



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 06:12 AM UTC

PDB ID : 5NIL / pdb_00005nil
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.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

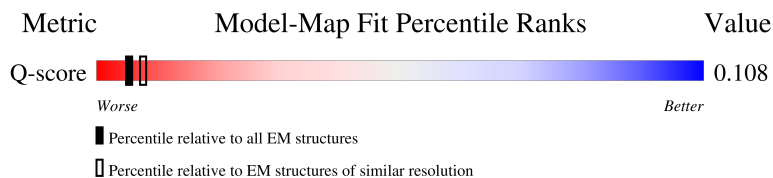
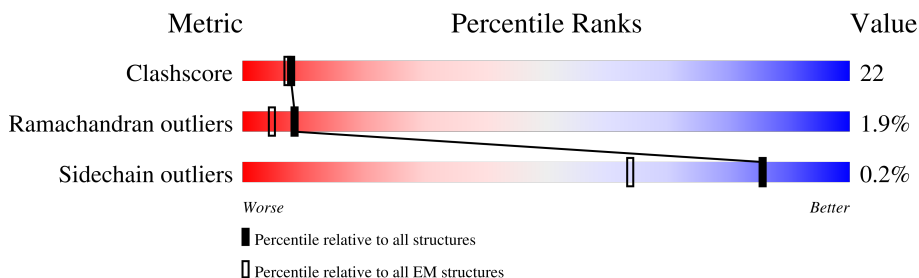
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	625 (4.80 - 5.80)

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	479	
1	B	479	
1	C	479	
2	D	371	

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Mol	Chain	Length	Quality of chain
2	E	371	<p>57% 67% 23% • 8%</p>
2	F	371	<p>59% 63% 27% • 8%</p>
2	G	371	<p>69% 64% 27% • 8%</p>
2	H	371	<p>58% 65% 26% • 8%</p>
2	I	371	<p>60% 63% 27% • 8%</p>
3	J	654	<p>19% 45% 50% • •</p>
3	K	654	<p>18% 46% 49% • •</p>

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		

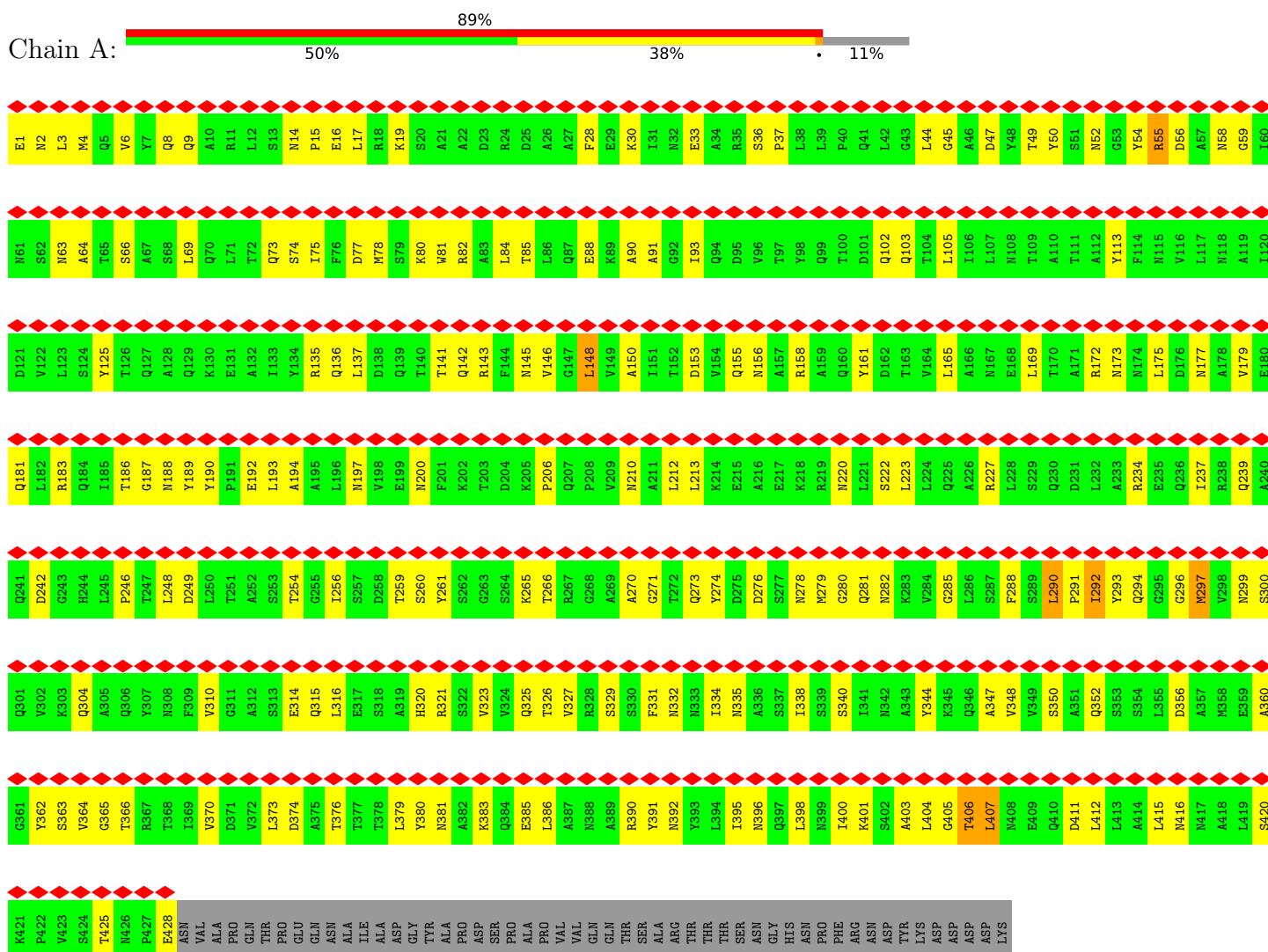
There are 12 discrepancies between the modelled and reference sequences:

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

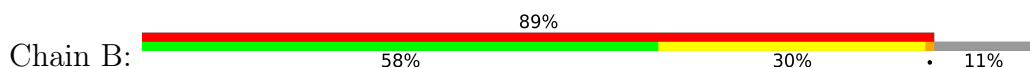
3 Residue-property plots

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

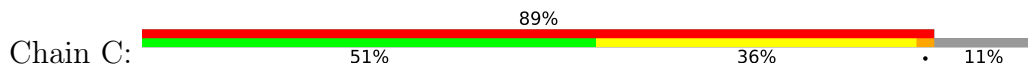


- Molecule 1: Outer membrane protein TolC

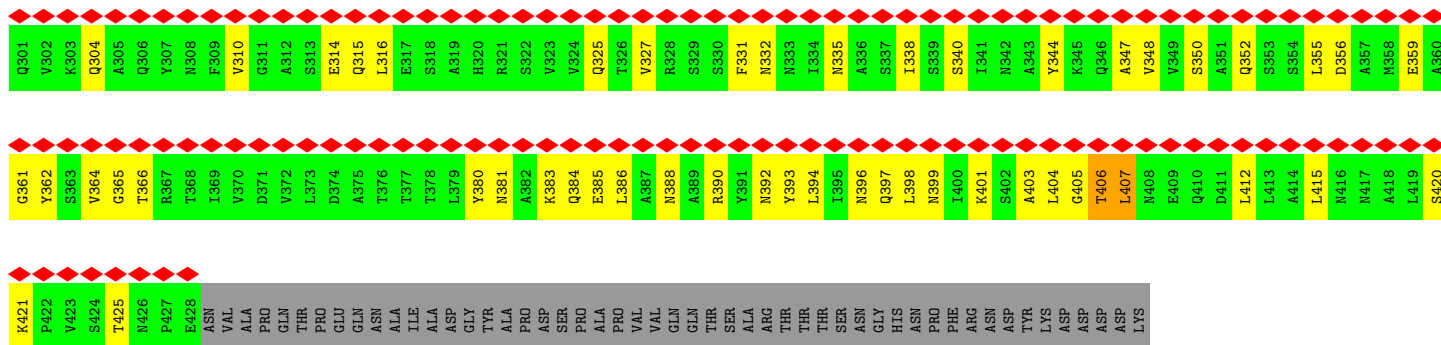


E1	N2	L3	M4	Q5	V6	Y7	Q8	Q9	A10	R11	L12	S13	M14	P15	E16	L17	R18	K19	S20	A21	A22	D23	R24	D25	A26	A27	F28	E29	K30	I31	N32	E33	A34	R35	S36	P37	L38	L39	P40	Q41	L42	G43	L44	G45	A46	D47	Y48	T49	Y50	S51	N52	G53	Y54	R55	D56	A57	N58	G59	I60	
M61	S62	M63	A64	T65	S66	A67	S68	L69	Q70	L71	T72	Q73	S74	I75	F76	D77	M78	S79	K80	M81	A82	A83	L84	T85	L86	Q87	E88	R89	A90	A91	G92	I93	Q94	D95	V96	T97	Y98	Q99	T100	D101	Q102	Q103	T104	L105	A106	L107	M108	T109	A110	T111	A112	Y113	F114	M115	V116	L117	M118	A119	T120	
D121	V122	L123	S124	Y125	T126	Q127	A128	Q129	K130	E131	A132	I133	Y134	R135	Q136	L137	D138	Q139	T140	T141	Q142	R143	F144	M145	L146	G147	L148	V149	A150	I151	T152	D153	V154	Q155	D156	M156	A157	R158	A159	Q160	Y161	D162	T163	V164	L165	A166	M167	E168	L169	T170	A171	L172	M173	M174	L175	D176	M177	V178	V179	E180
Q181	L182	R183	Q184	I185	T186	G187	M188	Y189	Y190	P191	E192	L193	A194	A195	L196	M197	V198	E199	N200	F201	K202	T203	D204	K205	P206	Q207	P208	V209	N210	A211	L212	L213	K214	E215	V216	A216	E217	K218	R219	N220	L221	S222	L223	L224	Q225	A226	R227	L228	S229	Q230	D231	L232	R234	E235	Q236	I237	R238	Q239	A240	
Q241	D242	G243	H244	L245	P246	T247	L248	D249	L250	T251	A252	S253	T254	G255	T256	S257	T258	S260	Y261	S262	G263	S264	K265	T266	R267	G268	A269	A270	G271	Q272	Q273	Y274	D275	D276	S277	N278	M279	G280	Q281	N282	K283	V284	G285	L286	S287	F288	S289	L290	P291	I292	Y293	Q294	G295	G296	M297	V298	N299	S300		
Q301	V302	K303	Q304	A305	Q306	Y307	M308	F309	V310	G311	A312	S313	E314	Q315	L316	E317	S318	A319	H320	A321	S322	V323	V324	Q325	T326	V327	R328	S329	S330	F331	N332	N333	I334	N335	D336	A336	S337	I338	S339	S340	T341	N342	A343	Y344	K345	Q346	A347	V348	V349	S350	A351	Q352	S353	S354	L355	D356	A357	M358	E359	A360
G361	Y362	S363	V364	G365	T366	R367	T368	I369	V370	D371	V372	L373	D374	A375	T376	T377	T378	L379	Y380	N381	A382	K383	Q384	E385	L386	A387	N388	A389	R390	Y391	N392	Y393	L394	I395	N396	Q397	L398	N399	I400	K401	A402	A403	L404	G405	A406	L407	N408	E409	Q410	D411	L412	L413	A414	L415	N416	M417	A418	L419	S420	
K421	P422	V423	S424	T425	N426	A427	E428	ASN	VAL	ALA	PRO	THR	GLN	PRO	GLU	ASN	ALA	ILE	ALA	ASP	TYR	PRO	ASP	SER	ALA	VAL	CLN	GLN	THR	SER	ALA	ARG	THR	THR	THR	SER	ASN	GLY	HIS	ASN	PRO	PHE	ARG	ASN	ASP	THR	LYS	ASP	ASP	ASP	LYS									

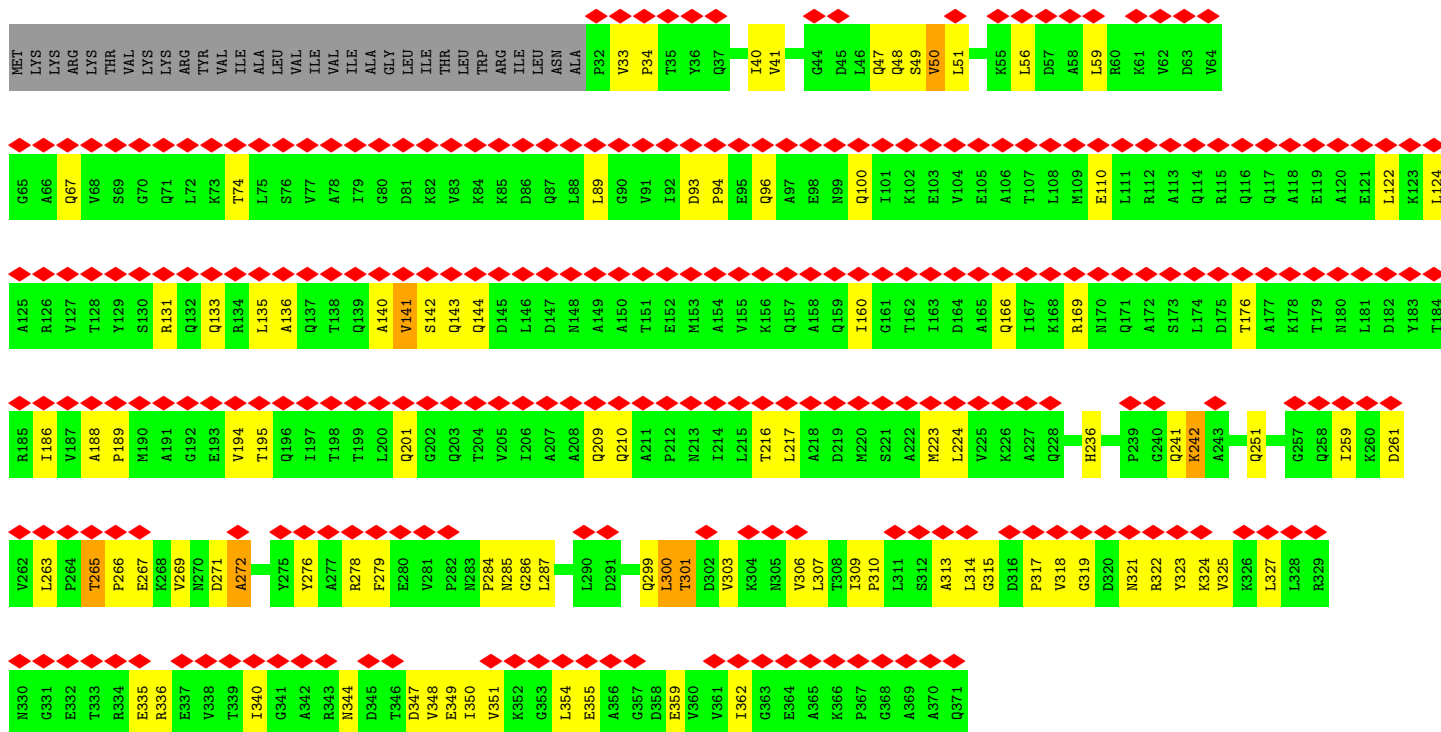
• Molecule 1: Outer membrane protein TolC



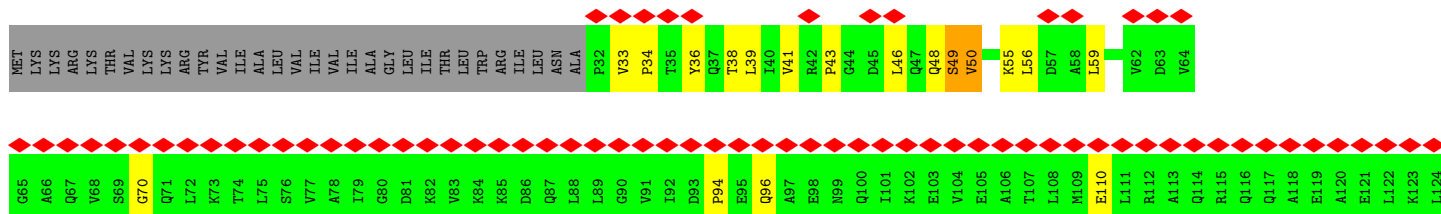
E1	N2	L3	M4	Q5	V6	Y7	Q8	Q9	A10	R11	L12	S13	M14	P15	E16	L17	R18	K19	S20	A21	A22	D23	R24	D25	A26	A27	F28	E29	K30	I31	N32	E33	A34	R35	S36	P37	L38	L39	P40	Q41	L42	G43	L44	G45	A46	D47	Y48	T49	Y50	S51	N52	G53	Y54	R55	D56	A57	N58	G59	I60	
M61	S62	M63	A64	T65	S66	A67	S68	L69	Q70	L71	T72	Q73	S74	I75	F76	D77	M78	S79	K80	M81	A82	A83	L84	T85	L86	Q87	E88	R89	A90	A91	G92	I93	Q94	D95	V96	T97	Y98	Q99	T100	D101	Q102	Q103	T104	L105	A106	L107	M108	T109	A110	T111	A112	Y113	F114	M115	V116	L117	M118	A119	T120	
D121	V122	L123	S124	Y125	T126	Q127	A128	Q129	K130	E131	A132	I133	Y134	R135	Q136	L137	D138	Q139	T140	T141	Q142	R143	F144	M145	L146	G147	L148	V149	A150	I151	T152	D153	V154	Q155	D156	M156	A157	R158	A159	Q160	Y161	D162	T163	V164	L165	A166	M167	E168	L169	T170	A171	L172	M173	M174	L175	D176	M177	V178	V179	E180
Q181	L182	R183	Q184	I185	T186	G187	M188	Y189	Y190	P191	E192	L193	A194	A195	L196	M197	V198	E199	N200	F201	K202	T203	D204	K205	P206	Q207	P208	V209	N210	A211	L212	L213	K214	E215	V216	A216	E217	K218	R219	N220	L221	S222	L223	L224	Q225	A226	R227	L228	S229	Q230	D231	L232	R234	E235	Q236	I237	R238	Q239	A240	
Q241	D242	G243	H244	L245	P246	T247	L248	D249	L250	T251	A252	S253	T254	G255	T256	S257	T258	S260	Y261	S262	G263	S264	K265	T266	R267	G268	A269	A270	G271	Q272	Q273	Y274	D275	D276	S277	N278	M279	G280	Q281	N282	K283	V284	G285	L286	S287	F288	S289	L290	P291	I292	Y293	Q294	G295	G296	M297	V298	N299	S300		

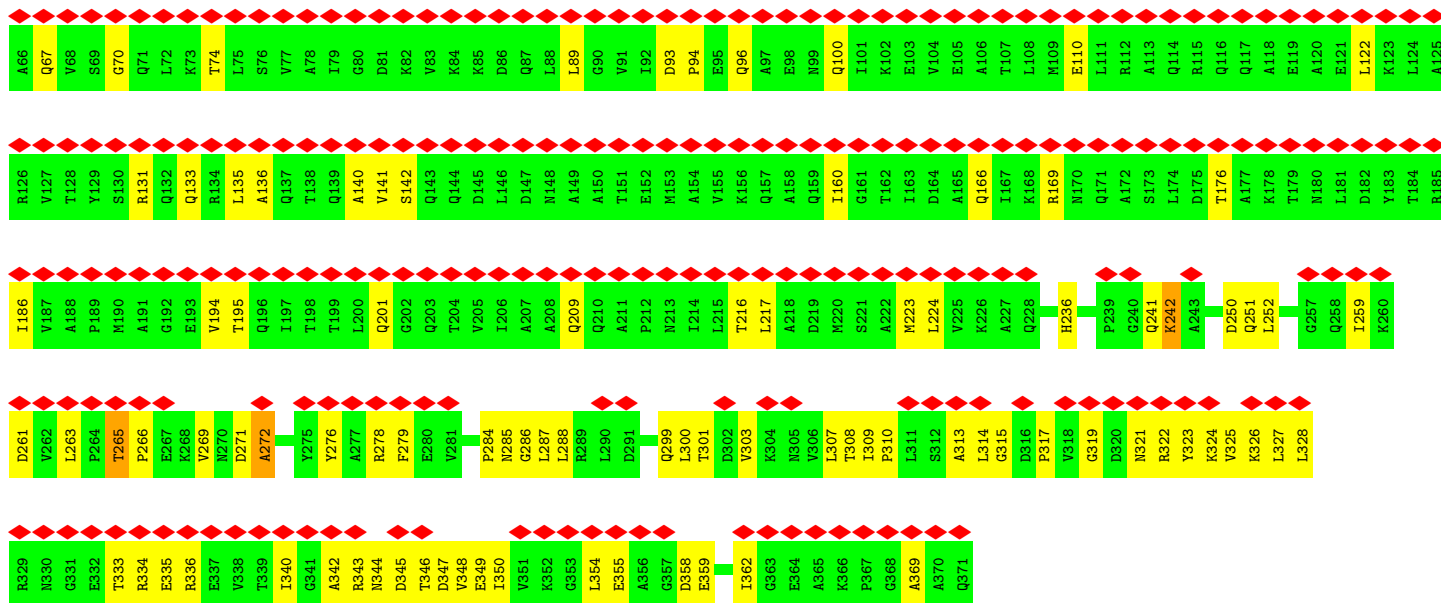


• Molecule 2: Macrolide export protein MacA

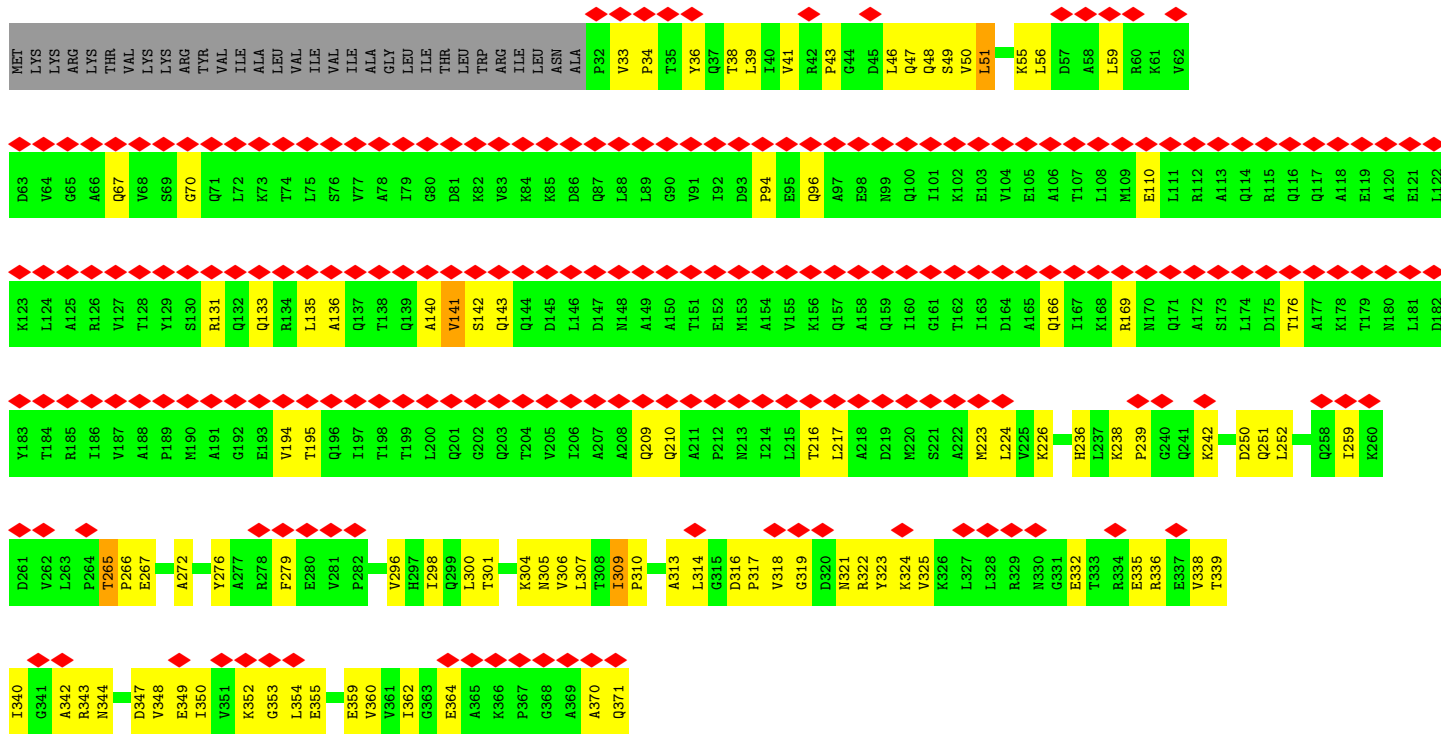


• Molecule 2: Macrolide export protein MacA



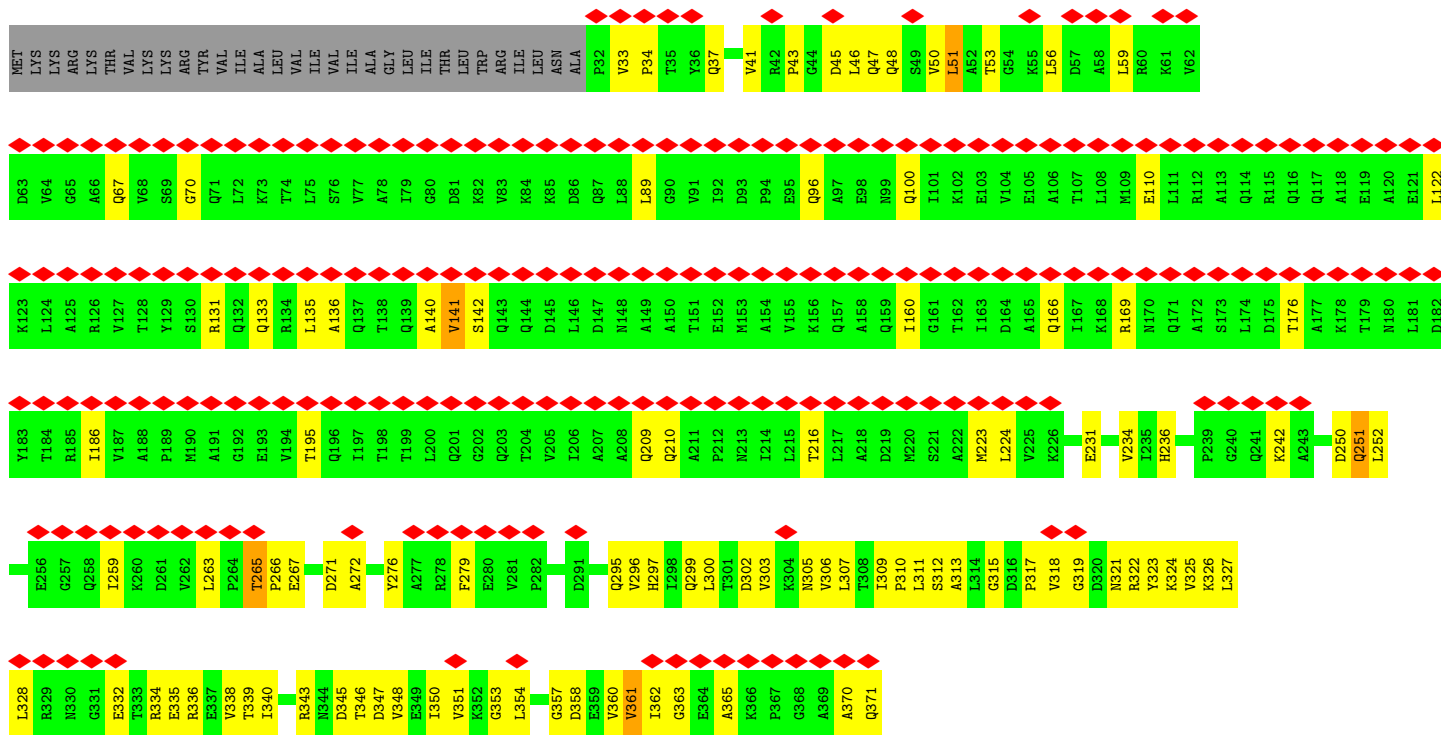


• Molecule 2: Macrolide export protein MacA

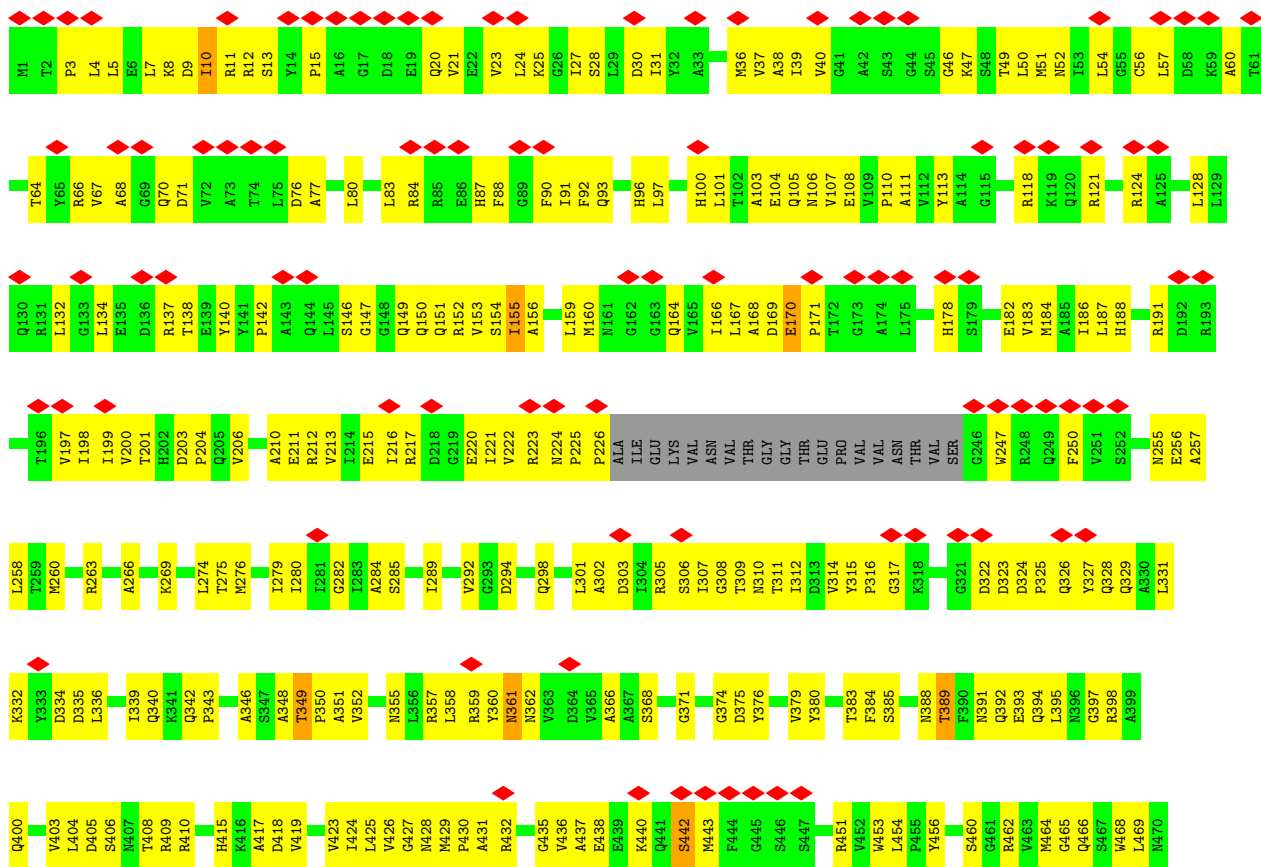


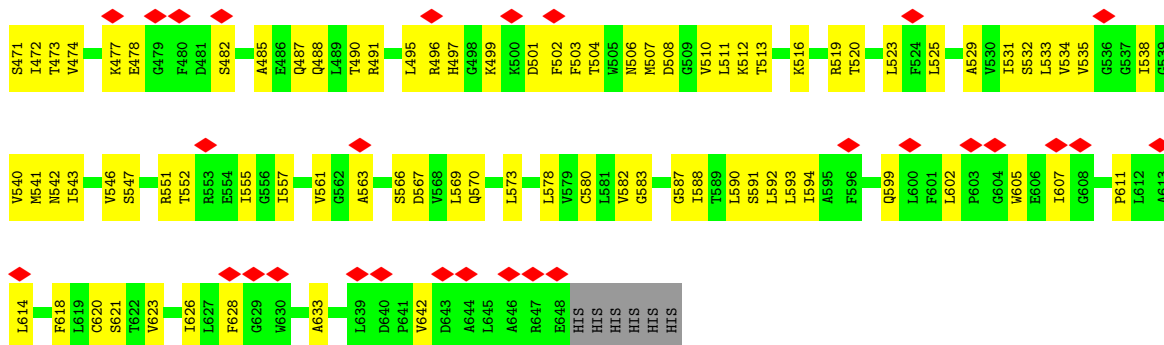
• Molecule 2: Macrolide export protein MacA



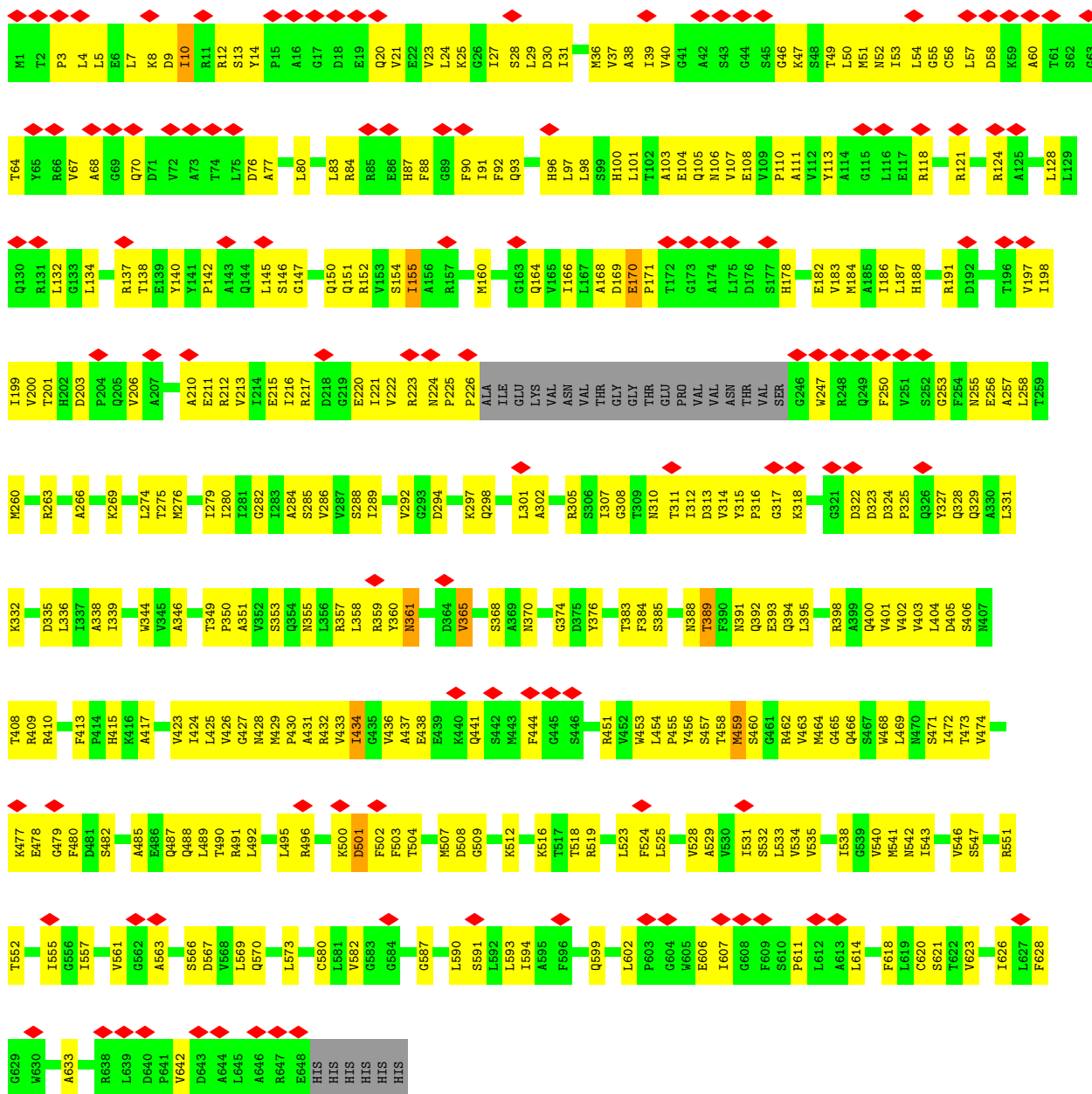


• Molecule 3: Macrolide export ATP-binding/permease protein MacB





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



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 (\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 (\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	0.55	0/3346	0.87	4/4545 (0.1%)
1	B	0.54	0/3346	0.85	3/4545 (0.1%)
1	C	0.54	0/3346	0.85	2/4545 (0.0%)
2	D	0.33	0/2631	0.78	2/3568 (0.1%)
2	E	0.33	0/2630	0.84	8/3565 (0.2%)
2	F	0.33	0/2630	0.79	2/3565 (0.1%)
2	G	0.32	0/2631	0.80	4/3568 (0.1%)
2	H	0.33	0/2631	0.84	7/3568 (0.2%)
2	I	0.33	0/2631	0.79	2/3568 (0.1%)
3	J	0.40	0/4914	0.82	3/6661 (0.0%)
3	K	0.40	0/4914	0.81	5/6661 (0.1%)
All	All	0.42	0/35650	0.82	42/48359 (0.1%)

There are no bond length outliers.

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	J	349	THR	CA-C-N	8.83	128.87	119.78
3	J	349	THR	C-N-CA	8.83	128.87	119.78
2	G	33	VAL	CA-C-N	8.39	128.12	119.56
2	G	33	VAL	C-N-CA	8.39	128.12	119.56
2	E	33	VAL	CA-C-N	8.04	128.12	119.28

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	173	0
1	B	3305	0	3256	148	0
1	C	3305	0	3256	164	0
2	D	2604	0	2678	137	0
2	E	2604	0	2678	95	0
2	F	2604	0	2677	139	0
2	G	2604	0	2679	134	0
2	H	2604	0	2678	87	0
2	I	2604	0	2679	125	0
3	J	4838	0	4930	317	0
3	K	4838	0	4930	323	0
All	All	35215	0	35697	1572	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 1572 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%)	6	30
1	B	426/479 (89%)	400 (94%)	20 (5%)	6 (1%)	9	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	426/479 (89%)	398 (93%)	19 (4%)	9 (2%)	5	28
2	D	338/371 (91%)	305 (90%)	25 (7%)	8 (2%)	4	25
2	E	336/371 (91%)	306 (91%)	21 (6%)	9 (3%)	4	24
2	F	336/371 (91%)	301 (90%)	25 (7%)	10 (3%)	3	22
2	G	338/371 (91%)	307 (91%)	26 (8%)	5 (2%)	8	38
2	H	338/371 (91%)	307 (91%)	24 (7%)	7 (2%)	5	28
2	I	338/371 (91%)	304 (90%)	27 (8%)	7 (2%)	5	28
3	J	623/654 (95%)	567 (91%)	48 (8%)	8 (1%)	9	40
3	K	623/654 (95%)	571 (92%)	41 (7%)	11 (2%)	6	32
All	All	4548/4971 (92%)	4167 (92%)	293 (6%)	88 (2%)	8	30

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%)	84	83
2	E	281/308 (91%)	281 (100%)	0	100	100
2	F	281/308 (91%)	280 (100%)	1 (0%)	84	83
2	G	281/308 (91%)	281 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	281/308 (91%)	279 (99%)	2 (1%)	76	80
2	I	281/308 (91%)	280 (100%)	1 (0%)	84	83
3	J	515/537 (96%)	513 (100%)	2 (0%)	84	83
3	K	515/537 (96%)	513 (100%)	2 (0%)	84	83
All	All	3790/4125 (92%)	3781 (100%)	9 (0%)	85	85

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	K	10	ILE
3	K	155	ILE
2	H	51	LEU
2	I	51	LEU
3	J	10	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 107 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	96	GLN
2	G	330	ASN
3	K	355	ASN
2	F	48	GLN
2	F	297	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 [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

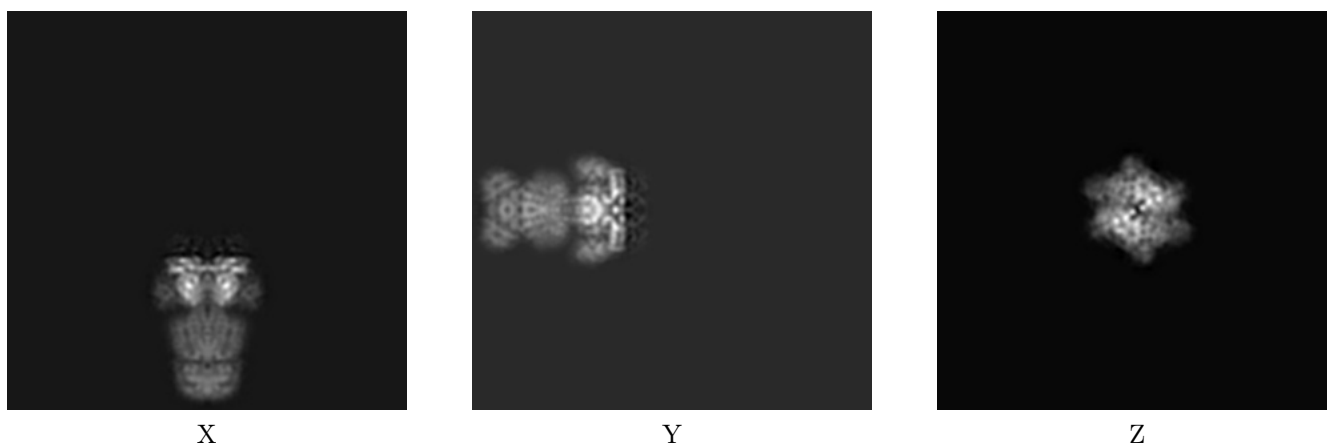
6 Map visualisation [i](#)

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](#)

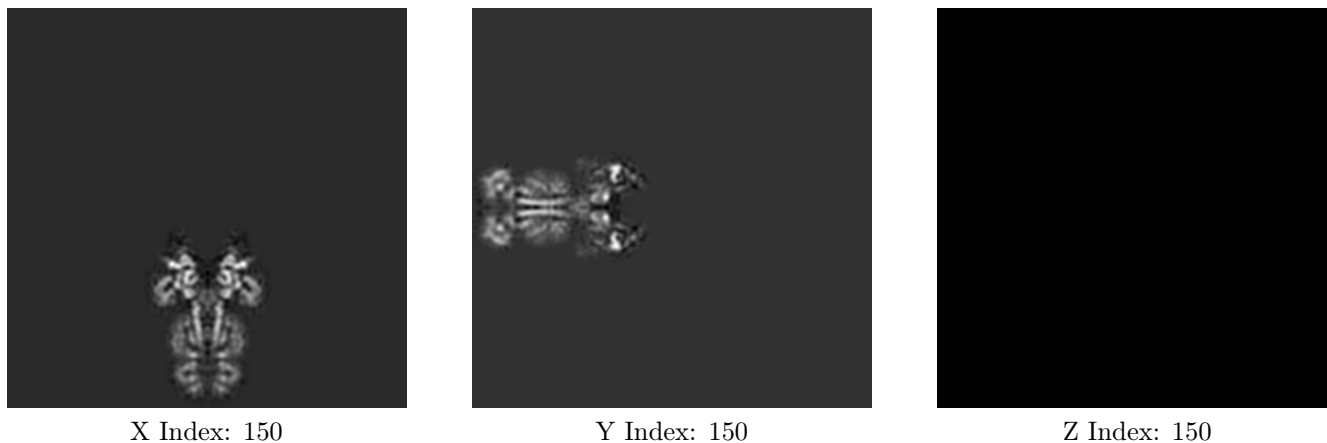
6.1.1 Primary map



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

6.2 Central slices [i](#)

6.2.1 Primary map



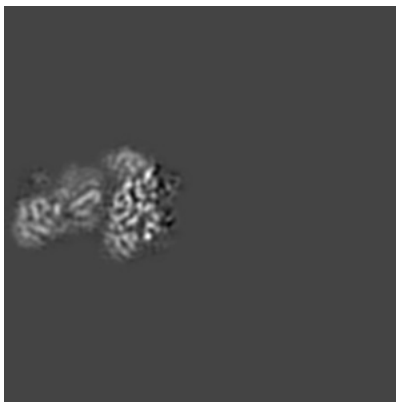
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

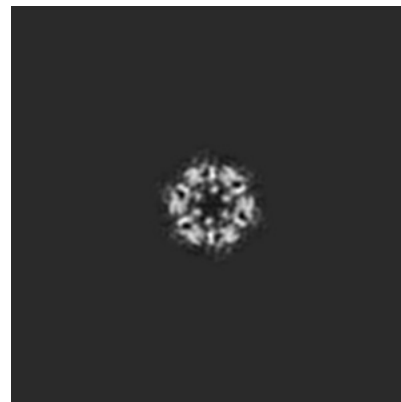
6.3.1 Primary map



X Index: 150



Y Index: 137



Z Index: 106

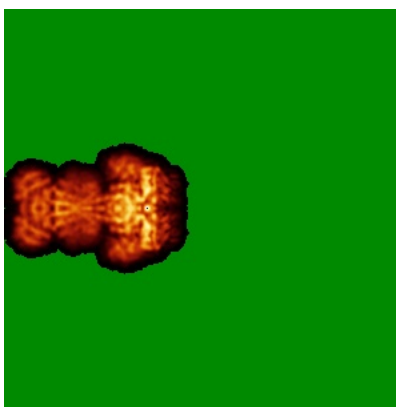
The images above show the largest variance slices of the map in three orthogonal directions.

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

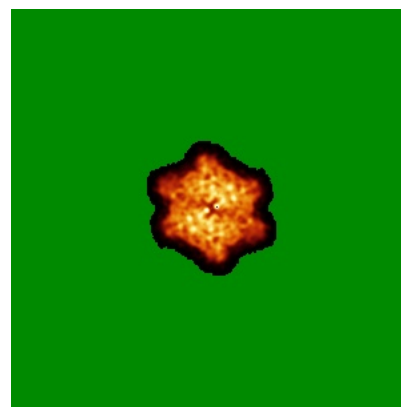
6.4.1 Primary map



X



Y

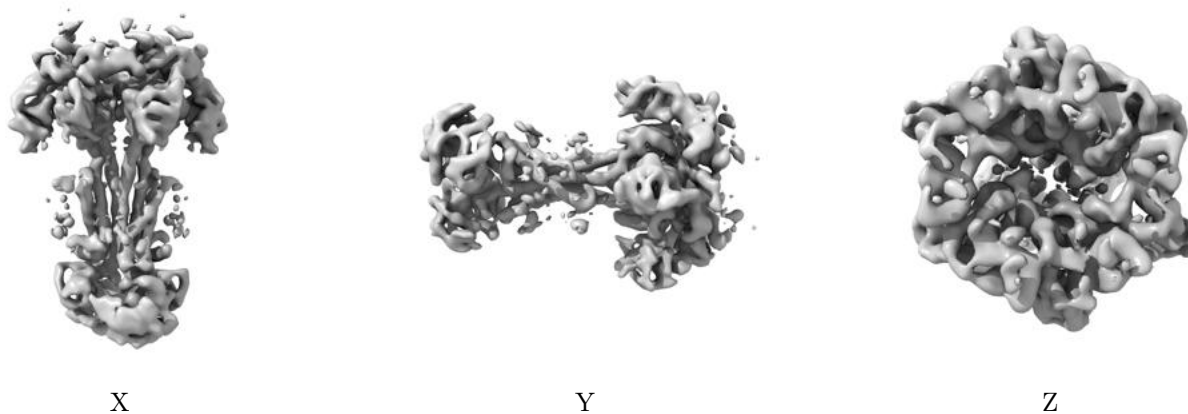


Z

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 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

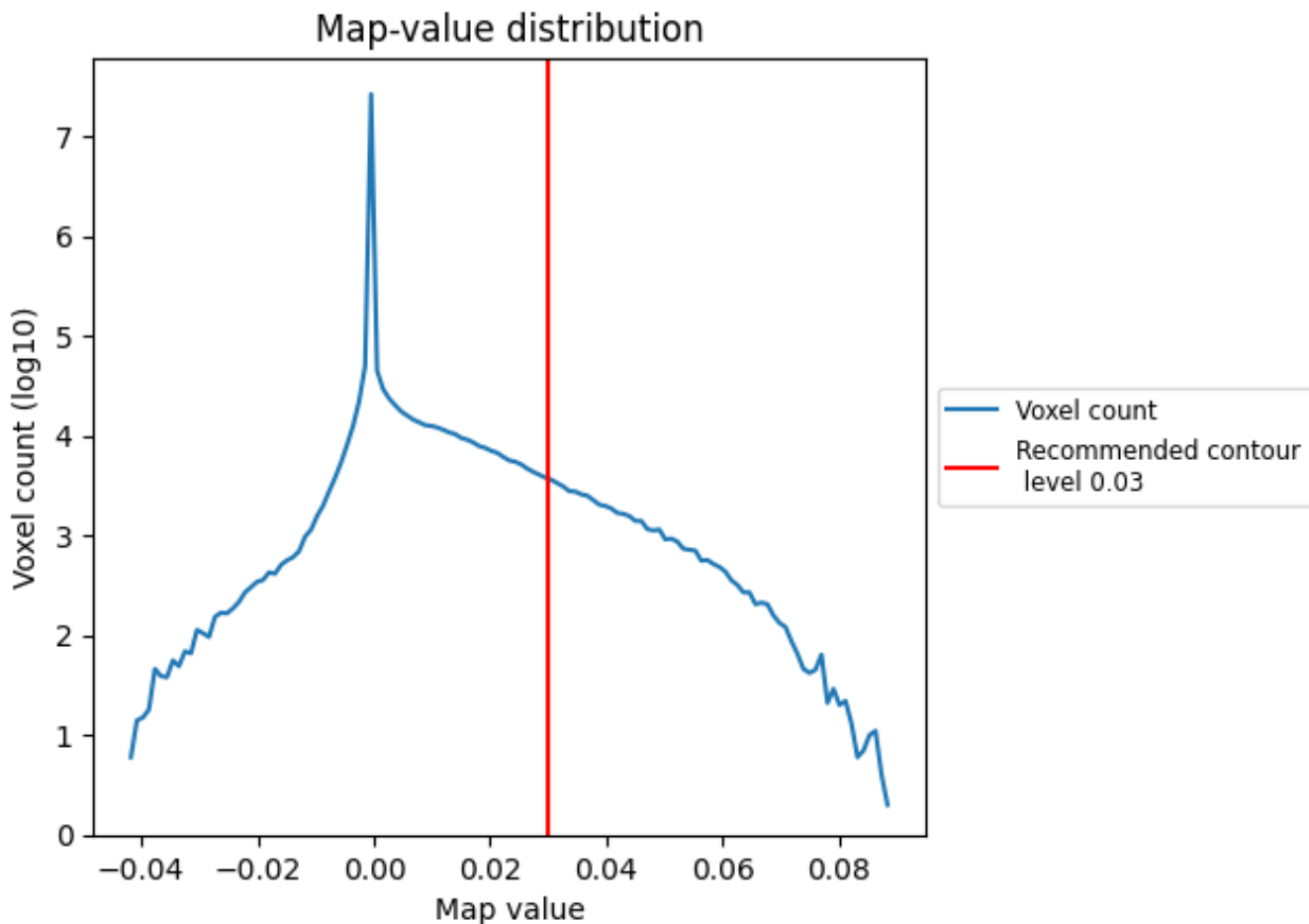
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

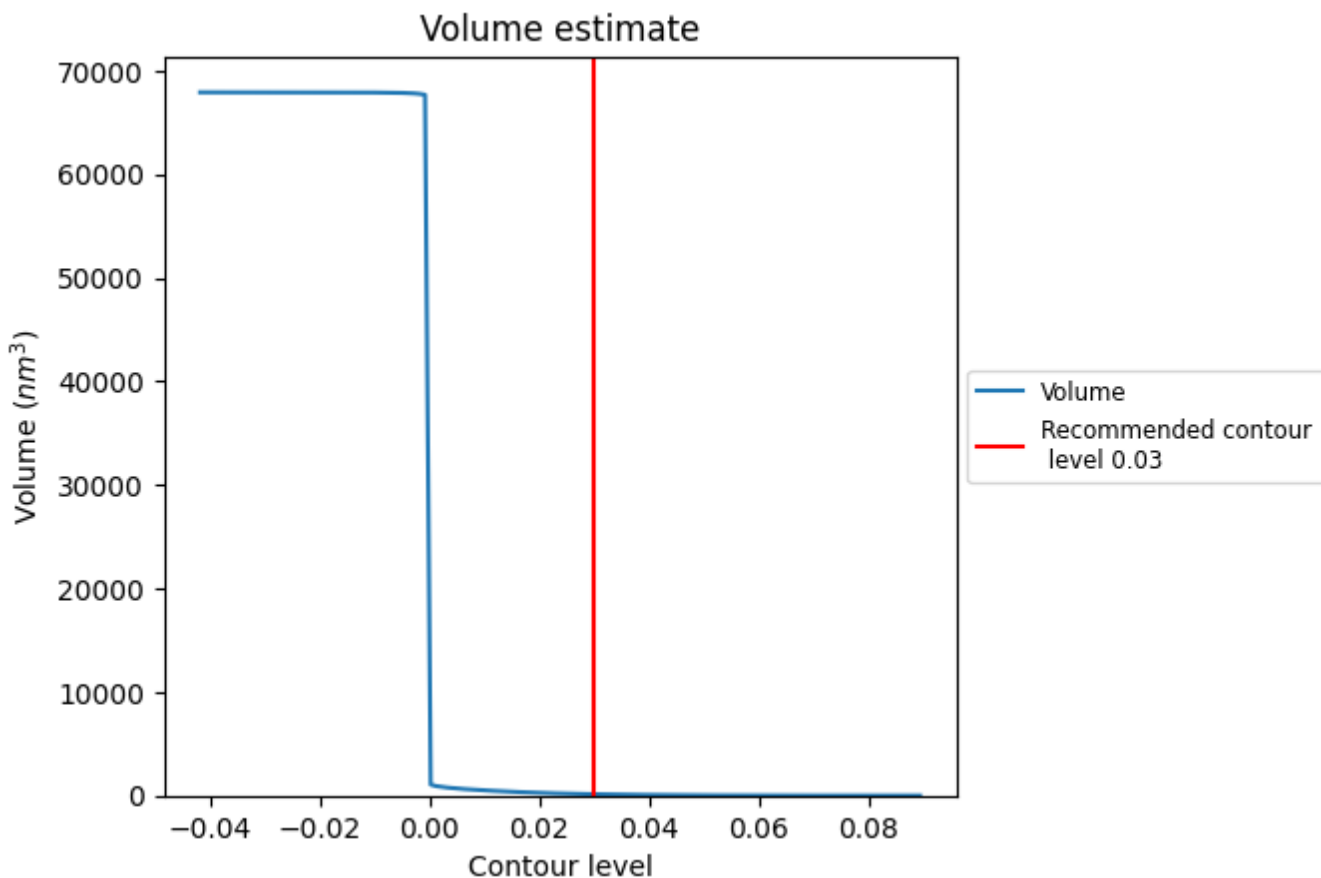
This section contains the results of statistical analysis of the map.

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.

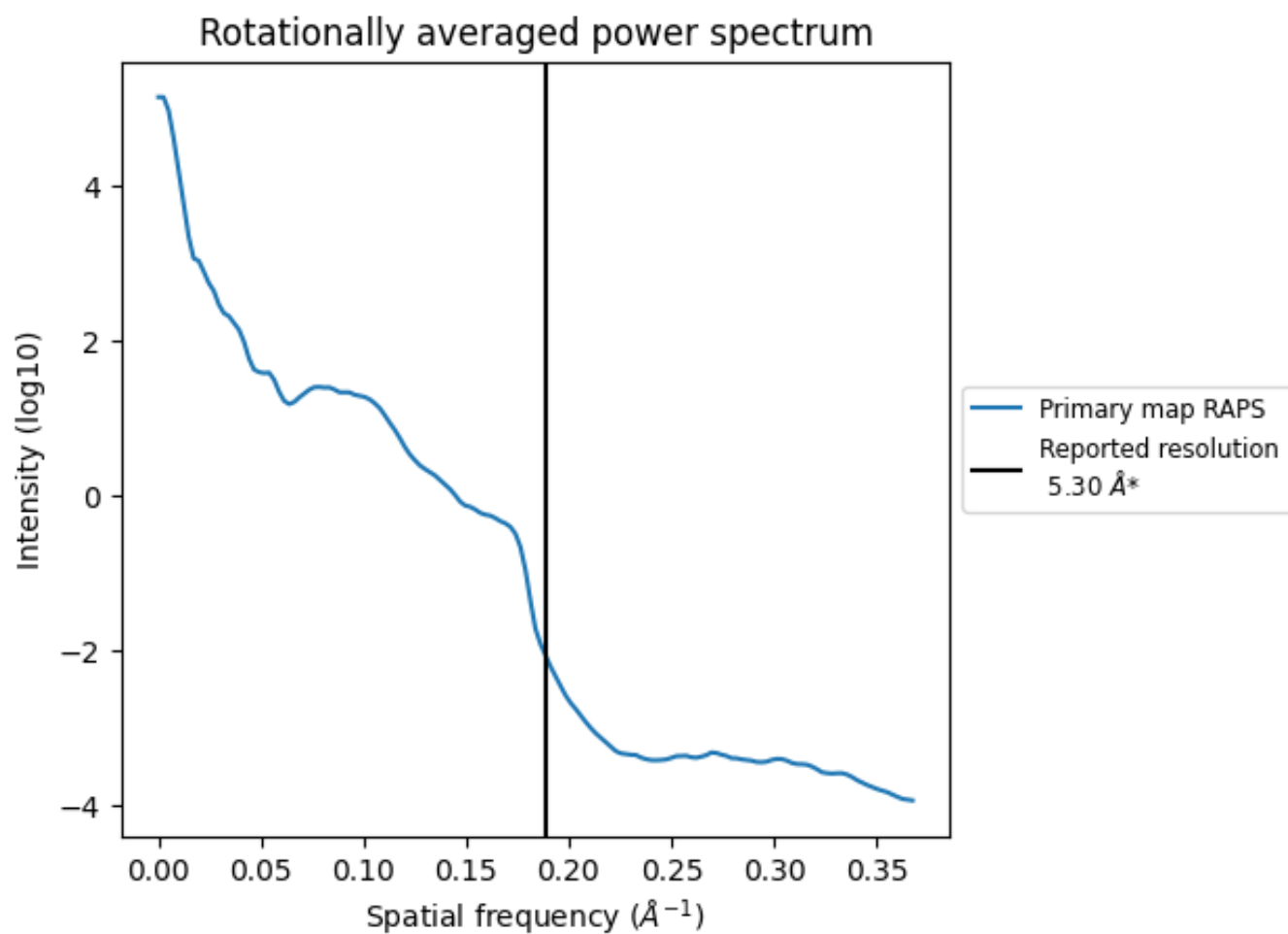
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 131 nm³; 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\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](#)

This section was not generated.

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

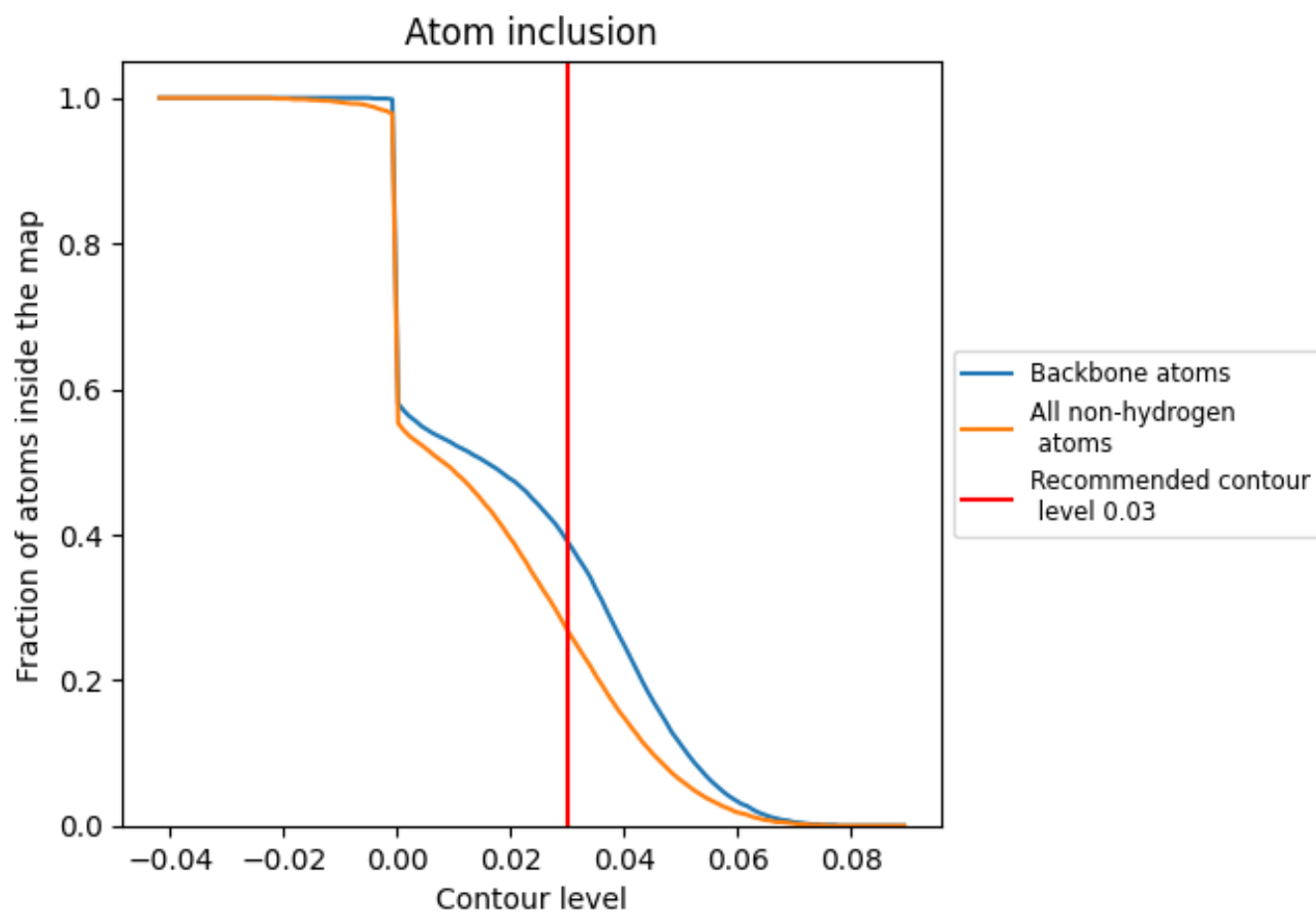


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

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	0.2690	0.1080
A	0.0000	0.0000
B	0.0000	0.0000
C	0.0000	0.0000
D	0.1950	0.1140
E	0.2760	0.1250
F	0.2760	0.1230
G	0.1990	0.1120
H	0.2800	0.1230
I	0.2740	0.1230
J	0.5760	0.1990
K	0.5770	0.2010

