



wwPDB EM Validation Summary Report ⓘ

Nov 10, 2024 – 02:48 pm GMT

PDB ID : 5V5S
EMDB ID : EMD-8636
Title : multi-drug efflux; membrane transport; RND superfamily; Drug resistance
Authors : wang, Z.; fan, G.; Hryc, C.F.; Blaza, J.N.; Serysheva, I.I.; Schmid, M.F.; Chiu, W.; Luisi, B.F.; Du, D.
Deposited on : 2017-03-15
Resolution : 6.50 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.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

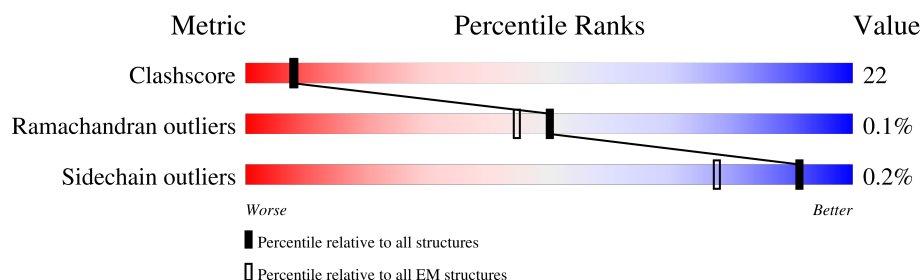
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.50 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	442	<div> <div>6%</div> <div>51%</div> <div>45%</div> <div>• •</div> </div>
1	B	442	<div> <div>5%</div> <div>52%</div> <div>44%</div> <div>•</div> </div>
1	C	442	<div> <div>6%</div> <div>54%</div> <div>43%</div> <div>•</div> </div>
2	D	397	<div> <div>18%</div> <div>54%</div> <div>30%</div> <div>• 14%</div> </div>
2	E	397	<div> <div>11%</div> <div>53%</div> <div>31%</div> <div>• 14%</div> </div>
2	F	397	<div> <div>19%</div> <div>52%</div> <div>33%</div> <div>• 14%</div> </div>
2	G	397	<div> <div>11%</div> <div>54%</div> <div>31%</div> <div>• 14%</div> </div>
2	H	397	<div> <div>19%</div> <div>53%</div> <div>32%</div> <div>• 14%</div> </div>

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Mol	Chain	Length	Quality of chain
2	I	397	<div><div></div><div>12%</div><div>51%</div><div>34%</div><div>•</div><div>14%</div></div>
3	J	1049	<div><div></div><div>5%</div><div>57%</div><div>42%</div><div>••</div></div>
3	K	1049	<div><div></div><div>•</div><div>54%</div><div>44%</div><div>••</div></div>
3	L	1049	<div><div></div><div>•</div><div>55%</div><div>43%</div><div>••</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 48705 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
1	A	428	Total	C	N	O	Se	0	0
			3304	2037	586	676	5		
1	B	428	Total	C	N	O	Se	0	0
			3304	2037	586	676	5		
1	C	428	Total	C	N	O	Se	0	0
			3304	2037	586	676	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	340	Total	C	N	O	S	0	0
			2556	1598	451	505	2		
2	E	340	Total	C	N	O	S	0	0
			2556	1598	451	505	2		
2	F	340	Total	C	N	O	S	0	0
			2556	1598	451	505	2		
2	G	340	Total	C	N	O	S	0	0
			2556	1598	451	505	2		
2	H	340	Total	C	N	O	S	0	0
			2556	1598	451	505	2		
2	I	340	Total	C	N	O	S	0	0
			2556	1598	451	505	2		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	273	CYS	SER	conflict	UNP P0AE07
E	273	CYS	SER	conflict	UNP P0AE07
F	273	CYS	SER	conflict	UNP P0AE07
G	273	CYS	SER	conflict	UNP P0AE07
H	273	CYS	SER	conflict	UNP P0AE07
I	273	CYS	SER	conflict	UNP P0AE07

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	1037	Total	C	N	O	S	0	0
			7819	5032	1290	1452	45		
3	K	1037	Total	C	N	O	S	0	0
			7819	5032	1290	1452	45		
3	L	1037	Total	C	N	O	S	0	0
			7819	5032	1290	1452	45		

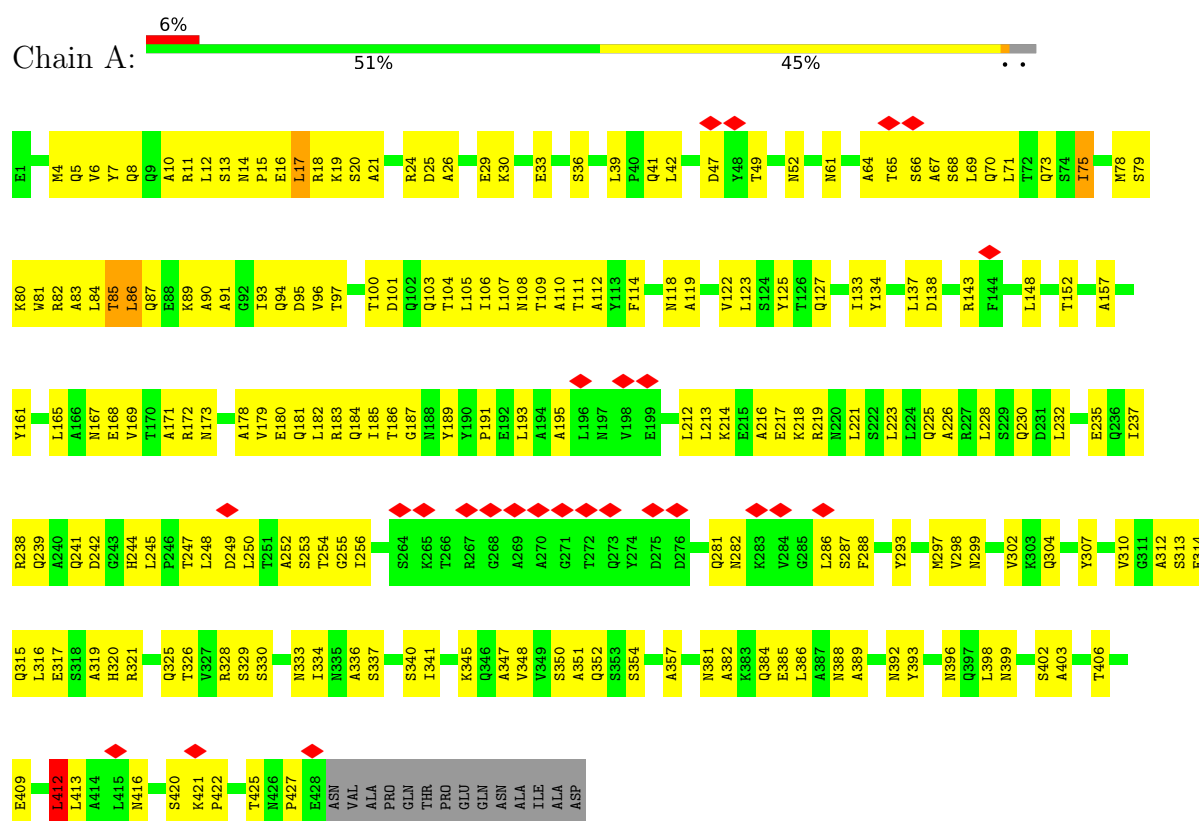
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	258	CYS	SER	conflict	UNP P31224
K	258	CYS	SER	conflict	UNP P31224
L	258	CYS	SER	conflict	UNP P31224

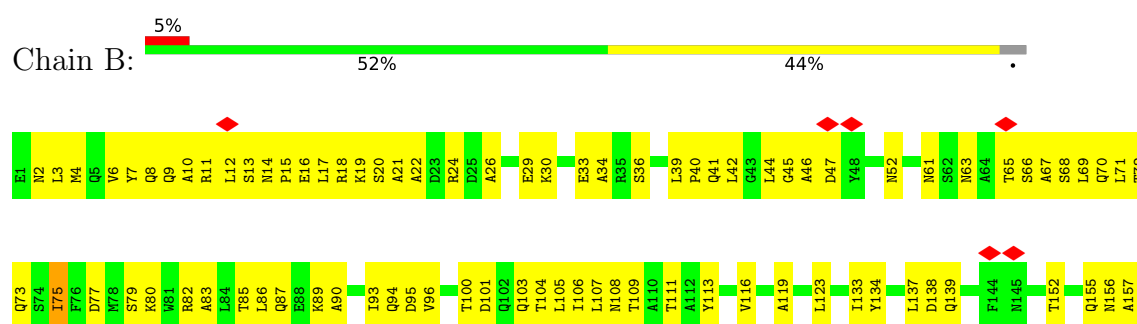
3 Residue-property plots

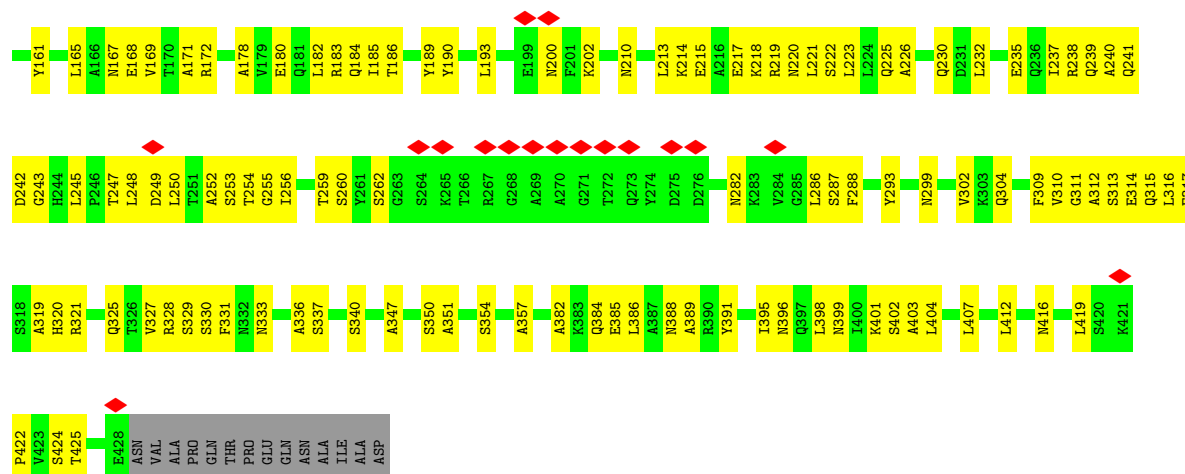
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

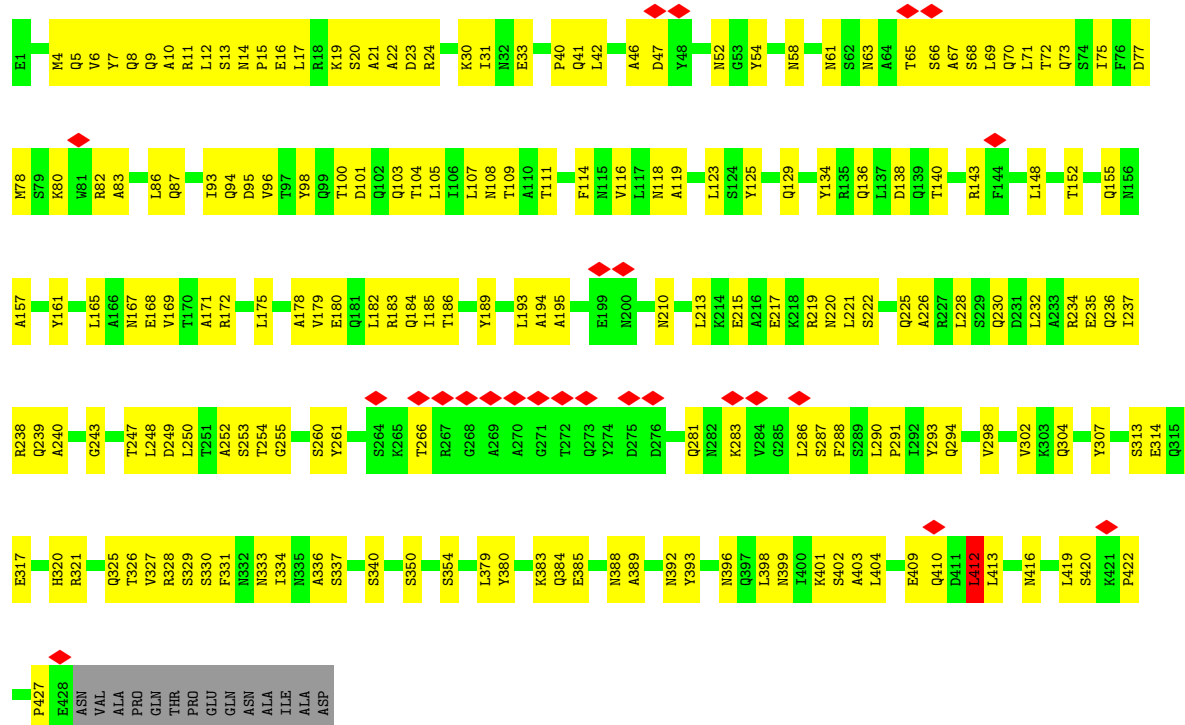


• Molecule 1: Outer membrane protein TolC

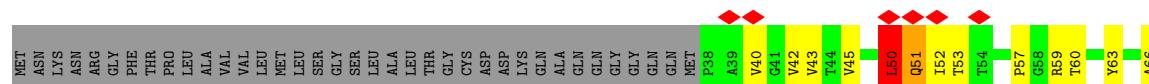


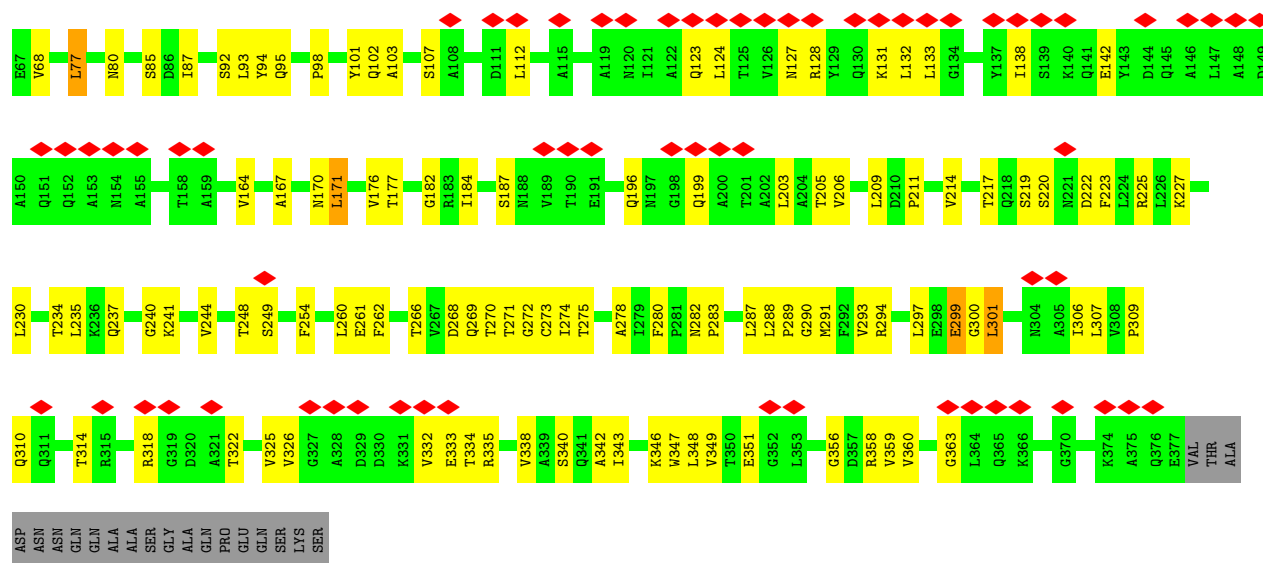


• Molecule 1: Outer membrane protein TolC

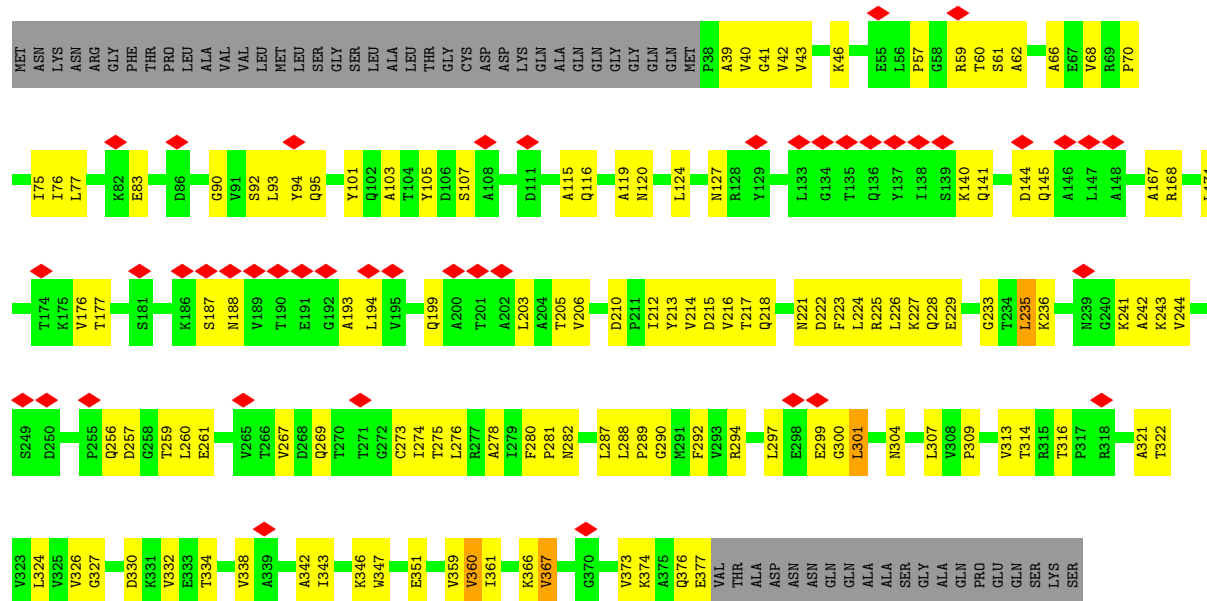


• Molecule 2: Multidrug efflux pump subunit AcrA

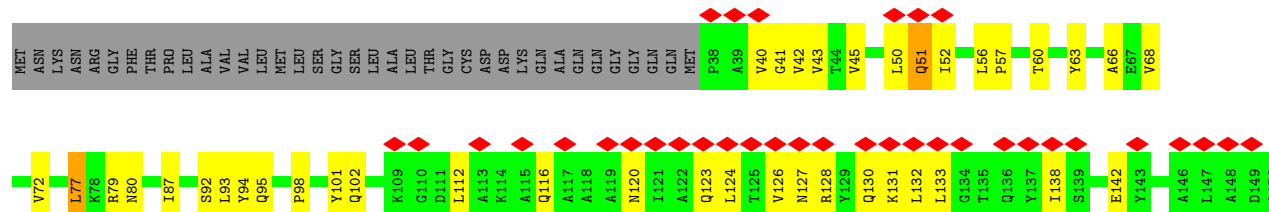


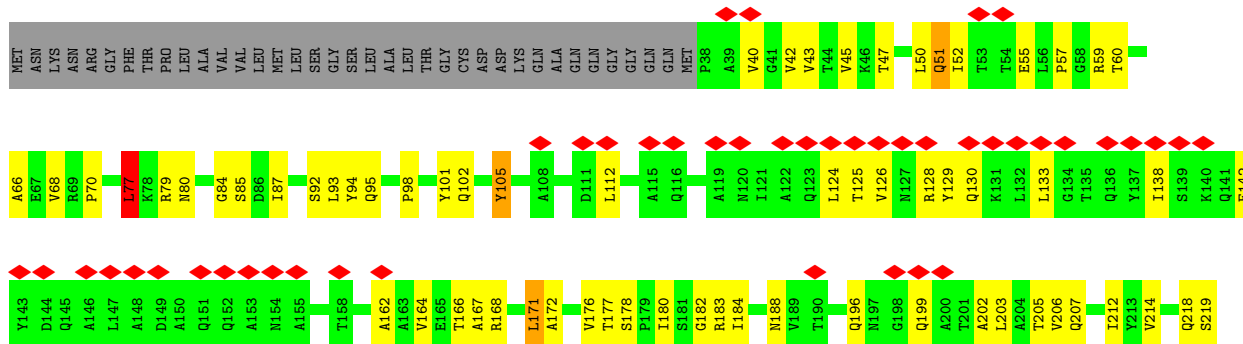


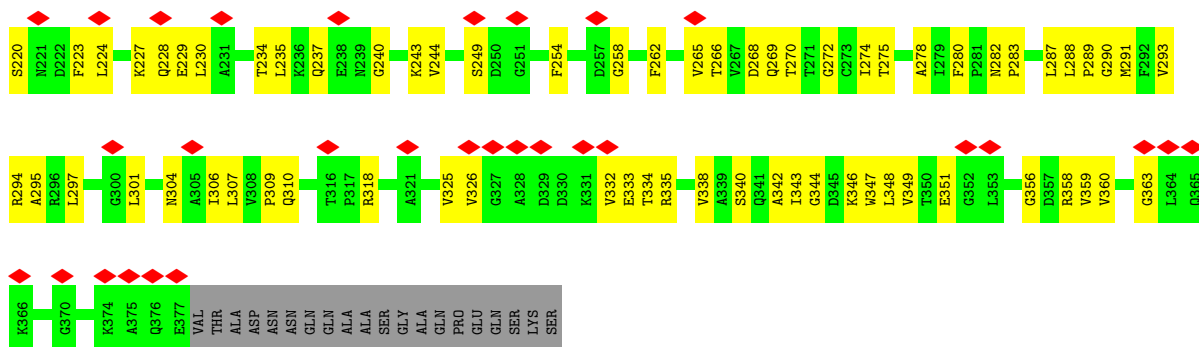
• Molecule 2: Multidrug efflux pump subunit AcrA



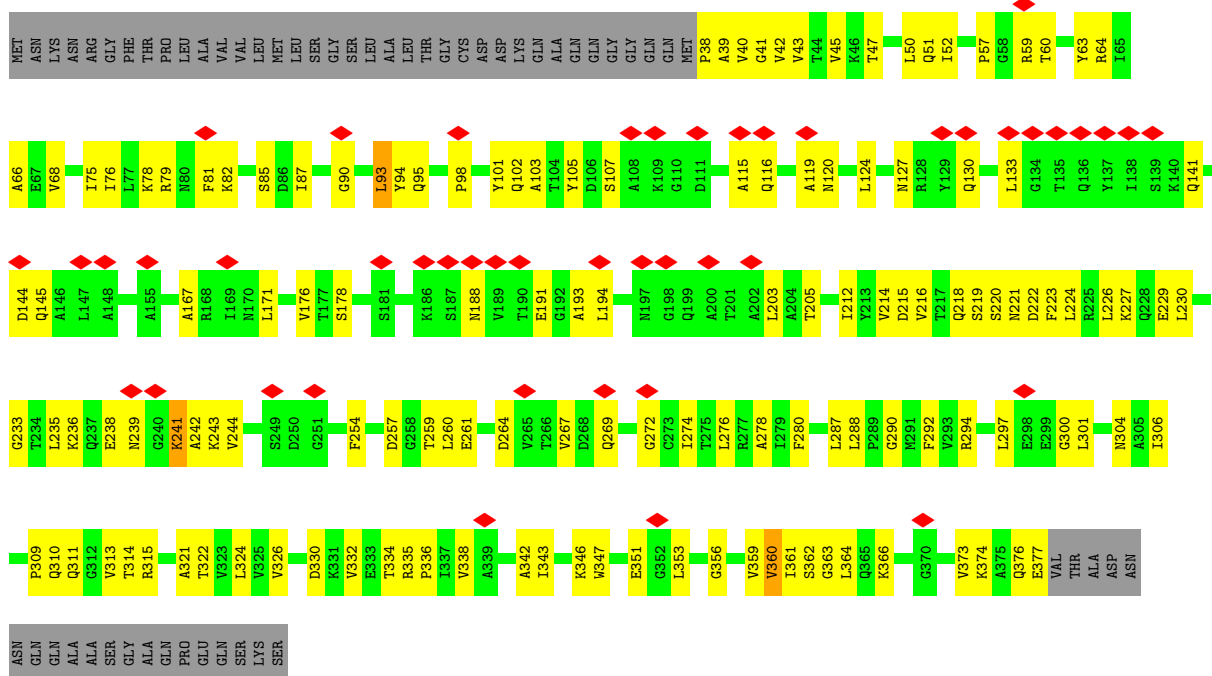
• Molecule 2: Multidrug efflux pump subunit AcrA



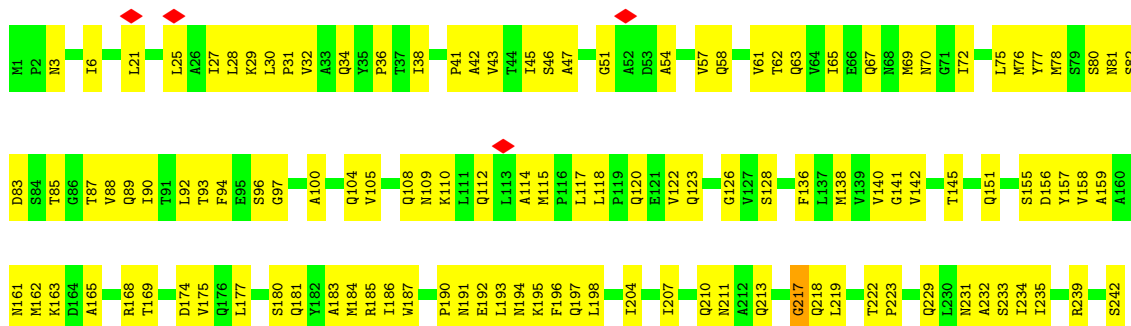


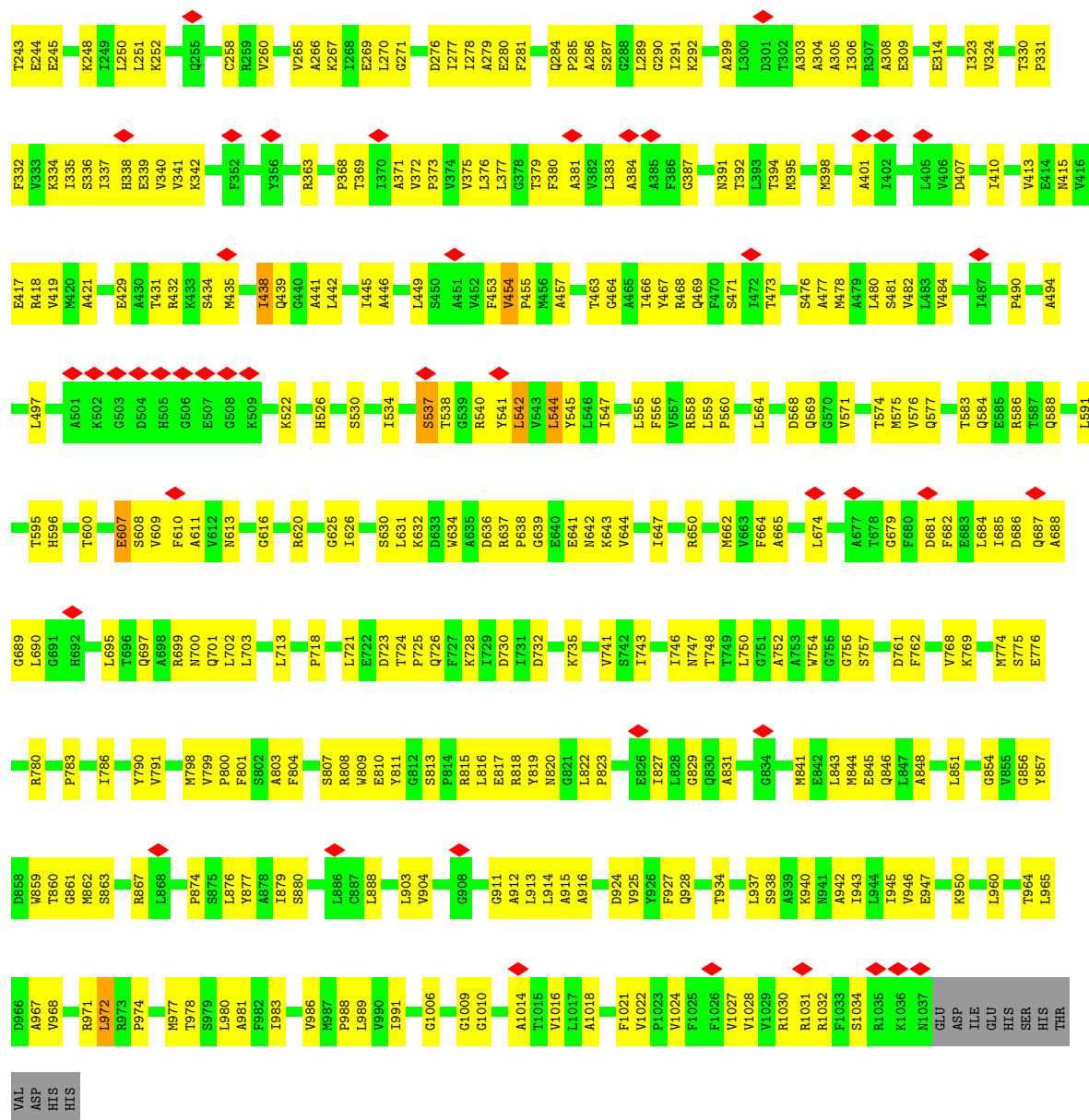


• Molecule 2: Multidrug efflux pump subunit AcrA



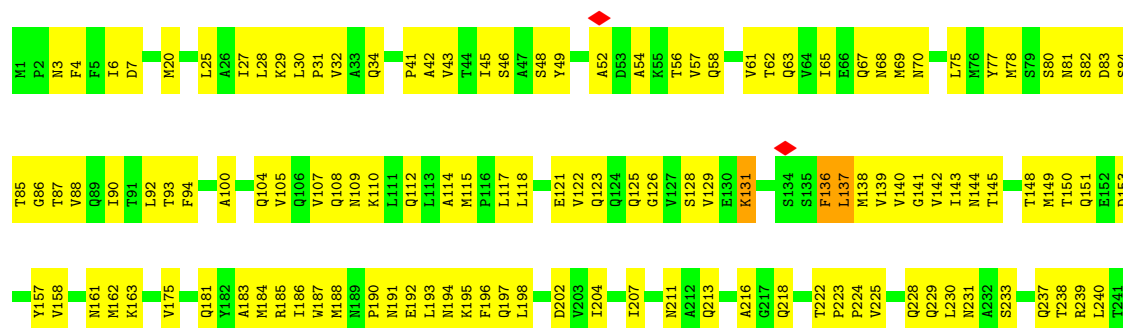
• Molecule 3: Multidrug efflux pump subunit AcrB

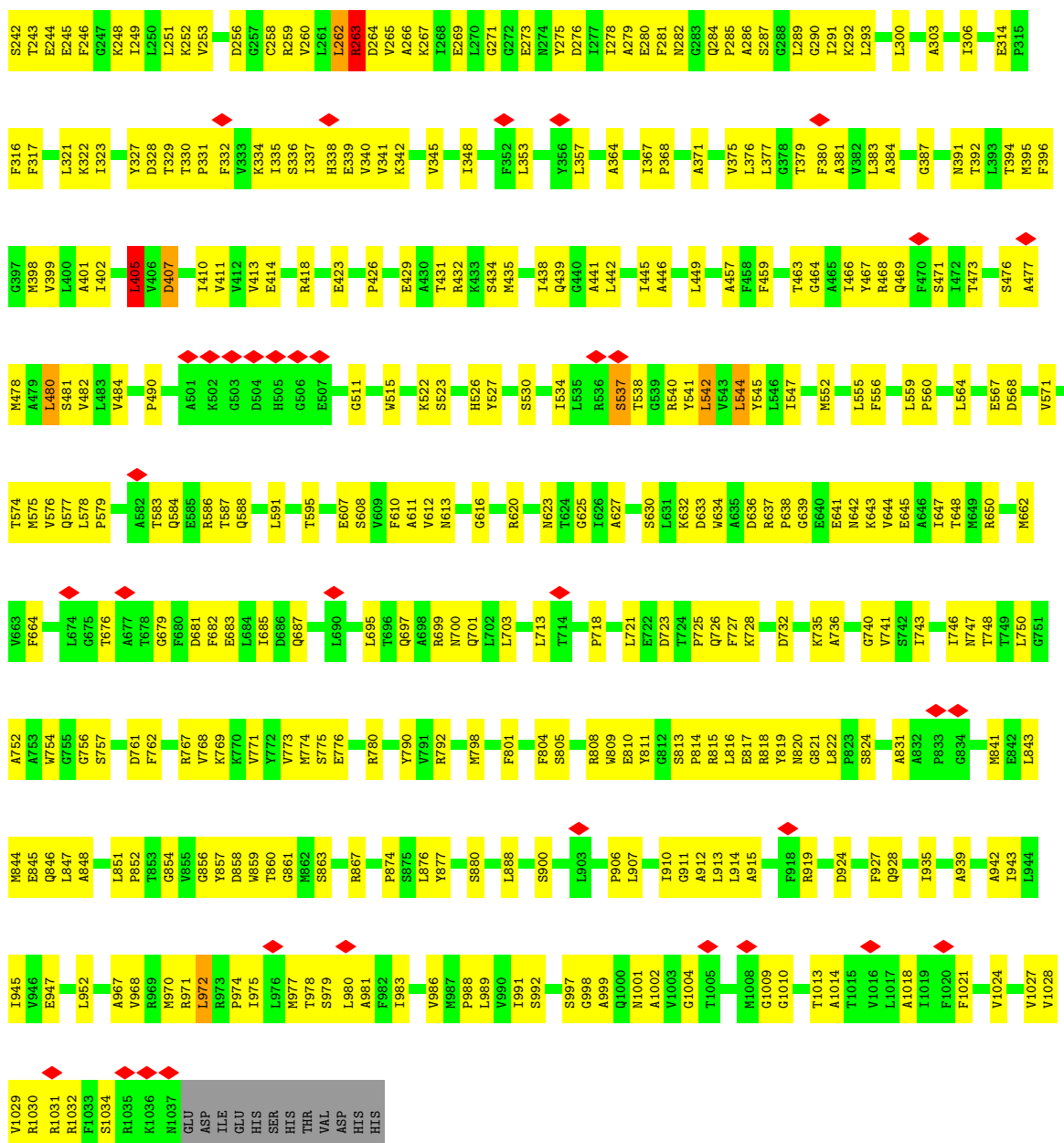




• Molecule 3: Multidrug efflux pump subunit AcrB

Chain K: 54% 44%





S1034	K940	P852	K769	E683	T583	L483	V406	P326	K248
R1035	N941	T853	K770	L684	Q584	V484	D407	Y327	I249
K1036	A942	G854	V771	I685	E585	A485	I410	T330	L250
N1037	I943	H855	V772	D686	R586	L486	V413	P331	L251
GLU	I945	G856	M773	Q687	T587	P490	E417	F332	K252
ASP	V946	H857	M774	A688	Q588	A494	R418	V333	V253
ILE	E947	D858	S775	G689	L591	T495	M419	K334	R254
GLU	F948	H859	E776	L690	T595	M496	M420	I337	Q255
SER	L952	C861	A777	L695	T596	L497	A421	H338	
HIS		M862	R780	Q697	T596	A501	G424	V340	C258
THR		S863	V790	A698	S608	K502	L425	V341	R260
VAL	A963	R867	V791	R699	F610	G503	P426	V342	R263
ASP	T964	P874	R792	N700	A611	D504	K428	V345	D264
HIS	L965	S875	G796	Q701	V612	H505	E429	I348	V265
HIS	A967	L876	M798	L702	G625	G506	A430	Y356	K267
	V968	H877	V799	L703	I626	E507	R432	F362	I268
		L879	P800	L713	A627	G508	K433	A364	E269
	R971	T879	F801	T714	F628	K509	S434	R363	L270
	L972	S880	P718	L631	V629	K510	M435	E272	G271
	M977	V883	L721	E722	K632	G511	T438	E273	
	L980	L896	D723	T724	D633	W515	Q439	D276	
	A981	A899	P725	Q726	D633	Y527	G440	A371	A279
	I983	F899	T727	F727	W634	S530	L442	F372	E280
	V986		Q726	F727	R637	T534	I445	P373	F281
	L989		F727	F727	P638	S537	A446	V374	N282
	S997		K728	K728	G439	T538	L449	G378	G283
	G998		L729	L729	E640	G539	S450	T379	P285
A999	N1001		D730	D730	E641	R540	A451	F380	A286
Q1000	G911		I731	I731	K643	Y541	V452	A381	G288
A1002	A912		D732	D732	V644	L542	F453	V382	L289
V1003	L913		K735	K735	E645	V543	F458	L383	G290
	L914		L739	L739	R650	L544	T463	K292	I291
G1010	A915		G740	G740	A651	L555	G464	L293	
			S742	S742	T652	L559	A466	A294	
A1014	F918		I743	I743	F655	P560	I467	G296	
A1018	A831		N744	N744	I658	F563	R468	A297	
I1019	A832		D745	D745	T655	L564	T473	N298	
F1020	P833		I746	I746	I658	D568	F396	E314	
F1021	G834		N747	N747	T658	Q569	G397	P315	
V1024	K835		T748	T748	V662	V571	V399	F317	
F1025	M841		A752	A752	F664	T574	M395	L321	
F1026	E842		G756	G756	F664	M575	F396	K322	
V1027	L843		S757	S757	E673	V576	G387	I323	
V1028	M844		T757	T757	L674	M575	N391	V324	
V1029	E845		D761	D761	A677	V482	T392	Y325	
R1030	Q846		F762	F762	D681		M395		
R1031	I847		V768	V768	F682		F396		
R1032	A848						G387		
F1033	L851						N391		
	A939						T392		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	13544	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1	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	0.092	Depositor
Minimum map value	-0.031	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0266	Depositor
Map size (\AA)	402.8, 402.8, 402.8	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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	0.34	0/3340	0.60	4/4529 (0.1%)
1	B	0.35	0/3340	0.58	0/4529
1	C	0.35	0/3340	0.58	1/4529 (0.0%)
2	D	0.36	0/2589	0.65	3/3521 (0.1%)
2	E	0.37	0/2589	0.65	3/3521 (0.1%)
2	F	0.35	0/2589	0.63	1/3521 (0.0%)
2	G	0.37	0/2589	0.64	2/3521 (0.1%)
2	H	2.48	7/2589 (0.3%)	0.68	4/3521 (0.1%)
2	I	0.37	0/2589	0.65	2/3521 (0.1%)
3	J	0.45	0/7968	0.68	3/10826 (0.0%)
3	K	0.46	0/7968	0.70	6/10826 (0.1%)
3	L	0.46	0/7968	0.70	5/10826 (0.0%)
All	All	0.69	7/49458 (0.0%)	0.66	34/67191 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	3
1	C	0	1
2	D	0	5
2	E	0	3
2	F	0	3
2	G	0	3
2	H	0	2
2	I	0	4
3	J	0	7
3	K	0	9
3	L	0	8
All	All	0	51

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	171	LEU	CG-CD2	89.71	4.83	1.51
2	H	105	TYR	CD2-CE2	47.26	2.10	1.39
2	H	105	TYR	CD1-CE1	43.32	2.04	1.39
2	H	105	TYR	CE2-CZ	33.06	1.81	1.38
2	H	105	TYR	CE1-CZ	32.37	1.80	1.38

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	405	LEU	CA-CB-CG	9.60	137.38	115.30
3	L	405	LEU	CA-CB-CG	9.29	136.66	115.30
2	H	171	LEU	CB-CG-CD2	8.53	125.49	111.00
2	E	367	VAL	C-N-CA	8.48	142.90	121.70
2	H	171	LEU	CA-CB-CG	7.59	132.75	115.30

There are no chirality outliers.

5 of 51 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	297	MSE	Peptide
1	A	75	ILE	Peptide
1	A	85	THR	Peptide
1	B	2	ASN	Peptide
1	B	75	ILE	Peptide

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	3304	0	3254	194	0
1	B	3304	0	3254	178	0
1	C	3304	0	3254	174	0
2	D	2556	0	2616	121	0
2	E	2556	0	2615	104	0
2	F	2556	0	2615	122	0
2	G	2556	0	2616	116	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	2556	0	2616	121	0
2	I	2556	0	2616	113	0
3	J	7819	0	7919	326	0
3	K	7819	0	7919	361	0
3	L	7819	0	7919	349	0
All	All	48705	0	49213	2161	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 2161 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:H:105:TYR:CZ	2:H:105:TYR:CE2	1.81	1.63
2:D:217:THR:HG23	2:D:273:CYS:SG	1.40	1.60
2:H:105:TYR:CZ	2:H:105:TYR:CE1	1.80	1.60
2:H:220:SER:HA	2:H:223:PHE:CE1	1.36	1.60
2:G:217:THR:HG23	2:G:273:CYS:SG	1.43	1.56

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	426/442 (96%)	407 (96%)	19 (4%)	0	100	100
1	B	426/442 (96%)	406 (95%)	20 (5%)	0	100	100
1	C	426/442 (96%)	407 (96%)	19 (4%)	0	100	100
2	D	338/397 (85%)	300 (89%)	36 (11%)	2 (1%)	22	60
2	E	338/397 (85%)	301 (89%)	37 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	338/397 (85%)	306 (90%)	30 (9%)	2 (1%)	22	60
2	G	338/397 (85%)	299 (88%)	39 (12%)	0	100	100
2	H	338/397 (85%)	306 (90%)	30 (9%)	2 (1%)	22	60
2	I	338/397 (85%)	306 (90%)	32 (10%)	0	100	100
3	J	1035/1049 (99%)	949 (92%)	86 (8%)	0	100	100
3	K	1035/1049 (99%)	948 (92%)	85 (8%)	2 (0%)	44	78
3	L	1035/1049 (99%)	952 (92%)	82 (8%)	1 (0%)	48	83
All	All	6411/6855 (94%)	5887 (92%)	515 (8%)	9 (0%)	50	83

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	52	ILE
2	F	52	ILE
2	H	52	ILE
3	K	264	ASP
3	K	263	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	358/364 (98%)	357 (100%)	1 (0%)	91	92
1	B	358/364 (98%)	358 (100%)	0	100	100
1	C	358/364 (98%)	357 (100%)	1 (0%)	91	92
2	D	274/318 (86%)	274 (100%)	0	100	100
2	E	274/318 (86%)	274 (100%)	0	100	100
2	F	274/318 (86%)	273 (100%)	1 (0%)	89	91
2	G	274/318 (86%)	274 (100%)	0	100	100
2	H	274/318 (86%)	274 (100%)	0	100	100
2	I	274/318 (86%)	274 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	J	826/855 (97%)	824 (100%)	2 (0%)	92	94
3	K	826/855 (97%)	823 (100%)	3 (0%)	89	91
3	L	826/855 (97%)	823 (100%)	3 (0%)	89	91
All	All	5196/5565 (93%)	5185 (100%)	11 (0%)	91	94

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	K	480	LEU
3	L	263	ARG
3	L	480	LEU
3	L	405	LEU
3	J	480	LEU

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	G	302	ASN
3	J	151	GLN
3	L	517	ASN
2	G	365	GLN
2	I	302	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 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](#)

There are no chain breaks in this entry.

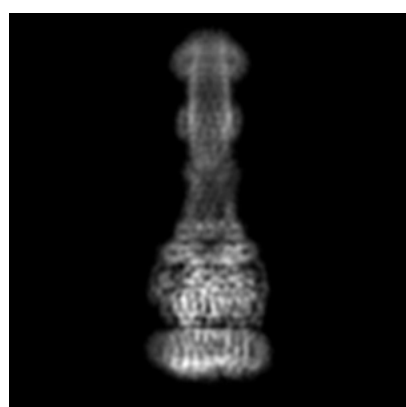
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8636. These allow visual inspection of the internal detail of the map and identification of artifacts.

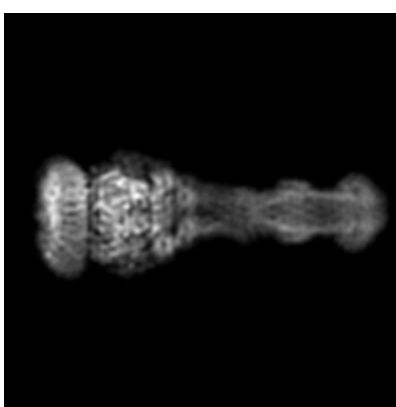
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

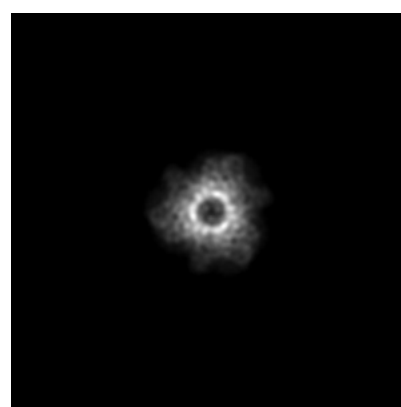
6.1.1 Primary map



X



Y



Z

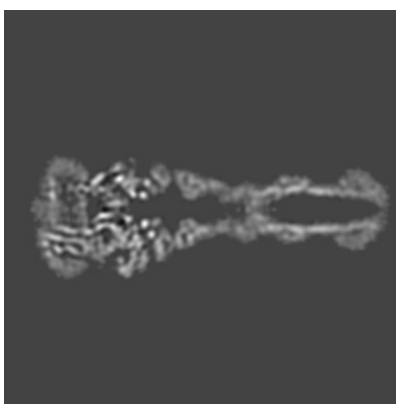
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

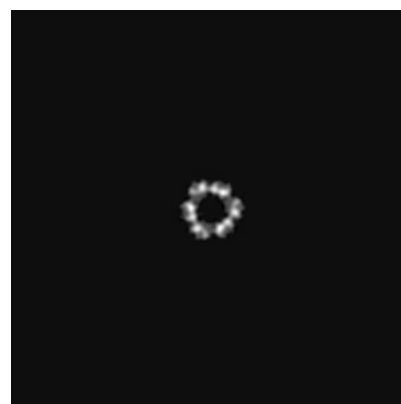
6.2.1 Primary map



X Index: 190



Y Index: 190



Z Index: 190

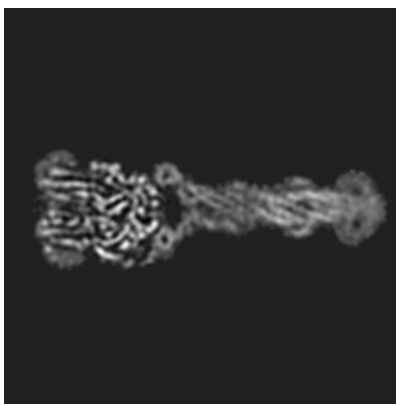
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

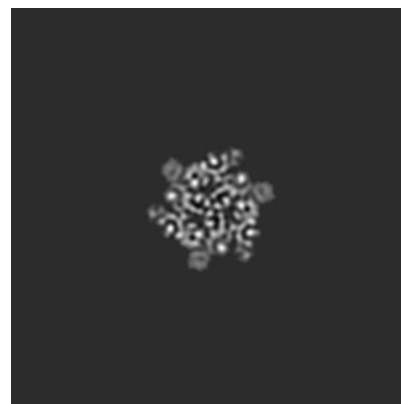
6.3.1 Primary map



X Index: 204



Y Index: 175

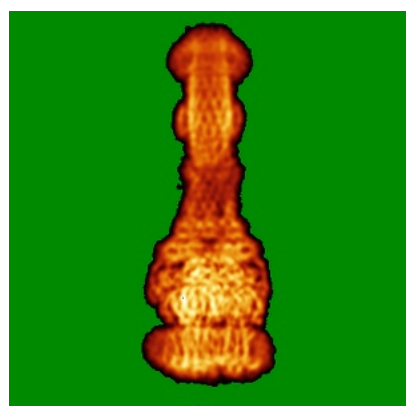


Z Index: 107

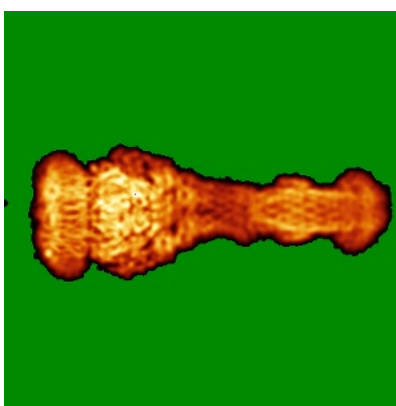
The images above show the largest variance slices of the map in three orthogonal directions.

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

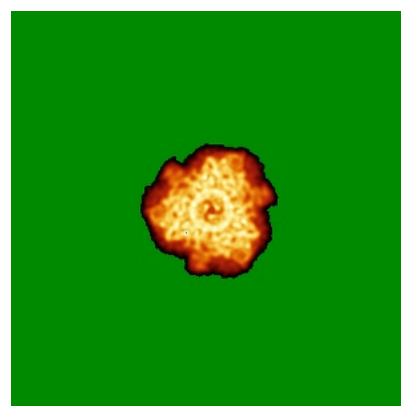
6.4.1 Primary map



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 0.0266. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

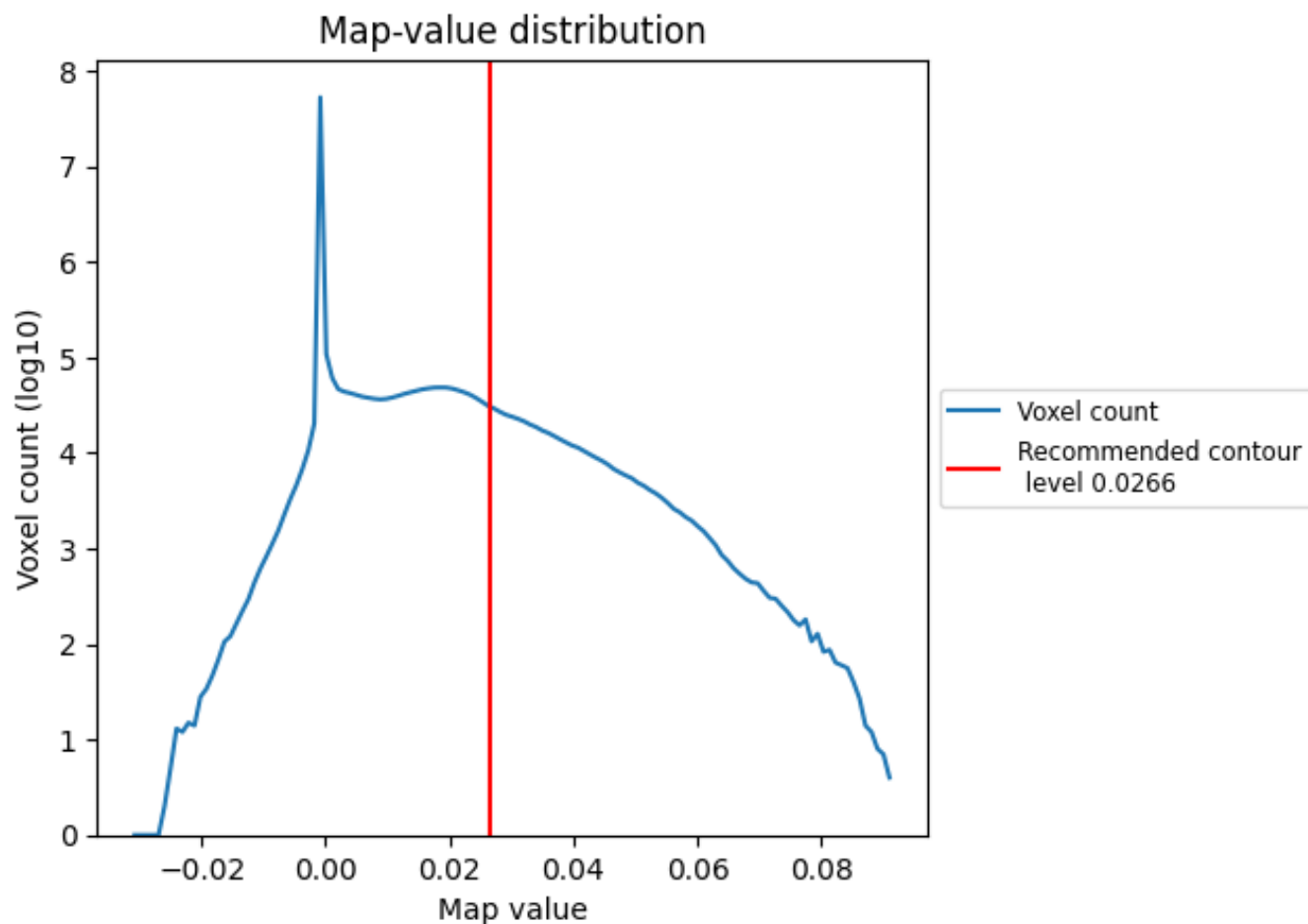
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

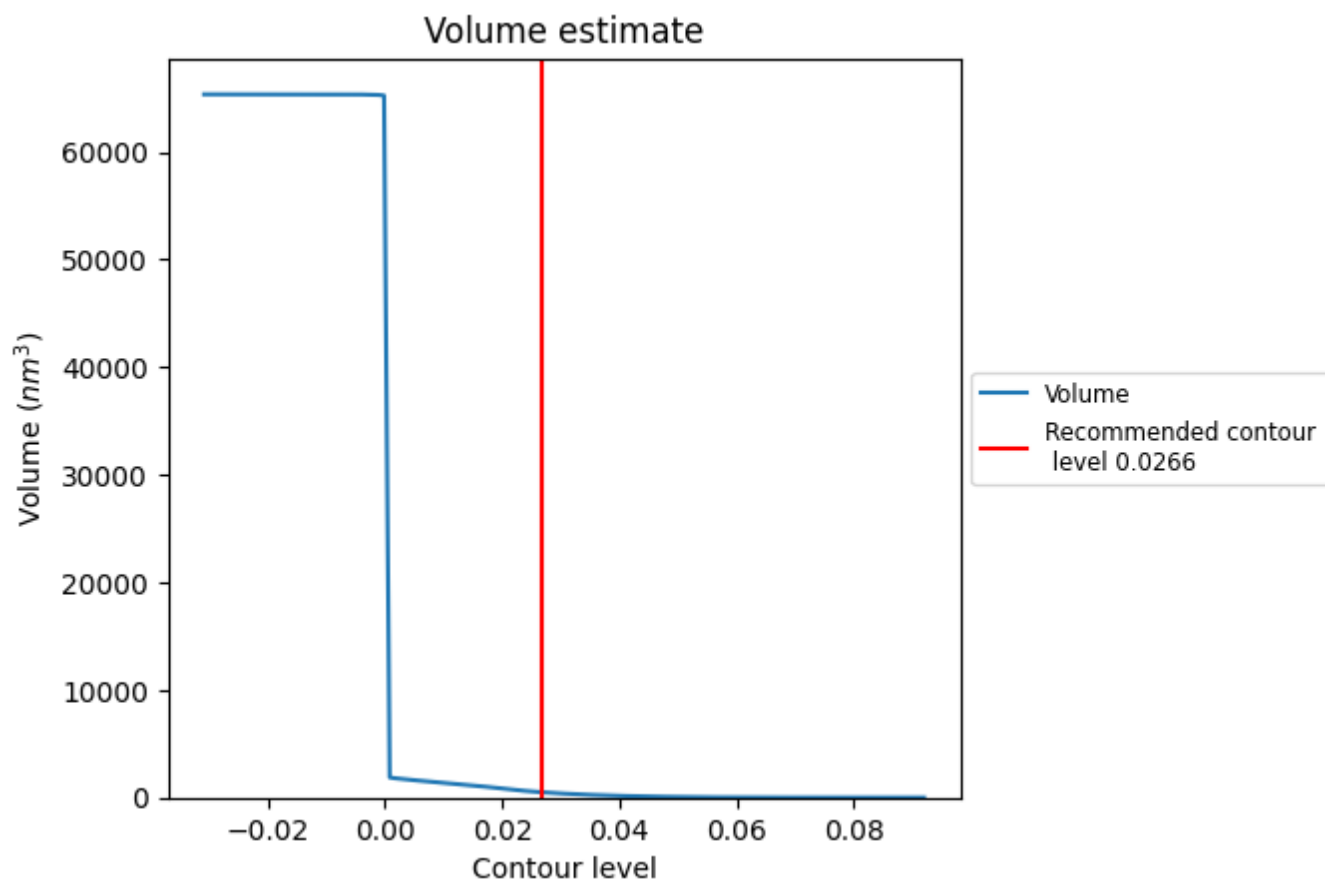
This section contains the results of statistical analysis of the map.

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.

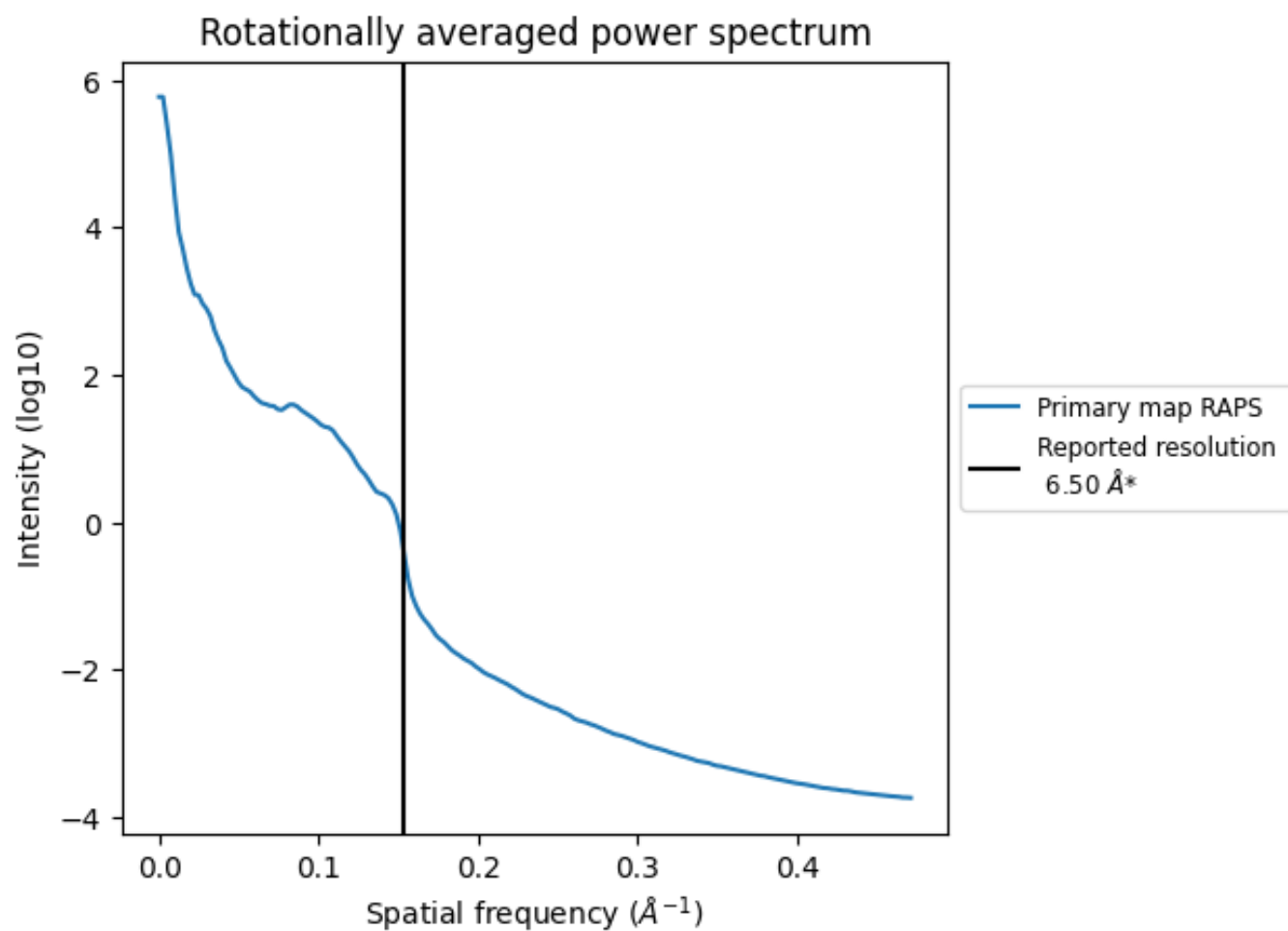
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 501 nm³; this corresponds to an approximate mass of 452 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

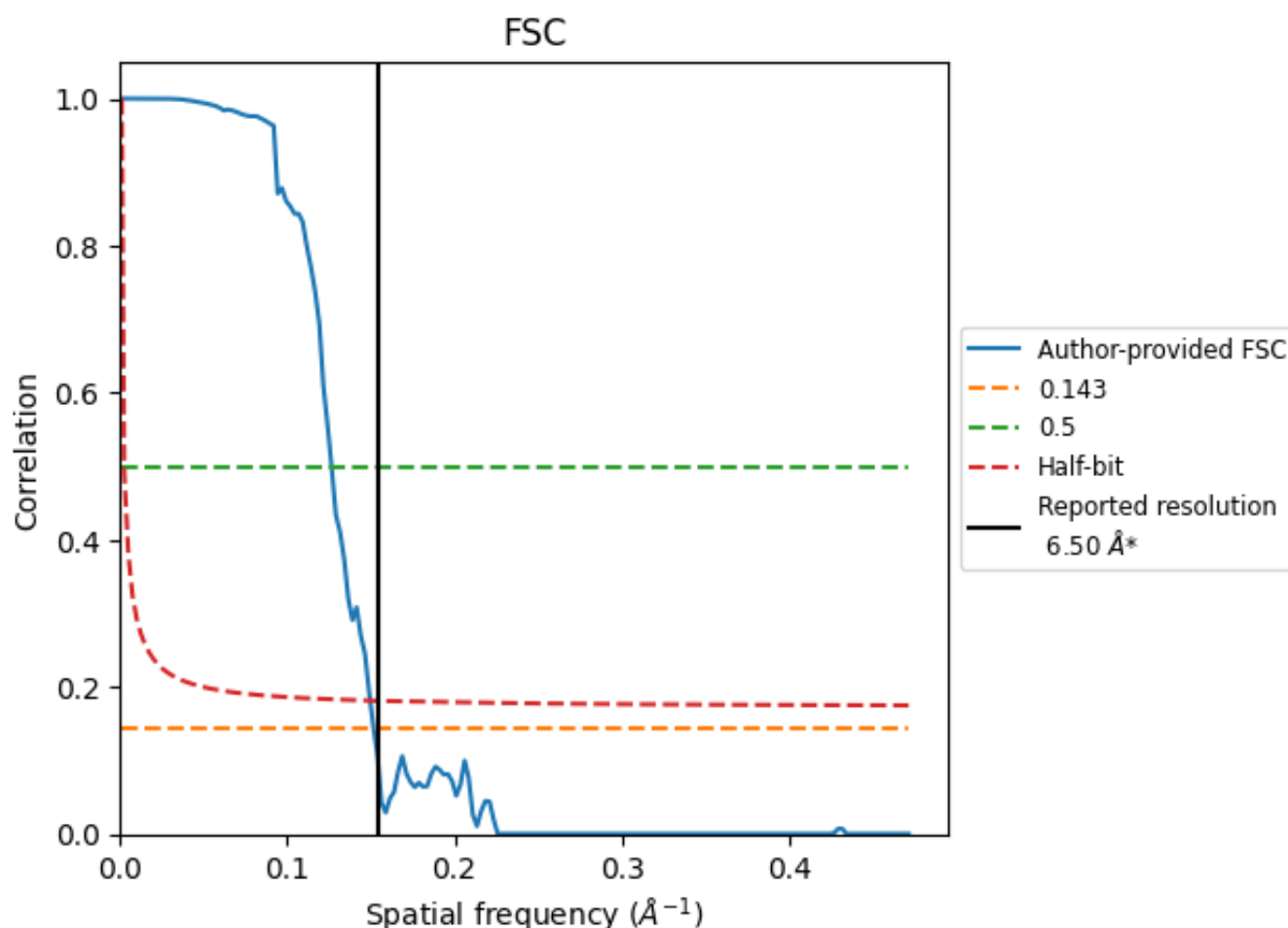


*Reported resolution corresponds to spatial frequency of 0.154 \AA^{-1}

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 0.154 Å⁻¹

8.2 Resolution estimates [i](#)

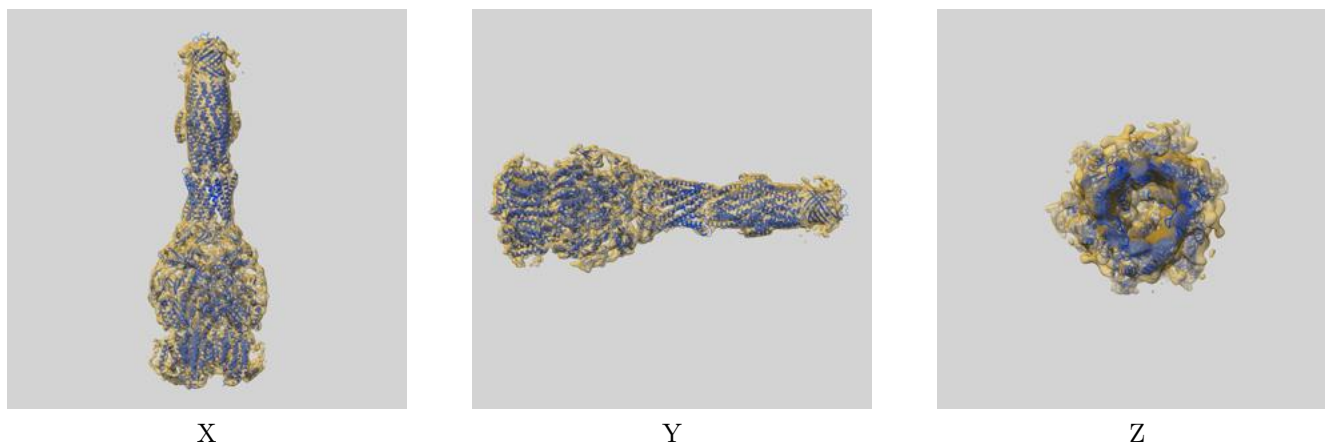
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.50	-	-
Author-provided FSC curve	6.59	7.91	6.68
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

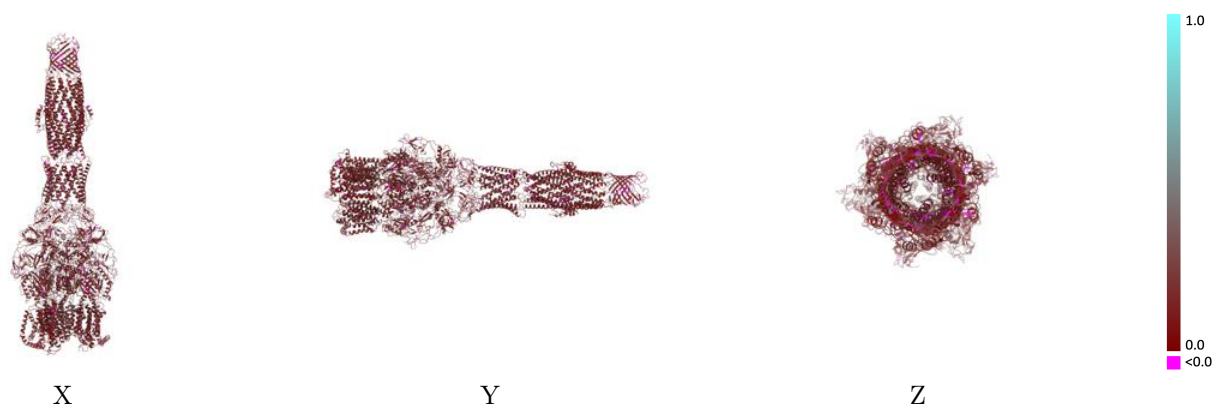
This section contains information regarding the fit between EMDB map EMD-8636 and PDB model 5V5S. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



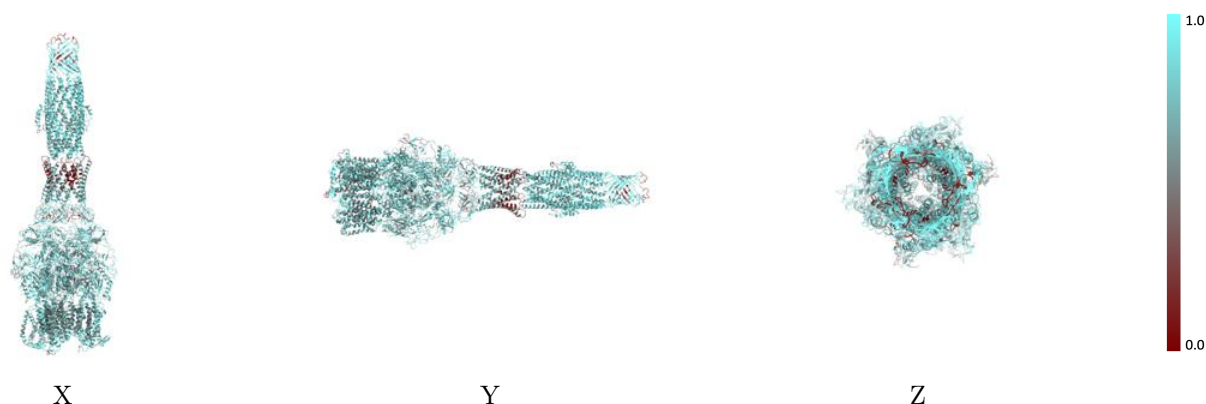
The images above show the 3D surface view of the map at the recommended contour level 0.0266 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



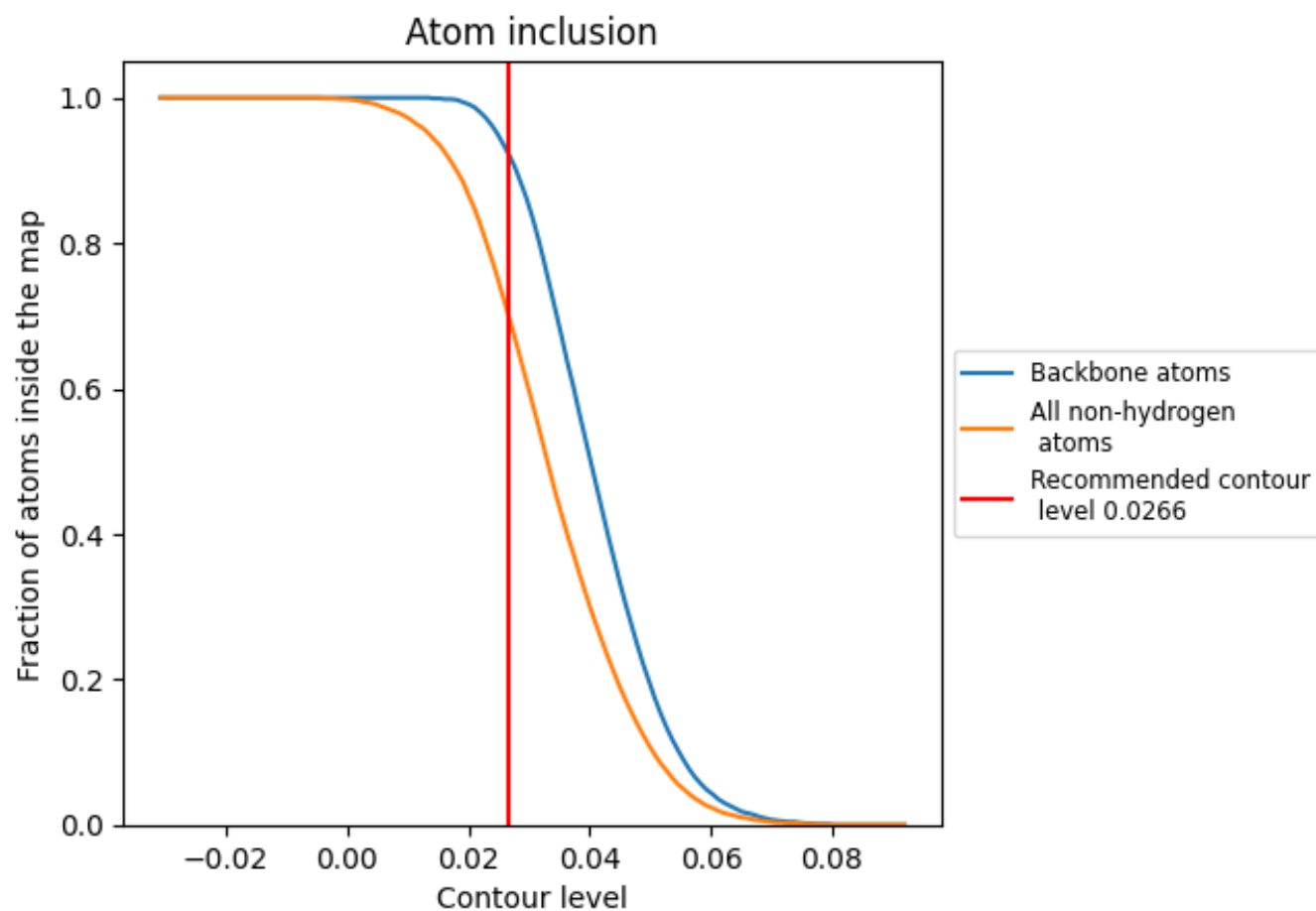
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0266).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0266) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.7010	<div><div></div></div> 0.1930
A	<div><div></div></div> 0.7600	<div><div></div></div> 0.1660
B	<div><div></div></div> 0.7520	<div><div></div></div> 0.1710
C	<div><div></div></div> 0.7480	<div><div></div></div> 0.1720
D	<div><div></div></div> 0.6180	<div><div></div></div> 0.1910
E	<div><div></div></div> 0.6480	<div><div></div></div> 0.2000
F	<div><div></div></div> 0.6070	<div><div></div></div> 0.1940
G	<div><div></div></div> 0.6480	<div><div></div></div> 0.1990
H	<div><div></div></div> 0.6150	<div><div></div></div> 0.1970
I	<div><div></div></div> 0.6480	<div><div></div></div> 0.2010
J	<div><div></div></div> 0.7190	<div><div></div></div> 0.2000
K	<div><div></div></div> 0.7280	<div><div></div></div> 0.1990
L	<div><div></div></div> 0.7270	<div><div></div></div> 0.2000

1.0

0.0

<0.0