



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 5, 2022 – 01:18 pm BST

PDB ID : 7O3N  
Title : Crystal Structure of AcrB Single Mutant - 2  
Authors : Ababou, A.  
Deposited on : 2021-04-02  
Resolution : 3.56 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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.27  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.27

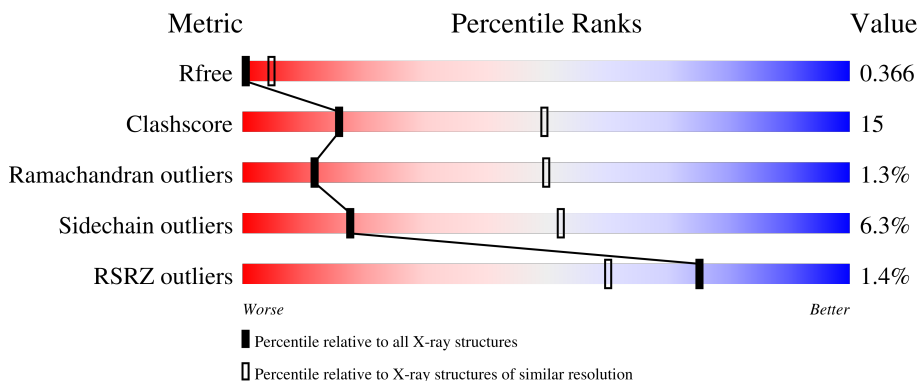
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.56 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.



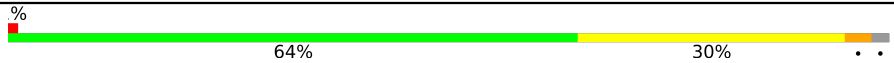
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1020 (3.62-3.50)
Clashscore	141614	1100 (3.62-3.50)
Ramachandran outliers	138981	1065 (3.62-3.50)
Sidechain outliers	138945	1066 (3.62-3.50)
RSRZ outliers	127900	1009 (3.64-3.48)

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  $\geq 3$ , 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	1069	
1	B	1069	
1	C	1069	
1	D	1069	
1	E	1069	

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Mol	Chain	Length	Quality of chain
1	F	1069	 A horizontal bar chart representing the quality of chain. The bar is divided into segments: a small red segment at the start, followed by a large green segment labeled '64%', then a yellow segment labeled '30%', and finally a small grey segment at the end. A '%' symbol is positioned above the bar.

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	A	2000	X	-	-	-
2	LMT	B	2000	X	-	-	-
2	LMT	C	2000	X	-	-	-
2	LMT	D	2000	X	-	-	-
2	LMT	E	2000	X	-	-	-
2	LMT	F	2000	X	-	-	-

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 47816 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 Efflux pump membrane transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1044	7940	5105	1313	1479	43	0	0	0
1	B	1042	7923	5095	1309	1476	43	0	0	0
1	C	1044	7940	5105	1313	1479	43	0	0	0
1	D	1044	7940	5105	1313	1479	43	0	0	0
1	E	1042	7923	5095	1309	1476	43	0	0	0
1	F	1044	7940	5105	1313	1479	43	0	0	0

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP E2QH56
A	-18	GLY	-	expression tag	UNP E2QH56
A	-17	SER	-	expression tag	UNP E2QH56
A	-16	SER	-	expression tag	UNP E2QH56
A	-15	HIS	-	expression tag	UNP E2QH56
A	-14	HIS	-	expression tag	UNP E2QH56
A	-13	HIS	-	expression tag	UNP E2QH56
A	-12	HIS	-	expression tag	UNP E2QH56
A	-11	HIS	-	expression tag	UNP E2QH56
A	-10	HIS	-	expression tag	UNP E2QH56
A	-9	SER	-	expression tag	UNP E2QH56
A	-8	SER	-	expression tag	UNP E2QH56
A	-7	GLY	-	expression tag	UNP E2QH56
A	-6	LEU	-	expression tag	UNP E2QH56
A	-5	VAL	-	expression tag	UNP E2QH56
A	-4	PRO	-	expression tag	UNP E2QH56
A	-3	ARG	-	expression tag	UNP E2QH56

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP E2QH56
A	-1	SER	-	expression tag	UNP E2QH56
A	0	HIS	-	expression tag	UNP E2QH56
A	620	LYS	ARG	engineered mutation	UNP E2QH56
B	-19	MET	-	initiating methionine	UNP E2QH56
B	-18	GLY	-	expression tag	UNP E2QH56
B	-17	SER	-	expression tag	UNP E2QH56
B	-16	SER	-	expression tag	UNP E2QH56
B	-15	HIS	-	expression tag	UNP E2QH56
B	-14	HIS	-	expression tag	UNP E2QH56
B	-13	HIS	-	expression tag	UNP E2QH56
B	-12	HIS	-	expression tag	UNP E2QH56
B	-11	HIS	-	expression tag	UNP E2QH56
B	-10	HIS	-	expression tag	UNP E2QH56
B	-9	SER	-	expression tag	UNP E2QH56
B	-8	SER	-	expression tag	UNP E2QH56
B	-7	GLY	-	expression tag	UNP E2QH56
B	-6	LEU	-	expression tag	UNP E2QH56
B	-5	VAL	-	expression tag	UNP E2QH56
B	-4	PRO	-	expression tag	UNP E2QH56
B	-3	ARG	-	expression tag	UNP E2QH56
B	-2	GLY	-	expression tag	UNP E2QH56
B	-1	SER	-	expression tag	UNP E2QH56
B	0	HIS	-	expression tag	UNP E2QH56
B	620	LYS	ARG	engineered mutation	UNP E2QH56
C	-19	MET	-	initiating methionine	UNP E2QH56
C	-18	GLY	-	expression tag	UNP E2QH56
C	-17	SER	-	expression tag	UNP E2QH56
C	-16	SER	-	expression tag	UNP E2QH56
C	-15	HIS	-	expression tag	UNP E2QH56
C	-14	HIS	-	expression tag	UNP E2QH56
C	-13	HIS	-	expression tag	UNP E2QH56
C	-12	HIS	-	expression tag	UNP E2QH56
C	-11	HIS	-	expression tag	UNP E2QH56
C	-10	HIS	-	expression tag	UNP E2QH56
C	-9	SER	-	expression tag	UNP E2QH56
C	-8	SER	-	expression tag	UNP E2QH56
C	-7	GLY	-	expression tag	UNP E2QH56
C	-6	LEU	-	expression tag	UNP E2QH56
C	-5	VAL	-	expression tag	UNP E2QH56
C	-4	PRO	-	expression tag	UNP E2QH56
C	-3	ARG	-	expression tag	UNP E2QH56

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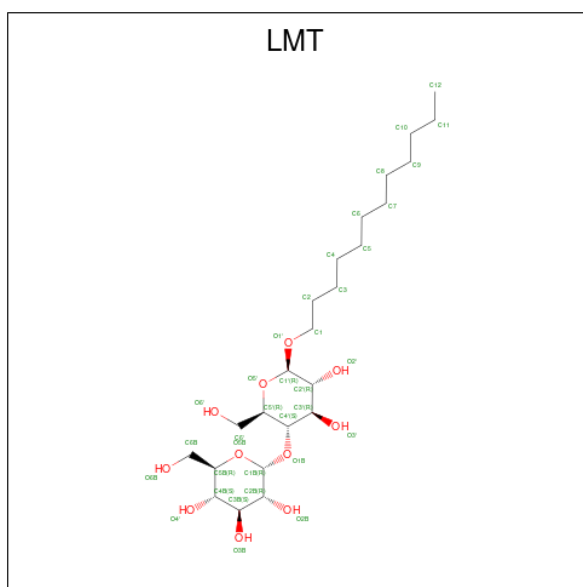
Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP E2QH56
C	-1	SER	-	expression tag	UNP E2QH56
C	0	HIS	-	expression tag	UNP E2QH56
C	620	LYS	ARG	engineered mutation	UNP E2QH56
D	-19	MET	-	initiating methionine	UNP E2QH56
D	-18	GLY	-	expression tag	UNP E2QH56
D	-17	SER	-	expression tag	UNP E2QH56
D	-16	SER	-	expression tag	UNP E2QH56
D	-15	HIS	-	expression tag	UNP E2QH56
D	-14	HIS	-	expression tag	UNP E2QH56
D	-13	HIS	-	expression tag	UNP E2QH56
D	-12	HIS	-	expression tag	UNP E2QH56
D	-11	HIS	-	expression tag	UNP E2QH56
D	-10	HIS	-	expression tag	UNP E2QH56
D	-9	SER	-	expression tag	UNP E2QH56
D	-8	SER	-	expression tag	UNP E2QH56
D	-7	GLY	-	expression tag	UNP E2QH56
D	-6	LEU	-	expression tag	UNP E2QH56
D	-5	VAL	-	expression tag	UNP E2QH56
D	-4	PRO	-	expression tag	UNP E2QH56
D	-3	ARG	-	expression tag	UNP E2QH56
D	-2	GLY	-	expression tag	UNP E2QH56
D	-1	SER	-	expression tag	UNP E2QH56
D	0	HIS	-	expression tag	UNP E2QH56
D	620	LYS	ARG	engineered mutation	UNP E2QH56
E	-19	MET	-	initiating methionine	UNP E2QH56
E	-18	GLY	-	expression tag	UNP E2QH56
E	-17	SER	-	expression tag	UNP E2QH56
E	-16	SER	-	expression tag	UNP E2QH56
E	-15	HIS	-	expression tag	UNP E2QH56
E	-14	HIS	-	expression tag	UNP E2QH56
E	-13	HIS	-	expression tag	UNP E2QH56
E	-12	HIS	-	expression tag	UNP E2QH56
E	-11	HIS	-	expression tag	UNP E2QH56
E	-10	HIS	-	expression tag	UNP E2QH56
E	-9	SER	-	expression tag	UNP E2QH56
E	-8	SER	-	expression tag	UNP E2QH56
E	-7	GLY	-	expression tag	UNP E2QH56
E	-6	LEU	-	expression tag	UNP E2QH56
E	-5	VAL	-	expression tag	UNP E2QH56
E	-4	PRO	-	expression tag	UNP E2QH56
E	-3	ARG	-	expression tag	UNP E2QH56

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP E2QH56
E	-1	SER	-	expression tag	UNP E2QH56
E	0	HIS	-	expression tag	UNP E2QH56
E	620	LYS	ARG	engineered mutation	UNP E2QH56
F	-19	MET	-	initiating methionine	UNP E2QH56
F	-18	GLY	-	expression tag	UNP E2QH56
F	-17	SER	-	expression tag	UNP E2QH56
F	-16	SER	-	expression tag	UNP E2QH56
F	-15	HIS	-	expression tag	UNP E2QH56
F	-14	HIS	-	expression tag	UNP E2QH56
F	-13	HIS	-	expression tag	UNP E2QH56
F	-12	HIS	-	expression tag	UNP E2QH56
F	-11	HIS	-	expression tag	UNP E2QH56
F	-10	HIS	-	expression tag	UNP E2QH56
F	-9	SER	-	expression tag	UNP E2QH56
F	-8	SER	-	expression tag	UNP E2QH56
F	-7	GLY	-	expression tag	UNP E2QH56
F	-6	LEU	-	expression tag	UNP E2QH56
F	-5	VAL	-	expression tag	UNP E2QH56
F	-4	PRO	-	expression tag	UNP E2QH56
F	-3	ARG	-	expression tag	UNP E2QH56
F	-2	GLY	-	expression tag	UNP E2QH56
F	-1	SER	-	expression tag	UNP E2QH56
F	0	HIS	-	expression tag	UNP E2QH56
F	620	LYS	ARG	engineered mutation	UNP E2QH56

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



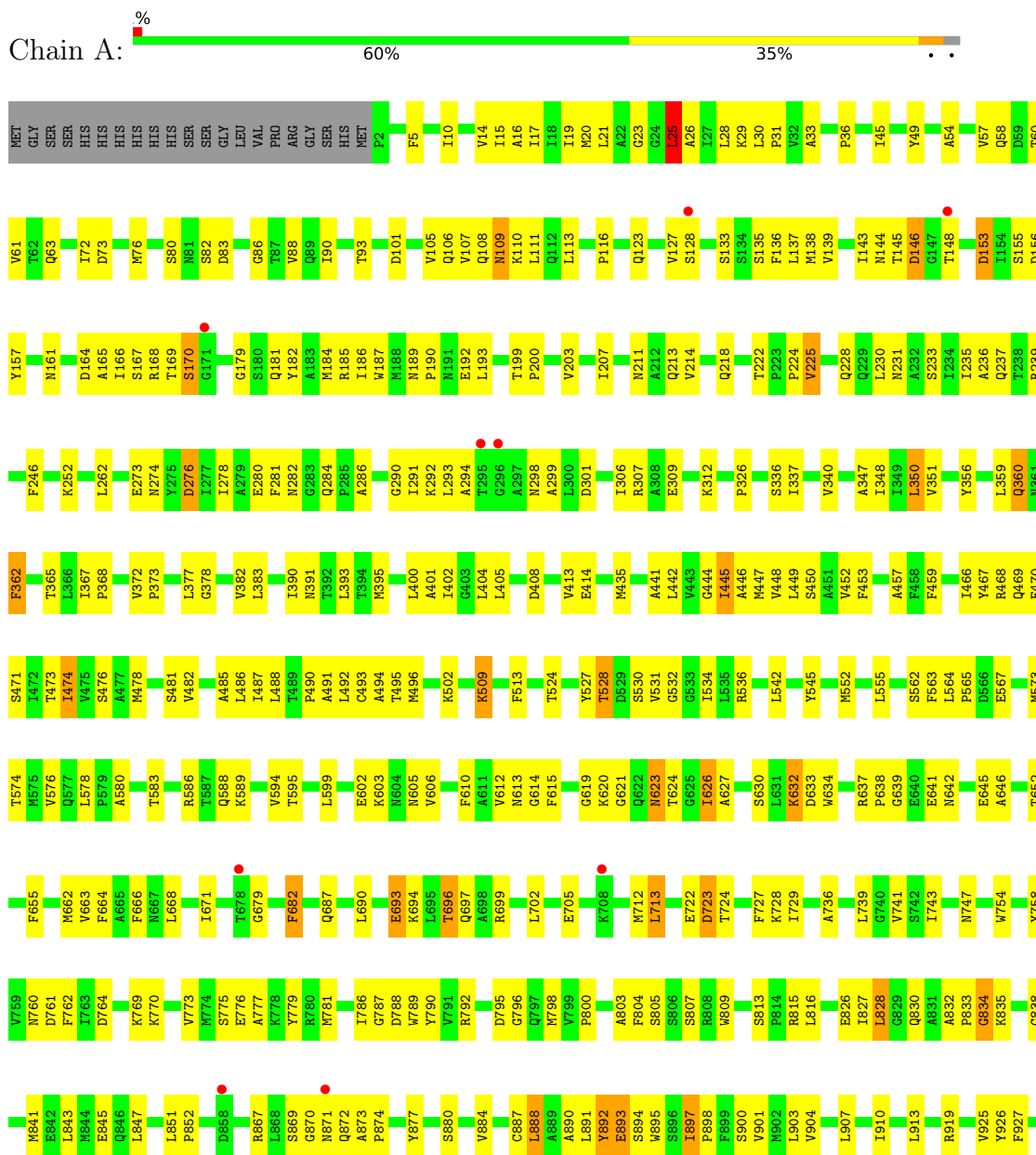
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			35	24	11		
2	B	1	Total	C	O	0	0
			35	24	11		
2	C	1	Total	C	O	0	0
			35	24	11		
2	D	1	Total	C	O	0	0
			35	24	11		
2	E	1	Total	C	O	0	0
			35	24	11		
2	F	1	Total	C	O	0	0
			35	24	11		



### 3 Residue-property plots [i](#)

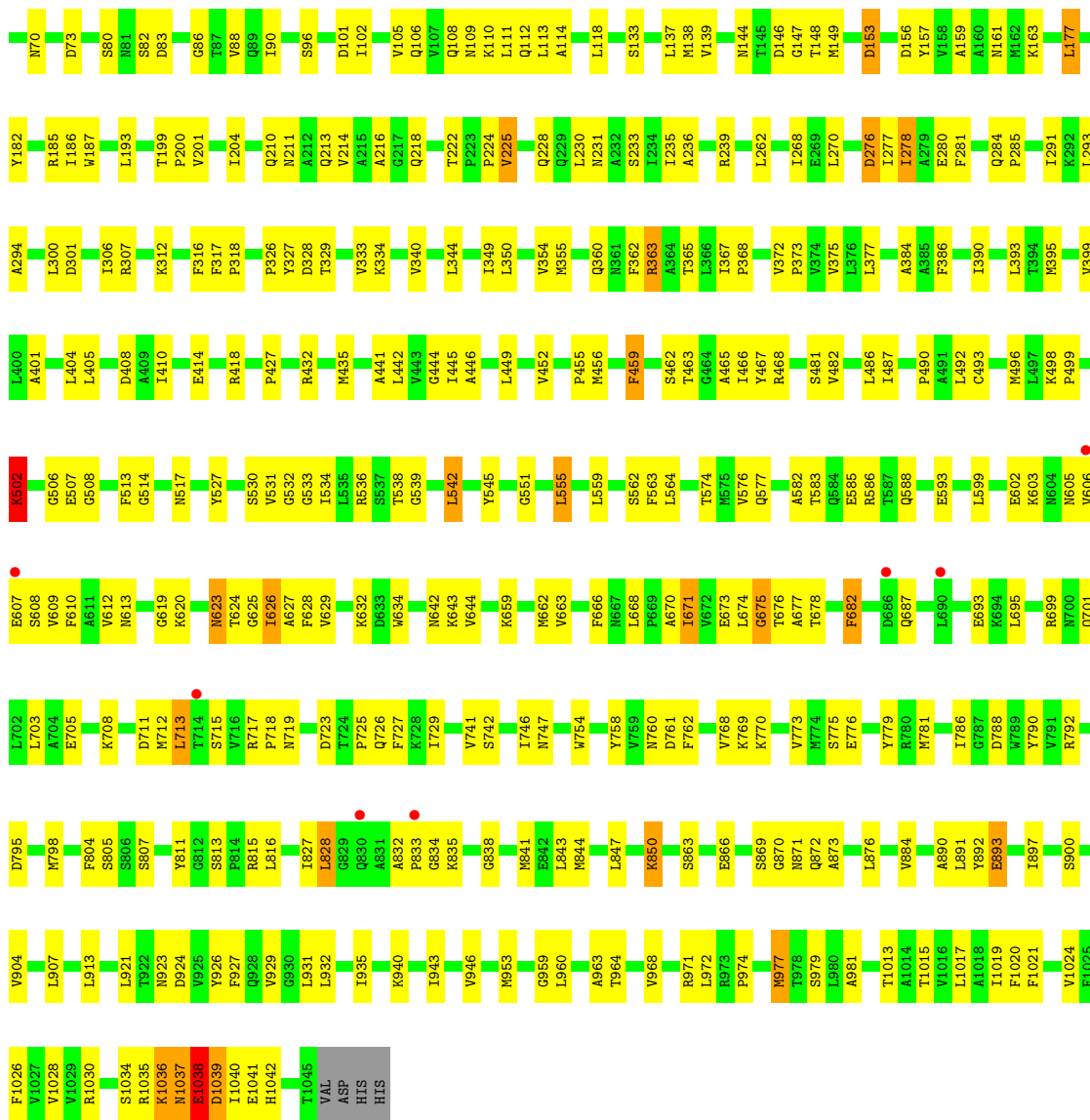
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

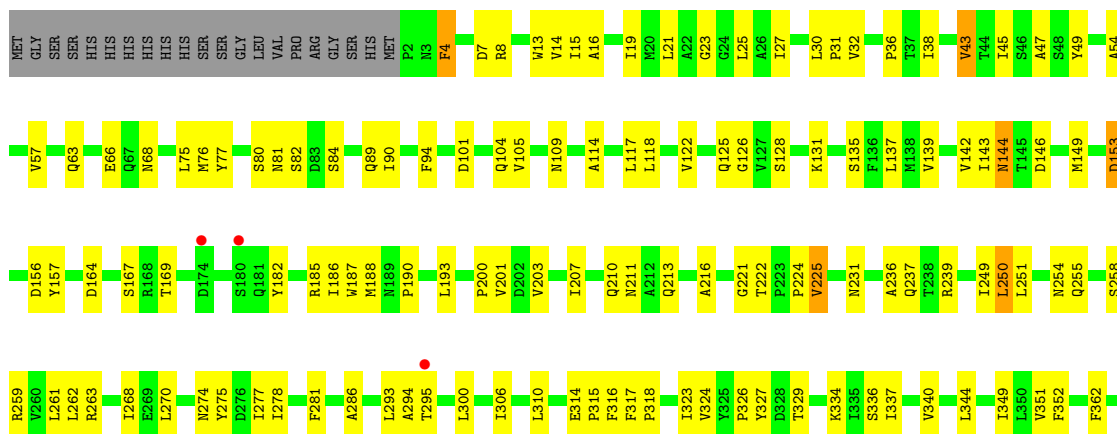




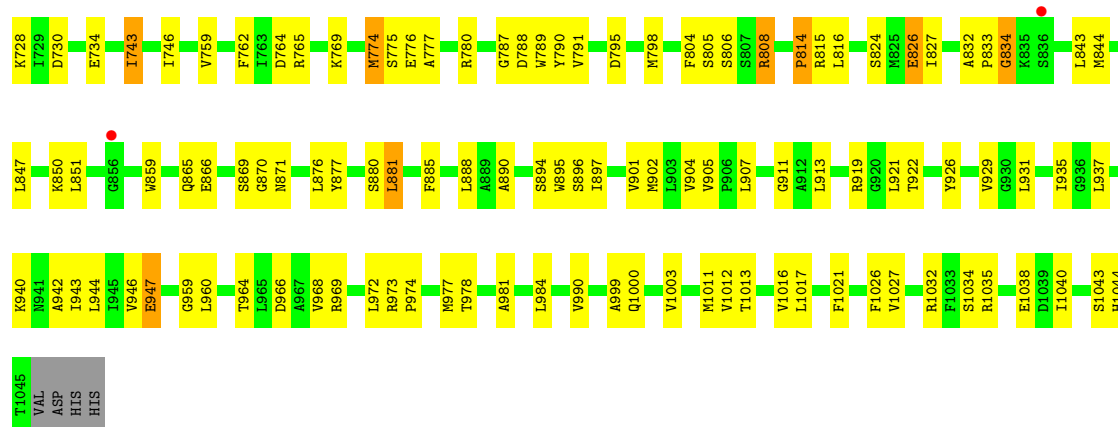




• Molecule 1: Efflux pump membrane transporter







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	152.34Å 157.10Å 218.86Å 90.00° 92.73° 90.00°	Depositor
Resolution (Å)	20.00 – 3.56 20.00 – 3.56	Depositor EDS
% Data completeness (in resolution range)	98.9 (20.00-3.56) 98.9 (20.00-3.56)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.94 (at 3.52Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, $R_{free}$	0.306 , 0.366 0.306 , 0.366	Depositor DCC
$R_{free}$ test set	6063 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	102.9	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.079 for -k,-h,-l 0.099 for k,h,-l 0.097 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	47816	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	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 52.24 % 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 5.0059e-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:  
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	0.25	0/8092	0.52	1/10987 (0.0%)
1	B	0.25	0/8074	0.51	1/10962 (0.0%)
1	C	0.26	0/8092	0.55	3/10987 (0.0%)
1	D	0.25	0/8092	0.50	1/10987 (0.0%)
1	E	0.25	0/8074	0.51	0/10962
1	F	0.25	0/8092	0.51	0/10987
All	All	0.25	0/48516	0.52	6/65872 (0.0%)

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	F	0	1
All	All	0	2

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	713	LEU	CA-CB-CG	6.31	129.82	115.30
1	A	25	LEU	CA-CB-CG	6.08	129.28	115.30
1	C	854	GLY	N-CA-C	-5.35	99.73	113.10
1	D	1038	GLU	C-N-CA	5.33	135.01	121.70
1	C	1038	GLU	C-N-CA	5.30	134.96	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	C	148	THR	Peptide
1	F	834	GLY	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	7940	0	8080	268	0
1	B	7923	0	8066	246	0
1	C	7940	0	8080	266	0
1	D	7940	0	8080	239	0
1	E	7923	0	8066	223	0
1	F	7940	0	8080	243	0
2	A	35	0	46	2	0
2	B	35	0	46	2	0
2	C	35	0	46	0	0
2	D	35	0	46	1	0
2	E	35	0	46	1	0
2	F	35	0	46	3	0
All	All	47816	0	48728	1407	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 15.

The worst 5 of 1407 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:C:446:ALA:HB2	1:C:482:VAL:HG21	1.50	0.94
1:A:105:VAL:HG21	1:B:105:VAL:HG13	1.52	0.89
1:C:1038:GLU:HA	1:C:1039:ASP:HB2	1.54	0.89
1:D:105:VAL:HG22	1:E:105:VAL:HG11	1.56	0.88
1:E:726:GLN:HG3	1:E:810:GLU:HG3	1.55	0.88

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	1042/1069 (98%)	908 (87%)	115 (11%)	19 (2%)	8	43
1	B	1040/1069 (97%)	909 (87%)	116 (11%)	15 (1%)	11	48
1	C	1042/1069 (98%)	898 (86%)	128 (12%)	16 (2%)	10	47
1	D	1042/1069 (98%)	904 (87%)	123 (12%)	15 (1%)	11	48
1	E	1040/1069 (97%)	913 (88%)	120 (12%)	7 (1%)	22	62
1	F	1042/1069 (98%)	905 (87%)	126 (12%)	11 (1%)	14	54
All	All	6248/6414 (97%)	5437 (87%)	728 (12%)	83 (1%)	12	50

5 of 83 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	133	SER
1	A	167	SER
1	A	833	PRO
1	A	871	ASN
1	A	893	GLU

### 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	850/872 (98%)	796 (94%)	54 (6%)	17	51
1	B	848/872 (97%)	792 (93%)	56 (7%)	16	50
1	C	850/872 (98%)	795 (94%)	55 (6%)	17	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	850/872 (98%)	803 (94%)	47 (6%)	21	56
1	E	848/872 (97%)	801 (94%)	47 (6%)	21	56
1	F	850/872 (98%)	789 (93%)	61 (7%)	14	47
All	All	5096/5232 (97%)	4776 (94%)	320 (6%)	18	52

5 of 320 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	418	ARG
1	F	562	SER
1	E	554	TYR
1	F	6	ILE
1	F	692	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	760	ASN
1	F	108	GLN
1	F	865	GLN
1	F	109	ASN
1	E	865	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 monosaccharides in this entry.

## 5.6 Ligand geometry

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	LMT	A	2000	-	36,36,36	1.75	9 (25%)	47,47,47	1.23	4 (8%)
2	LMT	F	2000	-	36,36,36	1.71	9 (25%)	47,47,47	1.29	4 (8%)
2	LMT	B	2000	-	36,36,36	1.74	8 (22%)	47,47,47	0.95	3 (6%)
2	LMT	C	2000	-	36,36,36	1.76	9 (25%)	47,47,47	1.26	4 (8%)
2	LMT	E	2000	-	36,36,36	1.73	8 (22%)	47,47,47	1.20	5 (10%)
2	LMT	D	2000	-	36,36,36	1.77	9 (25%)	47,47,47	0.93	1 (2%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LMT	A	2000	-	2/2/10/10	9/21/61/61	0/2/2/2
2	LMT	F	2000	-	3/3/10/10	13/21/61/61	0/2/2/2
2	LMT	B	2000	-	2/2/10/10	11/21/61/61	0/2/2/2
2	LMT	C	2000	-	3/3/10/10	7/21/61/61	0/2/2/2
2	LMT	E	2000	-	5/5/10/10	10/21/61/61	0/2/2/2
2	LMT	D	2000	-	2/2/10/10	12/21/61/61	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2000	LMT	O5'-C5'	4.04	1.54	1.44
2	B	2000	LMT	O5'-C5'	3.96	1.53	1.44
2	E	2000	LMT	O5'-C5'	3.92	1.53	1.44
2	C	2000	LMT	O5'-C5'	3.85	1.53	1.44
2	A	2000	LMT	O5'-C5'	3.82	1.53	1.44

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2000	LMT	C2'-C3'-C4'	4.78	120.59	109.68
2	C	2000	LMT	O5B-C5B-C4B	4.04	117.03	109.69
2	C	2000	LMT	C3B-C4B-C5B	3.96	117.30	110.24
2	A	2000	LMT	C3'-C4'-C5'	3.77	119.58	110.93
2	A	2000	LMT	C2'-C3'-C4'	3.74	118.23	109.68

5 of 17 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	2000	LMT	C3'
2	A	2000	LMT	C4B
2	B	2000	LMT	C3'
2	B	2000	LMT	C4B
2	C	2000	LMT	C3'

5 of 62 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2000	LMT	C2-C1-O1'-C1'
2	D	2000	LMT	C2'-C1'-O1'-C1
2	D	2000	LMT	O5'-C1'-O1'-C1
2	D	2000	LMT	C2-C1-O1'-C1'
2	E	2000	LMT	C2-C1-O1'-C1'

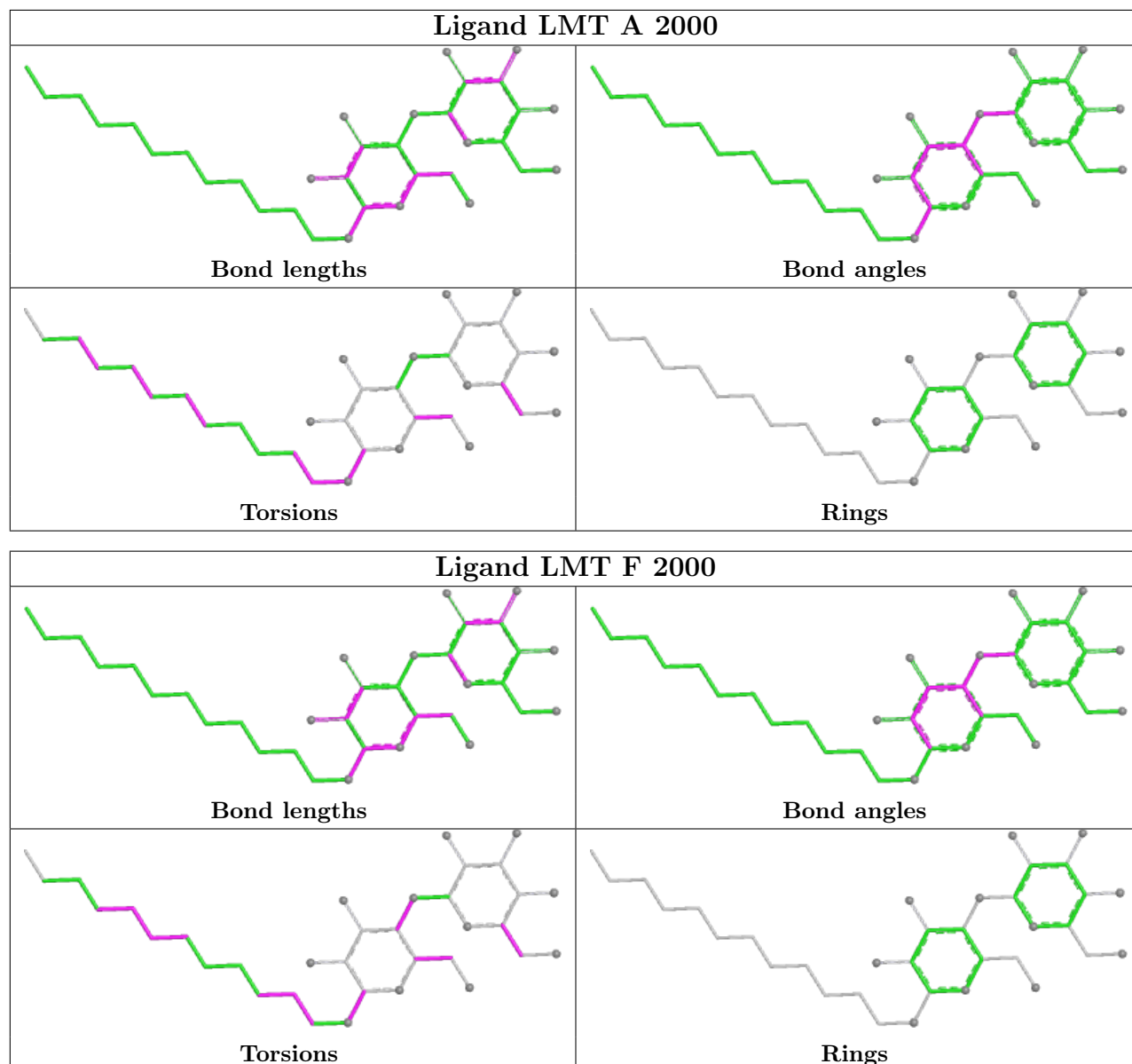
There are no ring outliers.

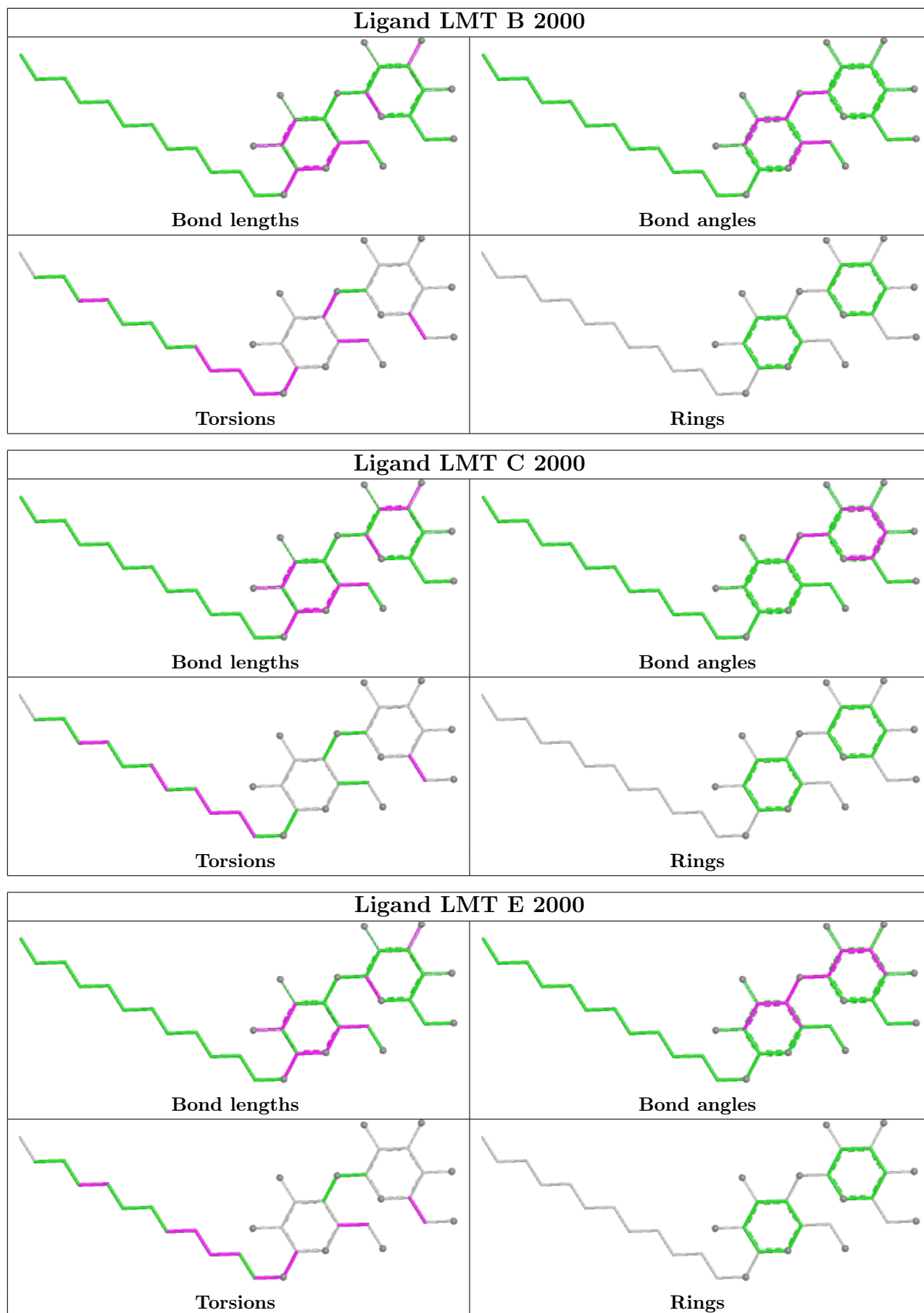
5 monomers are involved in 9 short contacts:

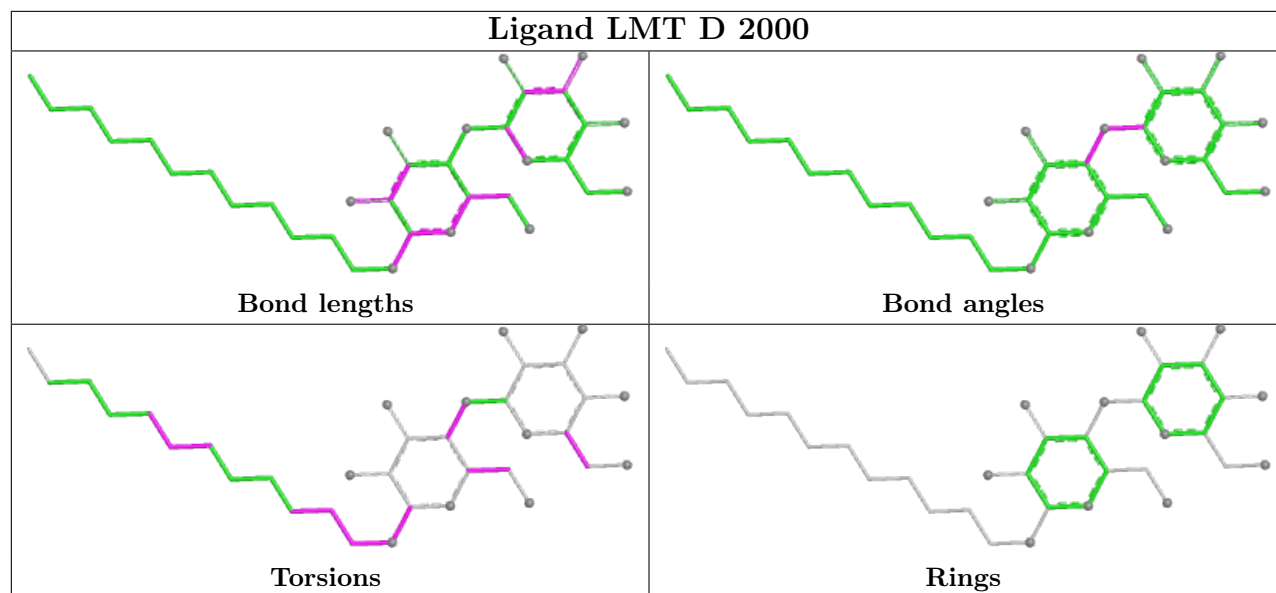
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2000	LMT	2	0
2	F	2000	LMT	3	0
2	B	2000	LMT	2	0
2	E	2000	LMT	1	0
2	D	2000	LMT	1	0

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	1044/1069 (97%)	-0.25	9 (0%) 84 72	15, 54, 96, 123	0
1	B	1042/1069 (97%)	-0.18	21 (2%) 65 49	8, 53, 102, 133	0
1	C	1044/1069 (97%)	-0.10	34 (3%) 46 32	10, 57, 103, 141	0
1	D	1044/1069 (97%)	-0.34	7 (0%) 87 78	13, 45, 89, 128	0
1	E	1042/1069 (97%)	-0.39	7 (0%) 87 78	10, 36, 75, 99	0
1	F	1044/1069 (97%)	-0.36	9 (0%) 84 72	6, 37, 71, 95	0
All	All	6260/6414 (97%)	-0.27	87 (1%) 75 60	6, 46, 93, 141	0

The worst 5 of 87 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	78	MET	5.5
1	C	171	GLY	5.2
1	C	116	PRO	4.7
1	B	870	GLY	4.5
1	C	856	GLY	4.2

### 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](#)

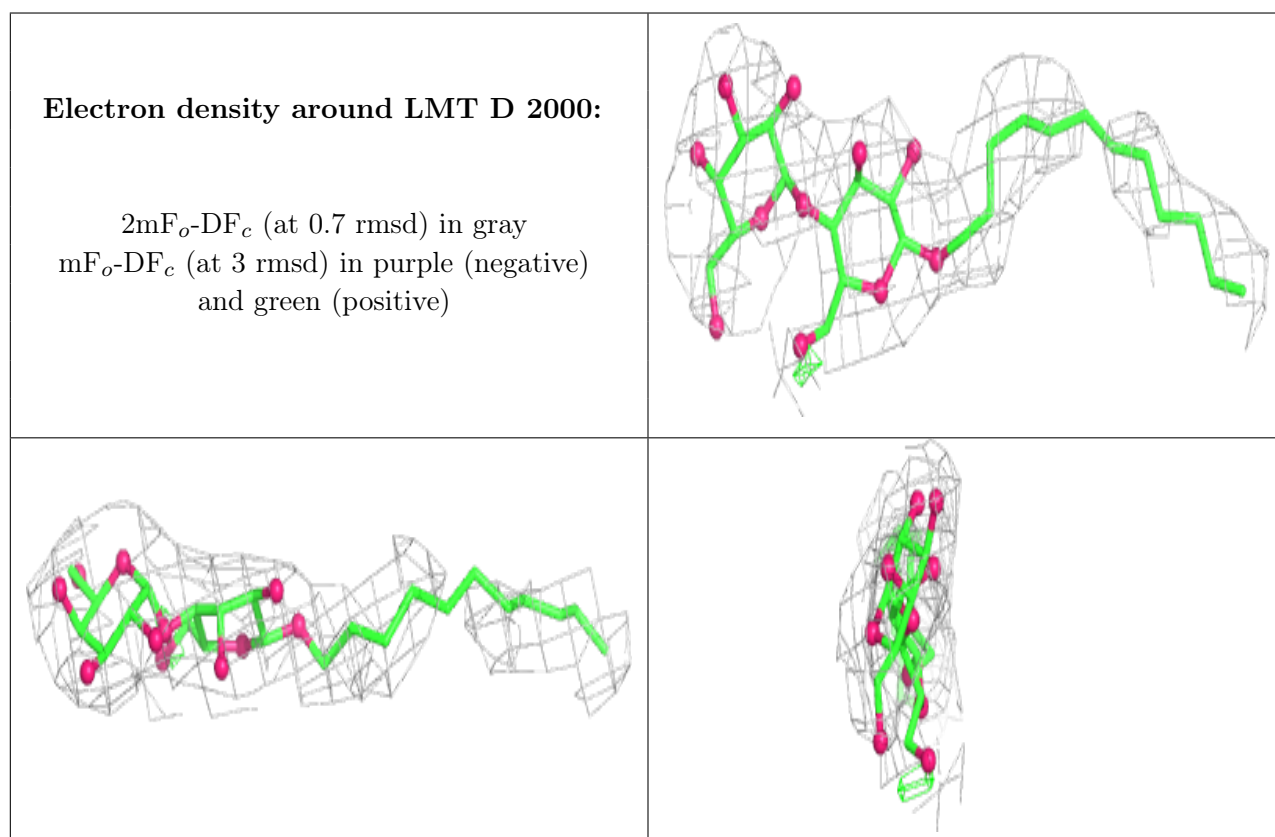
There are no monosaccharides in this entry.

## 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<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.

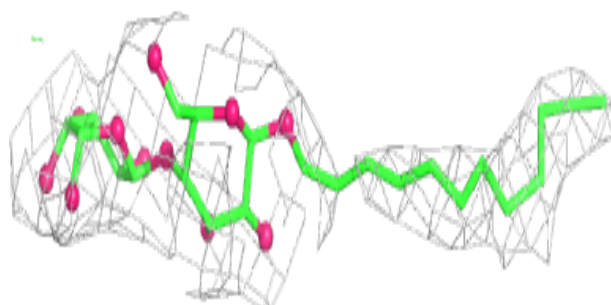
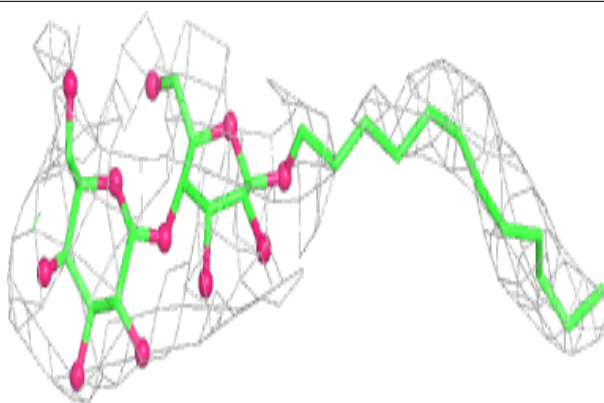
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	LMT	D	2000	35/35	0.81	0.33	21,41,61,68	0
2	LMT	A	2000	35/35	0.86	0.31	11,44,65,67	0
2	LMT	E	2000	35/35	0.86	0.34	3,42,59,66	0
2	LMT	C	2000	35/35	0.87	0.43	10,44,55,59	0
2	LMT	F	2000	35/35	0.87	0.39	6,45,57,63	0
2	LMT	B	2000	35/35	0.90	0.42	2,48,54,66	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.

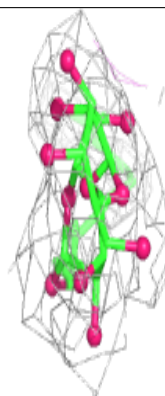
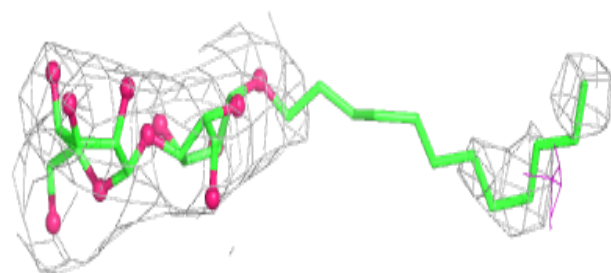
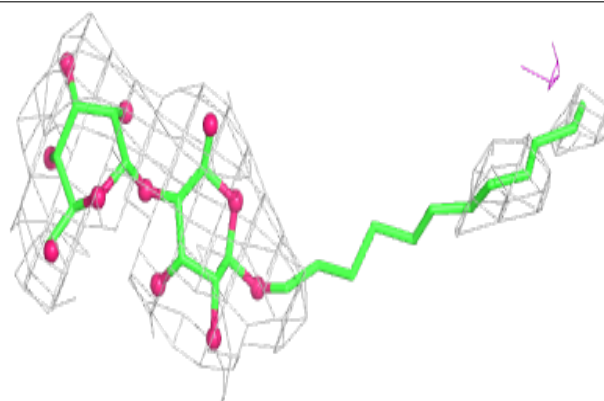


**Electron density around LMT A 2000:**

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

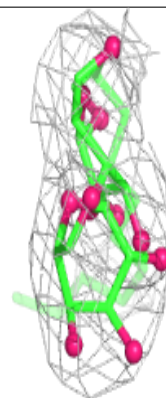
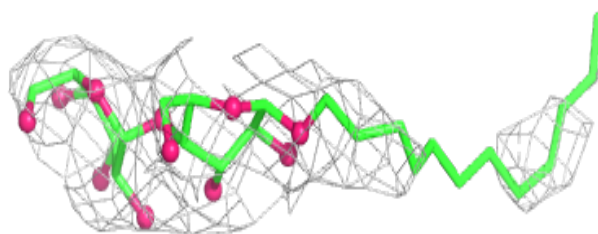
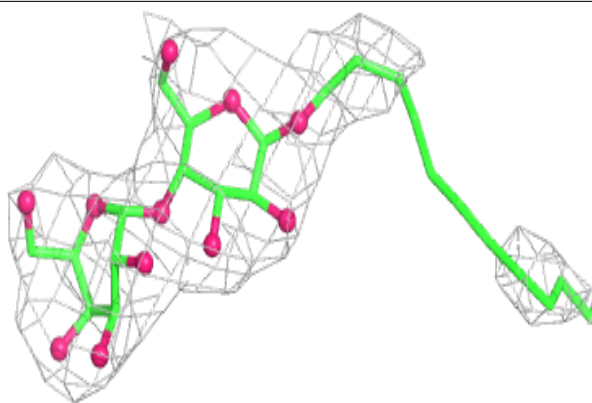
**Electron density around LMT E 2000:**

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

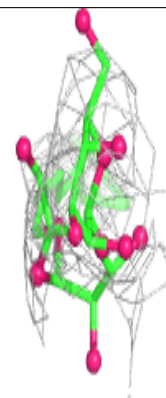
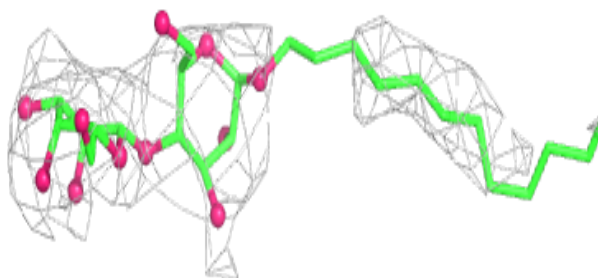
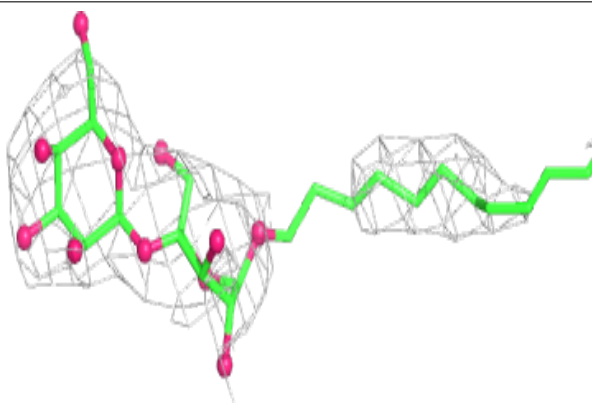


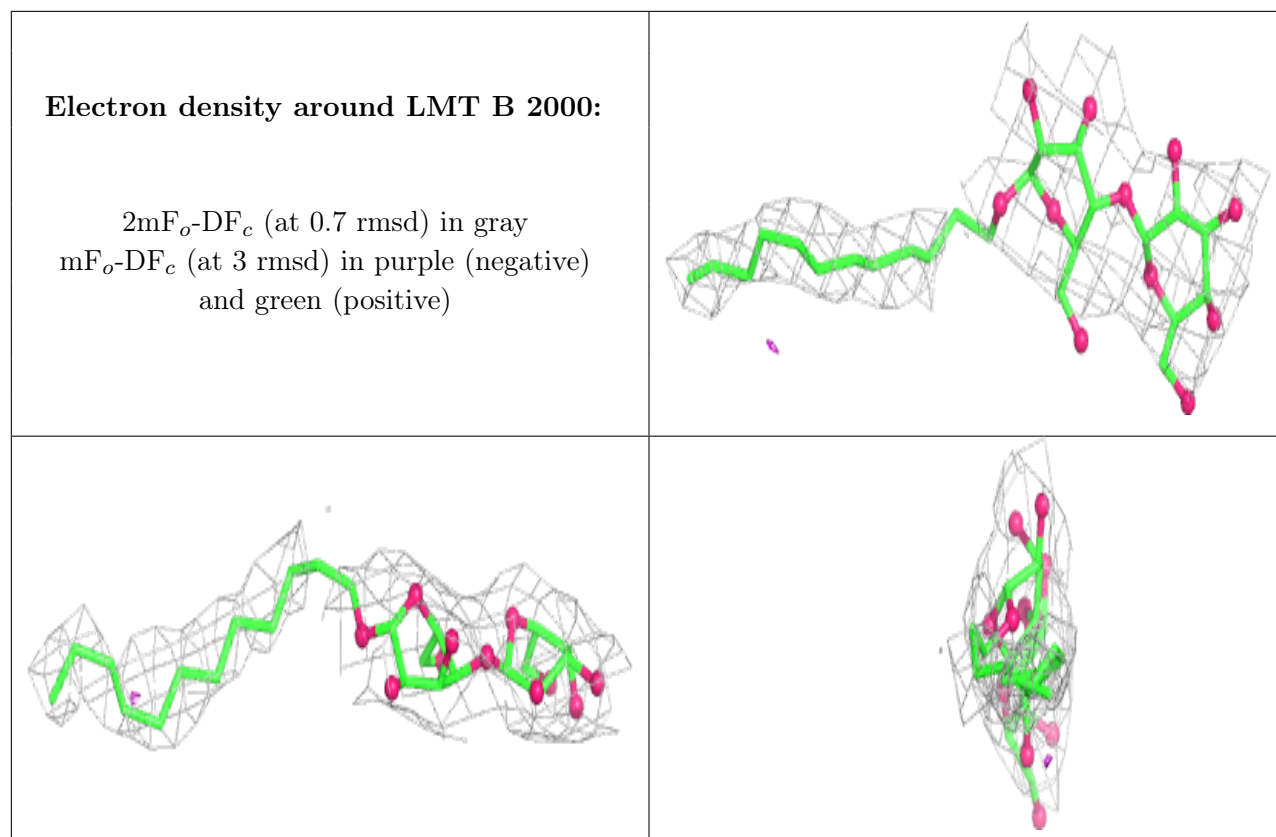
**Electron density around LMT C 2000:**

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

**Electron density around LMT 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.