



wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 05:48 pm GMT

PDB ID : 5O66
EMDB ID : EMD-8640
Title : Asymmetric AcrABZ-TolC
Authors : Du, D.; Luisi, B.F.
Deposited on : 2017-06-05
Resolution : 5.90 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

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.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

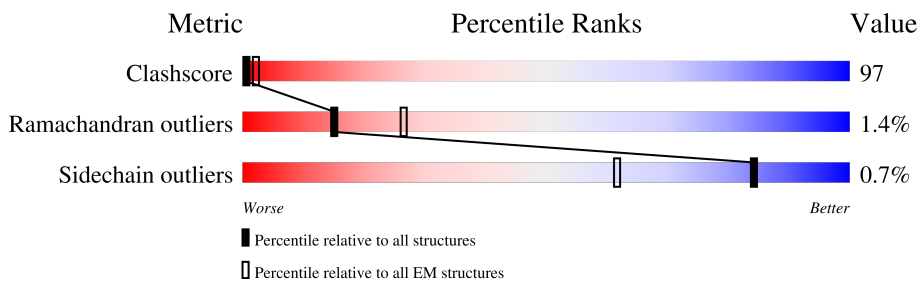
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.90 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 ≥ 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	493	
1	B	493	
1	C	493	
2	D	373	
2	E	373	
2	F	373	
2	G	373	
2	H	373	

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Mol	Chain	Length	Quality of chain
2	I	373	
3	J	1049	
3	K	1049	
3	L	1049	
4	M	54	
4	N	54	
4	O	54	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 49671 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	3304	2037	586	676	5	0	0
1	B	428	3304	2037	586	676	5	0	0
1	C	428	3304	2037	586	676	5	0	0

- Molecule 2 is a protein called Multidrug efflux pump subunit AcrA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	340	2553	1591	451	506	5	0	0
2	E	340	2553	1591	451	506	5	0	0
2	F	340	2553	1591	451	506	5	0	0
2	G	340	2553	1591	451	506	5	0	0
2	H	340	2553	1591	451	506	5	0	0
2	I	340	2553	1591	451	506	5	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	223	MET	PHE	conflict	UNP P0AE07
D	224	MET	LEU	conflict	UNP P0AE07
D	287	MET	LEU	conflict	UNP P0AE07
D	288	MET	LEU	conflict	UNP P0AE07
E	223	MET	PHE	conflict	UNP P0AE07
E	224	MET	LEU	conflict	UNP P0AE07
E	287	MET	LEU	conflict	UNP P0AE07

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Chain	Residue	Modelled	Actual	Comment	Reference
E	288	MET	LEU	conflict	UNP P0AE07
F	223	MET	PHE	conflict	UNP P0AE07
F	224	MET	LEU	conflict	UNP P0AE07
F	287	MET	LEU	conflict	UNP P0AE07
F	288	MET	LEU	conflict	UNP P0AE07
G	223	MET	PHE	conflict	UNP P0AE07
G	224	MET	LEU	conflict	UNP P0AE07
G	287	MET	LEU	conflict	UNP P0AE07
G	288	MET	LEU	conflict	UNP P0AE07
H	223	MET	PHE	conflict	UNP P0AE07
H	224	MET	LEU	conflict	UNP P0AE07
H	287	MET	LEU	conflict	UNP P0AE07
H	288	MET	LEU	conflict	UNP P0AE07
I	223	MET	PHE	conflict	UNP P0AE07
I	224	MET	LEU	conflict	UNP P0AE07
I	287	MET	LEU	conflict	UNP P0AE07
I	288	MET	LEU	conflict	UNP P0AE07

- Molecule 3 is a protein called Multidrug efflux pump subunit AcrB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	J	1044	Total	C	N	O	S	0	0
			7908	5086	1308	1470	44		
3	K	1033	Total	C	N	O	S	0	0
			7845	5049	1294	1458	44		
3	L	1033	Total	C	N	O	S	0	0
			7845	5049	1294	1458	44		

- Molecule 4 is a protein called Multidrug efflux pump accessory protein AcrZ.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	M	36	Total	C	N	O	S	0	0
			277	193	38	43	3		
4	N	37	Total	C	N	O	S	0	0
			283	196	39	45	3		
4	O	37	Total	C	N	O	S	0	0
			283	196	39	45	3		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	50	HIS	-	expression tag	UNP P0AAX1

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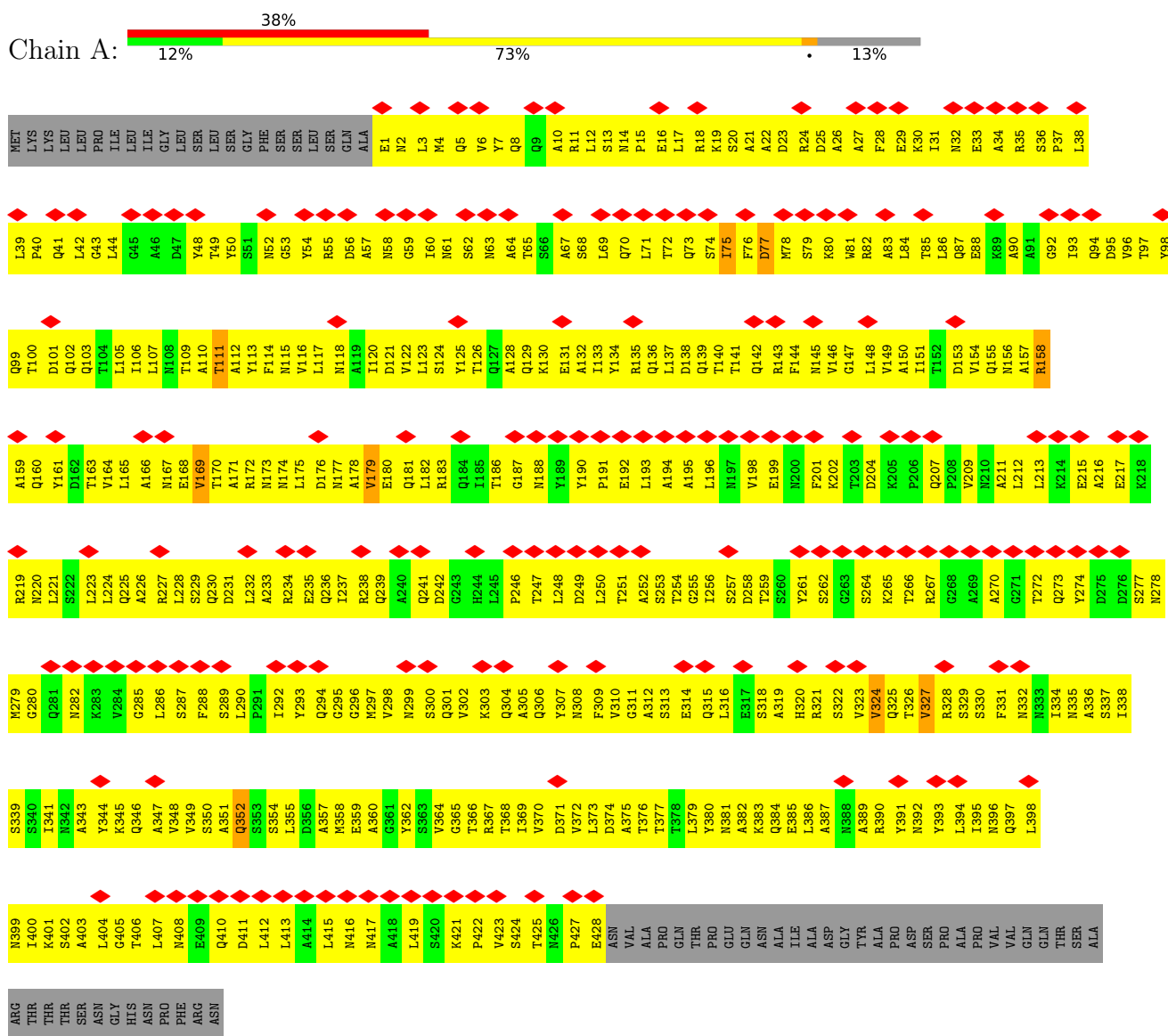
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Chain	Residue	Modelled	Actual	Comment	Reference
M	51	HIS	-	expression tag	UNP P0AAX1
M	52	HIS	-	expression tag	UNP P0AAX1
M	53	HIS	-	expression tag	UNP P0AAX1
M	54	HIS	-	expression tag	UNP P0AAX1
N	50	HIS	-	expression tag	UNP P0AAX1
N	51	HIS	-	expression tag	UNP P0AAX1
N	52	HIS	-	expression tag	UNP P0AAX1
N	53	HIS	-	expression tag	UNP P0AAX1
N	54	HIS	-	expression tag	UNP P0AAX1
O	50	HIS	-	expression tag	UNP P0AAX1
O	51	HIS	-	expression tag	UNP P0AAX1
O	52	HIS	-	expression tag	UNP P0AAX1
O	53	HIS	-	expression tag	UNP P0AAX1
O	54	HIS	-	expression tag	UNP P0AAX1

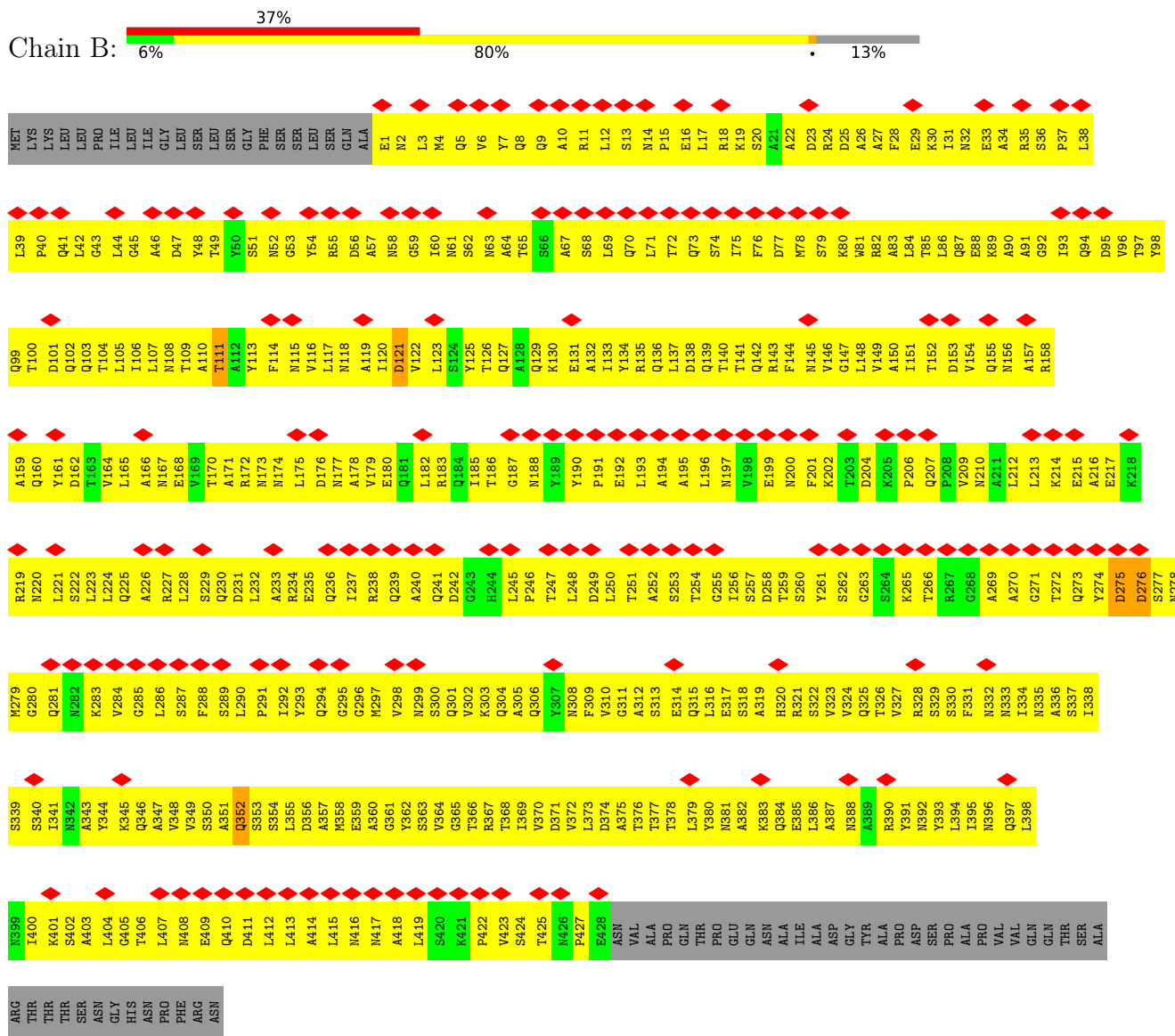
3 Residue-property plots [i](#)

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.

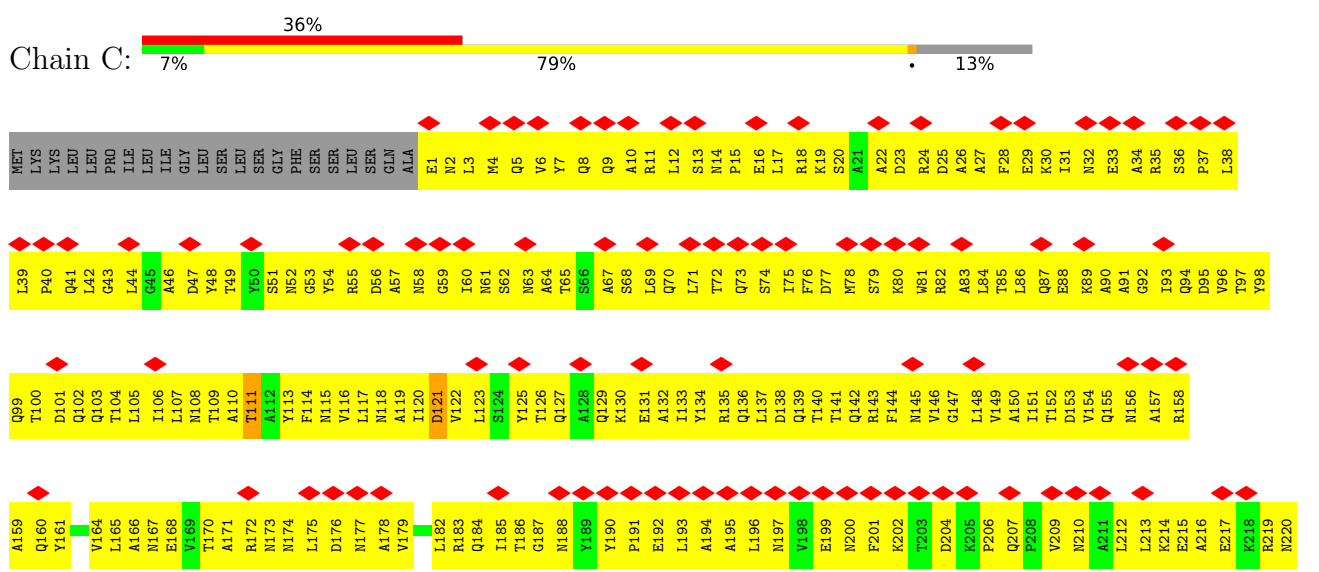
- Molecule 1: Outer membrane protein TolC



- Molecule 1: Outer membrane protein TolC

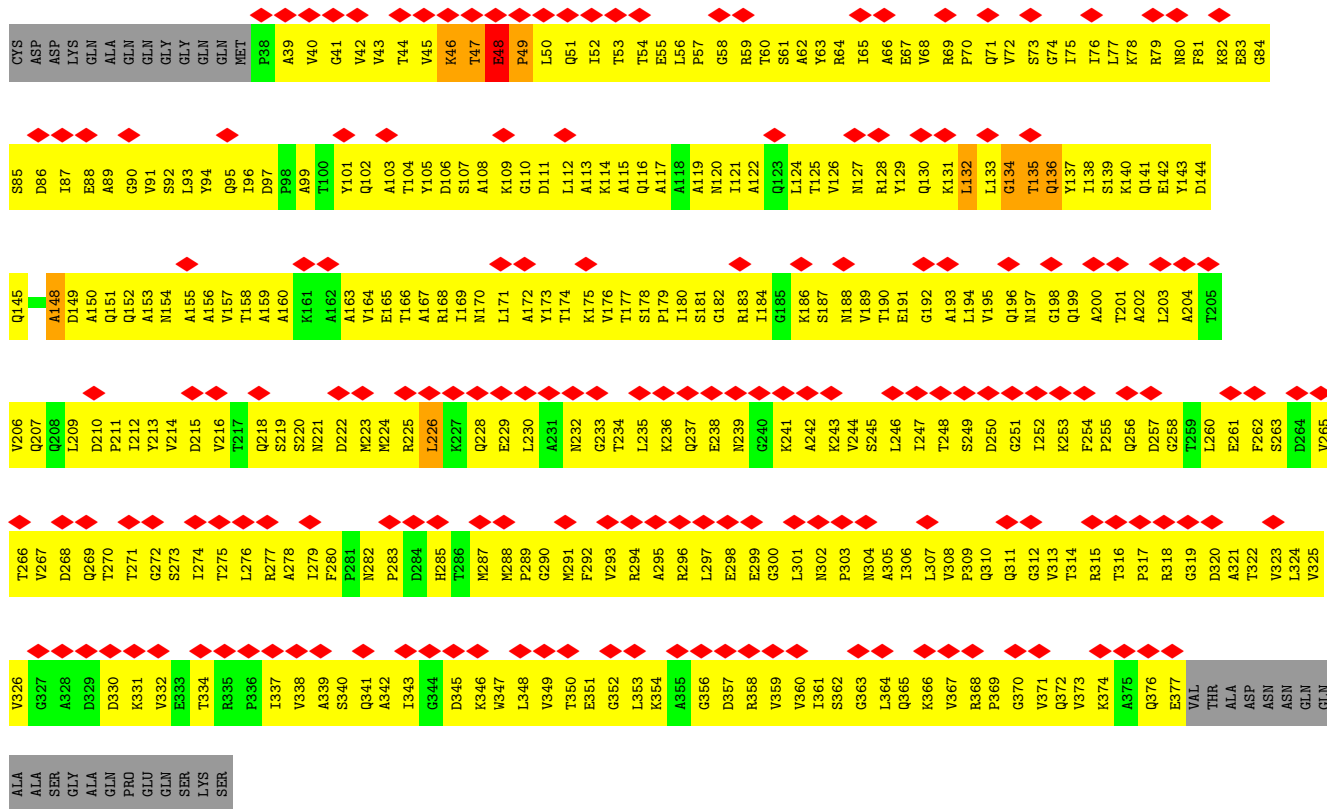


• Molecule 1: Outer membrane protein TolC

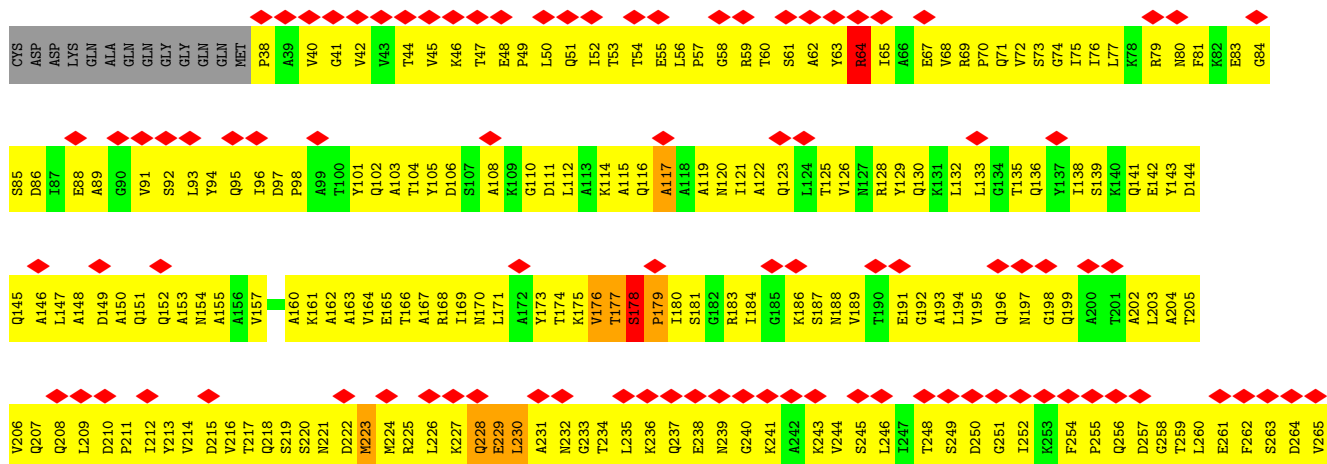
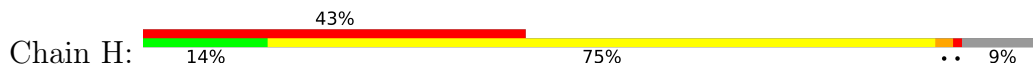


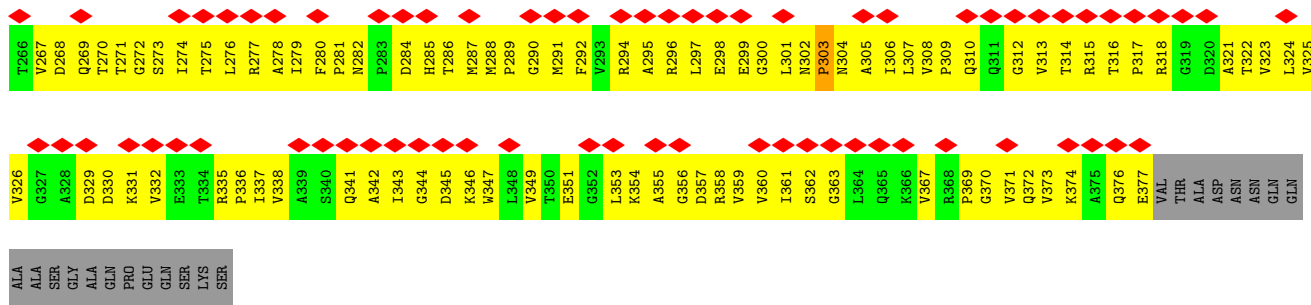
GLN
ALA
ALA
ASP
SER
GLY
GLN
ALA
GLN
GLN
PRO
GLU
GLY
GLN
SER
LYS
SER

• Molecule 2: Multidrug efflux pump subunit AcrA

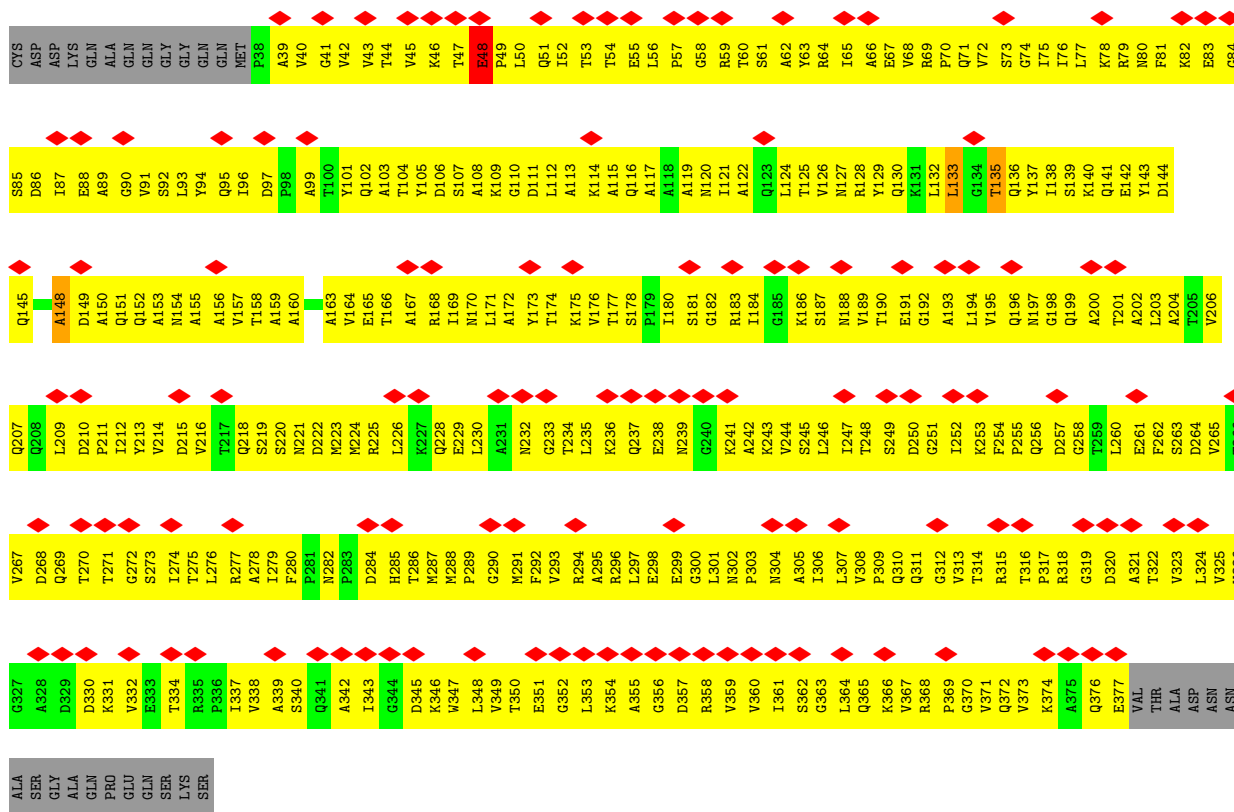


• Molecule 2: Multidrug efflux pump subunit AcrA

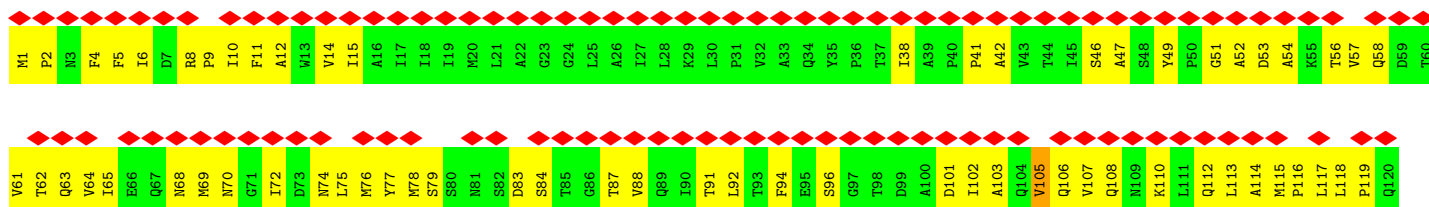
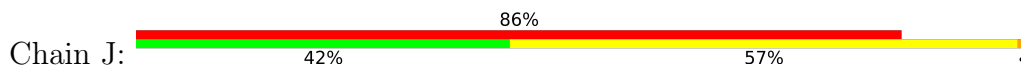


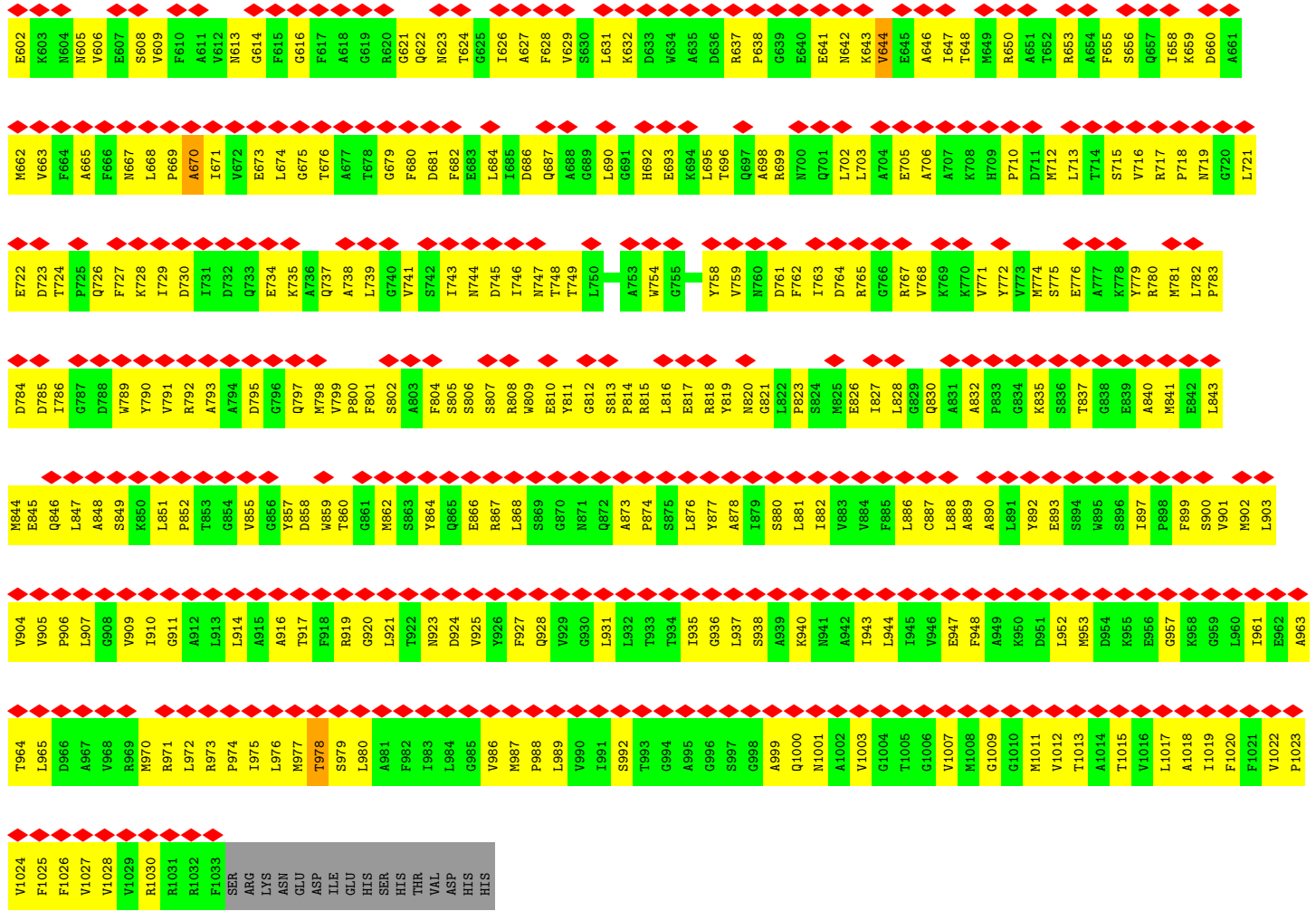


• Molecule 2: Multidrug efflux pump subunit AcrA

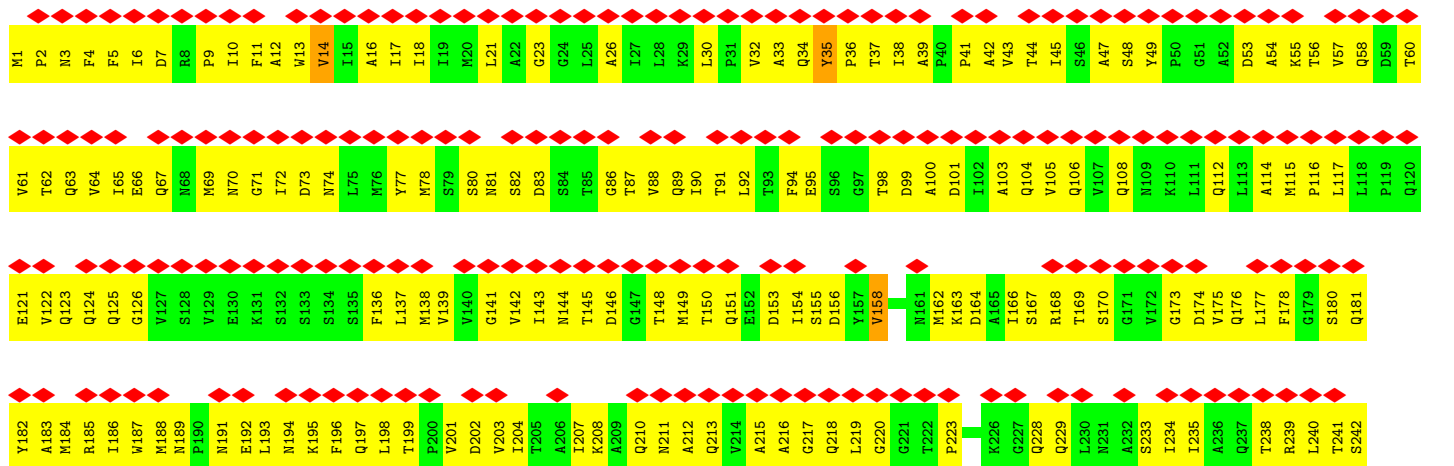
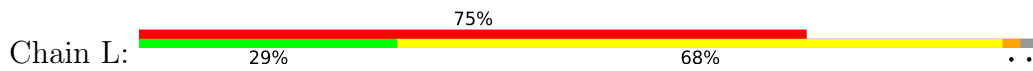


• Molecule 3: Multidrug efflux pump subunit AcrB

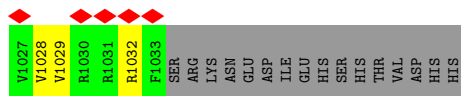




• Molecule 3: Multidrug efflux pump subunit AcrB



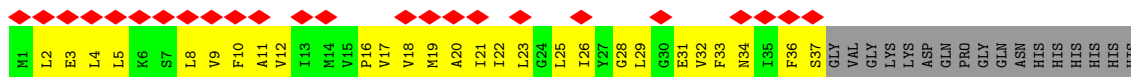
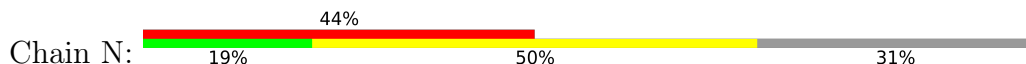
T243	A303	R363	E423	L483	V543	N603	F663	T723	D783	E843	V903
E244	A304	A364	E244	V484	L544	N604	A665	F725	L786	D846	P906
E245	A305	T365	E245	A485	Y645	V606	F666	F726	G787	L847	L907
F246	I306	T366	F246	L486	L546	E607	N667	Q727	D788	A848	G908
G247	R307	I367	G247	L487	I547	S608	L668	K728	D789	S849	V909
K248	A308	F368	K248	L488	I548	V609	P669	L729	W790	R850	T910
L249	E309	T369	L249	L489	F549	F610	A670	D730	V791	L851	G911
L250	L310	I370	L250	P490	V550	A611	L671	Q733	R792	P852	A912
L251	A311	A371	L251	A491	G511	N613	V672	E734	A793	T853	L913
K252	K312	V372	K252	L492	M552	G614	E673	K735	A794	G854	L914
V253	M313	P373	V253	C493	M553	F615	L674	A736	D795	A915	L915
K254	E314	V374	K254	A494	Y554	G616	G675	Q737	G796	G855	A916
Q255	P315	V375	Q255	M495	V555	F617	T676	A738	Q797	T856	T917
D256	F316	L376	D256	L497	V557	A618	A677	L739	W798	Y857	T918
G257	F317	L377	G257	L498	R558	A619	T678	G740	W799	D858	F918
S258	P318	G378	S258	I438	L559	R620	G679	V741	F800	W859	R919
R259	G319	T379	R259	Q439	P499	G621	F680	S742	F801	T860	G920
L261	G320	F380	L261	G440	I500	Q622	D681	N743	A803	S861	L921
L262	L321	F381	L262	A441	A501	N623	F682	N744	F804	S862	T922
R263	K322	V382	R263	L442	K502	T624	E683	I746	S805	S863	N923
D264	I323	L383	D264	L443	G503	G625	L684	N747	S806	Y864	L984
V265	V324	A384	V265	V443	D604	G626	L685	T748	S807	G865	Y925
A266	Y325	A385	A266	G444	H505	A627	L686	T749	R808	E866	Y926
K267	P326	F386	K267	I445	G506	F628	D686	T750	W809	R867	F927
I268	Y327	G387	I268	A446	E507	V629	E687	L751	E810	L868	L989
E269	D328	F388	E269	M447	S508	S630	A688	G751	Y811	G869	G930
L270	T329	F389	L270	M448	G509	L631	G689	A752	C812	S869	L931
G271	T330	S389	G271	V448	K510	L632	Q689	A753	S813	G870	L932
G272	T331	I390	G272	L449	G511	D633	Q690	A754	P814	N871	T933
E273	P331	N391	E273	S450	F512	W634	H691	G755	R815	G872	Y934
N274	F332	T392	N274	A451	F513	A635	H692	G756	L816	S757	I935
Y275	G333	L393	Y275	V452	G514	D636	E693	Y758	E817	F758	G936
D276	K334	T394	D276	F453	W515	R637	K694	V759	R818	W759	G937
I277	I335	T395	I277	V454	F516	F638	L695	N760	R819	N760	L937
I278	S336	M395	I278	P455	N517	Q639	T696	A761	N820	G761	S938
A279	G337	F396	A279	M456	R518	E640	Q697	F762	A698	F762	A939
E280	H338	G397	E280	A457	M519	E641	A698	L763	R699	L763	R940
F281	E339	M398	F281	F458	F520	N642	E641	D764	W700	D764	L941
N282	V340	V399	N282	F459	E521	K643	E642	G766	Q701	G766	A942
G283	V341	L400	G283	F459	K522	K644	E643	R767	L702	R765	L943
Q284	V342	A401	Q284	G460	S223	V644	E644	V768	L703	L703	L944
P285	K343	I402	P285	G461	T524	E645	A646	W768	A704	L704	I945
A286	T343	G403	A286	S462	H525	T648	L647	T648	E705	E705	V946
S287	L344	L404	S287	T463	Y527	T648	T648	T648	A706	A706	E947
C288	V345	L405	C288	G464	T528	R650	R650	R650	A707	A707	F948
L289	E346	V406	L289	A465	D529	Q688	A651	A651	K708	K708	A949
G290	A347	V407	G290	I466	S530	T587	T652	T652	M774	M774	K950
I291	I348	D407	I291	Y467	V531	K653	L591	L591	H709	H709	G951
K292	I349	D408	K292	R468	G532	A654	L592	E776	P710	P710	L952
L293	G350	A409	L293	Q469	G533	F655	N592	A777	D711	D711	L953
A294	L351	I410	A294	F470	I534	S656	E593	A777	M712	M712	M953
T295	F352	V411	T295	S471	L535	Q657	V594	K778	L713	L713	D954
C296	L353	V412	C296	I472	H536	R659	H596	Y779	L714	L714	K955
A297	V354	V413	A297	T473	S537	K659	H597	T714	Q657	Q657	E956
N298	F355	E414	N298	I474	T538	D660	V598	M781	S715	S715	G957
A299	M355	N415	A299	I475	G539	A661	L599	L782	V716	V716	K958
L300	L357	E417	L300	S476	R540	A661	T600	L783	R717	R717	F1020
D301	F358	R418	D301	A477	R541	E602	K601	P718	R718	R718	F1021
L302	V359	V419	L302	M478	Y541	E603	K602	P719	M719	M719	L1022
	Q360	M420		M479	L542			G720	G720	G720	L1023
	N361	A421		L480				E722	E722	E722	L1024
	F362	E422		S481				D723	D723	D723	F1026



• Molecule 4: Multidrug efflux pump accessory protein AcrZ



• Molecule 4: Multidrug efflux pump accessory protein AcrZ



• Molecule 4: Multidrug efflux pump accessory protein AcrZ



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	26950	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	0.143	Depositor
Minimum map value	-0.084	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.05	Depositor
Map size (\AA)	414.72, 414.72, 414.72	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.62, 1.62, 1.62	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	0.36	0/3345	0.51	0/4544
1	B	0.38	0/3345	0.50	0/4544
1	C	0.38	0/3345	0.50	0/4544
2	D	0.41	0/2585	0.60	0/3512
2	E	0.46	0/2585	0.61	2/3512 (0.1%)
2	F	0.41	0/2585	0.60	2/3512 (0.1%)
2	G	0.46	0/2585	0.61	2/3512 (0.1%)
2	H	0.40	0/2585	0.59	0/3512
2	I	0.44	0/2585	0.59	1/3512 (0.0%)
3	J	0.53	1/8060 (0.0%)	0.63	2/10947 (0.0%)
3	K	0.52	0/7995	0.62	0/10859
3	L	0.58	3/7995 (0.0%)	0.69	6/10859 (0.1%)
4	M	0.44	0/281	0.57	0/380
4	N	0.44	0/287	0.64	0/388
4	O	0.42	0/287	0.61	0/388
All	All	0.48	4/50450 (0.0%)	0.61	15/68525 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	283	GLY	C-N	-6.72	1.18	1.34
3	L	586	ARG	CZ-NH1	5.90	1.40	1.33
3	L	812	GLY	C-N	-5.81	1.20	1.34
3	J	117	LEU	C-N	-5.80	1.20	1.34

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	586	ARG	NE-CZ-NH2	-21.27	109.66	120.30
3	L	586	ARG	NH1-CZ-NH2	6.62	126.68	119.40
2	F	277	ARG	NE-CZ-NH1	-6.60	117.00	120.30
3	L	586	ARG	NE-CZ-NH1	6.58	123.59	120.30
3	J	250	LEU	CA-CB-CG	6.11	129.36	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3304	0	3251	929	0
1	B	3304	0	3254	1031	0
1	C	3304	0	3254	1011	0
2	D	2553	0	2607	803	0
2	E	2553	0	2610	857	0
2	F	2553	0	2608	776	0
2	G	2553	0	2610	861	0
2	H	2553	0	2610	732	0
2	I	2553	0	2610	928	0
3	J	7908	0	8018	708	0
3	K	7845	0	7990	755	0
3	L	7845	0	7988	1028	0
4	M	277	0	313	22	0
4	N	283	0	318	27	0
4	O	283	0	318	28	0
All	All	49671	0	50359	9656	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 97.

The worst 5 of 9656 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)
3:J:865:GLN:CG	3:J:868:LEU:HD11	1.23	1.65
2:H:63:TYR:CG	2:H:64:ARG:HD2	1.25	1.65
2:H:63:TYR:CB	2:H:64:ARG:HD2	1.28	1.62
2:H:93:LEU:H	2:H:176:VAL:CG1	1.07	1.62
2:H:63:TYR:CB	2:H:64:ARG:HB2	1.31	1.57

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	426/493 (86%)	371 (87%)	46 (11%)	9 (2%)	7	36
1	B	426/493 (86%)	377 (88%)	44 (10%)	5 (1%)	13	50
1	C	426/493 (86%)	378 (89%)	44 (10%)	4 (1%)	17	56
2	D	338/373 (91%)	296 (88%)	31 (9%)	11 (3%)	4	26
2	E	338/373 (91%)	287 (85%)	45 (13%)	6 (2%)	8	40
2	F	338/373 (91%)	294 (87%)	34 (10%)	10 (3%)	4	28
2	G	338/373 (91%)	283 (84%)	47 (14%)	8 (2%)	6	33
2	H	338/373 (91%)	302 (89%)	29 (9%)	7 (2%)	7	36
2	I	338/373 (91%)	288 (85%)	48 (14%)	2 (1%)	25	65
3	J	1042/1049 (99%)	971 (93%)	64 (6%)	7 (1%)	22	62
3	K	1031/1049 (98%)	982 (95%)	41 (4%)	8 (1%)	19	60
3	L	1031/1049 (98%)	953 (92%)	64 (6%)	14 (1%)	11	46
4	M	34/54 (63%)	32 (94%)	2 (6%)	0	100	100
4	N	35/54 (65%)	33 (94%)	2 (6%)	0	100	100
4	O	35/54 (65%)	33 (94%)	2 (6%)	0	100	100
All	All	6514/7026 (93%)	5880 (90%)	543 (8%)	91 (1%)	15	46

5 of 91 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	75	ILE
1	A	77	ASP
2	D	62	ALA
2	D	137	TYR
2	D	178	SER

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	358/412 (87%)	357 (100%)	1 (0%)	92	94
1	B	358/412 (87%)	358 (100%)	0	100	100
1	C	358/412 (87%)	357 (100%)	1 (0%)	92	94
2	D	274/299 (92%)	269 (98%)	5 (2%)	59	77
2	E	274/299 (92%)	272 (99%)	2 (1%)	84	90
2	F	274/299 (92%)	269 (98%)	5 (2%)	59	77
2	G	274/299 (92%)	270 (98%)	4 (2%)	65	80
2	H	274/299 (92%)	268 (98%)	6 (2%)	52	71
2	I	274/299 (92%)	270 (98%)	4 (2%)	65	80
3	J	840/855 (98%)	837 (100%)	3 (0%)	91	94
3	K	838/855 (98%)	834 (100%)	4 (0%)	88	93
3	L	838/855 (98%)	834 (100%)	4 (0%)	88	93
4	M	31/46 (67%)	31 (100%)	0	100	100
4	N	32/46 (70%)	32 (100%)	0	100	100
4	O	32/46 (70%)	32 (100%)	0	100	100
All	All	5329/5733 (93%)	5290 (99%)	39 (1%)	84	90

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	J	218	GLN
3	L	265	VAL
3	J	676	THR
3	K	230	LEU
3	L	509	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 104 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	304	ASN
3	J	254	ASN
3	L	254	ASN
2	I	51	GLN
3	J	68	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	L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	283:GLY	C	284:GLN	N	1.18

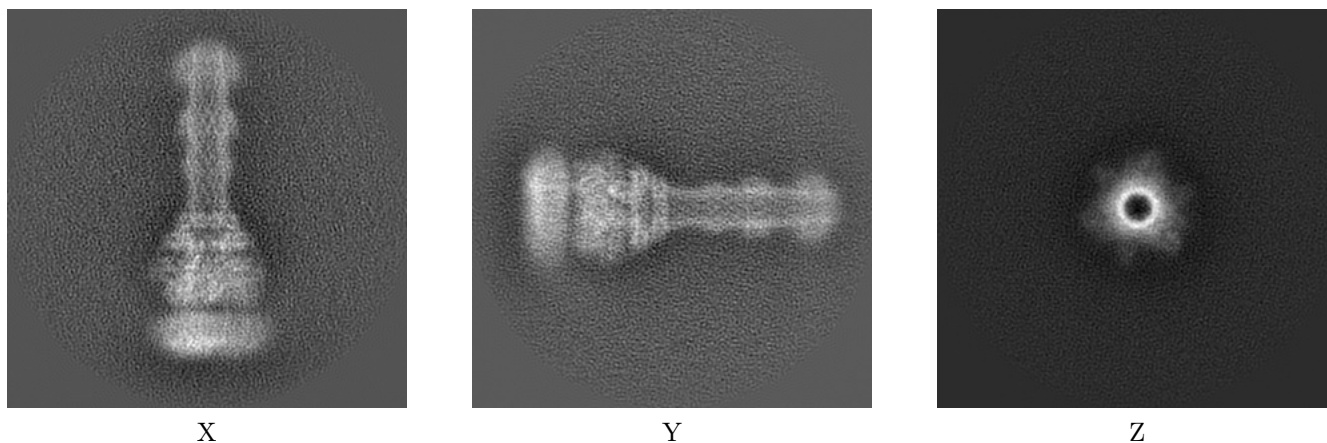
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8640. 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](#)

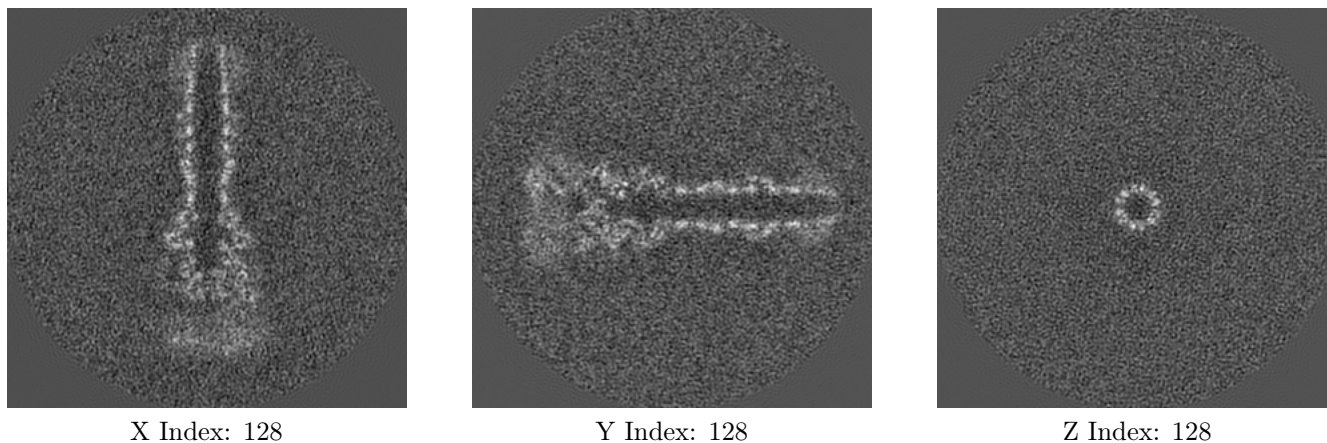
6.1.1 Primary map



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

6.2 Central slices [i](#)

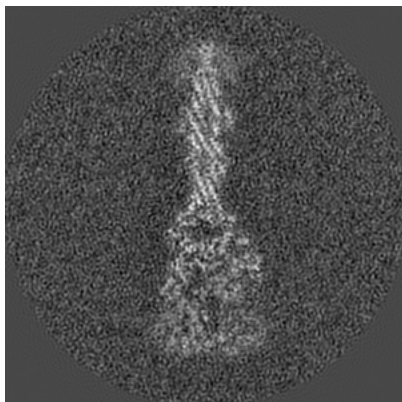
6.2.1 Primary map



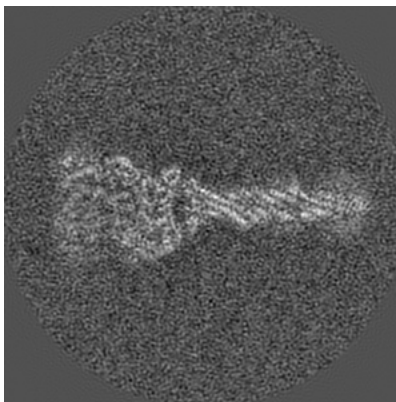
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

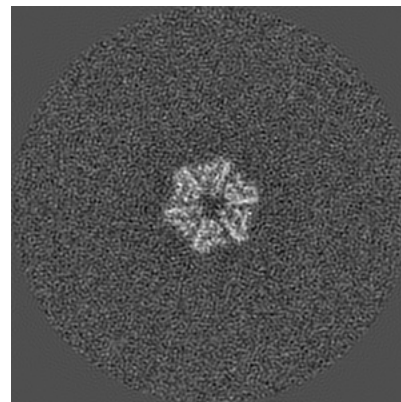
6.3.1 Primary map



X Index: 138



Y Index: 118

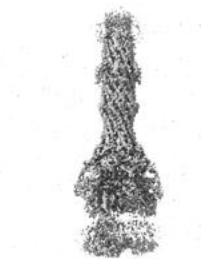


Z Index: 105

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

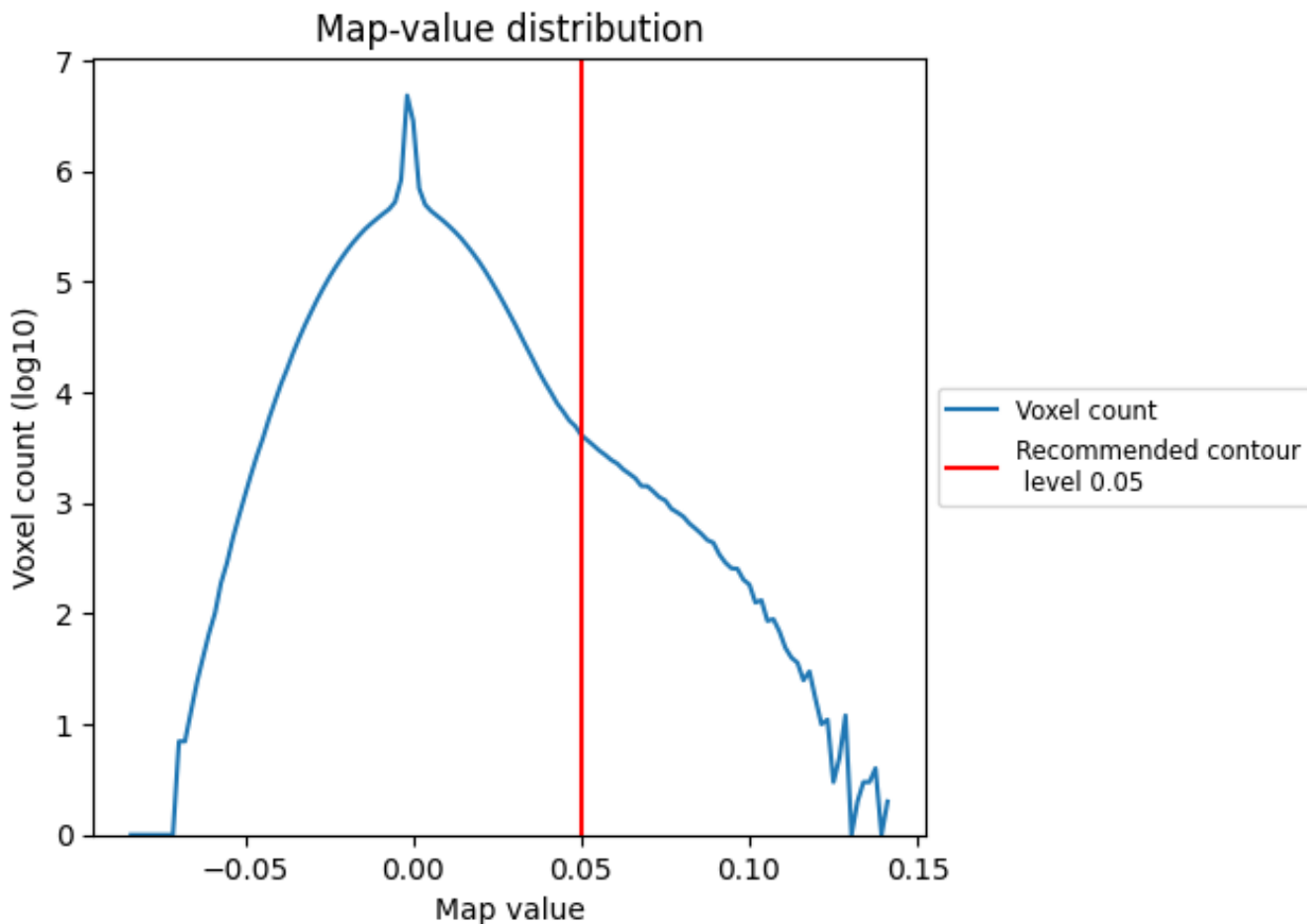
6.5 Mask visualisation

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

7 Map analysis [i](#)

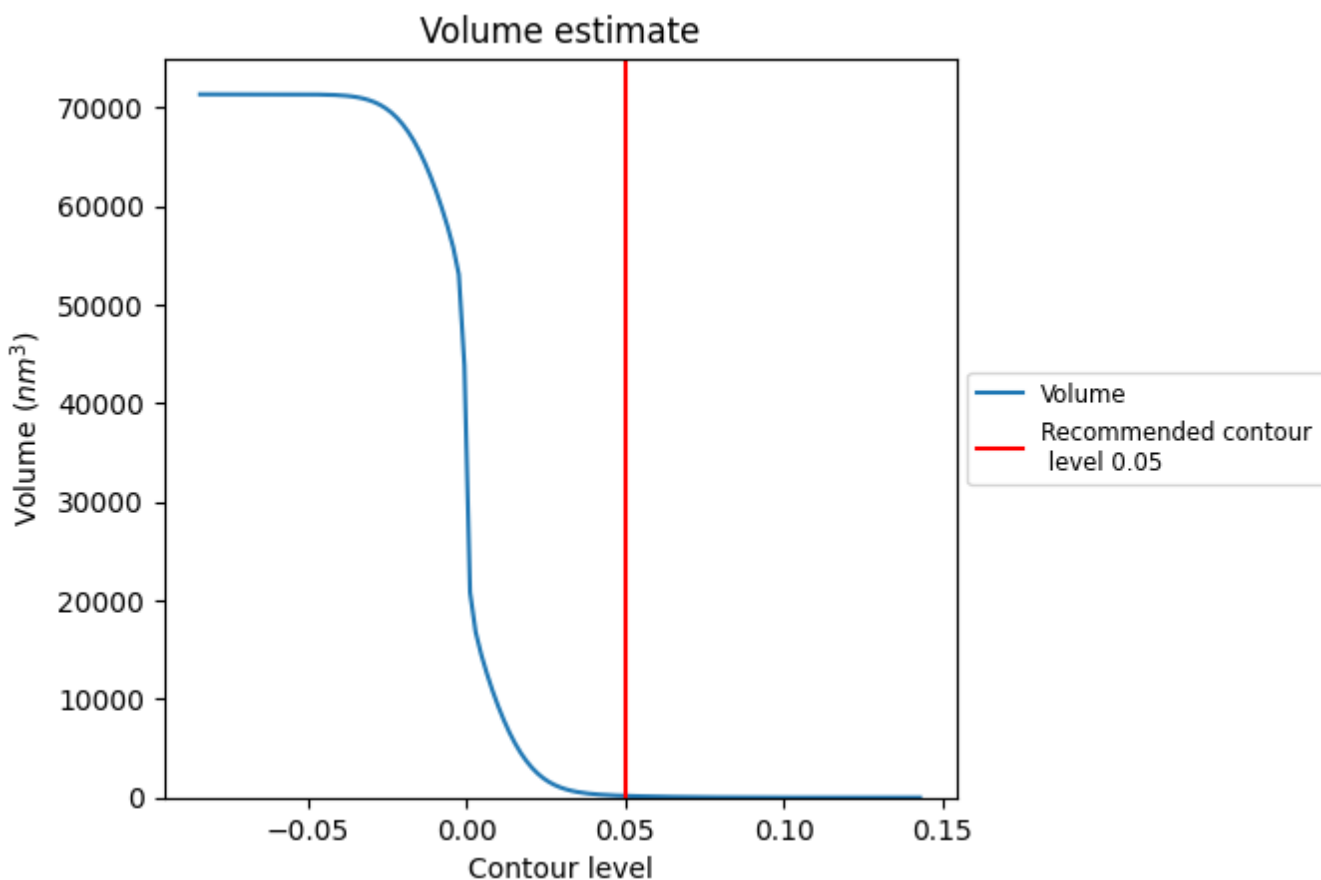
This section contains the results of statistical analysis of the map.

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.

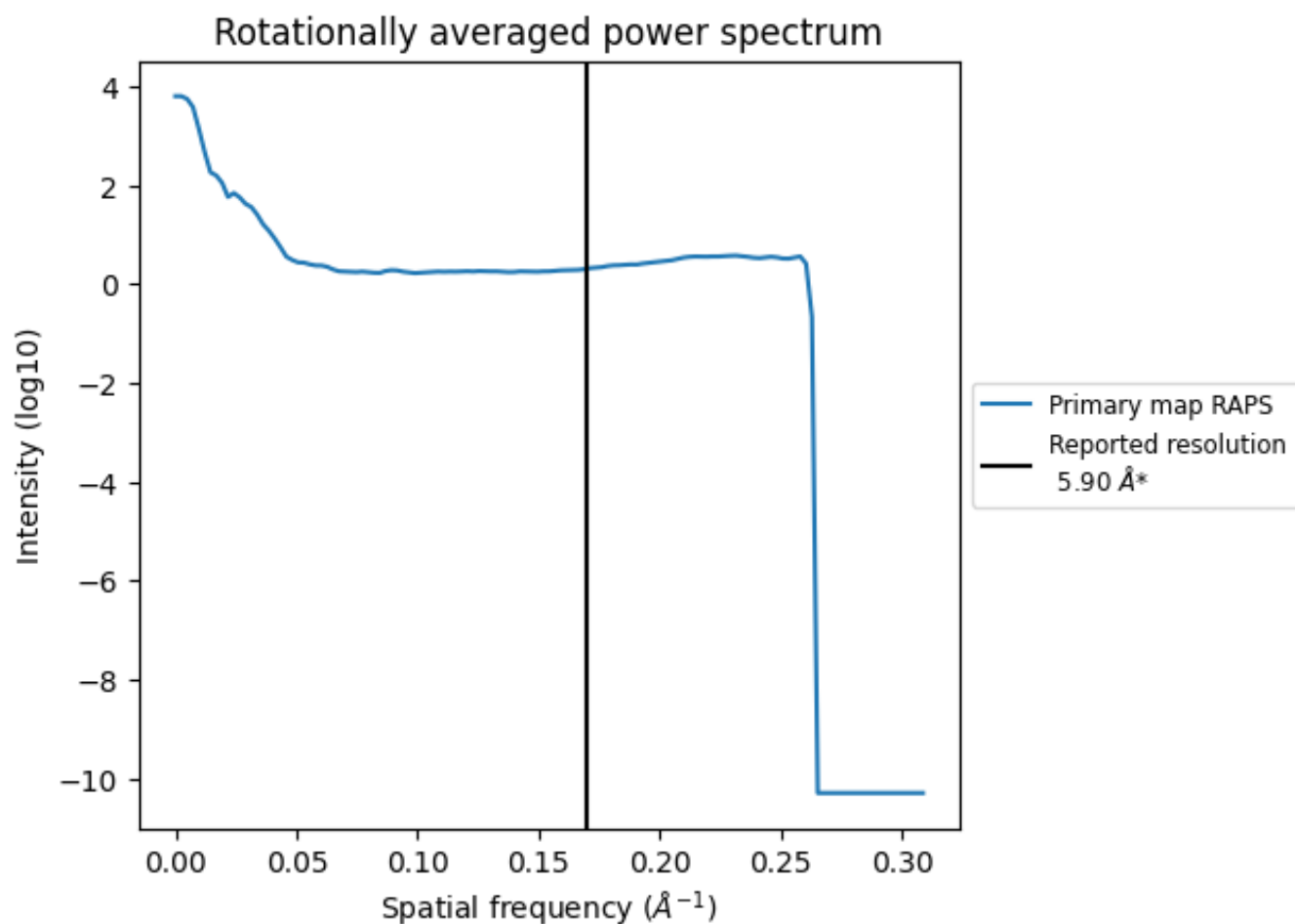
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 175 nm³; this corresponds to an approximate mass of 158 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 [\(i\)](#)

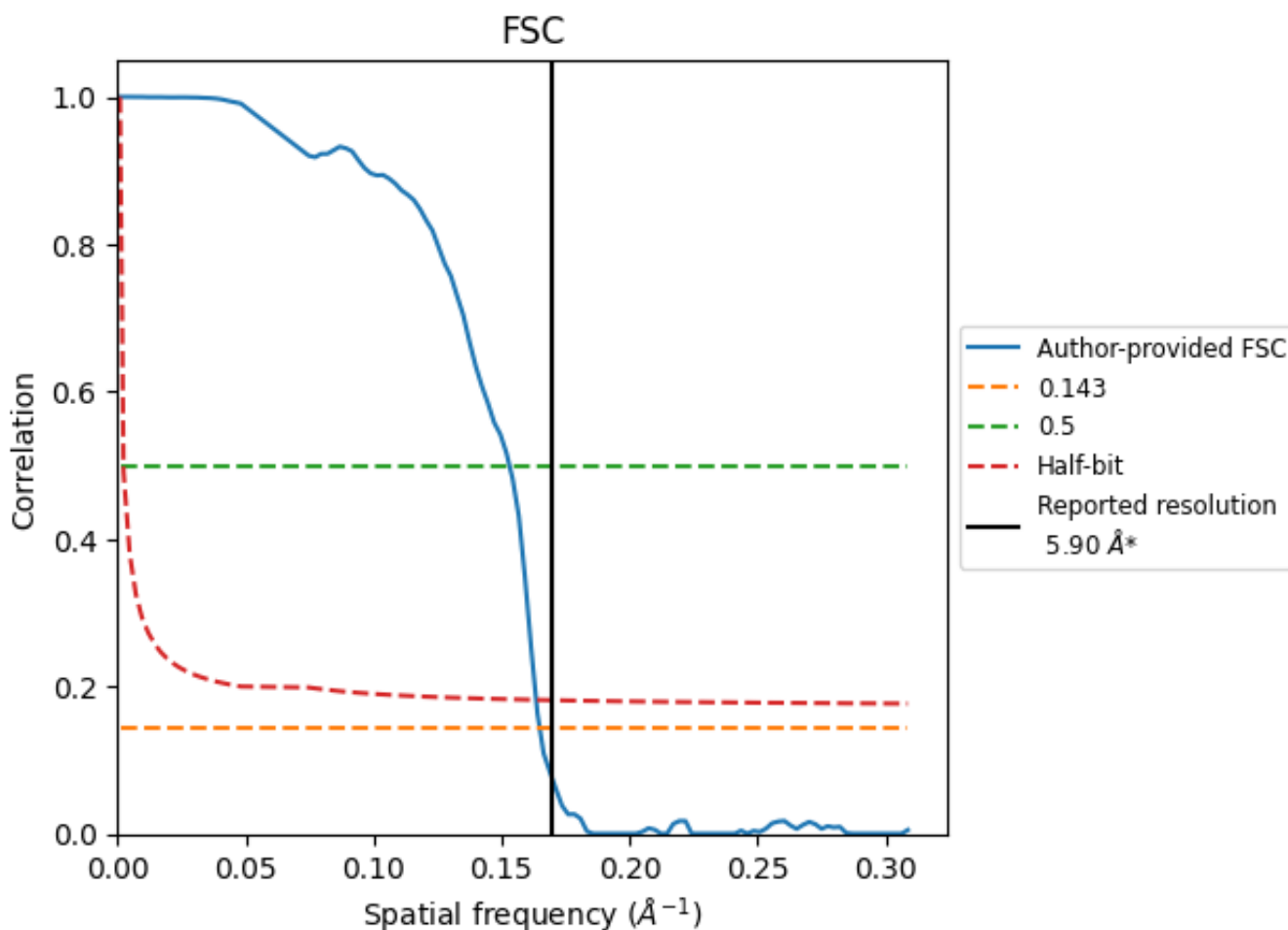


*Reported resolution corresponds to spatial frequency of 0.169 Å⁻¹

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 0.169 Å⁻¹

8.2 Resolution estimates [i](#)

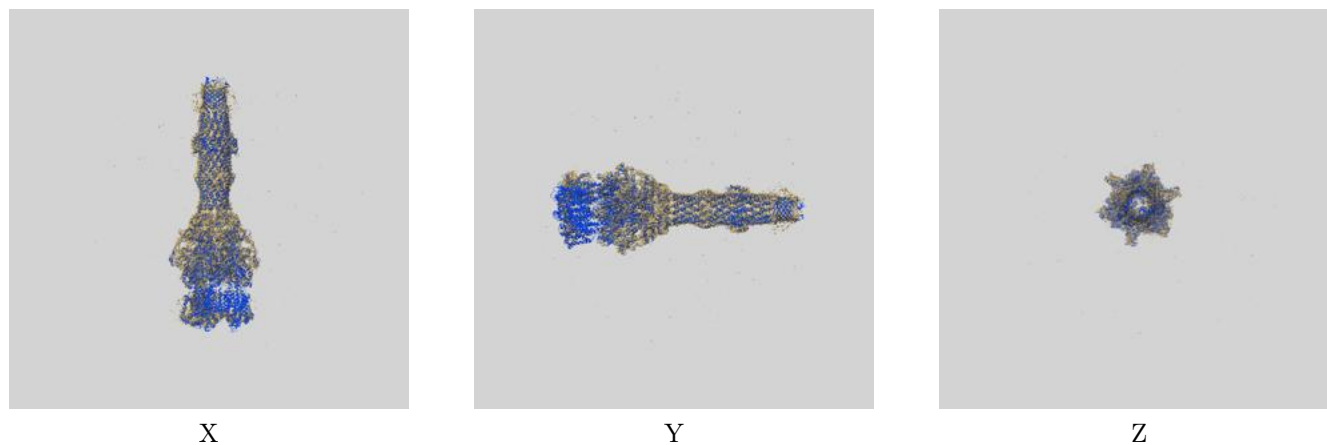
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.90	-	-
Author-provided FSC curve	6.06	6.54	6.12
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

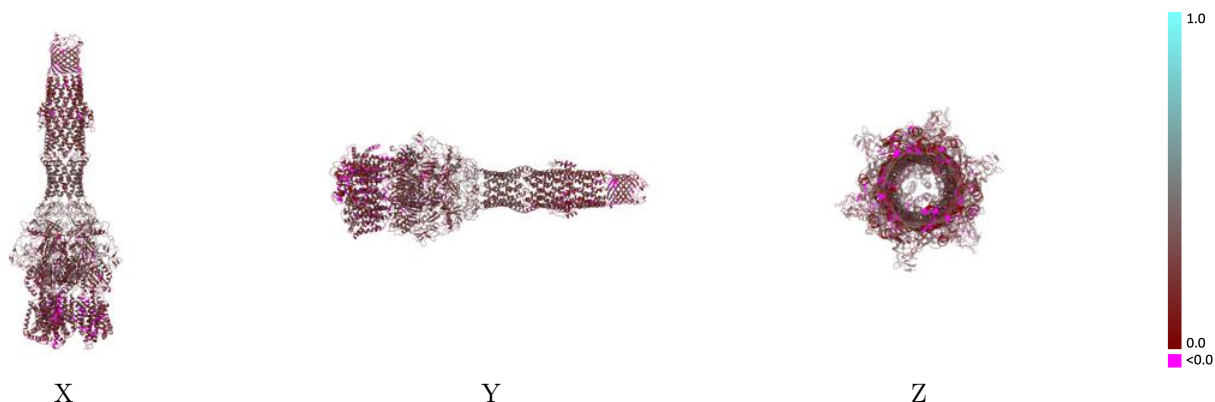
This section contains information regarding the fit between EMDB map EMD-8640 and PDB model 5O66. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



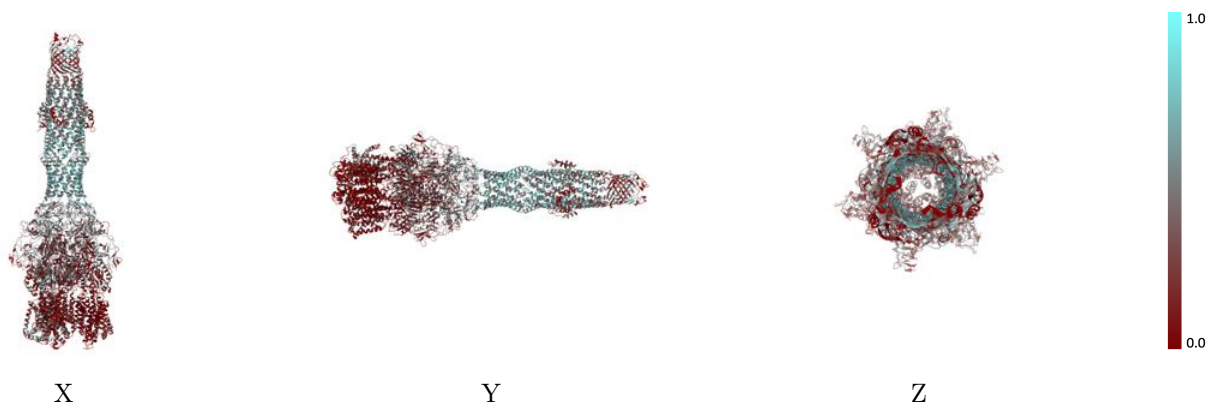
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



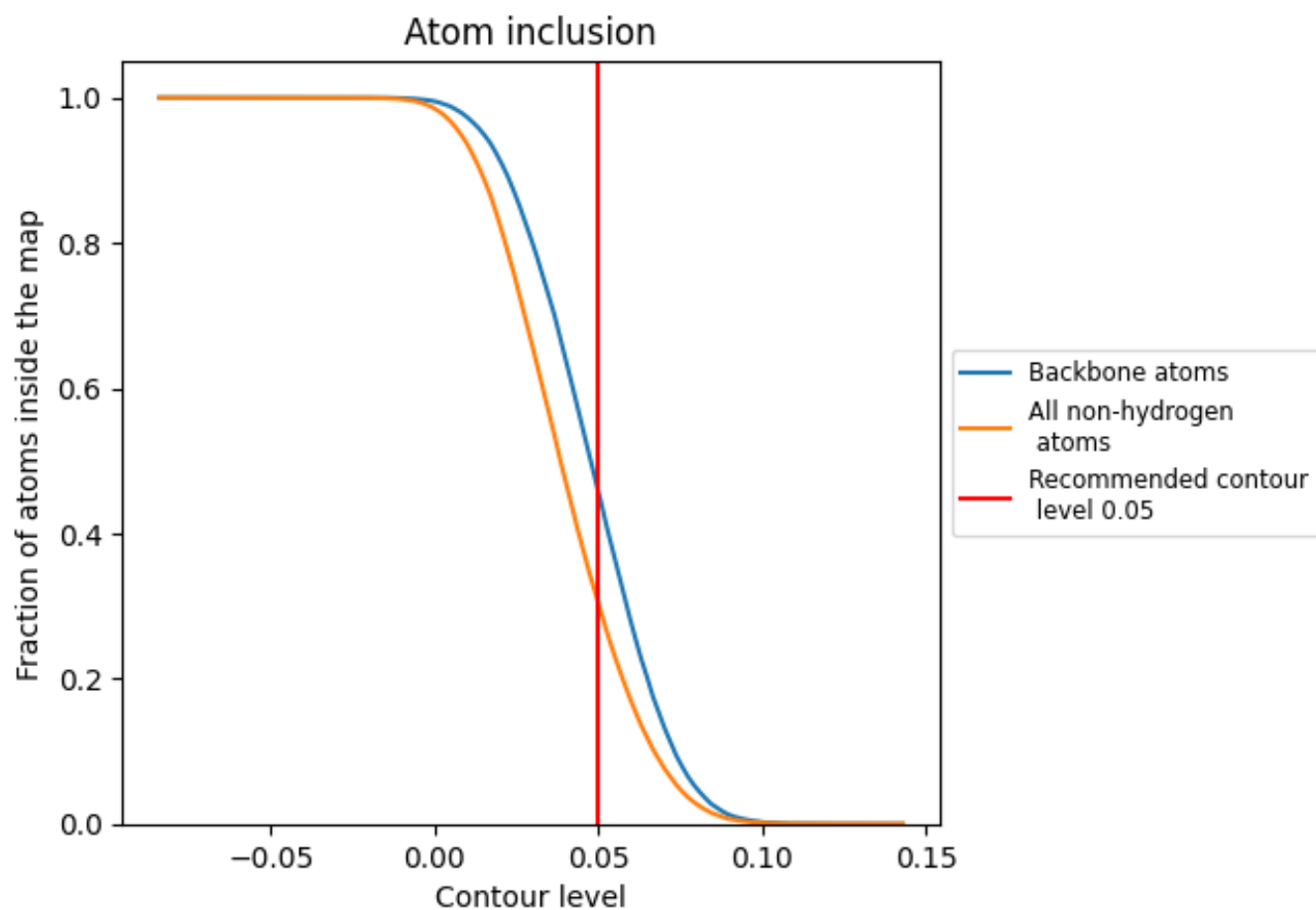
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

































9.4 Atom inclusion [i](#)



At the recommended contour level, 46% of all backbone atoms, 30% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3041	 0.2400
A	 0.4246	 0.2250
B	 0.4215	 0.2100
C	 0.4141	 0.2190
D	 0.4221	 0.3200
E	 0.4146	 0.2910
F	 0.4054	 0.3040
G	 0.3919	 0.2740
H	 0.4066	 0.3180
I	 0.4620	 0.2920
J	 0.1635	 0.2060
K	 0.1507	 0.2220
L	 0.2508	 0.2070
M	 0.0797	 0.2000
N	 0.2766	 0.1970
O	 0.0709	 0.1850

