



## wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 04:12 pm GMT

PDB ID : 5NIK  
EMDB ID : EMD-3652  
Title : Structure of the MacAB-TolC ABC-type tripartite multidrug efflux pump  
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 : 3.30 Å(reported)

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

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<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

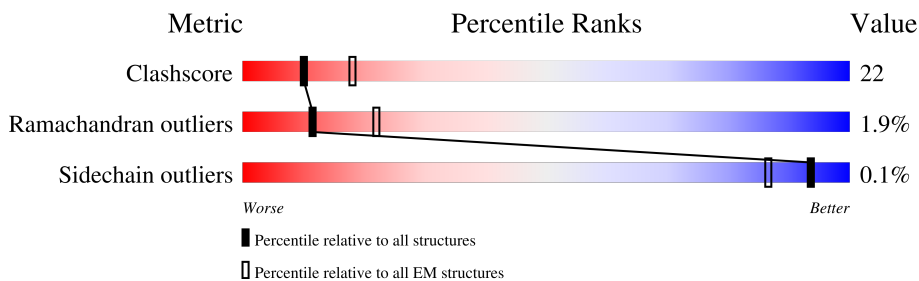
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.30 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	
1	B	479	
1	C	479	
2	D	371	
2	E	371	
2	F	371	
2	G	371	
2	H	371	

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Mol	Chain	Length	Quality of chain
2	I	371	
3	J	654	
3	K	654	

## 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	Total	C	N	O	S	0	0
			4838	3066	853	898	21		
3	K	629	Total	C	N	O	S	0	0
			4838	3066	853	898	21		

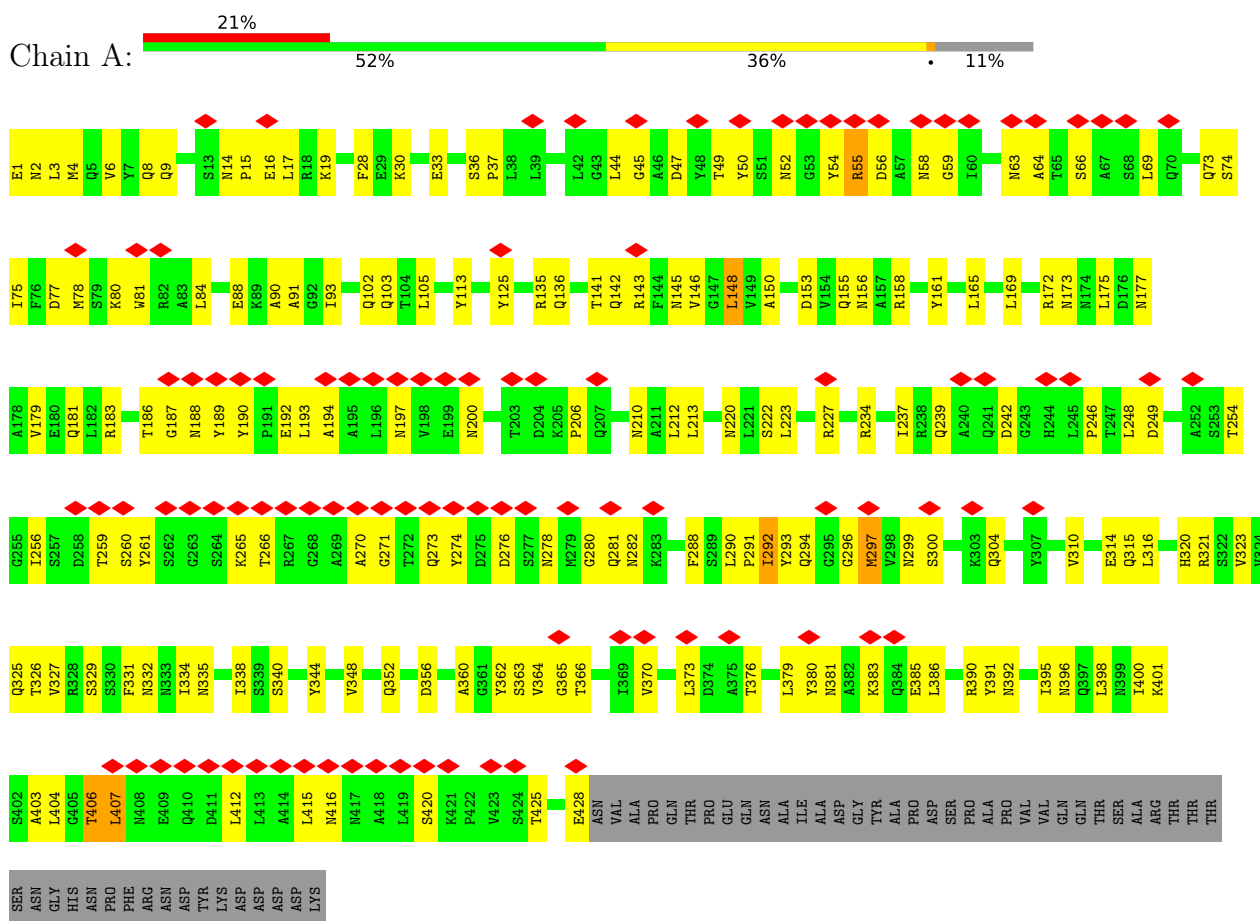
There are 12 discrepancies between the modelled and reference sequences:

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

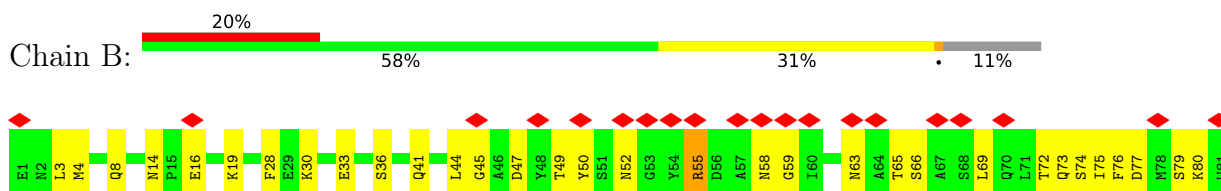
### 3 Residue-property plots

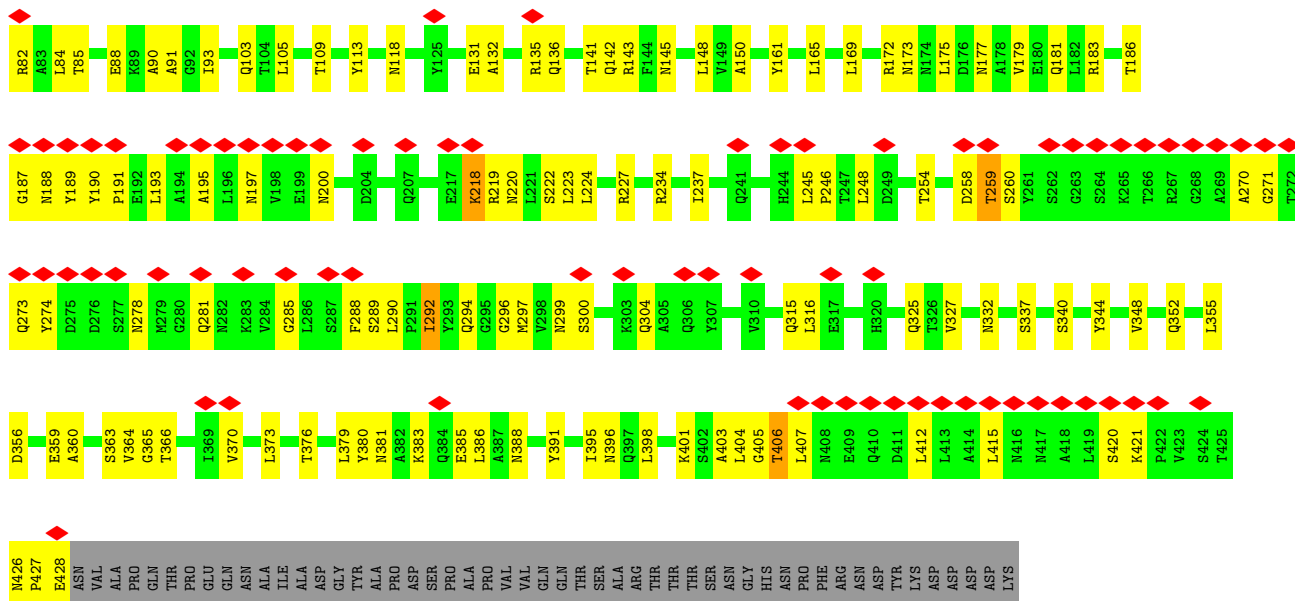
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

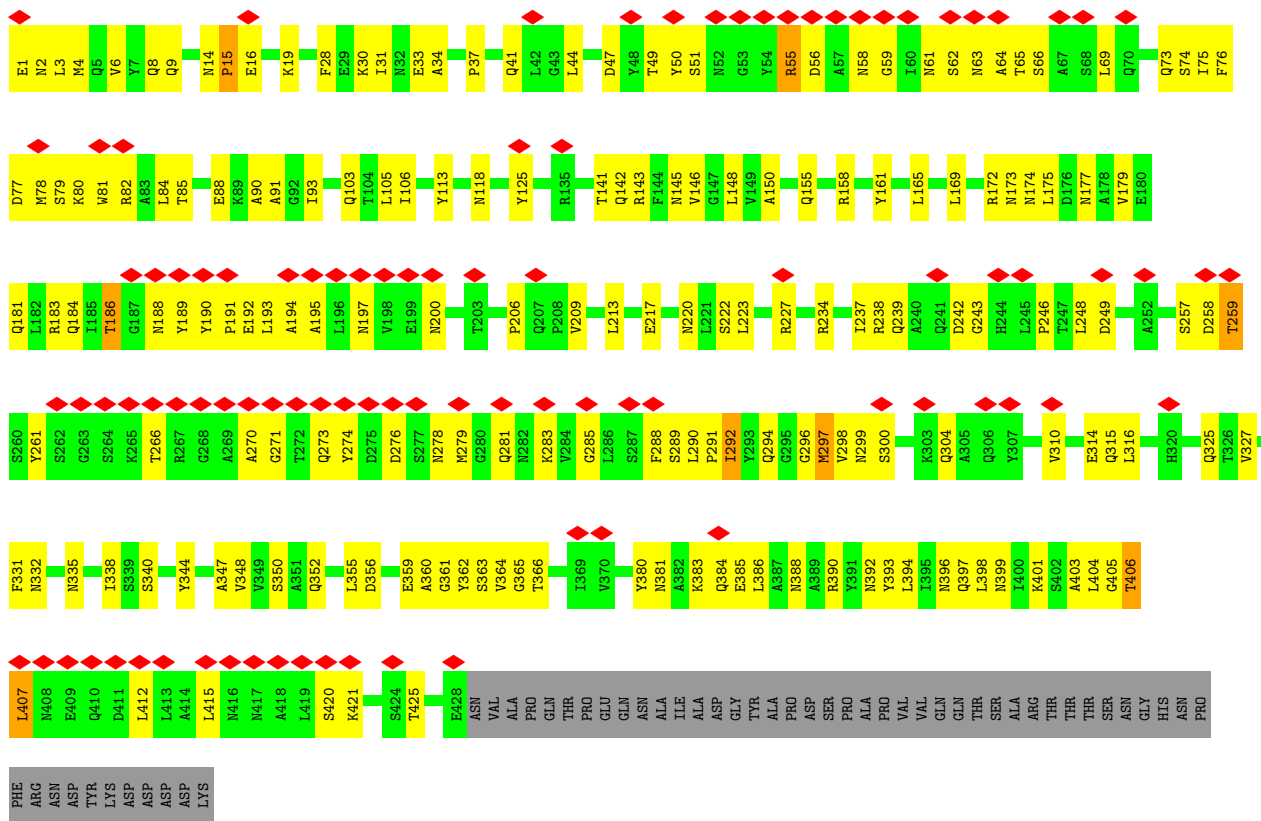


- Molecule 1: Outer membrane protein TolC





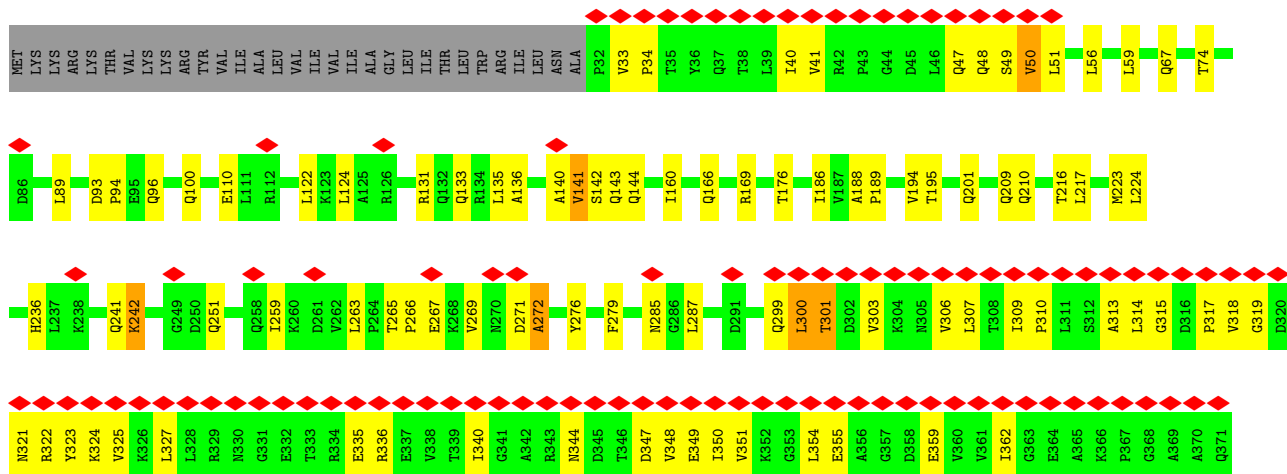
• Molecule 1: Outer membrane protein TolC



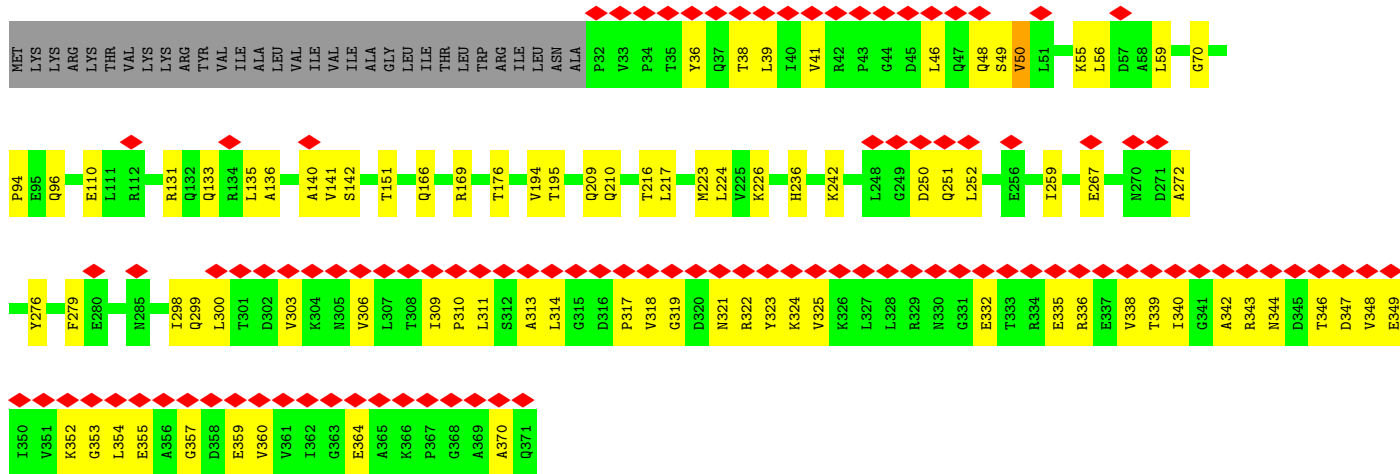
• Molecule 2: Macrolide export protein MacA



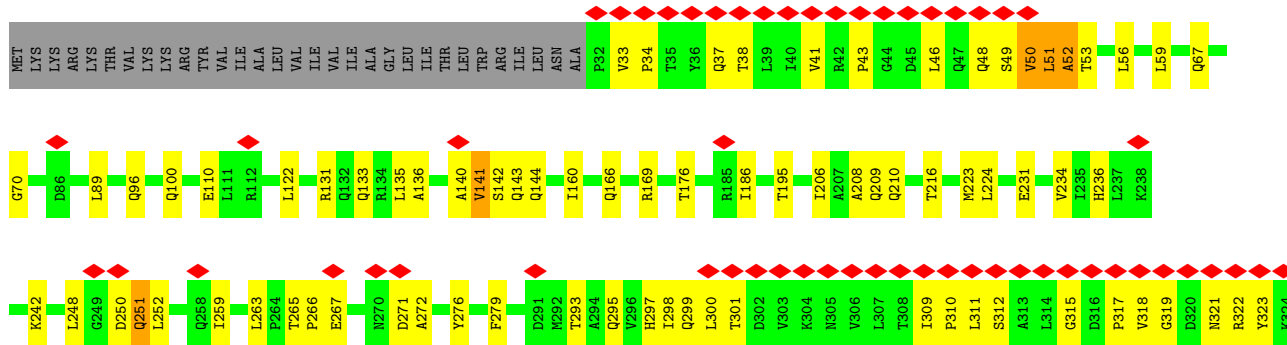




• Molecule 2: Macrolide export protein MacA

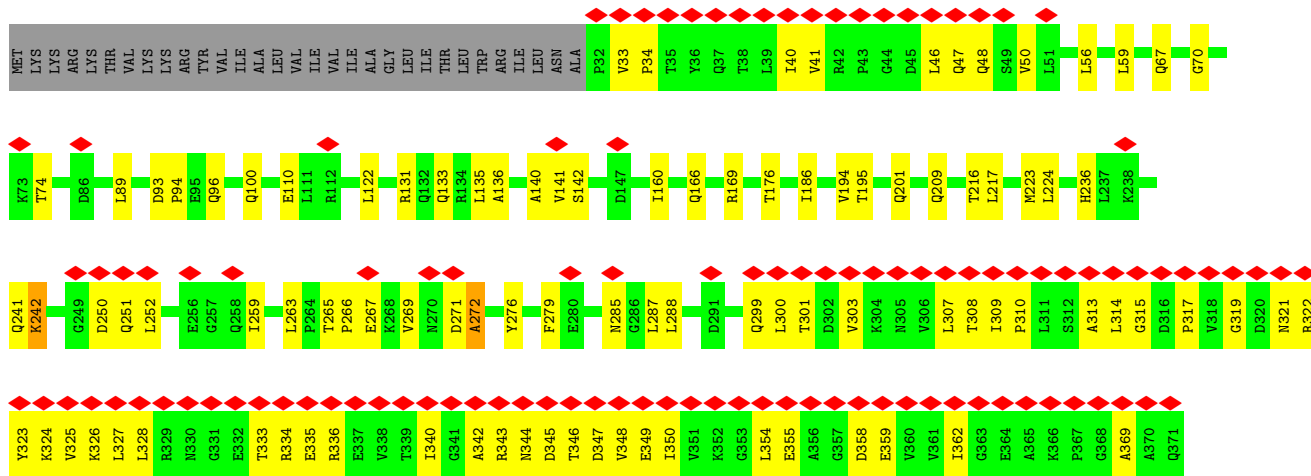


• Molecule 2: Macrolide export protein MacA

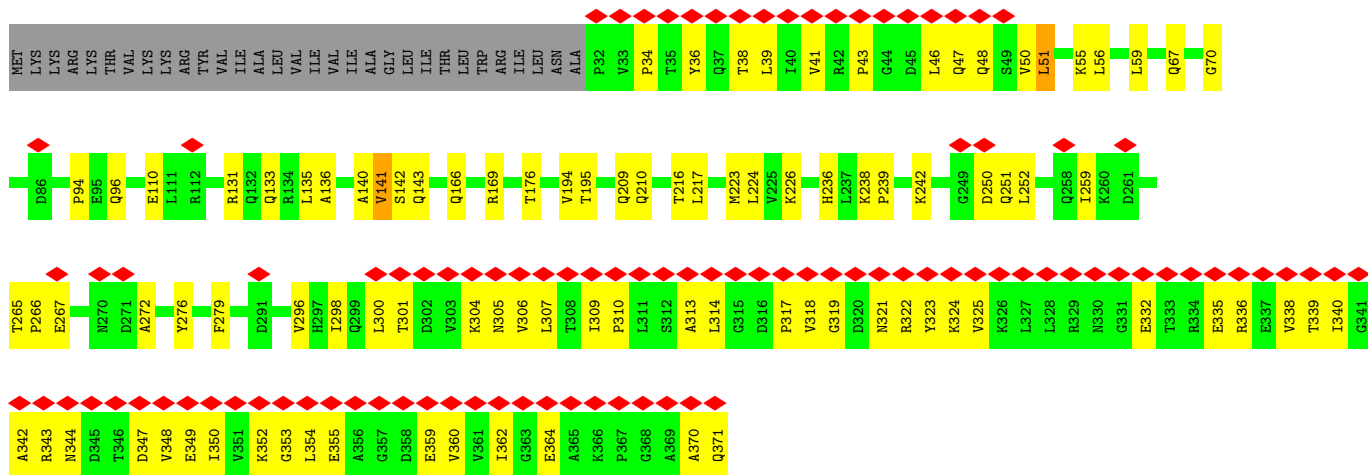




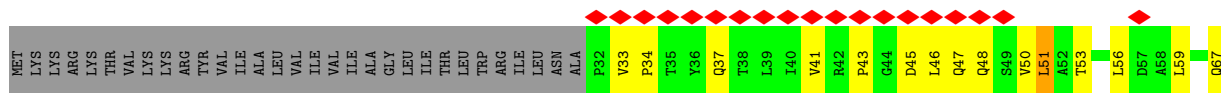
• Molecule 2: Macrolide export protein MacA

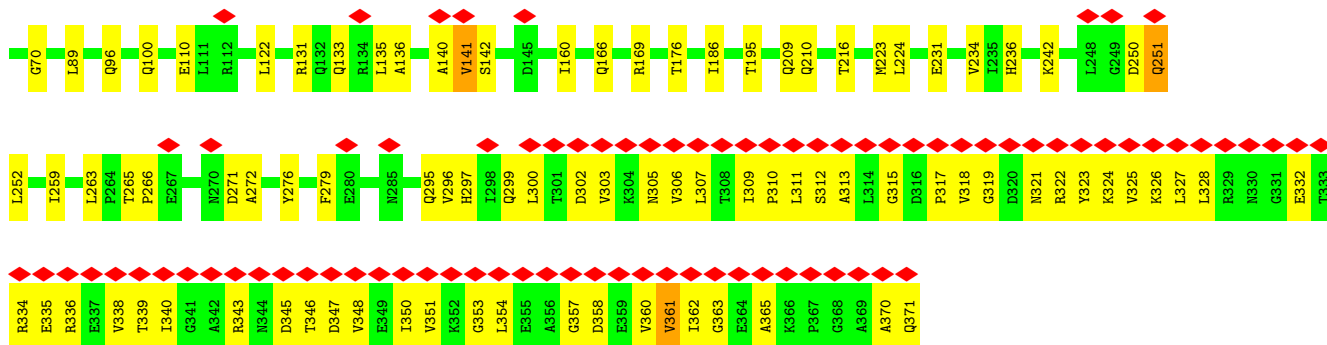


• Molecule 2: Macrolide export protein MacA

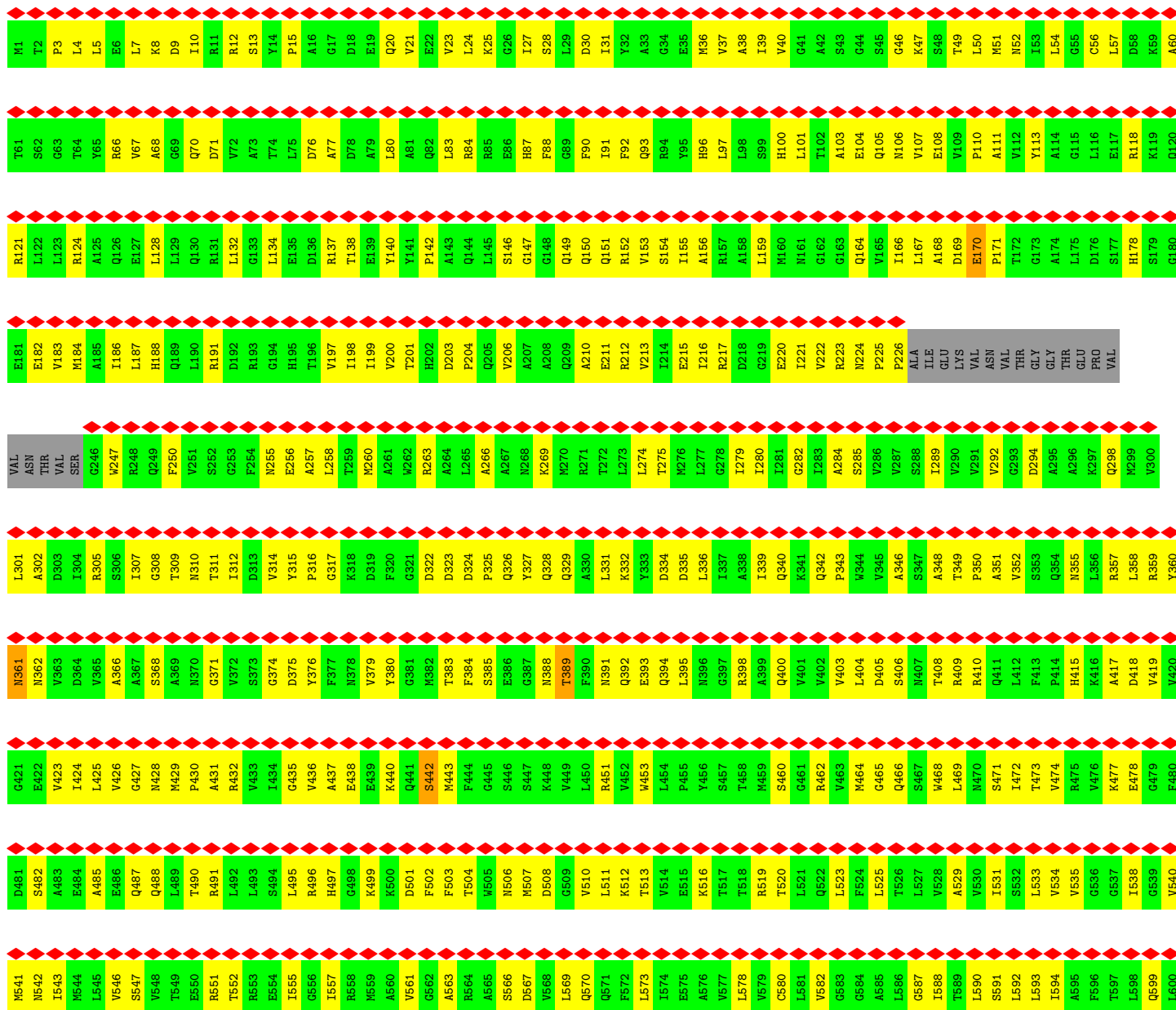


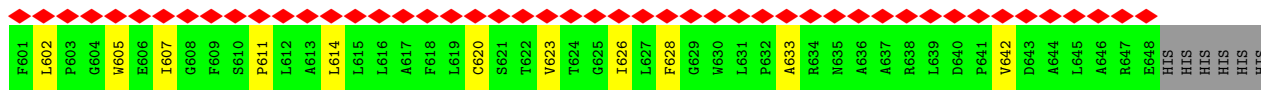
• Molecule 2: Macrolide export protein MacA





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





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



M1	T2	P3	L4	L5	E6	L7	K8	D9	S10	P611	L612	A613	L614	L615	L616	A617	F618	L619	C620	S621	T622	V623	T624	G625	I626	L627	F628	G629	W630	L631	P632	A633	R634	N635	A636	A637	R638	L639	D640	P641	V642	D643	A644	L645	A646	R647	E648	HIS	HIS	HIS	HIS	HIS	HIS																																																																		
T61	S62	G63	T64	V65	I66	V67	A68	G69	Q70	D71	V72	A73	T74	V75	A76	G77	D78	A79	L80	A81	E82	V83	L84	R85	E86	H87	F88	G89	F90	D91	L92	F93	A94	R95	H96	L97	L98	S99	H100	L101	T102	A103	E104	Q105	G106	K107	S108	V109	L110	M111	N112	Y113	L114	G115	L116	E117	R118	K119	Q120																																																												
R121	L122	L123	R124	A125	Q126	E127	L128	L129	Q130	R131	L132	G133	L134	E135	D136	R137	T138	E139	Y140	P141	L142	A143	Q144	L145	S146	G147	G148	Q149	Q150	Q151	R152	V153	S154	I155	A156	R157	A158	L159	M160	G161	G162	G163	Q164	V165	I166	L167	A168	D169	O170	E171	T172	G173	A174	L175	D176	S177	H178	S179	G180																																																												
E181	E182	V183	M184	A185	W186	L187	H188	Q189	L190	R191	D192	R193	G194	H195	T196	V197	I198	I199	V200	T201	H202	D203	P204	L205	Q206	A207	A208	Q209	A210	E211	R212	V213	T214	E215	L216	R217	D218	G219	E220	L221	V222	R223	N224	P225	A226	I227	A228	L229	V230	L231	V232	V233	G234	A235	L236	K237	Q238	V239	T240	R241	V242	G243	D244	A245	A246	K247	S248	T249	R250	L251	S252	G253	F254	S255	V256	G257	V258	G259	L260	A261	I262	R263	A264	L265	A266	A267	I268	K269	N270	Q271	R272	L273	L274	T275	N276	L277	G278	L279	L280	L281	G282	L283	A284	S285	V286	V287	S288	L289	V290	V291	V292	G293	D294	A295	A296	K297	Q298	V299	L300
L301	A302	D303	L304	R305	S306	L307	G308	T309	N310	T311	L312	D313	V314	Y315	P316	G317	K318	D319	F320	G321	D322	D323	D324	P325	Q326	Y327	Q328	Q329	A330	L331	K332	Y333	D334	D335	L336	L337	A338	L339	Q340	K341	P342	P343	V344	V345	A346	S347	A348	R349	P350	A351	V352	S353	Q354	N355	L356	R357	R358	R359	Y360																																																												
N361	N362	V363	D364	V365	A366	A367	S368	A369	N370	G371	V372	S373	G374	D375	V376	F377	N378	V379	Y380	G381	N382	T383	F384	S385	E386	G387	N388	T389	N391	Q392	E393	Q394	L395	N396	G397	R398	A399	Q400	V401	V402	V403	L404	D405	A406	N407	T408	R409	R410	Q411	L412	F413	P414	H415	K416	A417	V419	V420																																																														
G421	E422	V423	I424	L425	V426	G427	N428	M429	P430	A431	R432	V433	I434	G435	V436	A437	E438	E439	K440	Q441	S442	M443	F444	G445	S446	S447	K448	V449	L450	R451	V452	V453	L454	P455	V456	S457	T458	M459	S460	G461	R462	V463	M464	G465	Q466	S467	V468	L469	M470	S471	L472	T473	V474	R475	G476	K477	E478	G479	F480																																																												
D481	S482	A483	F484	A485	F486	Q487	Q488	L489	T490	R491	L492	L493	S494	L495	R496	H497	Q498	K499	K500	D501	F502	F503	T504	W505	M506	M507	D508	G509	V510	L511	K512	T513	V514	E515	K516	T517	T518	R519	T520	L521	O522	L523	F524	L525	T526	L527	V528	A529	V530	I531	S532	L533	V534	V535	G536	G537	L538	G539	V540																																																												
M541	N542	I543	M544	L545	V546	S547	V548	T549	E550	R551	T552	R553	E554	I555	G556	I557	R558	M559	A560	V561	G562	A563	R564	A565	S566	D567	V568	L569	Q570	Q571	F572	L573	I574	E575	A576	V577	L578	V579	C580	L581	V582	G583	G584	A585	L586	G587	I588	T589	L590	S591	L592	L593	I594	A595	F596	T597	L598	Q599	L600																																																												
F601	L602	P603	G604	W605	E606	I607	G608	F609	S610	P611	L612	A613	L614	L615	L616	A617	F618	L619	C620	S621	T622	V623	T624	G625	I626	L627	F628	G629	W630	L631	P632	A633	R634	N635	A636	A637	R638	L639	D640	P641	V642	D643	A644	L645	A646	R647	E648	HIS	HIS	HIS	HIS	HIS	HIS																																																																		

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	27614	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 ( $e^-/\text{\AA}^2$ )	45	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	0.345	Depositor
Minimum map value	-0.136	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.07	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%)	<b>8</b> 34
1	B	426/479 (89%)	400 (94%)	20 (5%)	6 (1%)	<b>11</b> 38
1	C	426/479 (89%)	398 (93%)	19 (4%)	9 (2%)	<b>7</b> 31
2	D	338/371 (91%)	305 (90%)	25 (7%)	8 (2%)	<b>6</b> 28
2	E	336/371 (91%)	306 (91%)	21 (6%)	9 (3%)	<b>5</b> 26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	336/371 (91%)	301 (90%)	25 (7%)	10 (3%)	4	24
2	G	338/371 (91%)	307 (91%)	26 (8%)	5 (2%)	10	38
2	H	338/371 (91%)	307 (91%)	24 (7%)	7 (2%)	7	31
2	I	338/371 (91%)	304 (90%)	27 (8%)	7 (2%)	7	31
3	J	623/654 (95%)	567 (91%)	48 (8%)	8 (1%)	12	40
3	K	623/654 (95%)	571 (92%)	41 (7%)	11 (2%)	8	35
All	All	4548/4971 (92%)	4167 (92%)	293 (6%)	88 (2%)	11	34

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	95
2	E	281/308 (91%)	281 (100%)	0	100	100
2	F	281/308 (91%)	280 (100%)	1 (0%)	91	95
2	G	281/308 (91%)	281 (100%)	0	100	100
2	H	281/308 (91%)	280 (100%)	1 (0%)	91	95
2	I	281/308 (91%)	280 (100%)	1 (0%)	91	95
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

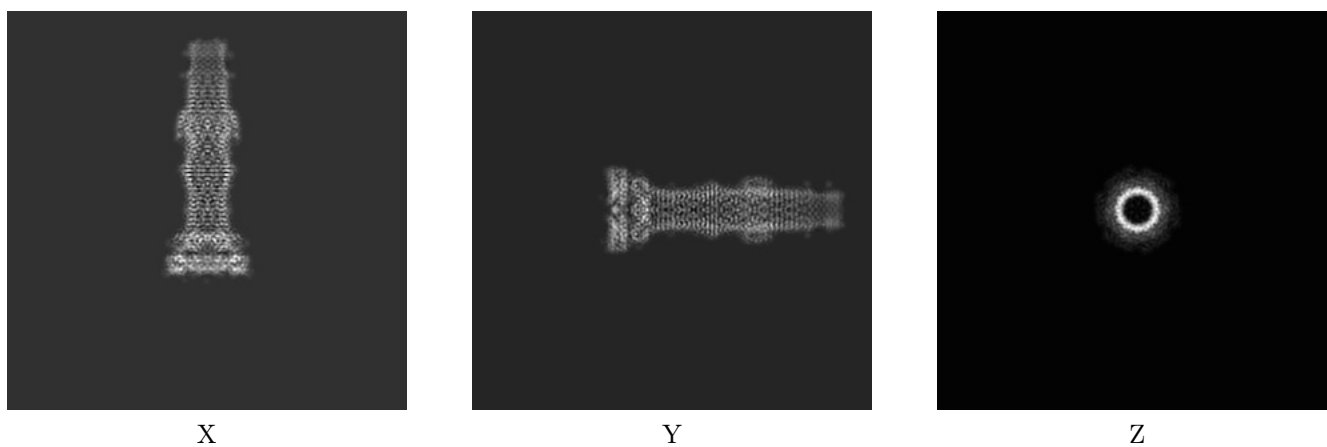
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3652. 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](#)

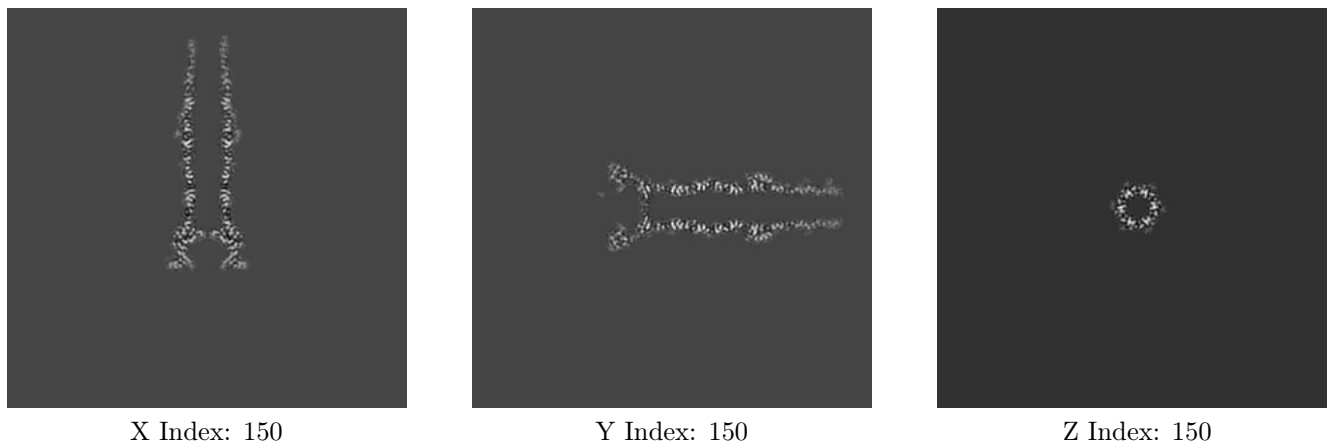
#### 6.1.1 Primary map



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

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

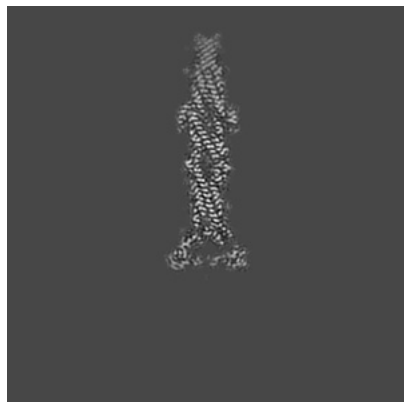
#### 6.2.1 Primary map



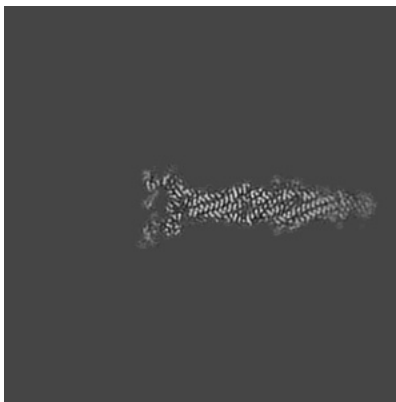
The images above show central slices of the map in three orthogonal directions.

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

### 6.3.1 Primary map



X Index: 162



Y Index: 163



Z Index: 128

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

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

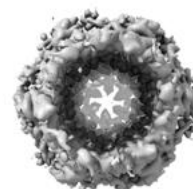
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

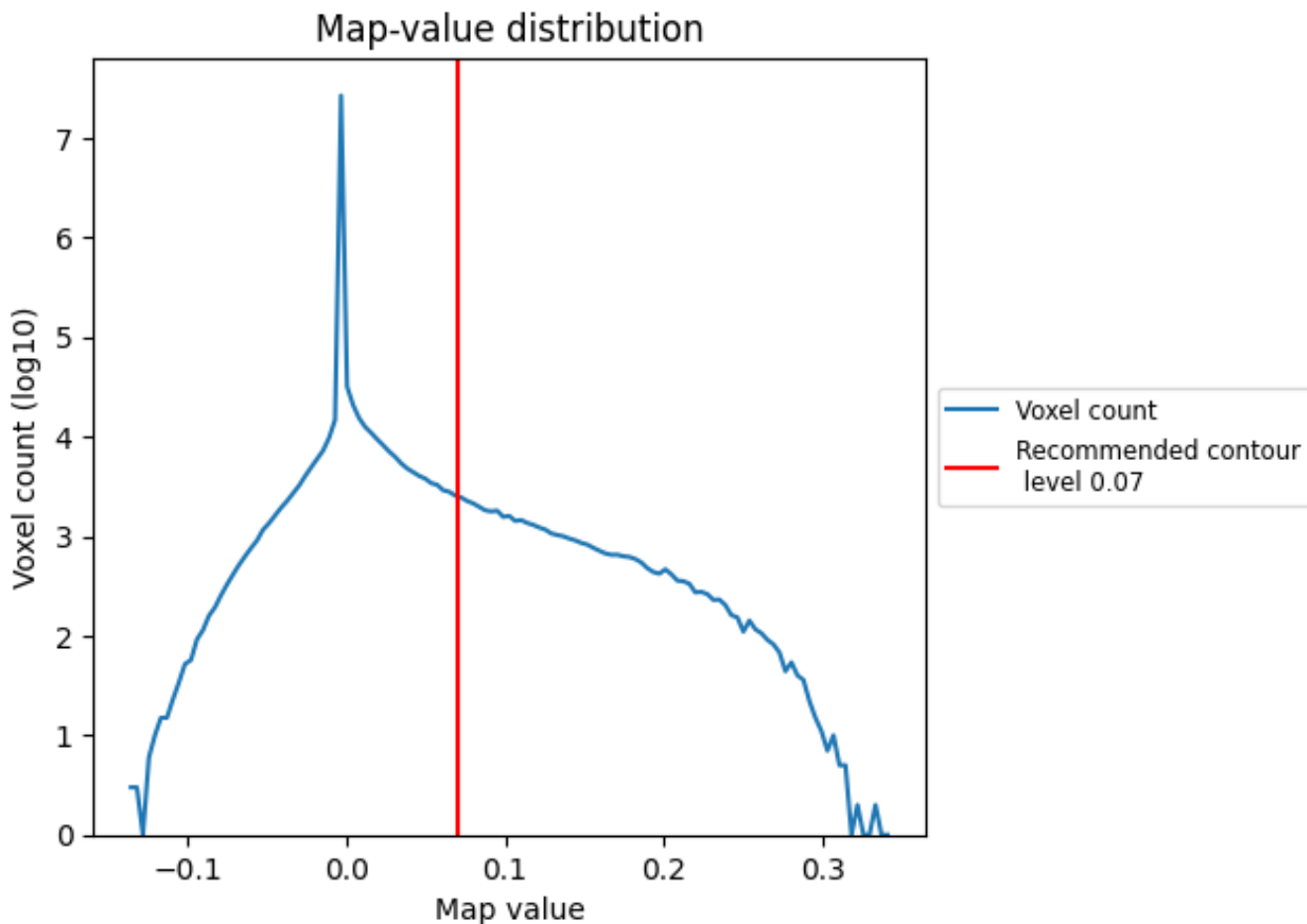
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

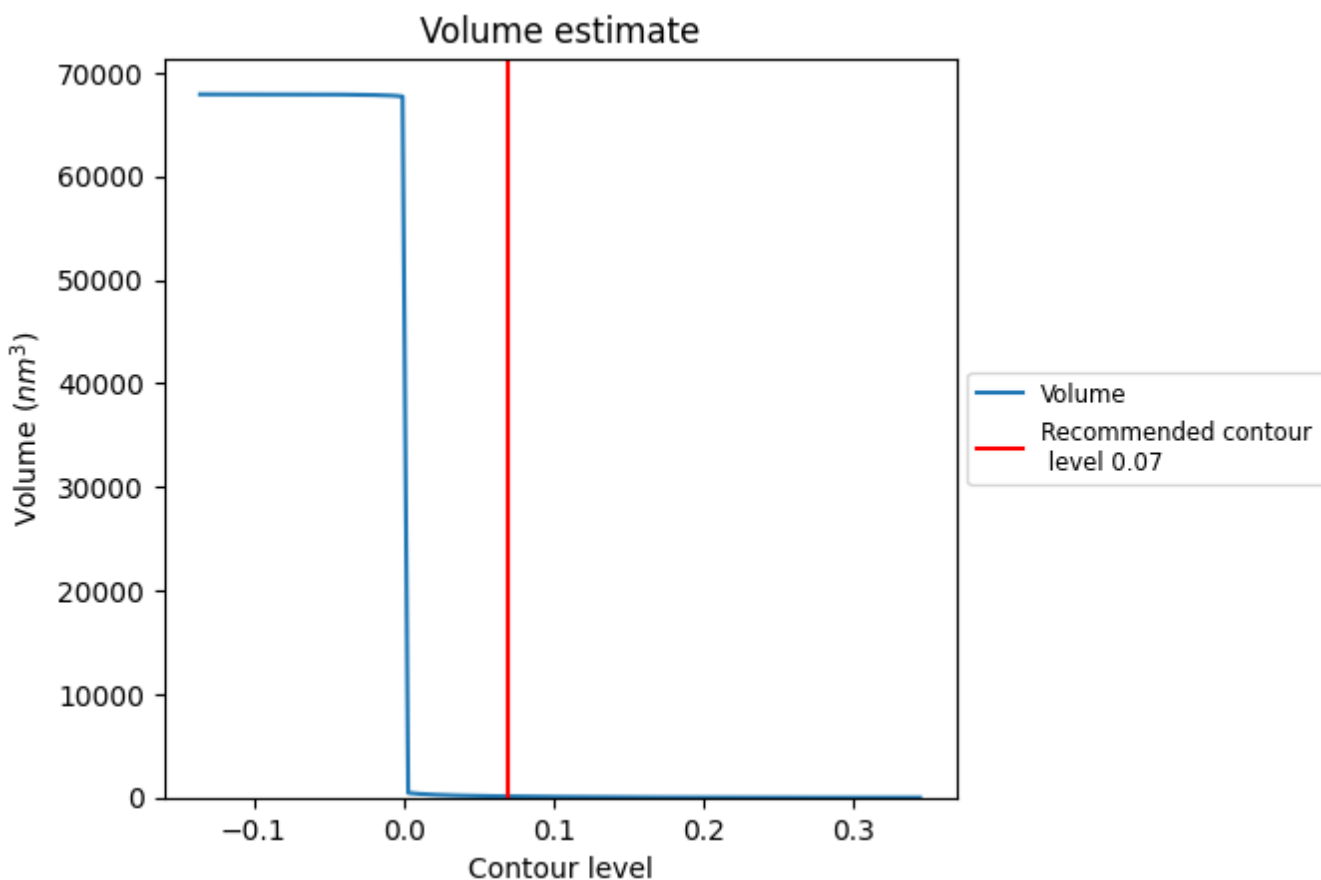
This section contains the results of statistical analysis of the map.

### 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.

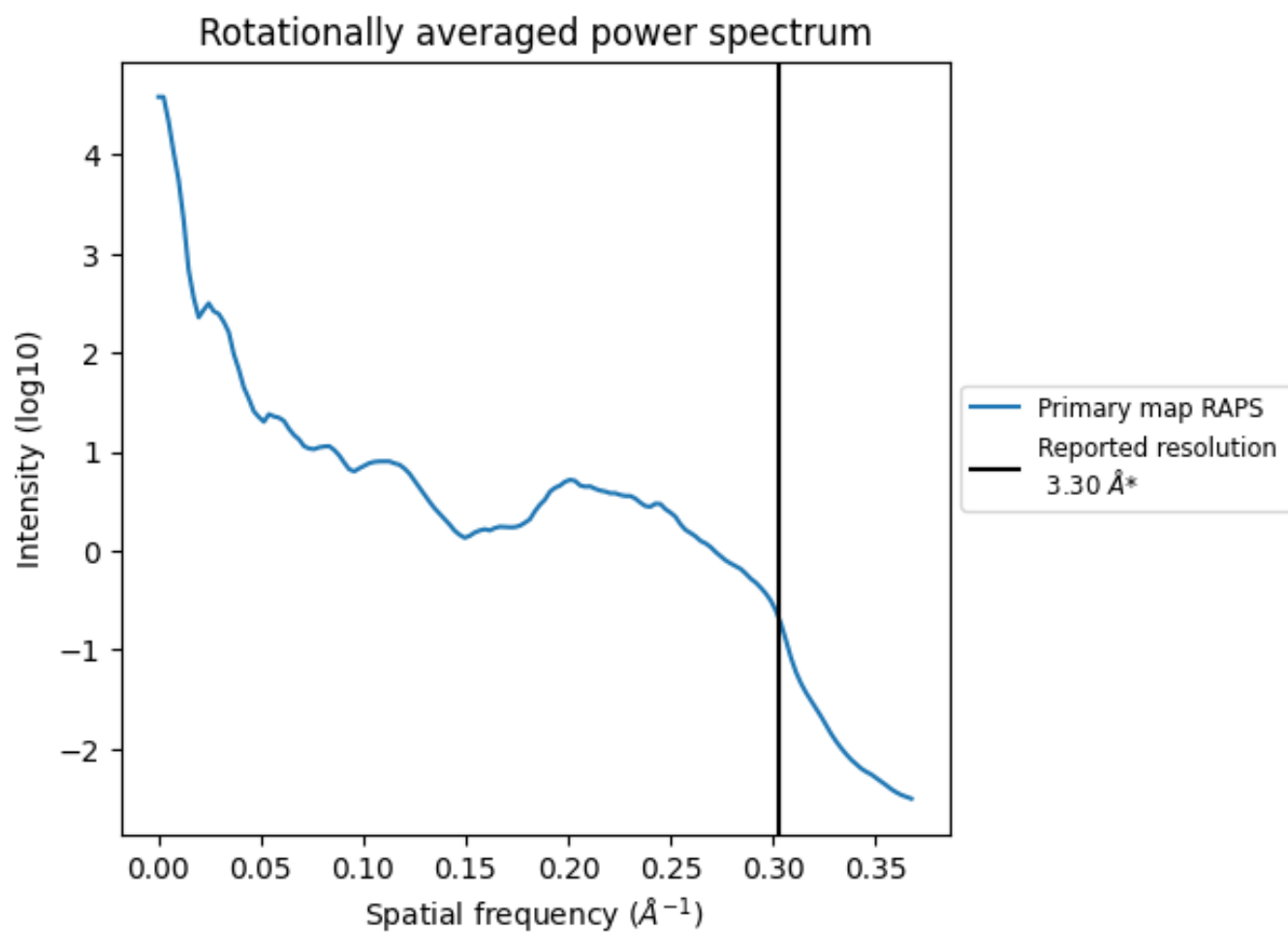
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 114 nm<sup>3</sup>; this corresponds to an approximate mass of 103 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 0.303 Å<sup>-1</sup>



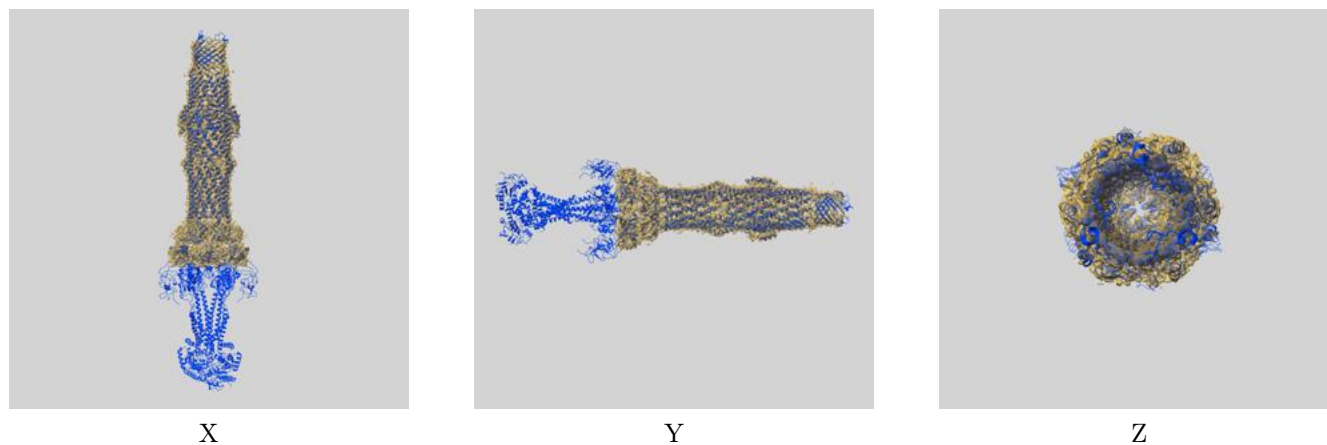
## 8 Fourier-Shell correlation

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-3652 and PDB model 5NIK. Per-residue inclusion information can be found in section [3](#) on page [7](#).

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



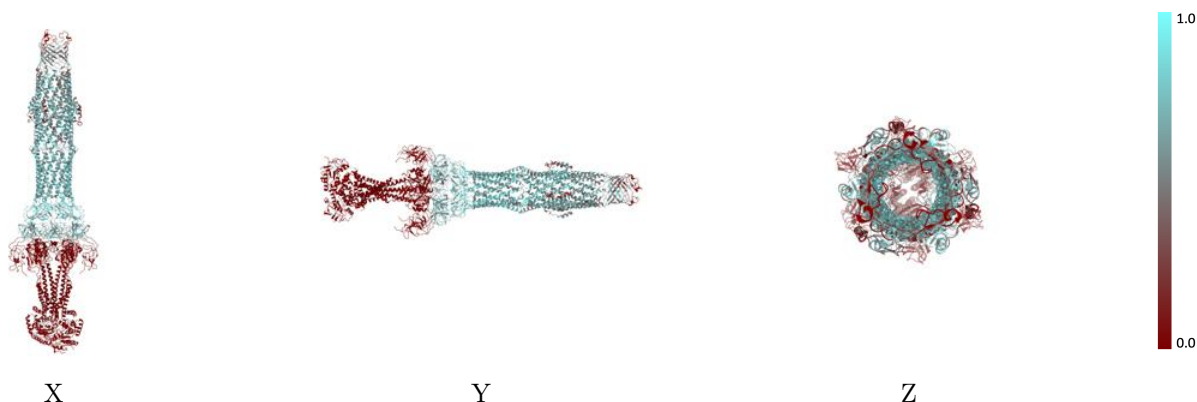
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



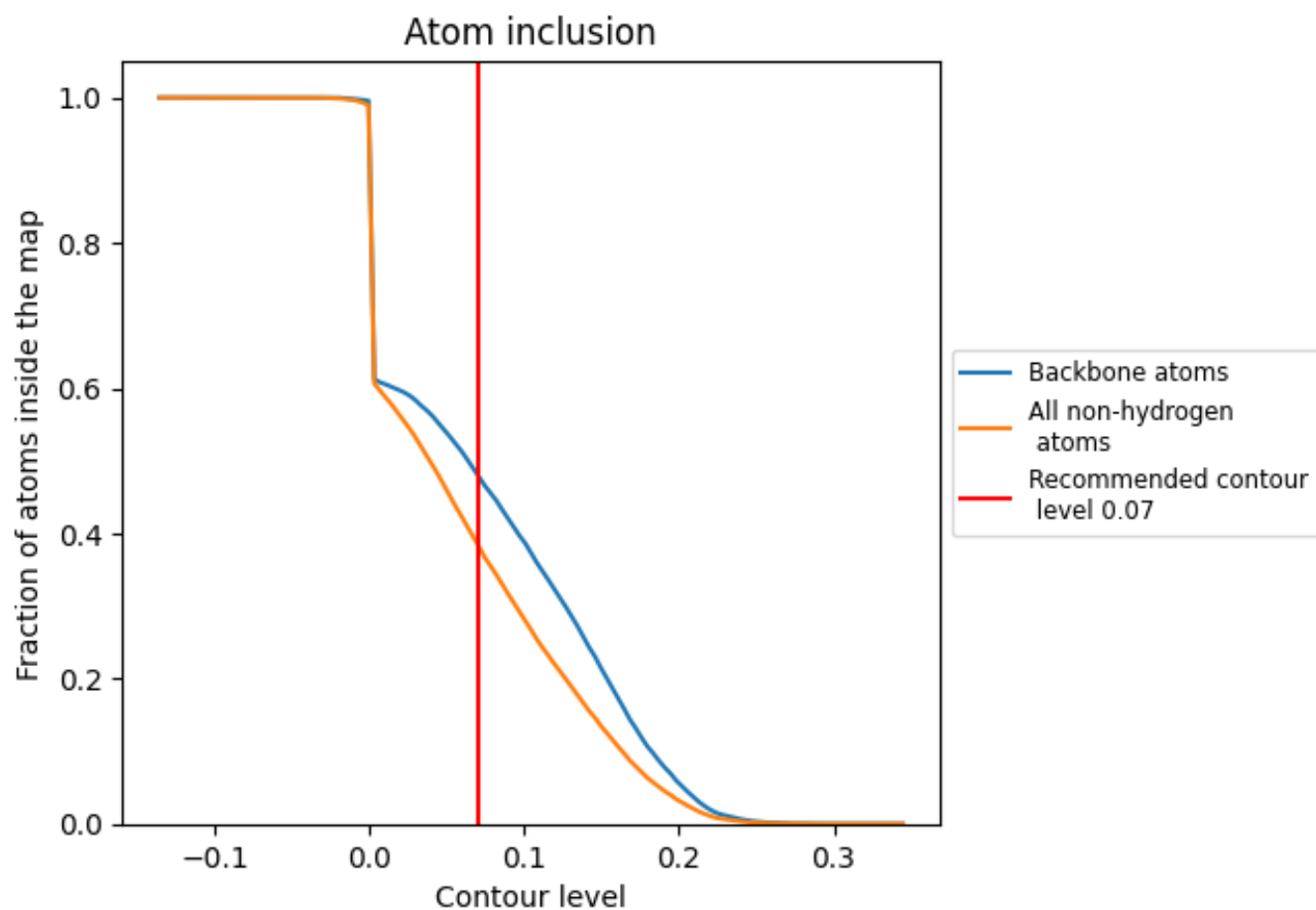
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

























## 9.4 Atom inclusion [i](#)



At the recommended contour level, 48% of all backbone atoms, 38% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3846	 0.2410
A	 0.5583	 0.3340
B	 0.5626	 0.3430
C	 0.5666	 0.3420
D	 0.5016	 0.3280
E	 0.5105	 0.3290
F	 0.5098	 0.3310
G	 0.5117	 0.3280
H	 0.5074	 0.3270
I	 0.5125	 0.3330
J	 0.0000	 -0.0030
K	 0.0000	 -0.0030

