wwPDB X-ray Structure Validation Summary Report (i)

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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

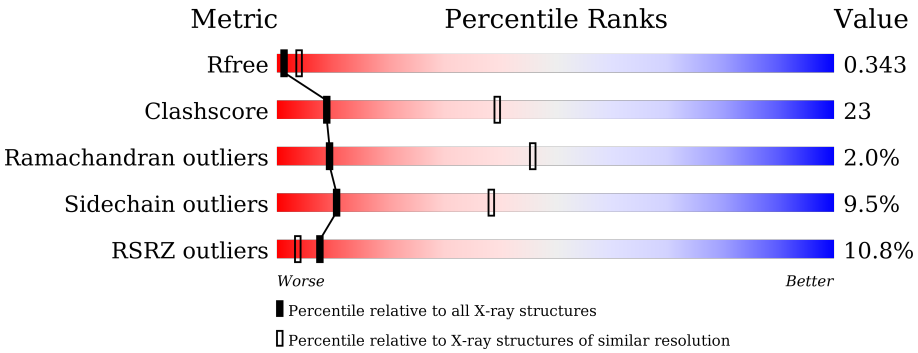
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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 <=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	8% 52% 43%
1	B	1049	7% 53% 39% 6%
1	C	1049	11% 53% 41% 6%
1	D	1049	11% 53% 41%
1	E	1049	13% 48% 43% 7%
1	F	1049	15% 52% 43%

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

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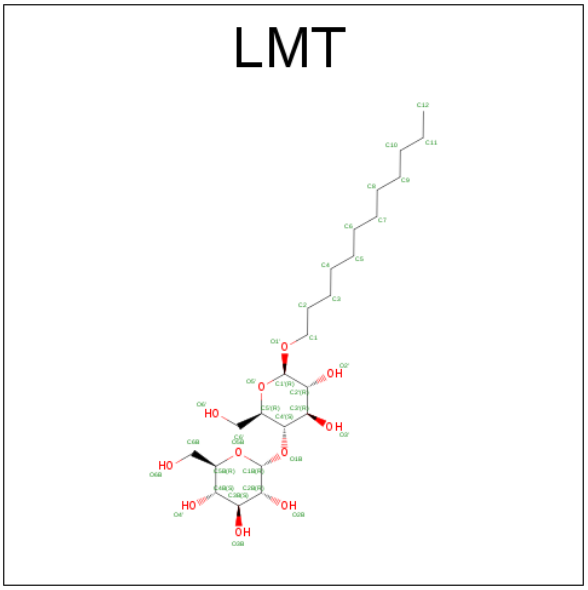
Chain	Residue	Modelled	Actual	Comment	Reference
F	620	ALA	ARG	engineered mutation	UNP P31224

- Molecule 2 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



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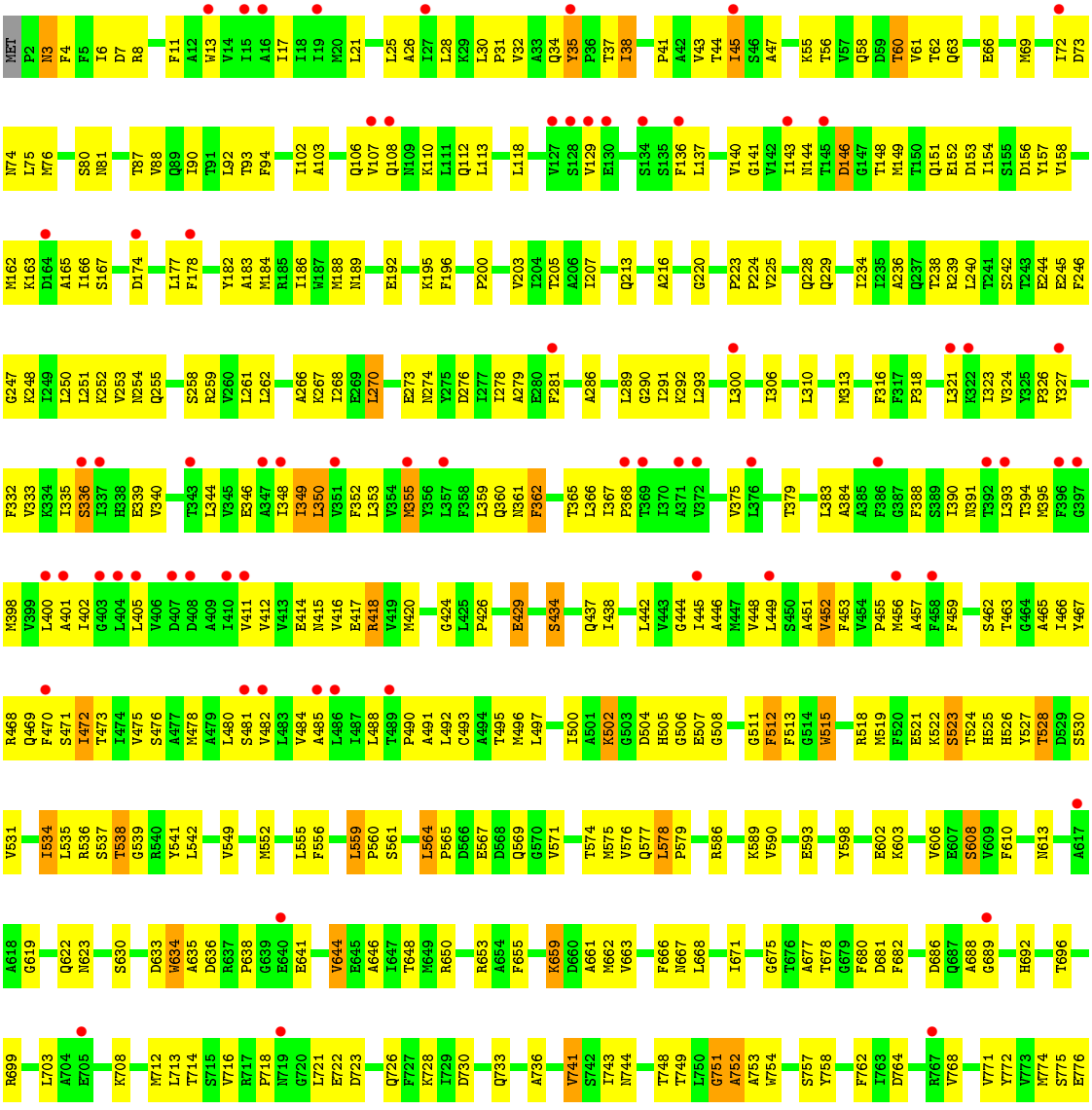
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total Ni 1 1	0	0

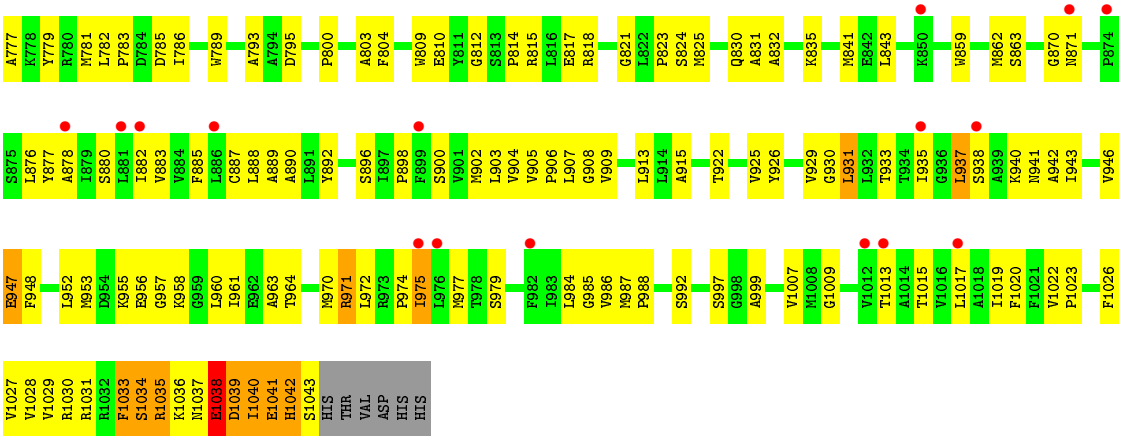
3 Residue-property plots (i)

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

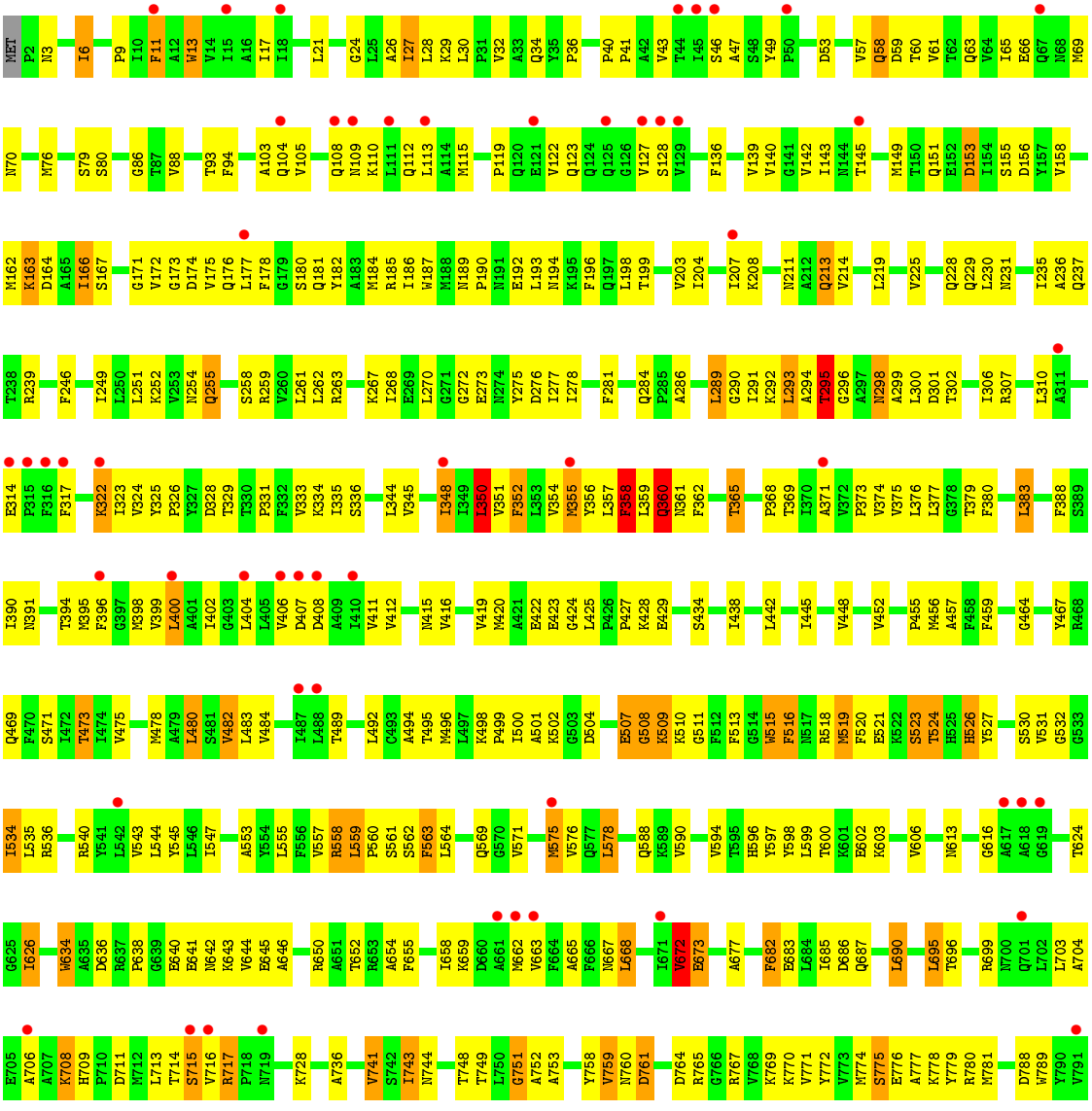
Chain A:

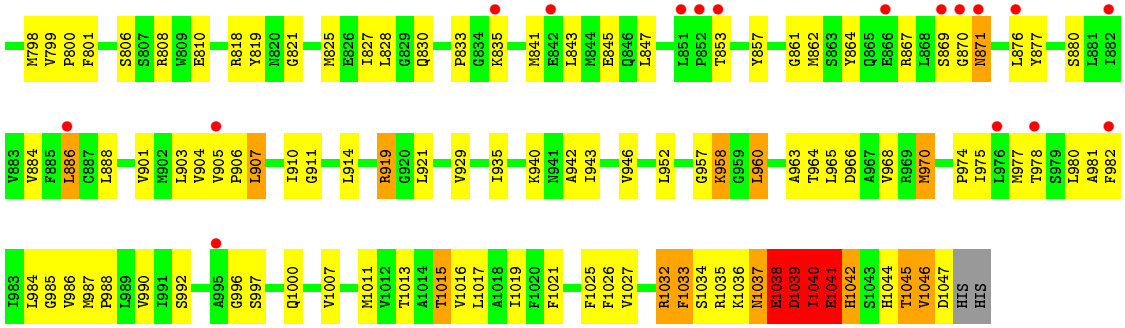




- Molecule 1: Multidrug efflux pump subunit AcrB

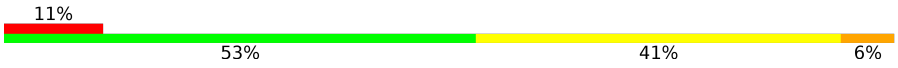
Chain B:

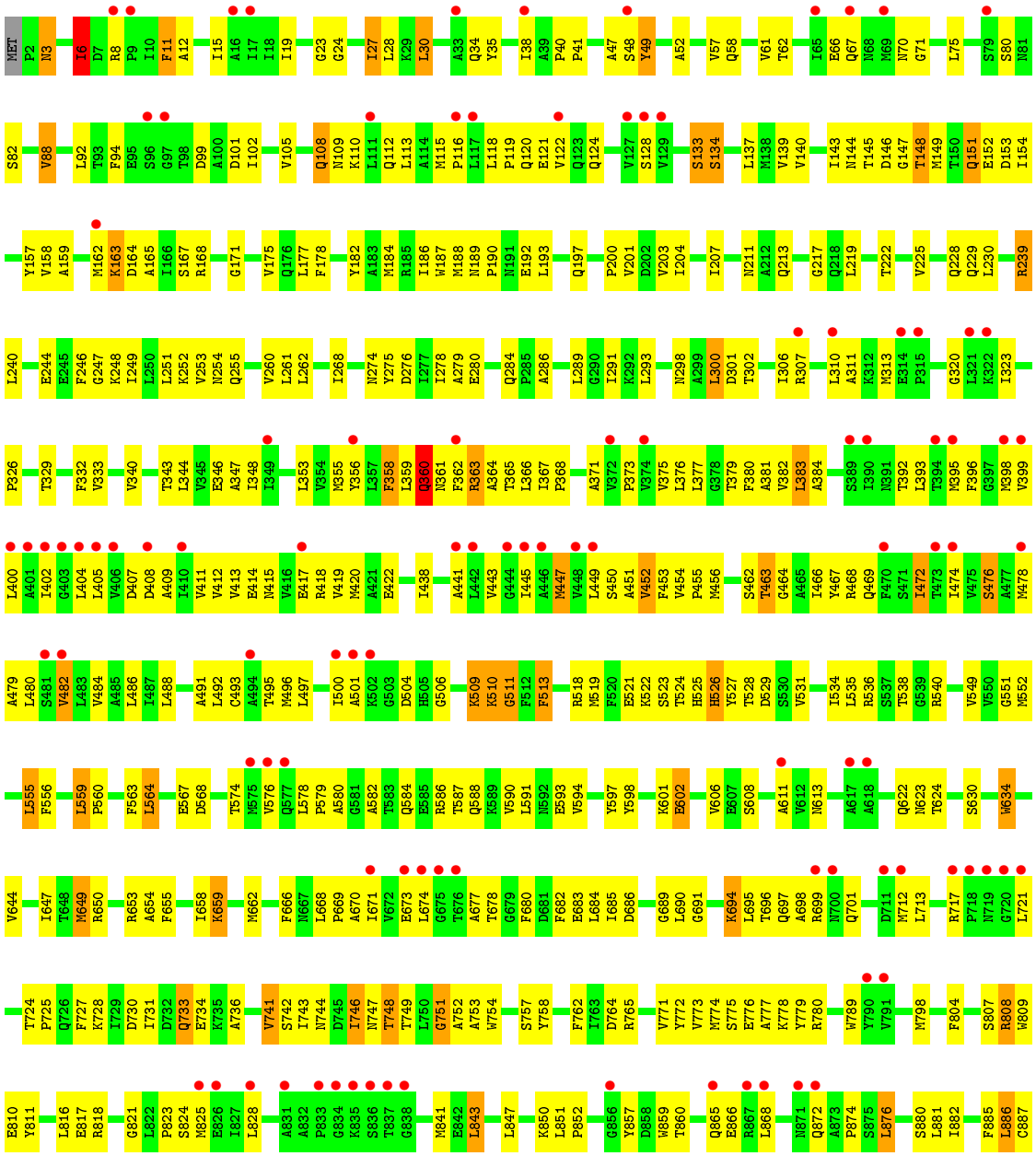


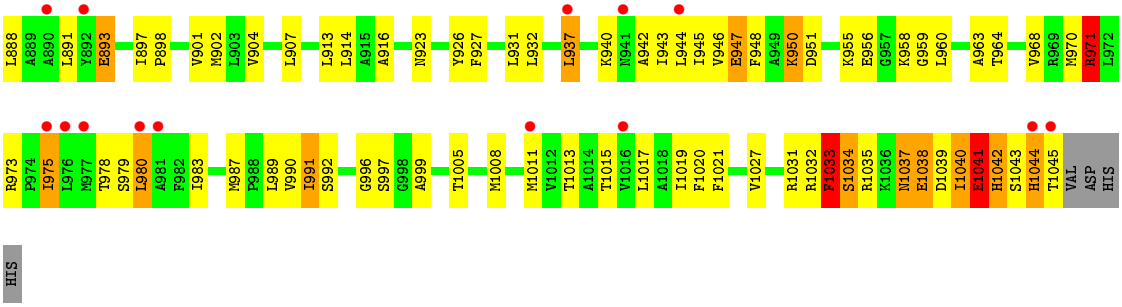


- Molecule 1: Multidrug efflux pump subunit AcrB

Chain C:

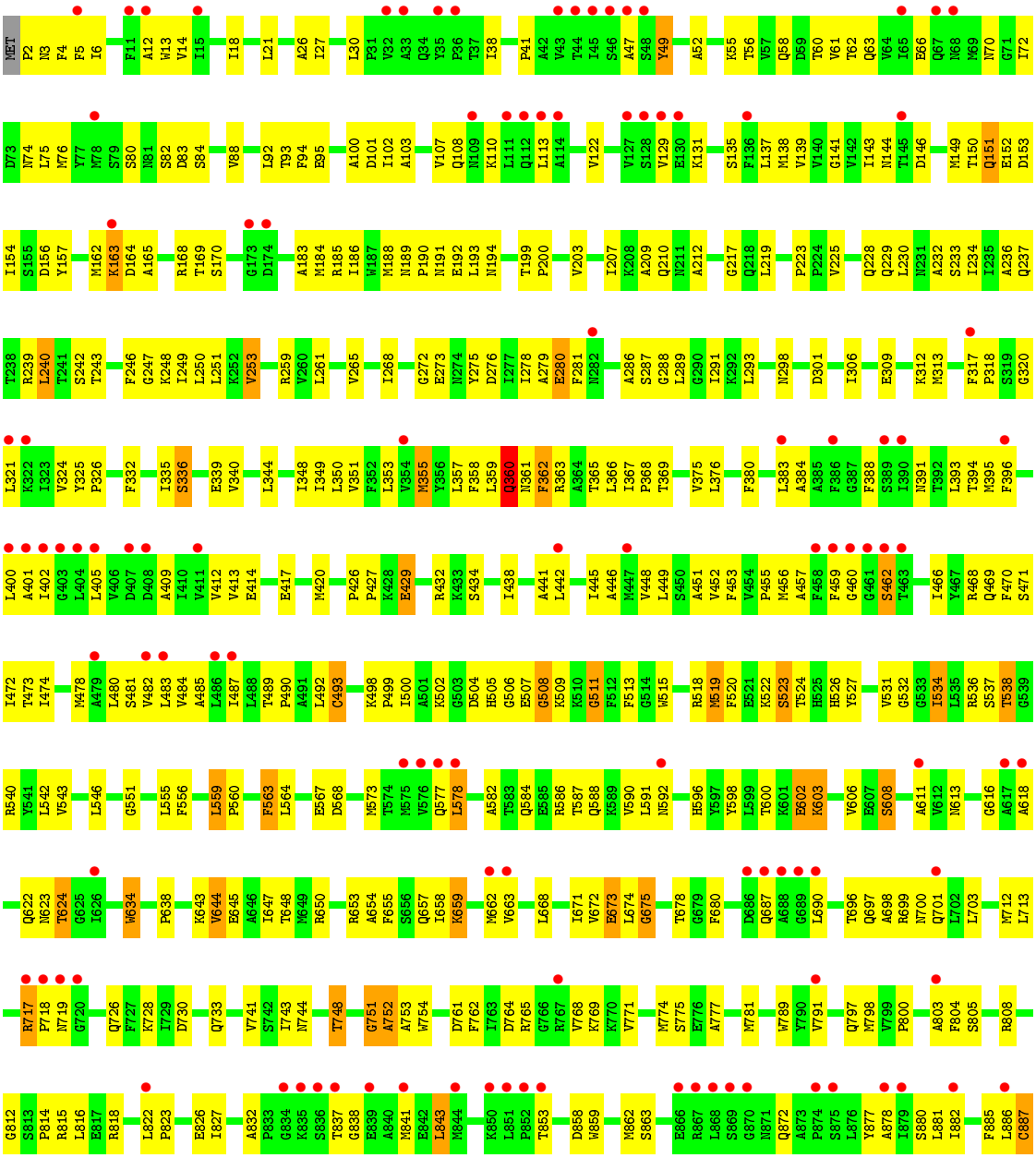


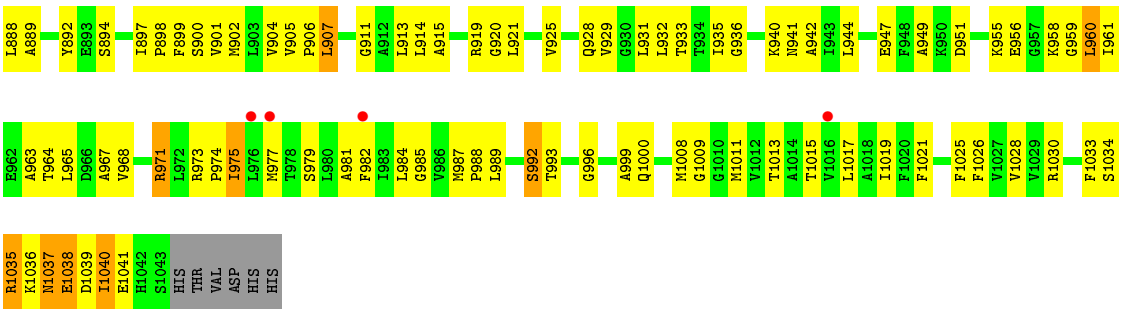




• Molecule 1: Multidrug efflux pump subunit AcrB

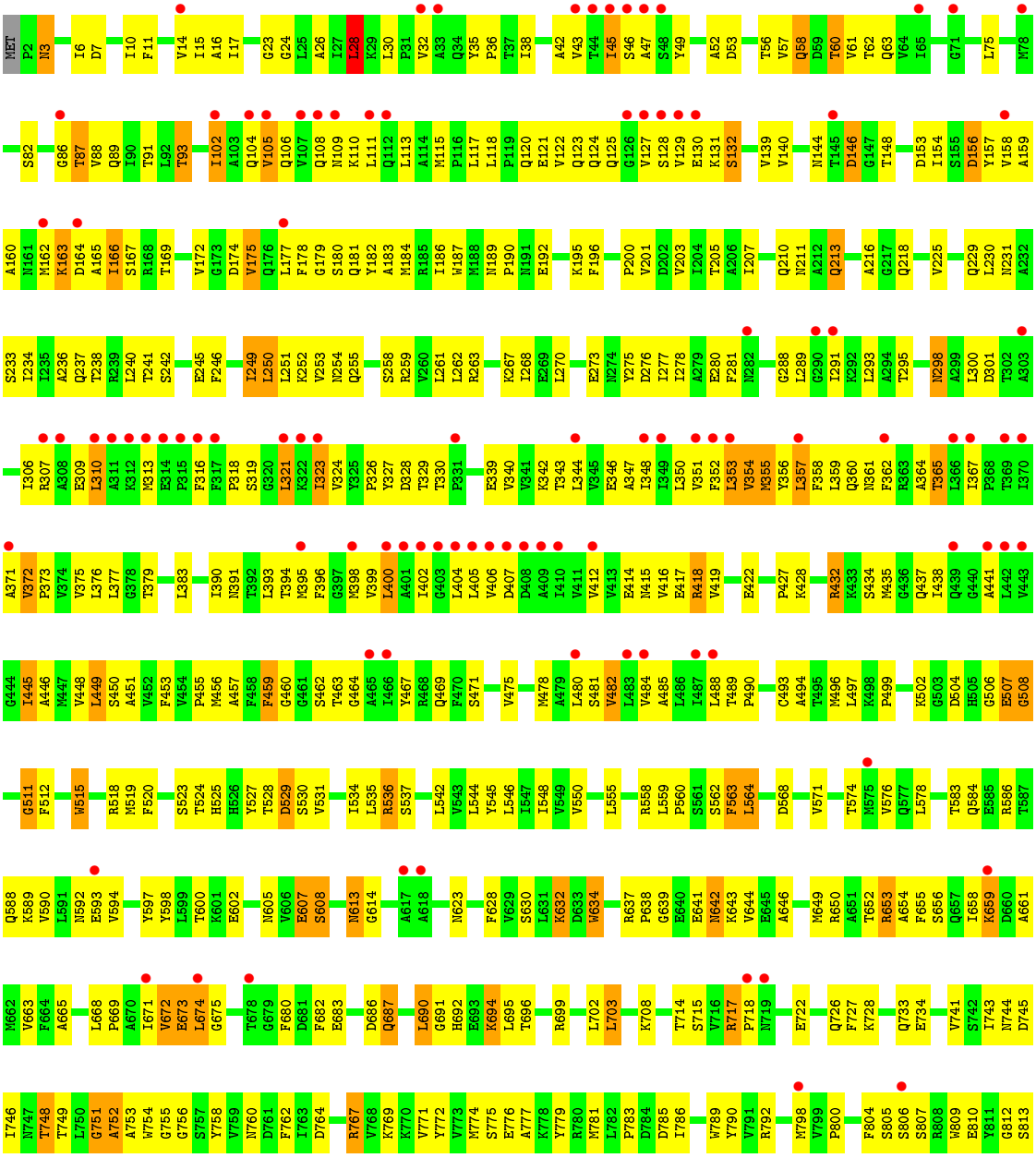
Chain D:

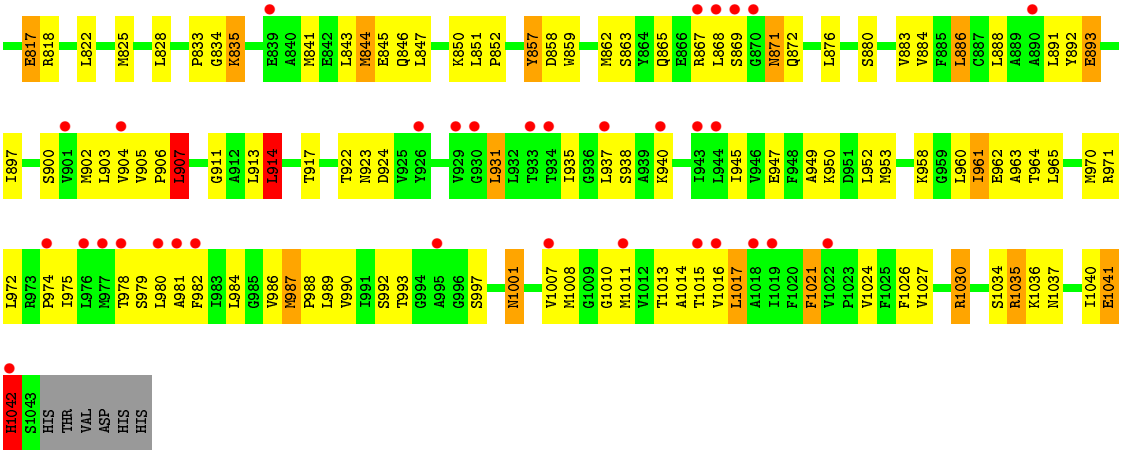




• Molecule 1: Multidrug efflux pump subunit AcrB

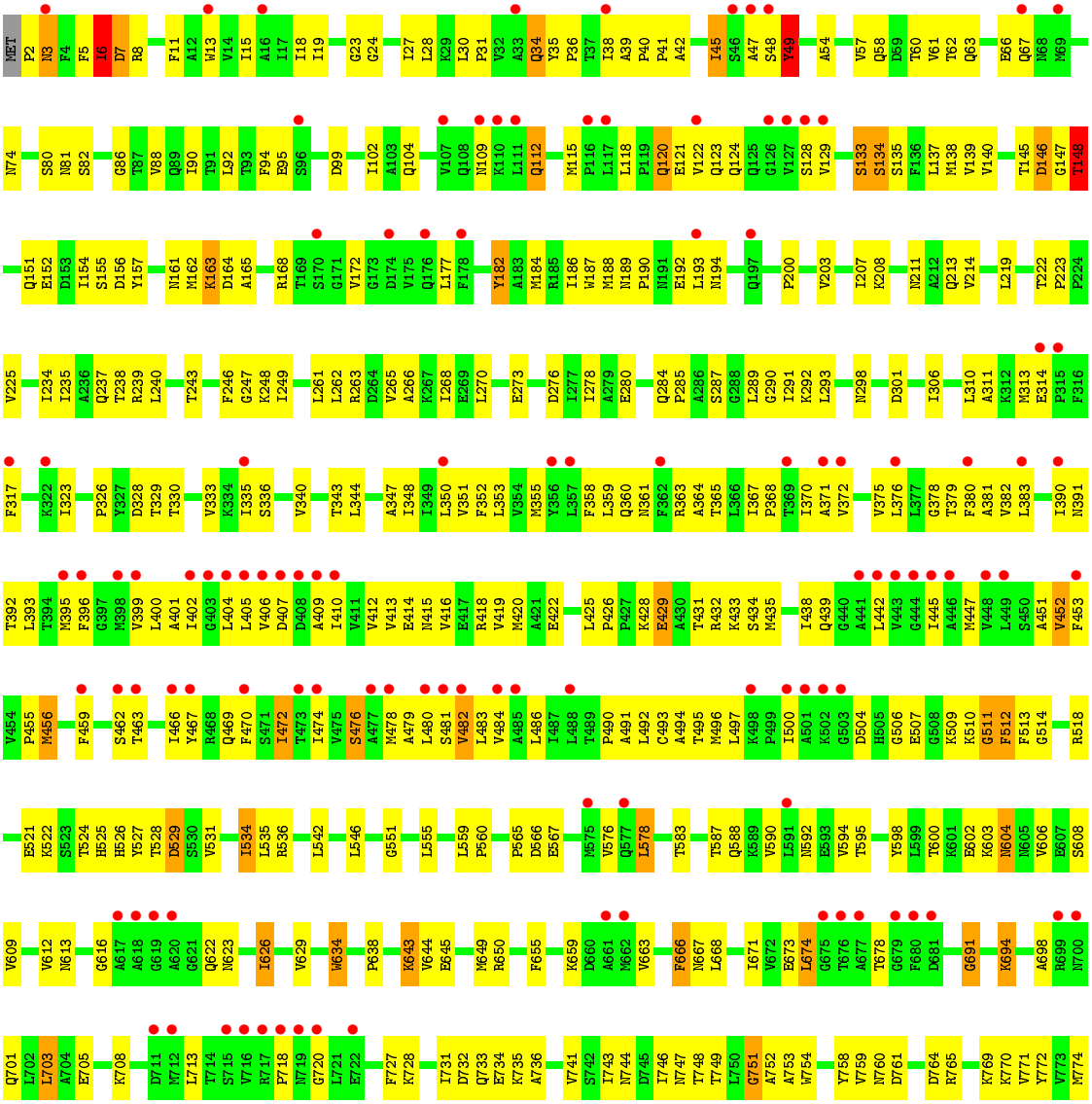
Chain E:

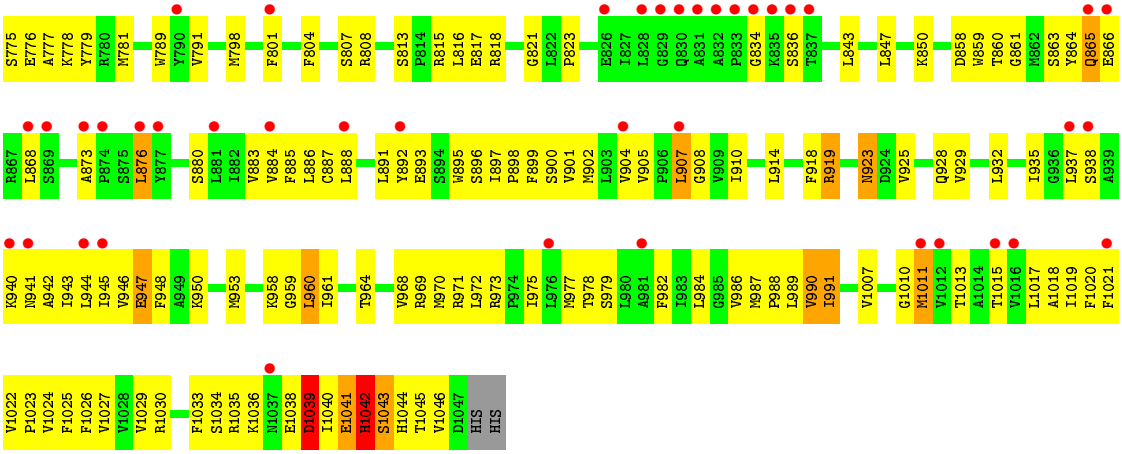




- Molecule 1: Multidrug efflux pump subunit AcrB

Chain F:




S775 E776 A777 K778 Y779 R780 M781 W789 Y790 V791 M798 F801 F804 S807 R808 S813 P814 R815 L816 E817 R818 G821 L822 P823 E826 I827 L828 G829 Q830 A831 A832 P833 G834 K835 S836 T837 L843 L847 K850 D858 W859 T860 G861 M862 S863 Y864 Q865 E866
R867 L868 S869 A873 P874 S875 L876 Y877 S880 L881 I882 V883 V884 F885 L886 C887 L888 L891 Y892 E893 S894 W895 S896 I897 P898 F899 S900 V901 M902 L903 V904 V905 P906 L907 G908 V909 I910 L914 F918 R919 N923 D924 V925 Q928 V929 L932 I935 G936 L937 S938 A939
K940 N941 A942 I943 L944 I945 V946 E947 F948 A949 K950 M953 K958 G959 L960 I961 T964 V968 R969 M970 R971 L972 R973 P974 I975 L976 M977 T978 S979 L980 A981 F982 I983 L984 G985 V986 M987 P988 L989 V990 I991 V1007 G1010 M1011 V1012 T1013 A1014 T1015 V1016 L1017 A1018 I1019 F1020 F1021
V1022 P1023 V1024 F1025 F1026 V1027 V1028 V1029 R1030 F1033 S1034 R1035 K1036 H1037 E1038 D1039 I1040 E1041 H1042 S1043 H1044 T1045 V1046 D1047 HIS HIS

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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(^{o})	Ideal(^{o})
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 (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	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 (i)

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

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 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(^{o})	Ideal(^{o})
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, 95^{th} 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, 95^{th} 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.