



Full wwPDB EM Validation Report ⓘ

Mar 22, 2026 – 09:51 PM UTC

PDB ID : 8AXK / pdb_00008axk
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 : 6RWY, 6RWX, 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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

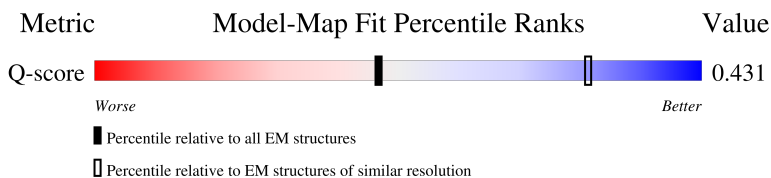
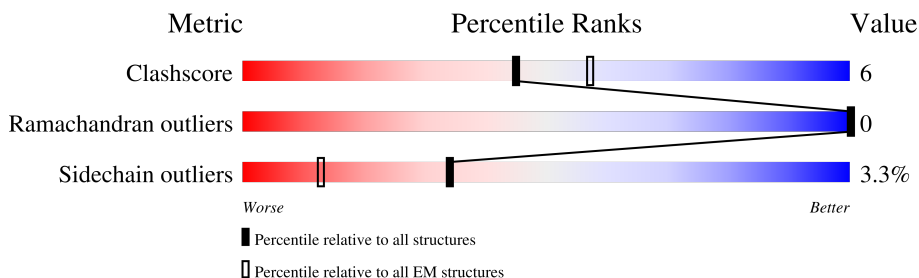
1 Overall quality at a glance

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.



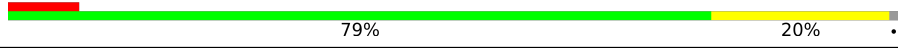
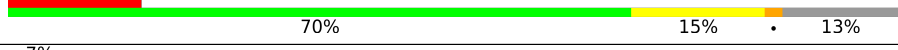
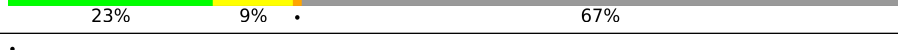
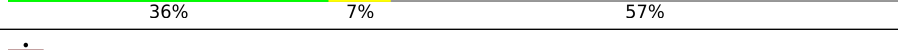
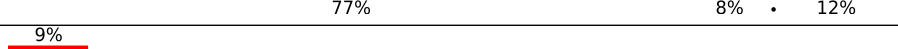
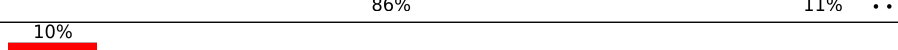
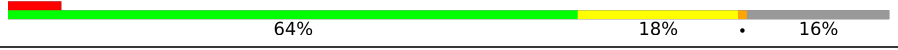
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6569 (3.55 - 4.55)

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	

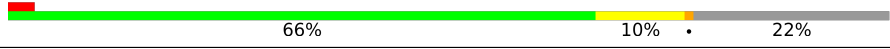
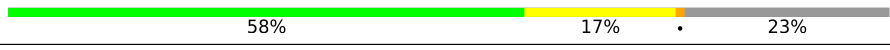
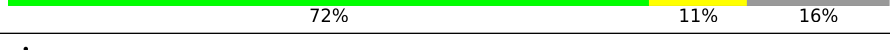
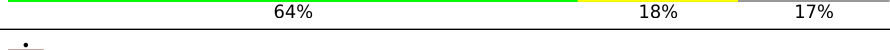
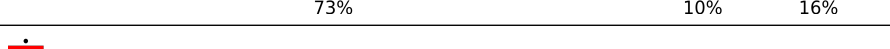
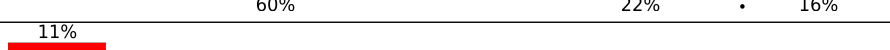
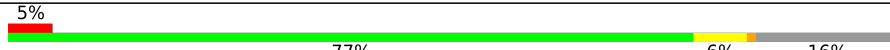
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Mol	Chain	Length	Quality of chain
1	E	216	
2	F	256	
3	G	86	
3	H	86	
3	I	86	
3	J	86	
4	K	342	
5	M	97	
5	N	97	
5	O	97	
5	P	97	
5	Q	97	
5	R	97	
6	S	98	
6	T	98	
6	U	98	
6	V	98	
6	W	98	
6	a	98	
6	b	98	
6	c	98	
6	d	98	
6	e	98	
6	f	98	
6	g	98	

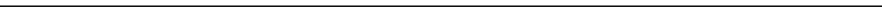
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Mol	Chain	Length	Quality of chain
6	h	98	
6	i	98	
6	j	98	
6	k	98	
6	l	98	
6	m	98	
6	n	98	
6	o	98	
6	p	98	
6	q	98	
6	r	98	
6	s	98	
6	t	98	
6	u	98	
6	v	98	
6	w	98	
7	0	566	
7	1	566	
7	2	566	
7	3	566	
7	4	566	
7	5	566	
7	6	566	
7	7	566	
7	8	566	

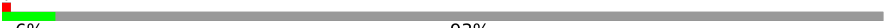
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Mol	Chain	Length	Quality of chain
7	9	566	 8% . 89%
7	X	566	 10% .. 89%
7	Y	566	 8% . 89%
7	Z	566	 10% . 89%
7	x	566	 10% . 89%
7	y	566	 9% . 89%
7	z	566	 9% . 89%
8	a0	241	 5% . 93%
8	b0	241	 5% . 93%
8	c0	241	 7% 93%
8	d0	241	 7% 93%
8	e0	241	 5% . 93%
8	f0	241	 6% . 93%
8	g0	241	 7% 93%
8	h0	241	 7% 93%
8	i0	241	 6% . 93%
8	j0	241	 5% . 93%
8	k0	241	 6% . 93%
8	l0	241	 7% 93%
8	m0	241	 7% 93%
8	n0	241	 7% 93%
8	o0	241	 6% . 93%
8	p0	241	 5% . 93%
8	q0	241	 6% . 93%
8	r0	241	 6% 93%

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Mol	Chain	Length	Quality of chain
8	s0	241	 7% 93%
8	t0	241	 5% 93%
8	u0	241	 6% 93%
8	v0	241	 6% 93%
8	w0	241	 7% 93%
8	x0	241	 6% 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 MxiL.

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

- Molecule 6 is a protein called Protein MxiH.

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

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

There are 420 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 8 is a protein called Lipoprotein MxiJ.

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

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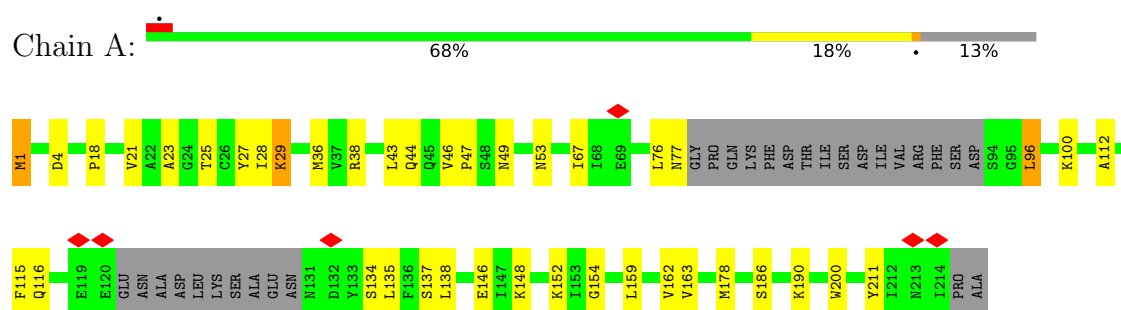
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Mol	Chain	Residues	Atoms				AltConf	Trace
8	e0	17	Total 131	C 82	N 24	O 25	0	0
8	f0	17	Total 131	C 82	N 24	O 25	0	0
8	g0	17	Total 131	C 82	N 24	O 25	0	0
8	h0	17	Total 131	C 82	N 24	O 25	0	0
8	i0	17	Total 131	C 82	N 24	O 25	0	0
8	j0	17	Total 131	C 82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

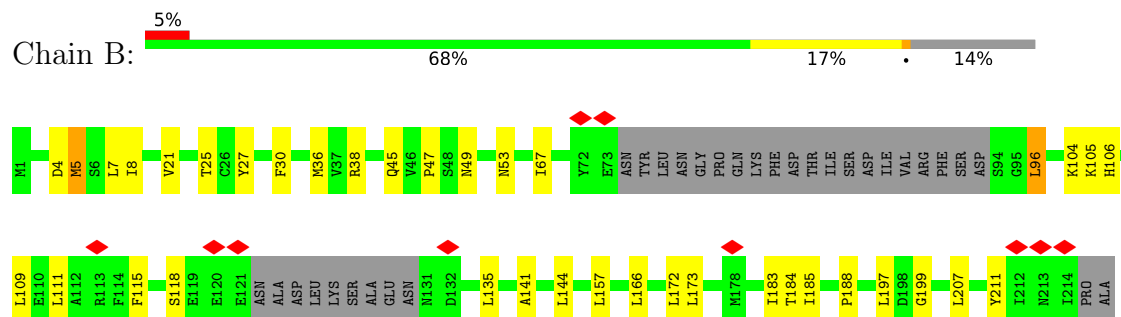
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

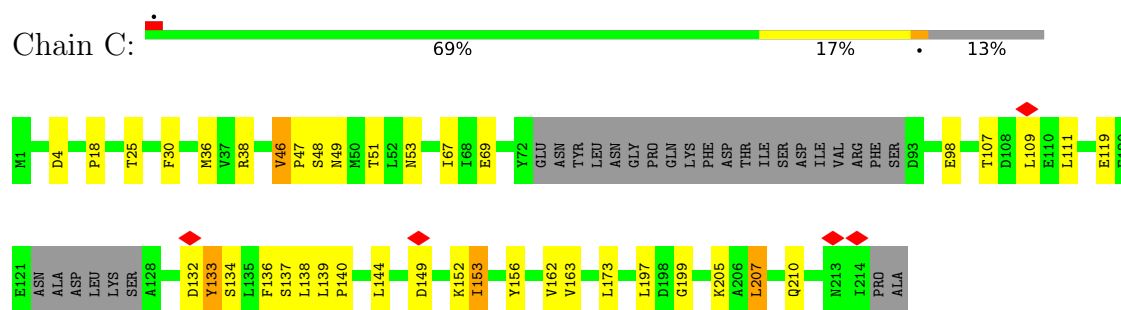
- Molecule 1: Surface presentation of antigens protein SpaP



- Molecule 1: Surface presentation of antigens protein SpaP

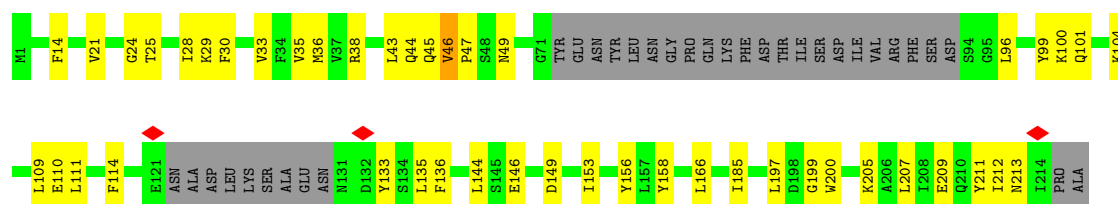


- Molecule 1: Surface presentation of antigens protein SpaP

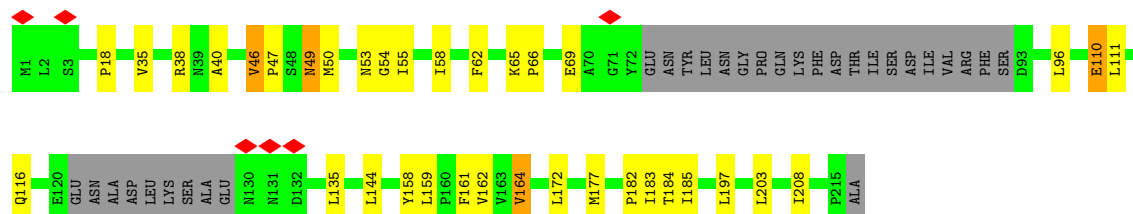


- Molecule 1: Surface presentation of antigens protein SpaP

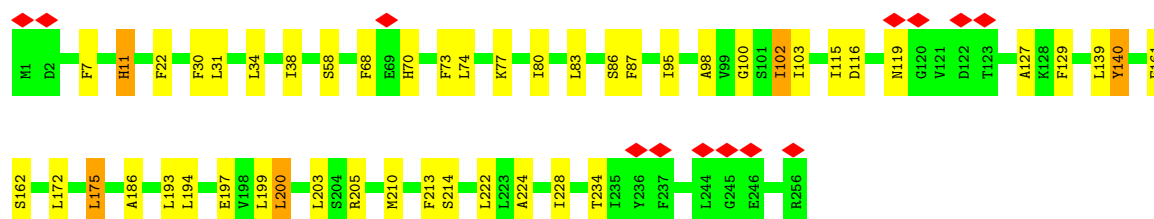
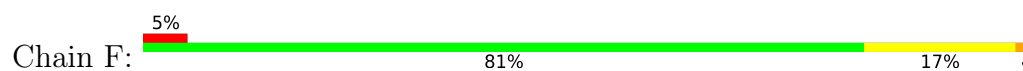




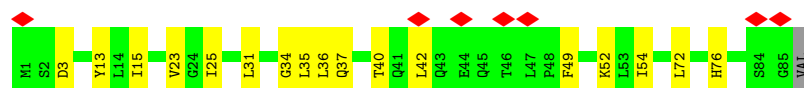
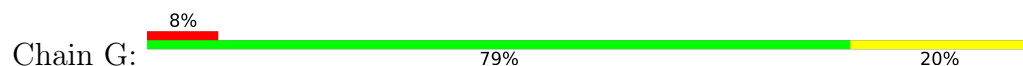
• Molecule 1: Surface presentation of antigens protein SpaP



• Molecule 2: Surface presentation of antigens protein SpaR



• Molecule 3: Surface presentation of antigens protein SpaQ

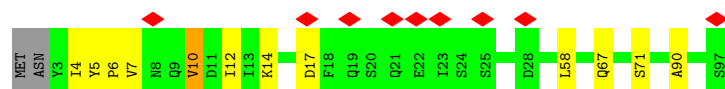
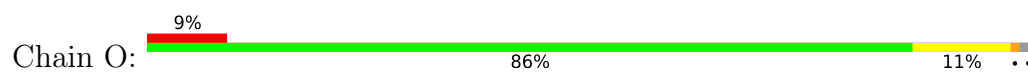


• Molecule 3: Surface presentation of antigens protein SpaQ

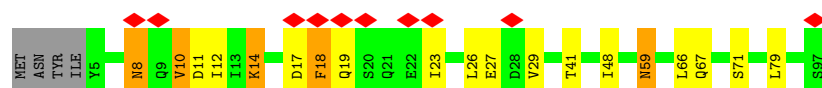
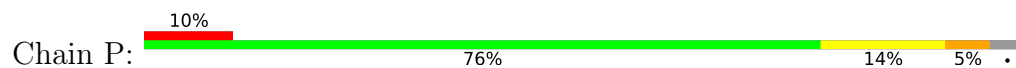


• Molecule 3: Surface presentation of antigens protein SpaQ

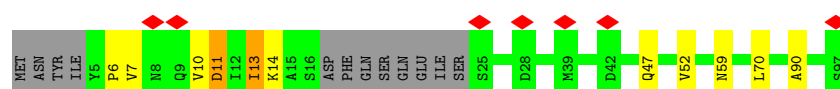
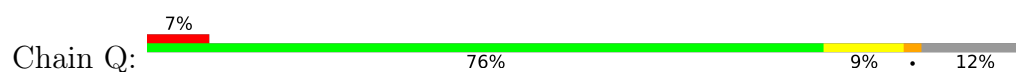




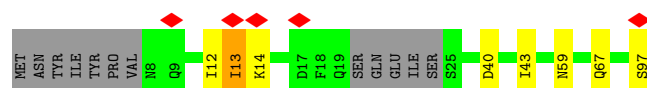
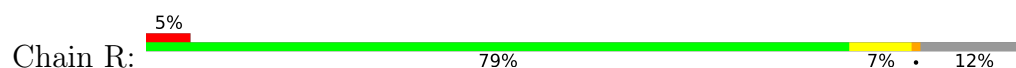
• Molecule 5: Protein MxiI



• Molecule 5: Protein MxiI



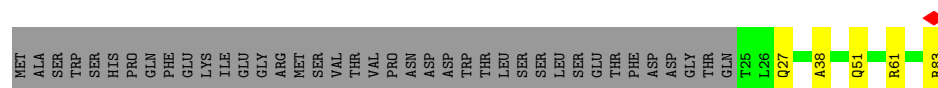
• Molecule 5: Protein MxiI



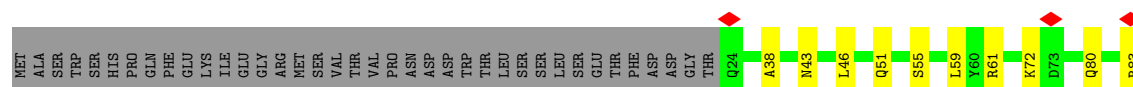
• Molecule 6: Protein MxiH



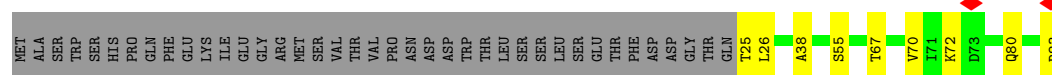
• Molecule 6: Protein MxiH



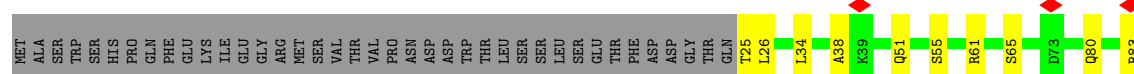
• Molecule 6: Protein MxiH



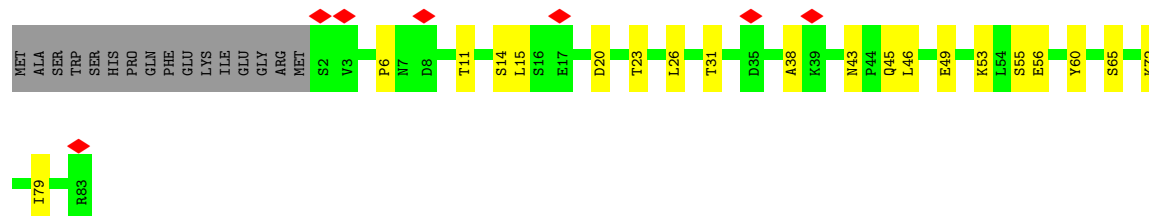
- Molecule 6: Protein MxiH



- Molecule 6: Protein MxiH



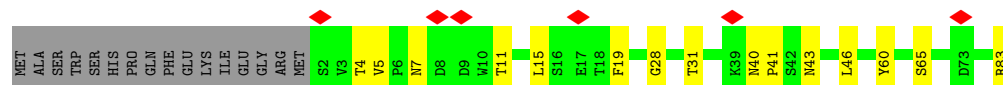
- Molecule 6: Protein MxiH



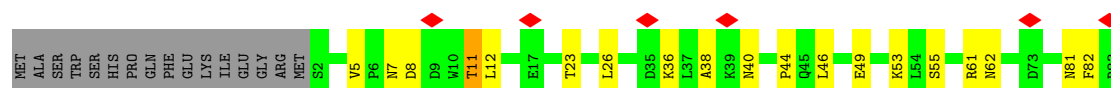
- Molecule 6: Protein MxiH



- Molecule 6: Protein MxiH



- Molecule 6: Protein MxiH



- Molecule 6: Protein MxiH

Chain e:  64% 18% 17%



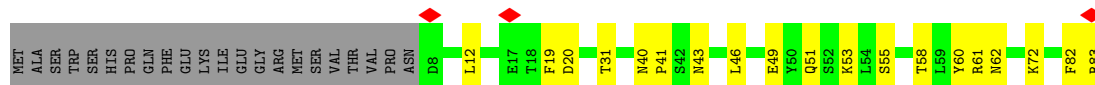
• Molecule 6: Protein MxiH

Chain f:  67% 15% 17%



• Molecule 6: Protein MxiH

Chain g:  58% 19% 22%



• Molecule 6: Protein MxiH

Chain h:  60% 16% 23%



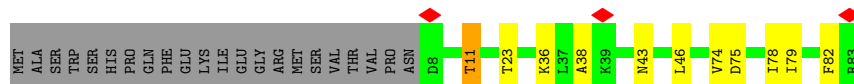
• Molecule 6: Protein MxiH

Chain i:  62% 12% 23%



• Molecule 6: Protein MxiH

Chain j:  66% 10% 22%

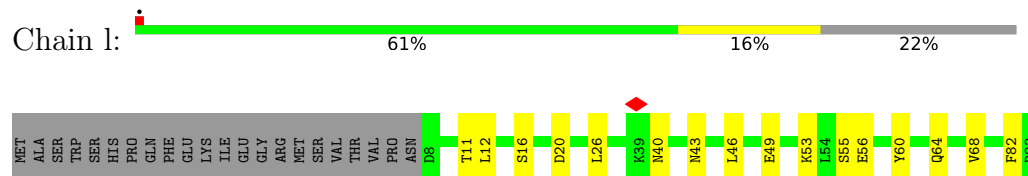


• Molecule 6: Protein MxiH

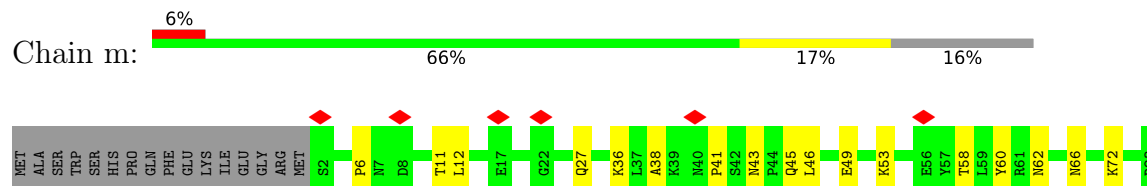
Chain k:  58% 17% 23%



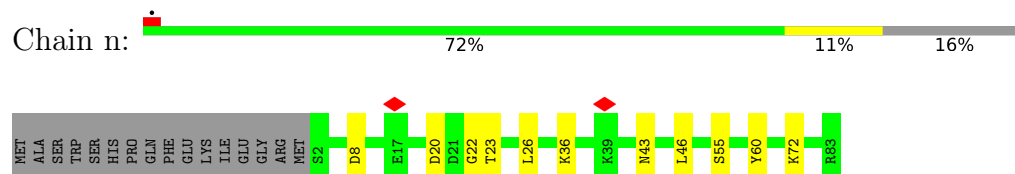
● Molecule 6: Protein MxiH



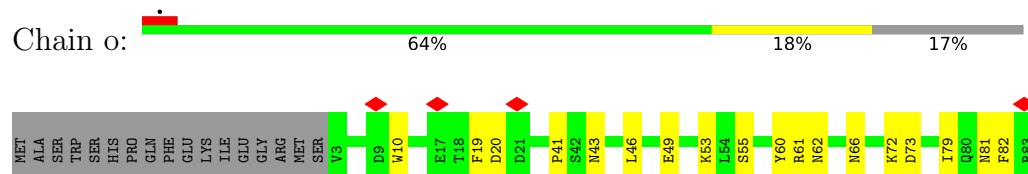
● Molecule 6: Protein MxiH



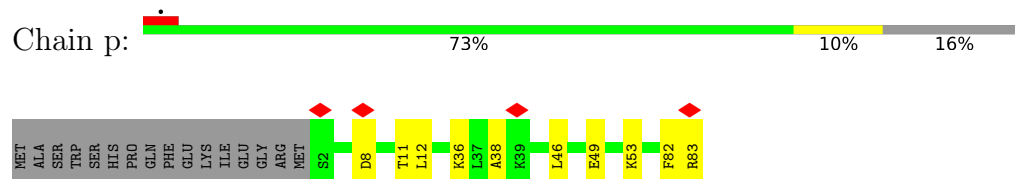
● Molecule 6: Protein MxiH



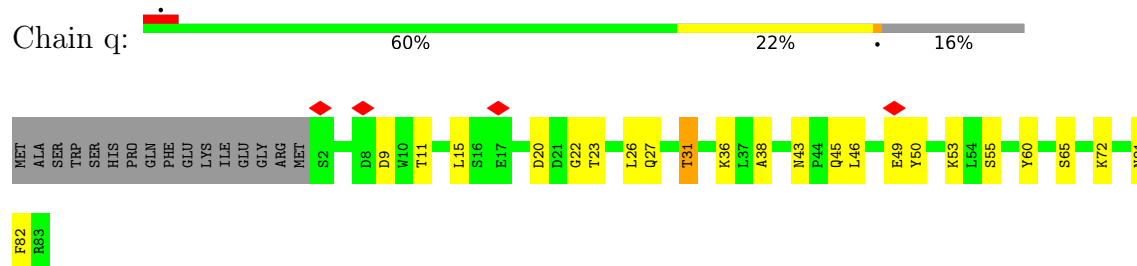
● Molecule 6: Protein MxiH



● Molecule 6: Protein MxiH



● Molecule 6: Protein MxiH

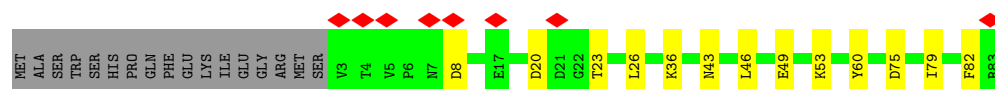


● Molecule 6: Protein MxiH

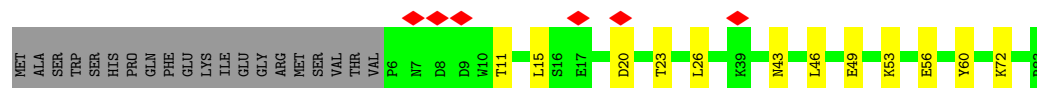




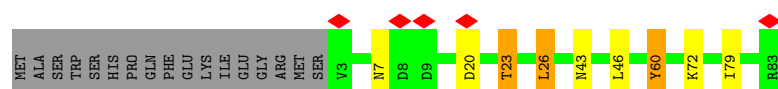
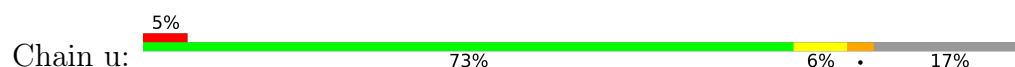
- Molecule 6: Protein MxiH



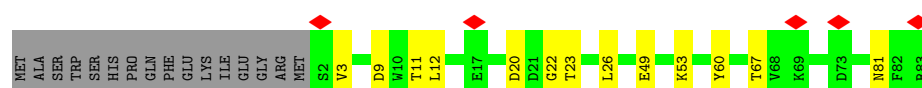
- Molecule 6: Protein MxiH



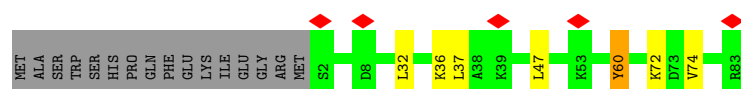
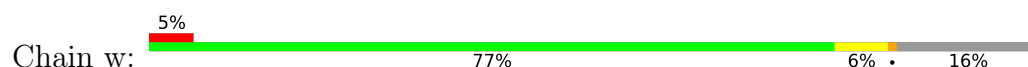
- Molecule 6: Protein MxiH



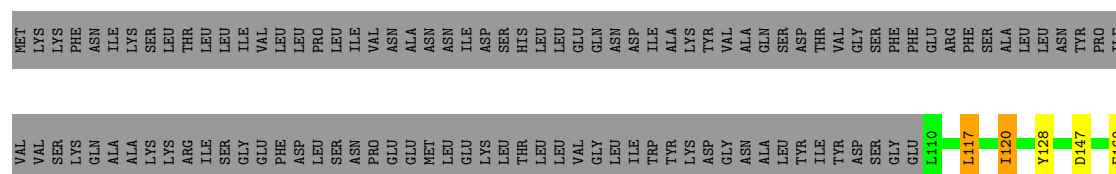
- Molecule 6: Protein MxiH

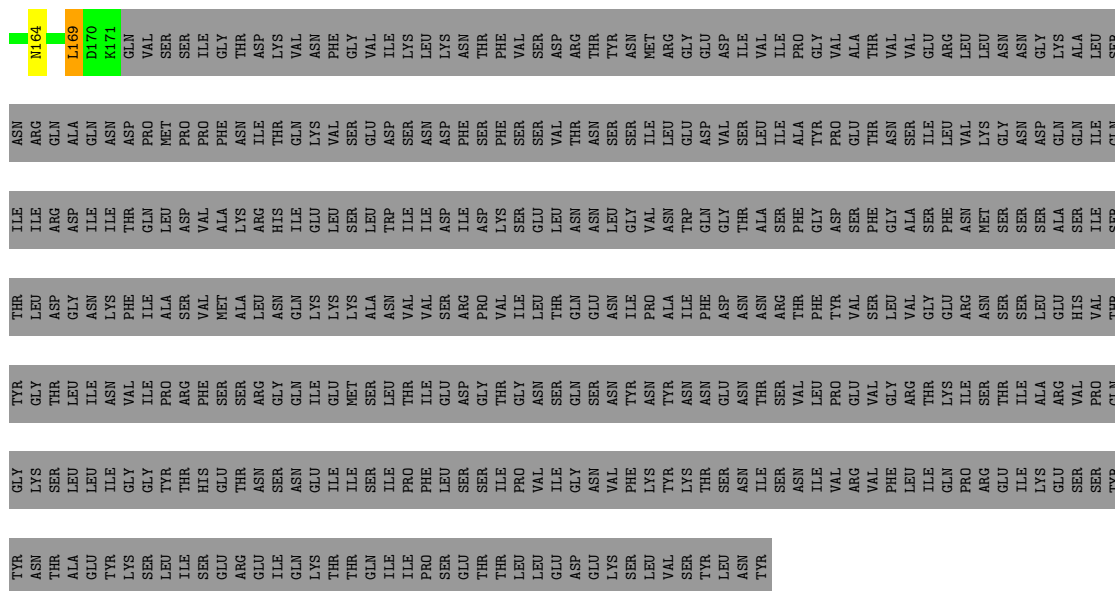


- Molecule 6: Protein MxiH



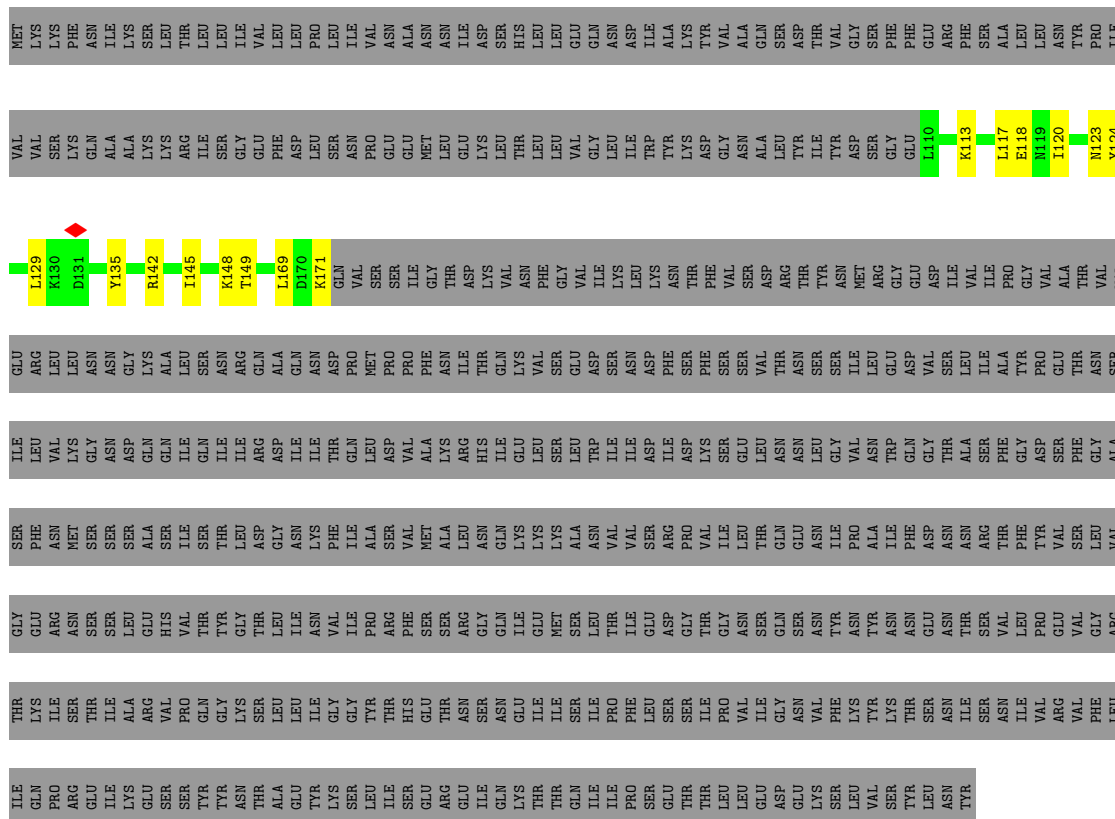
- Molecule 7: Outer membrane protein MxiD



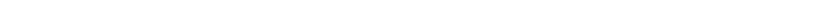


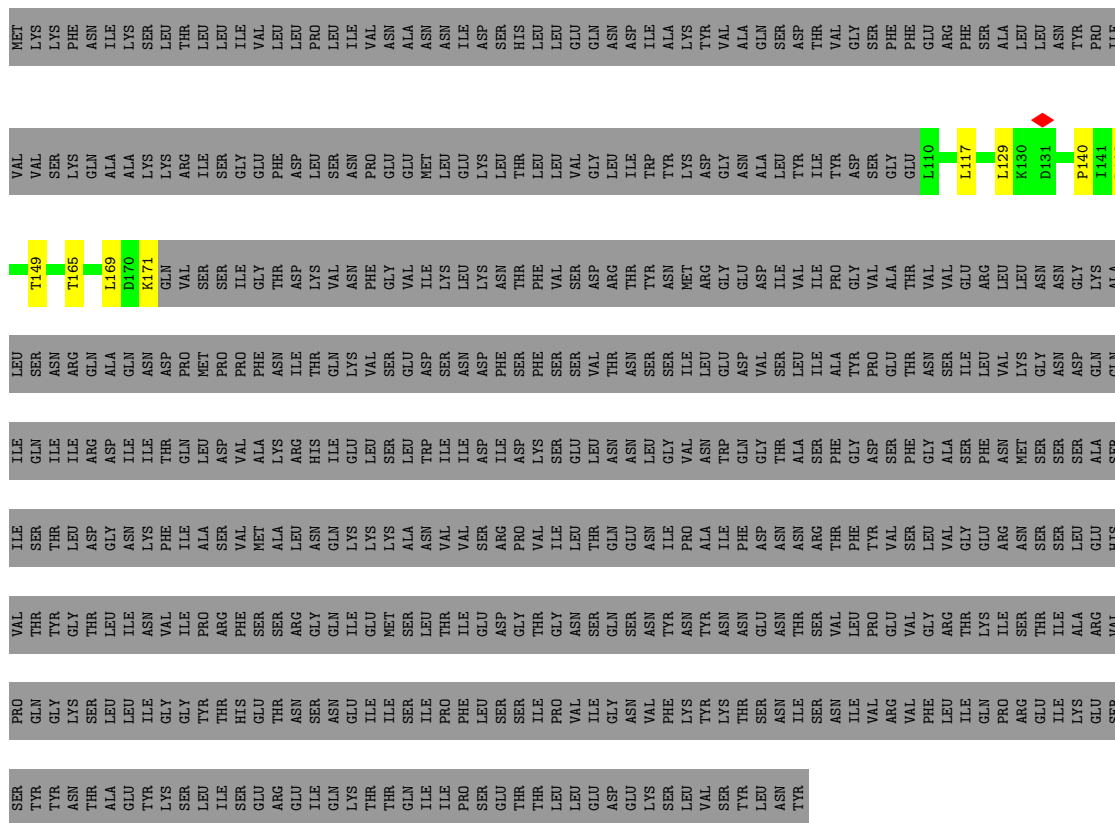
- Molecule 7: Outer membrane protein MxiD

Chain Y: 8% . 89%



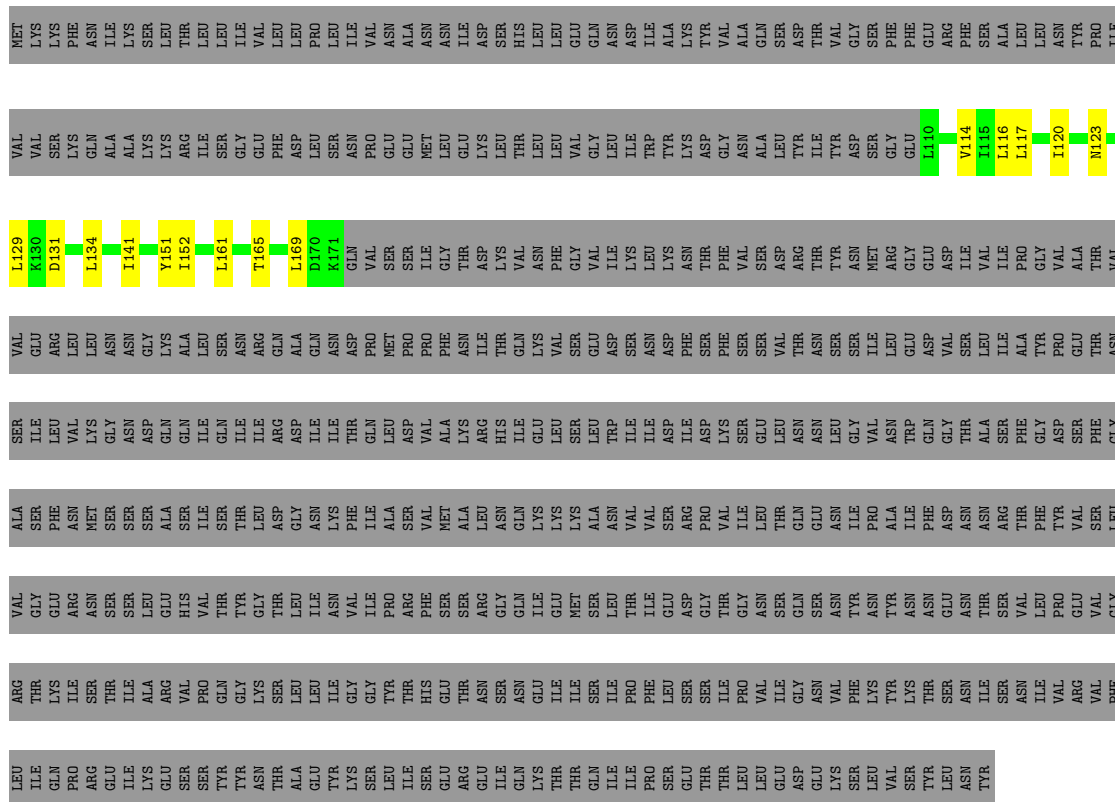
- Molecule 7: Outer membrane protein MxiD

Chain Z:  10% . 89%

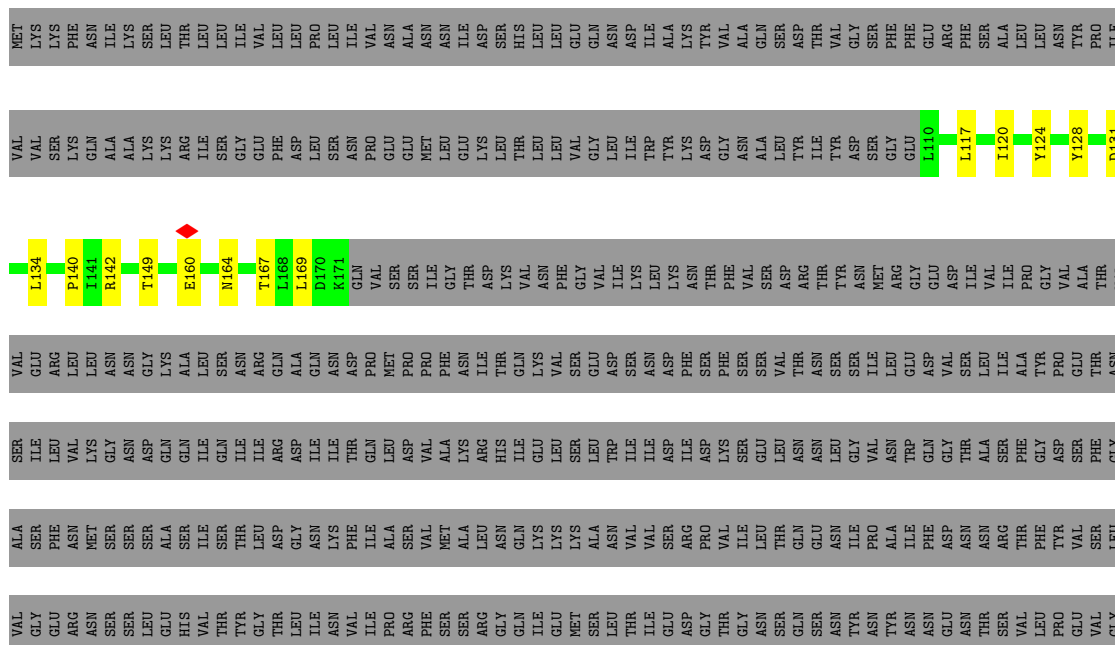


- Molecule 7: Outer membrane protein MxiD

Chain 0: 8% . 89%



Chain 2: 10% . 89%



[illegible]

- Molecule 7: Outer membrane protein MxiD

Chain 6: 8% . 89%

VAL	PHE	LEU	ILE	GLN	PRO	ARG	GLU	LYS	THR	GLY	SER	PHE	THR	THR	ASN	THR	D131	VAL	MET
LEU	LEU	THR	GLY	LYS	ILE	GLY	GLU	LYS	VAL	VAL	SER	ALA	VAL	ASN	ILE	GLY	L134	SER	LYS
ILE	GLN	THR	PHE	GLY	THR	GLY	ARG	ASN	VAL	VAL	LYS	ASN	LEU	LEU	ILE	GLY	P140	ASN	PHE
PRO	PRO	ILE	ARG	ASN	MET	ASN	VAL	VAL	LYS	ALA	VAL	ASN	LEU	LEU	ILE	GLY	I141	ILE	LYS
ARG	ARG	SER	ASN	GLY	GLY	GLY	ASN	LYS	LEU	ALA	THR	THR	ASN	LEU	ILE	GLY	R142	VAL	SER
GLU	ILE	THR	SER	SER	ASN	ASN	GLY	ASN	ASN	GLY	ASN	GLY	ASN	ASN	ILE	GLY	D147	LEU	THR
LYS	LYS	ALA	SER	SER	ASN	ALA	GLN	GLN	LYS	ALA	ALA	ALA	LYS	GLN	ILE	GLY	K148	ARG	LYS
GLY	SER	VAL	HIS	SER	ILE	ILE	VAL	THR	LEU	LEU	THR	THR	ASN	ASN	GLY	GLY	L161	SER	LEU
SER	SER	PRO	VAL	VAL	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	M164	ILE	VAL
THR	THR	GLN	TYR	TYR	TYR	TYR	TYR	TYR	TYR	TYR	TYR	TYR	TYR	TYR	TYR	TYR	T165	PHE	VAL
ASN	ASN	LYS	GLY	LYS	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	A166	LEU	LEU
ALA	ALA	LEU	THR	SER	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	T167	LEU	PRO
GLU	GLU	LEU	LEU	ILE	ILE	ILE	ASN	ASN	GLN	GLY	GLY	GLY	GLY	GLY	GLY	GLY	L168	SER	LEU
TYR	TYR	ILE	ASN	LYS	ILE	ASN	ASN	LYS	ASN	GLN	ASN	ASN	ASN	ASN	ASN	ASN	K171	ASN	VAL
LYS	LYS	GLY	VAL	PHE	THR	PHE	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLN	GLU	ASN
SER	SER	GLY	ILE	ILE	ILE	ILE	ILE	GLN	PRO	VAL	LEU	ALA	PRO	PRO	PRO	PRO	VAL	GLU	ALA
LEU	LEU	THR	ARG	SER	ASN	PHE	ARG	SER	ASN	VAL	VAL	ALA	VAL	VAL	VAL	VAL	SER	LEU	ASN
THR	THR	GLU	SER	THR	THR	SER	SER	MET	ALA	ALA	SER	ALA	PHE	PHE	PHE	PHE	GLY	LYS	ASP
ASN	ASN	ASN	GLY	GLY	GLY	GLY	GLY	GLY	LYS	LYS	LYS	LYS	ASN	ASN	ASN	ASN	THR	LEU	SER
GLN	GLN	ASN	GLN	GLN	GLN	GLN	GLN	GLN	ILE	ILE	ILE	ILE	HIS	HIS	ILE	ILE	ASN	LEU	HIS
LYS	LYS	ASN	ASN	ASN	ASN	ASN	ASN	ASN	GLY	GLY	GLY	GLY	THR	THR	THR	THR	LYS	LEU	SER
THR	THR	ILE	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	LEU	GLY
GLN	GLN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	LEU	ASN
THR	THR	ILE	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	GLY
ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	GLY	ASN
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
LEU	LEU	VAL	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	GLY	ALA
GLU	GLU	ILE	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	LEU
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	LEU
ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	THR	ASN
THR	THR	VAL	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	THR	THR

- Molecule 7: Outer membrane protein MxiD

Chain 8: 9% . 89%

GLN	GLN	LYS	ALA	LYS	VAL	MET
ILE	ILE	LEU	LEU	LYS	VAL	LYS
ILE	GLN	ASN	ASN	LYS	SER	PHE
ILE	ILE	ARG	ARG	ALA	ALA	ILE
ARG	ASP	GLN	GLN	LYS	LYS	SER
ILE	ILE	GLN	GLN	LYS	ARG	THR
THR	THR	ASP	ASP	ILE	ILE	LEU
GLN	GLN	PRO	PRO	VAL	SER	LEU
LEU	LEU	MET	SER	GLY	GLY	ILE
ASP	ASP	PRO	SER	PHE	GLU	VAL
VAL	VAL	PRO	ILE	GLY	LEU	VAL
ALA	ALA	PHE	PHE	ASP	LEU	ASP
LYS	LYS	ASN	ASN	THR	LEU	PRO
ARG	ARG	ILE	ILE	ASP	SER	LEU
ILE	ILE	THR	THR	LYS	ASN	ILE
HIS	HIS	THR	THR	VAL	PRO	VAL
ILE	ILE	GLN	GLN	VAL	ASN	ASN
GLU	GLU	LYS	VAL	PHE	GLU	ALA
LEU	LEU	VAL	VAL	GLY	MET	ASN
SER	SER	SER	GLY	VAL	LEU	ASN
SER	SER	GLU	GLU	VAL	LEU	ASN
ASP	ASP	ASP	ASP	VAL	LEU	ILE
ASP	ASP	PHE	PHE	THR	LEU	LEU
LYS	LYS	PHE	PHE	PHE	GLY	GLU
GLU	GLU	SER	SER	VAL	VAL	GLN
GLU	GLU	SER	SER	VAL	GLY	GLN
LEU	LEU	VAL	VAL	ASP	ASP	ASP
LEU	LEU	THR	THR	ARG	TRP	ILE
ASN	ASN	ASN	ASN	THR	TYR	ALA
ASN	ASN	SER	SER	TYR	LYS	LYS
GLY	GLY	SER	SER	ASN	ASP	TYR
VAL	VAL	ILE	ILE	MET	GLY	VAL
ASN	ASN	LEU	LEU	ARG	ASN	ALA
TRP	TRP	GLU	GLU	GLY	ALA	GLN
GLN	GLN	ASP	VAL	GLU	LEU	SER
GLY	GLY	VAL	ASP	ASP	TYR	ASP
THR	THR	SER	SER	ILE	ILE	THR
ALA	ALA	LEU	LEU	VAL	TYR	VAL
SER	SER	ILE	ILE	ILE	ASP	GLY
PHE	PHE	ALA	ALA	PRO	SER	SER
GLY	GLY	TYR	TYR	GLY	GLY	PHE
ASP	ASP	PRO	PRO	VAL	GLU	PHE
SER	SER	GLU	GLU	THR	GLU	ARG
PHE	PHE	THR	THR	ALA	L110	PHE
GLY	GLY	ASN	VAL	VAL	L117	ARG
ALA	ALA	SER	VAL	VAL	E118	SER
SER	SER	ILE	GLU	GLU	M119	ALA
PHE	PHE	LEU	ARG	ARG	I120	LEU
ASN	ASN	VAL	LEU	LEU	Y128	ASN
MET	MET	LYS	LYS	LEU	L129	TYR
SER	SER	GLY	ASN	ASN	E130	ASN
SER	SER	ASN	GLY	GLY	L139	PRO
THR	THR	ASP	THR	THR	THR	THR

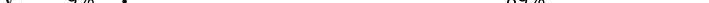
[illegible]

- Molecule 7: Outer membrane protein MxiD

Chain x: 10% . 89%

[illegible]

- Molecule 7: Outer membrane protein MxiD

Chain v:  9% . 89%

Y135	D136	H137	D147	E160	N164	T167	K171	GLN	VAL	SER	SER	GLY	ASP	LYS	VAL	VAL	ASN	ASN	ASN	ASN	ASP	SER	HIS	LEU	LEU	LEU	GLY	GLN	ASN	ASP	ILE	ALA	LYS	TYR	VAL	ALA	GLN	SER	ASP	THR	VAL	GLY	SER	PHE	PHE	GLU	ARG	PHE	SER	ALA	LEU	LEU	ASN	TYR	PRO	TIF
Met	Lys	Phe	Lys	Ala	Lys	Lys	Lys	Val	Phe	Leu	Ser	Gly	Asp	Leu	Pro	Val	Ala	Met	Val	Val	Asn	Ser	His	Leu	Leu	Leu	Gly	Gln	Asn	Asp	Leu	Ala	Lys	Tyr	Val	Ala	Gln	Ser	Asp	Thr	Val	Gly	Ser	Phe	Phe	Glu	Arg	Phe	Ser	Ala	Leu	Leu	Asn	Tyr	Pro	Tif

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

- Molecule 7: Outer membrane protein MxiD

Chain z: 9% : 89%

[illegible]

- Molecule 7: Outer membrane protein MxiD

Chain 1: 8% 89%

MET	LYS	LYS	LYS	ASN	ILE	LYS	SER	SER	LEU	LEU	THR	LEU	LEU	LEU	ILE	VAL	VAL	VAL	ASN	ASN	ALA	ALA	ASN	ASN	ILE	ASP	SER	SER	HIS	LEU	LEU	LEU	GLU	GLN	GLN	ASP	ASN	ASP	ILE	ALA	LYS	TYR	VAL	VAL	ALA	ALA	GLN	SER	SER	PHE	PHE	GLU	GLY	VAL	GLY	THR	THR	ASP	ASP	LYS	ALA	ALA	SER	SER	ASN	TYR	PRO	PRO	ILE
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ILE	GLN	THR	GLY	SER	THR	GLY	GLY	GLY	THR	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
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● Molecule 7: Outer membrane protein MxiD

Chain 3: 8% . 89%

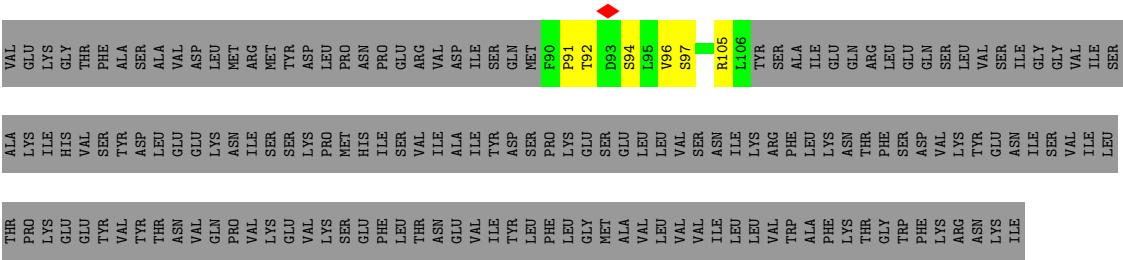
VAL	ARG	GLU	THR	VAL	ASP	TYR	PRO	THR	VAL	MET
VAL	PHE	VAL	GLY	SER	PHE	LEU	VAL	SER	LEU	LYS
ILE	LEU	ARG	THR	VAL	GLY	GLY	THR	ASN	VAL	PHE
GLN	GLN	GLY	THR	GLY	PHE	GLU	THR	ILE	GLU	ASN
PRO	ARG	ILE	ILE	ARG	ASN	ARG	ILE	VAL	LYS	SER
SER	ARG	SER	SER	SER	MET	ASN	THR	GLY	LEU	LEU
GLU	GLU	THR	THR	ASN	SER	THR	THR	ASN	ASN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

● Molecule 7: Outer membrane protein MxiD

[illegible]

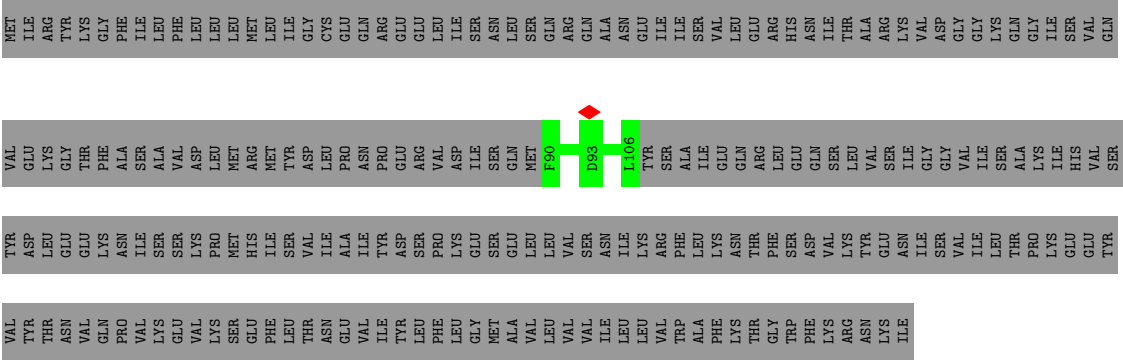
Chain 7: 9% . 89%

[illegible]



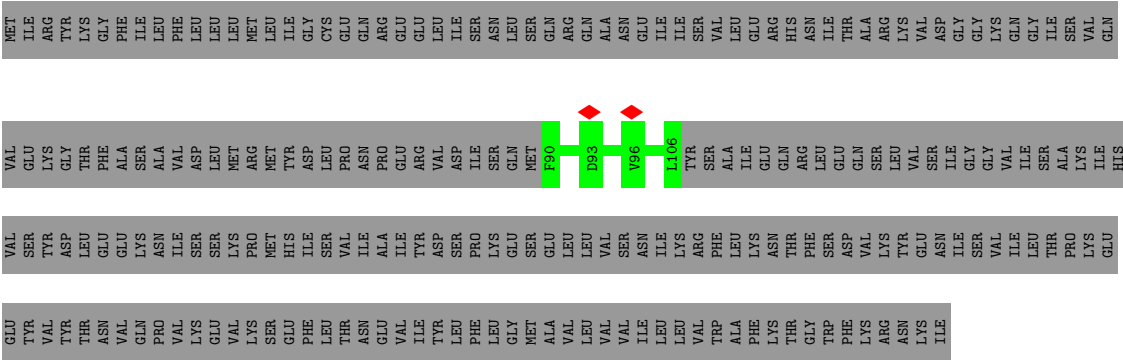
● Molecule 8: Lipoprotein MxiJ

Chain c0: 7% 93%



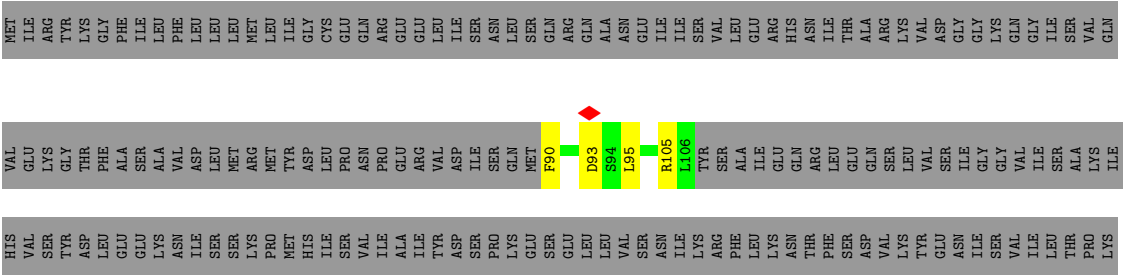
● Molecule 8: Lipoprotein MxiJ

Chain d0: 7% 93%



● Molecule 8: Lipoprotein MxiJ

Chain e0: 5% 93%



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

● Molecule 8: Lipoprotein MxiJ

Chain m0: 7% 93%

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

● Molecule 8: Lipoprotein MxiJ

Chain n0: 7% 93%

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

● Molecule 8: Lipoprotein MxiJ

Chain o0: 6% 93%

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

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

● Molecule 8: Lipoprotein MxiJ

[illegible][illegible][illegible]

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

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	90547	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	101179	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.306	Depositor
Minimum map value	-0.209	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	498.41714, 498.41714, 498.41714	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.038369, 1.038369, 1.038369	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.12	0/1516	0.29	0/2051
1	B	0.11	0/1488	0.30	0/2012
1	C	0.12	0/1509	0.31	0/2041
1	D	0.12	0/1466	0.28	0/1982
1	E	0.13	0/1494	0.29	0/2022
2	F	0.13	0/2071	0.29	0/2811
3	G	0.12	0/669	0.26	0/908
3	H	0.09	0/587	0.23	0/794
3	I	0.11	0/506	0.23	0/682
3	J	0.10	0/533	0.23	0/721
4	K	0.14	0/979	0.35	0/1324
5	M	0.12	0/309	0.32	0/417
5	N	0.12	0/648	0.26	0/876
5	O	0.14	0/734	0.38	0/994
5	P	0.11	0/713	0.29	0/965
5	Q	0.10	0/645	0.25	0/872
5	R	0.10	0/646	0.24	0/871
6	S	0.12	0/482	0.23	0/651
6	T	0.12	0/473	0.29	0/639
6	U	0.11	0/482	0.26	0/651
6	V	0.12	0/473	0.24	0/639
6	W	0.11	0/473	0.22	0/639
6	a	0.11	0/653	0.23	0/888
6	b	0.11	0/647	0.24	0/880
6	c	0.11	0/653	0.24	0/888
6	d	0.11	0/653	0.26	0/888
6	e	0.10	0/647	0.25	0/880
6	f	0.11	0/647	0.24	0/880
6	g	0.10	0/610	0.21	0/827
6	h	0.11	0/602	0.21	0/816
6	i	0.11	0/602	0.21	0/816
6	j	0.11	0/610	0.23	0/827
6	k	0.11	0/602	0.23	0/816
6	l	0.11	0/610	0.21	0/827

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	m	0.10	0/653	0.23	0/888
6	n	0.11	0/653	0.24	0/888
6	o	0.12	0/647	0.24	0/880
6	p	0.12	0/653	0.28	0/888
6	q	0.11	0/653	0.23	0/888
6	r	0.11	0/653	0.25	0/888
6	s	0.11	0/647	0.25	0/880
6	t	0.11	0/626	0.22	0/849
6	u	0.11	0/647	0.23	0/880
6	v	0.11	0/653	0.25	0/888
6	w	0.10	0/653	0.24	0/888
7	0	0.09	0/506	0.26	0/689
7	1	0.10	0/506	0.27	0/689
7	2	0.09	0/506	0.25	0/689
7	3	0.10	0/506	0.28	0/689
7	4	0.09	0/506	0.28	0/689
7	5	0.09	0/506	0.25	0/689
7	6	0.11	0/506	0.30	0/689
7	7	0.11	0/506	0.29	0/689
7	8	0.10	0/506	0.26	0/689
7	9	0.11	0/506	0.30	0/689
7	X	0.10	0/506	0.30	0/689
7	Y	0.11	0/506	0.29	0/689
7	Z	0.09	0/506	0.26	0/689
7	x	0.09	0/506	0.26	0/689
7	y	0.11	0/506	0.25	0/689
7	z	0.09	0/506	0.27	0/689
8	a0	0.16	0/133	0.38	0/179
8	b0	0.16	0/133	0.46	0/179
8	c0	0.12	0/133	0.39	0/179
8	d0	0.14	0/133	0.32	0/179
8	e0	0.15	0/133	0.35	0/179
8	f0	0.12	0/133	0.31	0/179
8	g0	0.12	0/133	0.37	0/179
8	h0	0.10	0/133	0.29	0/179
8	i0	0.11	0/133	0.26	0/179
8	j0	0.13	0/133	0.35	0/179
8	k0	0.13	0/133	0.29	0/179
8	l0	0.11	0/133	0.25	0/179
8	m0	0.11	0/133	0.30	0/179
8	n0	0.11	0/133	0.27	0/179
8	o0	0.14	0/133	0.43	0/179
8	p0	0.18	0/133	0.60	0/179

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
8	q0	0.13	0/133	0.30	0/179
8	r0	0.13	0/133	0.38	0/179
8	s0	0.14	0/133	0.32	0/179
8	t0	0.17	0/133	0.56	0/179
8	u0	0.13	0/133	0.33	0/179
8	v0	0.13	0/133	0.47	0/179
8	w0	0.14	0/133	0.45	0/179
8	x0	0.17	0/133	0.36	0/179
All	All	0.11	0/44858	0.28	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 ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1486	0	1557	29	0
1	B	1459	0	1531	23	0
1	C	1480	0	1546	31	0
1	D	1438	0	1516	30	0
1	E	1464	0	1536	27	0
2	F	2018	0	2086	37	0
3	G	656	0	704	13	0
3	H	575	0	624	9	0
3	I	494	0	527	13	0
3	J	521	0	558	6	0
4	K	953	0	995	22	0
5	M	308	0	327	7	0
5	N	644	0	665	8	0
5	O	727	0	736	11	0
5	P	707	0	716	18	0
5	Q	641	0	659	11	0
5	R	643	0	655	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	S	477	0	488	5	0
6	T	468	0	480	6	0
6	U	477	0	488	8	0
6	V	468	0	480	7	0
6	W	468	0	480	8	0
6	a	644	0	633	16	0
6	b	638	0	628	12	0
6	c	644	0	633	10	0
6	d	644	0	633	15	0
6	e	638	0	628	13	0
6	f	638	0	628	12	0
6	g	602	0	590	17	0
6	h	594	0	586	14	0
6	i	594	0	586	11	0
6	j	602	0	590	9	0
6	k	594	0	586	13	0
6	l	602	0	590	9	0
6	m	644	0	633	14	0
6	n	644	0	633	8	0
6	o	638	0	628	16	0
6	p	644	0	633	7	0
6	q	644	0	633	20	0
6	r	644	0	633	12	0
6	s	638	0	628	9	0
6	t	617	0	604	7	0
6	u	638	0	628	7	0
6	v	644	0	633	9	0
6	w	644	0	633	5	0
7	0	497	0	517	8	0
7	1	497	0	517	10	0
7	2	497	0	517	5	0
7	3	497	0	517	13	0
7	4	497	0	517	15	0
7	5	497	0	517	8	0
7	6	497	0	517	8	0
7	7	497	0	517	9	0
7	8	497	0	517	7	0
7	9	497	0	517	12	0
7	X	497	0	517	6	0
7	Y	497	0	517	10	0
7	Z	497	0	517	6	0
7	x	497	0	517	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	y	497	0	517	8	0
7	z	497	0	517	5	0
8	a0	131	0	134	3	0
8	b0	131	0	134	3	0
8	c0	131	0	134	0	0
8	d0	131	0	134	0	0
8	e0	131	0	134	2	0
8	f0	131	0	134	1	0
8	g0	131	0	134	1	0
8	h0	131	0	134	0	0
8	i0	131	0	134	1	0
8	j0	131	0	134	2	0
8	k0	131	0	134	1	0
8	l0	131	0	134	0	0
8	m0	131	0	134	0	0
8	n0	131	0	134	1	0
8	o0	131	0	134	3	0
8	p0	131	0	134	5	0
8	q0	131	0	134	1	0
8	r0	131	0	134	1	0
8	s0	131	0	134	1	0
8	t0	131	0	134	3	0
8	u0	131	0	134	2	0
8	v0	131	0	134	1	0
8	w0	131	0	134	0	0
8	x0	131	0	134	2	0
All	All	44141	0	45072	564	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (564) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:LEU:HA	1:A:138:LEU:HB3	1.68	0.74
5:Q:14:LYS:NZ	7:X:164:ASN:OD1	2.19	0.74
5:O:12:ILE:HD13	7:4:164:ASN:HD22	1.53	0.73
5:O:14:LYS:HZ2	7:4:160:GLU:HB3	1.54	0.71
6:a:72:LYS:HG3	6:g:55:SER:HB3	1.71	0.71
6:q:55:SER:HB3	6:w:72:LYS:HG3	1.73	0.71
6:U:80:GLN:OE1	6:U:83:ARG:NH1	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:14:LYS:NZ	7:7:164:ASN:OD1	2.24	0.70
6:S:81:ASN:HB2	6:T:83:ARG:HH21	1.54	0.70
1:E:46:VAL:HG13	1:E:47:PRO:HD3	1.74	0.69
5:O:4:ILE:HG23	5:O:6:PRO:HD2	1.73	0.69
2:F:77:LYS:NZ	2:F:162:SER:O	2.27	0.68
7:4:140:PRO:HG2	7:4:142:ARG:HH12	1.58	0.68
6:S:55:SER:HB3	6:k:72:LYS:HG3	1.74	0.68
6:U:55:SER:HB3	6:i:72:LYS:HG3	1.75	0.67
8:a0:91:PRO:HG2	8:a0:94:SER:HB2	1.75	0.67
1:C:205:LYS:NZ	1:D:110:GLU:OE2	2.26	0.67
3:G:40:THR:HG23	3:G:42:LEU:HG	1.77	0.66
1:A:163:VAL:HA	3:G:15:ILE:HD11	1.77	0.66
5:Q:10:VAL:HG22	7:9:116:LEU:HB3	1.78	0.66
6:W:65:SER:OG	6:h:81:ASN:ND2	2.28	0.66
1:A:38:ARG:HD2	1:A:47:PRO:HG2	1.77	0.66
6:e:72:LYS:HG3	6:k:55:SER:HB3	1.78	0.66
7:5:120:ILE:HD12	7:5:169:LEU:HB3	1.77	0.66
4:K:54:TYR:HB3	8:x0:95:LEU:HD23	1.77	0.66
6:o:55:SER:HB3	6:u:72:LYS:HG3	1.78	0.65
1:B:25:THR:HG23	1:B:27:TYR:H	1.60	0.65
5:P:23:ILE:HG22	5:P:29:VAL:HG22	1.77	0.65
6:k:43:ASN:OD1	6:k:43:ASN:N	2.30	0.65
6:g:83:ARG:NH2	6:h:81:ASN:OD1	2.30	0.65
7:y:160:GLU:O	7:y:164:ASN:ND2	2.29	0.64
7:9:129:LEU:HD21	7:9:165:THR:HG21	1.78	0.64
1:C:210:GLN:NE2	3:I:82:ILE:O	2.23	0.64
6:f:55:SER:HB3	6:m:72:LYS:HG3	1.79	0.64
6:W:38:ALA:O	6:h:23:THR:OG1	2.17	0.63
1:A:29:LYS:NZ	1:A:211:TYR:OH	2.32	0.63
1:D:205:LYS:NZ	1:E:110:GLU:OE2	2.28	0.63
6:o:81:ASN:OD1	6:p:83:ARG:NH2	2.31	0.63
1:E:203:LEU:HA	4:K:60:ASN:HD21	1.64	0.62
1:A:23:ALA:HA	1:A:28:ILE:HD11	1.80	0.62
8:j0:102:GLU:OE1	8:k0:100:ARG:NH1	2.32	0.62
7:4:128:TYR:HE1	7:3:144:ASN:H	1.48	0.62
7:1:129:LEU:HB3	7:1:135:TYR:HB2	1.82	0.61
6:u:23:THR:HG22	6:u:26:LEU:HB2	1.82	0.61
5:Q:11:ASP:HB2	7:9:115:ILE:HG23	1.82	0.61
1:A:49:ASN:O	1:A:53:ASN:ND2	2.27	0.61
6:c:65:SER:OG	6:o:81:ASN:ND2	2.31	0.61
1:A:38:ARG:NH2	1:A:44:GLN:O	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:5:171:LYS:H	7:5:171:LYS:HD3	1.66	0.60
6:e:31:THR:HB	6:m:6:PRO:HD3	1.83	0.60
7:7:134:LEU:HD13	7:7:161:LEU:HD21	1.84	0.60
1:C:134:SER:HB3	1:C:137:SER:HB3	1.83	0.60
6:q:38:ALA:O	6:v:23:THR:OG1	2.20	0.60
6:S:77:ALA:O	6:T:83:ARG:NH2	2.35	0.59
7:Z:149:THR:O	7:z:128:TYR:OH	2.19	0.59
5:N:10:VAL:HB	7:0:116:LEU:HB3	1.83	0.59
7:3:120:ILE:HD12	7:3:169:LEU:HB3	1.83	0.59
1:A:46:VAL:HG11	1:B:36:MET:HE2	1.84	0.59
5:P:59:ASN:N	5:P:59:ASN:OD1	2.33	0.59
8:t0:102:GLU:OE2	8:u0:100:ARG:NH1	2.33	0.59
6:U:43:ASN:HD22	6:U:46:LEU:HG	1.67	0.58
7:1:114:VAL:HG22	7:1:151:TYR:HD1	1.69	0.58
6:w:37:LEU:HD11	6:w:47:LEU:HD23	1.84	0.58
1:A:148:LYS:HA	2:F:139:LEU:HD21	1.84	0.58
1:D:100:LYS:HG2	1:D:104:LYS:HE3	1.85	0.58
5:O:10:VAL:HB	7:3:116:LEU:HB3	1.84	0.58
6:W:25:THR:OG1	6:W:26:LEU:N	2.37	0.58
6:a:23:THR:OG1	6:f:38:ALA:O	2.21	0.58
6:b:55:SER:HB3	6:q:72:LYS:HG3	1.86	0.58
1:A:96:LEU:HD22	1:A:100:LYS:HE3	1.83	0.58
6:k:40:ASN:HD22	6:m:11:THR:HB	1.68	0.58
1:A:162:VAL:HG21	2:F:129:PHE:HB2	1.86	0.58
5:P:8:ASN:N	5:P:8:ASN:OD1	2.36	0.58
5:P:8:ASN:ND2	5:P:11:ASP:OD2	2.28	0.58
5:R:12:ILE:O	7:Y:113:LYS:HA	2.04	0.58
1:C:107:THR:HG21	1:C:138:LEU:HD11	1.85	0.58
7:Y:123:ASN:HB2	7:Y:145:ILE:HD12	1.85	0.58
1:C:109:LEU:HD22	1:C:133:TYR:HE2	1.69	0.58
6:b:20:ASP:OD1	6:b:60:TYR:OH	2.22	0.58
6:h:43:ASN:ND2	6:p:8:ASP:O	2.37	0.58
3:G:37:GLN:HE22	3:G:42:LEU:HD12	1.68	0.58
6:V:38:ALA:O	6:i:23:THR:OG1	2.18	0.58
6:d:38:ALA:O	6:n:23:THR:OG1	2.21	0.58
7:4:164:ASN:HA	7:4:167:THR:HG22	1.86	0.57
1:D:21:VAL:O	1:D:25:THR:OG1	2.19	0.57
6:b:83:ARG:NH1	6:h:66:ASN:OD1	2.37	0.57
6:f:72:LYS:HG3	6:l:55:SER:HB3	1.87	0.57
8:o0:95:LEU:HA	8:p0:95:LEU:HD12	1.86	0.57
6:n:20:ASP:OD1	6:n:60:TYR:OH	2.23	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:q:50:TYR:HH	6:v:67:THR:HG1	1.50	0.57
2:F:11:HIS:HD2	5:M:73:TYR:HB3	1.70	0.57
3:G:72:LEU:O	3:G:76:HIS:ND1	2.36	0.57
5:P:10:VAL:HB	7:6:116:LEU:HB3	1.85	0.57
6:q:38:ALA:HB1	6:v:22:GLY:HA3	1.86	0.57
1:C:149:ASP:O	1:C:153:ILE:HG22	2.04	0.57
2:F:214:SER:OG	3:G:52:LYS:NZ	2.38	0.57
6:d:55:SER:HB3	6:o:72:LYS:HG3	1.87	0.57
6:n:55:SER:HB3	6:t:72:LYS:HG3	1.87	0.57
1:C:18:PRO:HG3	5:O:90:ALA:HA	1.85	0.57
6:e:55:SER:HB3	6:n:72:LYS:HG3	1.86	0.57
7:2:118:GLU:O	7:2:148:LYS:NZ	2.33	0.57
7:8:128:TYR:OH	7:7:149:THR:O	2.22	0.57
7:1:129:LEU:HD21	7:1:165:THR:HG21	1.87	0.57
1:A:18:PRO:HG3	5:Q:90:ALA:HA	1.86	0.56
1:A:21:VAL:O	1:A:25:THR:OG1	2.22	0.56
5:P:71:SER:HB3	6:V:72:LYS:HG2	1.85	0.56
6:T:38:ALA:HB1	6:k:22:GLY:HA3	1.87	0.56
6:f:23:THR:HG23	6:f:26:LEU:HD12	1.87	0.56
1:E:54:GLY:HA3	2:F:87:PHE:HZ	1.71	0.56
6:T:61:ARG:HG3	6:k:78:ILE:HD11	1.88	0.56
6:a:45:GLN:NE2	6:a:49:GLU:OE2	2.39	0.56
6:i:43:ASN:ND2	6:o:10:TRP:O	2.38	0.56
8:b0:91:PRO:HB2	8:b0:94:SER:HB2	1.87	0.56
7:Z:171:LYS:NZ	7:y:147:ASP:OD1	2.37	0.56
8:j0:91:PRO:O	8:j0:105:ARG:NH2	2.39	0.56
6:U:38:ALA:O	6:j:23:THR:OG1	2.23	0.55
7:9:129:LEU:HB3	7:9:135:TYR:HB2	1.89	0.55
6:h:51:GLN:HB2	6:p:82:PHE:HE1	1.71	0.55
1:C:163:VAL:HA	3:I:15:ILE:HD11	1.87	0.55
1:E:18:PRO:HG3	5:M:90:ALA:HA	1.88	0.55
7:4:120:ILE:HD12	7:4:169:LEU:HB3	1.88	0.55
6:k:26:LEU:HD11	6:k:56:GLU:HB3	1.88	0.55
1:D:46:VAL:HB	1:D:47:PRO:HD3	1.89	0.55
1:A:29:LYS:NZ	1:A:146:GLU:OE1	2.40	0.54
1:A:186:SER:HB3	1:A:190:LYS:HE3	1.88	0.54
5:M:85:ARG:NH1	5:R:97:SER:O	2.41	0.54
5:P:48:ILE:HG13	5:P:66:LEU:HD11	1.88	0.54
1:E:55:ILE:HG13	2:F:175:LEU:HD23	1.90	0.54
7:2:114:VAL:HG22	7:2:151:TYR:HD1	1.72	0.54
1:A:1:MET:HE3	1:A:77:ASN:HD22	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:38:ARG:NH1	1:D:49:ASN:OD1	2.41	0.54
7:X:120:ILE:HD12	7:X:169:LEU:HB3	1.89	0.54
1:C:30:PHE:HE1	1:C:207:LEU:HB3	1.74	0.54
1:D:44:GLN:HG2	1:D:45:GLN:H	1.73	0.54
7:1:160:GLU:O	7:1:164:ASN:ND2	2.41	0.54
6:e:43:ASN:ND2	6:s:8:ASP:O	2.41	0.54
5:O:10:VAL:HG11	7:3:116:LEU:HD23	1.90	0.53
6:u:20:ASP:OD1	6:u:60:TYR:OH	2.26	0.53
4:K:51:MET:HB2	4:K:81:ILE:HD11	1.91	0.53
4:K:68:LYS:HB2	8:v0:96:VAL:HB	1.90	0.53
6:m:38:ALA:O	6:r:23:THR:OG1	2.25	0.53
1:B:111:LEU:HD23	1:B:141:ALA:HA	1.89	0.53
2:F:103:ILE:HG21	2:F:228:ILE:HD11	1.89	0.53
5:Q:70:LEU:HD21	6:V:70:VAL:HG11	1.91	0.53
6:V:25:THR:OG1	6:V:26:LEU:N	2.42	0.53
7:X:117:LEU:HD22	7:X:120:ILE:HG22	1.89	0.53
6:k:43:ASN:HB2	6:k:46:LEU:HB2	1.90	0.53
7:7:136:ASP:N	7:7:136:ASP:OD1	2.42	0.53
6:s:36:LYS:HB3	6:s:46:LEU:HD11	1.90	0.53
6:W:34:LEU:HD11	6:h:15:LEU:HD11	1.90	0.52
6:a:20:ASP:OD1	6:a:60:TYR:OH	2.27	0.52
1:C:132:ASP:N	1:C:132:ASP:OD1	2.42	0.52
6:f:51:GLN:HB2	6:r:82:PHE:HE1	1.75	0.52
1:E:38:ARG:HH12	1:E:49:ASN:HB2	1.75	0.52
7:2:149:THR:O	7:3:128:TYR:OH	2.27	0.52
6:a:79:ILE:HG21	6:g:62:ASN:HB3	1.92	0.52
5:P:18:PHE:O	5:P:19:GLN:NE2	2.43	0.52
7:Y:142:ARG:HG3	7:y:134:LEU:HD21	1.91	0.52
7:Y:118:GLU:O	7:Y:148:LYS:NZ	2.41	0.52
6:d:23:THR:HG23	6:d:26:LEU:HD12	1.92	0.52
6:s:20:ASP:OD1	6:s:60:TYR:OH	2.27	0.52
5:Q:14:LYS:HZ2	7:X:160:GLU:C	2.17	0.52
1:D:209:GLU:HA	1:D:212:ILE:HG22	1.91	0.52
7:y:164:ASN:HA	7:y:167:THR:HG22	1.91	0.52
7:3:129:LEU:HB3	7:3:135:TYR:HB2	1.92	0.52
1:D:212:ILE:HG12	1:D:213:ASN:H	1.74	0.52
7:7:118:GLU:O	7:7:148:LYS:NZ	2.40	0.52
8:i0:93:ASP:OD1	8:i0:93:ASP:N	2.43	0.52
1:A:152:LYS:HD2	2:F:140:TYR:CE2	2.45	0.52
1:D:156:TYR:HB3	3:J:78:ILE:HD11	1.92	0.52
1:E:172:LEU:HD12	1:E:182:PRO:HG3	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:7:164:ASN:HA	7:7:167:THR:HG22	1.91	0.51
5:Q:13:ILE:HA	7:9:113:LYS:HG2	1.91	0.51
5:R:67:GLN:HB2	6:g:82:PHE:HE1	1.75	0.51
6:p:38:ALA:O	6:u:23:THR:OG1	2.28	0.51
1:C:156:TYR:HE1	3:I:7:MET:HG3	1.75	0.51
3:I:79:MET:HA	3:I:82:ILE:HD12	1.91	0.51
5:Q:59:ASN:OD1	5:Q:59:ASN:N	2.42	0.51
7:8:142:ARG:HG3	7:9:134:LEU:HD21	1.92	0.51
8:e0:93:ASP:OD1	8:e0:93:ASP:N	2.42	0.51
1:B:172:LEU:HD11	1:B:185:ILE:HD12	1.92	0.51
7:X:128:TYR:OH	7:9:149:THR:O	2.28	0.51
7:0:129:LEU:HD21	7:0:165:THR:HG21	1.93	0.51
6:g:51:GLN:HB2	6:q:82:PHE:HE1	1.75	0.51
7:7:120:ILE:HD12	7:7:169:LEU:HB3	1.91	0.51
6:a:38:ALA:O	6:q:23:THR:OG1	2.26	0.51
6:d:36:LYS:HB3	6:d:46:LEU:HD11	1.92	0.51
6:i:20:ASP:OD1	6:i:60:TYR:OH	2.27	0.51
1:D:146:GLU:OE1	1:D:211:TYR:OH	2.27	0.51
5:P:17:ASP:OD1	5:P:17:ASP:N	2.44	0.51
6:W:55:SER:HB3	6:g:72:LYS:HG3	1.93	0.51
6:o:62:ASN:O	6:o:66:ASN:ND2	2.33	0.51
5:N:8:ASN:OD1	5:N:8:ASN:N	2.44	0.51
7:8:117:LEU:HD22	7:8:120:ILE:HB	1.93	0.51
6:b:23:THR:HG23	6:b:26:LEU:HD12	1.93	0.51
1:E:164:VAL:HG23	4:K:52:LEU:HD13	1.93	0.50
6:w:32:LEU:HD11	6:w:36:LYS:HE3	1.92	0.50
3:J:3:ASP:OD1	3:J:3:ASP:N	2.44	0.50
7:5:135:TYR:HE1	7:5:141:ILE:HG13	1.76	0.50
6:d:44:PRO:HB2	6:o:61:ARG:HE	1.76	0.50
6:f:15:LEU:HD21	6:k:34:LEU:HD21	1.93	0.50
6:t:43:ASN:HB3	6:t:46:LEU:HB3	1.91	0.50
6:o:20:ASP:OD1	6:o:60:TYR:OH	2.30	0.50
1:B:5:MET:HE3	1:B:8:ILE:HD12	1.93	0.50
7:1:134:LEU:HB3	7:1:161:LEU:HD21	1.94	0.50
5:O:67:GLN:HB2	6:j:82:PHE:HE1	1.76	0.50
5:R:13:ILE:HG22	7:Y:113:LYS:HE2	1.94	0.50
8:u0:98:SER:O	8:u0:101:ALA:N	2.41	0.50
3:G:3:ASP:OD1	3:G:3:ASP:N	2.44	0.50
8:r0:96:VAL:HG13	8:s0:96:VAL:HG21	1.93	0.50
1:A:4:ASP:OD1	1:A:4:ASP:N	2.45	0.50
1:D:101:GLN:HA	1:D:104:LYS:HZ1	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:98:ALA:O	2:F:102:ILE:HG23	2.12	0.50
7:0:117:LEU:HD13	7:0:120:ILE:HG23	1.94	0.50
6:q:45:GLN:NE2	6:q:49:GLU:OE2	2.45	0.50
6:r:41:PRO:HG3	6:w:60:TYR:HB2	1.92	0.50
1:C:111:LEU:HD21	1:C:144:LEU:HD12	1.94	0.49
7:8:149:THR:O	7:9:128:TYR:OH	2.29	0.49
2:F:210:MET:HG3	3:G:34:GLY:HA3	1.95	0.49
3:G:36:LEU:O	3:G:40:THR:HG22	2.11	0.49
6:q:65:SER:OG	6:v:81:ASN:ND2	2.40	0.49
8:p0:94:SER:OG	8:p0:95:LEU:N	2.45	0.49
6:n:43:ASN:HB3	6:n:46:LEU:HB2	1.94	0.49
6:q:36:LYS:HB3	6:q:46:LEU:HD11	1.95	0.49
6:t:20:ASP:OD1	6:t:60:TYR:OH	2.27	0.49
3:H:18:PHE:O	3:H:67:TYR:OH	2.28	0.49
6:p:36:LYS:HB3	6:p:46:LEU:HD11	1.93	0.49
6:v:20:ASP:OD1	6:v:60:TYR:OH	2.28	0.49
7:4:128:TYR:HD2	7:4:169:LEU:HD11	1.77	0.49
3:H:72:LEU:O	3:H:76:HIS:ND1	2.33	0.49
4:K:51:MET:HB3	4:K:55:ARG:HH22	1.77	0.49
7:3:118:GLU:O	7:3:148:LYS:NZ	2.35	0.49
6:h:43:ASN:HB3	6:h:46:LEU:HB3	1.94	0.49
6:m:36:LYS:HB3	6:m:46:LEU:HD11	1.94	0.49
1:D:200:TRP:HB3	1:E:144:LEU:HD22	1.94	0.49
1:E:96:LEU:HD11	1:E:135:LEU:HD11	1.94	0.49
7:9:120:ILE:HD11	7:9:124:TYR:HD2	1.78	0.49
8:n0:102:GLU:OE1	8:o0:100:ARG:NE	2.37	0.49
5:N:10:VAL:HG11	7:0:116:LEU:HD23	1.94	0.49
7:8:129:LEU:HD21	7:8:165:THR:HG21	1.95	0.49
6:c:28:GLY:O	6:c:31:THR:OG1	2.29	0.49
6:e:36:LYS:HB3	6:e:46:LEU:HD11	1.95	0.49
1:A:27:TYR:OH	1:A:53:ASN:OD1	2.28	0.48
1:C:36:MET:HE2	1:C:36:MET:HB3	1.70	0.48
7:Y:149:THR:O	7:y:128:TYR:OH	2.30	0.48
7:4:149:THR:O	7:5:128:TYR:OH	2.31	0.48
6:f:20:ASP:OD1	6:f:60:TYR:OH	2.30	0.48
1:B:104:LYS:HG2	1:B:109:LEU:HD21	1.96	0.48
2:F:30:PHE:HB2	2:F:86:SER:HB3	1.96	0.48
7:4:134:LEU:HD21	7:3:142:ARG:HG3	1.96	0.48
6:l:16:SER:HA	6:l:64:GLN:HE21	1.79	0.48
1:B:21:VAL:O	1:B:25:THR:HG22	2.14	0.48
1:C:46:VAL:HG13	1:D:35:VAL:HB	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:92:GLU:OE2	5:N:96:LYS:NZ	2.31	0.48
6:j:36:LYS:HB3	6:j:46:LEU:HD11	1.96	0.48
6:l:26:LEU:HD11	6:l:56:GLU:HB3	1.95	0.48
6:q:27:GLN:O	6:q:31:THR:OG1	2.30	0.48
6:e:27:GLN:HB3	6:m:6:PRO:HG2	1.95	0.48
6:f:36:LYS:HB3	6:f:46:LEU:HD11	1.96	0.48
6:S:25:THR:HG23	6:S:28:GLY:H	1.79	0.48
6:j:74:VAL:O	6:j:78:ILE:HG12	2.13	0.48
1:C:173:LEU:HD23	3:H:49:PHE:CE1	2.49	0.47
7:0:141:ILE:HG12	7:0:152:ILE:HD13	1.94	0.47
7:4:120:ILE:HG23	7:4:124:TYR:HB3	1.96	0.47
6:t:49:GLU:O	6:t:53:LYS:HG2	2.14	0.47
6:o:41:PRO:HG3	6:t:60:TYR:HB2	1.95	0.47
8:t0:94:SER:OG	8:t0:95:LEU:N	2.43	0.47
5:O:71:SER:HB3	6:U:72:LYS:HG2	1.96	0.47
7:1:140:PRO:HB2	7:1:142:ARG:HH12	1.79	0.47
6:p:49:GLU:O	6:p:53:LYS:HG2	2.14	0.47
1:B:111:LEU:HD21	1:B:144:LEU:HD12	1.96	0.47
1:B:185:ILE:O	1:B:188:PRO:HD2	2.14	0.47
2:F:199:LEU:HD11	4:K:144:LEU:HD22	1.97	0.47
6:b:72:LYS:HG3	6:h:55:SER:HB3	1.96	0.47
6:i:51:GLN:HB2	6:o:82:PHE:HE1	1.79	0.47
6:q:23:THR:HG22	6:q:26:LEU:HB2	1.96	0.47
1:B:7:LEU:HD11	5:P:79:LEU:HD13	1.97	0.47
6:W:51:GLN:HB2	6:b:82:PHE:HE1	1.79	0.47
6:l:20:ASP:OD1	6:l:60:TYR:OH	2.33	0.47
6:m:49:GLU:O	6:m:53:LYS:HG2	2.14	0.47
6:v:9:ASP:OD1	6:v:9:ASP:N	2.47	0.47
3:H:66:TRP:O	3:H:69:GLU:HG3	2.15	0.47
4:K:53:LEU:HD13	4:K:53:LEU:HA	1.74	0.47
5:N:12:ILE:HG21	7:1:164:ASN:CG	2.40	0.47
7:2:129:LEU:HD21	7:2:165:THR:HG21	1.97	0.47
6:a:6:PRO:HD3	6:f:31:THR:HB	1.96	0.47
1:D:43:LEU:HB3	1:D:46:VAL:HG23	1.97	0.47
5:O:58:LEU:HB2	6:j:11:THR:HG23	1.96	0.47
7:0:114:VAL:HG22	7:0:151:TYR:HD1	1.80	0.47
6:j:43:ASN:ND2	6:n:8:ASP:O	2.48	0.47
6:o:49:GLU:O	6:o:53:LYS:HG2	2.15	0.47
1:A:200:TRP:HB3	1:B:144:LEU:HD22	1.96	0.47
6:b:36:LYS:HB3	6:b:46:LEU:HD11	1.96	0.47
6:c:5:VAL:HB	6:c:7:ASN:HD22	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:g:20:ASP:OD1	6:g:60:TYR:OH	2.33	0.47
1:D:197:LEU:HD22	3:J:75:CYS:HB3	1.97	0.46
1:E:184:THR:OG1	2:F:197:GLU:OE1	2.29	0.46
2:F:11:HIS:CD2	5:M:73:TYR:HB3	2.49	0.46
7:3:120:ILE:HG23	7:3:124:TYR:HB3	1.98	0.46
6:a:49:GLU:O	6:a:53:LYS:HG2	2.15	0.46
6:s:43:ASN:OD1	6:s:46:LEU:N	2.39	0.46
6:s:49:GLU:O	6:s:53:LYS:HG2	2.15	0.46
1:E:183:ILE:HD13	2:F:115:ILE:HD11	1.98	0.46
1:D:46:VAL:HG13	1:E:35:VAL:HB	1.97	0.46
7:X:147:ASP:OD1	7:x:171:LYS:NZ	2.43	0.46
6:c:4:THR:HG21	6:c:15:LEU:HD13	1.98	0.46
3:H:50:GLY:O	3:H:54:ILE:HG12	2.14	0.46
4:K:35:LEU:HD11	4:K:182:ILE:HD11	1.97	0.46
5:R:40:ASP:O	5:R:43:ILE:HG13	2.14	0.46
6:a:65:SER:OG	6:q:81:ASN:OD1	2.25	0.46
7:5:134:LEU:HD13	7:5:161:LEU:HD21	1.97	0.46
1:C:4:ASP:OD1	1:C:4:ASP:N	2.47	0.46
1:C:152:LYS:HE2	1:C:156:TYR:HE2	1.81	0.46
1:B:115:PHE:O	1:B:118:SER:OG	2.21	0.46
3:G:54:ILE:HG12	3:H:16:LEU:HD11	1.98	0.46
7:8:129:LEU:HB3	7:8:135:TYR:HB2	1.97	0.46
6:o:43:ASN:HB3	6:o:46:LEU:HB2	1.97	0.46
1:D:111:LEU:HD21	1:D:144:LEU:HD12	1.98	0.46
6:a:43:ASN:HB3	6:a:46:LEU:HB3	1.97	0.46
8:f0:92:THR:OG1	8:f0:93:ASP:N	2.50	0.46
5:Q:52:VAL:HG21	6:V:67:THR:HG21	1.97	0.45
6:m:11:THR:OG1	6:m:12:LEU:N	2.49	0.45
8:e0:90:PHE:O	8:e0:105:ARG:NH1	2.46	0.45
7:1:164:ASN:HA	7:1:167:THR:HG22	1.98	0.45
6:q:20:ASP:OD1	6:q:60:TYR:OH	2.34	0.45
6:r:26:LEU:HD23	6:r:26:LEU:HA	1.85	0.45
8:p0:91:PRO:O	8:p0:105:ARG:NH2	2.50	0.45
1:D:24:GLY:O	1:D:99:TYR:OH	2.32	0.45
4:K:132:LYS:H	4:K:132:LYS:HD3	1.82	0.45
7:2:171:LYS:NZ	7:1:147:ASP:OD1	2.47	0.45
7:x:129:LEU:HB3	7:x:135:TYR:HB2	1.98	0.45
6:i:43:ASN:ND2	6:o:10:TRP:H	2.14	0.45
6:k:15:LEU:HD21	6:k:67:THR:HG22	1.97	0.45
1:B:38:ARG:HG3	1:B:47:PRO:HG2	1.97	0.45
6:U:55:SER:OG	6:i:72:LYS:NZ	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:3:164:ASN:O	7:3:168:LEU:HB2	2.17	0.45
6:l:12:LEU:HD23	6:l:68:VAL:HG13	1.97	0.45
1:D:14:PHE:CD2	5:N:83:LEU:HD22	2.52	0.45
2:F:193:LEU:HD11	2:F:224:ALA:HB2	1.97	0.45
4:K:150:PHE:HD2	4:K:184:PHE:HZ	1.64	0.45
6:b:60:TYR:HB2	6:g:41:PRO:HG3	1.99	0.45
8:t:0:95:LEU:HD23	8:t:0:95:LEU:HA	1.86	0.45
1:A:43:LEU:HD22	1:A:46:VAL:HG21	1.99	0.45
2:F:102:ILE:HD11	2:F:186:ALA:HB1	1.99	0.45
6:a:60:TYR:HB2	6:f:41:PRO:HG3	1.99	0.45
6:d:5:VAL:HB	6:d:7:ASN:HD22	1.80	0.45
6:o:62:ASN:HB3	6:u:79:ILE:HG21	1.98	0.45
7:z:117:LEU:HD12	7:z:148:LYS:HB3	1.97	0.45
7:Y:129:LEU:HB3	7:Y:135:TYR:HB2	1.98	0.45
6:q:49:GLU:O	6:q:53:LYS:HG2	2.17	0.45
3:I:51:ILE:HA	3:I:54:ILE:HG22	1.99	0.45
4:K:144:LEU:O	4:K:148:THR:OG1	2.32	0.45
6:a:38:ALA:HB1	6:q:22:GLY:HA3	1.99	0.45
1:C:67:ILE:HD13	1:C:98:GLU:HG3	1.98	0.45
1:D:96:LEU:HD11	1:D:135:LEU:HD22	1.97	0.45
5:Q:7:VAL:HG12	7:9:167:THR:HG21	1.98	0.45
3:G:13:TYR:HE1	8:o:0:96:VAL:HB	1.81	0.44
5:O:17:ASP:N	5:O:17:ASP:OD1	2.50	0.44
7:4:128:TYR:OH	7:3:149:THR:O	2.35	0.44
7:z:164:ASN:O	7:z:168:LEU:HB2	2.17	0.44
6:e:23:THR:OG1	6:j:38:ALA:O	2.32	0.44
6:l:40:ASN:ND2	6:l:40:ASN:O	2.51	0.44
3:H:47:LEU:HD23	3:I:52:LYS:HE3	1.98	0.44
7:Z:140:PRO:O	7:Z:142:ARG:NH1	2.50	0.44
6:a:55:SER:HB3	6:r:72:LYS:HG3	1.99	0.44
5:N:61:GLU:OE2	6:T:27:GLN:NE2	2.50	0.44
6:b:79:ILE:HG21	6:h:62:ASN:HB3	1.98	0.44
6:c:40:ASN:O	6:c:40:ASN:ND2	2.51	0.44
6:c:41:PRO:HG3	6:o:60:TYR:HB2	2.00	0.44
6:d:40:ASN:O	6:d:40:ASN:ND2	2.50	0.44
6:g:40:ASN:ND2	6:q:9:ASP:OD1	2.50	0.44
4:K:52:LEU:HD12	4:K:55:ARG:NH1	2.33	0.44
6:V:80:GLN:OE1	6:V:83:ARG:NH2	2.50	0.44
1:D:33:VAL:HG11	1:D:207:LEU:HD11	2.00	0.44
5:R:59:ASN:N	5:R:59:ASN:OD1	2.50	0.44
6:m:43:ASN:HB3	6:m:46:LEU:HB2	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:b:6:PRO:HD3	6:g:31:THR:HB	2.00	0.44
6:v:11:THR:OG1	6:v:12:LEU:N	2.50	0.44
3:H:53:LEU:HA	3:H:56:VAL:HG22	1.98	0.44
5:Q:6:PRO:HG2	5:Q:47:GLN:OE1	2.17	0.44
7:4:140:PRO:HG2	7:4:142:ARG:HH22	1.82	0.44
6:r:58:THR:HG23	6:w:74:VAL:HG22	1.99	0.44
1:C:38:ARG:HG3	1:C:47:PRO:HG2	2.00	0.44
5:P:14:LYS:HE3	5:P:14:LYS:HB3	1.71	0.44
7:Z:129:LEU:HD21	7:Z:165:THR:HG21	2.00	0.44
6:m:45:GLN:NE2	6:s:20:ASP:OD2	2.42	0.44
6:p:11:THR:OG1	6:p:12:LEU:N	2.51	0.44
1:A:112:ALA:O	1:A:116:GLN:HG2	2.18	0.43
2:F:116:ASP:OD2	2:F:119:ASN:N	2.48	0.43
6:m:27:GLN:HB3	6:r:6:PRO:HG3	2.01	0.43
1:E:159:LEU:HD12	4:K:70:PHE:CE1	2.53	0.43
1:E:208:ILE:HG21	2:F:172:LEU:HD11	2.00	0.43
2:F:200:LEU:HD22	2:F:200:LEU:HA	1.91	0.43
4:K:47:LEU:O	4:K:51:MET:HG2	2.18	0.43
7:4:142:ARG:HG3	7:5:134:LEU:HD21	1.99	0.43
6:g:12:LEU:HD12	6:g:12:LEU:H	1.83	0.43
6:k:29:GLU:HG2	6:k:53:LYS:HE3	1.99	0.43
6:v:49:GLU:O	6:v:53:LYS:HG2	2.18	0.43
3:G:31:LEU:O	3:G:35:LEU:HG	2.18	0.43
7:Z:171:LYS:HE3	7:Z:171:LYS:HB2	1.82	0.43
3:I:13:TYR:CE1	8:g0:95:LEU:HD23	2.54	0.43
6:d:49:GLU:O	6:d:53:LYS:HG2	2.19	0.43
1:C:48:SER:O	1:C:51:THR:N	2.41	0.43
1:C:49:ASN:O	1:C:53:ASN:ND2	2.43	0.43
1:D:30:PHE:HE1	1:D:207:LEU:HB3	1.83	0.43
1:D:109:LEU:HD22	1:D:133:TYR:HE2	1.82	0.43
3:I:78:ILE:O	3:I:82:ILE:HG13	2.18	0.43
5:M:70:LEU:HD12	6:l:82:PHE:HE1	1.83	0.43
6:q:26:LEU:HD23	6:q:26:LEU:HA	1.85	0.43
1:A:46:VAL:HB	1:A:47:PRO:HD3	2.00	0.43
1:D:153:ILE:HD11	3:J:82:ILE:HD12	2.00	0.43
1:E:111:LEU:HD21	1:E:144:LEU:HD12	2.00	0.43
7:5:114:VAL:HG22	7:5:151:TYR:HD1	1.84	0.43
6:e:26:LEU:HD23	6:e:26:LEU:HA	1.84	0.43
6:i:49:GLU:O	6:i:53:LYS:HG2	2.19	0.43
6:s:23:THR:HG23	6:s:26:LEU:HD12	2.01	0.43
6:v:26:LEU:HD23	6:v:26:LEU:HA	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Z:140:PRO:HD2	7:Z:142:ARG:HH12	1.83	0.43
7:6:117:LEU:HD22	7:6:120:ILE:HG23	2.01	0.43
6:f:60:TYR:HB2	6:k:41:PRO:HG3	2.00	0.43
1:B:4:ASP:N	1:B:4:ASP:OD1	2.50	0.43
1:B:105:LYS:HG3	1:B:106:HIS:ND1	2.33	0.43
5:P:12:ILE:HG21	7:7:164:ASN:CG	2.44	0.43
6:V:55:SER:HB2	6:h:72:LYS:HG3	2.00	0.43
6:c:83:ARG:OXT	6:h:69:LYS:NZ	2.41	0.43
6:n:36:LYS:HB3	6:n:46:LEU:HD11	2.01	0.43
1:D:185:ILE:HG13	1:E:162:VAL:HG13	2.01	0.43
1:E:49:ASN:OD1	1:E:53:ASN:ND2	2.52	0.43
4:K:77:PHE:HA	4:K:80:ILE:HG22	1.99	0.43
6:c:43:ASN:HB3	6:c:46:LEU:HB2	2.01	0.43
6:e:51:GLN:HB2	6:s:82:PHE:HE1	1.84	0.43
6:g:40:ASN:HD22	6:q:11:THR:HG22	1.83	0.43
6:i:27:GLN:O	6:i:31:THR:OG1	2.33	0.43
6:k:74:VAL:O	6:k:78:ILE:HG12	2.19	0.43
8:q0:103:LYS:HE3	8:q0:103:LYS:HB2	1.86	0.43
2:F:74:LEU:HD11	2:F:161:PHE:HA	2.01	0.42
4:K:130:THR:HB	4:K:132:LYS:HD3	2.01	0.42
6:l:49:GLU:O	6:l:53:LYS:HG2	2.19	0.42
6:r:40:ASN:O	6:r:40:ASN:ND2	2.51	0.42
6:t:26:LEU:HD13	6:t:56:GLU:HG2	2.00	0.42
1:B:96:LEU:HD21	1:B:135:LEU:HD22	2.01	0.42
4:K:79:LYS:HA	4:K:79:LYS:HD3	1.83	0.42
7:0:134:LEU:HD13	7:0:161:LEU:HD21	2.01	0.42
7:y:117:LEU:HB2	7:y:120:ILE:HG22	2.00	0.42
6:a:56:GLU:OE1	6:r:13:SER:OG	2.36	0.42
1:C:136:PHE:HD2	5:P:27:GLU:HB2	1.84	0.42
7:6:164:ASN:HA	7:6:167:THR:HG22	2.00	0.42
6:g:40:ASN:OD1	6:g:40:ASN:N	2.53	0.42
1:E:40:ALA:HB1	1:E:161:PHE:HD2	1.84	0.42
7:5:117:LEU:HD13	7:5:120:ILE:O	2.20	0.42
6:c:60:TYR:HB2	6:h:41:PRO:HG3	2.01	0.42
6:m:62:ASN:O	6:m:66:ASN:ND2	2.32	0.42
1:B:173:LEU:HD23	3:G:49:PHE:CE1	2.54	0.42
4:K:168:ASP:OD1	4:K:168:ASP:N	2.49	0.42
8:p0:95:LEU:HB3	8:p0:96:VAL:H	1.68	0.42
5:R:14:LYS:HD2	7:y:160:GLU:HB3	2.02	0.42
7:0:169:LEU:HD23	7:0:169:LEU:HA	1.87	0.42
6:h:20:ASP:OD1	6:h:27:GLN:NE2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:LEU:O	1:A:162:VAL:HG12	2.20	0.42
3:I:3:ASP:O	3:I:7:MET:HG2	2.20	0.42
3:I:74:PHE:O	3:I:78:ILE:HG13	2.20	0.42
7:4:140:PRO:HG2	7:4:142:ARG:NH1	2.32	0.42
7:6:129:LEU:HD21	7:6:165:THR:HG21	2.02	0.42
6:e:16:SER:HA	6:e:64:GLN:HE21	1.85	0.42
6:g:43:ASN:OD1	6:g:46:LEU:N	2.39	0.42
6:m:58:THR:HG23	6:r:74:VAL:HG22	2.02	0.42
6:q:43:ASN:OD1	6:q:46:LEU:N	2.42	0.42
6:s:75:ASP:O	6:s:79:ILE:HG12	2.20	0.42
1:D:29:LYS:NZ	1:D:149:ASP:OD2	2.49	0.42
2:F:7:PHE:CD2	5:M:70:LEU:HD22	2.55	0.42
6:a:11:THR:H	6:a:14:SER:HB3	1.84	0.42
6:e:32:LEU:HG	6:e:36:LYS:HE3	2.01	0.42
6:l:43:ASN:HD22	6:l:46:LEU:HB2	1.85	0.42
1:D:36:MET:HE3	1:D:36:MET:HB3	1.88	0.42
6:W:80:GLN:HA	6:W:83:ARG:HG2	2.01	0.42
1:B:183:ILE:HD12	1:B:183:ILE:HA	1.94	0.41
5:M:63:LEU:HD23	5:M:63:LEU:HA	1.93	0.41
6:T:51:GLN:HB2	6:e:82:PHE:HE1	1.85	0.41
7:6:164:ASN:O	7:6:168:LEU:HB2	2.20	0.41
6:m:41:PRO:HG3	6:r:60:TYR:HB2	2.02	0.41
1:B:166:LEU:HD23	1:B:166:LEU:HA	1.85	0.41
1:C:156:TYR:CE1	3:I:7:MET:HG3	2.54	0.41
1:C:205:LYS:HG2	1:D:114:PHE:CE2	2.55	0.41
6:U:51:GLN:HB2	6:d:82:PHE:HE1	1.84	0.41
6:e:49:GLU:O	6:e:53:LYS:HG2	2.20	0.41
1:A:115:PHE:O	2:F:58:SER:OG	2.36	0.41
1:E:177:MET:HE2	2:F:205:ARG:HB2	2.02	0.41
7:z:120:ILE:HG23	7:z:124:TYR:HD2	1.85	0.41
7:9:136:ASP:OD1	7:9:136:ASP:N	2.52	0.41
6:d:61:ARG:HD3	6:d:61:ARG:HA	1.88	0.41
1:B:30:PHE:HE1	1:B:207:LEU:HB3	1.85	0.41
1:D:197:LEU:C	1:D:199:GLY:H	2.28	0.41
3:J:23:VAL:O	3:J:27:THR:OG1	2.34	0.41
7:6:134:LEU:HB3	7:6:161:LEU:HD21	2.02	0.41
6:a:26:LEU:HD21	6:a:56:GLU:HB3	2.02	0.41
6:d:81:ASN:ND2	6:i:65:SER:OG	2.35	0.41
8:b0:96:VAL:HG22	8:b0:97:SER:H	1.85	0.41
1:A:36:MET:SD	1:A:154:GLY:HA3	2.61	0.41
1:B:49:ASN:O	1:B:53:ASN:ND2	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:58:ILE:HD11	2:F:83:LEU:HB3	2.03	0.41
6:b:74:VAL:HG22	6:g:58:THR:HG23	2.02	0.41
6:c:43:ASN:ND2	6:u:7:ASN:O	2.51	0.41
6:j:43:ASN:HD22	6:j:46:LEU:HB2	1.86	0.41
8:b0:92:THR:HA	8:b0:105:ARG:HH21	1.86	0.41
4:K:153:ILE:HD13	4:K:153:ILE:HA	1.93	0.41
5:P:67:GLN:HB2	6:i:82:PHE:HE1	1.84	0.41
6:g:61:ARG:HD3	6:g:61:ARG:HA	1.91	0.41
1:A:178:MET:HE1	2:F:213:PHE:HE2	1.84	0.41
2:F:31:LEU:HD12	2:F:31:LEU:HA	1.90	0.41
4:K:77:PHE:CE2	8:x0:95:LEU:HD22	2.56	0.41
6:d:11:THR:HG22	6:d:12:LEU:H	1.86	0.41
6:g:49:GLU:O	6:g:53:LYS:HG2	2.20	0.41
1:B:185:ILE:HG23	1:C:162:VAL:HG21	2.03	0.41
1:C:139:LEU:HB3	1:C:140:PRO:HD3	2.03	0.41
3:H:54:ILE:HG23	3:I:16:LEU:HD11	2.02	0.41
3:J:75:CYS:HA	3:J:78:ILE:HG22	2.03	0.41
5:O:12:ILE:HG21	7:4:164:ASN:ND2	2.35	0.41
1:C:133:TYR:HD1	1:C:133:TYR:HA	1.65	0.41
1:C:197:LEU:C	1:C:199:GLY:H	2.29	0.41
1:E:65:LYS:HB3	1:E:66:PRO:HD3	2.03	0.41
1:E:185:ILE:HG23	2:F:194:LEU:HD11	2.02	0.41
5:N:5:TYR:N	5:N:6:PRO:HD2	2.35	0.41
7:Y:124:TYR:OH	7:x:147:ASP:OD1	2.38	0.41
7:Y:171:LYS:HE3	7:Y:171:LYS:HB2	1.92	0.41
7:8:171:LYS:HB2	7:8:171:LYS:HE3	1.88	0.41
7:y:136:ASP:OD1	7:y:136:ASP:N	2.53	0.41
7:3:134:LEU:HD13	7:3:161:LEU:HD21	2.03	0.41
6:j:75:ASP:O	6:j:79:ILE:HG12	2.21	0.41
8:a0:90:PHE:HA	8:a0:91:PRO:HD3	1.90	0.41
2:F:100:GLY:HA3	2:F:127:ALA:HA	2.02	0.41
3:I:73:SER:O	3:I:77:GLU:HG3	2.21	0.41
6:U:61:ARG:HD3	6:U:61:ARG:HA	1.88	0.41
7:1:135:TYR:HE1	7:1:141:ILE:HG13	1.85	0.41
7:3:169:LEU:HD23	7:3:169:LEU:HA	1.90	0.41
6:d:62:ASN:HB3	6:o:79:ILE:HG21	2.03	0.41
8:p0:93:ASP:OD1	8:p0:93:ASP:N	2.54	0.41
1:A:134:SER:O	1:A:137:SER:N	2.48	0.40
1:E:69:GLU:HA	2:F:73:PHE:CE1	2.56	0.40
5:P:12:ILE:HD12	7:7:164:ASN:HB3	2.03	0.40
7:6:140:PRO:HB2	7:6:142:ARG:NH1	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:z:148:LYS:HE2	7:z:148:LYS:HB2	1.91	0.40
6:d:8:ASP:OD1	6:d:8:ASP:N	2.53	0.40
6:d:38:ALA:HB1	6:n:22:GLY:HA3	2.03	0.40
6:f:40:ASN:O	6:f:40:ASN:ND2	2.53	0.40
1:C:4:ASP:OD2	5:P:41:THR:OG1	2.38	0.40
1:C:109:LEU:HB3	1:C:133:TYR:OH	2.21	0.40
1:C:119:GLU:OE2	5:P:26:LEU:N	2.45	0.40
1:E:62:PHE:CE1	2:F:80:ILE:HD11	2.55	0.40
2:F:77:LYS:HE2	2:F:77:LYS:HB3	1.88	0.40
2:F:222:LEU:HB2	3:G:23:VAL:HG11	2.04	0.40
7:6:118:GLU:O	7:6:148:LYS:NZ	2.37	0.40
6:r:20:ASP:OD1	6:r:60:TYR:OH	2.40	0.40
6:t:23:THR:HG23	6:t:26:LEU:HD12	2.03	0.40
6:u:43:ASN:HB3	6:u:46:LEU:HB3	2.04	0.40
1:A:148:LYS:HB2	2:F:139:LEU:HD11	2.02	0.40
6:W:61:ARG:HD3	6:W:61:ARG:HA	1.93	0.40
7:9:116:LEU:HD13	7:9:149:THR:OG1	2.21	0.40
1:B:197:LEU:C	1:B:199:GLY:H	2.29	0.40
4:K:73:VAL:HG21	8:a0:96:VAL:HG22	2.03	0.40
7:Y:169:LEU:HA	7:Y:169:LEU:HD23	1.86	0.40
6:b:49:GLU:O	6:b:53:LYS:HG2	2.21	0.40
1:E:50:MET:HE2	2:F:30:PHE:CE2	2.57	0.40
2:F:203:LEU:HD22	2:F:210:MET:HE1	2.02	0.40
6:S:27:GLN:H	6:S:27:GLN:CD	2.30	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	182/216 (84%)	171 (94%)	11 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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%)	160 (97%)	5 (3%)	36	57
1	B	162/189 (86%)	155 (96%)	7 (4%)	26	49
1	C	164/189 (87%)	158 (96%)	6 (4%)	30	52
1	D	160/189 (85%)	155 (97%)	5 (3%)	35	57
1	E	163/189 (86%)	156 (96%)	7 (4%)	26	49
2	F	230/230 (100%)	218 (95%)	12 (5%)	21	45
3	G	74/75 (99%)	73 (99%)	1 (1%)	59	71
3	H	64/75 (85%)	60 (94%)	4 (6%)	16	40
3	I	55/75 (73%)	54 (98%)	1 (2%)	51	68
3	J	58/75 (77%)	56 (97%)	2 (3%)	32	55
4	K	105/316 (33%)	90 (86%)	15 (14%)	3	16
5	M	36/89 (40%)	34 (94%)	2 (6%)	19	43
5	N	78/89 (88%)	75 (96%)	3 (4%)	29	51
5	O	87/89 (98%)	84 (97%)	3 (3%)	32	55
5	P	85/89 (96%)	80 (94%)	5 (6%)	18	42
5	Q	77/89 (86%)	75 (97%)	2 (3%)	40	61
5	R	77/89 (86%)	76 (99%)	1 (1%)	61	72
6	S	53/88 (60%)	52 (98%)	1 (2%)	50	67
6	T	52/88 (59%)	52 (100%)	0	100	100
6	U	53/88 (60%)	52 (98%)	1 (2%)	50	67
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%)	39	60
6	b	73/88 (83%)	70 (96%)	3 (4%)	27	50
6	c	74/88 (84%)	72 (97%)	2 (3%)	39	60
6	d	74/88 (84%)	73 (99%)	1 (1%)	59	71
6	e	73/88 (83%)	71 (97%)	2 (3%)	39	60
6	f	73/88 (83%)	72 (99%)	1 (1%)	59	71
6	g	68/88 (77%)	67 (98%)	1 (2%)	57	71
6	h	67/88 (76%)	65 (97%)	2 (3%)	36	57
6	i	67/88 (76%)	63 (94%)	4 (6%)	17	42
6	j	68/88 (77%)	67 (98%)	1 (2%)	57	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	k	67/88 (76%)	64 (96%)	3 (4%)	24	48
6	l	68/88 (77%)	67 (98%)	1 (2%)	57	71
6	m	74/88 (84%)	73 (99%)	1 (1%)	59	71
6	n	74/88 (84%)	73 (99%)	1 (1%)	59	71
6	o	73/88 (83%)	71 (97%)	2 (3%)	39	60
6	p	74/88 (84%)	74 (100%)	0	100	100
6	q	74/88 (84%)	72 (97%)	2 (3%)	39	60
6	r	74/88 (84%)	73 (99%)	1 (1%)	59	71
6	s	73/88 (83%)	73 (100%)	0	100	100
6	t	70/88 (80%)	68 (97%)	2 (3%)	37	58
6	u	73/88 (83%)	70 (96%)	3 (4%)	27	50
6	v	74/88 (84%)	73 (99%)	1 (1%)	59	71
6	w	74/88 (84%)	73 (99%)	1 (1%)	59	71
7	0	56/513 (11%)	54 (96%)	2 (4%)	31	53
7	1	56/513 (11%)	55 (98%)	1 (2%)	51	68
7	2	56/513 (11%)	56 (100%)	0	100	100
7	3	56/513 (11%)	55 (98%)	1 (2%)	51	68
7	4	56/513 (11%)	54 (96%)	2 (4%)	31	53
7	5	56/513 (11%)	54 (96%)	2 (4%)	31	53
7	6	56/513 (11%)	52 (93%)	4 (7%)	13	38
7	7	56/513 (11%)	54 (96%)	2 (4%)	31	53
7	8	56/513 (11%)	55 (98%)	1 (2%)	51	68
7	9	56/513 (11%)	55 (98%)	1 (2%)	51	68
7	X	56/513 (11%)	53 (95%)	3 (5%)	20	44
7	Y	56/513 (11%)	54 (96%)	2 (4%)	31	53
7	Z	56/513 (11%)	54 (96%)	2 (4%)	31	53
7	x	56/513 (11%)	53 (95%)	3 (5%)	20	44
7	y	56/513 (11%)	55 (98%)	1 (2%)	51	68
7	z	56/513 (11%)	53 (95%)	3 (5%)	20	44
8	a0	15/220 (7%)	15 (100%)	0	100	100
8	b0	15/220 (7%)	15 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	15	39
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%)	14 (93%)	1 (7%)	15	39
8	i0	15/220 (7%)	14 (93%)	1 (7%)	15	39
8	j0	15/220 (7%)	14 (93%)	1 (7%)	15	39
8	k0	15/220 (7%)	13 (87%)	2 (13%)	4	18
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%)	14 (93%)	1 (7%)	15	39
8	r0	15/220 (7%)	13 (87%)	2 (13%)	4	18
8	s0	15/220 (7%)	15 (100%)	0	100	100
8	t0	15/220 (7%)	14 (93%)	1 (7%)	15	39
8	u0	15/220 (7%)	15 (100%)	0	100	100
8	v0	15/220 (7%)	13 (87%)	2 (13%)	4	18
8	w0	15/220 (7%)	14 (93%)	1 (7%)	15	39
8	x0	15/220 (7%)	14 (93%)	1 (7%)	15	39
All	All	5011/18277 (27%)	4847 (97%)	164 (3%)	34	56

All (164) 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	B	5	MET
1	B	45	GLN

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Mol	Chain	Res	Type
1	B	67	ILE
1	B	96	LEU
1	B	157	LEU
1	B	184	THR
1	B	211	TYR
1	C	25	THR
1	C	46	VAL
1	C	69	GLU
1	C	133	TYR
1	C	153	ILE
1	C	207	LEU
1	D	28	ILE
1	D	46	VAL
1	D	136	PHE
1	D	158	TYR
1	D	166	LEU
1	E	46	VAL
1	E	49	ASN
1	E	110	GLU
1	E	116	GLN
1	E	158	TYR
1	E	164	VAL
1	E	197	LEU
2	F	11	HIS
2	F	22	PHE
2	F	34	LEU
2	F	38	ILE
2	F	68	PHE
2	F	70	HIS
2	F	95	ILE
2	F	102	ILE
2	F	140	TYR
2	F	175	LEU
2	F	200	LEU
2	F	234	THR
3	G	25	ILE
3	H	17	ILE
3	H	47	LEU
3	H	69	GLU
3	H	80	PHE
3	I	49	PHE
3	J	51	ILE

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Mol	Chain	Res	Type
3	J	78	ILE
4	K	39	PHE
4	K	42	ILE
4	K	52	LEU
4	K	53	LEU
4	K	58	ILE
4	K	74	VAL
4	K	130	THR
4	K	132	LYS
4	K	138	ILE
4	K	139	LEU
4	K	157	LYS
4	K	162	GLN
4	K	174	TRP
4	K	181	ILE
4	K	188	PHE
5	M	56	GLU
5	M	96	LYS
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	P	8	ASN
5	P	10	VAL
5	P	14	LYS
5	P	18	PHE
5	P	59	ASN
5	Q	11	ASP
5	Q	13	ILE
5	R	13	ILE
6	S	73	ASP
6	U	59	LEU
7	X	117	LEU
7	X	120	ILE
7	X	169	LEU
7	Y	117	LEU
7	Y	120	ILE
7	Z	117	LEU
7	Z	169	LEU
7	0	123	ASN

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Mol	Chain	Res	Type
7	0	131	ASP
7	4	117	LEU
7	4	131	ASP
7	6	111	ILE
7	6	117	LEU
7	6	131	ASP
7	6	147	ASP
7	8	131	ASP
7	x	117	LEU
7	x	120	ILE
7	x	137	HIS
7	y	117	LEU
7	z	117	LEU
7	z	131	ASP
7	z	171	LYS
7	1	117	LEU
7	3	117	LEU
7	5	117	LEU
7	5	131	ASP
7	7	117	LEU
7	7	125	LEU
7	9	117	LEU
6	a	15	LEU
6	a	31	THR
6	b	11	THR
6	b	31	THR
6	b	60	TYR
6	c	11	THR
6	c	19	PHE
6	d	11	THR
6	e	60	TYR
6	e	73	ASP
6	f	43	ASN
6	g	19	PHE
6	h	19	PHE
6	h	60	TYR
6	i	11	THR
6	i	19	PHE
6	i	31	THR
6	i	43	ASN
6	j	11	THR
6	k	11	THR

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Mol	Chain	Res	Type
6	k	19	PHE
6	k	43	ASN
6	l	11	THR
6	m	60	TYR
6	n	26	LEU
6	o	19	PHE
6	o	73	ASP
6	q	15	LEU
6	q	31	THR
6	r	11	THR
6	t	11	THR
6	t	15	LEU
6	u	23	THR
6	u	26	LEU
6	u	60	TYR
6	v	3	VAL
6	w	60	TYR
8	e0	95	LEU
8	h0	96	VAL
8	i0	90	PHE
8	j0	95	LEU
8	k0	92	THR
8	k0	96	VAL
8	q0	96	VAL
8	r0	95	LEU
8	r0	96	VAL
8	t0	93	ASP
8	v0	95	LEU
8	v0	96	VAL
8	w0	96	VAL
8	x0	96	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) 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
1	E	45	GLN
1	E	53	ASN

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Mol	Chain	Res	Type
2	F	105	ASN
2	F	163	GLN
3	G	37	GLN
4	K	60	ASN
5	O	8	ASN
5	P	67	GLN
6	T	27	GLN
7	0	123	ASN
7	2	127	GLN
7	1	164	ASN
7	5	119	ASN
6	c	64	GLN
6	e	64	GLN
6	f	40	ASN
6	f	43	ASN
6	g	81	ASN
6	i	43	ASN
6	j	43	ASN
6	k	40	ASN
6	l	40	ASN
6	l	43	ASN
6	n	40	ASN
6	o	27	GLN
6	q	64	GLN
6	r	24	GLN
6	r	40	ASN
6	s	27	GLN
6	s	64	GLN
6	u	81	ASN
6	v	64	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [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.

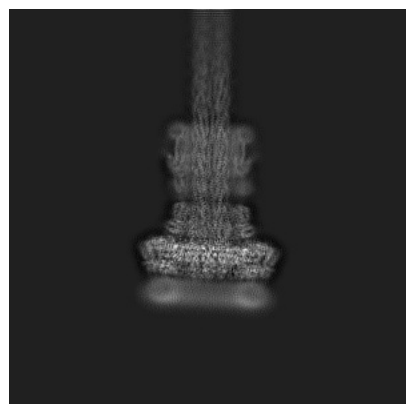
6 Map visualisation [i](#)

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.

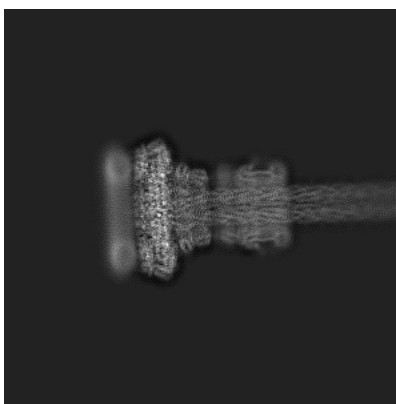
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

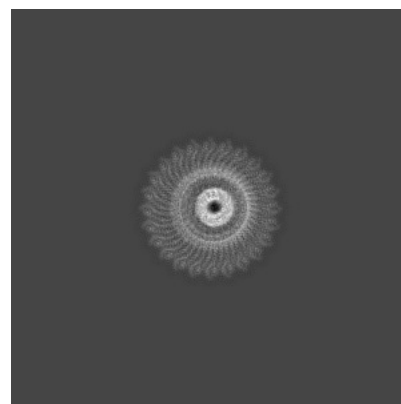
6.1.1 Primary map



X

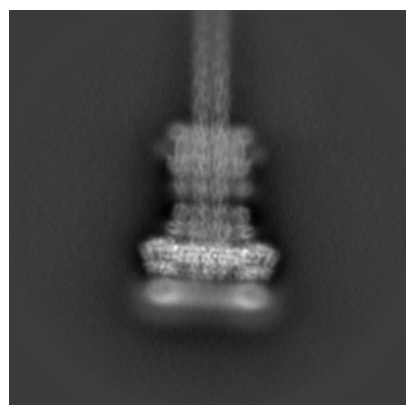


Y

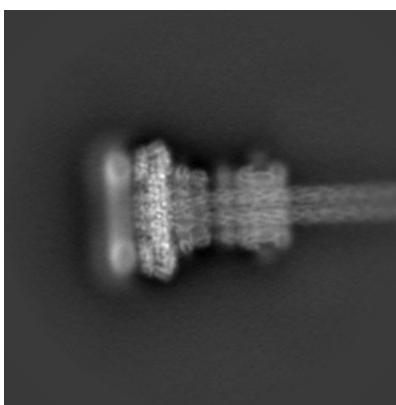


Z

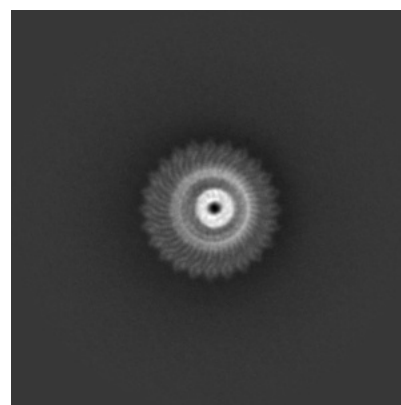
6.1.2 Raw map



X



Y

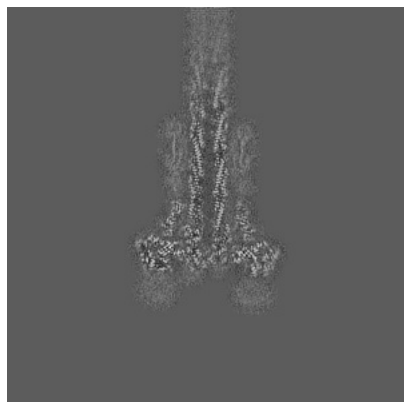


Z

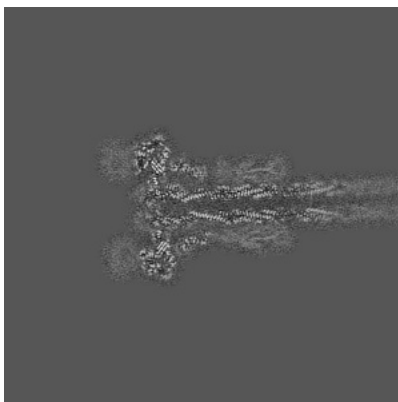
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

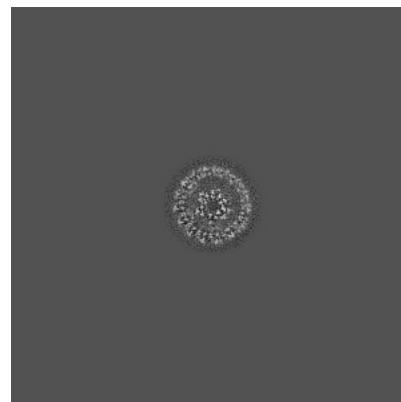
6.2.1 Primary map



X Index: 240

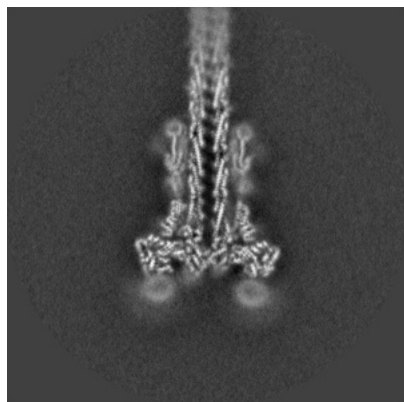


Y Index: 240

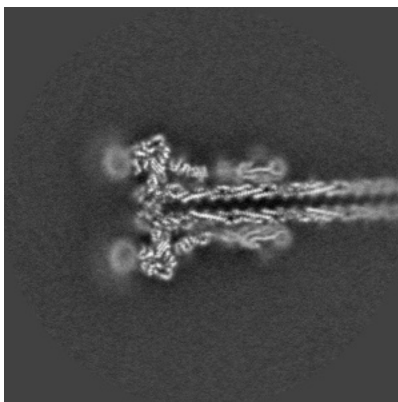


Z Index: 240

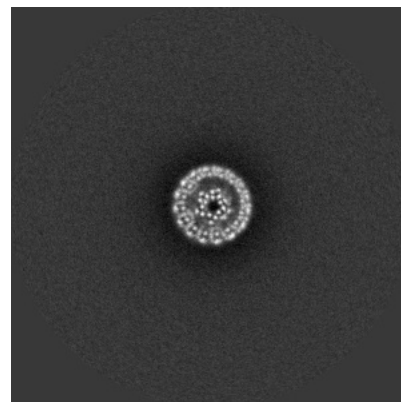
6.2.2 Raw map



X Index: 240



Y Index: 240

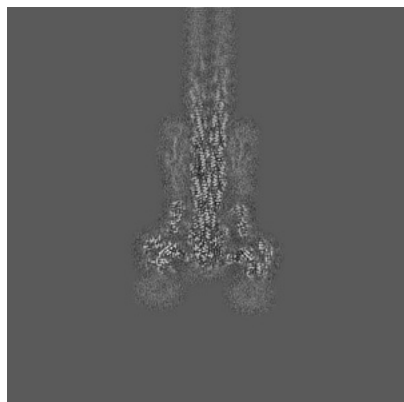


Z Index: 240

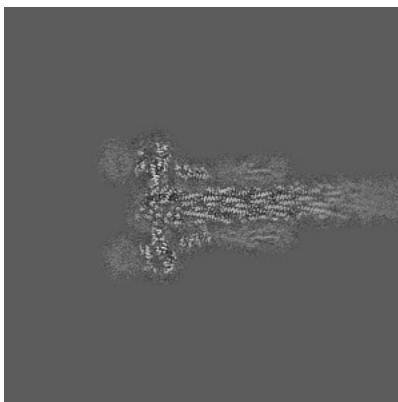
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

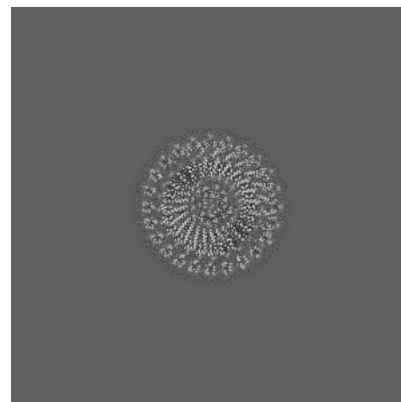
6.3.1 Primary map



X Index: 252

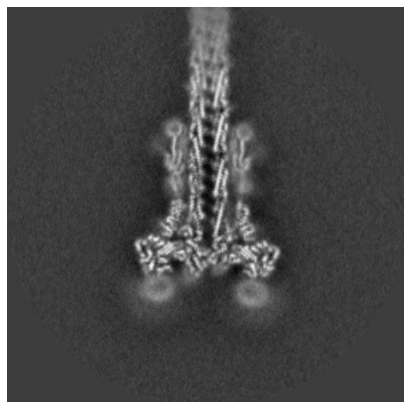


Y Index: 232

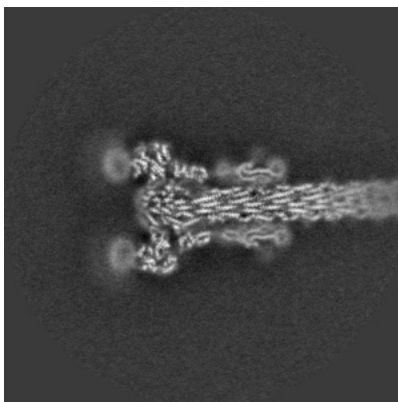


Z Index: 185

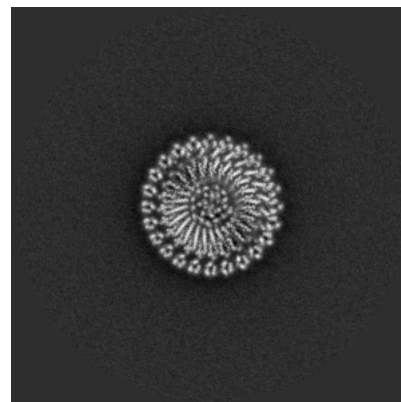
6.3.2 Raw map



X Index: 239



Y Index: 252

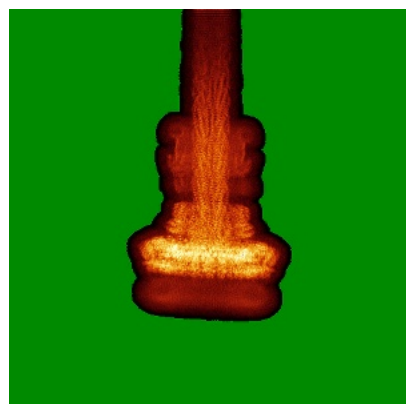


Z Index: 185

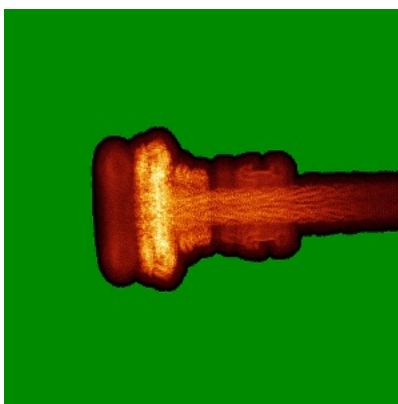
The images above show the largest variance slices of the map in three orthogonal directions.

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

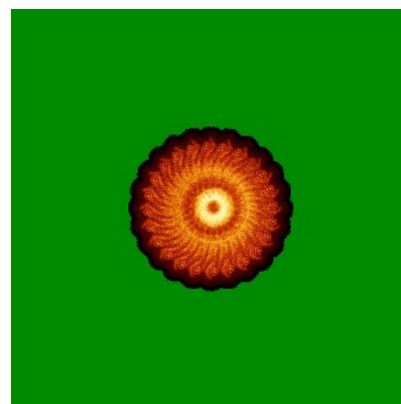
6.4.1 Primary map



X

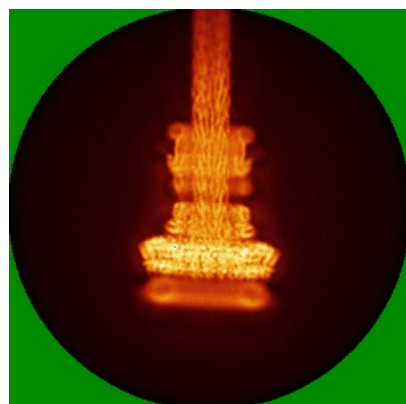


Y

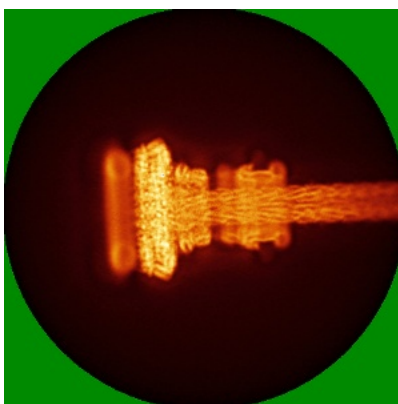


Z

6.4.2 Raw map



X



Y

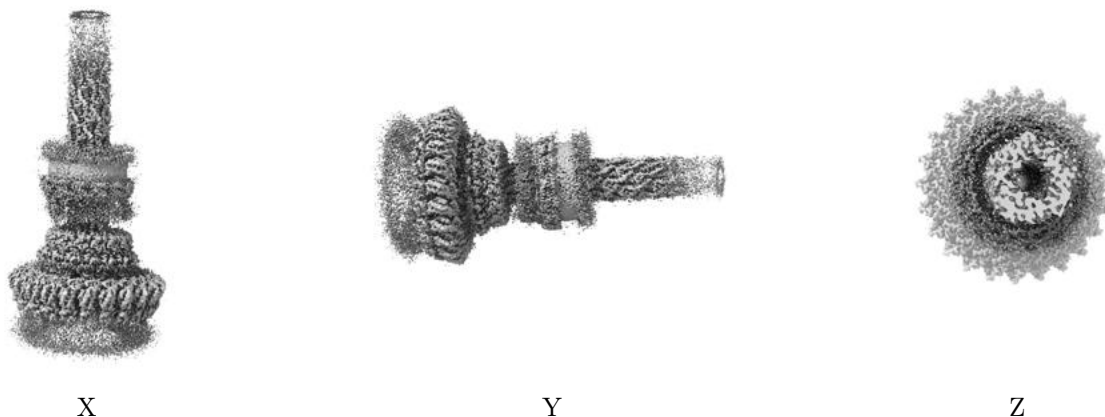


Z

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

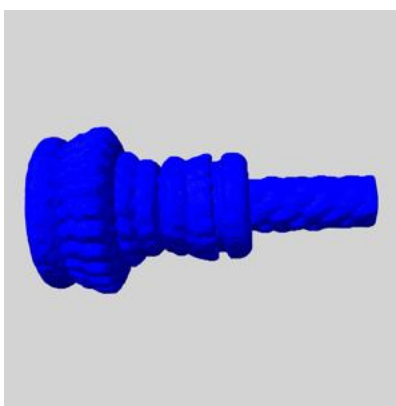
A mask typically either:

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

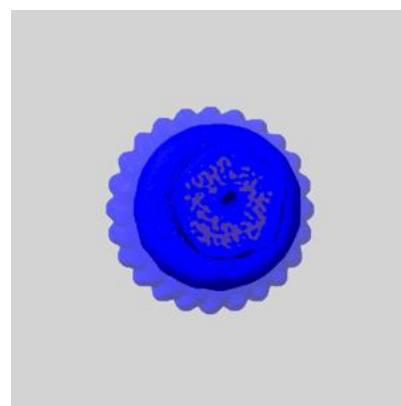
6.6.1 emd_15700_msk_1.map [i](#)



X



Y

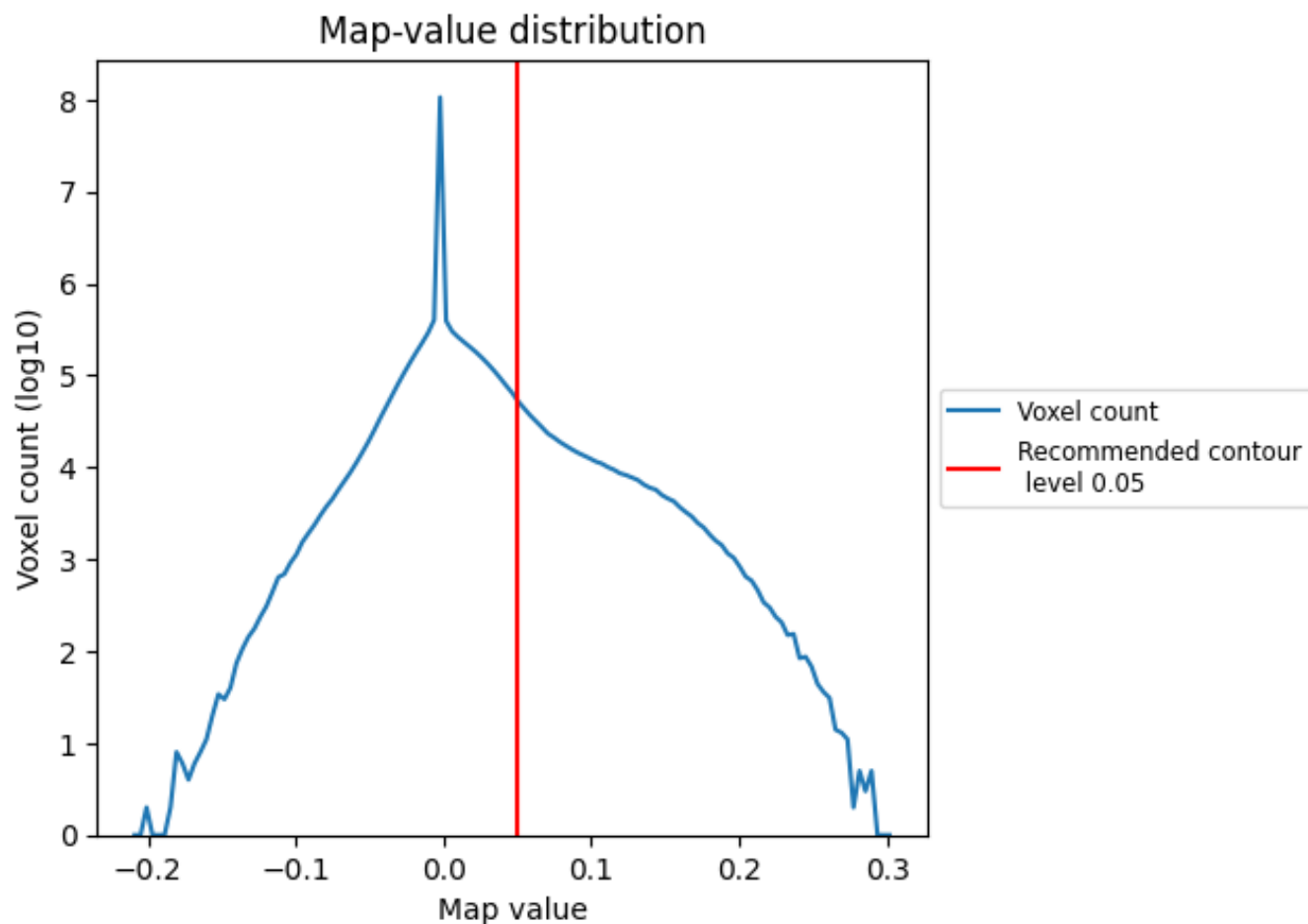


Z

7 Map analysis [i](#)

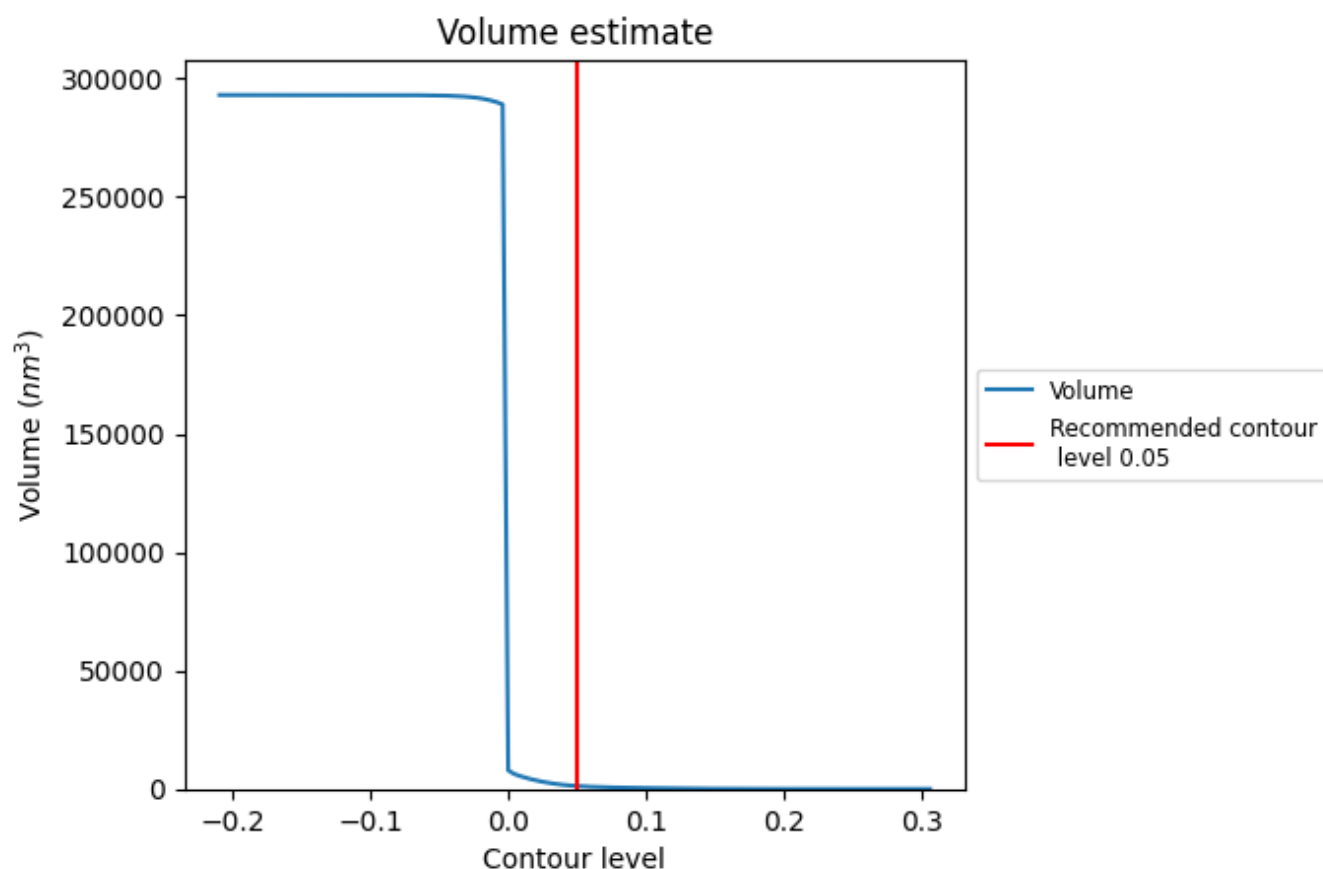
This section contains the results of statistical analysis of the map.

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.

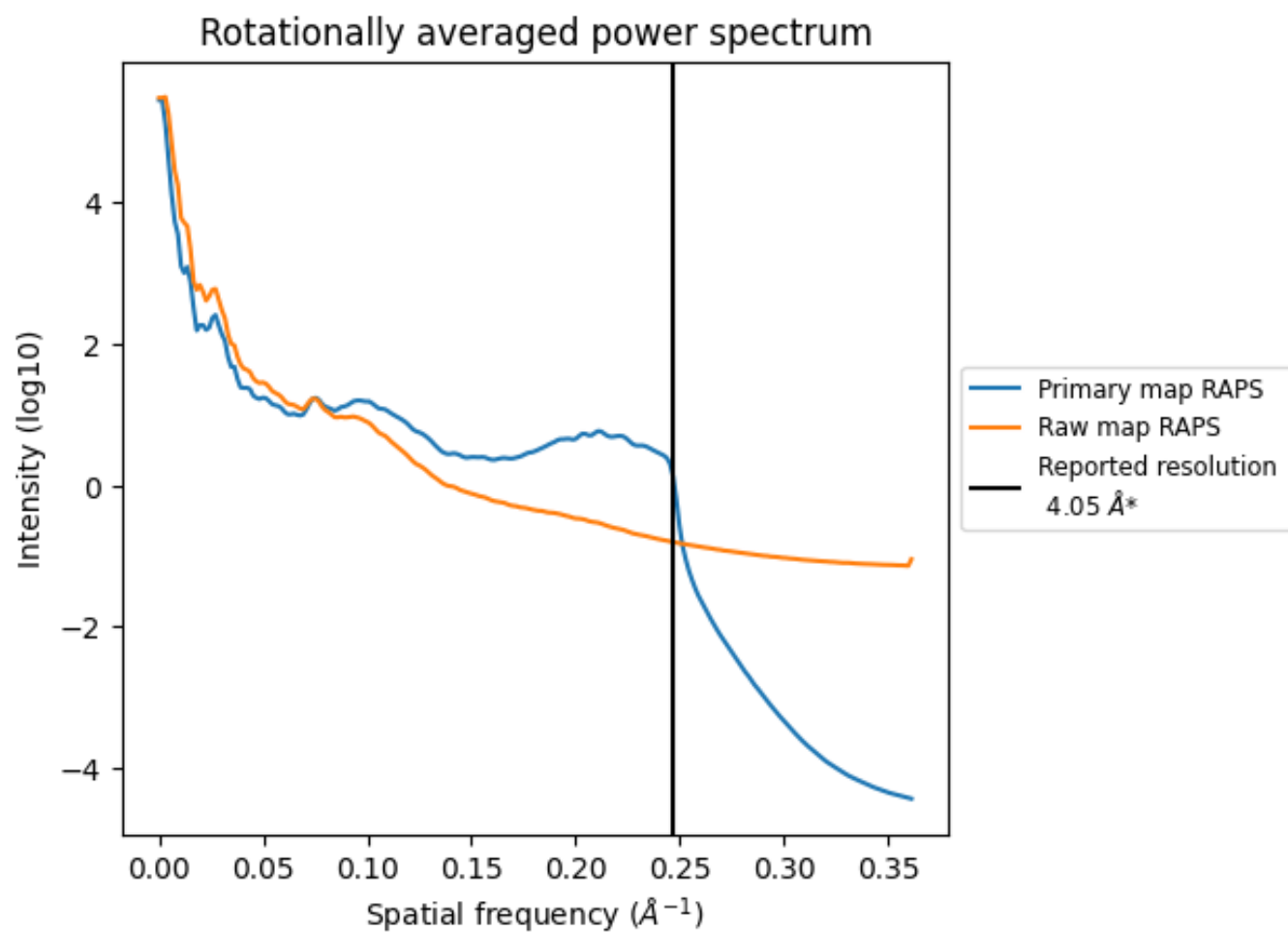
7.2 Volume estimate [i](#)



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 [i](#)

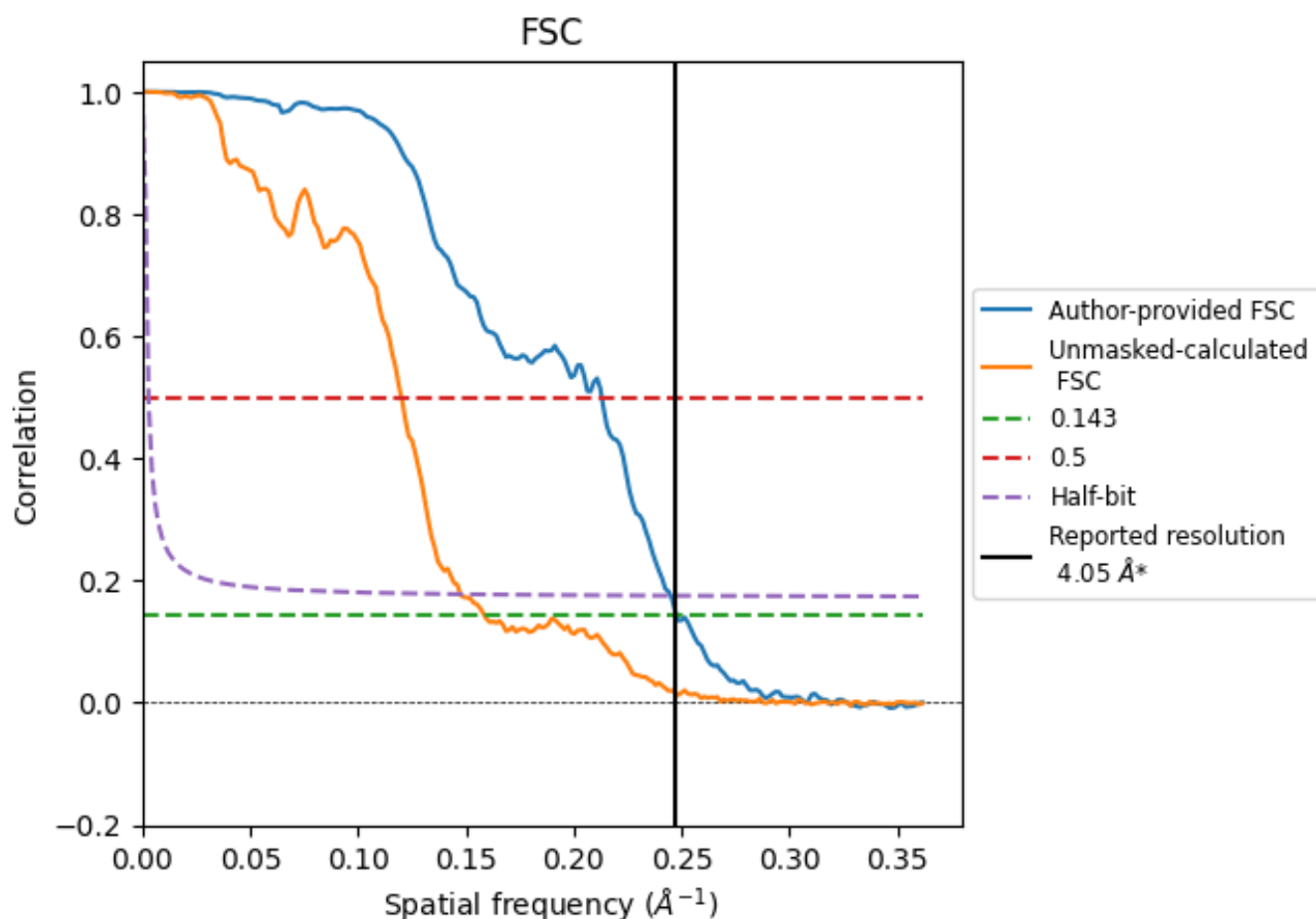


*Reported resolution corresponds to spatial frequency of 0.247 Å⁻¹

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 $0.247 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

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

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.31 differs from the reported value 4.05 by more than 10 %

9 Map-model fit [i](#)

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

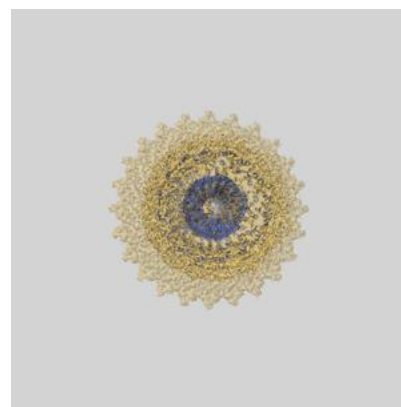
9.1 Map-model overlay [i](#)



X



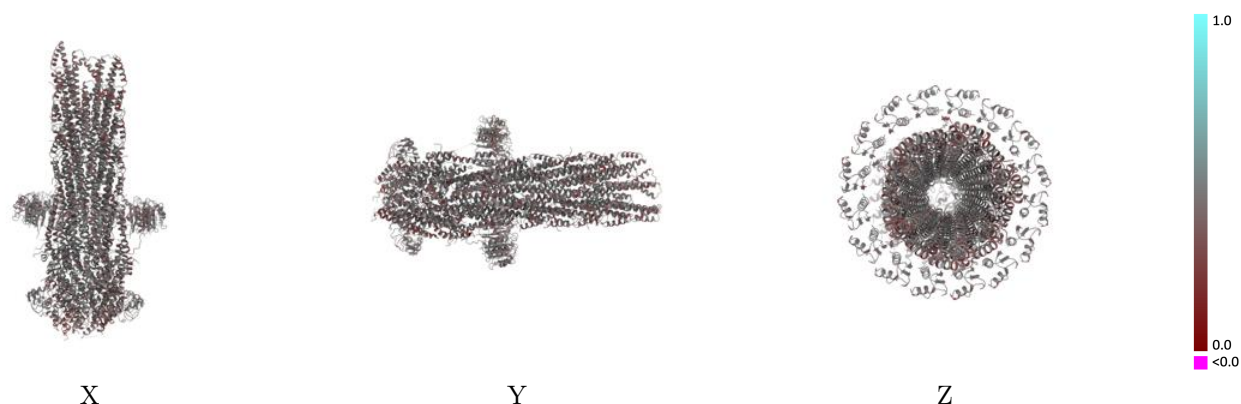
Y



Z

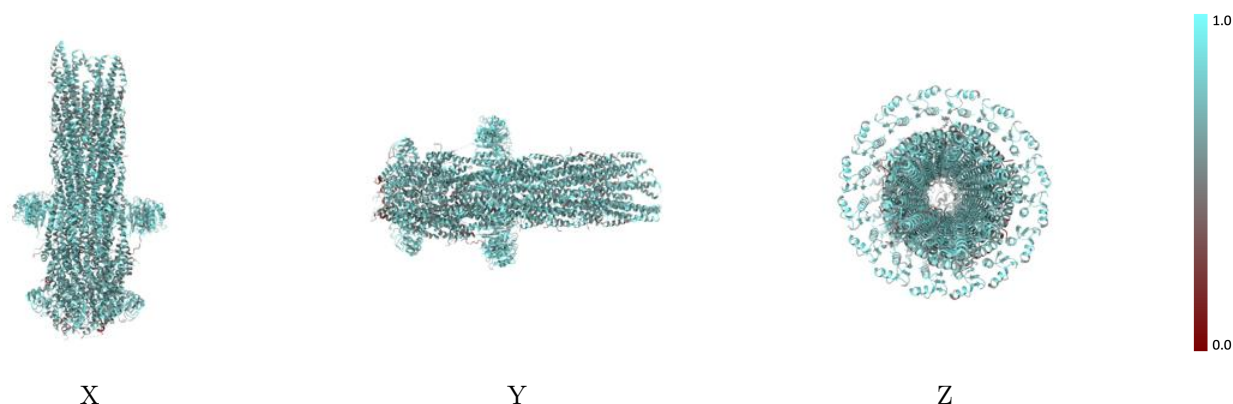
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



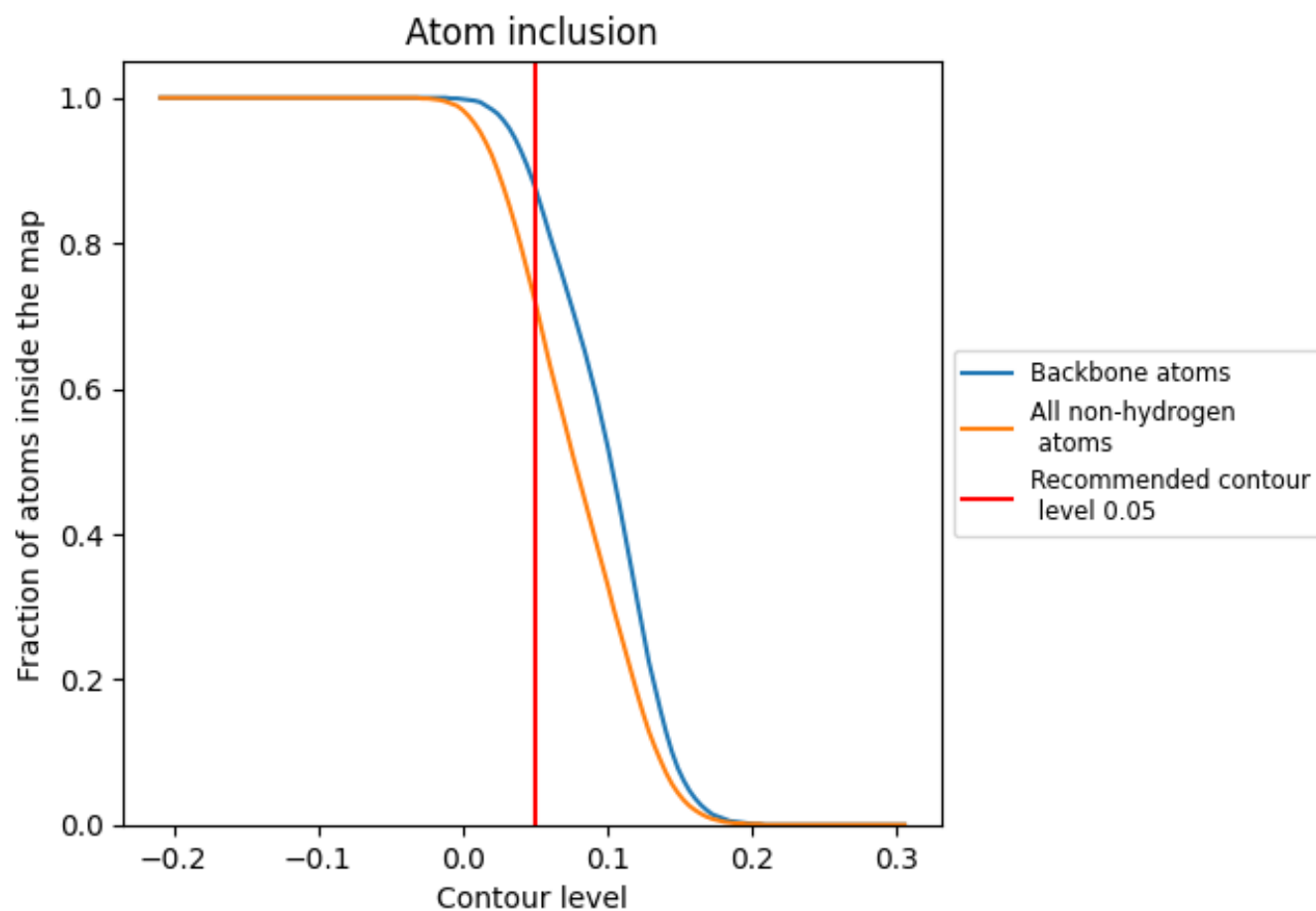
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

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



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

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