



## wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 04:13 pm GMT

PDB ID : 5NIL  
EMDB ID : EMD-3653  
Title : Structure of the MacAB-TolC ABC-type tripartite multidrug efflux pump-MacB section  
Authors : Fitzpatrick, A.W.P.; Llabres, S.; Neuberger, A.; Blaza, J.N.; Bai, X.-C.; Okada, U.; Murakami, S.; van Veen, H.W.; Zachariae, U.; Scheres, S.H.W.; Luisi, B.F.; Du, D.  
Deposited on : 2017-03-24  
Resolution : 5.30 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

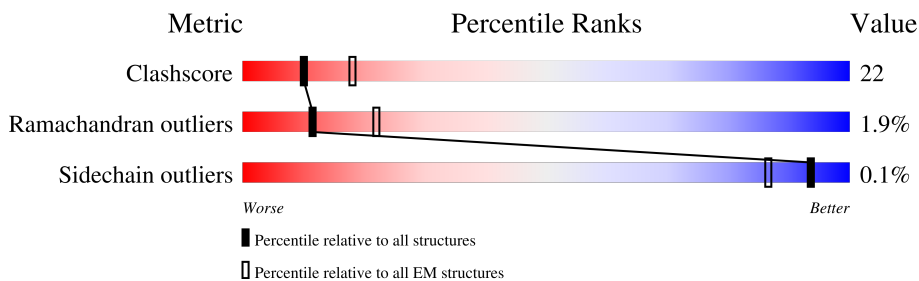
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 5.30 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	479	<p>89% 52% 36% 11%</p>
1	B	479	<p>89% 58% 31% 11%</p>
1	C	479	<p>89% 51% 37% 11%</p>
2	D	371	<p>70% 66% 24% 8%</p>
2	E	371	<p>57% 69% 23% 8%</p>
2	F	371	<p>59% 63% 27% 8%</p>
2	G	371	<p>69% 65% 26% 8%</p>
2	H	371	<p>58% 66% 25% 8%</p>

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Mol	Chain	Length	Quality of chain
2	I	371	60% 63% 27% 8%
3	J	654	19% 47% 48% 2%
3	K	654	18% 48% 47% 2%

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 35215 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 Outer membrane protein TolC.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	428	3305	2038	586	676	5	0	0
1	B	428	3305	2038	586	676	5	0	0
1	C	428	3305	2038	586	676	5	0	0

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	169	LEU	VAL	conflict	UNP P02930
A	472	ASP	-	expression tag	UNP P02930
A	473	TYR	-	expression tag	UNP P02930
A	474	LYS	-	expression tag	UNP P02930
A	475	ASP	-	expression tag	UNP P02930
A	476	ASP	-	expression tag	UNP P02930
A	477	ASP	-	expression tag	UNP P02930
A	478	ASP	-	expression tag	UNP P02930
A	479	LYS	-	expression tag	UNP P02930
B	169	LEU	VAL	conflict	UNP P02930
B	472	ASP	-	expression tag	UNP P02930
B	473	TYR	-	expression tag	UNP P02930
B	474	LYS	-	expression tag	UNP P02930
B	475	ASP	-	expression tag	UNP P02930
B	476	ASP	-	expression tag	UNP P02930
B	477	ASP	-	expression tag	UNP P02930
B	478	ASP	-	expression tag	UNP P02930
B	479	LYS	-	expression tag	UNP P02930
C	169	LEU	VAL	conflict	UNP P02930
C	472	ASP	-	expression tag	UNP P02930
C	473	TYR	-	expression tag	UNP P02930
C	474	LYS	-	expression tag	UNP P02930
C	475	ASP	-	expression tag	UNP P02930
C	476	ASP	-	expression tag	UNP P02930

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Chain	Residue	Modelled	Actual	Comment	Reference
C	477	ASP	-	expression tag	UNP P02930
C	478	ASP	-	expression tag	UNP P02930
C	479	LYS	-	expression tag	UNP P02930

- Molecule 2 is a protein called Macrolide export protein MacA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	340	Total	C	N	O	S	0	0
			2604	1622	462	514	6		
2	E	340	Total	C	N	O	S	0	0
			2604	1622	462	514	6		
2	F	340	Total	C	N	O	S	0	0
			2604	1622	462	514	6		
2	G	340	Total	C	N	O	S	0	0
			2604	1622	462	514	6		
2	H	340	Total	C	N	O	S	0	0
			2604	1622	462	514	6		
2	I	340	Total	C	N	O	S	0	0
			2604	1622	462	514	6		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	139	GLN	LYS	conflict	UNP P75830
D	148	ASN	THR	conflict	UNP P75830
D	251	GLN	PRO	conflict	UNP P75830
E	139	GLN	LYS	conflict	UNP P75830
E	148	ASN	THR	conflict	UNP P75830
E	251	GLN	PRO	conflict	UNP P75830
F	139	GLN	LYS	conflict	UNP P75830
F	148	ASN	THR	conflict	UNP P75830
F	251	GLN	PRO	conflict	UNP P75830
G	139	GLN	LYS	conflict	UNP P75830
G	148	ASN	THR	conflict	UNP P75830
G	251	GLN	PRO	conflict	UNP P75830
H	139	GLN	LYS	conflict	UNP P75830
H	148	ASN	THR	conflict	UNP P75830
H	251	GLN	PRO	conflict	UNP P75830
I	139	GLN	LYS	conflict	UNP P75830
I	148	ASN	THR	conflict	UNP P75830
I	251	GLN	PRO	conflict	UNP P75830

- Molecule 3 is a protein called Macrolide export ATP-binding/permease protein MacB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	J	629	4838	3066	853	898	21	0	0
3	K	629	4838	3066	853	898	21	0	0

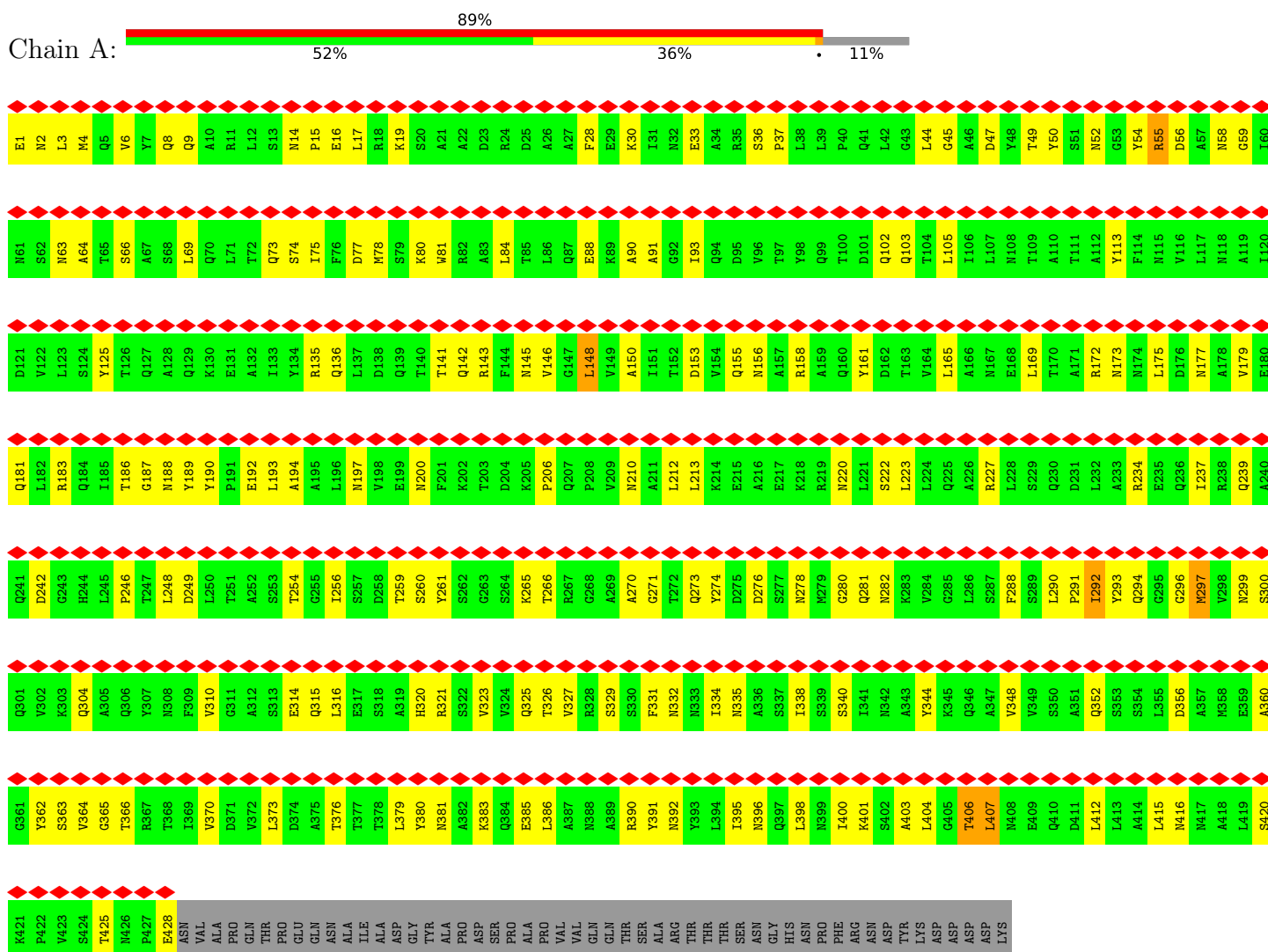
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	649	HIS	-	expression tag	UNP P75831
J	650	HIS	-	expression tag	UNP P75831
J	651	HIS	-	expression tag	UNP P75831
J	652	HIS	-	expression tag	UNP P75831
J	653	HIS	-	expression tag	UNP P75831
J	654	HIS	-	expression tag	UNP P75831
K	649	HIS	-	expression tag	UNP P75831
K	650	HIS	-	expression tag	UNP P75831
K	651	HIS	-	expression tag	UNP P75831
K	652	HIS	-	expression tag	UNP P75831
K	653	HIS	-	expression tag	UNP P75831
K	654	HIS	-	expression tag	UNP P75831

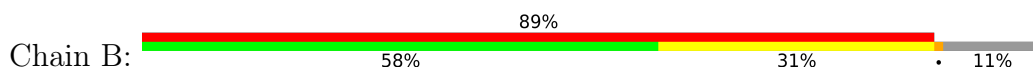
### 3 Residue-property plots

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: Outer membrane protein TolC

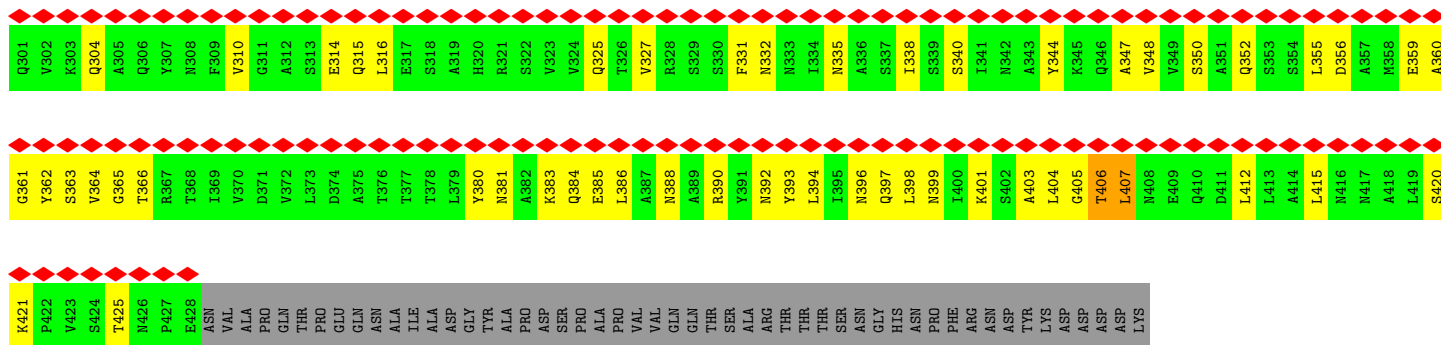


- Molecule 1: Outer membrane protein TolC

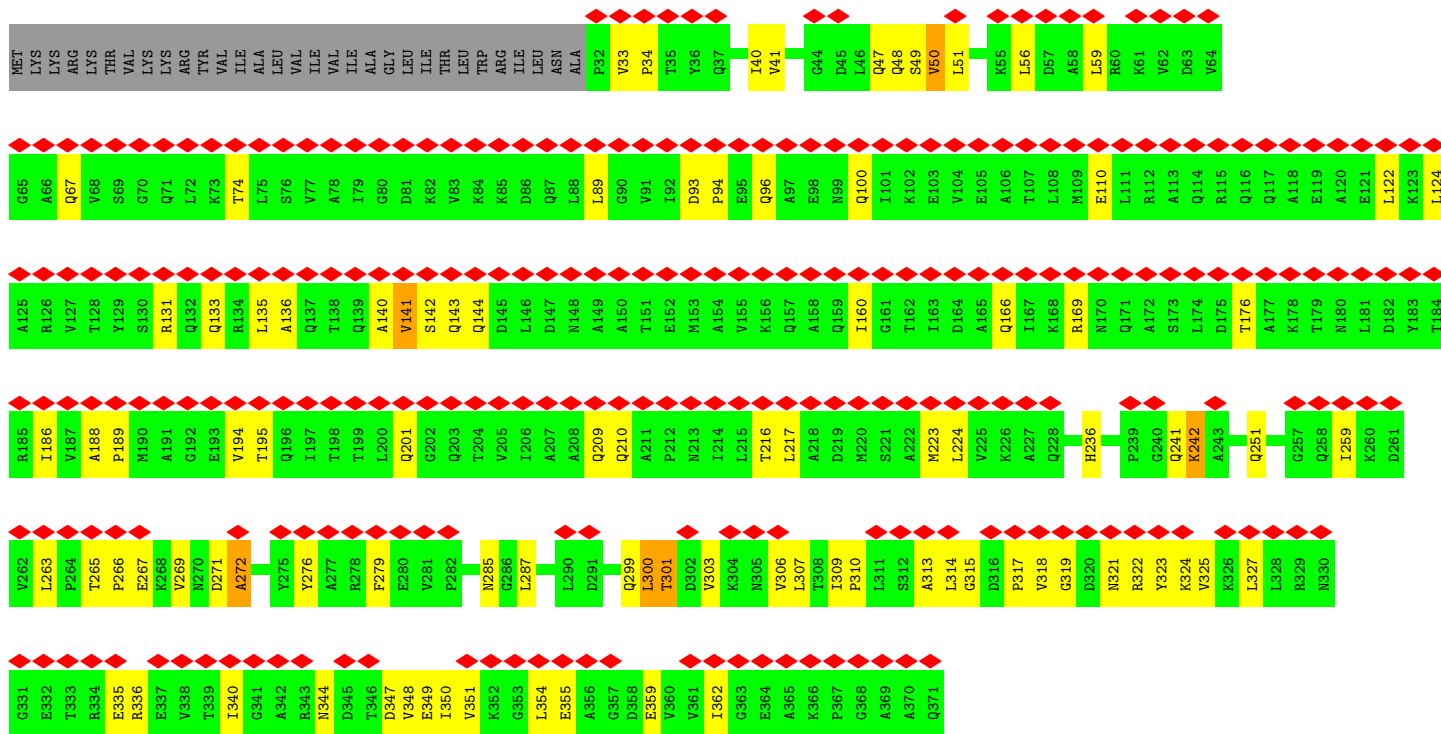




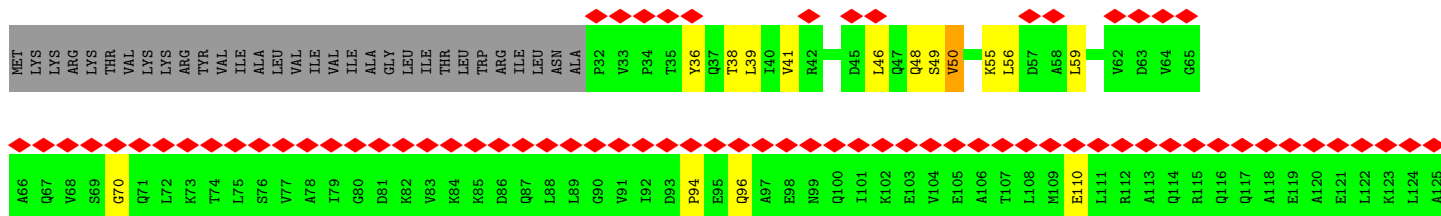




• Molecule 2: Macrolide export protein MacA

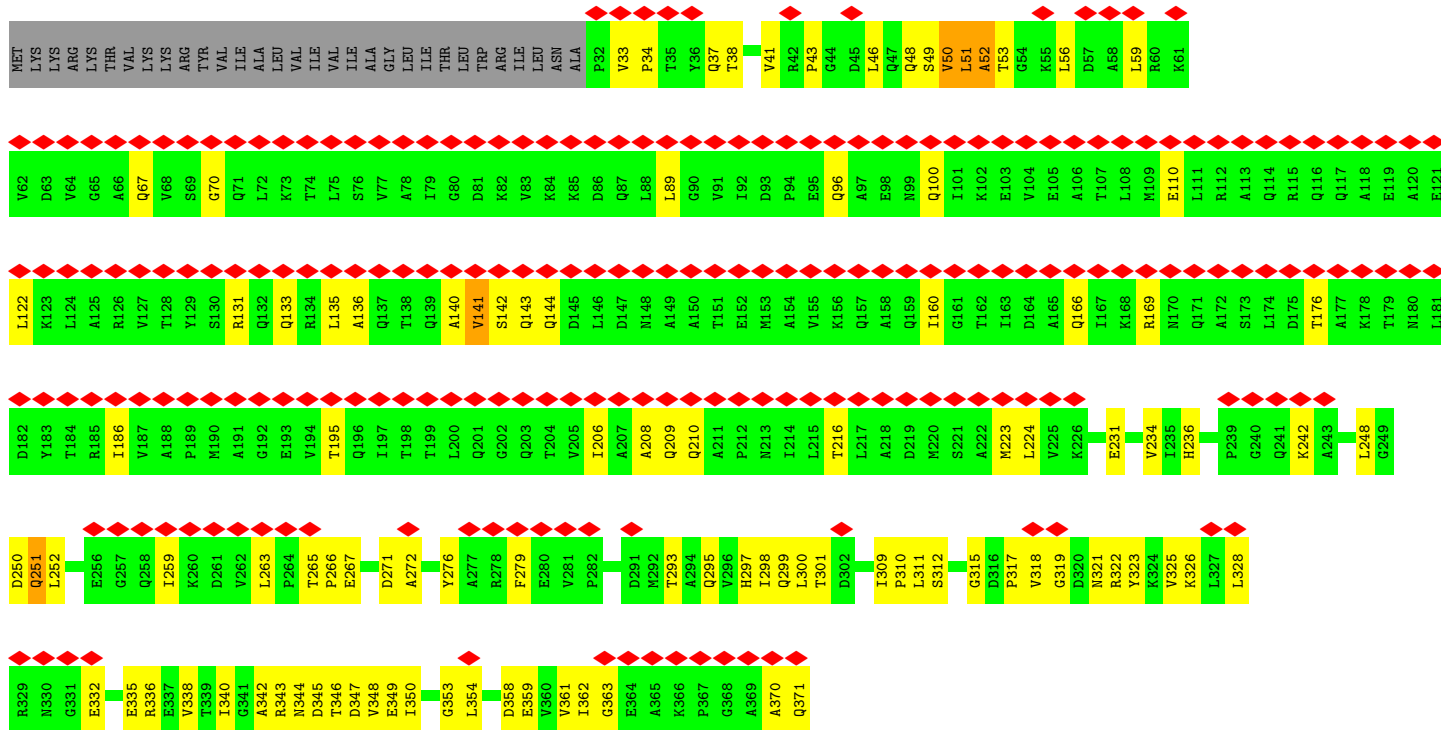


• Molecule 2: Macrolide export protein MacA





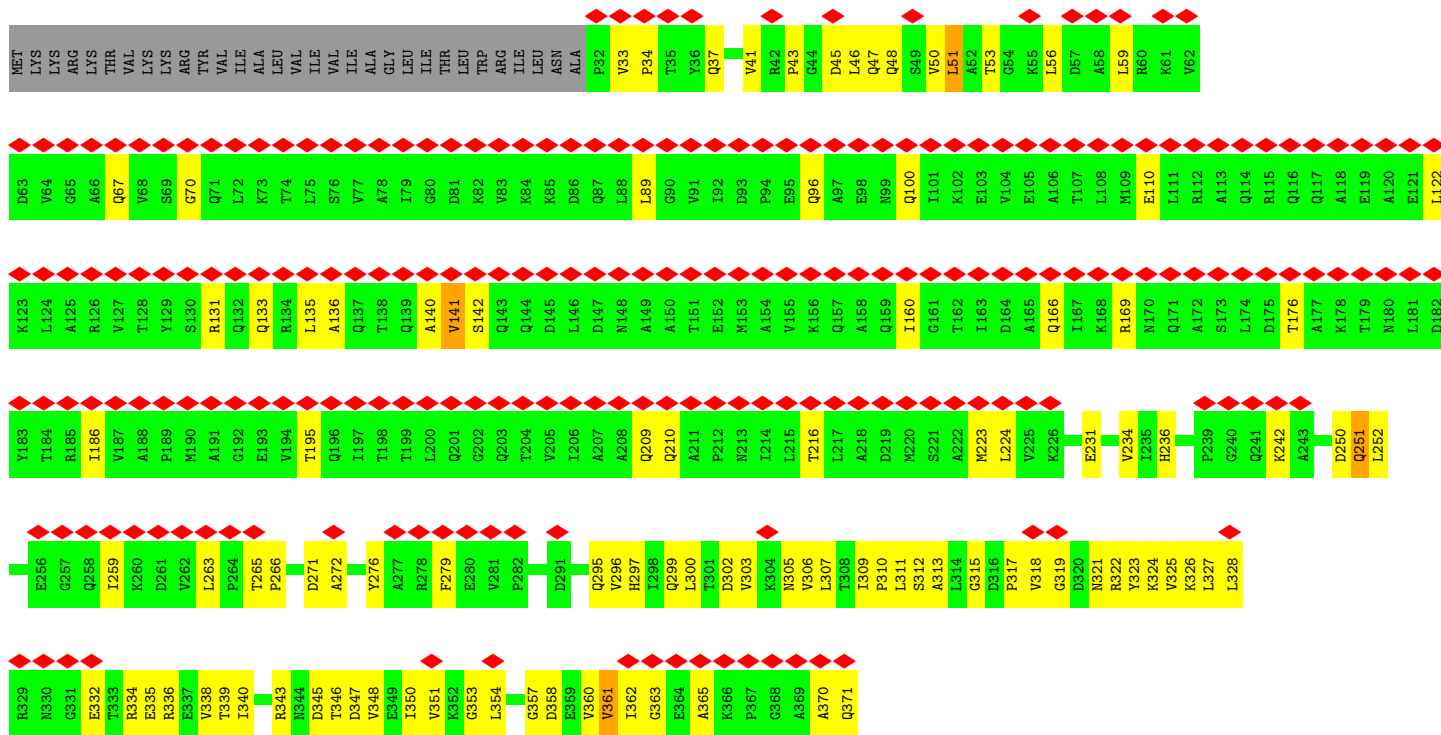
• Molecule 2: Macrolide export protein MacA



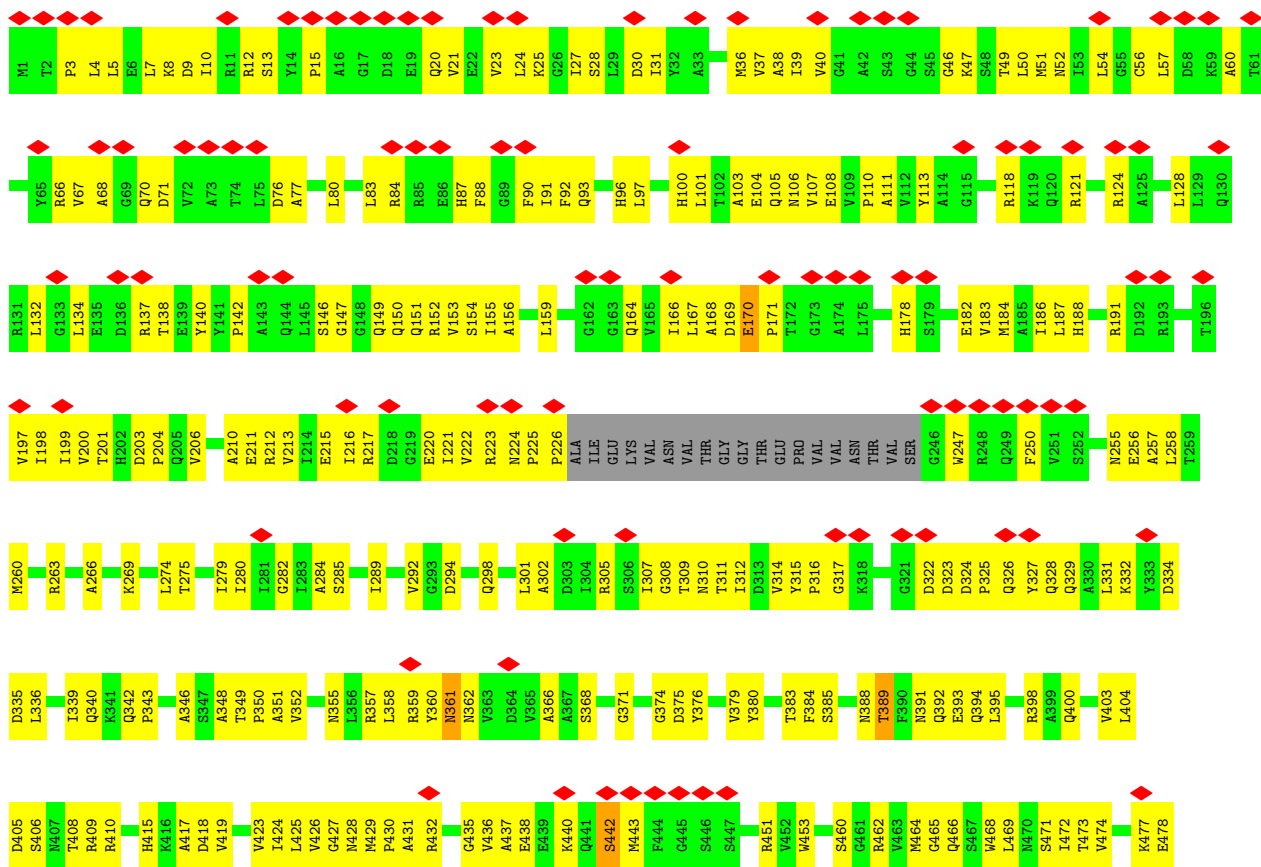
• Molecule 2: Macrolide export protein MacA







• Molecule 3: Macrolide export ATP-binding/permease protein MacB





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	17154	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.089	Depositor
Minimum map value	-0.042	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.03	Depositor
Map size ( $\text{\AA}$ )	408.0, 408.0, 408.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.36, 1.36, 1.36	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	0.39	0/3346	0.55	0/4545
1	B	0.40	0/3346	0.54	0/4545
1	C	0.39	0/3346	0.54	0/4545
2	D	0.24	0/2631	0.45	0/3568
2	E	0.24	0/2630	0.47	0/3565
2	F	0.25	0/2630	0.46	0/3565
2	G	0.24	0/2631	0.45	0/3568
2	H	0.24	0/2631	0.46	0/3568
2	I	0.24	0/2631	0.46	0/3568
3	J	0.29	0/4914	0.49	0/6661
3	K	0.29	0/4914	0.48	0/6661
All	All	0.30	0/35650	0.49	0/48359

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](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3305	0	3256	164	0
1	B	3305	0	3256	147	0
1	C	3305	0	3256	163	0
2	D	2604	0	2678	133	0
2	E	2604	0	2678	90	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	2604	0	2677	138	0
2	G	2604	0	2679	132	0
2	H	2604	0	2678	87	0
2	I	2604	0	2679	124	0
3	J	4838	0	4930	304	0
3	K	4838	0	4930	313	0
All	All	35215	0	35697	1532	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

The worst 5 of 1532 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:271:ASP:CB	3:K:357:ARG:HD2	1.13	1.61
2:D:271:ASP:HB2	3:K:357:ARG:CD	1.19	1.60
2:G:50:VAL:CG2	2:G:300:LEU:HD11	1.38	1.51
1:A:148:LEU:O	2:F:142:SER:CB	1.71	1.38
2:E:299:GLN:O	2:E:300:LEU:CA	1.76	1.33

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	426/479 (89%)	401 (94%)	17 (4%)	8 (2%)	8	40
1	B	426/479 (89%)	400 (94%)	20 (5%)	6 (1%)	11	46
1	C	426/479 (89%)	398 (93%)	19 (4%)	9 (2%)	7	38
2	D	338/371 (91%)	305 (90%)	25 (7%)	8 (2%)	6	35
2	E	336/371 (91%)	306 (91%)	21 (6%)	9 (3%)	5	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	336/371 (91%)	301 (90%)	25 (7%)	10 (3%)	4	30
2	G	338/371 (91%)	307 (91%)	26 (8%)	5 (2%)	10	46
2	H	338/371 (91%)	307 (91%)	24 (7%)	7 (2%)	7	38
2	I	338/371 (91%)	304 (90%)	27 (8%)	7 (2%)	7	38
3	J	623/654 (95%)	567 (91%)	48 (8%)	8 (1%)	12	48
3	K	623/654 (95%)	571 (92%)	41 (7%)	11 (2%)	8	41
All	All	4548/4971 (92%)	4167 (92%)	293 (6%)	88 (2%)	11	40

5 of 88 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	292	ILE
2	E	141	VAL
2	F	50	VAL
2	F	141	VAL
2	F	318	VAL

### 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	358/401 (89%)	358 (100%)	0	100	100
1	B	358/401 (89%)	358 (100%)	0	100	100
1	C	358/401 (89%)	358 (100%)	0	100	100
2	D	281/308 (91%)	280 (100%)	1 (0%)	91	94
2	E	281/308 (91%)	281 (100%)	0	100	100
2	F	281/308 (91%)	280 (100%)	1 (0%)	91	94
2	G	281/308 (91%)	281 (100%)	0	100	100
2	H	281/308 (91%)	280 (100%)	1 (0%)	91	94
2	I	281/308 (91%)	280 (100%)	1 (0%)	91	94
3	J	515/537 (96%)	515 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	K	515/537 (96%)	515 (100%)	0	100	100
All	All	3790/4125 (92%)	3786 (100%)	4 (0%)	93	97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	300	LEU
2	F	51	LEU
2	H	51	LEU
2	I	51	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 92 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	251	GLN
3	J	388	ASN
2	H	344	ASN
2	I	299	GLN
3	J	470	ASN

### 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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	K	1
3	J	1
2	F	1
2	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	K	309:THR	C	310:ASN	N	6.65
1	J	506:ASN	C	507:MET	N	4.22
1	F	299:GLN	C	300:LEU	N	3.26
1	E	299:GLN	C	300:LEU	N	2.88

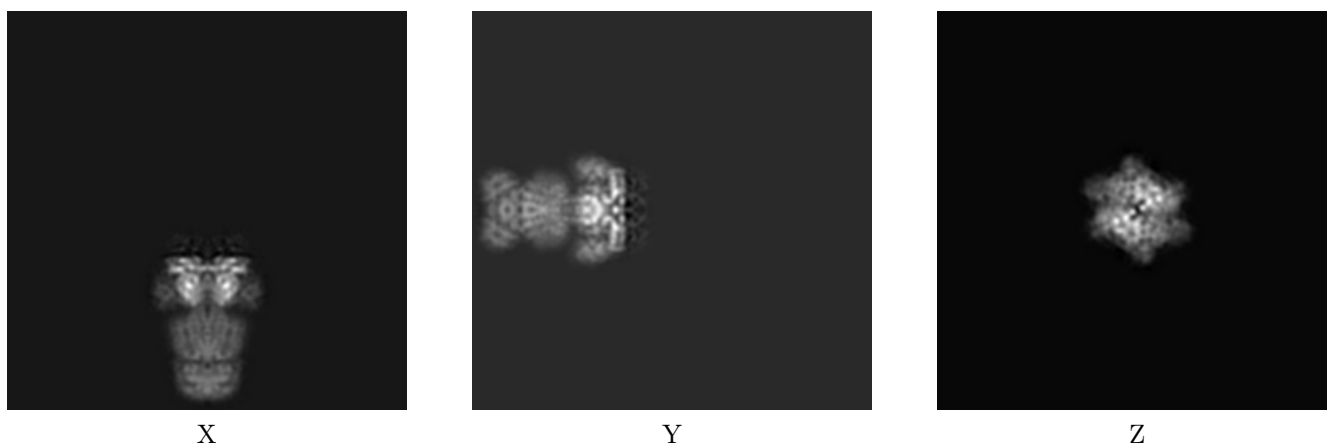
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3653. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

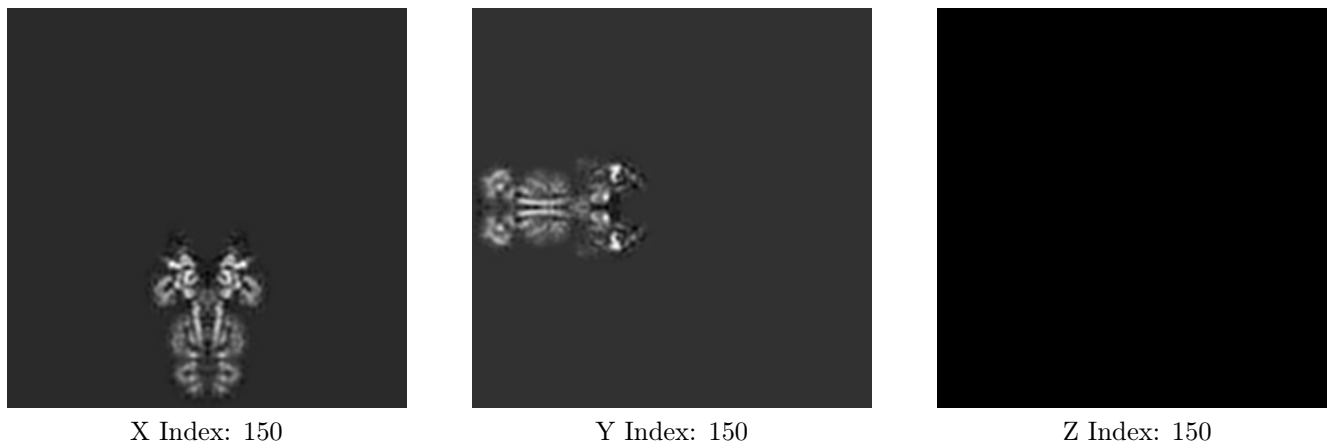
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

#### 6.2.1 Primary map



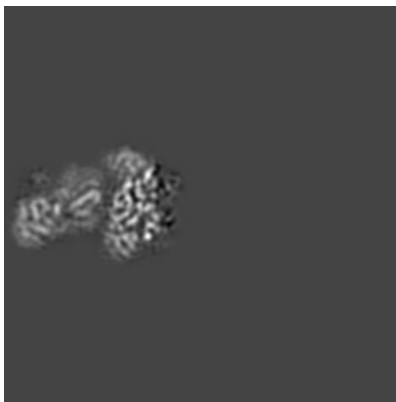
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

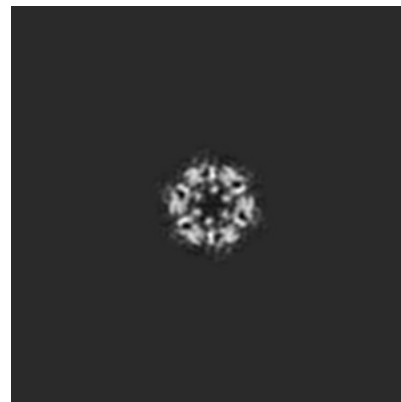
### 6.3.1 Primary map



X Index: 150



Y Index: 137



Z Index: 106

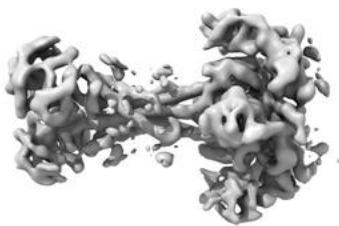
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

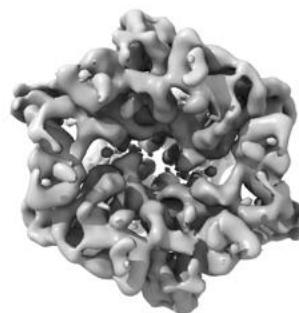
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

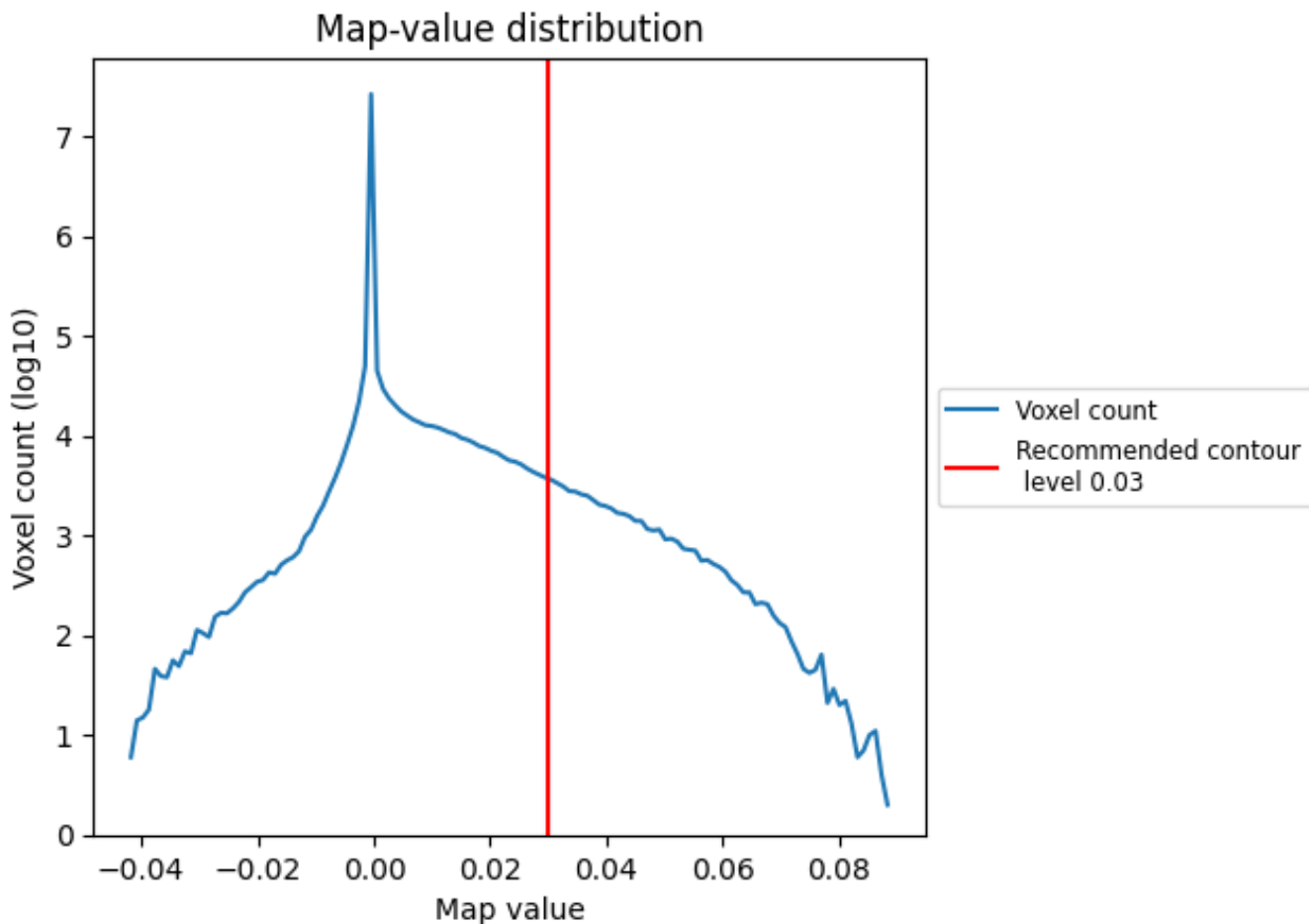
## 6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

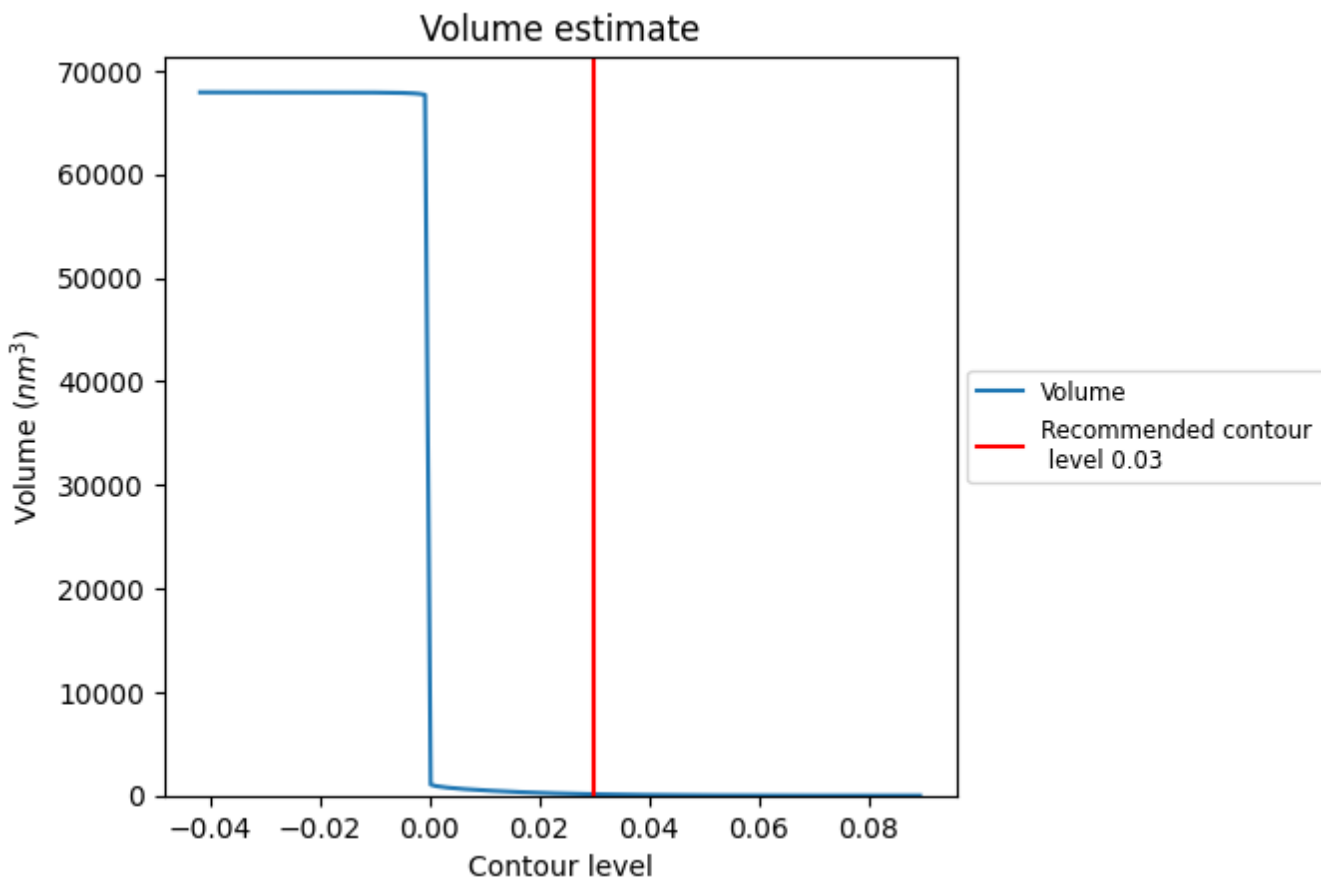
This section contains the results of statistical analysis of the map.

### 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 [\(i\)](#)

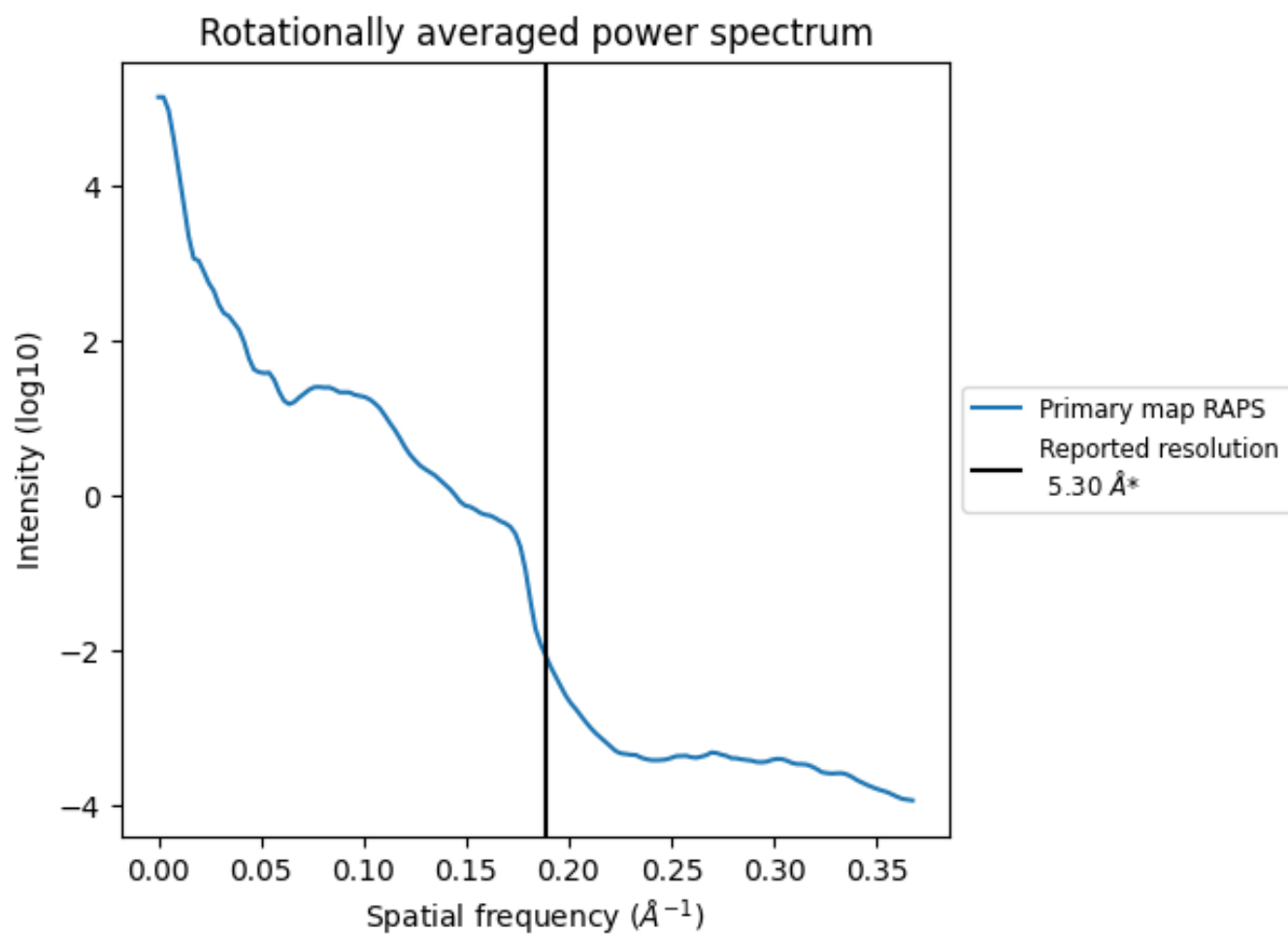


The volume at the recommended contour level is 131 nm<sup>3</sup>; this corresponds to an approximate mass of 118 kDa.

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  $0.189 \text{\AA}^{-1}$

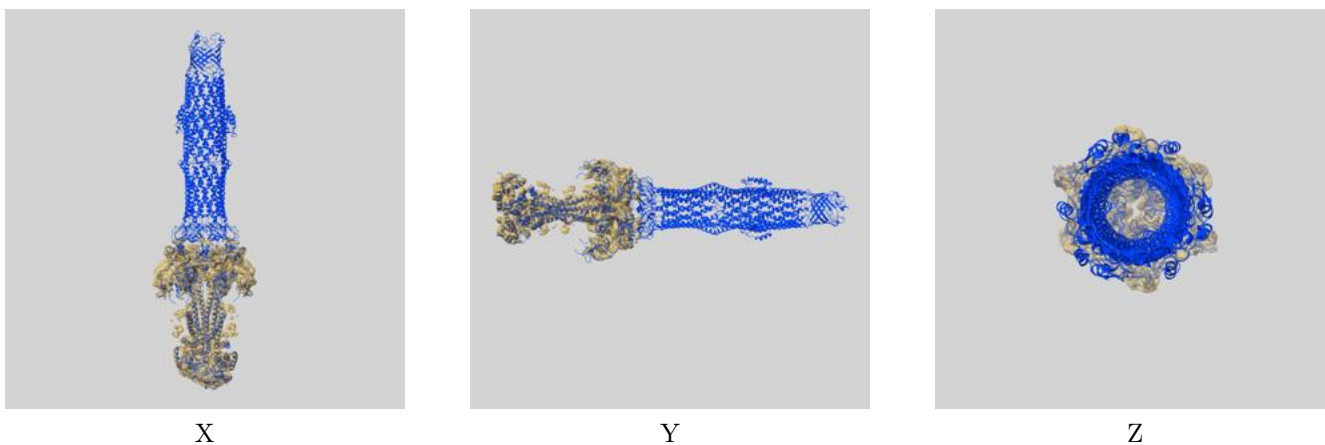
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3653 and PDB model 5NIL. Per-residue inclusion information can be found in section 3 on page 7.

### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.03 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 [\(i\)](#)



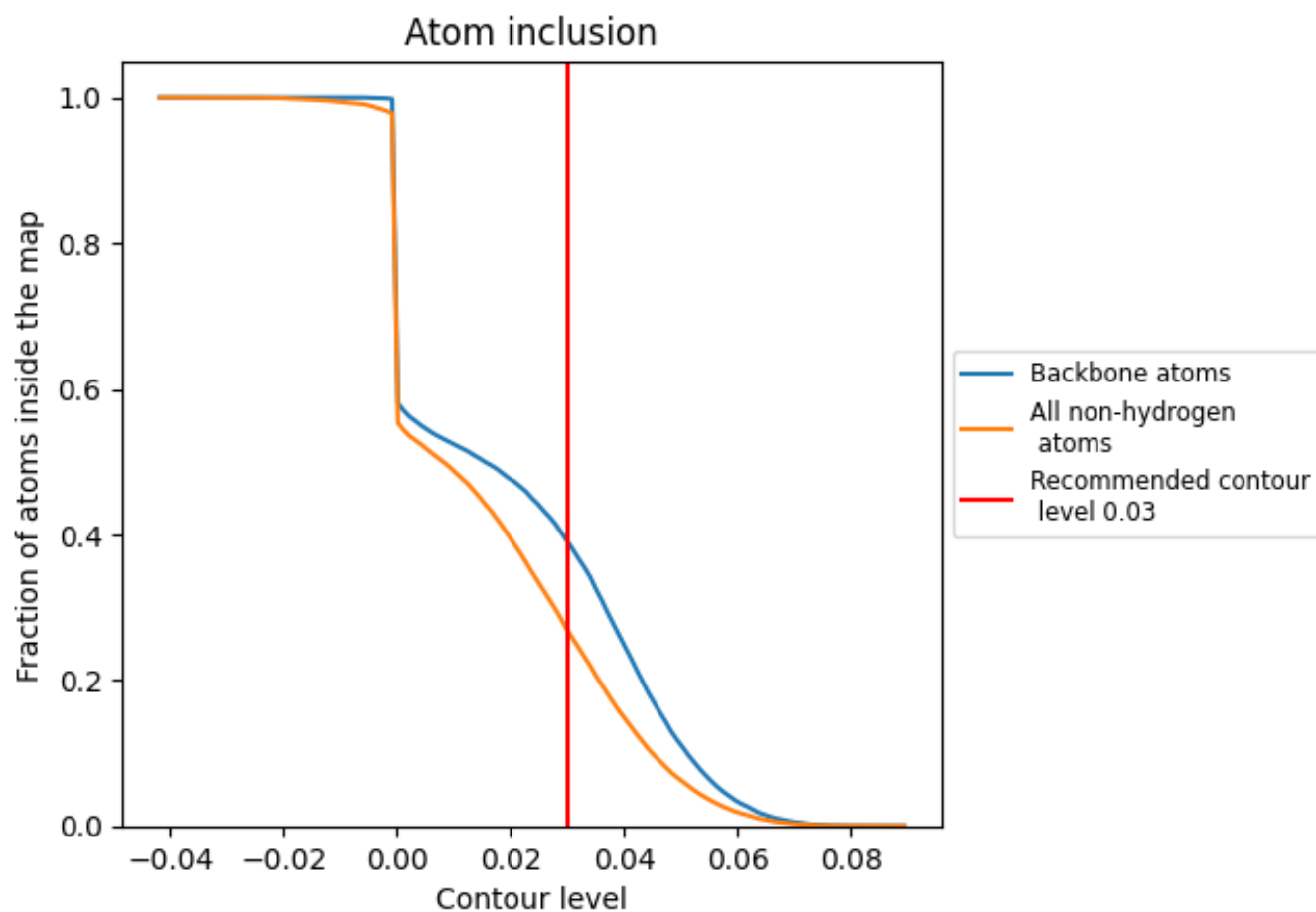
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 39% of all backbone atoms, 27% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.2689	0.1080
A	0.0000	0.0000
B	0.0000	0.0000
C	0.0000	0.0000
D	0.1948	0.1140
E	0.2763	0.1250
F	0.2763	0.1230
G	0.1987	0.1120
H	0.2799	0.1230
I	0.2736	0.1230
J	0.5758	0.1990
K	0.5765	0.2010

