



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 20, 2021 – 03:10 pm GMT

PDB ID : 7OUK  
Title : BDM88855 inhibitor bound to the transmembrane domain of AcrB  
Authors : Tam, H.K.; Foong, W.E.; Pos, K.M.  
Deposited on : 2021-06-12  
Resolution : 2.60 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 : 2.24  
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) : 2.24

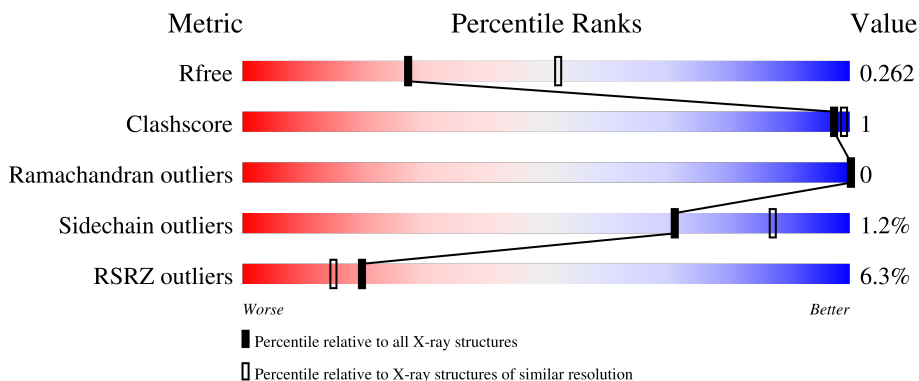
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	 7% 95%
1	B	1057	 5% 94%
1	C	1057	 3% 94%
2	D	169	 9% 91% 8%
2	E	169	 21% 89% 9%

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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
5	EDO	C	1712	-	-	-	X
6	OCT	C	1704	-	-	-	X
8	GOL	B	1512	-	-	-	X

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 26935 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
			Total	C	N	O	S			
1	A	1033	7873	5066	1299	1463	45	0	1	0
1	B	1036	7883	5072	1303	1463	45	0	1	0
1	C	1033	7874	5067	1303	1460	44	0	3	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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	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	1050	LEU	-	expression tag	UNP P31224
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

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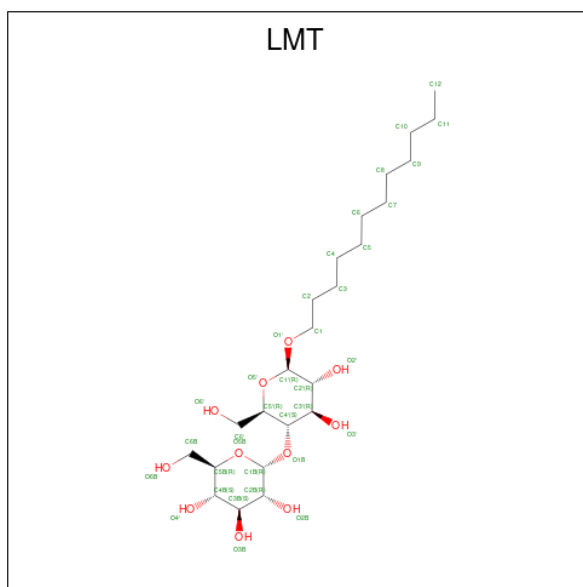
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Chain	Residue	Modelled	Actual	Comment	Reference
C	1057	HIS	-	expression tag	UNP P31224

- Molecule 2 is a protein called DARPIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	156	1182	745	207	229	1	0	0	0
2	E	153	1159	732	203	223	1	0	0	0

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



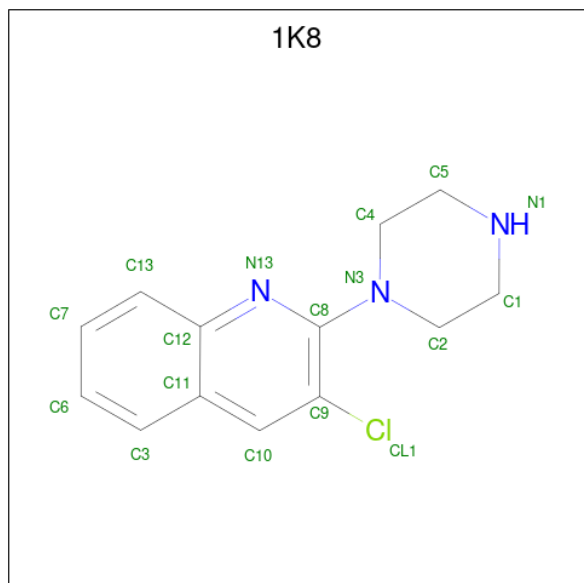
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	35	24	11	0	0
3	A	1	35	24	11	0	0
3	A	1	35	24	11	0	0
3	B	1	35	24	11	0	0
3	B	1	35	24	11	0	0
3	B	1	35	24	11	0	0

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

- Molecule 4 is 3-chloranyl-2-piperazin-1-yl-quinoline (three-letter code: 1K8) (formula:  $C_{13}H_{14}ClN_3$ ) (labeled as "Ligand of Interest" by depositor).



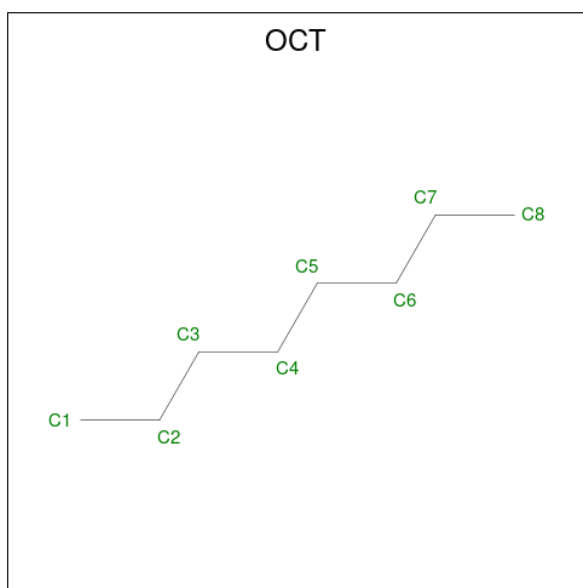
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	0	0
			17	13	1	3		
4	B	1	Total	C	Cl	N	0	0
			17	13	1	3		

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



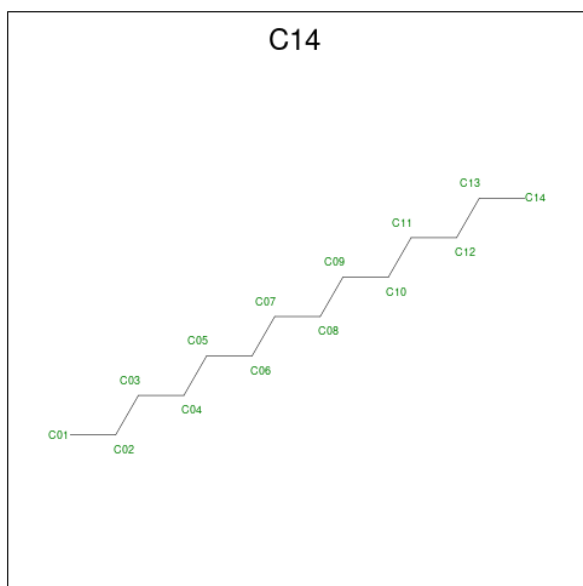
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0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

- Molecule 6 is N-OCTANE (three-letter code: OCT) (formula:  $C_8H_{18}$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C 8 8	0	0
6	C	1	Total C 8 8	0	0
6	C	1	Total C 8 8	0	0

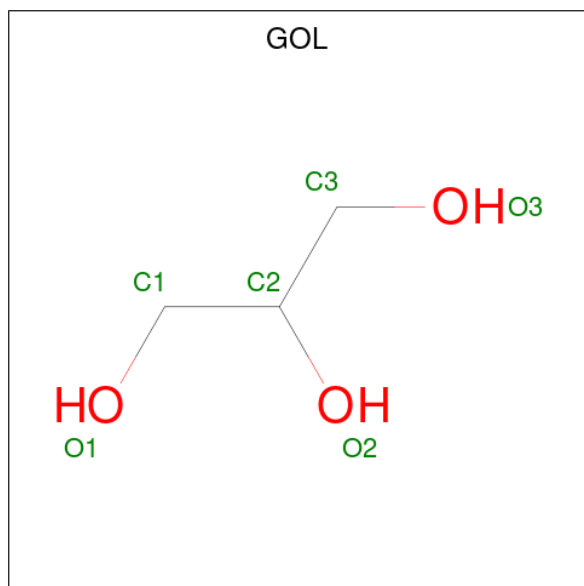
- Molecule 7 is TETRADECANE (three-letter code: C14) (formula:  $C_{14}H_{30}$ ).





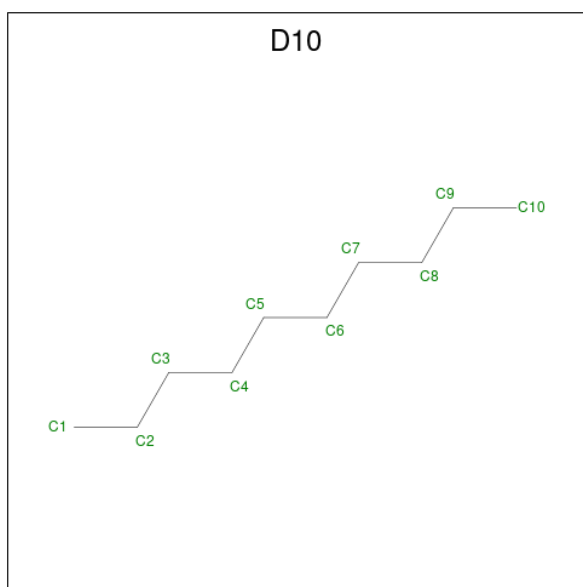
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C 14 14	0	0
7	A	1	Total C 14 14	0	0
7	C	1	Total C 14 14	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



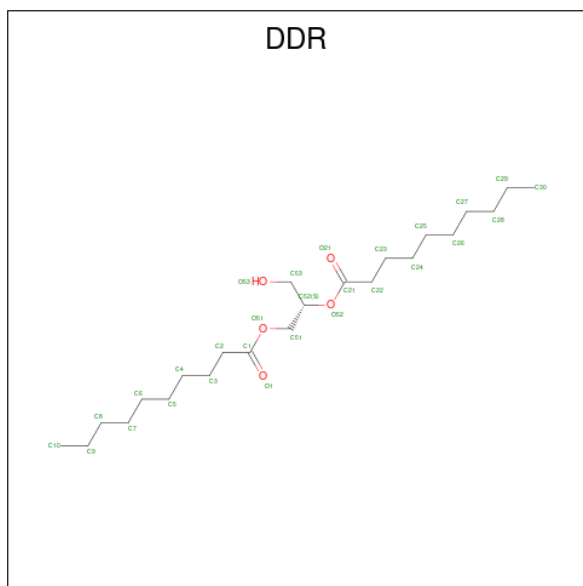
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 6 3 3	0	0
8	B	1	Total C O 6 3 3	0	0
8	B	1	Total C O 6 3 3	0	0
8	B	1	Total C O 6 3 3	0	0
8	B	1	Total C O 6 3 3	0	0
8	C	1	Total C O 6 3 3	0	0

- Molecule 9 is DECANE (three-letter code: D10) (formula:  $C_{10}H_{22}$ ).



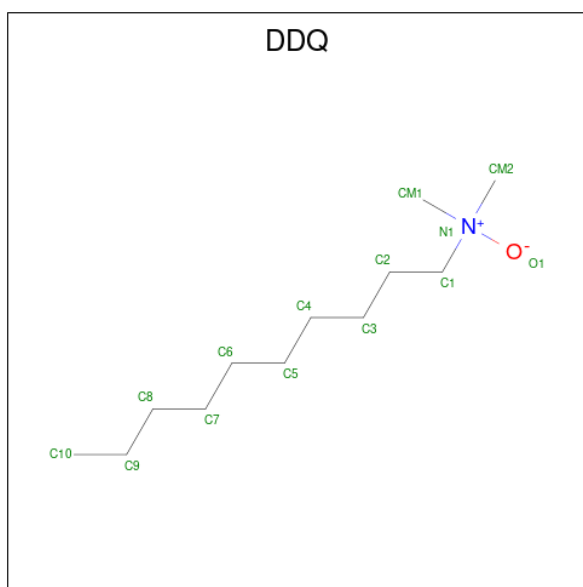
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C 10 10	0	0

- Molecule 10 is (2S)-3-hydroxypropane-1,2-diyl didecanoate (three-letter code: DDR) (formula:  $C_{23}H_{44}O_5$ ).



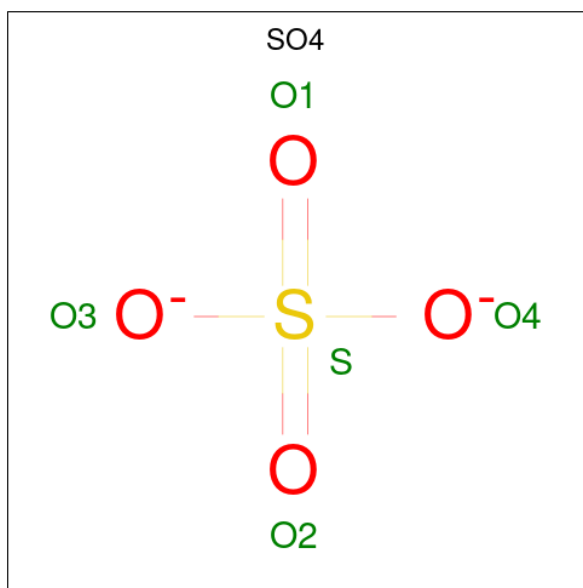
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total C O 28 23 5	0	0

- Molecule 11 is DECYLAMINE-N,N-DIMETHYL-N-OXIDE (three-letter code: DDQ) (formula:  $C_{12}H_{27}NO$ ).



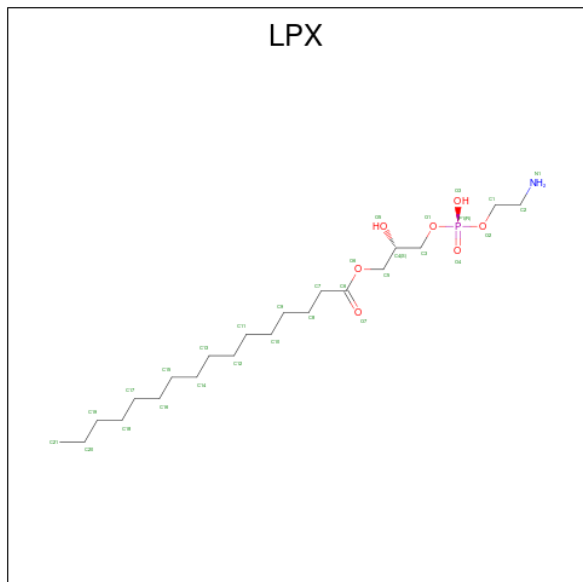
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
11	B	1	14	12	1	1	0	0

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



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

- Molecule 13 is (2S)-3-[[[(R)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy]-2-hydroxypropyl hexadecanoate (three-letter code: LPX) (formula: C<sub>21</sub>H<sub>44</sub>NO<sub>7</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
13	C	1	30	21	1	7	1	0	0
13	C	1	30	21	1	7	1	0	0

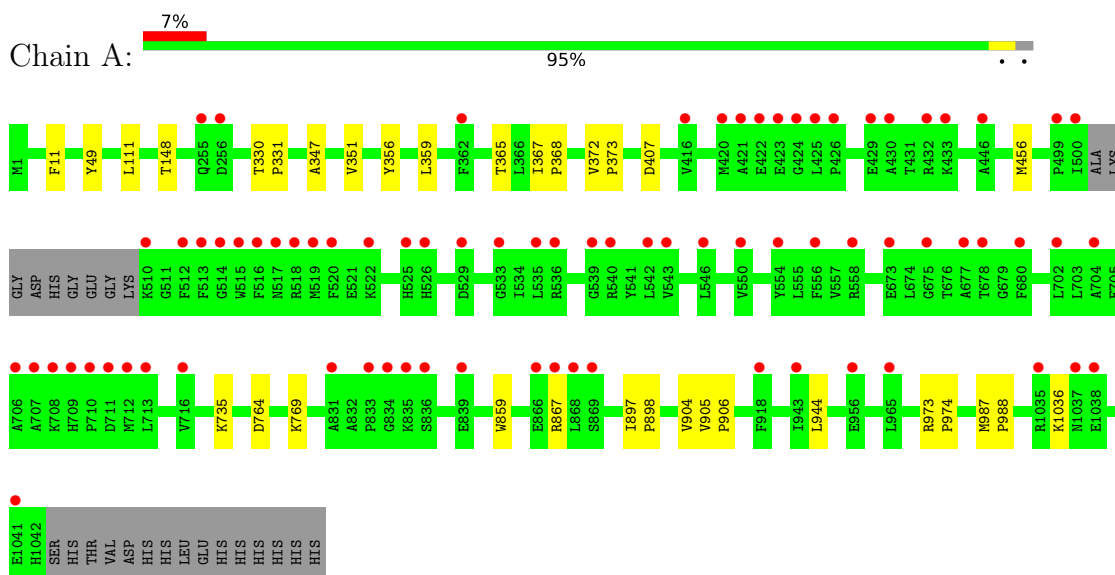
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	128	Total	O	0	0
			128	128		
14	B	94	Total	O	0	0
			94	94		
14	C	120	Total	O	0	0
			120	120		
14	D	14	Total	O	0	0
			14	14		
14	E	9	Total	O	0	0
			9	9		

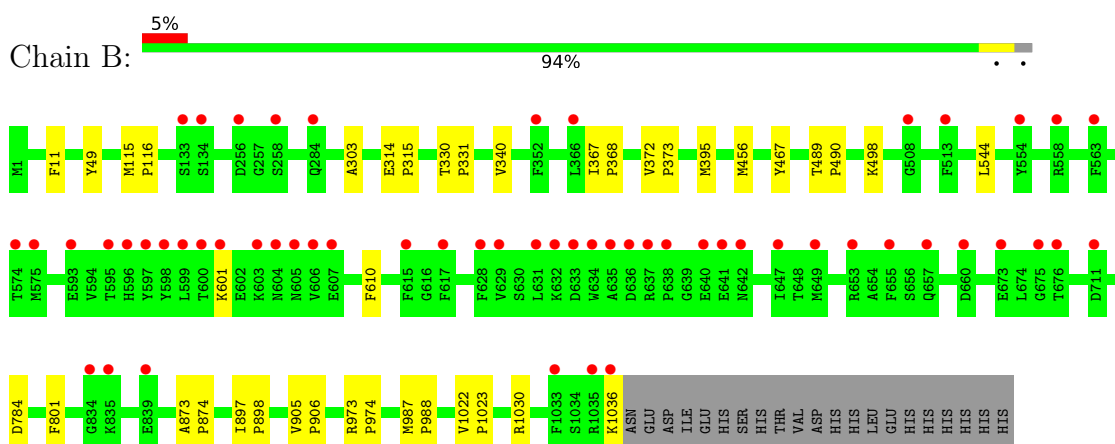
### 3 Residue-property plots [i](#)

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

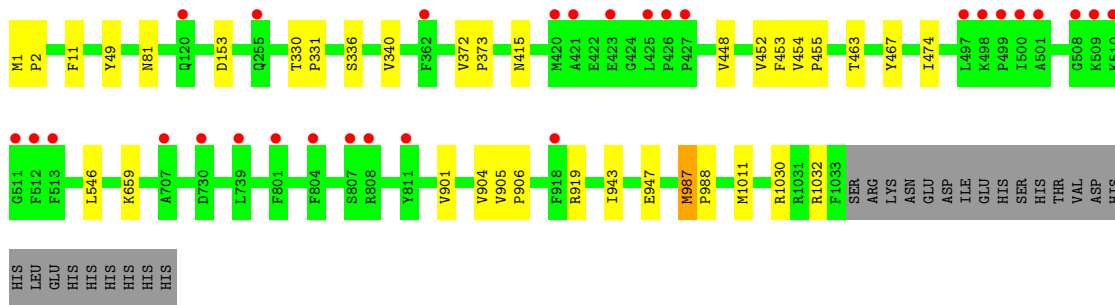


- Molecule 1: Multidrug efflux pump subunit AcrB

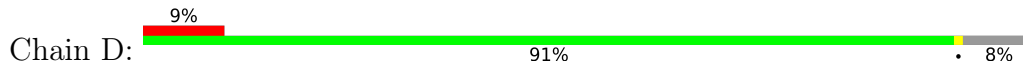


- Molecule 1: Multidrug efflux pump subunit AcrB

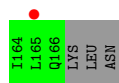
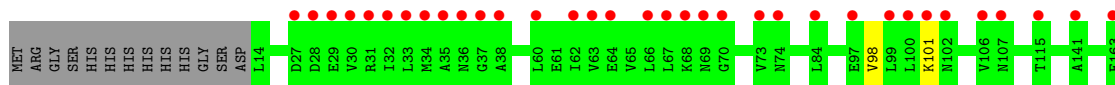
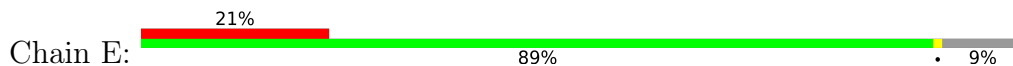




● Molecule 2: DARPIN



● Molecule 2: DARPIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	146.13Å 159.65Å 245.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.05 – 2.60 49.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.05-2.60) 99.9 (49.00-2.60)	Depositor EDS
$R_{merge}$	0.23	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.99 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.236 , 0.263 0.237 , 0.262	Depositor DCC
$R_{free}$ test set	8846 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.8	Xtriage
Anisotropy	0.528	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>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	26935	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.13% 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: D10, DDR, 1K8, LPX, OCT, GOL, DDQ, EDO, LMT, C14, SO4

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	0/8022	0.70	0/10893
1	B	0.67	0/8033	0.70	0/10906
1	C	0.67	0/8030	0.70	0/10904
2	D	0.68	0/1201	0.71	0/1632
2	E	0.68	0/1178	0.71	0/1602
All	All	0.67	0/26464	0.70	0/35937

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	7873	0	8022	12	0
1	B	7883	0	8040	17	0
1	C	7874	0	8035	12	0
2	D	1182	0	1169	1	0
2	E	1159	0	1147	1	0
3	A	105	0	138	0	0
3	B	105	0	138	0	0
3	C	70	0	92	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	17	0	0	0	0
4	B	17	0	0	1	0
5	A	20	0	30	0	0
5	B	20	0	30	0	0
5	C	16	0	24	0	0
6	A	8	0	18	0	0
6	C	16	0	36	0	0
7	A	28	0	60	0	0
7	C	14	0	30	0	0
8	A	6	0	8	0	0
8	B	24	0	32	0	0
8	C	6	0	8	0	0
9	B	10	0	22	0	0
10	B	28	0	44	0	0
11	B	14	0	27	0	0
12	B	10	0	0	0	0
12	C	5	0	0	0	0
13	C	60	0	86	0	0
14	A	128	0	0	0	0
14	B	94	0	0	0	0
14	C	120	0	0	0	0
14	D	14	0	0	0	0
14	E	9	0	0	0	0
All	All	26935	0	27236	44	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 1.

The worst 5 of 44 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:372:VAL:HB	1:C:373:PRO:HD3	1.88	0.56
1:A:356:TYR:HA	1:A:365:THR:HG21	1.87	0.55
1:C:454:VAL:HB	1:C:455:PRO:HD3	1.91	0.52
1:A:372:VAL:HB	1:A:373:PRO:HD3	1.94	0.49
1:C:901:VAL:O	1:C:904:VAL:HG12	2.12	0.49

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	1030/1057 (97%)	989 (96%)	41 (4%)	0	100	100
1	B	1035/1057 (98%)	1011 (98%)	24 (2%)	0	100	100
1	C	1034/1057 (98%)	1007 (97%)	27 (3%)	0	100	100
2	D	154/169 (91%)	151 (98%)	3 (2%)	0	100	100
2	E	151/169 (89%)	145 (96%)	6 (4%)	0	100	100
All	All	3404/3509 (97%)	3303 (97%)	101 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	844/863 (98%)	834 (99%)	10 (1%)	71	87
1	B	843/863 (98%)	833 (99%)	10 (1%)	71	87
1	C	842/863 (98%)	829 (98%)	13 (2%)	65	83
2	D	121/132 (92%)	121 (100%)	0	100	100
2	E	118/132 (89%)	118 (100%)	0	100	100
All	All	2768/2853 (97%)	2735 (99%)	33 (1%)	71	87

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	947	GLU
1	C	987	MET
1	C	1032	ARG
1	B	498	LYS
1	B	49	TYR

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](#)

44 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	$\# Z  > 2$
5	EDO	A	1110	-	3,3,3	0.06	0	2,2,2	0.17	0
8	GOL	B	1509	-	5,5,5	0.09	0	5,5,5	0.26	0
3	LMT	C	1708	-	36,36,36	0.58	1 (2%)	47,47,47	0.94	3 (6%)
5	EDO	C	1710	-	3,3,3	0.06	0	2,2,2	0.16	0
5	EDO	C	1702	-	3,3,3	0.07	0	2,2,2	0.19	0
8	GOL	A	1107	-	5,5,5	0.11	0	5,5,5	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	1K8	B	1516	-	19,19,19	2.79	4 (21%)	24,26,26	1.49	5 (20%)
5	EDO	C	1711	-	3,3,3	0.05	0	2,2,2	0.21	0
9	D10	B	1505	-	9,9,9	0.10	0	8,8,8	0.06	0
8	GOL	B	1511	-	5,5,5	0.09	0	5,5,5	0.31	0
4	1K8	A	1102	-	19,19,19	2.66	5 (26%)	24,26,26	1.37	2 (8%)
11	DDQ	B	1515	-	10,13,13	0.12	0	12,15,15	0.25	0
5	EDO	A	1109	-	3,3,3	0.05	0	2,2,2	0.18	0
10	DDR	B	1508	-	27,27,27	0.26	0	29,29,29	0.37	0
5	EDO	B	1513	-	3,3,3	0.06	0	2,2,2	0.17	0
5	EDO	A	1104	-	3,3,3	0.07	0	2,2,2	0.14	0
5	EDO	C	1712	-	3,3,3	0.08	0	2,2,2	0.30	0
8	GOL	C	1709	-	5,5,5	0.09	0	5,5,5	0.28	0
3	LMT	C	1703	-	36,36,36	0.45	0	47,47,47	0.49	0
6	OCT	C	1704	-	7,7,7	0.11	0	6,6,6	0.07	0
13	LPX	C	1707	-	29,29,29	0.29	0	31,33,33	0.35	0
7	C14	A	1106	-	13,13,13	0.08	0	12,12,12	0.05	0
8	GOL	B	1512	-	5,5,5	0.10	0	5,5,5	0.29	0
12	SO4	B	1518	-	4,4,4	0.40	0	6,6,6	0.04	0
5	EDO	B	1501	-	3,3,3	0.06	0	2,2,2	0.15	0
3	LMT	B	1510	-	36,36,36	0.51	0	47,47,47	0.97	3 (6%)
7	C14	C	1706	-	13,13,13	0.08	0	12,12,12	0.05	0
3	LMT	B	1503	-	36,36,36	0.46	0	47,47,47	0.57	0
5	EDO	A	1113	-	3,3,3	0.06	0	2,2,2	0.18	0
13	LPX	C	1705	-	29,29,29	0.28	0	31,33,33	0.35	0
5	EDO	B	1506	-	3,3,3	0.07	0	2,2,2	0.20	0
5	EDO	A	1112	-	3,3,3	0.06	0	2,2,2	0.17	0
6	OCT	C	1701	-	7,7,7	0.11	0	6,6,6	0.07	0
6	OCT	A	1105	-	7,7,7	0.11	0	6,6,6	0.07	0
3	LMT	A	1101	-	36,36,36	0.44	0	47,47,47	0.61	0
8	GOL	B	1502	-	5,5,5	0.10	0	5,5,5	0.26	0
12	SO4	C	1713	-	4,4,4	0.39	0	6,6,6	0.05	0
5	EDO	B	1514	-	3,3,3	0.06	0	2,2,2	0.21	0
7	C14	A	1108	-	13,13,13	0.09	0	12,12,12	0.07	0
3	LMT	A	1103	-	36,36,36	0.52	1 (2%)	47,47,47	0.83	2 (4%)
3	LMT	A	1111	-	36,36,36	0.50	1 (2%)	47,47,47	0.73	1 (2%)
12	SO4	B	1517	-	4,4,4	0.40	0	6,6,6	0.05	0
3	LMT	B	1504	-	36,36,36	0.52	0	47,47,47	0.98	2 (4%)
5	EDO	B	1507	-	3,3,3	0.06	0	2,2,2	0.18	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
5	EDO	A	1110	-	-	1/1/1/1	-
8	GOL	B	1509	-	-	0/4/4/4	-
3	LMT	C	1708	-	-	11/21/61/61	0/2/2/2
5	EDO	C	1710	-	-	0/1/1/1	-
5	EDO	C	1702	-	-	1/1/1/1	-
8	GOL	A	1107	-	-	2/4/4/4	-
4	1K8	B	1516	-	-	0/4/12/12	0/3/3/3
5	EDO	C	1711	-	-	1/1/1/1	-
9	D10	B	1505	-	-	4/7/7/7	-
8	GOL	B	1511	-	-	2/4/4/4	-
4	1K8	A	1102	-	-	2/4/12/12	0/3/3/3
11	DDQ	B	1515	-	-	5/11/11/11	-
5	EDO	A	1109	-	-	0/1/1/1	-
10	DDR	B	1508	-	-	15/29/29/29	-
5	EDO	B	1513	-	-	1/1/1/1	-
5	EDO	A	1104	-	-	1/1/1/1	-
5	EDO	C	1712	-	-	1/1/1/1	-
8	GOL	C	1709	-	-	4/4/4/4	-
3	LMT	C	1703	-	-	8/21/61/61	0/2/2/2
6	OCT	C	1704	-	-	1/5/5/5	-
13	LPX	C	1707	-	-	17/31/31/31	-
7	C14	A	1106	-	-	3/11/11/11	-
8	GOL	B	1512	-	-	2/4/4/4	-
5	EDO	B	1501	-	-	0/1/1/1	-
3	LMT	B	1510	-	-	10/21/61/61	0/2/2/2
7	C14	C	1706	-	-	6/11/11/11	-
3	LMT	B	1503	-	-	9/21/61/61	0/2/2/2
5	EDO	A	1113	-	-	1/1/1/1	-
13	LPX	C	1705	-	-	15/31/31/31	-
5	EDO	B	1506	-	-	1/1/1/1	-
5	EDO	A	1112	-	-	0/1/1/1	-
6	OCT	C	1701	-	-	1/5/5/5	-
6	OCT	A	1105	-	-	0/5/5/5	-
3	LMT	A	1101	-	-	7/21/61/61	0/2/2/2
8	GOL	B	1502	-	-	2/4/4/4	-
5	EDO	B	1514	-	-	0/1/1/1	-
7	C14	A	1108	-	-	5/11/11/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LMT	A	1103	-	-	11/21/61/61	0/2/2/2
3	LMT	A	1111	-	-	10/21/61/61	0/2/2/2
3	LMT	B	1504	-	-	12/21/61/61	0/2/2/2
5	EDO	B	1507	-	-	1/1/1/1	-

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1516	1K8	C9-C8	9.09	1.51	1.39
4	A	1102	1K8	C9-C8	8.46	1.50	1.39
4	A	1102	1K8	C11-C12	4.57	1.49	1.42
4	B	1516	1K8	C11-C12	4.52	1.49	1.42
4	B	1516	1K8	C8-N13	4.41	1.36	1.31

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1102	1K8	C4-N3-C2	4.67	121.83	111.52
3	B	1510	LMT	O1B-C4'-C3'	3.37	116.24	107.28
3	C	1708	LMT	C1'-C2'-C3'	3.35	116.97	110.00
4	B	1516	1K8	C8-N13-C12	3.03	122.51	116.11
4	B	1516	1K8	C5-C4-N3	-3.00	103.98	110.48

There are no chirality outliers.

5 of 173 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1101	LMT	C2'-C1'-O1'-C1
3	A	1101	LMT	O5'-C1'-O1'-C1
3	A	1103	LMT	O5'-C1'-O1'-C1
3	A	1111	LMT	C2'-C1'-O1'-C1
3	B	1503	LMT	C2'-C1'-O1'-C1

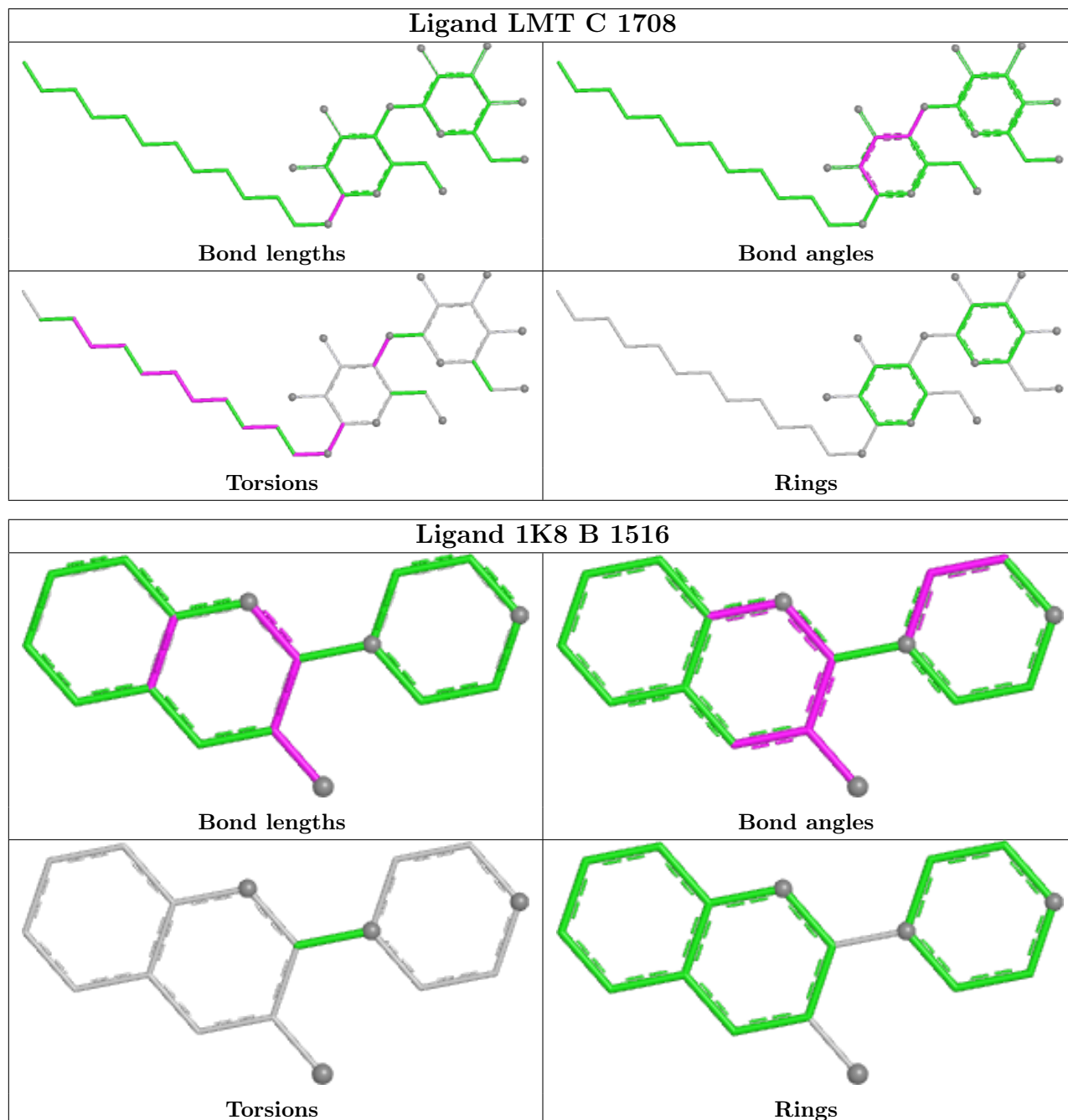
There are no ring outliers.

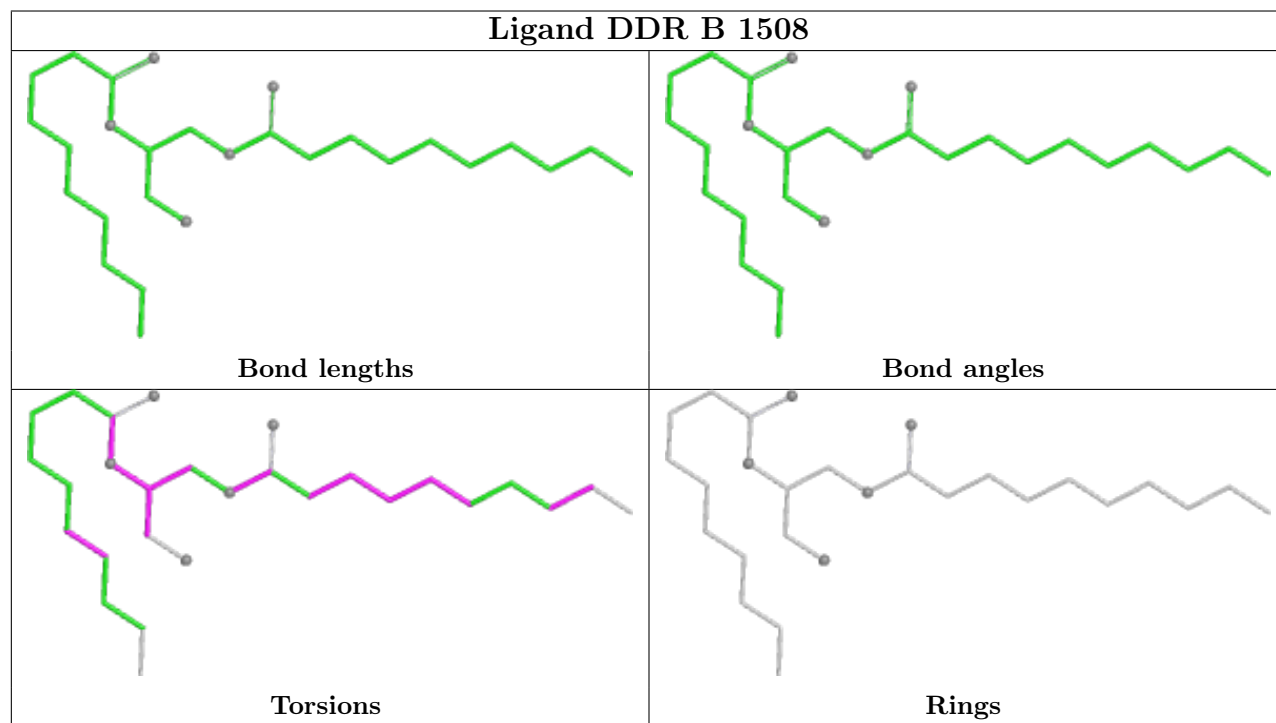
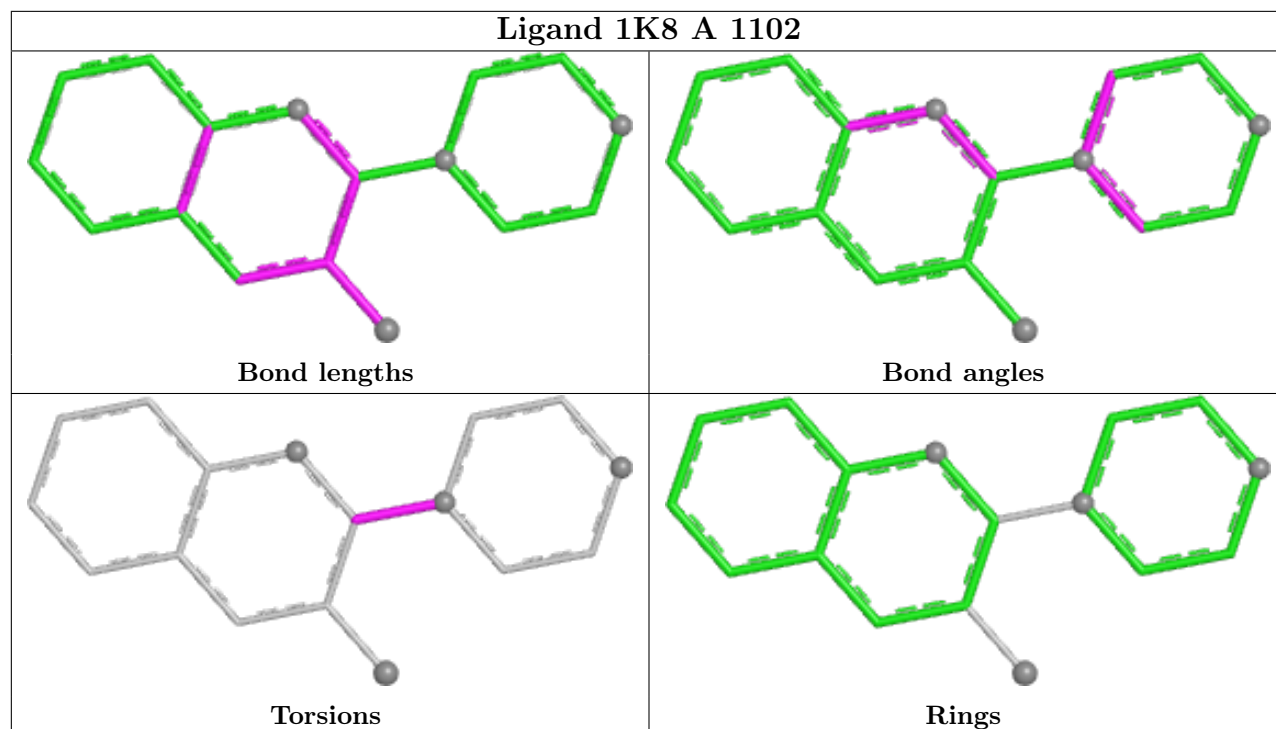
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1516	1K8	1	0

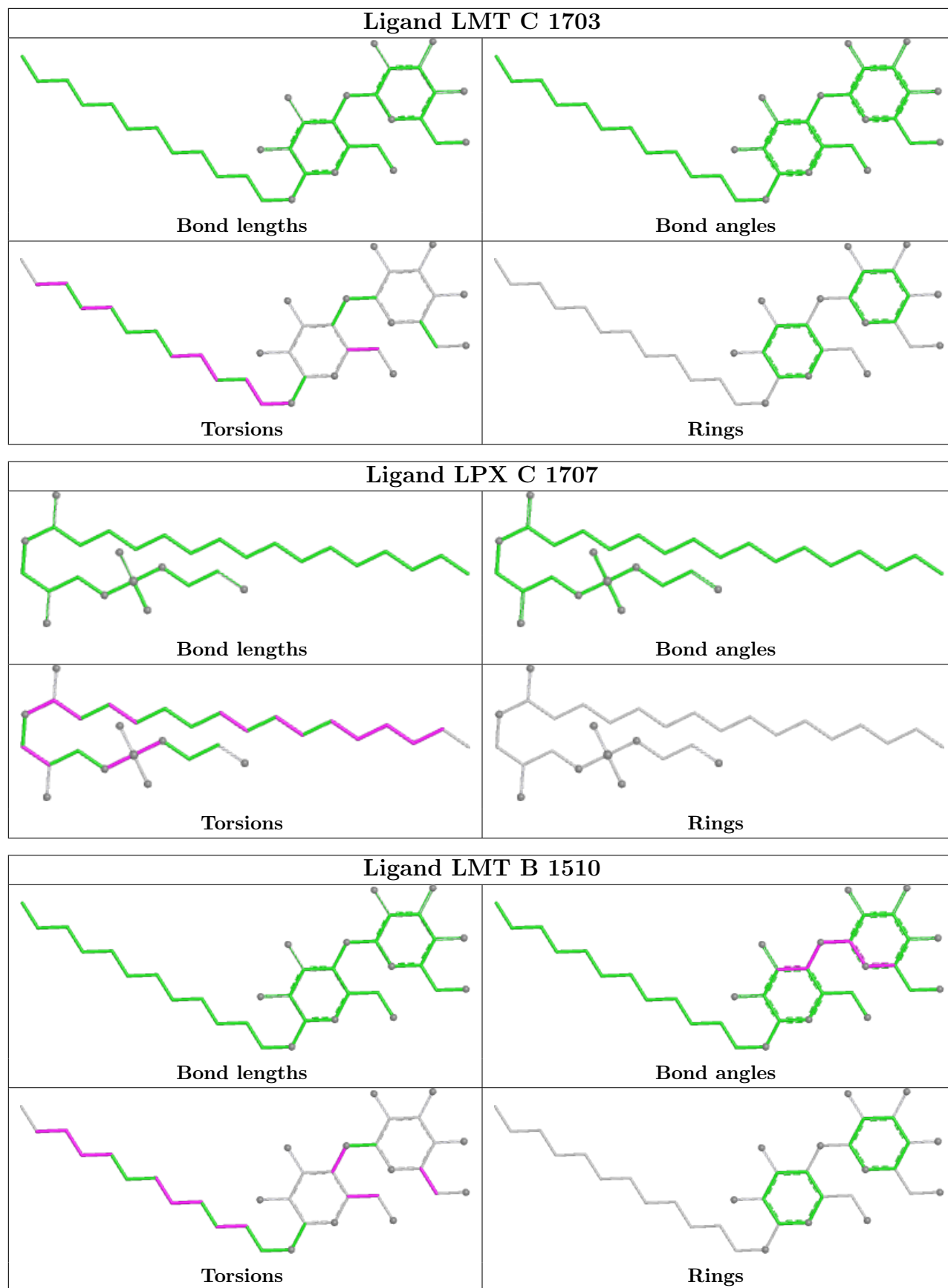
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

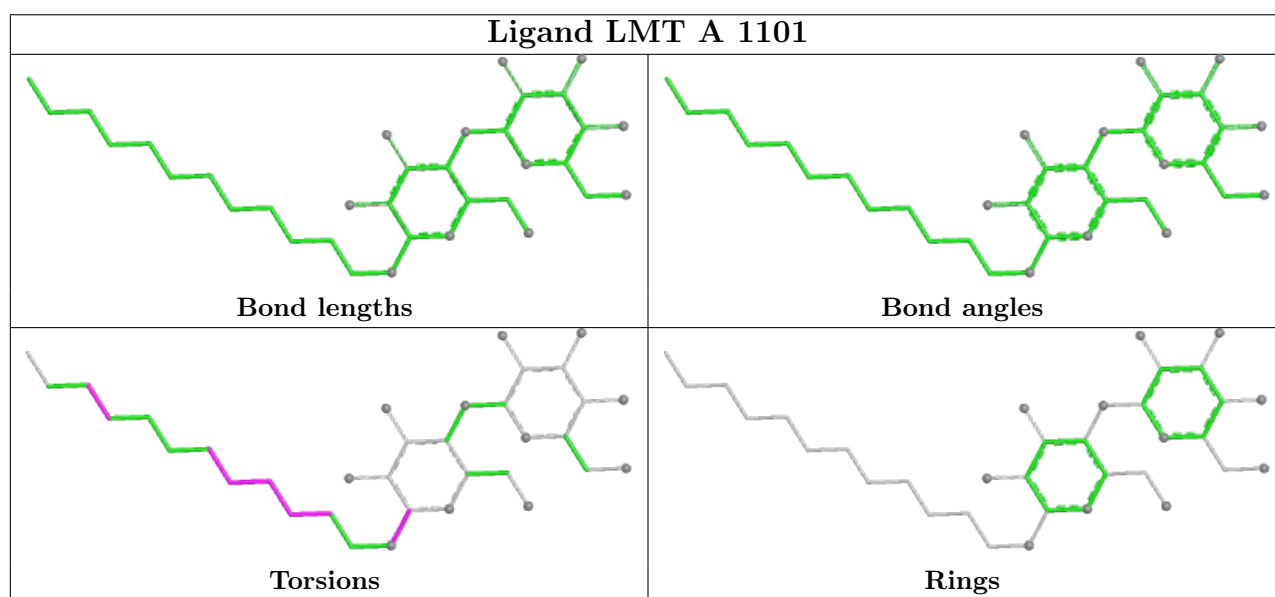
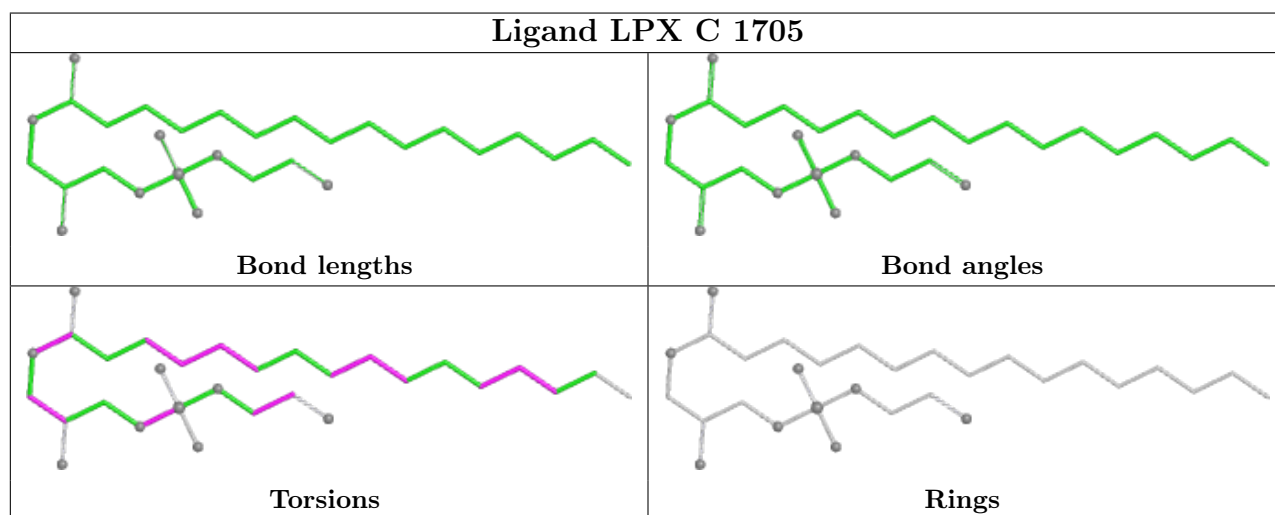
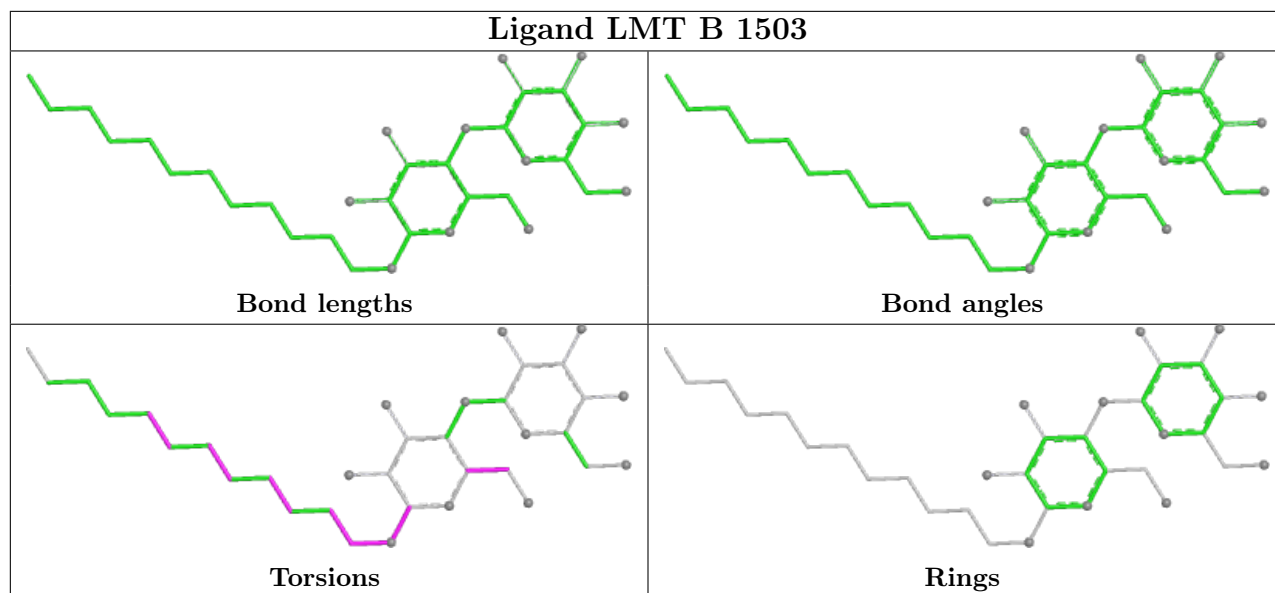
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.

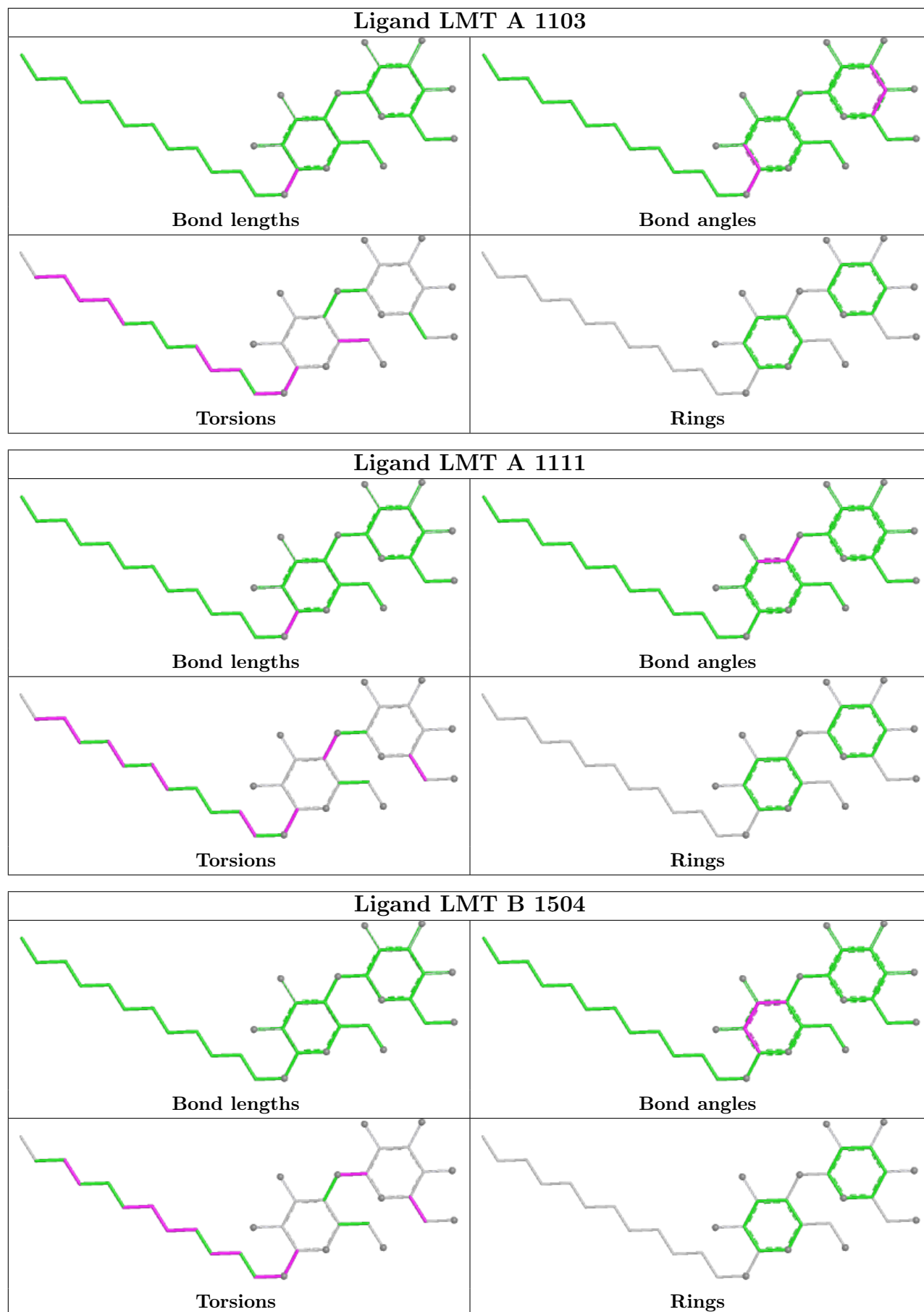












## 5.7 Other polymers [i](#)

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	1033/1057 (97%)	0.44	78 (7%) 13 10	39, 61, 115, 137	0
1	B	1036/1057 (98%)	0.21	58 (5%) 24 19	40, 59, 73, 80	0
1	C	1033/1057 (97%)	0.10	29 (2%) 53 46	39, 49, 67, 76	0
2	D	156/169 (92%)	0.37	15 (9%) 8 5	46, 58, 75, 83	0
2	E	153/169 (90%)	1.08	35 (22%) 0 0	52, 65, 85, 93	0
All	All	3411/3509 (97%)	0.29	215 (6%) 20 15	39, 56, 91, 137	0

The worst 5 of 215 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	424	GLY	7.5
2	E	66	LEU	6.7
1	A	868	LEU	6.0
2	E	33	LEU	6.0
1	C	510	LYS	5.8

### 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.

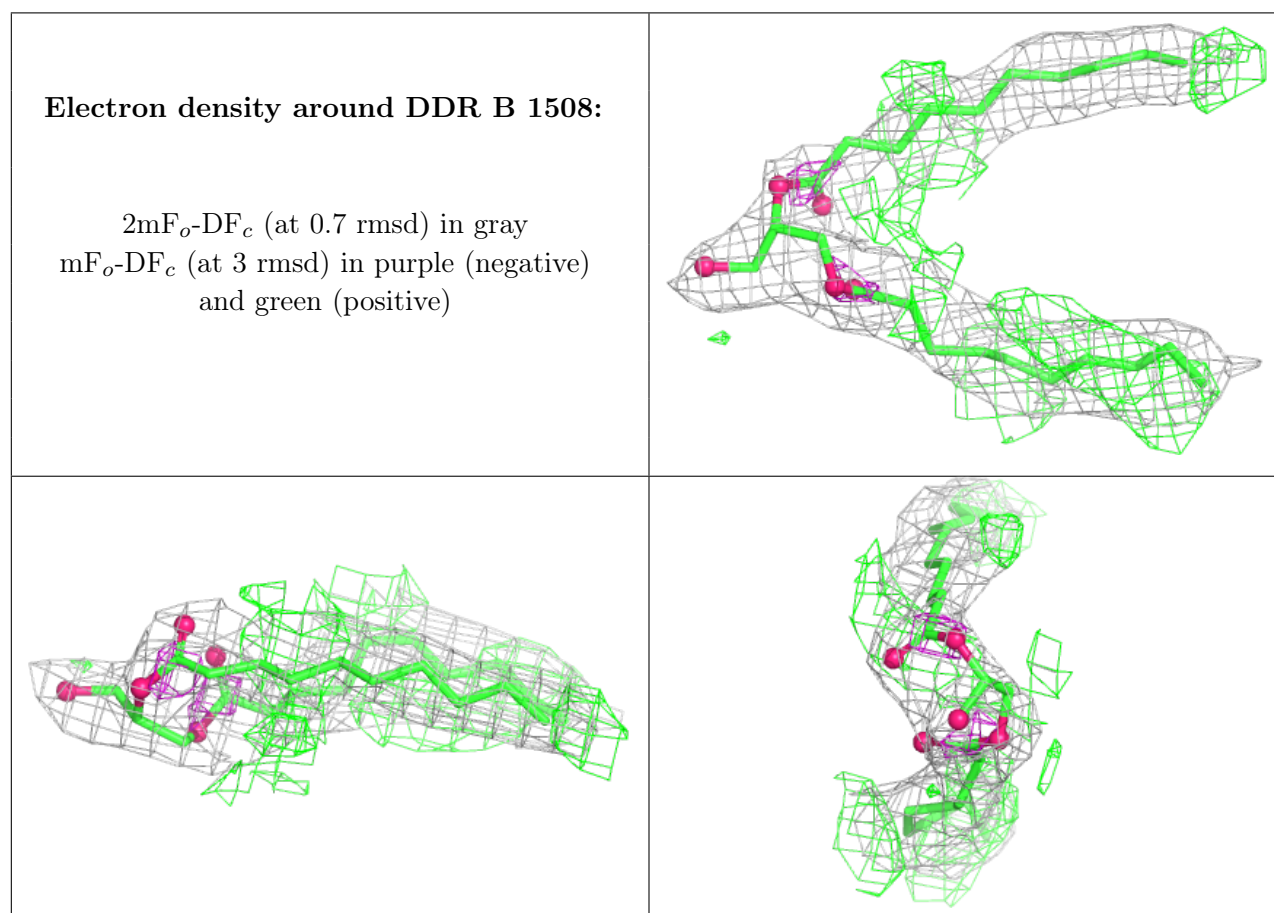
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	EDO	C	1712	4/4	0.58	0.40	59,59,59,60	0
10	DDR	B	1508	28/28	0.59	0.28	69,73,74,74	0
3	LMT	B	1504	35/35	0.72	0.29	71,75,80,80	0
6	OCT	C	1704	8/8	0.74	0.41	60,61,62,62	0
3	LMT	C	1708	35/35	0.74	0.25	66,77,79,80	0
5	EDO	A	1109	4/4	0.75	0.18	67,68,68,68	0
3	LMT	B	1510	35/35	0.76	0.38	69,76,79,80	0
7	C14	A	1106	14/14	0.76	0.18	75,83,91,93	0
8	GOL	B	1512	6/6	0.76	0.46	68,69,70,70	0
6	OCT	C	1701	8/8	0.76	0.28	83,87,92,92	0
11	DDQ	B	1515	14/14	0.76	0.25	62,64,66,67	0
9	D10	B	1505	10/10	0.77	0.19	66,68,69,69	0
4	1K8	A	1102	17/17	0.81	0.30	80,86,91,91	0
8	GOL	A	1107	6/6	0.81	0.31	66,67,67,67	0
6	OCT	A	1105	8/8	0.82	0.30	86,91,96,98	0
3	LMT	A	1101	35/35	0.82	0.30	66,69,72,73	0
3	LMT	A	1111	35/35	0.82	0.22	61,76,82,83	0
13	LPX	C	1705	30/30	0.82	0.37	66,70,75,76	0
4	1K8	B	1516	17/17	0.83	0.32	51,53,55,55	17
3	LMT	A	1103	35/35	0.84	0.32	73,76,81,83	0
5	EDO	A	1112	4/4	0.85	0.18	60,60,61,61	0
5	EDO	B	1501	4/4	0.85	0.26	58,58,59,60	0
5	EDO	B	1507	4/4	0.85	0.30	56,56,56,57	0
5	EDO	B	1514	4/4	0.85	0.13	75,75,75,76	0
3	LMT	B	1503	35/35	0.85	0.35	75,78,81,82	0
5	EDO	C	1702	4/4	0.86	0.23	63,64,64,64	0
5	EDO	B	1506	4/4	0.86	0.26	61,61,62,62	0
7	C14	A	1108	14/14	0.86	0.23	62,66,68,68	0
8	GOL	B	1511	6/6	0.87	0.23	61,61,61,62	0
5	EDO	A	1110	4/4	0.88	0.21	73,73,74,74	0
5	EDO	A	1113	4/4	0.88	0.20	63,63,64,65	0
12	SO4	B	1518	5/5	0.88	0.48	111,111,111,112	0
8	GOL	B	1509	6/6	0.88	0.34	70,70,71,71	0
8	GOL	B	1502	6/6	0.89	0.26	62,62,63,63	0
3	LMT	C	1703	35/35	0.90	0.22	60,65,68,68	0
7	C14	C	1706	14/14	0.90	0.18	57,58,59,59	0
5	EDO	A	1104	4/4	0.90	0.26	53,53,53,53	0
5	EDO	B	1513	4/4	0.91	0.16	78,78,78,78	0
13	LPX	C	1707	30/30	0.91	0.28	63,68,73,74	0
8	GOL	C	1709	6/6	0.92	0.19	52,52,53,53	0
12	SO4	C	1713	5/5	0.93	0.18	76,76,76,77	0

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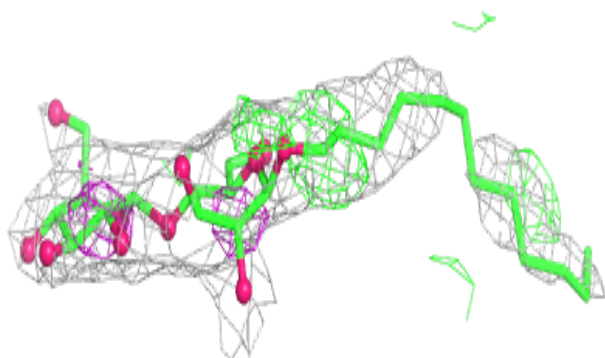
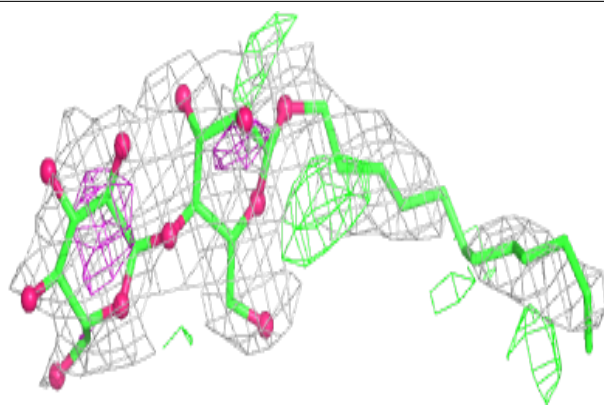
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	EDO	C	1711	4/4	0.94	0.26	57,57,57,58	0
12	SO4	B	1517	5/5	0.95	0.28	81,81,82,82	0
5	EDO	C	1710	4/4	0.96	0.36	56,56,56,57	0

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.

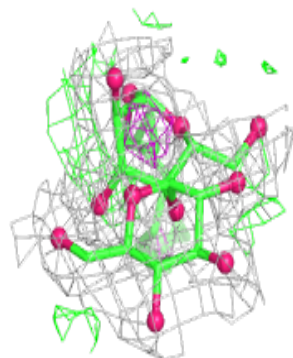
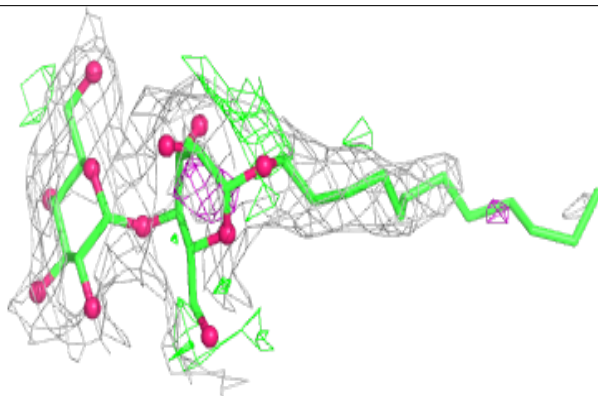
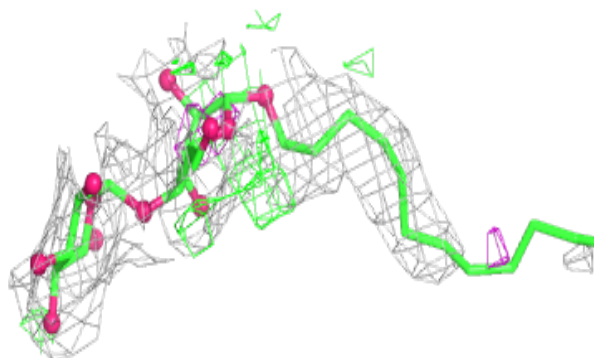


**Electron density around LMT B 1504:**

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

**Electron density around LMT C 1708:**

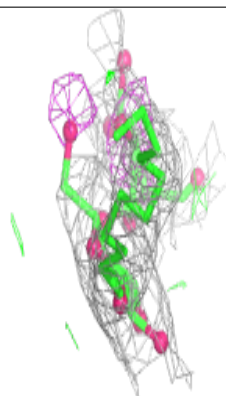
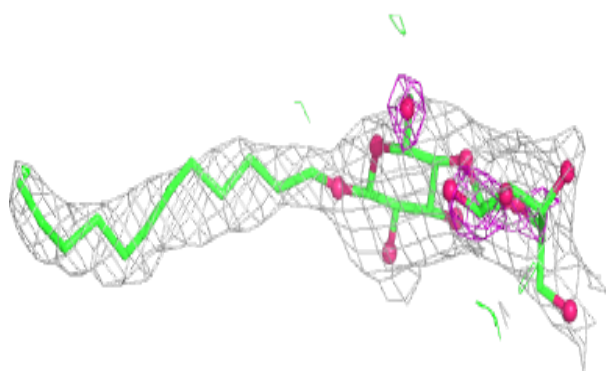
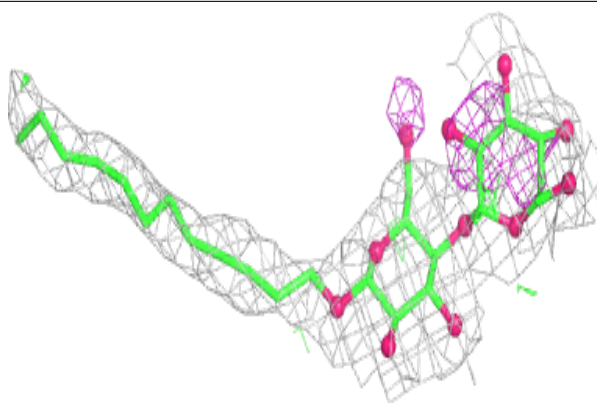
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



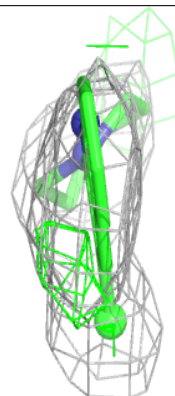
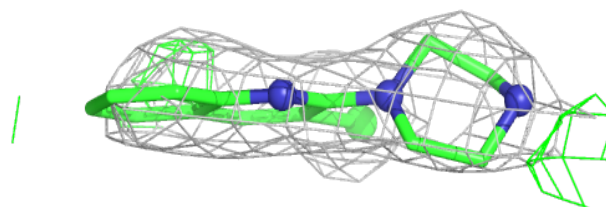
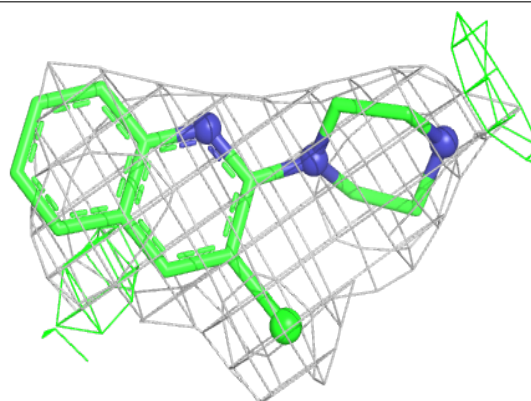


**Electron density around LMT B 1510:**

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

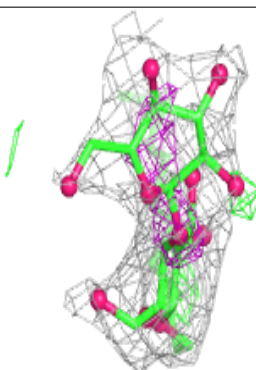
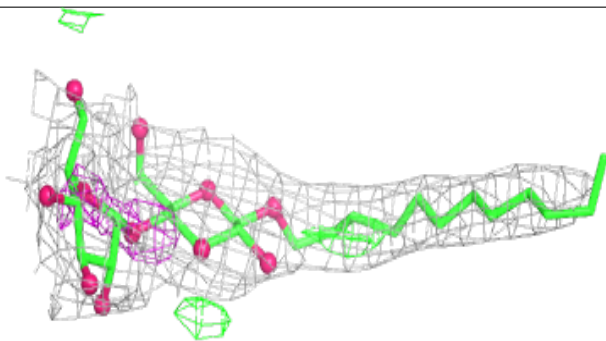
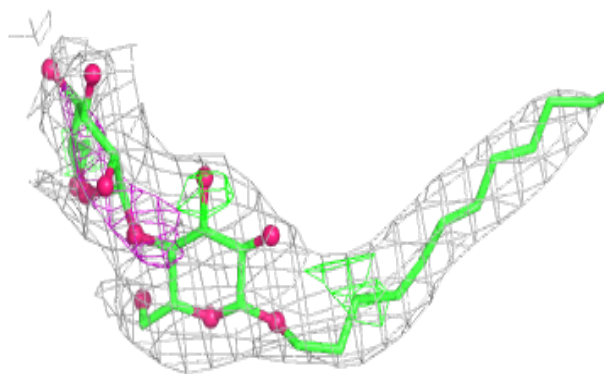
**Electron density around 1K8 A 1102:**

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

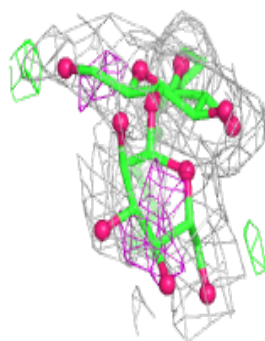
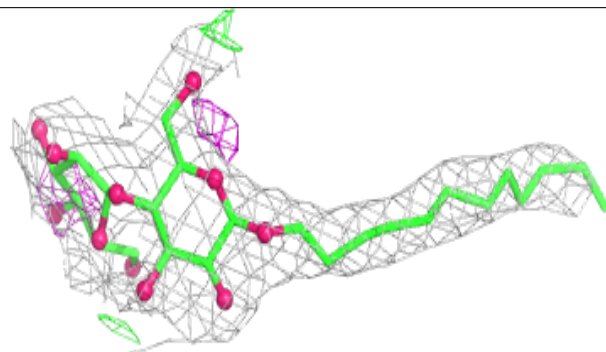
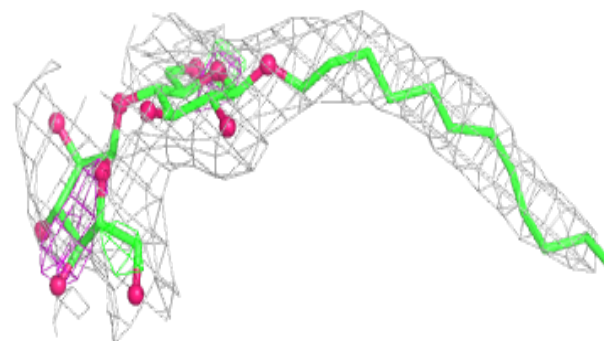


**Electron density around LMT A 1101:**

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

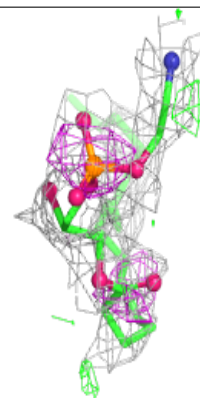
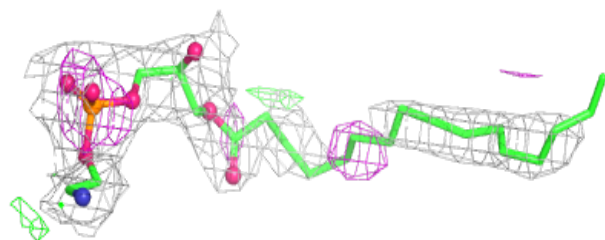
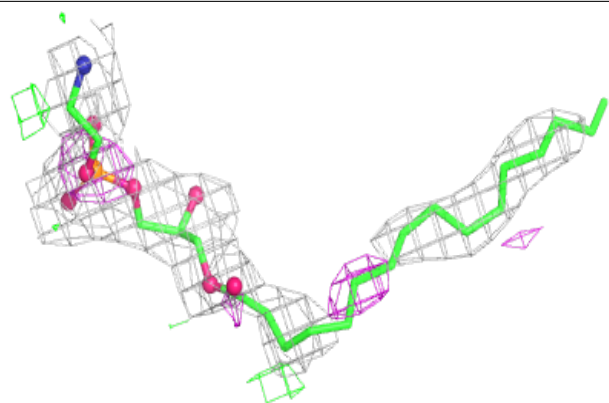
**Electron density around LMT A 1111:**

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

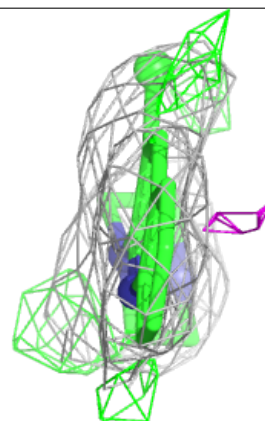
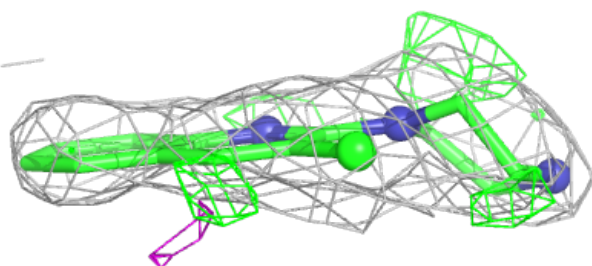
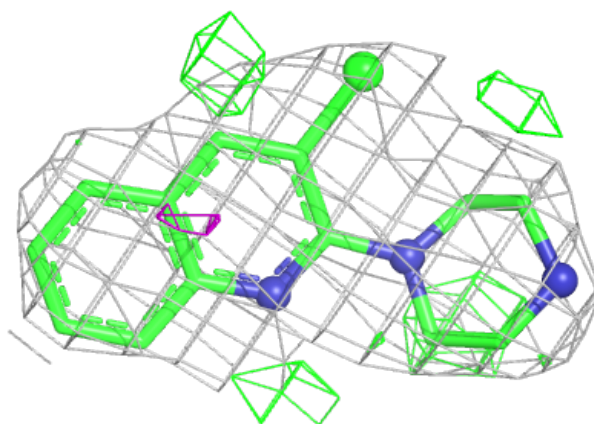


**Electron density around LPX C 1705:**

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

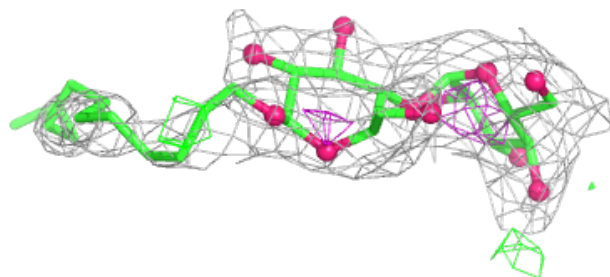
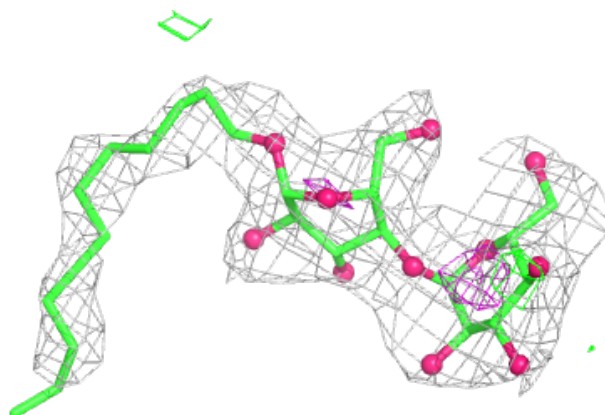
**Electron density around 1K8 B 1516:**

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

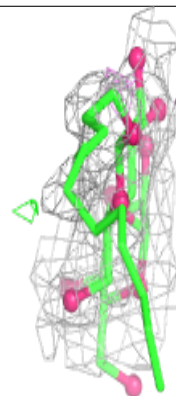
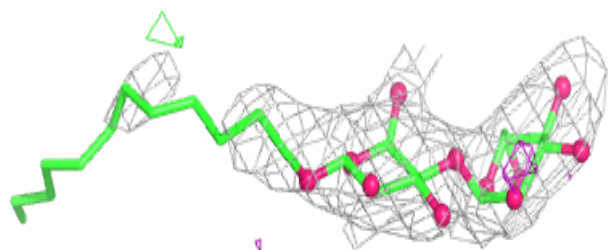
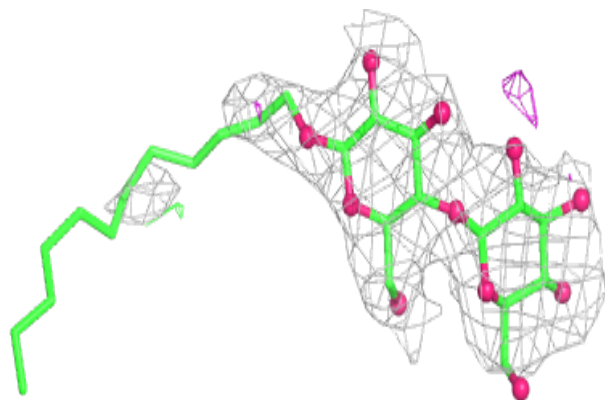


**Electron density around LMT A 1103:**

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

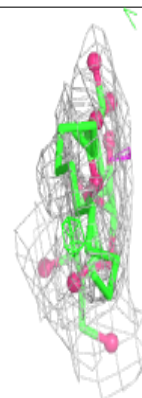
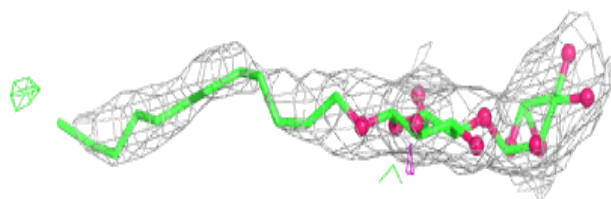
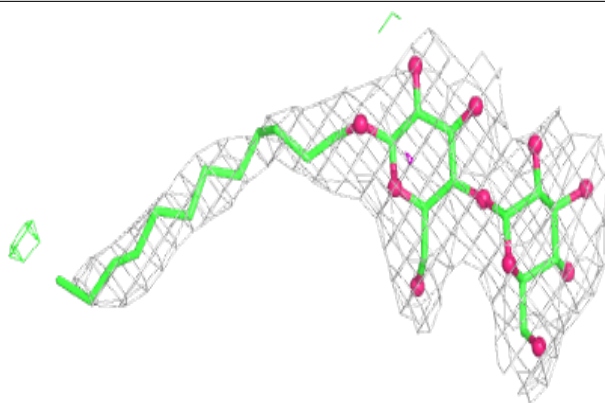
**Electron density around LMT B 1503:**

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

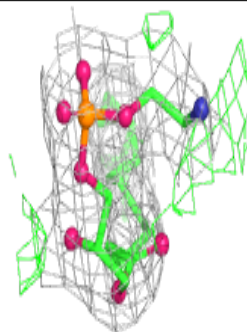
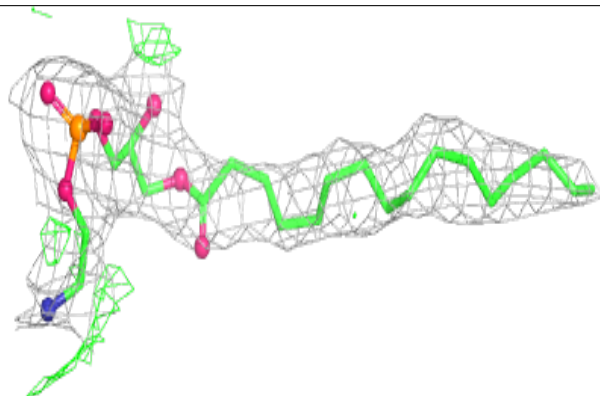
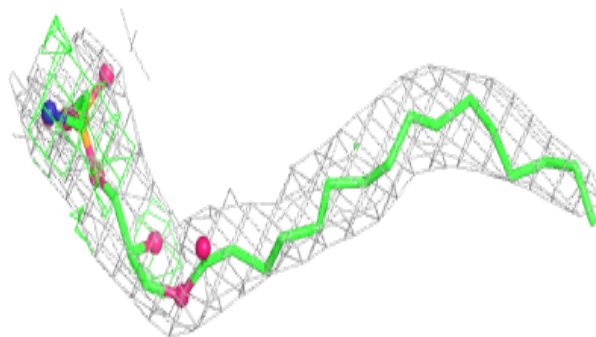


**Electron density around LMT C 1703:**

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

**Electron density around LPX C 1707:**

$2mF_o-DF_c$  (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.