



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 20, 2016 – 03:20 PM EDT

PDB ID : 4ZJO
Title : Crystal structure of AcrB triple mutant in complex with antibiotic in P21 space group
Authors : Ababou, A.; Koronakis, V.
Deposited on : 2015-04-29
Resolution : 3.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027939
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027939

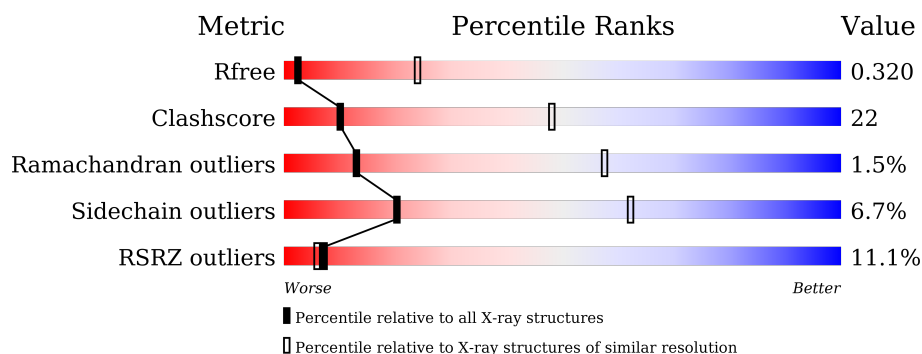
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1408 (3.80-3.40)
Clashscore	102246	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)
RSRZ outliers	91569	1003 (3.78-3.42)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1049	<div> <div>9%</div> <div>53%</div> <div>41%</div> <div>..</div> </div>
1	B	1049	<div> <div>7%</div> <div>56%</div> <div>39%</div> <div>..</div> </div>
1	C	1049	<div> <div>12%</div> <div>52%</div> <div>42%</div> <div>5% .</div> </div>
1	D	1049	<div> <div>11%</div> <div>55%</div> <div>39%</div> <div>5% .</div> </div>
1	E	1049	<div> <div>14%</div> <div>54%</div> <div>41%</div> <div>..</div> </div>
1	F	1049	<div> <div>14%</div> <div>54%</div> <div>41%</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ERY	A	1101	-	-	-	X
2	ERY	D	1101	-	-	-	X
3	LMT	A	1102	-	-	-	X
3	LMT	A	1103	-	-	-	X
3	LMT	B	1101	X	-	-	X
3	LMT	C	1101	-	-	-	X
3	LMT	D	1103	-	-	-	X
3	LMT	E	1101	-	-	-	X
3	LMT	F	1101	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 47876 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Multidrug efflux pump subunit AcrB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1042	Total	C	N	O	S	0	0	0
			7907	5080	1308	1476	43			
1	B	1042	Total	C	N	O	S	0	0	0
			7907	5080	1308	1476	43			
1	C	1044	Total	C	N	O	S	0	0	0
			7924	5090	1312	1479	43			
1	D	1042	Total	C	N	O	S	0	0	0
			7907	5080	1308	1476	43			
1	E	1042	Total	C	N	O	S	0	0	0
			7907	5080	1308	1476	43			
1	F	1046	Total	C	N	O	S	0	0	0
			7939	5099	1314	1483	43			

There are 18 discrepancies between the modelled and reference sequences:

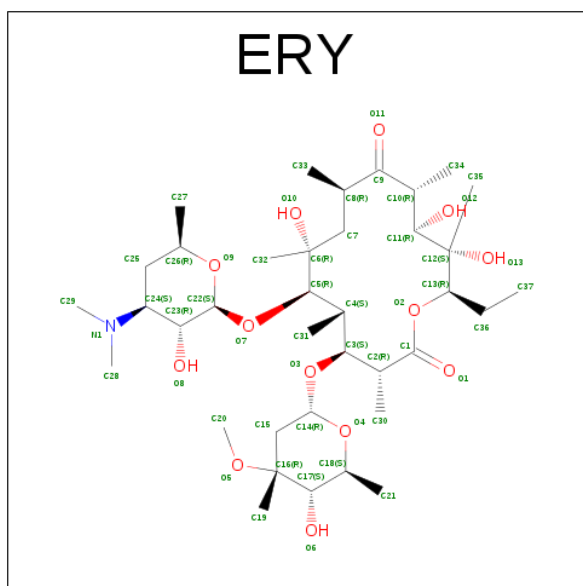
Chain	Residue	Modelled	Actual	Comment	Reference
A	615	ALA	PHE	engineered mutation	UNP P31224
A	617	ALA	PHE	engineered mutation	UNP P31224
A	620	ALA	ARG	engineered mutation	UNP P31224
B	615	ALA	PHE	engineered mutation	UNP P31224
B	617	ALA	PHE	engineered mutation	UNP P31224
B	620	ALA	ARG	engineered mutation	UNP P31224
C	615	ALA	PHE	engineered mutation	UNP P31224
C	617	ALA	PHE	engineered mutation	UNP P31224
C	620	ALA	ARG	engineered mutation	UNP P31224
D	615	ALA	PHE	engineered mutation	UNP P31224
D	617	ALA	PHE	engineered mutation	UNP P31224
D	620	ALA	ARG	engineered mutation	UNP P31224
E	615	ALA	PHE	engineered mutation	UNP P31224
E	617	ALA	PHE	engineered mutation	UNP P31224
E	620	ALA	ARG	engineered mutation	UNP P31224
F	615	ALA	PHE	engineered mutation	UNP P31224
F	617	ALA	PHE	engineered mutation	UNP P31224

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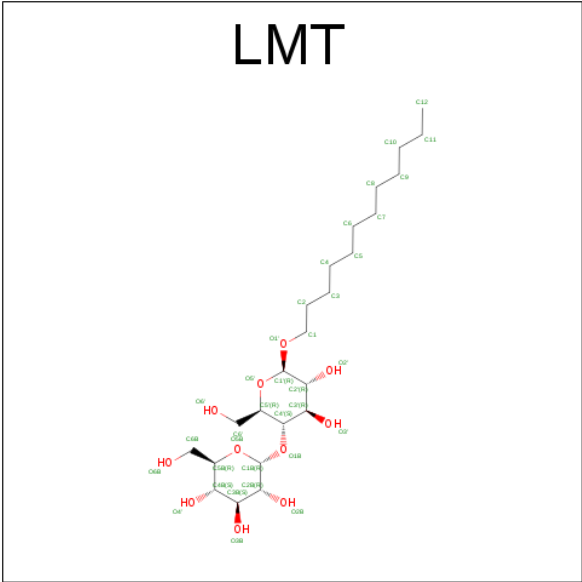
Chain	Residue	Modelled	Actual	Comment	Reference
F	620	ALA	ARG	engineered mutation	UNP P31224

- Molecule 2 is ERYTHROMYCIN A (three-letter code: ERY) (formula: $C_{37}H_{67}NO_{13}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			51	37	1	13		
2	D	1	Total	C	N	O	0	0
			51	37	1	13		

- Molecule 3 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			35	24	11		
3	A	1	Total	C	O	0	0
			35	24	11		
3	B	1	Total	C	O	0	0
			35	24	11		
3	C	1	Total	C	O	0	0
			35	24	11		
3	D	1	Total	C	O	0	0
			35	24	11		
3	D	1	Total	C	O	0	0
			35	24	11		
3	E	1	Total	C	O	0	0
			35	24	11		
3	F	1	Total	C	O	0	0
			35	24	11		

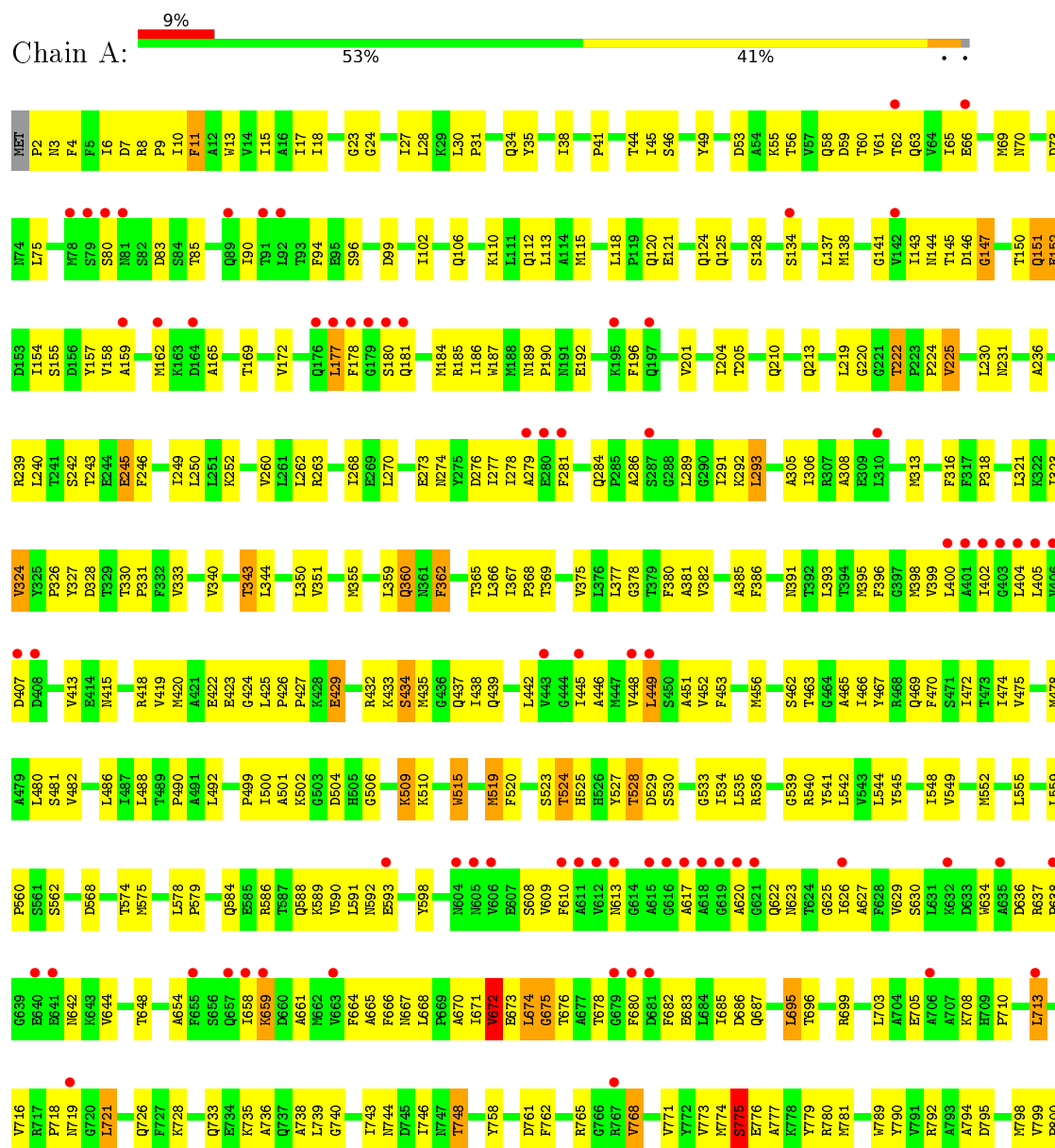
- Molecule 4 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

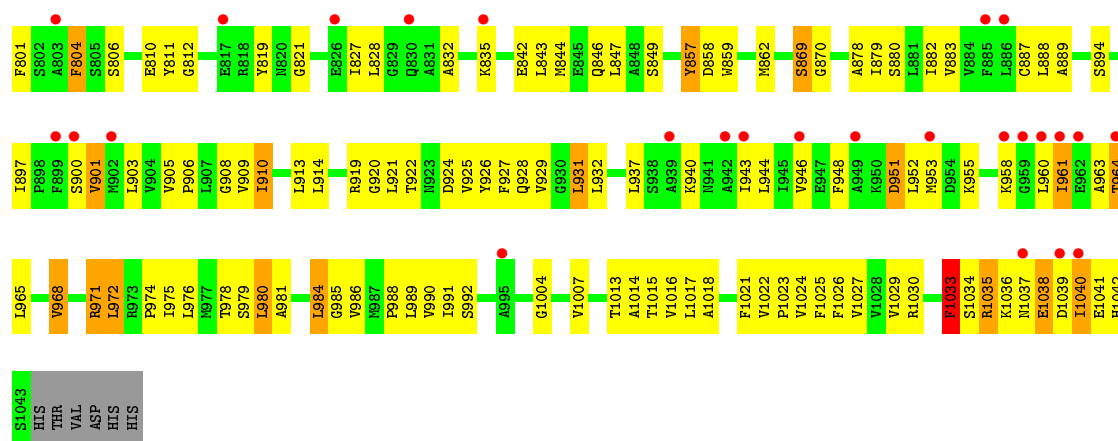
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ni	0	0
			1	1		
4	C	1	Total	Ni	0	0
			1	1		
4	E	1	Total	Ni	0	0
			1	1		

3 Residue-property plots

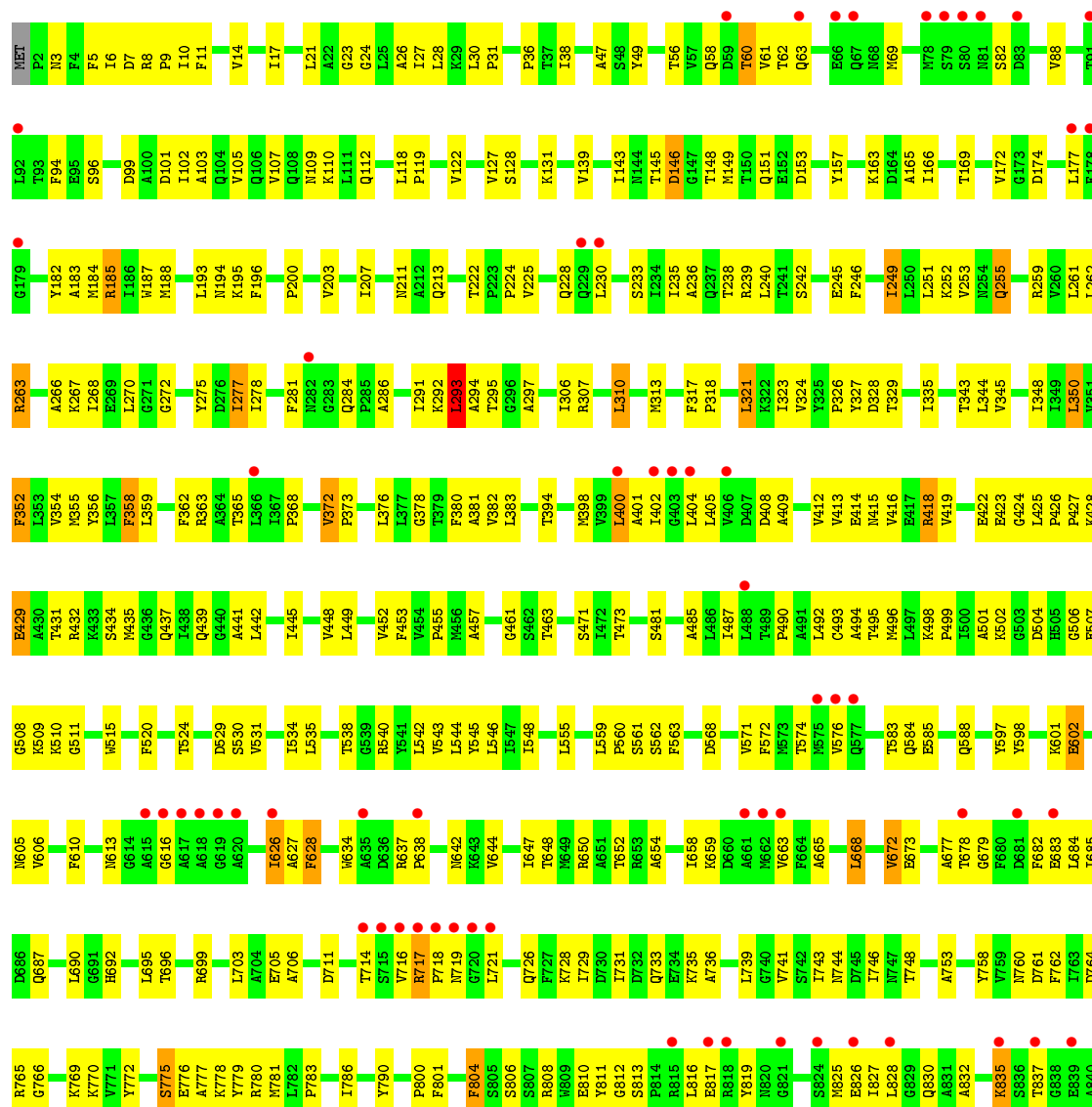
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

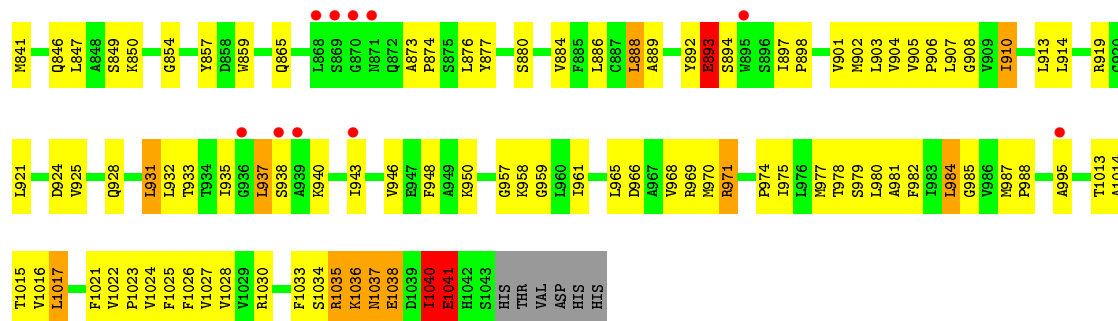
- Molecule 1: Multidrug efflux pump subunit AcrB



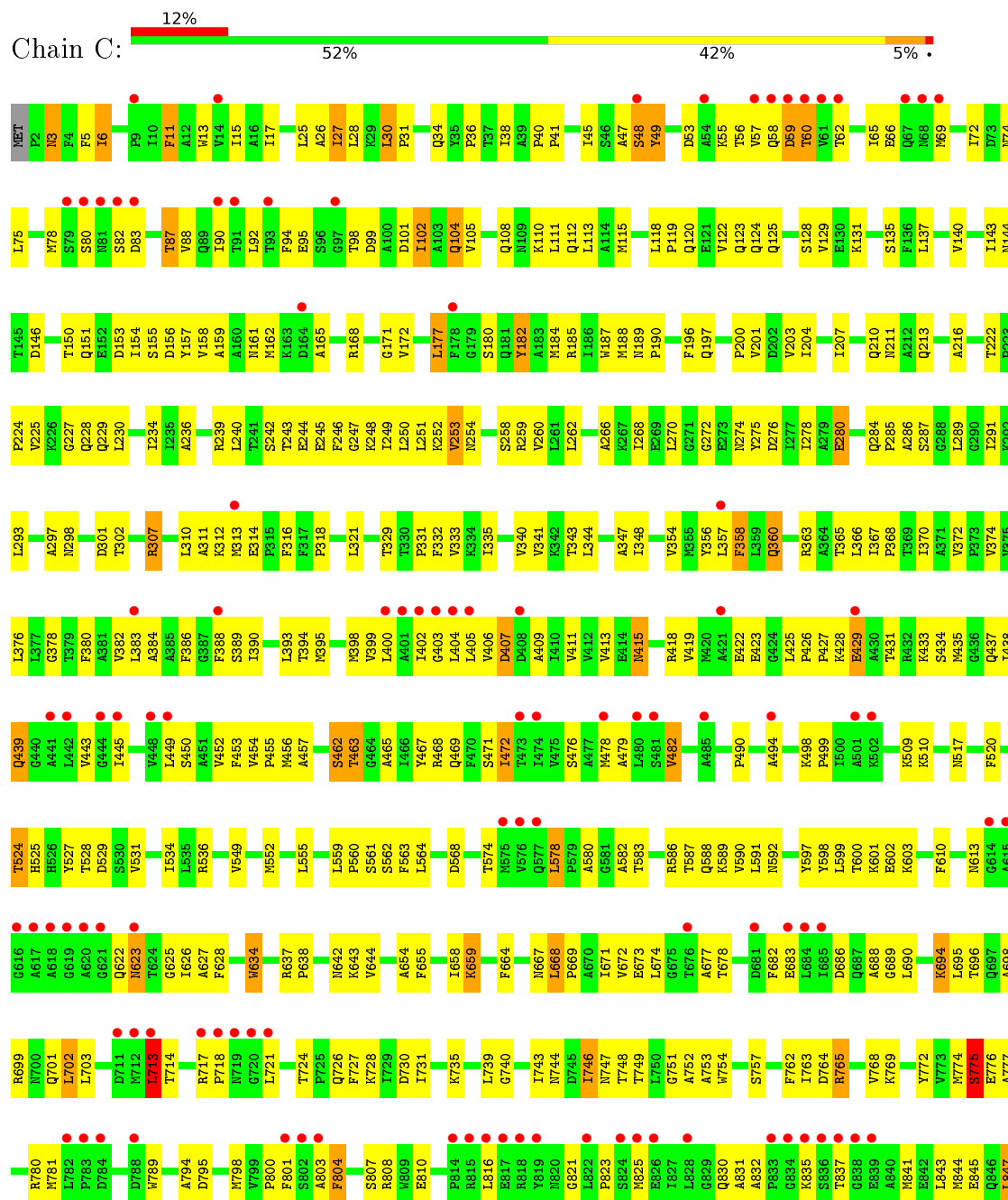


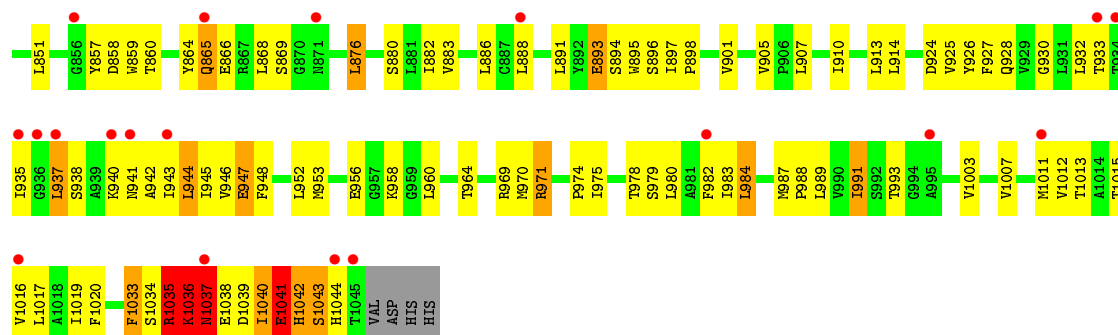
• Molecule 1: Multidrug efflux pump subunit AcrB



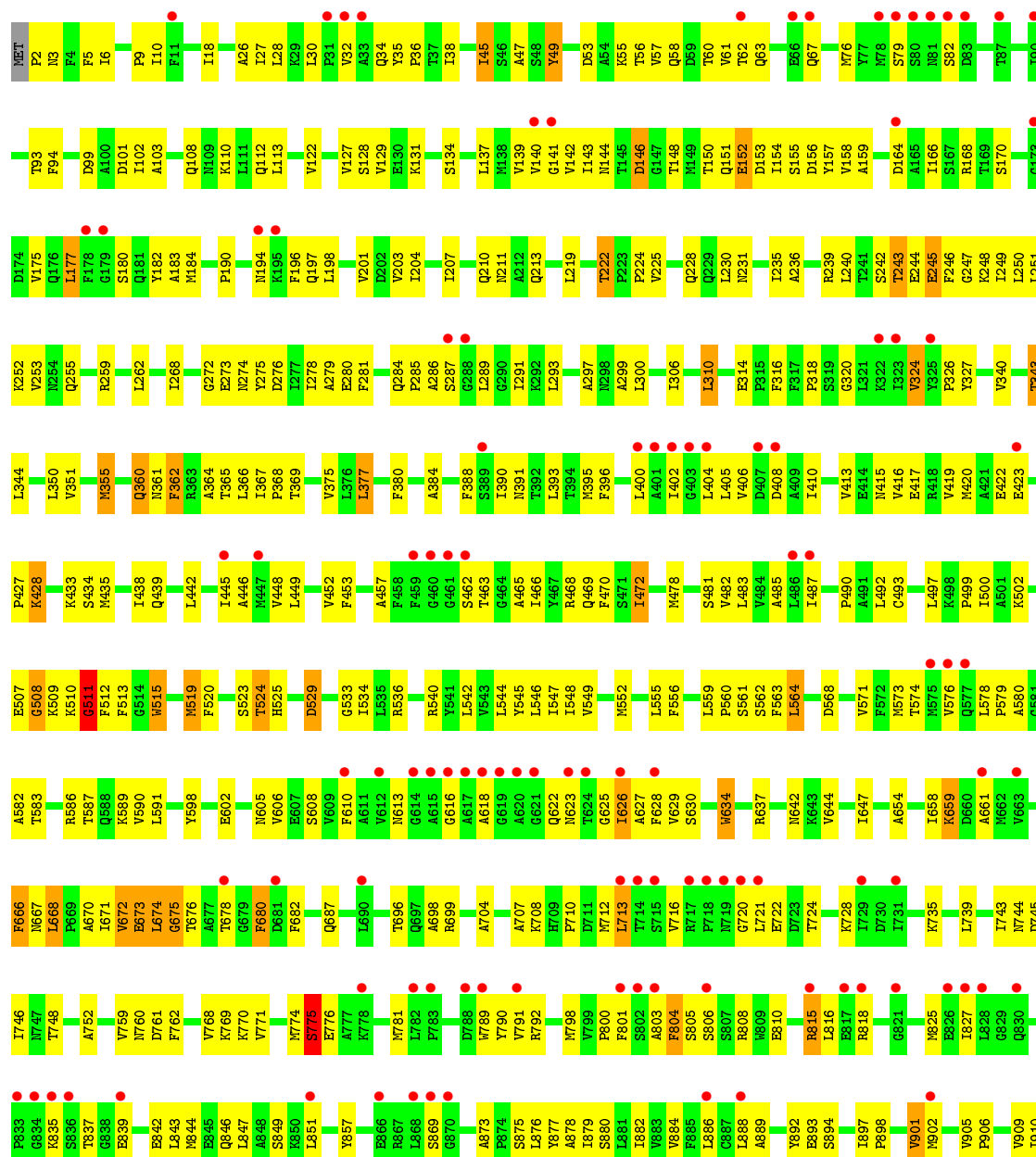


• Molecule 1: Multidrug efflux pump subunit AcrB

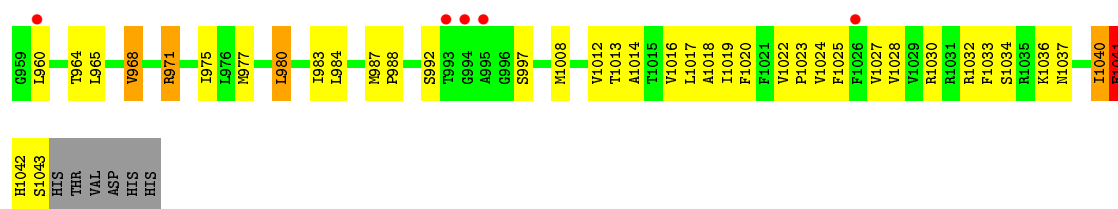




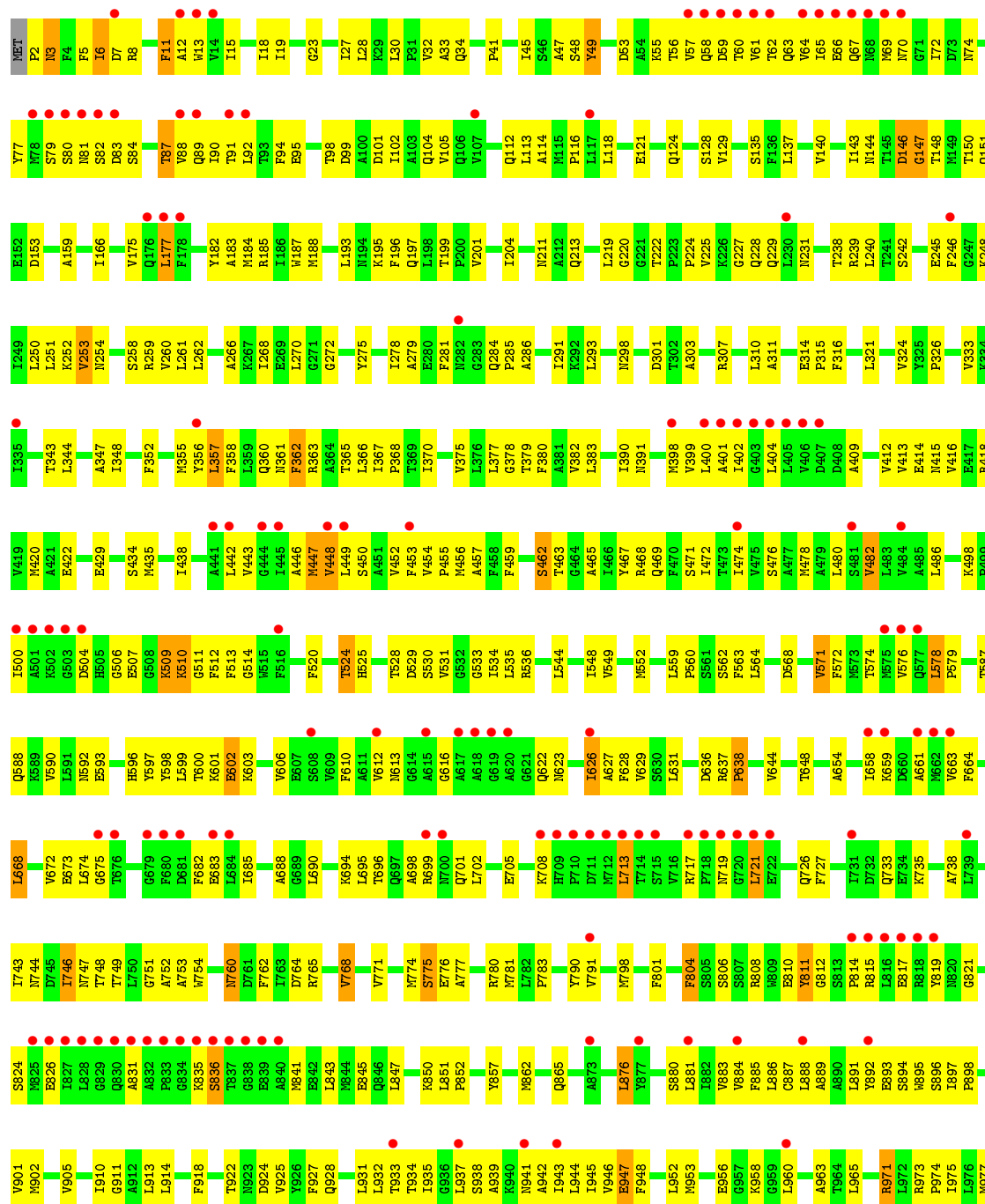
• Molecule 1: Multidrug efflux pump subunit AcrB







• Molecule 1: Multidrug efflux pump subunit AcrB



T978	S979	L980	A981	F982	I983	L984	G985	V986	M987	F988	L989	W990	I991	S992	T993	G994	A995	T1005	G1006	V1007	M1011	V1012	T1013	A1014	T1015	V1016	L1017	F1021	V1024	F1025	F1026	V1027	V1028	V1029	R1030	F1033	S1034	R1035	K1036	M1037	E1038	T1039	I1040	E1041	H1042	S1043	H1044	T1045	V1046	D1047	HIS	HIS
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	151.18Å 156.77Å 218.17Å 90.00° 93.09° 90.00°	Depositor
Resolution (Å)	19.96 – 3.60 108.93 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.96-3.60) 97.1 (108.93-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 3.58Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.238 , 0.307 0.247 , 0.320	Depositor DCC
R_{free} test set	5666 reflections (4.96%)	DCC
Wilson B-factor (Å ²)	101.2	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 70.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	47876	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.75 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.2566e-04.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NI, LMT, ERY

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	0.59	1/8056 (0.0%)	0.81	5/10940 (0.0%)
1	B	0.59	0/8056	0.81	9/10940 (0.1%)
1	C	0.58	1/8074 (0.0%)	0.84	11/10965 (0.1%)
1	D	0.55	1/8056 (0.0%)	0.80	9/10940 (0.1%)
1	E	0.56	1/8056 (0.0%)	0.80	7/10940 (0.1%)
1	F	0.57	0/8089	0.83	6/10986 (0.1%)
All	All	0.57	4/48387 (0.0%)	0.82	47/65711 (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	1
1	B	0	2
1	C	0	1
1	D	0	1
1	F	0	2
All	All	0	7

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	515	TRP	CB-CG	7.98	1.64	1.50
1	E	515	TRP	CB-CG	7.12	1.63	1.50
1	D	515	TRP	CB-CG	6.65	1.62	1.50
1	C	895	TRP	CB-CG	-5.62	1.40	1.50

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	529	ASP	CB-CG-OD1	11.89	129.00	118.30
1	B	529	ASP	CB-CG-OD1	11.82	128.94	118.30
1	C	529	ASP	CB-CG-OD1	9.63	126.97	118.30
1	B	293	LEU	CA-CB-CG	8.59	135.06	115.30
1	A	529	ASP	CB-CG-OD1	8.09	125.58	118.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1033	PHE	Peptide
1	B	1036	LYS	Peptide
1	B	1040	ILE	Peptide
1	C	1036	LYS	Peptide
1	D	1033	PHE	Peptide

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	7907	0	8050	386	0
1	B	7907	0	8050	338	0
1	C	7924	0	8064	394	1
1	D	7907	0	8050	344	1
1	E	7907	0	8050	345	0
1	F	7939	0	8077	376	0
2	A	51	0	67	10	0
2	D	51	0	67	5	0
3	A	70	0	92	5	0
3	B	35	0	46	5	0
3	C	35	0	46	1	0
3	D	70	0	92	9	0
3	E	35	0	46	3	0
3	F	35	0	46	5	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
All	All	47876	0	48843	2113	1

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 2113 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)
1:A:530:SER:OG	3:A:1102:LMT:O2'	1.59	1.15
1:A:427:PRO:HD3	1:A:499:PRO:HB3	1.41	1.03
1:C:831:ALA:HB3	1:C:835:LYS:HG3	1.42	0.98
1:E:340:VAL:HG21	1:E:395:MET:HB3	1.46	0.98
1:A:144:ASN:O	1:A:284:GLN:NE2	2.01	0.94

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:525:HIS:NE2	1:D:525:HIS:NE2[1_556]	2.02	0.18

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 X-ray entries followed by that with respect to entries of similar resolution.

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	1040/1049 (99%)	951 (91%)	75 (7%)	14 (1%)	15	60
1	B	1040/1049 (99%)	957 (92%)	70 (7%)	13 (1%)	15	60
1	C	1042/1049 (99%)	954 (92%)	72 (7%)	16 (2%)	13	57
1	D	1040/1049 (99%)	946 (91%)	79 (8%)	15 (1%)	14	59
1	E	1040/1049 (99%)	960 (92%)	63 (6%)	17 (2%)	12	56
1	F	1044/1049 (100%)	945 (90%)	83 (8%)	16 (2%)	13	57
All	All	6246/6294 (99%)	5713 (92%)	442 (7%)	91 (2%)	13	57

5 of 91 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	509	LYS
1	A	673	GLU
1	A	675	GLY
1	A	991	ILE
1	A	1040	ILE

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 X-ray entries followed by that with respect to entries of similar resolution.

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	845/852 (99%)	786 (93%)	59 (7%)	19	60
1	B	845/852 (99%)	788 (93%)	57 (7%)	20	62
1	C	847/852 (99%)	787 (93%)	60 (7%)	18	59
1	D	845/852 (99%)	795 (94%)	50 (6%)	24	66
1	E	845/852 (99%)	788 (93%)	57 (7%)	20	62
1	F	849/852 (100%)	791 (93%)	58 (7%)	20	61
All	All	5076/5112 (99%)	4735 (93%)	341 (7%)	20	62

5 of 341 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	713	LEU
1	D	360	GLN
1	F	695	LEU
1	C	795	ASP
1	C	1035	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	123	GLN
1	D	360	GLN
1	E	613	ASN
1	C	104	GLN

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Mol	Chain	Res	Type
1	C	274	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 ⓘ

Of 13 ligands modelled in this entry, 3 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	ERY	A	1101	-	53,53,53	1.26	4 (7%)	82,82,82	2.04	23 (28%)
3	LMT	A	1102	-	36,36,36	1.75	9 (25%)	47,47,47	1.18	5 (10%)
3	LMT	A	1103	-	36,36,36	1.88	8 (22%)	47,47,47	1.48	9 (19%)
3	LMT	B	1101	-	36,36,36	1.83	9 (25%)	47,47,47	1.95	11 (23%)
3	LMT	C	1101	-	36,36,36	1.72	9 (25%)	47,47,47	1.57	9 (19%)
2	ERY	D	1101	-	53,53,53	1.38	4 (7%)	82,82,82	2.02	22 (26%)
3	LMT	D	1102	-	36,36,36	1.81	10 (27%)	47,47,47	1.09	3 (6%)
3	LMT	D	1103	-	36,36,36	1.74	8 (22%)	47,47,47	1.60	10 (21%)
3	LMT	E	1101	-	36,36,36	1.81	10 (27%)	47,47,47	1.34	6 (12%)
3	LMT	F	1101	-	36,36,36	1.78	8 (22%)	47,47,47	1.38	8 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ERY	A	1101	-	-	0/72/107/107	0/3/3/3
3	LMT	A	1102	-	-	0/21/61/61	0/2/2/2
3	LMT	A	1103	-	-	0/21/61/61	0/2/2/2
3	LMT	B	1101	-	1/1/10/10	0/21/61/61	0/2/2/2
3	LMT	C	1101	-	-	0/21/61/61	0/2/2/2
2	ERY	D	1101	-	-	0/72/107/107	0/3/3/3
3	LMT	D	1102	-	-	0/21/61/61	0/2/2/2
3	LMT	D	1103	-	-	0/21/61/61	0/2/2/2
3	LMT	E	1101	-	-	0/21/61/61	0/2/2/2
3	LMT	F	1101	-	-	0/21/61/61	0/2/2/2

The worst 5 of 79 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1102	LMT	C6'-C5'	-3.24	1.40	1.51
3	F	1101	LMT	C6'-C5'	-3.11	1.40	1.51
3	E	1101	LMT	C3'-C2'	-3.10	1.44	1.52
3	D	1103	LMT	C6'-C5'	-3.04	1.41	1.51
3	A	1103	LMT	C6'-C5'	-2.96	1.41	1.51

The worst 5 of 106 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	ERY	O2-C1-O1	-4.68	114.81	123.88
3	D	1103	LMT	C1'-O5'-C5'	-4.32	105.26	113.74
3	B	1101	LMT	O5'-C5'-C4'	-4.14	100.94	109.78
2	A	1101	ERY	C13-O2-C1	-4.10	111.23	118.10
2	D	1101	ERY	C25-C24-N1	-3.56	104.97	115.68

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	1101	LMT	C3B

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	ERY	10	0
3	A	1102	LMT	3	0
3	A	1103	LMT	2	0
3	B	1101	LMT	5	0
3	C	1101	LMT	1	0
2	D	1101	ERY	5	0
3	D	1102	LMT	2	0
3	D	1103	LMT	7	0
3	E	1101	LMT	3	0
3	F	1101	LMT	5	0

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 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1042/1049 (99%)	0.39	99 (9%) 10 8	49, 83, 120, 150	0
1	B	1042/1049 (99%)	0.28	70 (6%) 21 13	45, 81, 117, 154	0
1	C	1044/1049 (99%)	0.58	121 (11%) 6 5	40, 83, 120, 176	0
1	D	1042/1049 (99%)	0.53	117 (11%) 7 6	43, 94, 130, 161	0
1	E	1042/1049 (99%)	0.55	144 (13%) 4 4	57, 94, 125, 151	0
1	F	1046/1049 (99%)	0.66	144 (13%) 4 4	44, 89, 124, 158	0
All	All	6258/6294 (99%)	0.50	695 (11%) 7 6	40, 87, 124, 176	0

The worst 5 of 695 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	719	ASN	14.3
1	C	720	GLY	14.2
1	F	80	SER	11.4
1	F	720	GLY	10.9
1	C	618	ALA	9.8

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	LMT	A	1103	35/35	0.84	1.05	6.48	58,93,104,107	0
2	ERY	A	1101	51/51	0.80	1.15	3.00	75,87,97,106	51
2	ERY	D	1101	51/51	0.67	1.13	2.62	73,92,103,104	51
3	LMT	F	1101	35/35	0.85	0.66	2.29	49,77,91,99	0
3	LMT	B	1101	35/35	0.84	0.57	1.87	49,76,101,110	0
3	LMT	A	1102	35/35	0.89	0.56	1.46	26,76,84,88	0
3	LMT	E	1101	35/35	0.83	0.54	1.05	57,76,88,116	0
3	LMT	D	1102	35/35	0.83	0.39	0.78	55,79,93,93	0
3	LMT	C	1101	35/35	0.81	0.46	0.73	55,72,93,98	0
3	LMT	D	1103	35/35	0.78	0.40	-0.17	79,94,108,110	0
4	NI	A	1104	1/1	0.99	0.15	-	54,54,54,54	0
4	NI	E	1102	1/1	0.98	0.13	-	94,94,94,94	0
4	NI	C	1102	1/1	0.99	0.12	-	62,62,62,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.