 22%




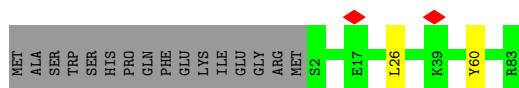
• Molecule 6: Protein MxiH

Chain m:  6% 83% 16%




• Molecule 6: Protein MxiH

Chain n:  82% 0% 16%




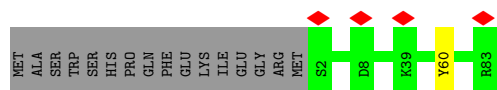
• Molecule 6: Protein MxiH

Chain o:  80% 0% 17%




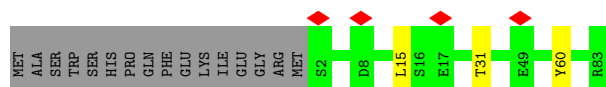
- Molecule 6: Protein MxiH

Chain p:  83% 16%




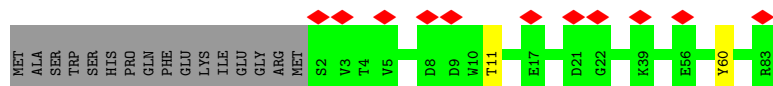
- Molecule 6: Protein MxiH

Chain q:  81% 16%




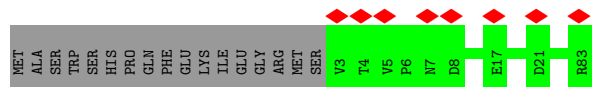
- Molecule 6: Protein MxiH

Chain r:  11% 82% 16%




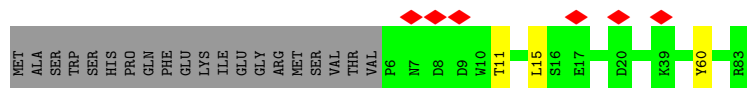
- Molecule 6: Protein MxiH

Chain s:  8% 83% 17%




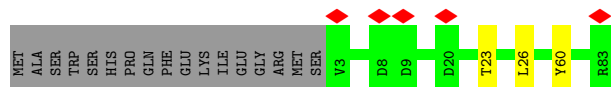
- Molecule 6: Protein MxiH

Chain t:  6% 77% 20%




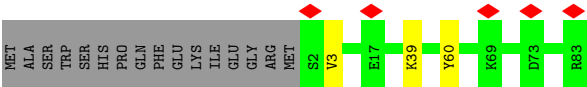
- Molecule 6: Protein MxiH

Chain u:  5% 80% 17%

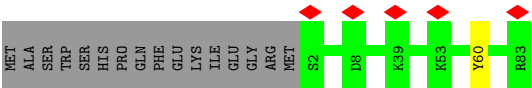
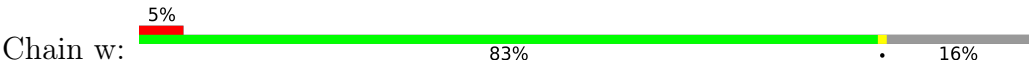


- Molecule 6: Protein MxiH

Chain v:  5% 81% 16%



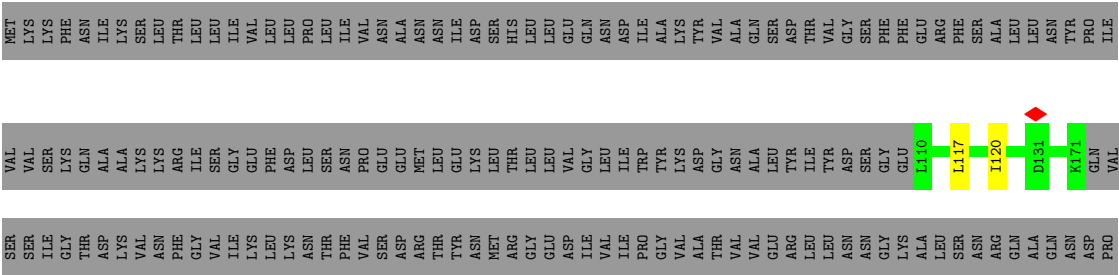
● Molecule 6: Protein MxiH



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

- Molecule 7: Outer membrane protein MxiD

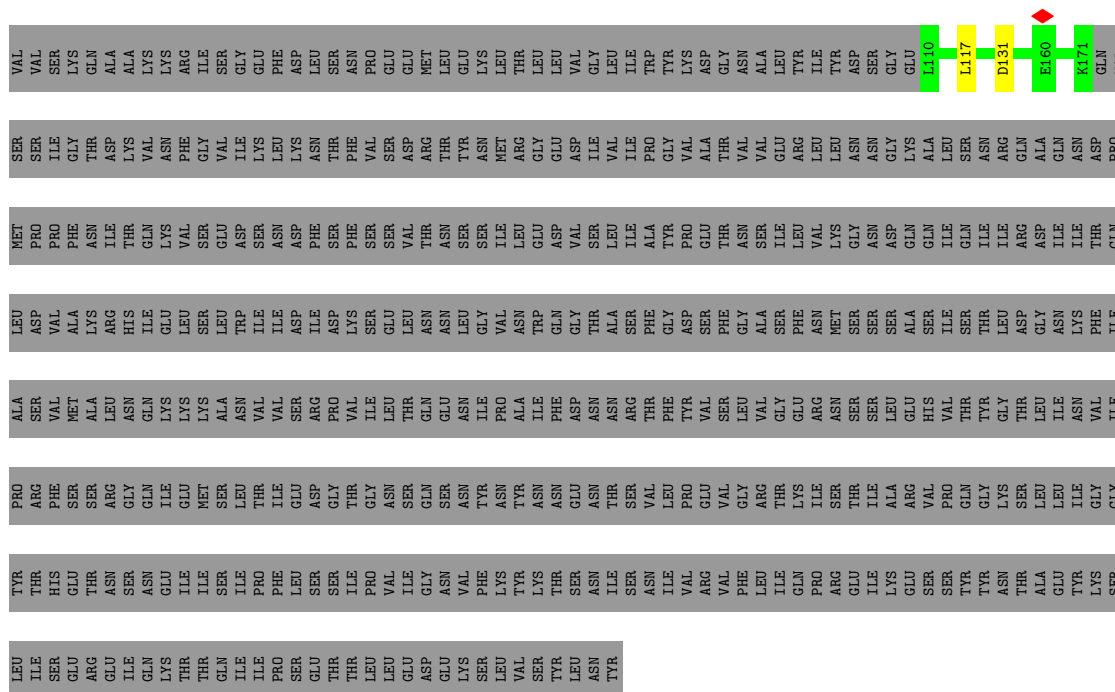
Chain 2:  11% 89%

[illegible]

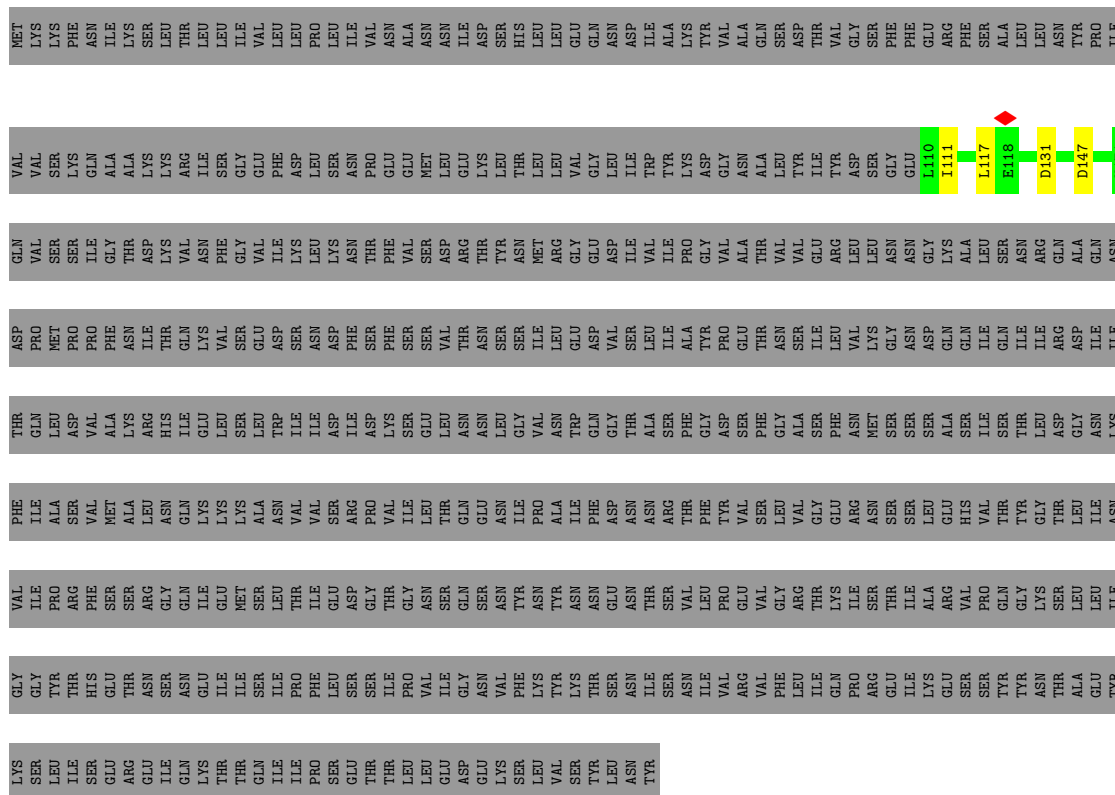
- Molecule 7: Outer membrane protein MxiD

Chain 4: 11% 89%

[illegible]



- Molecule 7: Outer membrane protein MxiD



- Molecule 7: Outer membrane protein MxiD

[illegible]

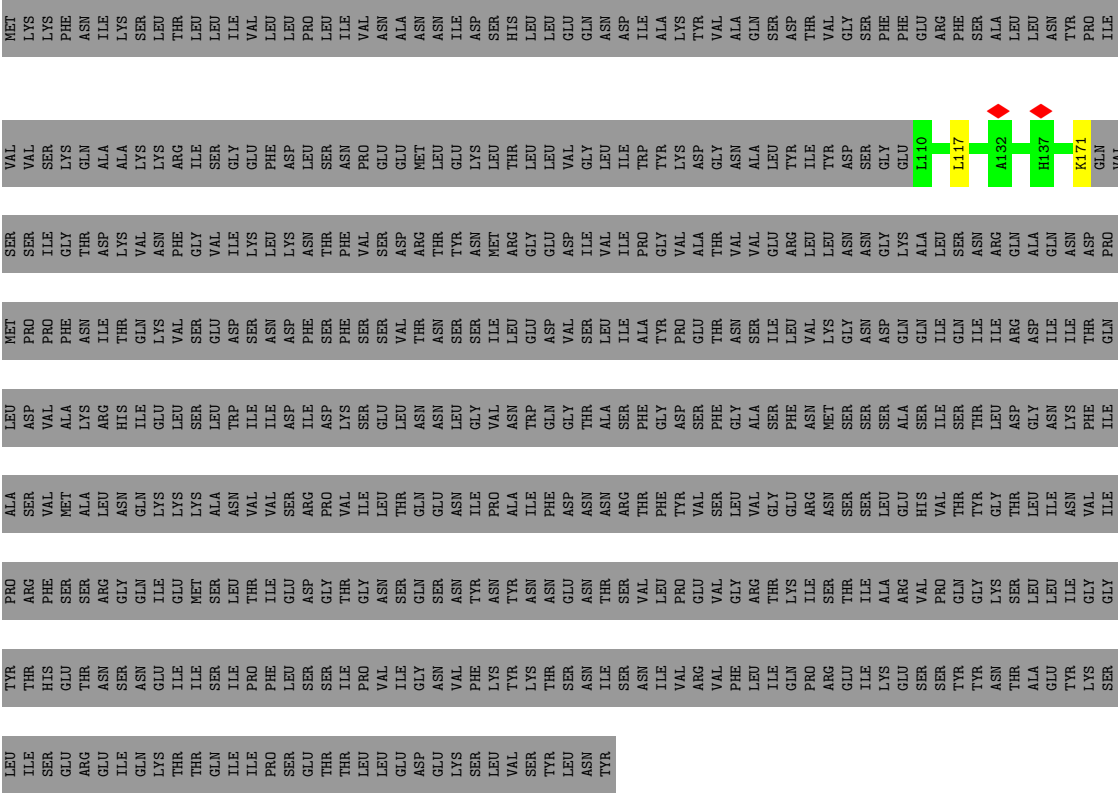
Chain x: 10% . 89%

HIS	PHE	VAL	VAL	PRO	TLE	VAL	MET
GLU	SER	MET	ALA	PHE	GLY	VAL	LYS
THR	SER	ALA	LYS	ASN	THR	SER	LYS
ASN	ARG	LEU	ARG	ILE	ASP	LYS	PHE
SER	GLY	ASN	HIS	THR	LYS	GLN	ASN
ASN	GLN	GLN	ILE	GLN	VAL	ALA	ILE
GLU	ILE	LYS	GLU	LYS	ASN	ALA	LYS
ILE	GLU	LYS	LEU	VAL	PHE	LYS	SER
ILE	MET	LYS	SER	SER	GLY	ARG	THR
SER	SER	ALA	LEU	GLU	VAL	ARG	LEU
ILE	LEU	ASN	THR	ASP	ILE	SER	LEU
PRO	THR	VAL	ILE	SER	LYS	ILE	LEU
PHE	ILE	VAL	ILE	ASN	GLY	ILE	ILE
LEU	GLU	SER	ASP	ASP	GLU	GLU	VAL
SER	GLY	PRO	ILE	PHE	THR	ASN	LEU
ILE	THR	VAL	LYS	PHE	PHE	LEU	PRO
PRO	GLY	ILE	SER	SER	VAL	SER	LEU
VAL	ASN	LEU	GLU	SER	SER	ASN	ILE
ILE	SER	THR	LEU	VAL	SER	ASN	VAL
GLY	GLN	GLN	ASN	THR	ARG	GLU	ASN
GLN	SER	GLU	ASN	ASN	THR	GLU	ALA
VAL	ASN	ASN	ILE	SER	TYR	MET	ALA
PHE	TYR	ILE	GLY	SER	ASN	LEU	ASN
LYS	ASN	PRO	VAL	ILE	MET	GLU	ASN
LYS	ASN	ALA	ASN	LEU	ARG	LEU	VAL
THR	ASN	PHE	THR	GLU	GLY	LEU	SER
SER	GLU	ASN	GLY	VAL	ASP	LEU	HIS
ASN	ASN	ASN	THR	SER	ASP	LEU	LEU
ILE	THR	ASN	ALA	ILE	ILE	VAL	GLN
ASN	SER	ARG	SER	ILE	ILE	GLN	GLN
ASN	VAL	PHE	LEU	GLY	GLY	ASP	TYR
ILE	LEU	THR	VAL	ILE	ILE	GLY	ASN
VAL	THR	TYR	GLY	PRO	VAL	TRP	ILE
ARG	GLU	VAL	SER	GLU	ALA	TYR	ALA
VAL	VAL	SER	PHE	THR	THR	LYS	LYS
PHE	GLY	LEU	GLY	ASN	VAL	ASP	TYR
LEU	ARG	VAL	ALA	SER	VAL	GLY	VAL
ILE	THR	GLY	SER	ILE	ARG	ASN	ALA
GLN	LYS	GLU	PHE	LEU	GLY	ALA	GLN
PRO	ILE	ARG	ASN	VAL	LEU	LEU	SER
ARG	SER	ASN	MET	LYS	LEU	TYR	ASP
GLU	THR	SER	SER	GLY	ASN	ILE	THR
LYS	ILE	SER	SER	ASN	GLY	ASP	VAL
ILE	ALA	LEU	SER	ASP	LYS	SER	GLY
GLU	ARG	GLU	ALA	GLN	ALA	GLY	PHE
SER	VAL	HIS	SER	GLN	ALA	GLY	THR
SER	PRO	VAL	ILE	ILE	LEU	GLU	PHE
TYR	GLN	THR	SER	GLN	SER	GLU	THR
TYR	GLY	TYR	THR	ILE	ASN	GLU	ARG
ASN	THR	GLY	GLY	ILE	ARG	PHE	ASN
ALA	LEU	THR	THR	ASP	ALA	+	SER
GLU	LEU	ILE	ASN	ILE	GLN	L110	ALA
LYS	GLY	VAL	ILE	ASP	ILE	L117	LEU
THR	ILE	ASN	GLY	ASP	GLN	+	LEU
ASN	GLY	LEU	GLY	ASP	ALA	H137	ASN
LYS	THR	ILE	ASN	ILE	GLN	K171	THR
SER	GLY	VAL	PHE	THR	ASP	GLN	TYR
LEU	GLY	ILE	ILE	GLN	MET	VAL	PRO
THR	TYR	ARG	SER	LEU	THR	SER	THR

SER
GLU
ARG
GLU
ILE
GLN
LYS
THR
THR
GLN
ILE
ILE
PRO
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TYR

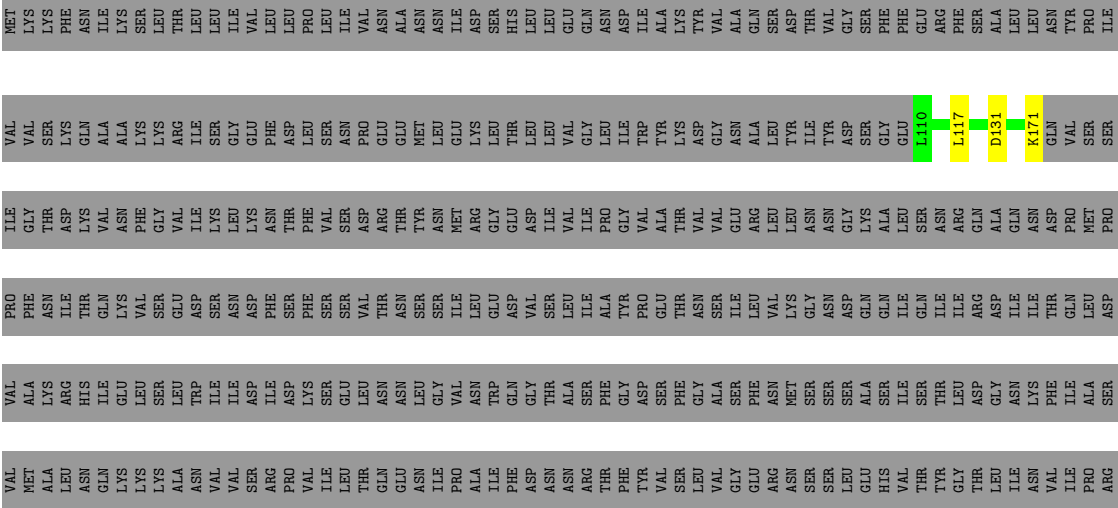
● Molecule 7: Outer membrane protein MxiD

Chain y: 11% 89%



● Molecule 7: Outer membrane protein MxiD

Chain z: 10% 89%



[illegible]

- Molecule 7: Outer membrane protein MxiD

Chain 5:  10% . 89%

LEU	TYR	PRO	ALA	LEU	MET	SER	VAL	MET
ILE	HIS	ARG	SER	ASP	PRO	SER	VAL	LYS
SER	HIS	PHE	VAL	VAL	PRO	SER	SER	LYS
GLU	GLU	SER	MET	ALA	PHE	GLY	LYS	PHE
ARG	THR	SER	ASN	LYS	ASN	THR	GLN	ASN
GLU	ASN	ARG	LEU	ARG	ILE	ASP	ALA	ILE
ILE	SER	GLY	ASN	HIS	THR	LYS	ALA	LYS
GLN	ASN	GLN	GLN	ILE	GLN	VAL	LYS	SER
THR	GLU	ILE	LYS	GLU	VAL	PHE	ARG	THR
THR	ILE	MET	LYS	SER	LYS	GLY	ILE	LEU
GLN	SER	SER	ALA	LEU	GLU	VAL	SER	LEU
ILE	ILE	LEU	ASN	TRP	ASP	ILE	GLY	ILE
ILE	PRO	THR	VAL	ILE	SER	ILE	PHE	VAL
PRO	PHE	ILE	VAL	ILE	ASN	LEU	PHE	LEU
SER	LEU	GLU	SER	ASP	ASP	LYS	ASP	VAL
GLU	SER	ASP	ARG	ILE	PHE	ASN	LEU	PRO
THR	SER	GLY	PRO	ASP	SER	THR	SER	LEU
THR	ILE	THR	VAL	LYS	PHE	PHE	ASN	ILE
LEU	PRO	GLY	ILE	SER	SER	VAL	PRO	VAL
LEU	VAL	ASN	LEU	GLU	SER	SER	GLU	ASN
GLU	ILE	SER	THR	LEU	VAL	ASP	GLU	ALA
ASP	GLY	GLN	GLN	ASN	THR	ARG	MET	ASN
GLU	ASN	SER	GLU	ASN	ASN	THR	LEU	ASN
LYS	VAL	ASN	ASN	LEU	SER	TYR	GLU	ILE
SER	PHE	TYR	ILE	GLY	SER	ASN	LYS	ASP
LEU	LYS	ASN	PRO	VAL	ILE	MET	LEU	SER
VAL	TYR	TYR	ALA	ASN	LEU	ARG	THR	HIS
SER	ASN	ASN	ILE	TRP	GLU	GLY	LEU	LEU
TYR	THR	ASN	PHE	GLN	ASP	GLU	LEU	LEU
LEU	SER	GLU	ASP	GLY	VAL	ASP	VAL	GLN
ASN	ASN	ASN	ASN	THR	SER	ILE	GLY	ASN
TYR	ILE	THR	ARG	SER	ILE	ILE	ILE	ILE
LYS	ASN	VAL	THR	PHE	ALA	PRO	TRP	ILE
VAL	ILE	LEU	PHE	GLY	TYR	GLY	TYR	ALA
ARG	VAL	GLU	VAL	SER	PRO	VAL	LYS	TYR
VAL	VAL	VAL	SER	PHE	GLU	ALA	GLY	VAL
PHE	PHE	GLY	GLY	GLY	ASN	VAL	ASN	ASN
LEU	LEU	ARG	VAL	ALA	SER	VAL	ALA	GLN
ILE	THR	THR	GLY	SER	ILE	GLU	LEU	SER
GLN	PRO	LYS	GLU	PHE	LEU	ARG	TYR	ASP
PRO	ILE	ILE	ASN	ASN	ASN	LYS	GLY	ASP
ARG	THR	ILE	VAL	SER	GLN	ALA	GLU	PHE
LYS	TYR	ILE	SER	SER	GLN	THR	PHE	SER
LEU	TYR	THR	THR	THR	ILE	ASN	ASN	PHE
ALA	ASN	LYS	GLY	LEU	ILE	ARG	ALA	ALA
GLU	THR	SER	THR	ASP	ASP	GLN	GLY	LEU
TYR	ASN	ARG	LEU	SER	ASN	LYS	GLU	ASN
ASN	GLU	VAL	HIS	SER	GLN	ALA	L110	ARG
TYR	TYR	PRO	VAL	SER	ILE	LEU	L117	PHE
LYS	GLY	GLN	THR	SER	GLN	SER	D131	SER
GLY	ASN	LYS	GLY	LEU	ILE	ARG	H137	ALA
THR	ASN	THR	THR	ASP	ILE	GLN	K171	LEU
ALA	THR	LYS	THR	GLY	ILE	ASN	K171	ASN
GLU	ASN	LEU	THR	ASN	ILE	ARG	GLN	TYR
ASN	ALA	LEU	THR	GLY	ASP	ALA	ASP	PRO
TYR	SER	GLY	ILE	PHE	THR	THR	ASN	THR

- Molecule 7: Outer membrane protein MxiD

Chain 7:  10% . 89%

[illegible]

[illegible]

- Molecule 7: Outer membrane protein MxiD

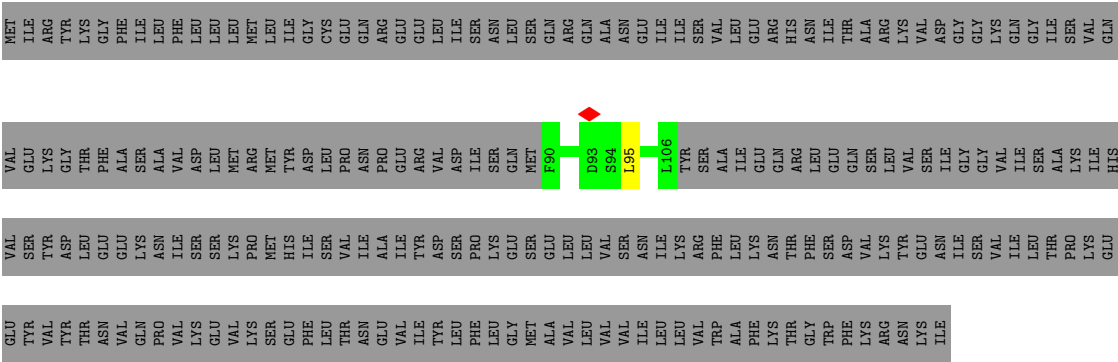
Chain 9:  11% 89%

ARG	GLU	ILE	GLN	LYS	THR	SER	ALA	LYS	ASN	THR	VAL	MET
GLU	ILE	GLN	LYS	THR	THR	ARG	LEU	ARG	ILE	ASP	VAL	LYS
ILE	ILE	GLN	LYS	THR	ILE	ILE	GLN	ILE	GLM	VAL	VAL	PHE
LYS	THR	ILE	THR	ILE	GLU	GLU	LYS	LEU	VAL	PHE	ALA	ILE
THR	THR	ILE	THR	ILE	MET	LYS	LYS	SER	SER	GLY	ALA	LYS
GLN	GLN	SER	SER	SER	THR	ASP	ALA	LEU	GLU	VAL	ALA	SER
ILE	ILE	ILE	ILE	PRO	LEU	THR	VAL	THR	ASP	ILE	LYS	THR
PRO	PRO	PRO	PRO	PHE	ILE	ILE	VAL	ILE	ASN	LEU	ILE	LEU
SER	SER	SER	SER	LEU	GLU	GLU	SER	ASP	ASP	LYS	SER	LEU
GLU	GLU	THR	THR	SER	ASP	ARG	ARG	ILE	PHE	ASN	GLY	ILE
THR	THR	THR	THR	ILE	GLY	PRO	PRO	ASP	SER	THR	GLU	VAL
LYS	LYS	LYS	LYS	PRO	GLN	ILE	VAL	LYS	PHE	LYS	ARG	THR
LEU	LEU	LEU	LEU	VAL	ASN	LEU	LEU	SER	SER	VAL	ASP	PRO
LEU	LEU	VAL	VAL	ILE	SER	THR	THR	LEU	VAL	ASP	SER	LEU
GLU	GLU	GLY	GLN	GLY	GLN	GLN	GLN	ASN	THR	ARG	ASN	ILE
ASP	GLU	ASN	GLU	ASN	SER	GLU	GLU	ASN	THR	ARG	PRO	VAL
GLU	LYS	PHE	VAL	PHE	ASN	ASN	ASN	GLY	SER	TYR	GLU	ALA
SER	SER	SER	SER	VAL	LYS	ASN	PRO	VAL	ILE	MET	MET	ASN
VAL	VAL	VAL	VAL	TYR	THR	THR	ALA	ASN	LEU	ARG	LEU	ASN
SER	SER	LYS	ASN	LYS	ASN	ASN	ILE	THR	GLU	GLY	GLU	ILE
TYR	TYR	THR	THR	THR	THR	ASN	PHE	GLN	ASP	GLU	VAL	GLU
ASN	ASN	ASN	ASN	ILE	THR	THR	ASN	ALA	SER	ILE	ILE	ASN
TYR	TYR	VAL	ARG	VAL	SER	VAL	ARG	THR	PHE	PRO	TRP	ILE
				PHE	GLY	GLY	LEU	GLY	ASN	VAL	TYR	LYS
				LEU	ARG	ARG	VAL	VAL	SER	VAL	LYS	ALA
				ILE	THR	THR	GLY	SER	ILE	GLU	ASP	TYR
				GLN	LYS	LYS	GLU	PHE	LEU	ARG	GLY	VAL
				PRO	ILE	ILE	ARG	ASN	VAL	LEU	ASN	ALA
				ARG	SER	SER	ASN	MET	LYS	LEU	ALA	GLN
				GLU	THR	THR	SER	SER	GLY	ASN	LEU	SER
				ILE	ILE	ILE	SER	SER	ASN	ASN	TYR	ASP
				GLU	THR	THR	LEU	ALA	ASP	GLY	ILE	THR
				LYS	GLY	GLY	GLY	ALA	ILE	THR	VAL	GLN
				THR	THR	THR	THR	GLU	ASN	GLY	THR	VAL
				SER	PRO	PRO	VAL	ILE	ILE	LEU	ASP	GLY
				TYR	GLN	GLN	THR	SER	GLN	SER	GLY	PHE
				TYR	GLY	GLY	TYR	THR	ILE	ASN	GLU	PHE
				ASN	LYS	LYS	GLY	LEU	ILE	ARG	L110	GLU
				ALA	LEU	LEU	ILE	GLY	ASP	GLN	L117	ARG
				TYR	GLU	GLU	ILE	ASN	ILE	GLN	L171	SER
				LYS	ILE	ILE	ASN	LYS	ILE	ASN	L171	ALA
				THR	GLY	VAL	VAL	PHE	THR	ASP	GLN	LEU
				LEU	ILE	ILE	ILE	ILE	GLM	PRO	VAL	LEU
				ILE	TYR	PRO	PRO	ALA	LEU	MET	SER	ASN
				THR	THR	ARG	ARG	SER	ASP	PRO	TYR	ASN
				GLU	THR	PHE	PHE	VAL	VAL	PRO	ILE	THR

- Molecule 8: Lipoprotein MxiJ

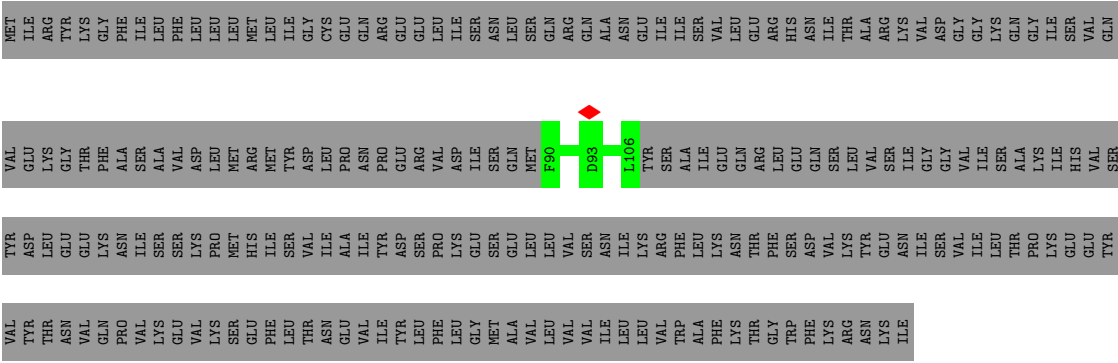
Chain a0: 7% 93%

[illegible]



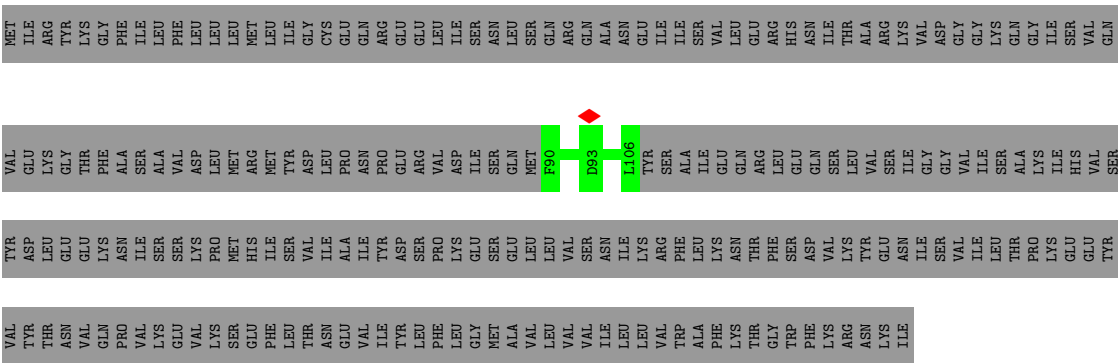
● Molecule 8: Lipoprotein MxiJ

Chain f0: 7% 93%



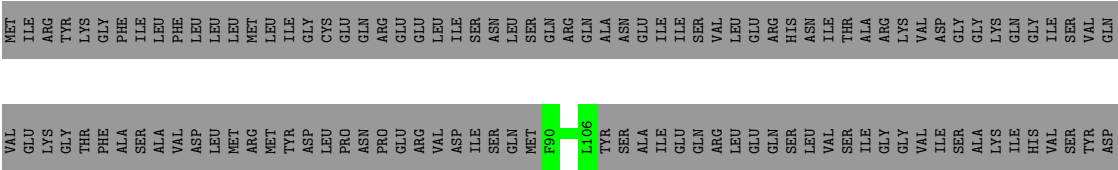
● Molecule 8: Lipoprotein MxiJ

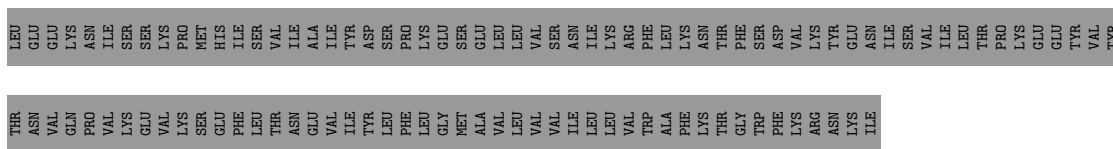
Chain g0: 7% 93%



● Molecule 8: Lipoprotein MxiJ

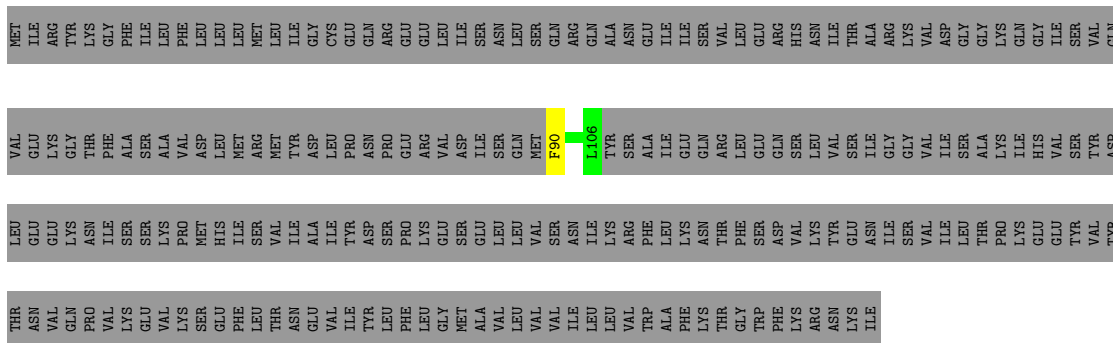
Chain h0: 7% 93%





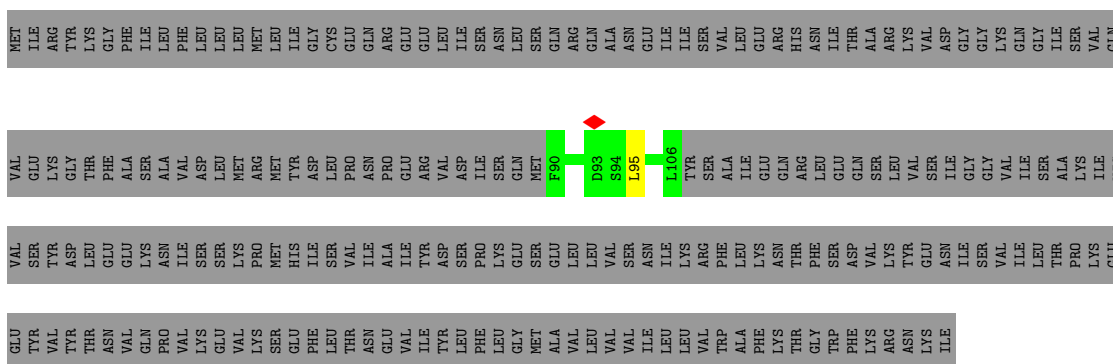
- Molecule 8: Lipoprotein MxiJ

Chain i0: 7% 93%



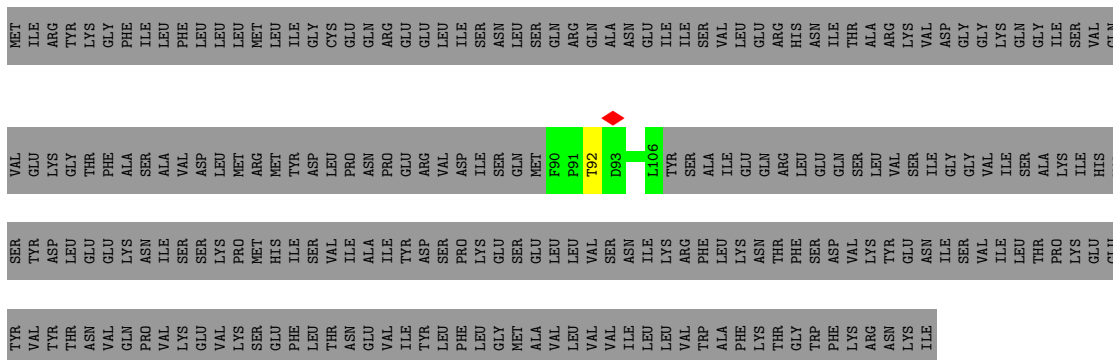
- Molecule 8: Lipoprotein MxiJ

Chain j0: 7% 93%

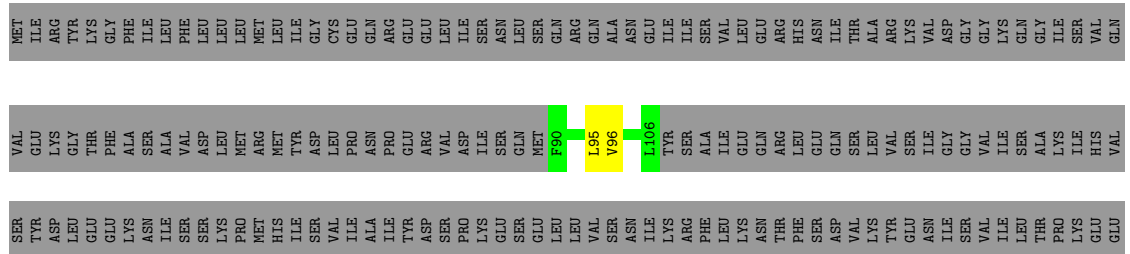


- Molecule 8: Lipoprotein MxiJ

Chain k0: 7% 93%



- Molecule 8: Lipoprotein MxiJ

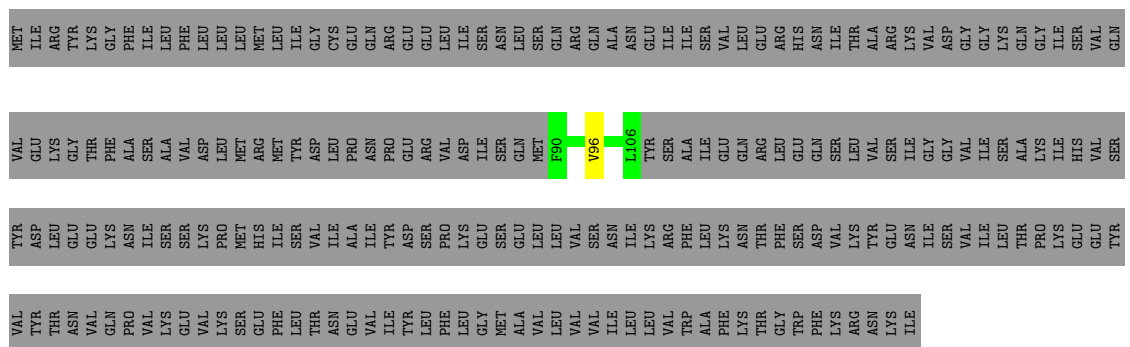


- Molecule 8: Lipoprotein MxiJ

Chain w0:  7% 93%

- Molecule 8: Lipoprotein MxiJ

Chain x0:  7% 93%



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

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.26	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

5 of 177 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	7	171	LYS
6	k	43	ASN
6	a	31	THR
6	g	60	TYR
6	o	60	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
6	i	43	ASN

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Mol	Chain	Res	Type
6	m	64	GLN
6	l	43	ASN
6	n	40	ASN
2	F	163	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

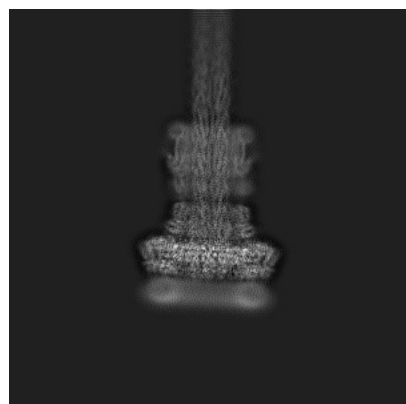
6 Map visualisation [i](#)

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

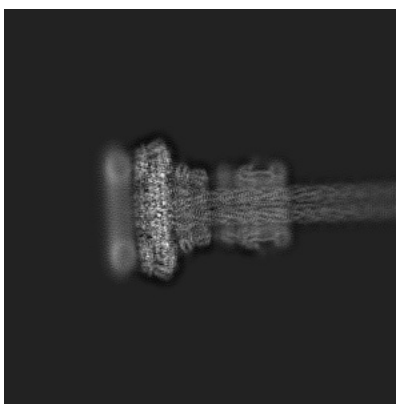
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

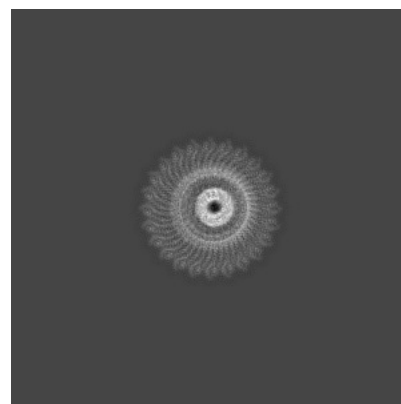
6.1.1 Primary map



X

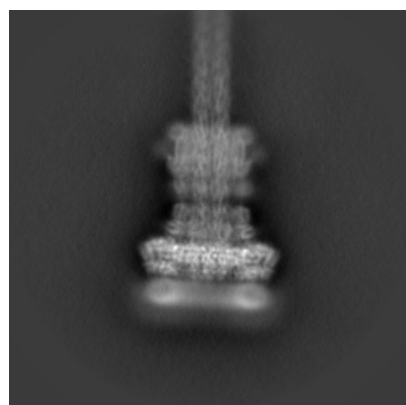


Y

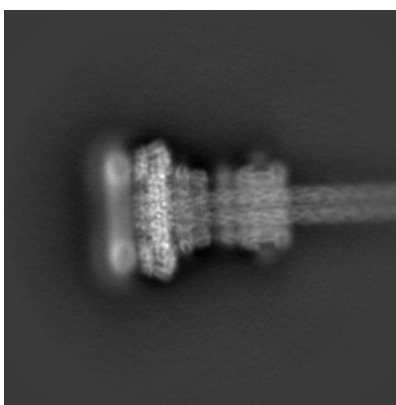


Z

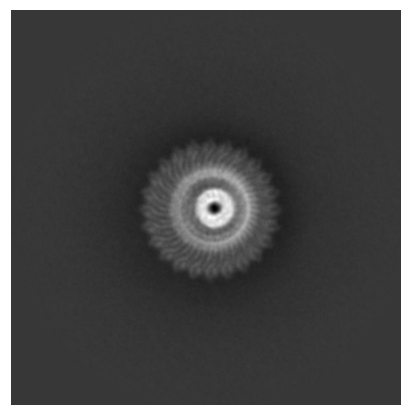
6.1.2 Raw map



X



Y

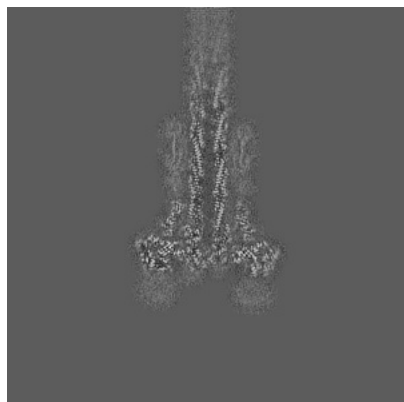


Z

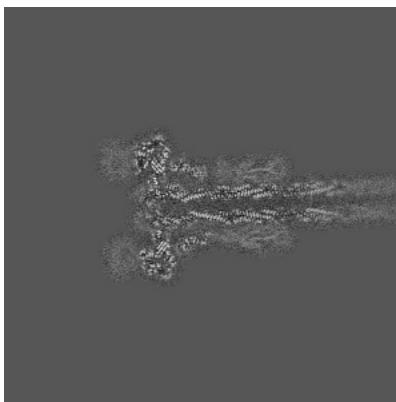
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

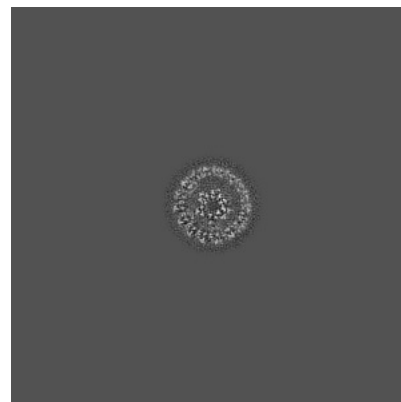
6.2.1 Primary map



X Index: 240

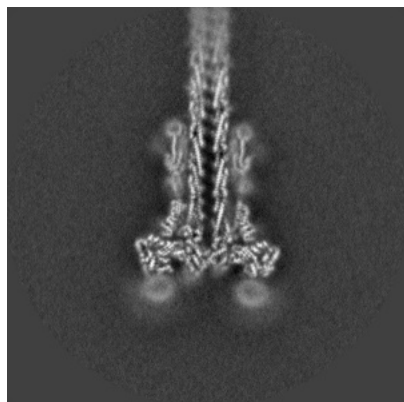


Y Index: 240

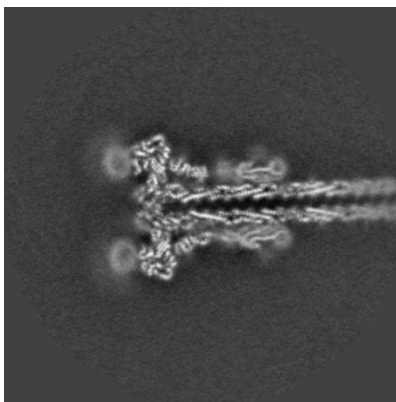


Z Index: 240

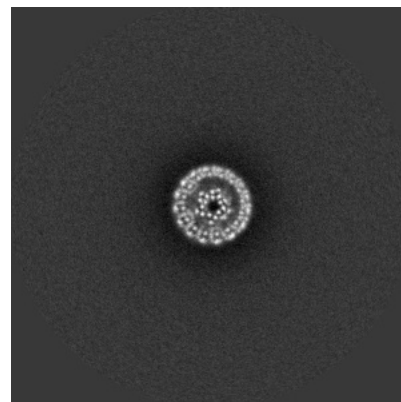
6.2.2 Raw map



X Index: 240



Y Index: 240

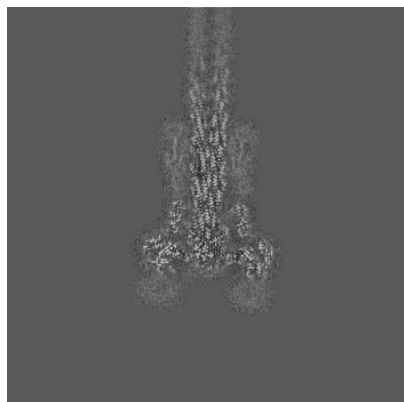


Z Index: 240

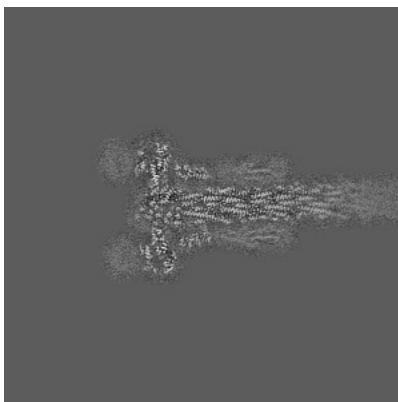
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

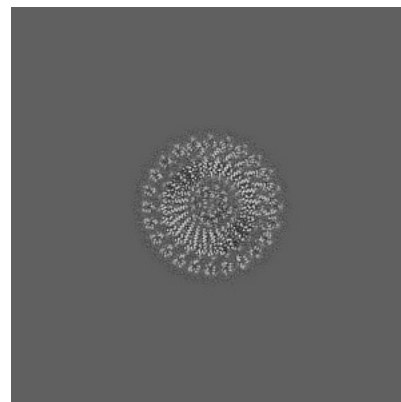
6.3.1 Primary map



X Index: 252

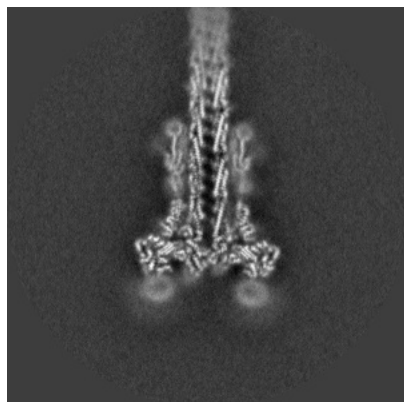


Y Index: 232

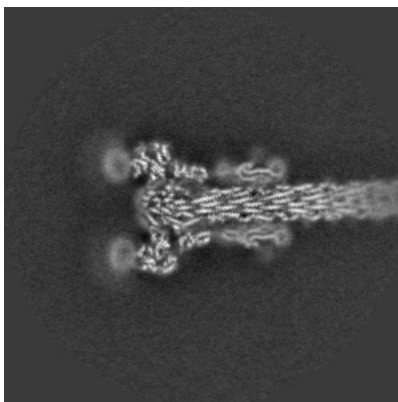


Z Index: 185

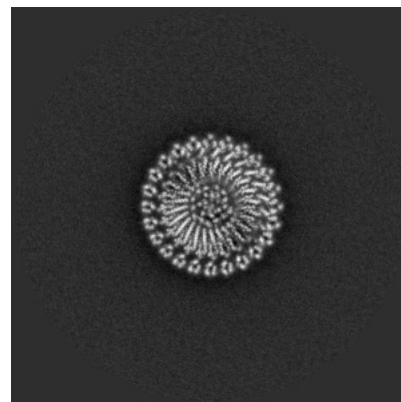
6.3.2 Raw map



X Index: 239



Y Index: 252

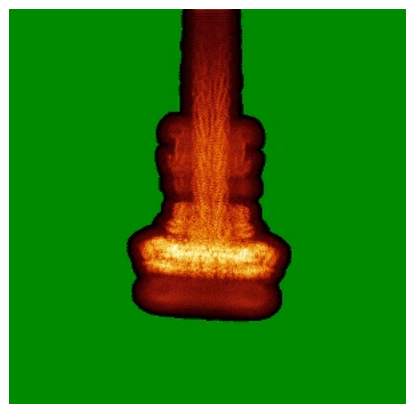


Z Index: 185

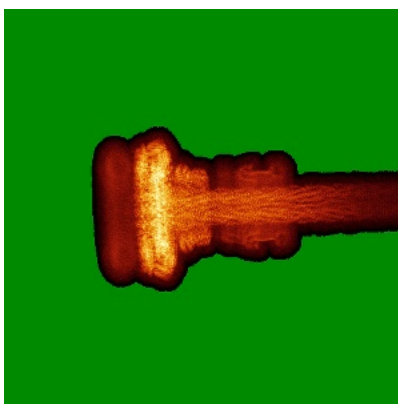
The images above show the largest variance slices of the map in three orthogonal directions.

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

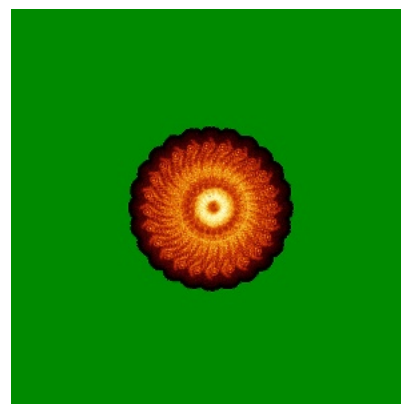
6.4.1 Primary map



X

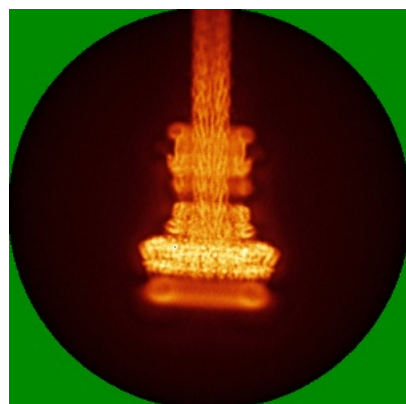


Y

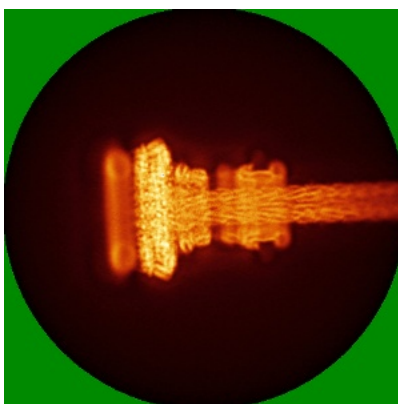


Z

6.4.2 Raw map



X



Y

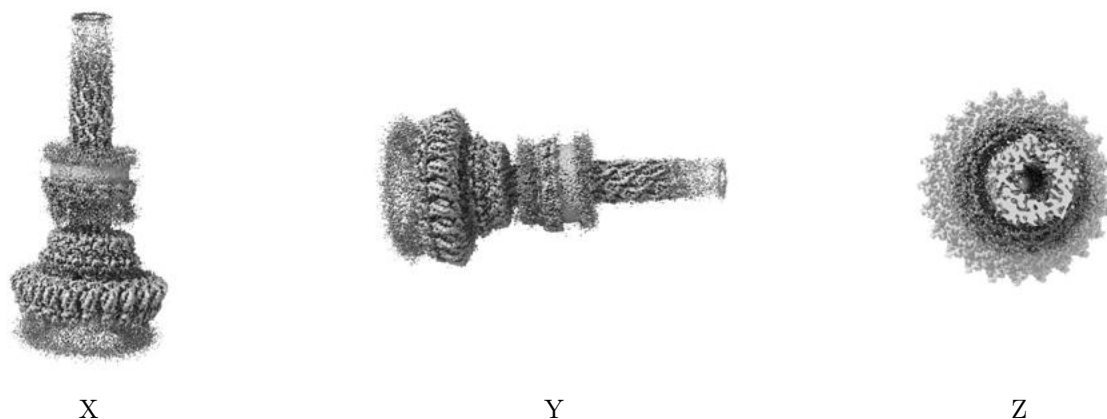


Z

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.

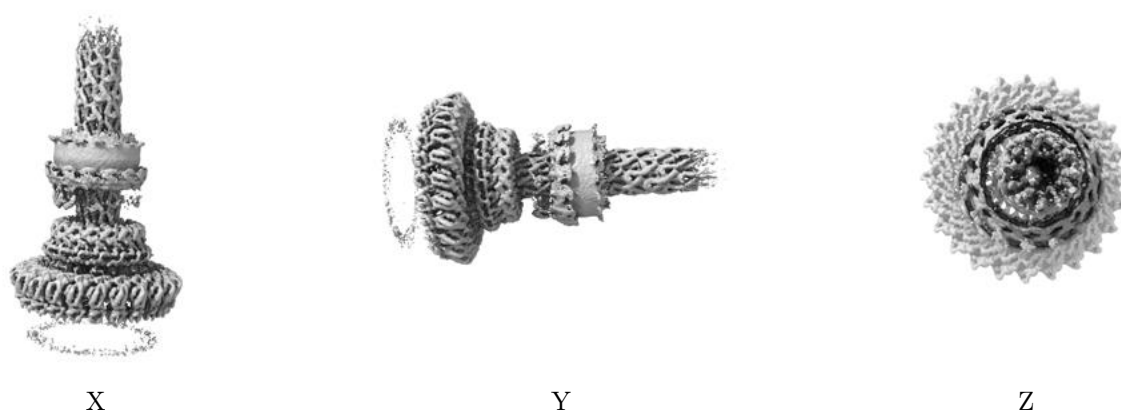
6.5 Orthogonal surface views [i](#)

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

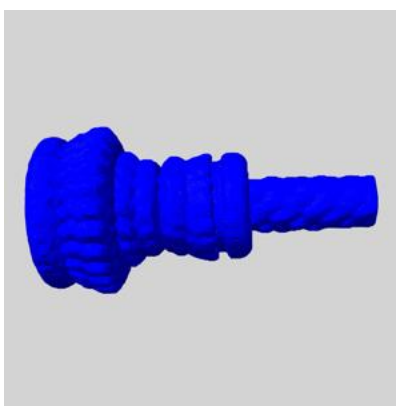
A mask typically either:

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

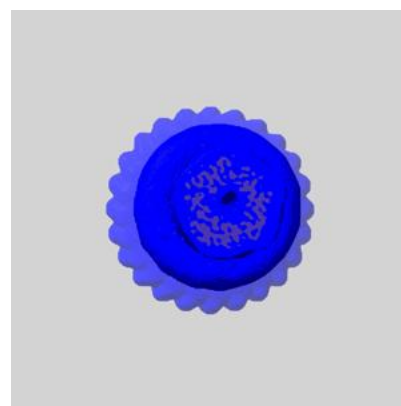
6.6.1 emd_15700_msk_1.map [i](#)



X



Y

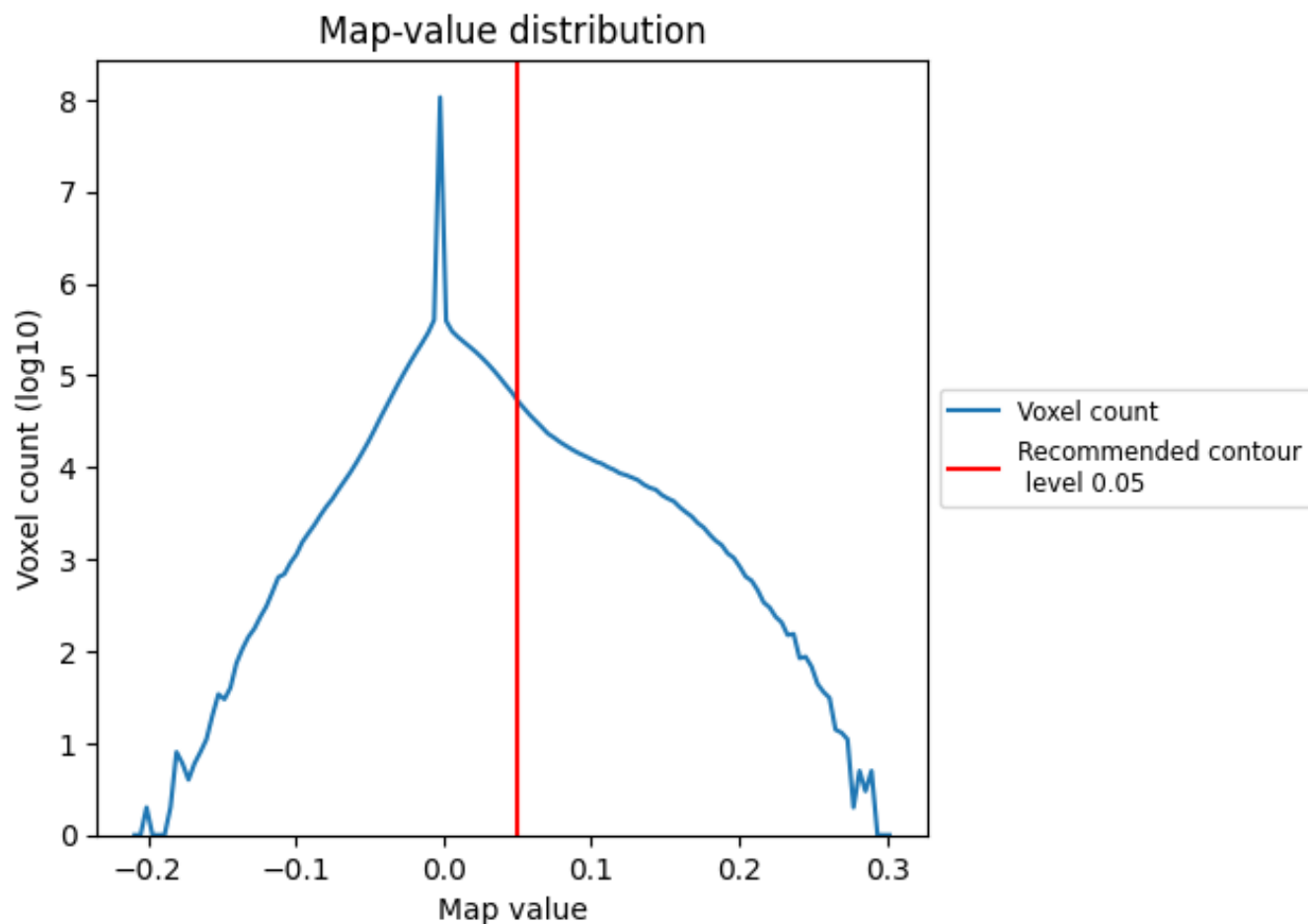


Z

7 Map analysis [i](#)

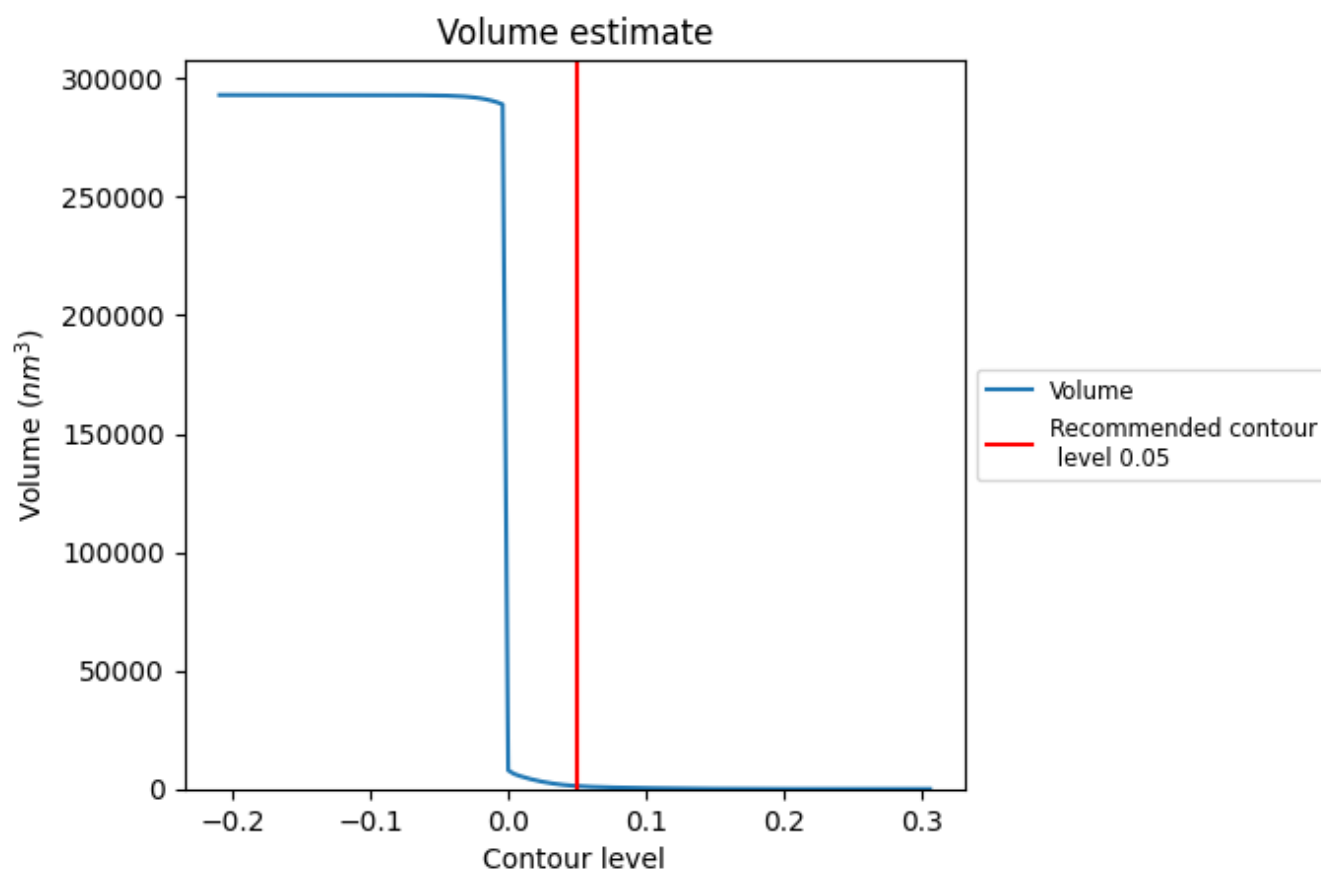
This section contains the results of statistical analysis of the map.

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.

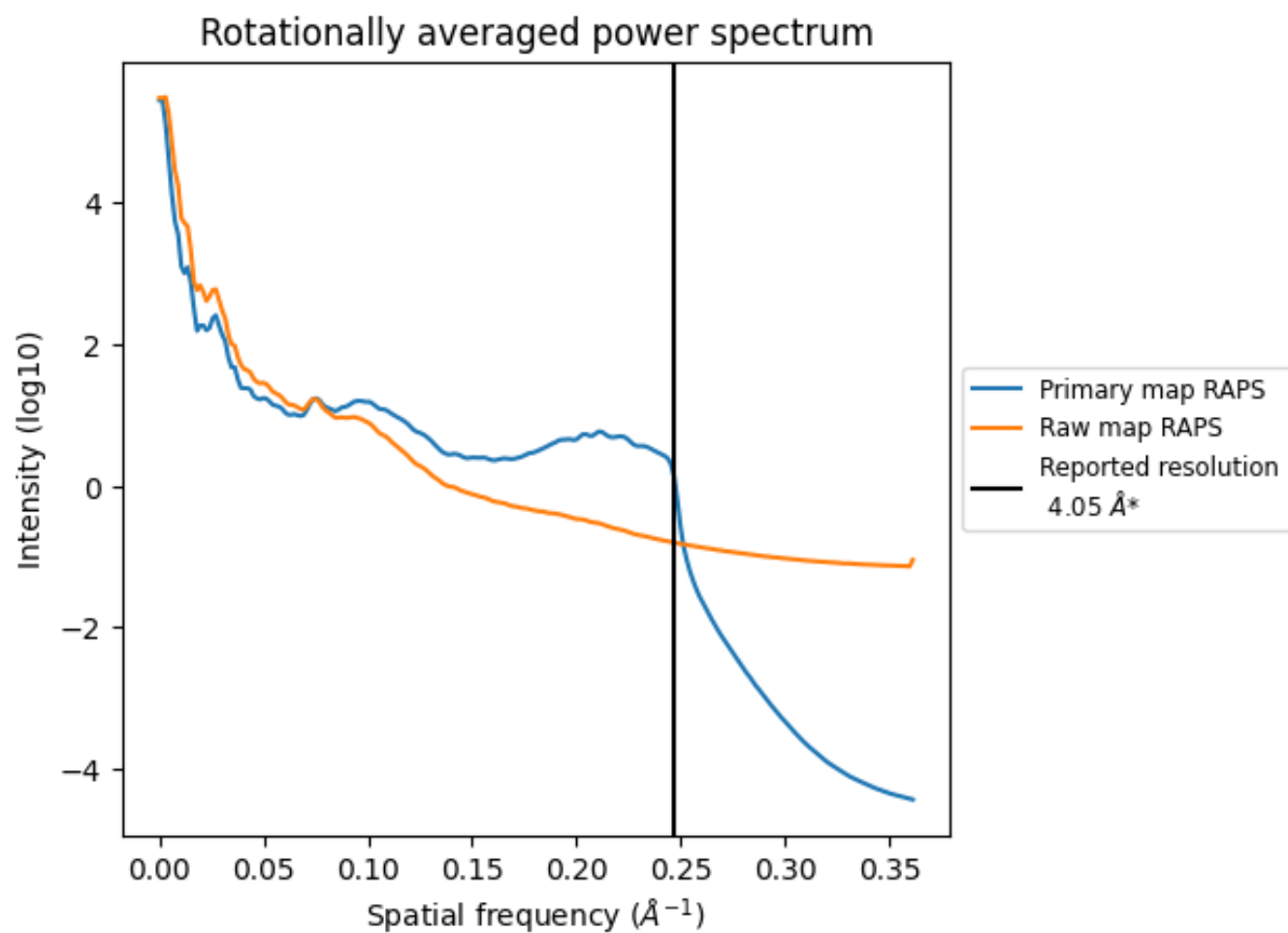
7.2 Volume estimate [i](#)



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 ⓘ

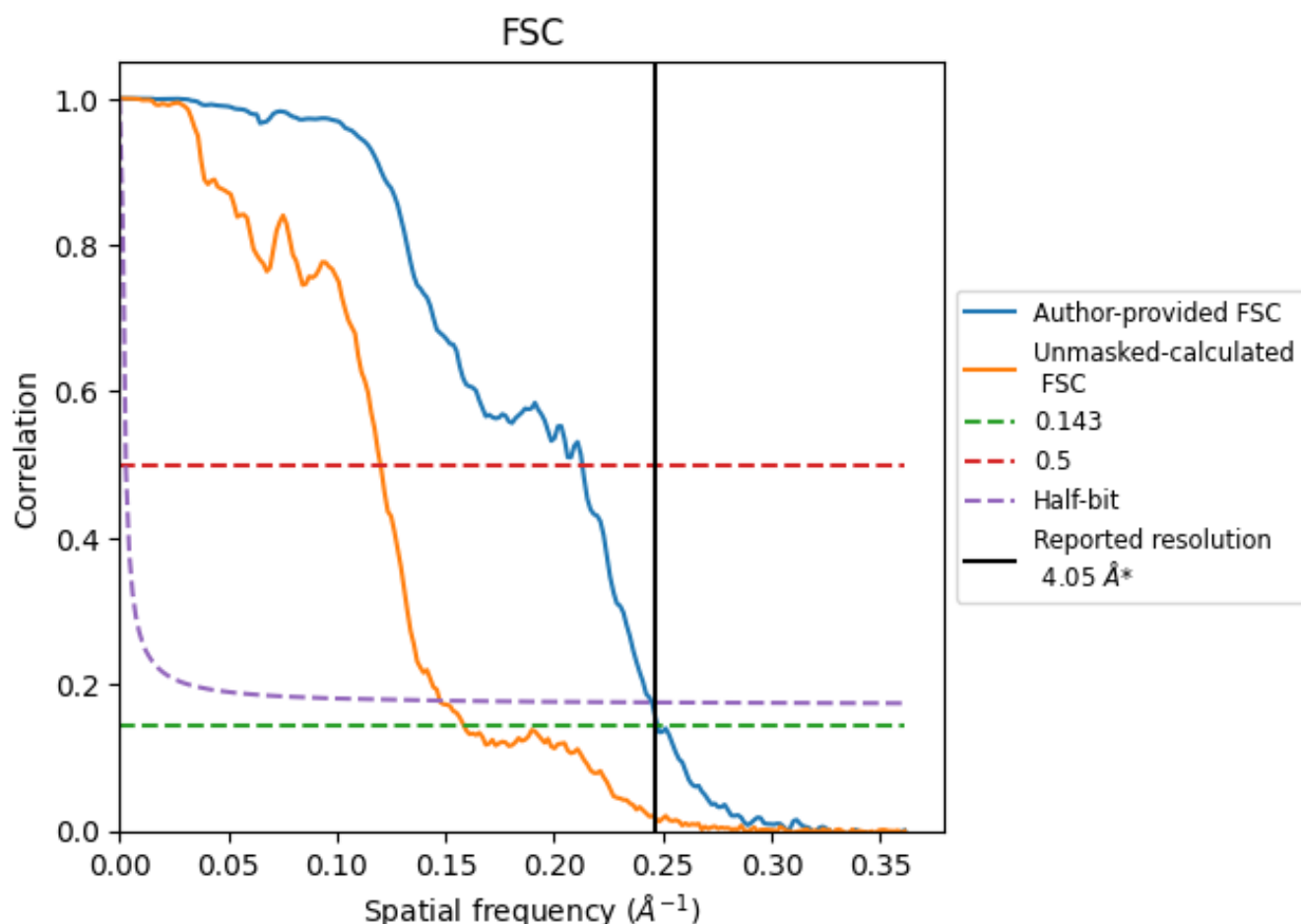


*Reported resolution corresponds to spatial frequency of 0.247 Å⁻¹

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](#)

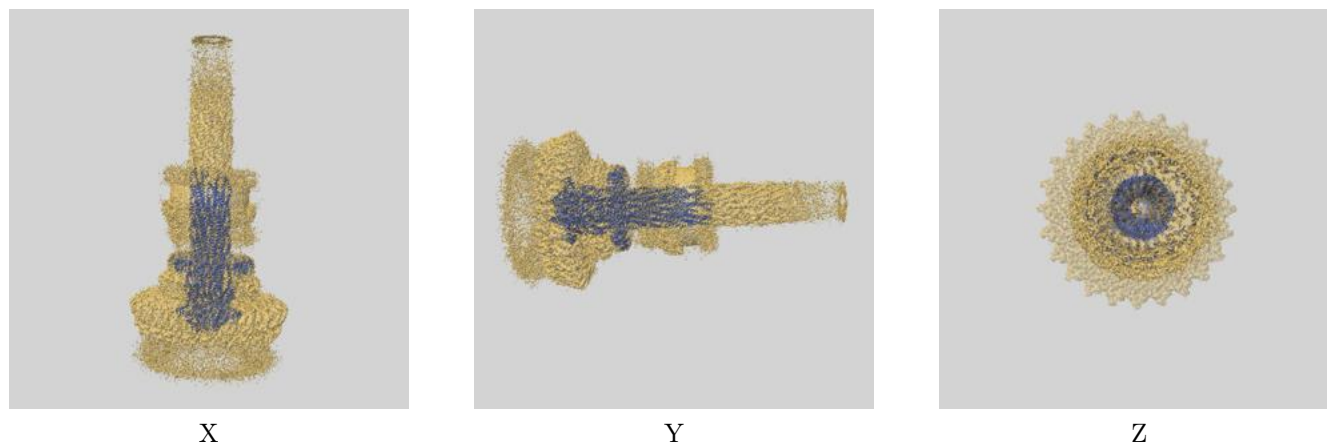
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.05	-	-
Author-provided FSC curve	4.04	4.69	4.08
Unmasked-calculated*	6.31	8.33	6.78

*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](#)

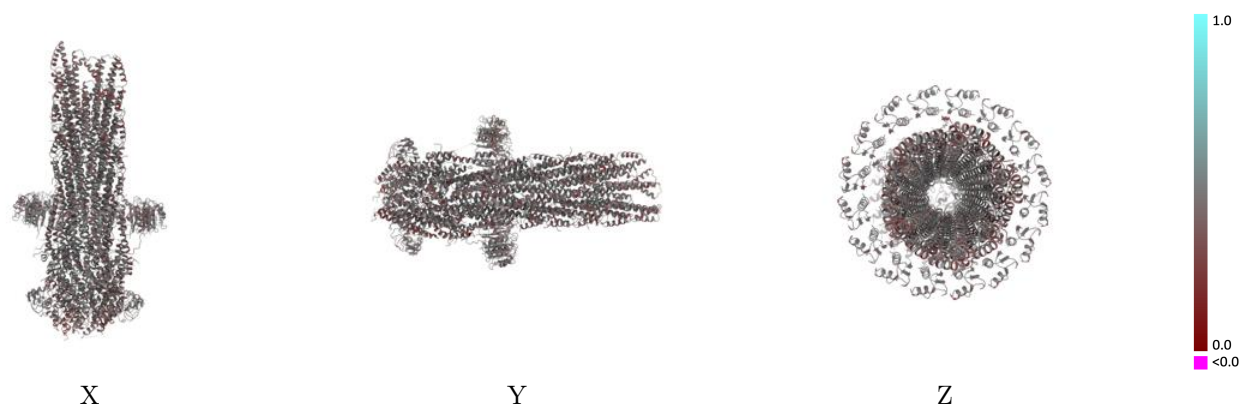
This section contains information regarding the fit between EMDB map EMD-15700 and PDB model 8AXK. Per-residue inclusion information can be found in [section 3](#) on [page 22](#).

9.1 Map-model overlay [i](#)



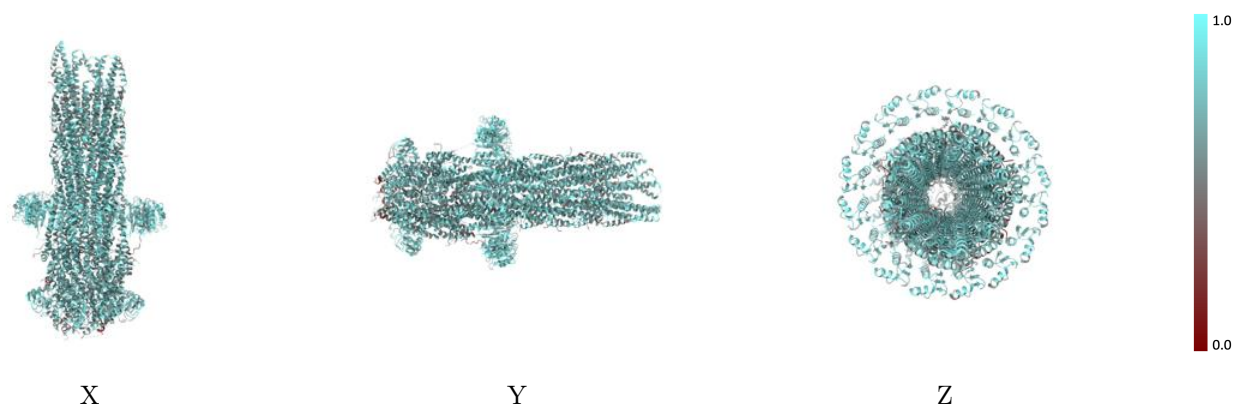
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



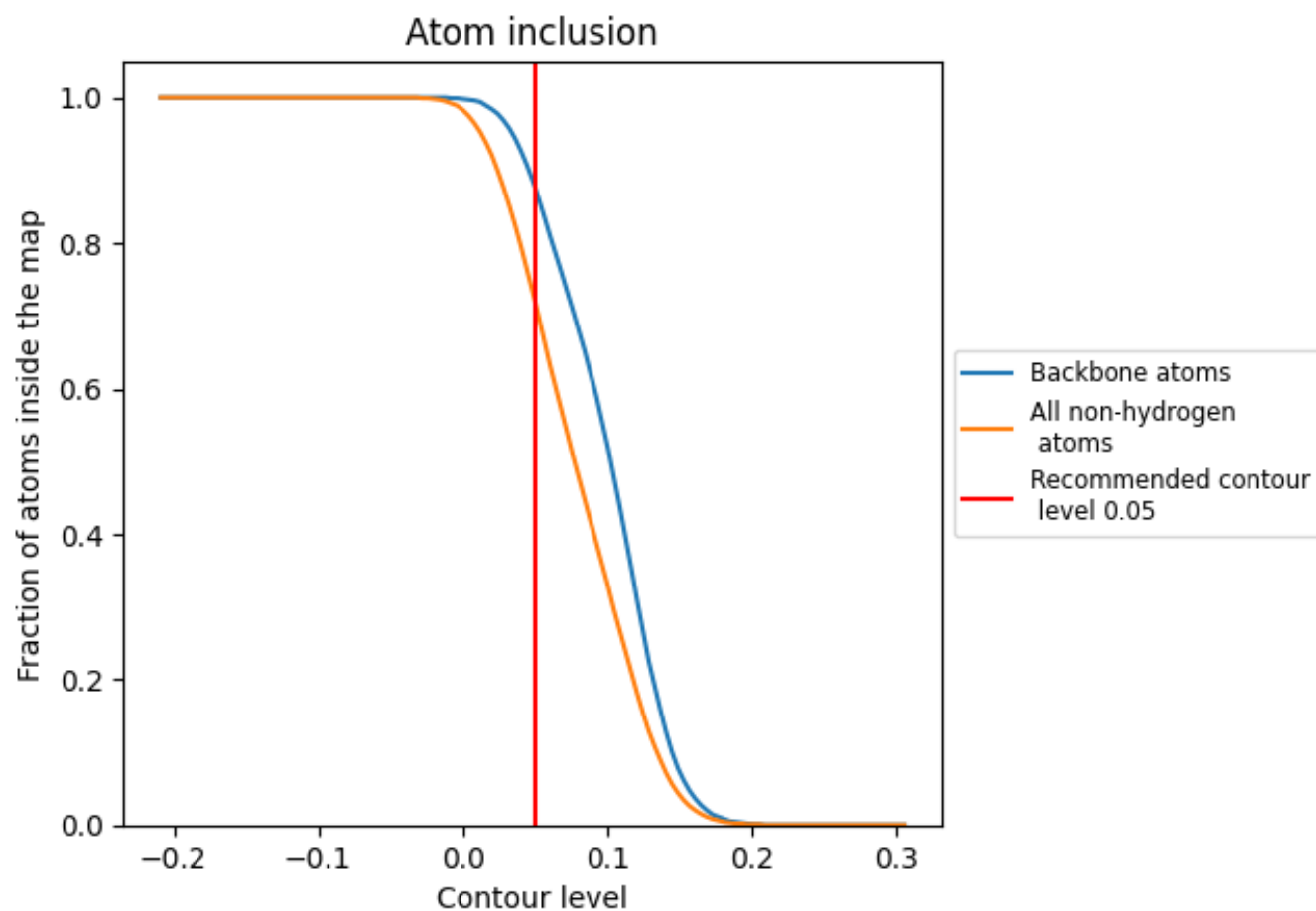
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.4230
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