wwPDB EM Validation Summary Report (i)

Oct 6, 2024 – 06:39 am BST

PDB ID	:	8AXN
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 (i) 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 (i)) were used in the production of this report:

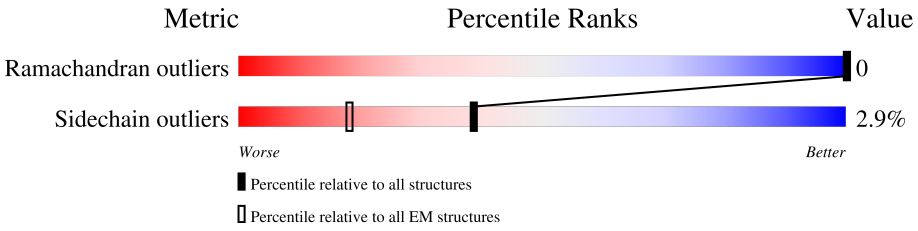
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	: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

1 Overall quality at a glance (i)

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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	57% · 41%
1	B	371	58% · 41%
1	C	371	6% 56% · 43%
1	D	371	57% · 41%
1	E	371	58% · 41%
1	F	371	5% 56% · 43%
1	G	371	57% · 41%
1	H	371	58% · 41%
1	I	371	6% 56% · 43%

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Mol	Chain	Length	Quality of chain
1	J	371	57% 41%
1	K	371	58% 41%
1	L	371	5% 56% 43%
1	M	371	57% 41%
1	N	371	58% 41%
1	O	371	5% 56% 43%
1	P	371	57% 41%
1	Q	371	58% 41%
1	R	371	6% 56% 43%
1	S	371	57% 41%
1	T	371	58% 41%
1	U	371	57% 41%
1	V	371	58% 41%
1	W	371	6% 56% 43%
1	X	371	6% 56% 43%
2	a	241	10% 73% 25%
2	b	241	11% 73% 25%
2	c	241	11% 71% 25%
2	d	241	10% 73% 25%
2	e	241	10% 73% 25%
2	f	241	11% 71% 25%
2	g	241	10% 73% 25%
2	h	241	10% 73% 25%
2	i	241	11% 71% 25%
2	j	241	10% 73% 25%

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Mol	Chain	Length	Quality of chain
2	k	241	10% 73% 25%
2	l	241	11% 71% 25%
2	m	241	9% 73% 25%
2	n	241	10% 73% 25%
2	o	241	11% 71% 25%
2	p	241	10% 73% 25%
2	q	241	11% 73% 25%
2	r	241	11% 71% 25%
2	s	241	9% 73% 25%
2	t	241	10% 73% 25%
2	u	241	11% 71% 25%
2	v	241	12% 71% 25%
2	w	241	10% 73% 25%
2	x	241	10% 73% 25%
3	0	566	24% 76%
3	1	566	24% 76%
3	2	566	24% 76%
3	3	566	24% 76%
3	4	566	24% 76%
3	5	566	24% 76%
3	6	566	24% 76%
3	7	566	24% 76%
3	8	566	24% 76%
3	9	566	24% 76%
3	Y	566	24% 76%

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Mol	Chain	Length	Quality of chain
3	Z	566	
3	a0	566	
3	b0	566	
3	y	566	
3	z	566	

2 Entry composition (i)

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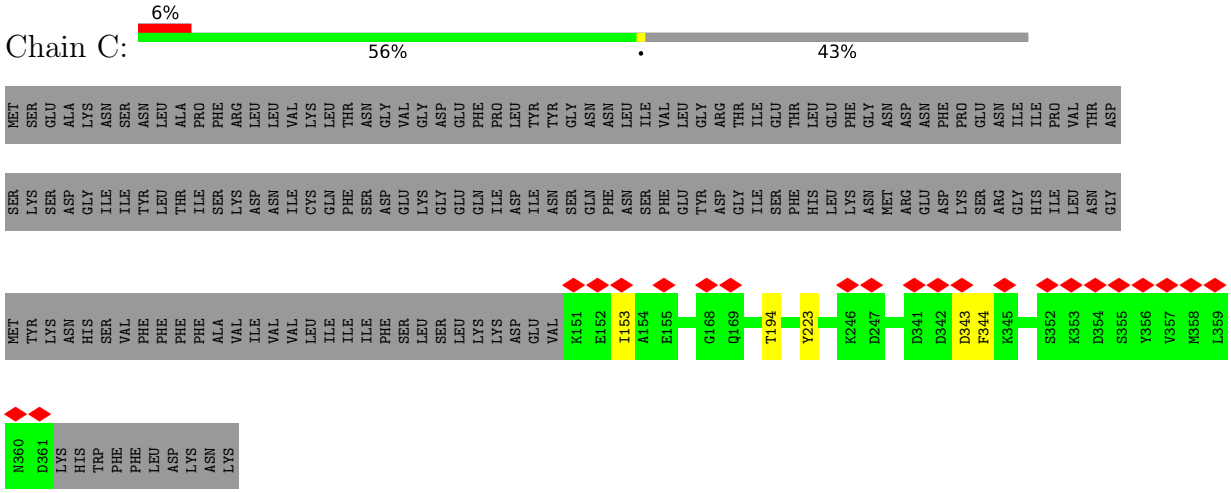
Mol	Chain	Residues	Atoms					AltConf	Trace
3	6	138	Total	C	N	O	S	0	0
			1102	718	174	209	1		
3	8	138	Total	C	N	O	S	0	0
			1102	718	174	209	1		
3	b0	138	Total	C	N	O	S	0	0
			1102	718	174	209	1		
3	y	138	Total	C	N	O	S	0	0
			1102	718	174	209	1		
3	z	138	Total	C	N	O	S	0	0
			1102	718	174	209	1		
3	3	138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

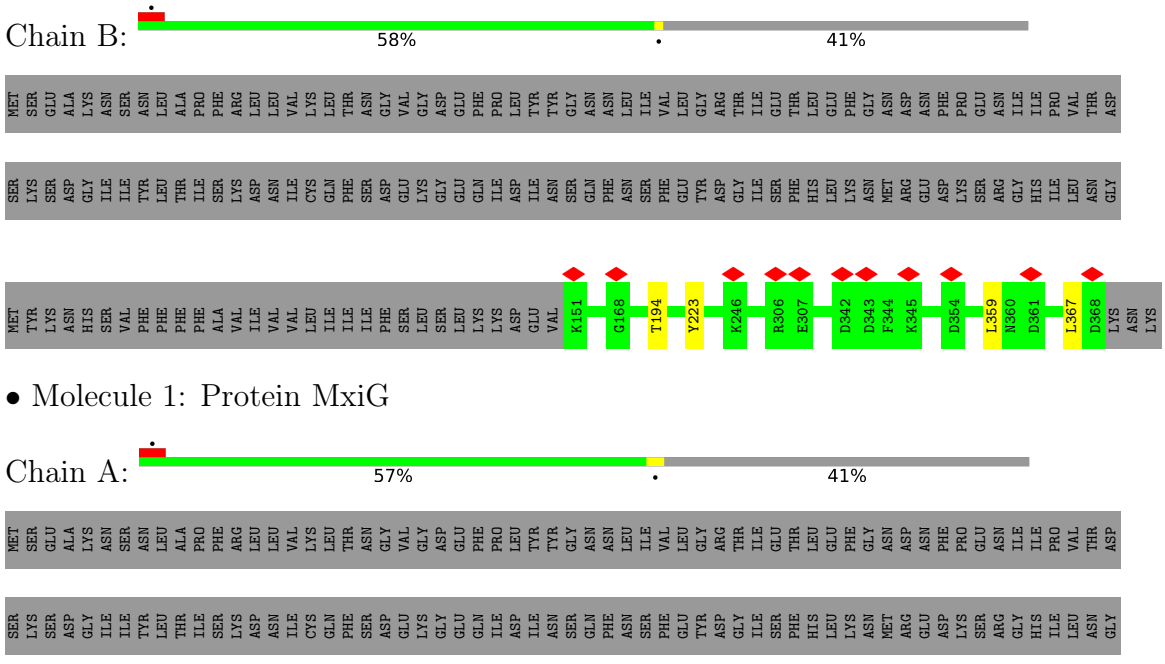
3 Residue-property plots

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.

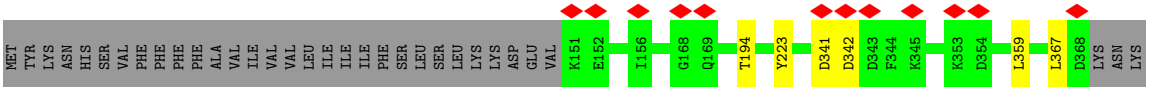
- Molecule 1: Protein MxiG



- Molecule 1: Protein MxiG

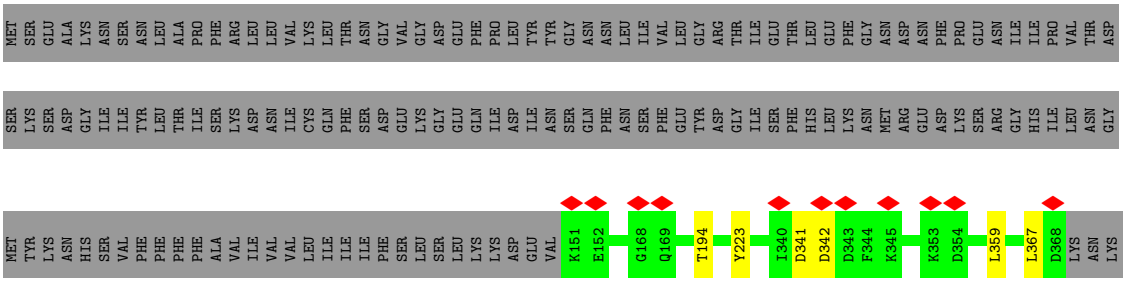


- Molecule 1: Protein MxiG



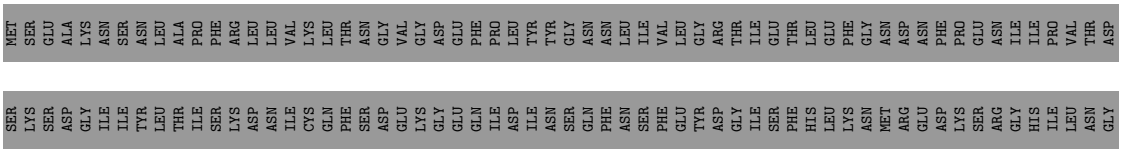
• Molecule 1: Protein MxiG

Chain S:



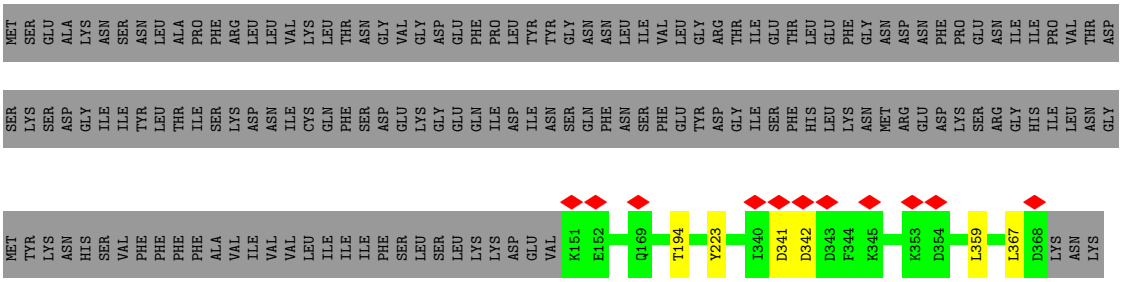
• Molecule 1: Protein MxiG

Chain P:



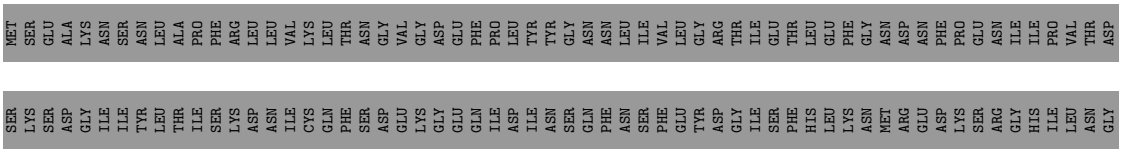
• Molecule 1: Protein MxiG

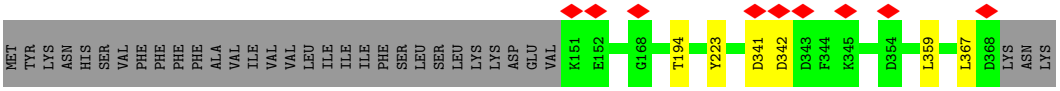
Chain M:



• Molecule 1: Protein MxiG

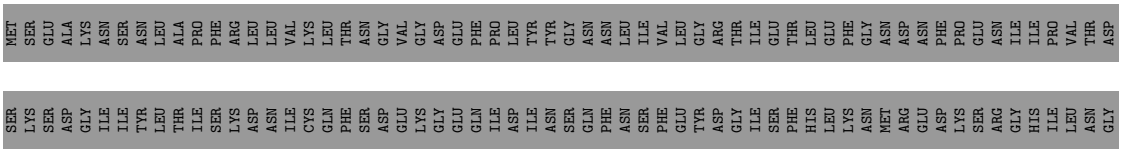
Chain J:

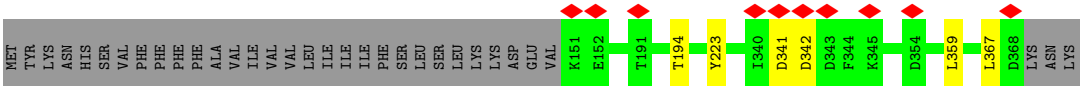




• Molecule 1: Protein MxiG

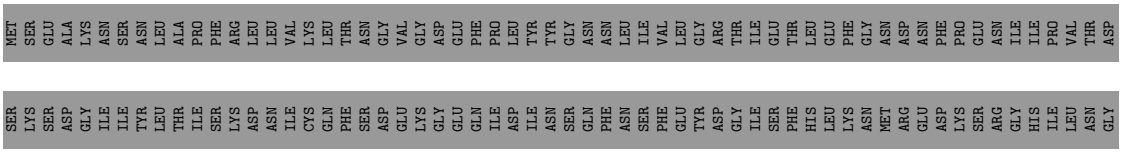
Chain G:

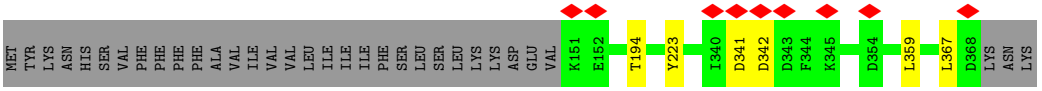




• Molecule 1: Protein MxiG

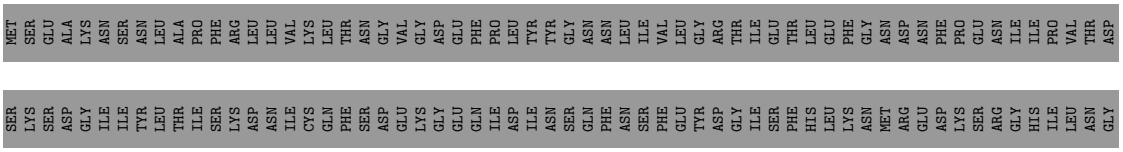
Chain D:

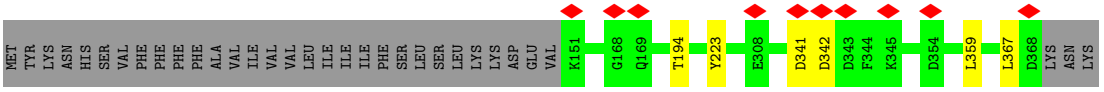




• Molecule 1: Protein MxiG

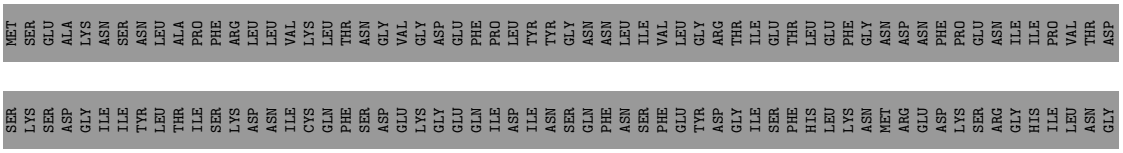
Chain U:

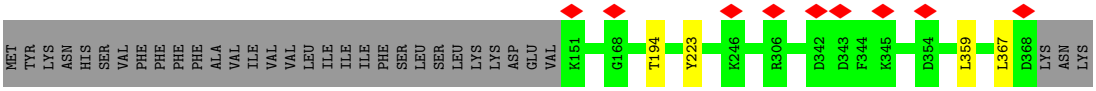




• Molecule 1: Protein MxiG

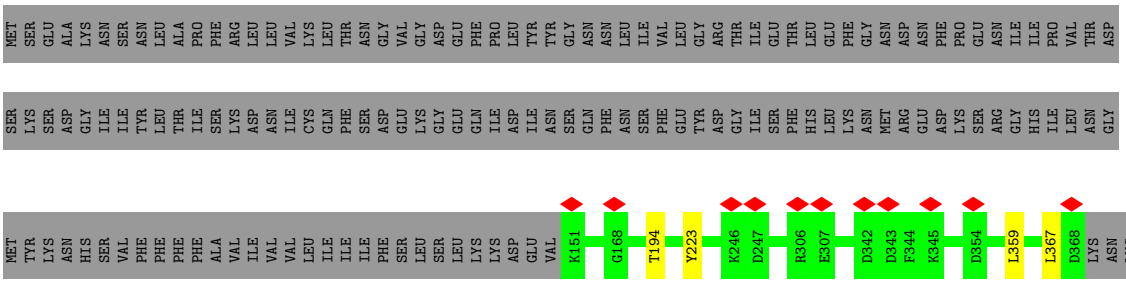
Chain T:





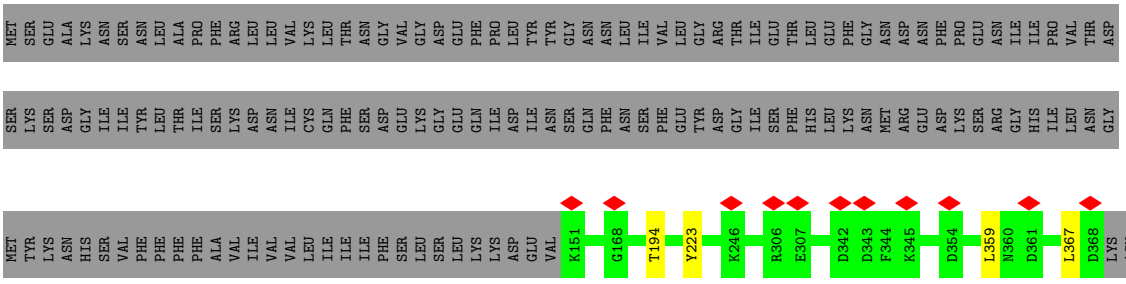
• Molecule 1: Protein MxiG

Chain Q:



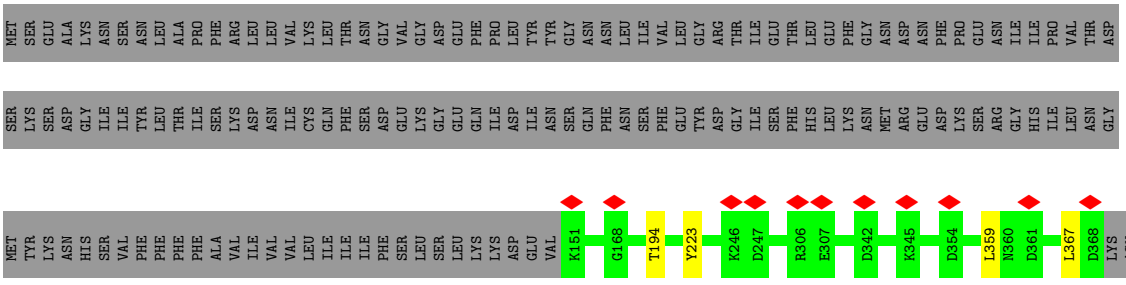
• Molecule 1: Protein MxiG

Chain N:



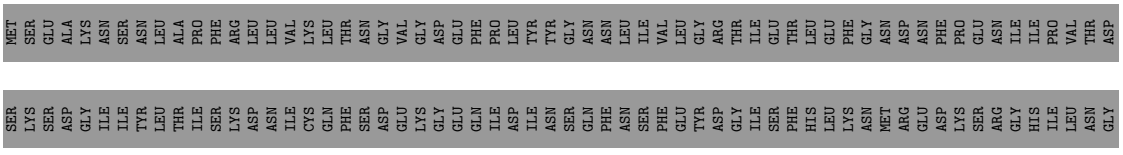
• Molecule 1: Protein MxiG

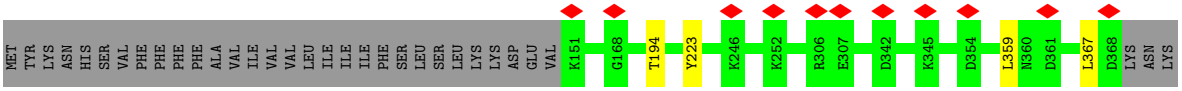
Chain K:



• Molecule 1: Protein MxiG

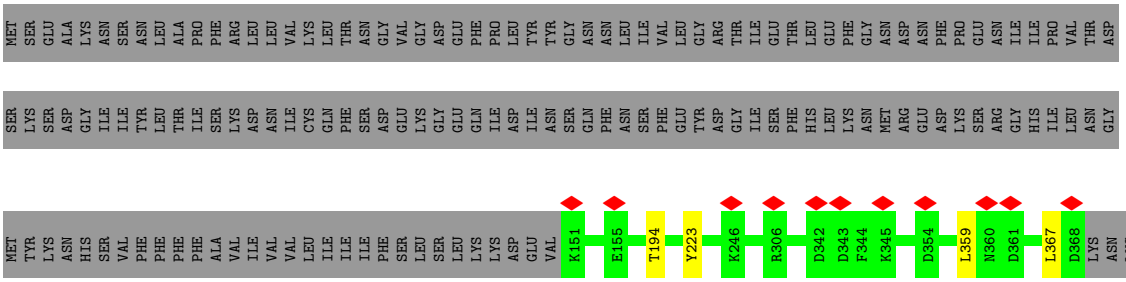
Chain H:





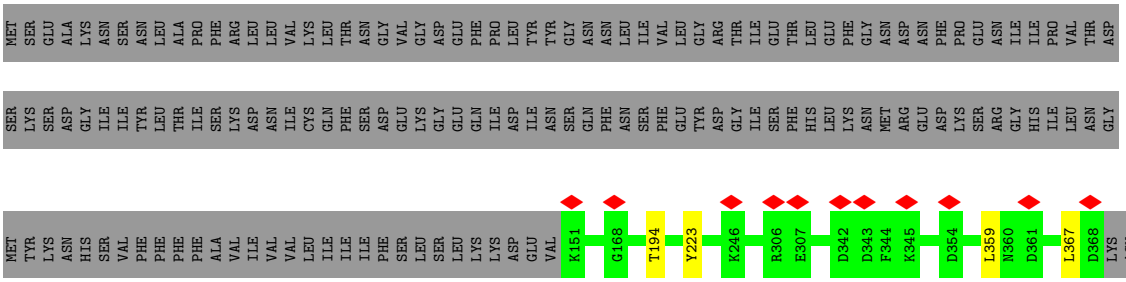
• Molecule 1: Protein MxiG

Chain E:



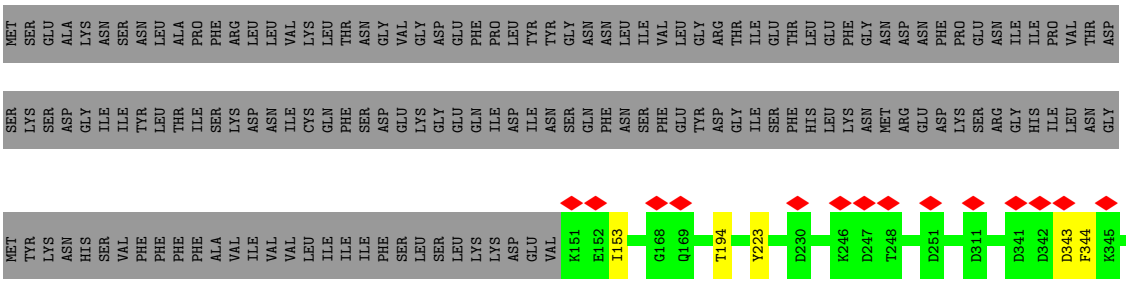
• Molecule 1: Protein MxiG

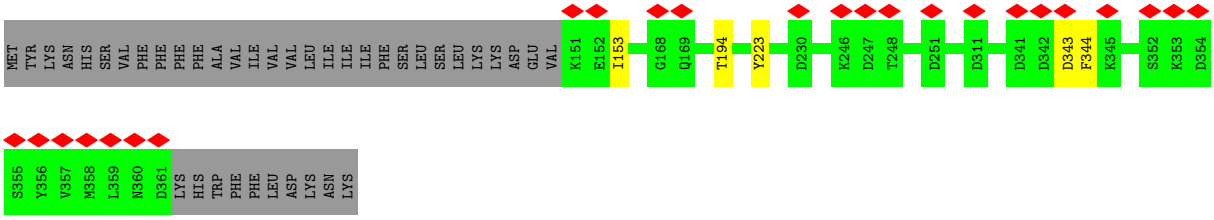
Chain V:



• Molecule 1: Protein MxiG

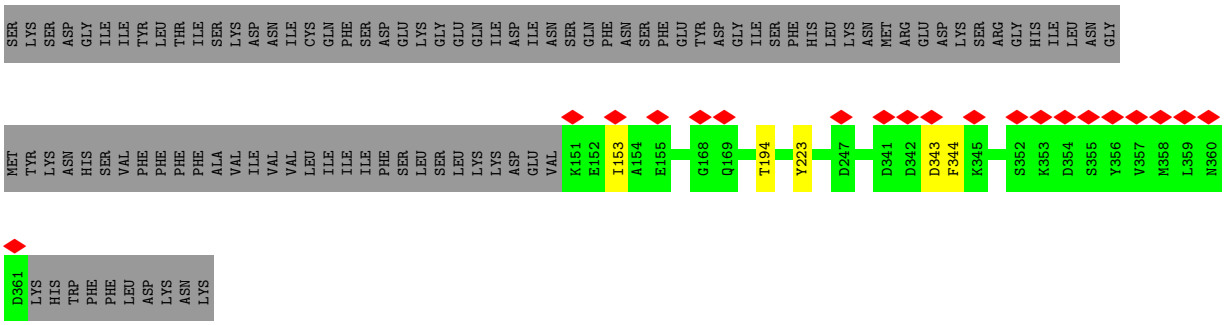
Chain R:





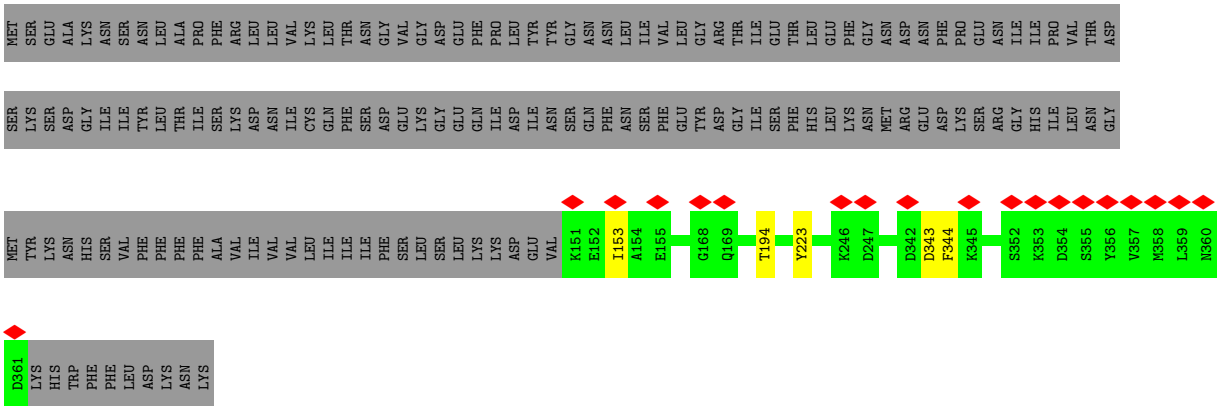
• Molecule 1: Protein MxiG

Chain O:



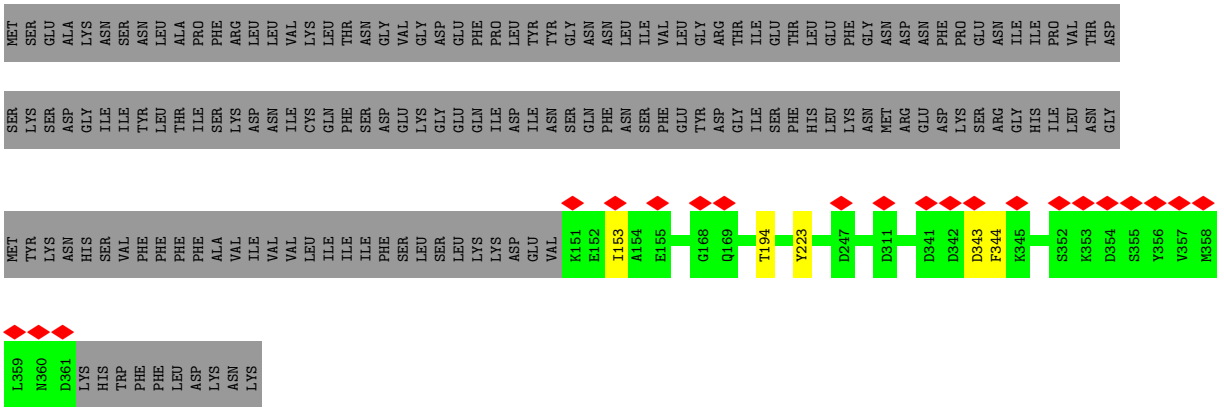
• Molecule 1: Protein MxiG

Chain L:



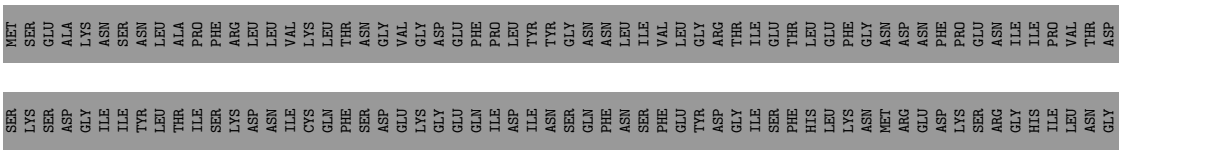
• Molecule 1: Protein MxiG

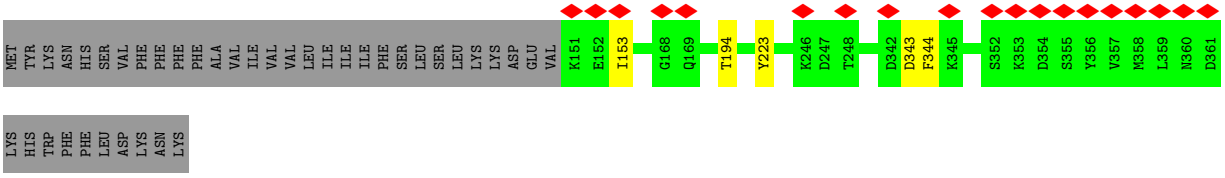
Chain I:



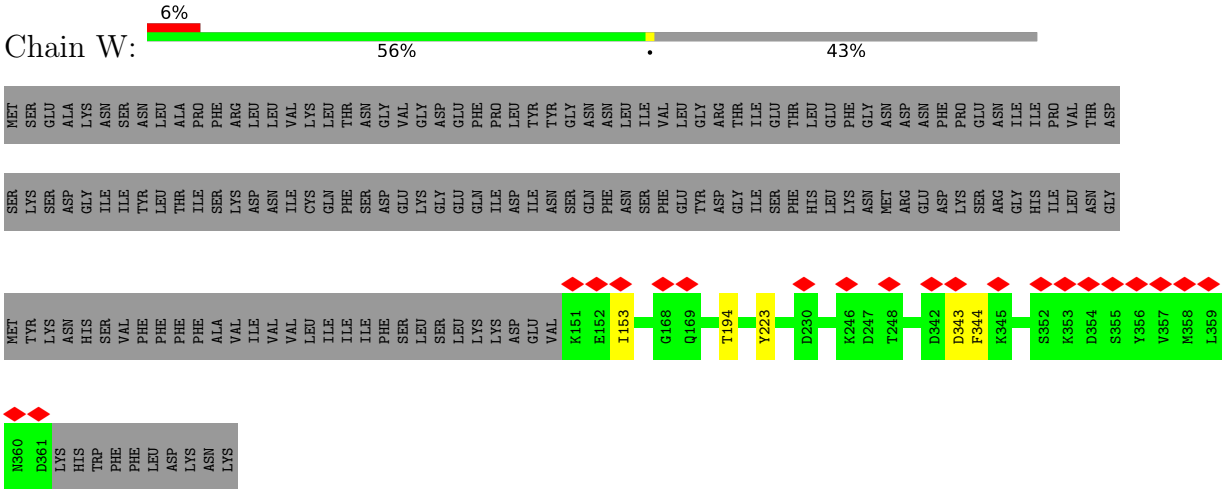
• Molecule 1: Protein MxiG

Chain F:

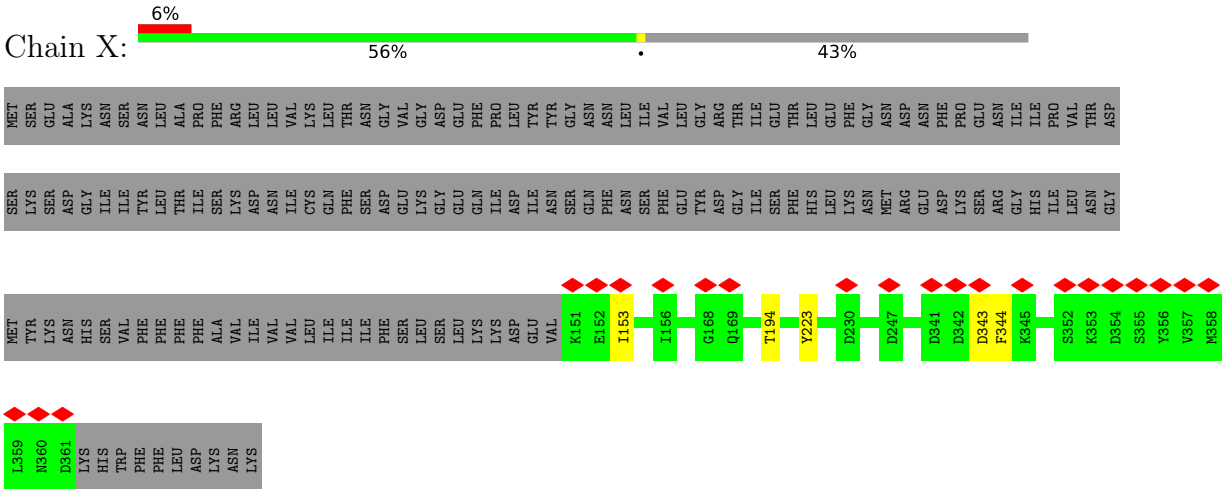




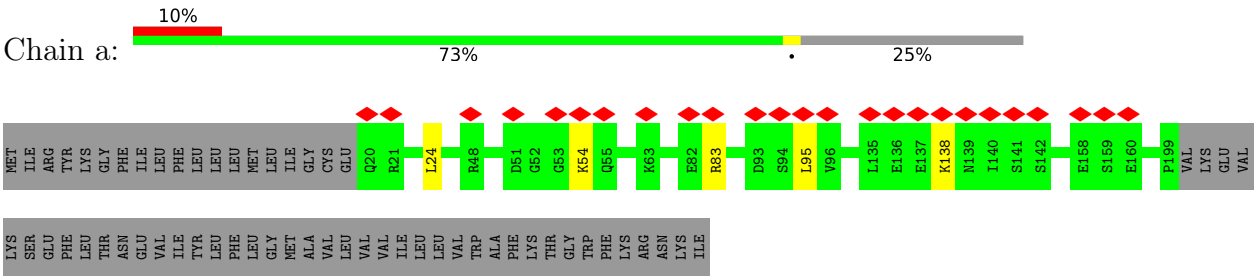
• Molecule 1: Protein MxiG



• Molecule 1: Protein MxiG

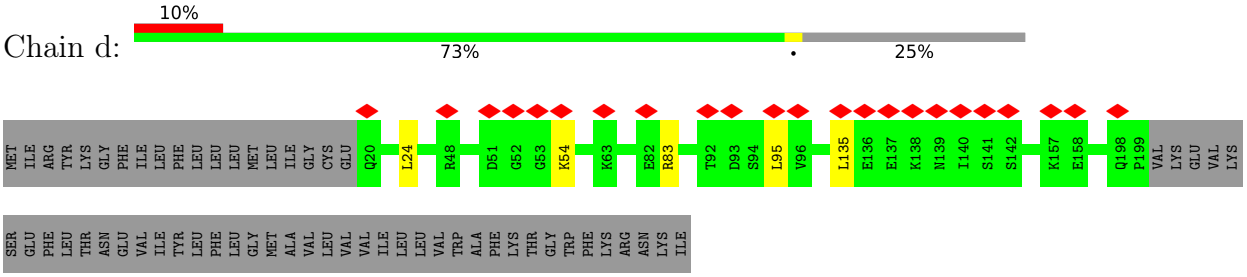


• Molecule 2: Lipoprotein MxiJ



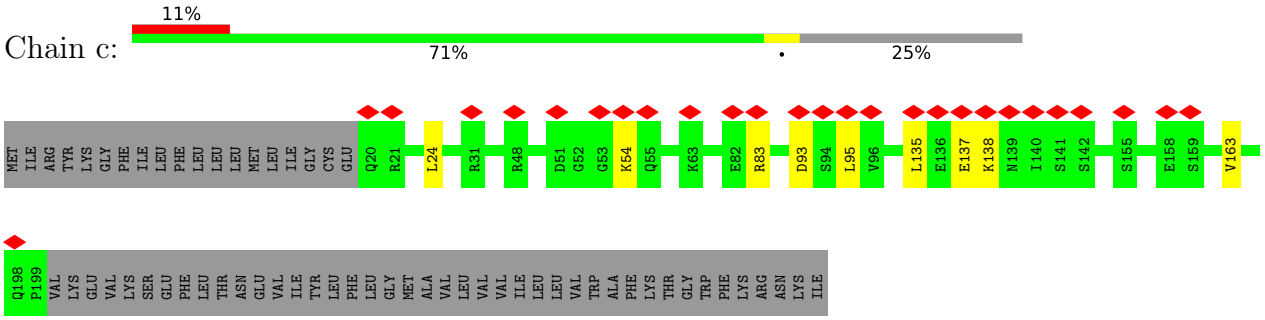
• Molecule 2: Lipoprotein MxiJ

Chain d:



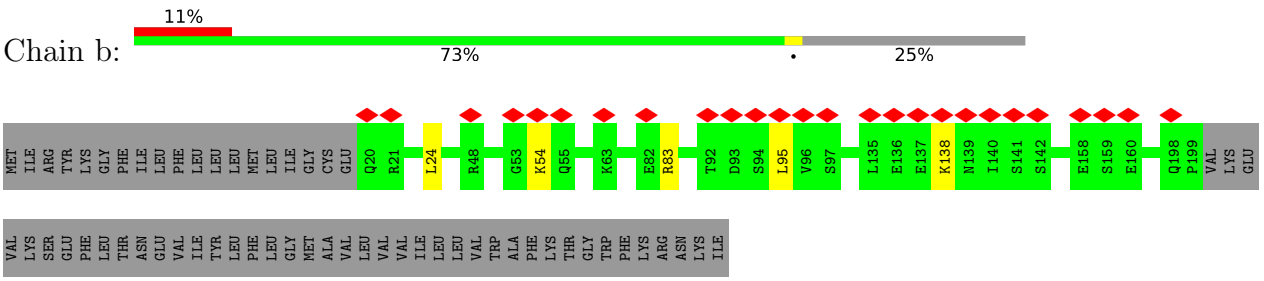
- Molecule 2: Lipoprotein MxiJ

Chain c:



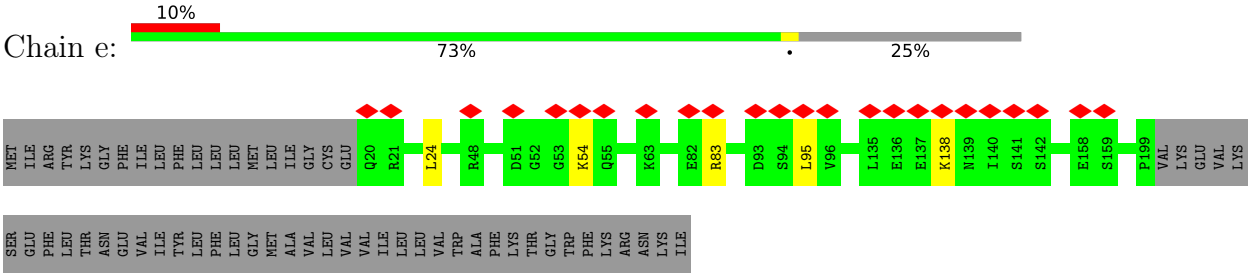
- Molecule 2: Lipoprotein MxiJ

Chain b:



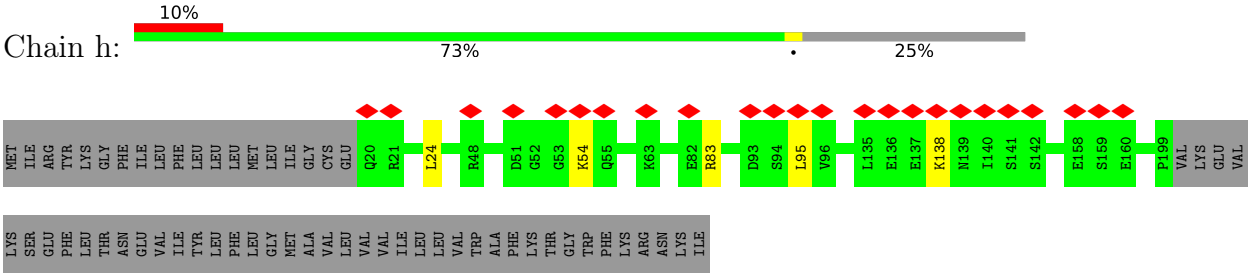
- Molecule 2: Lipoprotein MxiJ

Chain e:



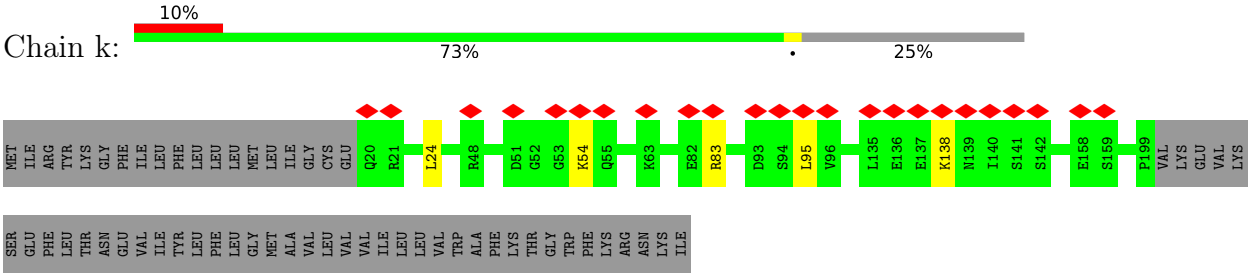
- Molecule 2: Lipoprotein MxiJ

Chain h:



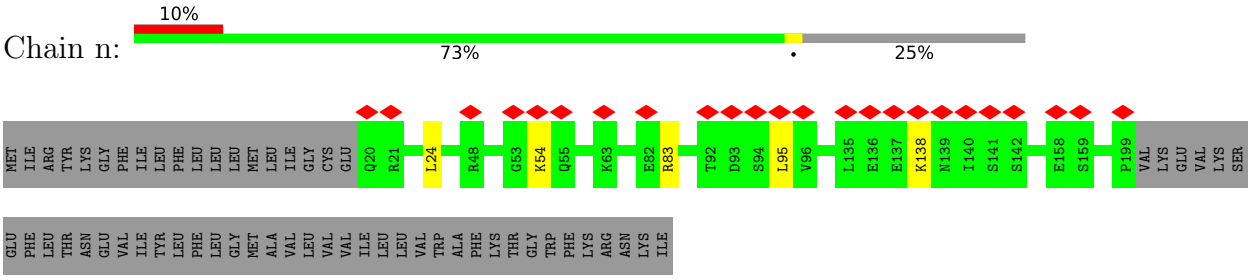
- Molecule 2: Lipoprotein MxiJ

Chain k:



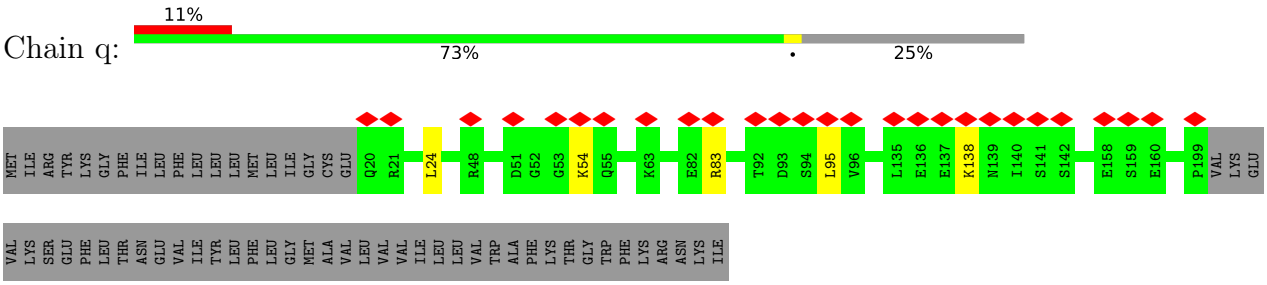
• Molecule 2: Lipoprotein MxiJ

Chain n:



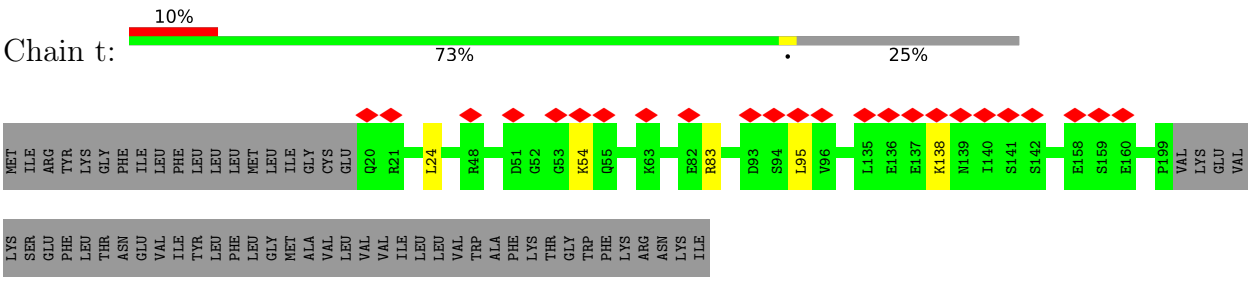
• Molecule 2: Lipoprotein MxiJ

Chain q:



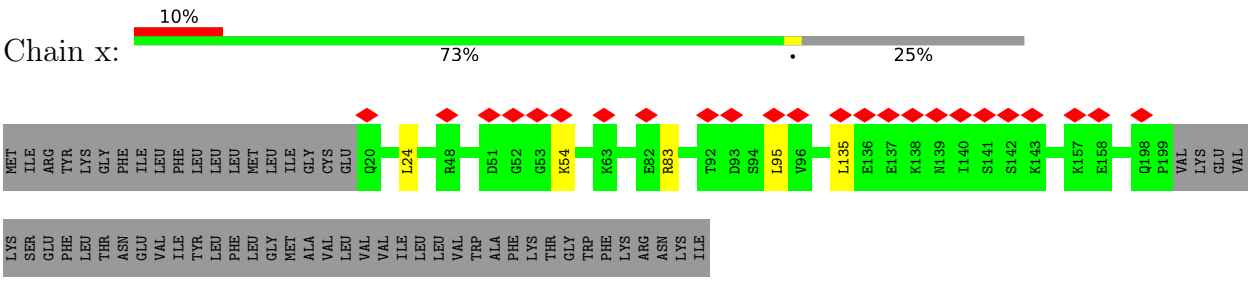
• Molecule 2: Lipoprotein MxiJ

Chain t:



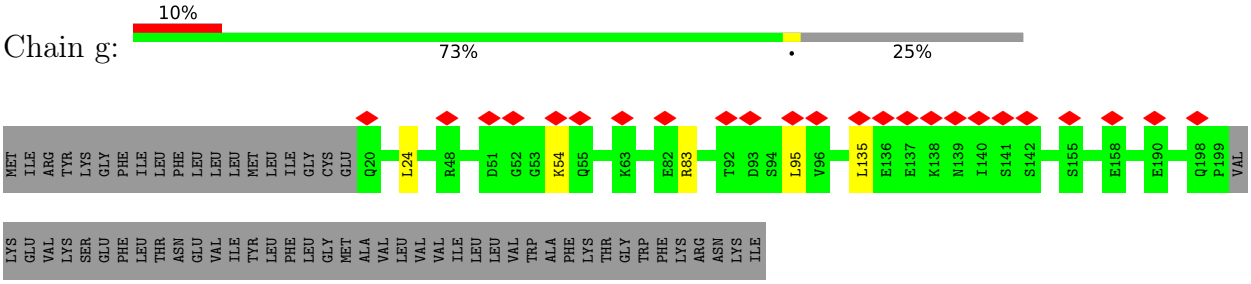
• Molecule 2: Lipoprotein MxiJ

Chain x:



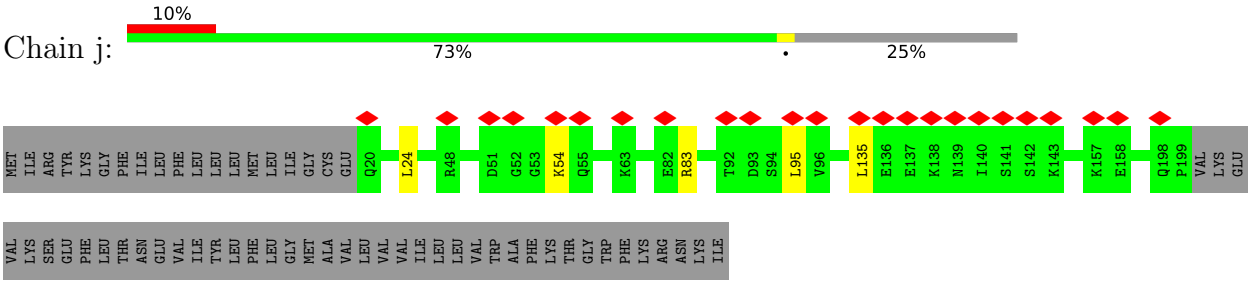
• Molecule 2: Lipoprotein MxiJ

Chain g:



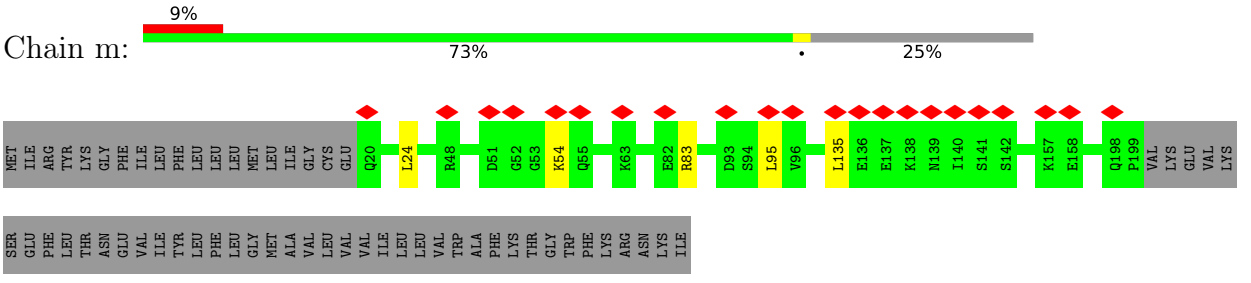
- Molecule 2: Lipoprotein MxiJ

Chain j:



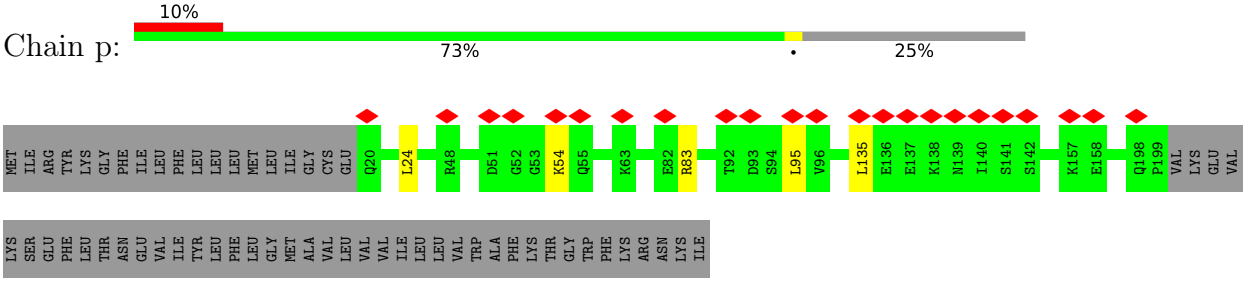
- Molecule 2: Lipoprotein MxiJ

Chain m:



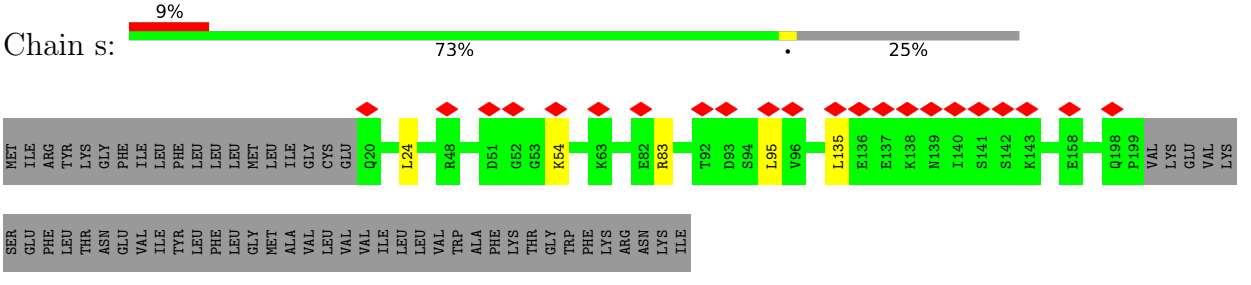
- Molecule 2: Lipoprotein MxiJ

Chain p:



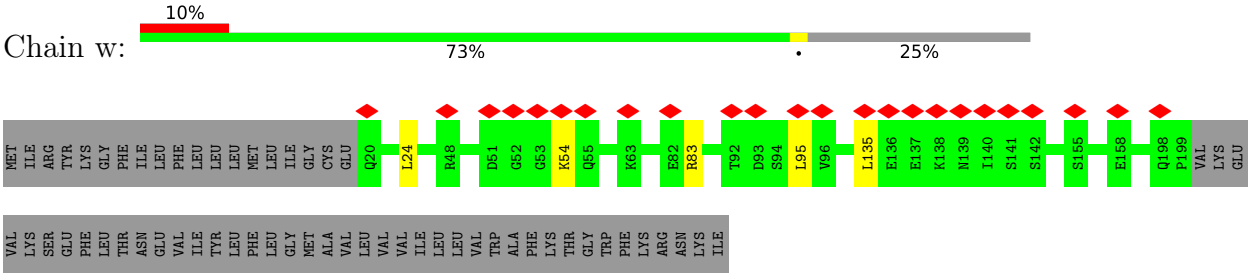
- Molecule 2: Lipoprotein MxiJ

Chain s:



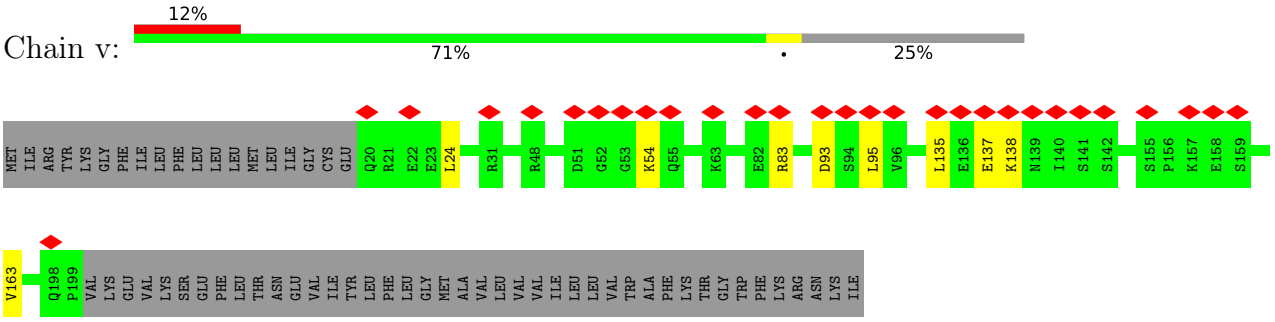
- Molecule 2: Lipoprotein MxiJ

Chain w:



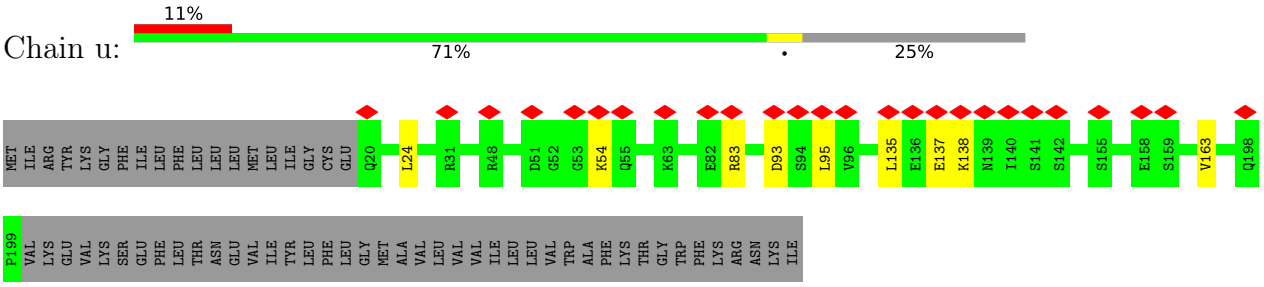
• Molecule 2: Lipoprotein MxiJ

Chain v:



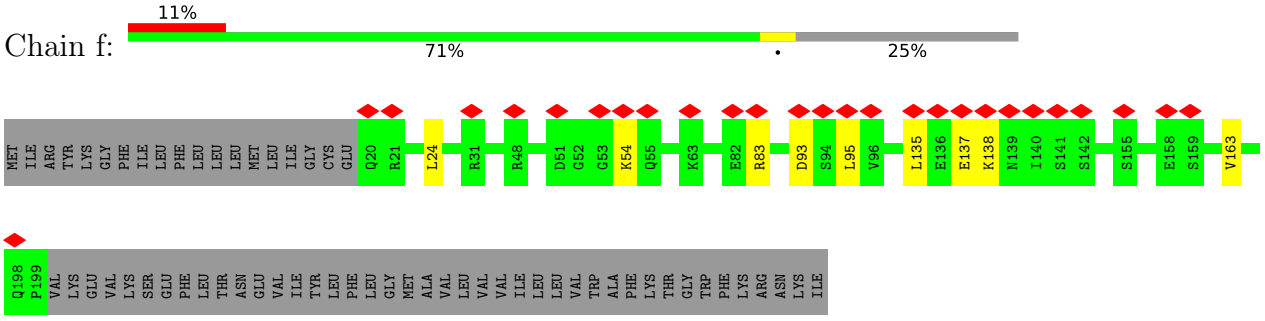
• Molecule 2: Lipoprotein MxiJ

Chain u:



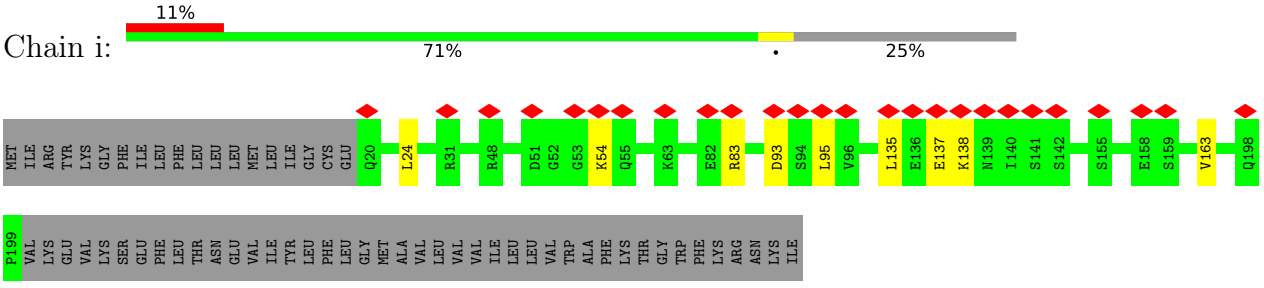
• Molecule 2: Lipoprotein MxiJ

Chain f:



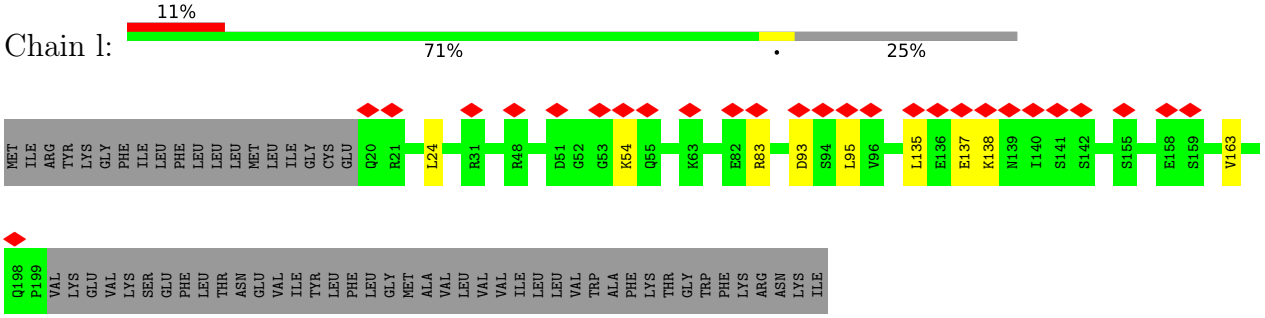
• Molecule 2: Lipoprotein MxiJ

Chain i:



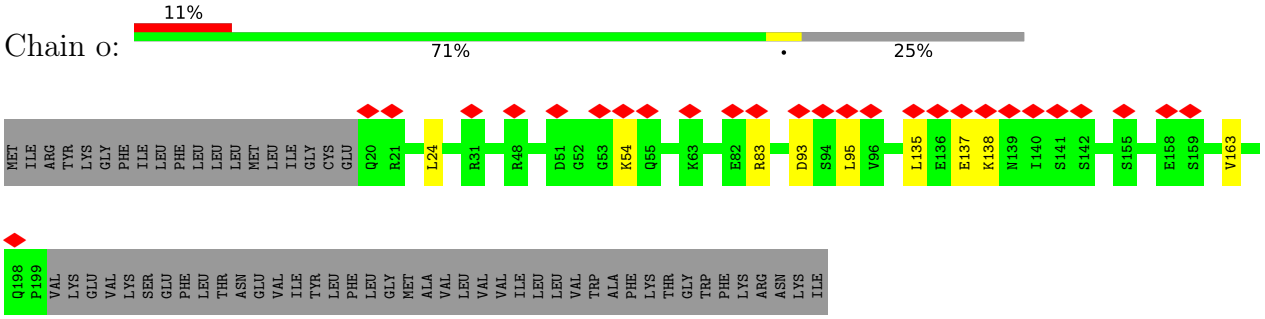
• Molecule 2: Lipoprotein MxiJ

Chain l:



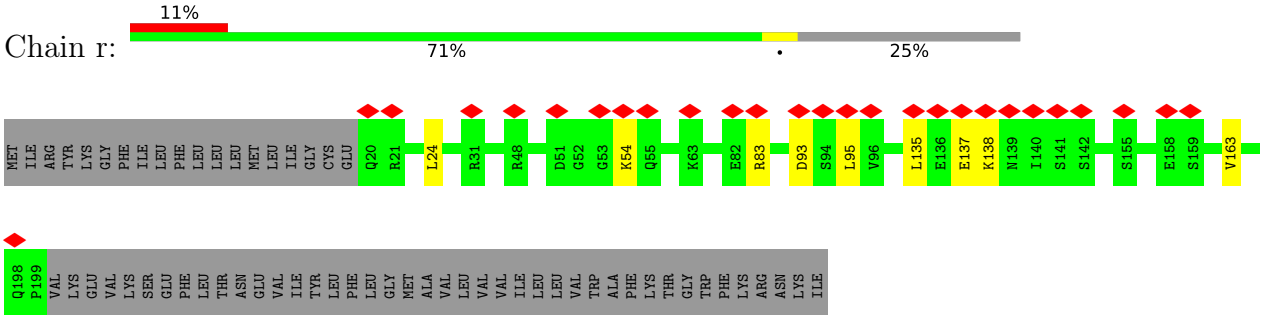
• Molecule 2: Lipoprotein MxiJ

Chain o:



• Molecule 2: Lipoprotein MxiJ

Chain r:



• Molecule 3: Outer membrane protein MxiD

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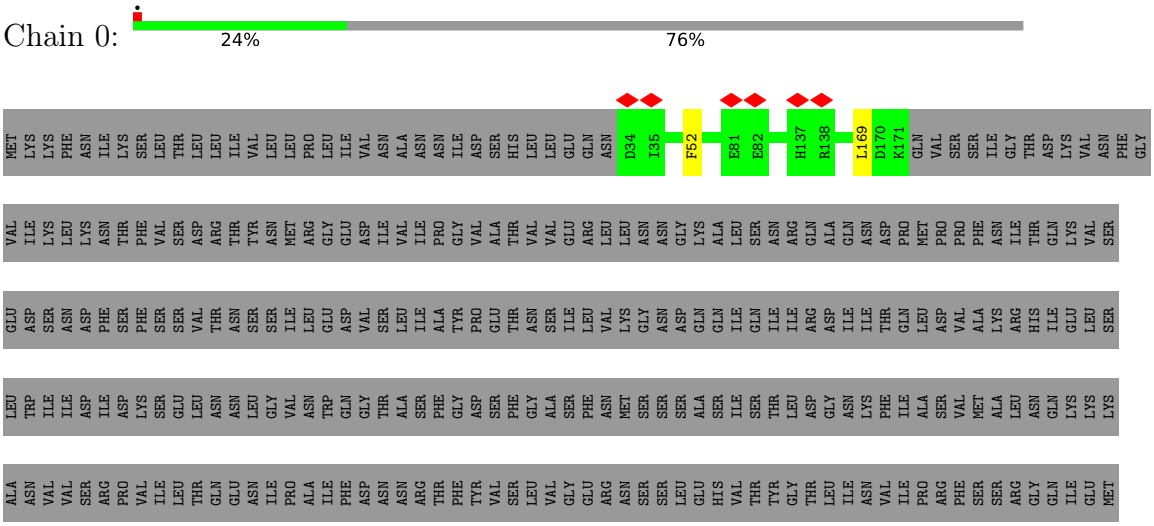
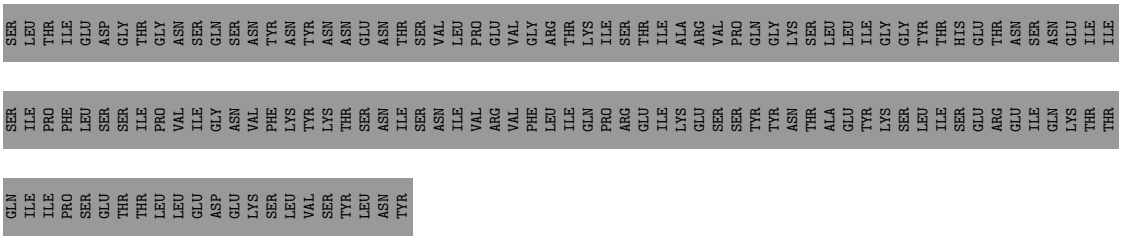


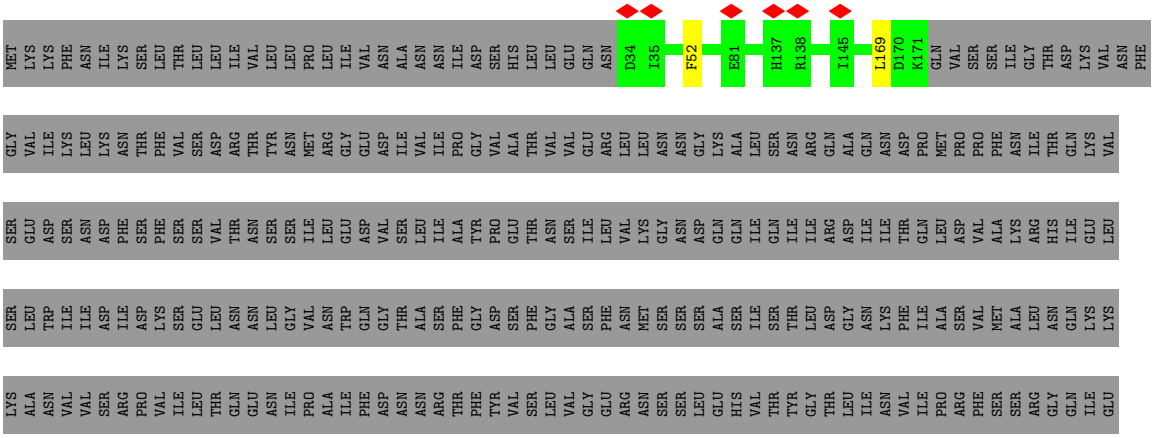


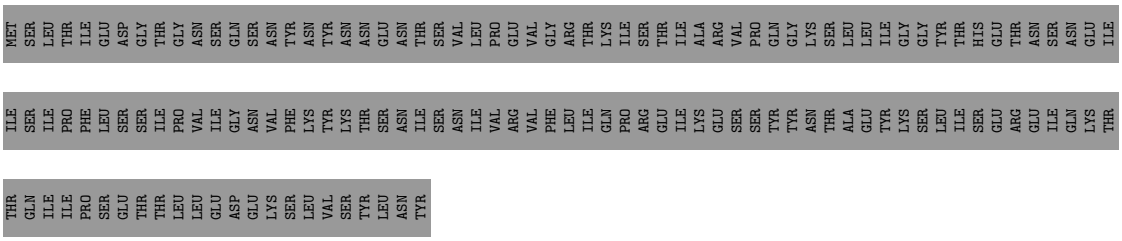
• Molecule 3: Outer membrane protein MxiD

Chain 1:

• Molecule 3: Outer membrane protein MxiD

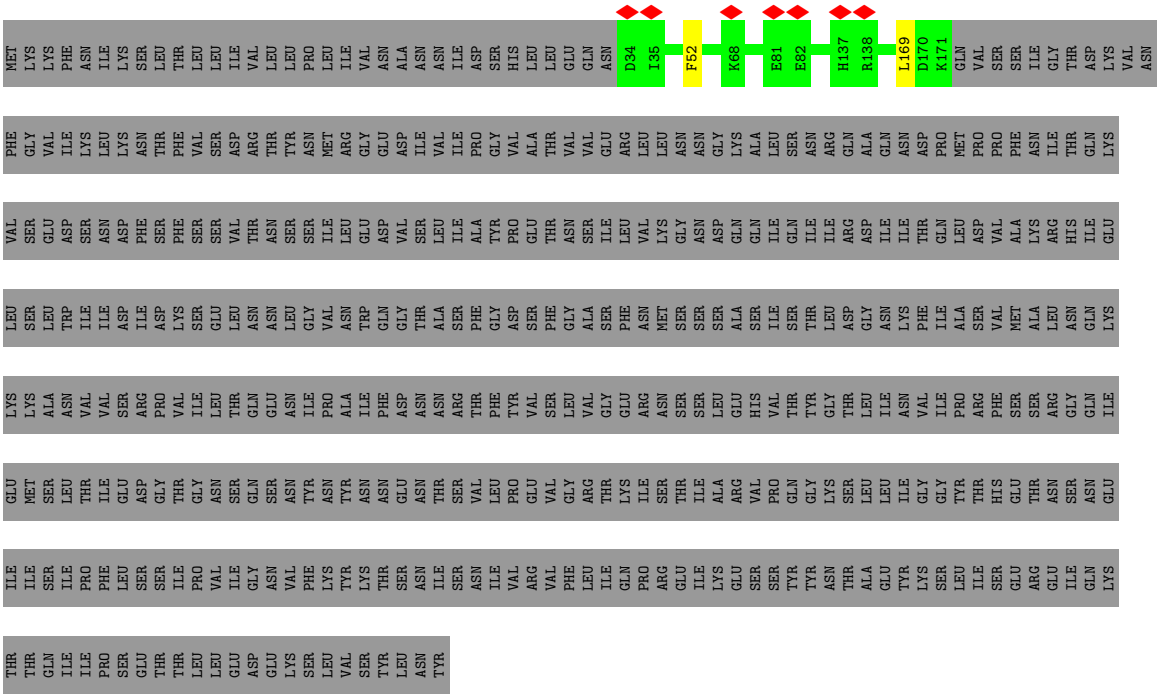
Chain a0:





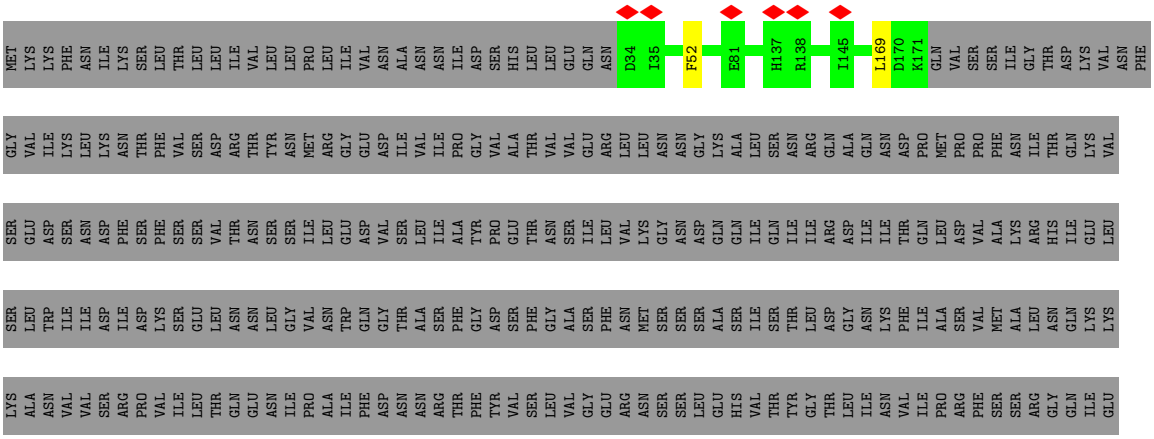
• Molecule 3: Outer membrane protein MxiD

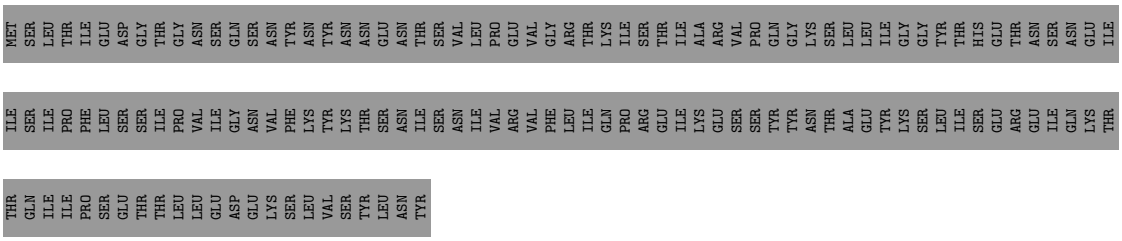
Chain Y:



• Molecule 3: Outer membrane protein MxiD

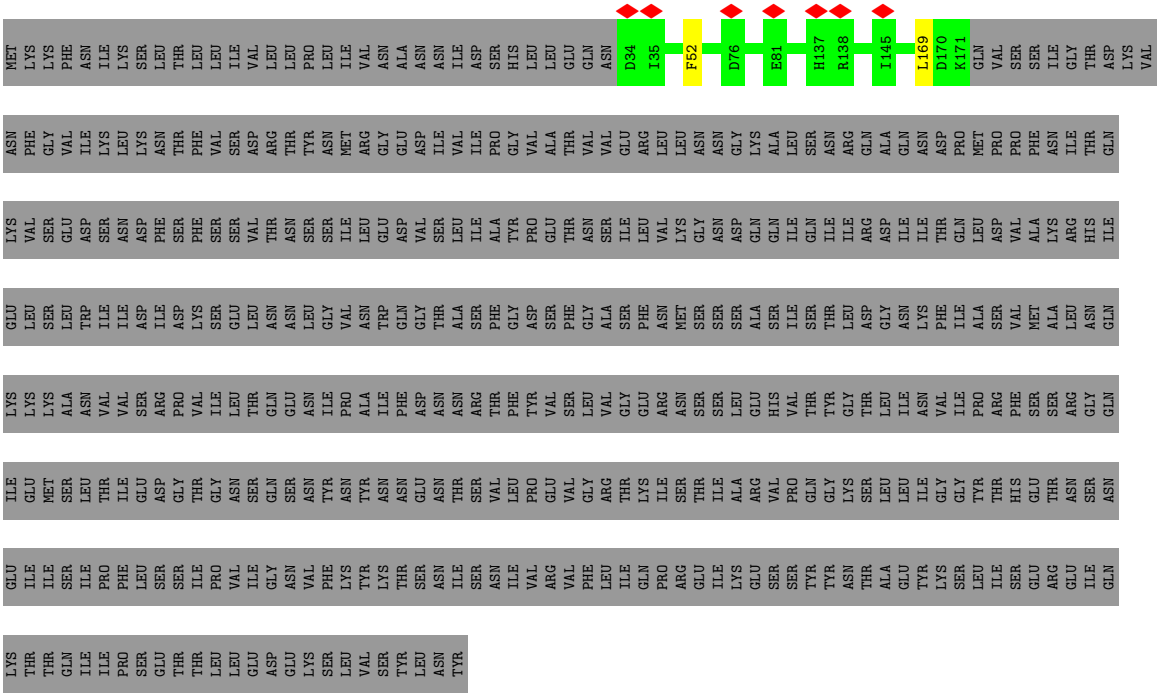
Chain Z:





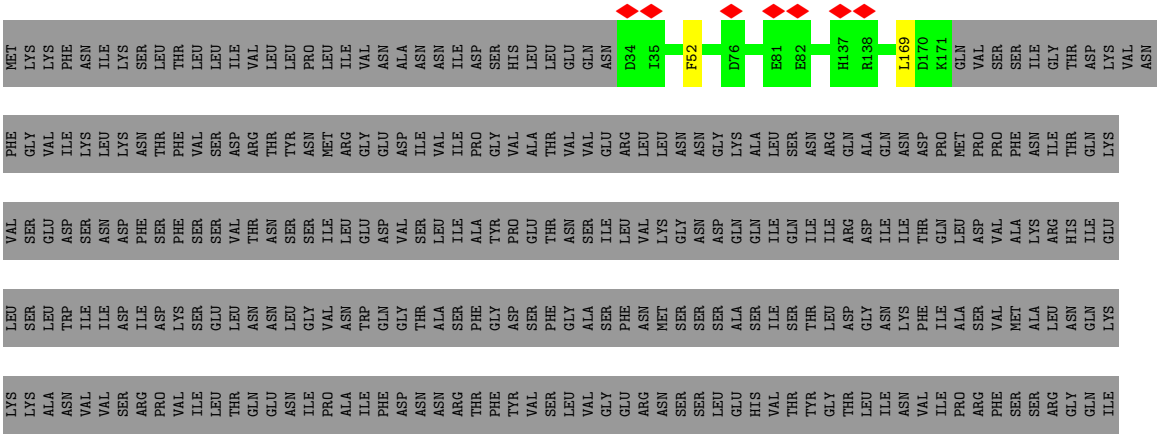
• Molecule 3: Outer membrane protein MxiD

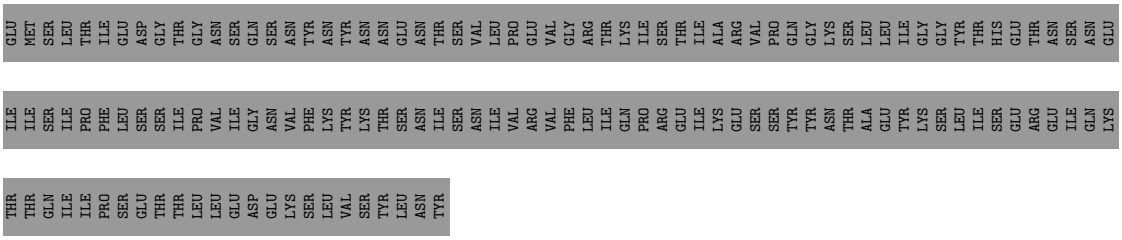
Chain 2:



• Molecule 3: Outer membrane protein MxiD

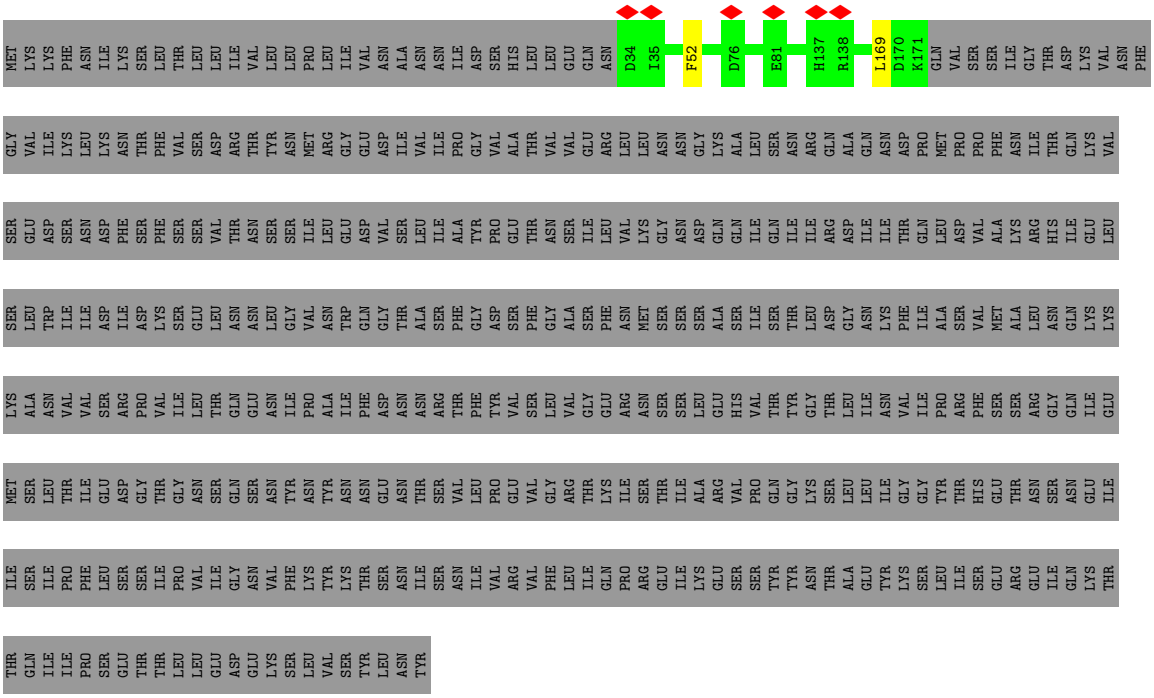
Chain 4:





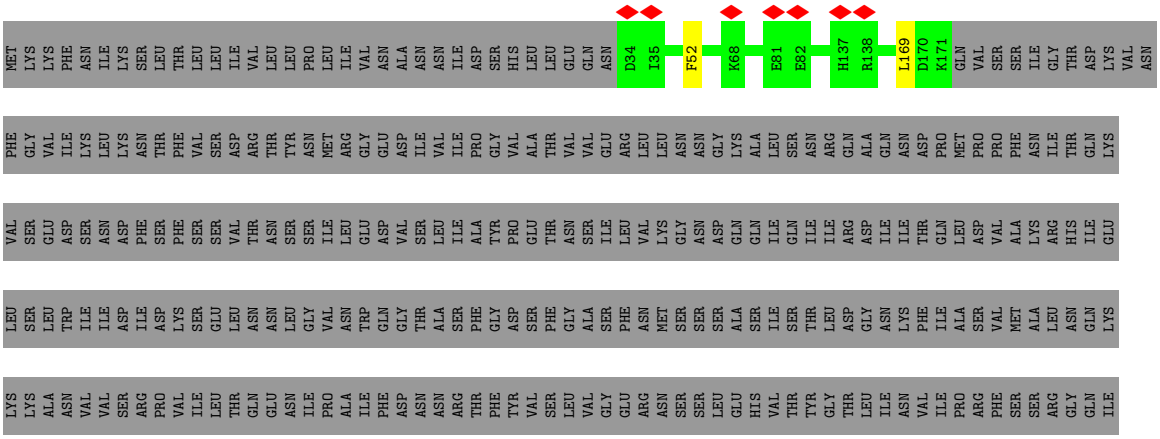
• Molecule 3: Outer membrane protein MxiD

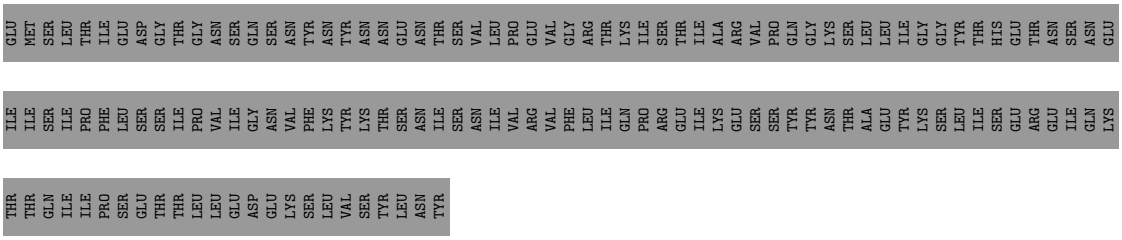
Chain 6:



• Molecule 3: Outer membrane protein MxiD

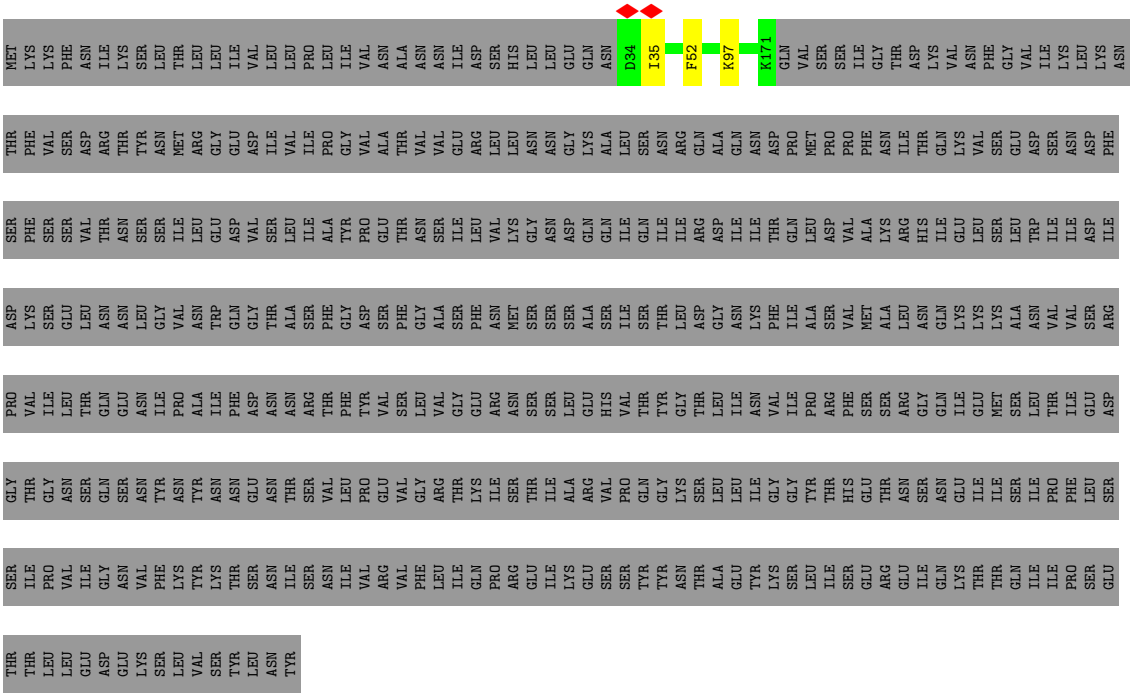
Chain 8:





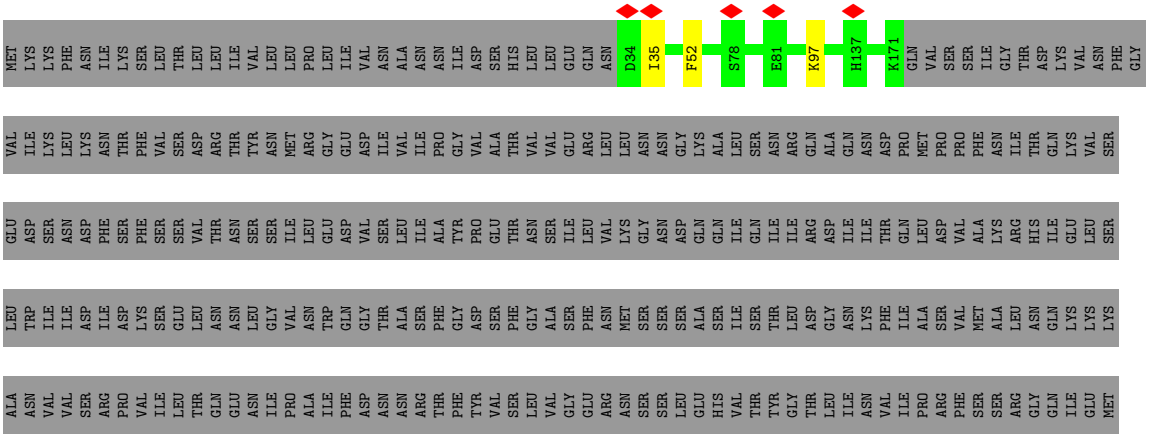
• Molecule 3: Outer membrane protein MxiD

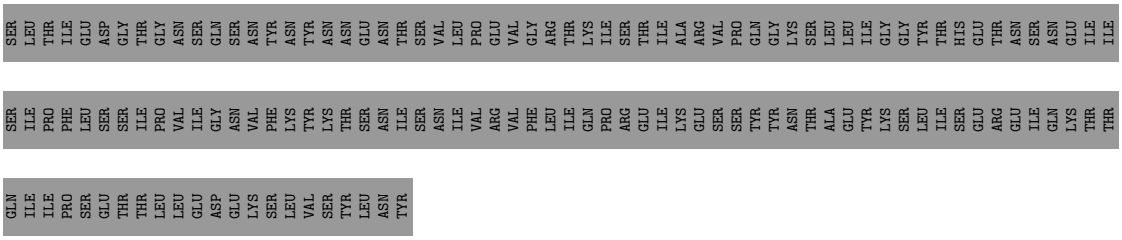
Chain b0:



• Molecule 3: Outer membrane protein MxiD

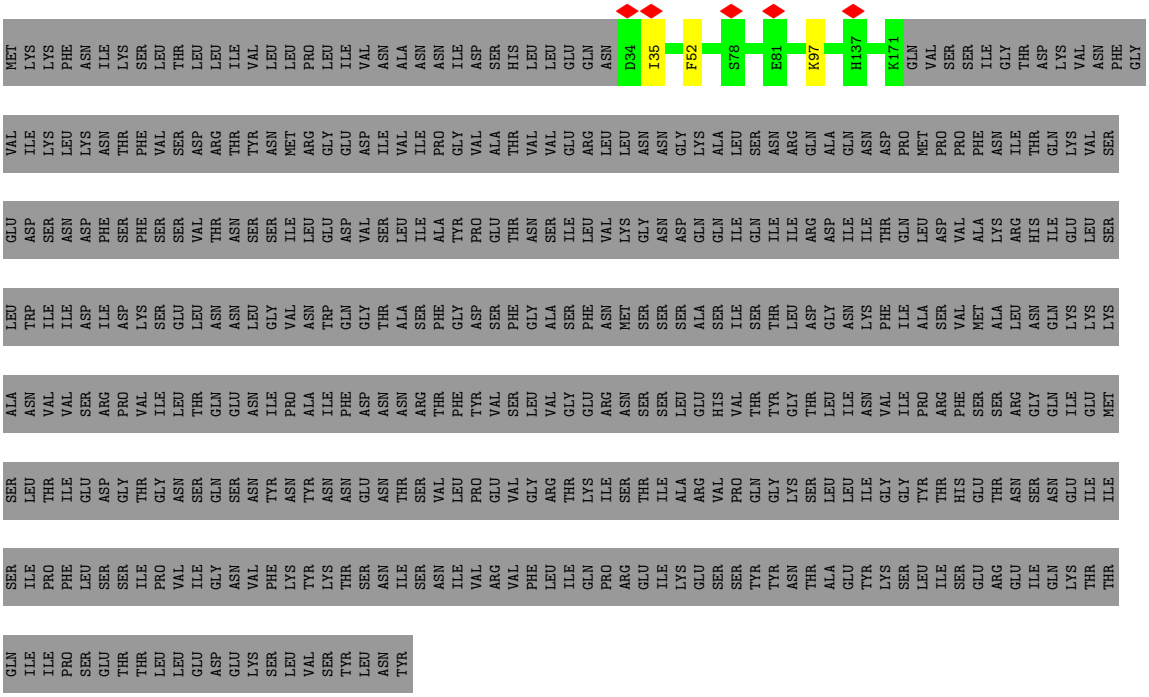
Chain y:





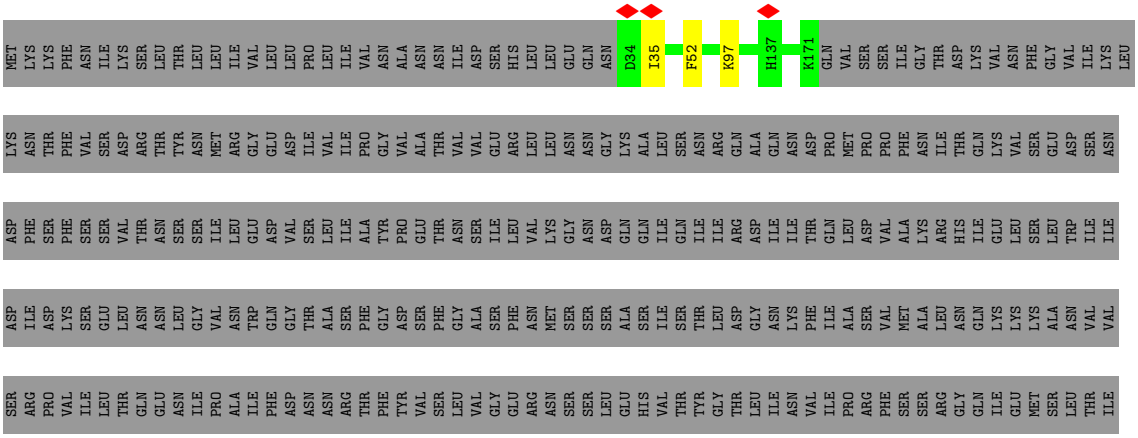
• Molecule 3: Outer membrane protein MxiD

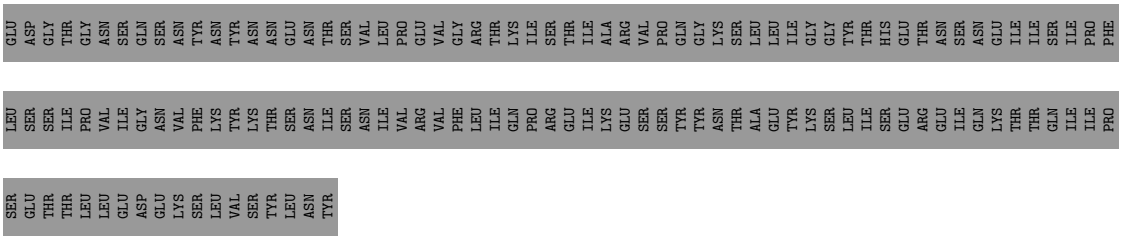
Chain z:



• Molecule 3: Outer membrane protein MxiD

Chain 3:



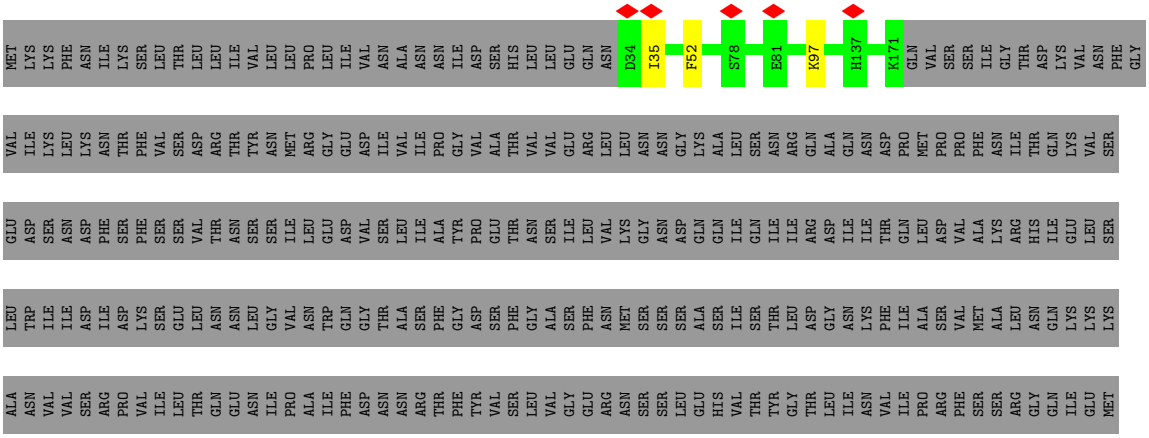


• Molecule 3: Outer membrane protein MxiD

Chain 5:

• Molecule 3: Outer membrane protein MxiD

Chain 7:



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

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

GLN ILE ILE PRO SER GLU THR THR LEU LEU GLU GLU ASP GLU LYS SER LEU VAL SER TYR LEU ASN TYR

- Molecule 3: Outer membrane protein MxiD

Chain 9:

MET LYS LYS PHE ASN ILE LYS SER LEU THR LEU LEU LEU ILE VAL LEU LEU PRO LEU ILE VAL ASN ALA ASN ASN ILE ASP SER HIS LEU LEU GLU GLN ASN D34 I35 F52 E81 K97 H137 K171 GLN VAL SER SER ILE GLY THR ASP LYS VAL ASN PHE GLY VAL ILE

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

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

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

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

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

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

ILE PRO SER GLU THR THR LEU LEU GLU GLU ASP GLU LYS SER LEU VAL SER TYR LEU ASN TYR

4 Experimental information (i)

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 ($e^-/Å^2$)	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

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.26	0/1837	0.42	0/2477
1	B	0.26	0/1837	0.42	0/2477
1	C	0.26	0/1761	0.40	0/2374
1	D	0.26	0/1837	0.42	0/2477
1	E	0.26	0/1837	0.42	0/2477
1	F	0.25	0/1761	0.40	0/2374
1	G	0.26	0/1837	0.42	0/2477
1	H	0.26	0/1837	0.42	0/2477
1	I	0.26	0/1761	0.40	0/2374
1	J	0.26	0/1837	0.42	0/2477
1	K	0.26	0/1837	0.42	0/2477
1	L	0.25	0/1761	0.40	0/2374
1	M	0.26	0/1837	0.42	0/2477
1	N	0.26	0/1837	0.42	0/2477
1	O	0.26	0/1761	0.40	0/2374
1	P	0.26	0/1837	0.42	0/2477
1	Q	0.26	0/1837	0.42	0/2477
1	R	0.26	0/1761	0.40	0/2374
1	S	0.26	0/1837	0.42	0/2477
1	T	0.26	0/1837	0.42	0/2477
1	U	0.26	0/1837	0.42	0/2477
1	V	0.26	0/1837	0.42	0/2477
1	W	0.26	0/1761	0.40	0/2374
1	X	0.26	0/1761	0.40	0/2374
2	a	0.26	0/1449	0.42	0/1957
2	b	0.26	0/1449	0.42	0/1957
2	c	0.26	0/1449	0.42	0/1957
2	d	0.25	0/1449	0.42	0/1957
2	e	0.26	0/1449	0.42	0/1957
2	f	0.26	0/1449	0.42	0/1957
2	g	0.25	0/1449	0.42	0/1957
2	h	0.26	0/1449	0.42	0/1957
2	i	0.26	0/1449	0.42	0/1957
2	j	0.25	0/1449	0.42	0/1957

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
2	k	0.26	0/1449	0.42	0/1957
2	l	0.26	0/1449	0.42	0/1957
2	m	0.25	0/1449	0.42	0/1957
2	n	0.26	0/1449	0.42	0/1957
2	o	0.26	0/1449	0.42	0/1957
2	p	0.25	0/1449	0.42	0/1957
2	q	0.26	0/1449	0.42	0/1957
2	r	0.25	0/1449	0.42	0/1957
2	s	0.25	0/1449	0.42	0/1957
2	t	0.26	0/1449	0.42	0/1957
2	u	0.26	0/1449	0.42	0/1957
2	v	0.25	0/1449	0.42	0/1957
2	w	0.25	0/1449	0.42	0/1957
2	x	0.25	0/1449	0.42	0/1957
3	0	0.26	0/1124	0.42	0/1525
3	1	0.26	0/1124	0.42	0/1525
3	2	0.26	0/1124	0.42	0/1525
3	3	0.26	0/1124	0.42	0/1525
3	4	0.25	0/1124	0.42	0/1525
3	5	0.26	0/1124	0.42	0/1525
3	6	0.26	0/1124	0.42	0/1525
3	7	0.26	0/1124	0.42	0/1525
3	8	0.26	0/1124	0.42	0/1525
3	9	0.26	0/1124	0.42	0/1525
3	Y	0.25	0/1124	0.42	0/1525
3	Z	0.26	0/1124	0.42	0/1525
3	a0	0.26	0/1124	0.42	0/1525
3	b0	0.26	0/1124	0.42	0/1525
3	y	0.26	0/1124	0.42	0/1525
3	z	0.26	0/1124	0.41	0/1525
All	All	0.26	0/96240	0.42	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 (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	202/342 (59%)	196 (97%)	6 (3%)	36	62
1	B	202/342 (59%)	198 (98%)	4 (2%)	50	72
1	C	195/342 (57%)	190 (97%)	5 (3%)	41	66
1	D	202/342 (59%)	196 (97%)	6 (3%)	36	62
1	E	202/342 (59%)	198 (98%)	4 (2%)	50	72
1	F	195/342 (57%)	190 (97%)	5 (3%)	41	66
1	G	202/342 (59%)	196 (97%)	6 (3%)	36	62
1	H	202/342 (59%)	198 (98%)	4 (2%)	50	72
1	I	195/342 (57%)	190 (97%)	5 (3%)	41	66
1	J	202/342 (59%)	196 (97%)	6 (3%)	36	62
1	K	202/342 (59%)	198 (98%)	4 (2%)	50	72
1	L	195/342 (57%)	190 (97%)	5 (3%)	41	66
1	M	202/342 (59%)	196 (97%)	6 (3%)	36	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	202/342 (59%)	198 (98%)	4 (2%)	50	72
1	O	195/342 (57%)	190 (97%)	5 (3%)	41	66
1	P	202/342 (59%)	196 (97%)	6 (3%)	36	62
1	Q	202/342 (59%)	198 (98%)	4 (2%)	50	72
1	R	195/342 (57%)	190 (97%)	5 (3%)	41	66
1	S	202/342 (59%)	196 (97%)	6 (3%)	36	62
1	T	202/342 (59%)	198 (98%)	4 (2%)	50	72
1	U	202/342 (59%)	196 (97%)	6 (3%)	36	62
1	V	202/342 (59%)	198 (98%)	4 (2%)	50	72
1	W	195/342 (57%)	190 (97%)	5 (3%)	41	66
1	X	195/342 (57%)	190 (97%)	5 (3%)	41	66
2	a	165/220 (75%)	160 (97%)	5 (3%)	36	62
2	b	165/220 (75%)	160 (97%)	5 (3%)	36	62
2	c	165/220 (75%)	156 (94%)	9 (6%)	18	46
2	d	165/220 (75%)	160 (97%)	5 (3%)	36	62
2	e	165/220 (75%)	160 (97%)	5 (3%)	36	62
2	f	165/220 (75%)	156 (94%)	9 (6%)	18	46
2	g	165/220 (75%)	160 (97%)	5 (3%)	36	62
2	h	165/220 (75%)	160 (97%)	5 (3%)	36	62
2	i	165/220 (75%)	156 (94%)	9 (6%)	18	46
2	j	165/220 (75%)	160 (97%)	5 (3%)	36	62
2	k	165/220 (75%)	160 (97%)	5 (3%)	36	62
2	l	165/220 (75%)	156 (94%)	9 (6%)	18	46
2	m	165/220 (75%)	160 (97%)	5 (3%)	36	62
2	n	165/220 (75%)	160 (97%)	5 (3%)	36	62
2	o	165/220 (75%)	156 (94%)	9 (6%)	18	46
2	p	165/220 (75%)	160 (97%)	5 (3%)	36	62
2	q	165/220 (75%)	160 (97%)	5 (3%)	36	62
2	r	165/220 (75%)	156 (94%)	9 (6%)	18	46
2	s	165/220 (75%)	160 (97%)	5 (3%)	36	62
2	t	165/220 (75%)	160 (97%)	5 (3%)	36	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	u	165/220 (75%)	156 (94%)	9 (6%)	18	46
2	v	165/220 (75%)	156 (94%)	9 (6%)	18	46
2	w	165/220 (75%)	160 (97%)	5 (3%)	36	62
2	x	165/220 (75%)	160 (97%)	5 (3%)	36	62
3	0	121/513 (24%)	119 (98%)	2 (2%)	56	75
3	1	121/513 (24%)	118 (98%)	3 (2%)	42	67
3	2	121/513 (24%)	119 (98%)	2 (2%)	56	75
3	3	121/513 (24%)	118 (98%)	3 (2%)	42	67
3	4	121/513 (24%)	119 (98%)	2 (2%)	56	75
3	5	121/513 (24%)	118 (98%)	3 (2%)	42	67
3	6	121/513 (24%)	119 (98%)	2 (2%)	56	75
3	7	121/513 (24%)	118 (98%)	3 (2%)	42	67
3	8	121/513 (24%)	119 (98%)	2 (2%)	56	75
3	9	121/513 (24%)	118 (98%)	3 (2%)	42	67
3	Y	121/513 (24%)	119 (98%)	2 (2%)	56	75
3	Z	121/513 (24%)	119 (98%)	2 (2%)	56	75
3	a0	121/513 (24%)	119 (98%)	2 (2%)	56	75
3	b0	121/513 (24%)	118 (98%)	3 (2%)	42	67
3	y	121/513 (24%)	118 (98%)	3 (2%)	42	67
3	z	121/513 (24%)	118 (98%)	3 (2%)	42	67
All	All	10688/21696 (49%)	10376 (97%)	312 (3%)	39	63

5 of 312 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	u	163	VAL
3	4	169	LEU
2	f	137	GLU
2	o	54	LYS
3	3	35	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	171	ASN
2	t	130	HIS
1	G	298	ASN
2	g	130	HIS
1	I	298	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

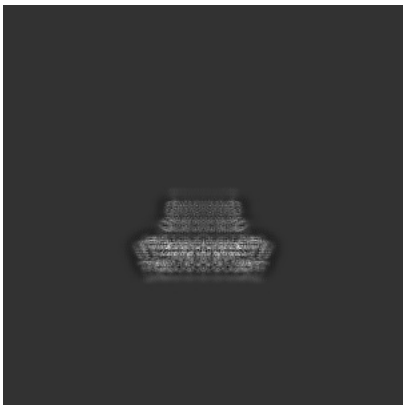
6 Map visualisation

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.

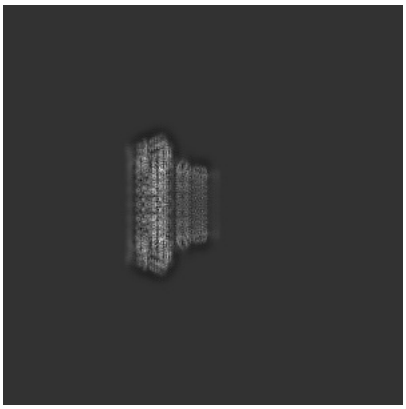
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

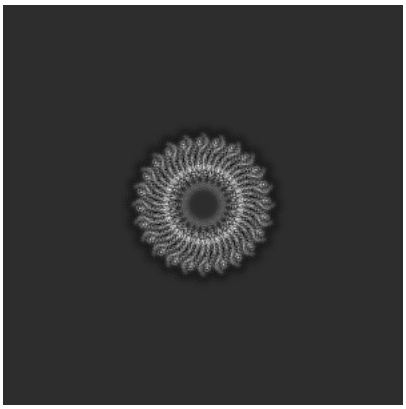
6.1.1 Primary map



X



Y

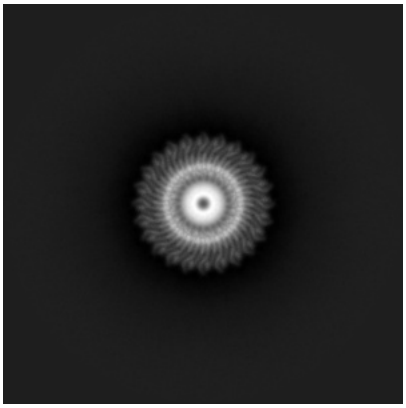


Z

6.1.2 Raw map

X

Y



Z

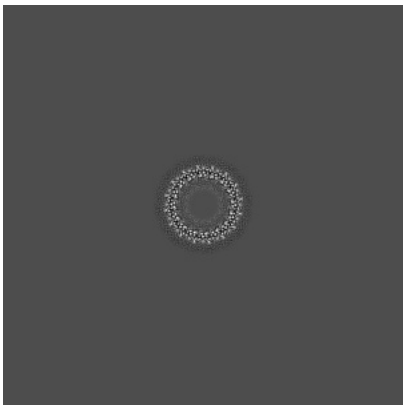
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map

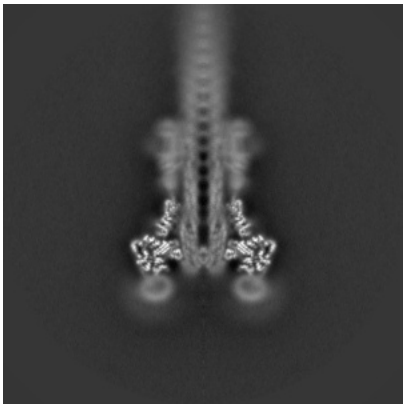
X Index: 240

Y Index: 240

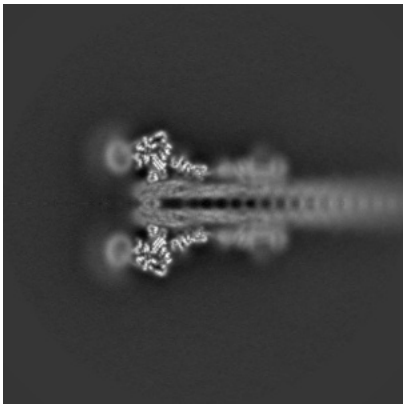


Z Index: 240

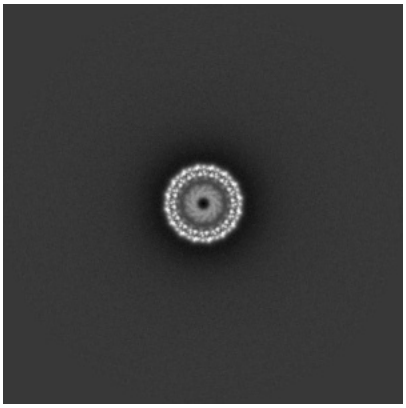
6.2.2 Raw map



X Index: 240



Y Index: 240

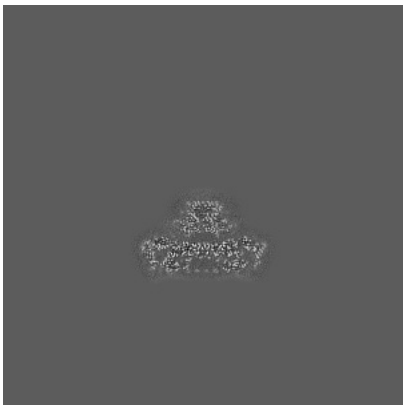


Z Index: 240

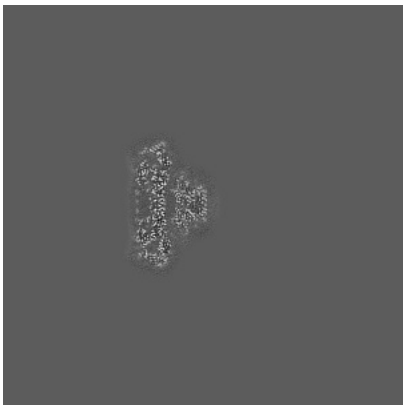
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

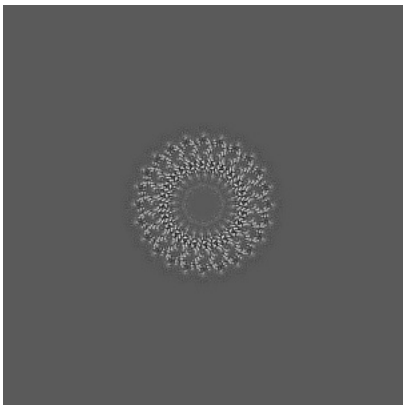
6.3.1 Primary map



X Index: 281

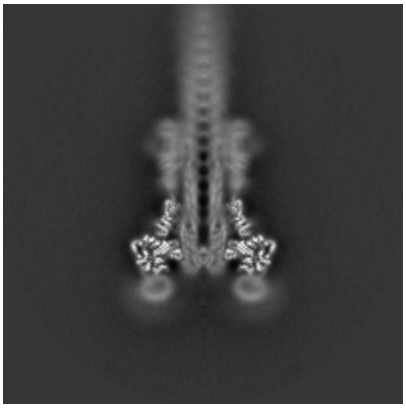


Y Index: 199

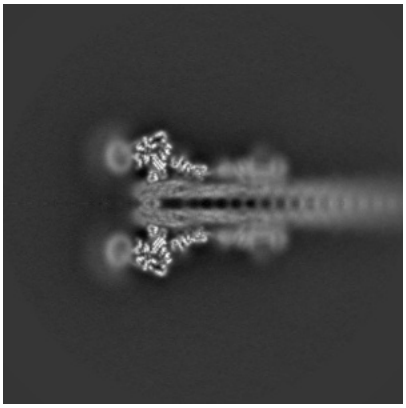


Z Index: 188

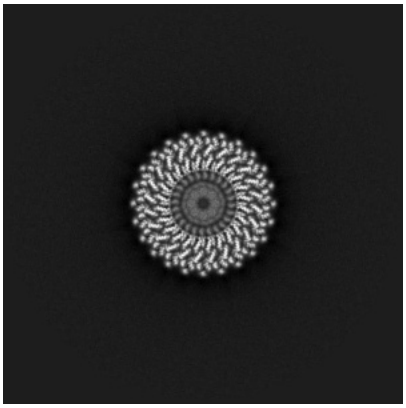
6.3.2 Raw map



X Index: 240



Y Index: 240

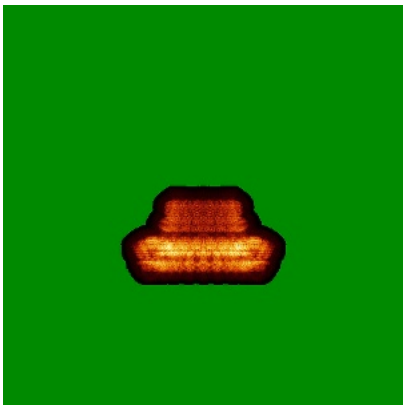


Z Index: 189

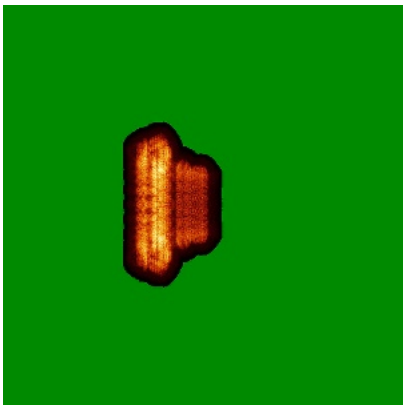
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

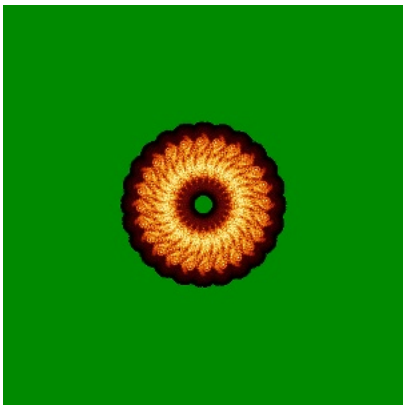
6.4.1 Primary map



X

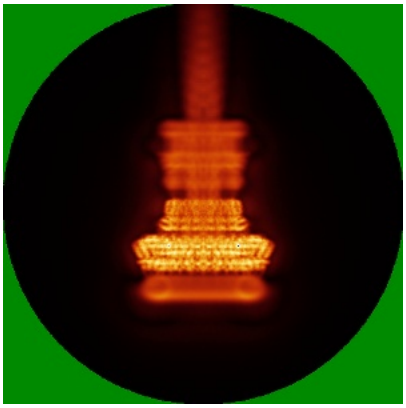


Y

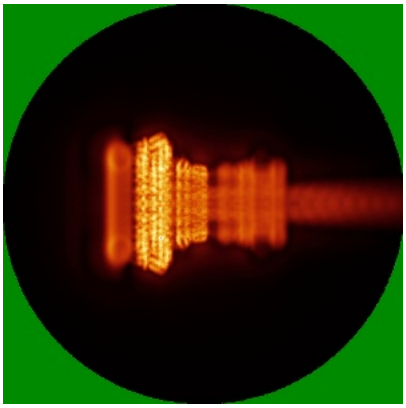


Z

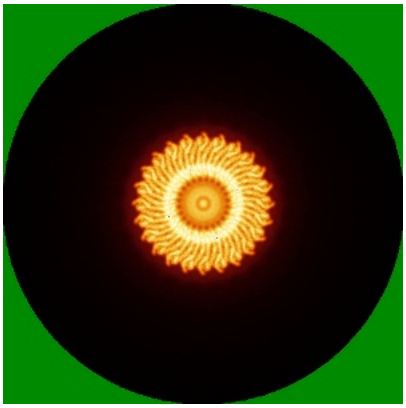
6.4.2 Raw map



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

X Y Z

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

X Y Z

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.

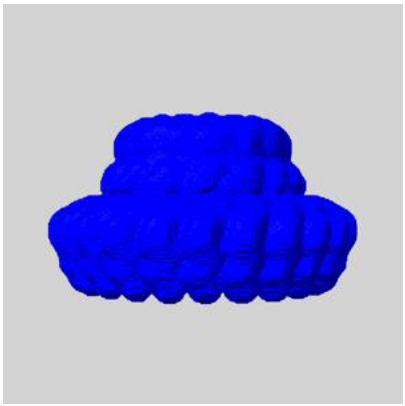
6.6 Mask visualisation (i)

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

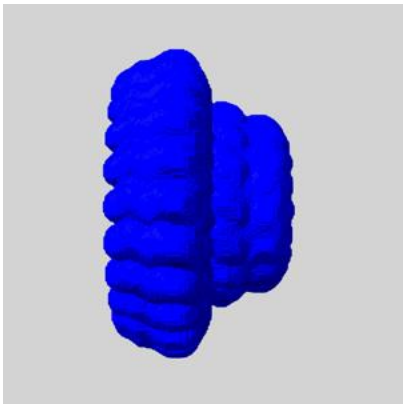
A mask typically either:

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

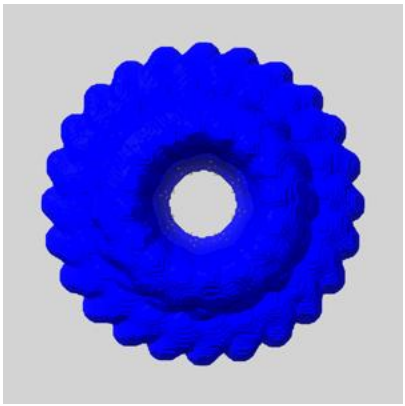
6.6.1 emd_15702_msk_1.map (i)



X



Y

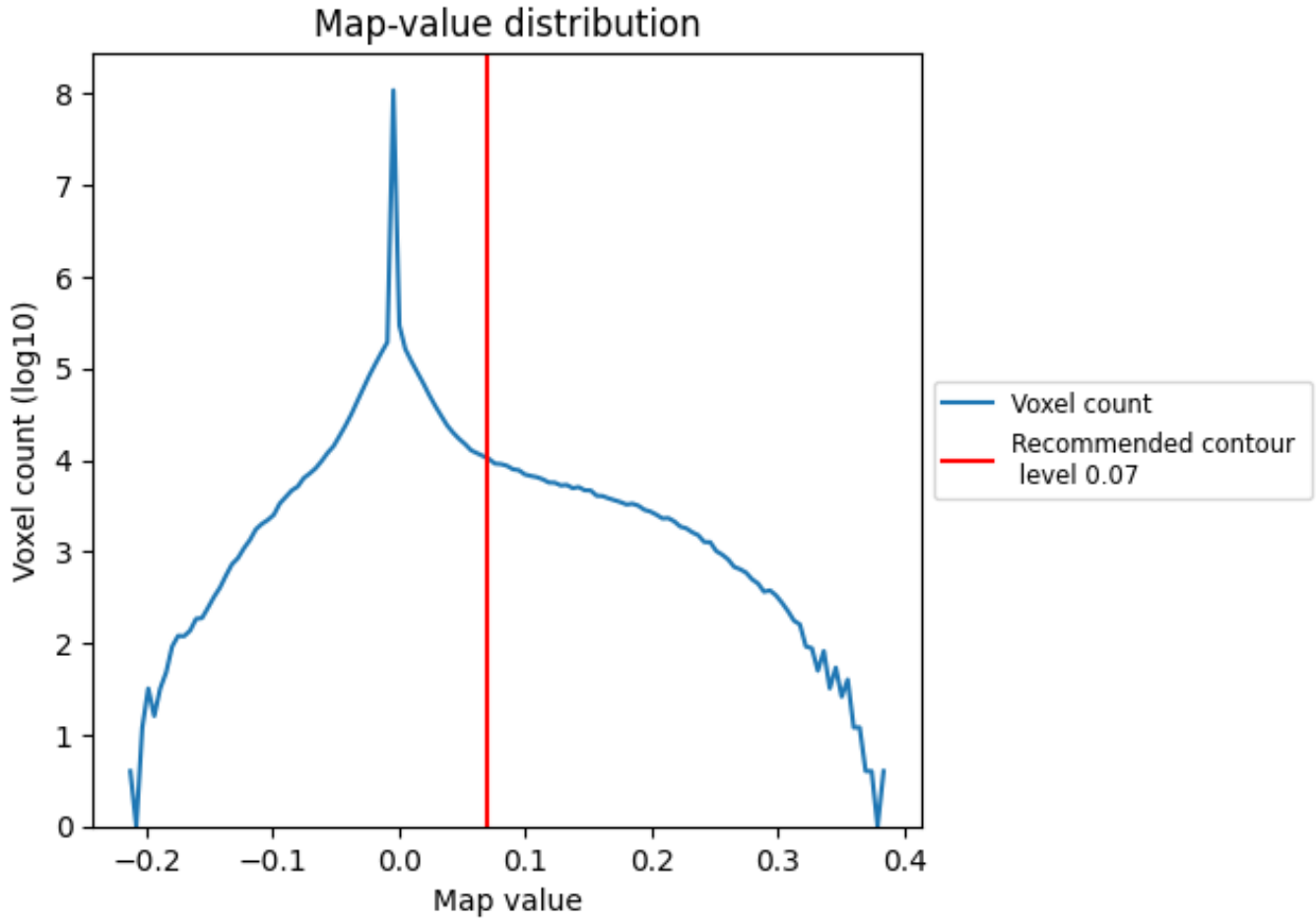


Z

7 Map analysis

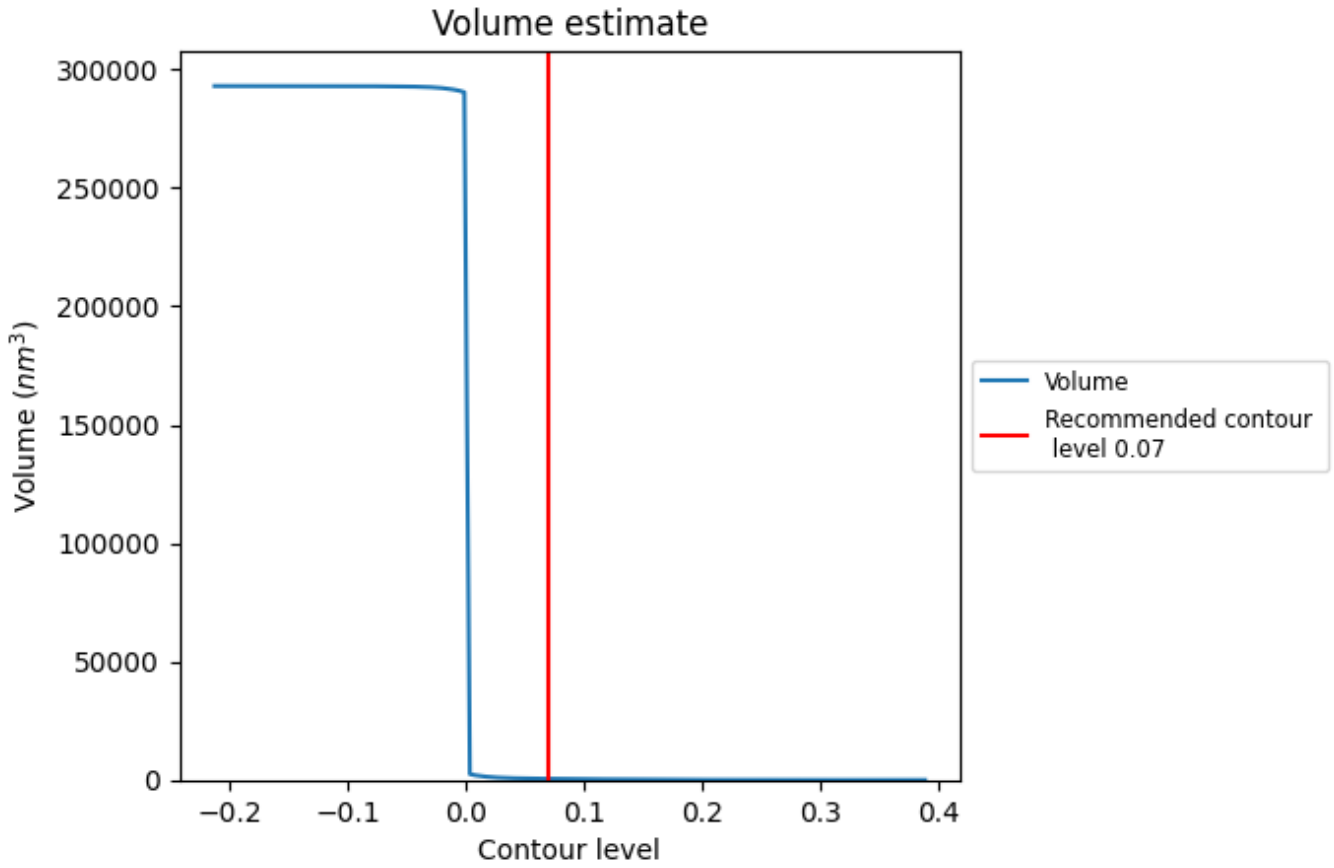
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

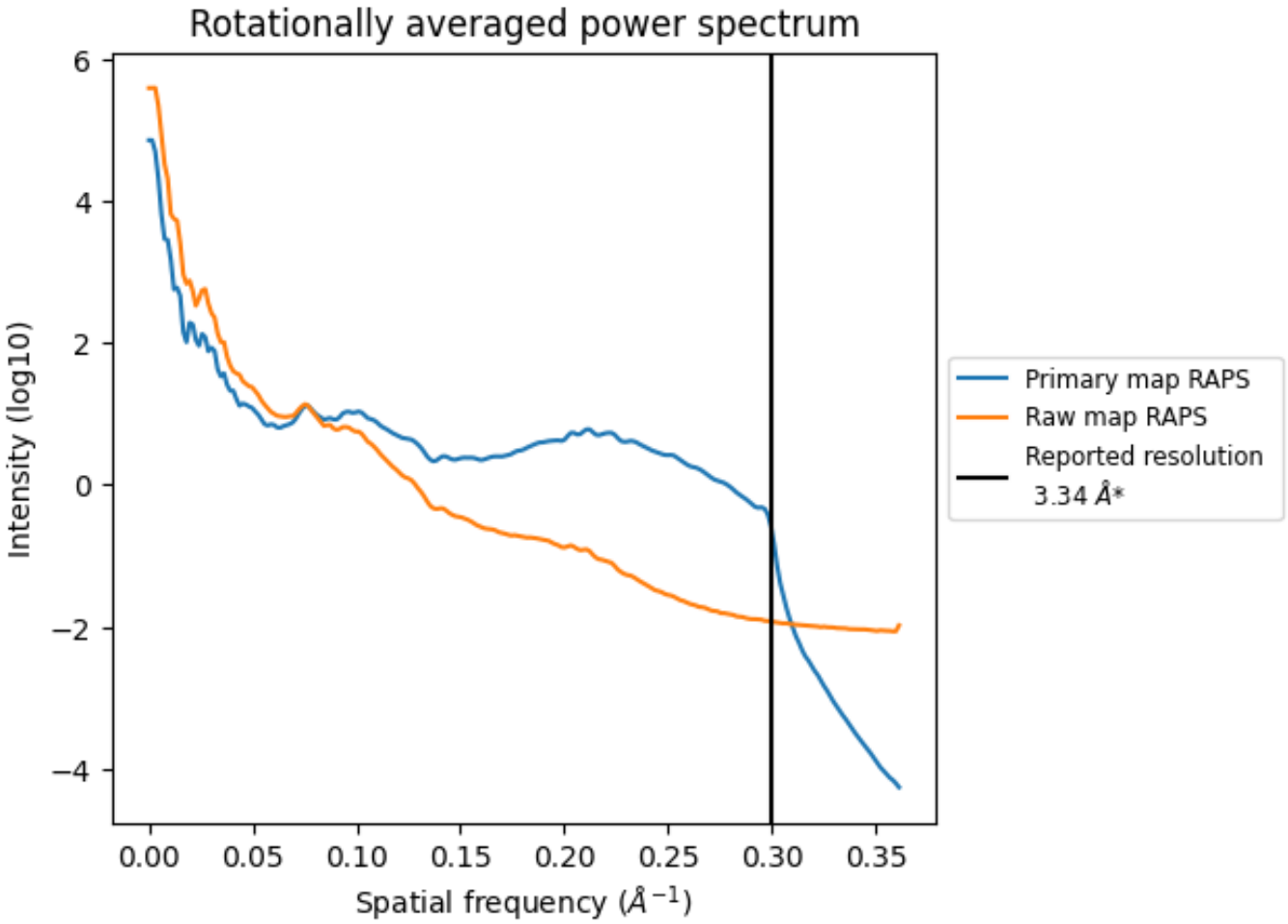
7.2 Volume estimate (i)



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 (i)

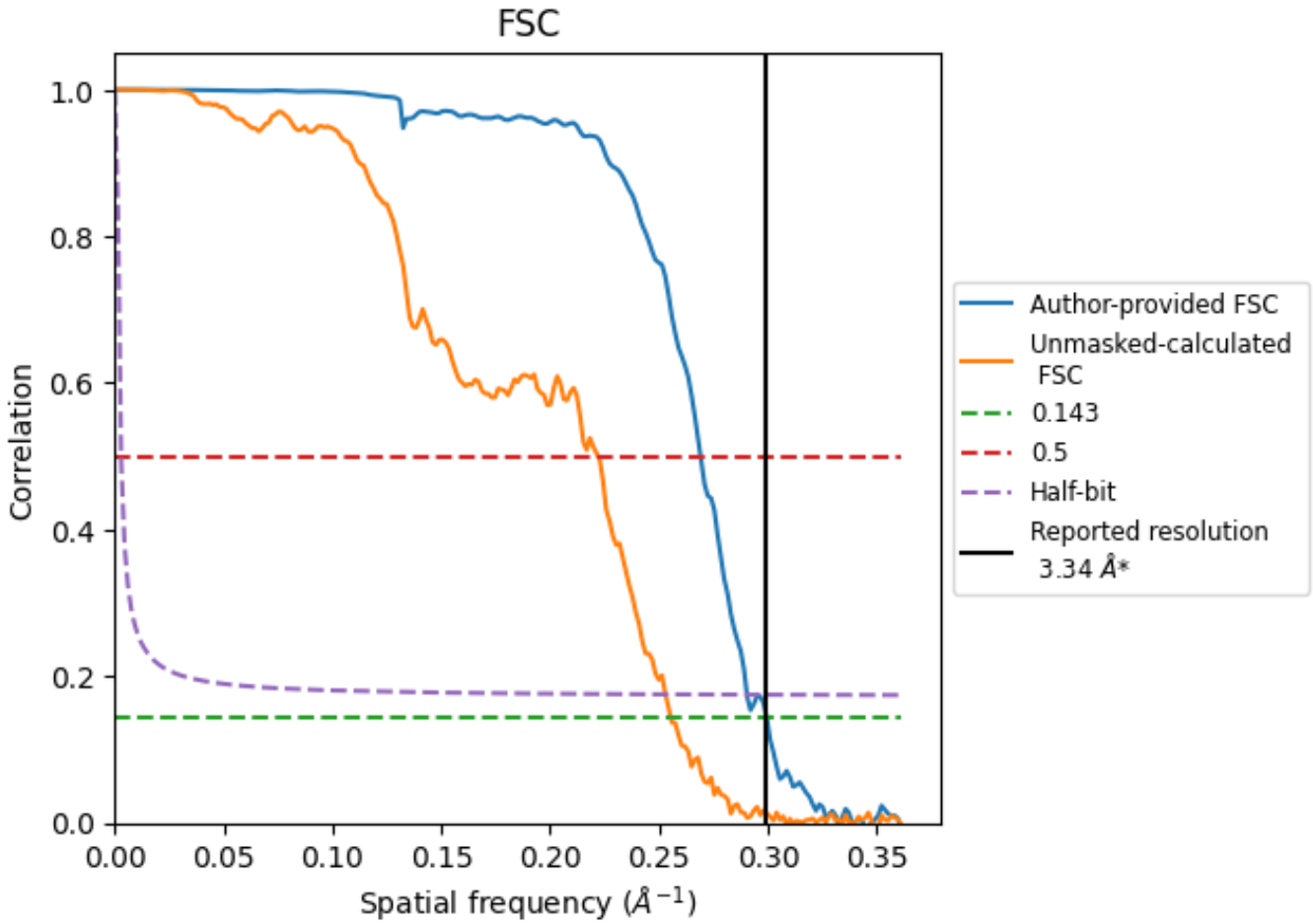


*Reported resolution corresponds to spatial frequency of 0.299 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.299 Å^{-1}

8.2 Resolution estimates (i)

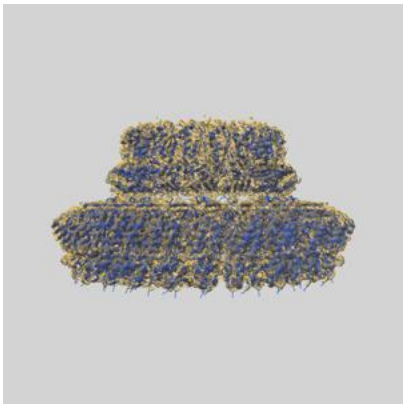
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.34	-	-
Author-provided FSC curve	3.34	3.71	3.44
Unmasked-calculated*	3.91	4.50	3.95

*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 %

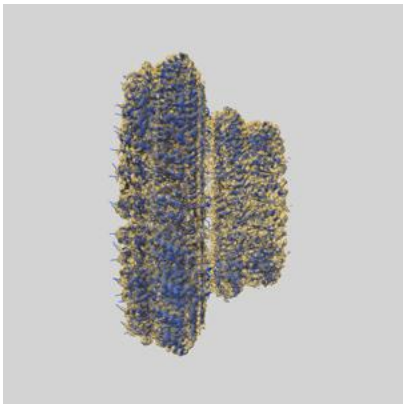
9 Map-model fit

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.

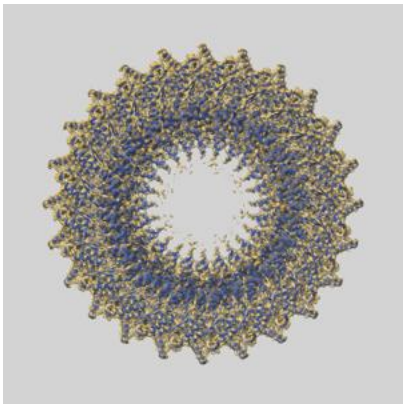
9.1 Map-model overlay



X



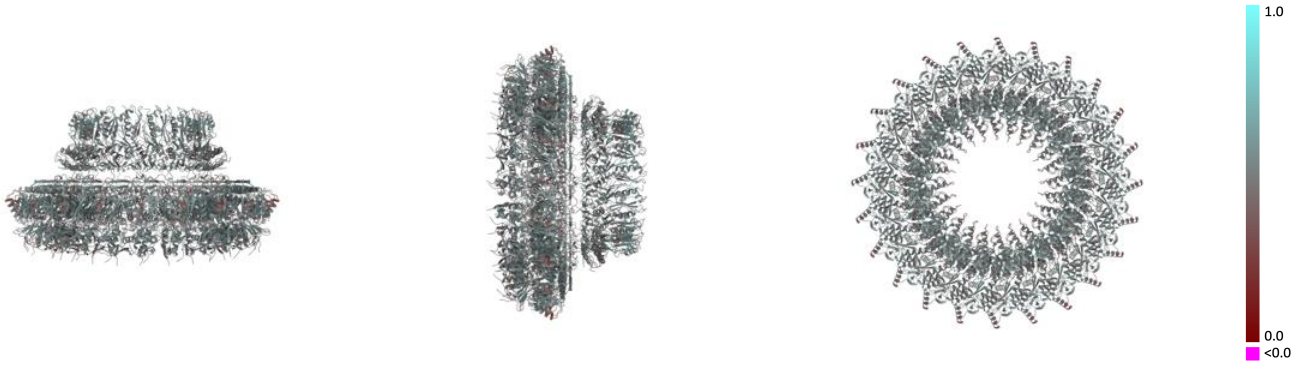
Y



Z

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.

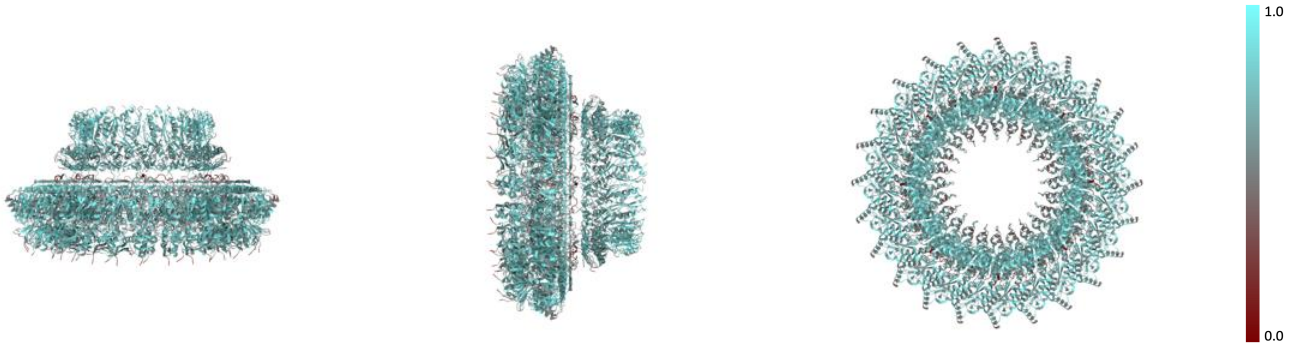
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

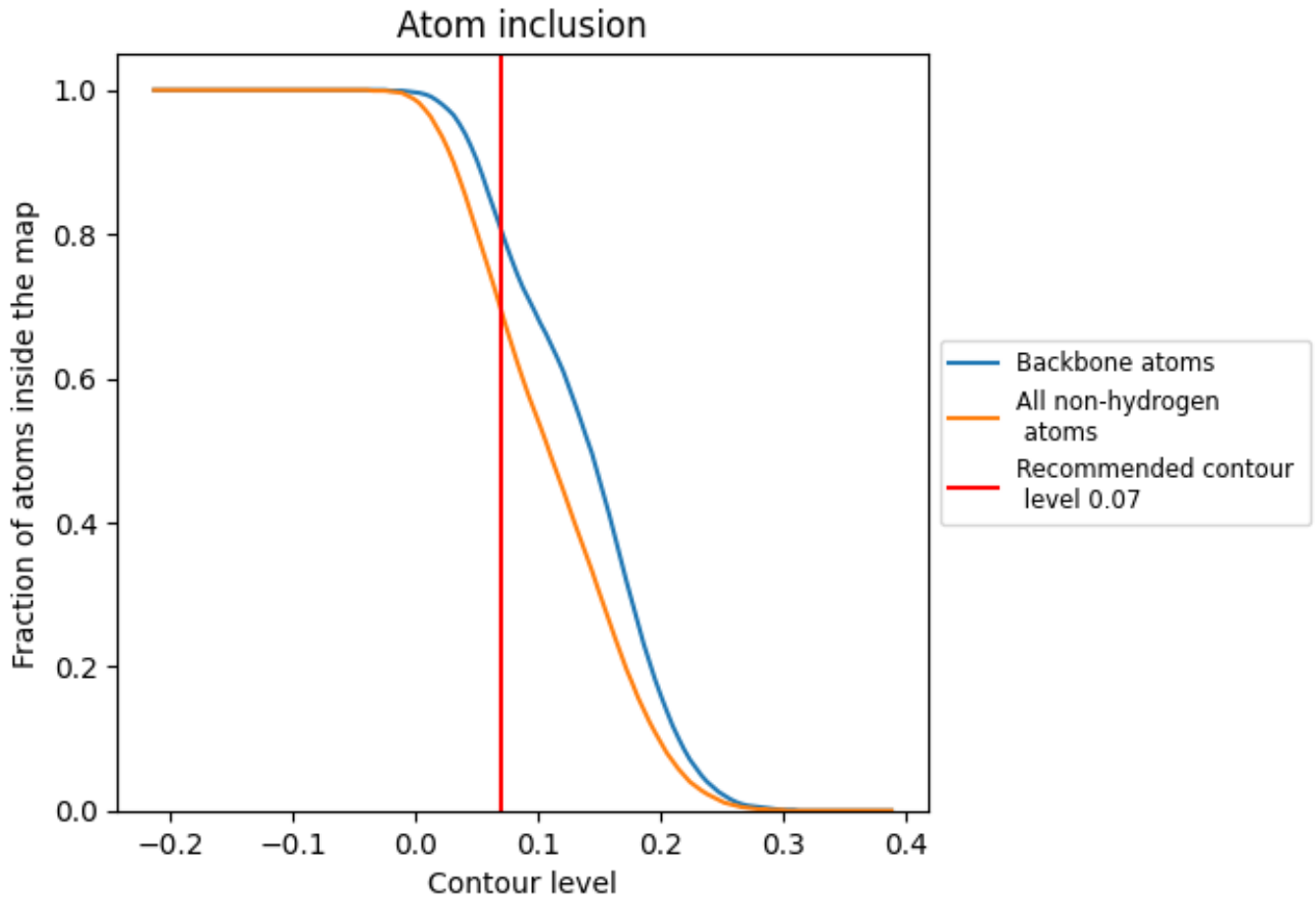
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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

Continued on next page...

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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