



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 05:30 pm BST

PDB ID : 4ZIW  
Title : Crystal structure of AcrB deletion mutant in P21 space group  
Authors : Ababou, A.; Koronakis, V.  
Deposited on : 2015-04-28  
Resolution : 3.40 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

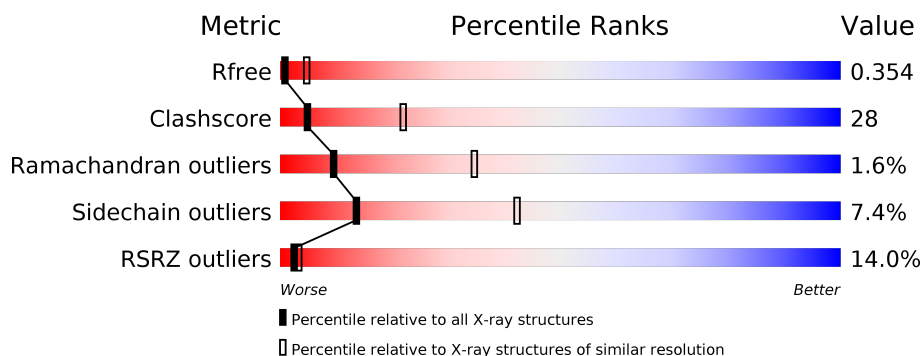
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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	1044	<div> <div>12%</div> <div>47%</div> <div>47%</div> <div>5%</div> </div>
1	B	1044	<div> <div>10%</div> <div>50%</div> <div>45%</div> <div>5%</div> </div>
1	C	1044	<div> <div>12%</div> <div>47%</div> <div>47%</div> <div>5%</div> </div>
1	D	1044	<div> <div>16%</div> <div>44%</div> <div>50%</div> <div>5%</div> </div>
1	E	1044	<div> <div>17%</div> <div>47%</div> <div>47%</div> <div>5%</div> </div>
1	F	1044	<div> <div>17%</div> <div>46%</div> <div>48%</div> <div>5%</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	2000	-	-	-	X
2	LMT	D	2000	X	-	-	-
2	LMT	E	1101	X	-	-	X

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 47532 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	1039	Total	C	N	O	S	0	0	0
			7900	5076	1307	1474	43			
1	C	1035	Total	C	N	O	S	0	0	0
			7867	5057	1299	1468	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:

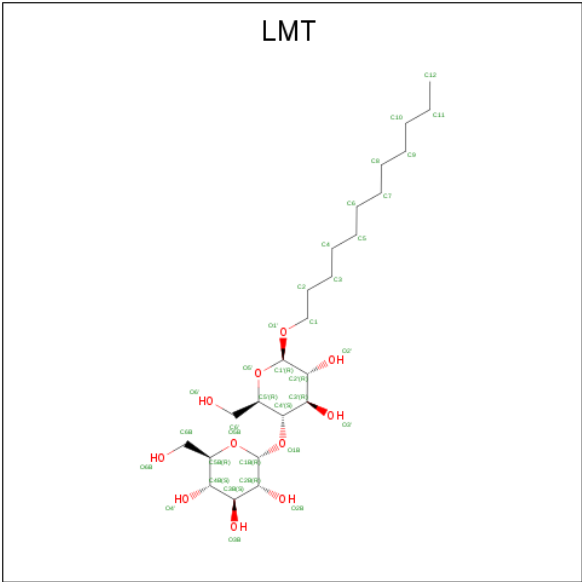
Chain	Residue	Modelled	Actual	Comment	Reference
A	615	GLY	PHE	engineered mutation	UNP P31224
A	?	-	GLY	deletion	UNP P31224
A	?	-	PHE	deletion	UNP P31224
A	?	-	ALA	deletion	UNP P31224
A	?	-	GLY	deletion	UNP P31224
A	?	-	ARG	deletion	UNP P31224
B	615	GLY	PHE	engineered mutation	UNP P31224
B	?	-	GLY	deletion	UNP P31224
B	?	-	PHE	deletion	UNP P31224
B	?	-	ALA	deletion	UNP P31224
B	?	-	GLY	deletion	UNP P31224
B	?	-	ARG	deletion	UNP P31224
C	615	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	615	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	615	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	615	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 DODECYL-BETA-D-MALTOSE (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		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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		

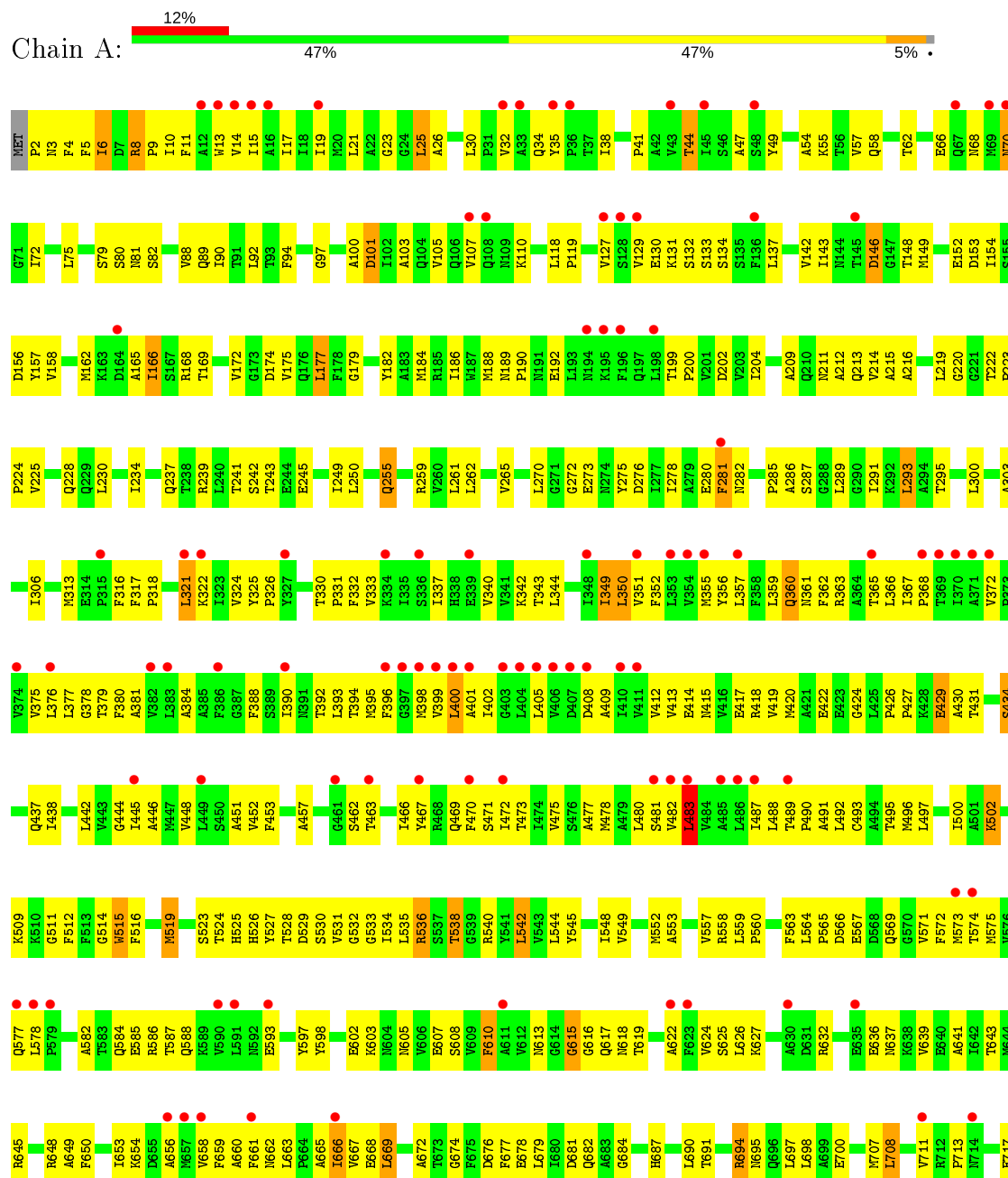
- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

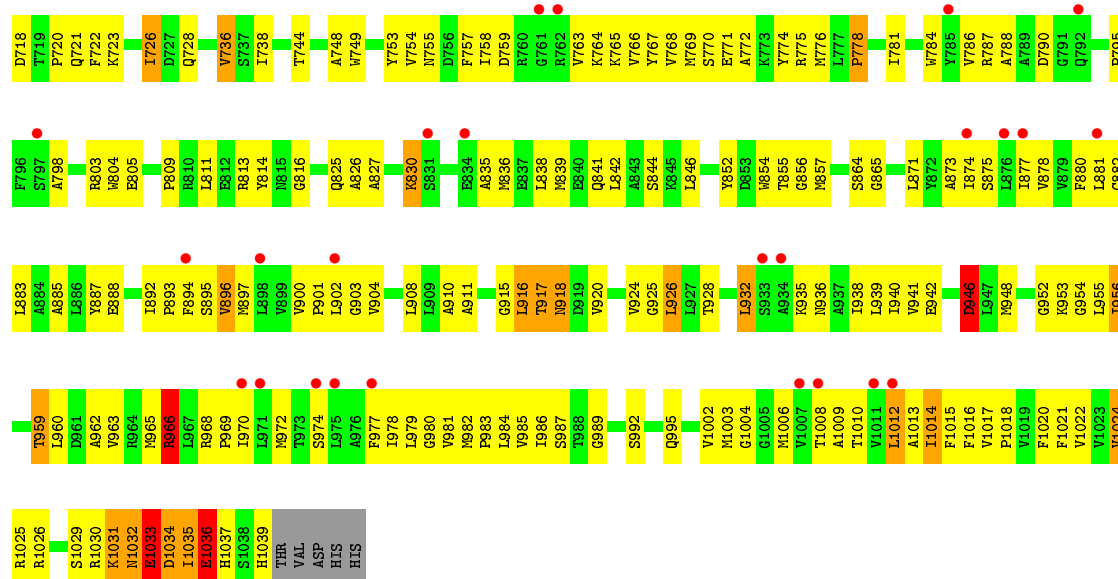
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ni	0	0
			1	1		
3	C	1	Total	Ni	0	0
			1	1		
3	E	1	Total	Ni	0	0
			1	1		

### 3 Residue-property plots

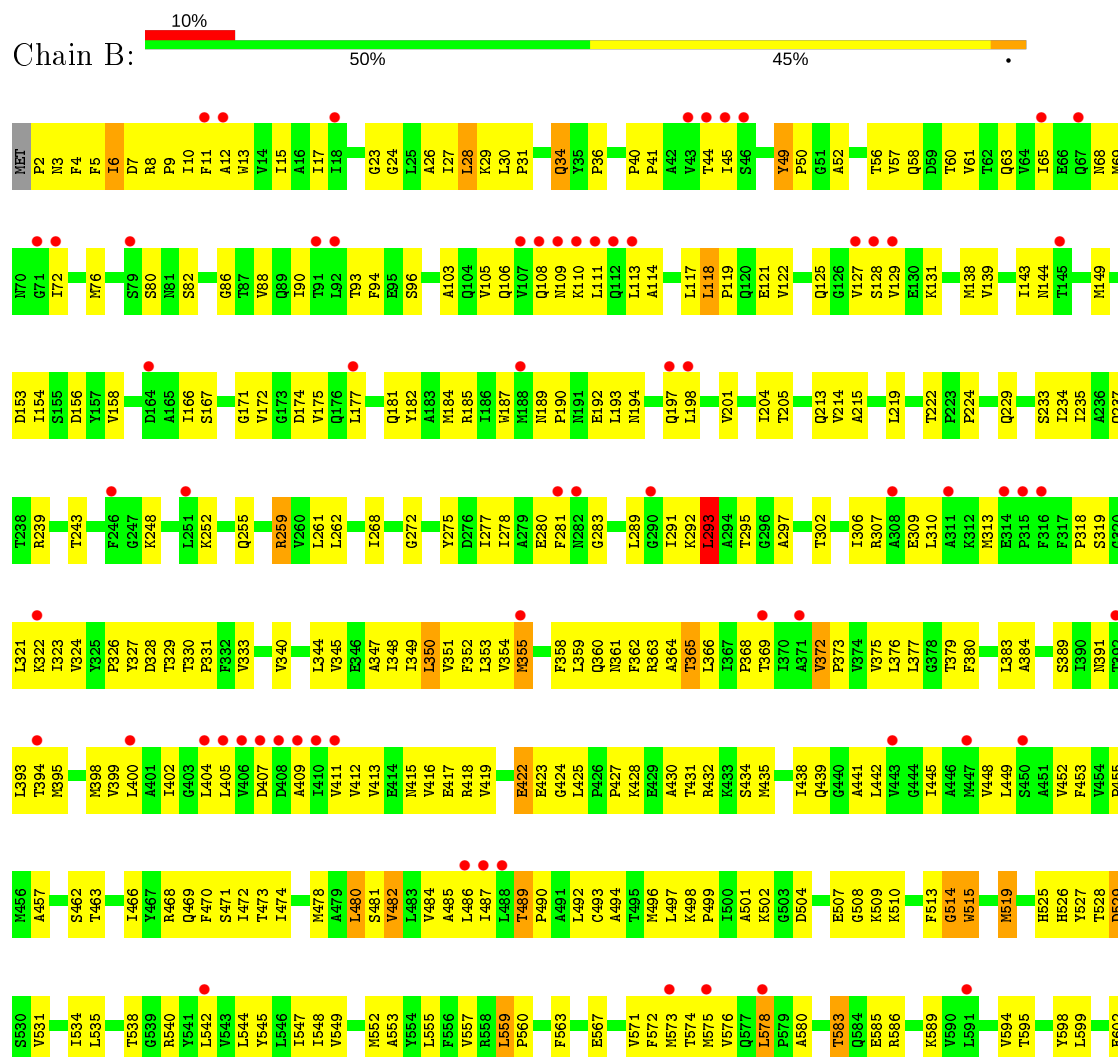
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

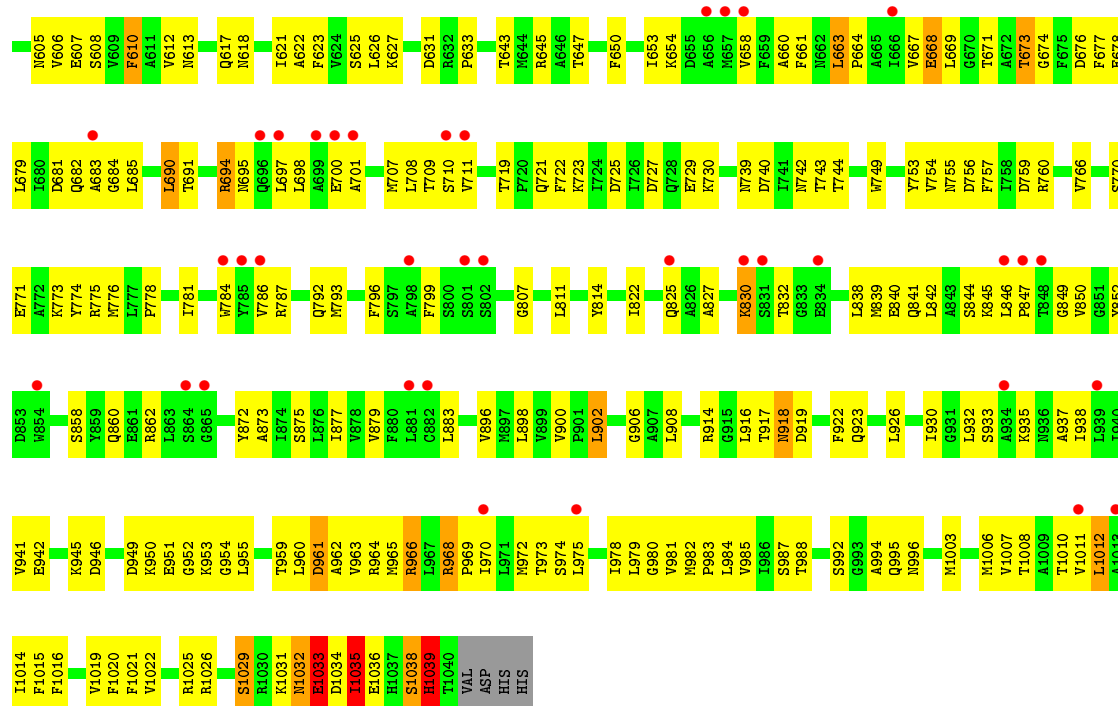




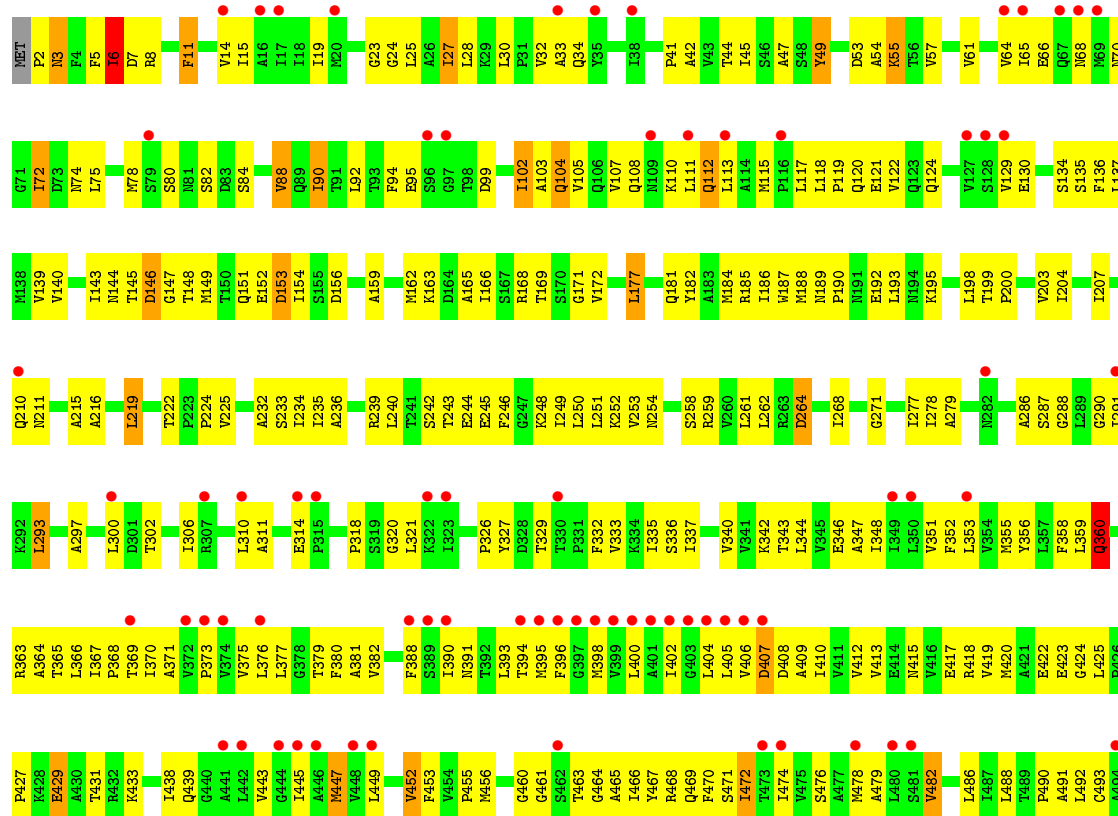
### • Molecule 1: Multidrug efflux pump subunit AcrB

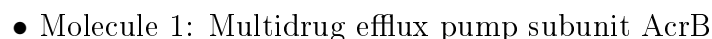


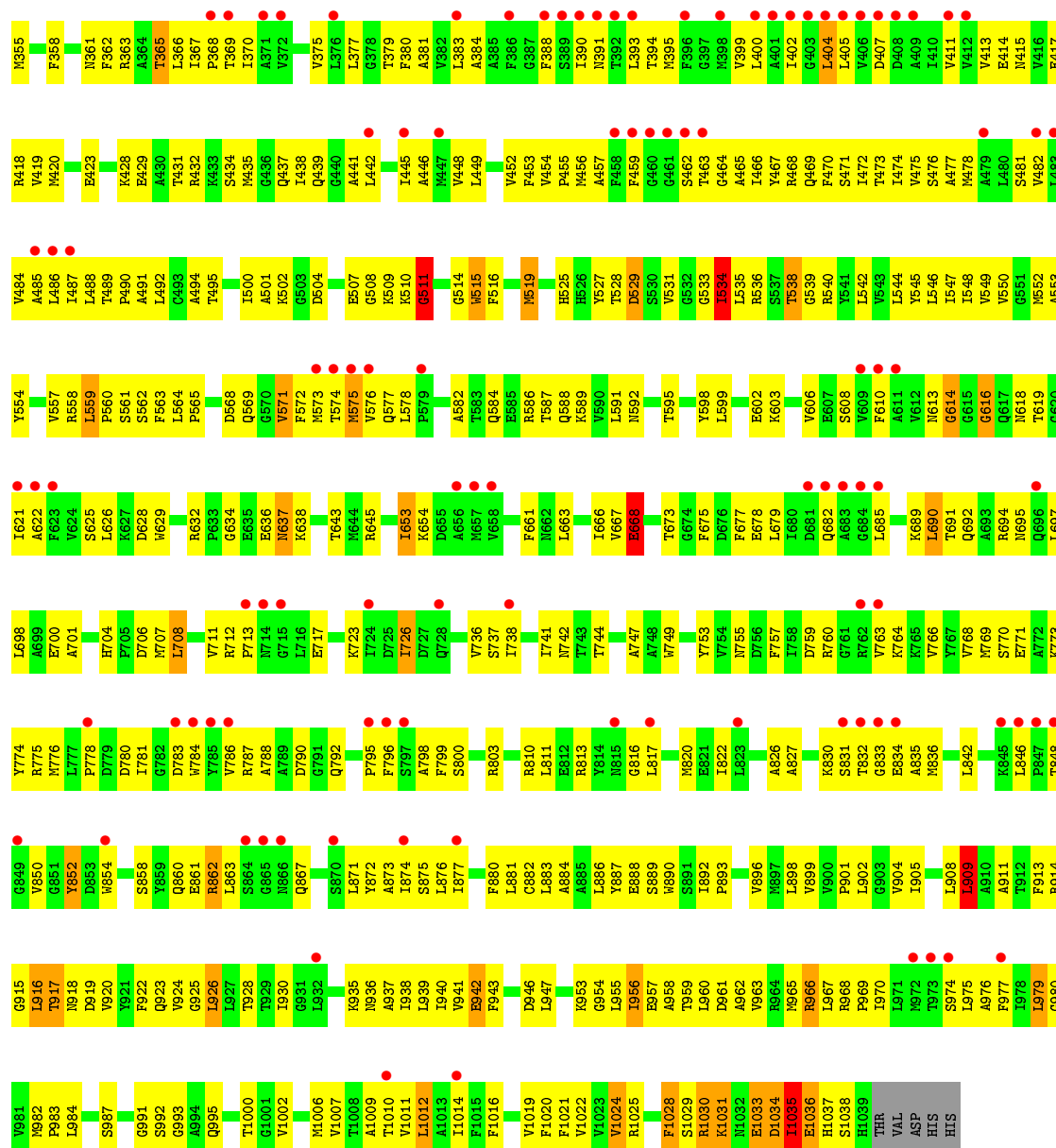




• Molecule 1: Multidrug efflux pump subunit AcrB



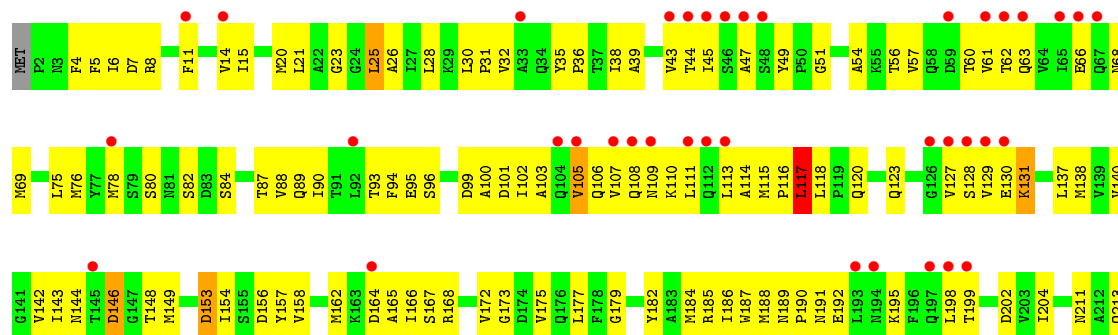




### • Molecule 1: Multidrug efflux pump subunit AcrB



Chain E:







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	152.07Å 157.78Å 219.39Å 90.00° 93.14° 90.00°	Depositor
Resolution (Å)	20.00 – 3.40 109.53 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-3.40) 97.9 (109.53-3.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.93 (at 3.41Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, $R_{free}$	0.275 , 0.349 0.285 , 0.354	Depositor DCC
$R_{free}$ test set	7110 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	98.9	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 74.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.80	EDS
Total number of atoms	47532	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	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 47.48 % 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 9.8623e-05.*

<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	0.65	1/8043 (0.0%)	0.89	11/10922 (0.1%)
1	B	0.65	1/8050 (0.0%)	0.89	9/10932 (0.1%)
1	C	0.67	1/8015 (0.0%)	0.91	9/10884 (0.1%)
1	D	0.60	1/8043 (0.0%)	0.89	15/10922 (0.1%)
1	E	0.60	1/8032 (0.0%)	0.87	12/10907 (0.1%)
1	F	0.60	0/8032	0.89	7/10907 (0.1%)
All	All	0.63	5/48215 (0.0%)	0.89	63/65474 (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	3
1	B	0	2
1	C	0	1
1	D	0	1
1	F	0	1
All	All	0	8

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	515	TRP	CB-CG	7.50	1.63	1.50
1	A	515	TRP	CB-CG	6.68	1.62	1.50
1	E	515	TRP	CB-CG	5.77	1.60	1.50
1	B	515	TRP	CB-CG	5.72	1.60	1.50
1	C	515	TRP	CB-CG	5.07	1.59	1.50

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	939	LEU	CA-CB-CG	-8.38	96.02	115.30
1	C	529	ASP	CB-CG-OD1	8.07	125.56	118.30
1	F	529	ASP	CB-CG-OD1	7.98	125.48	118.30
1	A	529	ASP	CB-CG-OD1	7.69	125.22	118.30
1	D	350	LEU	CA-CB-CG	-7.26	98.61	115.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1033	GLU	Peptide
1	A	1034	ASP	Peptide
1	A	1036	GLU	Peptide
1	B	1033	GLU	Peptide
1	B	1035	ILE	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	7893	0	8034	457	0
1	B	7900	0	8041	384	0
1	C	7867	0	8015	444	0
1	D	7893	0	8034	515	0
1	E	7883	0	8027	461	0
1	F	7883	0	8027	477	0
2	A	35	0	46	4	0
2	B	35	0	46	3	0
2	C	35	0	46	1	0
2	D	35	0	46	3	0
2	E	35	0	46	8	0
2	F	35	0	46	1	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
All	All	47532	0	48454	2651	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 2651 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:E:536:ARG:NE	2:E:1101:LMT:O3B	1.81	1.13
1:A:424:GLY:HA3	1:A:502:LYS:HG2	1.38	1.04
1:D:954:GLY:HA2	1:D:1034:ASP:H	1.23	1.03
1:C:686:GLY:HA3	1:C:689:LYS:HD3	1.42	1.01
1:D:533:GLY:HA2	1:D:536:ARG:HD3	1.48	0.95

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%)	942 (91%)	79 (8%)	15 (1%)	11	37
1	B	1037/1044 (99%)	942 (91%)	85 (8%)	10 (1%)	15	46
1	C	1033/1044 (99%)	931 (90%)	84 (8%)	18 (2%)	9	34
1	D	1036/1044 (99%)	934 (90%)	83 (8%)	19 (2%)	8	32
1	E	1035/1044 (99%)	937 (90%)	87 (8%)	11 (1%)	14	44
1	F	1035/1044 (99%)	926 (90%)	84 (8%)	25 (2%)	6	28
All	All	6212/6264 (99%)	5612 (90%)	502 (8%)	98 (2%)	9	34

5 of 98 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	672	ALA
1	A	986	ILE
1	A	1029	SER
1	A	1033	GLU
1	B	617	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	846/852 (99%)	781 (92%)	65 (8%)	13	40
1	B	847/852 (99%)	789 (93%)	58 (7%)	16	45
1	C	843/852 (99%)	774 (92%)	69 (8%)	11	37
1	D	846/852 (99%)	789 (93%)	57 (7%)	16	46
1	E	845/852 (99%)	775 (92%)	70 (8%)	11	36
1	F	845/852 (99%)	789 (93%)	56 (7%)	16	46
All	All	5072/5112 (99%)	4697 (93%)	375 (7%)	13	42

5 of 375 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	689	LYS
1	D	358	PHE
1	F	538	THR
1	C	842	LEU
1	C	1035	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	742	ASN
1	E	231	ASN
1	F	704	HIS
1	E	34	GLN
1	E	67	GLN

### 5.3.3 RNA ⓘ

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	D	2000	-	36,36,36	1.87	9 (25%)	47,47,47	1.70	8 (17%)
2	LMT	F	2000	-	36,36,36	1.85	8 (22%)	47,47,47	1.14	4 (8%)
2	LMT	B	2000	-	36,36,36	1.81	12 (33%)	47,47,47	1.50	8 (17%)
2	LMT	A	1101	-	36,36,36	1.80	11 (30%)	47,47,47	1.37	6 (12%)
2	LMT	C	1101	-	36,36,36	1.85	10 (27%)	47,47,47	1.40	6 (12%)
2	LMT	E	1101	-	36,36,36	1.83	10 (27%)	47,47,47	1.92	9 (19%)

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	D	2000	-	1/1/10/10	12/21/61/61	0/2/2/2
2	LMT	F	2000	-	-	15/21/61/61	0/2/2/2
2	LMT	B	2000	-	-	13/21/61/61	0/2/2/2
2	LMT	A	1101	-	-	8/21/61/61	0/2/2/2
2	LMT	C	1101	-	-	12/21/61/61	0/2/2/2
2	LMT	E	1101	-	1/1/10/10	12/21/61/61	0/2/2/2

The worst 5 of 60 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1101	LMT	O1'-C1'	4.20	1.47	1.40
2	C	1101	LMT	O5'-C5'	4.10	1.54	1.44
2	F	2000	LMT	O5'-C1'	4.07	1.52	1.41
2	F	2000	LMT	O5'-C5'	3.97	1.54	1.44
2	B	2000	LMT	O5'-C5'	3.97	1.54	1.44

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1101	LMT	O1B-C4'-C5'	-5.21	95.18	109.45
2	D	2000	LMT	O1'-C1'-C2'	5.11	116.28	108.30
2	C	1101	LMT	O1'-C1'-C2'	4.87	115.91	108.30
2	E	1101	LMT	C4B-C3B-C2B	4.82	119.23	110.82
2	E	1101	LMT	C3B-C4B-C5B	4.70	118.63	110.24

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	2000	LMT	C3B
2	E	1101	LMT	C2B

5 of 72 torsion outliers are listed below:

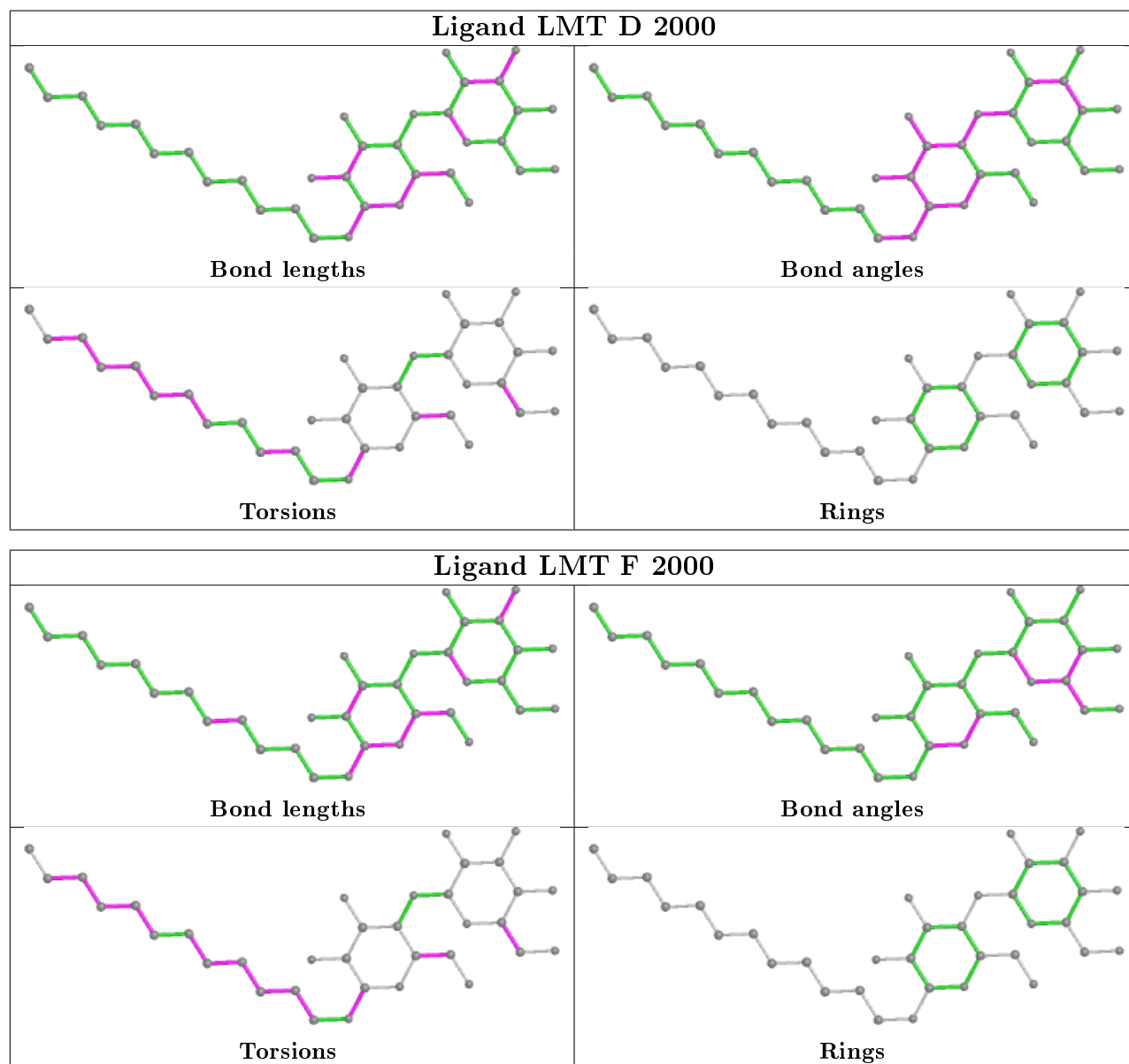
Mol	Chain	Res	Type	Atoms
2	F	2000	LMT	C2'-C1'-O1'-C1
2	C	1101	LMT	C2'-C1'-O1'-C1
2	C	1101	LMT	O5'-C1'-O1'-C1
2	E	1101	LMT	C2-C1-O1'-C1'
2	E	1101	LMT	C4B-C5B-C6B-O6B

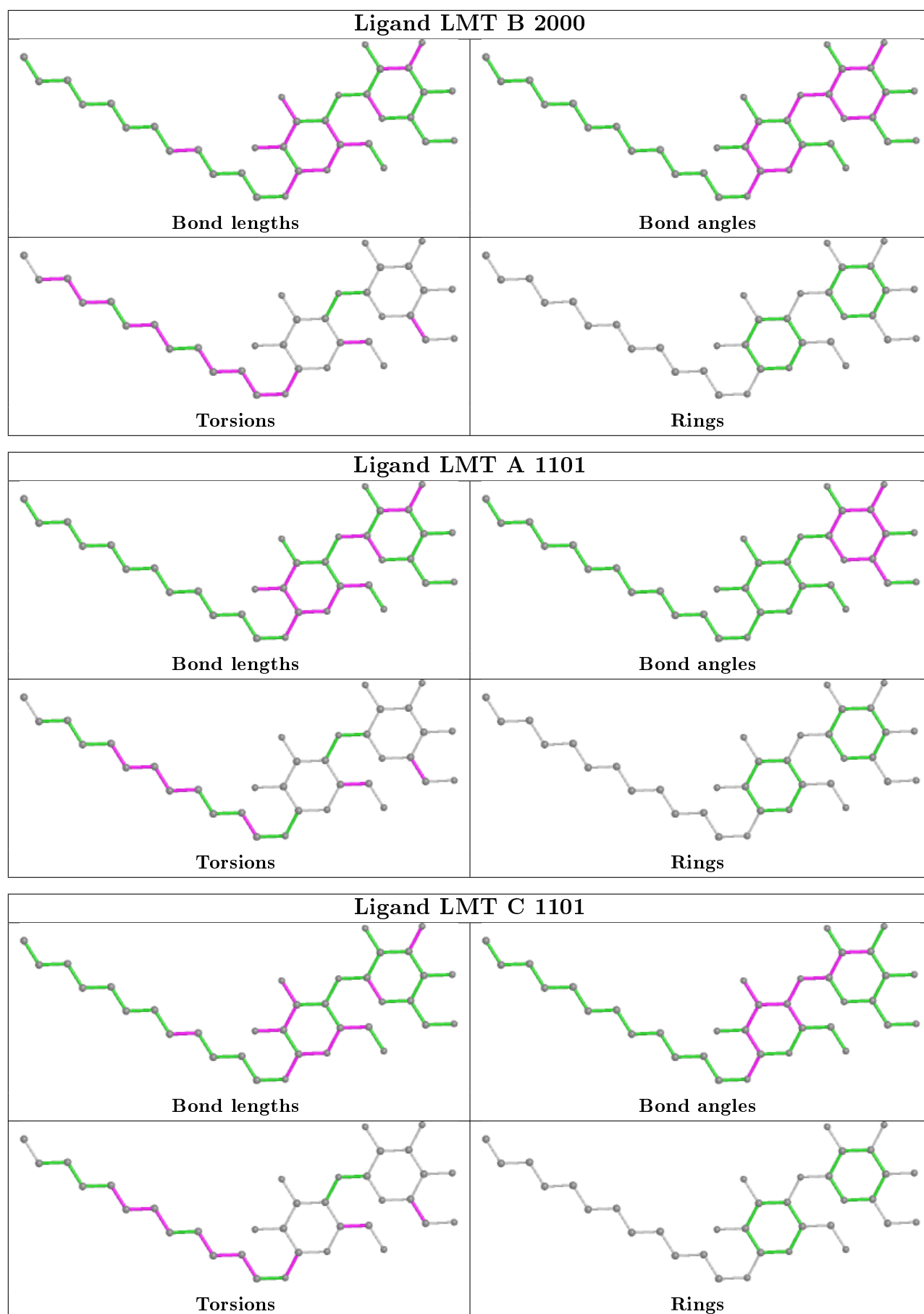
There are no ring outliers.

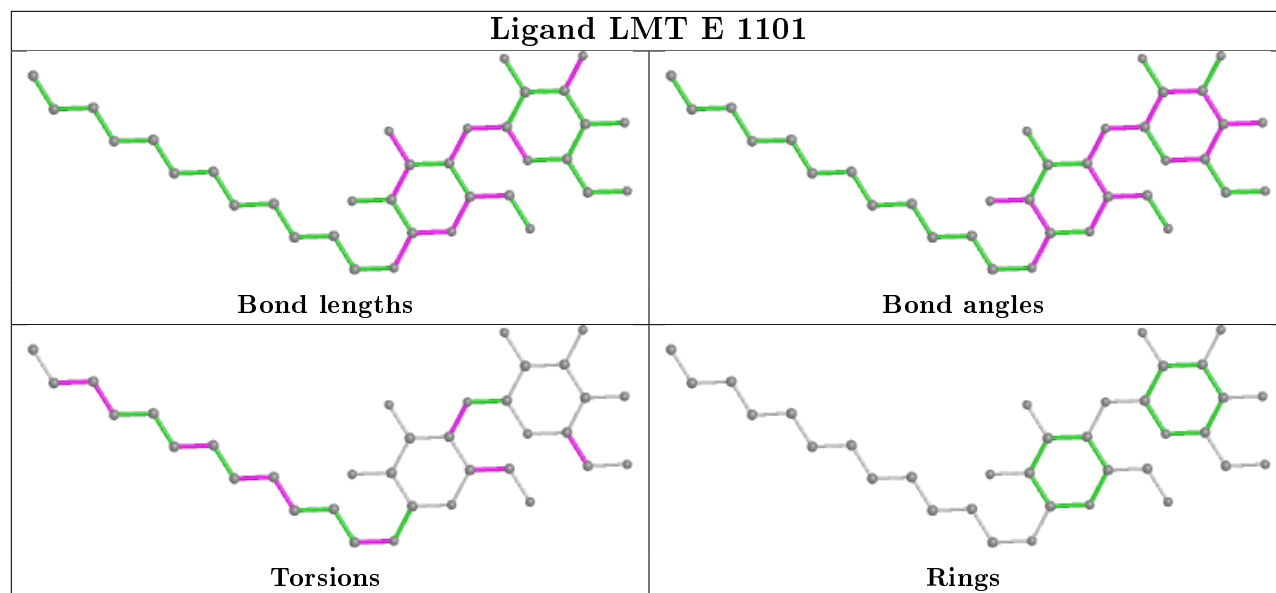
6 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2000	LMT	3	0
2	F	2000	LMT	1	0
2	B	2000	LMT	3	0
2	A	1101	LMT	4	0
2	C	1101	LMT	1	0
2	E	1101	LMT	8	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	1038/1044 (99%)	0.42	127 (12%) 4 5	27, 75, 109, 132	0
1	B	1039/1044 (99%)	0.37	102 (9%) 7 9	18, 68, 104, 130	0
1	C	1035/1044 (99%)	0.49	125 (12%) 4 5	17, 69, 104, 126	0
1	D	1038/1044 (99%)	0.59	162 (15%) 2 2	16, 90, 130, 173	0
1	E	1037/1044 (99%)	0.69	180 (17%) 1 1	40, 91, 115, 134	0
1	F	1037/1044 (99%)	0.73	177 (17%) 1 2	24, 84, 118, 142	0
All	All	6224/6264 (99%)	0.55	873 (14%) 2 3	16, 80, 115, 173	0

The worst 5 of 873 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	128	SER	16.7
1	E	314	GLU	14.0
1	E	315	PRO	12.2
1	F	714	ASN	11.8
1	F	442	LEU	11.2

### 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.

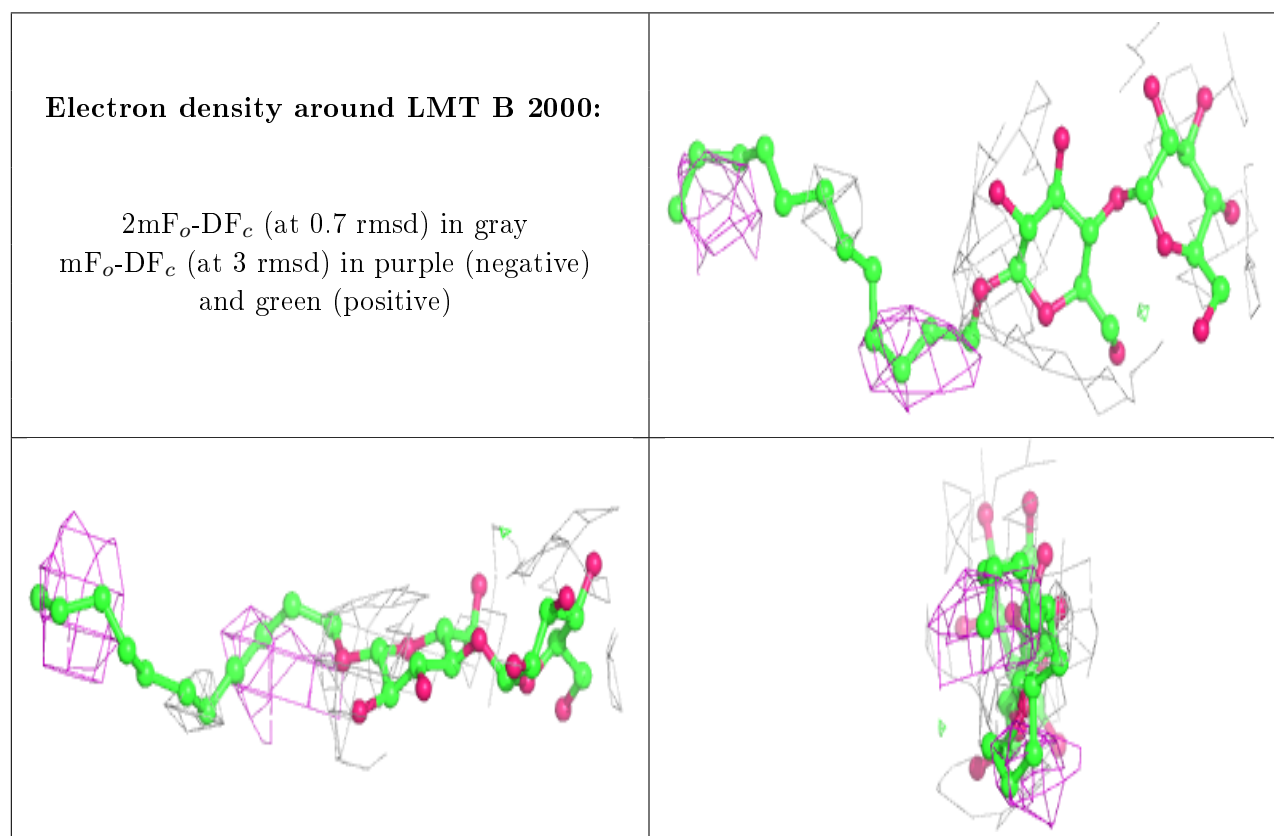


## 6.4 Ligands ⓘ

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.

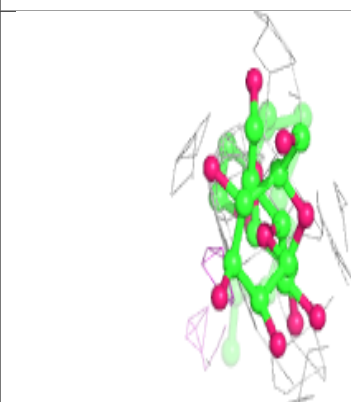
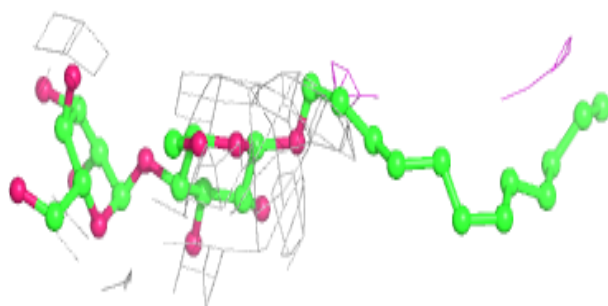
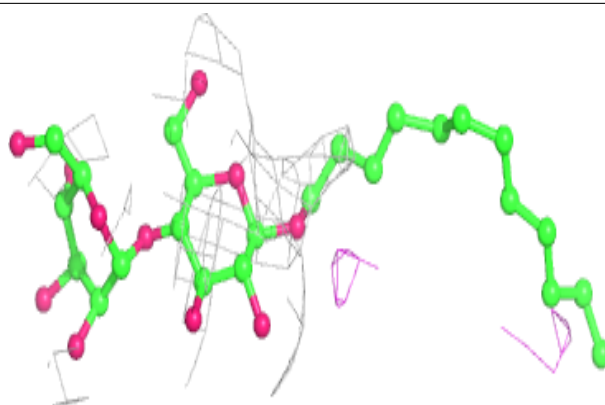
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	LMT	B	2000	35/35	0.73	0.43	31,50,60,69	0
2	LMT	E	1101	35/35	0.78	0.42	41,74,104,107	0
2	LMT	D	2000	35/35	0.82	0.34	21,41,56,63	0
2	LMT	C	1101	35/35	0.82	0.33	12,41,56,72	0
2	LMT	F	2000	35/35	0.82	0.39	40,64,89,94	0
2	LMT	A	1101	35/35	0.86	0.32	31,41,90,99	0
3	NI	E	1102	1/1	0.96	0.15	170,170,170,170	0
3	NI	A	1102	1/1	0.97	0.19	154,154,154,154	0
3	NI	C	1102	1/1	0.98	0.09	41,41,41,41	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.

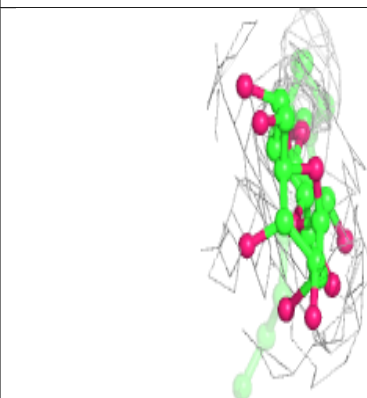
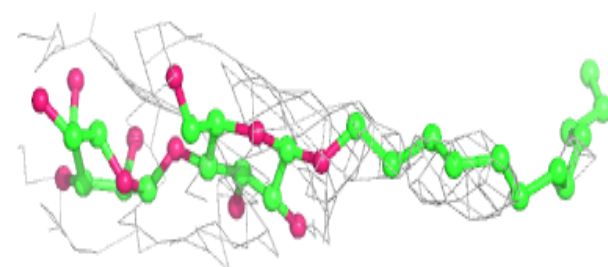
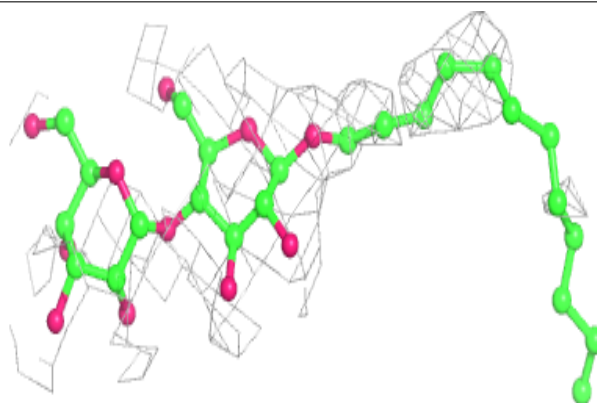


**Electron density around LMT E 1101:**

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

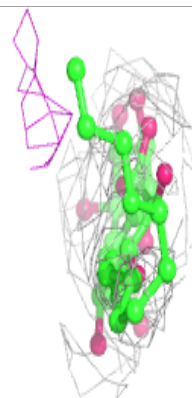
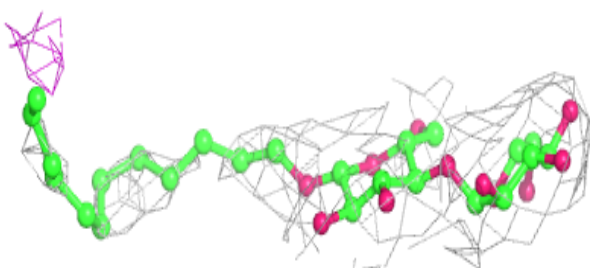
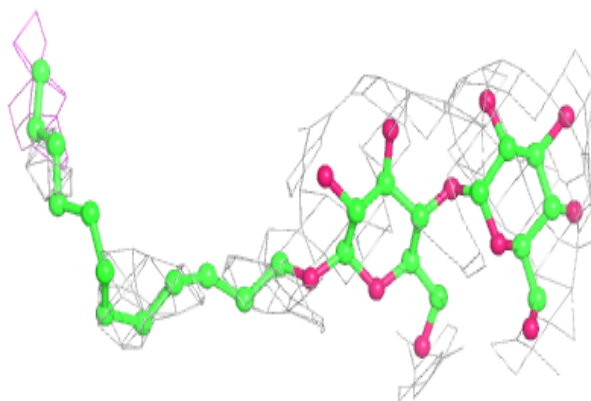
**Electron density around LMT D 2000:**

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

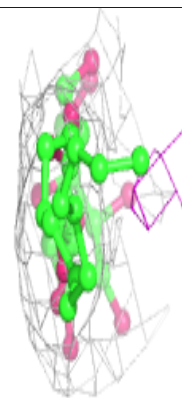
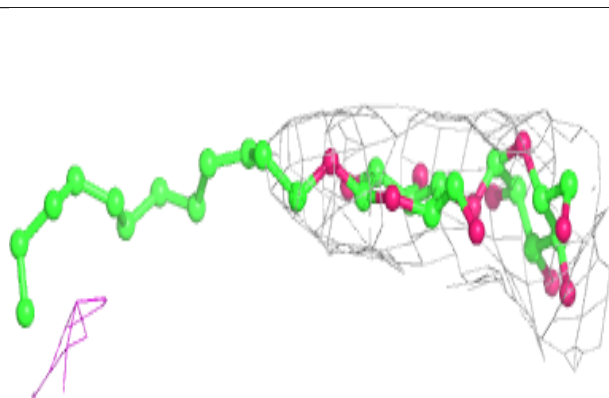
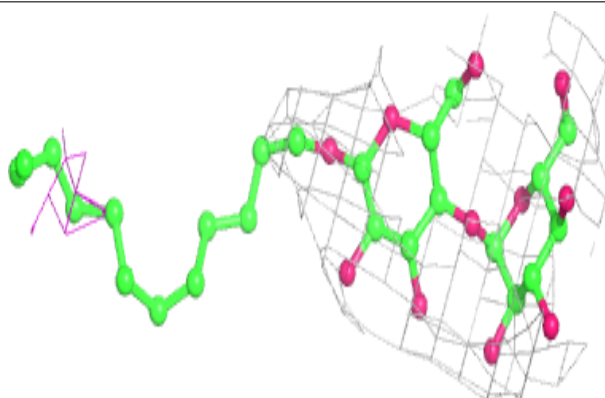


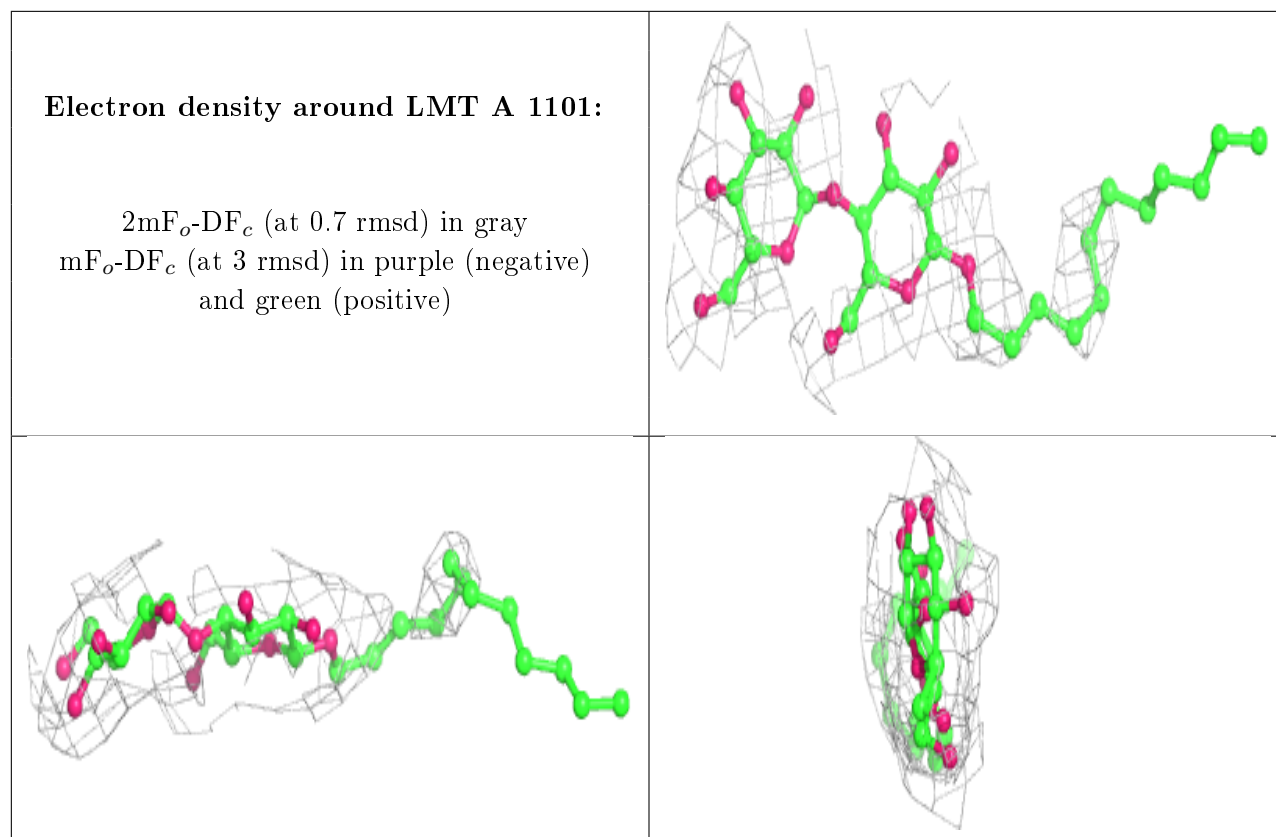
**Electron density around LMT C 1101:**

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

**Electron density around LMT F 2000:**

$2mF_o-DF_c$  (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.