



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 25, 2024 – 12:17 AM EDT

PDB ID : 6ZOG  
Title : Minocycline binding to the deep binding pocket of AcrB-I38F\_I671T  
Authors : Tam, H.K.; Foong, W.E.; Pos, K.M.  
Deposited on : 2020-07-07  
Resolution : 2.75 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

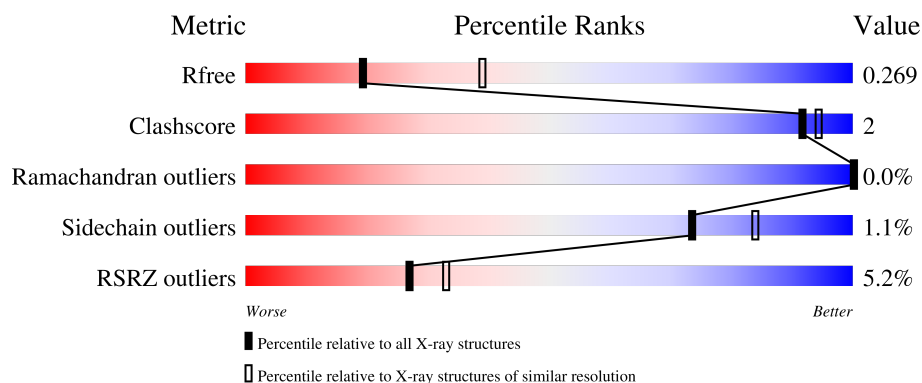
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	1057	<div> <div>5%</div> <div>92%</div> <div>6%</div> </div>
1	B	1057	<div> <div>4%</div> <div>93%</div> <div>5%</div> </div>
1	C	1057	<div> <div>3%</div> <div>92%</div> <div>6%</div> </div>
2	D	169	<div> <div>5%</div> <div>92%</div> <div>7%</div> </div>
2	E	169	<div> <div>22%</div> <div>89%</div> <div>9%</div> </div>

## 2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 26599 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	1034	Total	C	N	O	S	0	2	0
			7874	5066	1300	1464	44			
1	B	1034	Total	C	N	O	S	0	2	0
			7872	5065	1298	1464	45			
1	C	1034	Total	C	N	O	S	0	2	0
			7876	5069	1299	1464	44			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	PHE	ILE	engineered mutation	UNP P31224
A	671	THR	ILE	engineered mutation	UNP P31224
A	1050	LEU	-	expression tag	UNP P31224
A	1051	GLU	-	expression tag	UNP P31224
A	1052	HIS	-	expression tag	UNP P31224
A	1053	HIS	-	expression tag	UNP P31224
A	1054	HIS	-	expression tag	UNP P31224
A	1055	HIS	-	expression tag	UNP P31224
A	1056	HIS	-	expression tag	UNP P31224
A	1057	HIS	-	expression tag	UNP P31224
B	38	PHE	ILE	engineered mutation	UNP P31224
B	671	THR	ILE	engineered mutation	UNP P31224
B	1050	LEU	-	expression tag	UNP P31224
B	1051	GLU	-	expression tag	UNP P31224
B	1052	HIS	-	expression tag	UNP P31224
B	1053	HIS	-	expression tag	UNP P31224
B	1054	HIS	-	expression tag	UNP P31224
B	1055	HIS	-	expression tag	UNP P31224
B	1056	HIS	-	expression tag	UNP P31224
B	1057	HIS	-	expression tag	UNP P31224
C	38	PHE	ILE	engineered mutation	UNP P31224
C	671	THR	ILE	engineered mutation	UNP P31224
C	1050	LEU	-	expression tag	UNP P31224

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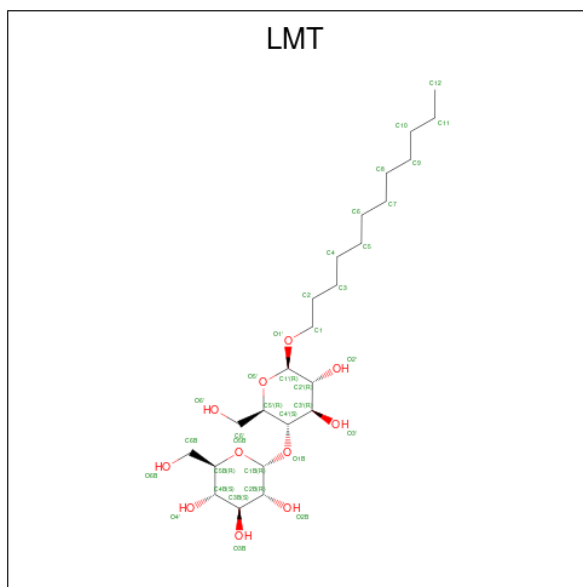
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Chain	Residue	Modelled	Actual	Comment	Reference
C	1051	GLU	-	expression tag	UNP P31224
C	1052	HIS	-	expression tag	UNP P31224
C	1053	HIS	-	expression tag	UNP P31224
C	1054	HIS	-	expression tag	UNP P31224
C	1055	HIS	-	expression tag	UNP P31224
C	1056	HIS	-	expression tag	UNP P31224
C	1057	HIS	-	expression tag	UNP P31224

- Molecule 2 is a protein called DARPIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	157	Total	C	N	O	S	0	0	0
			1186	747	208	230	1			
2	E	154	Total	C	N	O	S	0	0	0
			1167	736	204	226	1			

- Molecule 3 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



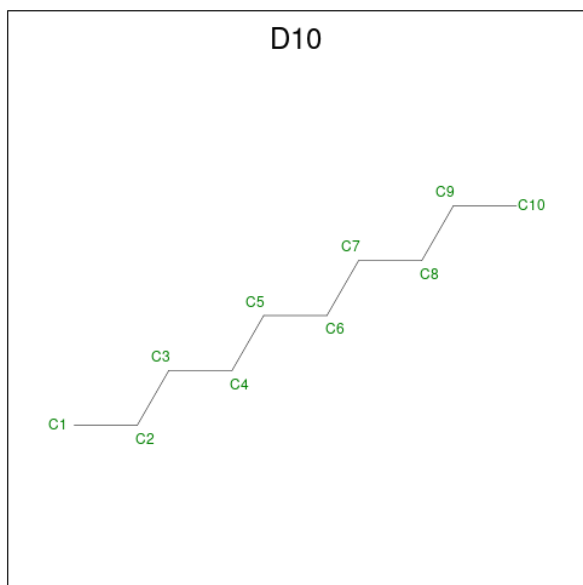
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			35	24	11		
3	A	1	Total	C	O	0	0
			35	24	11		
3	A	1	Total	C	O	0	0
			35	24	11		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			35	24	11		
3	B	1	Total	C	O	0	0
			35	24	11		
3	C	1	Total	C	O	0	0
			35	24	11		

- Molecule 4 is DECANE (three-letter code: D10) (formula:  $C_{10}H_{22}$ ).



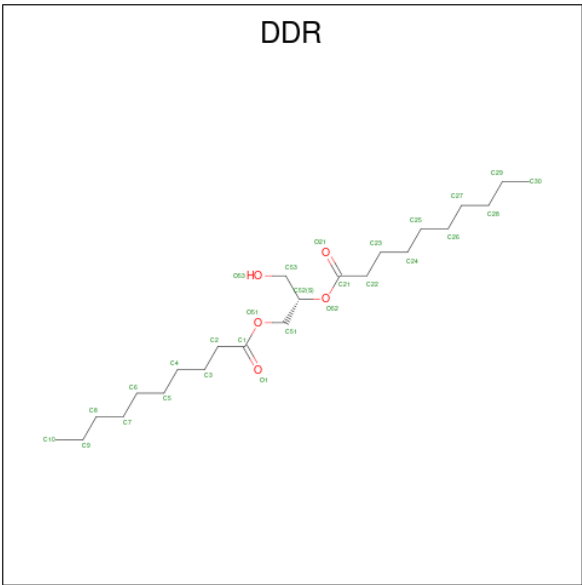
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	C	0	0
			10	10		
4	C	1	Total	C	0	0
			10	10		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



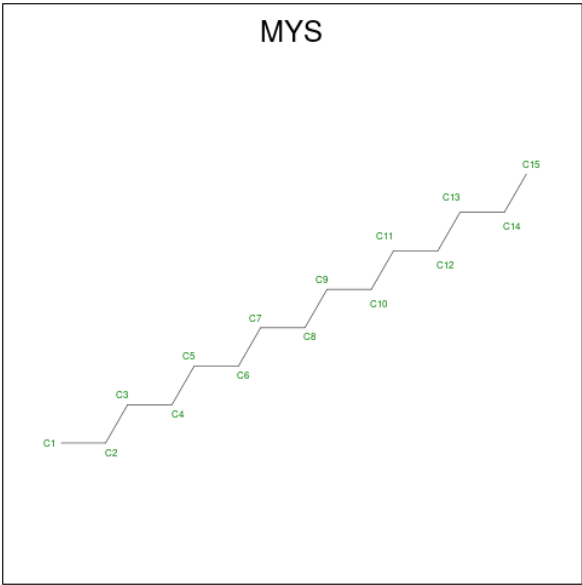
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is (2S)-3-hydroxypropane-1,2-diyl didecanoate (three-letter code: DDR) (formula:  $C_{23}H_{44}O_5$ ).



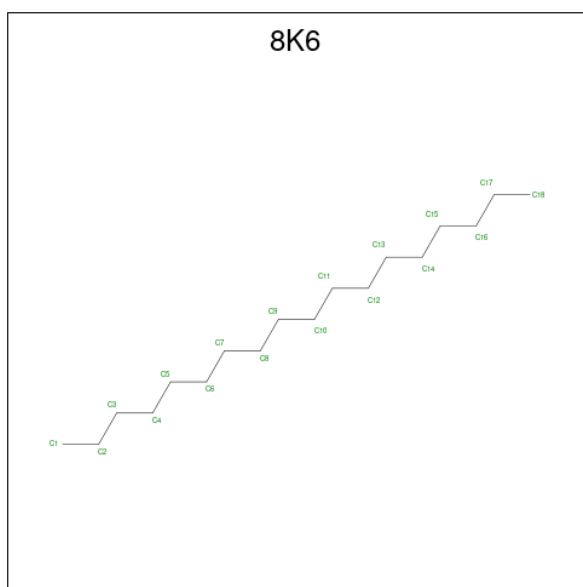
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			28	23	5		

- Molecule 7 is PENTADECANE (three-letter code: MYS) (formula: C<sub>15</sub>H<sub>32</sub>).



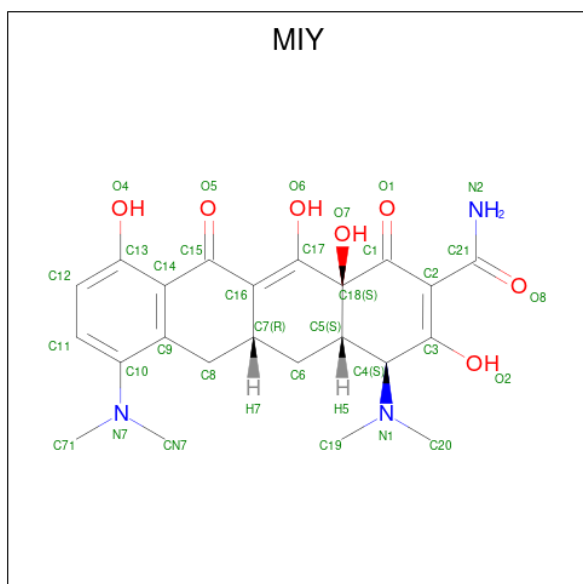
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	C	0	0
			15	15		

- Molecule 8 is Octadecane (three-letter code: 8K6) (formula: C<sub>18</sub>H<sub>38</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C		0	0
			18	18			

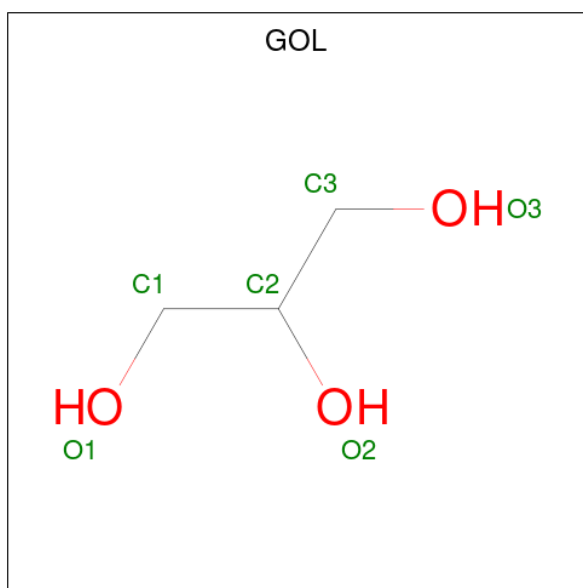
- Molecule 9 is (4S,4AS,5AR,12AS)-4,7-BIS(DIMETHYLAMINO)-3,10,12,12A-TETRAHYDROXY-1,11-DIOXO-1,4,4A,5,5A,6,11,12A-OCTAHYDROTETRACENE-2-CARBOXAMIDE (three-letter code: MIY) (formula:  $C_{23}H_{27}N_3O_7$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	N	O	0	0
			33	23	3	7		

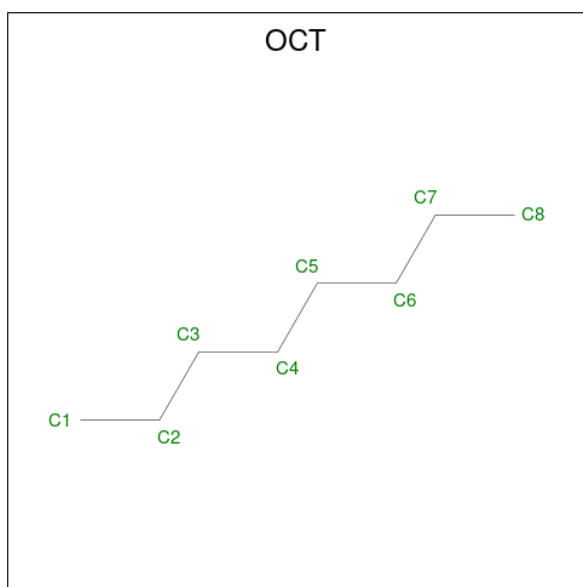


- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



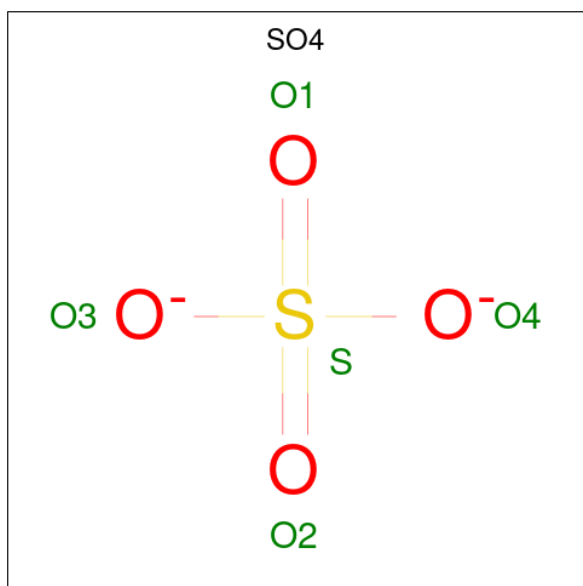
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	0	0
			6	3	3		
10	C	1	Total	C	O	0	0
			6	3	3		
10	C	1	Total	C	O	0	0
			6	3	3		
10	C	1	Total	C	O	0	0
			6	3	3		
10	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 11 is N-OCTANE (three-letter code: OCT) (formula:  $C_8H_{18}$ ).



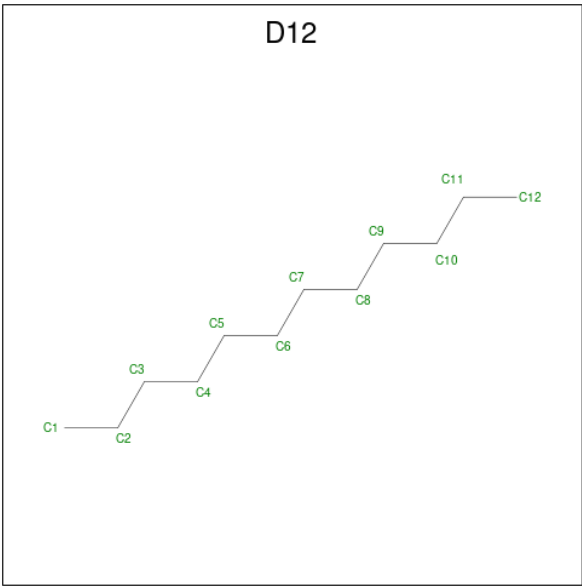
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	B	1	Total	C	0	0
			8	8		

- Molecule 12 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



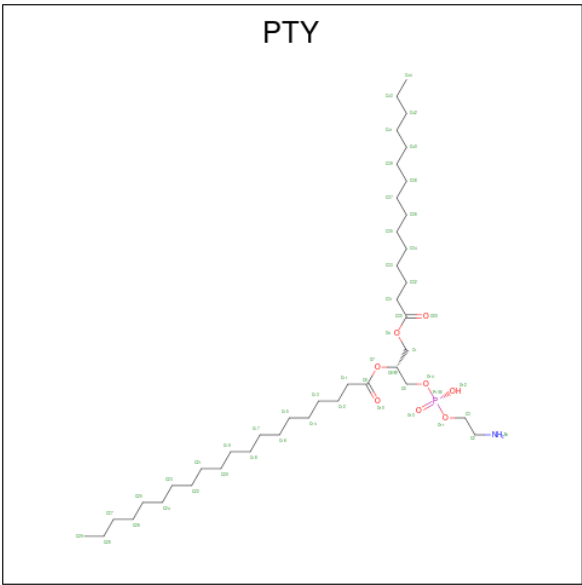
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	B	1	Total	O	S	0	0
			5	4	1		
12	B	1	Total	O	S	0	0
			5	4	1		
12	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 13 is DODECANE (three-letter code: D12) (formula: C<sub>12</sub>H<sub>26</sub>).



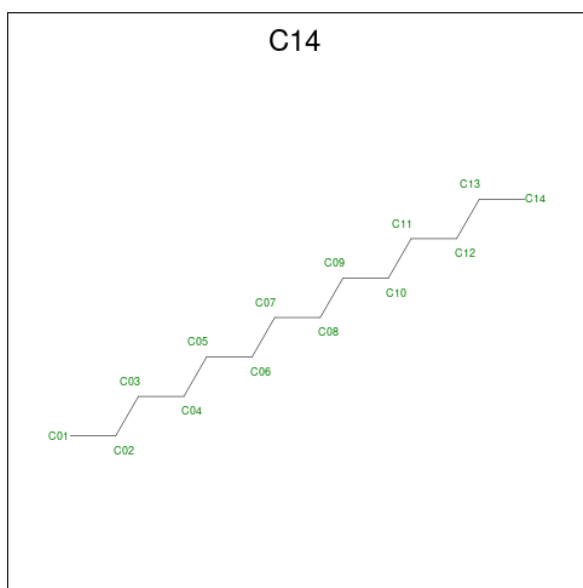
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	C	1	Total	C	0	0
			12	12		

- Molecule 14 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: C<sub>40</sub>H<sub>80</sub>NO<sub>8</sub>P).



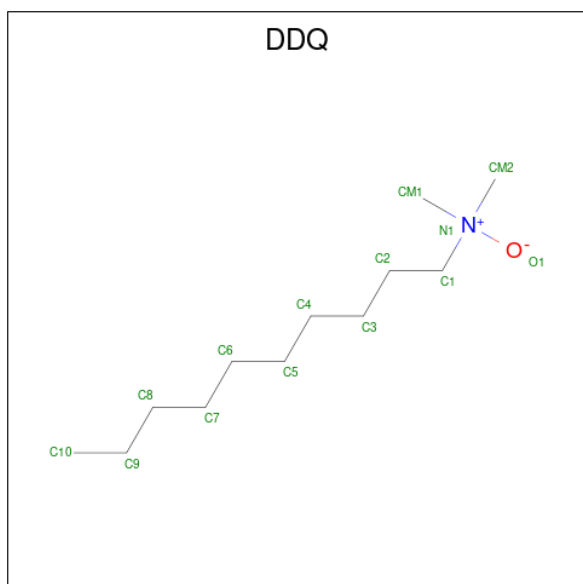
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	C	1	Total	C	N	O	P	0	0
			50	40	1	8	1		

- Molecule 15 is TETRADECANE (three-letter code: C14) (formula:  $C_{14}H_{30}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	C	1	Total	C		0	0
			14	14			

- Molecule 16 is DECYLAMINE-N,N-DIMETHYL-N-OXIDE (three-letter code: DDQ) (formula:  $C_{12}H_{27}NO$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	C	1	Total	C	N	O	0	0
			14	12	1	1		

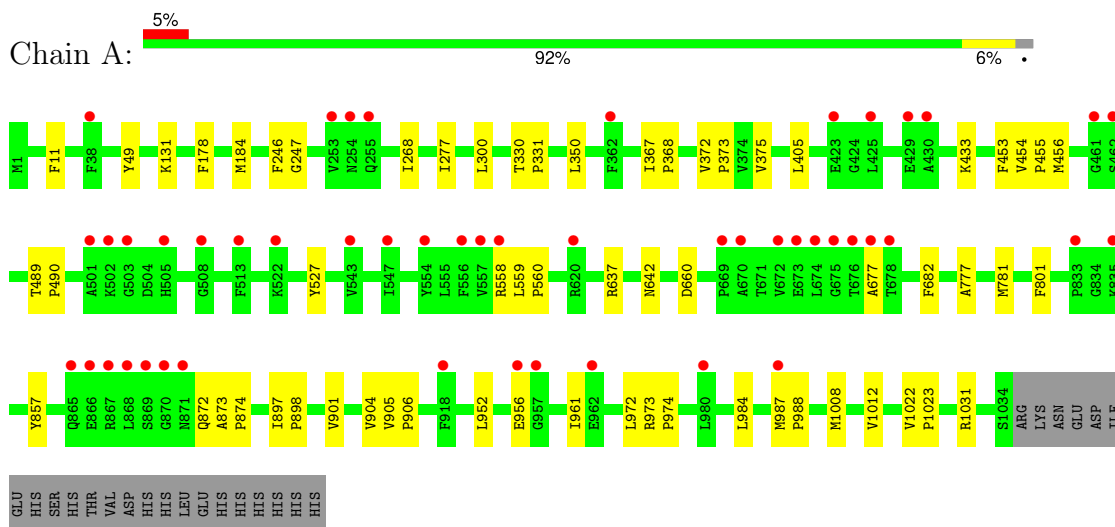
- Molecule 17 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	49	Total 49	O 49	0	0
17	B	35	Total 35	O 35	0	0
17	C	43	Total 43	O 43	0	0
17	D	5	Total 5	O 5	0	0
17	E	1	Total 1	O 1	0	0

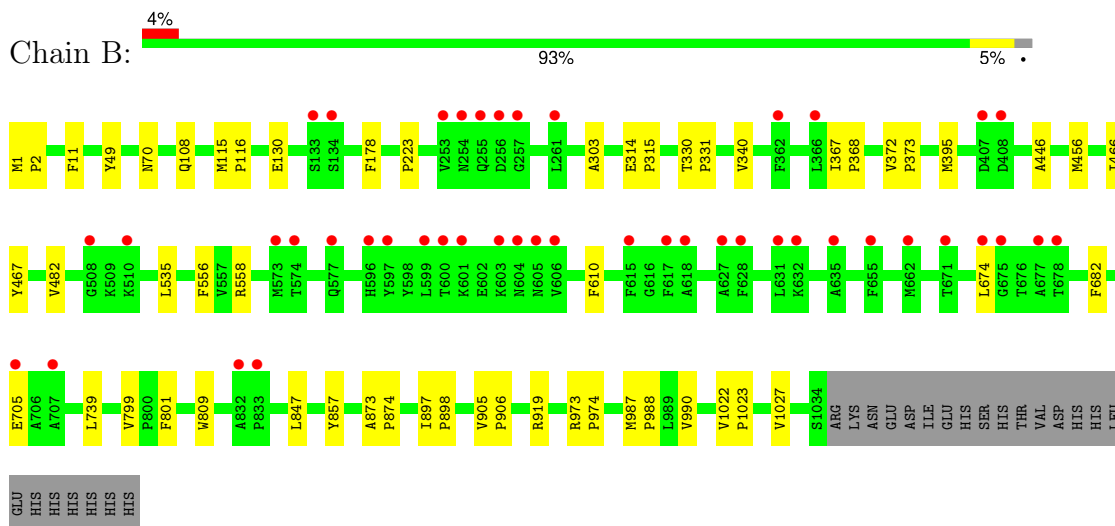
### 3 Residue-property plots [i](#)

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

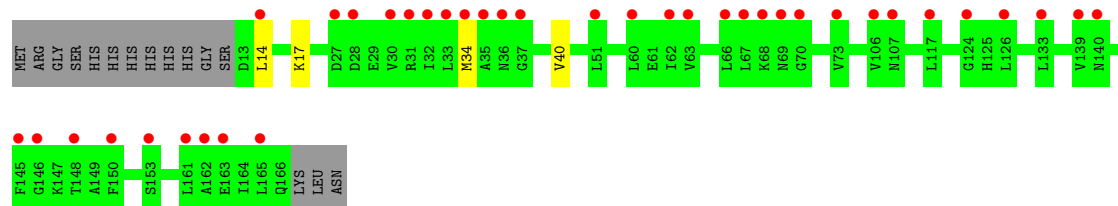


- Molecule 1: Multidrug efflux pump subunit AcrB



- Molecule 1: Multidrug efflux pump subunit AcrB





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	145.97Å 161.95Å 245.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.59 – 2.75 49.59 – 2.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.59-2.75) 100.0 (49.59-2.75)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.65 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.230 , 0.268 0.232 , 0.269	Depositor DCC
$R_{free}$ test set	7492 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.3	Xtriage
Anisotropy	0.699	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 34.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	26599	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: EDO, SO4, D10, D12, 8K6, DDQ, DDR, LMT, C14, OCT, GOL, PTY, MYS, MIY

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	0.67	0/8028	0.71	0/10901
1	B	0.67	0/8023	0.70	0/10895
1	C	0.67	0/8028	0.70	0/10902
2	D	0.68	0/1205	0.71	0/1637
2	E	0.68	0/1186	0.72	0/1613
All	All	0.67	0/26470	0.71	0/35948

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	7874	0	8018	27	0
1	B	7872	0	8014	32	0
1	C	7876	0	8013	27	0
2	D	1186	0	1172	1	0
2	E	1167	0	1151	1	0
3	A	140	0	184	0	0
3	B	35	0	46	0	0
3	C	35	0	46	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	10	0	22	0	0
4	C	10	0	22	0	0
5	A	4	0	6	0	0
5	B	4	0	6	0	0
5	C	8	0	12	0	0
5	E	8	0	12	0	0
6	B	28	0	44	0	0
7	B	15	0	32	0	0
8	B	18	0	38	0	0
9	B	33	0	24	5	0
10	B	6	0	8	0	0
10	C	18	0	24	0	0
10	D	6	0	8	0	0
11	B	8	0	18	0	0
12	B	10	0	0	0	0
12	C	5	0	0	0	0
13	C	12	0	26	0	0
14	C	50	0	79	0	0
15	C	14	0	30	0	0
16	C	14	0	27	0	0
17	A	49	0	0	0	0
17	B	35	0	0	0	0
17	C	43	0	0	0	0
17	D	5	0	0	0	0
17	E	1	0	0	0	0
All	All	26599	0	27082	88	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 2.

The worst 5 of 88 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)
9:B:1105:MIY:H713	9:B:1105:MIY:H81	1.65	0.79
1:B:395[B]:MET:HA	1:B:395[B]:MET:HE2	1.78	0.64
1:B:873:ALA:HB3	1:B:874:PRO:HD3	1.80	0.64
1:B:303:ALA:HB2	1:B:330:THR:HG21	1.84	0.59
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.84	0.58

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	1034/1057 (98%)	1004 (97%)	29 (3%)	1 (0%)	51	75
1	B	1034/1057 (98%)	1004 (97%)	30 (3%)	0	100	100
1	C	1034/1057 (98%)	1010 (98%)	24 (2%)	0	100	100
2	D	155/169 (92%)	150 (97%)	5 (3%)	0	100	100
2	E	152/169 (90%)	146 (96%)	6 (4%)	0	100	100
All	All	3409/3509 (97%)	3314 (97%)	94 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	677	ALA

### 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	842/863 (98%)	834 (99%)	8 (1%)	76	85
1	B	842/863 (98%)	834 (99%)	8 (1%)	76	85
1	C	842/863 (98%)	831 (99%)	11 (1%)	69	81
2	D	121/132 (92%)	120 (99%)	1 (1%)	81	88
2	E	119/132 (90%)	117 (98%)	2 (2%)	60	76
All	All	2766/2853 (97%)	2736 (99%)	30 (1%)	73	84

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	610	PHE
2	D	31	ARG
1	C	49	TYR
2	E	17	LYS
1	C	862	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

31 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	$\# Z  > 2$
7	MYS	B	1103	-	14,14,14	0.09	0	13,13,13	0.06	0
3	LMT	A	1106	-	36,36,36	0.49	0	47,47,47	0.61	0
4	D10	C	1303	-	9,9,9	0.10	0	8,8,8	0.08	0
12	SO4	B	1109	-	4,4,4	0.34	0	6,6,6	0.07	0
15	C14	C	1305	-	13,13,13	0.09	0	12,12,12	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	LMT	C	1302	-	36,36,36	0.44	0	47,47,47	0.49	0
10	GOL	C	1310	-	5,5,5	0.09	0	5,5,5	0.25	0
6	DDR	B	1102	-	27,27,27	0.24	0	29,29,29	0.25	0
9	MIY	B	1105	-	36,36,36	1.09	2 (5%)	42,58,58	1.16	4 (9%)
11	OCT	B	1107	-	7,7,7	0.10	0	6,6,6	0.05	0
8	8K6	B	1104	-	17,17,17	0.07	0	16,16,16	0.06	0
3	LMT	A	1105	-	36,36,36	0.51	0	47,47,47	1.08	3 (6%)
5	EDO	B	1108	-	3,3,3	0.08	0	2,2,2	0.07	0
16	DDQ	C	1311	-	11,13,13	0.20	0	12,15,15	0.20	0
5	EDO	A	1104	-	3,3,3	0.07	0	2,2,2	0.10	0
10	GOL	C	1308	-	5,5,5	0.08	0	5,5,5	0.27	0
5	EDO	C	1306	-	3,3,3	0.08	0	2,2,2	0.06	0
5	EDO	E	202	-	3,3,3	0.06	0	2,2,2	0.13	0
10	GOL	D	201	-	5,5,5	0.09	0	5,5,5	0.28	0
3	LMT	A	1101	-	36,36,36	0.48	0	47,47,47	0.64	0
3	LMT	A	1103	-	36,36,36	0.46	0	47,47,47	0.57	0
3	LMT	B	1101	-	36,36,36	0.43	0	47,47,47	0.46	0
5	EDO	C	1307	-	3,3,3	0.06	0	2,2,2	0.10	0
5	EDO	E	201	-	3,3,3	0.07	0	2,2,2	0.11	0
13	D12	C	1301	-	11,11,11	0.09	0	10,10,10	0.08	0
14	PTY	C	1304	-	49,49,49	0.26	0	52,54,54	0.32	0
10	GOL	C	1309	-	5,5,5	0.09	0	5,5,5	0.28	0
4	D10	A	1102	-	9,9,9	0.10	0	8,8,8	0.09	0
10	GOL	B	1106	-	5,5,5	0.10	0	5,5,5	0.26	0
12	SO4	C	1312	-	4,4,4	0.34	0	6,6,6	0.08	0
12	SO4	B	1110	-	4,4,4	0.34	0	6,6,6	0.08	0

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
7	MYS	B	1103	-	-	2/12/12/12	-
3	LMT	A	1106	-	-	13/21/61/61	0/2/2/2
4	D10	C	1303	-	-	0/7/7/7	-
15	C14	C	1305	-	-	5/11/11/11	-
3	LMT	C	1302	-	-	7/21/61/61	0/2/2/2
10	GOL	C	1310	-	-	0/4/4/4	-
6	DDR	B	1102	-	-	14/29/29/29	-
9	MIY	B	1105	-	-	0/12/70/70	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	OCT	B	1107	-	-	2/5/5/5	-
8	8K6	B	1104	-	-	8/15/15/15	-
3	LMT	A	1105	-	-	13/21/61/61	0/2/2/2
5	EDO	B	1108	-	-	1/1/1/1	-
16	DDQ	C	1311	-	-	2/11/11/11	-
5	EDO	A	1104	-	-	0/1/1/1	-
10	GOL	C	1308	-	-	0/4/4/4	-
5	EDO	C	1306	-	-	1/1/1/1	-
5	EDO	E	202	-	-	0/1/1/1	-
10	GOL	D	201	-	-	2/4/4/4	-
3	LMT	A	1101	-	-	8/21/61/61	0/2/2/2
3	LMT	A	1103	-	-	11/21/61/61	0/2/2/2
3	LMT	B	1101	-	-	6/21/61/61	0/2/2/2
5	EDO	C	1307	-	-	1/1/1/1	-
5	EDO	E	201	-	-	0/1/1/1	-
13	D12	C	1301	-	-	3/9/9/9	-
14	PTY	C	1304	-	-	30/53/53/53	-
10	GOL	C	1309	-	-	2/4/4/4	-
4	D10	A	1102	-	-	1/7/7/7	-
10	GOL	B	1106	-	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	1105	MIY	C21-N2	5.17	1.48	1.33
9	B	1105	MIY	O5-C15	2.27	1.28	1.23

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1105	LMT	C4B-C3B-C2B	3.98	117.82	110.83
3	A	1105	LMT	C3B-C4B-C5B	3.11	115.87	110.23
3	A	1105	LMT	C1B-C2B-C3B	2.94	116.20	110.01
9	B	1105	MIY	C19-N1-C4	2.65	120.14	114.10
9	B	1105	MIY	C18-C1-C2	2.41	119.58	115.75

There are no chirality outliers.

5 of 132 torsion outliers are listed below:

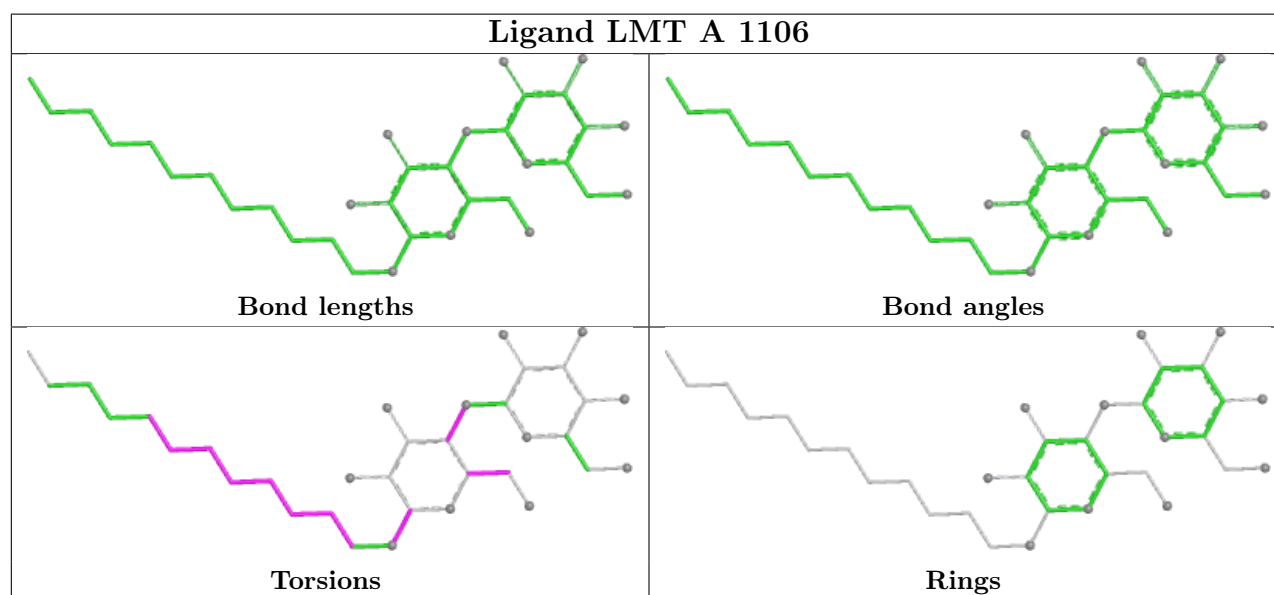
Mol	Chain	Res	Type	Atoms
3	A	1105	LMT	C2'-C1'-O1'-C1
3	A	1105	LMT	O5'-C1'-O1'-C1
10	C	1309	GOL	C1-C2-C3-O3
10	D	201	GOL	C1-C2-C3-O3
14	C	1304	PTY	N1-C2-C3-O11

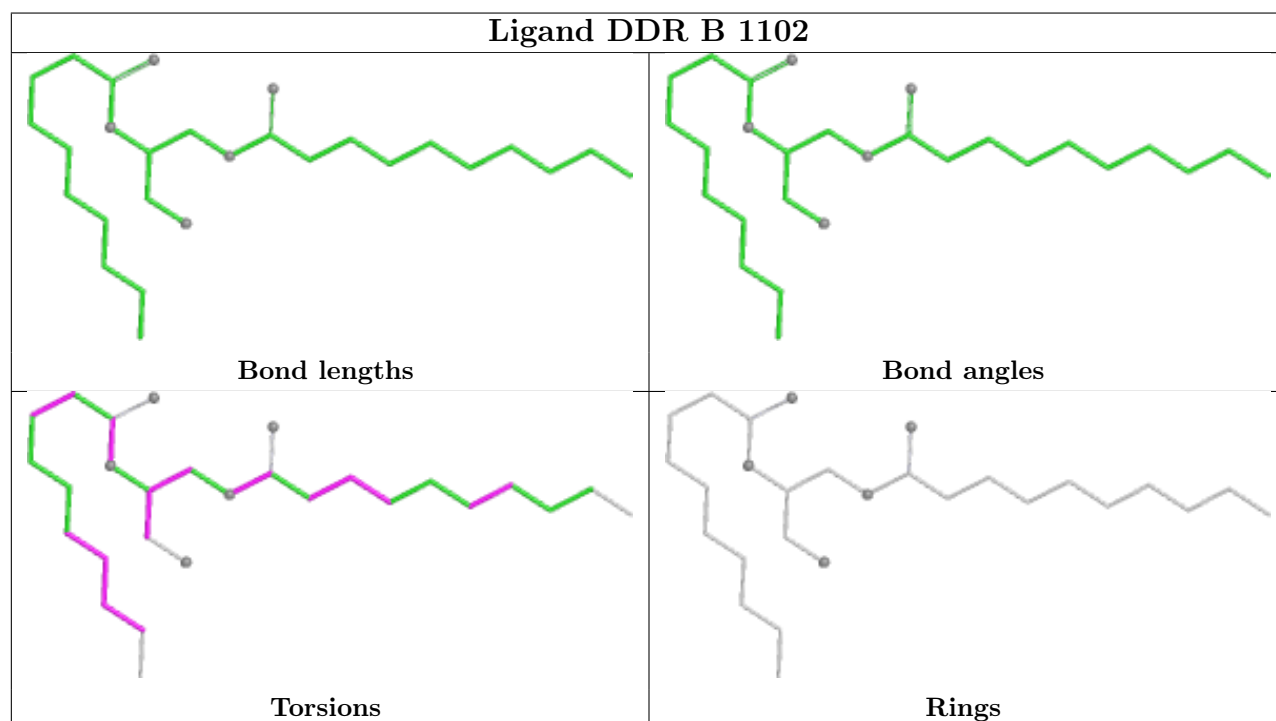
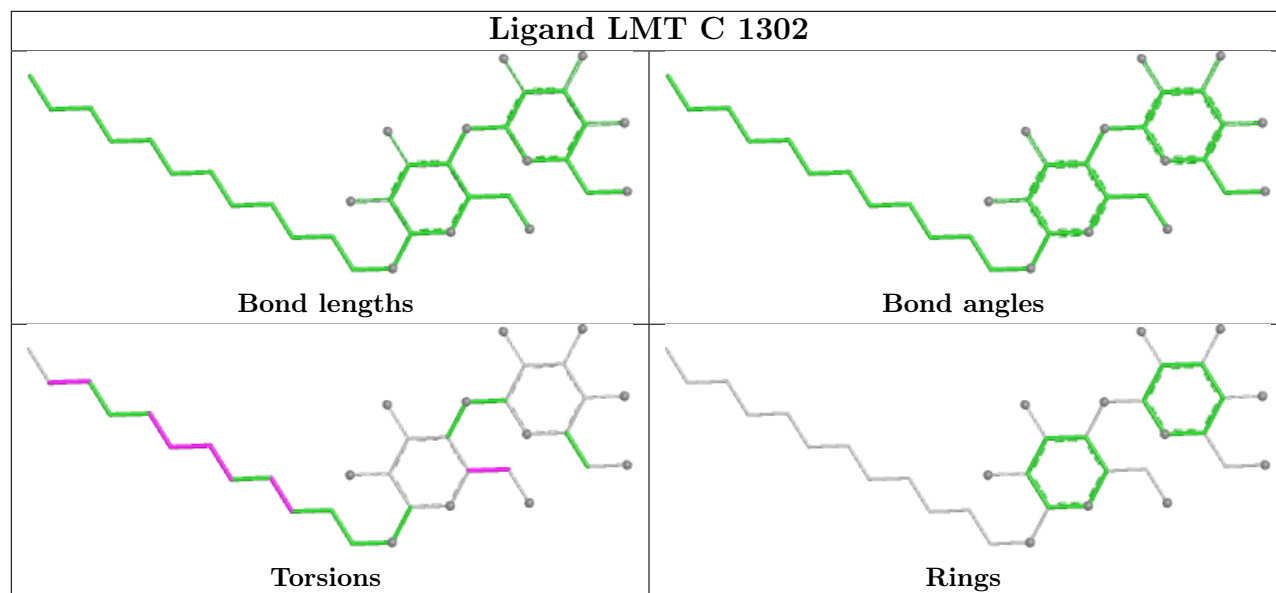
There are no ring outliers.

1 monomer is involved in 5 short contacts:

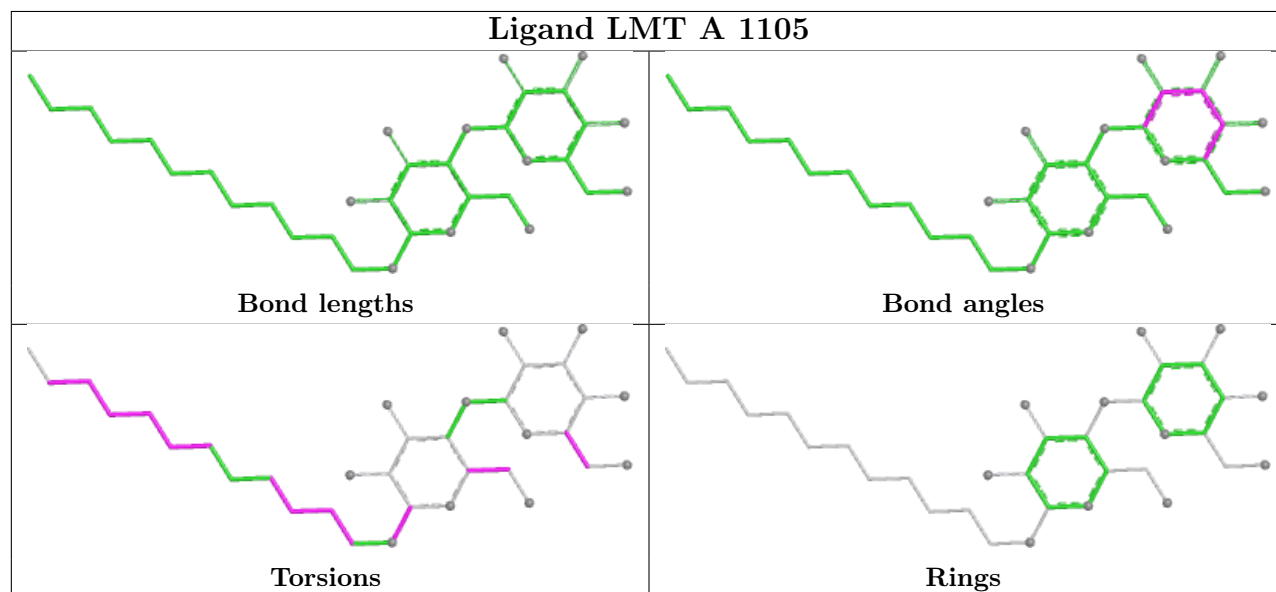
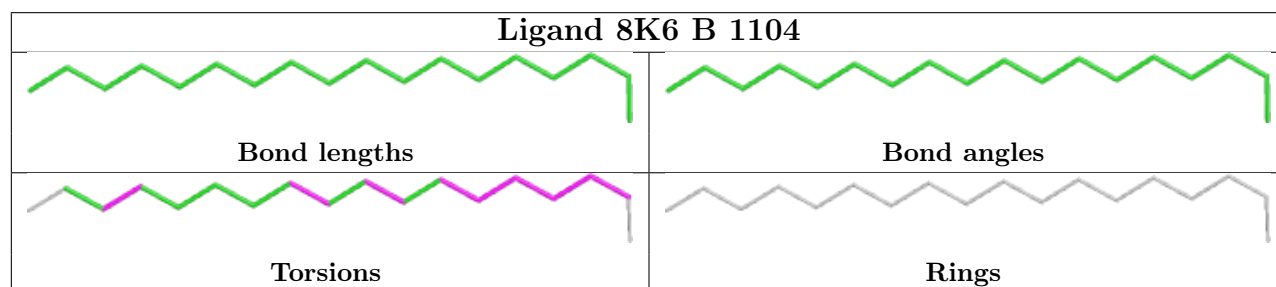
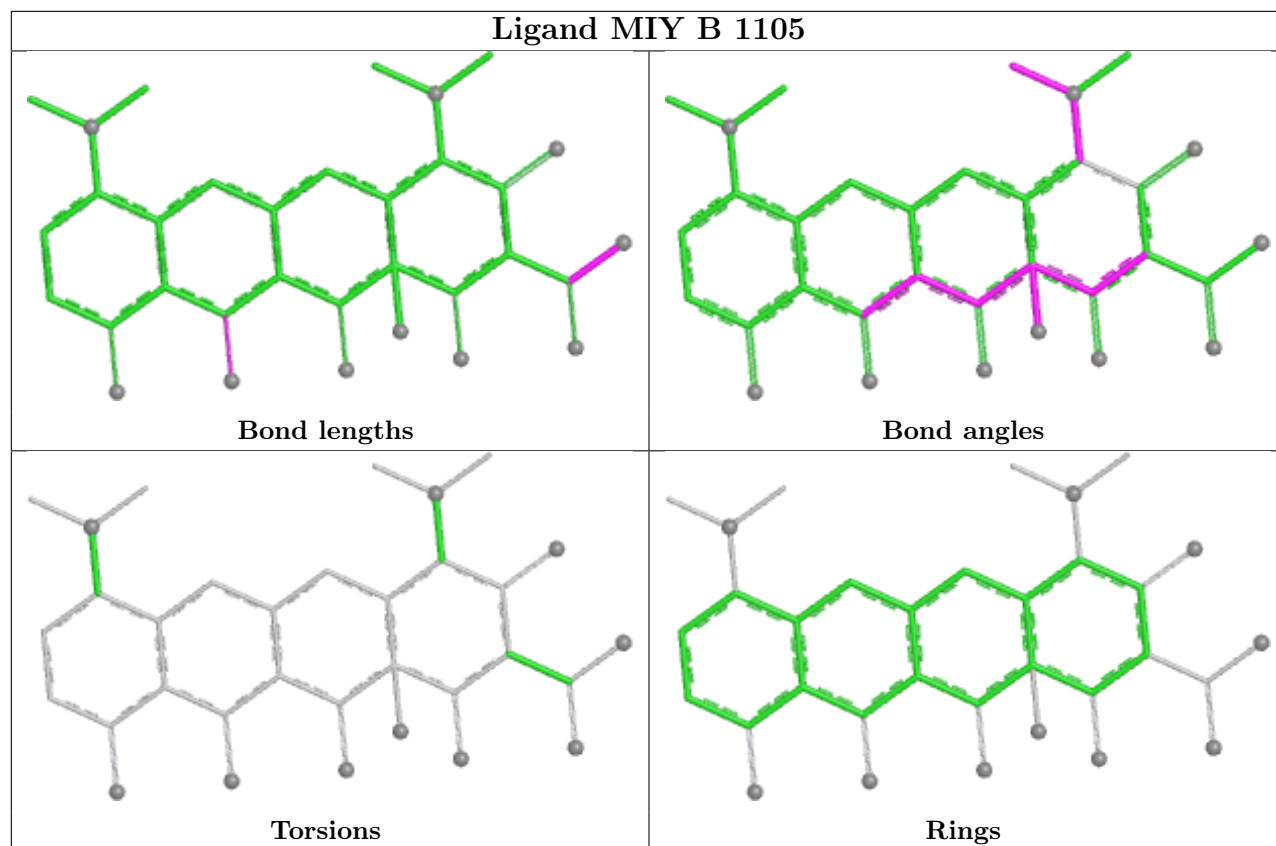
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	1105	MIY	5	0

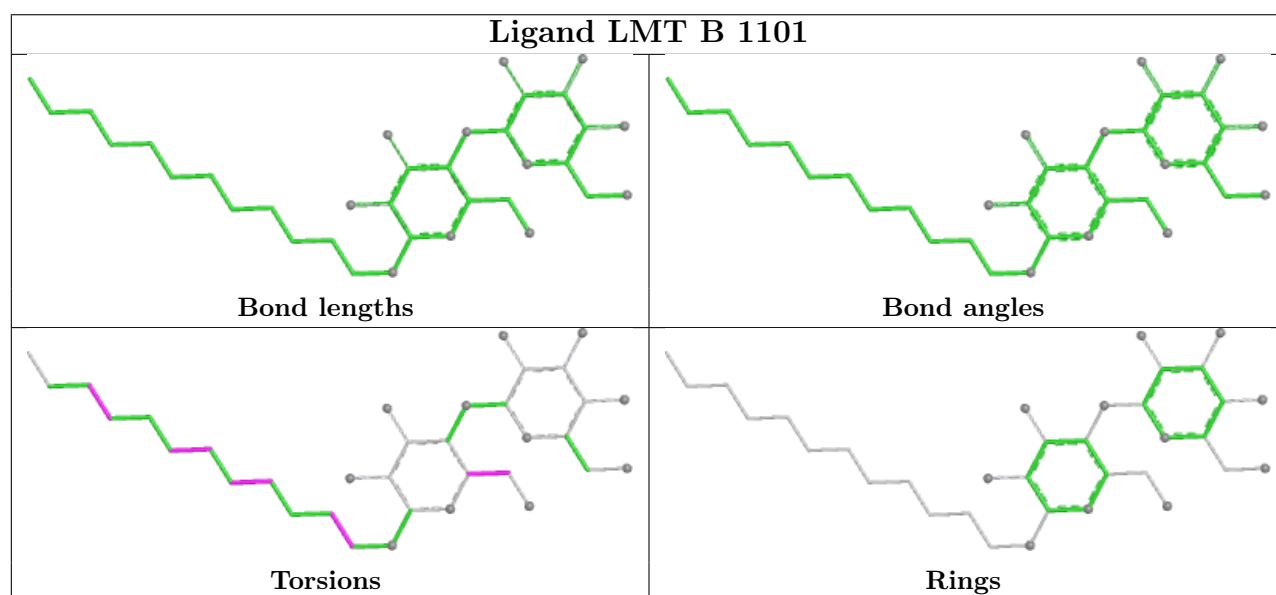
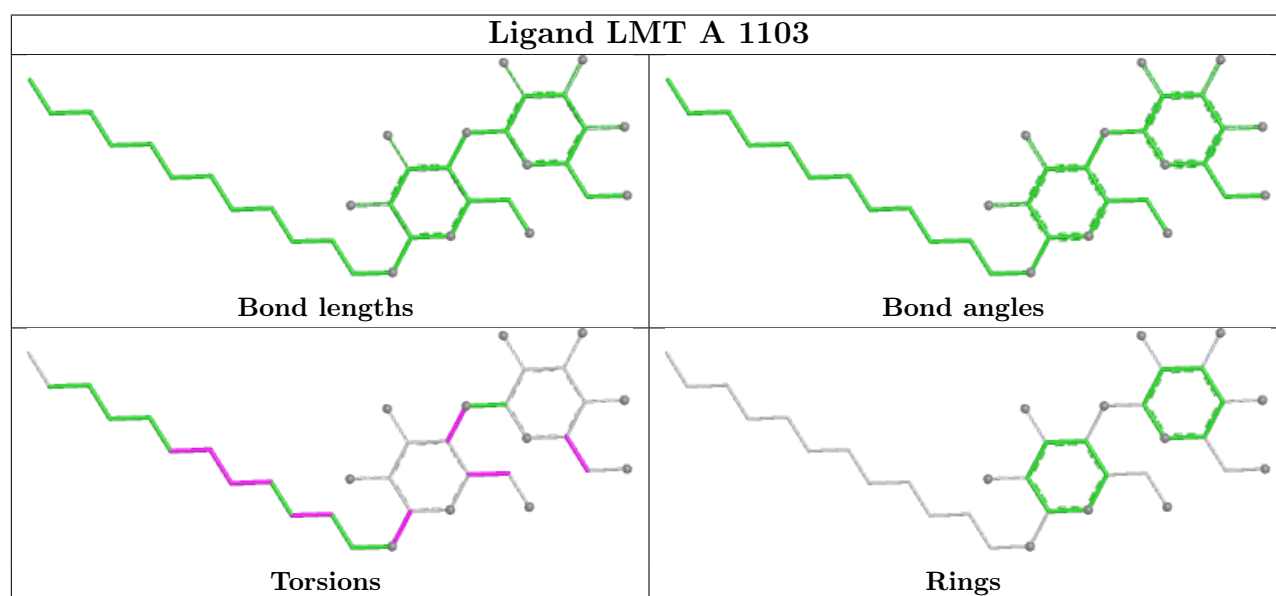
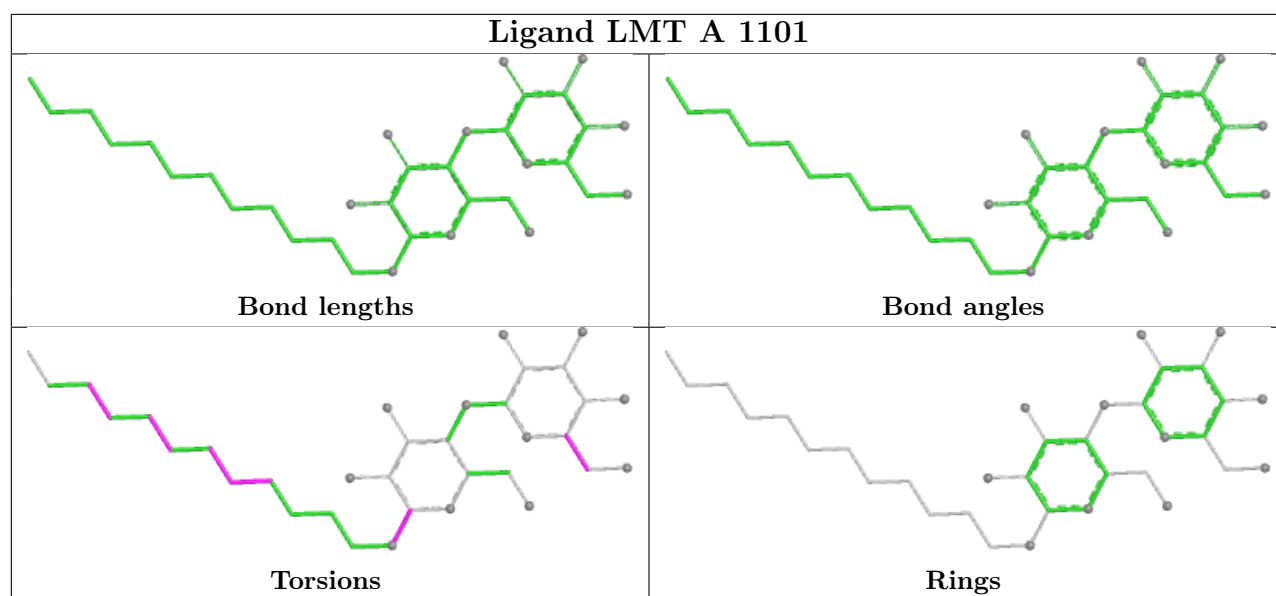
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

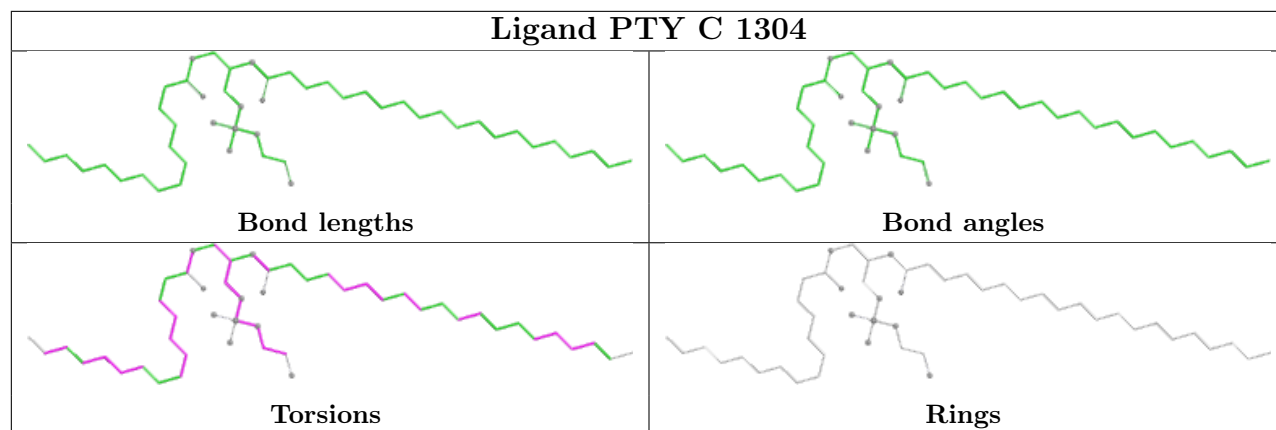












## 5.7 Other polymers [i](#)

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	1034/1057 (97%)	0.34	49 (4%)	31 37	39, 67, 108, 151	0
1	B	1034/1057 (97%)	0.25	45 (4%)	34 41	40, 64, 88, 101	0
1	C	1034/1057 (97%)	0.22	36 (3%)	44 52	42, 59, 82, 98	0
2	D	157/169 (92%)	0.46	8 (5%)	28 34	55, 66, 89, 105	0
2	E	154/169 (91%)	1.31	38 (24%)	0 0	58, 75, 100, 106	0
All	All	3413/3509 (97%)	0.33	176 (5%)	27 33	39, 63, 96, 151	0

The worst 5 of 176 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	35	ALA	8.5
1	A	675	GLY	8.5
1	A	673	GLU	8.0
2	E	68	LYS	6.1
1	A	677	ALA	5.9

### 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,

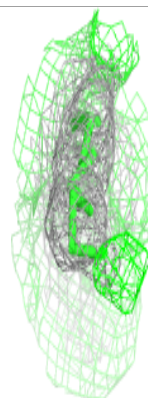
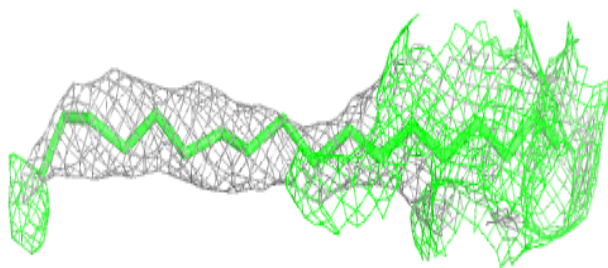
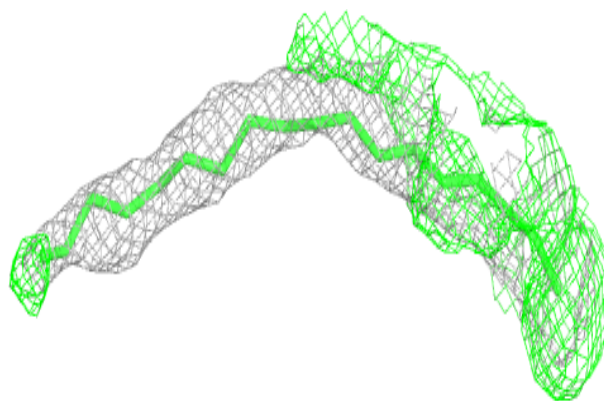
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
10	GOL	C	1310	6/6	0.68	0.20	77,77,78,78	0
8	8K6	B	1104	18/18	0.71	0.27	85,90,91,91	0
3	LMT	A	1105	35/35	0.72	0.26	89,117,121,122	0
5	EDO	C	1307	4/4	0.75	0.35	67,68,68,68	0
10	GOL	C	1309	6/6	0.80	0.22	82,82,83,83	0
3	LMT	A	1103	35/35	0.81	0.25	95,110,121,121	0
3	LMT	A	1106	35/35	0.81	0.27	92,101,112,112	0
14	PTY	C	1304	50/50	0.82	0.34	93,97,102,103	0
4	D10	A	1102	10/10	0.83	0.34	80,81,82,82	0
13	D12	C	1301	12/12	0.83	0.26	81,83,84,85	0
3	LMT	A	1101	35/35	0.83	0.32	121,123,125,125	0
15	C14	C	1305	14/14	0.83	0.26	70,73,76,76	0
12	SO4	B	1109	5/5	0.84	0.24	120,121,121,121	0
5	EDO	A	1104	4/4	0.84	0.29	63,63,64,64	0
3	LMT	B	1101	35/35	0.85	0.33	94,98,113,113	0
5	EDO	C	1306	4/4	0.85	0.25	49,49,49,50	0
10	GOL	D	201	6/6	0.85	0.36	88,88,89,89	0
11	OCT	B	1107	8/8	0.85	0.22	77,78,78,78	0
16	DDQ	C	1311	14/14	0.85	0.28	70,70,70,70	0
6	DDR	B	1102	28/28	0.86	0.28	86,90,94,94	0
10	GOL	C	1308	6/6	0.87	0.17	81,82,82,82	0
4	D10	C	1303	10/10	0.87	0.26	77,79,81,81	0
7	MYS	B	1103	15/15	0.88	0.42	84,85,86,86	0
9	MIY	B	1105	33/33	0.88	0.23	88,89,90,90	0
3	LMT	C	1302	35/35	0.89	0.22	75,79,90,90	0
5	EDO	E	201	4/4	0.89	0.23	82,82,82,82	0
12	SO4	B	1110	5/5	0.90	0.18	105,106,106,106	0
5	EDO	E	202	4/4	0.93	0.18	61,61,61,61	0
5	EDO	B	1108	4/4	0.93	0.10	59,59,59,59	0
10	GOL	B	1106	6/6	0.94	0.20	65,65,66,66	0
12	SO4	C	1312	5/5	0.95	0.11	87,87,87,87	0

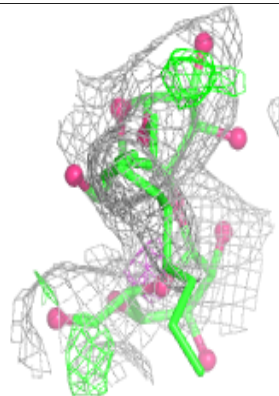
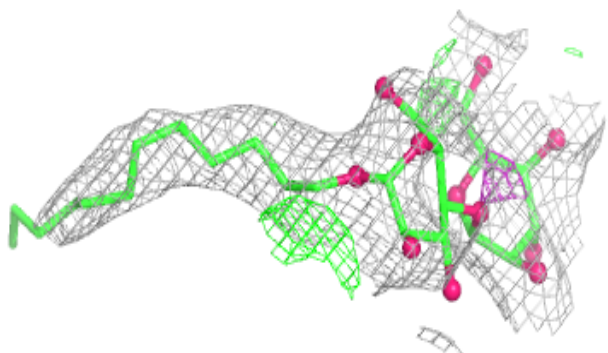
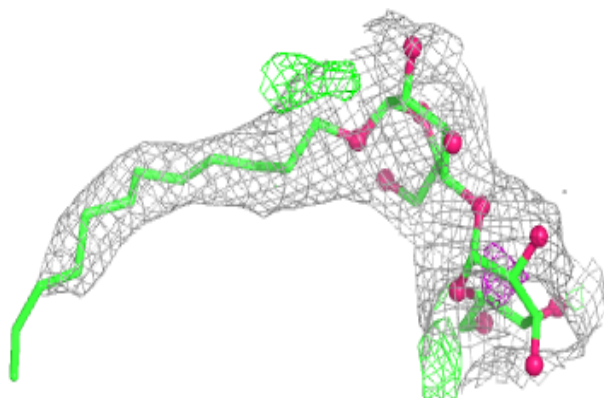
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 8K6 B 1104:**

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

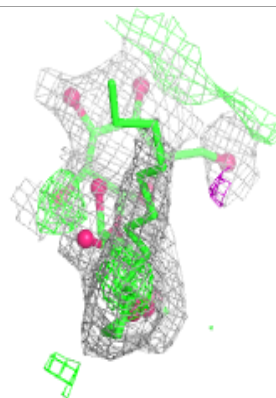
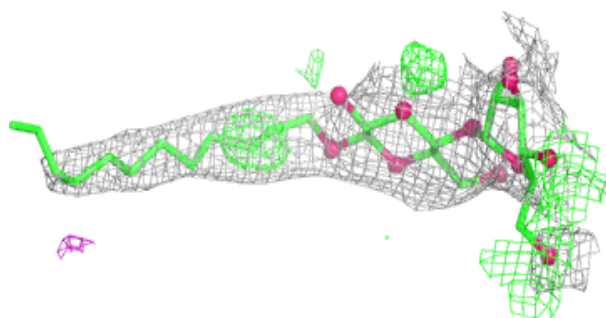
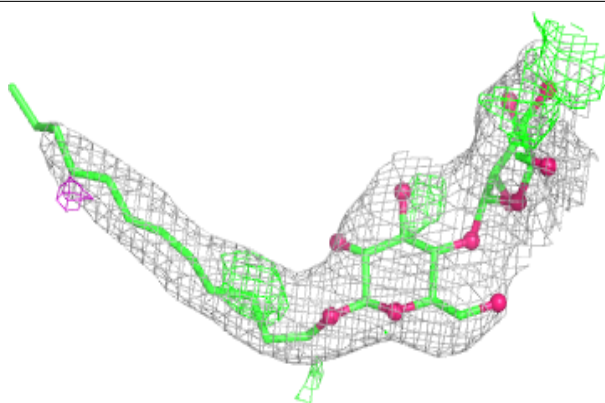
**Electron density around LMT A 1105:**

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

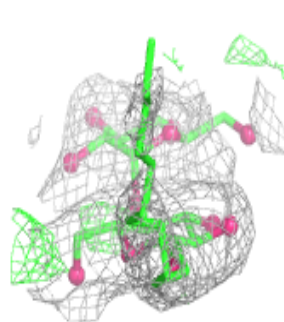
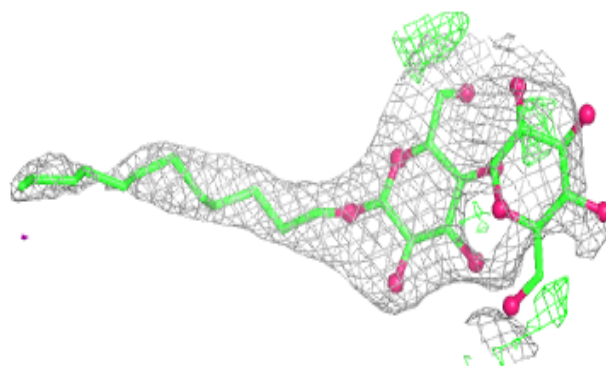
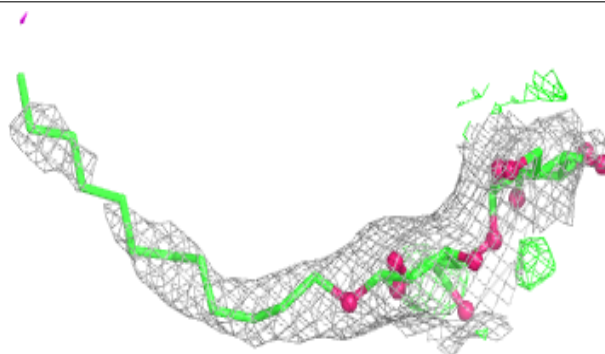


**Electron density around LMT A 1103:**

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

**Electron density around LMT A 1106:**

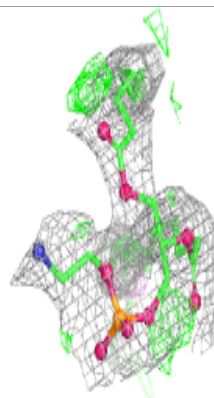
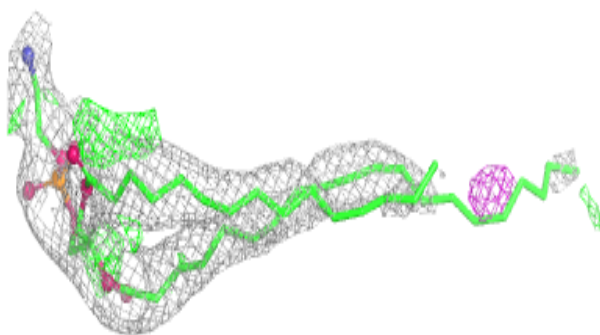
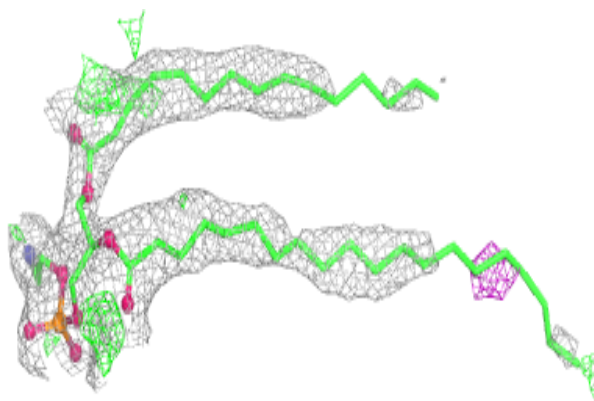
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



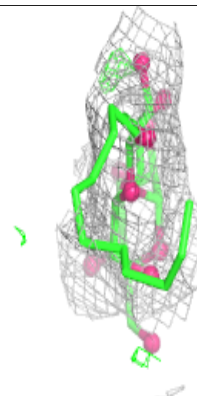
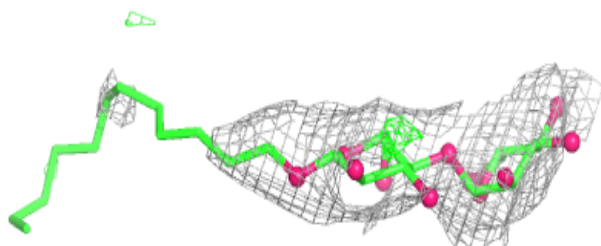
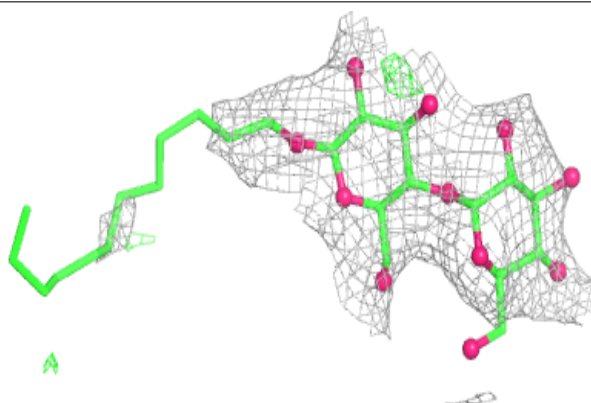


**Electron density around PTY C 1304:**

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

**Electron density around LMT A 1101:**

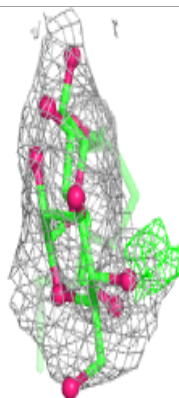
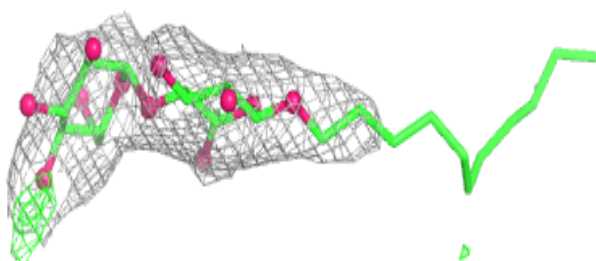
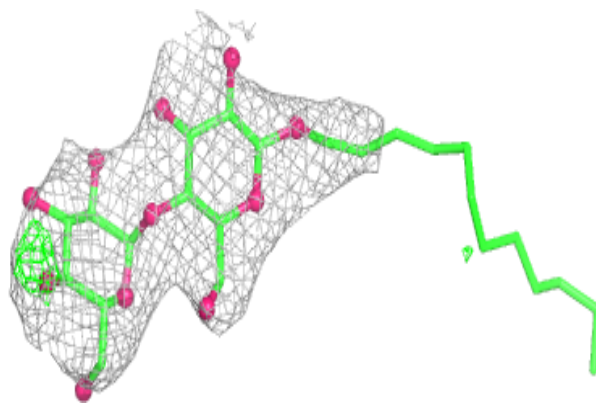
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



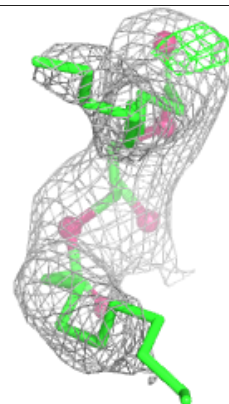
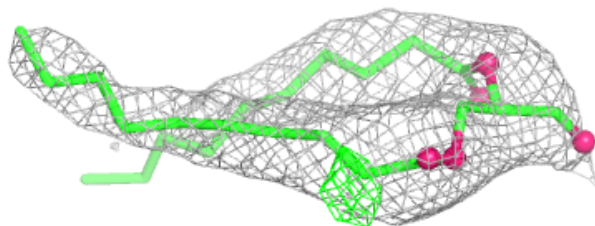
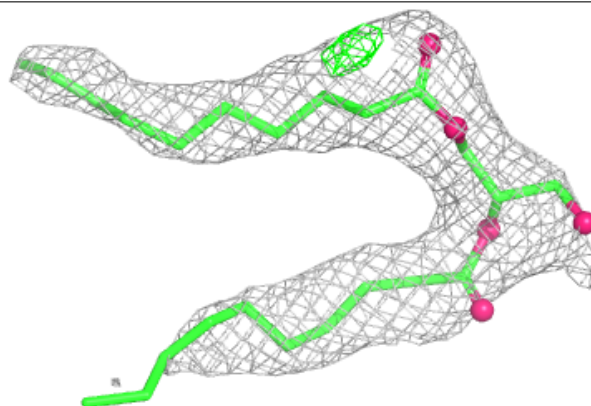


**Electron density around LMT B 1101:**

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

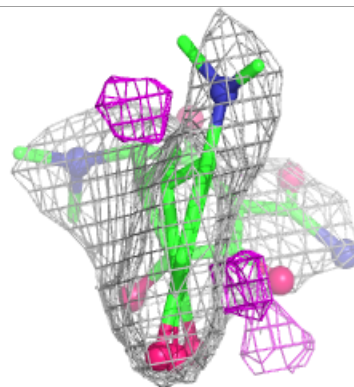
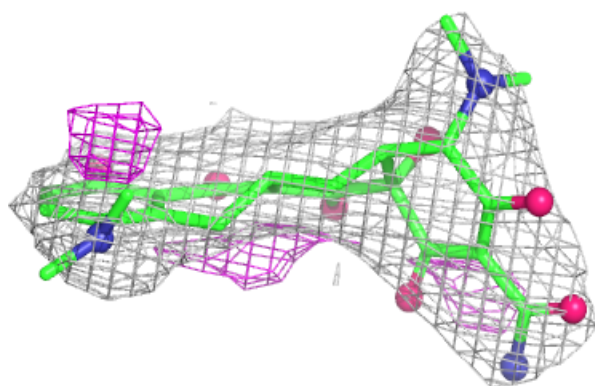
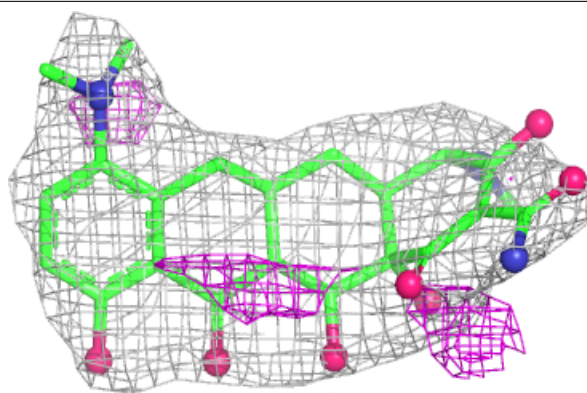
**Electron density around DDR B 1102:**

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

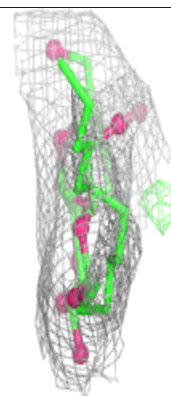
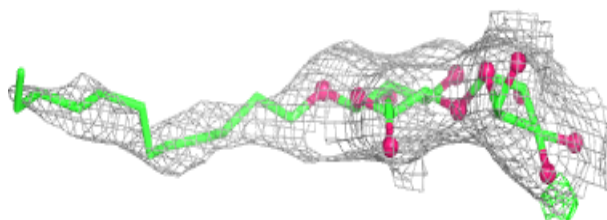
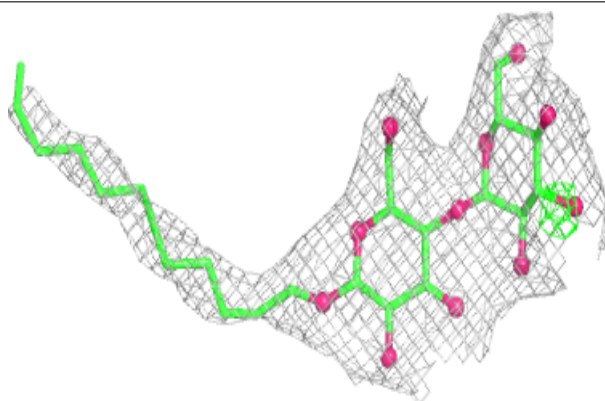


**Electron density around MIY B 1105:**

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

**Electron density around LMT C 1302:**

$2mF_o-DF_c$  (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.