



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 20, 2016 – 06:01 PM EDT

PDB ID : 4ZIV
Title : Crystal structure of AcrB triple mutant in P21 space group
Authors : Ababou, A.; Koronakis, V.
Deposited on : 2015-04-28
Resolution : 3.16 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

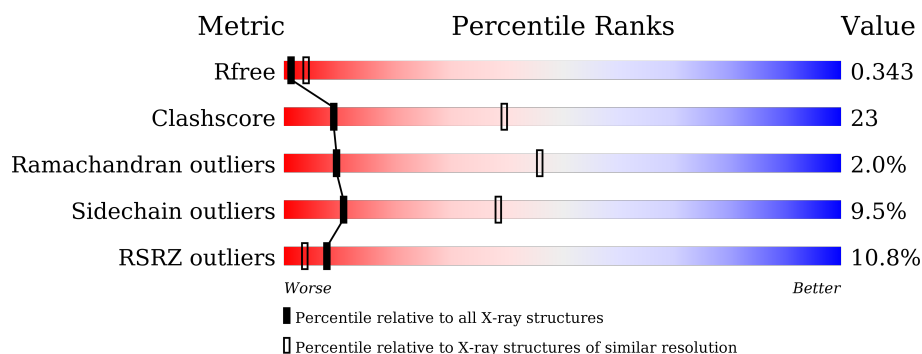
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.16 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	1112 (3.20-3.12)
Clashscore	102246	1249 (3.20-3.12)
Ramachandran outliers	100387	1222 (3.20-3.12)
Sidechain outliers	100360	1221 (3.20-3.12)
RSRZ outliers	91569	1117 (3.20-3.12)

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>8%</div> <div>52%</div> <div>43%</div> <div>..</div> </div>
1	B	1049	<div> <div>7%</div> <div>53%</div> <div>39%</div> <div>6%</div> <div>.</div> </div>
1	C	1049	<div> <div>11%</div> <div>53%</div> <div>41%</div> <div>6%</div> </div>
1	D	1049	<div> <div>11%</div> <div>53%</div> <div>41%</div> <div>..</div> </div>
1	E	1049	<div> <div>13%</div> <div>48%</div> <div>43%</div> <div>7%</div> <div>.</div> </div>
1	F	1049	<div> <div>15%</div> <div>52%</div> <div>43%</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	LMT	B	1101	X	-	-	-
2	LMT	C	1101	X	-	-	-
2	LMT	E	1101	-	-	-	X

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 47736 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	1046	Total	C	N	O	S	0	0	0
			7939	5099	1314	1483	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:

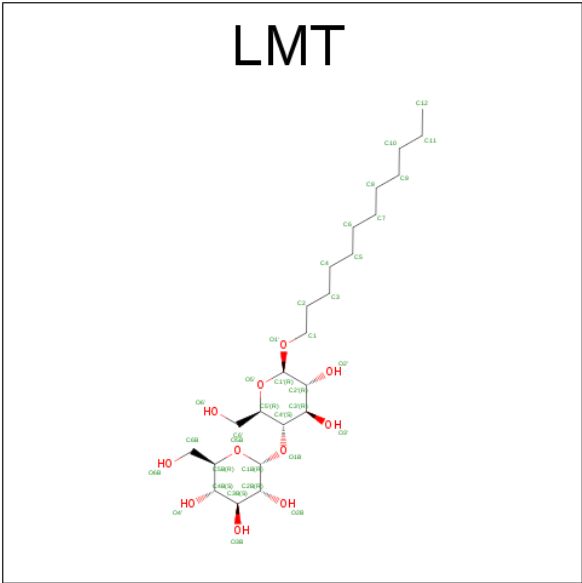
Chain	Residue	Modelled	Actual	Comment	Reference
A	615	ALA	PHE	engineered mutation	UNP P31224
A	617	ALA	PHE	engineered mutation	UNP P31224
A	620	ALA	ARG	engineered mutation	UNP P31224
B	615	ALA	PHE	engineered mutation	UNP P31224
B	617	ALA	PHE	engineered mutation	UNP P31224
B	620	ALA	ARG	engineered mutation	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 DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



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

- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

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

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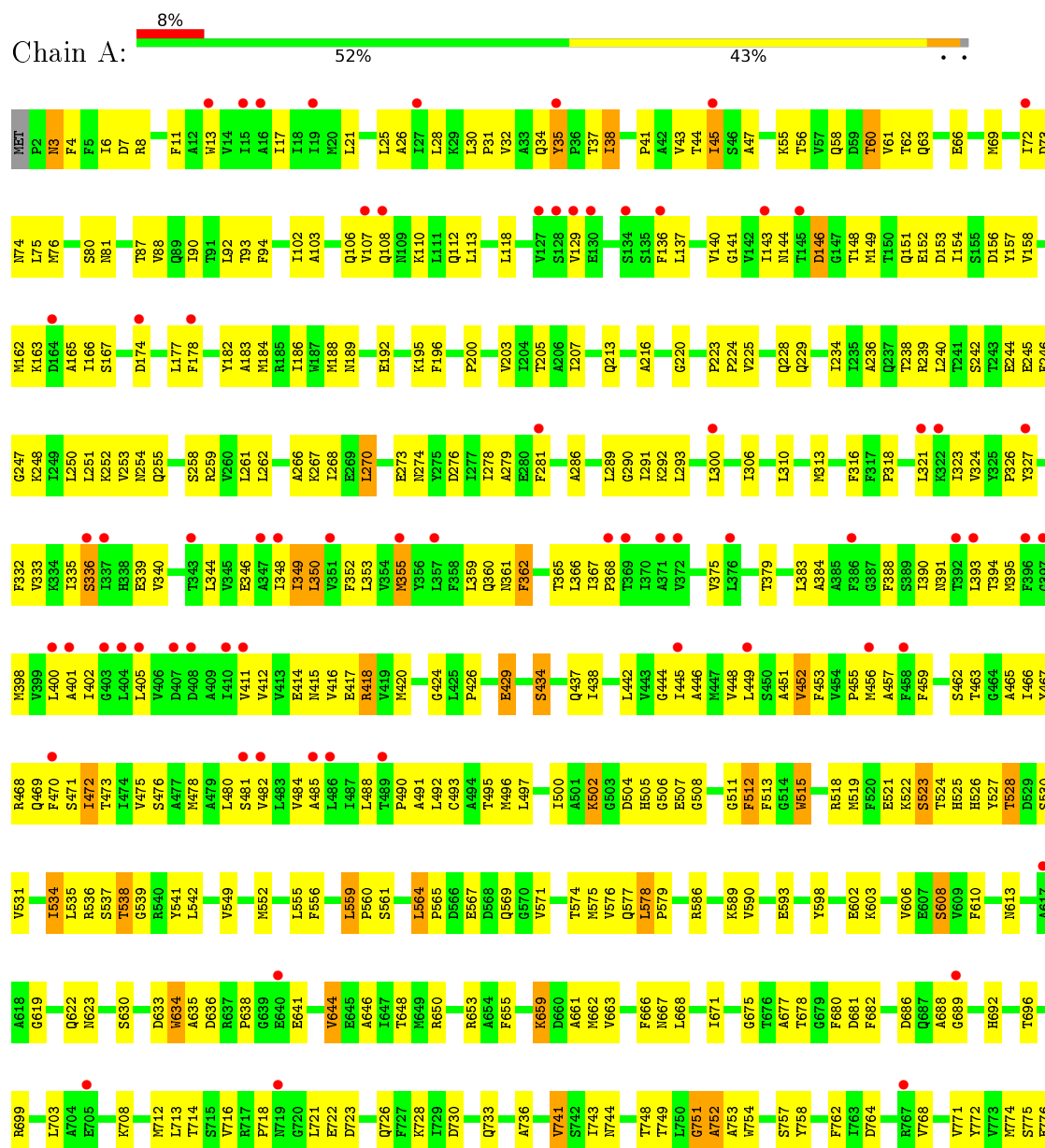
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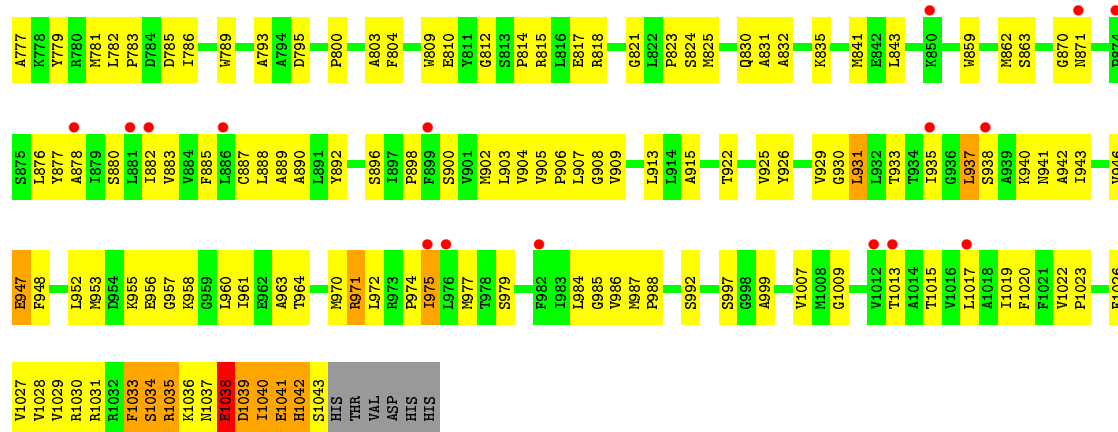
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	1	Total	Ni	0	0
			1	1		

3 Residue-property plots

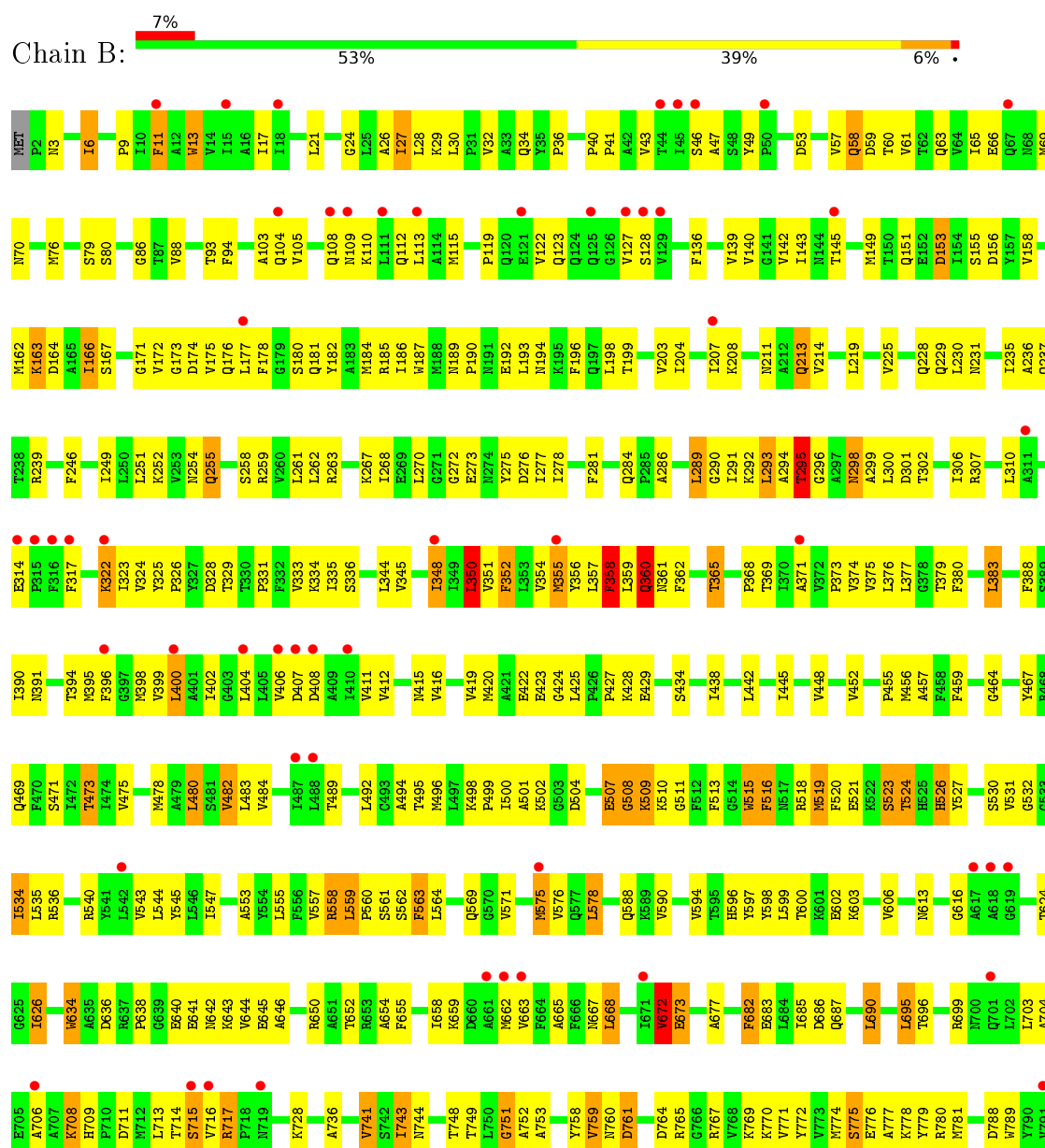
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

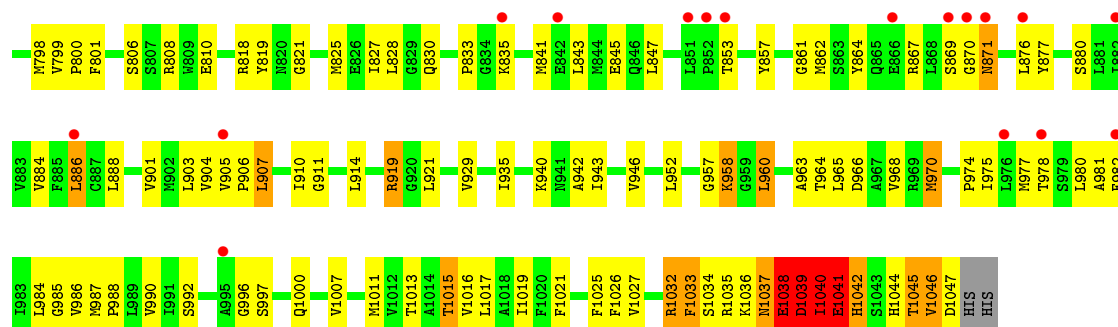
- Molecule 1: Multidrug efflux pump subunit AcrB



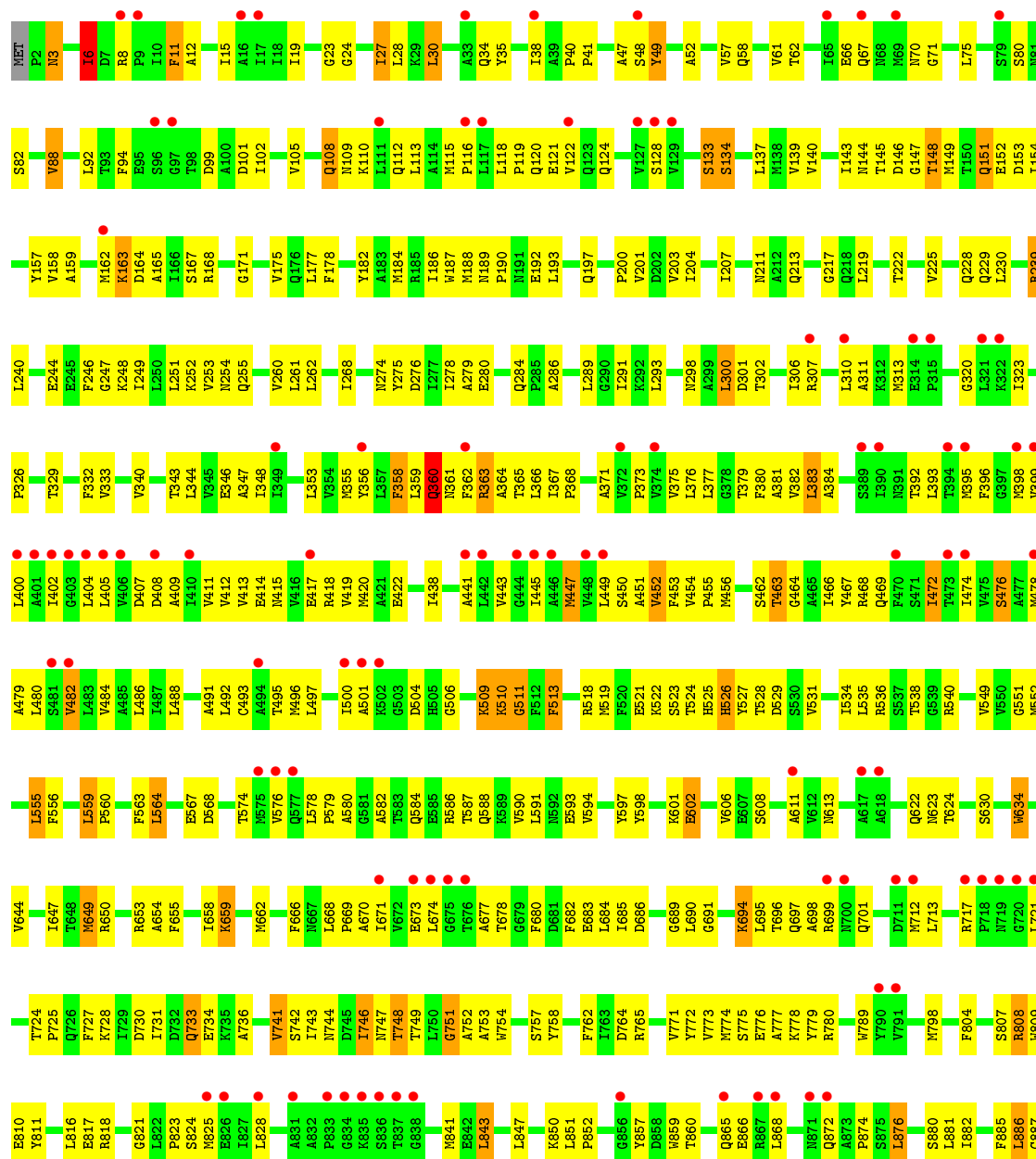


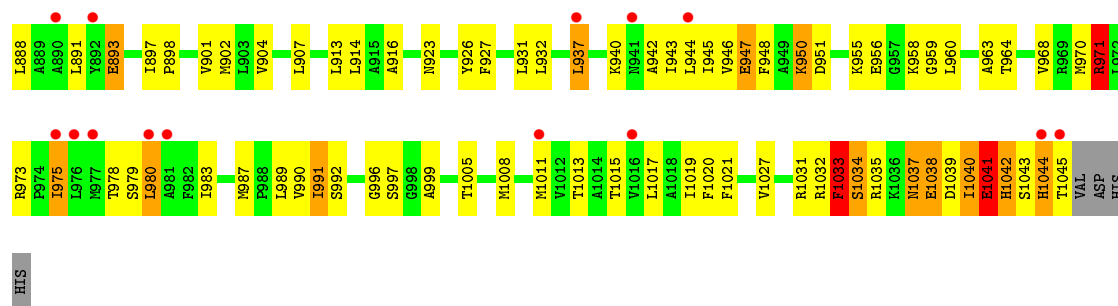
● Molecule 1: Multidrug efflux pump subunit AcrB



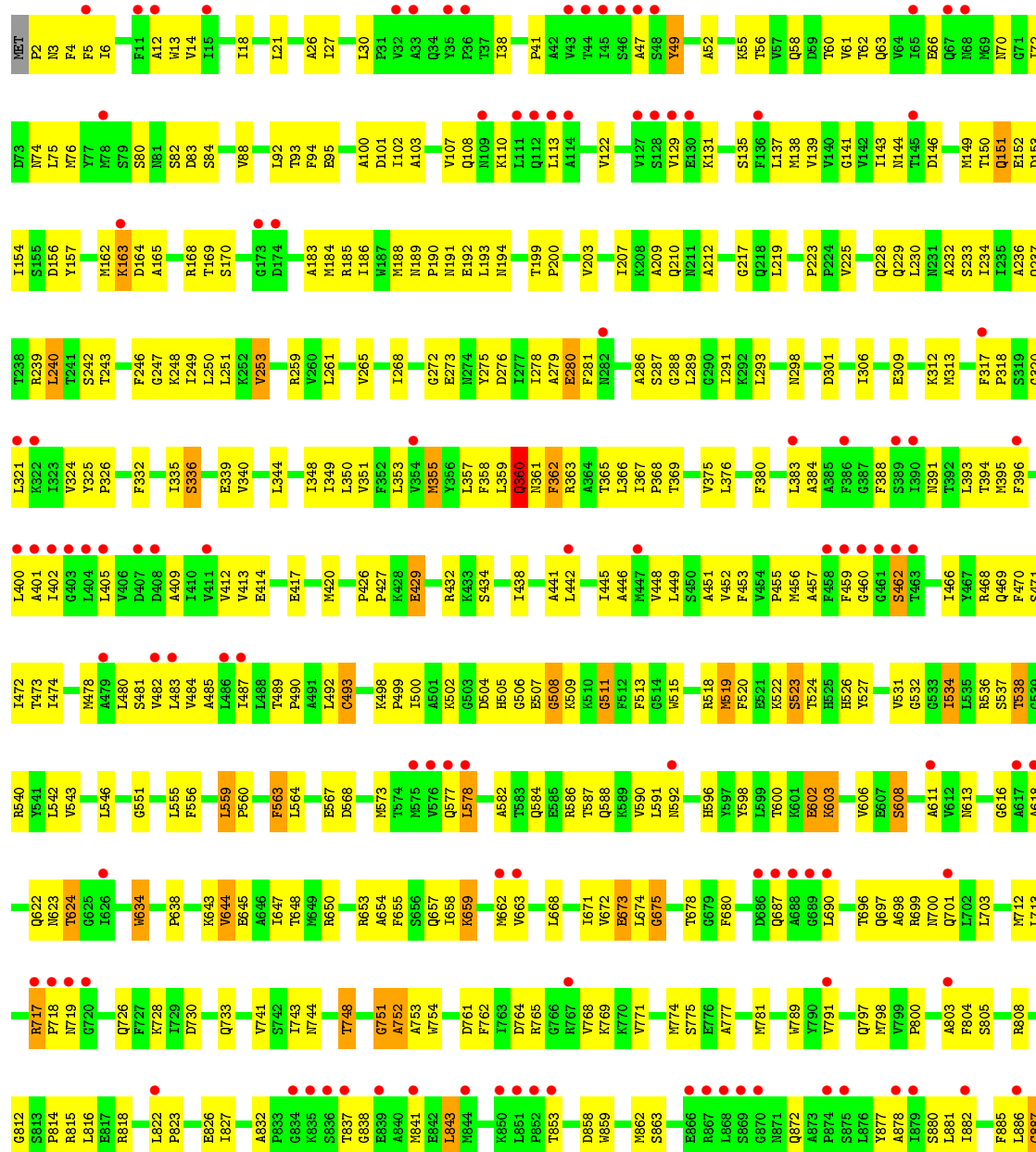


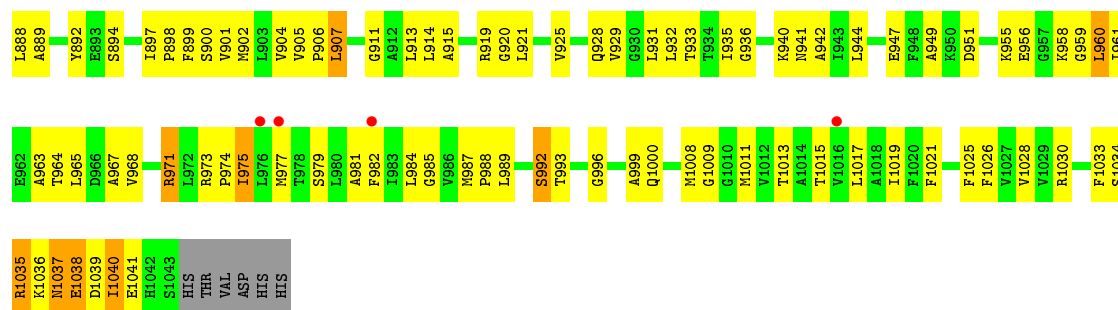
● Molecule 1: Multidrug efflux pump subunit AcrB



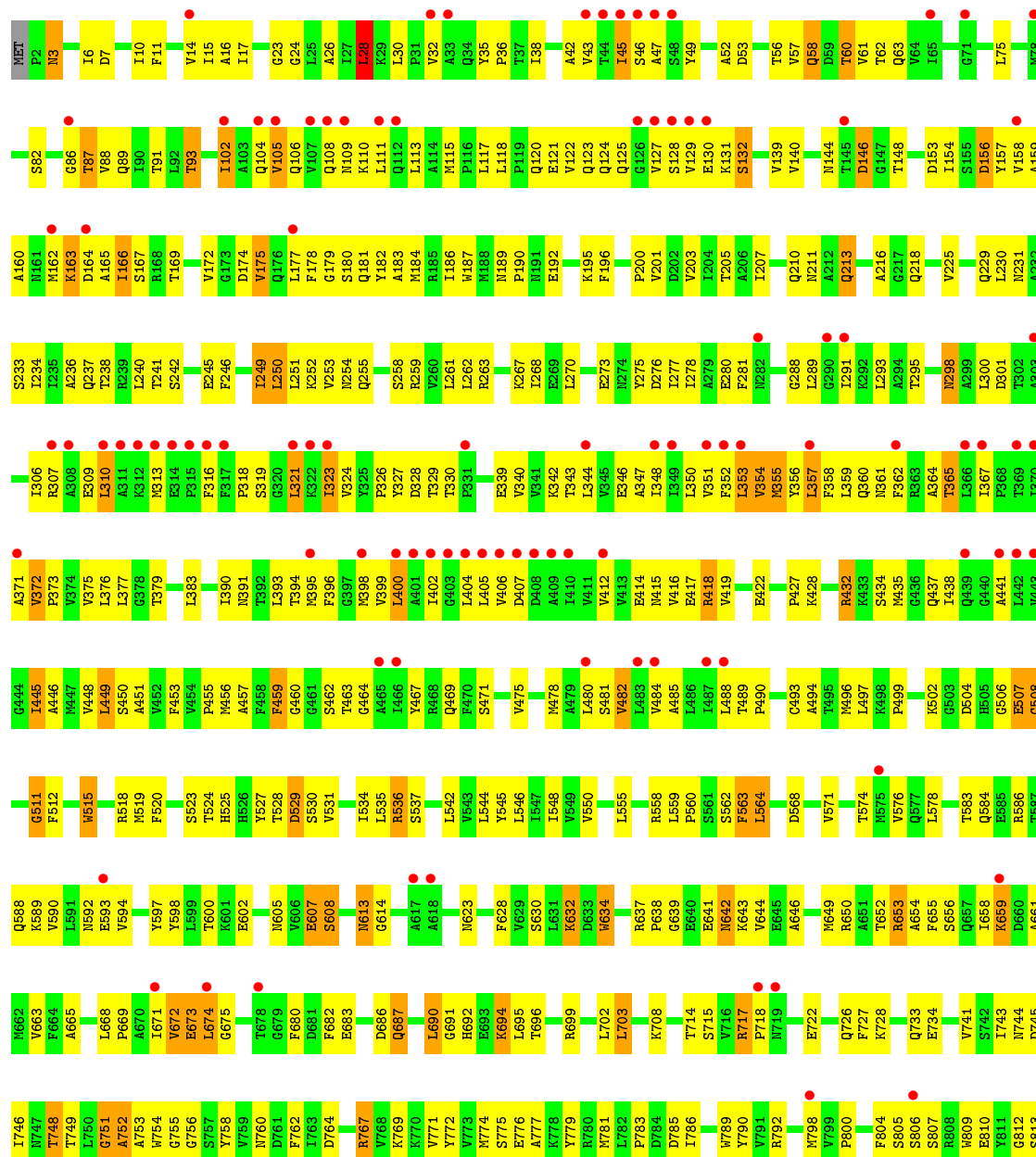


• Molecule 1: Multidrug efflux pump subunit AcrB





• Molecule 1: Multidrug efflux pump subunit AcrB





V1022	S775	R867	I940	S776	L868	I941	F1023	E776	L869	A942	F1024	A777	K778	A873	R780	R781	W789	Y790	Y791	M798	F801	F804	S807	R808	S813	P814	R815	L816	E817	R818	G821	L822	P823	E826	L827	L828	G829	Q830	A831	A832	P833	G834	K835	S836	T837	L843	L847	K850	D858	W859	T860	G861	W862	S863	Y864	Q865	E866
P1023	I941	L868	I942	A777	S869	I943	F1025	K778	A873	R780	R781	W789	Y790	Y791	M798	F801	F804	S807	R808	S813	P814	R815	L816	E817	R818	G821	L822	P823	E826	L827	L828	G829	Q830	A831	A832	P833	G834	K835	S836	T837	L843	L847	K850	D858	W859	T860	G861	W862	S863	Y864	Q865	E866					
V1024	I942	L869	I943	A778	S870	I944	F1026	K779	A874	R781	R782	W790	Y791	Y792	M799	F802	F805	S808	R809	S814	P815	R816	E818	R819	G822	L823	P824	E827	L829	G830	Q831	A832	A833	P834	G835	K836	S837	T838	L844	L848	K851	D859	W860	T861	G862	W863	S864	Y865	Q866	E867							
F1025	I943	L870	F1026	A779	A875	R782	F1027	K780	R783	W791	Y792	Y793	M800	F803	F806	S810	R811	S815	P816	R817	L817	E820	R821	G823	L824	P825	E828	L830	G831	Q832	A834	A835	P835	G836	K837	S838	T839	L845	L849	K852	D860	W861	T862	G863	W864	S865	Y866	Q867	E868								
V1027	I945	L871	V1028	A780	R784	R785	V1027	K781	R786	W792	Y794	Y795	M801	F804	F807	S811	R812	S816	P817	R818	L818	E821	R822	G824	L825	P826	E829	L831	G832	Q833	A836	A837	P836	G837	K838	S839	T840	L846	L850	K853	D861	W862	T863	G864	W865	S866	Y867	Q868	E869								
V1029	I946	L872	V1029	A781	R785	R786	V1029	K782	R787	W793	Y796	Y797	M802	F805	F808	S812	R813	S817	P818	R819	L819	E822	R823	G825	L826	P827	E830	L832	G833	Q834	A838	A839	P837	G838	K839	S840	T841	L847	L851	K854	D862	W863	T864	G865	W866	S867	Y868	Q869	E870								
R1030	I947	L873	R1030	A782	R786	R787	R1030	K783	R788	W794	Y798	Y799	M803	F806	F809	S813	R814	S818	P819	R820	L820	E823	R824	G826	L827	P828	E831	L833	G834	Q835	A839	A840	P838	G839	K840	S841	T842	L848	L852	K855	D863	W864	T865	G866	W867	S868	Y869	Q870	E871								
F1033	I948	L874	S1034	A783	R787	R788	S1034	K784	R789	W795	Y800	Y801	M804	F807	F810	S814	R815	S819	P820	R821	L821	E824	R825	G827	L828	P829	E832	L834	G835	Q836	A840	A841	P839	G840	K841	S842	T843	L849	L853	K856	D864	W865	T866	G867	W868	S869	Y870	Q871	E872								
S1034	I949	L875	R1035	A784	R788	R789	R1035	K785	R790	W796	Y801	Y802	M805	F808	F811	S815	R816	S820	P821	R822	L822	E825	R826	G828	L829	P830	E833	L835	G836	Q837	A841	A842	P840	G841	K842	S843	T844	L850	L854	K857	D865	W866	T867	G868	W869	S870	Y871	Q872	E873								
R1035	I950	L876	R1036	A785	R789	R790	R1036	K786	R791	W797	Y802	Y803	M806	F809	F812	S816	R817	S821	P822	R823	L823	E826	R827	G829	L830	P831	E834	L836	G837	Q838	A842	A843	P841	G842	K843	S844	T845	L851	L855	K858	D866	W867	T868	G869	W870	S871	Y872	Q873	E874								
NI037	I951	L877	R1037	A786	R790	R791	NI037	K787	R792	W798	Y803	Y804	M807	F810	F813	S817	R818	S822	P823	R824	L824	E827	R828	G830	L831	P832	E835	L837	G838	Q839	A843	A844	P842	G843	K844	S845	T846	L852	L856	K859	D867	W868	T869	G870	W871	S872	Y873	Q874	E875								
E1038	I952	L878	R1038	A787	R791	R792	E1038	K788	R793	W799	Y804	Y805	M808	F811	F814	S818	R819	S823	P824	R825	L825	E828	R829	G831	L832	P833	E836	L838	G839	Q840	A844	A845	P843	G844	K845	S846	T847	L853	L857	K860	D868	W869	T870	G871	W872	S873	Y874	Q875	E876								
D1039	I953	L879	R1039	A788	R792	R793	D1039	K789	R794	W800	Y805	Y806	M809	F812	F815	S819	R820	S824	P825	R826	L826	E829	R830	G832	L833	P834	E837	L839	G840	Q841	A845	A846	P844	G845	K846	S847	T848	L854	L858	K861	D869	W870	T871	G872	W873	S874	Y875	Q876	E877								
I1040	I954	L880	R1040	A789	R793	R794	I1040	K790	R795	W801	Y806	Y807	M810	F813	F816	S820	R821	S825	P826	R827	L827	E830	R831	G833	L834	P835	E838	L840	G841	Q842	A846	A847	P845	G846	K847	S848	T849	L855	L859	K862	D870	W871	T872	G873	W874	S875	Y876	Q877	E878								
E1041	I955	L881	R1041	A790	R794	R795	E1041	K791	R796	W802	Y807	Y808	M811	F814	F817	S821	R822	S826	P827	R828	L828	E831	R832	G834	L835	P836	E839	L841	G842	Q843	A847	A848	P846	G847	K848	S849	T850	L856	L860	K863	D871	W872	T873	G874	W875	S876	Y877	Q878	E879								
HI042	I956	L882	R1042	A791	R795	R796	HI042	K792	R797	W803	Y808	Y809	M812	F815	F818	S822	R823	S827	P828	R829	L829	E832	R833	G835	L836	P837	E840	L842	G843	Q844	A848	A849	P847	G848	K849	S850	T851	L857	L861	K864	D872	W873	T874	G875	W876	S877	Y878	Q879	E880								
S1043	I957	L883	R1043	A792	R796	R797	S1043	K793	R798	W804	Y809	Y810	M813	F816	F819	S823	R824	S828	P829	R830	L831	E833	R834	G836	L837	P838	E841	L843	G844	Q845	A849	A850	P848	G849	K850	S851	T852	L858	L862	K865	D873	W874	T875	G876	W877	S878	Y879	Q880	E881								
H1044	I958	L884	R1044	A793	R797	R798	H1044	K794	R799	W805	Y810	Y811	M814	F817	F820	S824	R825	S829	P830	R831	L832	E834	R835	G837	L838	P839	E842	L844	G845	Q846	A850	A851	P849	G850	K851	S852	T853	L859	L863	K866	D874	W875	T876	G877	W878	S879	Y880	Q881	E882								
V1046	I959	L885	R1045	A794	R798	R799	V1046	K795	R800	W806	Y811	Y812	M815	F818	F821	S826	R827	S830	P831	R832	L832	E835	R836	G838	L839	P840	E843	L845	G846	Q847	A851	A852	P849	G850	K851	S853	T854	L860	L864	K867	D875	W876	T877	G878	W879	S880	Y881	Q882	E883								
D1047	I960	L886	R1046	A795	R799	R800	D1047	K796	R801	W807	Y812	Y813	M816	F819	F822	S827	R828	S831	P832	R833	L833	E836	R837	G839	L840	P841	E844	L846	G847	Q848	A852	A853	P850	G851	K852	S854	T855	L861	L865	K868	D876	W877	T878	G879	W880	S881	Y882	Q883	E884								
HIS	I961	L887	R1047	A796	R800	R801	HIS	K797	R802	W808	Y813	Y814	M817	F820	F823	S828	R829	S832	P833	R834	L834	E837	R838	G840	L841	P842	E845	L847	G848	Q849	A853	A854	P851	G852	K853	S855	T856	L862	L866	K869	D877	W878	T879	G880	W881	S882	Y883	Q884	E885								

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	152.28Å 157.49Å 219.16Å 90.00° 92.74° 90.00°	Depositor
Resolution (Å)	19.98 – 3.16 109.45 – 3.16	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.98-3.16) 97.7 (109.45-3.16)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 3.13Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.270 , 0.335 0.280 , 0.343	Depositor DCC
R_{free} test set	8594 reflections (4.98%)	DCC
Wilson B-factor (Å ²)	95.0	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 63.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.076 for -k,-h,-l 0.095 for k,h,-l 0.089 for h,-k,-l	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	47736	wwPDB-VP
Average B, all atoms (Å ²)	70.0	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 50.23 % 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 6.6624e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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

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	0.61	1/8056 (0.0%)	0.83	5/10940 (0.0%)
1	B	0.63	1/8089 (0.0%)	0.86	6/10986 (0.1%)
1	C	0.63	0/8074	0.89	16/10965 (0.1%)
1	D	0.56	2/8056 (0.0%)	0.82	8/10940 (0.1%)
1	E	0.57	2/8056 (0.0%)	0.83	9/10940 (0.1%)
1	F	0.58	0/8089	0.85	7/10986 (0.1%)
All	All	0.60	6/48420 (0.0%)	0.85	51/65757 (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	C	0	1
1	D	0	2
1	F	0	2
All	All	0	5

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	515	TRP	CB-CG	7.82	1.64	1.50
1	E	515	TRP	CB-CG	6.85	1.62	1.50
1	D	515	TRP	CB-CG	6.71	1.62	1.50
1	B	515	TRP	CB-CG	6.47	1.61	1.50
1	E	493	CYS	CB-SG	-6.06	1.72	1.82

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	529	ASP	CB-CG-OD1	9.33	126.69	118.30
1	E	914	LEU	CA-CB-CG	7.93	133.55	115.30
1	A	972	LEU	CA-CB-CG	7.92	133.50	115.30
1	E	529	ASP	CB-CG-OD1	7.63	125.17	118.30
1	B	357	LEU	CA-CB-CG	7.55	132.67	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	6	ILE	Peptide
1	D	1034	SER	Peptide
1	D	992	SER	Peptide
1	F	1036	LYS	Peptide
1	F	1039	ASP	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	393	0
1	B	7939	0	8077	355	0
1	C	7924	0	8064	396	0
1	D	7907	0	8050	369	0
1	E	7907	0	8050	414	1
1	F	7939	0	8077	397	1
2	A	35	0	46	4	0
2	B	35	0	46	3	0
2	C	35	0	46	4	0
2	D	35	0	46	1	0
2	E	35	0	46	4	0
2	F	35	0	46	4	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
All	All	47736	0	48644	2245	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 23.

The worst 5 of 2245 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:D:446:ALA:HB2	1:D:482:VAL:HG21	1.39	0.99
1:A:957:GLY:HA2	1:A:1042:HIS:HB2	1.41	0.99
1:A:578:LEU:HD21	1:A:590:VAL:HG21	1.46	0.98
1:D:536:ARG:NH2	2:D:1101:LMT:O3B	1.97	0.97
1:F:578:LEU:HG	1:F:587:THR:HG22	1.46	0.95

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:E:529:ASP:OD1	1:F:529:ASP:OD2[2_555]	2.08	0.12

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%)	939 (90%)	82 (8%)	19 (2%)	11	49
1	B	1044/1049 (100%)	925 (89%)	92 (9%)	27 (3%)	7	38
1	C	1042/1049 (99%)	931 (89%)	91 (9%)	20 (2%)	10	48
1	D	1040/1049 (99%)	941 (90%)	83 (8%)	16 (2%)	13	53
1	E	1040/1049 (99%)	919 (88%)	97 (9%)	24 (2%)	8	42
1	F	1044/1049 (100%)	936 (90%)	87 (8%)	21 (2%)	9	46
All	All	6250/6294 (99%)	5591 (90%)	532 (8%)	127 (2%)	9	46

5 of 127 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	360	GLN
1	A	675	GLY
1	A	1038	GLU
1	B	163	LYS
1	B	360	GLN

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%)	789 (93%)	56 (7%)	21	59
1	B	849/852 (100%)	735 (87%)	114 (13%)	5	22
1	C	847/852 (99%)	769 (91%)	78 (9%)	11	40
1	D	845/852 (99%)	786 (93%)	59 (7%)	19	57
1	E	845/852 (99%)	735 (87%)	110 (13%)	5	23
1	F	849/852 (100%)	783 (92%)	66 (8%)	16	51
All	All	5080/5112 (99%)	4597 (90%)	483 (10%)	11	38

5 of 483 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	694	LYS
1	D	502	LYS
1	F	482	VAL
1	C	741	VAL
1	C	1040	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	70	ASN
1	D	505	HIS
1	F	63	GLN
1	D	151	GLN

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Mol	Chain	Res	Type
1	E	34	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 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	LMT	A	1101	-	36,36,36	1.82	10 (27%)	47,47,47	1.27	6 (12%)
2	LMT	B	1101	-	36,36,36	1.78	9 (25%)	47,47,47	1.34	8 (17%)
2	LMT	C	1101	-	36,36,36	1.71	7 (19%)	47,47,47	1.61	10 (21%)
2	LMT	D	1101	-	36,36,36	1.74	9 (25%)	47,47,47	1.37	7 (14%)
2	LMT	E	1101	-	36,36,36	1.81	11 (30%)	47,47,47	1.45	7 (14%)
2	LMT	F	1101	-	36,36,36	1.93	10 (27%)	47,47,47	1.45	7 (14%)

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	LMT	A	1101	-	-	0/21/61/61	0/2/2/2
2	LMT	B	1101	-	1/1/10/10	0/21/61/61	0/2/2/2
2	LMT	C	1101	-	1/1/10/10	0/21/61/61	0/2/2/2
2	LMT	D	1101	-	-	0/21/61/61	0/2/2/2
2	LMT	E	1101	-	-	0/21/61/61	0/2/2/2
2	LMT	F	1101	-	-	0/21/61/61	0/2/2/2

The worst 5 of 56 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1101	LMT	C6'-C5'	-3.46	1.39	1.51
2	C	1101	LMT	C6'-C5'	-3.35	1.40	1.51
2	B	1101	LMT	C6'-C5'	-3.19	1.40	1.51
2	F	1101	LMT	C6'-C5'	-3.11	1.40	1.51
2	A	1101	LMT	C6'-C5'	-3.04	1.41	1.51

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1101	LMT	O3B-C3B-C2B	-4.15	101.01	110.36
2	A	1101	LMT	C1B-O1B-C4'	-3.76	107.99	118.00
2	D	1101	LMT	C1B-O1B-C4'	-3.59	108.46	118.00
2	C	1101	LMT	O5B-C5B-C4B	-3.47	103.05	109.67
2	A	1101	LMT	C1'-C2'-C3'	-2.97	104.09	109.98

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1101	LMT	C3B
2	C	1101	LMT	C3B

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	LMT	4	0
2	B	1101	LMT	3	0
2	C	1101	LMT	4	0
2	D	1101	LMT	1	0
2	E	1101	LMT	4	0
2	F	1101	LMT	4	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

6.1 Protein, DNA and RNA chains

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%)	0.32	85 (8%) 14 7	28, 63, 113, 139	0
1	B	1046/1049 (99%)	0.18	71 (6%) 20 10	26, 57, 100, 161	0
1	C	1044/1049 (99%)	0.46	117 (11%) 7 3	17, 56, 98, 173	0
1	D	1042/1049 (99%)	0.46	115 (11%) 7 3	21, 81, 133, 168	0
1	E	1042/1049 (99%)	0.53	132 (12%) 5 2	38, 77, 119, 154	0
1	F	1046/1049 (99%)	0.63	154 (14%) 3 2	29, 73, 120, 143	0
All	All	6262/6294 (99%)	0.43	674 (10%) 8 4	17, 68, 116, 173	0

The worst 5 of 674 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	314	GLU	16.2
1	E	315	PRO	15.9
1	D	869	SER	14.3
1	F	481	SER	12.4
1	E	128	SER	12.3

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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
2	LMT	F	1101	35/35	0.81	0.37	1.33	19,65,82,87	0
2	LMT	B	1101	35/35	0.82	0.37	0.90	40,61,68,70	0
2	LMT	A	1101	35/35	0.88	0.32	0.83	40,56,74,75	0
2	LMT	D	1101	35/35	0.86	0.31	0.75	35,48,67,83	0
2	LMT	C	1101	35/35	0.84	0.33	0.72	29,44,62,65	0
2	LMT	E	1101	35/35	0.73	0.40	0.69	43,83,98,109	0
3	NI	A	1102	1/1	0.97	0.08	-	31,31,31,31	0
3	NI	E	1102	1/1	0.99	0.08	-	64,64,64,64	0
3	NI	C	1102	1/1	0.99	0.12	-	33,33,33,33	0

6.5 Other polymers

There are no such residues in this entry.