



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 19, 2020 – 07:20 am BST

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](mailto: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 ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

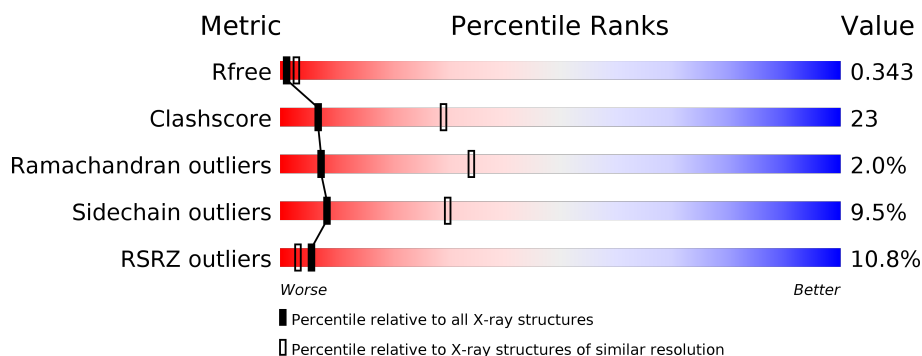
# 1 Overall quality at a glance

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))
$R_{free}$	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (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  $\geq 3$ , 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  $\leq 5\%$ . 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>
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>12%</div> <div>48%</div> <div>43%</div> <div>7% •</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:

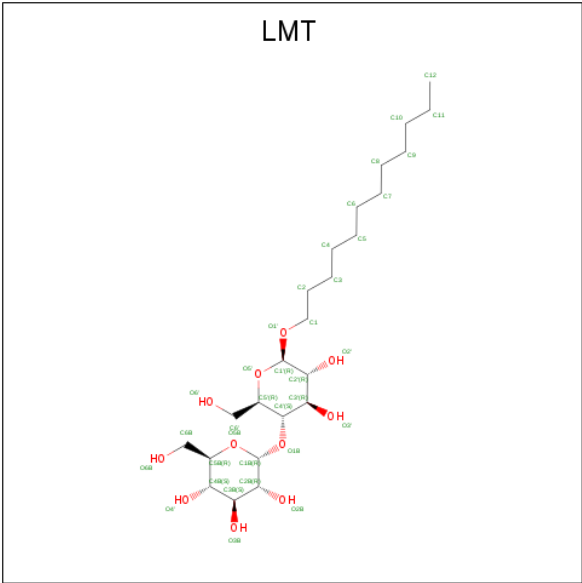
Chain	Residue	Modelled	Actual	Comment	Reference
A	615	ALA	PHE	engineered mutation	UNP P31224
A	617	ALA	PHE	engineered mutation	UNP P31224
A	620	ALA	ARG	engineered mutation	UNP P31224
B	615	ALA	PHE	engineered mutation	UNP P31224
B	617	ALA	PHE	engineered mutation	UNP P31224
B	620	ALA	ARG	engineered mutation	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-MALTOSIDE (three-letter code: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



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

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

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

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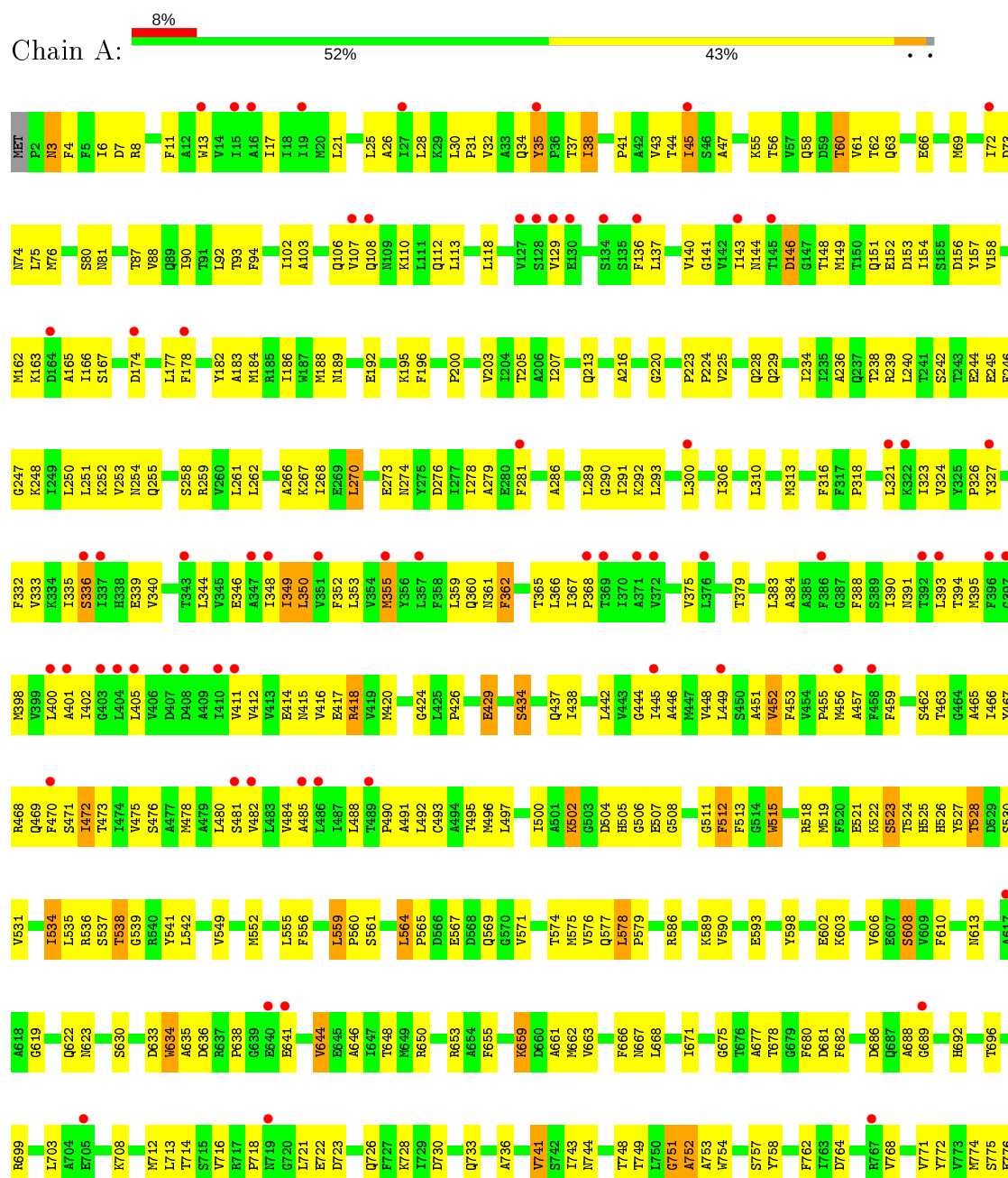
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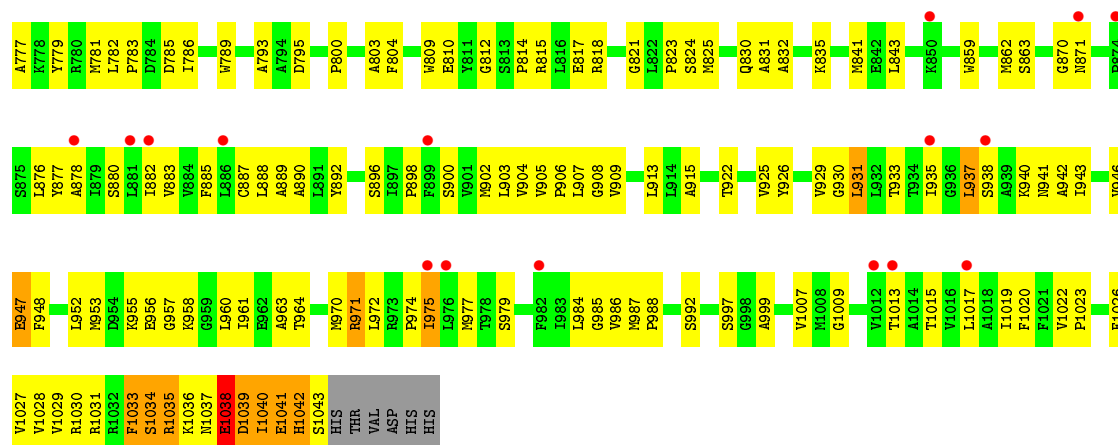
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	1	Total	Ni	0	0
			1	1		

### 3 Residue-property plots

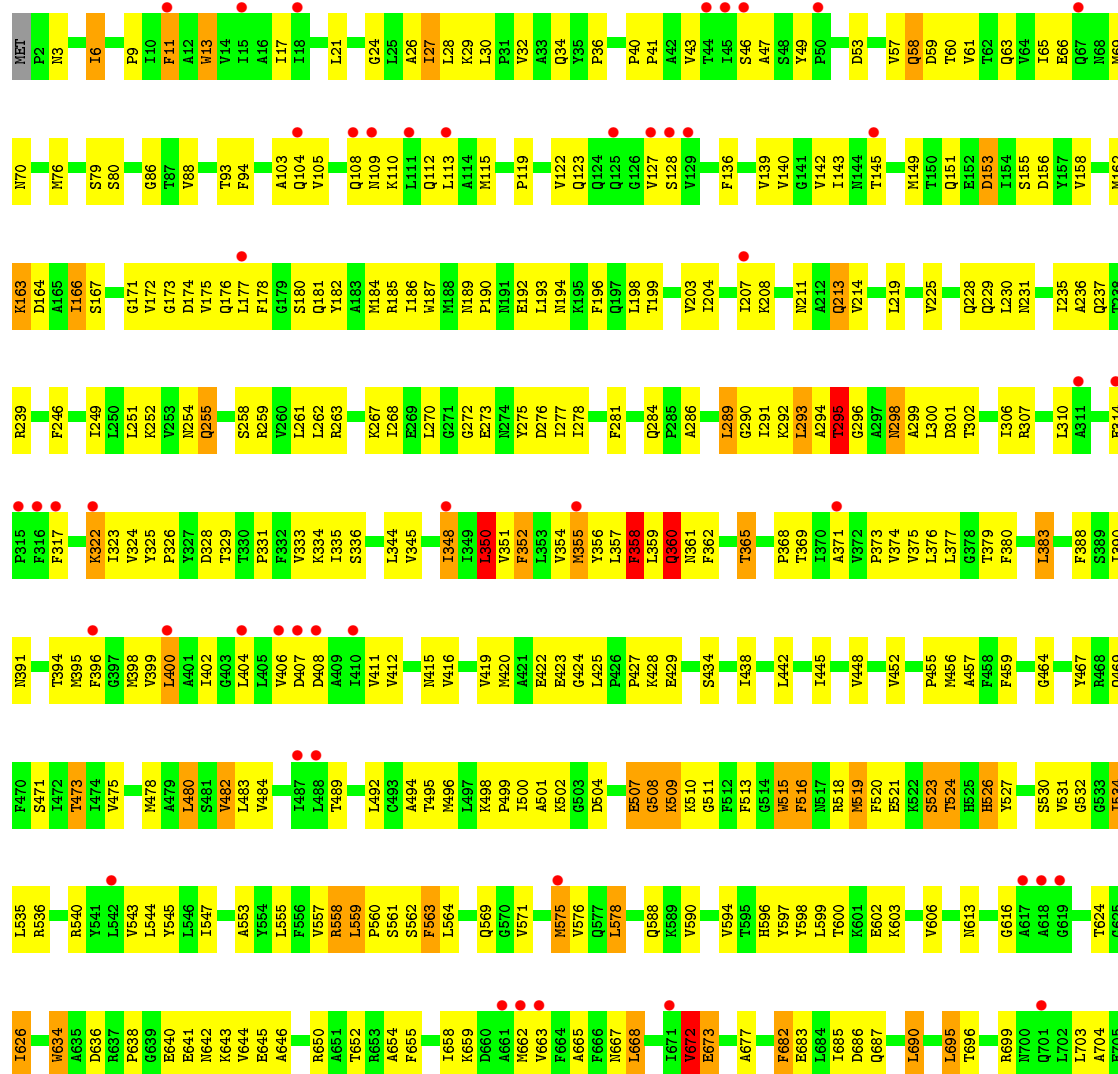
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

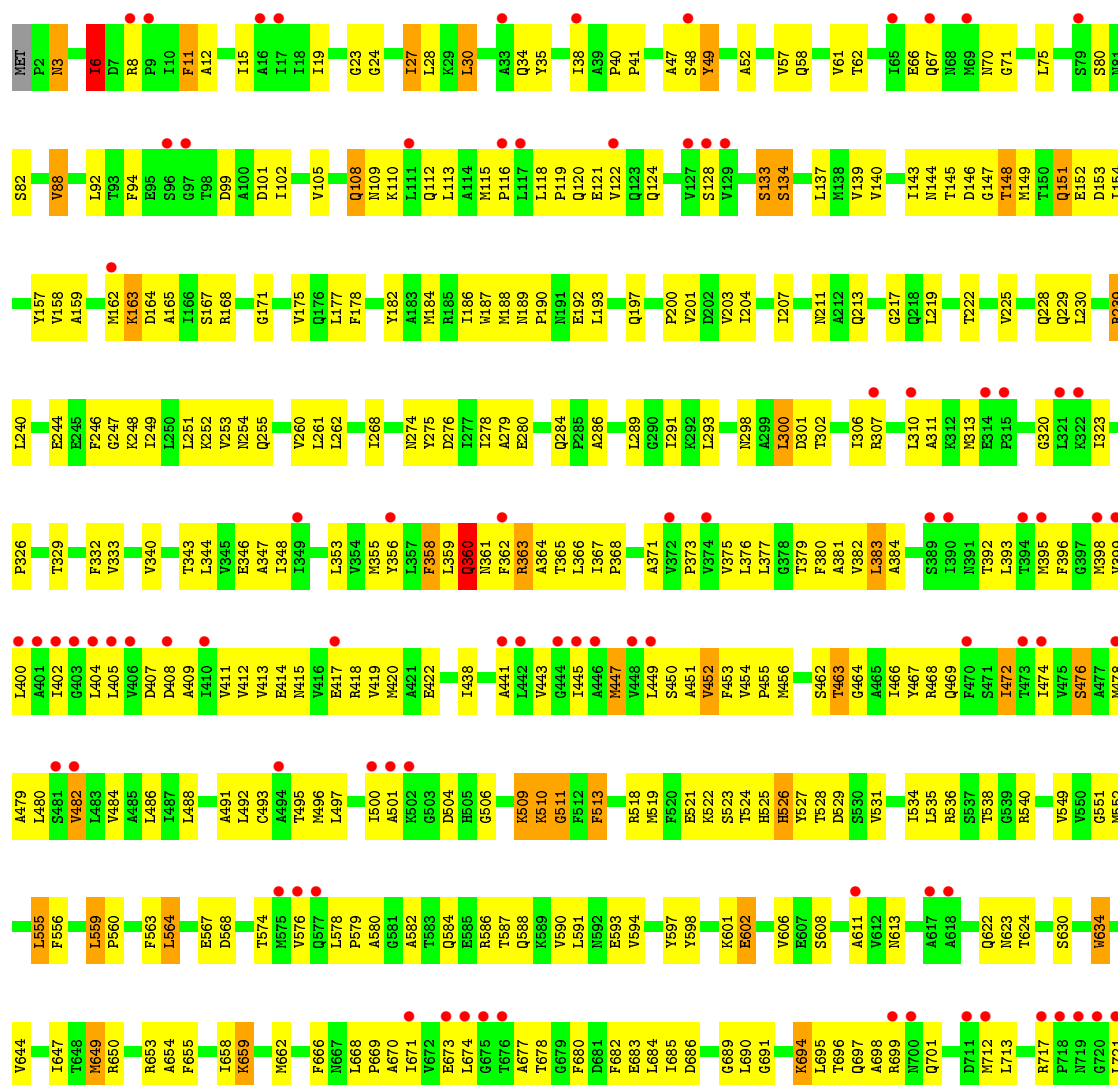


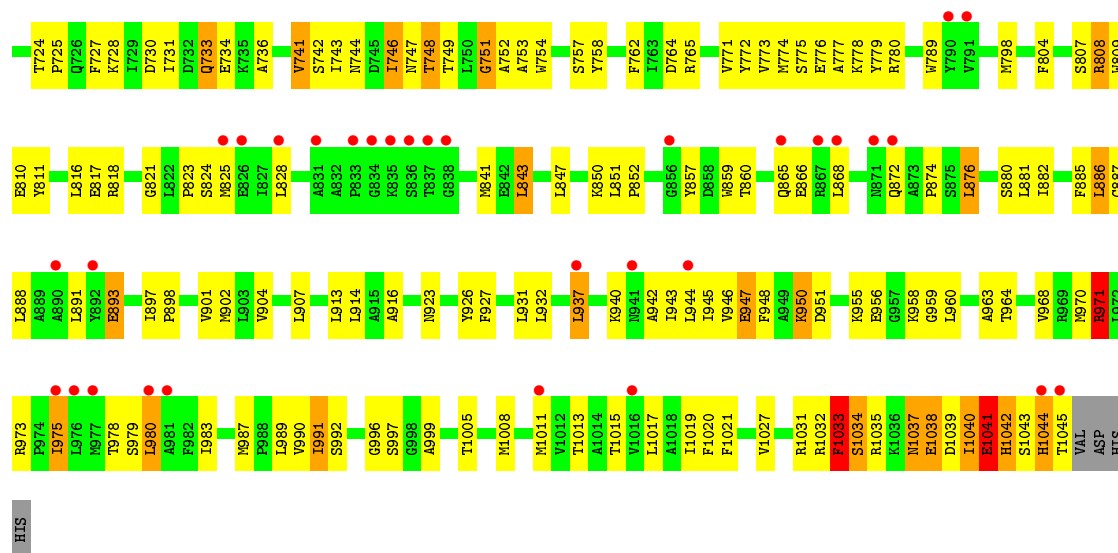


• Molecule 1: Multidrug efflux pump subunit AcrB

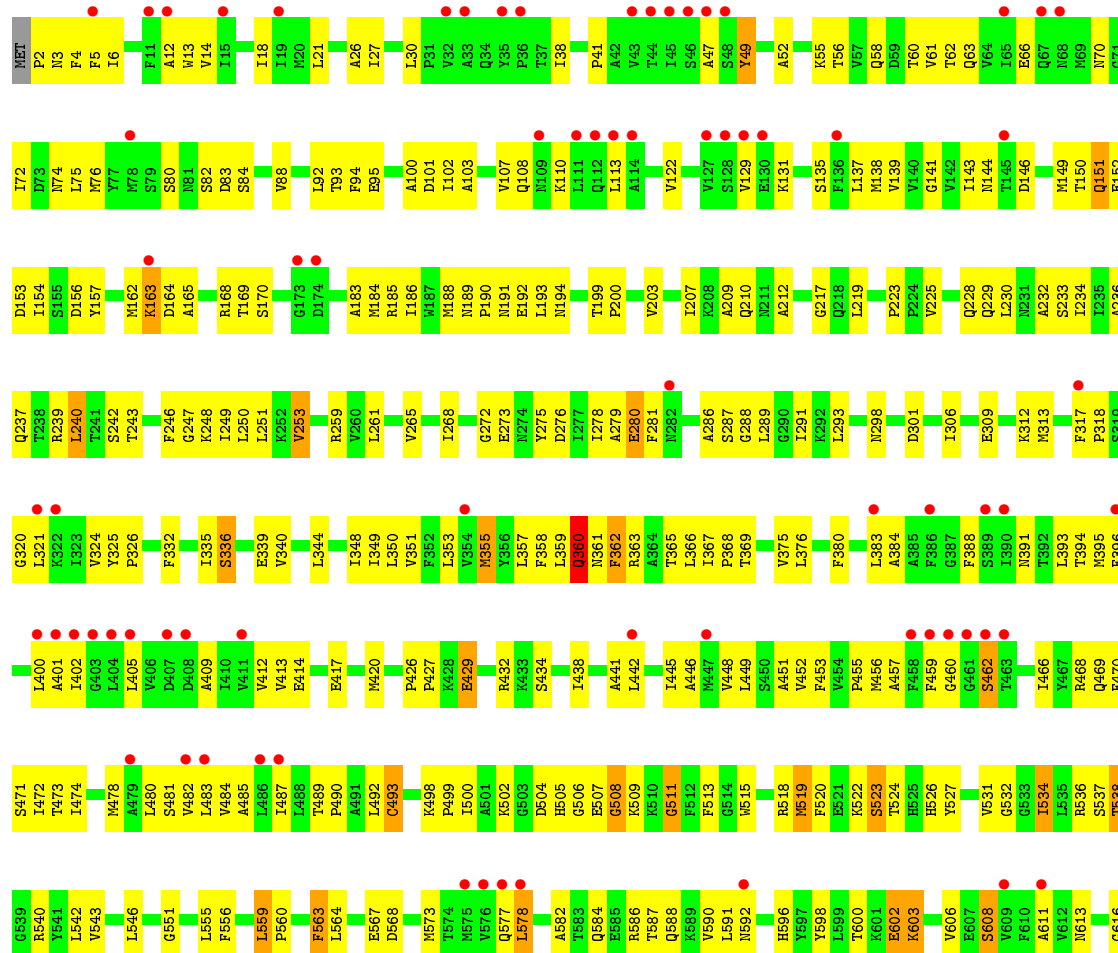






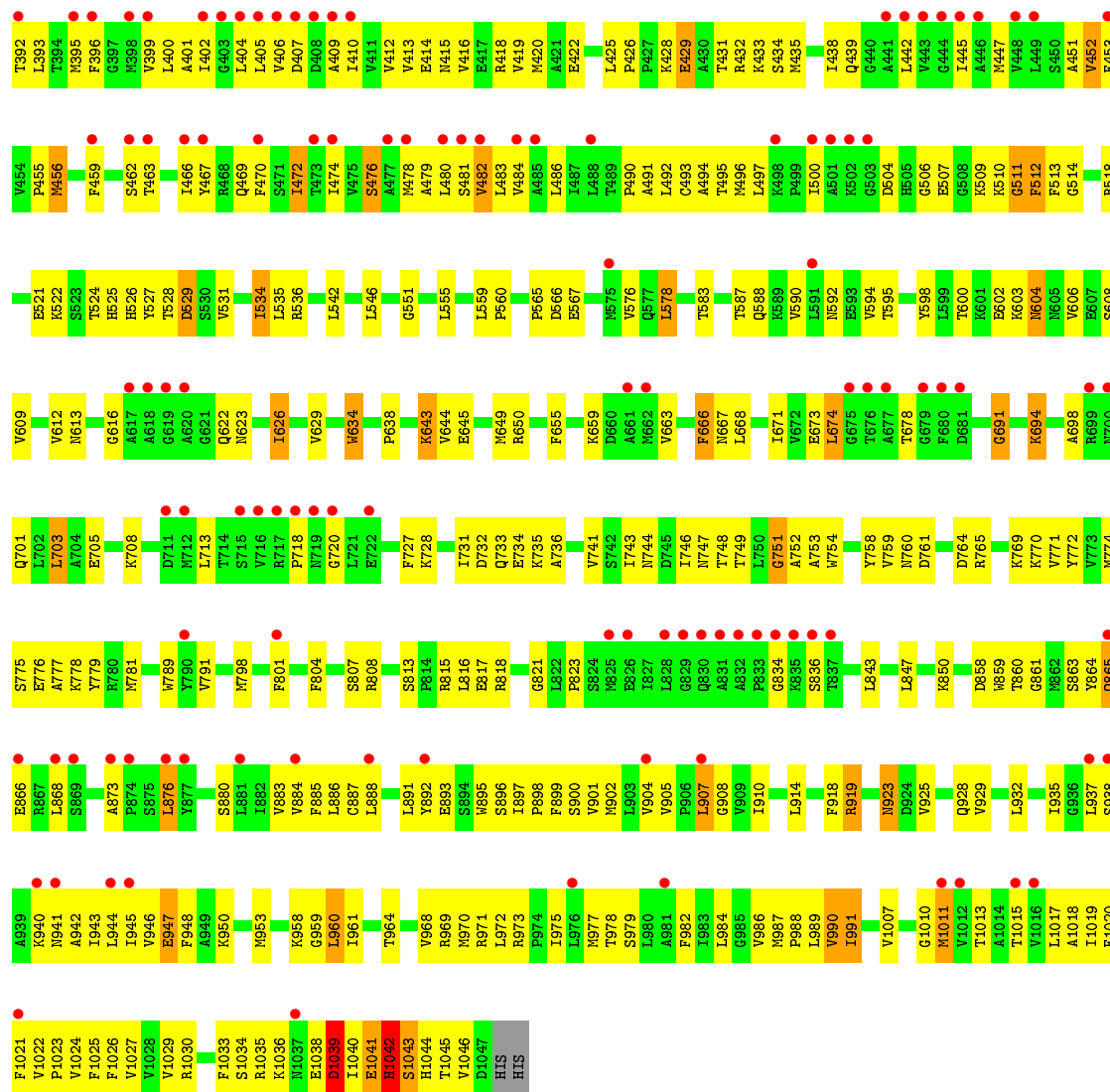


• Molecule 1: Multidrug efflux pump subunit AcrB









## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.78 (at 3.13Å)	Xtriage
Refinement program	PHENIX 1.8.2 _1309	Depositor
R, $R_{free}$	0.270 , 0.335 0.280 , 0.343	Depositor DCC
$R_{free}$ test set	8816 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	95.8	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 63.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.075 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 <sup>2</sup> )	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 50.20 % 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 6.6875e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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%)	8	37
1	B	1044/1049 (100%)	925 (89%)	92 (9%)	27 (3%)	5	28
1	C	1042/1049 (99%)	931 (89%)	91 (9%)	20 (2%)	8	36
1	D	1040/1049 (99%)	941 (90%)	83 (8%)	16 (2%)	10	41
1	E	1040/1049 (99%)	919 (88%)	97 (9%)	24 (2%)	6	31
1	F	1044/1049 (100%)	936 (90%)	87 (8%)	21 (2%)	7	34
All	All	6250/6294 (99%)	5591 (90%)	532 (8%)	127 (2%)	7	34

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%)	16	47
1	B	849/852 (100%)	735 (87%)	114 (13%)	4	17
1	C	847/852 (99%)	769 (91%)	78 (9%)	9	31
1	D	845/852 (99%)	786 (93%)	59 (7%)	15	45
1	E	845/852 (99%)	735 (87%)	110 (13%)	4	18
1	F	849/852 (100%)	783 (92%)	66 (8%)	12	40
All	All	5080/5112 (99%)	4597 (90%)	483 (10%)	8	30

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	F	1101	-	36,36,36	1.97	10 (27%)	47,47,47	1.43	7 (14%)
2	LMT	B	1101	-	36,36,36	1.81	9 (25%)	47,47,47	1.32	8 (17%)
2	LMT	C	1101	-	36,36,36	1.75	7 (19%)	47,47,47	1.59	9 (19%)
2	LMT	E	1101	-	36,36,36	1.85	11 (30%)	47,47,47	1.46	6 (12%)
2	LMT	A	1101	-	36,36,36	1.85	10 (27%)	47,47,47	1.24	5 (10%)
2	LMT	D	1101	-	36,36,36	1.77	10 (27%)	47,47,47	1.37	6 (12%)

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	F	1101	-	-	15/21/61/61	0/2/2/2
2	LMT	B	1101	-	1/1/10/10	12/21/61/61	0/2/2/2
2	LMT	C	1101	-	1/1/10/10	14/21/61/61	0/2/2/2
2	LMT	E	1101	-	-	10/21/61/61	0/2/2/2
2	LMT	A	1101	-	-	8/21/61/61	0/2/2/2
2	LMT	D	1101	-	-	16/21/61/61	0/2/2/2

The worst 5 of 57 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1101	LMT	O5'-C5'	4.73	1.55	1.44
2	F	1101	LMT	O1'-C1'	4.59	1.48	1.40
2	A	1101	LMT	O5'-C5'	4.41	1.55	1.44
2	E	1101	LMT	O5'-C5'	4.10	1.54	1.44
2	E	1101	LMT	O1'-C1'	4.05	1.47	1.40

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1101	LMT	C4B-C3B-C2B	4.91	119.39	110.82
2	E	1101	LMT	O5B-C5B-C4B	4.50	117.86	109.69
2	D	1101	LMT	O3B-C3B-C2B	-4.04	101.01	110.35
2	A	1101	LMT	C1B-O1B-C4'	-4.03	107.99	117.96
2	F	1101	LMT	O5B-C5B-C4B	4.02	116.99	109.69

All (2) chirality outliers are listed below:

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

5 of 75 torsion outliers are listed below:

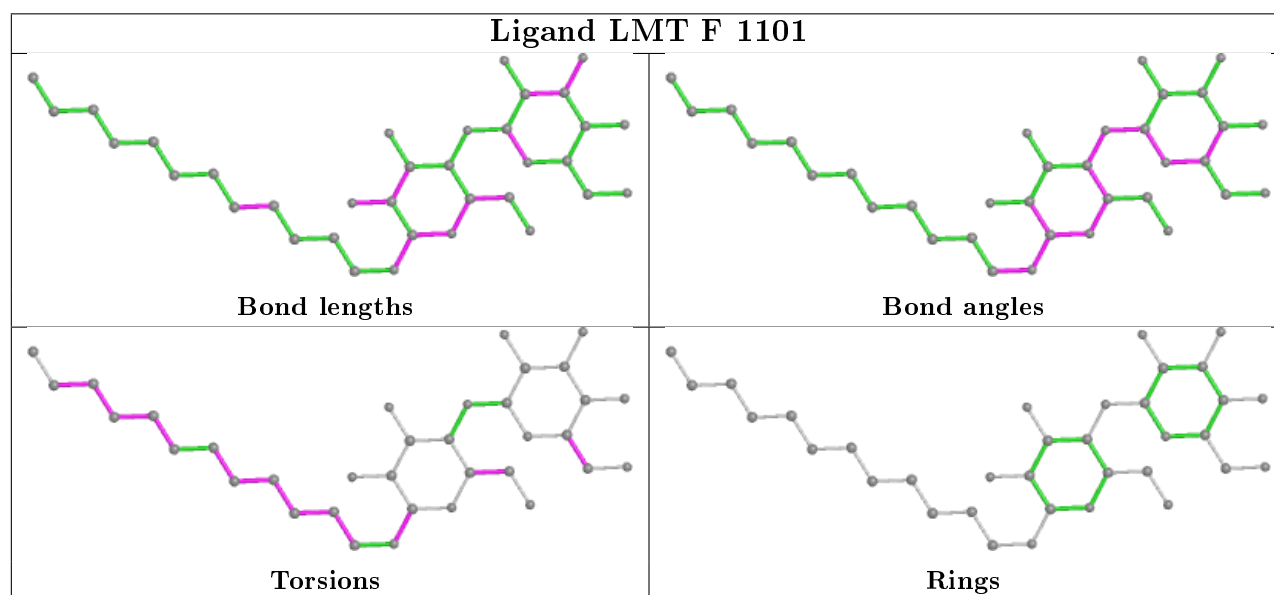
Mol	Chain	Res	Type	Atoms
2	B	1101	LMT	O5'-C1'-O1'-C1
2	C	1101	LMT	C2'-C1'-O1'-C1
2	C	1101	LMT	O5'-C1'-O1'-C1
2	E	1101	LMT	C2'-C1'-O1'-C1
2	B	1101	LMT	O5B-C5B-C6B-O6B

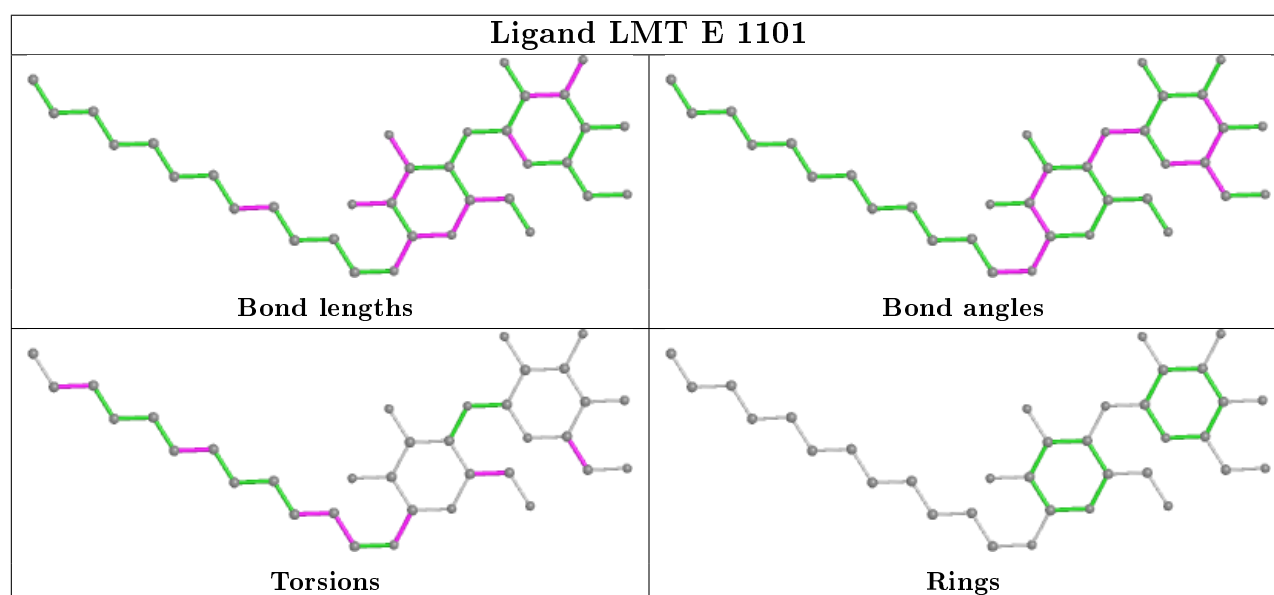
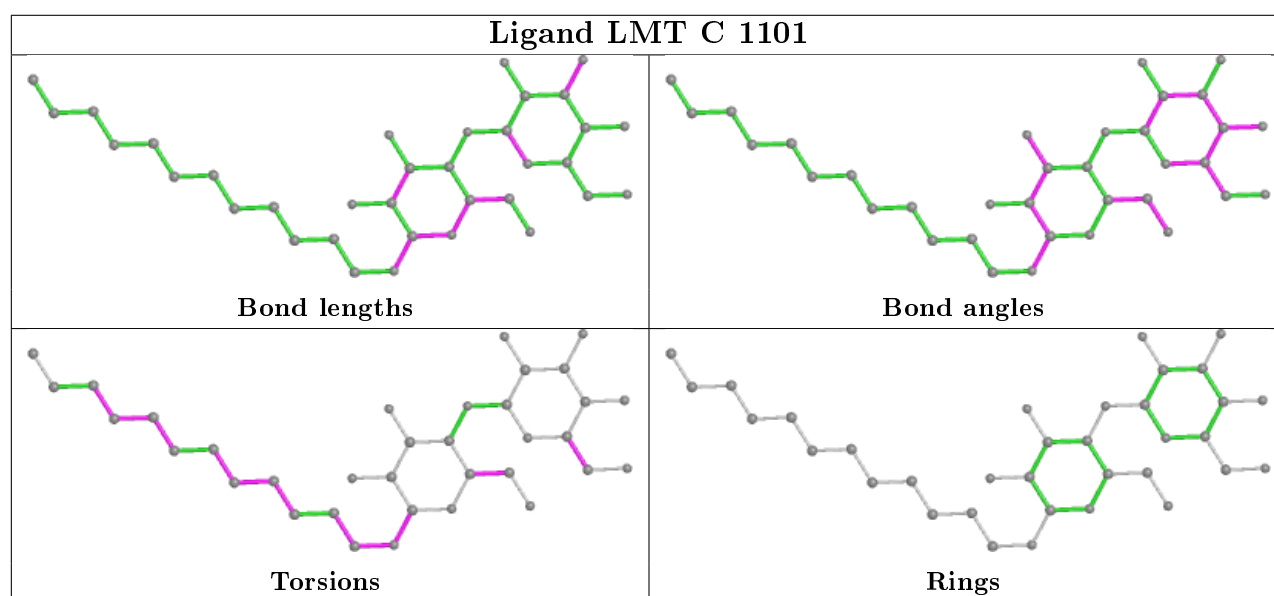
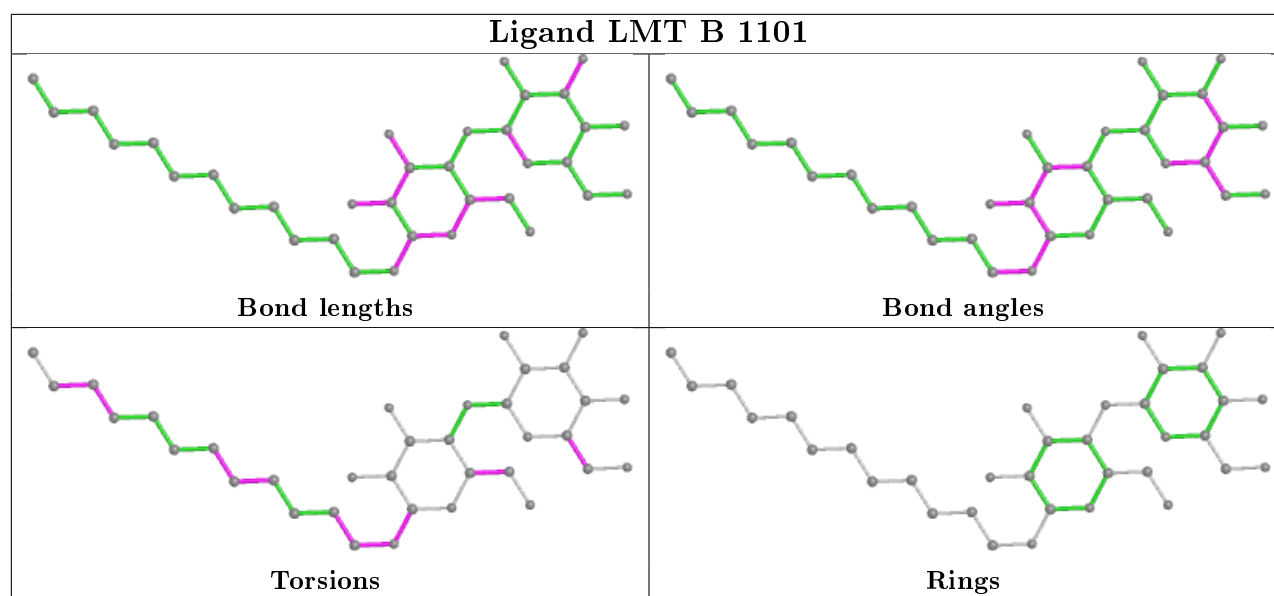
There are no ring outliers.

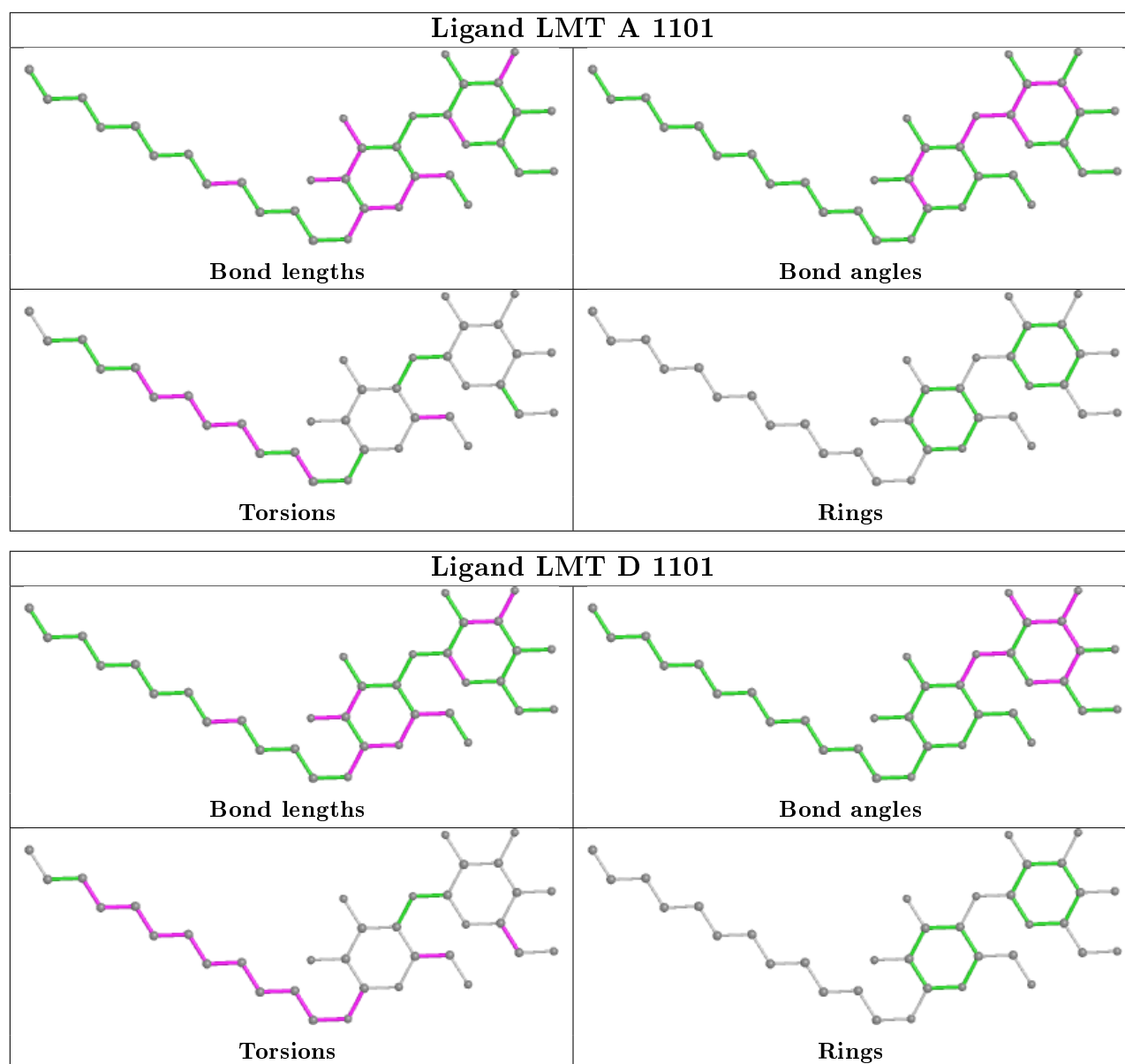
6 monomers are involved in 20 short contacts:

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







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1042/1049 (99%)	0.32	86 (8%) 11 6	28, 63, 113, 139	0
1	B	1046/1049 (99%)	0.18	70 (6%) 17 9	26, 57, 100, 161	0
1	C	1044/1049 (99%)	0.46	117 (11%) 5 3	17, 56, 98, 173	0
1	D	1042/1049 (99%)	0.45	115 (11%) 5 3	21, 81, 133, 168	0
1	E	1042/1049 (99%)	0.53	131 (12%) 3 2	38, 77, 119, 154	0
1	F	1046/1049 (99%)	0.62	155 (14%) 2 1	29, 73, 120, 143	0
All	All	6262/6294 (99%)	0.43	674 (10%) 5 3	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	12.3
1	E	128	SER	12.1

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

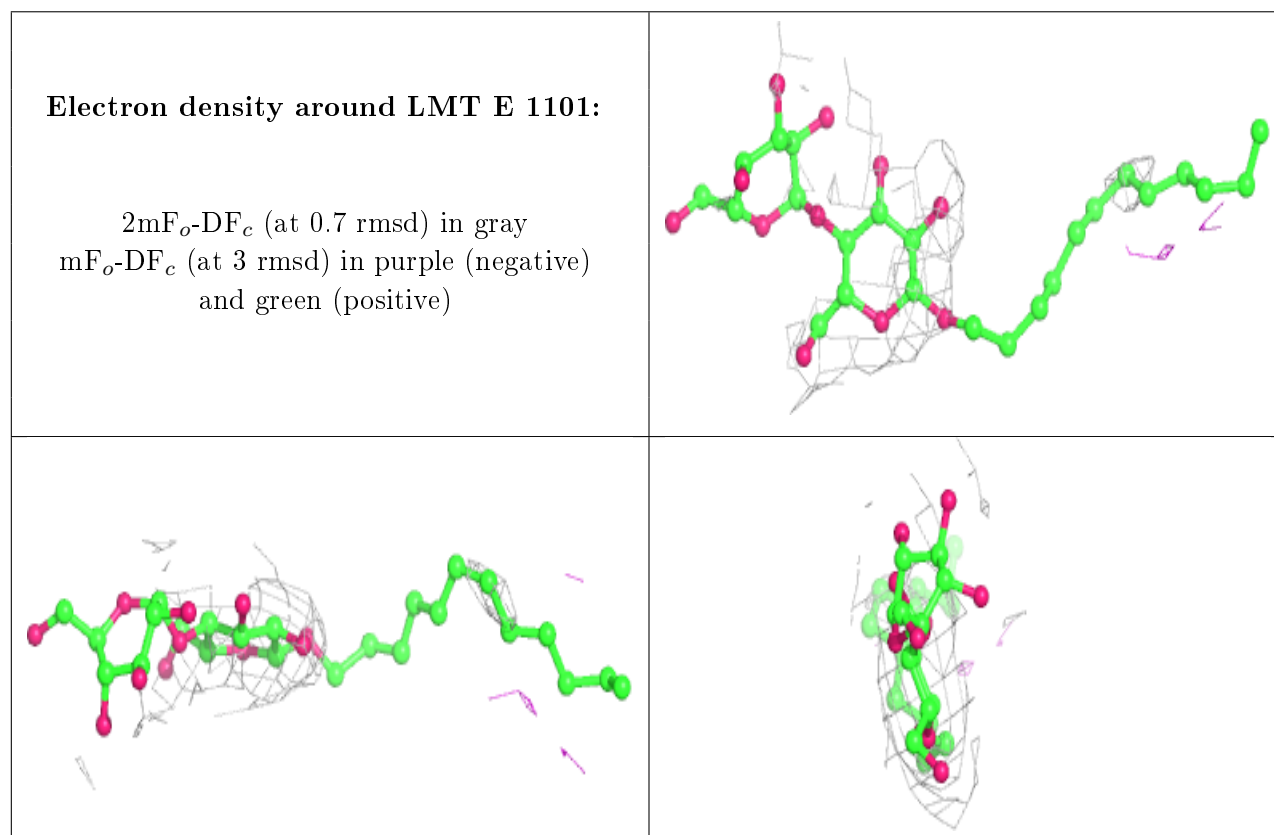


## 6.4 Ligands ⓘ

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<sup>th</sup> 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.

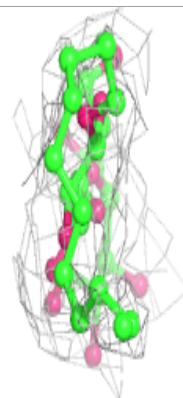
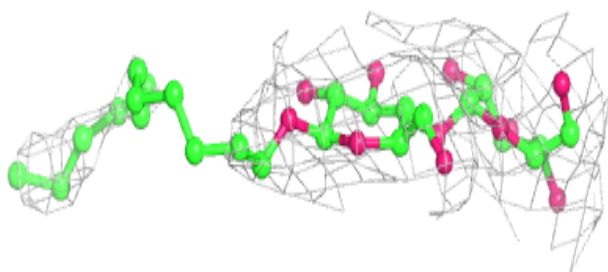
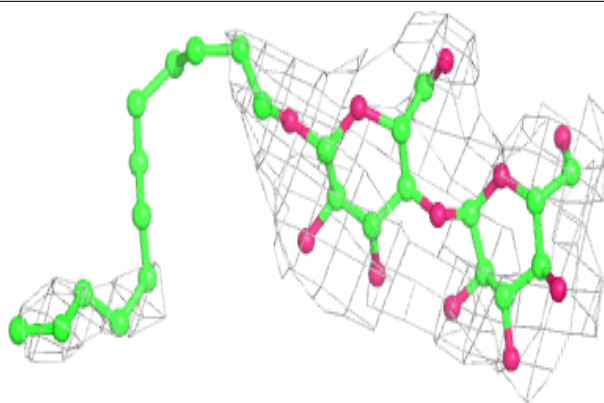
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	LMT	E	1101	35/35	0.73	0.40	43,83,98,109	0
2	LMT	F	1101	35/35	0.81	0.37	19,65,82,87	0
2	LMT	B	1101	35/35	0.82	0.37	40,61,68,70	0
2	LMT	C	1101	35/35	0.84	0.33	29,44,62,65	0
2	LMT	D	1101	35/35	0.86	0.31	35,48,67,83	0
2	LMT	A	1101	35/35	0.88	0.32	40,56,74,75	0
3	NI	A	1102	1/1	0.97	0.08	31,31,31,31	0
3	NI	C	1102	1/1	0.99	0.12	33,33,33,33	0
3	NI	E	1102	1/1	0.99	0.08	64,64,64,64	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.

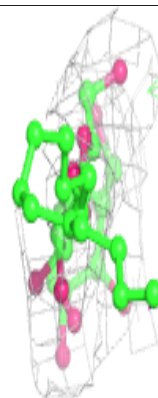
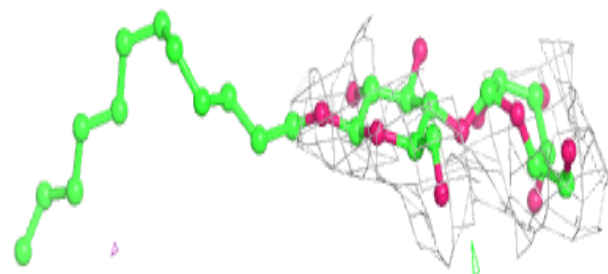
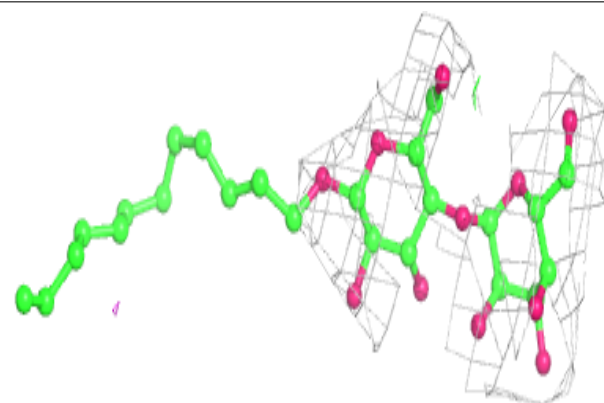


**Electron density around LMT F 1101:**

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

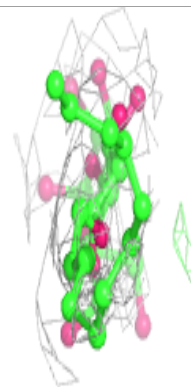
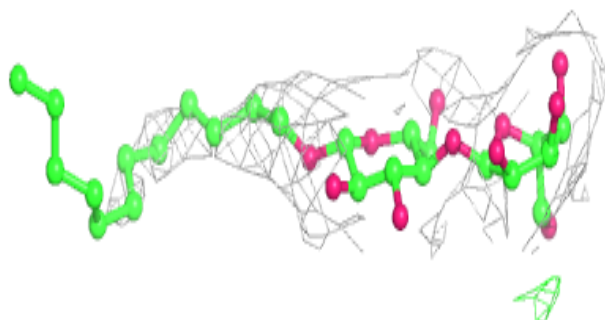
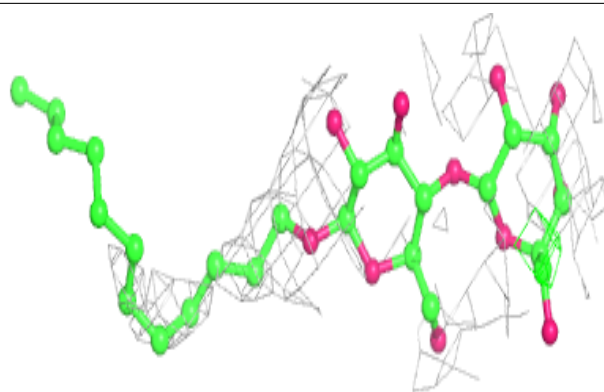
**Electron density around LMT B 1101:**

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

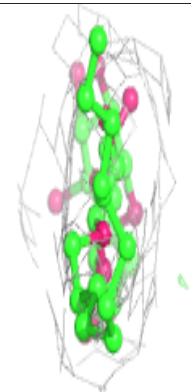
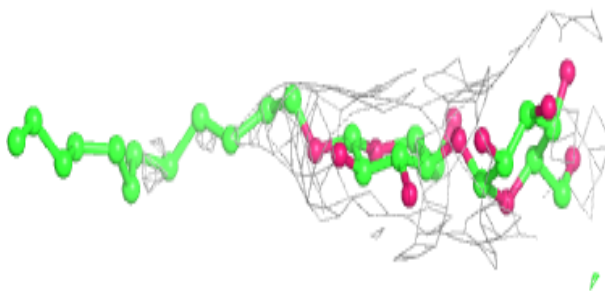
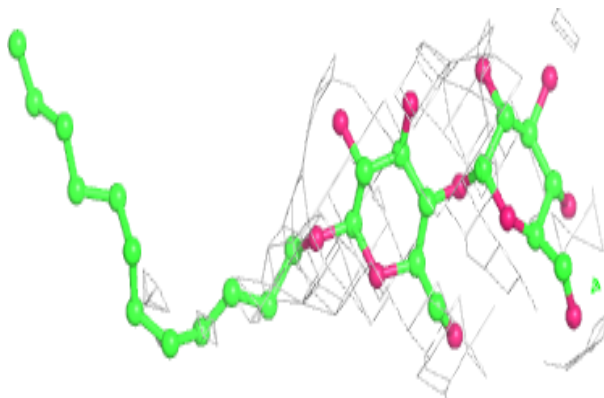


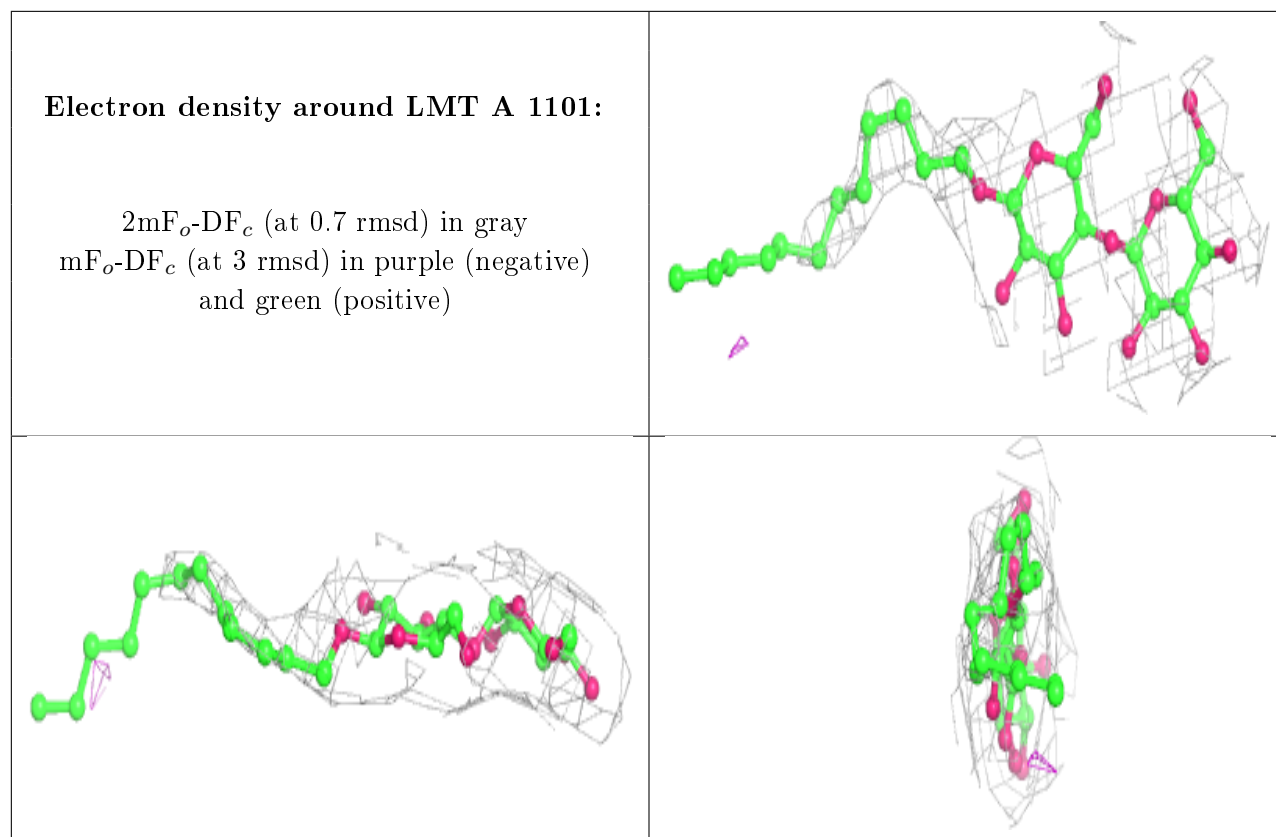
**Electron density around LMT C 1101:**

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

**Electron density around LMT 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.