Full wwPDB X-ray Structure Validation Report ⓘ

May 11, 2021 – 09:17 am BST

PDB ID	:	6ZOA
Title	:	Partially induced AcrB T protomer and DDM binding to the TM8/PC2 pathway of AcrB L2 protomer
Authors	:	Tam, H.K.; Foong, W.E.; Pos, K.M.
Deposited on	:	2020-07-07
Resolution	:	3.05 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *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 following versions of software and data (see references ⓘ) were used in the production of this report:

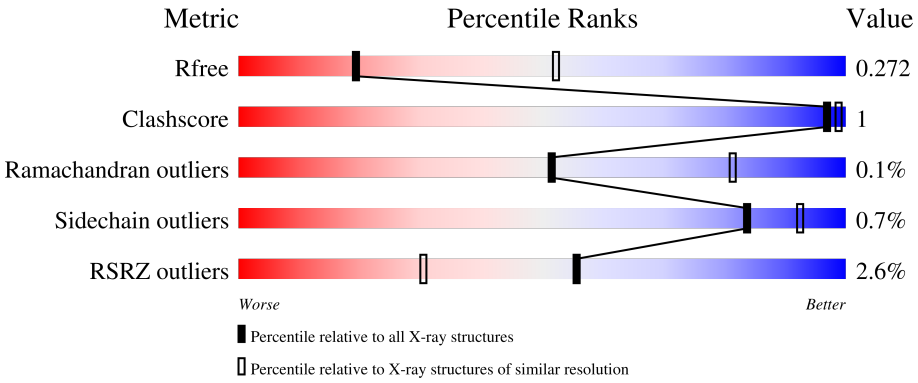
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.18
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.18

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

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 >=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 <=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	3% 94% 5%
1	B	1057	2% 94%
1	C	1057	% 95%
2	D	169	6% 92% 8%
2	E	169	9% 91% 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:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	OCT	B	1108	-	-	-	X
3	LMT	A	1104	-	-	-	X

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 26771 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Multidrug efflux pump subunit AcrB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1042	Total	C	N	O	S	0	1	0
			7932	5099	1314	1475	44			
1	B	1024	Total	C	N	O	S	0	0	0
			7800	5024	1286	1446	44			
1	C	1035	Total	C	N	O	S	0	0	0
			7866	5061	1300	1461	44			

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

Continued on next page...

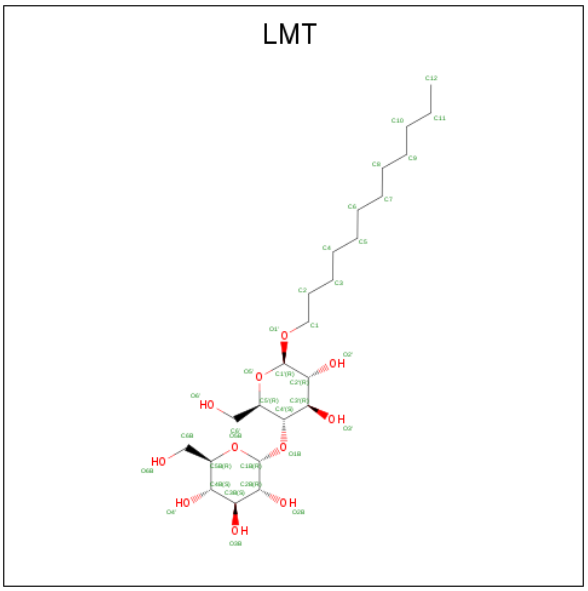
Continued from previous page...

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

- Molecule 2 is a protein called DARPIN.

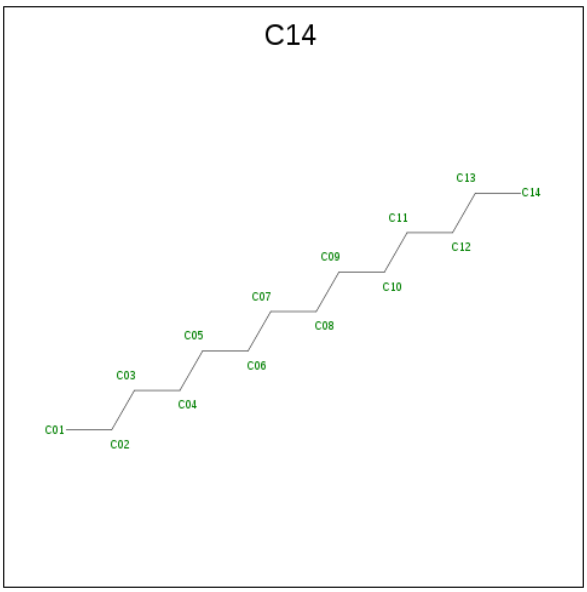
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	156	Total	C	N	O	S	0	0	0
			1177	741	206	229	1			
2	E	154	Total	C	N	O	S	0	0	0
			1167	736	204	226	1			

- Molecule 3 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).



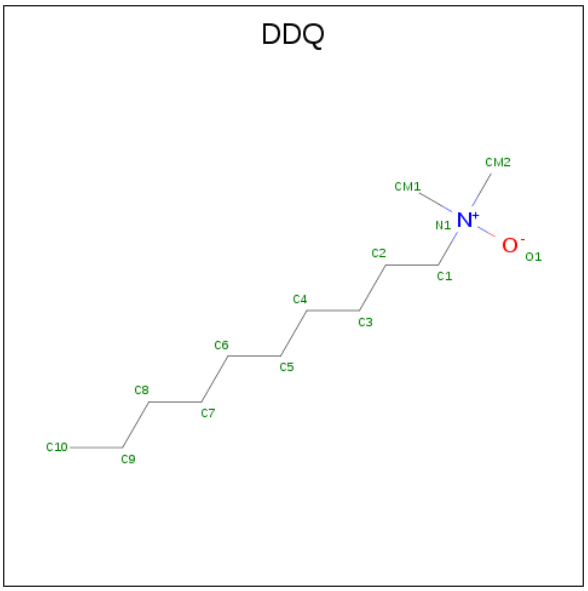
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			35	24	11		
3	A	1	Total	C	O	0	0
			35	24	11		
3	A	1	Total	C	O	0	0
			35	24	11		
3	A	1	Total	C	O	0	0
			35	24	11		
3	B	1	Total	C	O	0	0
			35	24	11		
3	C	1	Total	C	O	0	0
			35	24	11		

- Molecule 4 is TETRADECANE (three-letter code: C14) (formula: $C_{14}H_{30}$).



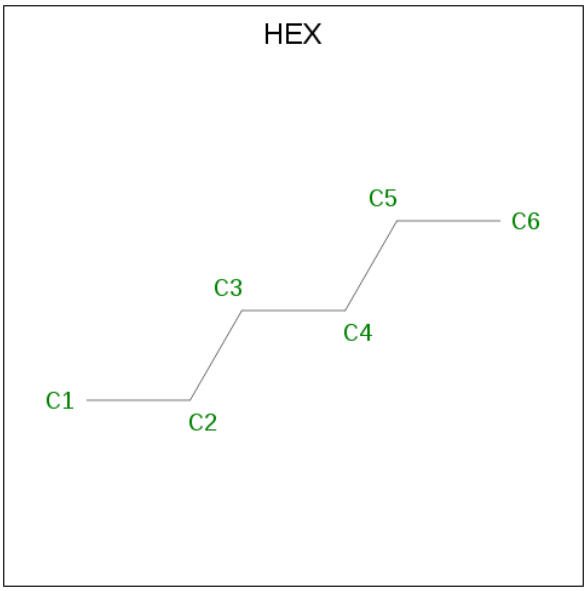
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C 14 14	0	0
4	B	1	Total C 14 14	0	0
4	B	1	Total C 14 14	0	0
4	B	1	Total C 14 14	0	0

- Molecule 5 is DECYLAMINE-N,N-DIMETHYL-N-OXIDE (three-letter code: DDQ) (formula: $C_{12}H_{27}NO$).



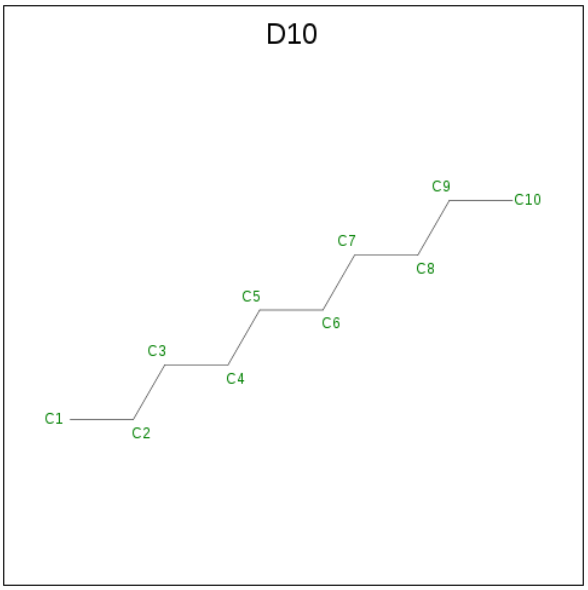
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 14 12 1 1	0	0
5	A	1	Total C N O 14 12 1 1	0	0
5	B	1	Total C N O 14 12 1 1	0	0
5	B	1	Total C N O 14 12 1 1	0	0
5	C	1	Total C N O 14 12 1 1	0	0
5	C	1	Total C N O 14 12 1 1	0	0
5	C	1	Total C N O 14 12 1 1	0	0

- Molecule 6 is HEXANE (three-letter code: HEX) (formula: C_6H_{14}).



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

- Molecule 7 is DECANE (three-letter code: D10) (formula: $C_{10}H_{22}$).

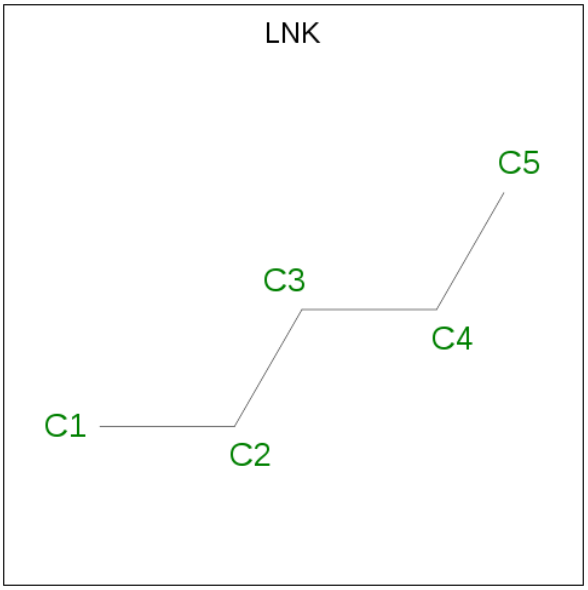


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C 10 10	0	0

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

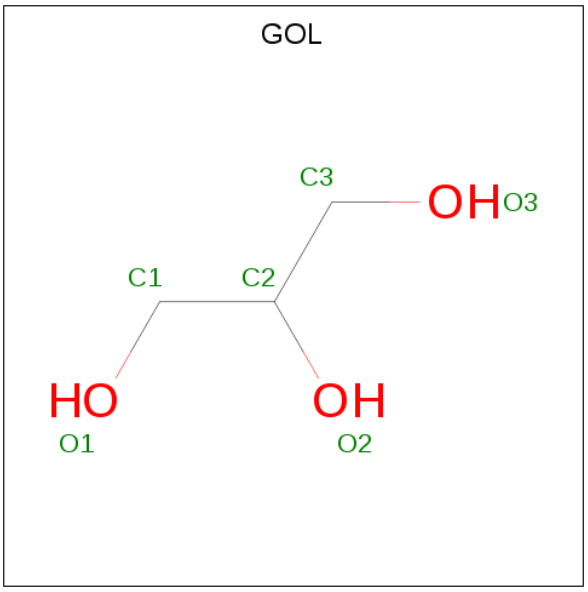
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Cl 1 1	0	0

- Molecule 9 is PENTANE (three-letter code: LNK) (formula: C_5H_{12}).



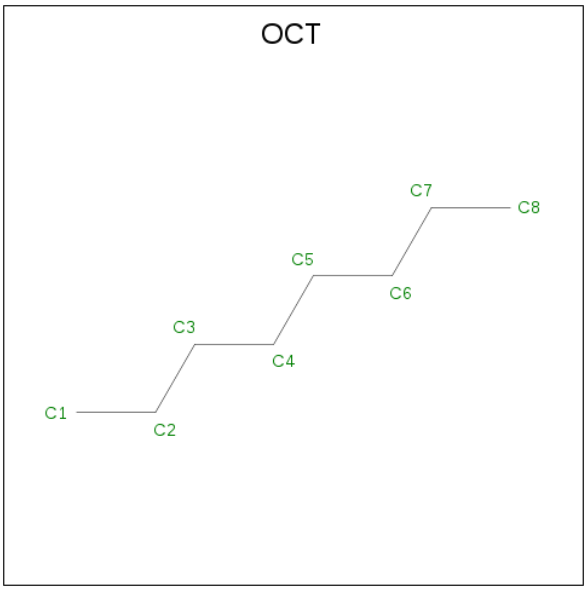
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C 5 5	0	0

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



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

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



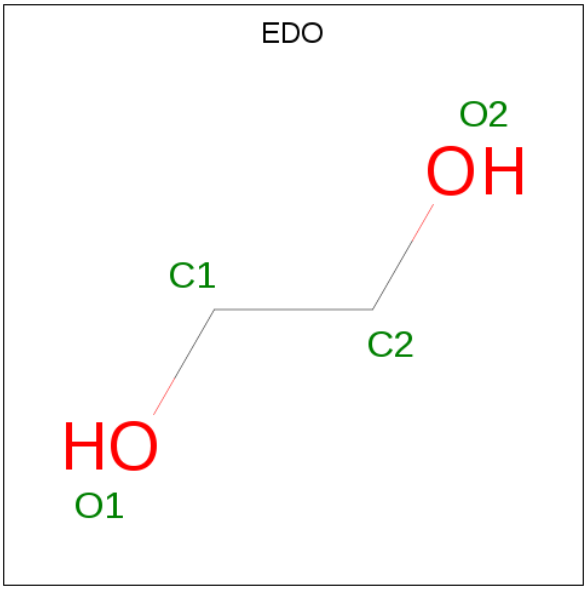
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	1	Total C 8 8	0	0

Continued on next page...

Continued from previous page...

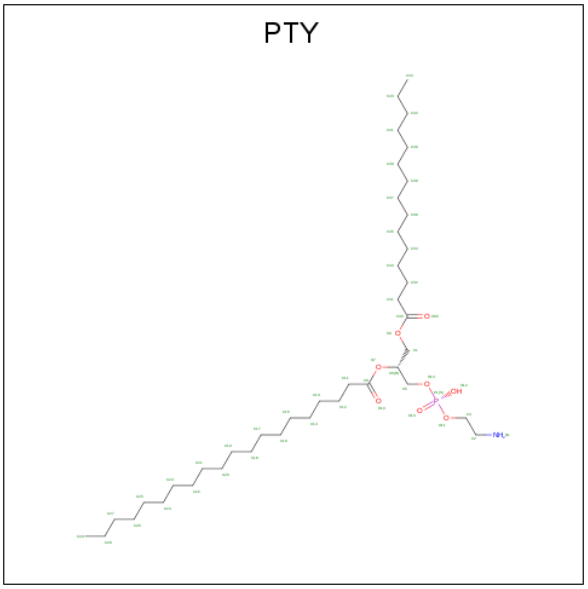
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	C	1	Total C 8 8	0	0

- Molecule 12 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



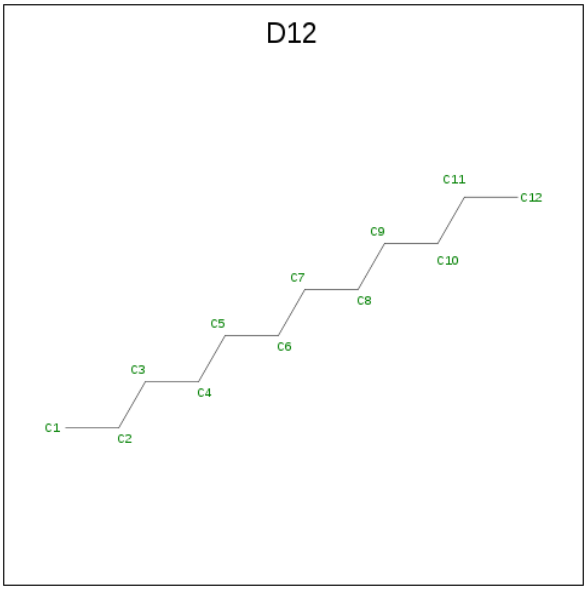
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	B	1	Total C O 4 2 2	0	0

- Molecule 13 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$).



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

- Molecule 14 is DODECANE (three-letter code: D12) (formula: $C_{12}H_{26}$).



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

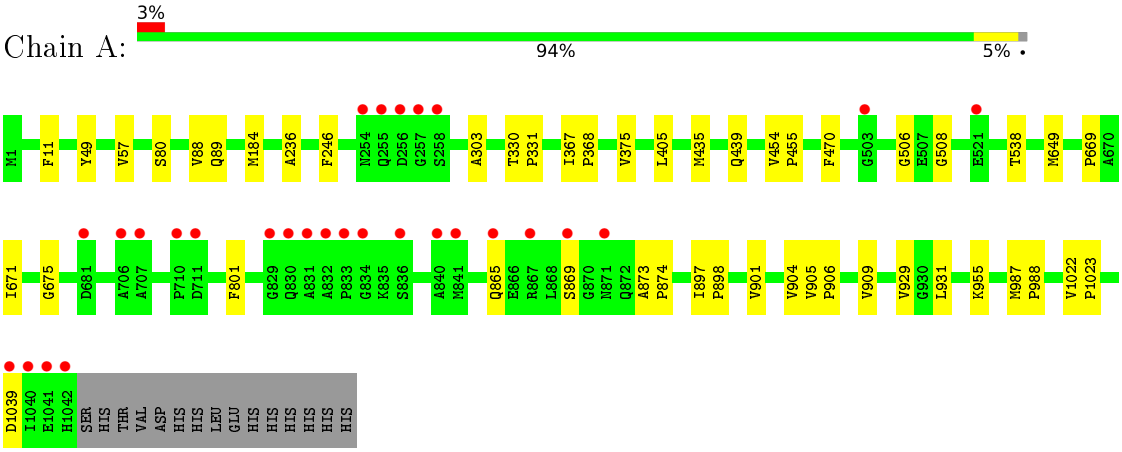
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	86	Total	O	0	0
			86	86		
15	B	83	Total	O	0	0
			83	83		
15	C	86	Total	O	0	0
			86	86		
15	D	15	Total	O	0	0
			15	15		
15	E	5	Total	O	0	0
			5	5		

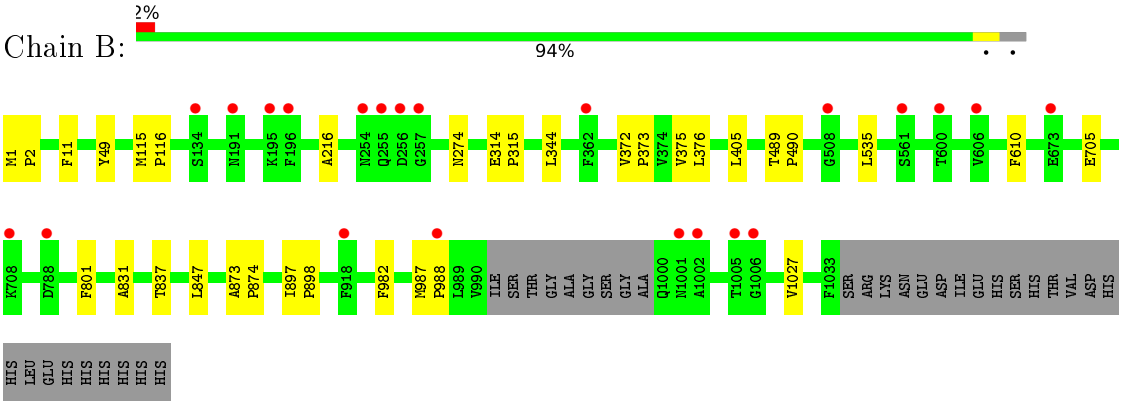
3 Residue-property plots (i)

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.

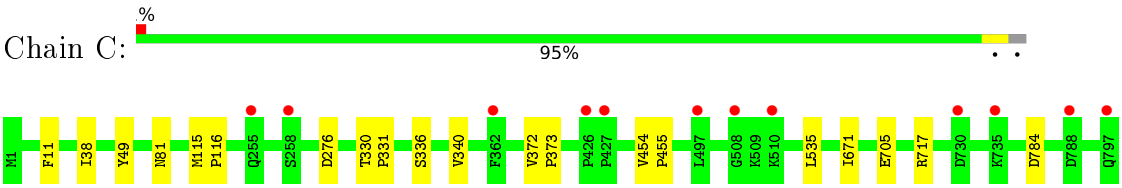
- Molecule 1: Multidrug efflux pump subunit AcrB

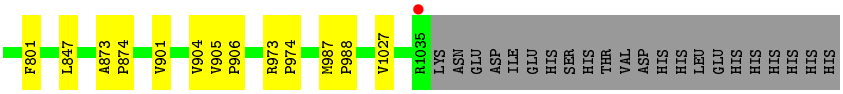


- Molecule 1: Multidrug efflux pump subunit AcrB



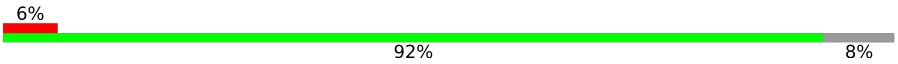
- Molecule 1: Multidrug efflux pump subunit AcrB

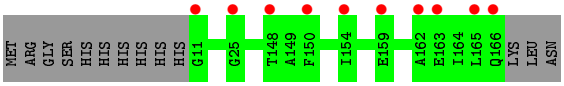




- Molecule 2: DARPIN

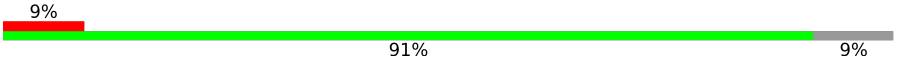
Chain D:

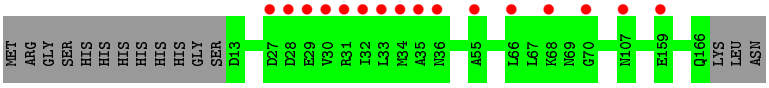




- Molecule 2: DARPIN

Chain E:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	145.60Å 162.99Å 246.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.68 – 3.05 49.68 – 3.05	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.68-3.05) 99.7 (49.68-3.05)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.50 (at 3.07Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.240 , 0.272 0.243 , 0.272	Depositor DCC
R_{free} test set	5610 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	56.9	Xtriage
Anisotropy	0.751	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 51.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	26771	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.97% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, HEX, D10, LMT, DDQ, PTY, GOL, LNK, D12, C14, EDO, OCT

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	0/8086	0.70	0/10978
1	B	0.67	0/7949	0.70	0/10794
1	C	0.67	0/8016	0.70	0/10885
2	D	0.68	0/1196	0.71	0/1626
2	E	0.68	0/1186	0.70	0/1613
All	All	0.67	0/26433	0.70	0/35896

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

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	7932	0	8076	20	0
1	B	7800	0	7953	14	0
1	C	7866	0	8019	13	0
2	D	1177	0	1159	0	0
2	E	1167	0	1151	0	0
3	A	140	0	184	0	0
3	B	35	0	46	0	0
3	C	35	0	46	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	14	0	30	0	0
4	B	42	0	90	0	0
5	A	28	0	54	0	0
5	B	28	0	54	0	0
5	C	42	0	81	0	0
6	A	12	0	28	0	0
6	B	6	0	14	0	0
6	C	6	0	14	0	0
7	A	10	0	22	0	0
8	A	1	0	0	0	0
9	A	5	0	12	0	0
10	A	12	0	16	0	0
10	B	6	0	8	0	0
11	B	8	0	18	0	0
11	C	8	0	18	0	0
12	B	4	0	6	0	0
13	C	100	0	158	0	0
14	C	12	0	26	0	0
15	A	86	0	0	0	0
15	B	83	0	0	0	0
15	C	86	0	0	0	0
15	D	15	0	0	0	0
15	E	5	0	0	0	0
All	All	26771	0	27283	47	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.

All (47) 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:A:375:VAL:HG11	1:A:405:LEU:HD22	1.76	0.66
1:C:372:VAL:HB	1:C:373:PRO:HD3	1.86	0.57
1:C:38:ILE:HD11	1:C:671:ILE:HD12	1.89	0.55
1:B:873:ALA:HB3	1:B:874:PRO:HD3	1.88	0.55
1:B:375:VAL:HG11	1:B:405:LEU:HD22	1.90	0.54
1:A:470:PHE:CZ	1:A:929:VAL:HB	2.43	0.53
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.91	0.51
1:B:897:ILE:N	1:B:898:PRO:HD2	2.28	0.49
1:C:115:MET:N	1:C:116:PRO:HD2	2.28	0.48
1:B:831:ALA:HB2	1:B:837:THR:HA	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:VAL:HB	1:B:373:PRO:HD3	1.97	0.47
1:A:303:ALA:HB2	1:A:330:THR:HG21	1.96	0.46
1:C:535:LEU:HD22	1:C:1027:VAL:HG21	1.98	0.46
1:A:330:THR:N	1:A:331:PRO:CD	2.79	0.45
1:B:987:MET:N	1:B:988:PRO:CD	2.79	0.45
1:C:987:MET:N	1:C:988:PRO:CD	2.80	0.45
1:B:115:MET:N	1:B:116:PRO:CD	2.80	0.44
1:C:454:VAL:HB	1:C:455:PRO:HD3	2.00	0.44
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.98	0.44
1:B:535:LEU:HD22	1:B:1027:VAL:HG21	2.00	0.44
1:C:705:GLU:HB3	1:C:847:LEU:HD22	2.00	0.43
1:B:344:LEU:HD13	1:B:376:LEU:HD12	1.99	0.43
1:A:897:ILE:N	1:A:898:PRO:CD	2.82	0.43
1:A:901:VAL:O	1:A:904:VAL:HG22	2.19	0.42
1:A:873:ALA:HB3	1:A:874:PRO:HD3	2.00	0.42
1:C:905:VAL:HB	1:C:906:PRO:HD3	2.01	0.42
1:A:435:MET:O	1:A:439:GLN:HB2	2.19	0.42
1:A:80:SER:HA	1:A:89:GLN:O	2.20	0.42
1:A:987:MET:HB3	1:A:988:PRO:HD3	2.02	0.42
1:C:330:THR:N	1:C:331:PRO:CD	2.83	0.42
1:C:973:ARG:N	1:C:974:PRO:HD2	2.34	0.42
1:B:489:THR:N	1:B:490:PRO:CD	2.83	0.42
1:B:705:GLU:HB3	1:B:847:LEU:HD22	2.02	0.42
1:A:57:VAL:CG1	1:A:88:VAL:HG22	2.49	0.42
1:B:1:MET:HB3	1:B:2:PRO:HD3	2.02	0.41
1:A:865:GLN:O	1:A:869:SER:HB3	2.20	0.41
1:C:336:SER:O	1:C:340:VAL:HG23	2.19	0.41
1:A:909:VAL:HG22	1:A:931:LEU:HD11	2.02	0.41
1:A:454:VAL:N	1:A:455:PRO:CD	2.84	0.41
1:A:506:GLY:O	1:A:508:GLY:N	2.54	0.41
1:A:1022:VAL:N	1:A:1023:PRO:HD2	2.36	0.41
1:B:987:MET:N	1:B:988:PRO:HD2	2.35	0.41
1:A:184:MET:HG2	1:A:246:PHE:CE2	2.56	0.41
1:C:901:VAL:O	1:C:904:VAL:HG12	2.20	0.41
1:B:314:GLU:N	1:B:315:PRO:HD2	2.36	0.40
1:A:669:PRO:HD2	1:A:675:GLY:O	2.21	0.40
1:C:873:ALA:HB3	1:C:874:PRO:HD3	2.02	0.40

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	1041/1057 (98%)	1004 (96%)	34 (3%)	3 (0%)	41 70
1	B	1020/1057 (96%)	987 (97%)	32 (3%)	1 (0%)	51 81
1	C	1033/1057 (98%)	1001 (97%)	32 (3%)	0	100 100
2	D	154/169 (91%)	148 (96%)	6 (4%)	0	100 100
2	E	152/169 (90%)	148 (97%)	4 (3%)	0	100 100
All	All	3400/3509 (97%)	3288 (97%)	108 (3%)	4 (0%)	51 81

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	236	ALA
1	B	216	ALA
1	A	538	THR
1	A	671	ILE

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	848/863 (98%)	842 (99%)	6 (1%)	84 92
1	B	835/863 (97%)	829 (99%)	6 (1%)	84 92
1	C	841/863 (98%)	834 (99%)	7 (1%)	81 91
2	D	120/132 (91%)	120 (100%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	E	119/132 (90%)	119 (100%)	0	100 100
All	All	2763/2853 (97%)	2744 (99%)	19 (1%)	84 92

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	PHE
1	A	49	TYR
1	A	649	MET
1	A	801	PHE
1	A	955	LYS
1	A	1039	ASP
1	B	11	PHE
1	B	49	TYR
1	B	274	ASN
1	B	610	PHE
1	B	801	PHE
1	B	982	PHE
1	C	11	PHE
1	C	49	TYR
1	C	81	ASN
1	C	276	ASP
1	C	717	ARG
1	C	784	ASP
1	C	801	PHE

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

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 33 ligands modelled in this entry, 1 is monoatomic - leaving 32 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	HEX	A	1109	-	5,5,5	0.13	0	4,4,4	0.08	0
6	HEX	A	1108	-	5,5,5	0.13	0	4,4,4	0.08	0
13	PTY	C	1102	-	49,49,49	0.26	0	52,54,54	0.36	0
3	LMT	C	1101	-	36,36,36	0.48	1 (2%)	47,47,47	0.62	0
5	DDQ	B	1105	-	10,13,13	2.27	1 (10%)	12,15,15	0.55	0
10	GOL	B	1109	-	5,5,5	0.10	0	5,5,5	0.26	0
4	C14	B	1103	-	13,13,13	0.08	0	12,12,12	0.06	0
6	HEX	C	1107	-	5,5,5	0.13	0	4,4,4	0.08	0
10	GOL	A	1113	-	5,5,5	0.10	0	5,5,5	0.25	0
3	LMT	A	1102	-	36,36,36	0.46	0	47,47,47	0.62	0
12	EDO	B	1110	-	3,3,3	0.07	0	2,2,2	0.18	0
11	OCT	B	1108	-	7,7,7	0.11	0	6,6,6	0.07	0
13	PTY	C	1103	-	49,49,49	0.26	0	52,54,54	0.31	0
3	LMT	B	1101	-	36,36,36	0.53	1 (2%)	47,47,47	1.14	4 (8%)
3	LMT	A	1104	-	36,36,36	0.47	0	47,47,47	0.65	0
11	OCT	C	1108	-	7,7,7	0.11	0	6,6,6	0.07	0
9	LNK	A	1112	-	4,4,4	0.15	0	3,3,3	0.20	0
4	C14	B	1102	-	13,13,13	0.08	0	12,12,12	0.05	0
10	GOL	A	1114	-	5,5,5	0.09	0	5,5,5	0.25	0
14	D12	C	1109	-	11,11,11	0.24	0	10,10,10	0.54	0
4	C14	B	1104	-	13,13,13	0.08	0	12,12,12	0.06	0
7	D10	A	1110	-	9,9,9	0.10	0	8,8,8	0.09	0
5	DDQ	C	1104	-	10,13,13	2.27	1 (10%)	12,15,15	0.51	0
4	C14	A	1105	-	13,13,13	0.08	0	12,12,12	0.08	0
3	LMT	A	1103	-	36,36,36	0.50	0	47,47,47	0.71	0
3	LMT	A	1101	-	36,36,36	0.45	0	47,47,47	0.50	0
5	DDQ	C	1106	-	10,13,13	2.28	1 (10%)	12,15,15	0.53	0
6	HEX	B	1107	-	5,5,5	0.13	0	4,4,4	0.08	0
5	DDQ	C	1105	-	10,13,13	2.27	1 (10%)	12,15,15	0.57	0
5	DDQ	B	1106	-	10,13,13	2.27	1 (10%)	12,15,15	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	DDQ	A	1106	-	10,13,13	2.29	1 (10%)	12,15,15	0.55	0
5	DDQ	A	1107	-	10,13,13	2.27	1 (10%)	12,15,15	0.46	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
6	HEX	A	1109	-	-	0/3/3/3	-
6	HEX	A	1108	-	-	0/3/3/3	-
13	PTY	C	1102	-	-	30/53/53/53	-
3	LMT	C	1101	-	-	12/21/61/61	0/2/2/2
5	DDQ	B	1105	-	-	3/11/11/11	-
10	GOL	B	1109	-	-	0/4/4/4	-
4	C14	B	1103	-	-	3/11/11/11	-
6	HEX	C	1107	-	-	0/3/3/3	-
10	GOL	A	1113	-	-	2/4/4/4	-
3	LMT	A	1102	-	-	8/21/61/61	0/2/2/2
12	EDO	B	1110	-	-	1/1/1/1	-
11	OCT	B	1108	-	-	0/5/5/5	-
13	PTY	C	1103	-	-	19/53/53/53	-
3	LMT	B	1101	-	-	15/21/61/61	0/2/2/2
3	LMT	A	1104	-	-	4/21/61/61	0/2/2/2
11	OCT	C	1108	-	-	0/5/5/5	-
9	LNK	A	1112	-	-	0/2/2/2	-
4	C14	B	1102	-	-	2/11/11/11	-
10	GOL	A	1114	-	-	0/4/4/4	-
14	D12	C	1109	-	-	1/9/9/9	-
4	C14	B	1104	-	-	6/11/11/11	-
7	D10	A	1110	-	-	2/7/7/7	-
5	DDQ	C	1104	-	-	4/11/11/11	-
4	C14	A	1105	-	-	2/11/11/11	-
3	LMT	A	1103	-	-	11/21/61/61	0/2/2/2
3	LMT	A	1101	-	-	12/21/61/61	0/2/2/2
5	DDQ	C	1106	-	-	3/11/11/11	-
6	HEX	B	1107	-	-	0/3/3/3	-
5	DDQ	C	1105	-	-	2/11/11/11	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DDQ	B	1106	-	-	2/11/11/11	-
5	DDQ	A	1106	-	-	2/11/11/11	-
5	DDQ	A	1107	-	-	3/11/11/11	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1106	DDQ	O1-N1	-7.21	1.25	1.42
5	C	1106	DDQ	O1-N1	-7.15	1.25	1.42
5	B	1106	DDQ	O1-N1	-7.14	1.25	1.42
5	C	1105	DDQ	O1-N1	-7.14	1.25	1.42
5	A	1107	DDQ	O1-N1	-7.13	1.25	1.42
5	C	1104	DDQ	O1-N1	-7.13	1.25	1.42
5	B	1105	DDQ	O1-N1	-7.12	1.25	1.42
3	B	1101	LMT	O1'-C1'	2.15	1.43	1.40
3	C	1101	LMT	O1'-C1'	2.07	1.43	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1101	LMT	C1B-O5B-C5B	3.25	120.06	113.69
3	B	1101	LMT	C1'-C2'-C3'	2.19	114.56	110.00
3	B	1101	LMT	C3B-C4B-C5B	2.17	114.11	110.24
3	B	1101	LMT	O5B-C5B-C6B	2.08	111.60	106.44

There are no chirality outliers.

All (149) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1102	LMT	C2'-C1'-O1'-C1
3	A	1102	LMT	O5'-C1'-O1'-C1
3	A	1103	LMT	C2'-C1'-O1'-C1
3	A	1103	LMT	O5'-C1'-O1'-C1
3	B	1101	LMT	O5'-C1'-O1'-C1
3	C	1101	LMT	C2-C1-O1'-C1'
5	A	1107	DDQ	C2-C1-N1-CM2
5	C	1104	DDQ	C2-C1-N1-CM2
5	C	1105	DDQ	N1-C1-C2-C3
5	C	1106	DDQ	N1-C1-C2-C3
13	C	1102	PTY	C11-C8-O7-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	C	1102	PTY	C3-O11-P1-O13
13	C	1102	PTY	C3-O11-P1-O14
13	C	1102	PTY	C5-O14-P1-O13
13	C	1103	PTY	C5-O14-P1-O11
3	A	1103	LMT	O5B-C1B-O1B-C4'
13	C	1102	PTY	O30-C30-O4-C1
13	C	1102	PTY	O10-C8-O7-C6
13	C	1102	PTY	C31-C30-O4-C1
3	B	1101	LMT	O5B-C5B-C6B-O6B
13	C	1103	PTY	C11-C8-O7-C6
3	B	1101	LMT	C4B-C5B-C6B-O6B
13	C	1103	PTY	C8-C11-C12-C13
3	C	1101	LMT	O5B-C5B-C6B-O6B
3	A	1101	LMT	O1'-C1-C2-C3
3	A	1103	LMT	O1'-C1-C2-C3
3	B	1101	LMT	C5'-C4'-O1B-C1B
13	C	1103	PTY	O10-C8-O7-C6
13	C	1102	PTY	C5-O14-P1-O11
13	C	1103	PTY	C3-O11-P1-O14
3	B	1101	LMT	O5'-C5'-C6'-O6'
3	A	1102	LMT	C4-C5-C6-C7
3	A	1101	LMT	C2-C3-C4-C5
3	B	1101	LMT	O1'-C1-C2-C3
14	C	1109	D12	C5-C6-C7-C8
4	B	1103	C14	C05-C06-C07-C08
5	B	1106	DDQ	C5-C6-C7-C8
3	A	1103	LMT	C4-C5-C6-C7
5	A	1107	DDQ	C4-C5-C6-C7
3	C	1101	LMT	C2'-C1'-O1'-C1
3	C	1101	LMT	C2-C3-C4-C5
5	A	1106	DDQ	C5-C6-C7-C8
3	A	1103	LMT	C11-C10-C9-C8
10	A	1113	GOL	O1-C1-C2-C3
13	C	1102	PTY	C11-C12-C13-C14
13	C	1103	PTY	C14-C15-C16-C17
3	C	1101	LMT	O5'-C1'-O1'-C1
13	C	1103	PTY	C24-C25-C26-C27
5	C	1105	DDQ	C5-C6-C7-C8
13	C	1102	PTY	C33-C34-C35-C36
3	A	1101	LMT	C2-C1-O1'-C1'
3	A	1101	LMT	C7-C8-C9-C10
5	B	1106	DDQ	C2-C3-C4-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	1101	LMT	C7-C8-C9-C10
4	A	1105	C14	C04-C05-C06-C07
3	A	1101	LMT	C1-C2-C3-C4
13	C	1102	PTY	C18-C19-C20-C21
4	B	1104	C14	C03-C04-C05-C06
3	B	1101	LMT	C3'-C4'-O1B-C1B
12	B	1110	EDO	O1-C1-C2-O2
13	C	1103	PTY	C32-C33-C34-C35
5	C	1106	DDQ	C5-C6-C7-C8
3	C	1101	LMT	C5-C6-C7-C8
13	C	1102	PTY	C21-C22-C23-C24
3	A	1102	LMT	C2-C3-C4-C5
3	B	1101	LMT	C2'-C1'-O1'-C1
3	A	1104	LMT	C2-C3-C4-C5
3	A	1104	LMT	C5-C6-C7-C8
13	C	1102	PTY	C40-C41-C42-C43
5	C	1106	DDQ	C1-C2-C3-C4
4	B	1104	C14	C09-C10-C11-C12
4	B	1104	C14	C05-C06-C07-C08
3	C	1101	LMT	C6-C7-C8-C9
13	C	1102	PTY	C23-C24-C25-C26
3	A	1101	LMT	O5B-C5B-C6B-O6B
3	B	1101	LMT	C3-C4-C5-C6
3	A	1103	LMT	C3-C4-C5-C6
4	B	1103	C14	C09-C10-C11-C12
4	B	1102	C14	C07-C08-C09-C10
5	A	1106	DDQ	N1-C1-C2-C3
5	B	1105	DDQ	C1-C2-C3-C4
3	A	1101	LMT	C5-C6-C7-C8
3	A	1102	LMT	C2-C1-O1'-C1'
3	A	1103	LMT	C9-C10-C11-C12
13	C	1102	PTY	C26-C27-C28-C29
3	B	1101	LMT	C2-C3-C4-C5
3	C	1101	LMT	C1-C2-C3-C4
13	C	1102	PTY	C32-C33-C34-C35
3	B	1101	LMT	C4'-C5'-C6'-O6'
13	C	1103	PTY	C16-C17-C18-C19
13	C	1102	PTY	C36-C37-C38-C39
13	C	1102	PTY	C20-C21-C22-C23
3	B	1101	LMT	C6-C7-C8-C9
5	B	1105	DDQ	C2-C3-C4-C5
13	C	1102	PTY	C14-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	1102	LMT	C1-C2-C3-C4
5	A	1107	DDQ	C2-C1-N1-CM1
5	C	1104	DDQ	C2-C1-N1-CM1
4	B	1102	C14	C02-C03-C04-C05
3	A	1104	LMT	O5'-C5'-C6'-O6'
13	C	1102	PTY	C6-C5-O14-P1
13	C	1103	PTY	C6-C5-O14-P1
13	C	1102	PTY	C5-O14-P1-O12
13	C	1103	PTY	C3-O11-P1-O13
13	C	1103	PTY	C5-O14-P1-O12
4	B	1103	C14	C02-C03-C04-C05
13	C	1102	PTY	C2-C3-O11-P1
3	C	1101	LMT	O5'-C5'-C6'-O6'
13	C	1103	PTY	O14-C5-C6-O7
3	C	1101	LMT	C4B-C5B-C6B-O6B
3	A	1102	LMT	C6-C7-C8-C9
3	C	1101	LMT	C4-C5-C6-C7
13	C	1103	PTY	C22-C23-C24-C25
13	C	1103	PTY	O14-C5-C6-C1
3	A	1101	LMT	C6-C7-C8-C9
13	C	1103	PTY	C13-C14-C15-C16
5	B	1105	DDQ	C5-C6-C7-C8
10	A	1113	GOL	O1-C1-C2-O2
13	C	1103	PTY	C31-C30-O4-C1
13	C	1103	PTY	O30-C30-O4-C1
3	A	1104	LMT	C6-C7-C8-C9
3	B	1101	LMT	C5-C6-C7-C8
4	B	1104	C14	C02-C03-C04-C05
13	C	1103	PTY	C12-C13-C14-C15
3	A	1102	LMT	C4B-C5B-C6B-O6B
4	B	1104	C14	C10-C11-C12-C13
3	A	1103	LMT	C2-C3-C4-C5
3	A	1103	LMT	C3'-C4'-O1B-C1B
13	C	1102	PTY	O4-C30-C31-C32
13	C	1102	PTY	C12-C13-C14-C15
4	A	1105	C14	C06-C07-C08-C09
3	A	1101	LMT	C4-C5-C6-C7
7	A	1110	D10	C7-C8-C9-C10
13	C	1102	PTY	C1-C6-O7-C8
13	C	1102	PTY	O14-C5-C6-O7
3	A	1103	LMT	C5'-C4'-O1B-C1B
3	C	1101	LMT	O1'-C1-C2-C3

Continued on next page...

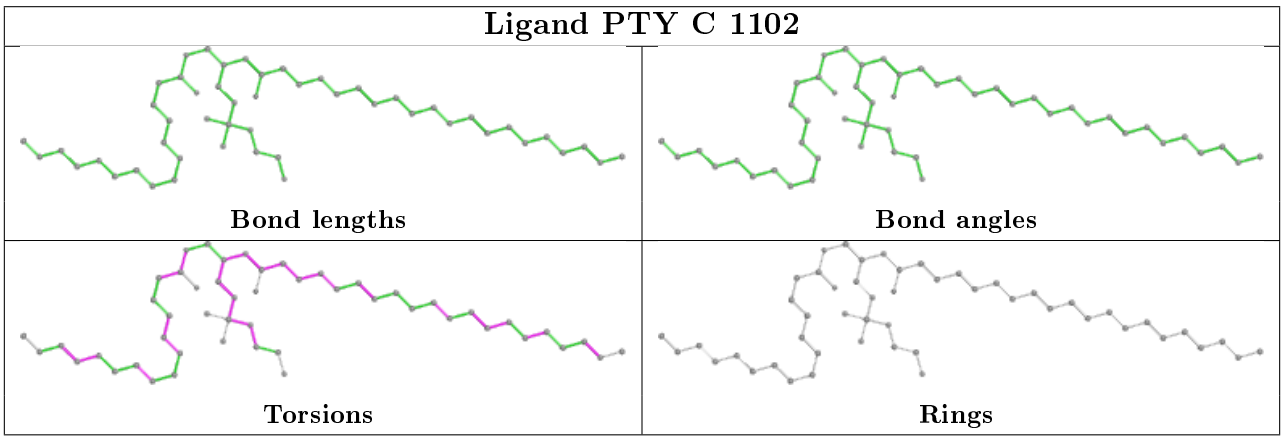
Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	A	1110	D10	C6-C7-C8-C9
13	C	1102	PTY	O14-C5-C6-C1
5	C	1104	DDQ	C5-C6-C7-C8
5	C	1104	DDQ	C6-C7-C8-C9
3	A	1101	LMT	O5B-C1B-O1B-C4'
4	B	1104	C14	C01-C02-C03-C04
13	C	1102	PTY	C39-C40-C41-C42
3	B	1101	LMT	C1-C2-C3-C4
13	C	1102	PTY	C8-C11-C12-C13
13	C	1102	PTY	C12-C11-C8-O7
3	A	1101	LMT	O5'-C5'-C6'-O6'
3	A	1101	LMT	C2B-C1B-O1B-C4'

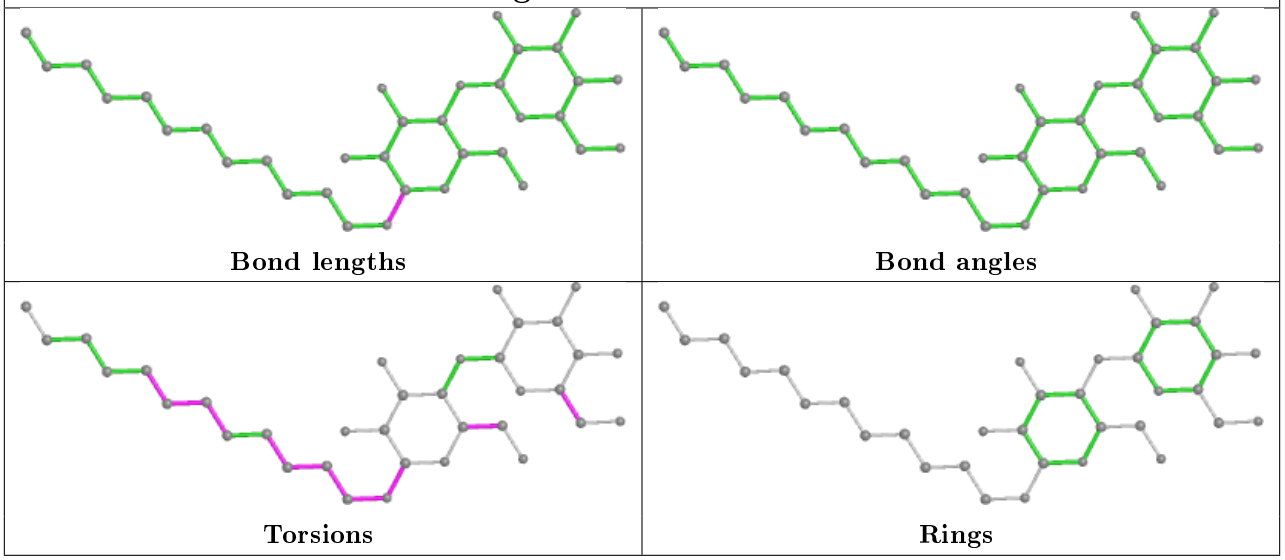
There are no ring outliers.

No monomer is involved in short contacts.

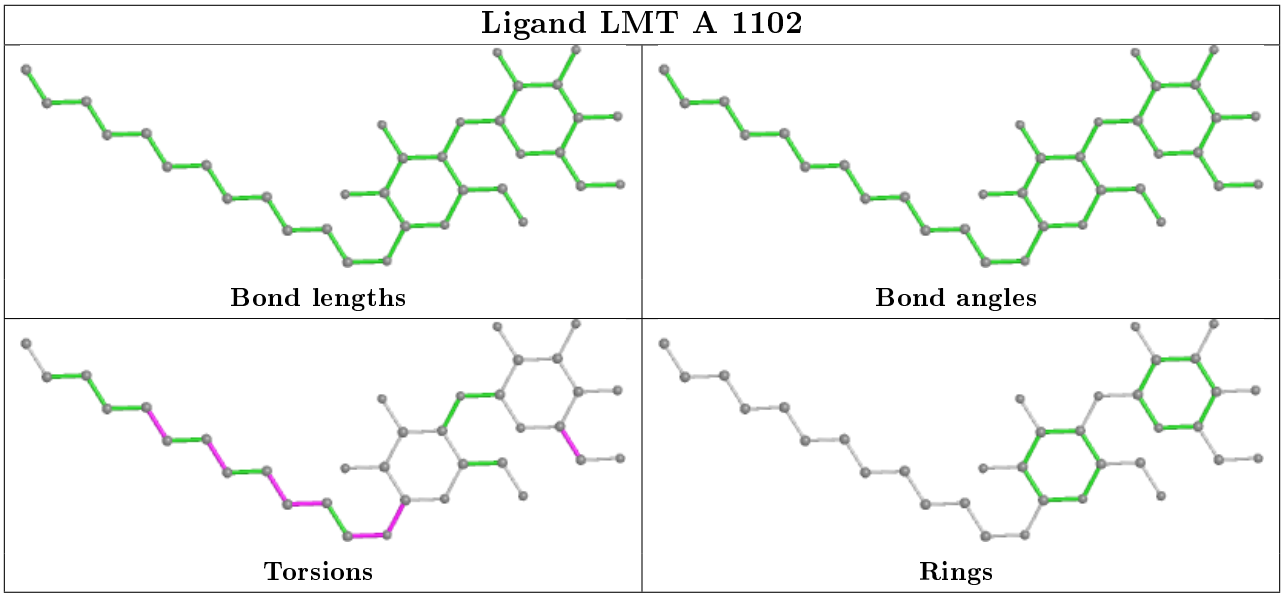
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



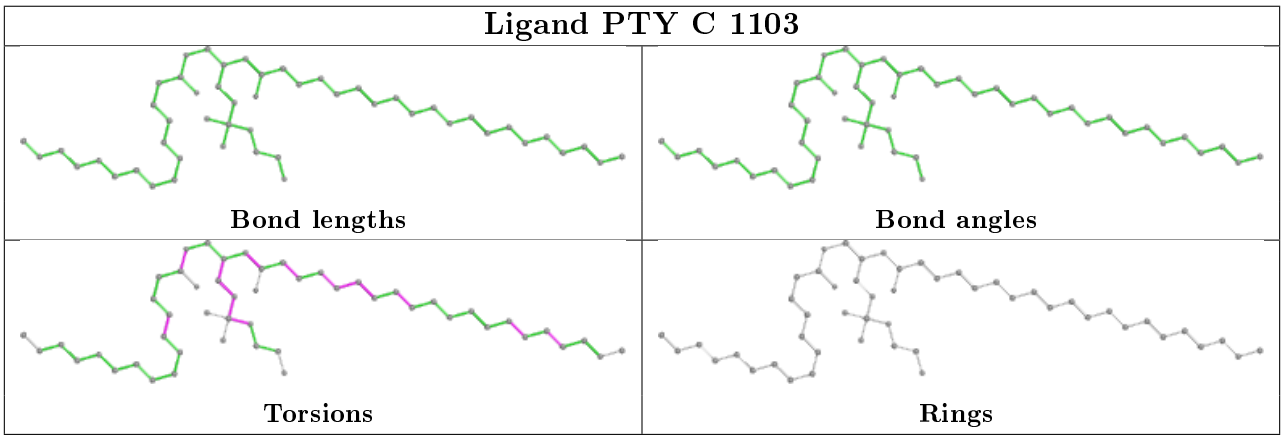
Ligand LMT C 1101



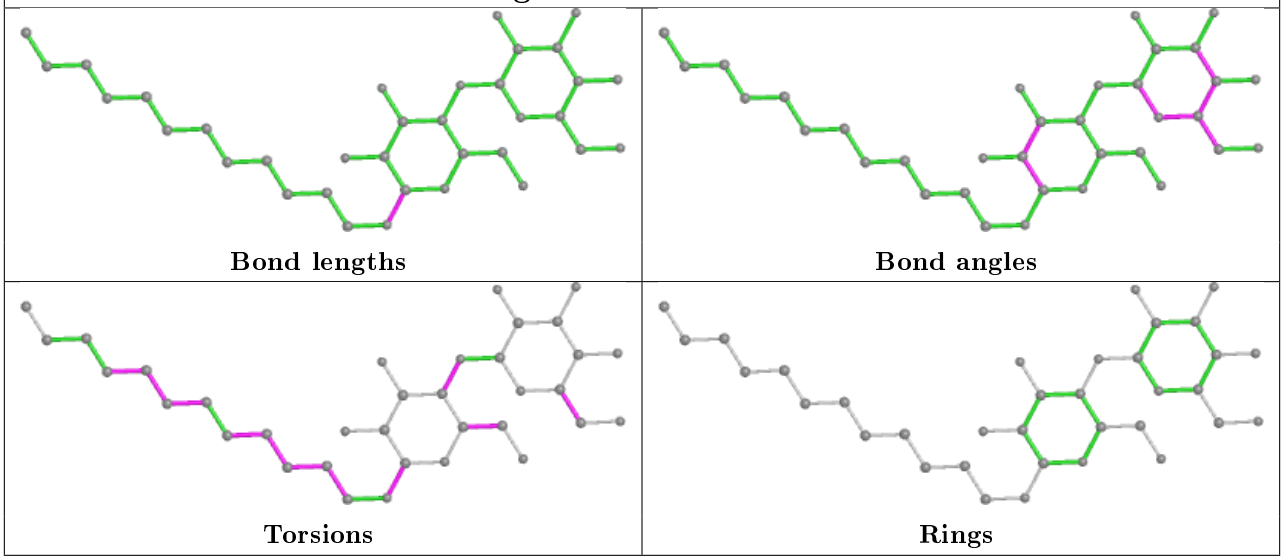
Ligand LMT A 1102



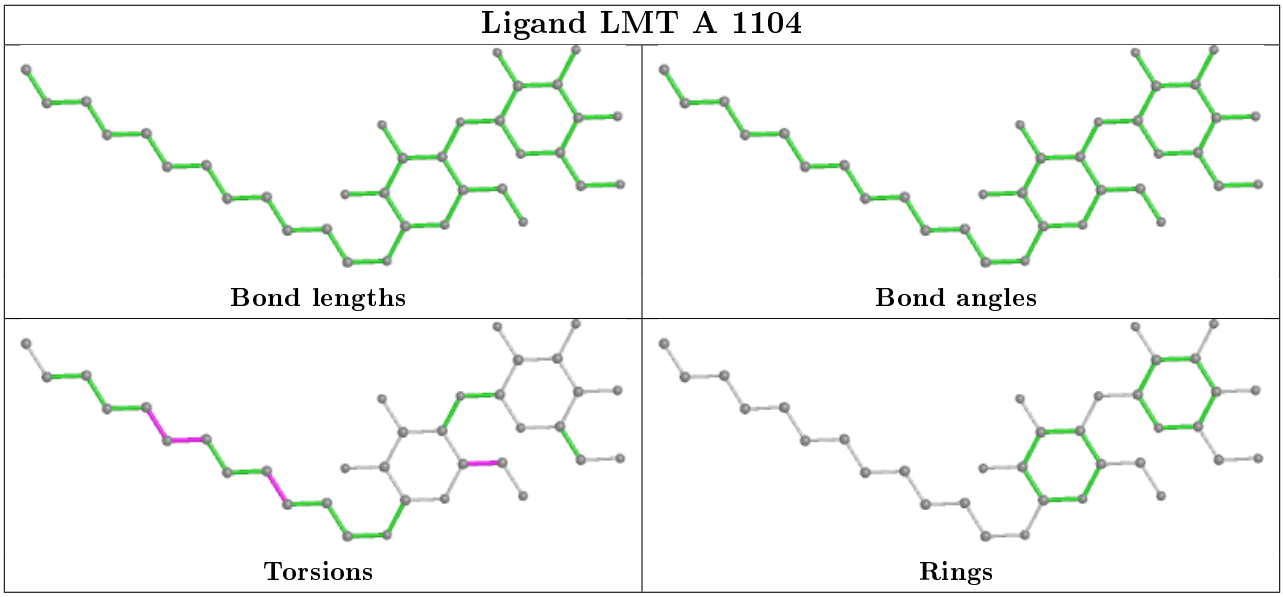
Ligand PTY C 1103



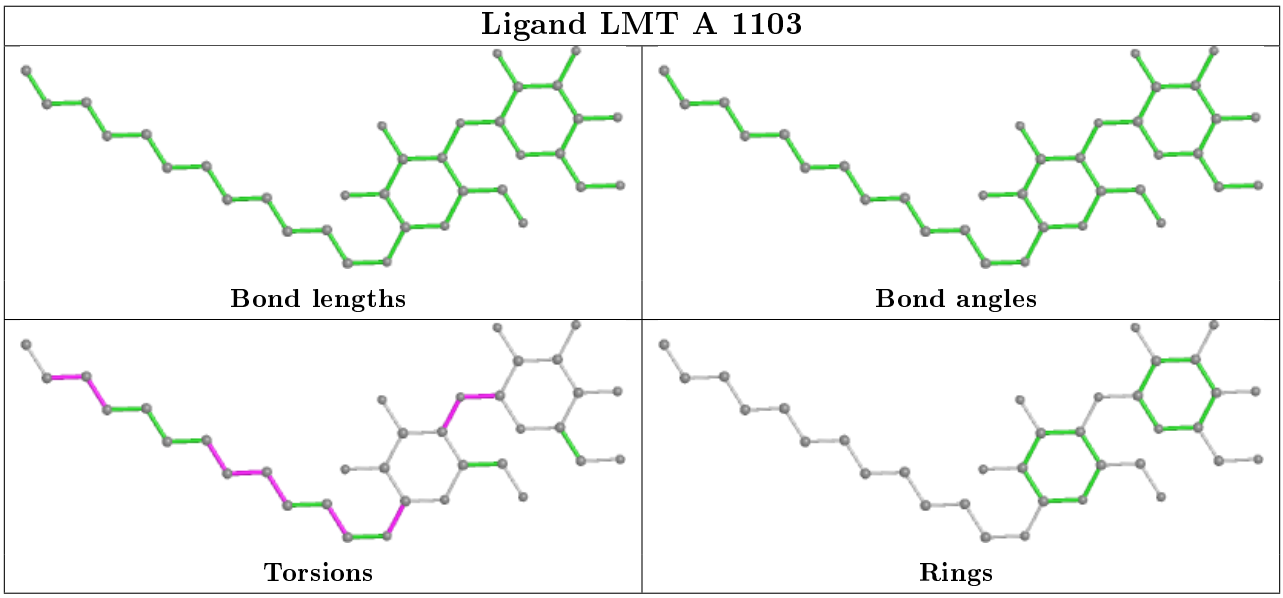
Ligand LMT B 1101



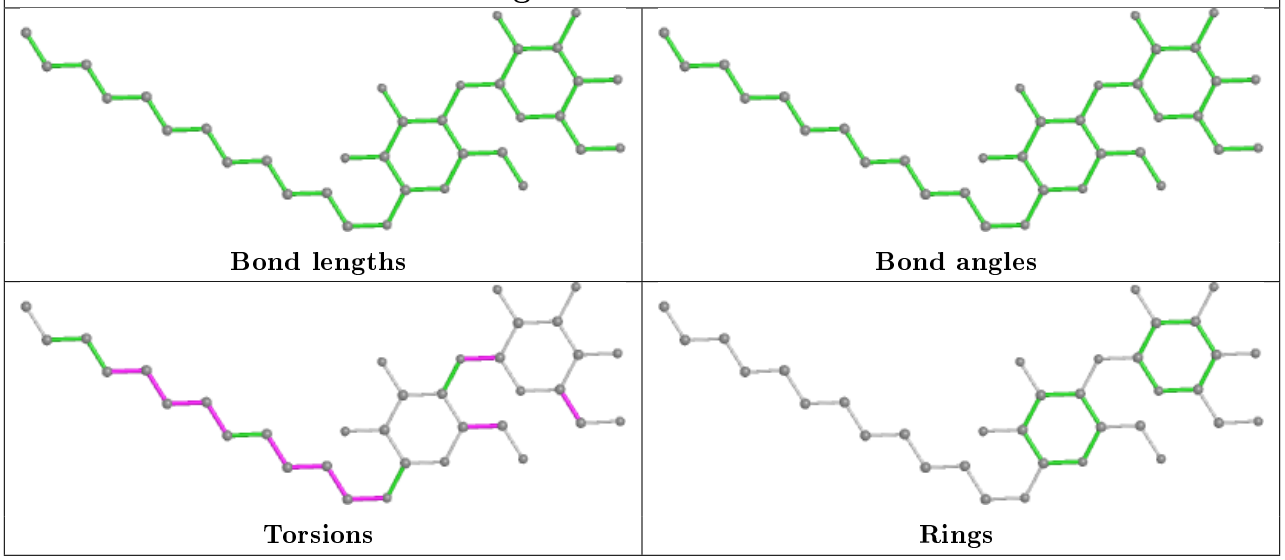
Ligand LMT A 1104



Ligand LMT A 1103



Ligand LMT A 1101



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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^{th} 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^2)	Q<0.9
1	A	1042/1057 (98%)	0.00	29 (2%) 53 28	48, 64, 98, 112	0
1	B	1024/1057 (96%)	-0.03	22 (2%) 63 39	48, 62, 79, 93	0
1	C	1035/1057 (97%)	-0.17	13 (1%) 77 56	45, 55, 72, 81	0
2	D	156/169 (92%)	0.27	10 (6%) 19 7	52, 63, 76, 87	0
2	E	154/169 (91%)	0.80	16 (10%) 6 2	55, 69, 90, 95	0
All	All	3411/3509 (97%)	-0.01	90 (2%) 56 30	45, 61, 85, 112	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	833	PRO	4.8
2	D	166	GLN	4.5
1	B	255	GLN	4.4
2	E	31	ARG	4.1
2	E	35	ALA	3.9
2	D	11	GLY	3.9
1	B	1005	THR	3.9
2	E	32	ILE	3.8
1	A	256	ASP	3.6
2	E	66	LEU	3.6
2	D	162	ALA	3.6
1	A	832	ALA	3.5
1	B	134	SER	3.4
1	A	254	ASN	3.3
1	A	258	SER	3.2
2	E	29	GLU	3.2
2	E	27	ASP	3.2
1	A	710	PRO	3.2
1	A	834	GLY	3.1
1	B	673	GLU	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	867	ARG	2.9
2	E	28	ASP	2.9
2	D	165	LEU	2.9
1	B	195	LYS	2.9
1	A	1041	GLU	2.9
1	C	427	PRO	2.8
2	E	30	VAL	2.8
1	A	869	SER	2.8
1	B	600	THR	2.8
1	A	836	SER	2.8
1	B	256	ASP	2.8
2	E	34	MET	2.7
2	D	25	GLY	2.7
2	E	36	ASN	2.7
1	C	1035	ARG	2.7
1	B	257	GLY	2.7
2	E	33	LEU	2.7
1	A	871	ASN	2.7
1	A	841	MET	2.6
1	A	865	GLN	2.6
1	A	706	ALA	2.6
2	D	150	PHE	2.6
1	B	708	LYS	2.6
1	C	510	LYS	2.6
1	A	1040	ILE	2.5
2	D	159	GLU	2.5
1	A	255	GLN	2.5
1	A	831	ALA	2.5
1	B	1006	GLY	2.5
1	B	788	ASP	2.5
1	A	503	GLY	2.5
1	A	711	ASP	2.5
1	A	830	GLN	2.5
1	C	508	GLY	2.4
1	C	730	ASP	2.4
2	E	70	GLY	2.4
1	B	196	PHE	2.4
1	B	1002	ALA	2.4
1	A	829	GLY	2.4
1	C	797	GLN	2.4
2	D	154	ILE	2.4
1	A	521	GLU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	840	ALA	2.3
1	C	735	LYS	2.3
1	B	561	SER	2.3
1	C	426	PRO	2.3
1	B	918	PHE	2.2
1	C	255	GLN	2.2
1	A	257	GLY	2.2
1	B	362	PHE	2.2
1	A	1042	HIS	2.2
1	C	258	SER	2.2
1	B	254	ASN	2.2
2	D	148	THR	2.2
1	A	681	ASP	2.2
1	A	1039	ASP	2.2
1	C	788	ASP	2.2
2	E	107	ASN	2.2
2	E	159	GLU	2.2
1	B	988	PRO	2.2
1	C	362	PHE	2.1
2	E	55	ALA	2.1
1	B	508	GLY	2.1
1	A	707	ALA	2.1
2	D	163	GLU	2.1
1	C	497	LEU	2.1
1	B	1001	ASN	2.1
1	B	606	VAL	2.0
2	E	68	LYS	2.0
1	B	191	ASN	2.0

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,

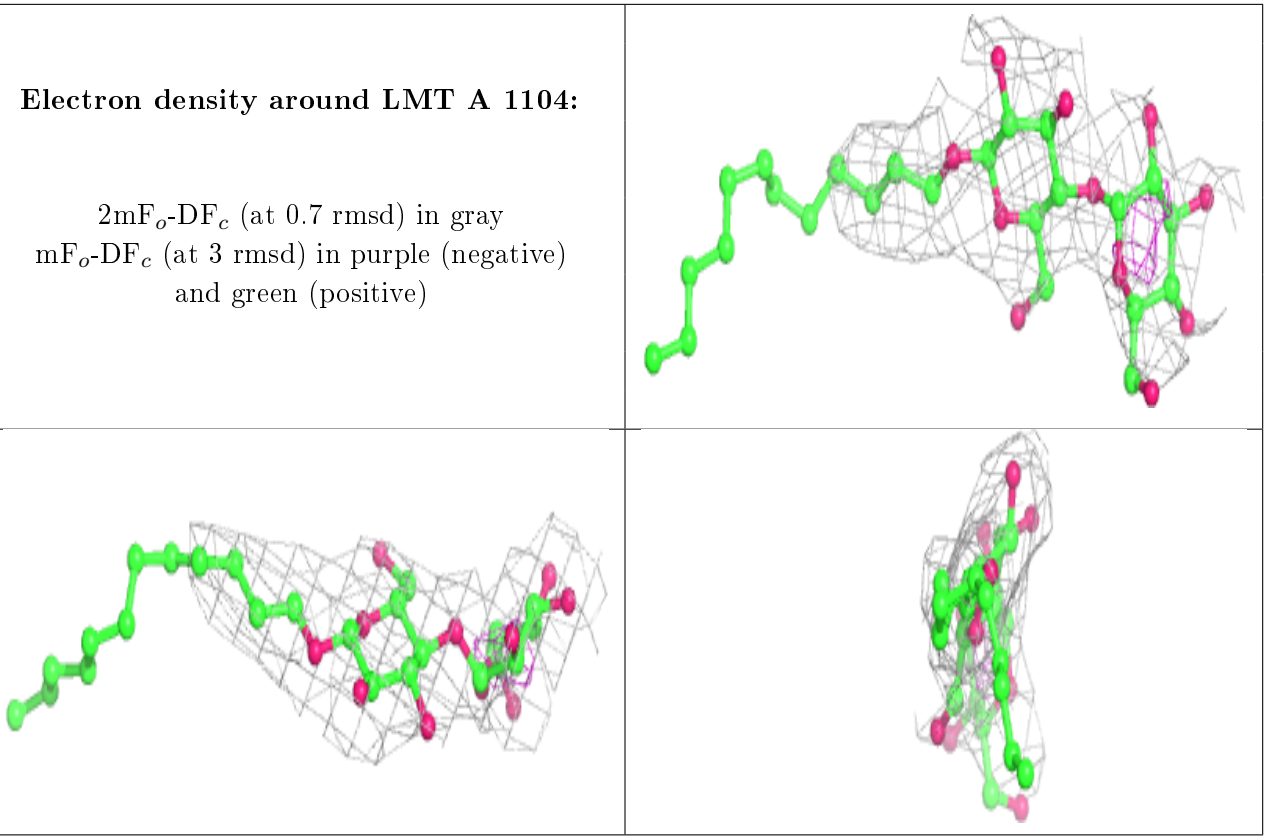
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	DDQ	C	1105	14/14	0.63	0.38	84,86,88,88	0
10	GOL	A	1114	6/6	0.66	0.25	83,83,83,83	0
5	DDQ	B	1106	14/14	0.68	0.33	87,88,90,90	0
9	LNK	A	1112	5/5	0.70	0.38	70,70,71,71	0
3	LMT	A	1104	35/35	0.70	0.41	90,97,102,102	0
5	DDQ	C	1104	14/14	0.71	0.33	82,85,87,88	0
5	DDQ	A	1107	14/14	0.74	0.34	88,89,91,91	0
4	C14	A	1105	14/14	0.77	0.29	79,80,80,80	0
13	PTY	C	1103	50/50	0.78	0.31	75,79,82,82	0
13	PTY	C	1102	50/50	0.79	0.30	82,88,102,102	0
3	LMT	A	1102	35/35	0.79	0.32	72,84,92,93	0
14	D12	C	1109	12/12	0.79	0.25	70,71,72,72	0
3	LMT	C	1101	35/35	0.80	0.37	71,74,81,82	0
8	CL	A	1111	1/1	0.80	0.17	66,66,66,66	0
11	OCT	B	1108	8/8	0.80	0.48	71,72,72,72	0
4	C14	B	1104	14/14	0.81	0.26	78,78,79,79	0
3	LMT	A	1103	35/35	0.81	0.28	83,87,90,91	0
3	LMT	B	1101	35/35	0.81	0.43	88,90,91,92	0
4	C14	B	1103	14/14	0.81	0.31	82,83,83,83	0
5	DDQ	C	1106	14/14	0.82	0.31	84,85,85,86	0
5	DDQ	A	1106	14/14	0.82	0.34	74,75,76,76	0
6	HEX	A	1109	6/6	0.83	0.27	78,78,78,78	0
10	GOL	B	1109	6/6	0.83	0.24	87,87,87,87	0
10	GOL	A	1113	6/6	0.83	0.30	70,70,70,70	0
4	C14	B	1102	14/14	0.84	0.22	76,77,78,78	0
5	DDQ	B	1105	14/14	0.84	0.30	68,72,76,76	0
3	LMT	A	1101	35/35	0.86	0.27	65,71,74,74	35
7	D10	A	1110	10/10	0.86	0.27	70,70,70,70	0
11	OCT	C	1108	8/8	0.86	0.33	73,74,75,75	0
6	HEX	B	1107	6/6	0.87	0.30	67,68,68,68	0
6	HEX	A	1108	6/6	0.88	0.23	74,74,75,75	0
12	EDO	B	1110	4/4	0.92	0.18	72,72,73,73	0
6	HEX	C	1107	6/6	0.94	0.26	71,71,71,71	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.

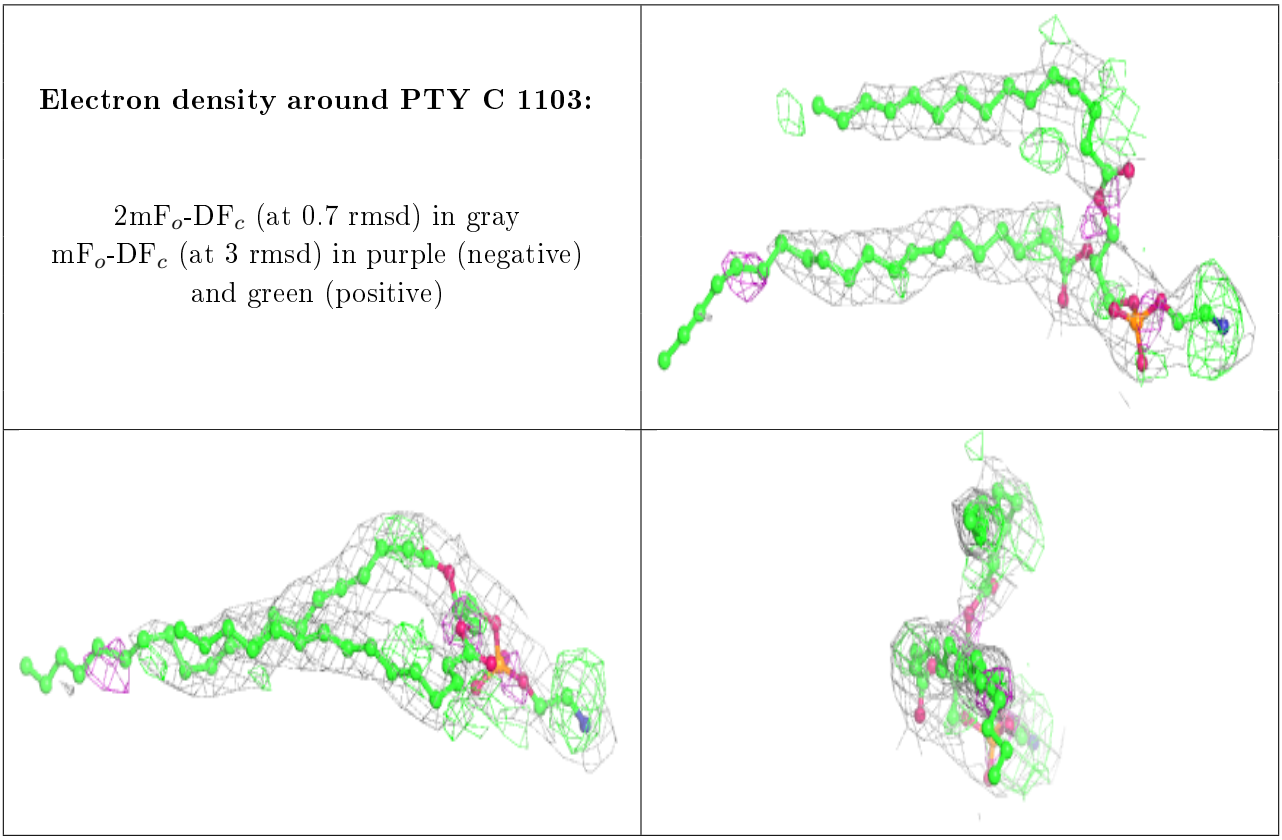
Electron density around LMT A 1104:

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



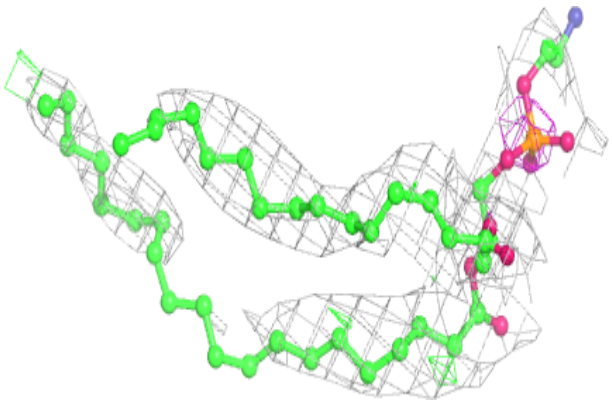
Electron density around PTY C 1103:

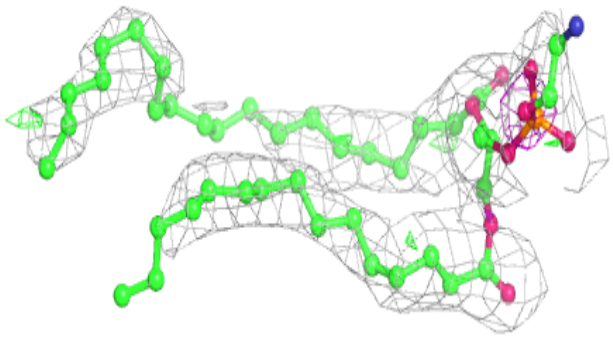
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

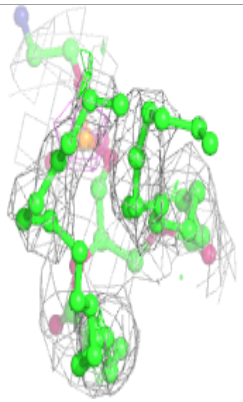


Electron density around PTY C 1102:

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

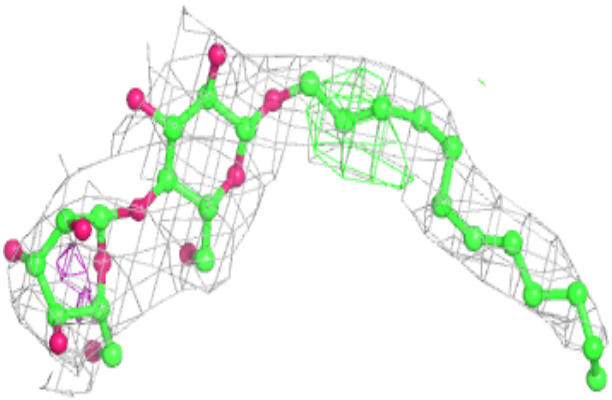


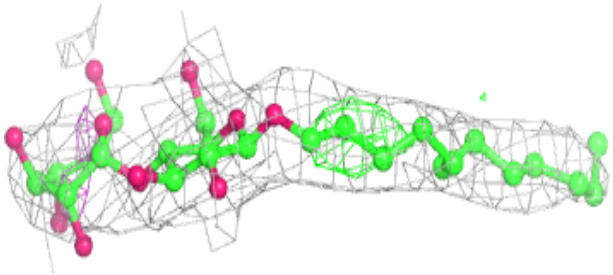


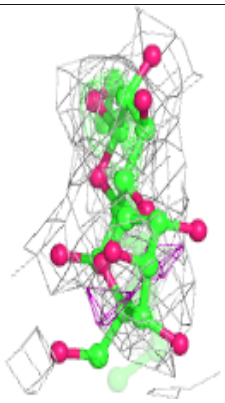


Electron density around LMT A 1102:

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

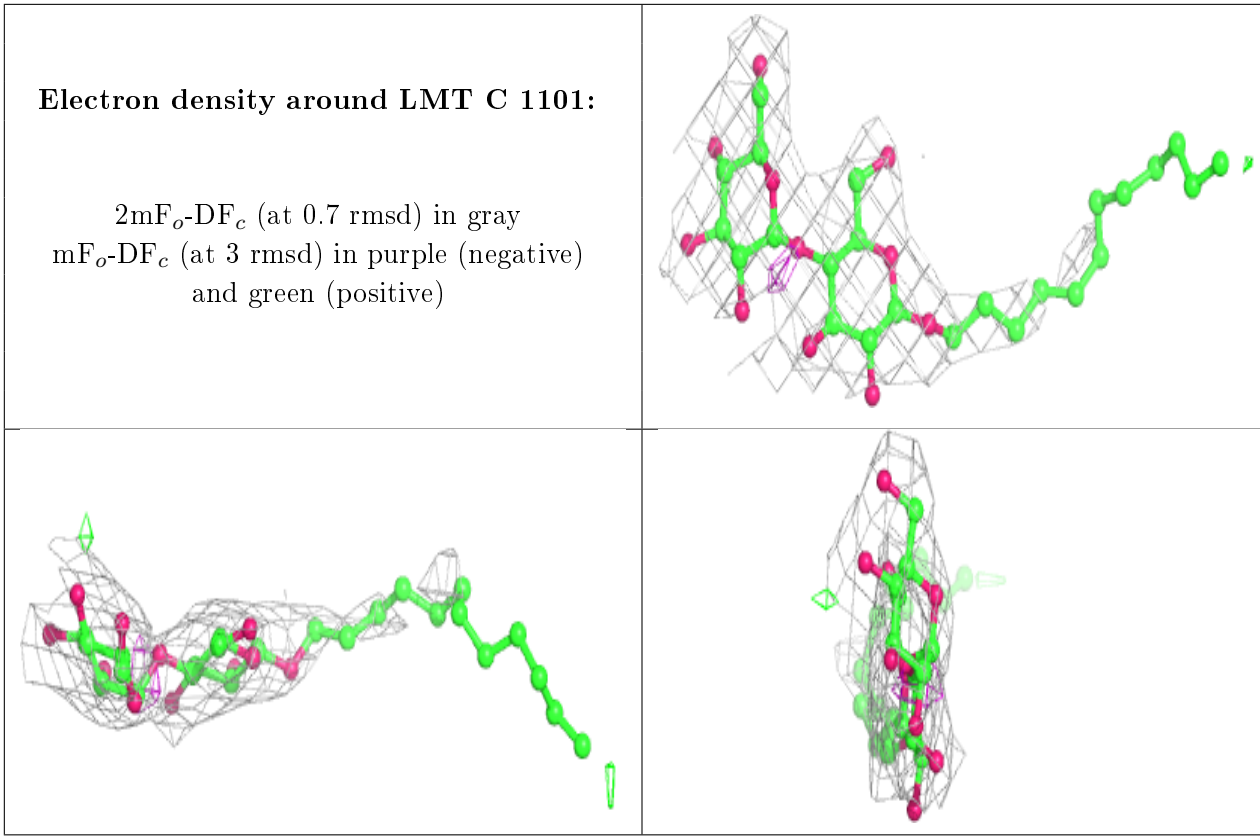






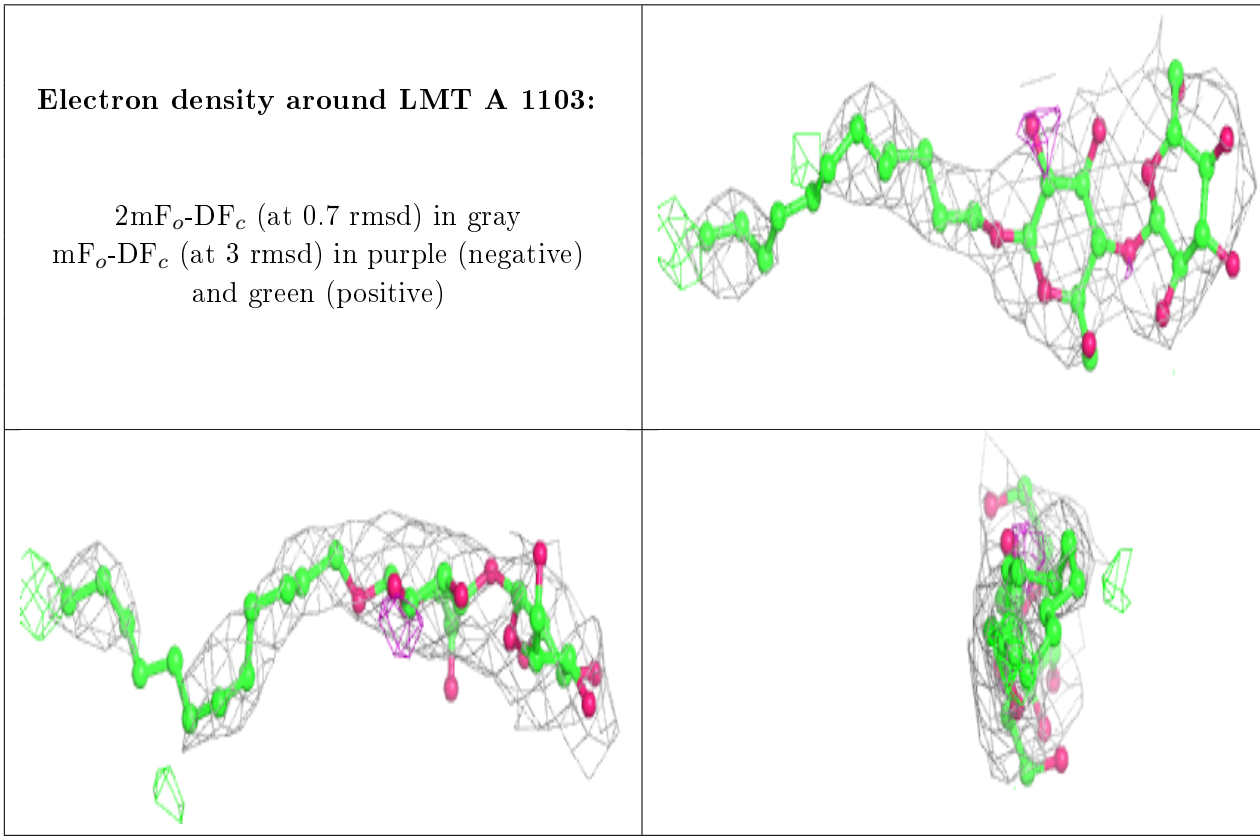
Electron density around LMT C 1101:

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



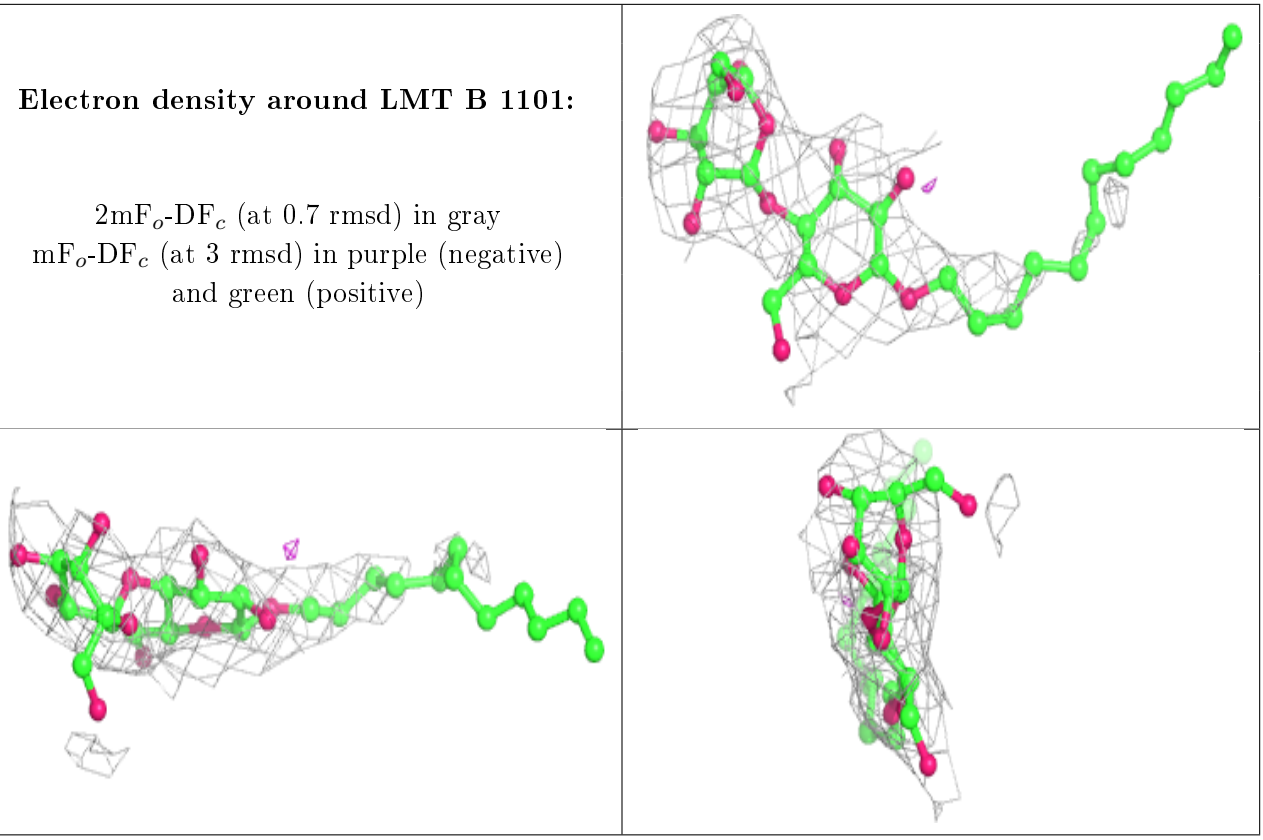
Electron density around LMT A 1103:

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



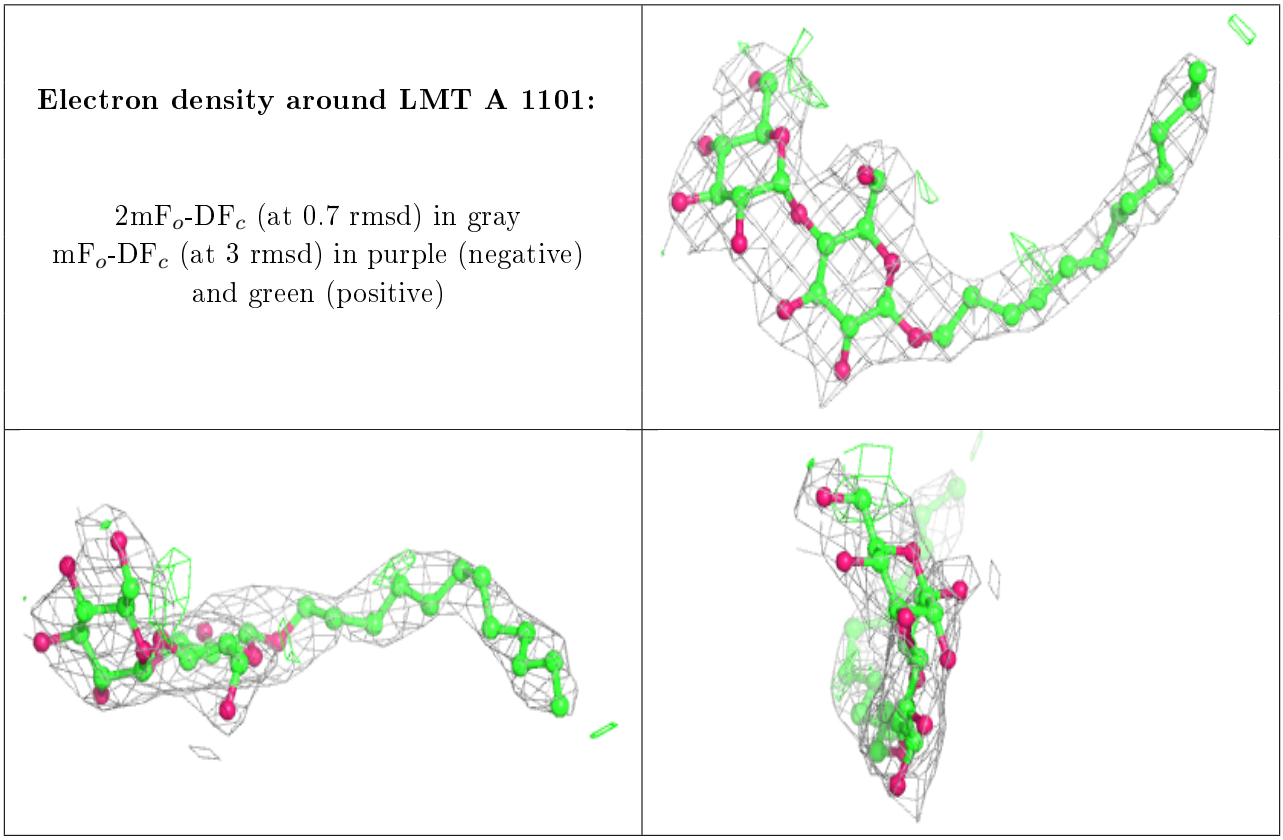
Electron density around LMT B 1101:

$2mF_o$-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 1101:

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



6.5 Other polymers (i)

There are no such residues in this entry.