wwPDB X-ray Structure Validation Summary Report (i)

Jan 2, 2024 – 08:54 pm GMT

PDB ID	:	4ZJQ
Title	:	Crystal structure of AcrB deletion mutant in complex with antibiotic in P21 space group
Authors	:	Ababou, A.; Koronakis, V.
Deposited on	:	2015-04-29
Resolution	:	3.59 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

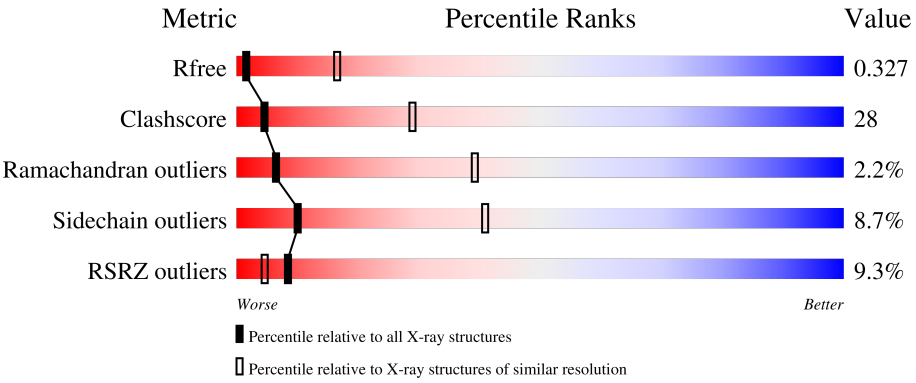
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.59 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}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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 of the lower 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 <=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	1044	7% 48% 47%
1	B	1044	7% 48% 46% 6%
1	C	1044	9% 45% 48% 6%
1	D	1044	7% 48% 45% 6%
1	E	1044	11% 47% 46% 6%

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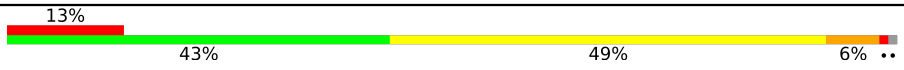
Mol	Chain	Length	Quality of chain
1	F	1044	

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	B	2100	-	-	-	X
3	LMT	C	1101	-	-	-	X
3	LMT	D	1102	-	-	-	X
3	LMT	D	1103	-	-	-	X
3	LMT	F	2100	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 47697 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	1038	Total	C	N	O	S	0	0	0
			7893	5072	1306	1472	43			
1	B	1037	Total	C	N	O	S	0	0	0
			7883	5066	1303	1471	43			
1	C	1036	Total	C	N	O	S	0	0	0
			7877	5063	1302	1469	43			
1	D	1038	Total	C	N	O	S	0	0	0
			7893	5072	1306	1472	43			
1	E	1037	Total	C	N	O	S	0	0	0
			7883	5066	1303	1471	43			
1	F	1037	Total	C	N	O	S	0	0	0
			7883	5066	1303	1471	43			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	GLY	PHE	engineered mutation	UNP P31224
A	?	-	GLY	deletion	UNP P31224
A	?	-	PHE	deletion	UNP P31224
A	?	-	ALA	deletion	UNP P31224
A	?	-	GLY	deletion	UNP P31224
A	?	-	ARG	deletion	UNP P31224
B	?	GLY	PHE	engineered mutation	UNP P31224
B	?	-	GLY	deletion	UNP P31224
B	?	-	PHE	deletion	UNP P31224
B	?	-	ALA	deletion	UNP P31224
B	?	-	GLY	deletion	UNP P31224
B	?	-	ARG	deletion	UNP P31224
C	?	GLY	PHE	engineered mutation	UNP P31224
C	?	-	GLY	deletion	UNP P31224
C	?	-	PHE	deletion	UNP P31224
C	?	-	ALA	deletion	UNP P31224
C	?	-	GLY	deletion	UNP P31224

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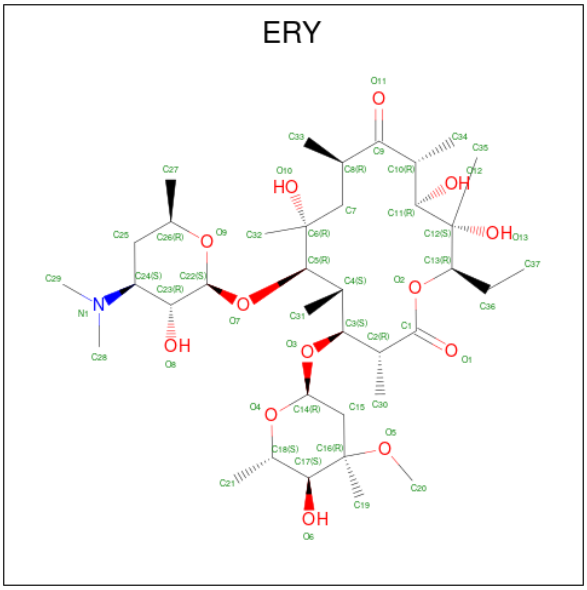
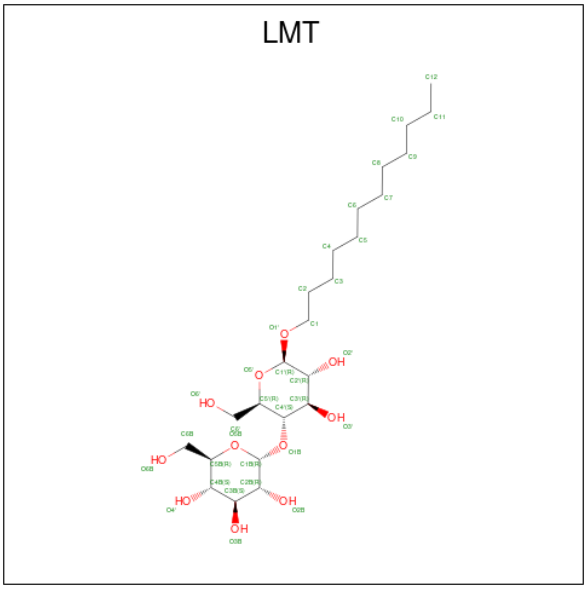
Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	ARG	deletion	UNP P31224
D	?	GLY	PHE	engineered mutation	UNP P31224
D	?	-	GLY	deletion	UNP P31224
D	?	-	PHE	deletion	UNP P31224
D	?	-	ALA	deletion	UNP P31224
D	?	-	GLY	deletion	UNP P31224
D	?	-	ARG	deletion	UNP P31224
E	?	GLY	PHE	engineered mutation	UNP P31224
E	?	-	GLY	deletion	UNP P31224
E	?	-	PHE	deletion	UNP P31224
E	?	-	ALA	deletion	UNP P31224
E	?	-	GLY	deletion	UNP P31224
E	?	-	ARG	deletion	UNP P31224
F	?	GLY	PHE	engineered mutation	UNP P31224
F	?	-	GLY	deletion	UNP P31224
F	?	-	PHE	deletion	UNP P31224
F	?	-	ALA	deletion	UNP P31224
F	?	-	GLY	deletion	UNP P31224
F	?	-	ARG	deletion	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 35 24 11	0	0
3	A	1	Total C O 35 24 11	0	0
3	B	1	Total C O 35 24 11	0	0
3	C	1	Total C O 35 24 11	0	0
3	D	1	Total C O 35 24 11	0	0
3	D	1	Total C O 35 24 11	0	0
3	E	1	Total C O 35 24 11	0	0
3	F	1	Total C O 35 24 11	0	0

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

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

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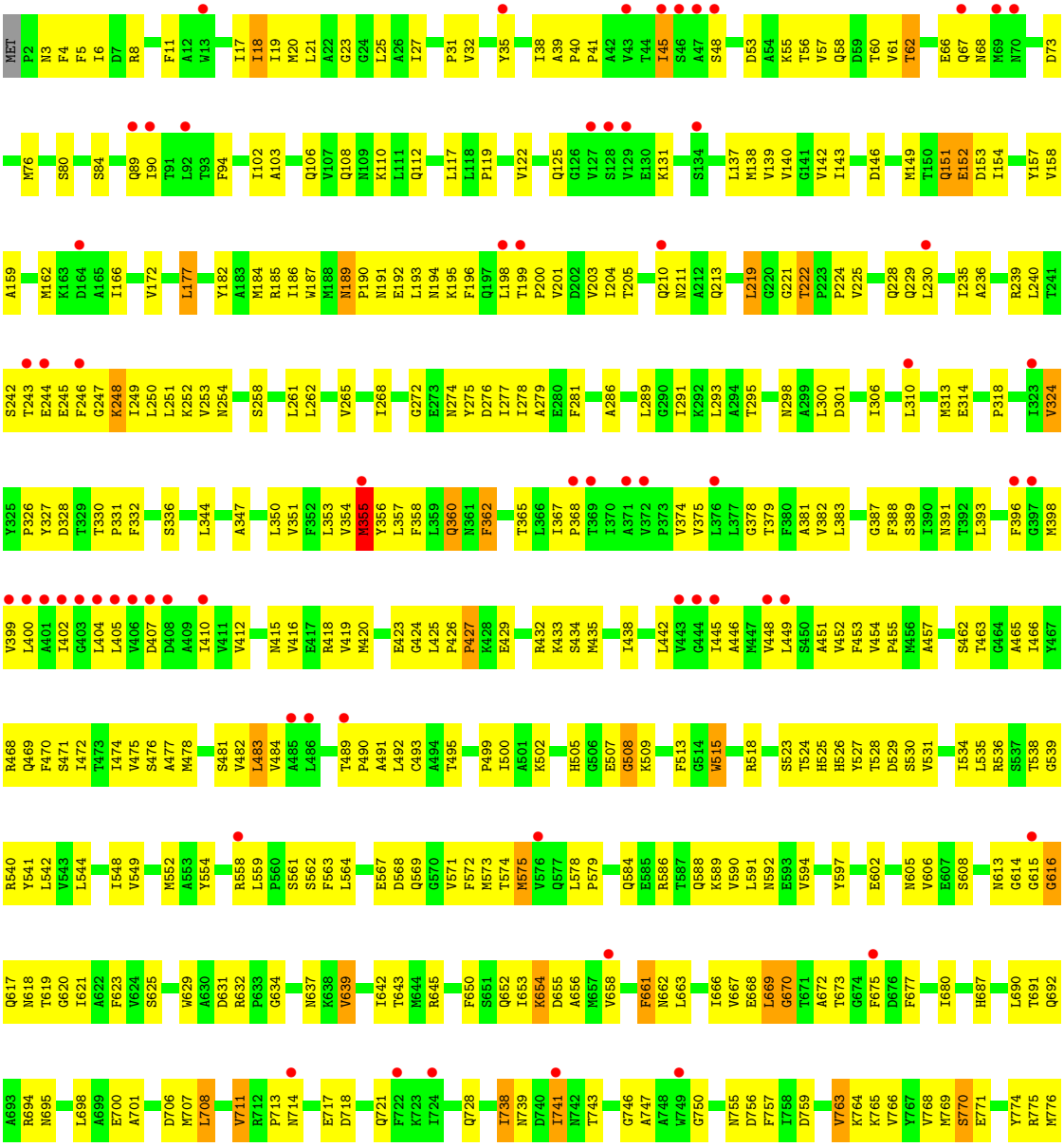
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ni		
4	E	1	1	1	0	0

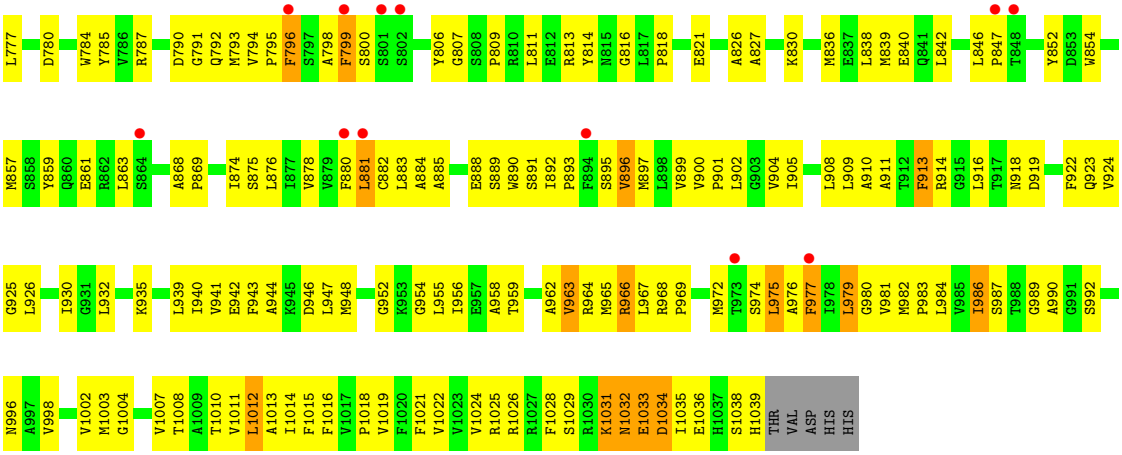
3 Residue-property plots (i)

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 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

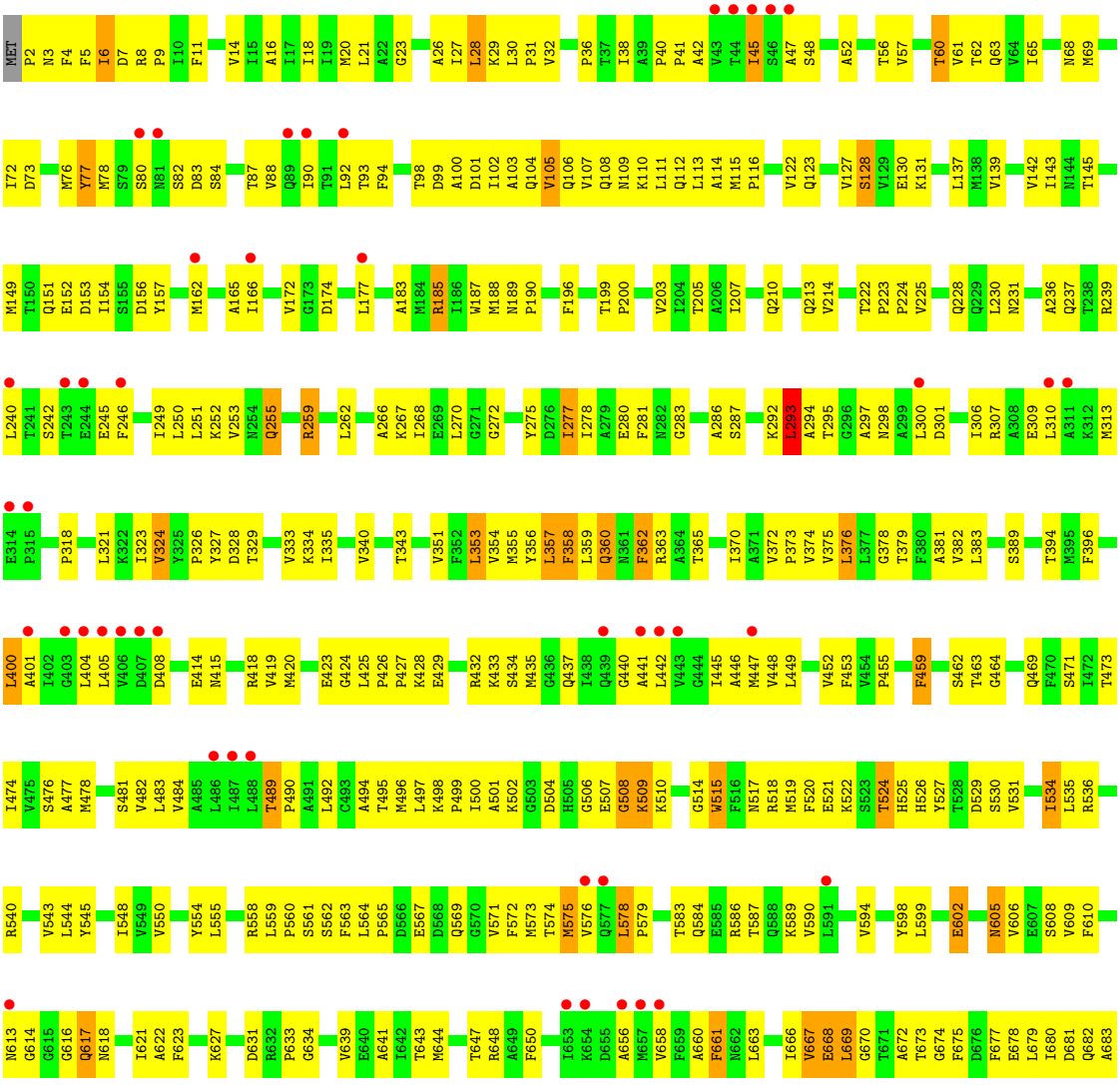
Chain A:

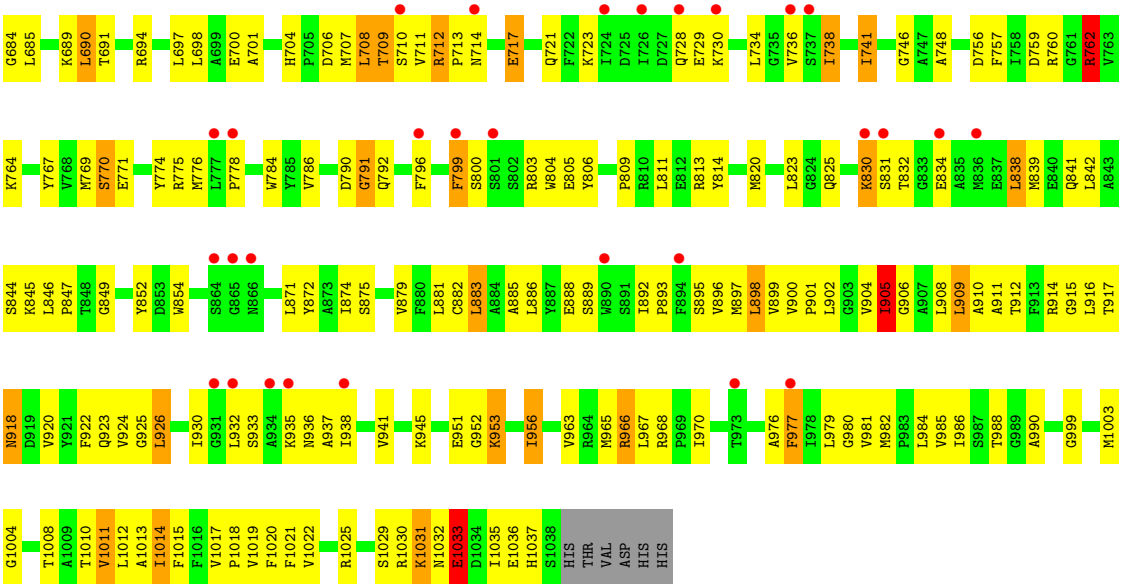




• Molecule 1: Multidrug efflux pump subunit AcrB

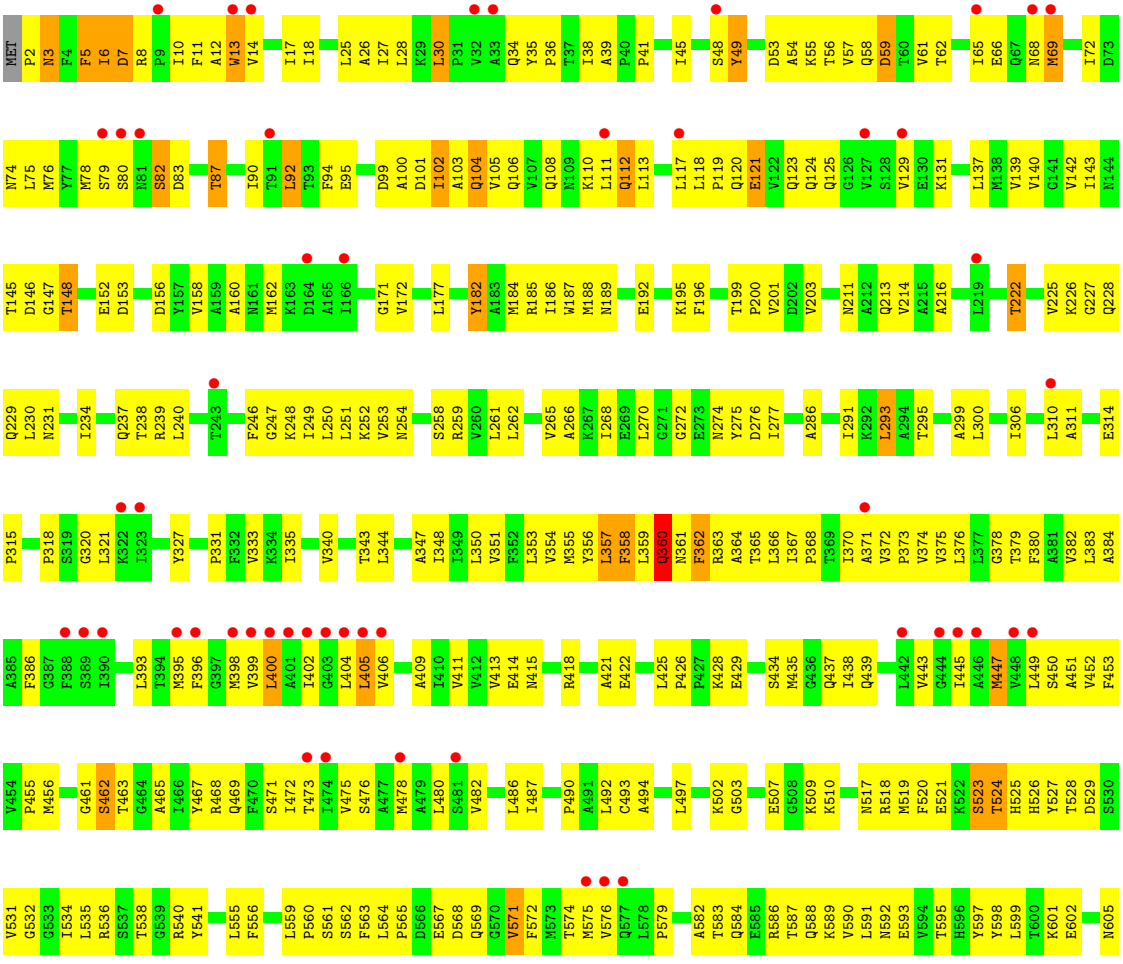
Chain B:

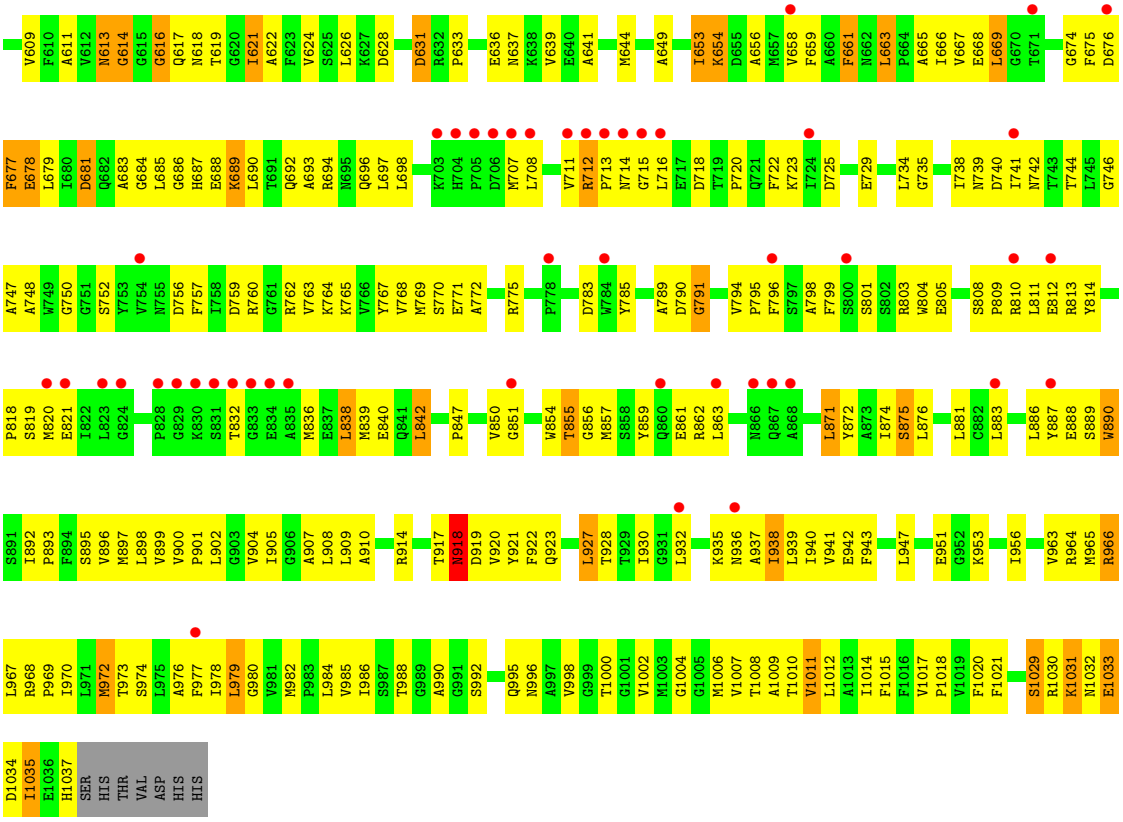




• Molecule 1: Multidrug efflux pump subunit AcrB

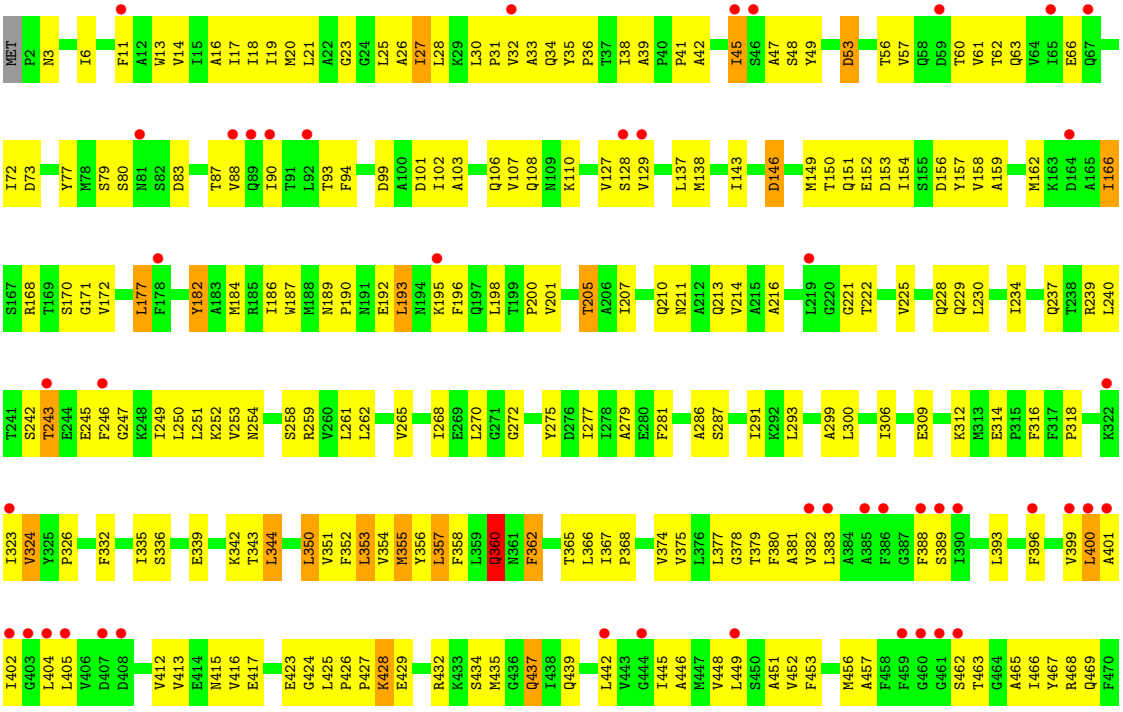
Chain C:

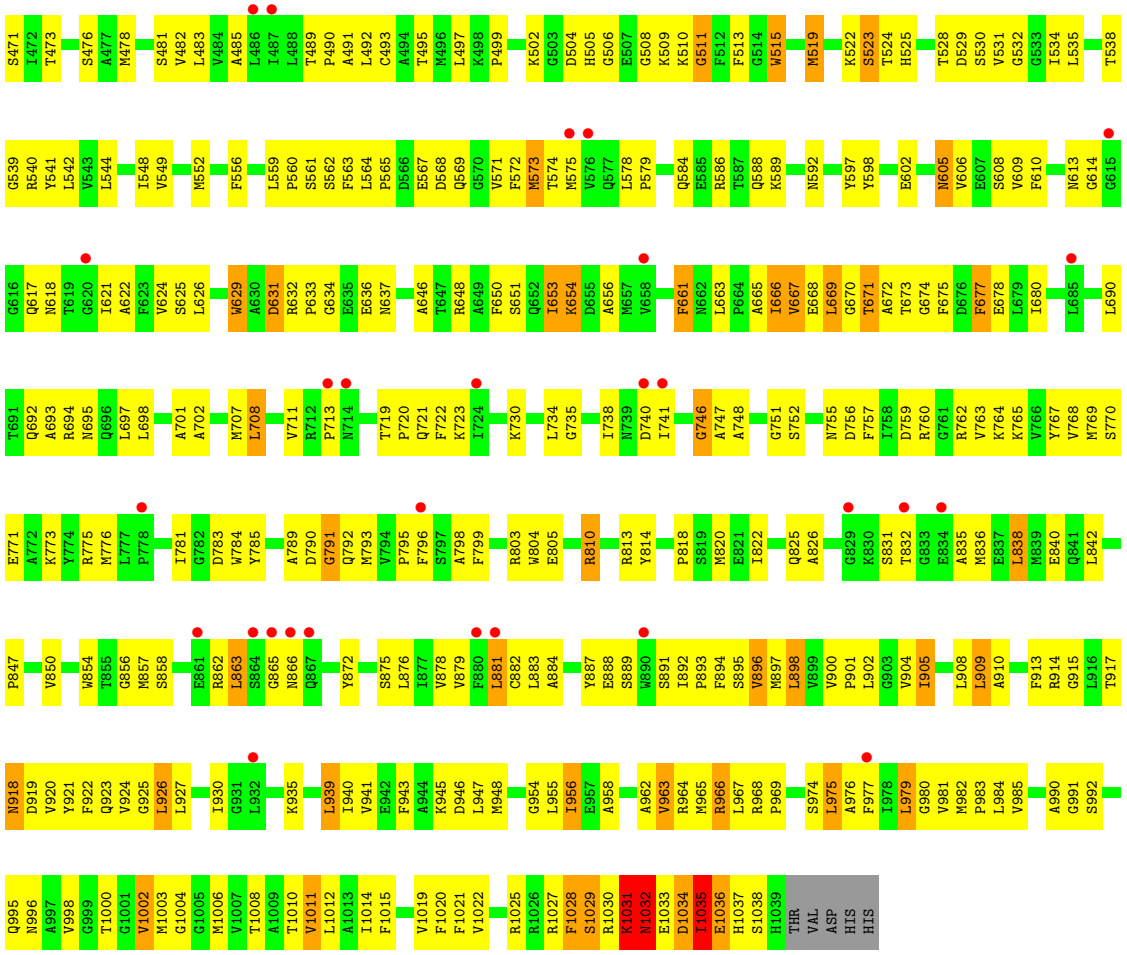




• Molecule 1: Multidrug efflux pump subunit AcrB

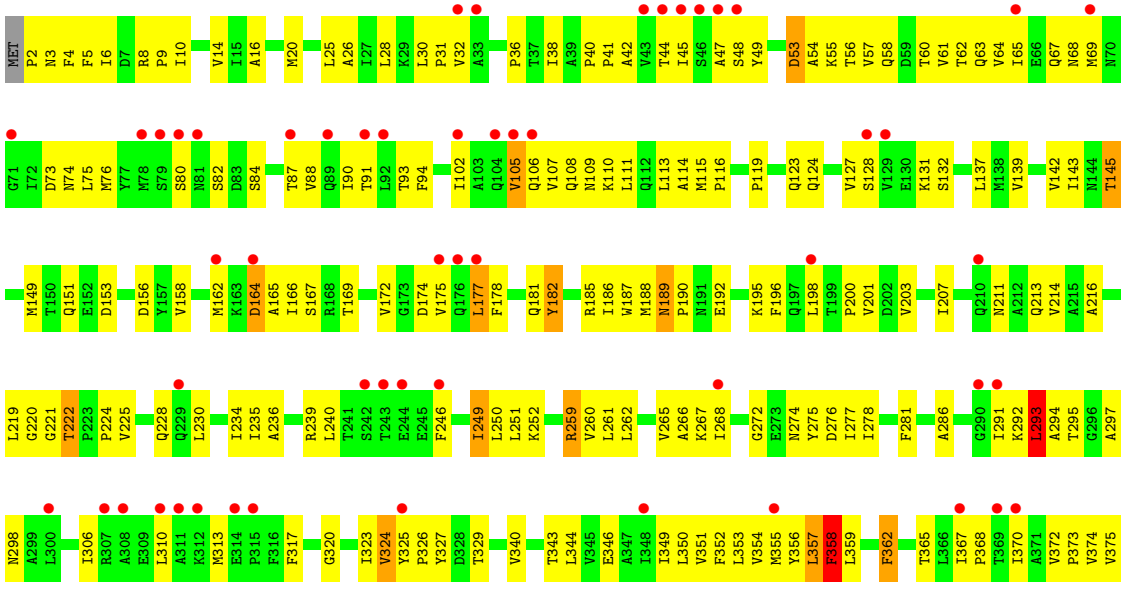
Chain D:

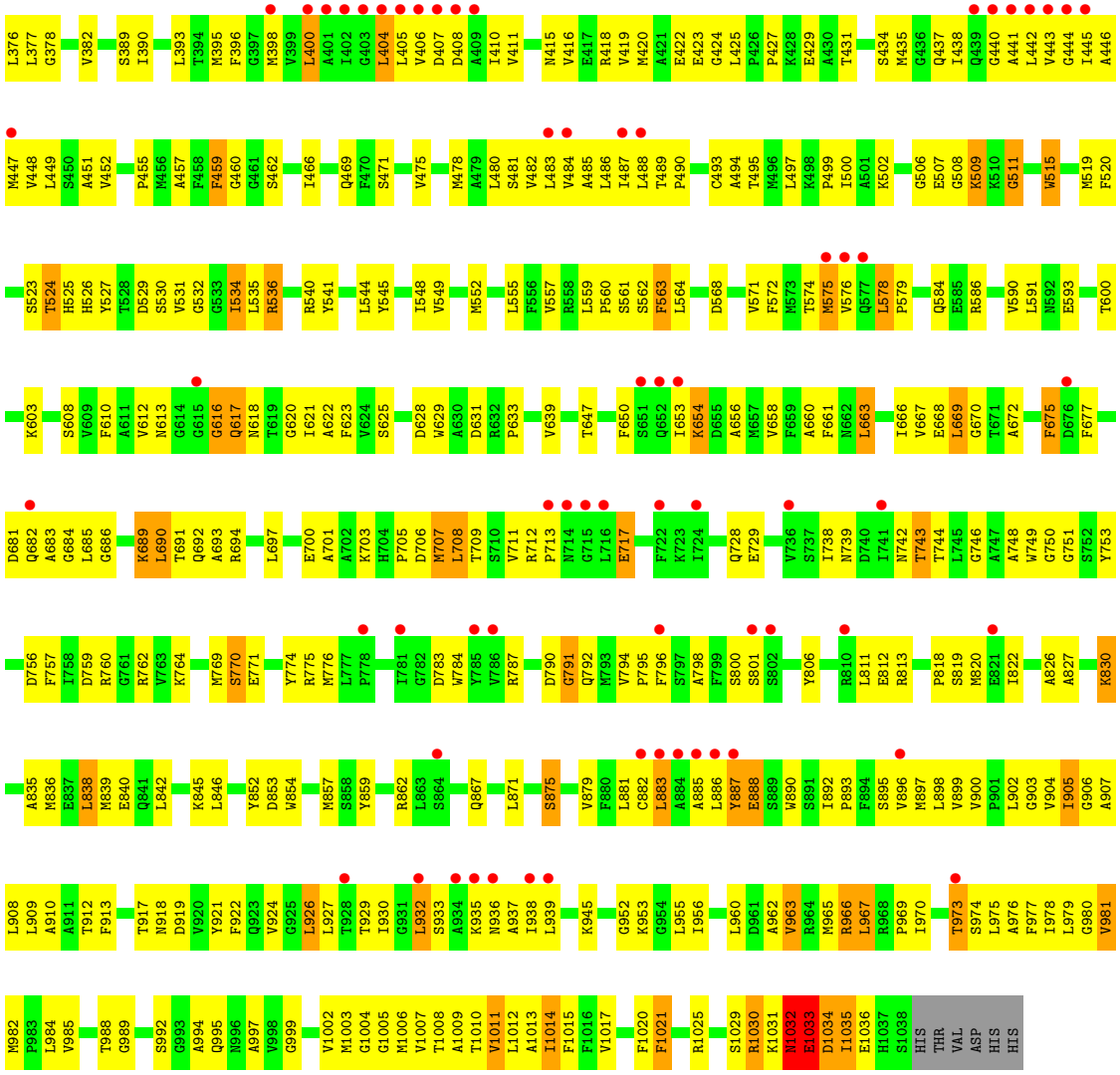




• Molecule 1: Multidrug efflux pump subunit AcrB

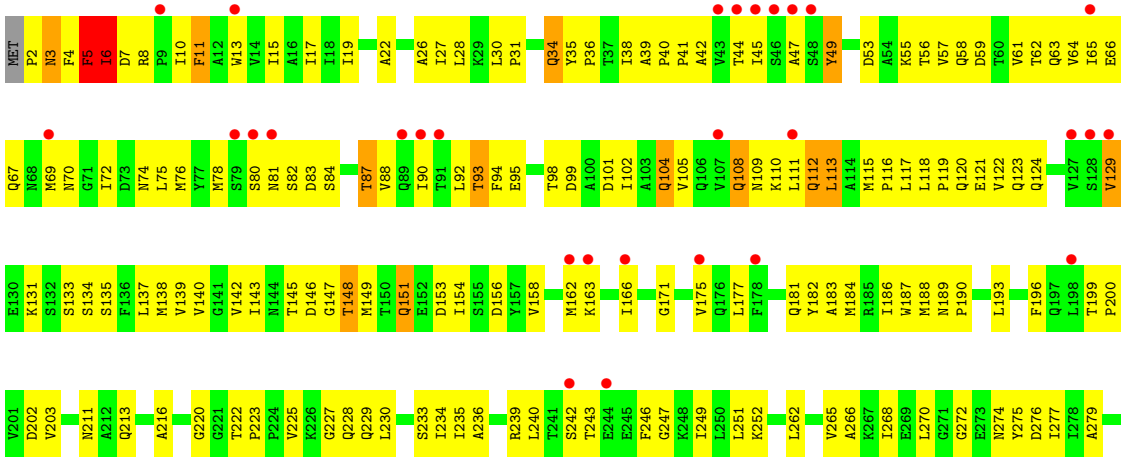
Chain E:

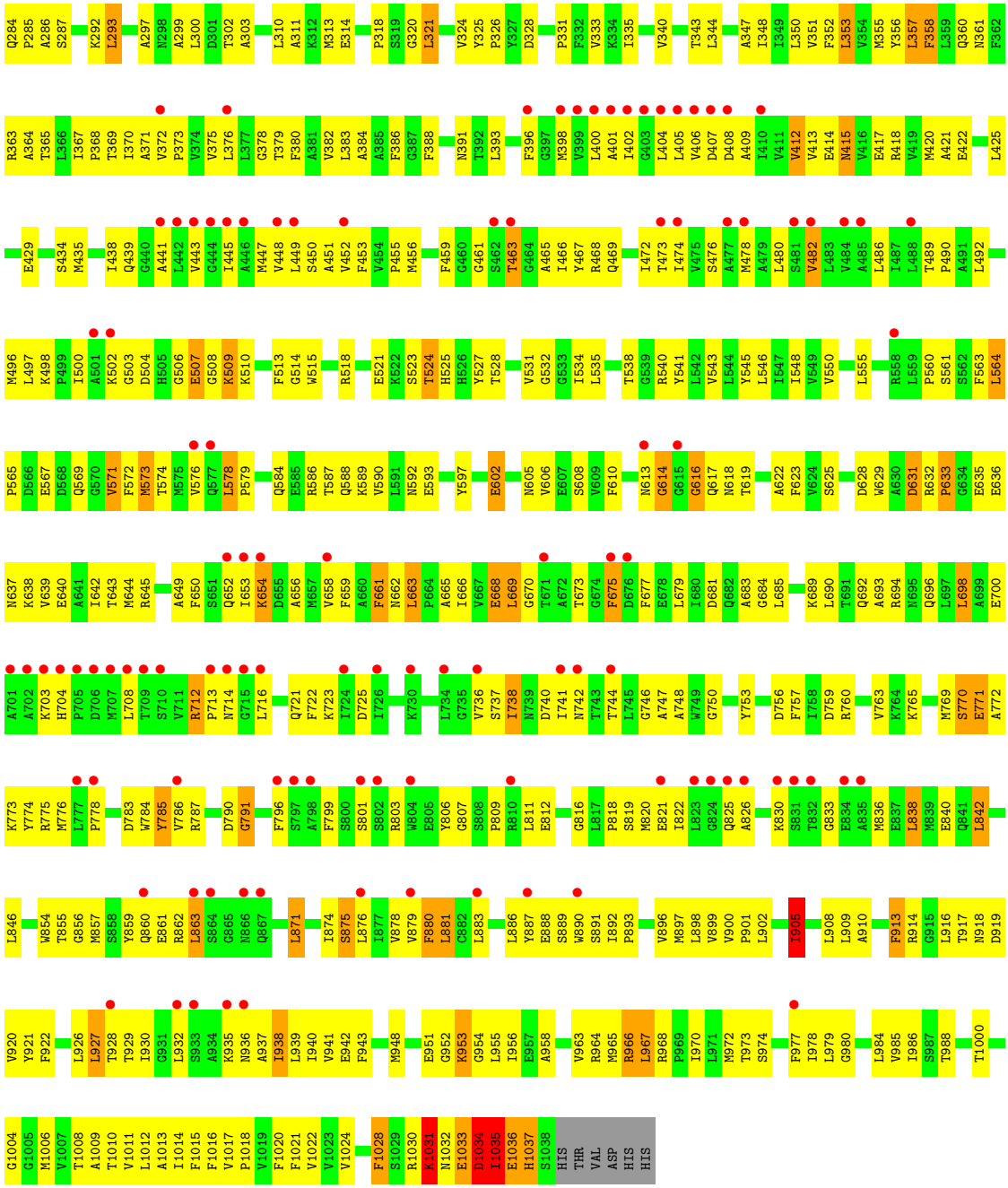




• Molecule 1: Multidrug efflux pump subunit AcrB

Chain F:




Q284 P285 A286 S287 K292 L293 A297 N298 A299 L300 D301 T302 A303 L310 A311 K312 M313 E314 P318 S319 G320 L321 V324 Y325 P326 Y327 D328 P331 F332 V333 K334 I335 V340 T343 L344 A347 I348 I349 L350 V351 F352 L353 V354 M355 Y356 L357 F358 L359 Q360 N361 F362
R363 A364 T365 L366 I367 P368 T369 I370 A371 V372 P373 V374 V375 L376 L377 G378 T379 F380 A381 V382 L383 A384 A385 F386 G387 F388 N391 T392 L393 F396 G397 M398 V399 L400 A401 I402 G403 L404 L405 V406 D407 D408 A409 I410 V411 V412 V413 E414 N415 V416 E417 R418 V419 M420 A421 E422 L425
E429 S434 M435 I438 Q439 G440 A441 L442 V443 G444 I445 A446 M447 V448 L449 S450 A451 V452 F453 V454 P455 M456 F459 G460 G461 S462 T463 G464 A465 I466 Y467 R468 Q469 I472 T473 I474 V475 S476 A477 M478 A479 L480 S481 V482 L483 V484 A485 L486 I487 L488 T489 P490 A491 L492
M496 L497 K498 P499 I500 A501 K502 Q503 D504 H505 G506 E507 G508 K509 K510 F513 G514 W515 R518 E521 K522 S523 T524 H525 H526 Y527 T528 V531 G532 G533 I534 L535 T538 G539 R540 Y541 L542 V543 L544 Y545 L546 I547 I548 V549 V550 L555 R558 L559 P560 S561 S562 F563 L564
P565 D566 E567 D568 Q569 G570 V571 F572 M573 T574 M575 V576 Q577 I578 P579 Q584 E585 R586 T587 Q588 K589 V590 L591 N592 E593 Y597 E602 N605 V606 E607 S608 V609 F610 N613 G614 G615 G616 Q617 N618 T619 A622 F623 V624 S625 D628 W629 A630 D631 R632 P633 G634 E635 E636
N637 K638 V639 E640 A641 I642 T643 M644 R645 A649 F650 S651 Q652 I653 K654 D655 A656 M657 V658 F659 A660 F661 N662 L663 P664 A665 I666 V667 E668 L669 G670 T671 A672 T673 G674 F675 D676 F677 E678 L679 T680 D681 Q682 A683 G684 L685 K689 L690 T691 Q692 A693 R694 N695 Q696 L697 L698 A699 E700
A701 A702 K703 H704 P705 D706 M707 L708 T709 S710 V711 R712 P713 N714 G715 L716 Q721 F722 K723 I724 D725 I726 K730 L734 G735 V736 S737 T738 N739 D740 I741 N742 T743 T744 L745 G746 A747 A748 W749 G750 Y753 D756 F757 T758 D759 R760 V763 K764 K765 M769 S770 E771 A772
K773 Y774 R775 W776 L777 P778 D783 W784 Y785 V786 R787 D790 G791 F796 S797 A798 F799 S800 S801 S802 R803 W804 E805 Y806 G807 S808 P809 R810 L811 E812 G816 L817 P818 S819 M820 E821 I822 L823 G824 Q825 A826 K830 S831 T832 G833 E834 A835 M836 E837 L838 M839 E840 Q841 L842
L846 W854 T855 G856 M857 S858 Y859 Q860 E861 R862 L863 S864 G865 N866 Q867 L871 I874 S875 L876 I877 V878 V879 F880 L881 G882 L883 L886 Y887 E888 S889 W890 S891 I892 P893 V896 M897 L898 V899 V900 P901 L902 I905 L908 L909 A910 F913 R914 G915 L916 T917 N918 D919
V920 Y921 F922 L926 L927 T928 T929 I930 G931 L932 S933 A934 K935 N936 A937 I938 L939 I940 V941 E942 F943 M948 E951 G952 K953 G954 L955 I956 E957 A958 V963 R964 M965 R966 L967 R968 P969 I970 L971 M972 T973 S974 F977 I978 L979 G980 L984 V985 I986 S987 T988 T1000
G1004 G1005 M1006 V1007 T1008 A1009 T1010 V1011 L1012 A1013 I1014 F1015 F1016 V1017 P1018 V1019 F1020 F1021 V1022 V1023 V1024 F1028 S1029 R1030 K1031 N1032 E1033 D1034 I1035 E1036 H1037 S1038 HIS THR VAL ASP 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	150.06Å 154.57Å 215.74Å 90.00° 92.42° 90.00°	Depositor
Resolution (Å)	19.96 – 3.59 125.61 – 3.59	Depositor EDS
% Data completeness (in resolution range)	99.2 (19.96-3.59) 96.5 (125.61-3.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 3.58Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.246 , 0.319 0.258 , 0.327	Depositor DCC
R_{free} test set	5715 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	110.6	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 61.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.055 for -k,-h,-l 0.070 for k,h,-l 0.068 for h,-k,-l	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	47697	wwPDB-VP
Average B, all atoms (Å^2)	81.0	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 51.06 % 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 5.9200e-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: LMT, ERY, NI

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	0/8043	0.85	10/10922 (0.1%)
1	B	0.59	0/8032	0.83	11/10907 (0.1%)
1	C	0.59	0/8026	0.87	7/10899 (0.1%)
1	D	0.56	1/8043 (0.0%)	0.81	9/10922 (0.1%)
1	E	0.57	1/8032 (0.0%)	0.82	10/10907 (0.1%)
1	F	0.56	0/8032	0.83	5/10907 (0.0%)
All	All	0.57	2/48208 (0.0%)	0.84	52/65464 (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	1
1	D	0	1
1	F	0	2
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	515	TRP	CB-CG	7.12	1.63	1.50
1	D	515	TRP	CB-CG	6.58	1.62	1.50

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	529	ASP	CB-CG-OD1	10.28	127.55	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	529	ASP	CB-CG-OD1	9.49	126.84	118.30
1	F	113	LEU	CA-CB-CG	9.17	136.39	115.30
1	A	529	ASP	CB-CG-OD1	8.95	126.36	118.30
1	E	529	ASP	CB-CG-OD1	7.96	125.46	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1034	ASP	Peptide
1	B	1033	GLU	Peptide
1	D	1032	ASN	Peptide
1	F	1033	GLU	Peptide
1	F	1034	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	7893	0	8034	443	0
1	B	7883	0	8027	442	0
1	C	7877	0	8022	481	0
1	D	7893	0	8034	470	0
1	E	7883	0	8027	467	0
1	F	7883	0	8027	497	0
2	A	51	0	67	5	0
2	D	51	0	67	4	0
3	A	70	0	92	7	0
3	B	35	0	46	7	0
3	C	35	0	46	1	0
3	D	70	0	92	13	0
3	E	35	0	46	10	0
3	F	35	0	46	2	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
All	All	47697	0	48673	2723	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 28.

The worst 5 of 2723 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:F:34:GLN:HB2	1:F:333:VAL:HG22	1.45	0.98
1:A:225:VAL:H	1:B:776:MET:HE1	1.25	0.97
1:D:344:LEU:HD22	1:D:402:ILE:HD11	1.45	0.97
1:A:776:MET:HE1	1:C:225:VAL:H	1.29	0.96
1:B:213:GLN:HG2	1:B:239:ARG:HG3	1.44	0.96

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 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	1036/1044 (99%)	902 (87%)	117 (11%)	17 (2%)	9	46
1	B	1035/1044 (99%)	896 (87%)	117 (11%)	22 (2%)	7	40
1	C	1034/1044 (99%)	896 (87%)	119 (12%)	19 (2%)	8	43
1	D	1036/1044 (99%)	894 (86%)	116 (11%)	26 (2%)	5	36
1	E	1035/1044 (99%)	894 (86%)	116 (11%)	25 (2%)	6	37
1	F	1035/1044 (99%)	891 (86%)	118 (11%)	26 (2%)	5	36
All	All	6211/6264 (99%)	5373 (86%)	703 (11%)	135 (2%)	6	39

5 of 135 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	987	SER
1	A	1033	GLU
1	B	357	LEU

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Mol	Chain	Res	Type
1	B	508	GLY
1	B	672	ALA

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	846/852 (99%)	782 (92%)	64 (8%)	13 45
1	B	845/852 (99%)	772 (91%)	73 (9%)	10 41
1	C	844/852 (99%)	766 (91%)	78 (9%)	9 39
1	D	846/852 (99%)	779 (92%)	67 (8%)	12 44
1	E	845/852 (99%)	775 (92%)	70 (8%)	11 42
1	F	845/852 (99%)	758 (90%)	87 (10%)	7 34
All	All	5071/5112 (99%)	4632 (91%)	439 (9%)	10 41

5 of 439 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	353	LEU
1	E	53	ASP
1	F	1037	HIS
1	F	652	GLN
1	D	463	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	613	ASN
1	E	732	GLN
1	D	825	GLN
1	E	123	GLN
1	F	109	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
3	LMT	F	2100	-	36,36,36	1.74	8 (22%)	47,47,47	1.11	4 (8%)
3	LMT	C	1101	-	36,36,36	1.79	8 (22%)	47,47,47	1.43	6 (12%)
3	LMT	D	1102	-	36,36,36	1.81	9 (25%)	47,47,47	1.41	7 (14%)
3	LMT	D	1103	-	36,36,36	1.92	8 (22%)	47,47,47	1.31	7 (14%)
3	LMT	B	2100	-	36,36,36	1.73	9 (25%)	47,47,47	1.93	14 (29%)
3	LMT	A	1103	-	36,36,36	1.89	10 (27%)	47,47,47	1.58	9 (19%)
2	ERY	A	1101	-	53,53,53	1.14	2 (3%)	82,82,82	1.86	18 (21%)
3	LMT	E	1101	-	36,36,36	1.89	11 (30%)	47,47,47	1.63	8 (17%)
3	LMT	A	1102	-	36,36,36	1.76	9 (25%)	47,47,47	1.14	4 (8%)
2	ERY	D	1101	-	53,53,53	1.28	2 (3%)	82,82,82	2.03	27 (32%)

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
3	LMT	F	2100	-	-	12/21/61/61	0/2/2/2
3	LMT	C	1101	-	-	12/21/61/61	0/2/2/2
3	LMT	D	1102	-	-	11/21/61/61	0/2/2/2
3	LMT	D	1103	-	-	14/21/61/61	0/2/2/2
3	LMT	B	2100	-	-	11/21/61/61	0/2/2/2
3	LMT	A	1103	-	-	14/21/61/61	0/2/2/2
2	ERY	A	1101	-	-	33/72/107/107	0/3/3/3
3	LMT	E	1101	-	-	11/21/61/61	0/2/2/2
3	LMT	A	1102	-	-	13/21/61/61	0/2/2/2
2	ERY	D	1101	-	-	48/72/107/107	0/3/3/3

The worst 5 of 76 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1101	ERY	O2-C1	5.43	1.47	1.34
2	A	1101	ERY	O2-C1	5.17	1.46	1.34
3	A	1103	LMT	O5'-C5'	4.58	1.55	1.44
3	D	1103	LMT	O5'-C5'	4.51	1.55	1.44
3	D	1102	LMT	O3B-C3B	4.36	1.53	1.43

The worst 5 of 104 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1103	LMT	O5B-C5B-C4B	5.53	119.73	109.69
3	E	1101	LMT	C1B-C2B-C3B	-5.51	98.53	110.00
2	D	1101	ERY	C20-O5-C16	5.24	128.48	117.55
3	C	1101	LMT	C4B-C3B-C2B	5.07	119.67	110.82
2	A	1101	ERY	C20-O5-C16	4.72	127.40	117.55

There are no chirality outliers.

5 of 179 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	ERY	C11-C12-C13-O2
2	A	1101	ERY	C11-C12-C13-C36
2	A	1101	ERY	C35-C12-C13-O2
2	A	1101	ERY	C35-C12-C13-C36
2	A	1101	ERY	O13-C12-C13-O2

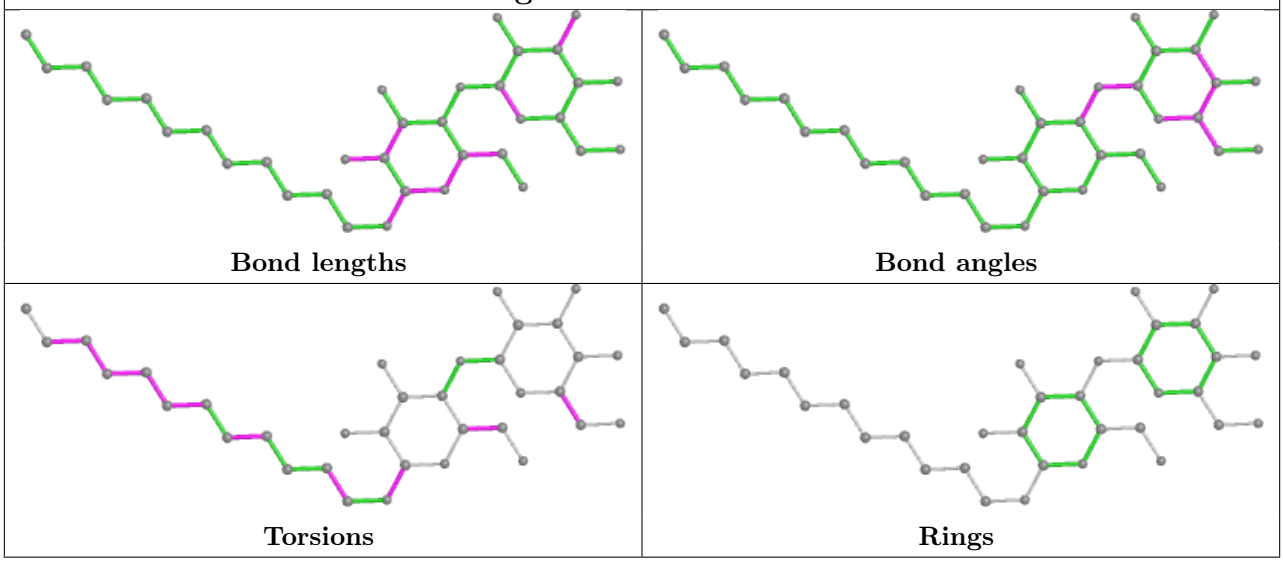
There are no ring outliers.

10 monomers are involved in 49 short contacts:

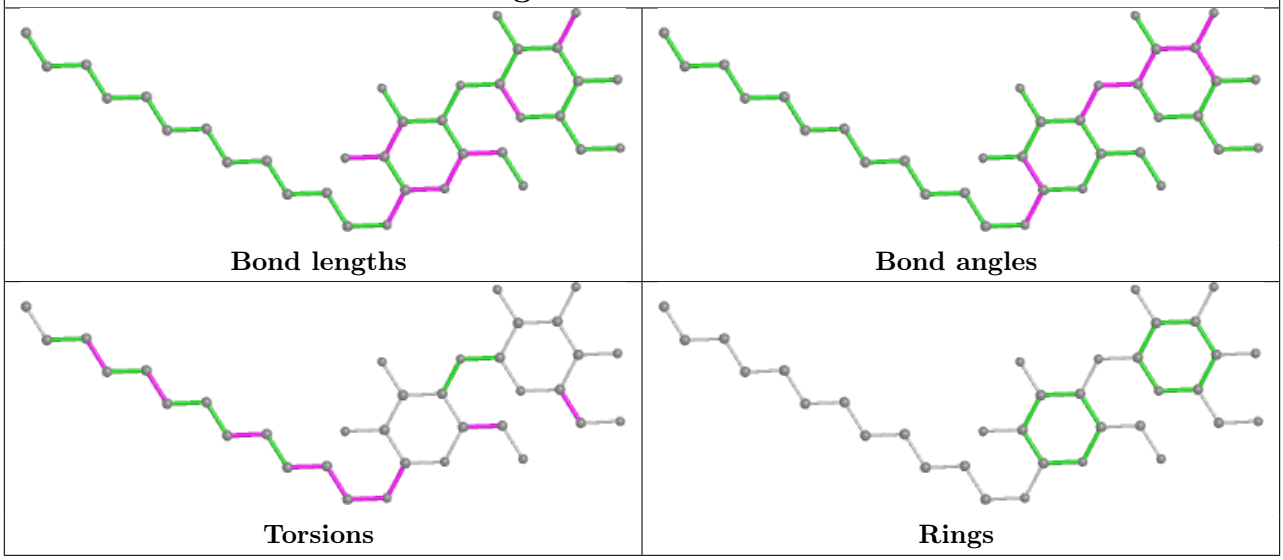
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	2100	LMT	2	0
3	C	1101	LMT	1	0
3	D	1102	LMT	7	0
3	D	1103	LMT	6	0
3	B	2100	LMT	7	0
3	A	1103	LMT	2	0
2	A	1101	ERY	5	0
3	E	1101	LMT	10	0
3	A	1102	LMT	5	0
2	D	1101	ERY	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

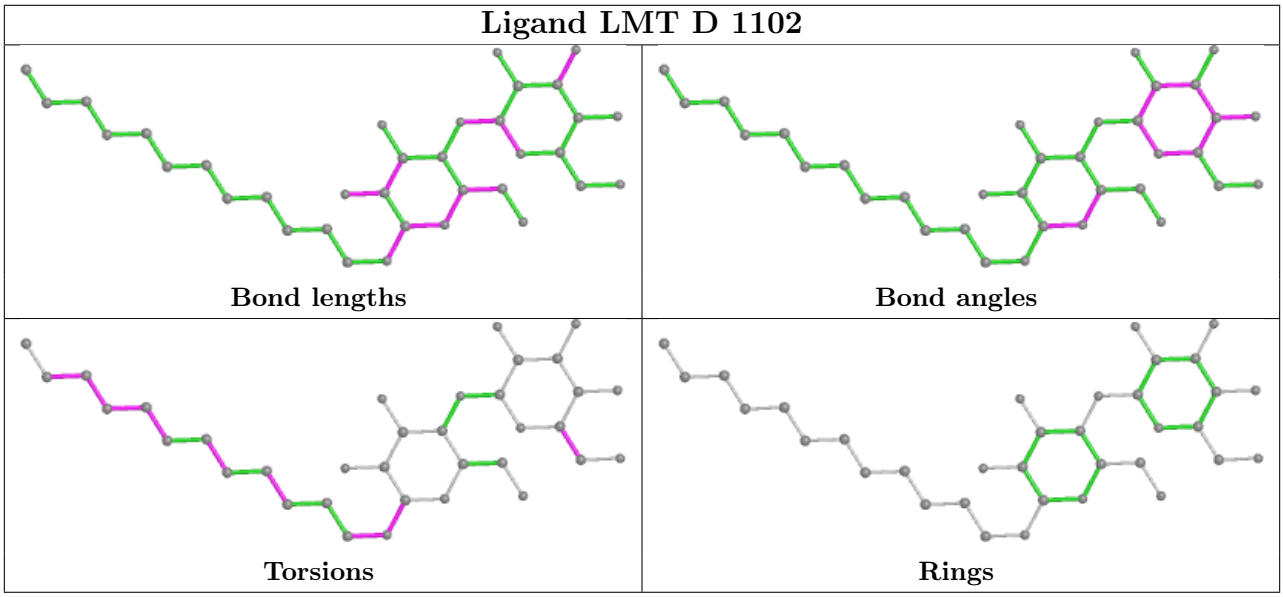
Ligand LMT F 2100



Ligand LMT C 1101



Ligand LMT D 1102



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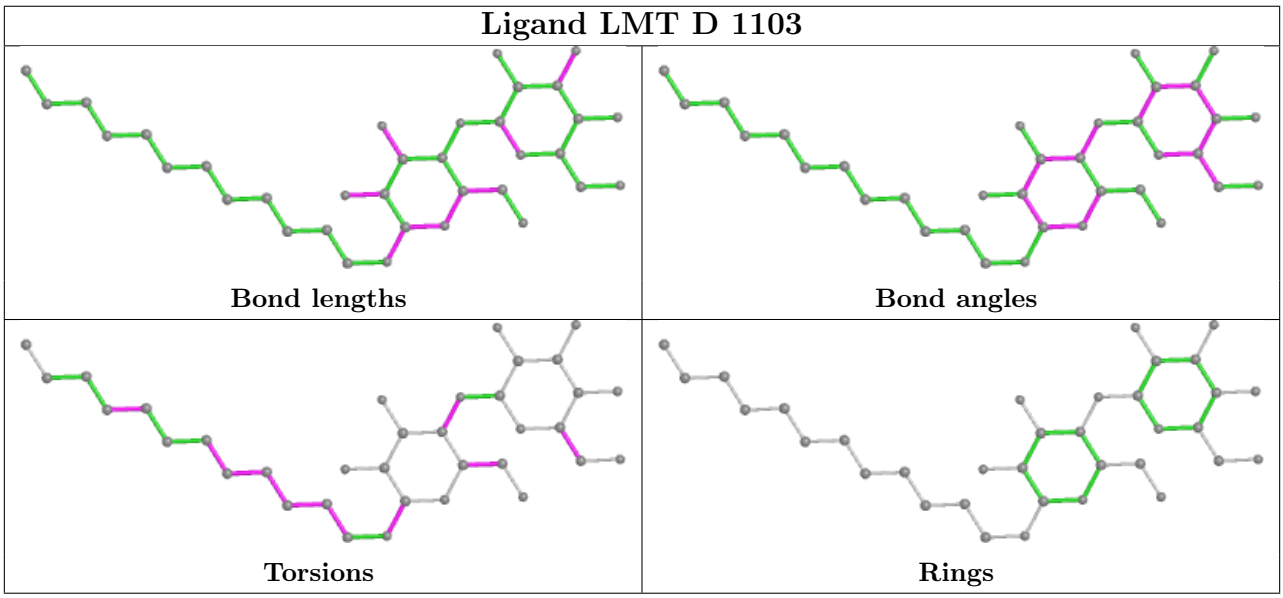
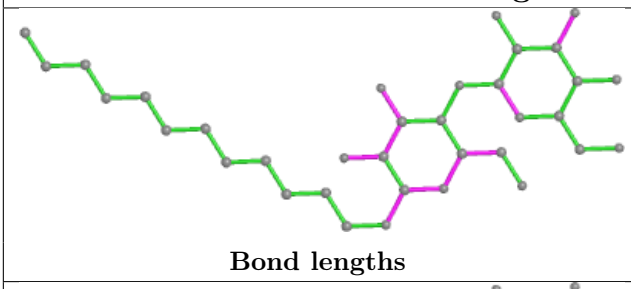
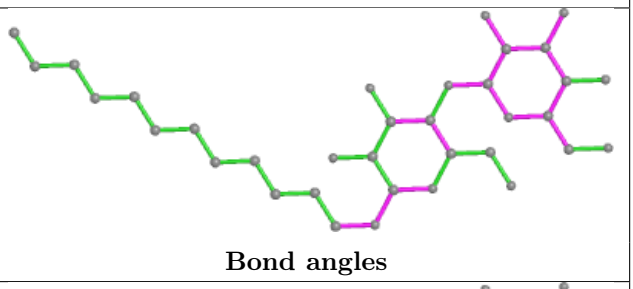


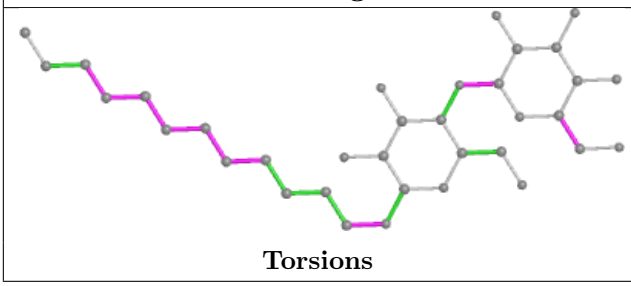
Ligand LMT B 2100



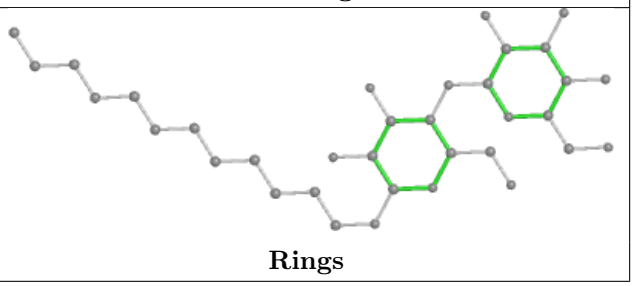
Bond lengths



Bond angles

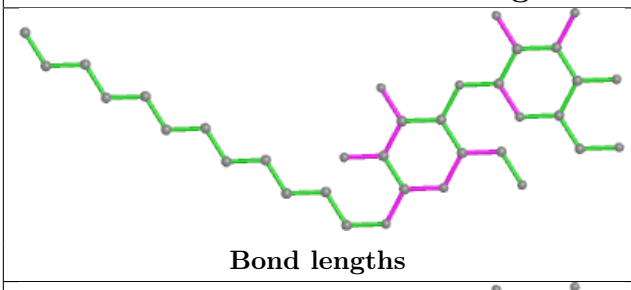


Torsions

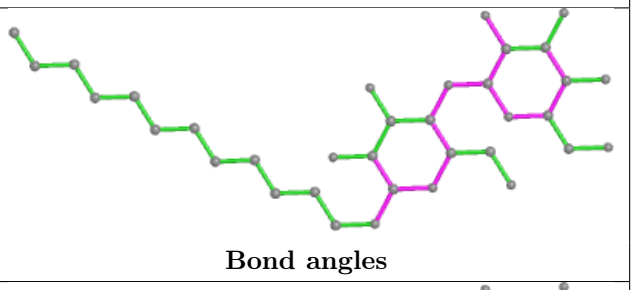


Rings

Ligand LMT A 1103



Bond lengths



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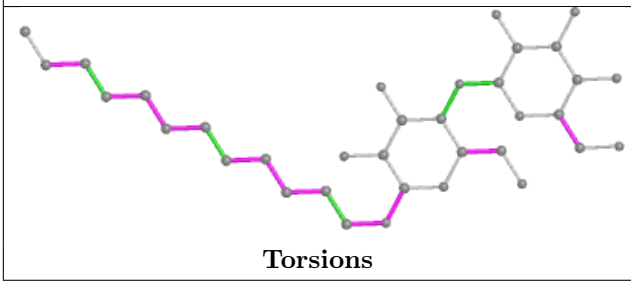
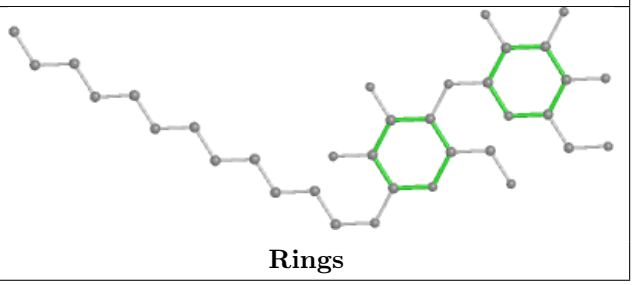
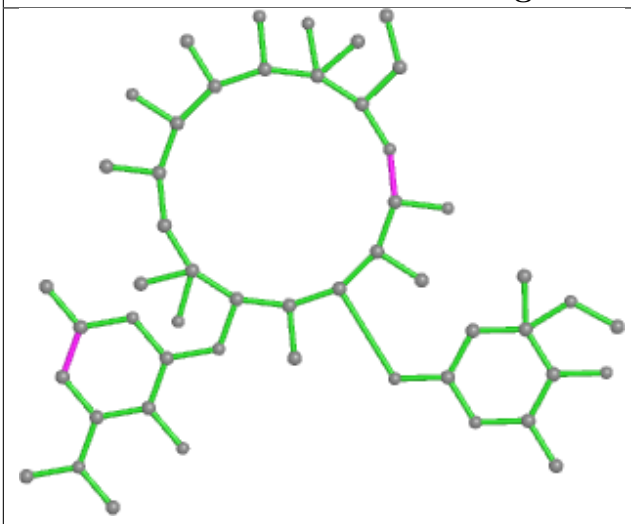


Torsions

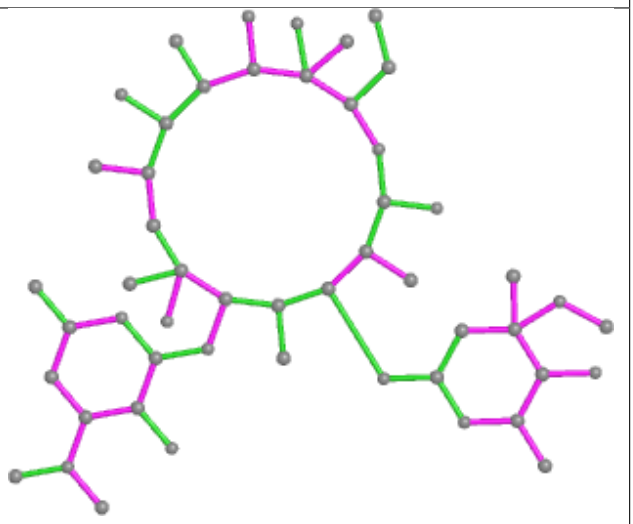


Rings

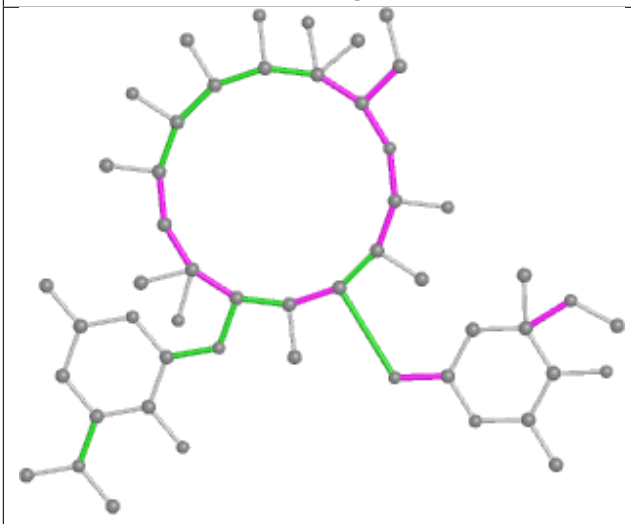
Ligand ERY A 1101



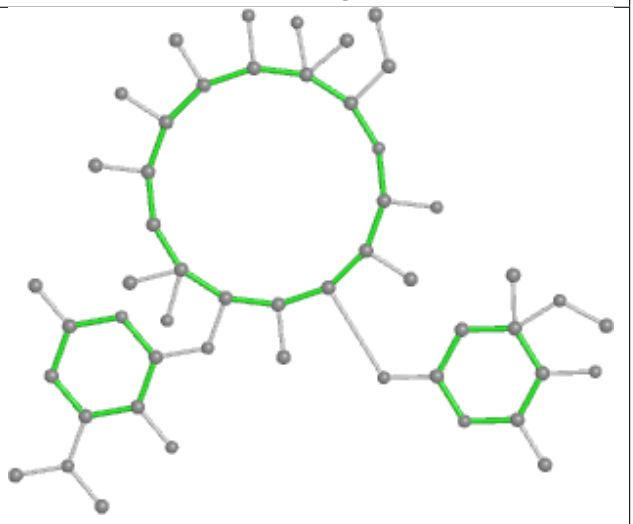
Bond lengths



Bond angles

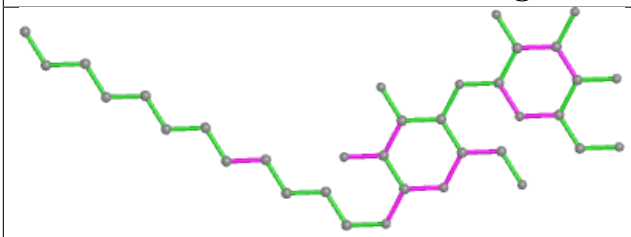


Torsions

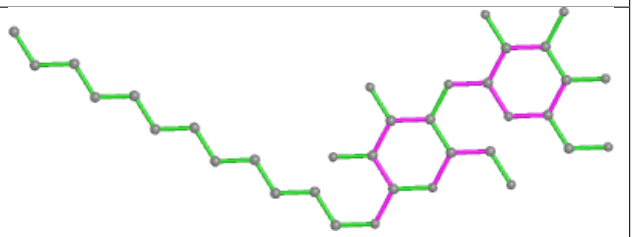


Rings

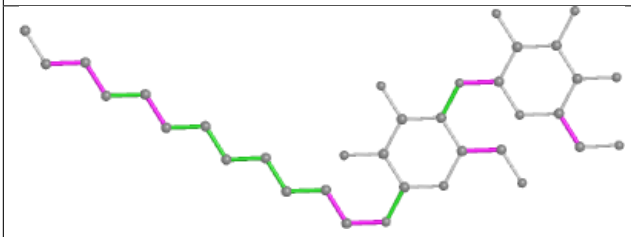
Ligand LMT E 1101



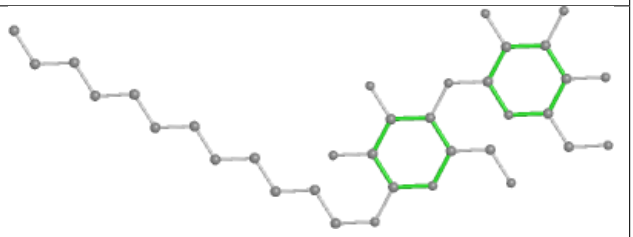
Bond lengths



Bond angles

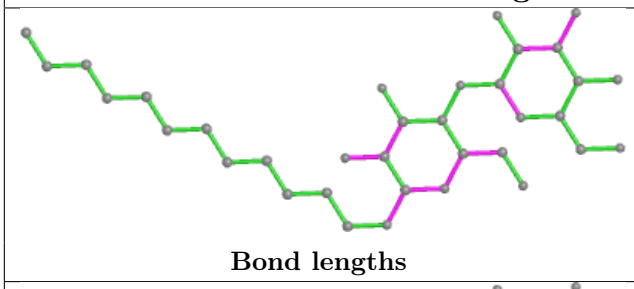


Torsions

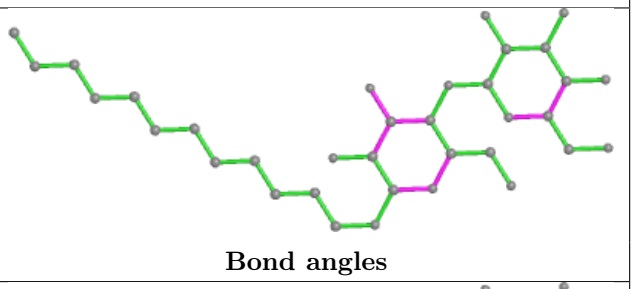


Rings

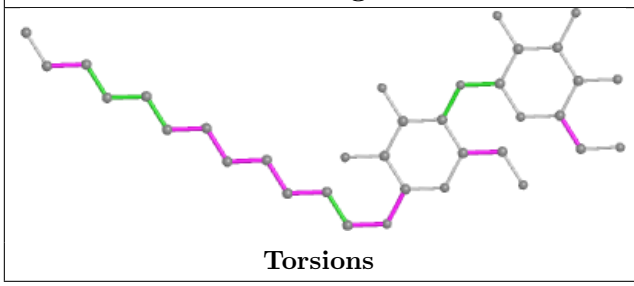
Ligand LMT A 1102



Bond lengths



Bond angles



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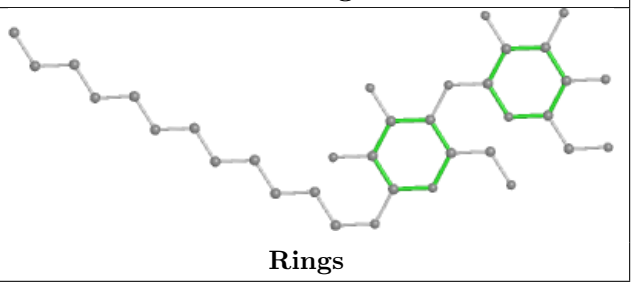
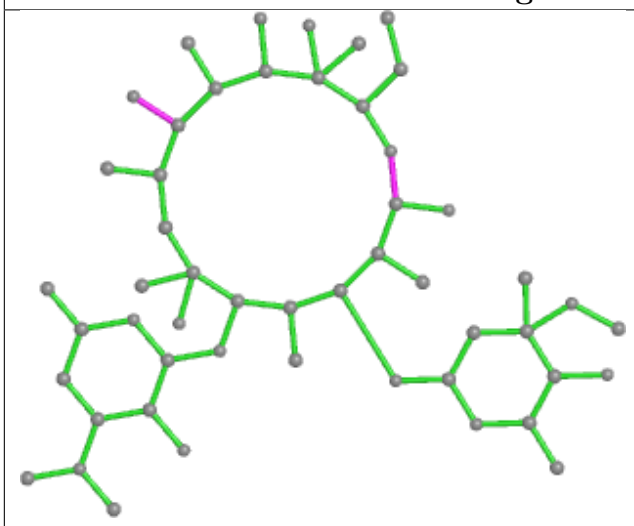
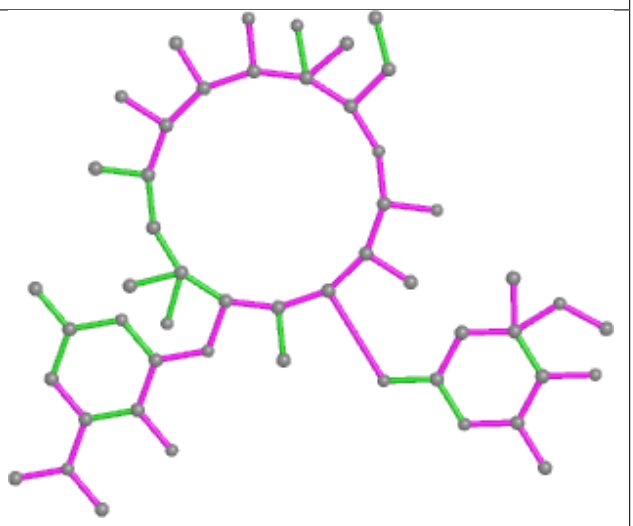


Rings

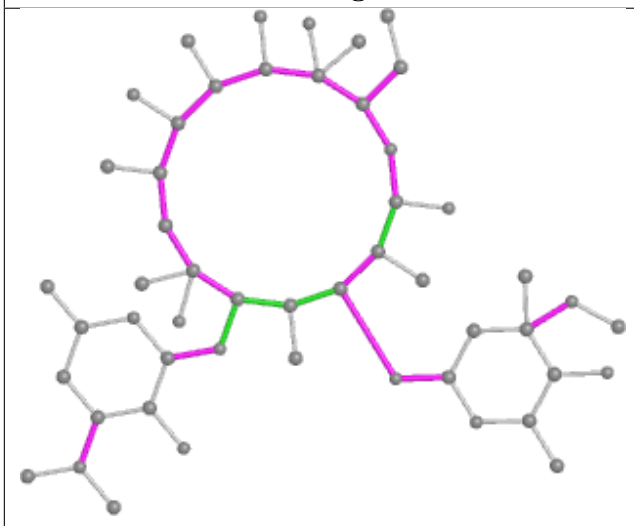
Ligand ERY D 1101



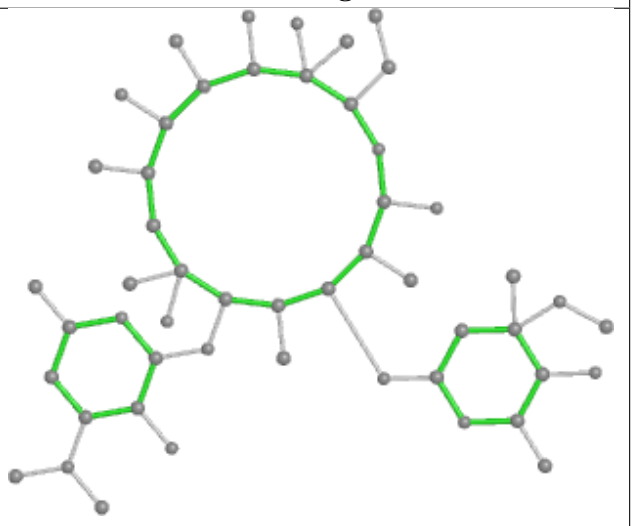
Bond lengths



Bond angles



Torsions



Rings

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	1038/1044 (99%)	0.17	76 (7%) 15 9	36, 75, 109, 154	0
1	B	1037/1044 (99%)	0.13	75 (7%) 15 9	31, 73, 111, 150	0
1	C	1036/1044 (99%)	0.33	99 (9%) 8 4	35, 76, 112, 139	0
1	D	1038/1044 (99%)	0.15	74 (7%) 16 9	34, 84, 123, 154	0
1	E	1037/1044 (99%)	0.32	119 (11%) 4 3	46, 87, 118, 148	0
1	F	1037/1044 (99%)	0.47	136 (13%) 3 2	41, 85, 119, 143	0
All	All	6223/6264 (99%)	0.26	579 (9%) 8 4	31, 81, 116, 154	0

The worst 5 of 579 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	714	ASN	10.9
1	C	714	ASN	10.3
1	C	715	GLY	9.4
1	E	314	GLU	9.1
1	A	404	LEU	9.0

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 monosaccharides in this entry.

6.4 Ligands (i)

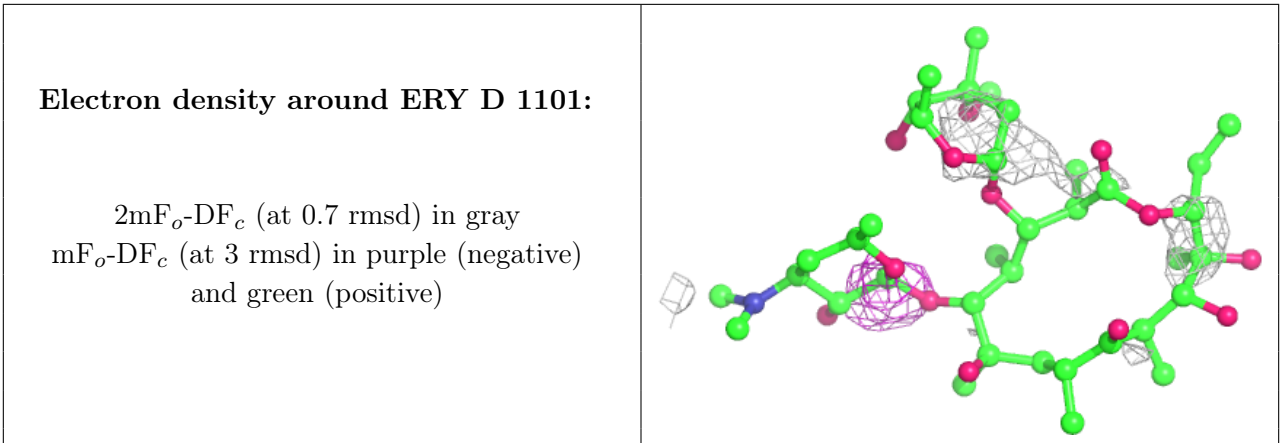
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

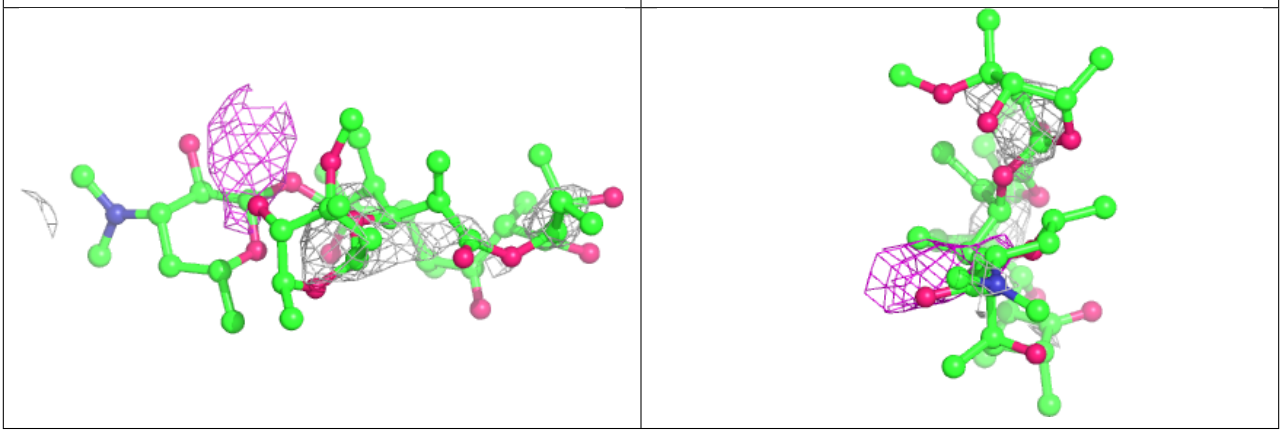
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ERY	D	1101	51/51	0.68	1.24	62,93,101,108	51
3	LMT	D	1103	35/35	0.73	0.41	77,92,105,106	0
3	LMT	D	1102	35/35	0.76	0.43	38,74,82,84	0
2	ERY	A	1101	51/51	0.77	1.26	81,93,101,104	51
3	LMT	F	2100	35/35	0.77	0.51	49,75,87,96	0
3	LMT	A	1102	35/35	0.79	0.41	49,70,79,82	0
3	LMT	B	2100	35/35	0.79	0.48	34,66,78,87	0
3	LMT	C	1101	35/35	0.79	0.41	62,75,83,87	0
3	LMT	E	1101	35/35	0.80	0.45	63,72,86,108	0
3	LMT	A	1103	35/35	0.85	0.80	65,90,106,109	0
4	NI	A	1104	1/1	0.99	0.21	67,67,67,67	0
4	NI	C	1102	1/1	0.99	0.21	77,77,77,77	0
4	NI	E	1102	1/1	0.99	0.21	73,73,73,73	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ERY D 1101:

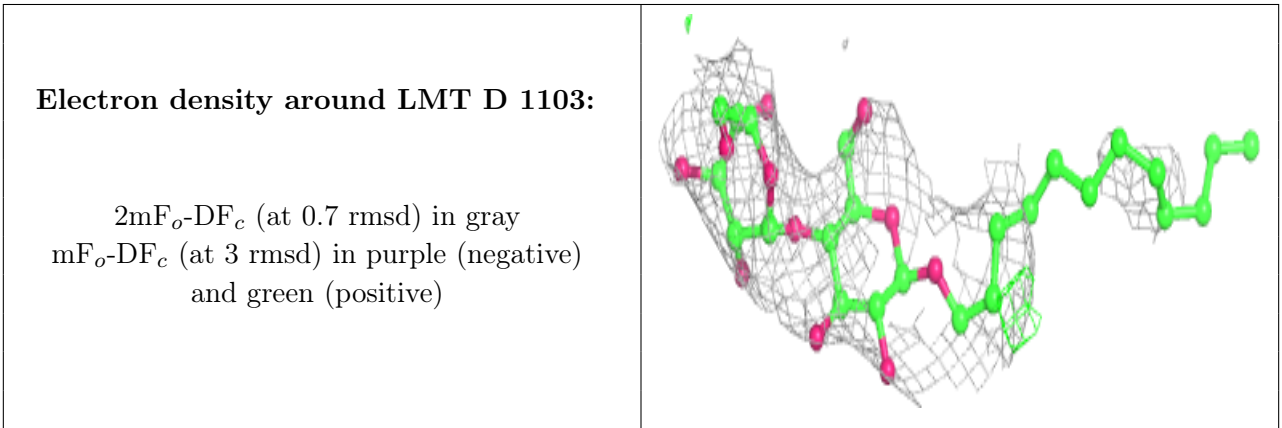
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

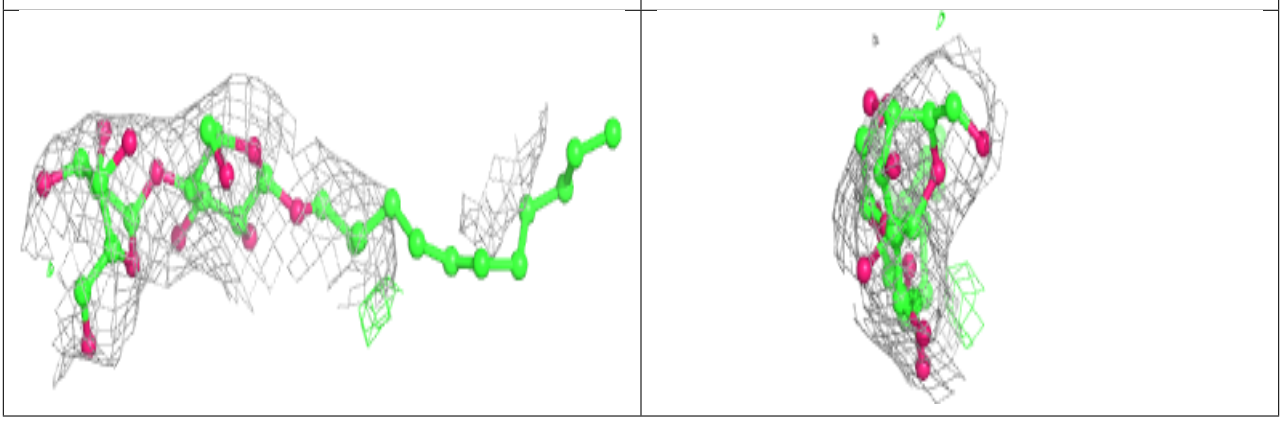




Electron density around LMT D 1103:

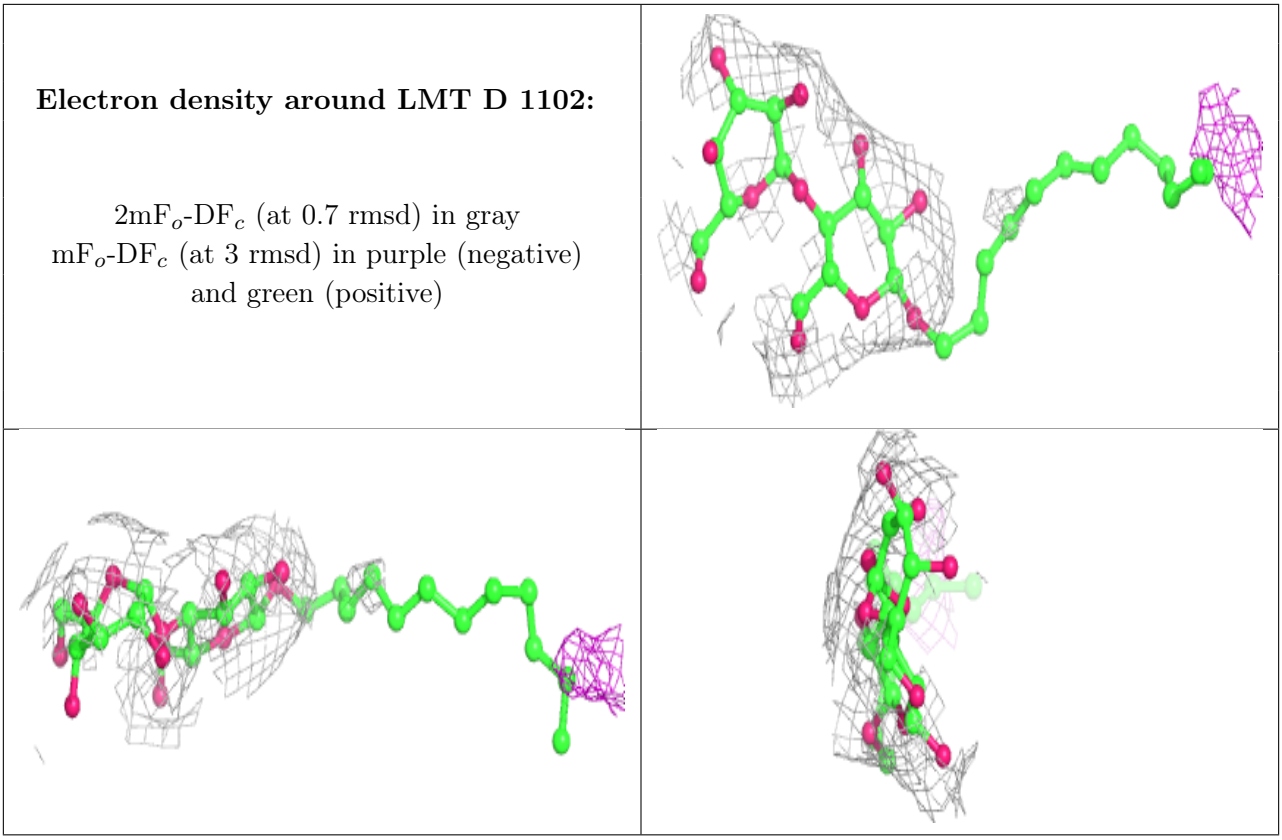
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





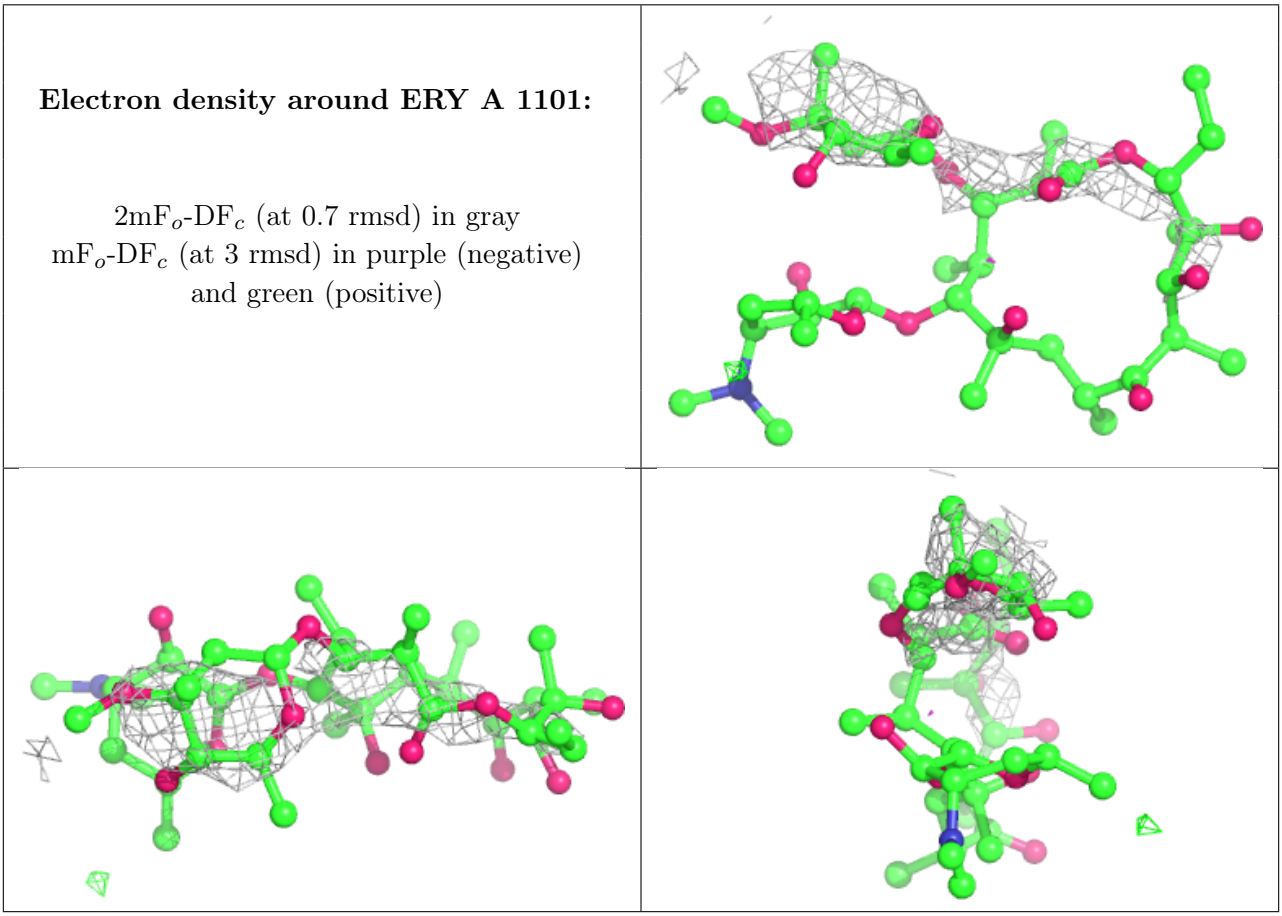
Electron density around LMT D 1102:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



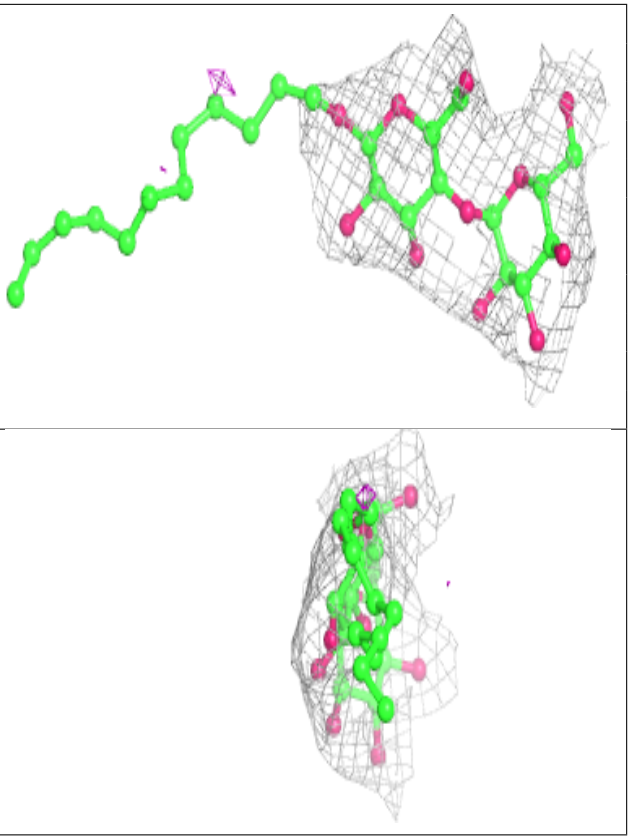
Electron density around ERY A 1101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



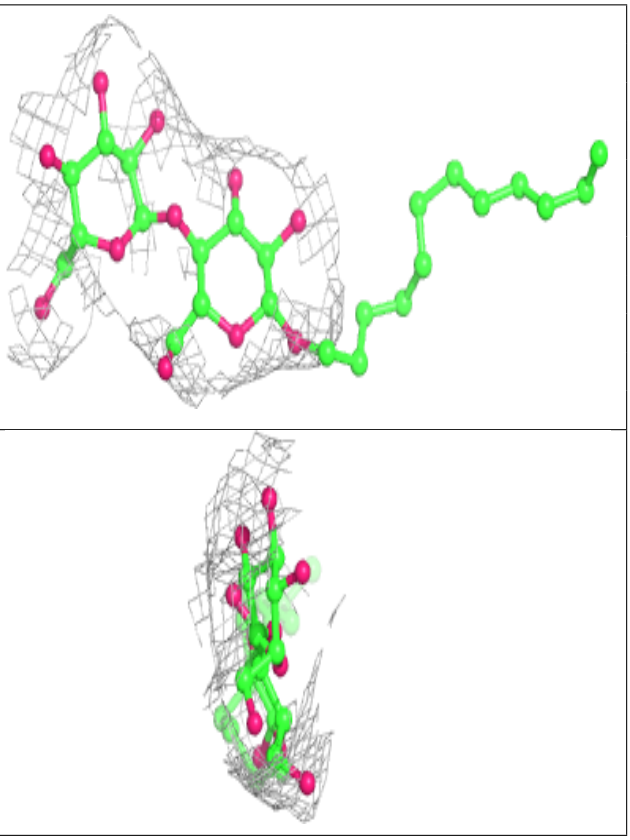
Electron density around LMT F 2100:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



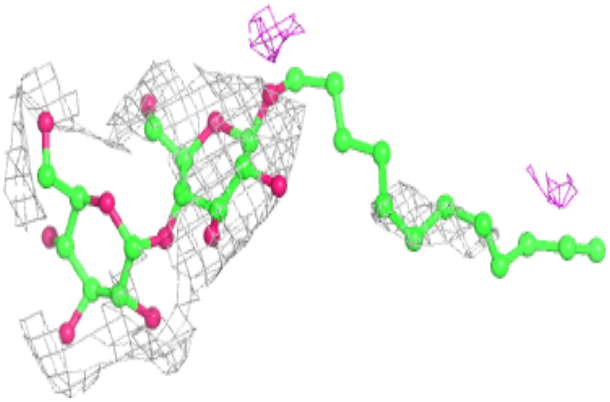
Electron density around LMT A 1102:

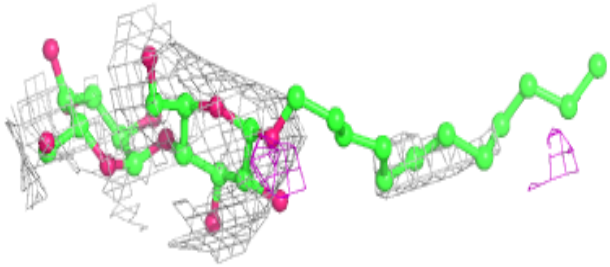
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

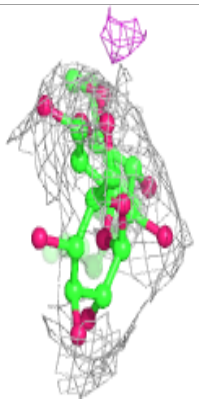


Electron density around LMT B 2100:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

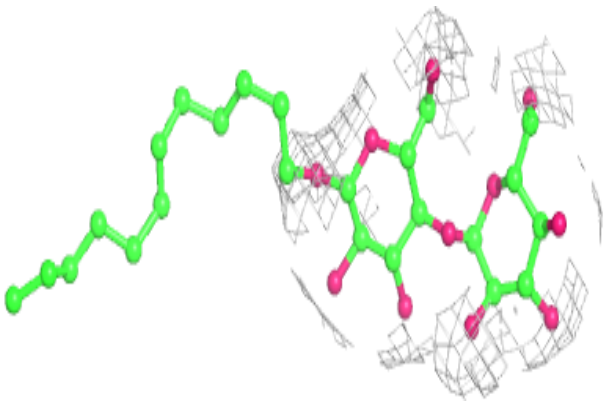


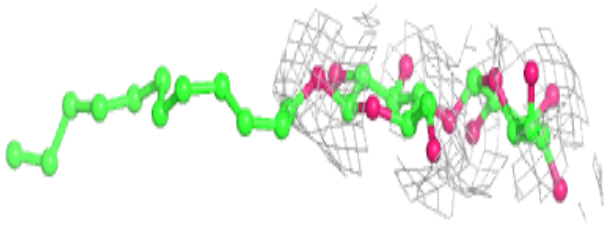




Electron density around LMT C 1101:

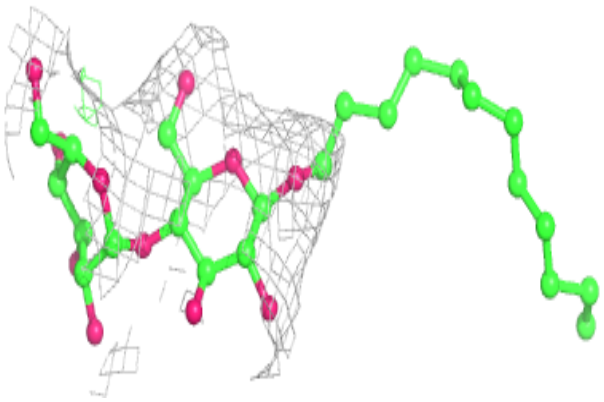
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

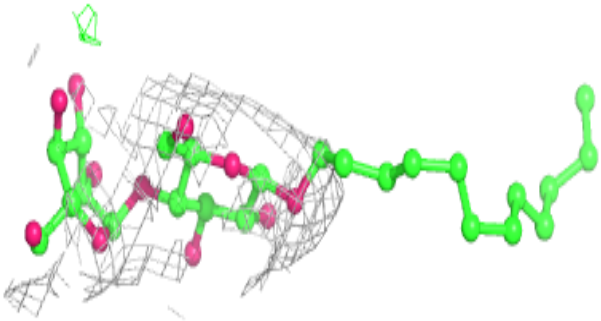


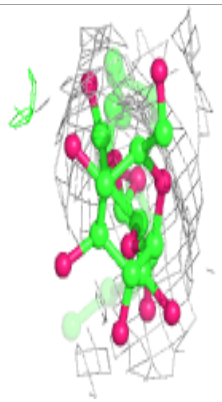


Electron density around LMT E 1101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

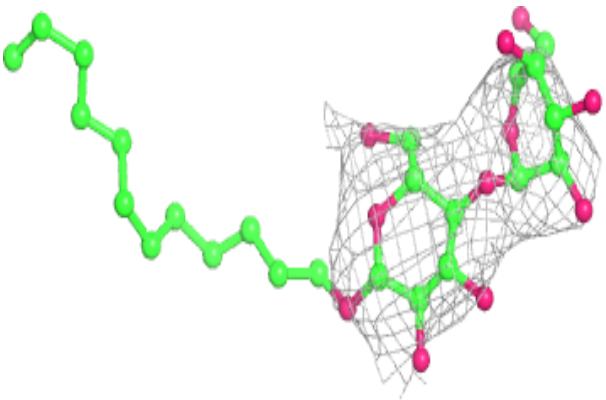


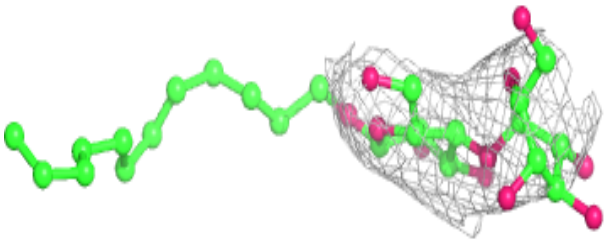


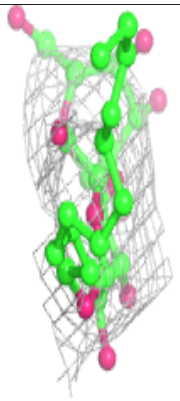


Electron density around LMT A 1103:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.