



Full wwPDB EM Validation Report ⓘ

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

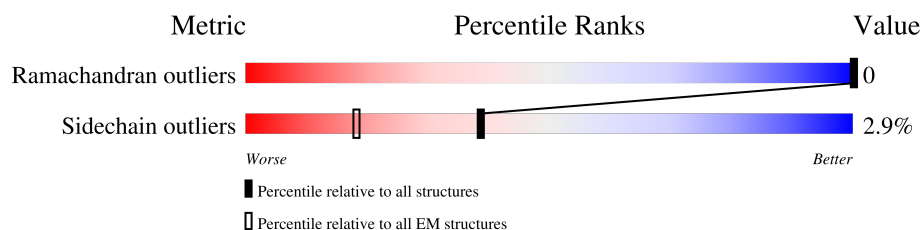
EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) :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

1 Overall quality at a glance

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

The reported resolution of this entry is 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.









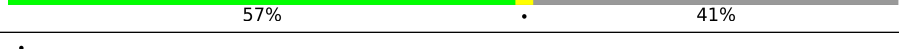
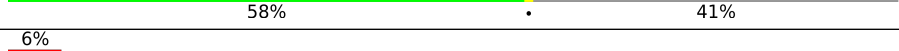
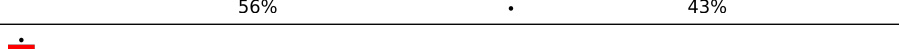
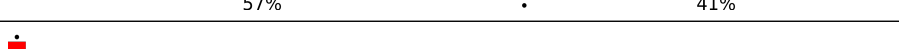
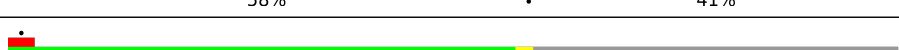

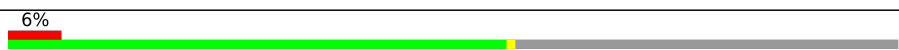

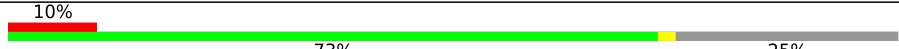





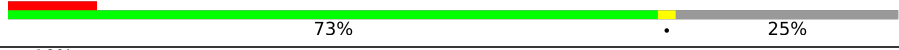
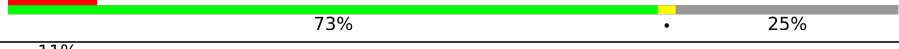



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 $\leq 5\%$. 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	 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	
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	
2	f	241	
2	g	241	
2	h	241	
2	i	241	
2	j	241	

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Mol	Chain	Length	Quality of chain
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	
3	6	566	
3	7	566	
3	8	566	
3	9	566	
3	Y	566	

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Mol	Chain	Length	Quality of chain
3	Z	566	<div><div></div><div>24%76%</div></div>
3	a0	566	<div><div></div><div>24%76%</div></div>
3	b0	566	<div><div></div><div>24%76%</div></div>
3	y	566	<div><div></div><div>24%76%</div></div>
3	z	566	<div><div></div><div>24%76%</div></div>

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.

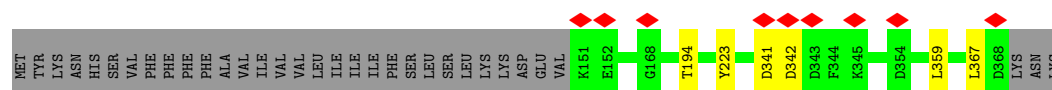
Mol	Chain	Residues	Atoms					AltConf	Trace
3	0	138	Total	C	N	O	S	0	0
			1102	718	174	209	1		
3	1	138	Total	C	N	O	S	0	0
			1102	718	174	209	1		
3	a0	138	Total	C	N	O	S	0	0
			1102	718	174	209	1		
3	Y	138	Total	C	N	O	S	0	0
			1102	718	174	209	1		
3	Z	138	Total	C	N	O	S	0	0
			1102	718	174	209	1		
3	2	138	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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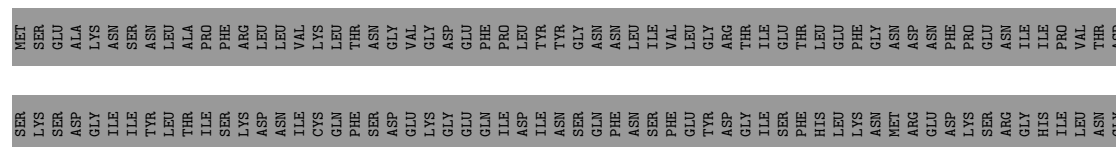
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Mol	Chain	Residues	Atoms					AltConf	Trace
3	6	138	Total	C	N	O	S	0	0
			1102	718	174	209	1		
3	8	138	Total	C	N	O	S	0	0
			1102	718	174	209	1		
3	b0	138	Total	C	N	O	S	0	0
			1102	718	174	209	1		
3	y	138	Total	C	N	O	S	0	0
			1102	718	174	209	1		
3	z	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		

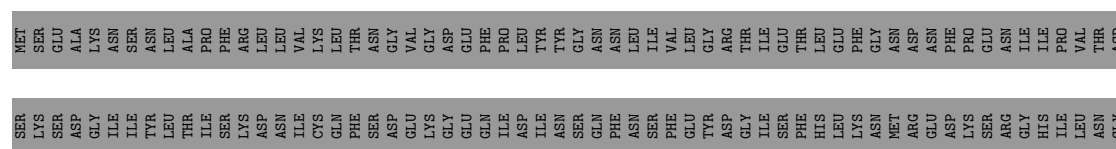




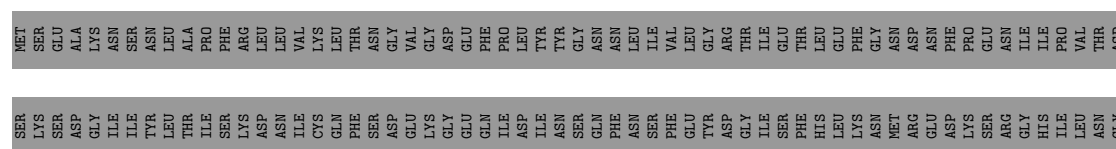
• Molecule 1: Protein MxiG



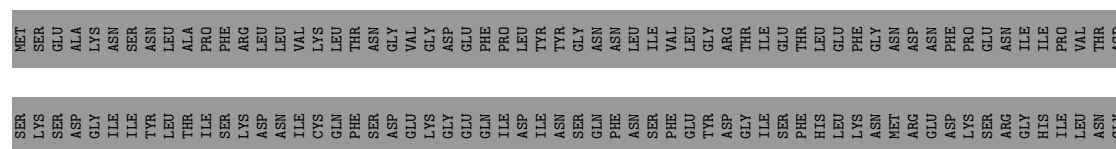
• Molecule 1: Protein MxiG

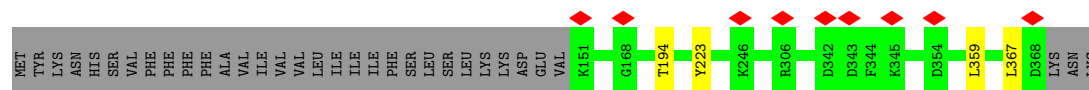


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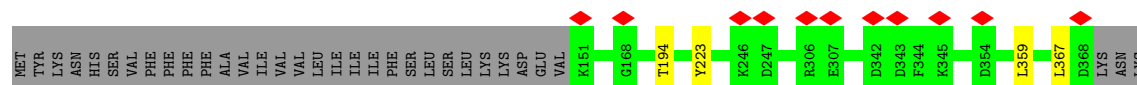
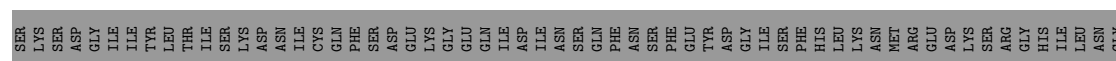
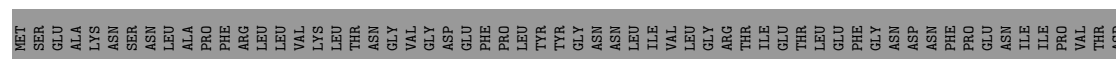


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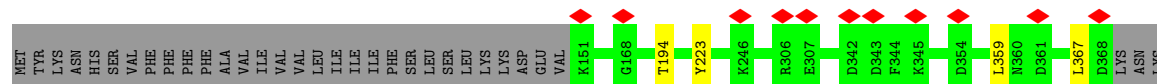
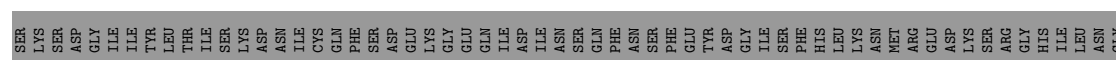
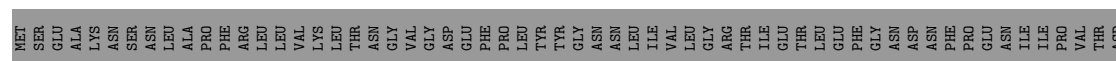




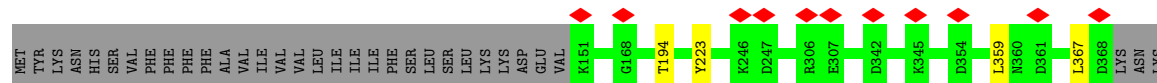
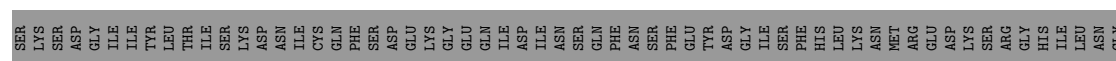
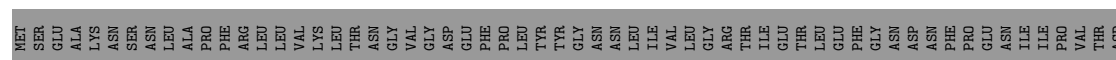
• Molecule 1: Protein MxiG



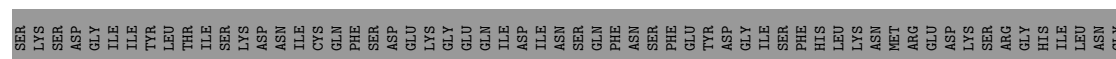
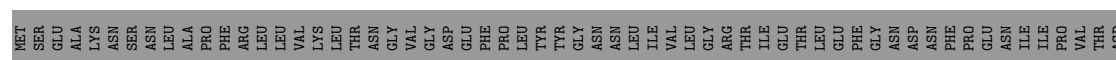
• Molecule 1: Protein MxiG

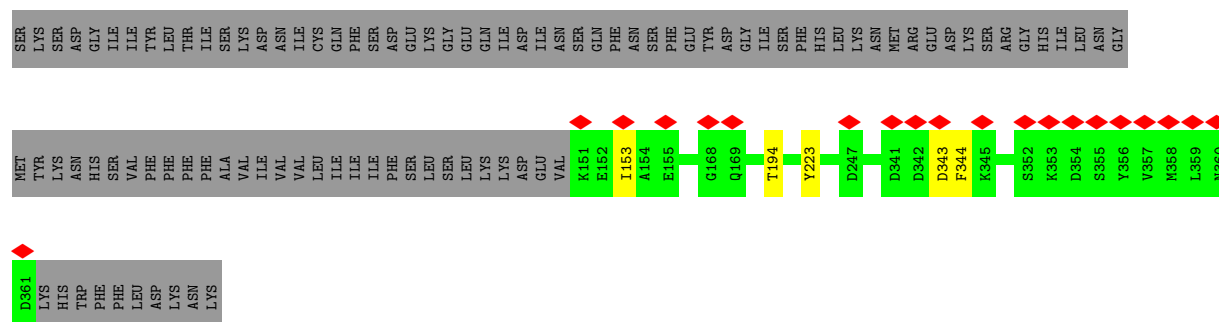


• Molecule 1: Protein MxiG

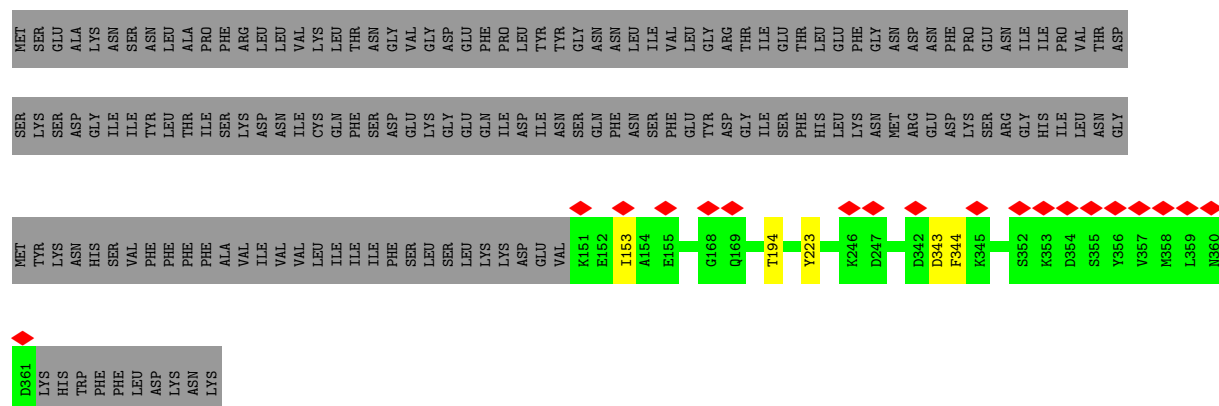


• Molecule 1: Protein MxiG

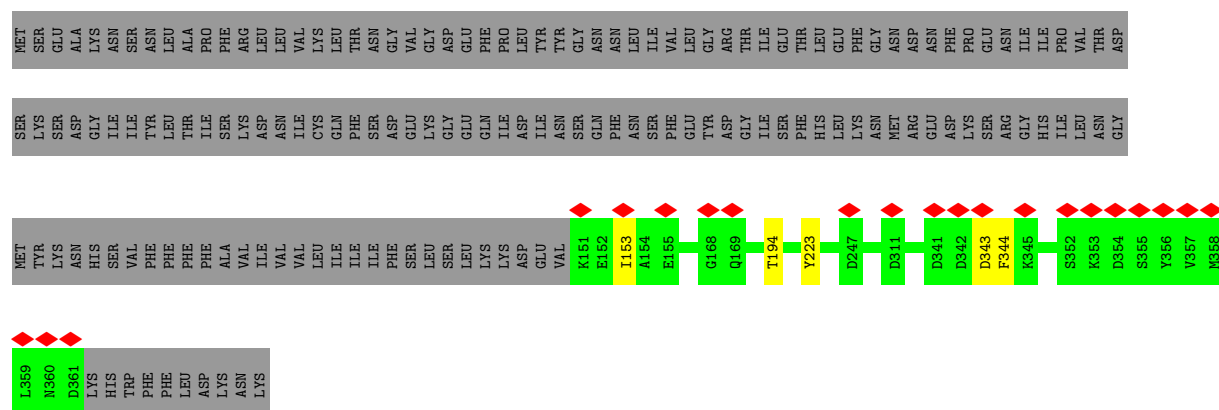




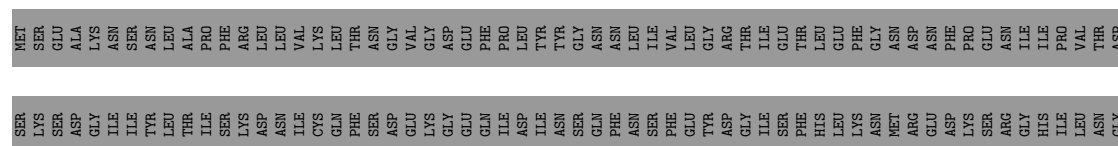
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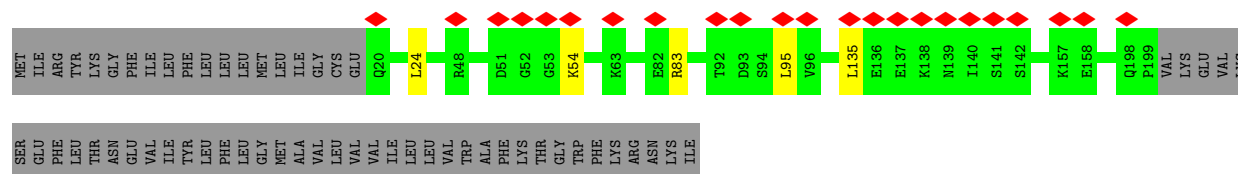
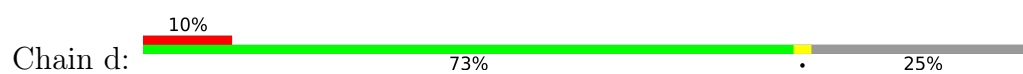


• Molecule 1: Protein MxiG

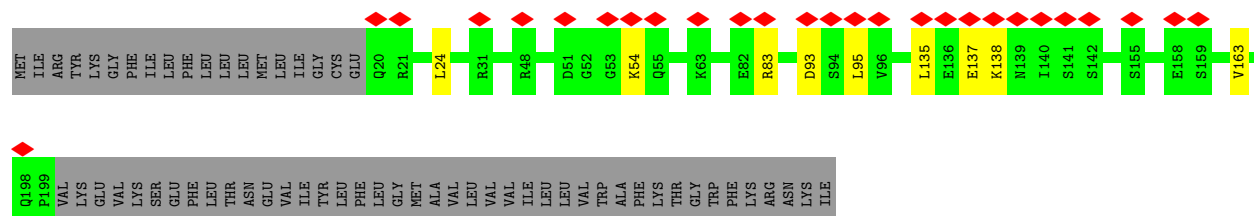


• Molecule 1: Protein MxiG

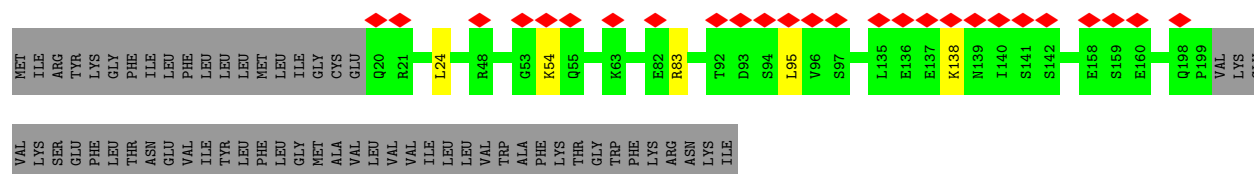
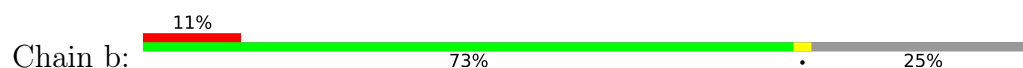




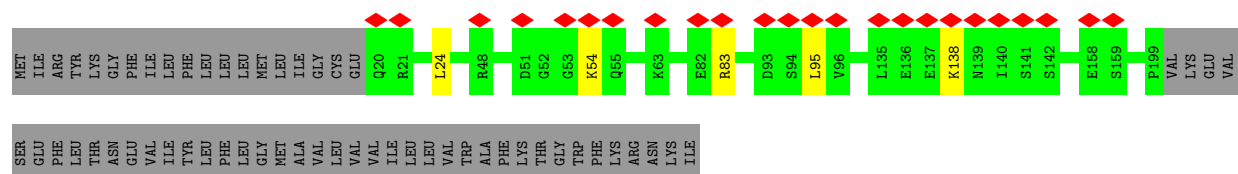
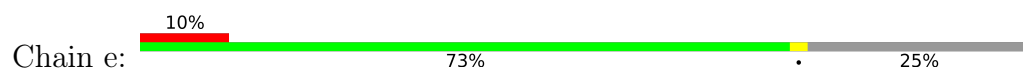
- Molecule 2: Lipoprotein MxiJ



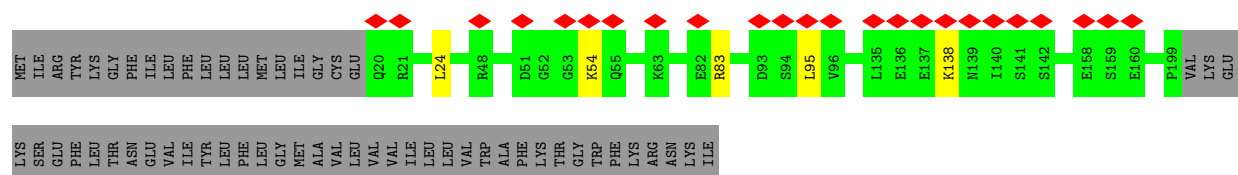
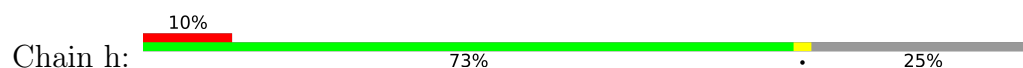
- Molecule 2: Lipoprotein MxiJ



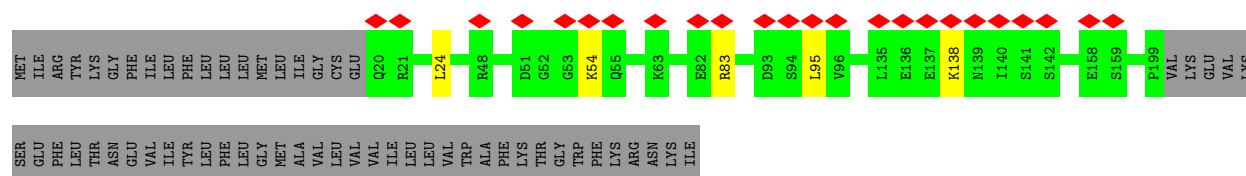
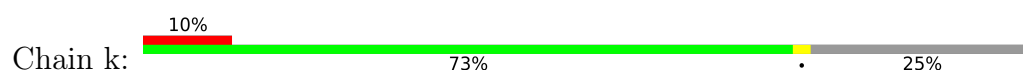
- Molecule 2: Lipoprotein MxiJ



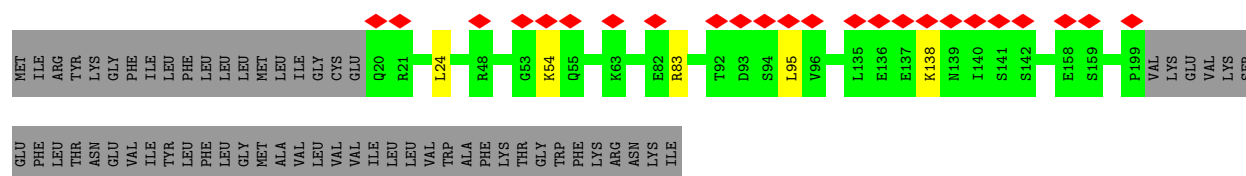
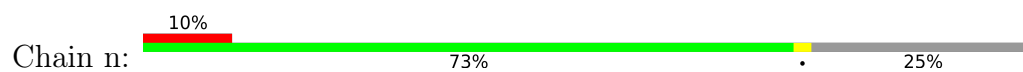
- Molecule 2: Lipoprotein MxiJ



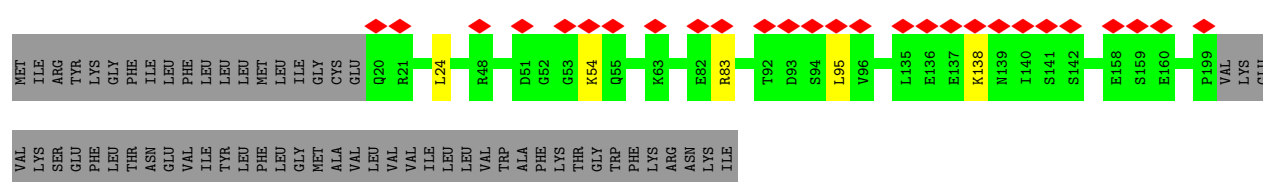
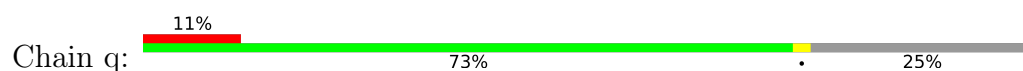
- Molecule 2: Lipoprotein MxiJ



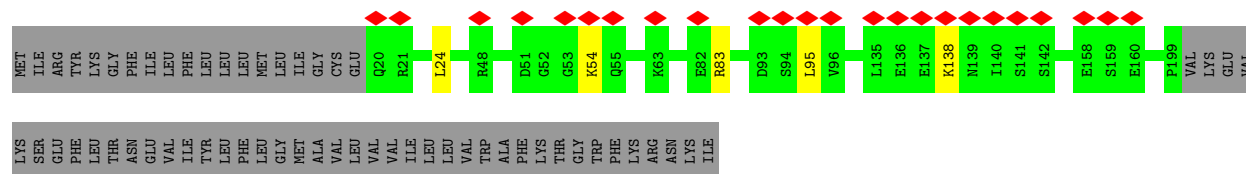
• Molecule 2: Lipoprotein MxiJ



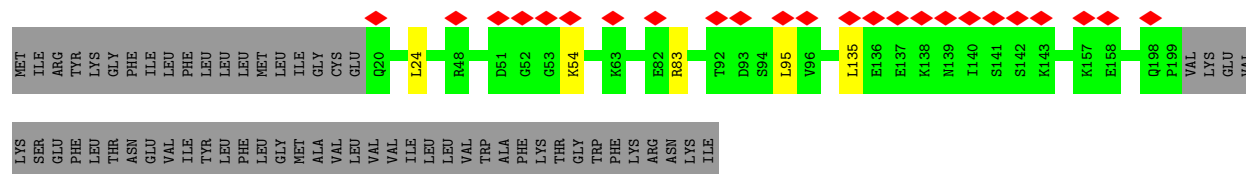
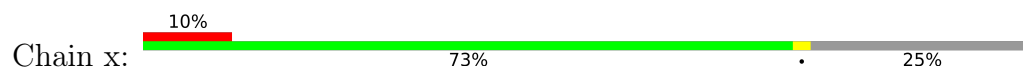
• Molecule 2: Lipoprotein MxiJ



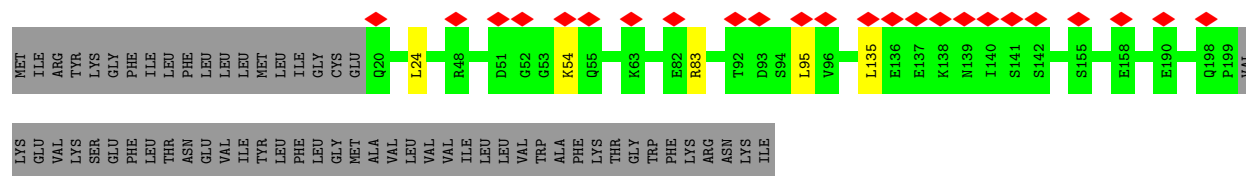
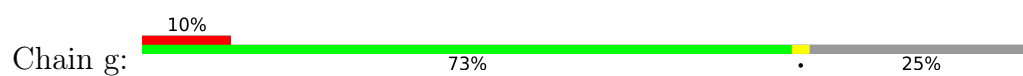
• Molecule 2: Lipoprotein MxiJ



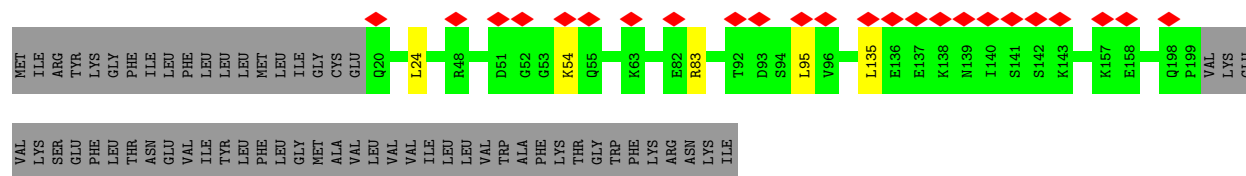
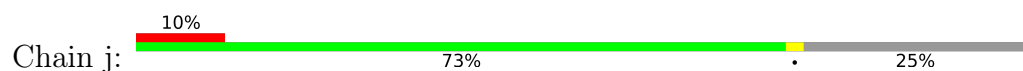
• Molecule 2: Lipoprotein MxiJ



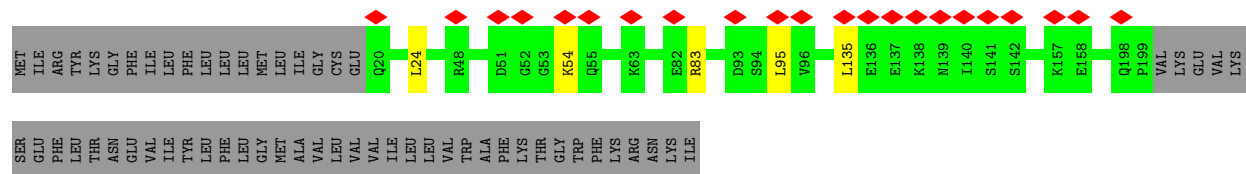
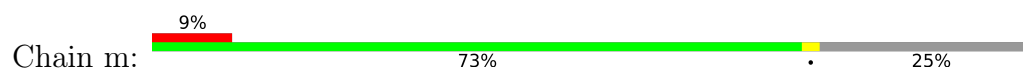
• Molecule 2: Lipoprotein MxiJ



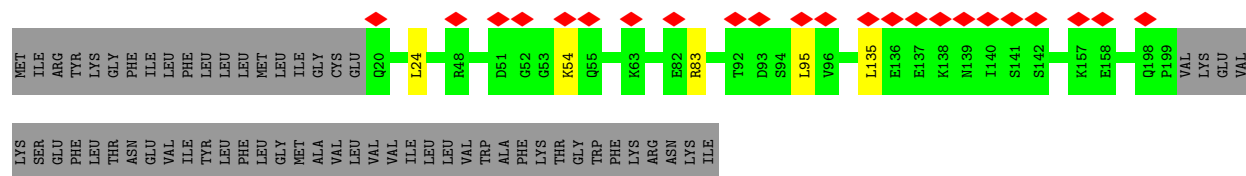
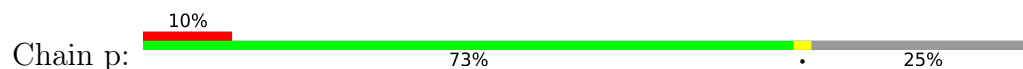
• Molecule 2: Lipoprotein MxiJ



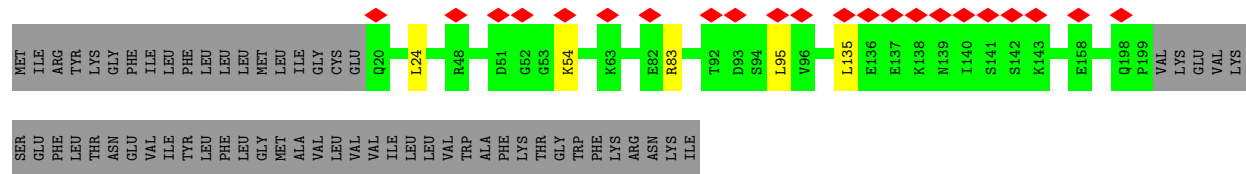
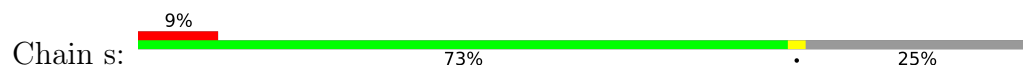
• Molecule 2: Lipoprotein MxiJ



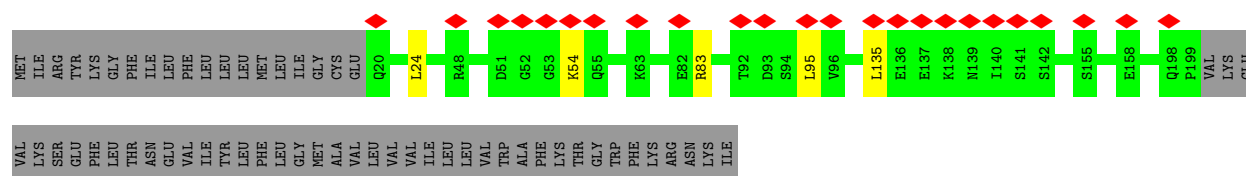
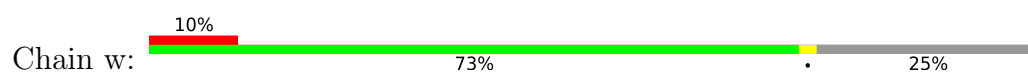
• Molecule 2: Lipoprotein MxiJ



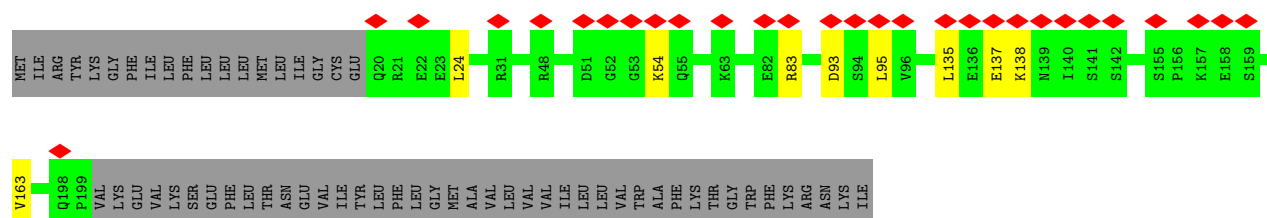
• Molecule 2: Lipoprotein MxiJ



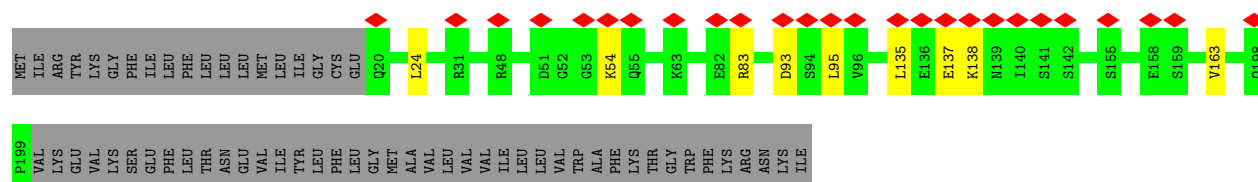
• Molecule 2: Lipoprotein MxiJ



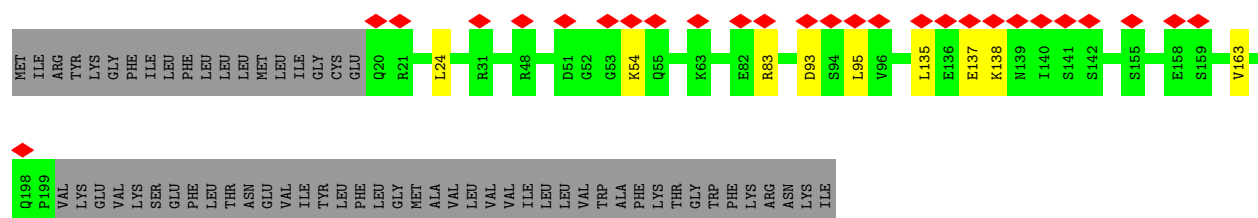
• Molecule 2: Lipoprotein MxiJ



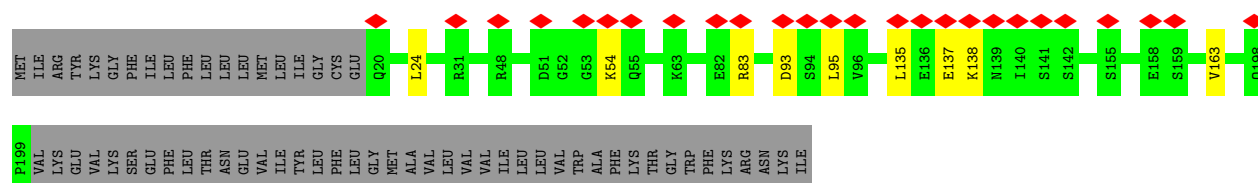
• Molecule 2: Lipoprotein MxiJ



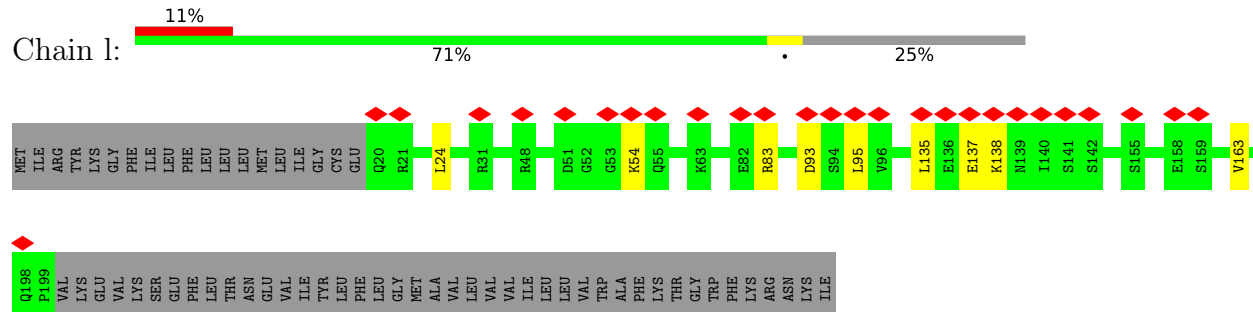
• Molecule 2: Lipoprotein MxiJ



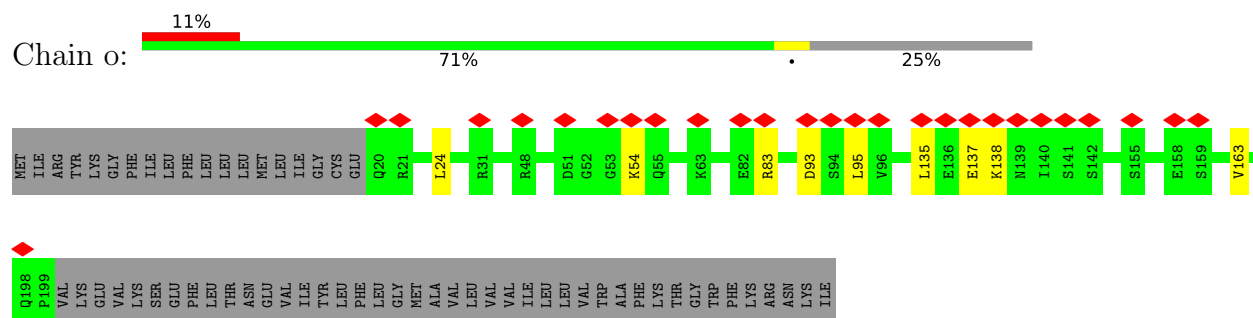
• Molecule 2: Lipoprotein MxiJ



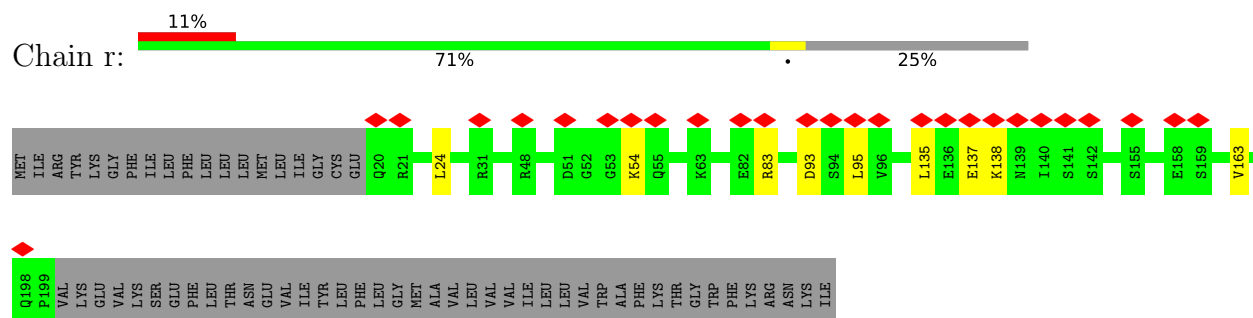
• Molecule 2: Lipoprotein MxiJ



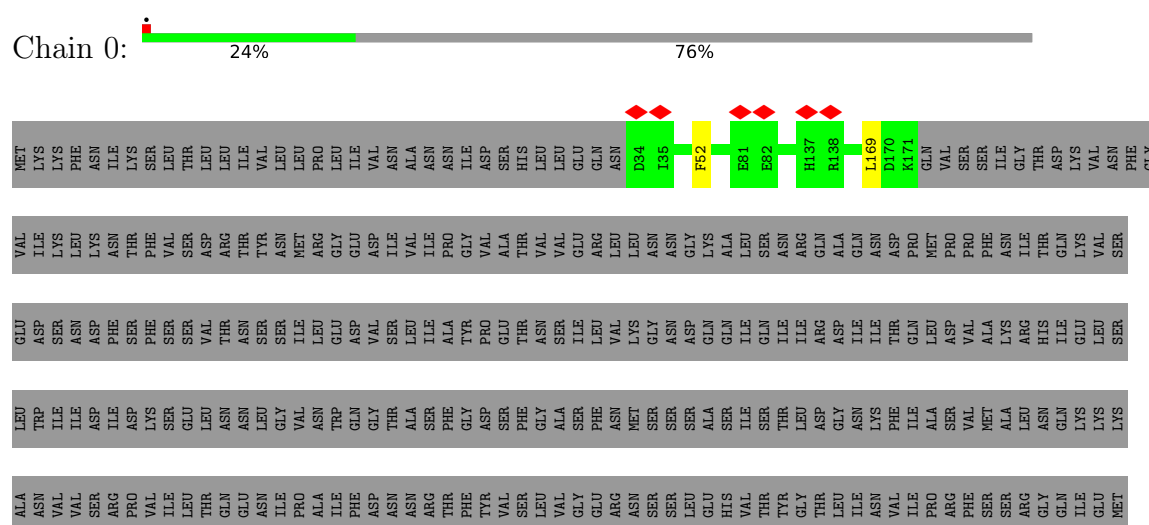
• Molecule 2: Lipoprotein MxiJ



• Molecule 2: Lipoprotein MxiJ



• Molecule 3: Outer membrane protein MxiD





[illegible]

- Molecule 3: Outer membrane protein MxiD



ILE	PRO	THR	VAL	ILE	SER	LYS	MET
PRO	PHE	ILE	VAL	ILE	ASN	LEU	LYS
GLU	LEU	GLU	SER	ASP	ASP	LYS	LYS
THR	SER	ASP	ARG	ILE	PHE	ASN	PHE
LEU	ILE	THR	VAL	LYS	PHE	THR	ASN
LEU	PRO	GLY	ILE	SER	SER	VAL	ILE
LEU	VAL	ASN	LEU	GLU	SER	SER	LYS
GLU	ILE	SER	THR	LEU	VAL	ASP	LEU
ASP	GLY	GLN	GLN	ASN	THR	ARG	THR
LYS	ASN	SER	GLU	ASN	ASN	THR	LEU
GLU	VAL	ASN	ASN	LEU	ASN	TYR	LEU
SER	PHE	TYR	ILE	GLY	SER	ASN	ILE
LEU	ASN	ASN	PRO	VAL	ILE	MET	VAL
VAL	TYR	THR	ALA	ASN	LEU	ARG	VAL
SER	LYS	ASN	ILE	TRP	GLU	GLY	LEU
TYR	THR	ASN	PHE	GLN	ASN	ASP	PRO
LEU	SER	GLU	GLY	GLY	VAL	ASP	LEU
ASN	ASN	ASN	ASN	THR	SER	ILE	ILE
ASN	ILE	THR	ASN	ALA	LEU	VAL	VAL
SER	ASN	SER	ARG	SER	ILE	ILE	ASN
ASN	ILE	VAL	THR	PHE	ALA	PRO	ALA
VAL	VAL	PRO	PHE	GLY	TYR	GLY	ASN
ARG	VAL	GLU	VAL	ASP	PRO	VAL	ASN
VAL	VAL	VAL	SER	PHE	GLU	ALA	ILE
PHE	PHE	GLY	LEU	SER	THR	ASP	ASP
LEU	LEU	ARG	VAL	GLY	ASN	VAL	SER
ILE	ILE	THR	GLY	ALA	VAL	VAL	HIS
GLU	GLN	LYS	GLY	SER	ILE	GLU	LEU
PRO	PRO	ILE	GLU	ASN	VAL	ARG	GLU
ARG	GLU	SER	ASN	MET	LYS	LEU	GLN
GLU	ARG	THR	SER	SER	GLY	ASN	ASN
ILE	ILE	ILE	SER	SER	ASN	ASN	ASN
LYS	GLU	ALA	LEU	SER	ASP	GLY	D84
SER	SER	ARG	GLU	ALA	GLN	LYS	I35
THR	SER	VAL	HIS	ILE	SER	ALA	F52
TYR	TYR	PRO	VAL	ILE	ILE	LEU	LYS
GLN	THR	GLN	THR	SER	GLN	SER	E81
ASN	ASN	LYS	GLY	THR	ILE	ASN	K97
THR	THR	LYS	GLY	LEU	ILE	ARG	K97
ALA	ALA	SER	THR	ASP	ARG	GLN	K171
GLU	GLU	LEU	LEU	GLY	ASP	ALA	H137
LEU	LEU	LEU	ILE	ASN	ILE	GLN	K171
TYR	TYR	GLY	VAL	PHE	THR	ASP	PRO
LEU	SER	GLY	ILE	ILE	GLN	PRO	MET
ILE	ILE	TYR	ARG	SER	LEU	MET	VAL
SER	SER	HIS	PHE	VAL	ASP	PRO	VAL
GLU	GLU	GLU	SER	VAL	VAL	PRO	SER
ARG	ARG	THR	SER	MET	ALA	PHE	ILE
GLU	GLU	ASN	ARG	ALA	LYS	ASN	GLY
ILE	ILE	SER	ASN	LEU	ARG	ILE	THR
GLN	GLN	ASN	GLY	ASN	HIS	THR	ASP
LYS	LYS	GLU	ILE	GLN	ILE	GLN	LYS
THR	THR	ILE	ILE	LYS	GLU	VAL	VAL
THR	THR	ILE	MET	LYS	LEU	VAL	ASN
GLN	GLN	SER	SER	ALA	LEU	SER	PHE
ILE	ILE	ILE	LEU	THR	ALA	GLU	GLY
				ASN	TRP	ASP	VAL

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	0.26	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 ⓘ

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

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	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

All (312) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	153	ILE
1	C	194	THR
1	C	223	TYR
1	C	343	ASP
1	C	344	PHE
1	B	194	THR
1	B	223	TYR
1	B	359	LEU
1	B	367	LEU
1	A	194	THR

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Mol	Chain	Res	Type
1	A	223	TYR
1	A	341	ASP
1	A	342	ASP
1	A	359	LEU
1	A	367	LEU
2	a	24	LEU
2	a	54	LYS
2	a	83	ARG
2	a	95	LEU
2	a	138	LYS
3	0	52	PHE
3	0	169	LEU
3	1	35	ILE
3	1	52	PHE
3	1	97	LYS
2	d	24	LEU
2	d	54	LYS
2	d	83	ARG
2	d	95	LEU
2	d	135	LEU
2	c	24	LEU
2	c	54	LYS
2	c	83	ARG
2	c	93	ASP
2	c	95	LEU
2	c	135	LEU
2	c	137	GLU
2	c	138	LYS
2	c	163	VAL
1	S	194	THR
1	S	223	TYR
1	S	341	ASP
1	S	342	ASP
1	S	359	LEU
1	S	367	LEU
1	P	194	THR
1	P	223	TYR
1	P	341	ASP
1	P	342	ASP
1	P	359	LEU
1	P	367	LEU
1	M	194	THR

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Mol	Chain	Res	Type
1	M	223	TYR
1	M	341	ASP
1	M	342	ASP
1	M	359	LEU
1	M	367	LEU
1	J	194	THR
1	J	223	TYR
1	J	341	ASP
1	J	342	ASP
1	J	359	LEU
1	J	367	LEU
1	G	194	THR
1	G	223	TYR
1	G	341	ASP
1	G	342	ASP
1	G	359	LEU
1	G	367	LEU
1	D	194	THR
1	D	223	TYR
1	D	341	ASP
1	D	342	ASP
1	D	359	LEU
1	D	367	LEU
1	U	194	THR
1	U	223	TYR
1	U	341	ASP
1	U	342	ASP
1	U	359	LEU
1	U	367	LEU
1	T	194	THR
1	T	223	TYR
1	T	359	LEU
1	T	367	LEU
1	Q	194	THR
1	Q	223	TYR
1	Q	359	LEU
1	Q	367	LEU
1	N	194	THR
1	N	223	TYR
1	N	359	LEU
1	N	367	LEU
1	K	194	THR

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Mol	Chain	Res	Type
1	K	223	TYR
1	K	359	LEU
1	K	367	LEU
1	H	194	THR
1	H	223	TYR
1	H	359	LEU
1	H	367	LEU
1	E	194	THR
1	E	223	TYR
1	E	359	LEU
1	E	367	LEU
1	V	194	THR
1	V	223	TYR
1	V	359	LEU
1	V	367	LEU
1	R	153	ILE
1	R	194	THR
1	R	223	TYR
1	R	343	ASP
1	R	344	PHE
1	O	153	ILE
1	O	194	THR
1	O	223	TYR
1	O	343	ASP
1	O	344	PHE
1	L	153	ILE
1	L	194	THR
1	L	223	TYR
1	L	343	ASP
1	L	344	PHE
1	I	153	ILE
1	I	194	THR
1	I	223	TYR
1	I	343	ASP
1	I	344	PHE
1	F	153	ILE
1	F	194	THR
1	F	223	TYR
1	F	343	ASP
1	F	344	PHE
1	W	153	ILE
1	W	194	THR

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Mol	Chain	Res	Type
1	W	223	TYR
1	W	343	ASP
1	W	344	PHE
1	X	153	ILE
1	X	194	THR
1	X	223	TYR
1	X	343	ASP
1	X	344	PHE
2	b	24	LEU
2	b	54	LYS
2	b	83	ARG
2	b	95	LEU
2	b	138	LYS
2	e	24	LEU
2	e	54	LYS
2	e	83	ARG
2	e	95	LEU
2	e	138	LYS
2	h	24	LEU
2	h	54	LYS
2	h	83	ARG
2	h	95	LEU
2	h	138	LYS
2	k	24	LEU
2	k	54	LYS
2	k	83	ARG
2	k	95	LEU
2	k	138	LYS
2	n	24	LEU
2	n	54	LYS
2	n	83	ARG
2	n	95	LEU
2	n	138	LYS
2	q	24	LEU
2	q	54	LYS
2	q	83	ARG
2	q	95	LEU
2	q	138	LYS
2	t	24	LEU
2	t	54	LYS
2	t	83	ARG
2	t	95	LEU

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Mol	Chain	Res	Type
2	t	138	LYS
2	x	24	LEU
2	x	54	LYS
2	x	83	ARG
2	x	95	LEU
2	x	135	LEU
2	g	24	LEU
2	g	54	LYS
2	g	83	ARG
2	g	95	LEU
2	g	135	LEU
2	j	24	LEU
2	j	54	LYS
2	j	83	ARG
2	j	95	LEU
2	j	135	LEU
2	m	24	LEU
2	m	54	LYS
2	m	83	ARG
2	m	95	LEU
2	m	135	LEU
2	p	24	LEU
2	p	54	LYS
2	p	83	ARG
2	p	95	LEU
2	p	135	LEU
2	s	24	LEU
2	s	54	LYS
2	s	83	ARG
2	s	95	LEU
2	s	135	LEU
2	w	24	LEU
2	w	54	LYS
2	w	83	ARG
2	w	95	LEU
2	w	135	LEU
2	v	24	LEU
2	v	54	LYS
2	v	83	ARG
2	v	93	ASP
2	v	95	LEU
2	v	135	LEU

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Mol	Chain	Res	Type
2	v	137	GLU
2	v	138	LYS
2	v	163	VAL
2	u	24	LEU
2	u	54	LYS
2	u	83	ARG
2	u	93	ASP
2	u	95	LEU
2	u	135	LEU
2	u	137	GLU
2	u	138	LYS
2	u	163	VAL
2	f	24	LEU
2	f	54	LYS
2	f	83	ARG
2	f	93	ASP
2	f	95	LEU
2	f	135	LEU
2	f	137	GLU
2	f	138	LYS
2	f	163	VAL
2	i	24	LEU
2	i	54	LYS
2	i	83	ARG
2	i	93	ASP
2	i	95	LEU
2	i	135	LEU
2	i	137	GLU
2	i	138	LYS
2	i	163	VAL
2	l	24	LEU
2	l	54	LYS
2	l	83	ARG
2	l	93	ASP
2	l	95	LEU
2	l	135	LEU
2	l	137	GLU
2	l	138	LYS
2	l	163	VAL
2	o	24	LEU
2	o	54	LYS
2	o	83	ARG

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Mol	Chain	Res	Type
2	o	93	ASP
2	o	95	LEU
2	o	135	LEU
2	o	137	GLU
2	o	138	LYS
2	o	163	VAL
2	r	24	LEU
2	r	54	LYS
2	r	83	ARG
2	r	93	ASP
2	r	95	LEU
2	r	135	LEU
2	r	137	GLU
2	r	138	LYS
2	r	163	VAL
3	a0	52	PHE
3	a0	169	LEU
3	Y	52	PHE
3	Y	169	LEU
3	Z	52	PHE
3	Z	169	LEU
3	2	52	PHE
3	2	169	LEU
3	4	52	PHE
3	4	169	LEU
3	6	52	PHE
3	6	169	LEU
3	8	52	PHE
3	8	169	LEU
3	b0	35	ILE
3	b0	52	PHE
3	b0	97	LYS
3	y	35	ILE
3	y	52	PHE
3	y	97	LYS
3	z	35	ILE
3	z	52	PHE
3	z	97	LYS
3	3	35	ILE
3	3	52	PHE
3	3	97	LYS
3	5	35	ILE

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Mol	Chain	Res	Type
3	5	52	PHE
3	5	97	LYS
3	7	35	ILE
3	7	52	PHE
3	7	97	LYS
3	9	35	ILE
3	9	52	PHE
3	9	97	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	171	ASN
2	c	130	HIS
1	S	171	ASN
1	P	171	ASN
1	M	171	ASN
1	J	171	ASN
1	J	298	ASN
1	G	171	ASN
1	G	298	ASN
1	D	171	ASN
1	U	171	ASN
1	I	298	ASN
1	F	298	ASN
2	t	130	HIS
2	g	130	HIS

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

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.

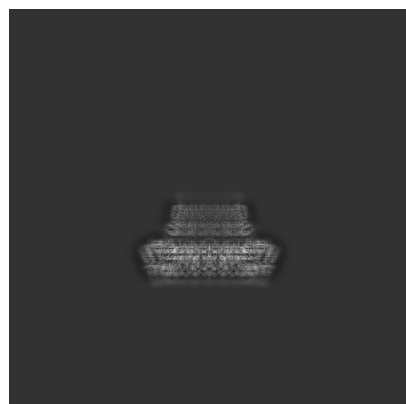
6 Map visualisation [i](#)

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.

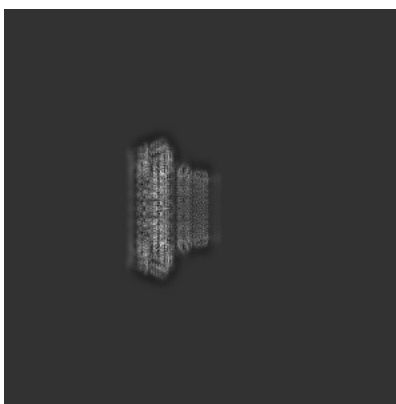
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

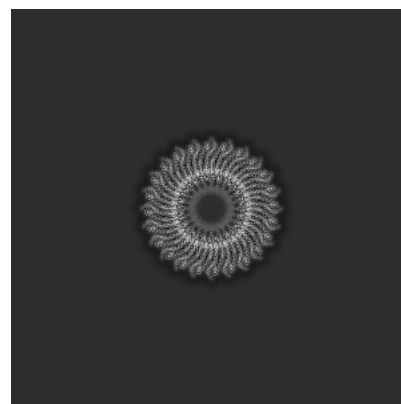
6.1.1 Primary map



X



Y

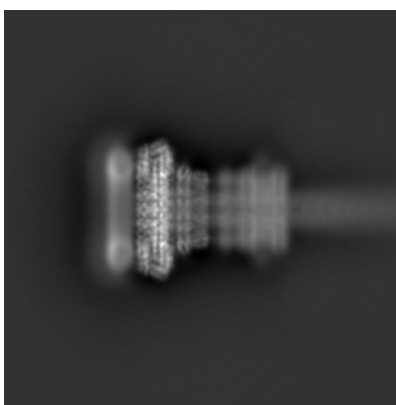


Z

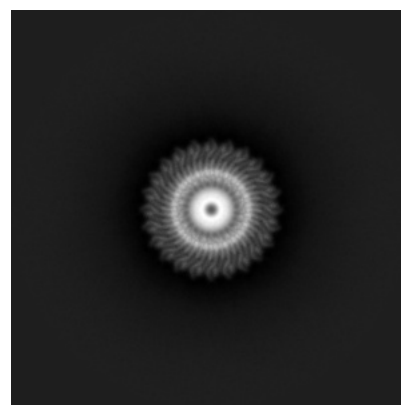
6.1.2 Raw map



X



Y

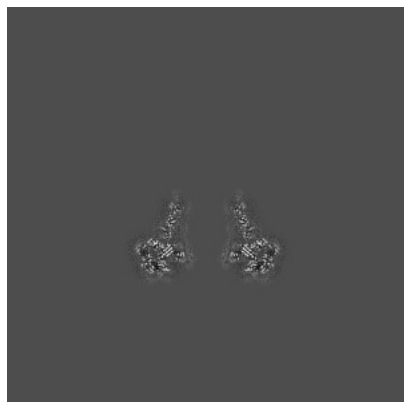


Z

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

6.2 Central slices [i](#)

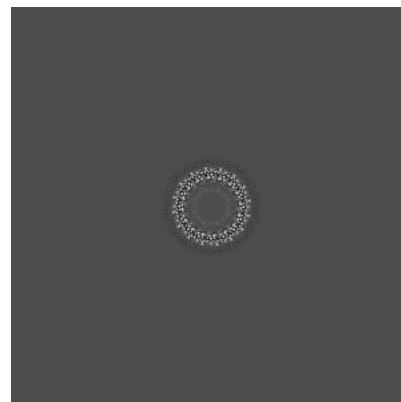
6.2.1 Primary map



X Index: 240

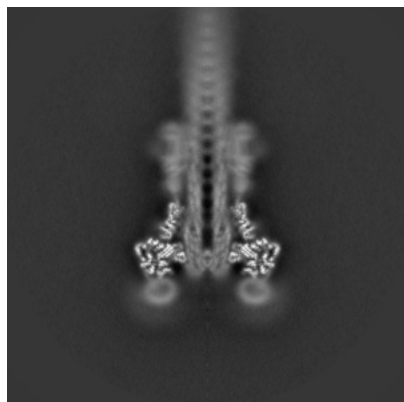


Y Index: 240

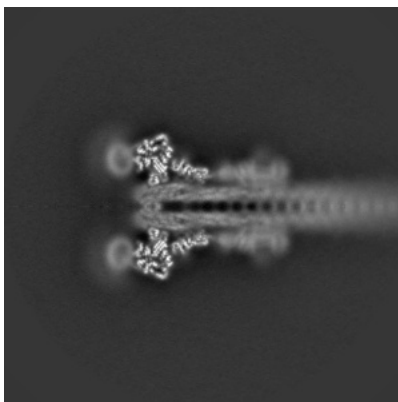


Z Index: 240

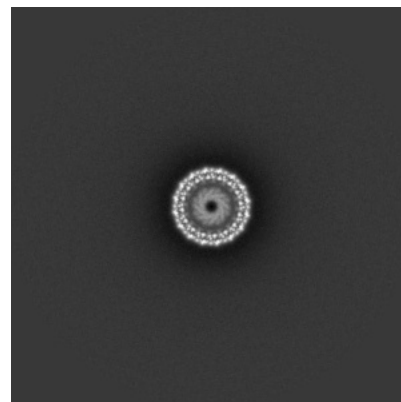
6.2.2 Raw map



X Index: 240



Y Index: 240

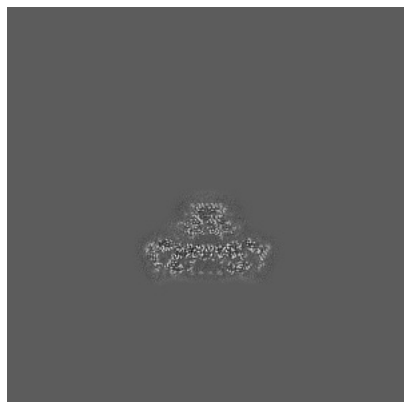


Z Index: 240

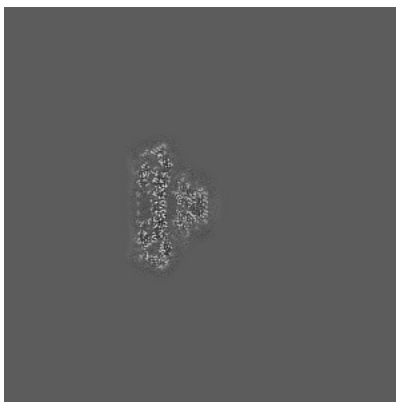
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

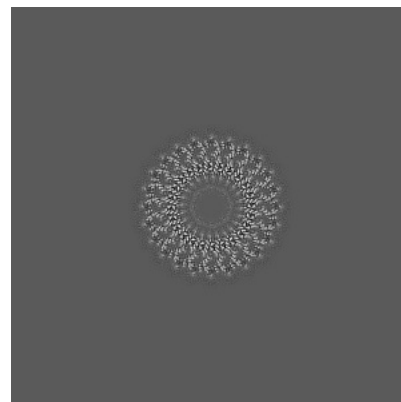
6.3.1 Primary map



X Index: 281

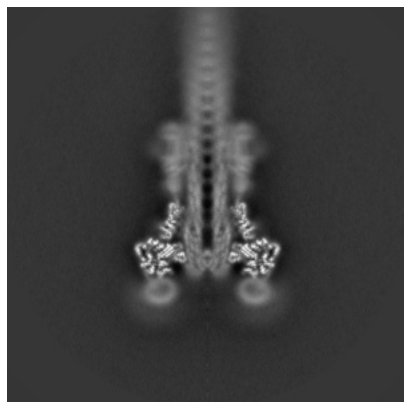


Y Index: 199

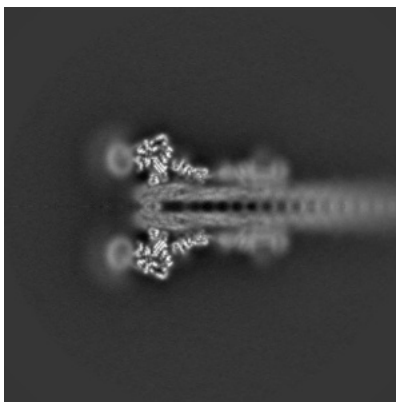


Z Index: 188

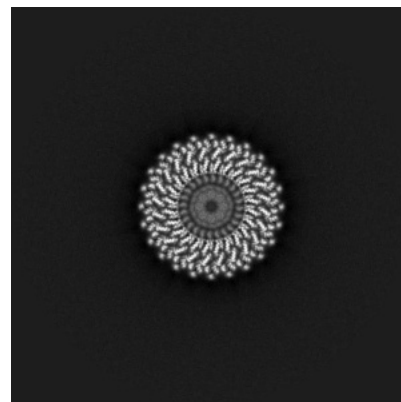
6.3.2 Raw map



X Index: 240



Y Index: 240

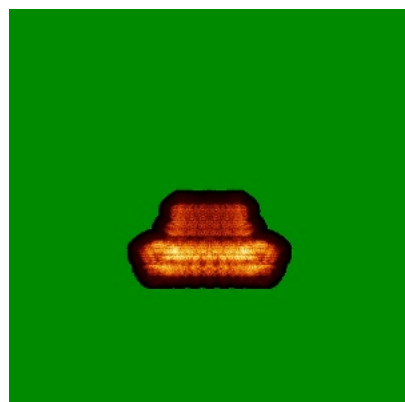


Z Index: 189

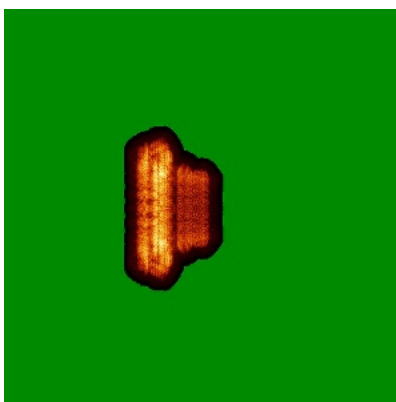
The images above show the largest variance slices of the map in three orthogonal directions.

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

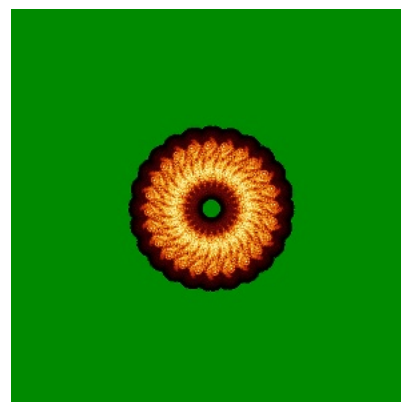
6.4.1 Primary map



X

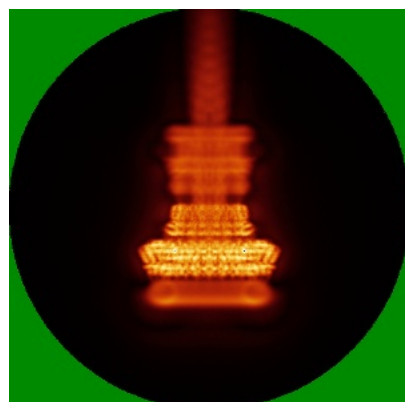


Y

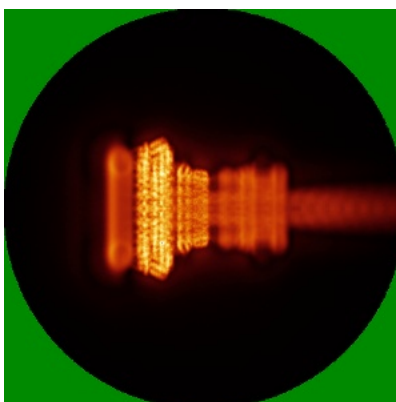


Z

6.4.2 Raw map



X



Y

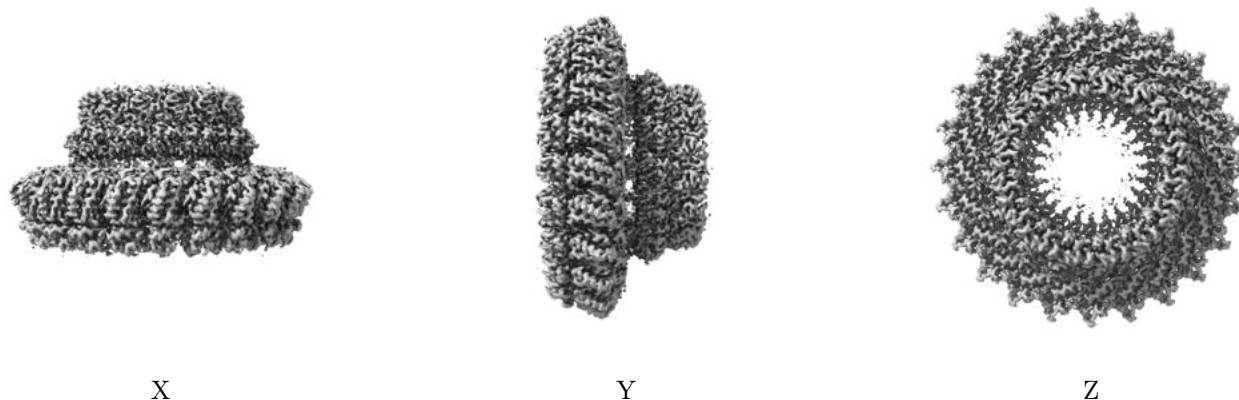


Z

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.

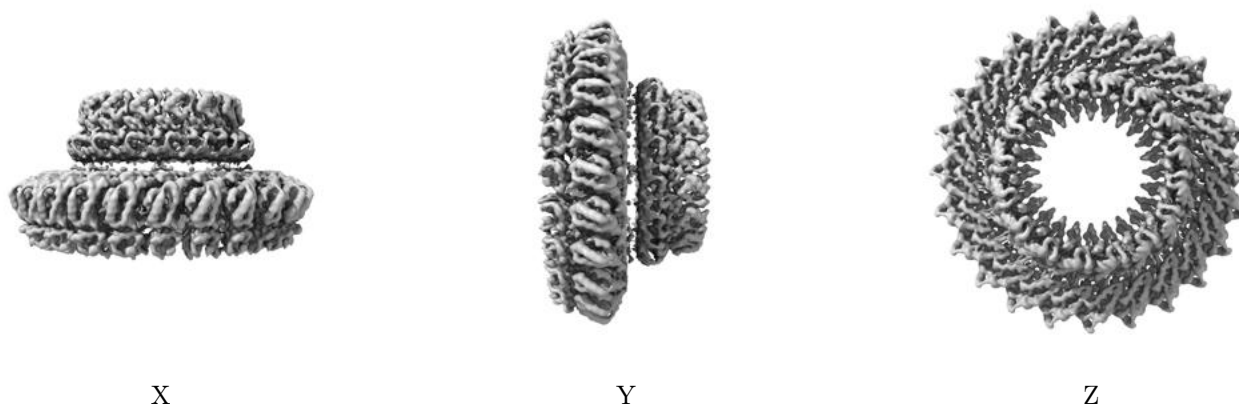
6.5 Orthogonal surface views [i](#)

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.

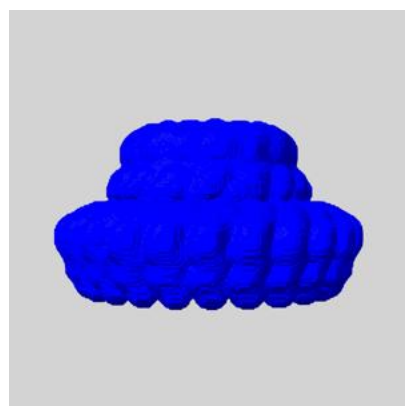
6.6 Mask visualisation [i](#)

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

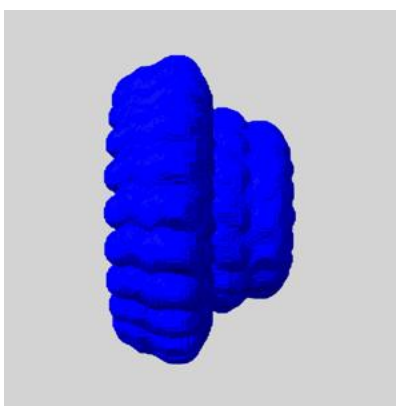
A mask typically either:

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

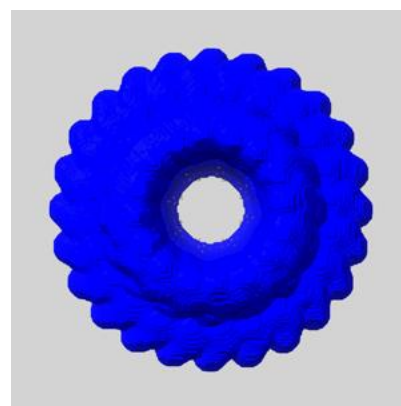
6.6.1 emd_15702_msk_1.map [i](#)



X



Y

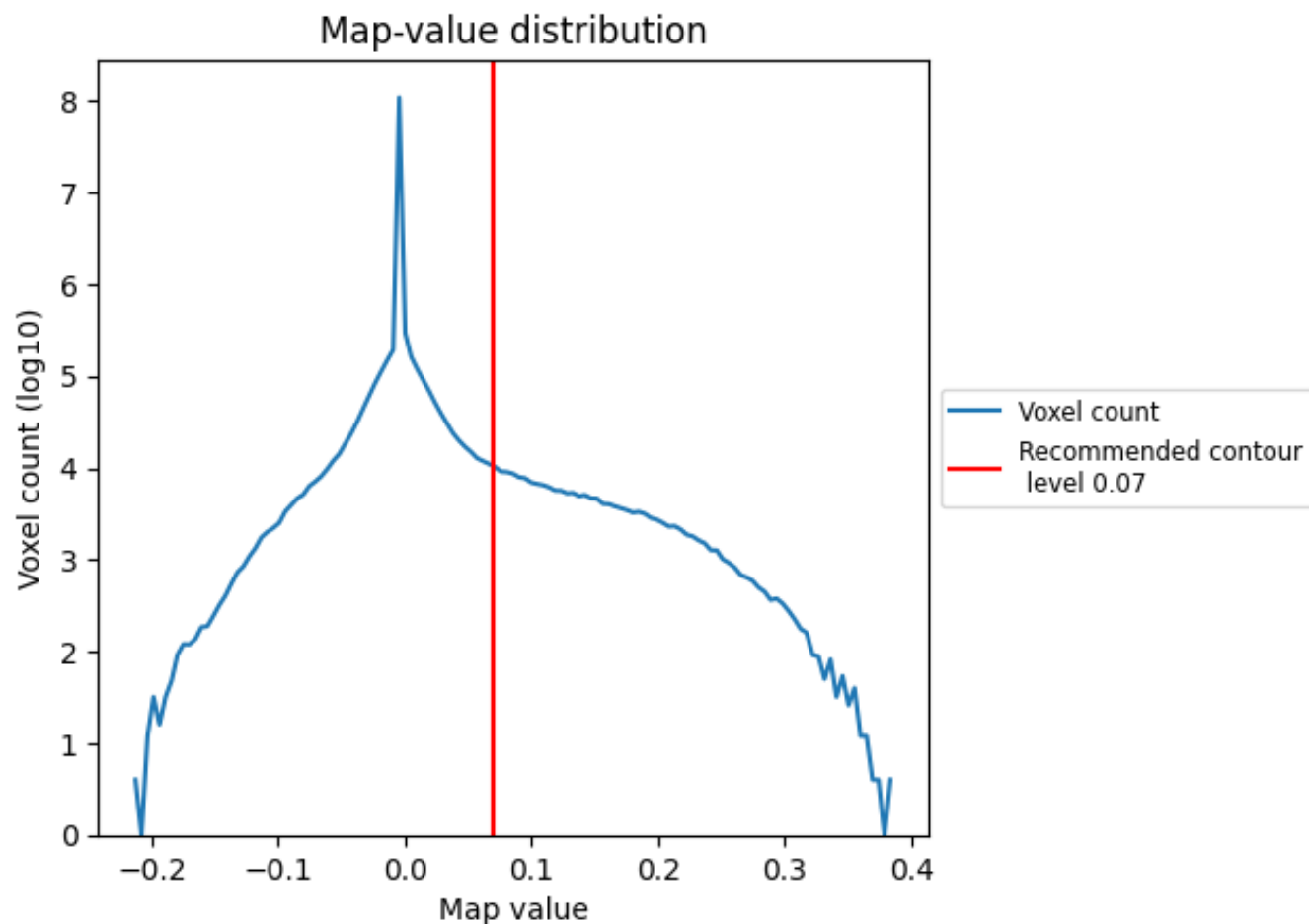


Z

7 Map analysis [i](#)

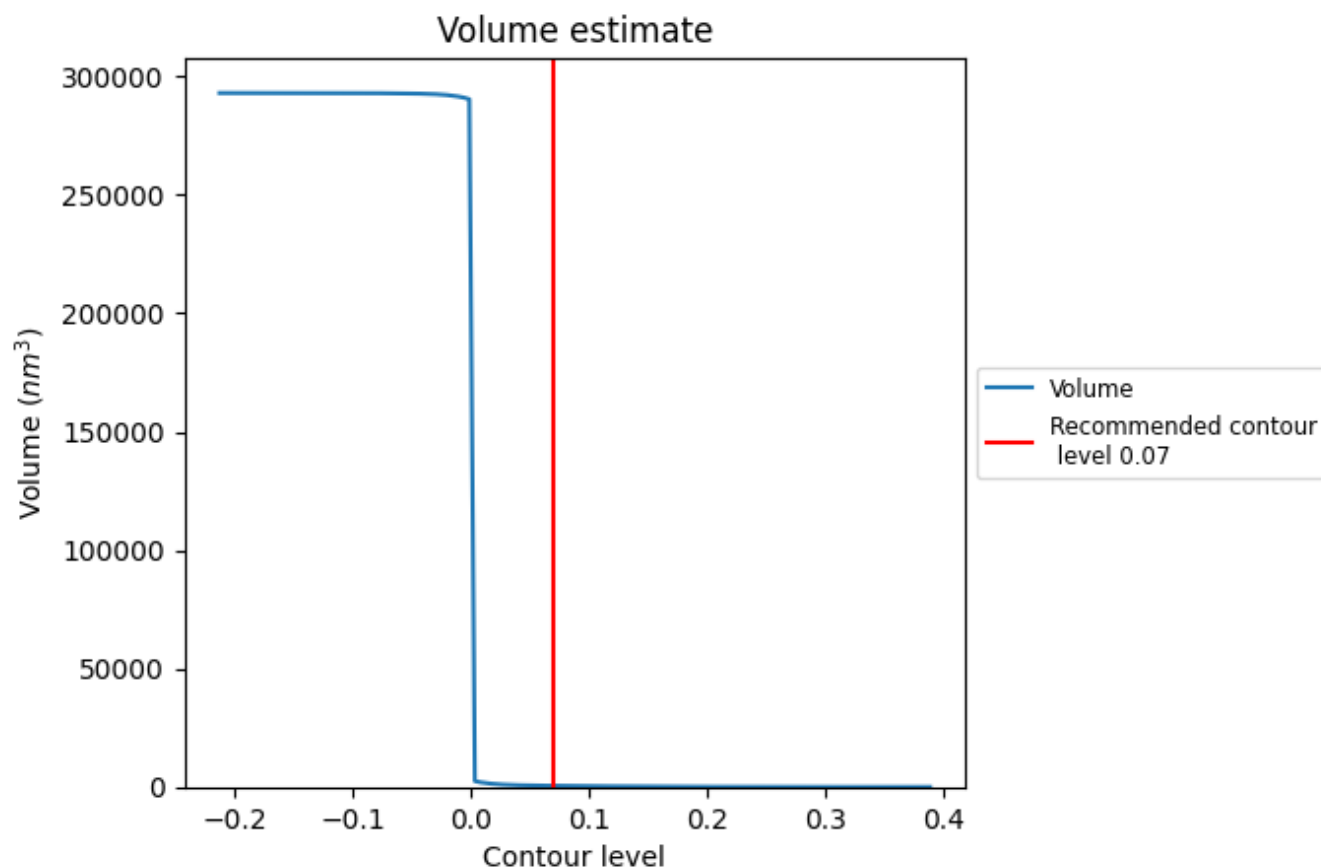
This section contains the results of statistical analysis of the map.

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.

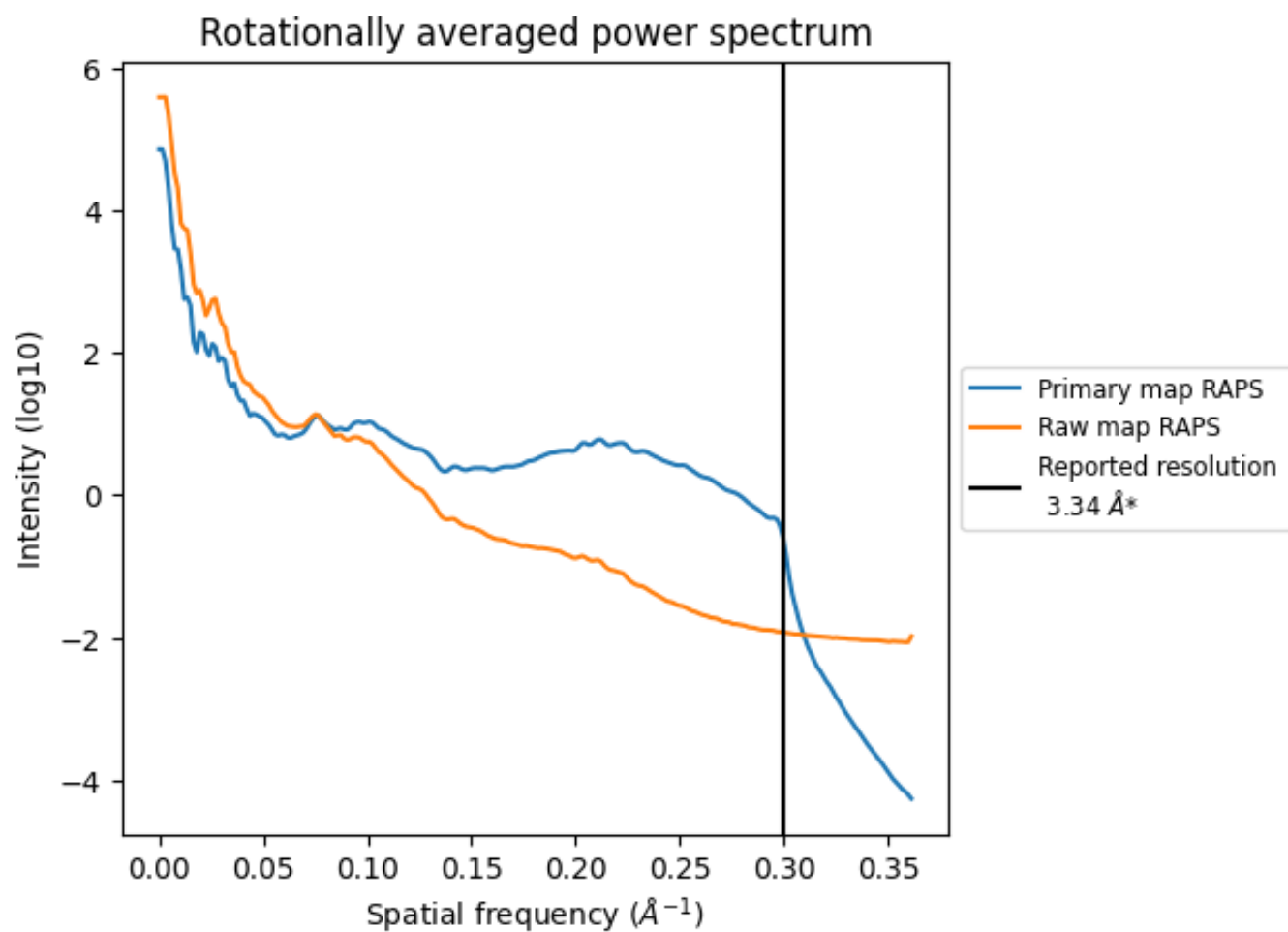
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 488 nm³; 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 ⓘ

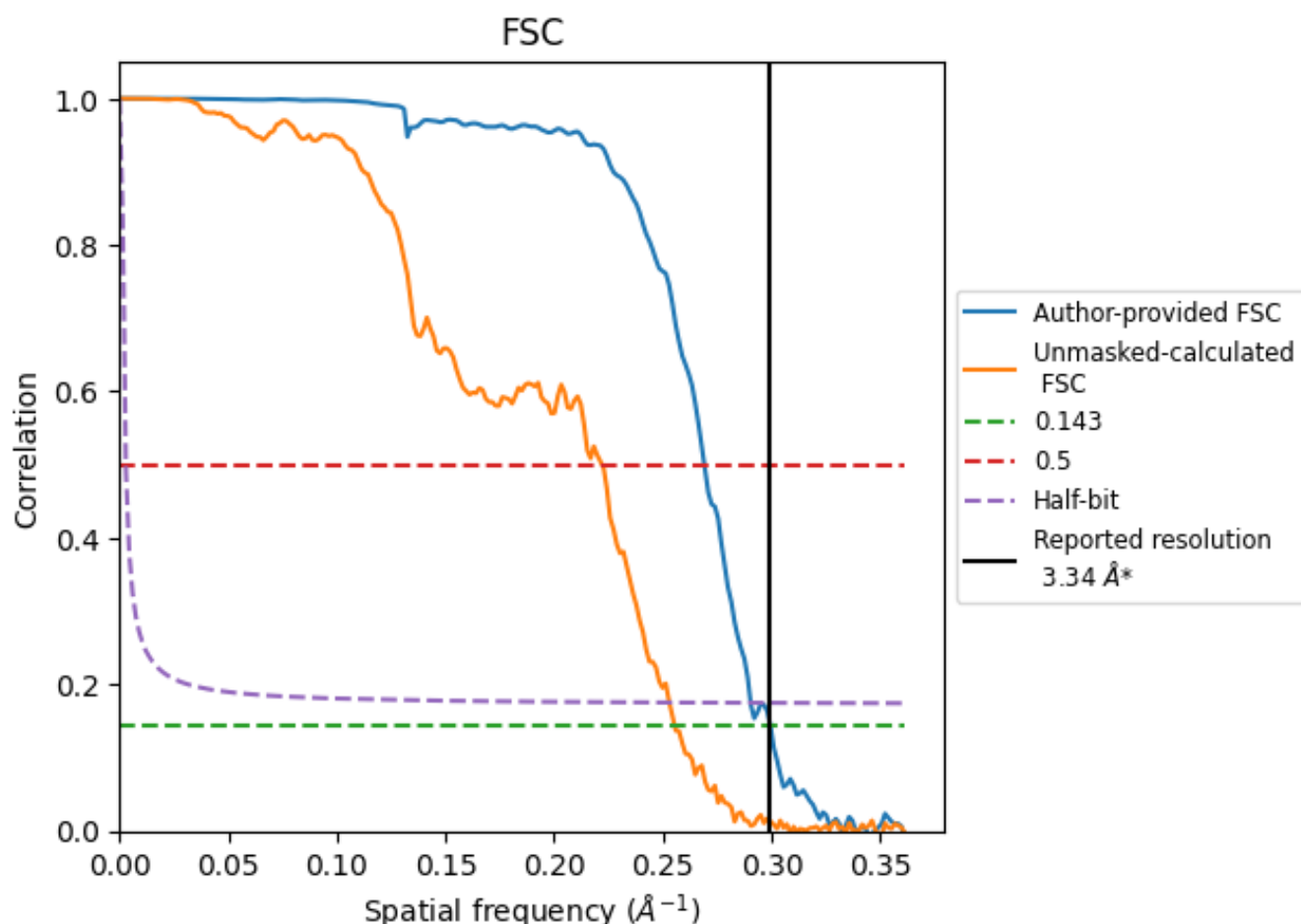


*Reported resolution corresponds to spatial frequency of 0.299 Å⁻¹

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 Å⁻¹

8.2 Resolution estimates [i](#)

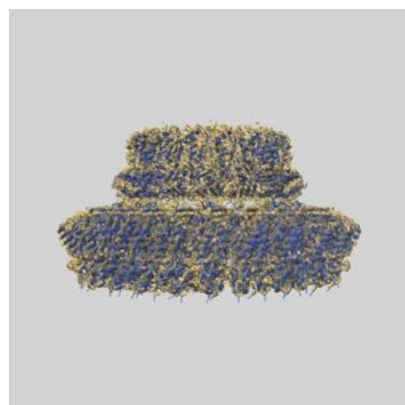
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.34	-	-
Author-provided FSC curve	3.34	3.71	3.44
Unmasked-calculated*	3.91	4.50	3.95

*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 %

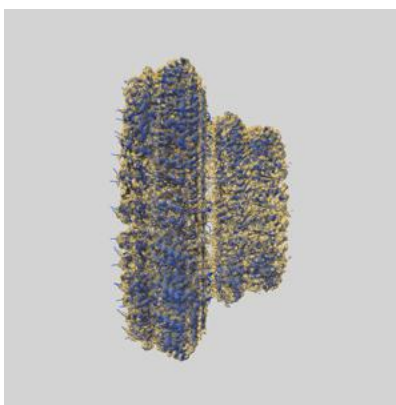
9 Map-model fit [i](#)

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](#).

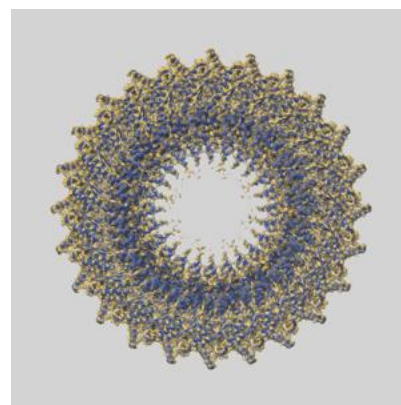
9.1 Map-model overlay [i](#)



X



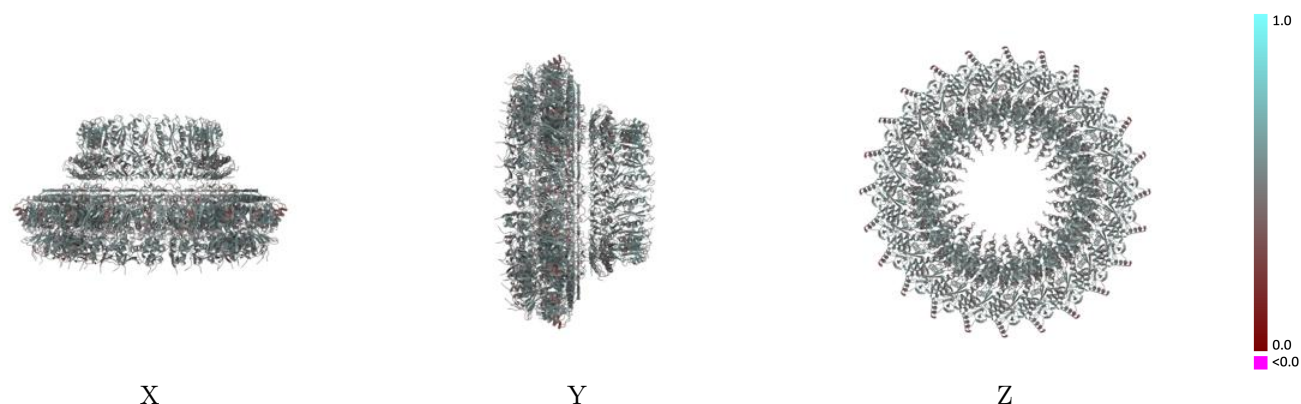
Y



Z

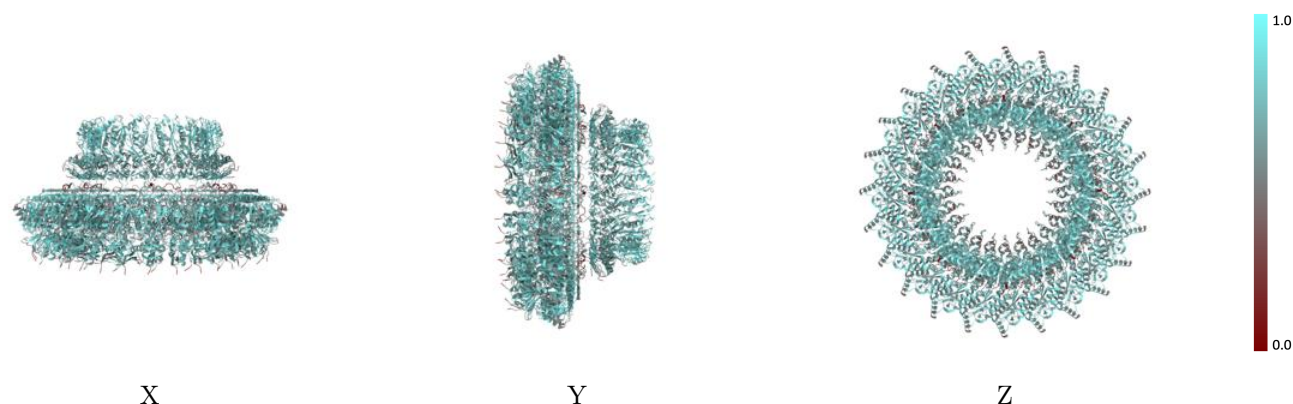
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



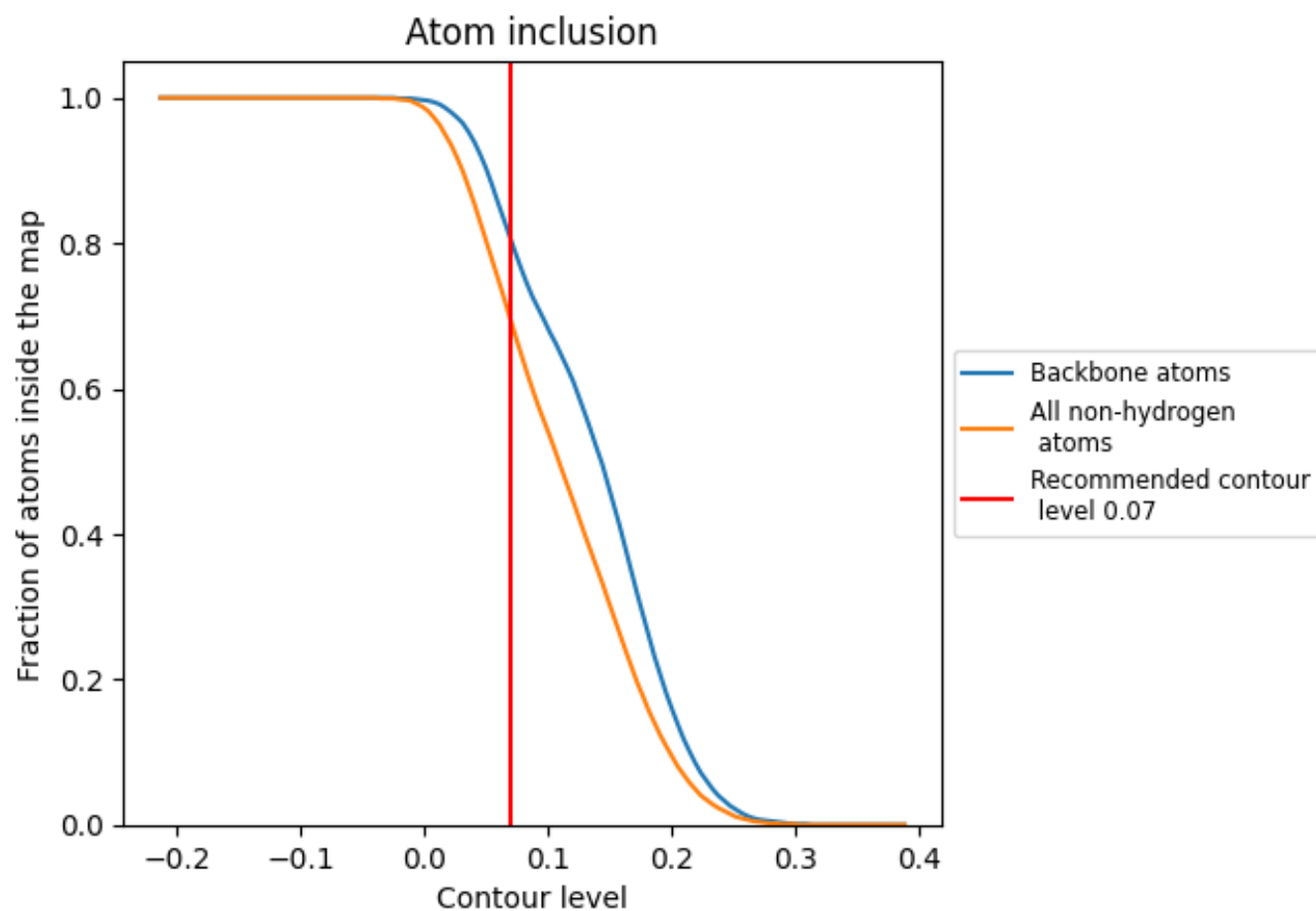
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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