



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Jul 24, 2017 – 04:47 AM EDT

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 : unknown
Resolution : 6.50 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

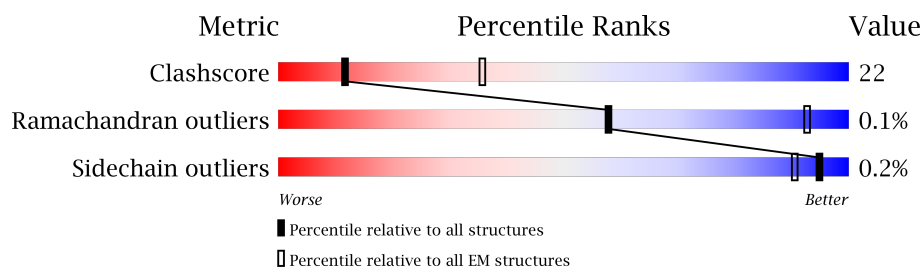
1 Overall quality at a glance

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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	442	51% 45% ..
1	B	442	52% 44% .
1	C	442	54% 43% .
2	D	397	54% 30% . 14%
2	E	397	53% 31% . 14%
2	F	397	52% 33% . 14%
2	G	397	54% 31% . 14%
2	H	397	53% 32% . 14%
2	I	397	51% 34% . 14%

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Mol	Chain	Length	Quality of chain
3	J	1049	<div><div></div><div>57%</div><div>42%</div><div>..</div></div>
3	K	1049	<div><div></div><div>54%</div><div>44%</div><div>..</div></div>
3	L	1049	<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		

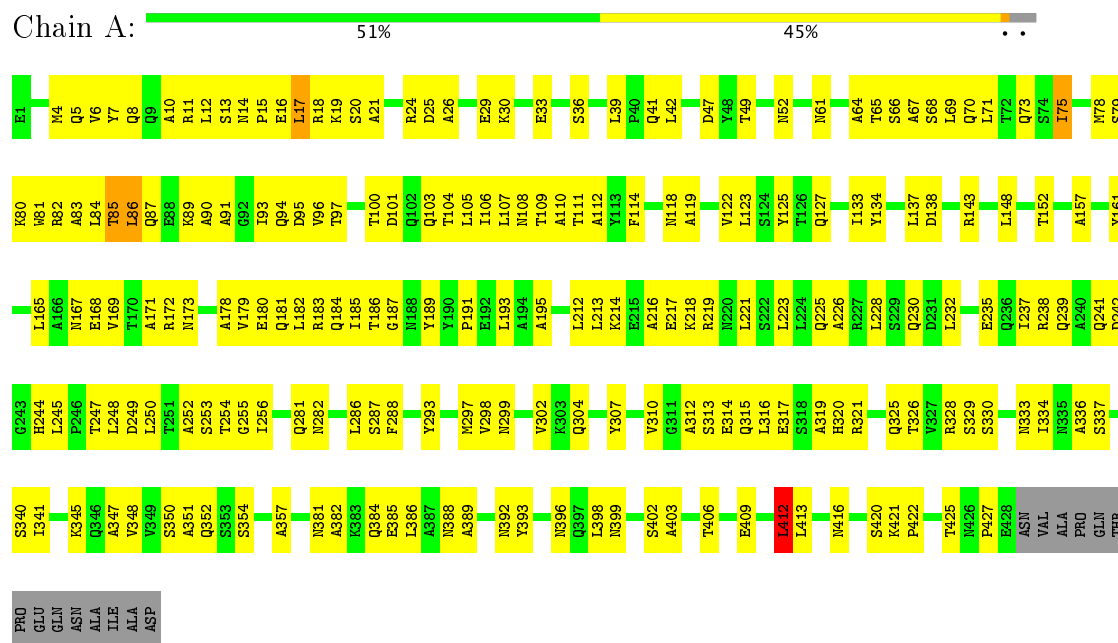
There are 3 discrepancies between the modelled and reference sequences:

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

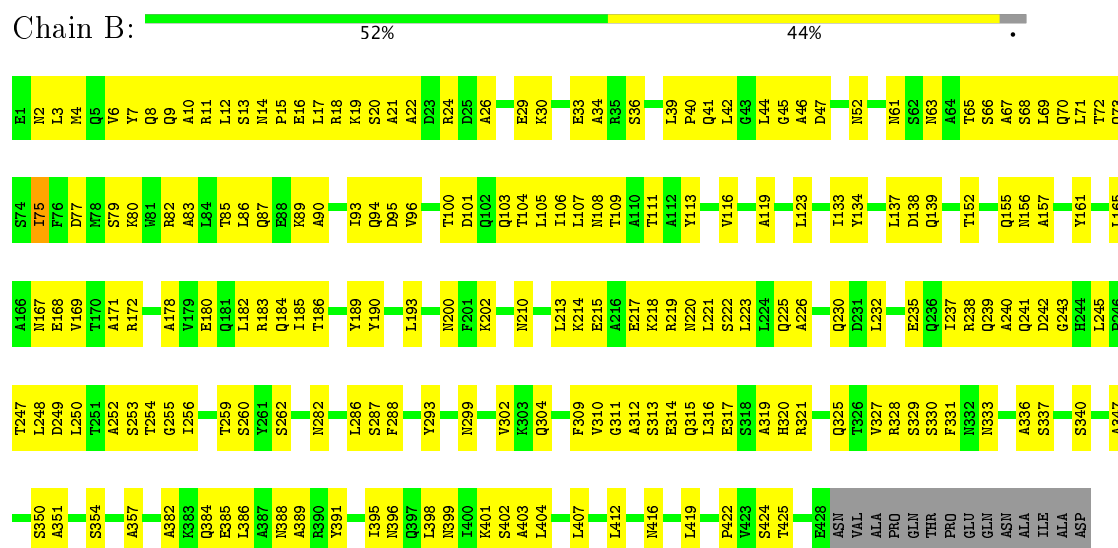
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

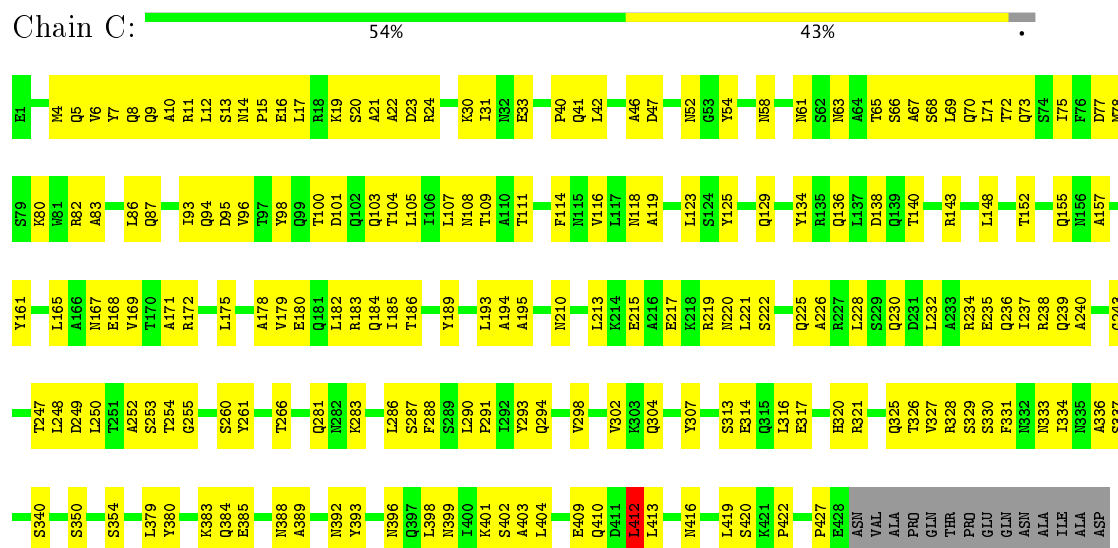
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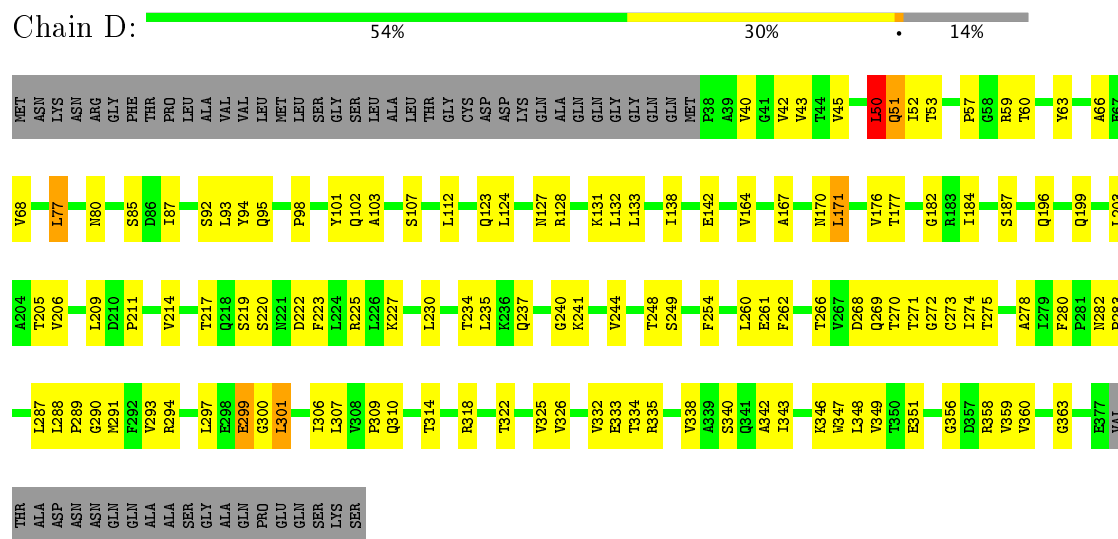
• Molecule 1: Outer membrane protein TolC



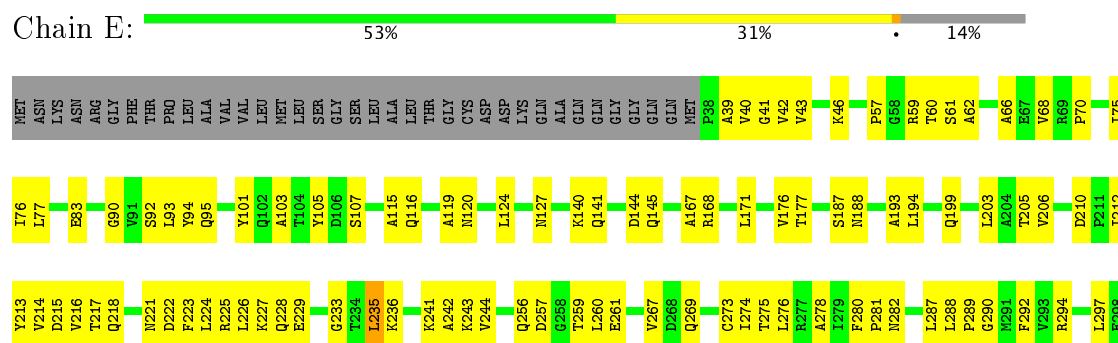
- Molecule 1: Outer membrane protein TolC



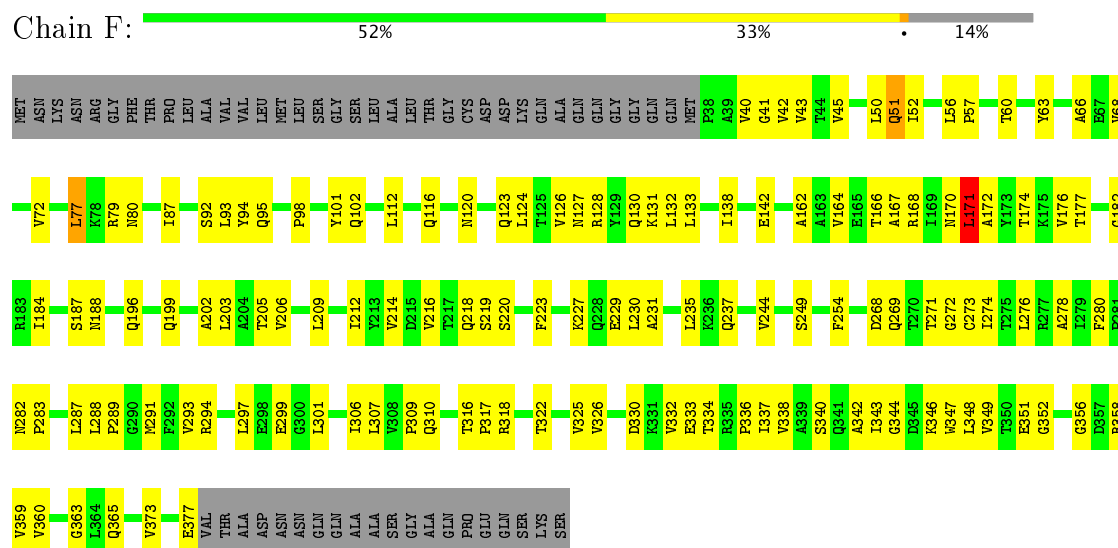
- Molecule 2: Multidrug efflux pump subunit AcrA



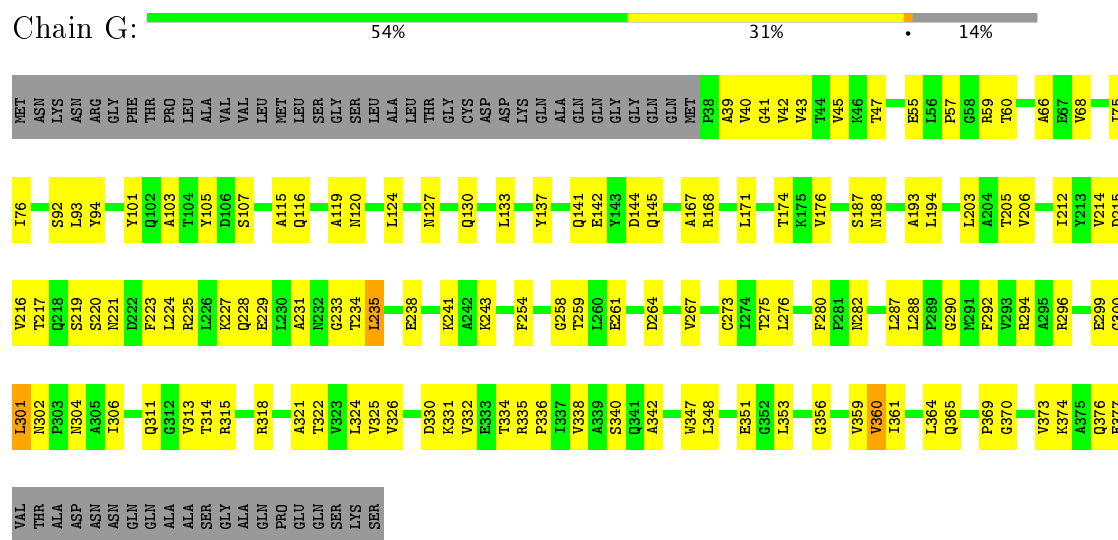
- Molecule 2: Multidrug efflux pump subunit AcrA



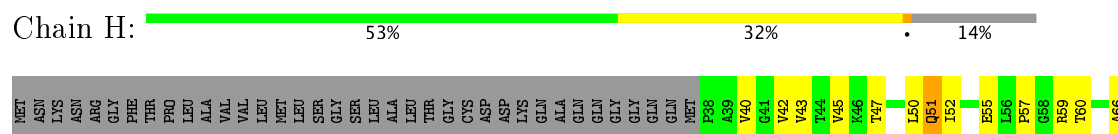
- Molecule 2: Multidrug efflux pump subunit AcrA

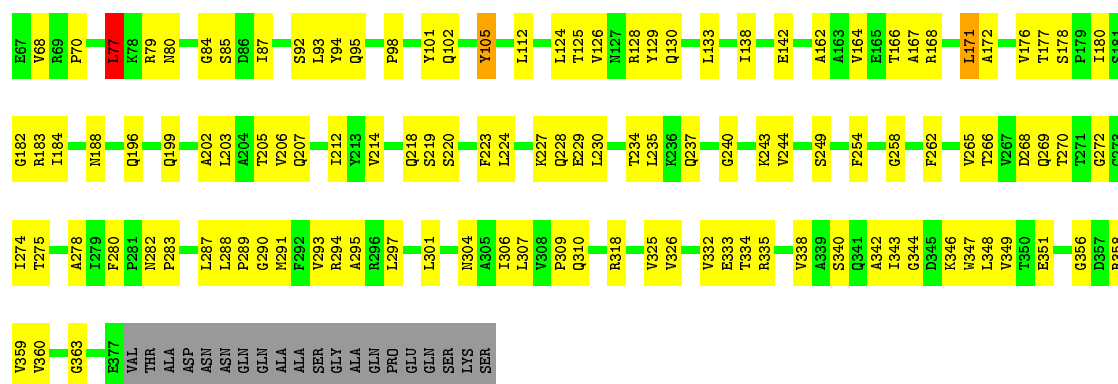


- Molecule 2: Multidrug efflux pump subunit AcrA

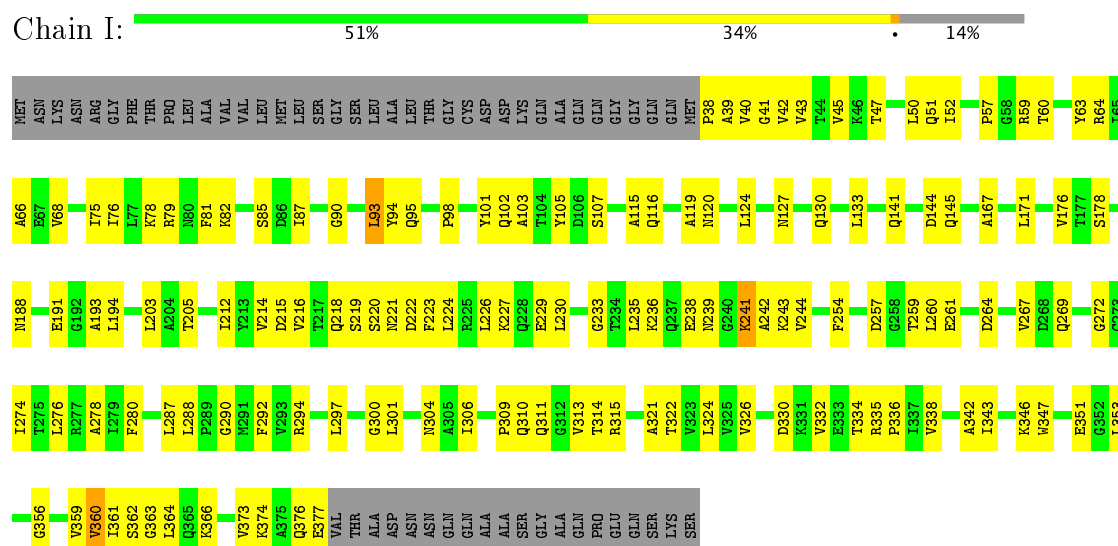


- Molecule 2: Multidrug efflux pump subunit AcrA

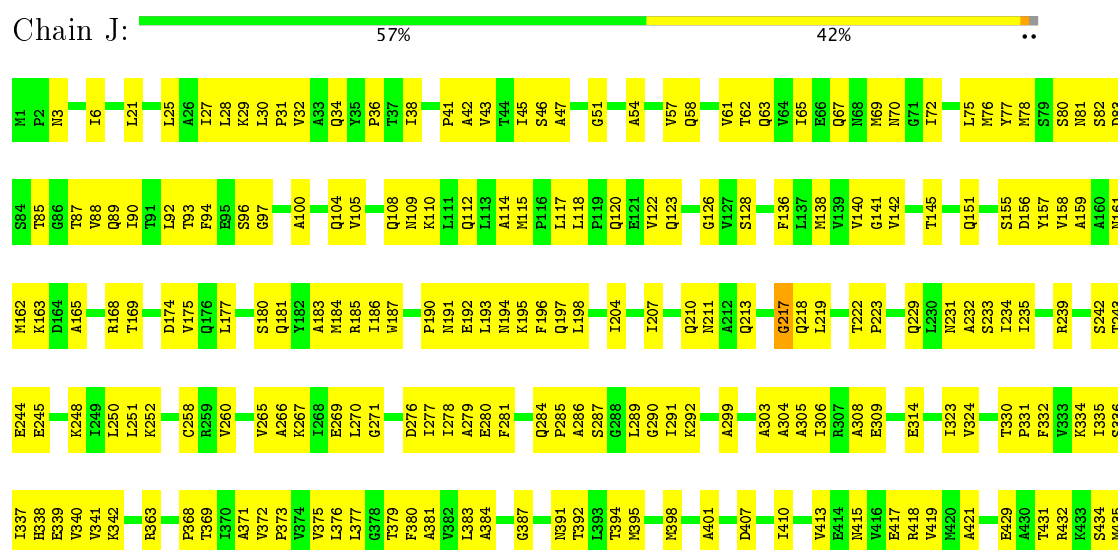


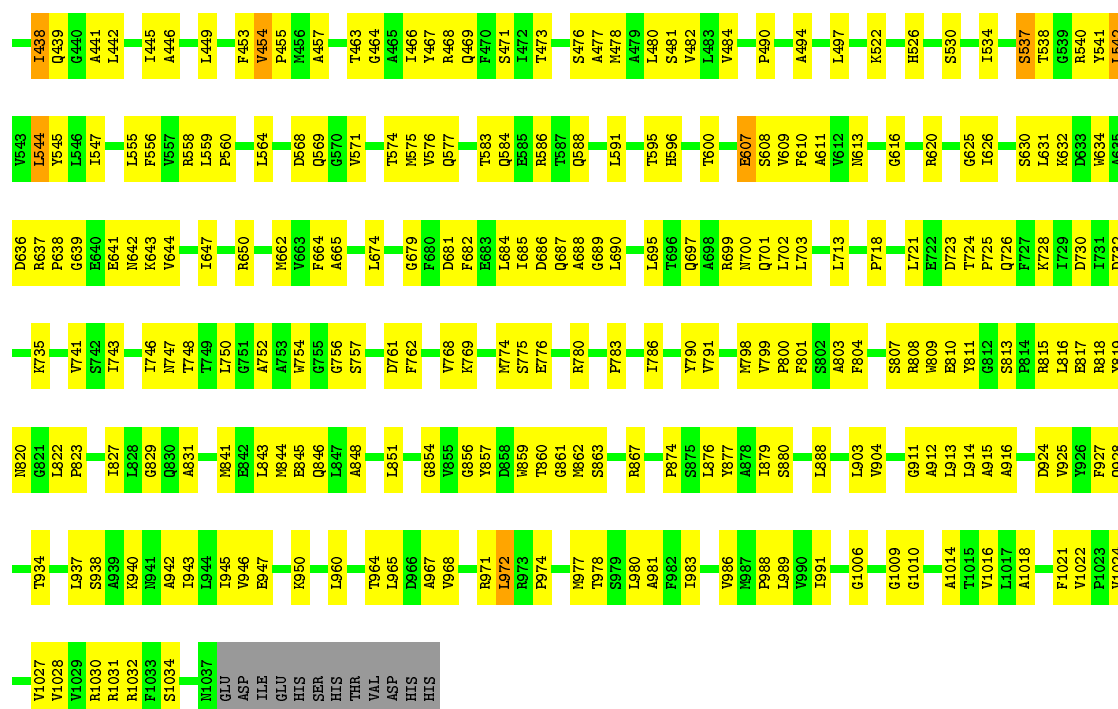


• Molecule 2: Multidrug efflux pump subunit AcrA

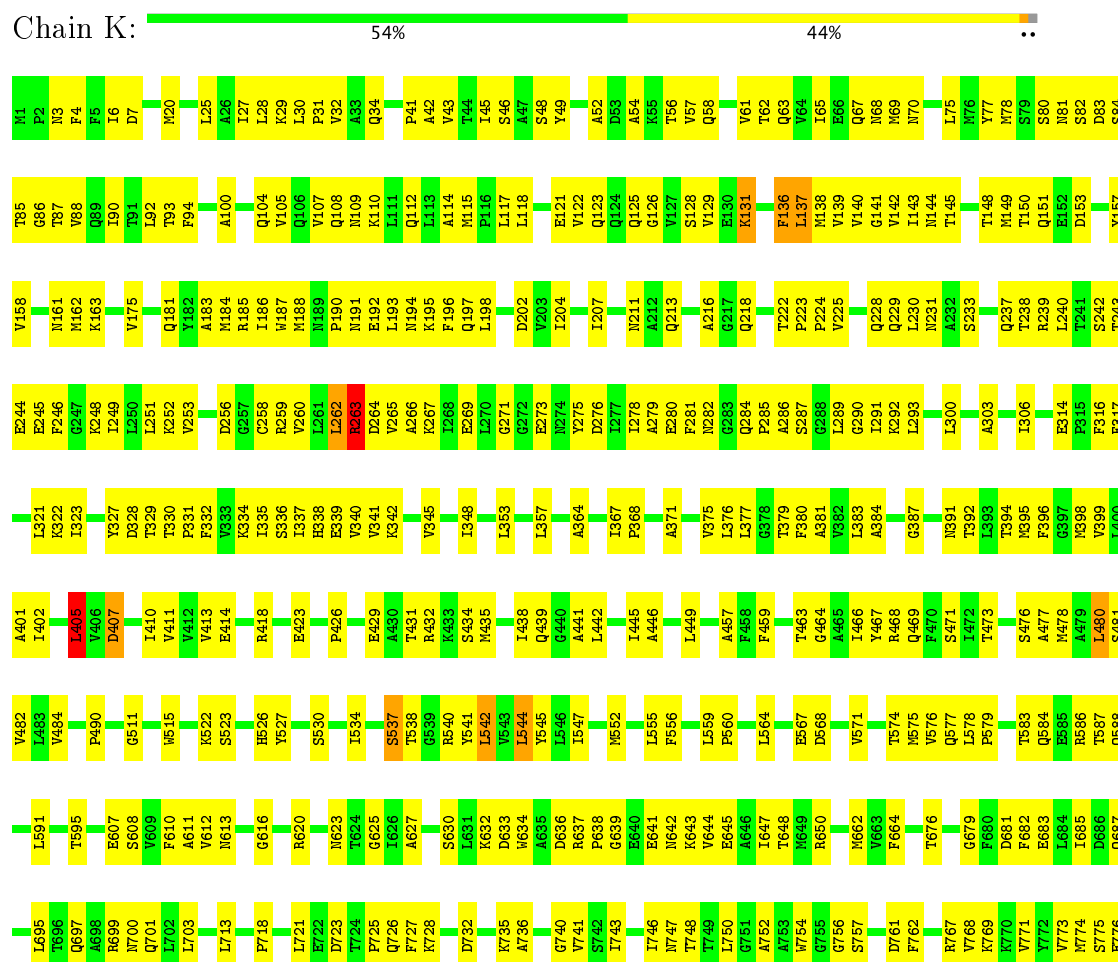


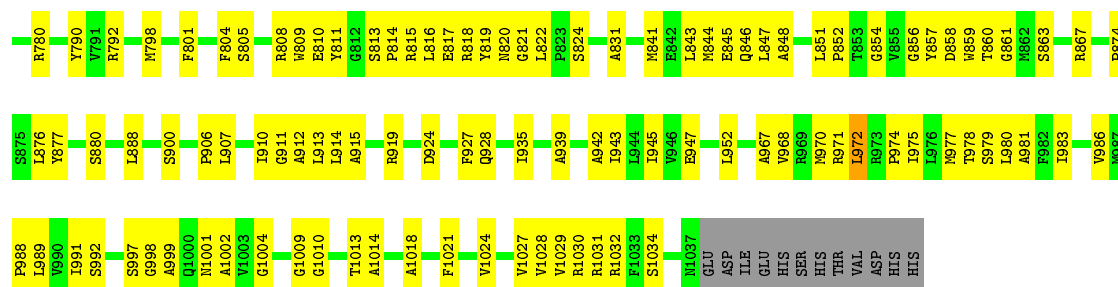
• Molecule 3: Multidrug efflux pump subunit AcrB





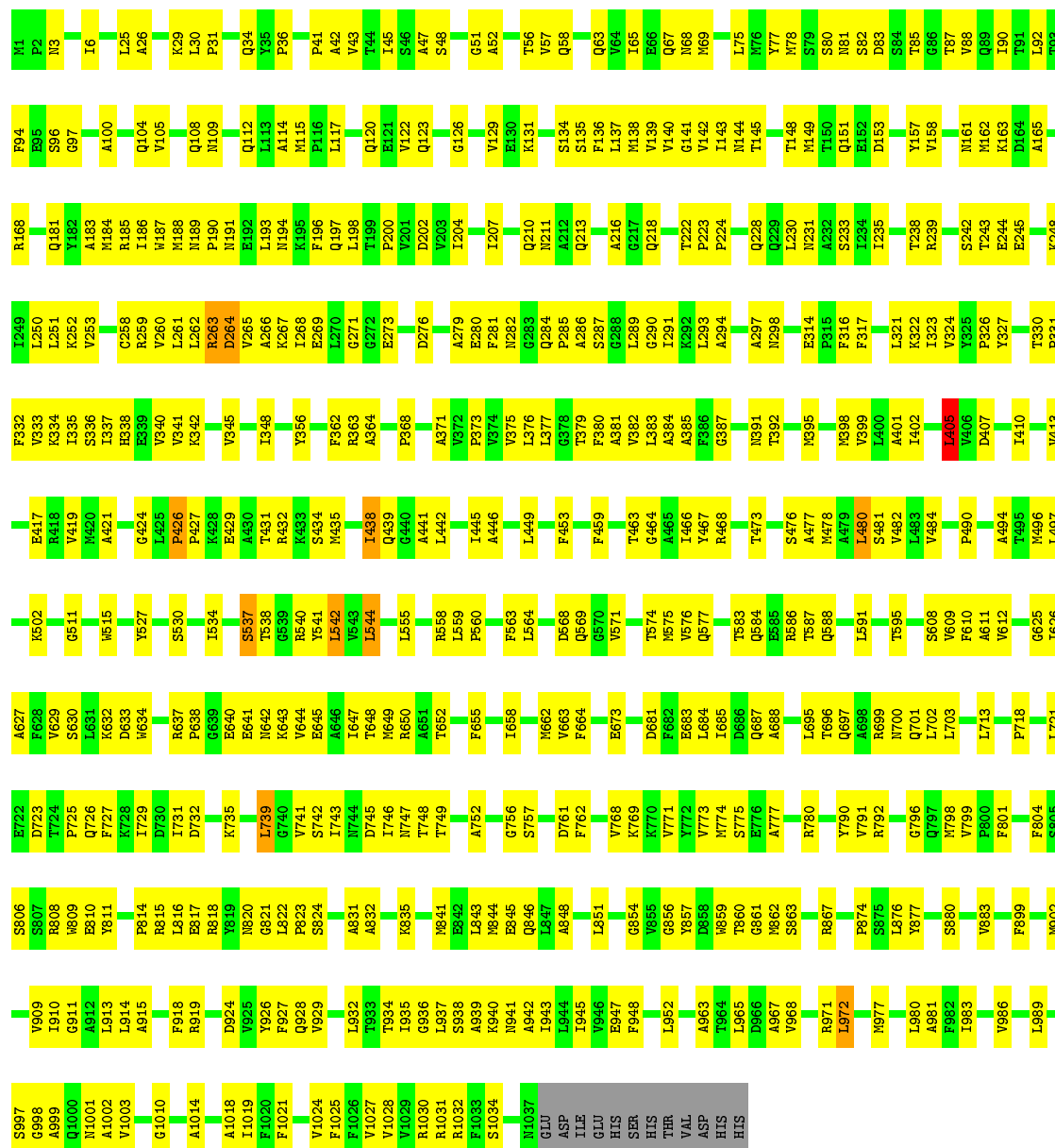
- Molecule 3: Multidrug efflux pump subunit AcrB





• Molecule 3: Multidrug efflux pump subunit AcrB

Chain L: 55% 43% ..



4 Experimental information

Property	Value	Source
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	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	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 > 2$	RMSZ	# $ Z > 2$
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:CE1	2:H:105:TYR:CZ	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%)	28	71
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%)	28	71
2	G	338/397 (85%)	299 (88%)	39 (12%)	0	100	100
2	H	338/397 (85%)	306 (90%)	30 (9%)	2 (1%)	28	71
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%)	51	84
3	L	1035/1049 (99%)	952 (92%)	82 (8%)	1 (0%)	55	88
All	All	6411/6855 (94%)	5887 (92%)	515 (8%)	9 (0%)	58	88

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%)	94	96
1	B	358/364 (98%)	358 (100%)	0	100	100
1	C	358/364 (98%)	357 (100%)	1 (0%)	94	96
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%)	93	95
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%)	94	97
3	K	826/855 (97%)	823 (100%)	3 (0%)	93	95
3	L	826/855 (97%)	823 (100%)	3 (0%)	93	95
All	All	5196/5565 (93%)	5185 (100%)	11 (0%)	95	97

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

Mol	Chain	Res	Type
3	J	480	LEU
3	K	263	ARG
3	L	263	ARG
3	J	454	VAL
3	K	480	LEU

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

Mol	Chain	Res	Type
2	F	80	ASN
2	G	311	GLN
3	L	191	ASN
2	F	127	ASN
2	G	127	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates 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.