



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 12:56 PM UTC

PDB ID : 8AXN / pdb_00008axn
EMDB ID : EMD-15702
Title : Inner membrane ring and secretin N0 N1 domains of the type 3 secretion system of *Shigella flexneri*
Authors : Lunelli, M.
Deposited on : 2022-08-31
Resolution : 3.34 Å(reported)
Based on initial model : 6RWK

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

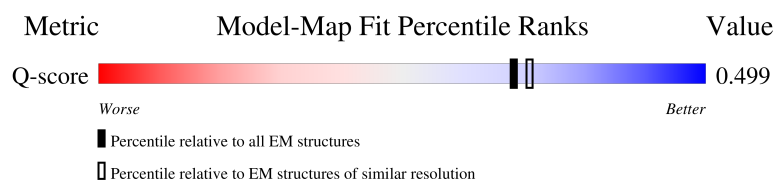
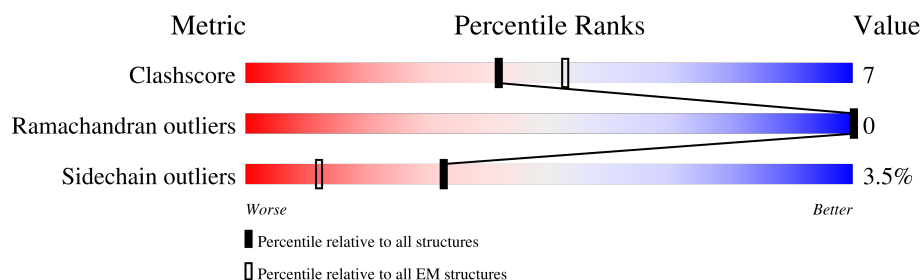
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.34 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.



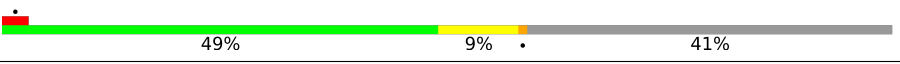
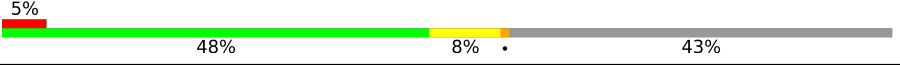
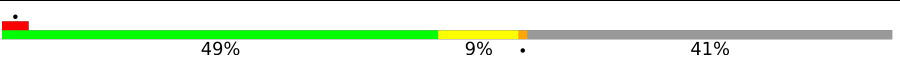
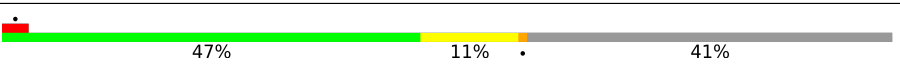
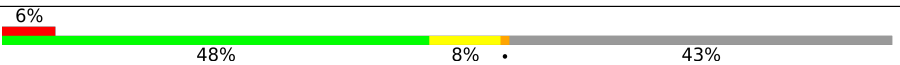
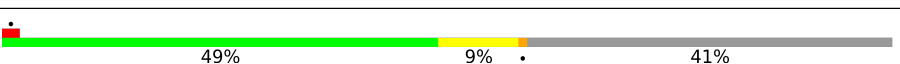
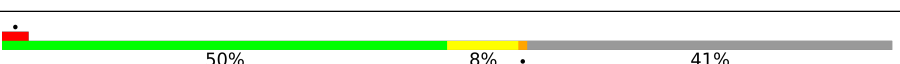
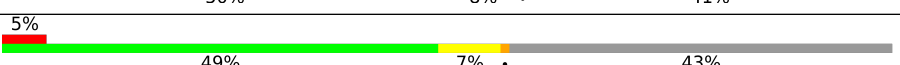
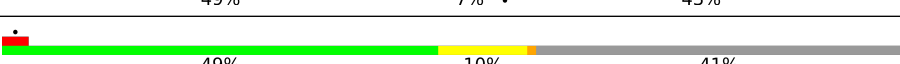
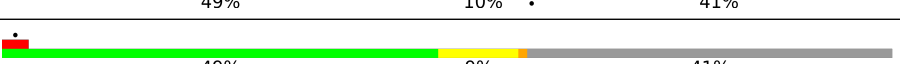
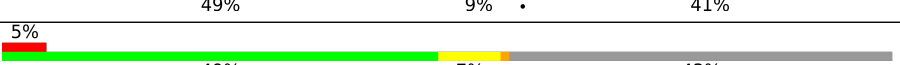
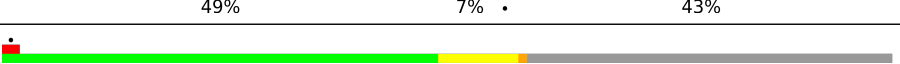
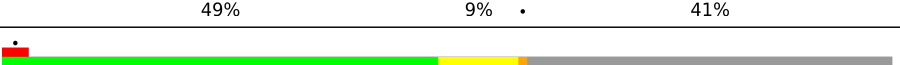
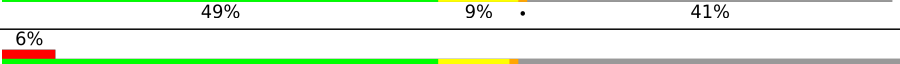
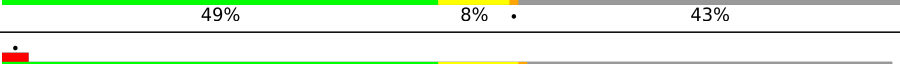
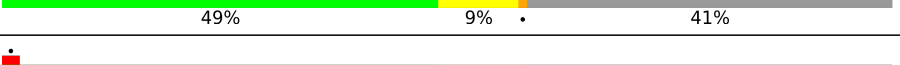
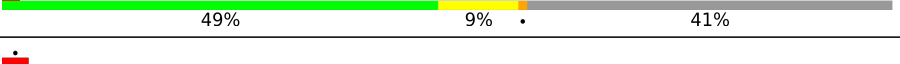
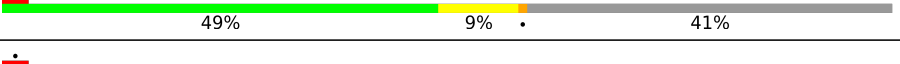
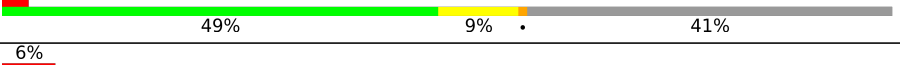
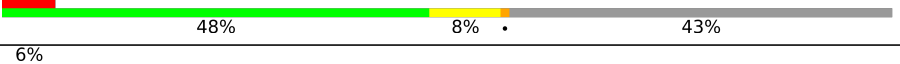
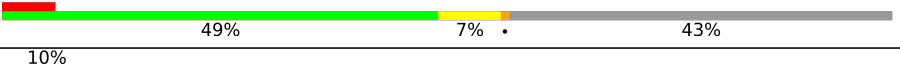
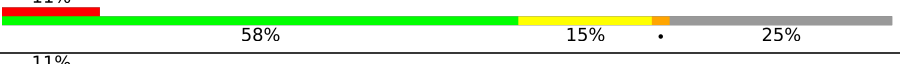
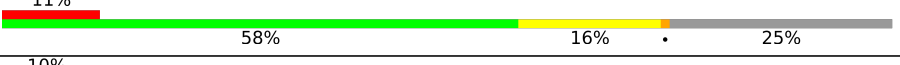
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14446 (2.84 - 3.84)

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	371	
1	B	371	
1	C	371	
1	D	371	

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Mol	Chain	Length	Quality of chain
1	E	371	
1	F	371	
1	G	371	
1	H	371	
1	I	371	
1	J	371	
1	K	371	
1	L	371	
1	M	371	
1	N	371	
1	O	371	
1	P	371	
1	Q	371	
1	R	371	
1	S	371	
1	T	371	
1	U	371	
1	V	371	
1	W	371	
1	X	371	
2	a	241	
2	b	241	
2	c	241	
2	d	241	
2	e	241	

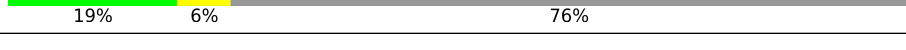
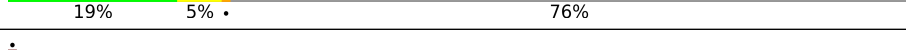
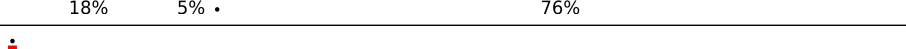
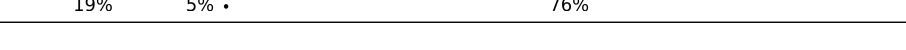
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Mol	Chain	Length	Quality of chain
2	f	241	
2	g	241	
2	h	241	
2	i	241	
2	j	241	
2	k	241	
2	l	241	
2	m	241	
2	n	241	
2	o	241	
2	p	241	
2	q	241	
2	r	241	
2	s	241	
2	t	241	
2	u	241	
2	v	241	
2	w	241	
2	x	241	
3	0	566	
3	1	566	
3	2	566	
3	3	566	
3	4	566	
3	5	566	

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Mol	Chain	Length	Quality of chain
3	6	566	 19% 5% 76%
3	7	566	 18% 5% 76%
3	8	566	 19% 6% 76%
3	9	566	 19% 5% 76%
3	Y	566	 19% 6% 76%
3	Z	566	 18% 6% 76%
3	a0	566	 19% 6% 76%
3	b0	566	 19% 5% 76%
3	y	566	 18% 5% 76%
3	z	566	 19% 5% 76%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 94656 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 Protein MxiG.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	211	Total	C	N	O	S	0	0
			1734	1106	289	335	4		
1	B	218	Total	C	N	O	S	0	0
			1805	1157	300	344	4		
1	A	218	Total	C	N	O	S	0	0
			1805	1157	300	344	4		
1	S	218	Total	C	N	O	S	0	0
			1805	1157	300	344	4		
1	P	218	Total	C	N	O	S	0	0
			1805	1157	300	344	4		
1	M	218	Total	C	N	O	S	0	0
			1805	1157	300	344	4		
1	J	218	Total	C	N	O	S	0	0
			1805	1157	300	344	4		
1	G	218	Total	C	N	O	S	0	0
			1805	1157	300	344	4		
1	D	218	Total	C	N	O	S	0	0
			1805	1157	300	344	4		
1	U	218	Total	C	N	O	S	0	0
			1805	1157	300	344	4		
1	T	218	Total	C	N	O	S	0	0
			1805	1157	300	344	4		
1	Q	218	Total	C	N	O	S	0	0
			1805	1157	300	344	4		
1	N	218	Total	C	N	O	S	0	0
			1805	1157	300	344	4		
1	K	218	Total	C	N	O	S	0	0
			1805	1157	300	344	4		
1	H	218	Total	C	N	O	S	0	0
			1805	1157	300	344	4		
1	E	218	Total	C	N	O	S	0	0
			1805	1157	300	344	4		
1	V	218	Total	C	N	O	S	0	0
			1805	1157	300	344	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	211	Total	C	N	O	S	0	0
			1734	1106	289	335	4		
1	O	211	Total	C	N	O	S	0	0
			1734	1106	289	335	4		
1	L	211	Total	C	N	O	S	0	0
			1734	1106	289	335	4		
1	I	211	Total	C	N	O	S	0	0
			1734	1106	289	335	4		
1	F	211	Total	C	N	O	S	0	0
			1734	1106	289	335	4		
1	W	211	Total	C	N	O	S	0	0
			1734	1106	289	335	4		
1	X	211	Total	C	N	O	S	0	0
			1734	1106	289	335	4		

- Molecule 2 is a protein called Lipoprotein MxiJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	a	180	Total	C	N	O	S	0	0
			1428	897	246	281	4		
2	d	180	Total	C	N	O	S	0	0
			1428	897	246	281	4		
2	c	180	Total	C	N	O	S	0	0
			1428	897	246	281	4		
2	b	180	Total	C	N	O	S	0	0
			1428	897	246	281	4		
2	e	180	Total	C	N	O	S	0	0
			1428	897	246	281	4		
2	h	180	Total	C	N	O	S	0	0
			1428	897	246	281	4		
2	k	180	Total	C	N	O	S	0	0
			1428	897	246	281	4		
2	n	180	Total	C	N	O	S	0	0
			1428	897	246	281	4		
2	q	180	Total	C	N	O	S	0	0
			1428	897	246	281	4		
2	t	180	Total	C	N	O	S	0	0
			1428	897	246	281	4		
2	x	180	Total	C	N	O	S	0	0
			1428	897	246	281	4		
2	g	180	Total	C	N	O	S	0	0
			1428	897	246	281	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	j	180	Total	C	N	O	S	0	0
			1428	897	246	281	4		
2	m	180	Total	C	N	O	S	0	0
			1428	897	246	281	4		
2	p	180	Total	C	N	O	S	0	0
			1428	897	246	281	4		
2	s	180	Total	C	N	O	S	0	0
			1428	897	246	281	4		
2	w	180	Total	C	N	O	S	0	0
			1428	897	246	281	4		
2	v	180	Total	C	N	O	S	0	0
			1428	897	246	281	4		
2	u	180	Total	C	N	O	S	0	0
			1428	897	246	281	4		
2	f	180	Total	C	N	O	S	0	0
			1428	897	246	281	4		
2	i	180	Total	C	N	O	S	0	0
			1428	897	246	281	4		
2	l	180	Total	C	N	O	S	0	0
			1428	897	246	281	4		
2	o	180	Total	C	N	O	S	0	0
			1428	897	246	281	4		
2	r	180	Total	C	N	O	S	0	0
			1428	897	246	281	4		

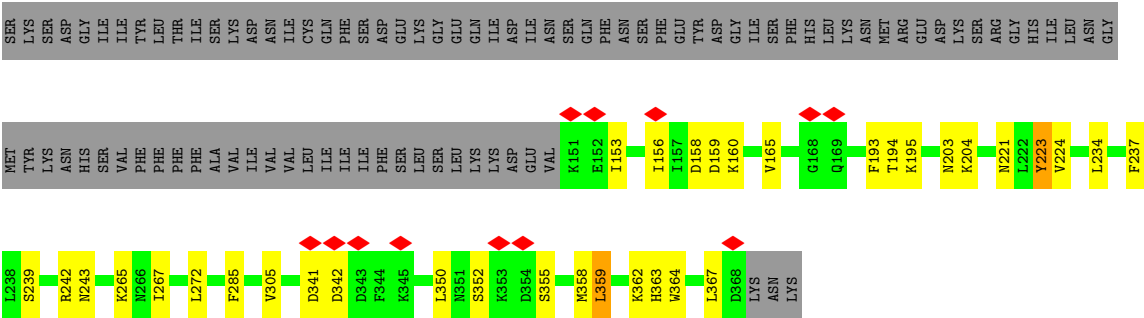
- Molecule 3 is a protein called Outer membrane protein MxiD.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	0	138	Total	C	N	O	S	0	0
			1102	718	174	209	1		
3	1	138	Total	C	N	O	S	0	0
			1102	718	174	209	1		
3	a0	138	Total	C	N	O	S	0	0
			1102	718	174	209	1		
3	Y	138	Total	C	N	O	S	0	0
			1102	718	174	209	1		
3	Z	138	Total	C	N	O	S	0	0
			1102	718	174	209	1		
3	2	138	Total	C	N	O	S	0	0
			1102	718	174	209	1		
3	4	138	Total	C	N	O	S	0	0
			1102	718	174	209	1		

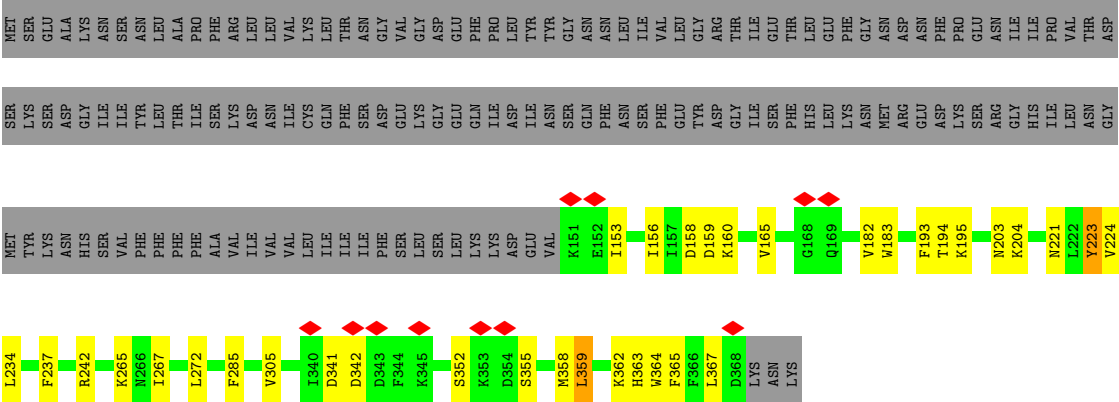
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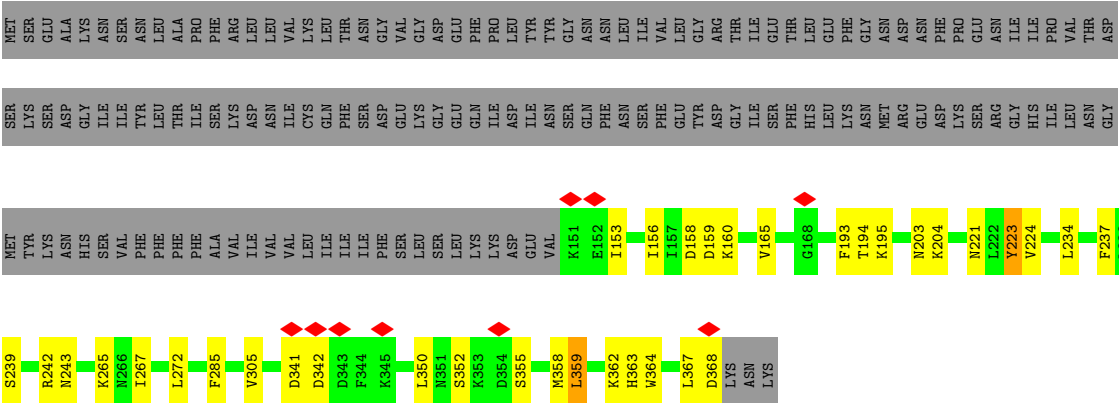
Mol	Chain	Residues	Atoms					AltConf	Trace
3	6	138	Total	C	N	O	S	0	0
			1102	718	174	209	1		
3	8	138	Total	C	N	O	S	0	0
			1102	718	174	209	1		
3	b0	138	Total	C	N	O	S	0	0
			1102	718	174	209	1		
3	y	138	Total	C	N	O	S	0	0
			1102	718	174	209	1		
3	z	138	Total	C	N	O	S	0	0
			1102	718	174	209	1		
3	3	138	Total	C	N	O	S	0	0
			1102	718	174	209	1		
3	5	138	Total	C	N	O	S	0	0
			1102	718	174	209	1		
3	7	138	Total	C	N	O	S	0	0
			1102	718	174	209	1		
3	9	138	Total	C	N	O	S	0	0
			1102	718	174	209	1		



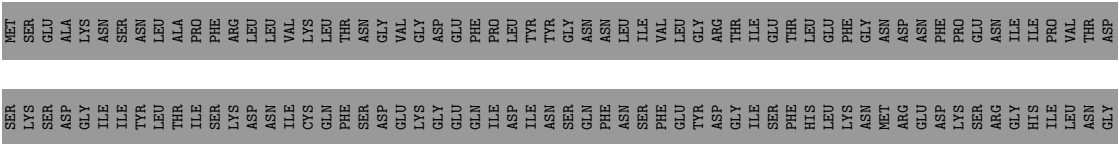
● Molecule 1: Protein MxiG

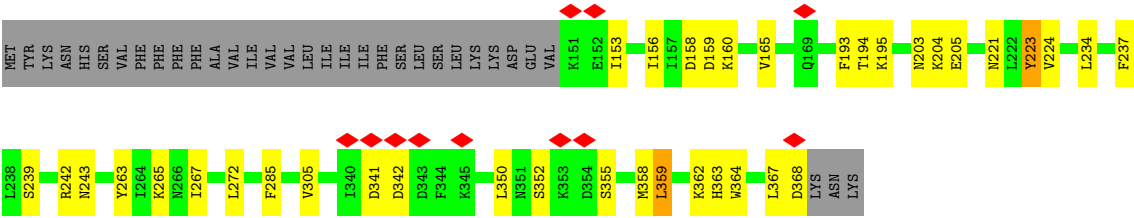


● Molecule 1: Protein MxiG

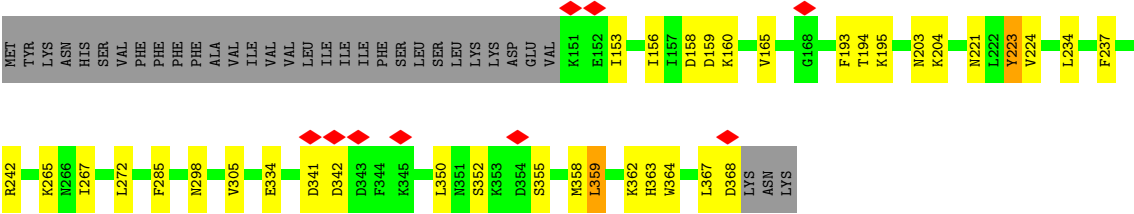
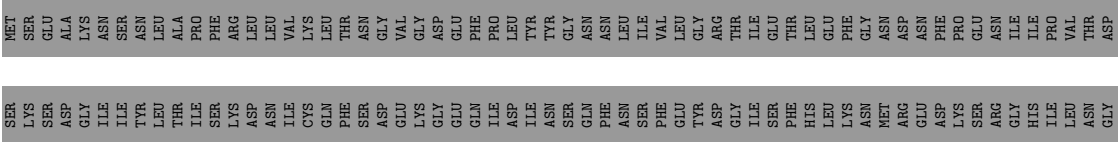


● Molecule 1: Protein MxiG

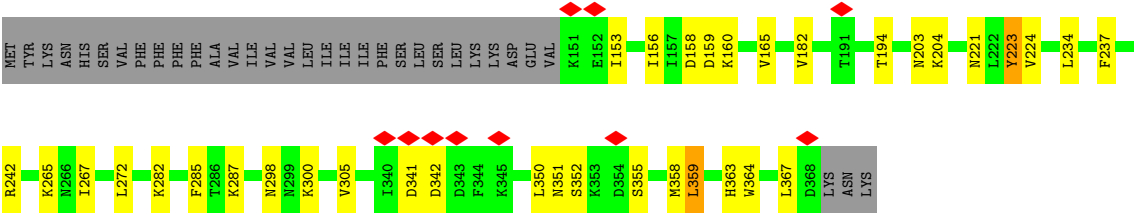
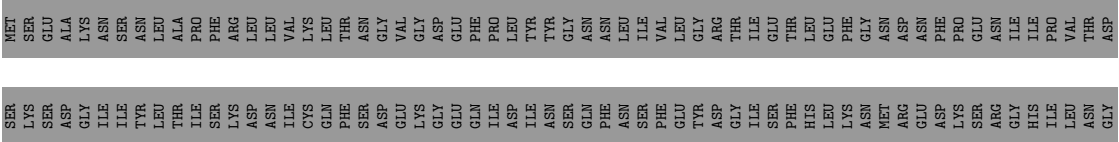




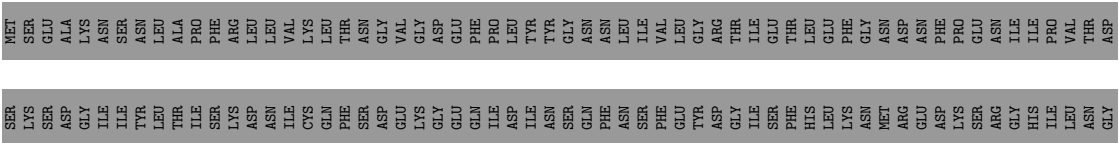
• Molecule 1: Protein MxiG

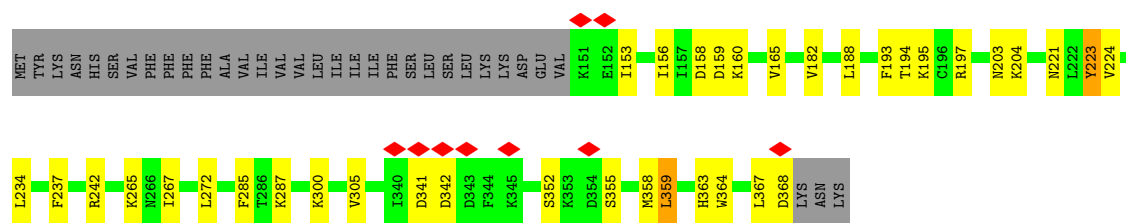


• Molecule 1: Protein MxiG



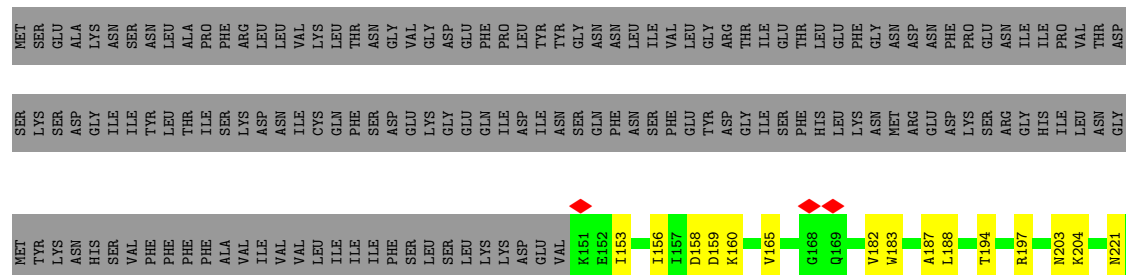
• Molecule 1: Protein MxiG





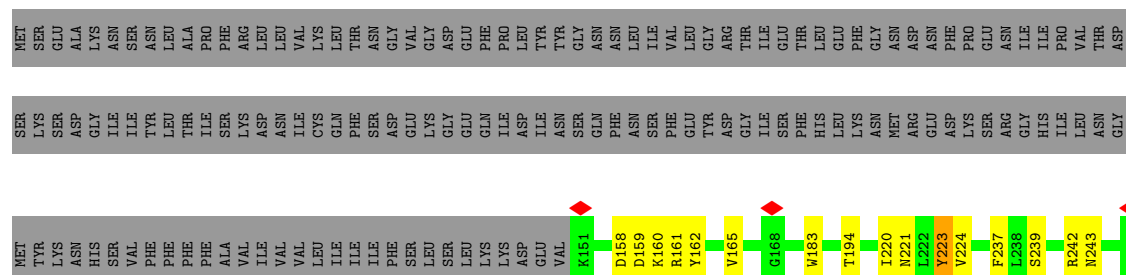
• Molecule 1: Protein MxiG

Chain U: 49% 9% 41%



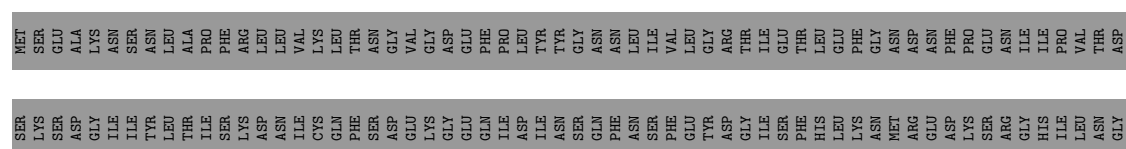
• Molecule 1: Protein MxiG

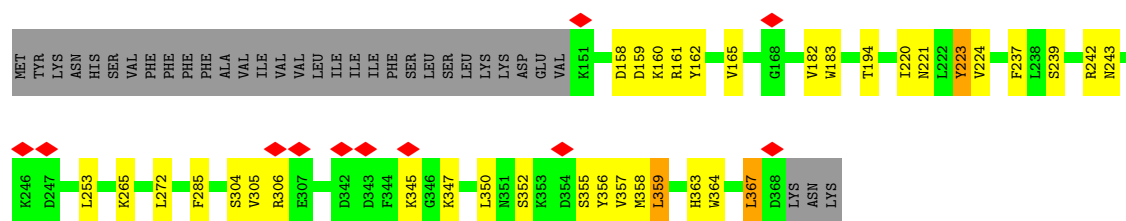
Chain T: 49% 9% 41%



• Molecule 1: Protein MxiG

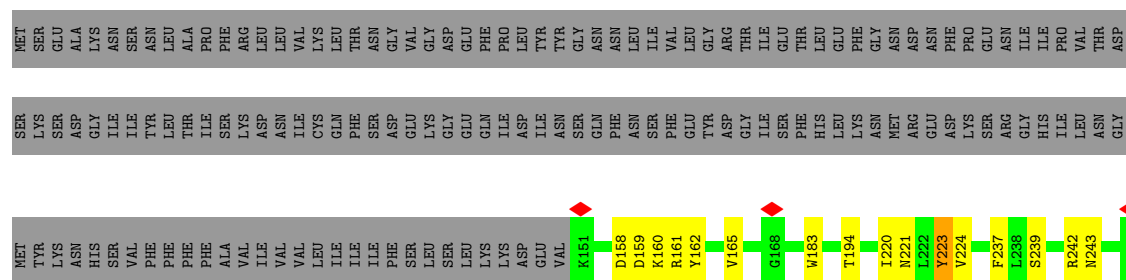
Chain Q: 49% 9% 41%





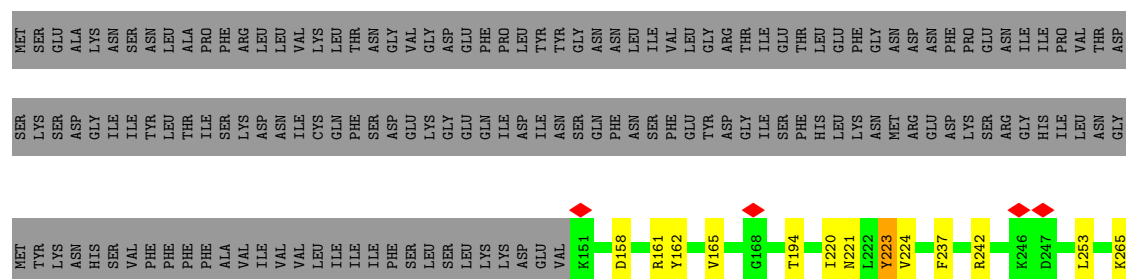
• Molecule 1: Protein MxiG

Chain N: 49% 9% 41%



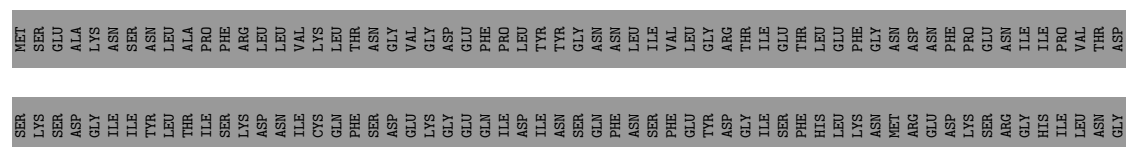
• Molecule 1: Protein MxiG

Chain K: 50% 8% 41%

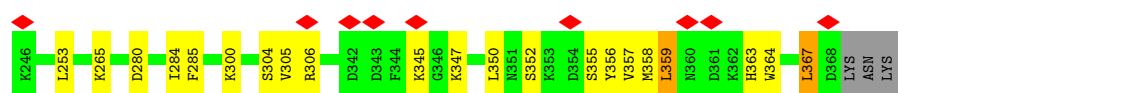


• Molecule 1: Protein MxiG

Chain H: 47% 11% 41%



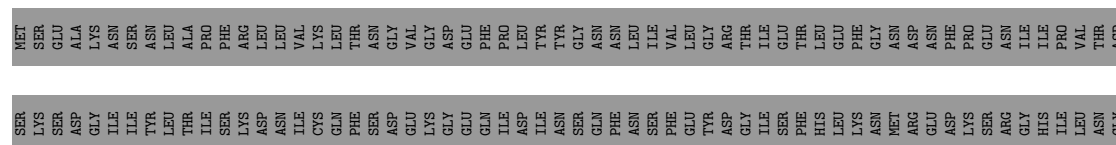
- Molecule 1: Protein MxiG

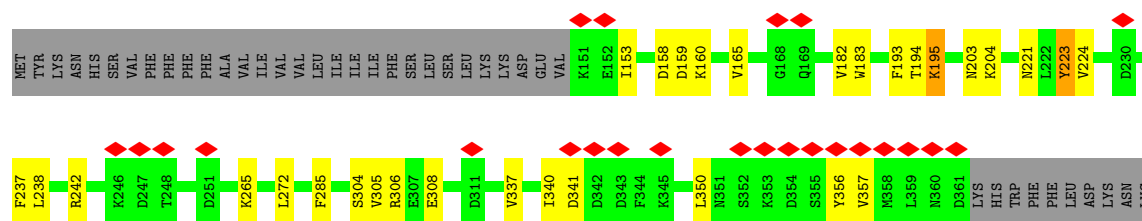


- Molecule 1: Protein MxiG

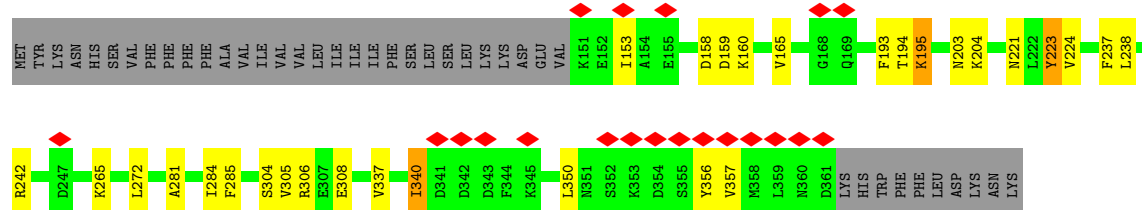
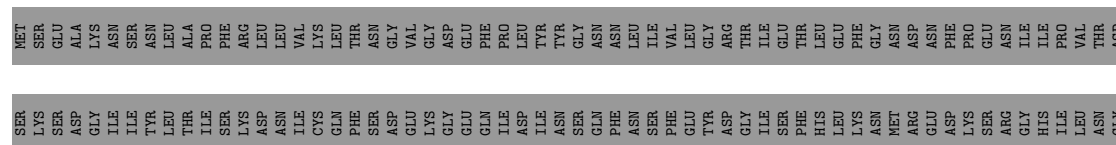


- Molecule 1: Protein MxiG

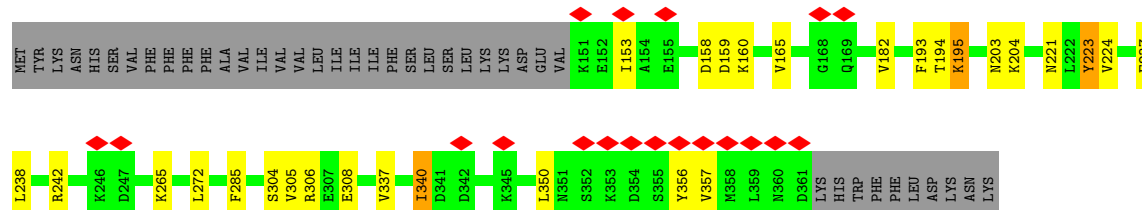
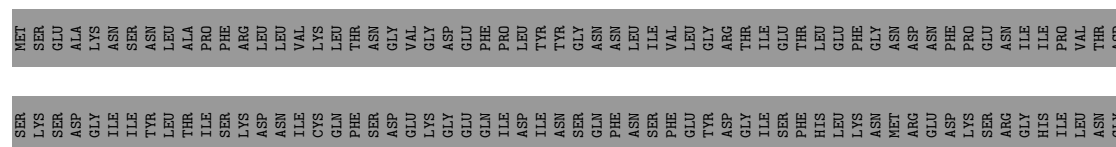




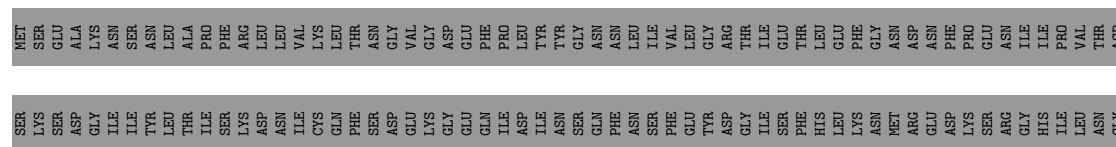
• Molecule 1: Protein MxiG

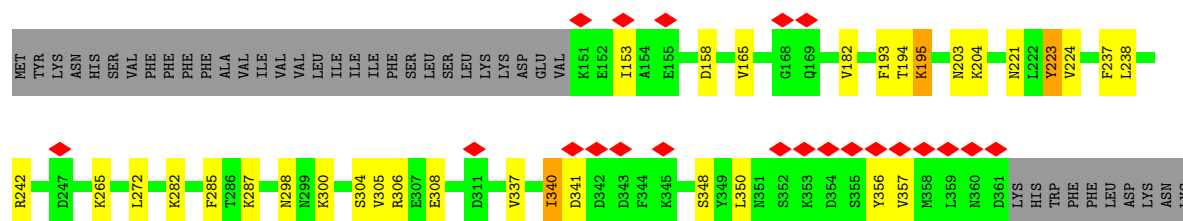


• Molecule 1: Protein MxiG

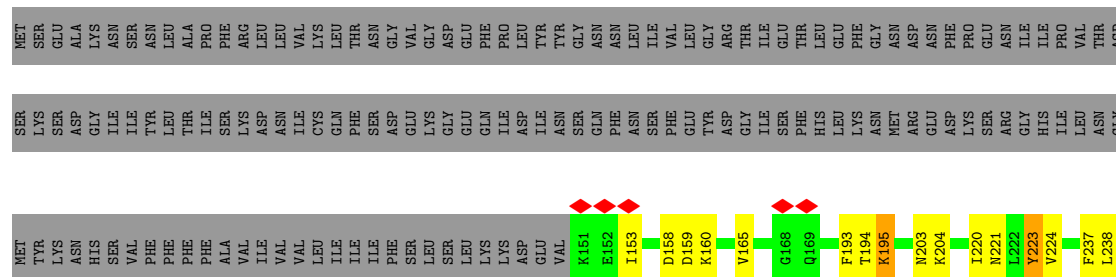


• Molecule 1: Protein MxiG

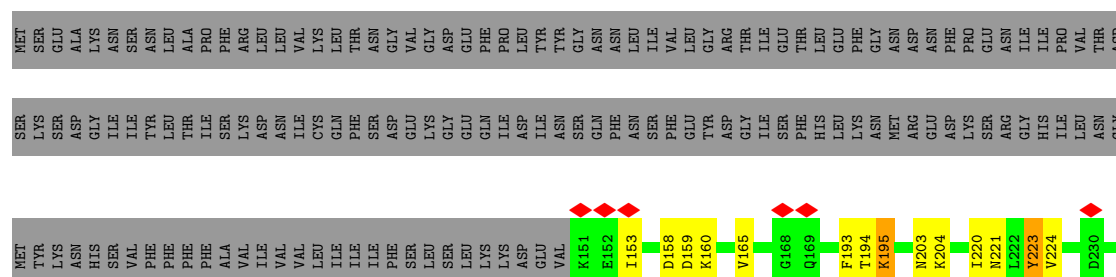




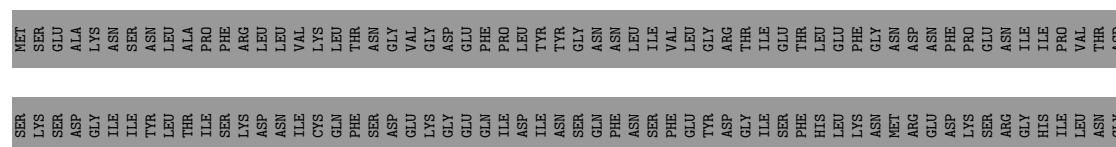
• Molecule 1: Protein MxiG



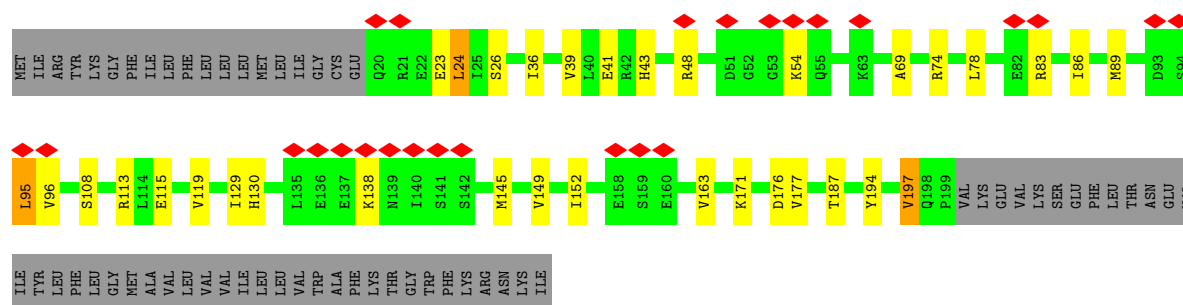
• Molecule 1: Protein MxiG



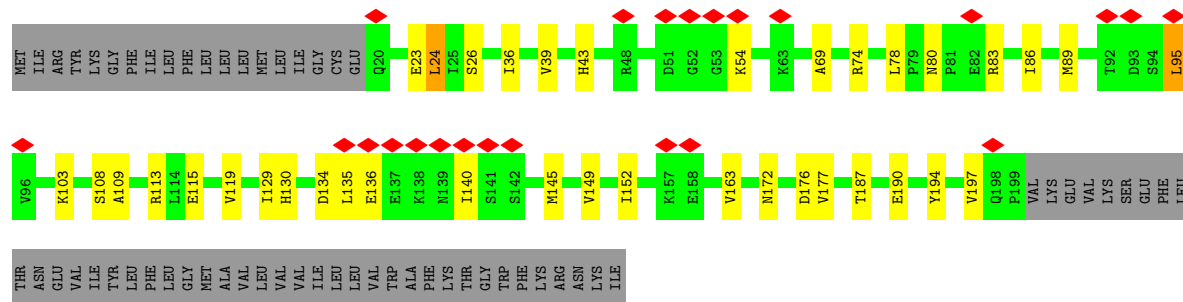
• Molecule 1: Protein MxiG



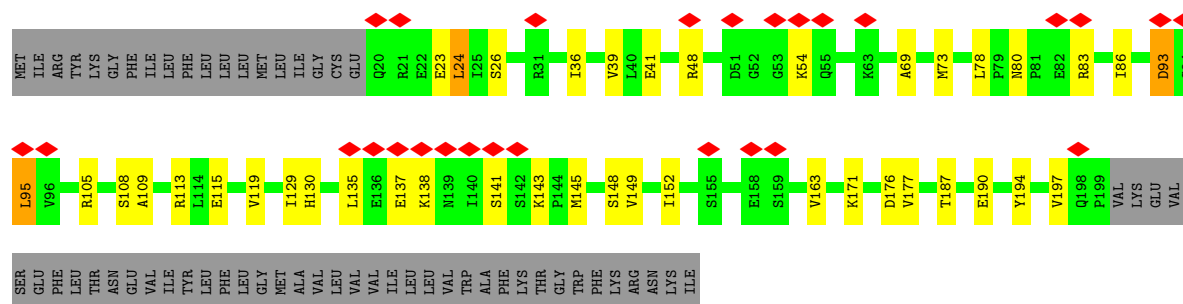
- Molecule 2: Lipoprotein MxiJ



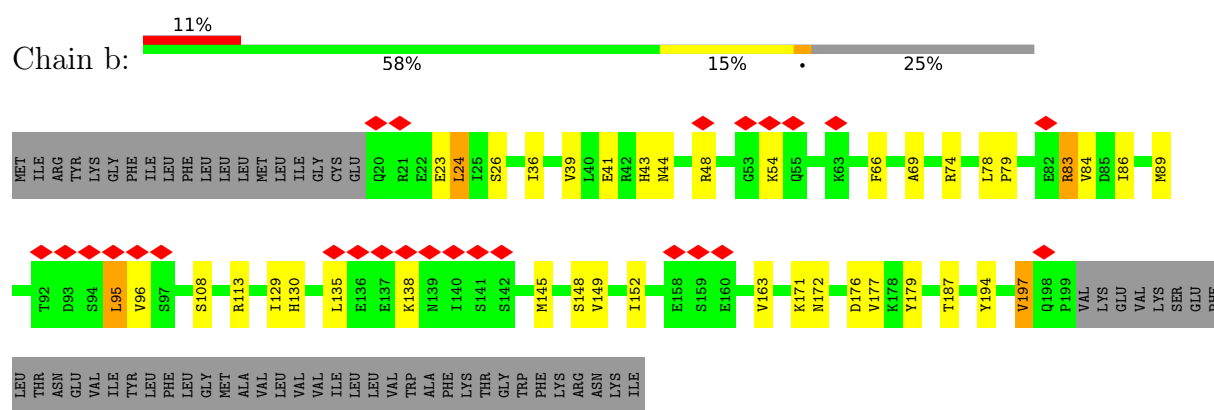
- Molecule 2: Lipoprotein MxiJ



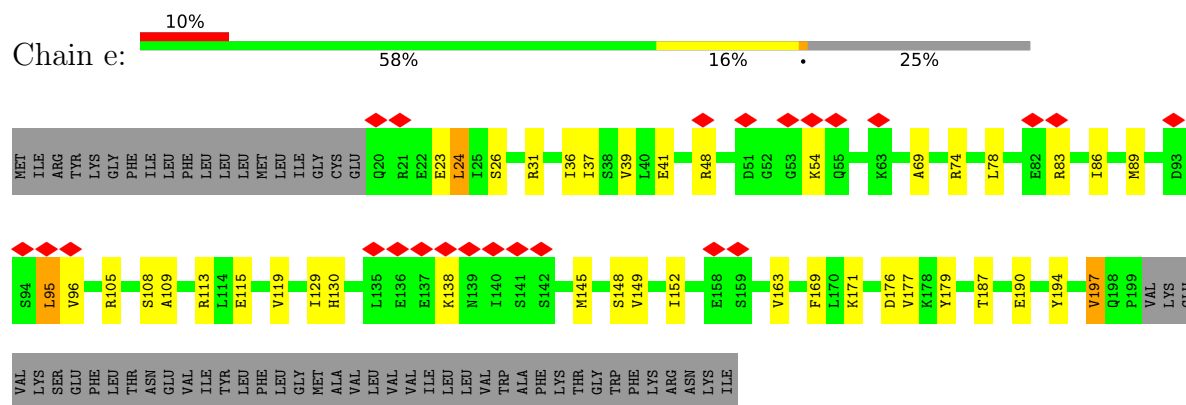
- Molecule 2: Lipoprotein MxiJ



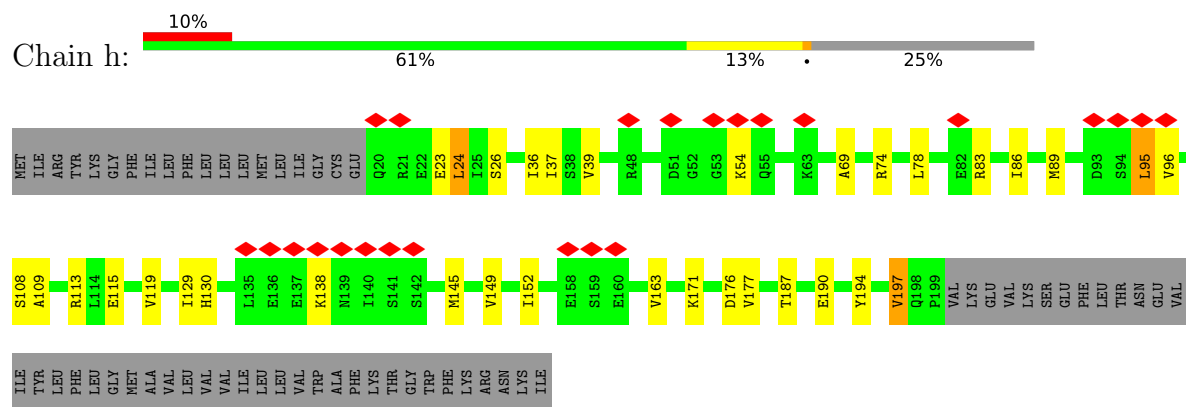
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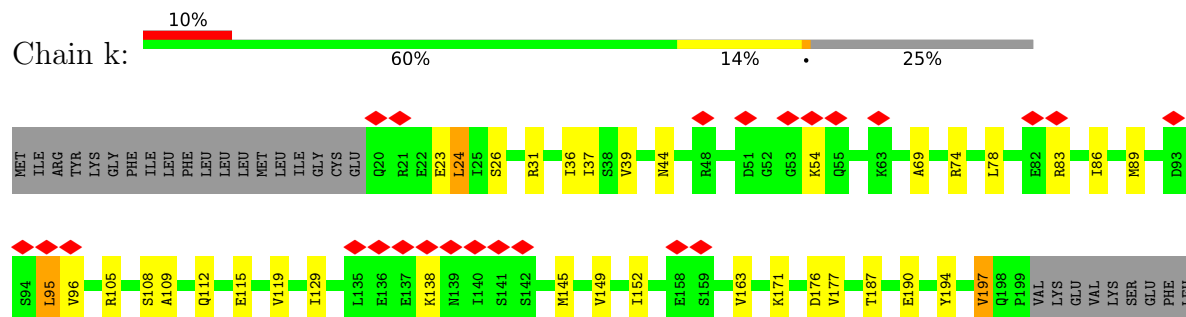
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• Molecule 2: Lipoprotein MxiJ



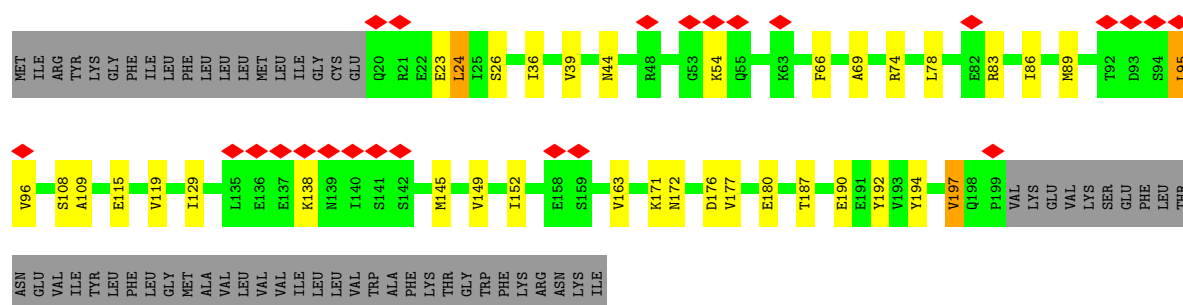
• Molecule 2: Lipoprotein MxiJ



THR ASN
GLU VAL
ILE TYR
LEU PHE
GLY MET
MET MET
VAL VAL
LEU VAL
VAL ILE
ILE ILE
CYS LEU
LEU VAL
TRP TRP
PHE PHE
PHE PHE
LYS THR
GLY GLY
TRP TRP
PHE PHE
LYS LYS
ASN ARG
LYS LYS
ILE ILE

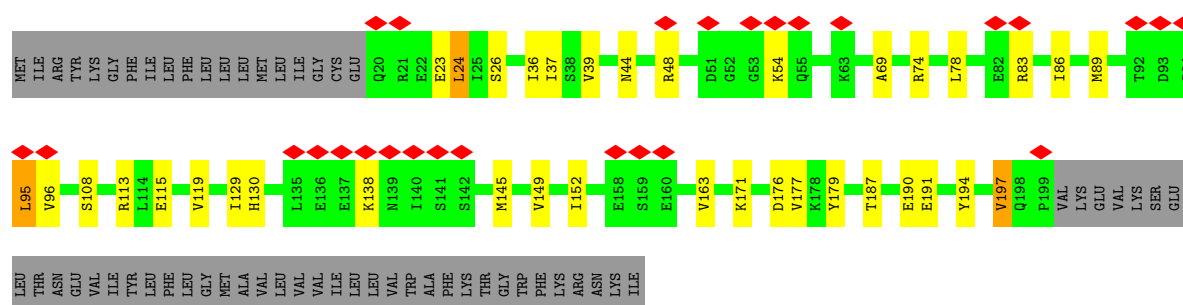
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Chain n: 



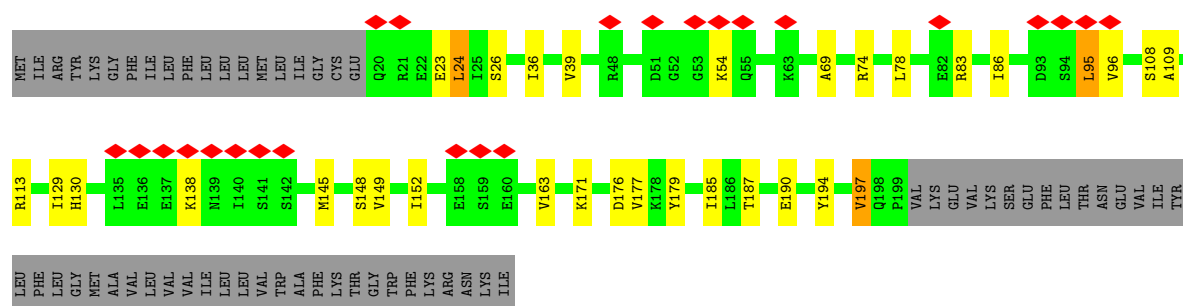
• Molecule 2: Lipoprotein MxiJ

Chain q: 



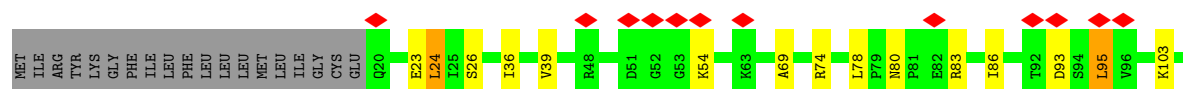
• Molecule 2: Lipoprotein MxiJ

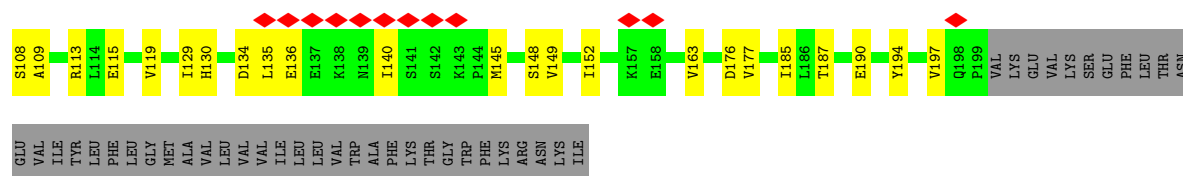
Chain t: 



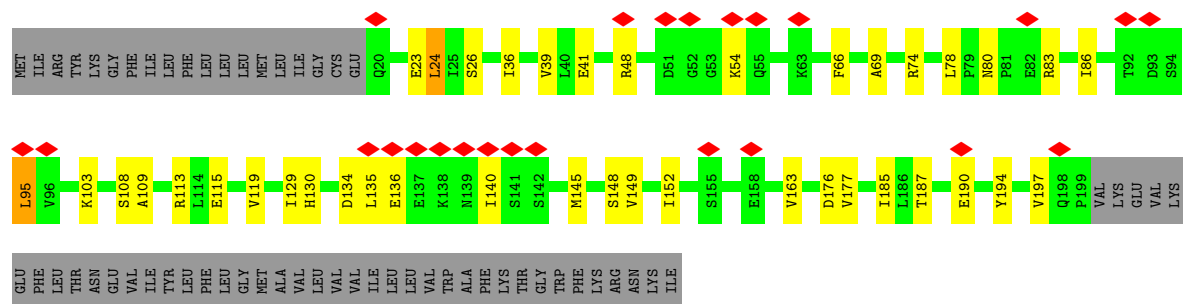
• Molecule 2: Lipoprotein MxiJ

Chain x: 

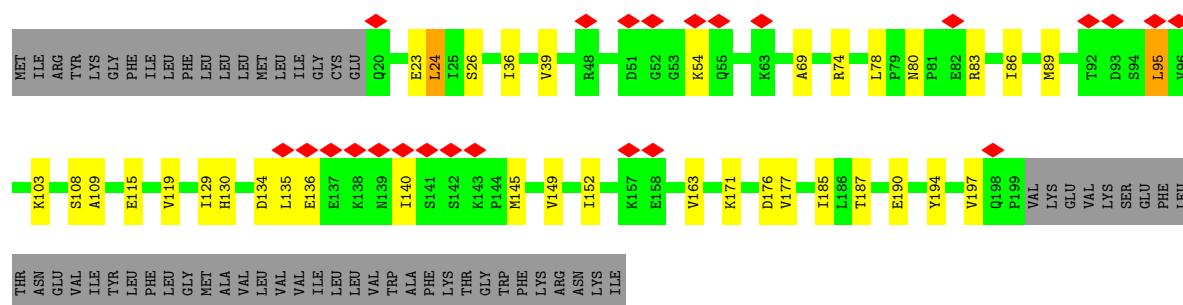




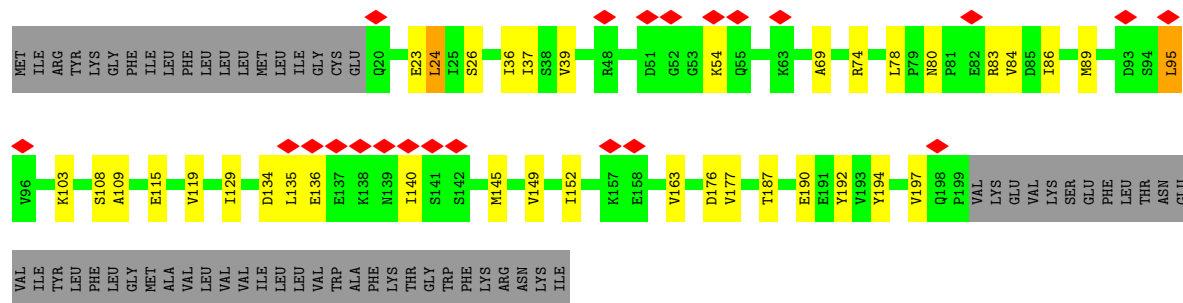
- Molecule 2: Lipoprotein MxiJ



- Molecule 2: Lipoprotein MxiJ

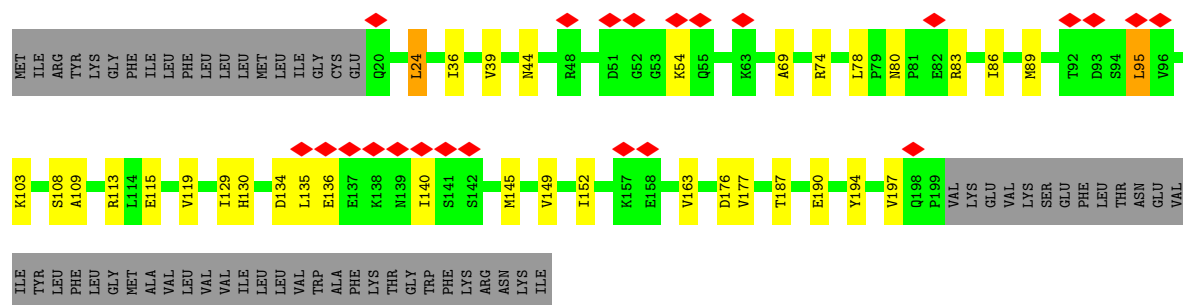


- Molecule 2: Lipoprotein MxiJ



- Molecule 2: Lipoprotein MxiJ





• Molecule 2: Lipoprotein MxiJ



• Molecule 2: Lipoprotein MxiJ

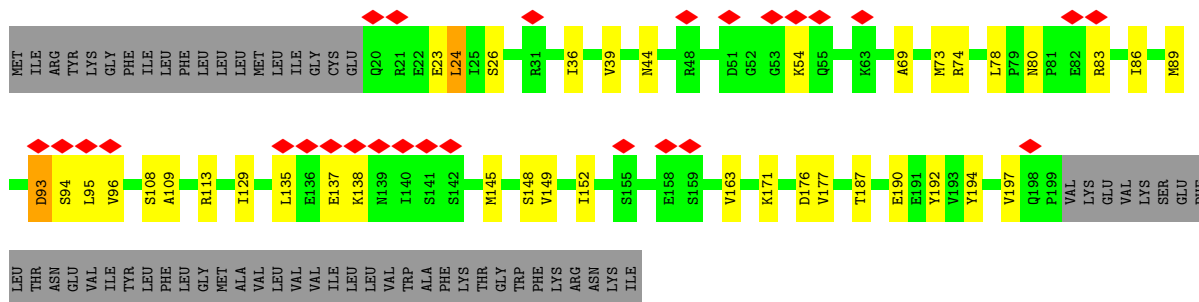


• Molecule 2: Lipoprotein MxiJ

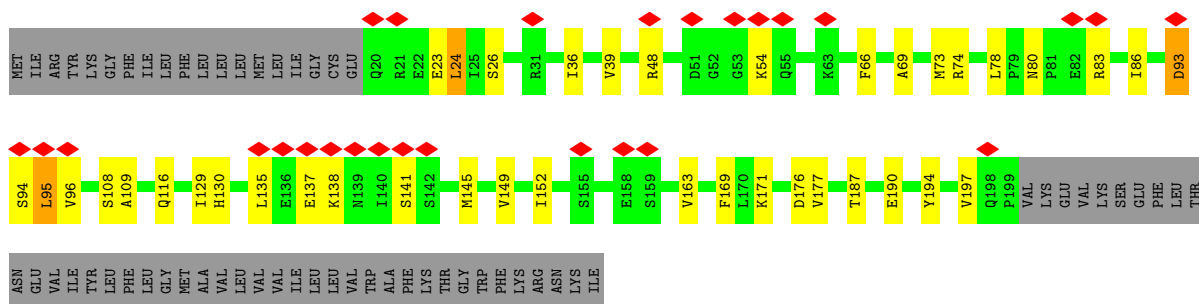




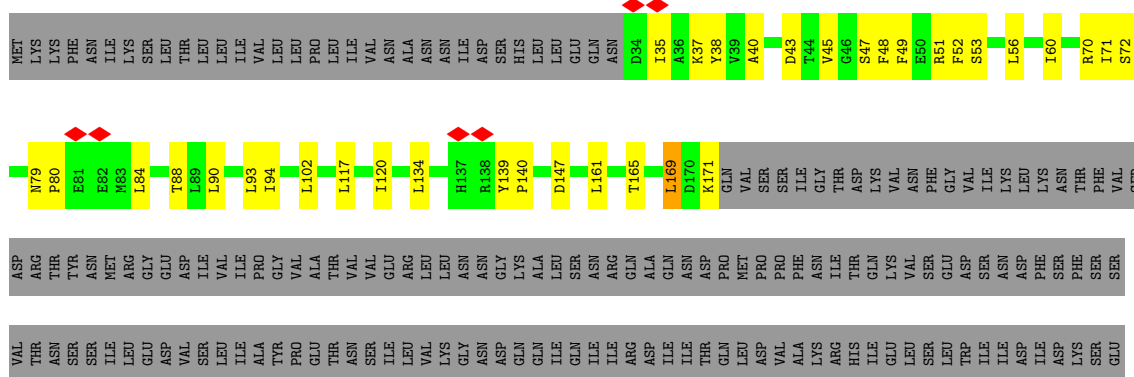
- Molecule 2: Lipoprotein MxiJ



- Molecule 2: Lipoprotein MxiJ

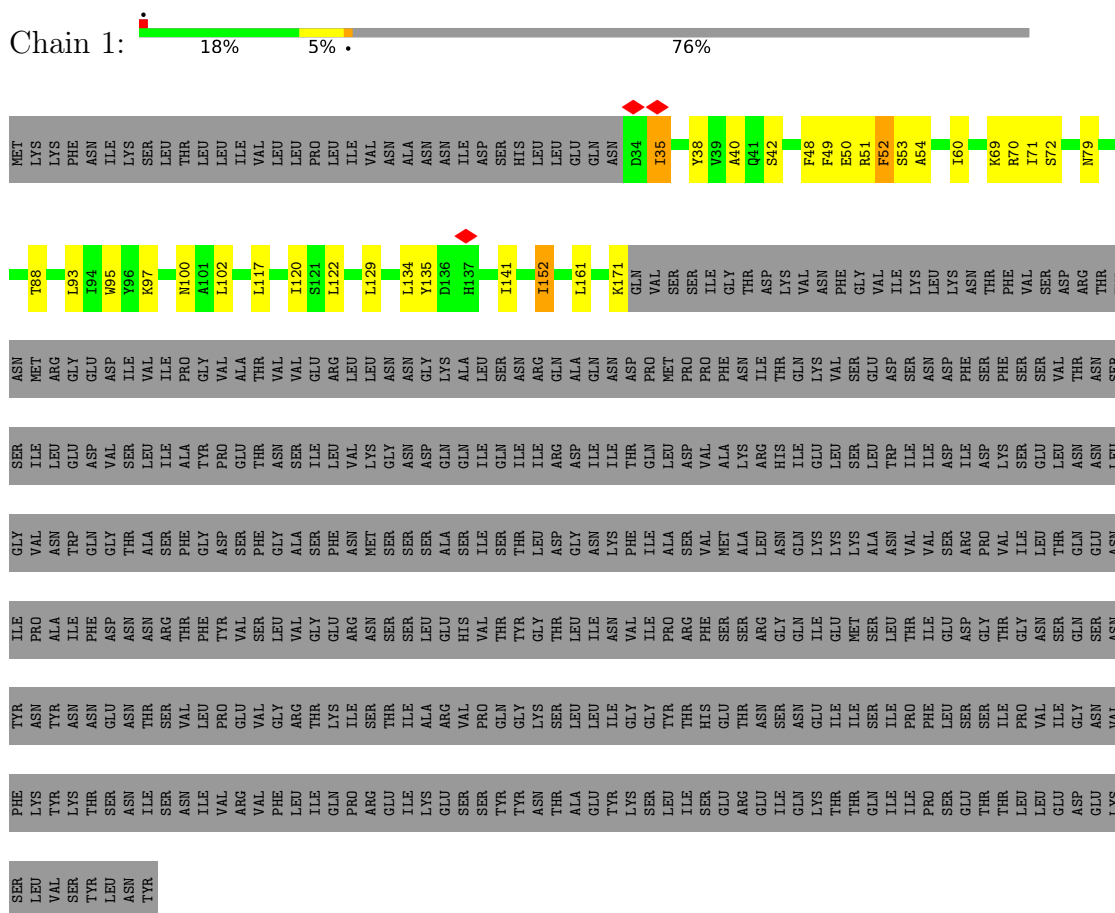


- Molecule 3: Outer membrane protein MxiD

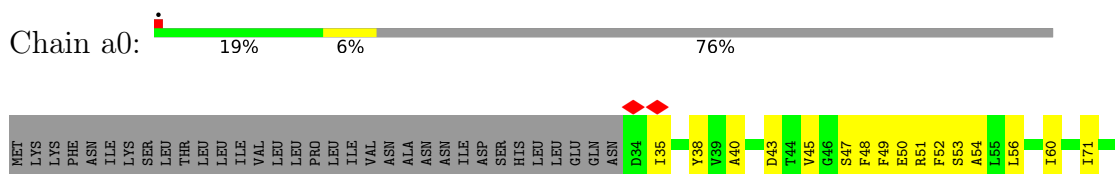


[illegible]

- Molecule 3: Outer membrane protein MxiD



- Molecule 3: Outer membrane protein MxiD





ASP	GLU	LYS	SER	LEU	VAL	THR	ASN	ASN	THR	ASN	THR	ARG	S72
GLU	LYS	SER	LEU	VAL	PHE	TYR	ASN	ASN	THR	SER	TYR	THR	N79
LEU	VAL	SER	SER	THR	THR	ASN	ASN	LEU	LEU	ILE	MET	ARG	E81
LEU	VAL	THR	THR	ASN	ASN	ASN	GLN	GLY	GLY	GLU	GLU	ASP	L84
ASN	ASN	ASN	ASN	THR	ASN	ASN	GLY	VAL	VAL	ASP	THR	ILE	T88
TYR	ASN	SER	ASN	THR	SER	VAL	ALA	LEU	THR	ASN	VAL	ILE	L93
	ASN	ASN	VAL	VAL	ASN	THR	PHE	ILE	ILE	PRO	PRO	ILE	I94
	VAL	VAL	VAL	THR	THR	THR	GLY	THR	GLY	TYR	GLY	GLY	L102
	PHE	PHE	VAL	GLU	GLU	GLU	ASP	VAL	VAL	PRO	VAL	ALA	L117
	THR	THR	THR	THR	THR	THR	PHE	THR	THR	THR	THR	VAL	I120
	THR	THR	THR	THR	THR	THR	GLY	ASN	ASN	ASN	VAL	VAL	L134
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	THR	THR	THR	THR	THR	THR	THR						

● Molecule 3: Outer membrane protein MxiD



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

● Molecule 3: Outer membrane protein MxiD

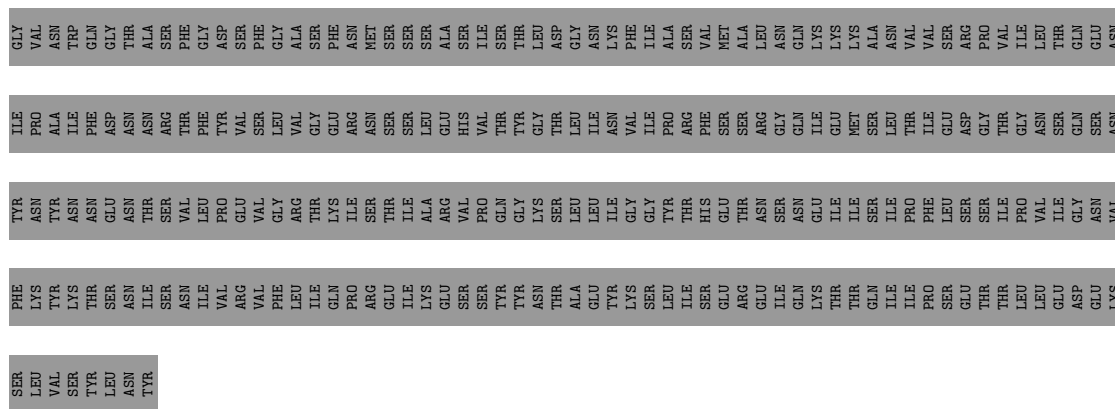


MET	LYS	LYS	PHE	ASN	ILE	LYS	SER	THR	LEU	THR	LEU	LEU	ILE	VAL	ASN	ALA	ASN	ASN	ILE	ASP	SER	HIS	LEU	LEU	GLN	GLN	ASN	D34	I35	Y38	V39	A40	D43	T44	V45	G46	S47	F48	F49	E50	R51	F52	S53	L56	I60	R70	I71	S72				
G76	N79	P80	E81	E82	M83	L84	T88	L89	L90	L93	I94	L102	L117	I120	L134	H137	R138	Y139	P140	D147	L161	T165	L169	D170	K171	GLN	VAL	SER	SER	PRO	PHE	PRO	ILE	ASN	GLY	THR	ASP	LYS	VAL	LEU	SER	ASP	VAL	ILE	LYS	LEU	ASN	THR	PHE	VAL		
SER	ASP	ARG	THR	TYR	ASN	MET	ARG	GLY	GLU	ASP	ILE	VAL	ILE	PRO	GLY	VAL	ASN	GLY	LYS	ALA	LEU	SER	ASN	GLN	GLN	ASN	ARG	ALA	ASN	ASP	PRO	MET	PRO	PHE	PRO	ASN	ILE	THR	THR	GLN	VAL	ALA	LYS	ARG	HIS	THR	ASP	LYS	VAL	SER	GLY	THR
SER	VAL	THR	ASN	SER	SER	ILE	LEU	GLU	ASP	VAL	SER	ILE	ASN	ALA	THR	GLY	ASN	ASP	GLN	GLN	ILE	GLN	ILE	ASP	ILE	GLN	ASP	ILE	ASN	THR	GLN	VAL	ASP	ALA	LYS	ARG	THR	ASN	GLN	ILE	GLY	LEU	SER	TRP	ASP	ILE	ASP	LYS	THR	SER		
GLU	LEU	ASN	ASN	GLY	VAL	ASN	TRP	GLN	GLY	THR	ALA	SER	SER	PHE	GLY	ALA	SER	SER	ALA	GLU	ILE	THR	LEU	GLY	ASN	LYS	PHE	VAL	ASN	GLY	ASN	ALA	VAL	VAL	MET	ALA	LEU	ARG	THR	ASN	GLN	ILE	GLY	LEU	SER	THR	VAL	ARG	PRO	VAL	ILE	
LEU	THR	GLN	GLU	ASN	ILE	PRO	ALA	ASN	PHE	THR	THR	ASN	VAL	VAL	ARG	SER	SER	SER	ALA	GLU	VAL	HIS	THR	TYR	THR	LEU	ASN	ILE	ASN	VAL	GLY	THR	ARG	PHE	SER	ARG	THR	ASN	GLN	ILE	GLY	LEU	ILE	THR	THR	GLY	ASP	GLY	THR	VAL	GLY	
ASN	SER	GLN	SER	ASN	TYR	ASN	TYR	ASN	ASN	ASN	THR	SER	VAL	VAL	LEU	THR	ALA	THR	ARG	GLY	THR	GLY	GLN	LYS	ILE	THR	ASN	GLU	VAL	ASN	GLY	THR	TYR	THR	GLN	PRO	GLY	GLN	ASN	THR	ILE	THR	ALA	GLU	THR	ASN	ILE	THR	THR	PRO		
VAL	ILE	GLY	ASN	VAL	PHE	LYS	TYR	THR	THR	ASN	ILE	SER	ASN	PHE	VAL	ARG	ILE	GLN	PRO	GLU	GLY	THR	ASN	GLY	THR	ASN	ALA	GLU	VAL	ASN	GLY	THR	ILE	ILE	SER	GLU	ARG	THR	ASN	GLN	LYS	THR	THR	GLN	ILE	THR	THR	THR	LEU			
LEU	GLU	ASP	GLU	LYS	SER	SER	VAL	LEU	VAL	ASN	TYR																																									

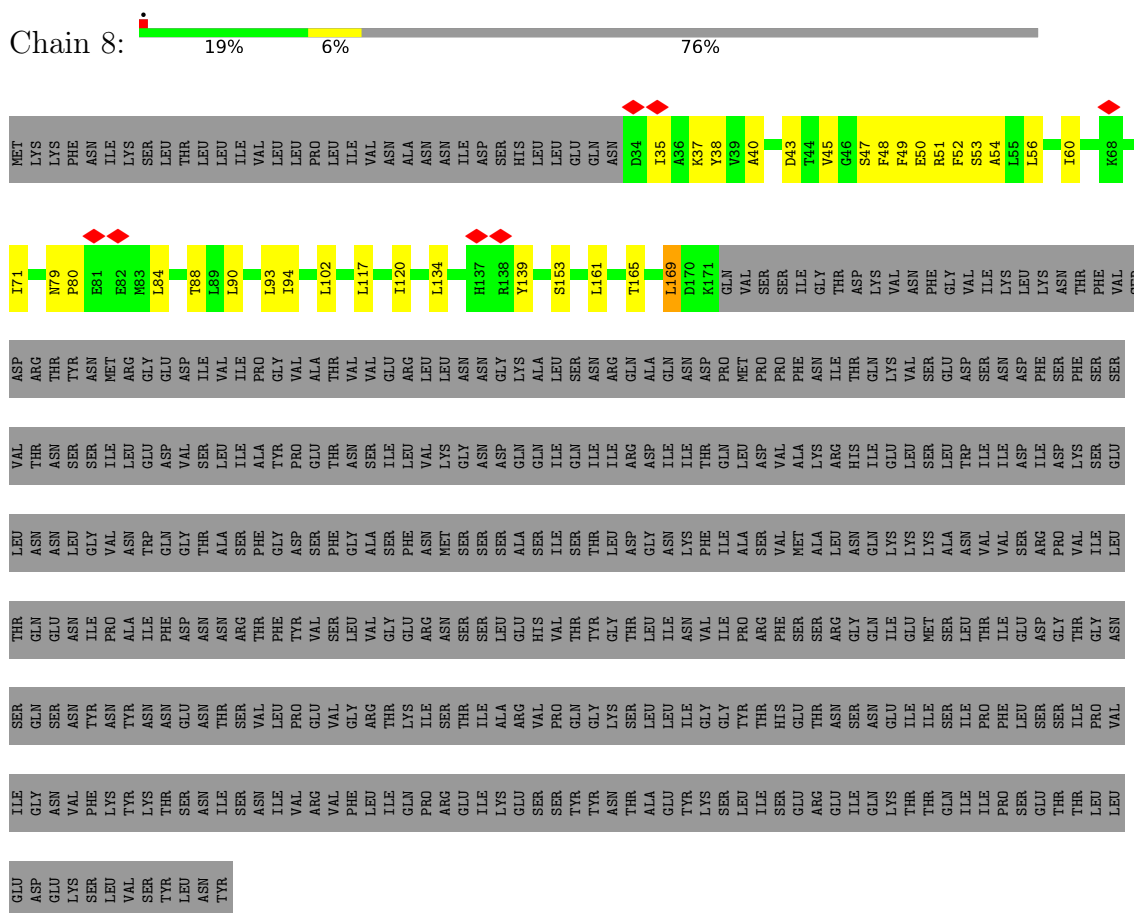
● Molecule 3: Outer membrane protein MxiD



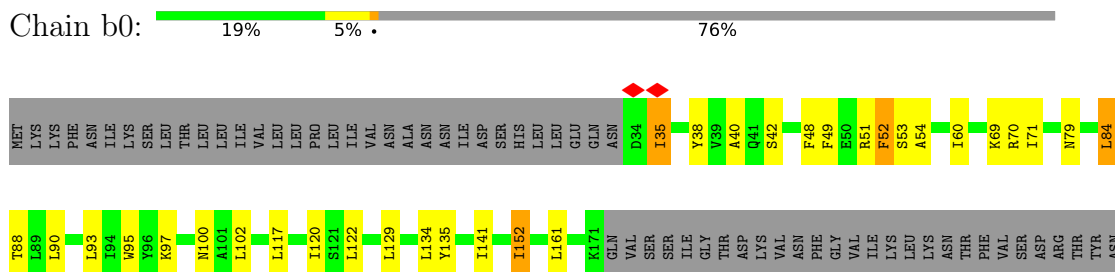
MET	LYS	PHE	ASN	ILE	LYS	SER	THR	LEU	THR	LEU	PRO	LEU	ILE	VAL	ASN	ALA	ASN	ASN	ILE	ASP	SER	HIS	LEU	LEU	GLU	GLN	ASN	D34	I35	Y38	V39	A40	D43	T44	V45	G46	S47	F48	F49	E50	R51	F52	S53	L56	I60	I71	D76																			
N79	P80	E81	L84	T88	L93	I94	L102	L117	I120	L134	H137	R138	Y139	P140	D147	L161	T165	L169	D170	K171	GLN	VAL	SER	SER	ILE	GLY	THR	ASP	LYS	VAL	ASN	PHE	GLY	VAL	ILE	LYS	LEU	LYS	ASN	THR	PHE	VAL	SER	THR	ASP	ARG	TYR																			
ASN	MET	ARG	GLY	GLU	ASP	ILE	VAL	ILE	PRO	GLY	VAL	ALA	THR	ASN	VAL	VAL	GLU	ARG	LEU	VAL	GLY	ASN	ASN	GLY	LYS	ALA	LEU	ILE	SER	ASN	GLN	ARG	ALA	GLN	ASN	ASP	THR	GLN	PRO	MET	PRO	PRO	PHE	ASN	GLY	ASP	THR	GLN	LYS	VAL	SER	GLU	TRP	ILE	ASN	ASP	ILE	ASN	PHE	SER	GLU	VAL	THR	ASN	ASN	LEU
SER	ILE	LEU	GLU	ASP	VAL	SER	LEU	ALA	TYP	PRO	PRO	GLU	THR	ASN	ASN	GLN	GLN	GLN	ILE	GLN	ILE	ILE	ILE	ARG	ASP	ILE	THR	ASN	GLN	LYS	GLU	LEU	SER	THR	TRP	LEU	ILE	ASN	ASP	ILE	ASN	ASP	LYS	SER	SER	GLU	LEU	ASN	ASN	LEU																



- Molecule 3: Outer membrane protein MxiD



- Molecule 3: Outer membrane protein MxiD



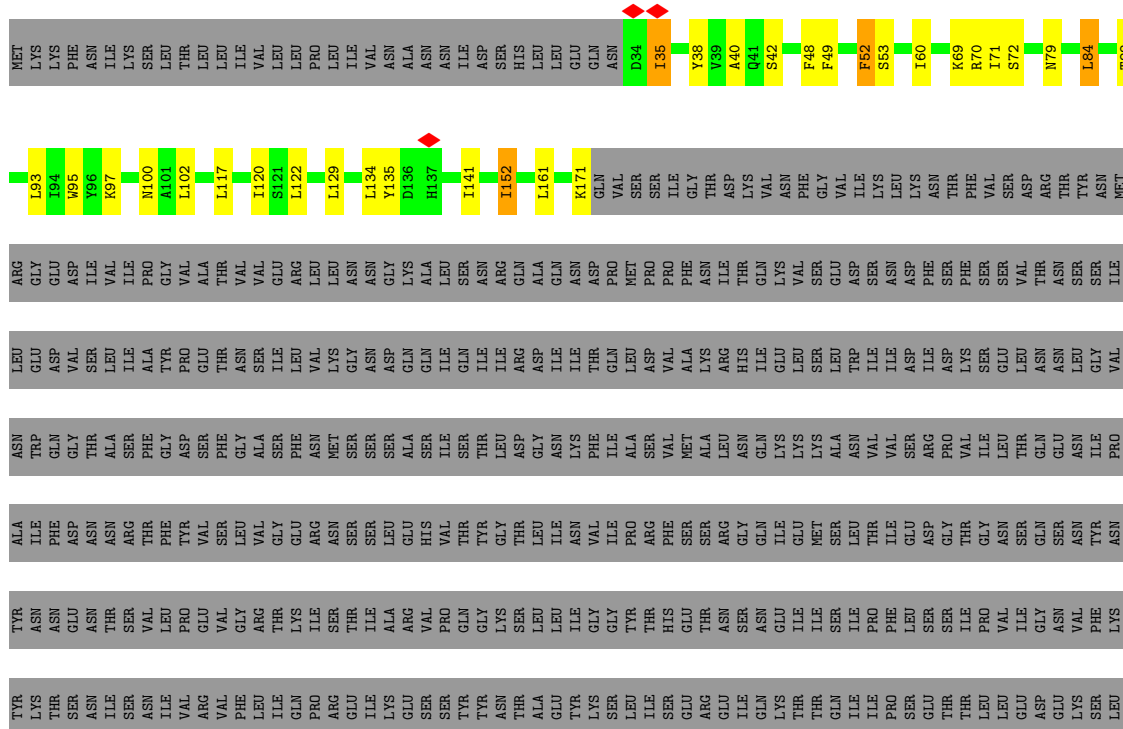
LEU	LYS	ASN	PRO	VAL	IIE
VAL	TYR	TYR	ALA	ASN	LEU
SER	LYS	ASN	IIE	TRP	GLY
TYR	THR	ASN	PHE	GLN	ASP
ASN	SER	GLU	ASP	GLY	VAL
ASN	ASN	ASN	ASN	THR	SER
TYR	IIE	THR	ASN	ALA	LEU
	SER	SER	ASN	THR	VAL
	ASN	VAL	THR	PHE	IIE
	IIE	LEU	PHE	GLY	TYR
	VAL	PRO	TYR	ASP	PRO
	ARG	VAL	VAL	SER	ALA
	VAL	VAL	SER	PHE	THR
	PHE	GLY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

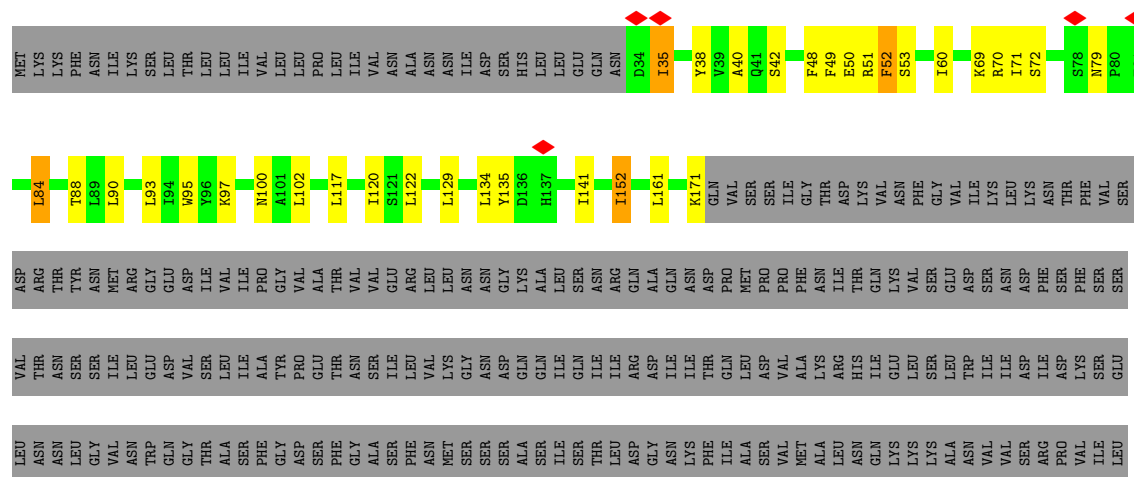
- Molecule 3: Outer membrane protein MxiD

[illegible]

- Molecule 3: Outer membrane protein MxiD

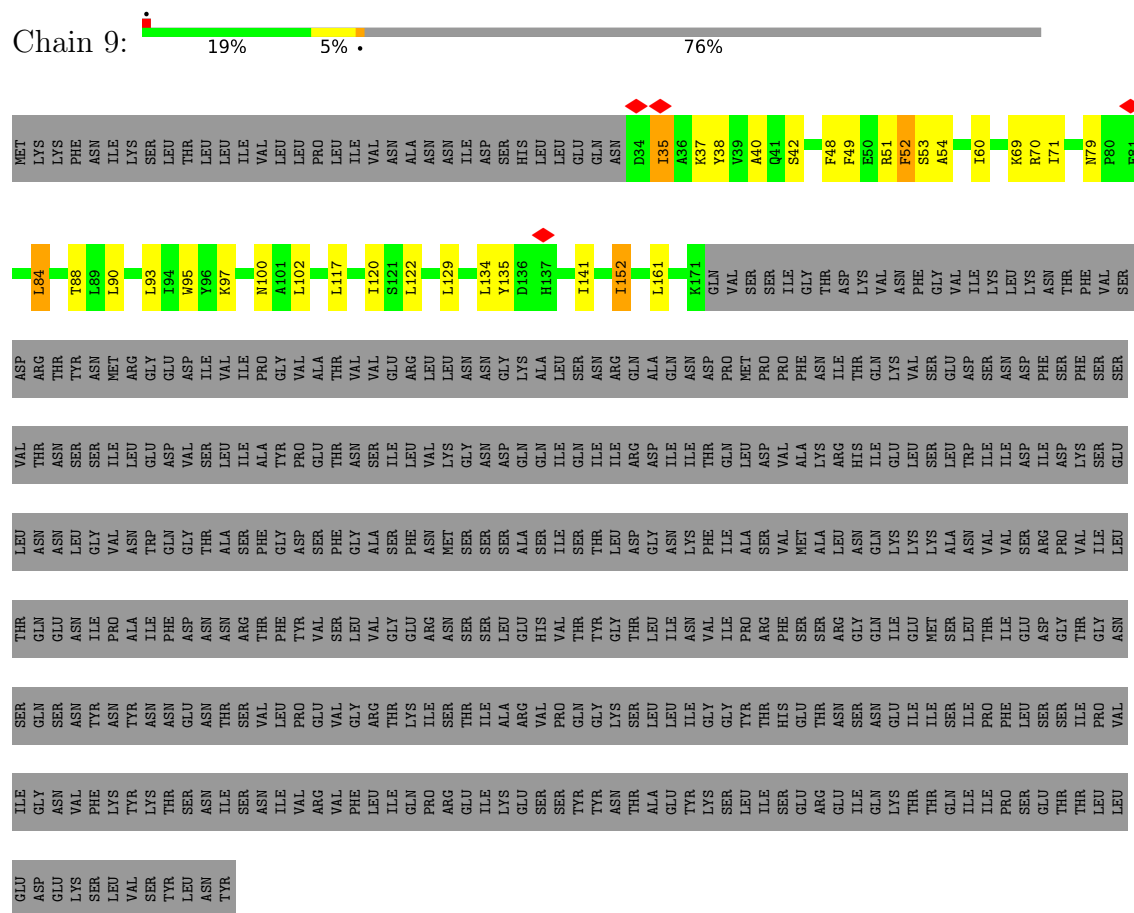






GLU	GLY	ILE	SER	THR
ASP	GLY	GLN	GLN	GLN
GLU	ASN	SER	SER	ASN
LYS	VAL	PHE	THR	ILE
SER	ASN	THR	ASN	PRO
LEU	LYS	THR	ASN	THR
VAL	TYR	TYR	TYR	ALA
SER	LYS	ASN	ASN	ILE
TYR	THR	THR	ASN	PHE
LEU	THR	SER	GLU	ASP
ASN	ASN	ASN	ASN	ASN
TYR	ILE	ILE	THR	ASN
	SER	SER	SER	ARG
	ASN	ASN	VAL	THR
	ILE	ILE	LEU	PHE
	VAL	VAL	PRO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

- Molecule 3: Outer membrane protein MxiD



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C8	Depositor
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	0.389	Depositor
Minimum map value	-0.213	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	664.1712, 664.1712, 664.1712	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.38369, 1.38369, 1.38369	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	0.14	0/1837	0.35	0/2477
1	B	0.14	0/1837	0.34	0/2477
1	C	0.13	0/1761	0.31	0/2374
1	D	0.14	0/1837	0.35	0/2477
1	E	0.14	0/1837	0.34	0/2477
1	F	0.13	0/1761	0.32	0/2374
1	G	0.14	0/1837	0.35	0/2477
1	H	0.14	0/1837	0.34	0/2477
1	I	0.13	0/1761	0.32	0/2374
1	J	0.14	0/1837	0.35	0/2477
1	K	0.14	0/1837	0.34	0/2477
1	L	0.13	0/1761	0.31	0/2374
1	M	0.14	0/1837	0.35	0/2477
1	N	0.14	0/1837	0.34	0/2477
1	O	0.13	0/1761	0.31	0/2374
1	P	0.14	0/1837	0.36	0/2477
1	Q	0.14	0/1837	0.34	0/2477
1	R	0.13	0/1761	0.32	0/2374
1	S	0.14	0/1837	0.35	0/2477
1	T	0.14	0/1837	0.34	0/2477
1	U	0.14	0/1837	0.35	0/2477
1	V	0.14	0/1837	0.34	0/2477
1	W	0.13	0/1761	0.31	0/2374
1	X	0.13	0/1761	0.31	0/2374
2	a	0.16	0/1449	0.42	0/1957
2	b	0.16	0/1449	0.42	0/1957
2	c	0.16	0/1449	0.43	0/1957
2	d	0.16	0/1449	0.45	0/1957
2	e	0.16	0/1449	0.42	0/1957
2	f	0.16	0/1449	0.43	0/1957
2	g	0.16	0/1449	0.45	0/1957
2	h	0.16	0/1449	0.42	0/1957
2	i	0.16	0/1449	0.43	0/1957
2	j	0.16	0/1449	0.45	0/1957

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	k	0.16	0/1449	0.42	0/1957
2	l	0.16	0/1449	0.43	0/1957
2	m	0.16	0/1449	0.45	0/1957
2	n	0.16	0/1449	0.42	0/1957
2	o	0.16	0/1449	0.43	0/1957
2	p	0.16	0/1449	0.45	0/1957
2	q	0.16	0/1449	0.42	0/1957
2	r	0.16	0/1449	0.43	0/1957
2	s	0.16	0/1449	0.45	0/1957
2	t	0.16	0/1449	0.42	0/1957
2	u	0.16	0/1449	0.43	0/1957
2	v	0.16	0/1449	0.43	0/1957
2	w	0.16	0/1449	0.45	0/1957
2	x	0.16	0/1449	0.45	0/1957
3	0	0.13	0/1124	0.37	0/1525
3	1	0.14	0/1124	0.35	0/1525
3	2	0.13	0/1124	0.37	0/1525
3	3	0.14	0/1124	0.35	0/1525
3	4	0.13	0/1124	0.37	0/1525
3	5	0.15	0/1124	0.35	0/1525
3	6	0.13	0/1124	0.38	0/1525
3	7	0.15	0/1124	0.35	0/1525
3	8	0.14	0/1124	0.37	0/1525
3	9	0.14	0/1124	0.35	0/1525
3	Y	0.13	0/1124	0.37	0/1525
3	Z	0.13	0/1124	0.37	0/1525
3	a0	0.13	0/1124	0.37	0/1525
3	b0	0.14	0/1124	0.35	0/1525
3	y	0.15	0/1124	0.35	0/1525
3	z	0.14	0/1124	0.35	0/1525
All	All	0.15	0/96240	0.38	0/129992

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	1805	0	1799	20	0
1	B	1805	0	1799	26	0
1	C	1734	0	1736	20	0
1	D	1805	0	1799	24	0
1	E	1805	0	1799	26	0
1	F	1734	0	1736	20	0
1	G	1805	0	1799	25	0
1	H	1805	0	1799	31	0
1	I	1734	0	1736	23	0
1	J	1805	0	1799	21	0
1	K	1805	0	1799	24	0
1	L	1734	0	1736	17	0
1	M	1805	0	1799	21	0
1	N	1805	0	1799	25	0
1	O	1734	0	1736	17	0
1	P	1805	0	1799	21	0
1	Q	1805	0	1799	25	0
1	R	1734	0	1736	18	0
1	S	1805	0	1799	25	0
1	T	1805	0	1799	26	0
1	U	1805	0	1799	25	0
1	V	1805	0	1799	24	0
1	W	1734	0	1736	16	0
1	X	1734	0	1736	15	0
2	a	1428	0	1451	22	0
2	b	1428	0	1451	30	0
2	c	1428	0	1451	25	0
2	d	1428	0	1451	27	0
2	e	1428	0	1451	27	0
2	f	1428	0	1451	31	0
2	g	1428	0	1451	28	0
2	h	1428	0	1451	22	0
2	i	1428	0	1451	30	0
2	j	1428	0	1451	29	0
2	k	1428	0	1451	23	0
2	l	1428	0	1451	26	0
2	m	1428	0	1451	24	0
2	n	1428	0	1451	24	0
2	o	1428	0	1451	24	0
2	p	1428	0	1451	23	0
2	q	1428	0	1451	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	r	1428	0	1451	27	0
2	s	1428	0	1451	29	0
2	t	1428	0	1451	23	0
2	u	1428	0	1451	27	0
2	v	1428	0	1451	22	0
2	w	1428	0	1451	31	0
2	x	1428	0	1451	27	0
3	0	1102	0	1118	25	0
3	1	1102	0	1118	25	0
3	2	1102	0	1118	24	0
3	3	1102	0	1118	25	0
3	4	1102	0	1118	24	0
3	5	1102	0	1118	23	0
3	6	1102	0	1118	20	0
3	7	1102	0	1118	26	0
3	8	1102	0	1118	22	0
3	9	1102	0	1118	23	0
3	Y	1102	0	1118	25	0
3	Z	1102	0	1118	24	0
3	a0	1102	0	1118	24	0
3	b0	1102	0	1118	23	0
3	y	1102	0	1118	26	0
3	z	1102	0	1118	21	0
All	All	94656	0	95384	1296	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 7.

The worst 5 of 1296 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:S:363:HIS:HE2	3:3:72:SER:HG	1.04	0.95
1:U:363:HIS:HE2	3:5:72:SER:HG	1.25	0.83
2:j:136:GLU:HB2	2:j:140:ILE:HD13	1.64	0.80
2:s:136:GLU:HB2	2:s:140:ILE:HD13	1.64	0.80
2:m:136:GLU:HB2	2:m:140:ILE:HD13	1.64	0.80

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	216/371 (58%)	204 (94%)	12 (6%)	0	100	100
1	B	216/371 (58%)	207 (96%)	9 (4%)	0	100	100
1	C	209/371 (56%)	203 (97%)	6 (3%)	0	100	100
1	D	216/371 (58%)	205 (95%)	11 (5%)	0	100	100
1	E	216/371 (58%)	207 (96%)	9 (4%)	0	100	100
1	F	209/371 (56%)	202 (97%)	7 (3%)	0	100	100
1	G	216/371 (58%)	203 (94%)	13 (6%)	0	100	100
1	H	216/371 (58%)	207 (96%)	9 (4%)	0	100	100
1	I	209/371 (56%)	202 (97%)	7 (3%)	0	100	100
1	J	216/371 (58%)	205 (95%)	11 (5%)	0	100	100
1	K	216/371 (58%)	207 (96%)	9 (4%)	0	100	100
1	L	209/371 (56%)	202 (97%)	7 (3%)	0	100	100
1	M	216/371 (58%)	205 (95%)	11 (5%)	0	100	100
1	N	216/371 (58%)	207 (96%)	9 (4%)	0	100	100
1	O	209/371 (56%)	202 (97%)	7 (3%)	0	100	100
1	P	216/371 (58%)	204 (94%)	12 (6%)	0	100	100
1	Q	216/371 (58%)	207 (96%)	9 (4%)	0	100	100
1	R	209/371 (56%)	202 (97%)	7 (3%)	0	100	100
1	S	216/371 (58%)	205 (95%)	11 (5%)	0	100	100
1	T	216/371 (58%)	207 (96%)	9 (4%)	0	100	100
1	U	216/371 (58%)	204 (94%)	12 (6%)	0	100	100
1	V	216/371 (58%)	207 (96%)	9 (4%)	0	100	100
1	W	209/371 (56%)	203 (97%)	6 (3%)	0	100	100
1	X	209/371 (56%)	203 (97%)	6 (3%)	0	100	100
2	a	178/241 (74%)	166 (93%)	12 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	b	178/241 (74%)	166 (93%)	12 (7%)	0	100	100
2	c	178/241 (74%)	165 (93%)	13 (7%)	0	100	100
2	d	178/241 (74%)	164 (92%)	14 (8%)	0	100	100
2	e	178/241 (74%)	167 (94%)	11 (6%)	0	100	100
2	f	178/241 (74%)	165 (93%)	13 (7%)	0	100	100
2	g	178/241 (74%)	164 (92%)	14 (8%)	0	100	100
2	h	178/241 (74%)	167 (94%)	11 (6%)	0	100	100
2	i	178/241 (74%)	165 (93%)	13 (7%)	0	100	100
2	j	178/241 (74%)	163 (92%)	15 (8%)	0	100	100
2	k	178/241 (74%)	167 (94%)	11 (6%)	0	100	100
2	l	178/241 (74%)	165 (93%)	13 (7%)	0	100	100
2	m	178/241 (74%)	164 (92%)	14 (8%)	0	100	100
2	n	178/241 (74%)	167 (94%)	11 (6%)	0	100	100
2	o	178/241 (74%)	165 (93%)	13 (7%)	0	100	100
2	p	178/241 (74%)	164 (92%)	14 (8%)	0	100	100
2	q	178/241 (74%)	167 (94%)	11 (6%)	0	100	100
2	r	178/241 (74%)	165 (93%)	13 (7%)	0	100	100
2	s	178/241 (74%)	164 (92%)	14 (8%)	0	100	100
2	t	178/241 (74%)	167 (94%)	11 (6%)	0	100	100
2	u	178/241 (74%)	165 (93%)	13 (7%)	0	100	100
2	v	178/241 (74%)	165 (93%)	13 (7%)	0	100	100
2	w	178/241 (74%)	164 (92%)	14 (8%)	0	100	100
2	x	178/241 (74%)	164 (92%)	14 (8%)	0	100	100
3	0	136/566 (24%)	130 (96%)	6 (4%)	0	100	100
3	1	136/566 (24%)	129 (95%)	7 (5%)	0	100	100
3	2	136/566 (24%)	130 (96%)	6 (4%)	0	100	100
3	3	136/566 (24%)	129 (95%)	7 (5%)	0	100	100
3	4	136/566 (24%)	130 (96%)	6 (4%)	0	100	100
3	5	136/566 (24%)	129 (95%)	7 (5%)	0	100	100
3	6	136/566 (24%)	130 (96%)	6 (4%)	0	100	100
3	7	136/566 (24%)	129 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	8	136/566 (24%)	130 (96%)	6 (4%)	0	100	100
3	9	136/566 (24%)	129 (95%)	7 (5%)	0	100	100
3	Y	136/566 (24%)	130 (96%)	6 (4%)	0	100	100
3	Z	136/566 (24%)	130 (96%)	6 (4%)	0	100	100
3	a0	136/566 (24%)	130 (96%)	6 (4%)	0	100	100
3	b0	136/566 (24%)	129 (95%)	7 (5%)	0	100	100
3	y	136/566 (24%)	129 (95%)	7 (5%)	0	100	100
3	z	136/566 (24%)	129 (95%)	7 (5%)	0	100	100
All	All	11576/23744 (49%)	10947 (95%)	629 (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	202/342 (59%)	196 (97%)	6 (3%)	36	61
1	B	202/342 (59%)	198 (98%)	4 (2%)	48	67
1	C	195/342 (57%)	188 (96%)	7 (4%)	31	58
1	D	202/342 (59%)	196 (97%)	6 (3%)	36	61
1	E	202/342 (59%)	198 (98%)	4 (2%)	48	67
1	F	195/342 (57%)	188 (96%)	7 (4%)	31	58
1	G	202/342 (59%)	196 (97%)	6 (3%)	36	61
1	H	202/342 (59%)	198 (98%)	4 (2%)	48	67
1	I	195/342 (57%)	188 (96%)	7 (4%)	31	58
1	J	202/342 (59%)	196 (97%)	6 (3%)	36	61
1	K	202/342 (59%)	198 (98%)	4 (2%)	48	67
1	L	195/342 (57%)	188 (96%)	7 (4%)	31	58
1	M	202/342 (59%)	196 (97%)	6 (3%)	36	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	202/342 (59%)	198 (98%)	4 (2%)	48	67
1	O	195/342 (57%)	188 (96%)	7 (4%)	31	58
1	P	202/342 (59%)	196 (97%)	6 (3%)	36	61
1	Q	202/342 (59%)	198 (98%)	4 (2%)	48	67
1	R	195/342 (57%)	188 (96%)	7 (4%)	31	58
1	S	202/342 (59%)	196 (97%)	6 (3%)	36	61
1	T	202/342 (59%)	198 (98%)	4 (2%)	48	67
1	U	202/342 (59%)	196 (97%)	6 (3%)	36	61
1	V	202/342 (59%)	198 (98%)	4 (2%)	48	67
1	W	195/342 (57%)	188 (96%)	7 (4%)	31	58
1	X	195/342 (57%)	188 (96%)	7 (4%)	31	58
2	a	165/220 (75%)	158 (96%)	7 (4%)	26	55
2	b	165/220 (75%)	158 (96%)	7 (4%)	26	55
2	c	165/220 (75%)	156 (94%)	9 (6%)	19	48
2	d	165/220 (75%)	159 (96%)	6 (4%)	31	58
2	e	165/220 (75%)	158 (96%)	7 (4%)	26	55
2	f	165/220 (75%)	156 (94%)	9 (6%)	19	48
2	g	165/220 (75%)	159 (96%)	6 (4%)	31	58
2	h	165/220 (75%)	158 (96%)	7 (4%)	26	55
2	i	165/220 (75%)	156 (94%)	9 (6%)	19	48
2	j	165/220 (75%)	159 (96%)	6 (4%)	31	58
2	k	165/220 (75%)	158 (96%)	7 (4%)	26	55
2	l	165/220 (75%)	156 (94%)	9 (6%)	19	48
2	m	165/220 (75%)	159 (96%)	6 (4%)	31	58
2	n	165/220 (75%)	158 (96%)	7 (4%)	26	55
2	o	165/220 (75%)	156 (94%)	9 (6%)	19	48
2	p	165/220 (75%)	159 (96%)	6 (4%)	31	58
2	q	165/220 (75%)	158 (96%)	7 (4%)	26	55
2	r	165/220 (75%)	156 (94%)	9 (6%)	19	48
2	s	165/220 (75%)	159 (96%)	6 (4%)	31	58
2	t	165/220 (75%)	158 (96%)	7 (4%)	26	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	u	165/220 (75%)	156 (94%)	9 (6%)	19	48
2	v	165/220 (75%)	156 (94%)	9 (6%)	19	48
2	w	165/220 (75%)	159 (96%)	6 (4%)	31	58
2	x	165/220 (75%)	159 (96%)	6 (4%)	31	58
3	0	121/513 (24%)	118 (98%)	3 (2%)	42	64
3	1	121/513 (24%)	116 (96%)	5 (4%)	27	55
3	2	121/513 (24%)	118 (98%)	3 (2%)	42	64
3	3	121/513 (24%)	116 (96%)	5 (4%)	27	55
3	4	121/513 (24%)	118 (98%)	3 (2%)	42	64
3	5	121/513 (24%)	116 (96%)	5 (4%)	27	55
3	6	121/513 (24%)	118 (98%)	3 (2%)	42	64
3	7	121/513 (24%)	116 (96%)	5 (4%)	27	55
3	8	121/513 (24%)	118 (98%)	3 (2%)	42	64
3	9	121/513 (24%)	116 (96%)	5 (4%)	27	55
3	Y	121/513 (24%)	118 (98%)	3 (2%)	42	64
3	Z	121/513 (24%)	118 (98%)	3 (2%)	42	64
3	a0	121/513 (24%)	118 (98%)	3 (2%)	42	64
3	b0	121/513 (24%)	116 (96%)	5 (4%)	27	55
3	y	121/513 (24%)	116 (96%)	5 (4%)	27	55
3	z	121/513 (24%)	116 (96%)	5 (4%)	27	55
All	All	10688/21696 (49%)	10312 (96%)	376 (4%)	32	58

5 of 376 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	j	135	LEU
2	i	83	ARG
2	m	163	VAL
2	v	93	ASP
2	l	138	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	324	HIS
1	X	210	GLN
1	I	331	GLN
1	F	331	GLN
1	X	331	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

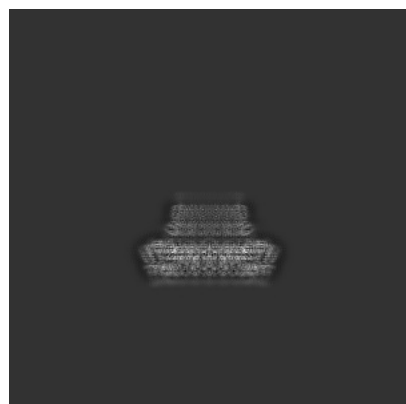
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15702. These allow visual inspection of the internal detail of the map and identification of artifacts.

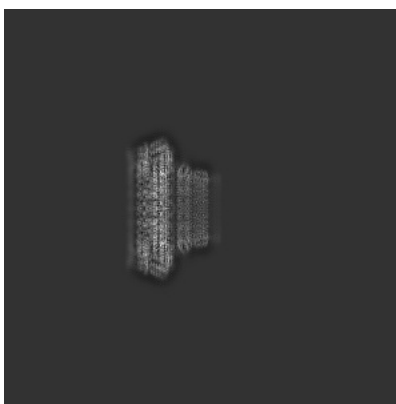
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

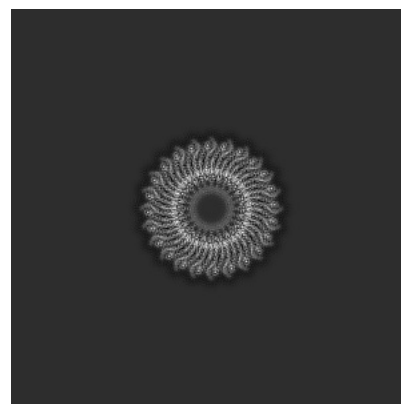
6.1.1 Primary map



X



Y

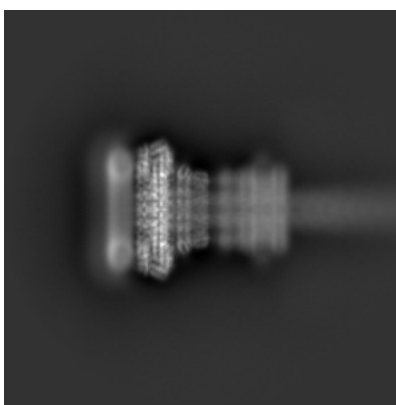


Z

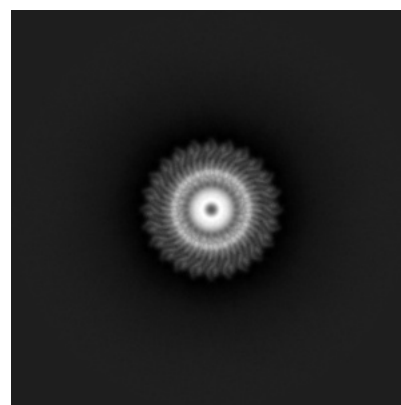
6.1.2 Raw map



X



Y

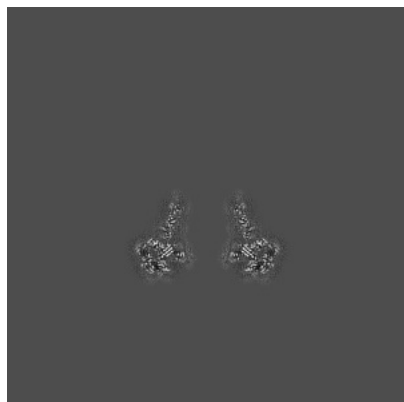


Z

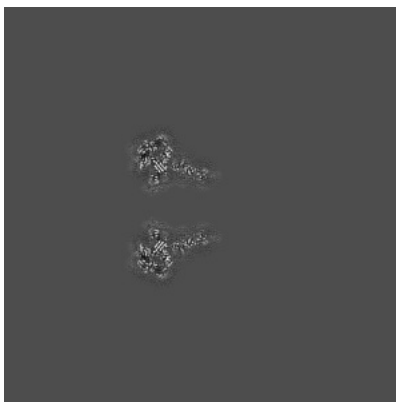
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

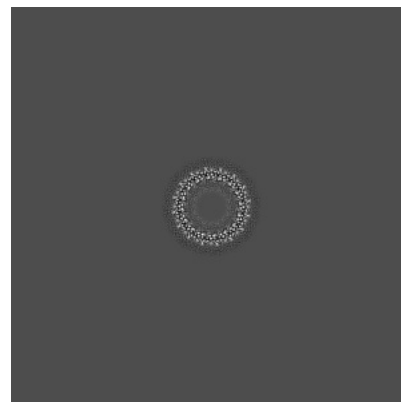
6.2.1 Primary map



X Index: 240

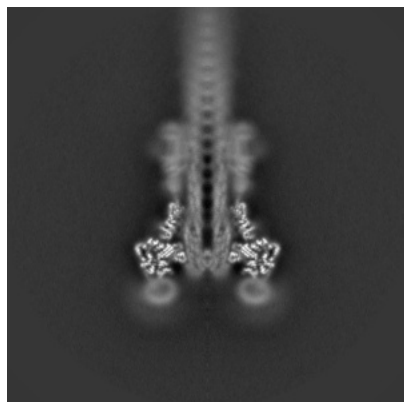


Y Index: 240

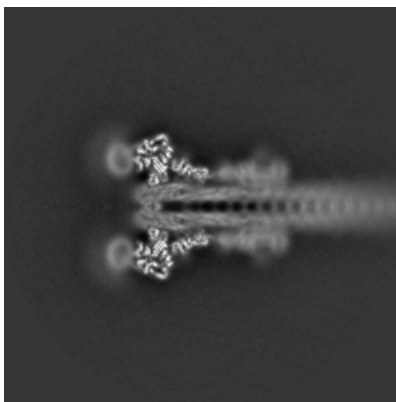


Z Index: 240

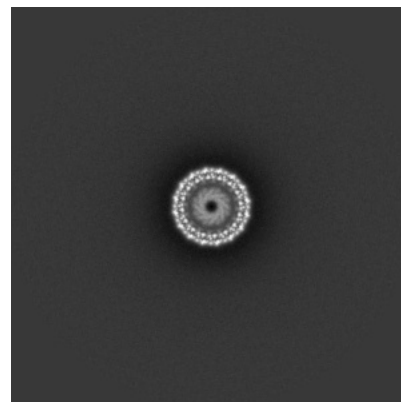
6.2.2 Raw map



X Index: 240



Y Index: 240

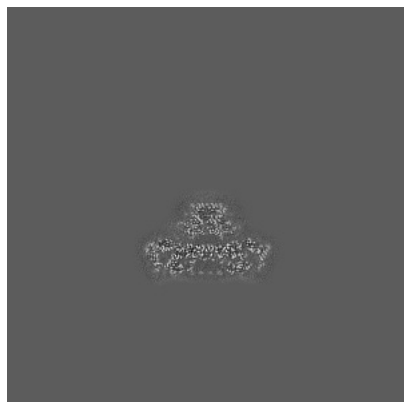


Z Index: 240

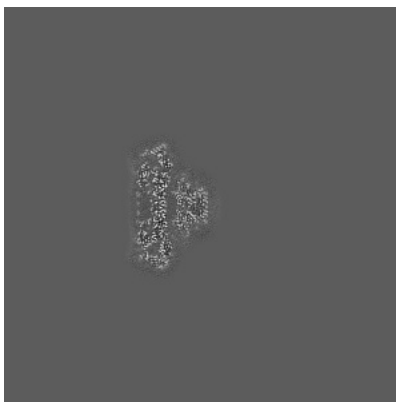
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

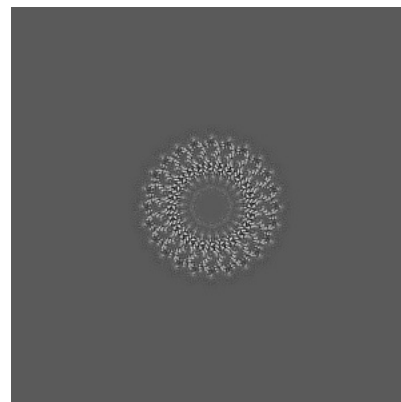
6.3.1 Primary map



X Index: 281

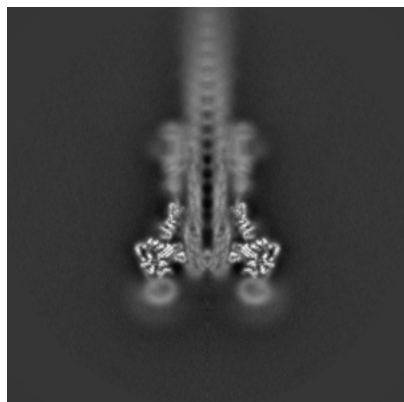


Y Index: 199

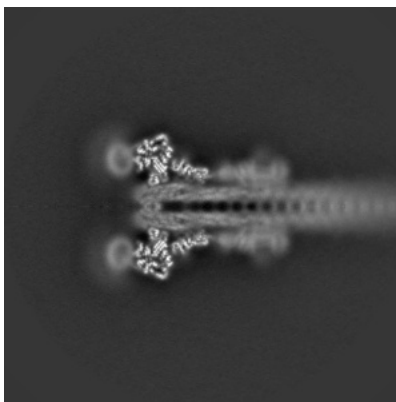


Z Index: 188

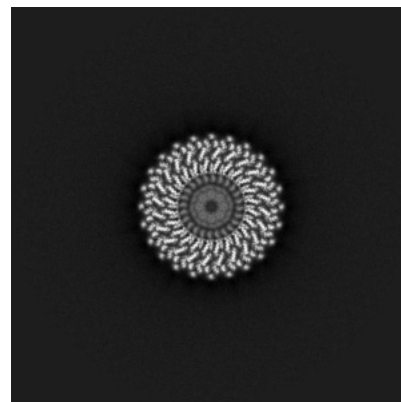
6.3.2 Raw map



X Index: 240



Y Index: 240

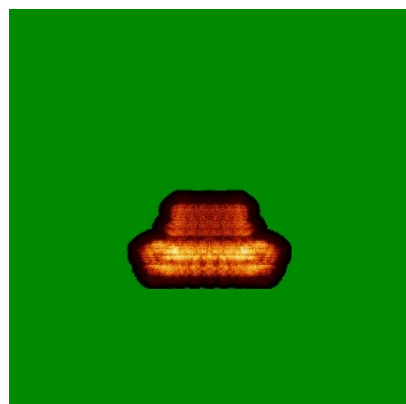


Z Index: 189

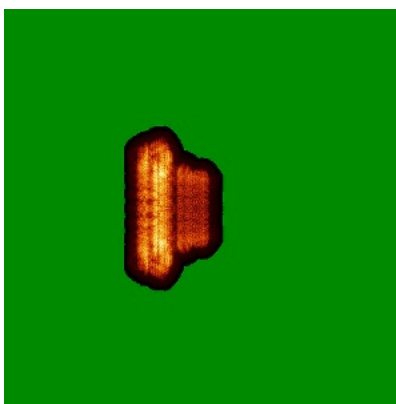
The images above show the largest variance slices of the map in three orthogonal directions.

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

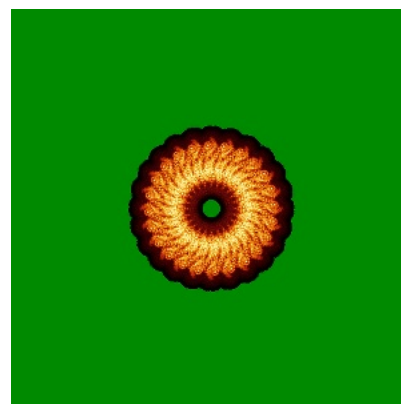
6.4.1 Primary map



X

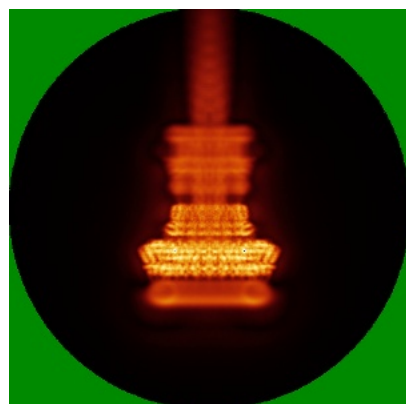


Y

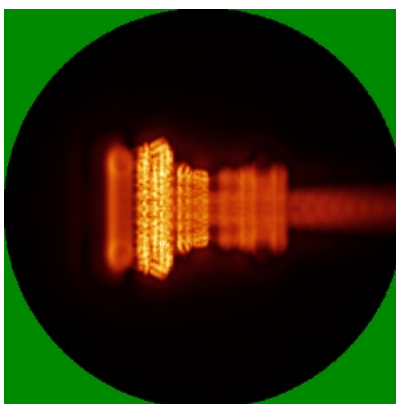


Z

6.4.2 Raw map



X



Y

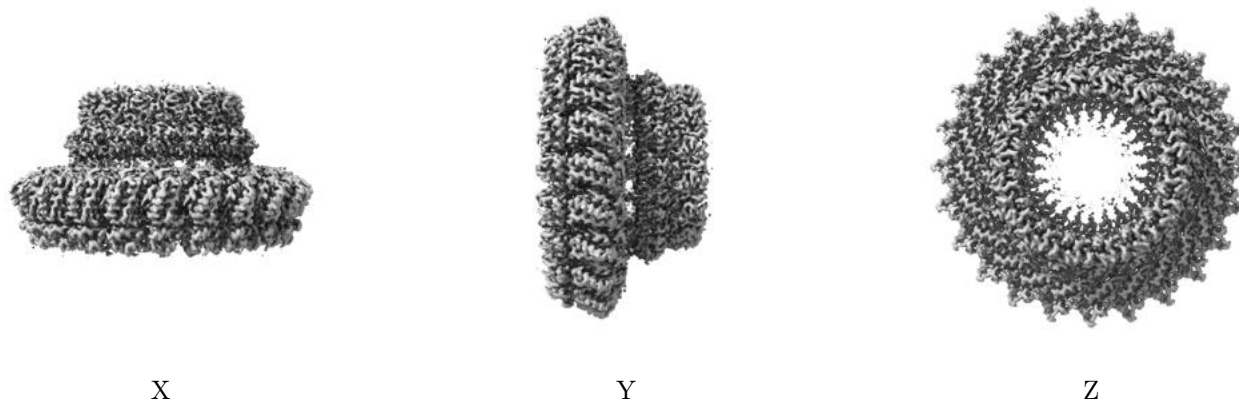


Z

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.

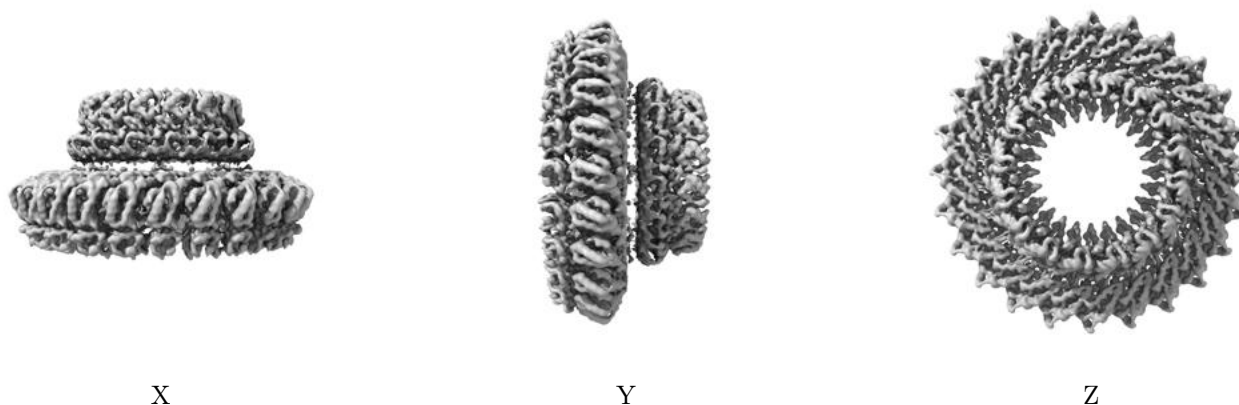
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.07. 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.

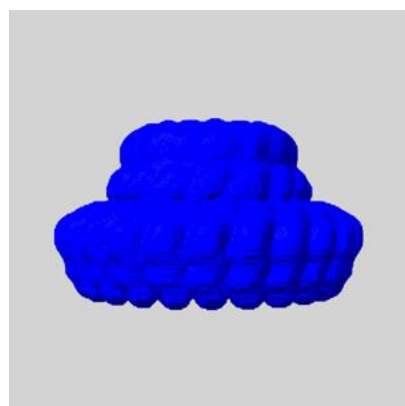
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

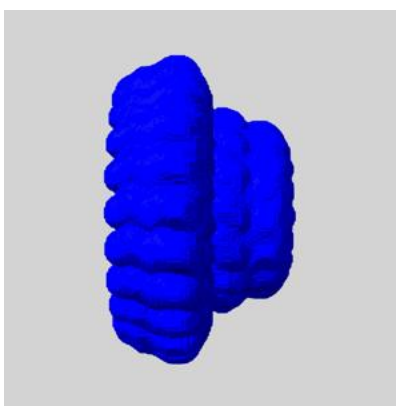
A mask typically either:

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

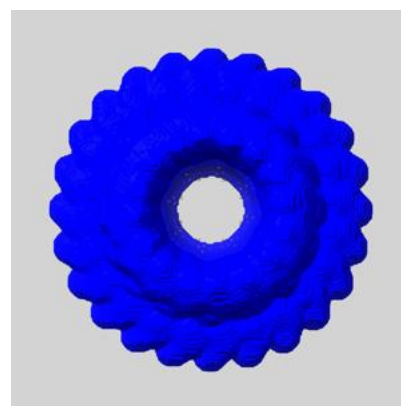
6.6.1 emd_15702_msk_1.map [i](#)



X



Y

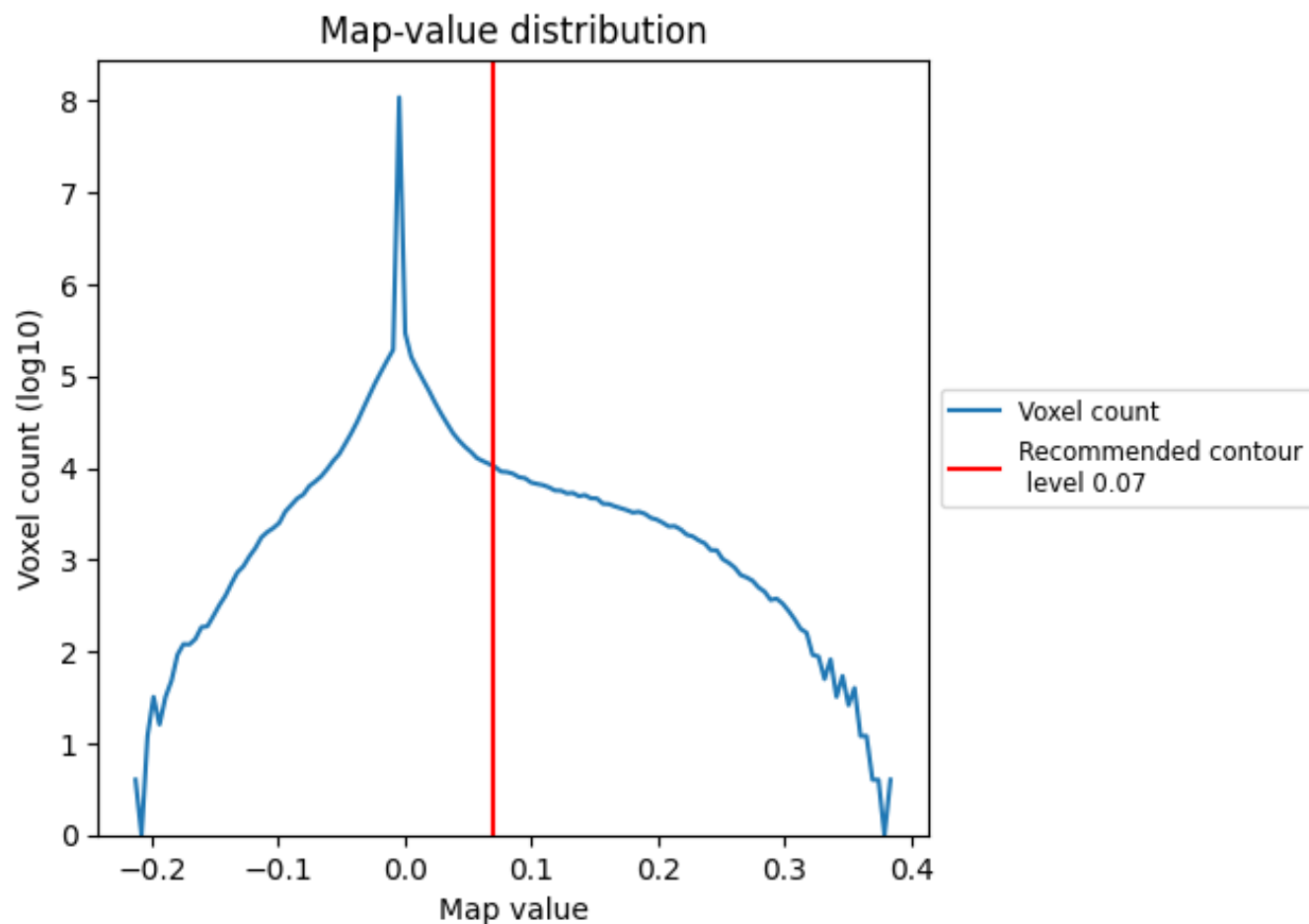


Z

7 Map analysis [i](#)

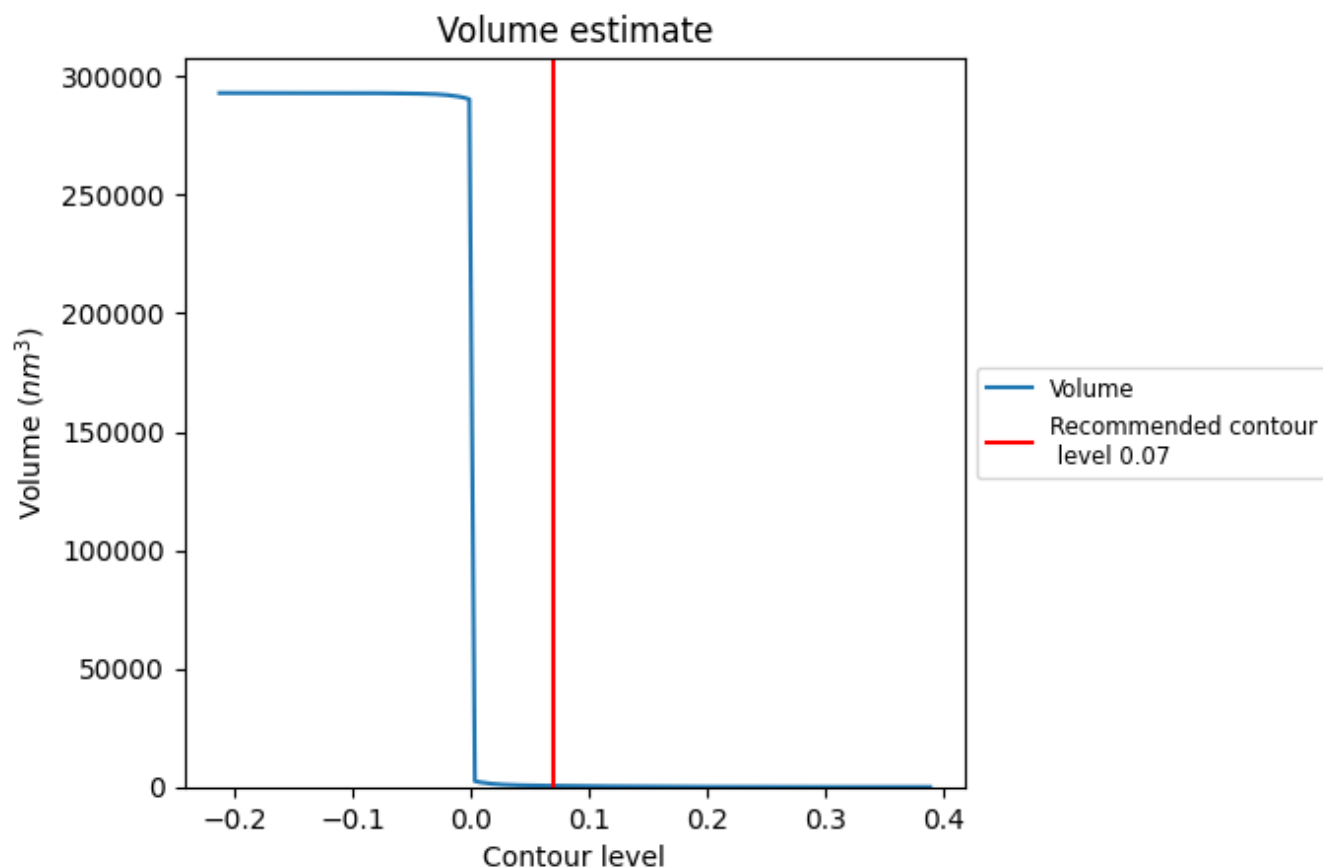
This section contains the results of statistical analysis of the map.

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.

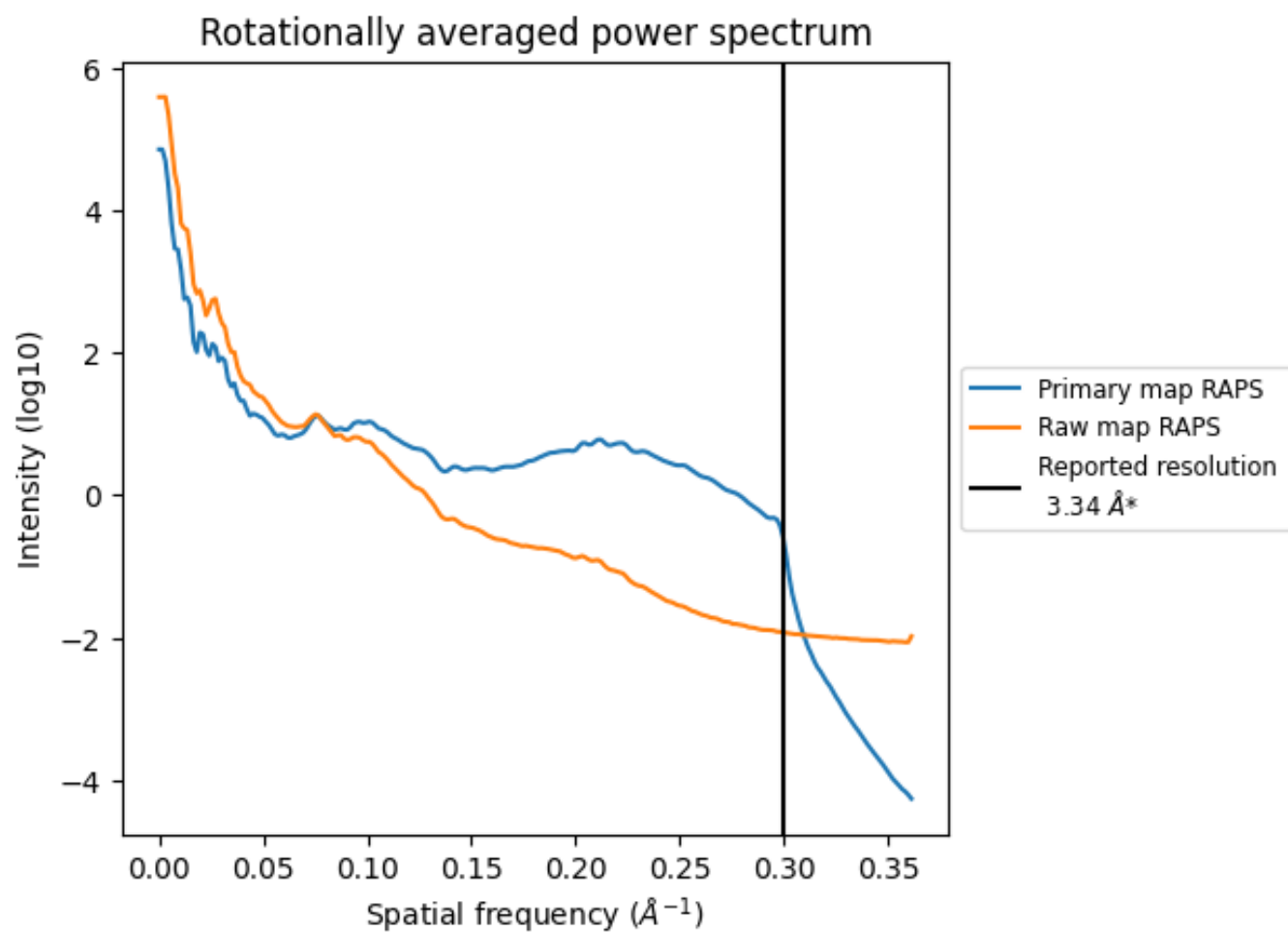
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 488 nm^3 ; this corresponds to an approximate mass of 441 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

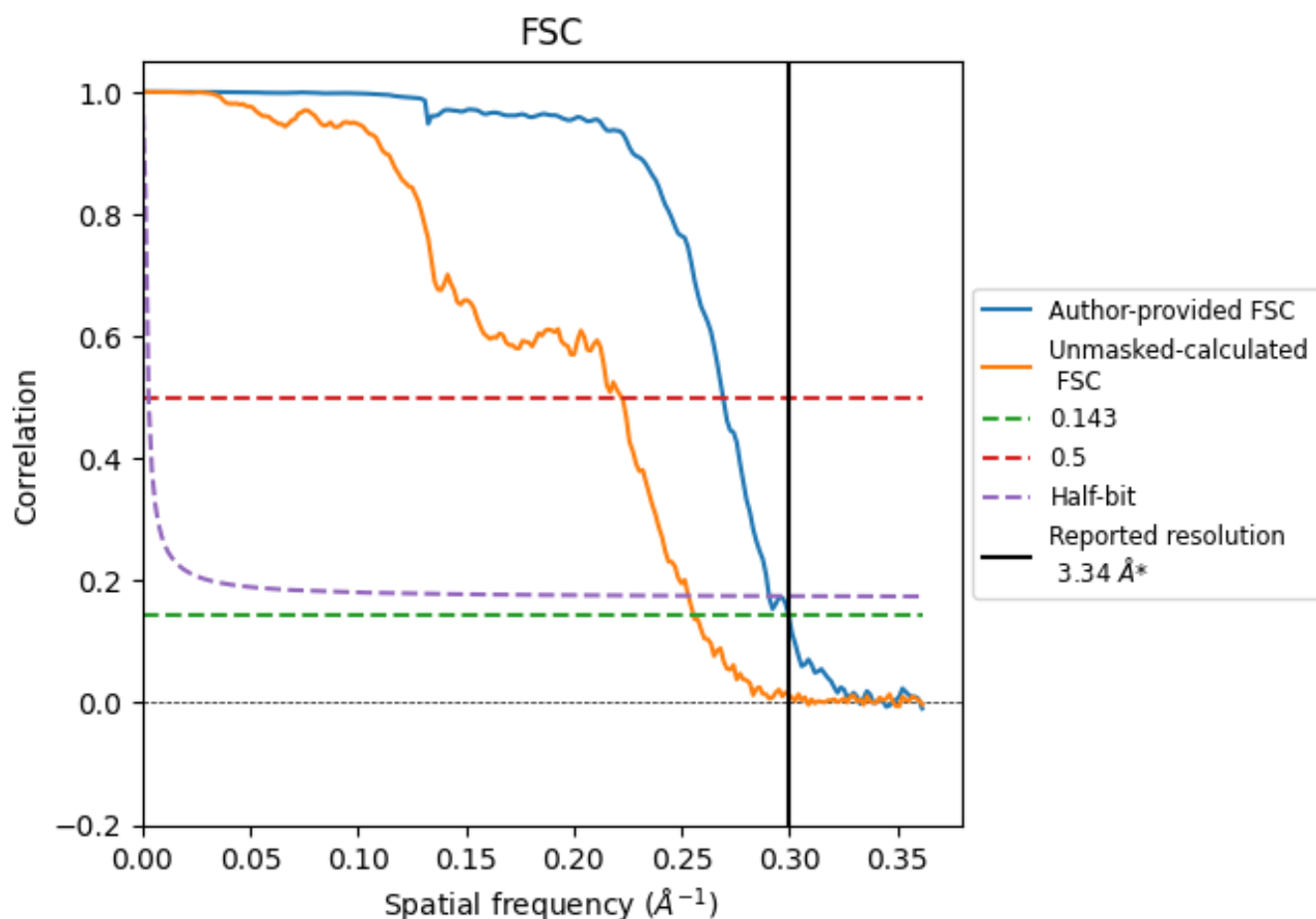


*Reported resolution corresponds to spatial frequency of 0.299 Å⁻¹

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 $0.299 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

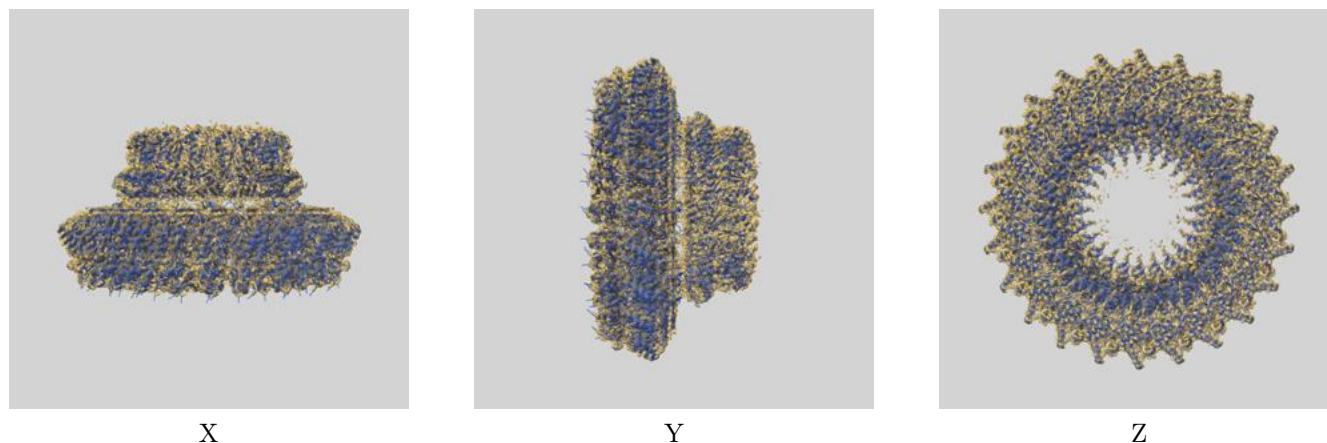
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.34	-	-
Author-provided FSC curve	3.34	3.71	3.44
Unmasked-calculated*	3.91	4.50	3.95

*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 3.91 differs from the reported value 3.34 by more than 10 %

9 Map-model fit [i](#)

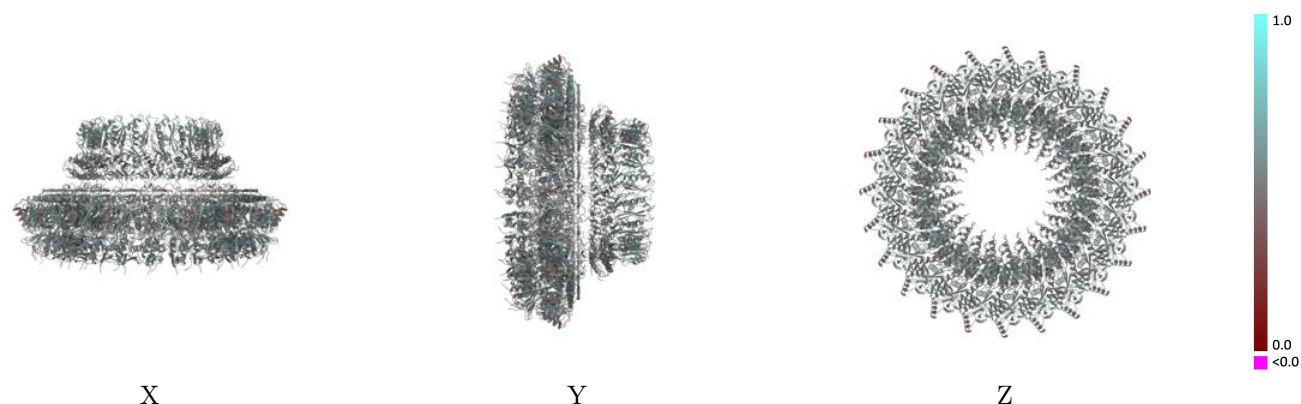
This section contains information regarding the fit between EMDB map EMD-15702 and PDB model 8AXN. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



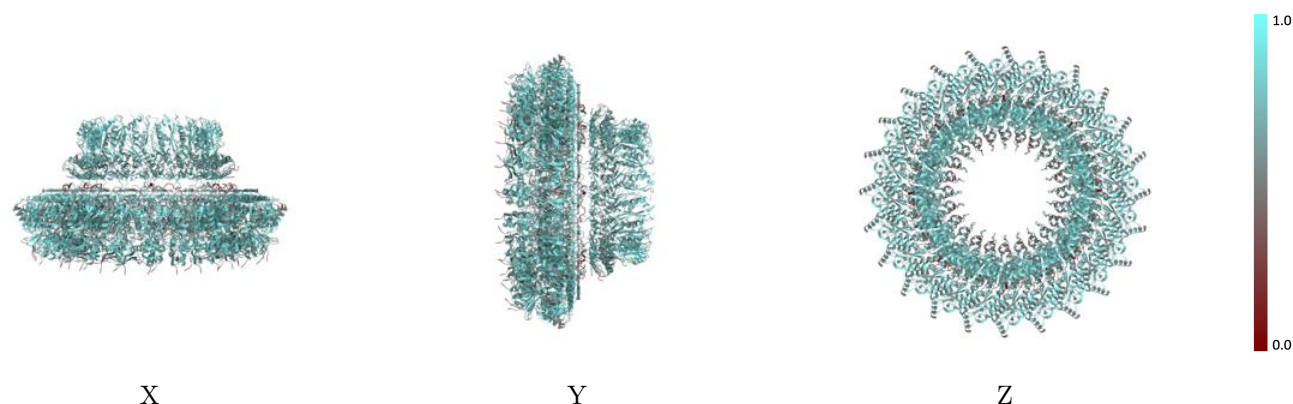
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



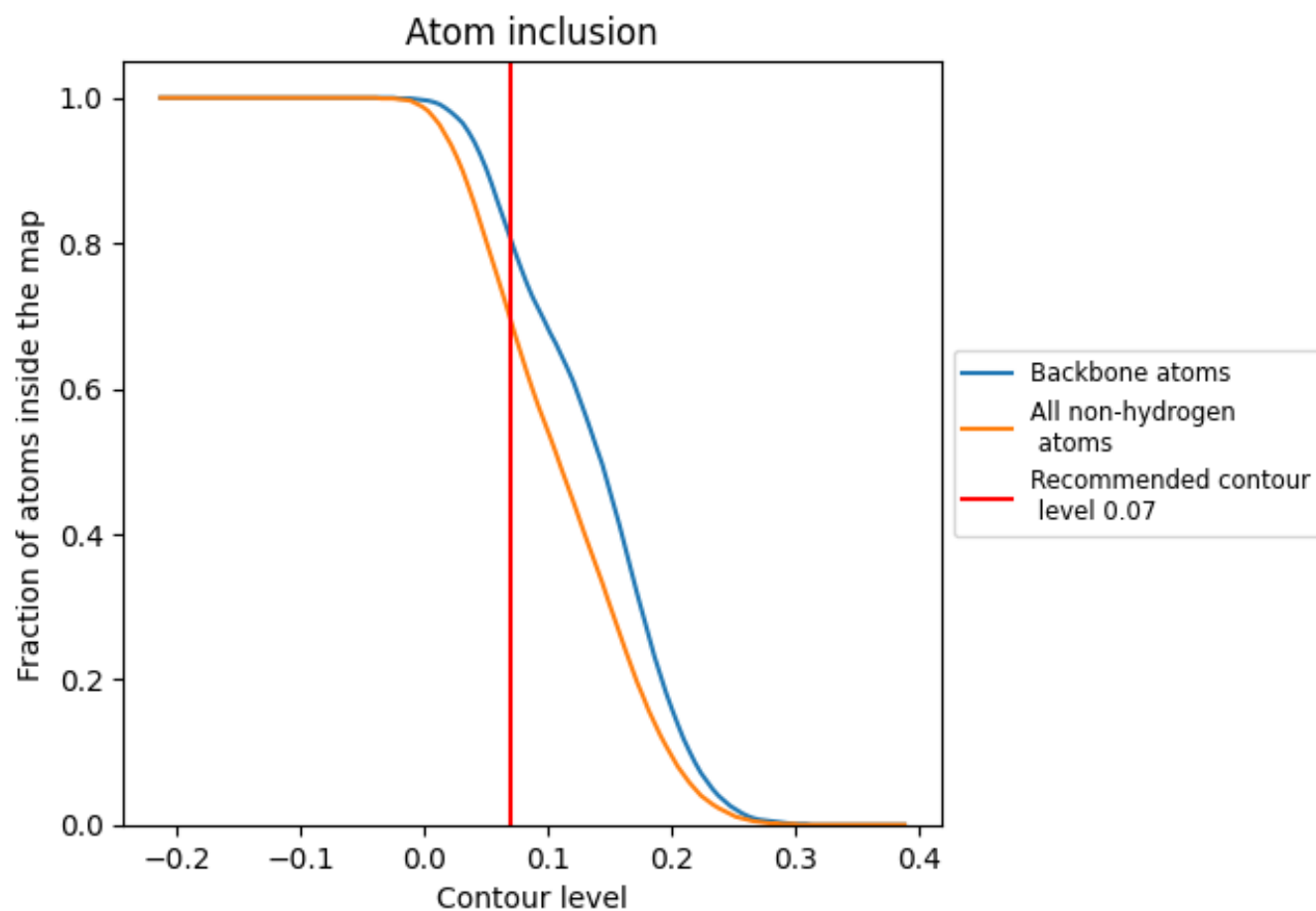
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 70% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6950	 0.4990
0	 0.7130	 0.5110
1	 0.7230	 0.5120
2	 0.7220	 0.5090
3	 0.7260	 0.5120
4	 0.7140	 0.5120
5	 0.7270	 0.5140
6	 0.7200	 0.5100
7	 0.7220	 0.5150
8	 0.7140	 0.5120
9	 0.7220	 0.5130
A	 0.7140	 0.5060
B	 0.7200	 0.5020
C	 0.6640	 0.5020
D	 0.7170	 0.5000
E	 0.7140	 0.4960
F	 0.6630	 0.4940
G	 0.7170	 0.5000
H	 0.7130	 0.4920
I	 0.6700	 0.4930
J	 0.7180	 0.5040
K	 0.7180	 0.4970
L	 0.6740	 0.5010
M	 0.7150	 0.5060
N	 0.7210	 0.5040
O	 0.6700	 0.5000
P	 0.7140	 0.5030
Q	 0.7180	 0.5000
R	 0.6560	 0.4910
S	 0.7150	 0.4990
T	 0.7130	 0.4930
U	 0.7110	 0.5000
V	 0.7200	 0.5040
W	 0.6710	 0.5000
X	 0.6580	 0.4920



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Chain	Atom inclusion	Q-score
Y	 0.7160	 0.5110
Z	 0.7200	 0.5070
a	 0.6810	 0.4930
a0	 0.7240	 0.5090
b	 0.6640	 0.4880
b0	 0.7270	 0.5140
c	 0.6650	 0.4950
d	 0.6830	 0.4930
e	 0.6780	 0.4910
f	 0.6740	 0.4970
g	 0.6870	 0.4890
h	 0.6790	 0.4960
i	 0.6610	 0.4960
j	 0.6820	 0.4920
k	 0.6800	 0.4950
l	 0.6720	 0.4940
m	 0.6770	 0.4890
n	 0.6780	 0.4940
o	 0.6690	 0.4970
p	 0.6760	 0.4920
q	 0.6710	 0.4930
r	 0.6720	 0.4980
s	 0.6820	 0.4850
t	 0.6800	 0.4940
u	 0.6660	 0.4970
v	 0.6670	 0.4910
w	 0.6760	 0.4890
x	 0.6820	 0.4920
y	 0.7190	 0.5120
z	 0.7290	 0.5130