wwPDB X-ray Structure Validation Summary Report (i)

Aug 25, 2020 – 05:22 PM BST

PDB ID	:	5JMN
Title	:	Fusidic acid bound AcrB
Authors	:	Oswald, C.; Tam, H.K.; Pos, K.M.
Deposited on	:	2016-04-29
Resolution	:	2.50 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

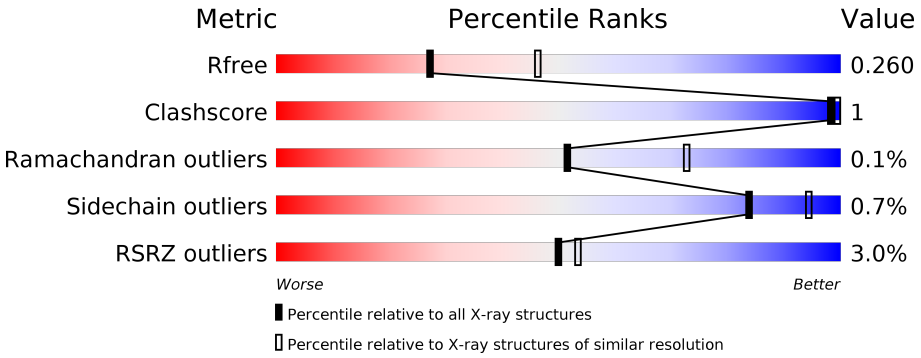
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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	5% 95%
1	B	1057	2% 96%
1	C	1057	% 95%
2	D	169	3% 93% 7%
2	E	169	11% 90% 9%

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 27640 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	3	0
			7874	5068	1299	1462	45			
1	B	1034	Total	C	N	O	S	0	0	0
			7855	5055	1296	1460	44			
1	C	1033	Total	C	N	O	S	0	1	0
			7855	5056	1295	1460	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

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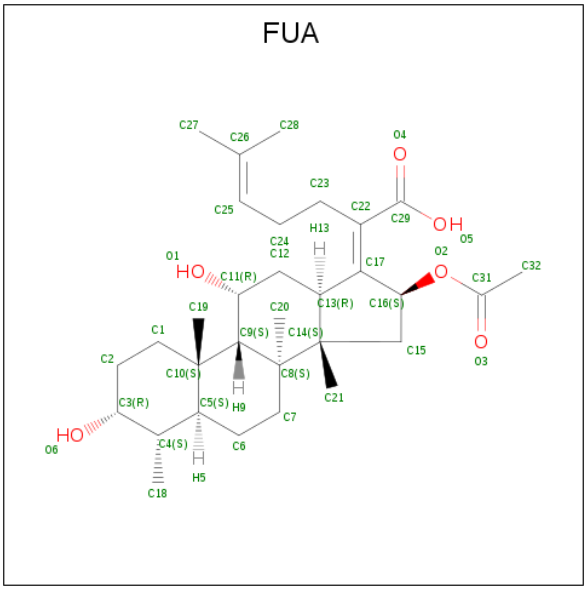
Chain	Residue	Modelled	Actual	Comment	Reference
C	1057	HIS	-	expression tag	UNP P31224

- Molecule 2 is a protein called DARPin.

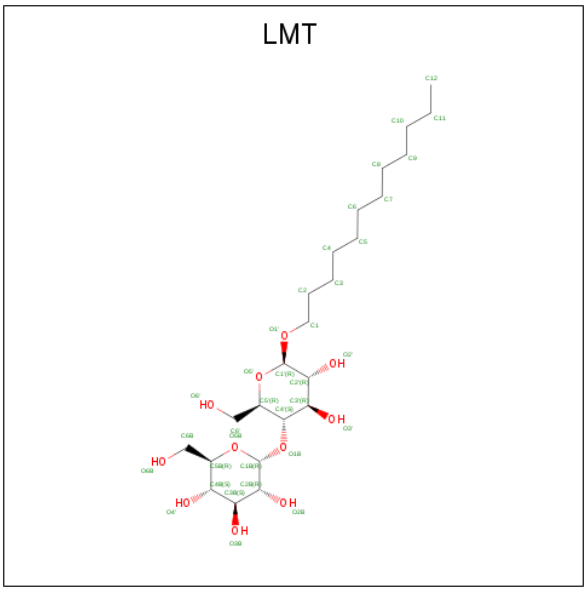
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	158	Total	C	N	O	S	0	0	0
			1194	753	209	231	1			
2	E	154	Total	C	N	O	S	0	1	0
			1173	740	204	228	1			

- Molecule 3 is FUSIDIC ACID (three-letter code: FUA) (formula: $C_{31}H_{48}O_6$).



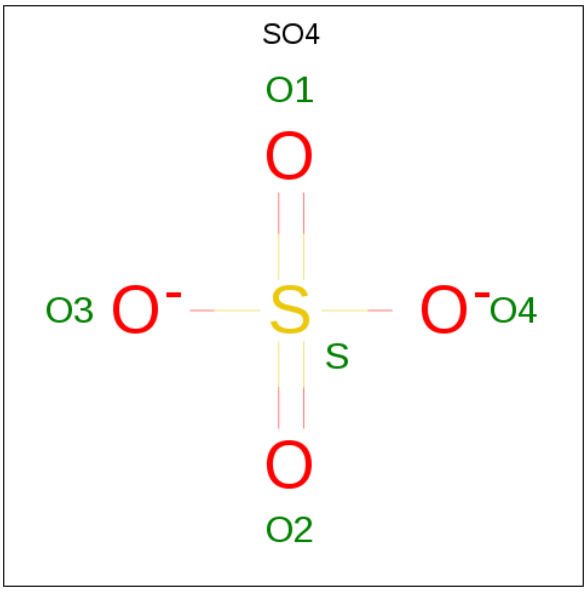
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			37	31	6		
3	B	1	Total	C	O	0	0
			37	31	6		
3	C	1	Total	C	O	0	0
			37	31	6		

- Molecule 4 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



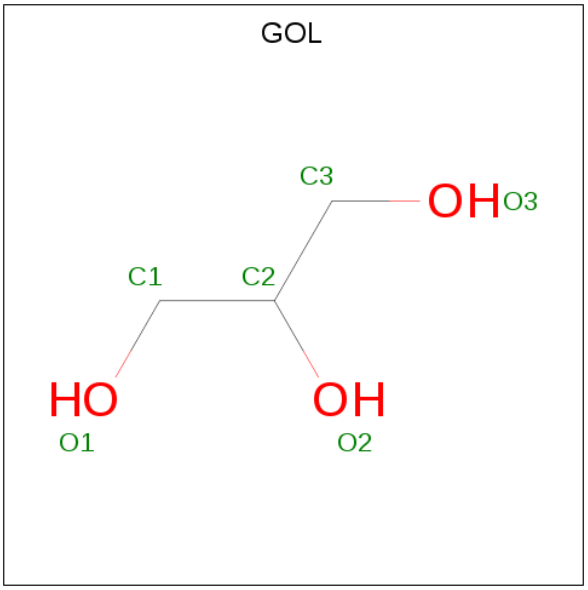
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 35 24 11	0	0
4	A	1	Total C O 35 24 11	0	0
4	A	1	Total C O 35 24 11	0	0
4	B	1	Total C O 35 24 11	0	0
4	B	1	Total C O 35 24 11	0	0
4	B	1	Total C O 35 24 11	0	0
4	C	1	Total C O 35 24 11	0	0
4	C	1	Total C O 35 24 11	0	0
4	C	1	Total C O 35 24 11	0	0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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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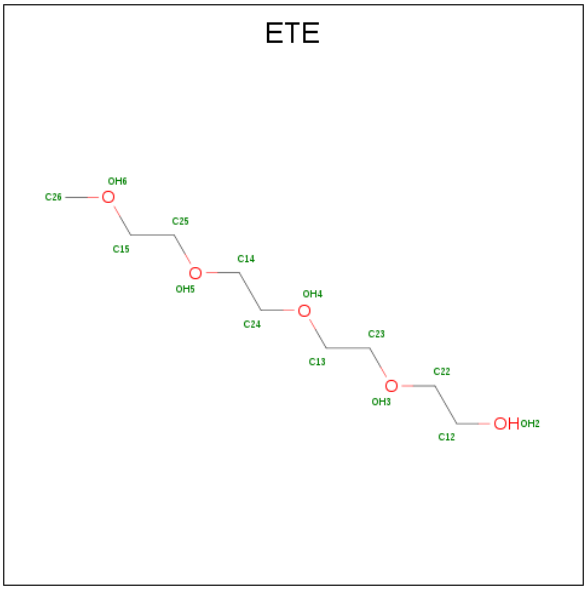
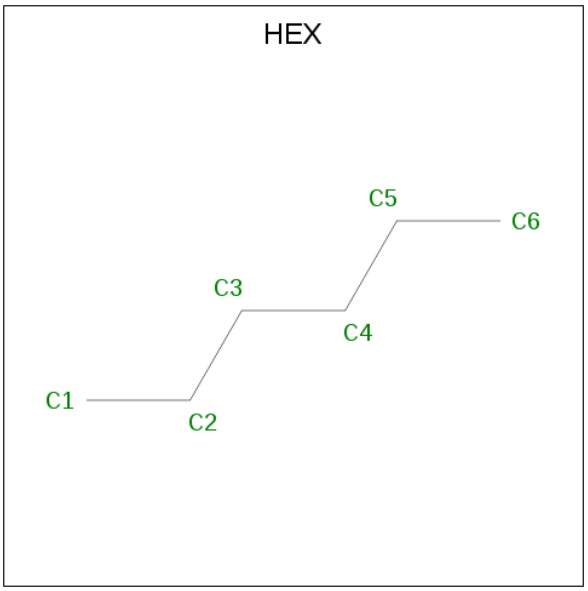
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 6 3 3	0	0
6	C	1	Total C O 6 3 3	0	0
6	C	1	Total C O 6 3 3	0	0
6	D	1	Total C O 6 3 3	0	0
6	E	1	Total C O 6 3 3	0	0
6	E	1	Total C O 6 3 3	0	0

- Molecule 7 is 2-{2-[2-2-(METHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (three-letter code: ETE) (formula: $C_9H_{20}O_5$).



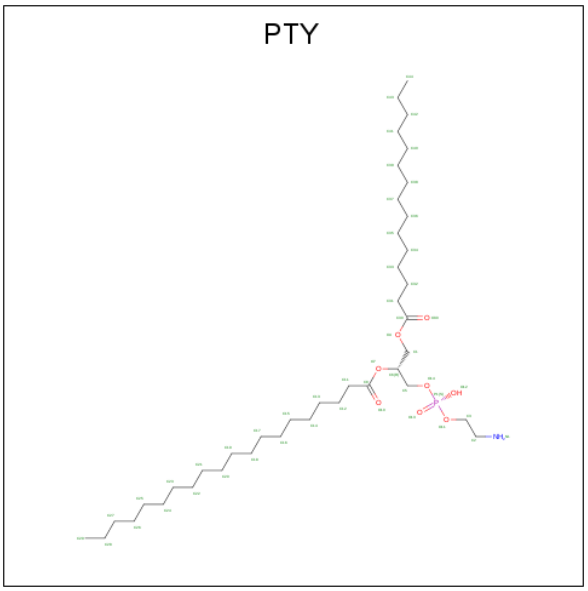
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 14 9 5	0	0
7	A	1	Total C O 14 9 5	0	0
7	C	1	Total C O 14 9 5	0	0

- Molecule 8 is HEXANE (three-letter code: HEX) (formula: C_6H_{14}).



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

- Molecule 9 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$).



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

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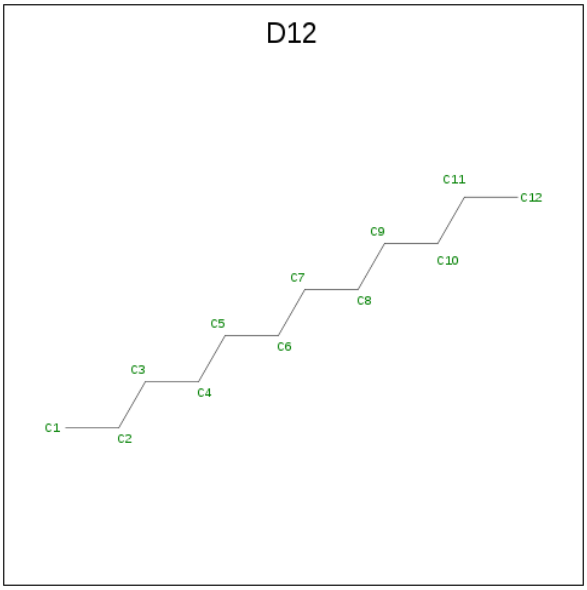
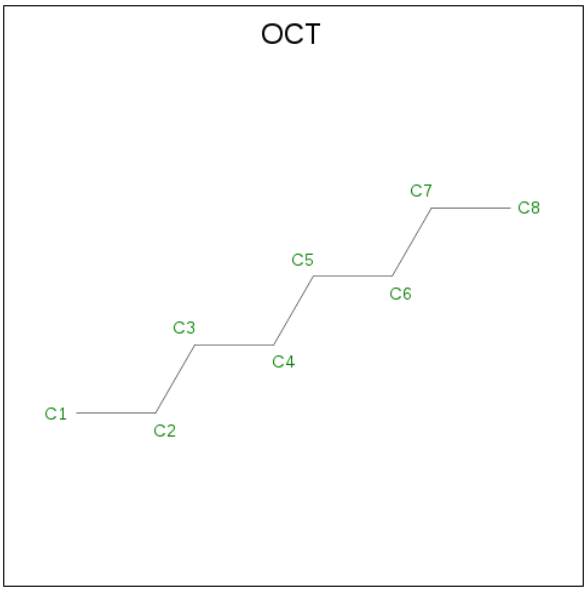
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	C	1	Total	C	N	O	P	0	0
			50	40	1	8	1		
9	C	1	Total	C	N	O	P	0	0
			50	40	1	8	1		
9	C	1	Total	C	N	O	P	0	0
			50	40	1	8	1		

- Molecule 10 is DODECANE (three-letter code: D12) (formula: $C_{12}H_{26}$).



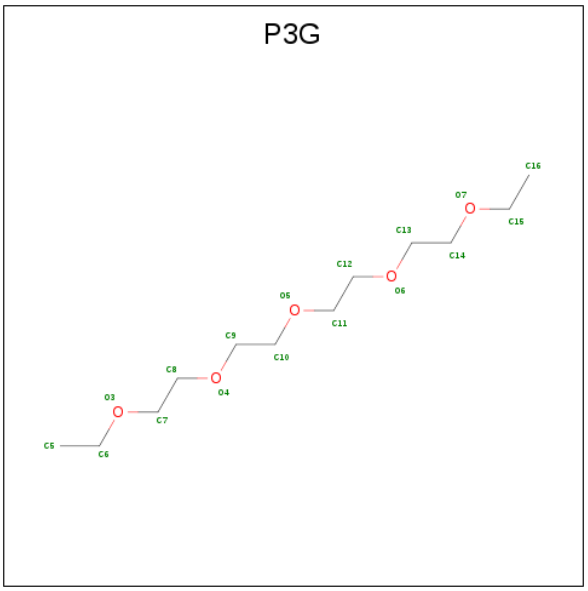
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	1	Total	C	0	0
			12	12		
10	C	1	Total	C	0	0
			12	12		
10	C	1	Total	C	0	0
			12	12		
10	C	1	Total	C	0	0
			12	12		

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



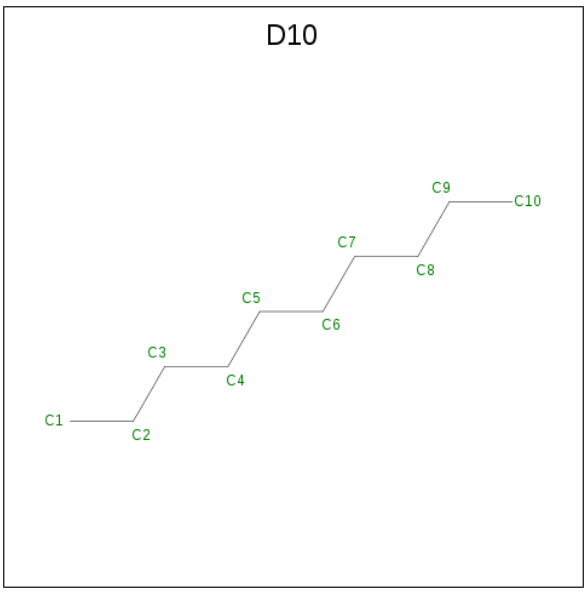
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	1	Total C 8 8	0	0
11	C	1	Total C 8 8	0	0

- Molecule 12 is 3,6,9,12,15-PENTAOXAHEPTADECANE (three-letter code: P3G) (formula: $C_{12}H_{26}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	B	1	Total C O 17 12 5	0	0

- Molecule 13 is DECANE (three-letter code: D10) (formula: $C_{10}H_{22}$).



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

- Molecule 14 is water.

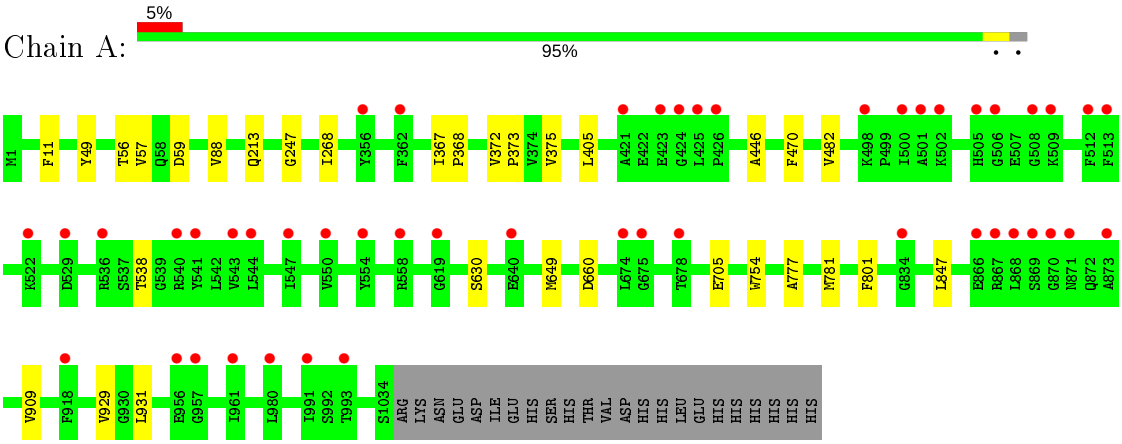
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	265	Total O 265 265	0	0
14	B	223	Total O 223 223	0	0
14	C	271	Total O 271 271	0	0
14	D	28	Total O 28 28	0	0
14	E	28	Total O 28 28	0	0

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.

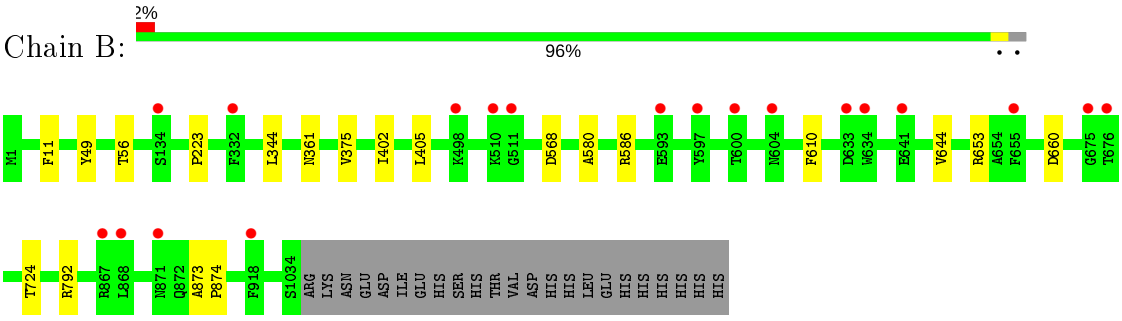
- Molecule 1: Multidrug efflux pump subunit AcrB

Chain A:



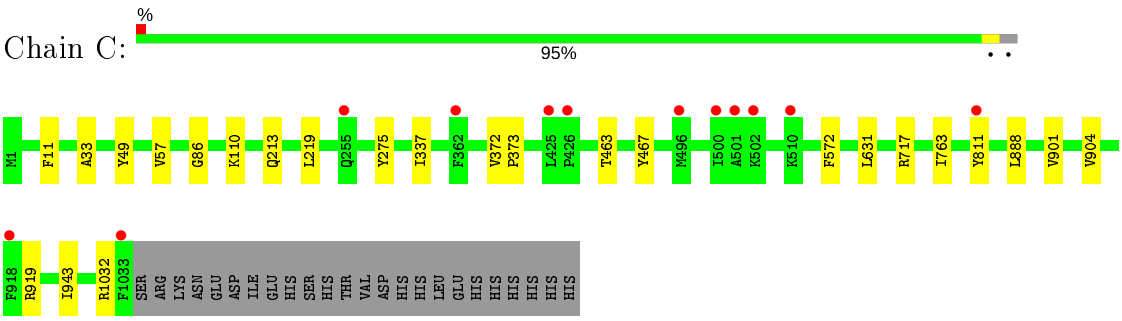
- Molecule 1: Multidrug efflux pump subunit AcrB

Chain B:



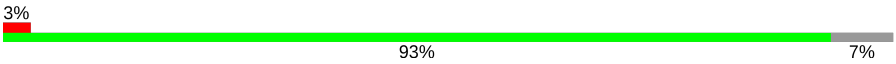
- Molecule 1: Multidrug efflux pump subunit AcrB

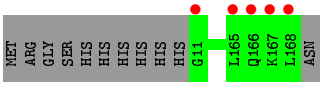
Chain C:



- Molecule 2: DARPin

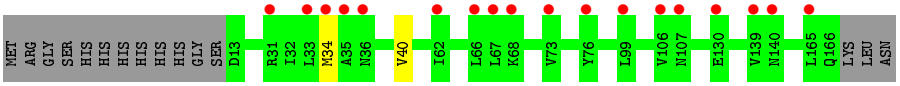
Chain D:





- 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	145.65Å 163.25Å 246.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.15 – 2.50 49.12 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.15-2.50) 100.0 (49.12-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.38 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.225 , 0.261 0.225 , 0.260	Depositor DCC
R_{free} test set	12949 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	37.9	Xtriage
Anisotropy	0.450	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 36.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	27640	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 1.89% 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: GOL, D10, D12, LMT, ETE, HEX, P3G, SO4, PTY, FUA, 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	0.37	0/8033	0.54	0/10907
1	B	0.36	0/8005	0.53	1/10871 (0.0%)
1	C	0.36	0/8008	0.54	0/10875
2	D	0.35	0/1213	0.51	0/1648
2	E	0.37	0/1195	0.51	0/1625
All	All	0.36	0/26454	0.53	1/35926 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	792	ARG	NE-CZ-NH1	5.07	122.84	120.30

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	7874	0	8034	14	0
1	B	7855	0	8006	7	0
1	C	7855	0	8007	11	0
2	D	1194	0	1183	0	0
2	E	1173	0	1157	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	37	0	47	1	0
3	B	37	0	47	2	0
3	C	37	0	47	1	0
4	A	105	0	138	0	0
4	B	105	0	138	0	0
4	C	140	0	184	0	0
5	A	5	0	0	0	0
5	C	5	0	0	0	0
6	A	6	0	8	0	0
6	B	12	0	16	0	0
6	C	12	0	16	0	0
6	D	6	0	8	0	0
6	E	12	0	16	0	0
7	A	28	0	40	0	0
7	C	14	0	20	0	0
8	A	6	0	14	0	0
8	C	6	0	14	0	0
9	B	50	0	79	0	0
9	C	150	0	237	0	0
10	B	12	0	26	0	0
10	C	36	0	78	0	0
11	B	8	0	18	0	0
11	C	8	0	18	0	0
12	B	17	0	26	0	0
13	B	20	0	44	0	0
14	A	265	0	0	1	0
14	B	223	0	0	0	0
14	C	271	0	0	0	0
14	D	28	0	0	0	0
14	E	28	0	0	0	0
All	All	27640	0	27666	32	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 32 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	1.84	0.58
1:C:57:VAL:HG21	1:C:86:GLY:HA2	1.87	0.56
1:C:901:VAL:O	1:C:904:VAL:HG12	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:375:VAL:HG11	1:B:405:LEU:HD22	1.88	0.54
3:B:1101:FUA:H202	3:B:1101:FUA:H5	1.89	0.54

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	1035/1057 (98%)	1011 (98%)	23 (2%)	1 (0%)	51 73
1	B	1032/1057 (98%)	1011 (98%)	20 (2%)	1 (0%)	51 73
1	C	1032/1057 (98%)	1012 (98%)	20 (2%)	0	100 100
2	D	156/169 (92%)	152 (97%)	4 (3%)	0	100 100
2	E	153/169 (90%)	150 (98%)	3 (2%)	0	100 100
All	All	3408/3509 (97%)	3336 (98%)	70 (2%)	2 (0%)	51 73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	660	ASP
1	A	538	THR

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	843/863 (98%)	836 (99%)	7 (1%)	81 93
1	B	840/863 (97%)	834 (99%)	6 (1%)	84 94
1	C	840/863 (97%)	833 (99%)	7 (1%)	81 93
2	D	122/132 (92%)	122 (100%)	0	100 100
2	E	120/132 (91%)	120 (100%)	0	100 100
All	All	2765/2853 (97%)	2745 (99%)	20 (1%)	84 94

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	361	ASN
1	B	586	ARG
1	C	717	ARG
1	B	11	PHE
1	B	49	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	361	ASN

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)

41 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	$\#\|Z\| > 2$
6	GOL	C	1108	-	5,5,5	0.36	0	5,5,5	0.24	0
9	PTY	C	1110	-	49,49,49	0.96	2 (4%)	52,54,54	0.96	2 (3%)
10	D12	C	1112	-	11,11,11	0.29	0	10,10,10	0.43	0
10	D12	B	1108	-	11,11,11	0.30	0	10,10,10	0.42	0
4	LMT	B	1102	-	36,36,36	0.51	1 (2%)	47,47,47	0.63	1 (2%)
13	D10	B	1111	-	9,9,9	0.27	0	8,8,8	0.45	0
3	FUA	C	1101	-	36,40,40	1.11	1 (2%)	46,64,64	1.56	8 (17%)
4	LMT	C	1103	-	36,36,36	0.50	1 (2%)	47,47,47	0.62	0
4	LMT	B	1104	-	36,36,36	0.53	1 (2%)	47,47,47	0.95	1 (2%)
10	D12	C	1114	-	11,11,11	0.26	0	10,10,10	0.50	0
4	LMT	B	1103	-	36,36,36	0.57	1 (2%)	47,47,47	0.81	0
7	ETE	A	1108	-	13,13,13	0.52	0	12,12,12	0.18	0
6	GOL	C	1107	-	5,5,5	0.26	0	5,5,5	0.15	0
6	GOL	B	1105	-	5,5,5	0.33	0	5,5,5	0.30	0
9	PTY	C	1111	-	49,49,49	0.99	2 (4%)	52,54,54	0.92	3 (5%)
3	FUA	A	1101	-	36,40,40	1.04	1 (2%)	46,64,64	1.52	7 (15%)
4	LMT	A	1103	-	36,36,36	0.51	0	47,47,47	0.86	1 (2%)
11	OCT	B	1109	-	7,7,7	0.26	0	6,6,6	0.42	0
6	GOL	D	201	-	5,5,5	0.34	0	5,5,5	0.24	0
6	GOL	E	201	-	5,5,5	0.30	0	5,5,5	0.19	0
6	GOL	E	202	-	5,5,5	0.25	0	5,5,5	0.25	0
12	P3G	B	1110	-	16,16,16	0.53	0	15,15,15	0.24	0
9	PTY	C	1109	-	49,49,49	1.00	2 (4%)	52,54,54	0.95	2 (3%)
4	LMT	C	1102	-	36,36,36	0.52	1 (2%)	47,47,47	0.66	0
7	ETE	C	1115	-	13,13,13	0.52	0	12,12,12	0.22	0
6	GOL	B	1106	-	5,5,5	0.35	0	5,5,5	0.26	0
5	SO4	C	1106	-	4,4,4	0.33	0	6,6,6	0.08	0
4	LMT	C	1104	-	36,36,36	0.49	0	47,47,47	0.60	0
4	LMT	A	1102	-	36,36,36	0.51	1 (2%)	47,47,47	0.66	0
5	SO4	A	1105	-	4,4,4	0.32	0	6,6,6	0.19	0
3	FUA	B	1101	-	36,40,40	0.99	1 (2%)	46,64,64	1.49	5 (10%)
7	ETE	A	1107	-	13,13,13	0.51	0	12,12,12	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	OCT	C	1116	-	7,7,7	0.27	0	6,6,6	0.42	0
6	GOL	A	1106	-	5,5,5	0.35	0	5,5,5	0.26	0
4	LMT	A	1104	-	36,36,36	0.49	0	47,47,47	0.67	0
13	D10	B	1112	-	9,9,9	0.28	0	8,8,8	0.40	0
9	PTY	B	1107	-	49,49,49	0.98	2 (4%)	52,54,54	0.91	2 (3%)
8	HEX	C	1117	-	5,5,5	0.26	0	4,4,4	0.29	0
8	HEX	A	1109	-	5,5,5	0.28	0	4,4,4	0.26	0
10	D12	C	1113	-	11,11,11	0.29	0	10,10,10	0.41	0
4	LMT	C	1105	-	36,36,36	0.57	1 (2%)	47,47,47	0.91	1 (2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	C	1108	-	-	2/4/4/4	-
9	PTY	C	1110	-	-	32/53/53/53	-
10	D12	C	1112	-	-	3/9/9/9	-
10	D12	B	1108	-	-	2/9/9/9	-
4	LMT	B	1102	-	-	5/21/61/61	0/2/2/2
13	D10	B	1111	-	-	1/7/7/7	-
3	FUA	C	1101	-	-	2/11/92/92	0/4/4/4
4	LMT	C	1103	-	-	10/21/61/61	0/2/2/2
4	LMT	B	1104	-	-	9/21/61/61	0/2/2/2
10	D12	C	1114	-	-	3/9/9/9	-
4	LMT	B	1103	-	-	10/21/61/61	0/2/2/2
7	ETE	A	1108	-	-	6/11/11/11	-
6	GOL	C	1107	-	-	2/4/4/4	-
6	GOL	B	1105	-	-	1/4/4/4	-
9	PTY	C	1111	-	-	24/53/53/53	-
3	FUA	A	1101	-	-	4/11/92/92	0/4/4/4
4	LMT	A	1103	-	-	9/21/61/61	0/2/2/2
11	OCT	B	1109	-	-	2/5/5/5	-
6	GOL	D	201	-	-	2/4/4/4	-
6	GOL	E	201	-	-	2/4/4/4	-
6	GOL	E	202	-	-	0/4/4/4	-
12	P3G	B	1110	-	-	4/14/14/14	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	PTY	C	1109	-	-	19/53/53/53	-
4	LMT	C	1102	-	-	12/21/61/61	0/2/2/2
7	ETE	C	1115	-	-	6/11/11/11	-
6	GOL	B	1106	-	-	0/4/4/4	-
4	LMT	C	1104	-	-	2/21/61/61	0/2/2/2
4	LMT	A	1102	-	-	6/21/61/61	0/2/2/2
7	ETE	A	1107	-	-	4/11/11/11	-
3	FUA	B	1101	-	-	2/11/92/92	0/4/4/4
11	OCT	C	1116	-	-	1/5/5/5	-
6	GOL	A	1106	-	-	2/4/4/4	-
4	LMT	A	1104	-	-	6/21/61/61	0/2/2/2
13	D10	B	1112	-	-	2/7/7/7	-
9	PTY	B	1107	-	-	24/53/53/53	-
8	HEX	C	1117	-	-	0/3/3/3	-
8	HEX	A	1109	-	-	1/3/3/3	-
10	D12	C	1113	-	-	3/9/9/9	-
4	LMT	C	1105	-	-	11/21/61/61	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1101	FUA	O2-C31	5.07	1.46	1.35
3	B	1101	FUA	O2-C31	4.99	1.46	1.35
3	A	1101	FUA	O2-C31	4.97	1.46	1.35
9	C	1111	PTY	O4-C30	4.65	1.46	1.33
9	C	1109	PTY	O7-C8	4.50	1.47	1.34

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1101	FUA	O2-C31-C32	4.90	120.10	111.09
3	A	1101	FUA	O2-C31-C32	4.70	119.73	111.09
3	C	1101	FUA	O2-C31-C32	4.19	118.80	111.09
9	C	1110	PTY	O7-C8-C11	4.17	120.50	111.50
9	C	1109	PTY	O7-C8-C11	4.02	120.17	111.50

There are no chirality outliers.

5 of 236 torsion outliers are listed below:

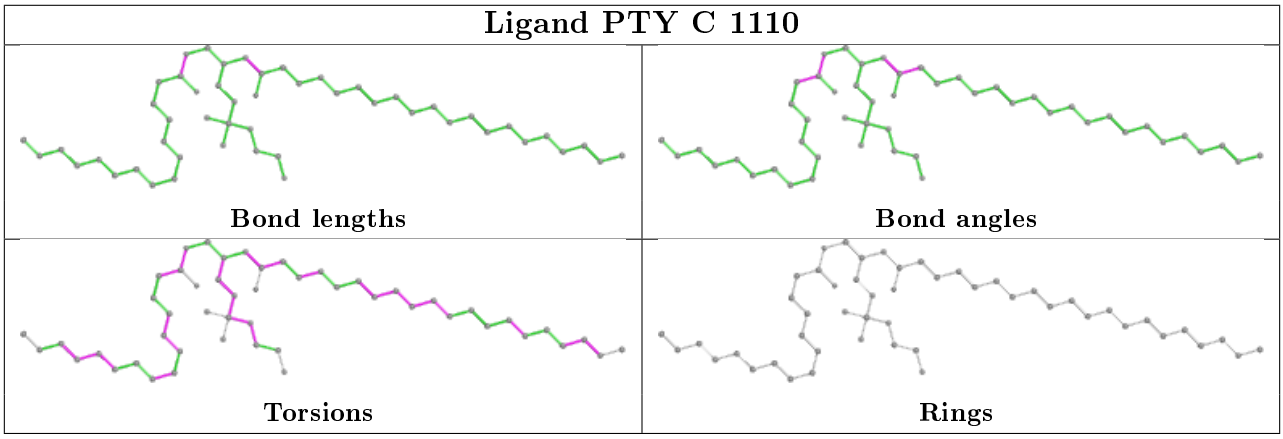
Mol	Chain	Res	Type	Atoms
9	C	1110	PTY	C11-C8-O7-C6
9	C	1110	PTY	C3-O11-P1-O13
4	B	1104	LMT	O5'-C1'-O1'-C1
4	B	1103	LMT	O5'-C1'-O1'-C1
4	B	1103	LMT	C2-C1-O1'-C1'

There are no ring outliers.

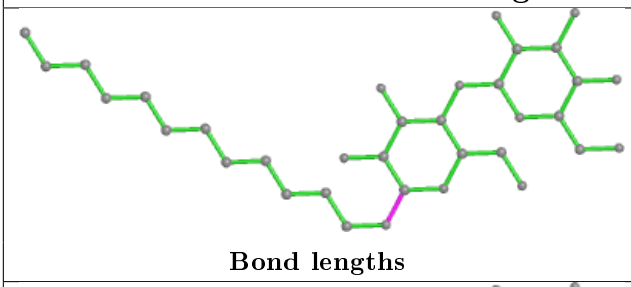
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1101	FUA	1	0
3	A	1101	FUA	1	0
3	B	1101	FUA	2	0

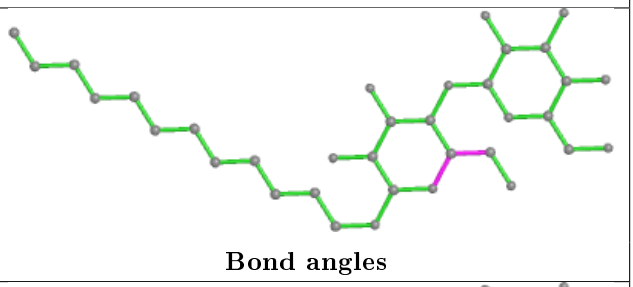
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



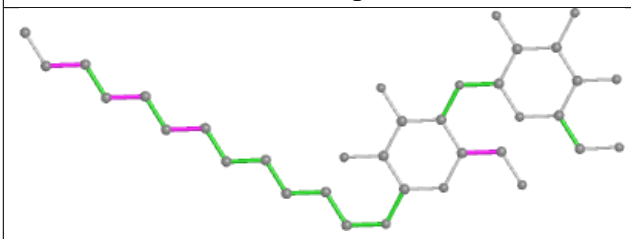
Ligand LMT B 1102



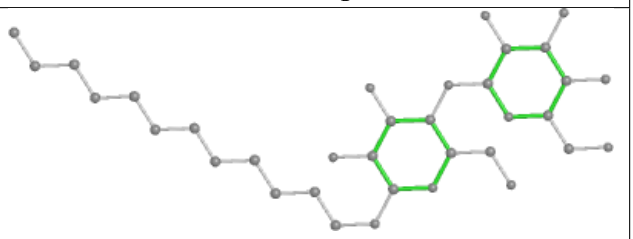
Bond lengths



Bond angles

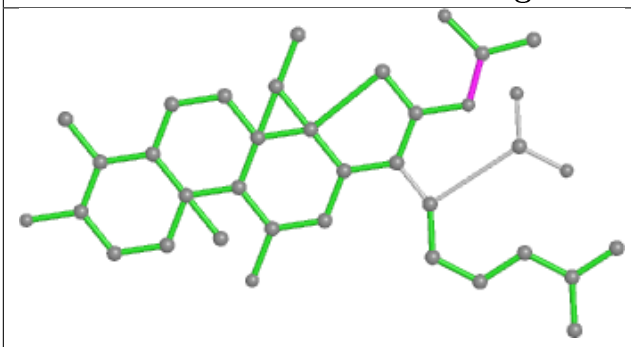


Torsions

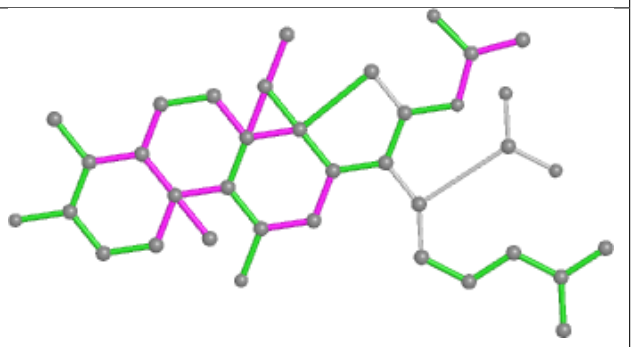


Rings

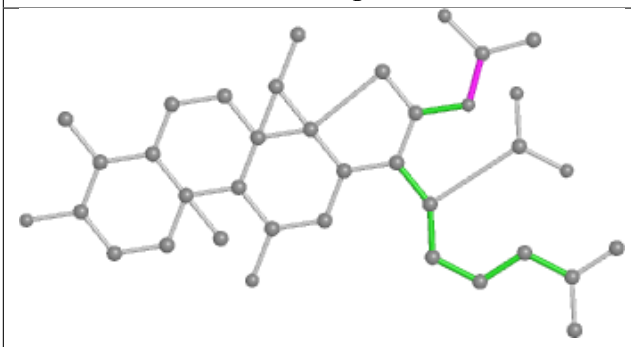
Ligand FUA C 1101



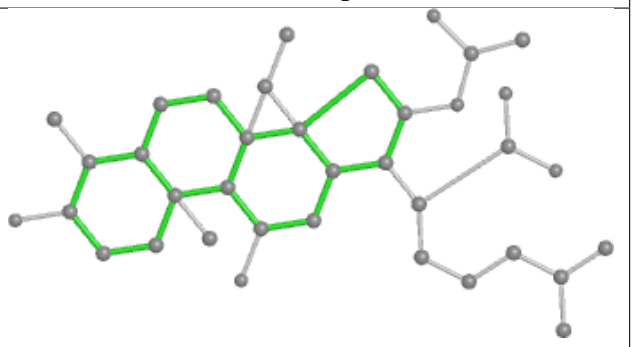
Bond lengths



Bond angles

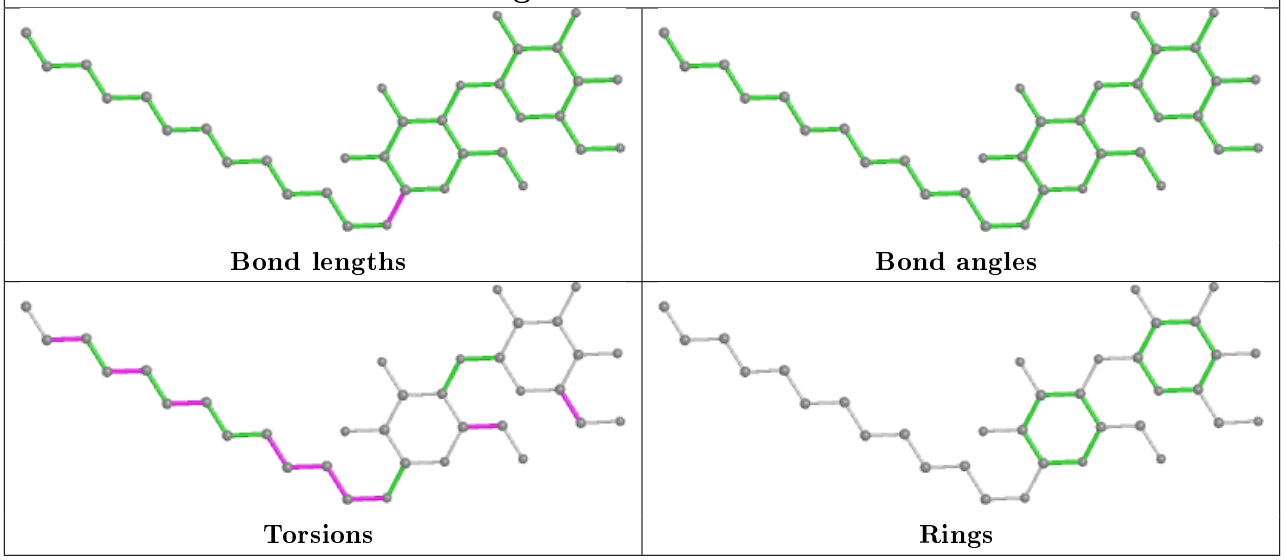


Torsions

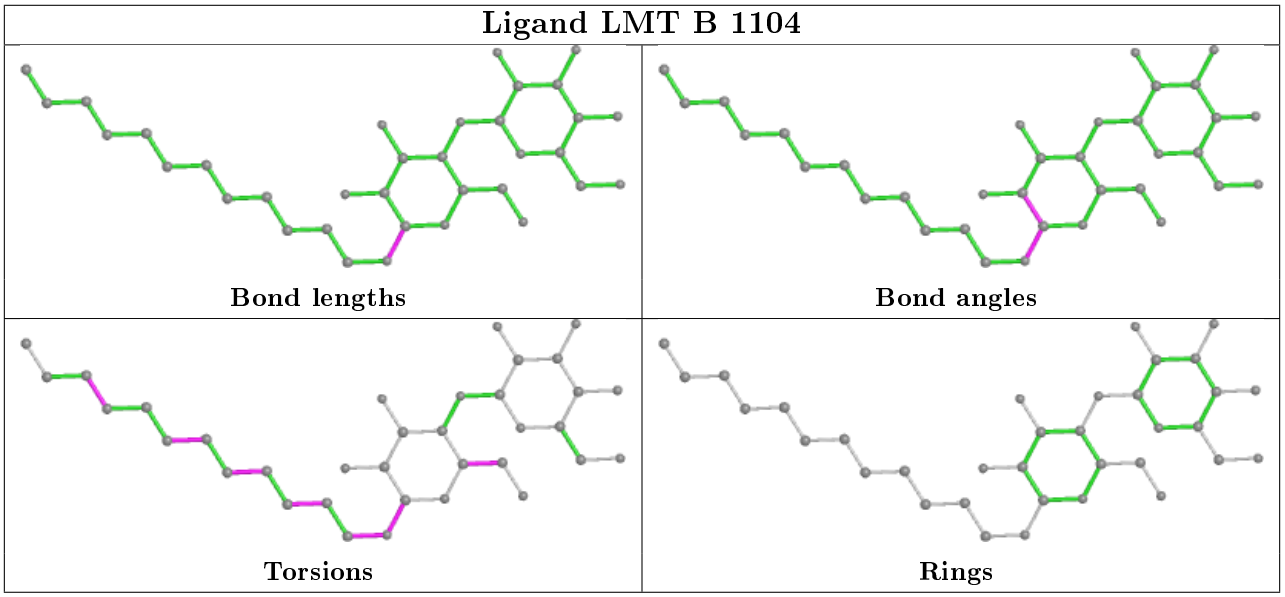


Rings

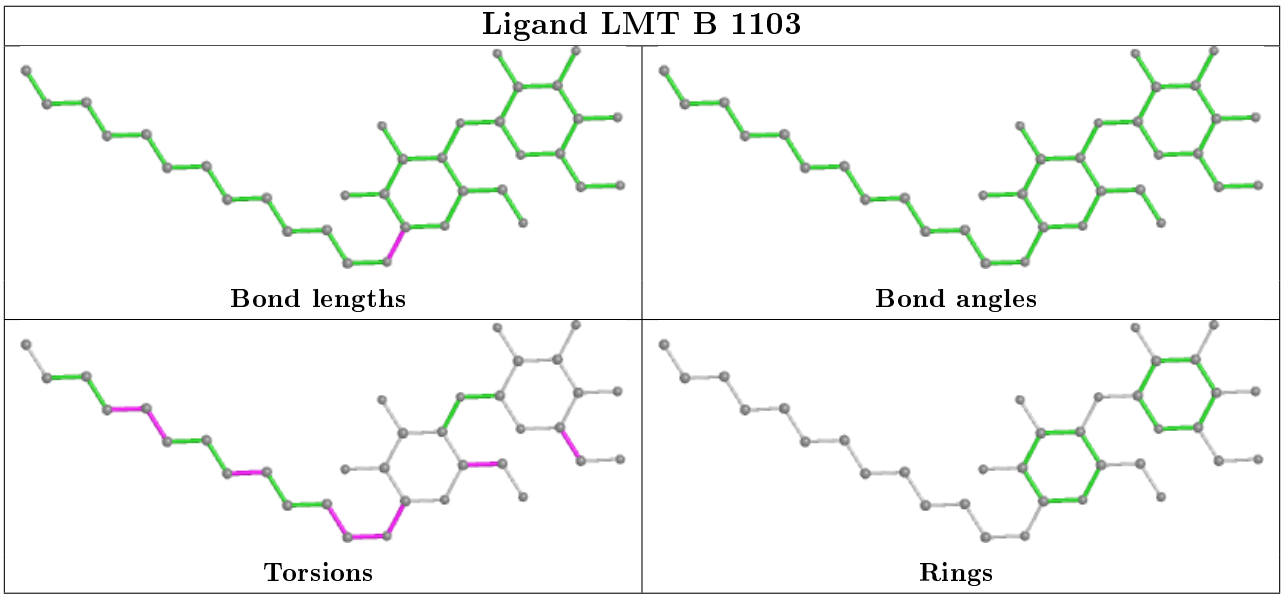
Ligand LMT C 1103



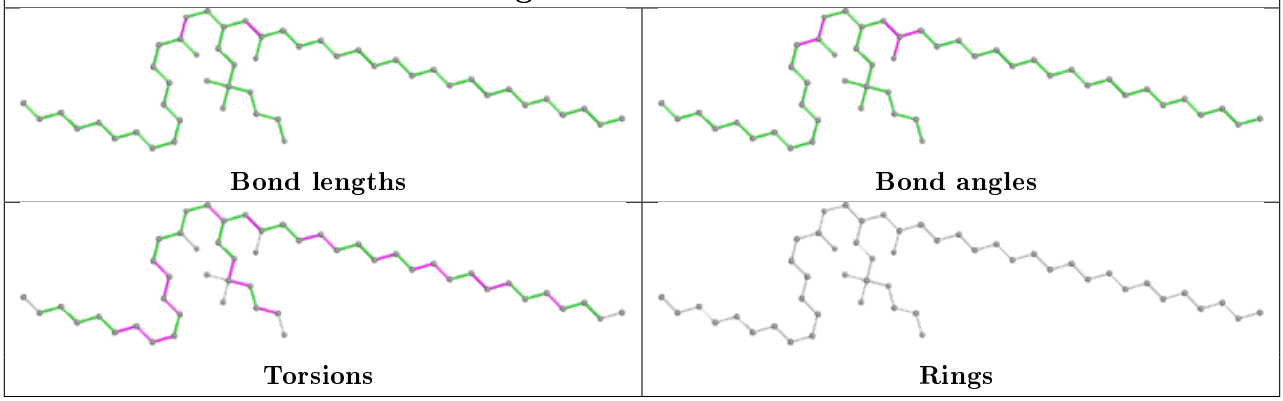
Ligand LMT B 1104



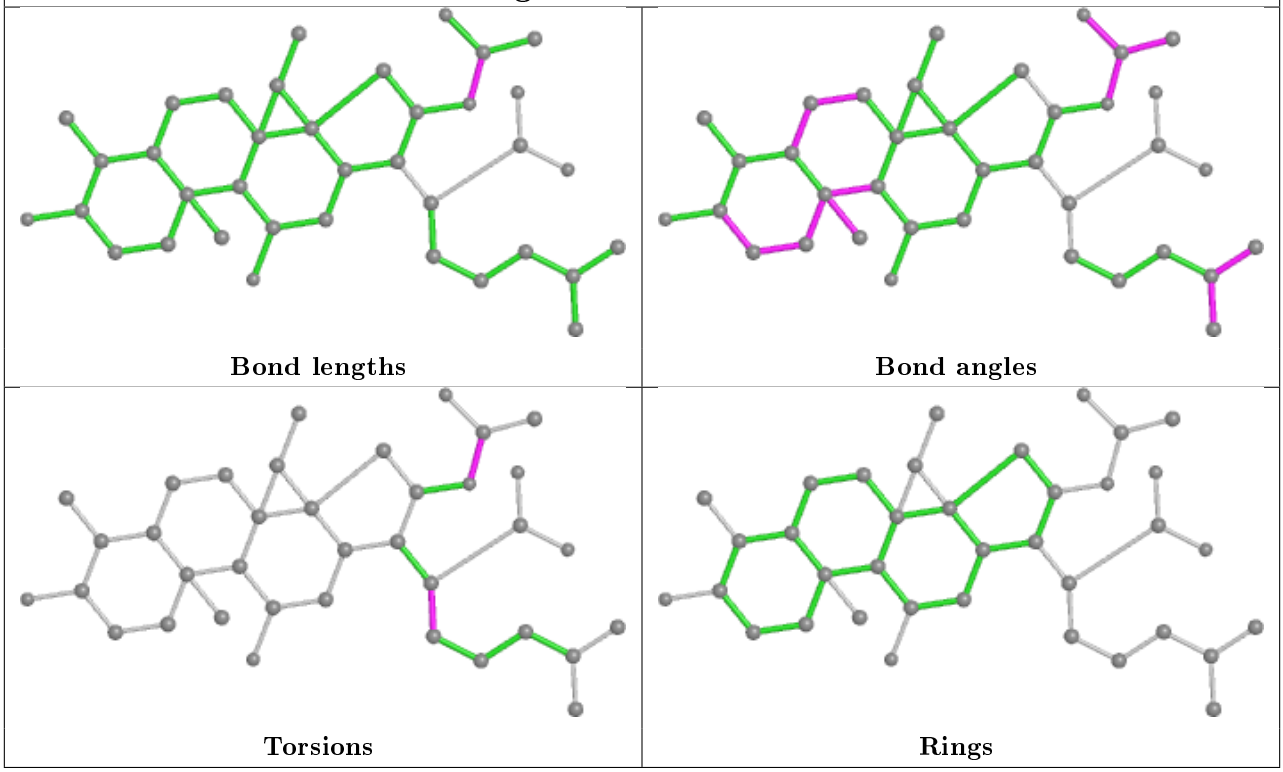
Ligand LMT B 1103



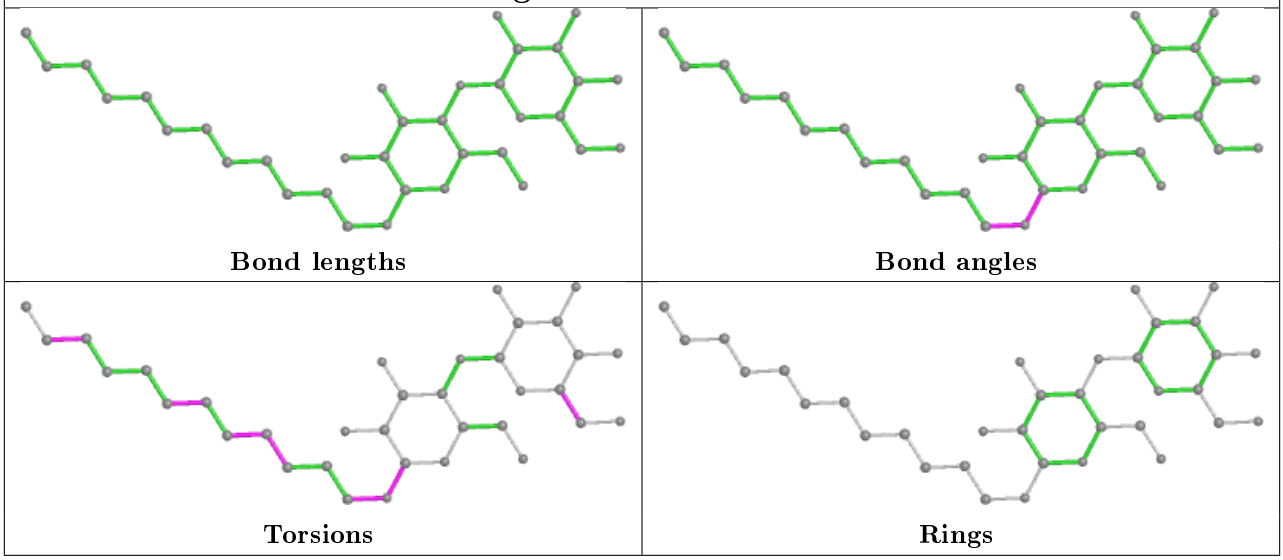
Ligand PTY C 1111



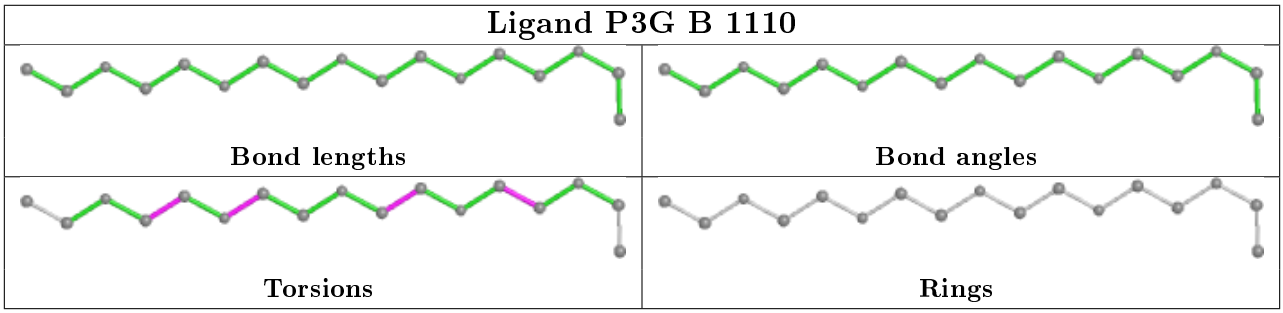
Ligand FUA A 1101



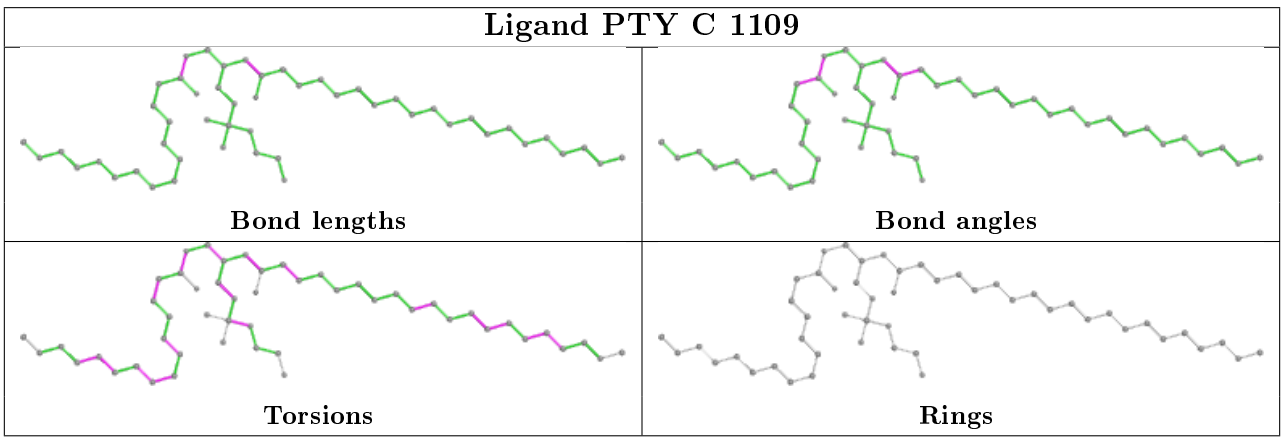
Ligand LMT A 1103



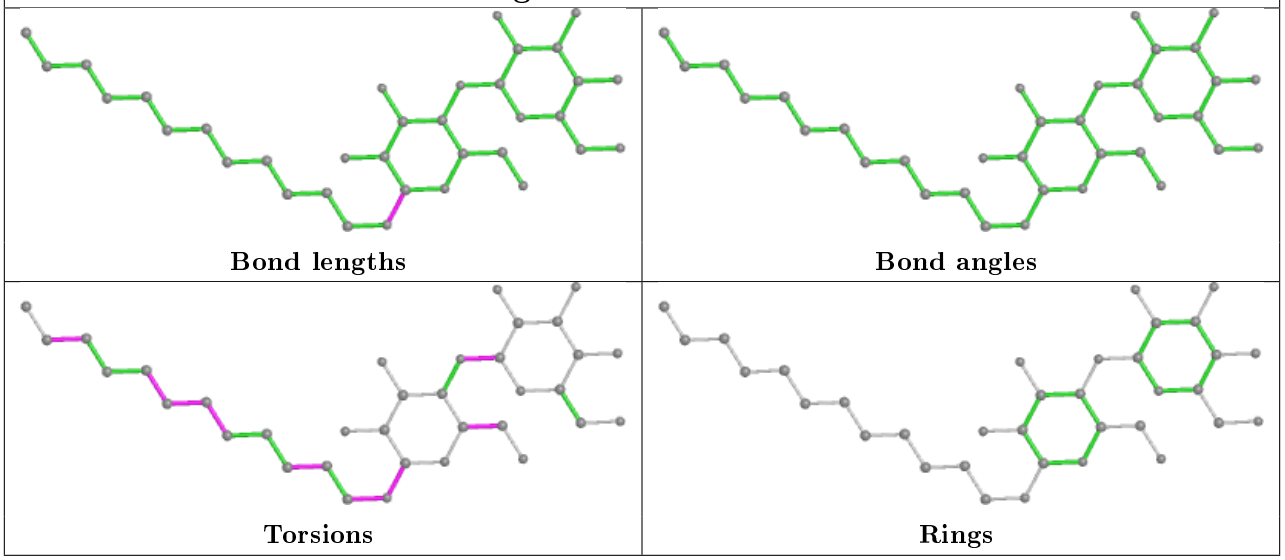
Ligand P3G B 1110



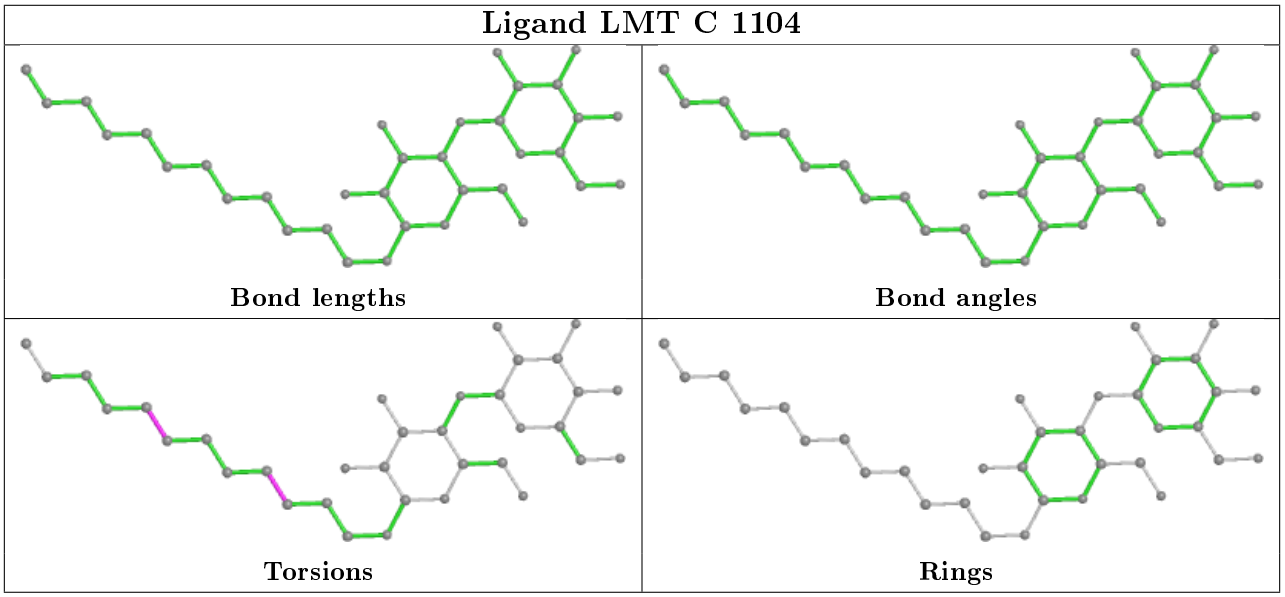
Ligand PTY C 1109



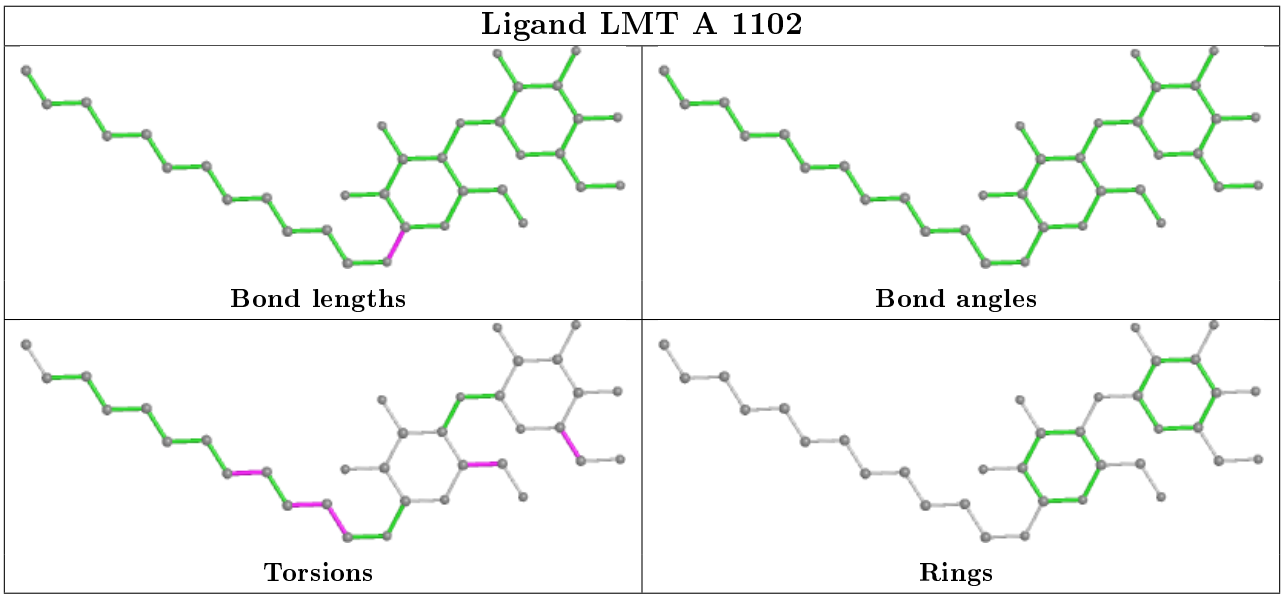
Ligand LMT C 1102



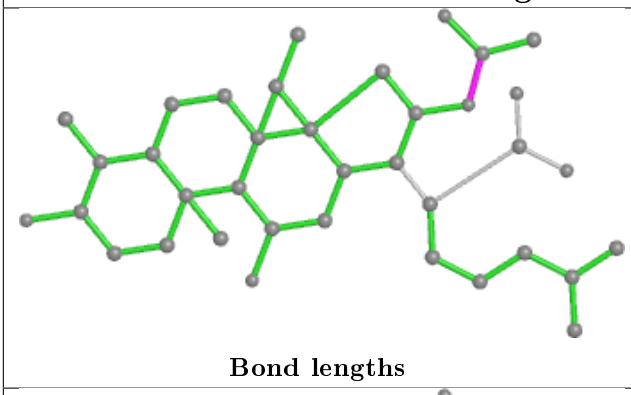
Ligand LMT C 1104



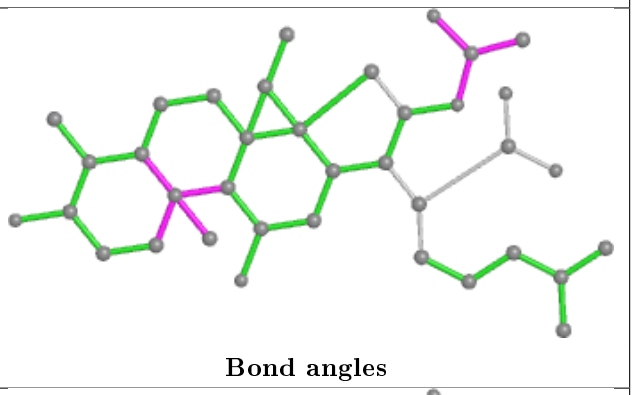
Ligand LMT A 1102



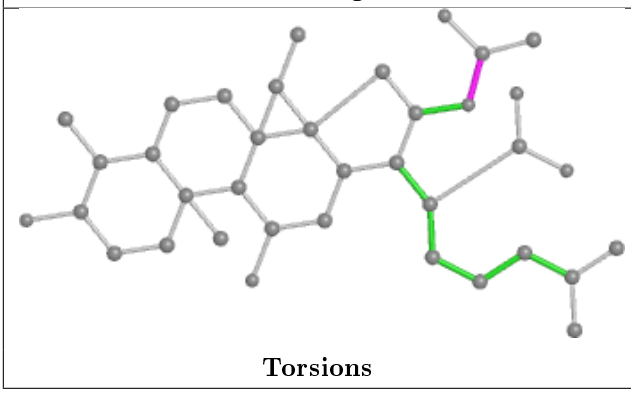
Ligand FUA B 1101



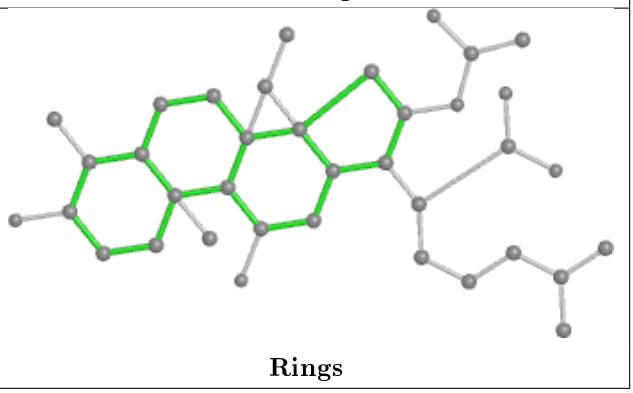
Bond lengths



Bond angles

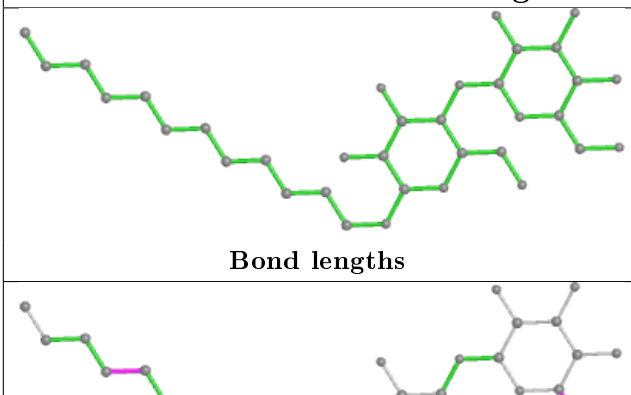


Torsions

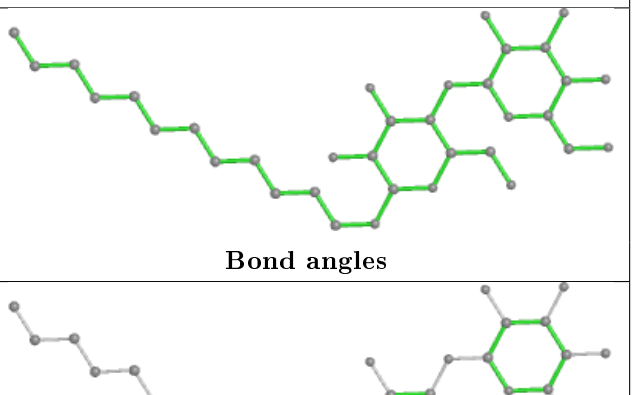


Rings

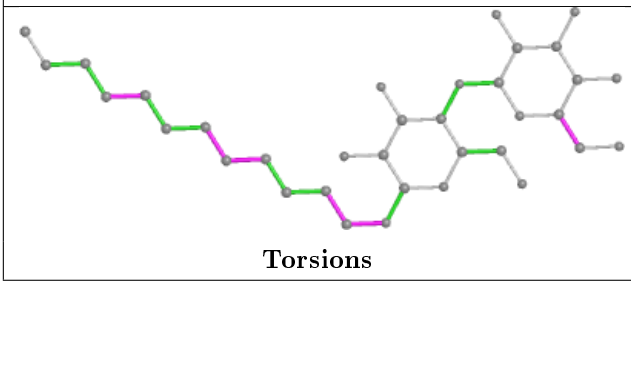
Ligand LMT A 1104



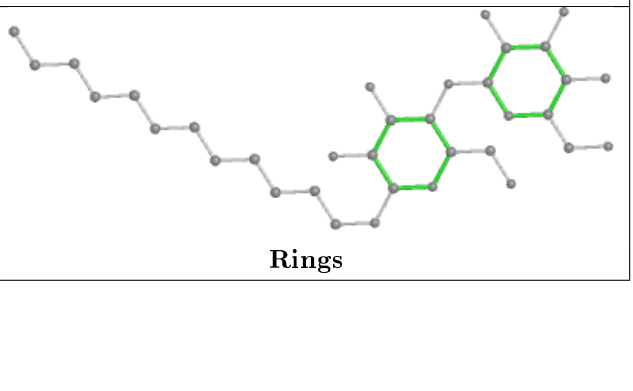
Bond lengths



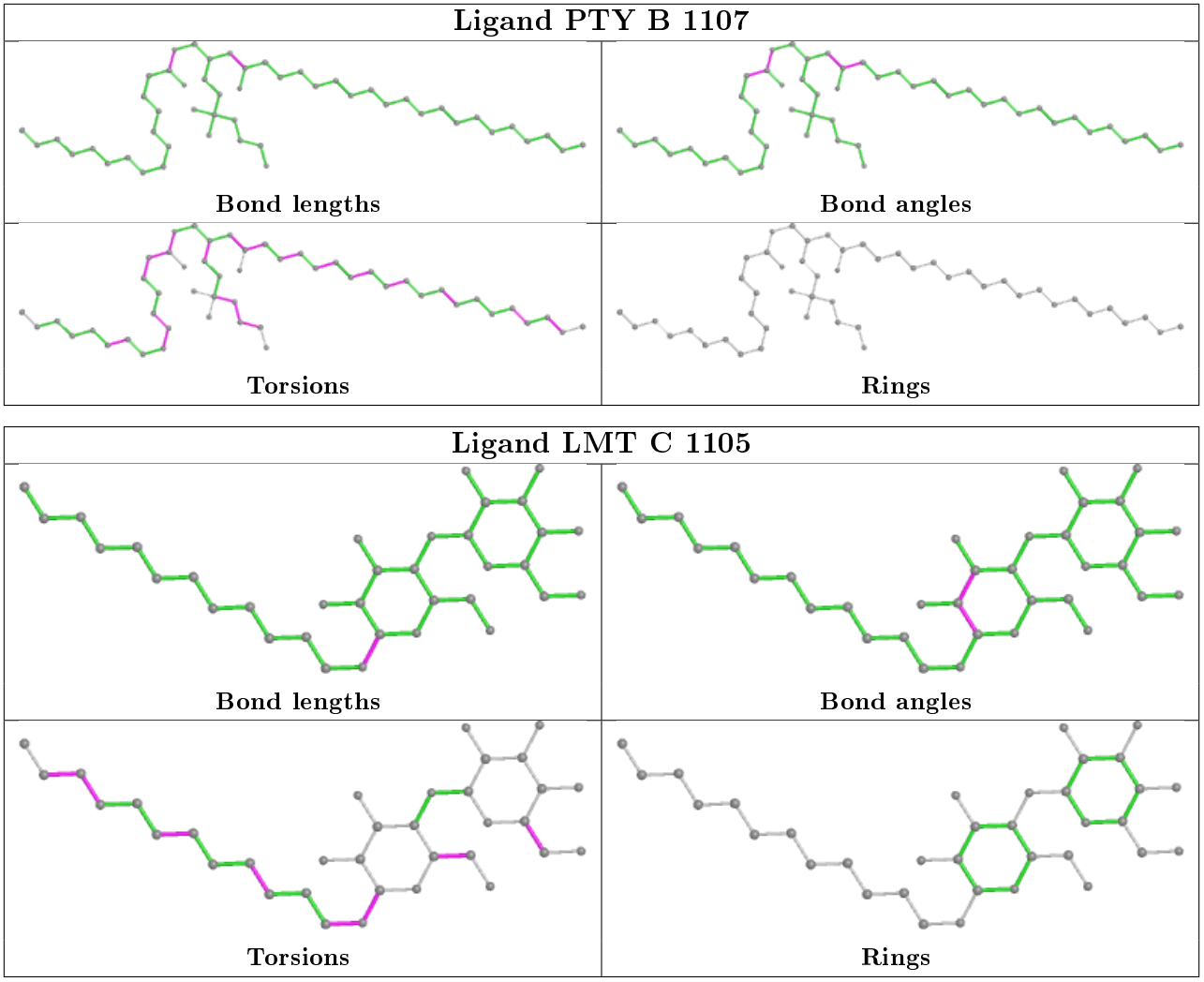
Bond angles



Torsions



Rings



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	1034/1057 (97%)	-0.05	48 (4%) 32 34	31, 63, 115, 150	0
1	B	1034/1057 (97%)	-0.19	19 (1%) 68 71	33, 60, 91, 125	0
1	C	1033/1057 (97%)	-0.26	12 (1%) 79 80	34, 52, 85, 110	0
2	D	158/169 (93%)	-0.11	5 (3%) 47 51	48, 60, 90, 134	0
2	E	154/169 (91%)	0.49	18 (11%) 4 4	49, 71, 100, 112	0
All	All	3413/3509 (97%)	-0.13	102 (2%) 50 53	31, 58, 100, 150	0

The worst 5 of 102 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	168	LEU	7.7
1	A	868	LEU	7.4
1	A	871	ASN	7.3
1	B	868	LEU	6.2
1	A	502	LYS	5.8

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

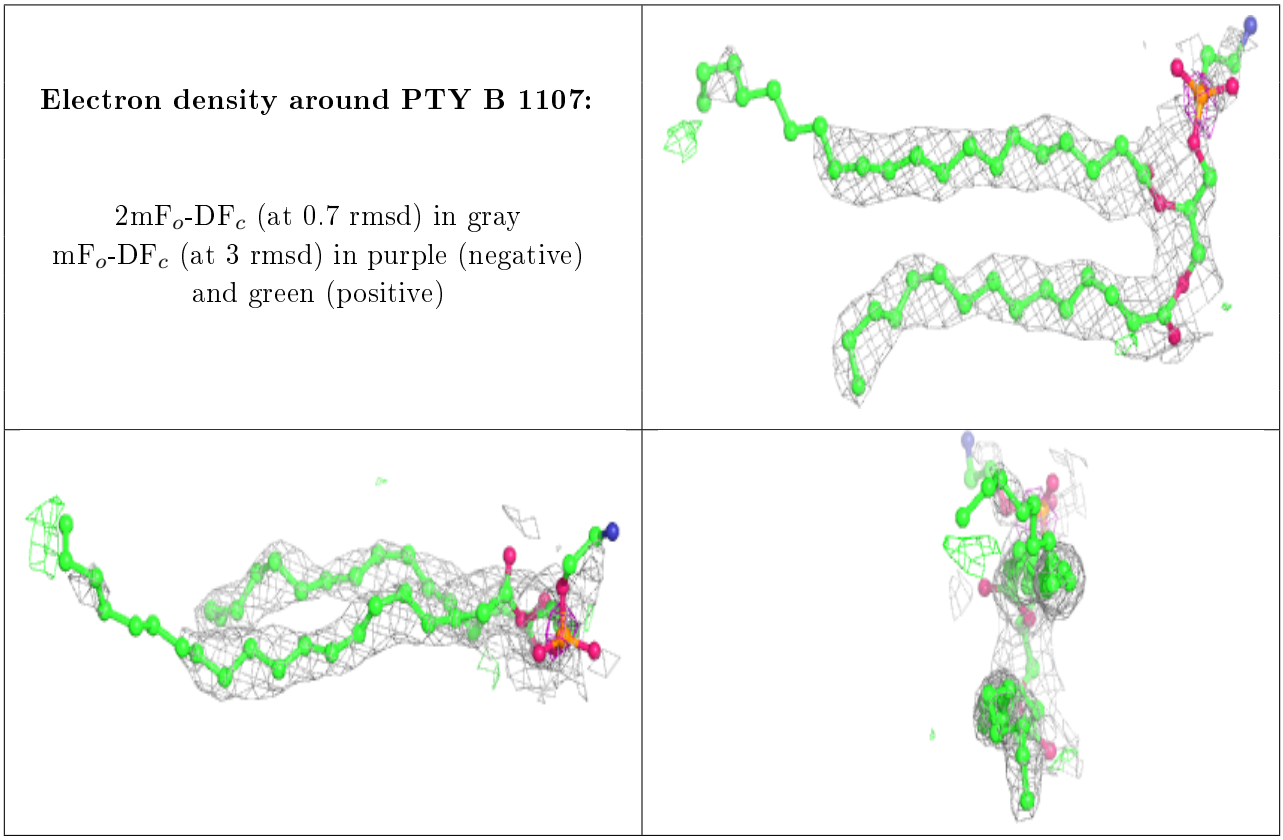
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	PTY	B	1107	50/50	0.61	0.33	92,107,159,165	0
11	OCT	C	1116	8/8	0.65	0.21	89,91,93,94	0
4	LMT	C	1104	35/35	0.66	0.27	98,132,157,157	0
4	LMT	A	1104	35/35	0.69	0.27	84,121,151,152	0
7	ETE	A	1107	14/14	0.69	0.14	111,115,122,122	0
4	LMT	C	1102	35/35	0.71	0.26	114,142,153,155	0
3	FUA	A	1101	37/37	0.71	0.34	122,146,149,149	0
3	FUA	C	1101	37/37	0.72	0.36	122,147,159,162	0
11	OCT	B	1109	8/8	0.72	0.21	93,94,96,97	0
12	P3G	B	1110	17/17	0.73	0.13	109,120,121,121	0
9	PTY	C	1109	50/50	0.73	0.26	76,111,132,138	0
10	D12	C	1113	12/12	0.73	0.36	84,89,90,90	0
9	PTY	C	1110	50/50	0.74	0.28	88,118,139,144	0
8	HEX	A	1109	6/6	0.75	0.25	68,70,71,72	0
9	PTY	C	1111	50/50	0.75	0.26	79,97,115,120	0
4	LMT	A	1103	35/35	0.76	0.24	80,107,132,133	0
7	ETE	A	1108	14/14	0.76	0.20	95,98,100,100	0
4	LMT	B	1104	35/35	0.78	0.20	86,95,102,102	0
8	HEX	C	1117	6/6	0.78	0.26	82,84,84,84	0
10	D12	C	1112	12/12	0.79	0.32	68,72,75,76	0
4	LMT	C	1105	35/35	0.79	0.30	122,130,133,134	0
10	D12	C	1114	12/12	0.80	0.20	89,92,94,95	0
13	D10	B	1111	10/10	0.80	0.17	88,92,94,95	0
6	GOL	C	1108	6/6	0.81	0.23	68,71,71,72	0
4	LMT	B	1103	35/35	0.82	0.38	114,125,131,133	0
7	ETE	C	1115	14/14	0.82	0.16	91,97,99,99	0
4	LMT	A	1102	35/35	0.83	0.22	96,115,129,133	0
13	D10	B	1112	10/10	0.84	0.18	81,83,83,84	0
6	GOL	D	201	6/6	0.84	0.18	67,70,70,72	0
10	D12	B	1108	12/12	0.84	0.17	71,74,75,75	0
6	GOL	B	1106	6/6	0.86	0.17	62,66,68,68	0
6	GOL	B	1105	6/6	0.87	0.25	67,68,72,74	0
6	GOL	A	1106	6/6	0.88	0.15	80,82,82,85	0
6	GOL	E	201	6/6	0.88	0.21	72,74,76,77	0
4	LMT	B	1102	35/35	0.89	0.23	93,101,111,111	0
3	FUA	B	1101	37/37	0.89	0.17	94,96,103,105	0
5	SO4	A	1105	5/5	0.90	0.19	86,90,92,92	0
4	LMT	C	1103	35/35	0.91	0.16	73,81,91,92	0
6	GOL	C	1107	6/6	0.92	0.16	43,44,45,45	0
6	GOL	E	202	6/6	0.94	0.14	64,65,66,67	0
5	SO4	C	1106	5/5	0.97	0.07	76,76,77,78	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.

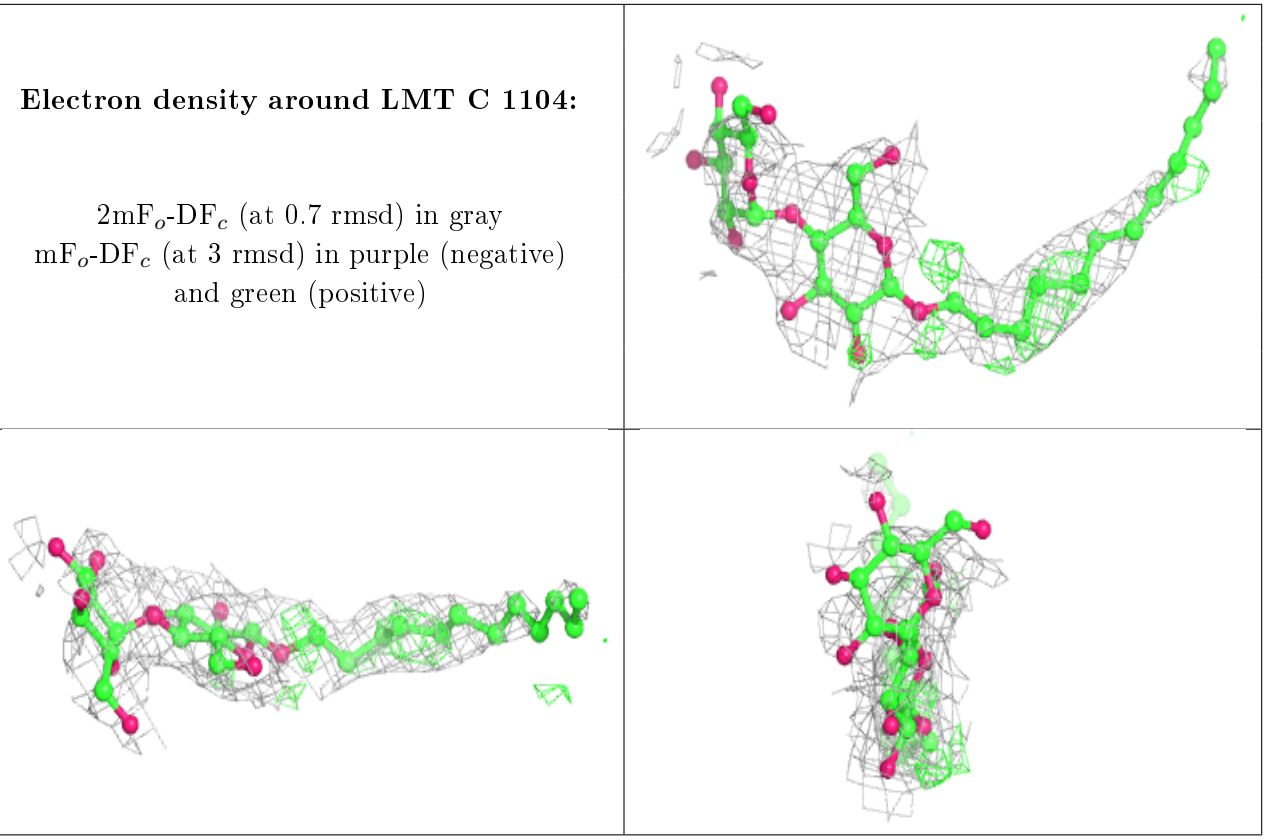
Electron density around PTY B 1107:

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



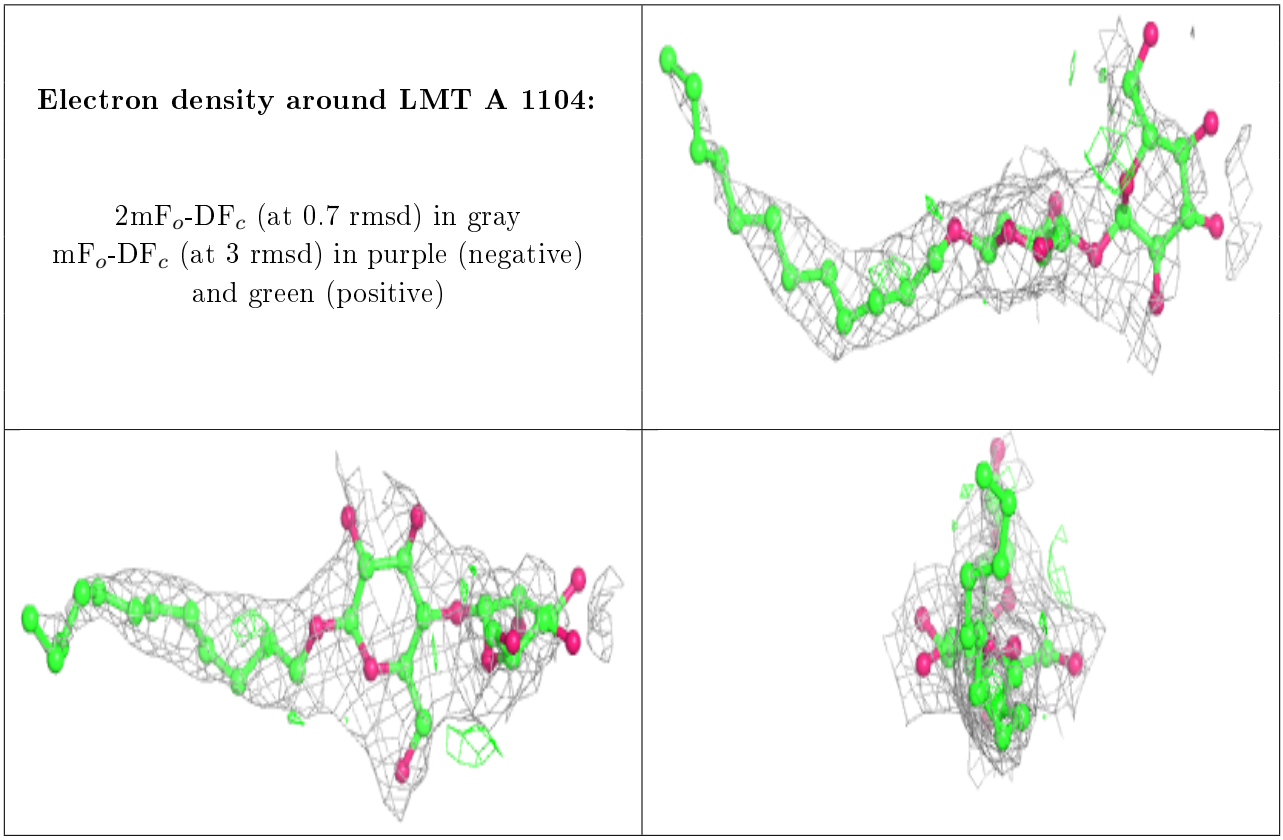
Electron density around LMT C 1104:

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



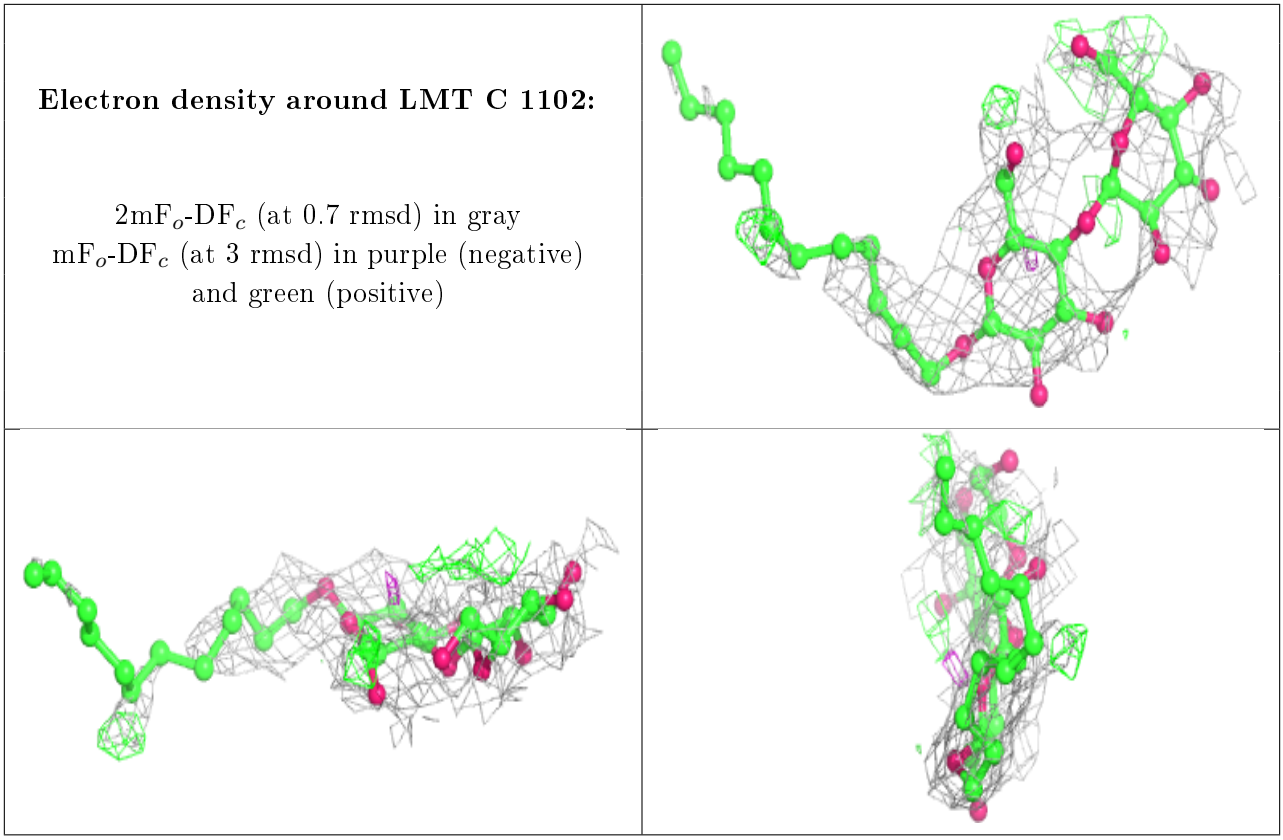
Electron density around LMT A 1104:

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



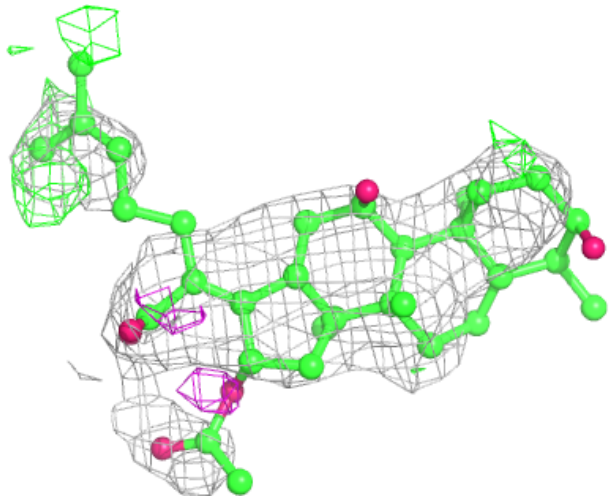
Electron density around LMT C 1102:

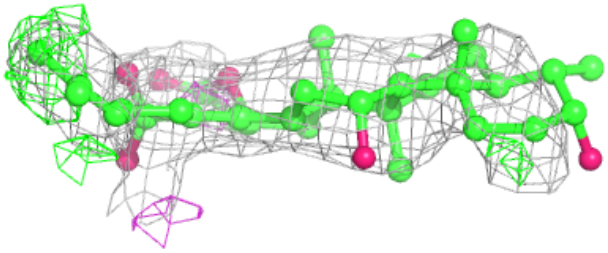
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

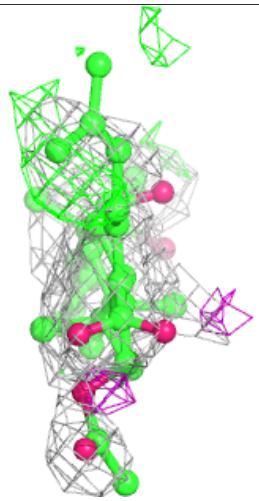


Electron density around FUA A 1101:

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

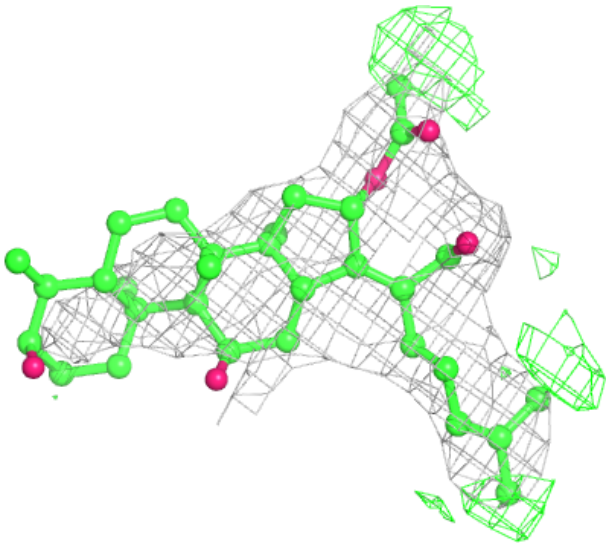


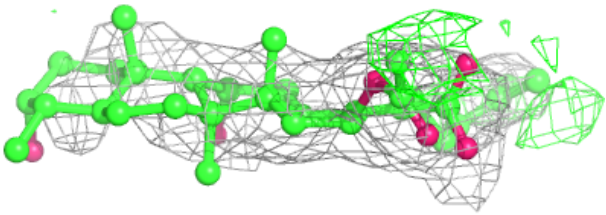


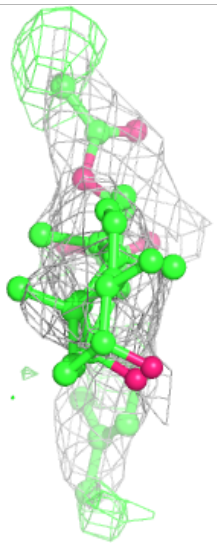


Electron density around FUA C 1101:

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

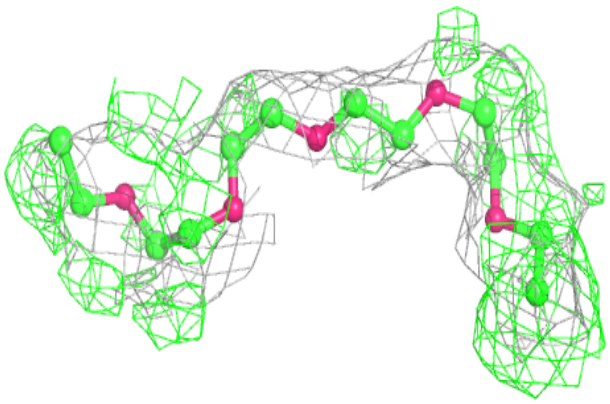


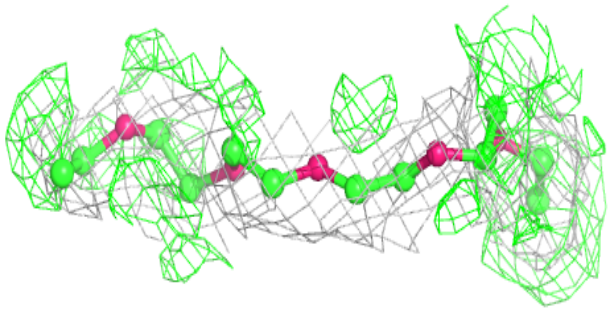


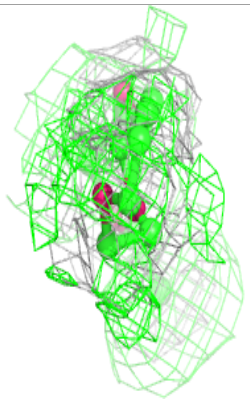


Electron density around P3G B 1110:

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

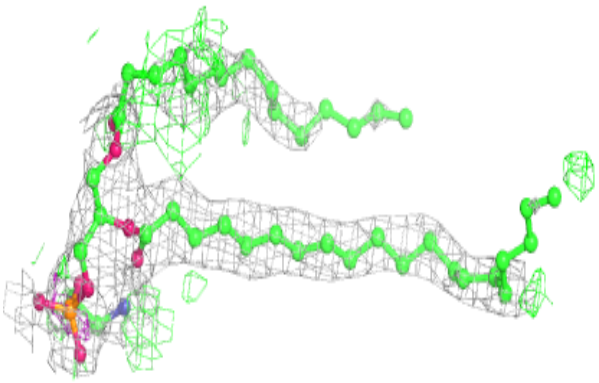


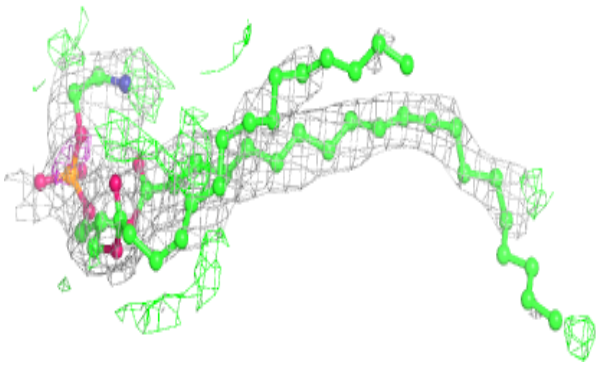


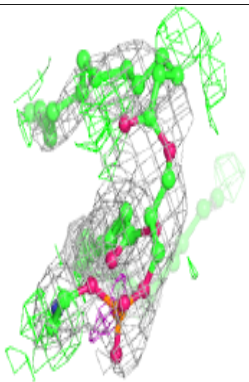


Electron density around PTY C 1109:

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

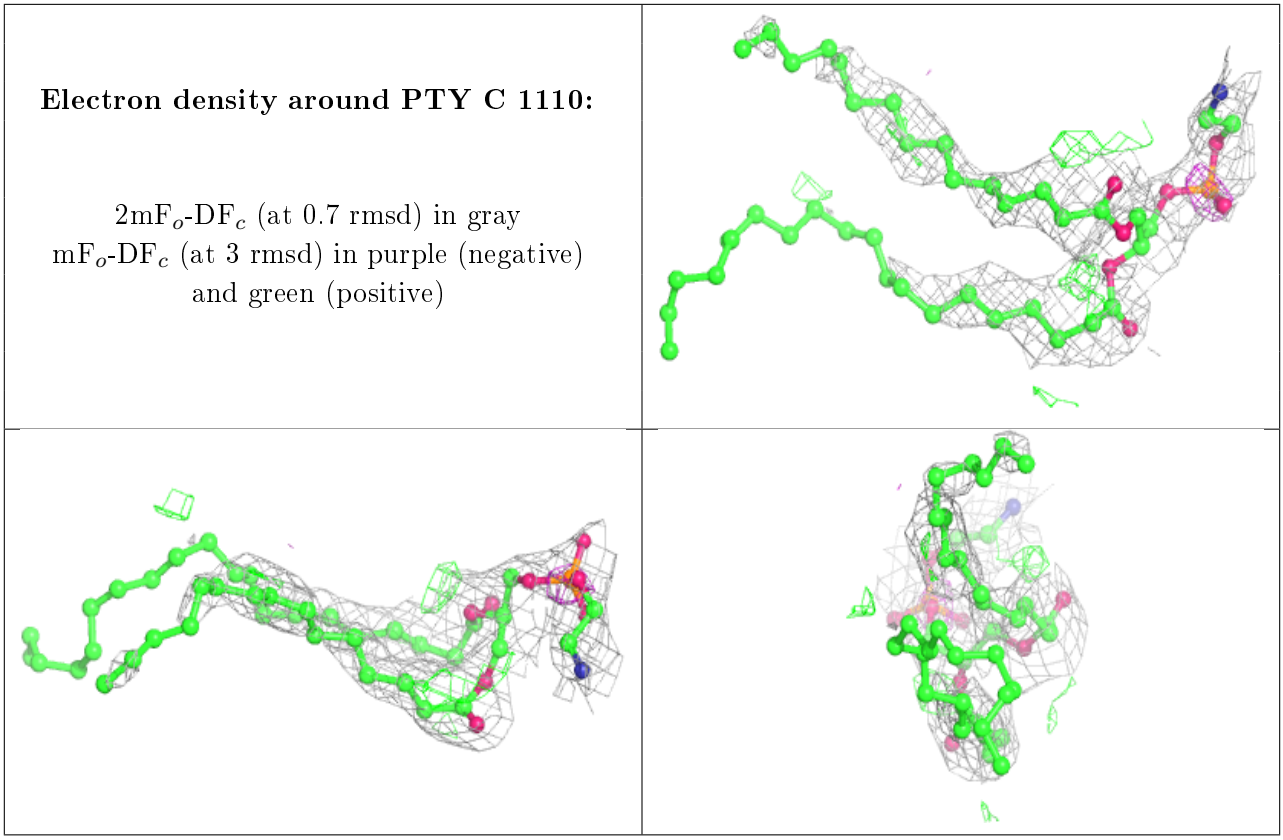






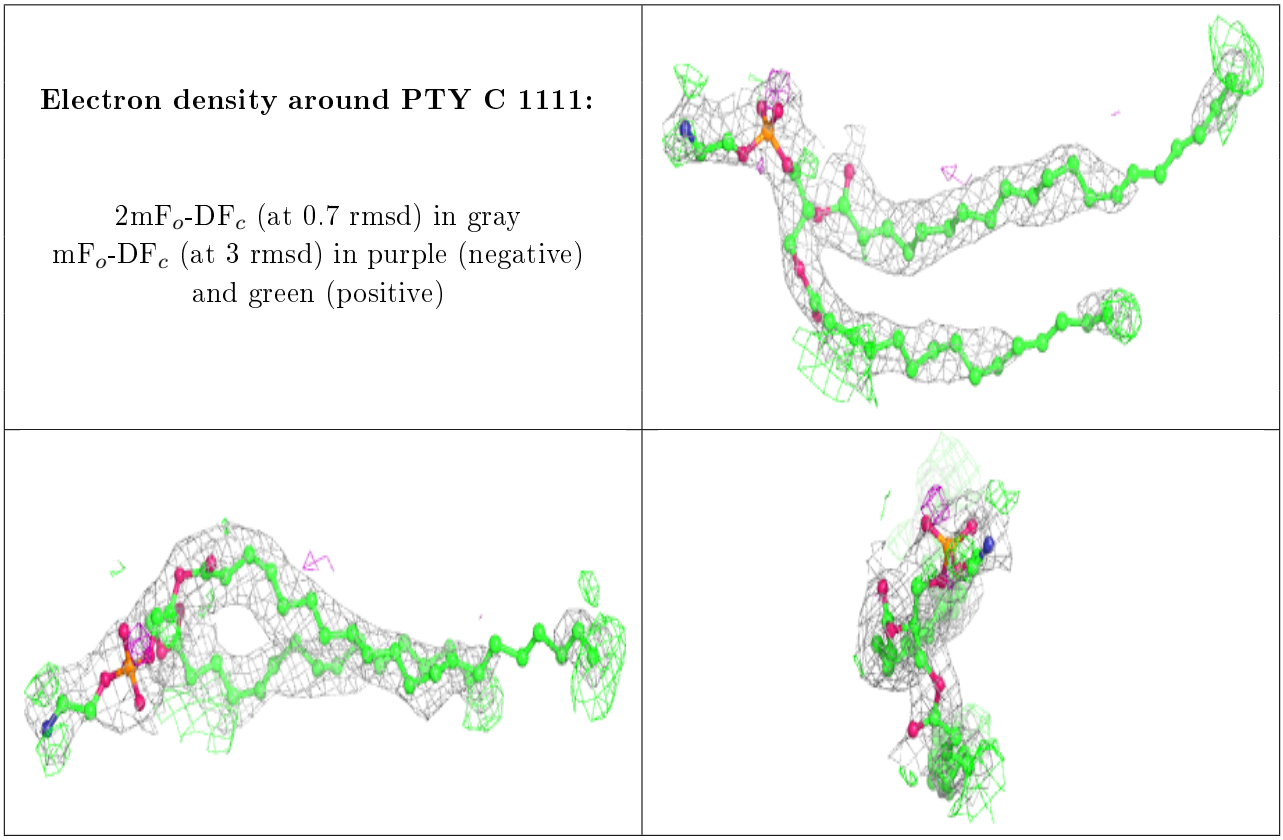
Electron density around PTY C 1110:

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



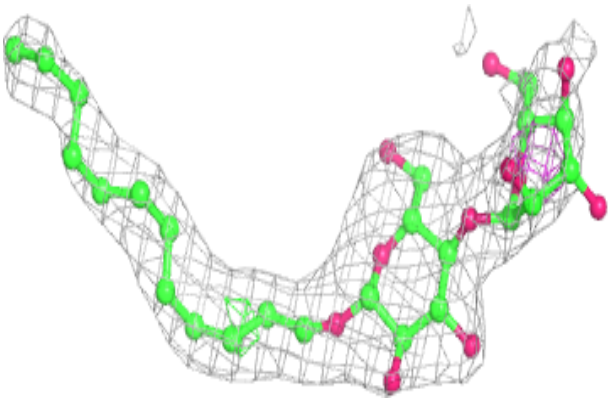
Electron density around PTY C 1111:

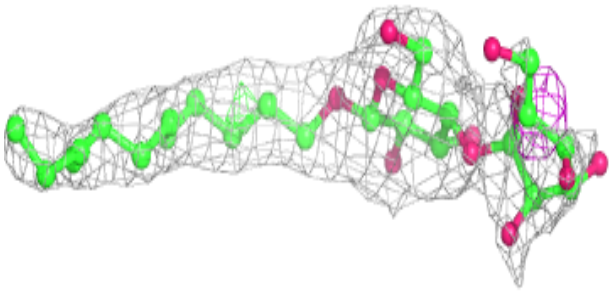
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

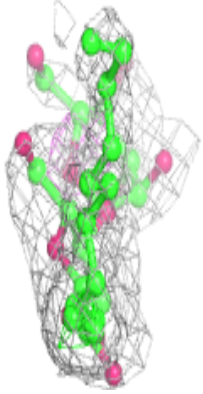


Electron density around LMT A 1103:

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

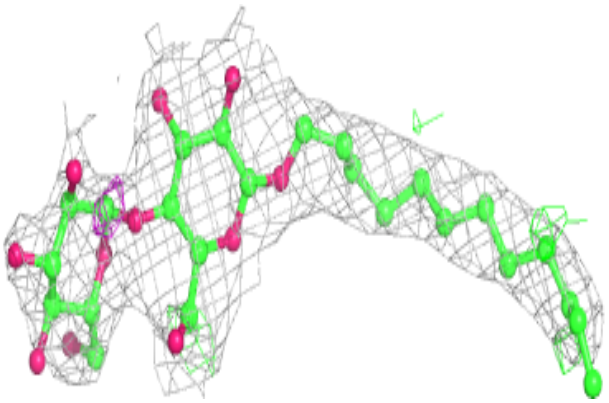


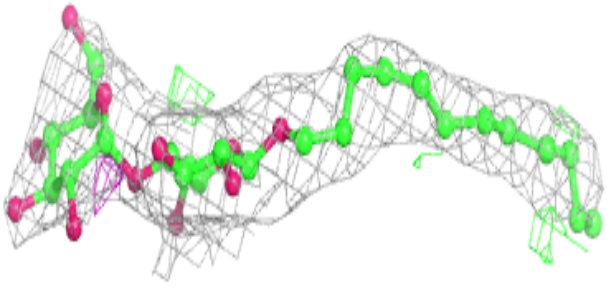


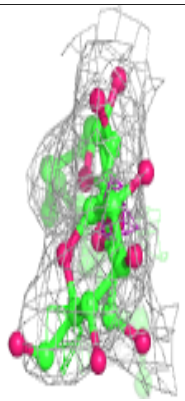


Electron density around LMT B 1104:

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

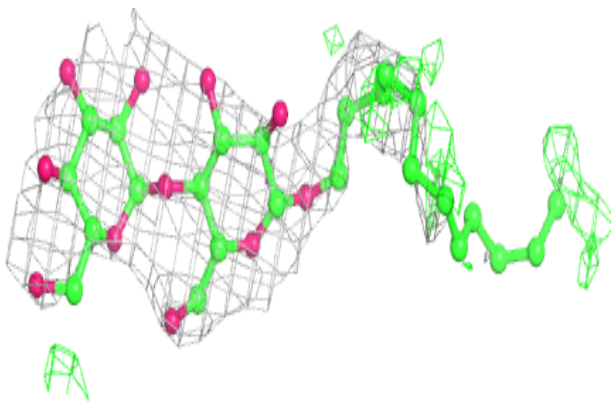


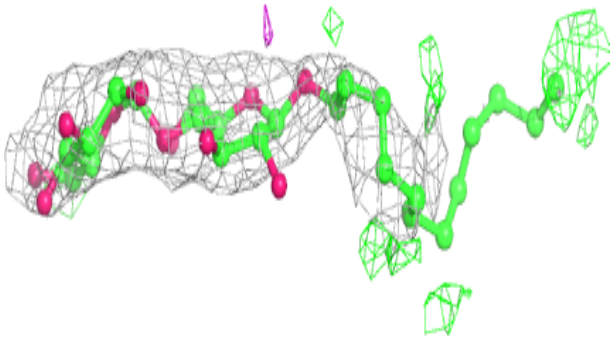


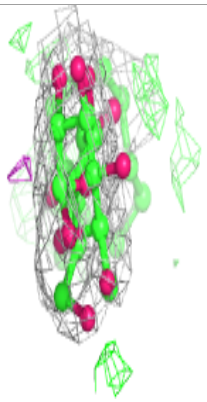


Electron density around LMT C 1105:

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

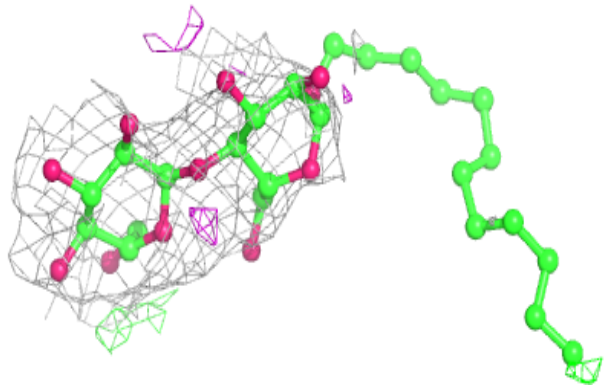


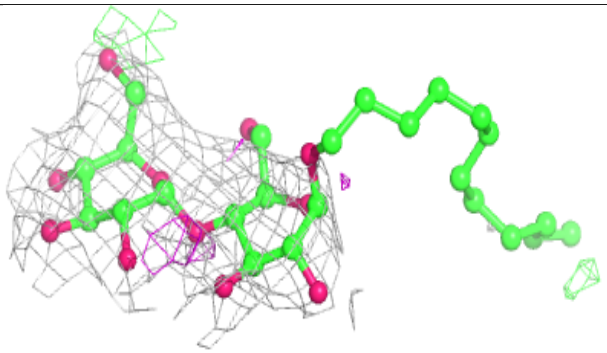


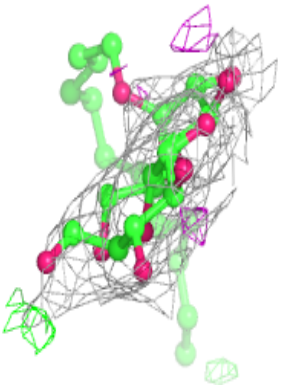


Electron density around LMT B 1103:

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

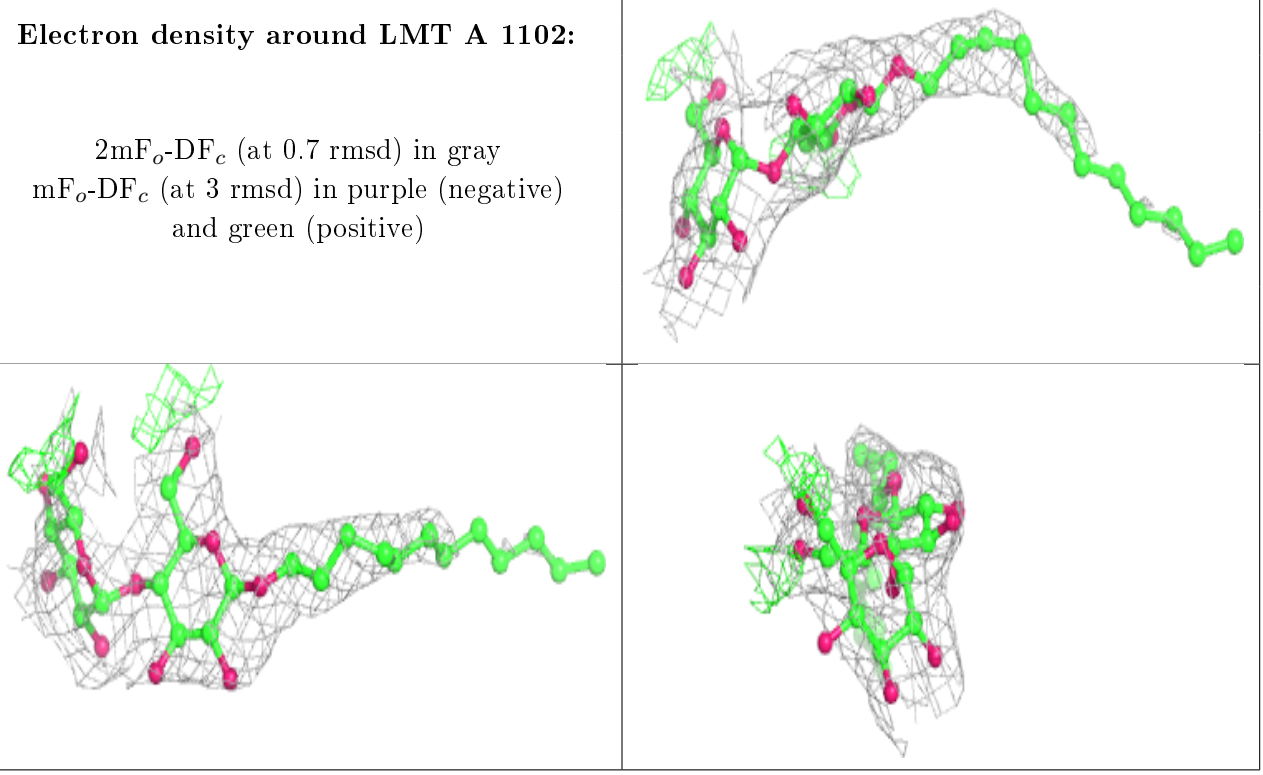






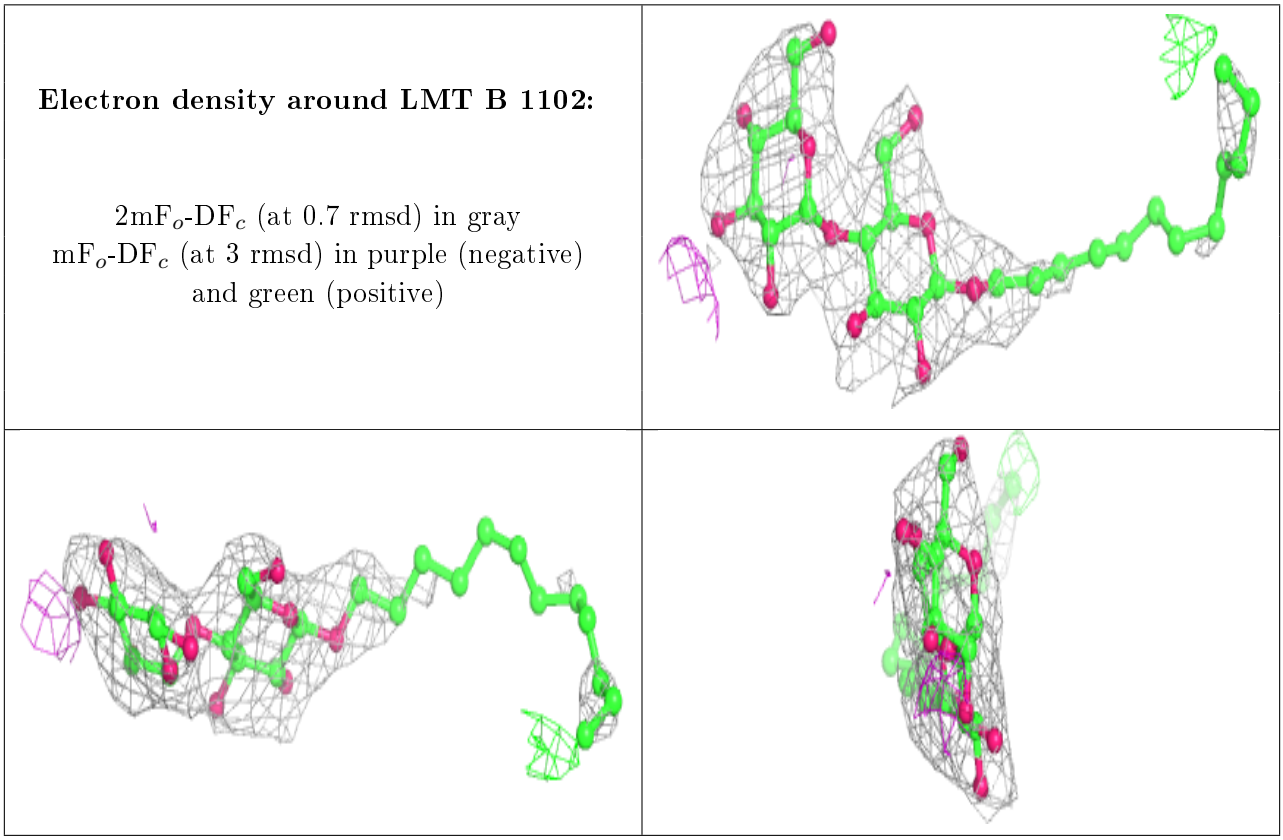
Electron density around LMT A 1102:

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



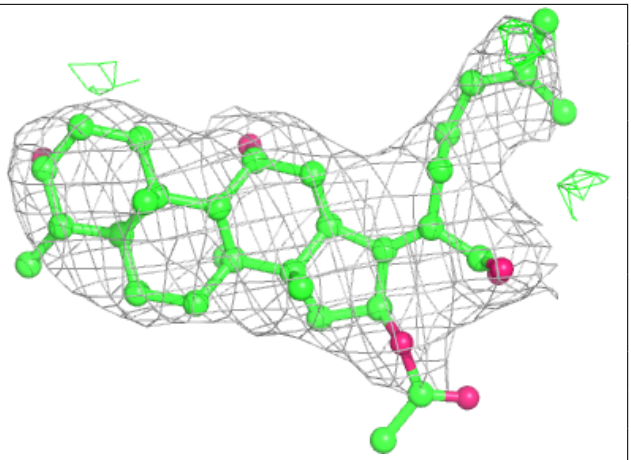
Electron density around LMT B 1102:

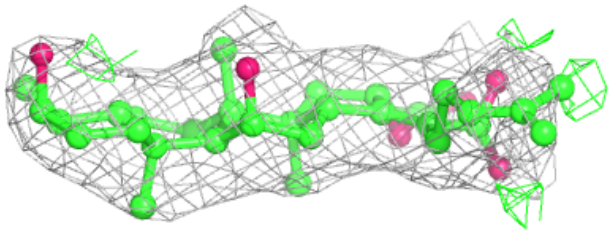
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

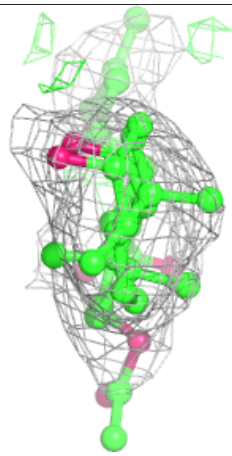


Electron density around FUA B 1101:

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

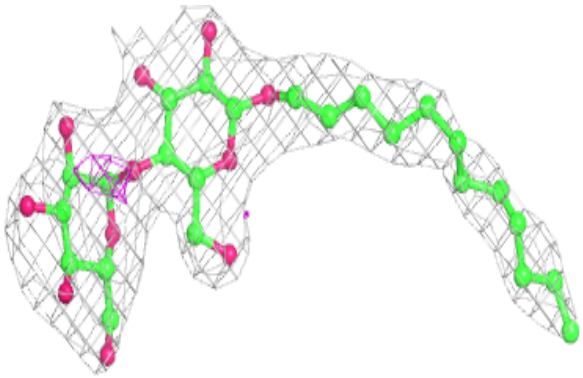


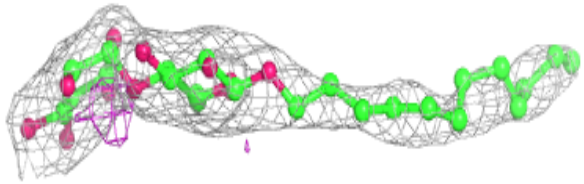


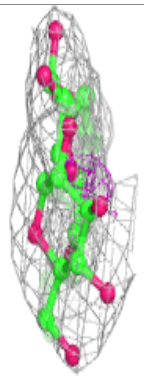


Electron density around LMT C 1103:

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







6.5 Other polymers (i)

There are no such residues in this entry.