Full wwPDB X-ray Structure Validation Report ⓘ

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 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:

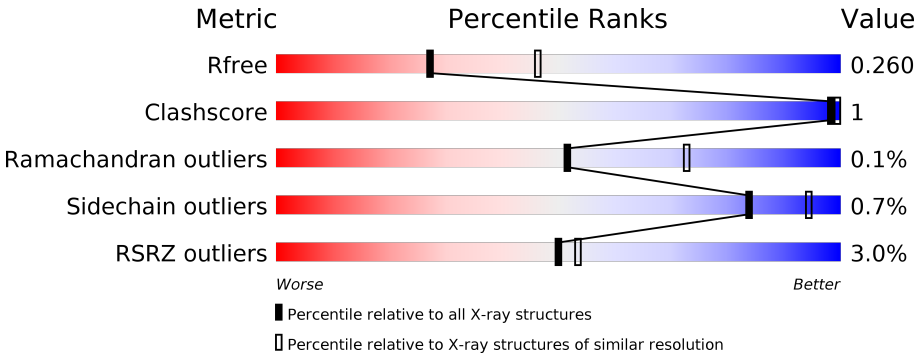
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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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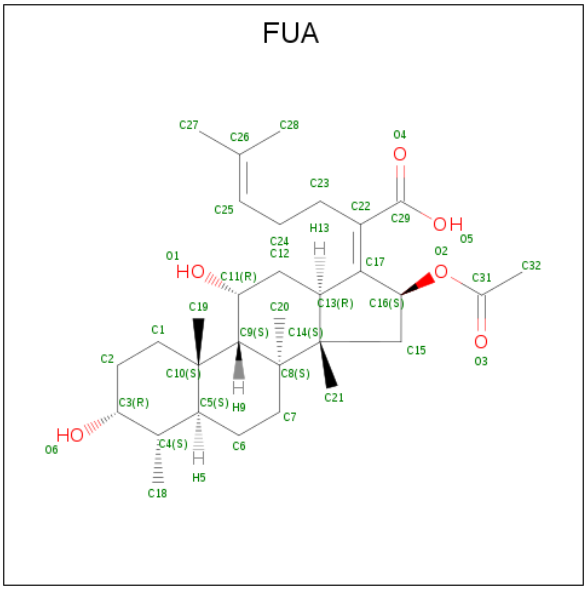
Chain	Residue	Modelled	Actual	Comment	Reference
C	1057	HIS	-	expression tag	UNP P31224

- Molecule 2 is a protein called DARPin.

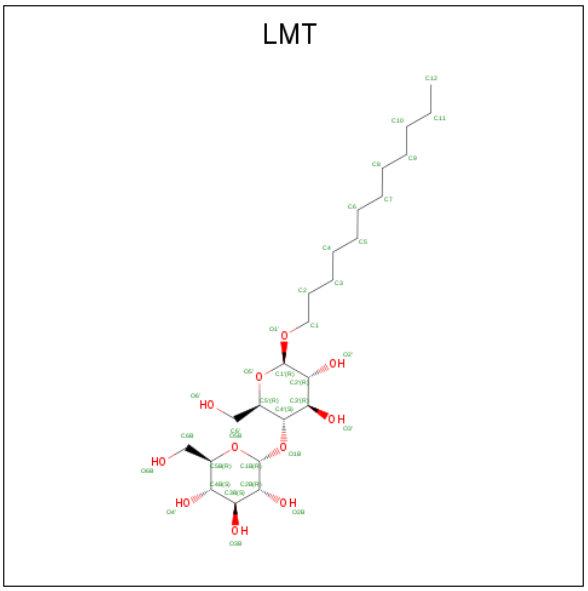
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	158	Total	C	N	O	S	0	0	0
			1194	753	209	231	1			
2	E	154	Total	C	N	O	S	0	1	0
			1173	740	204	228	1			

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



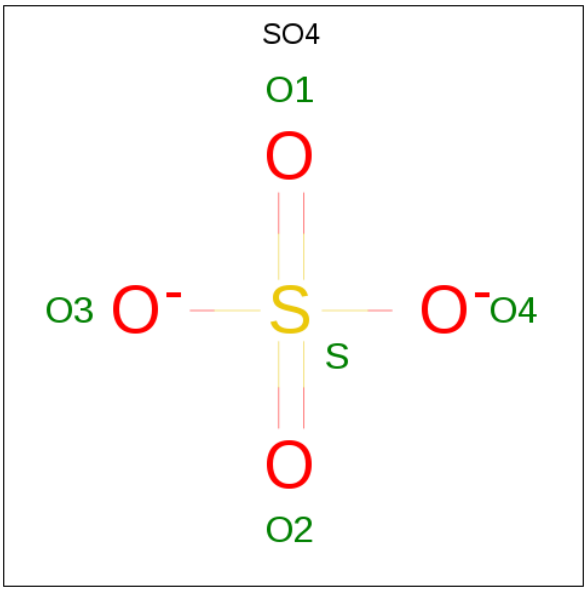
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			37	31	6		
3	B	1	Total	C	O	0	0
			37	31	6		
3	C	1	Total	C	O	0	0
			37	31	6		

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



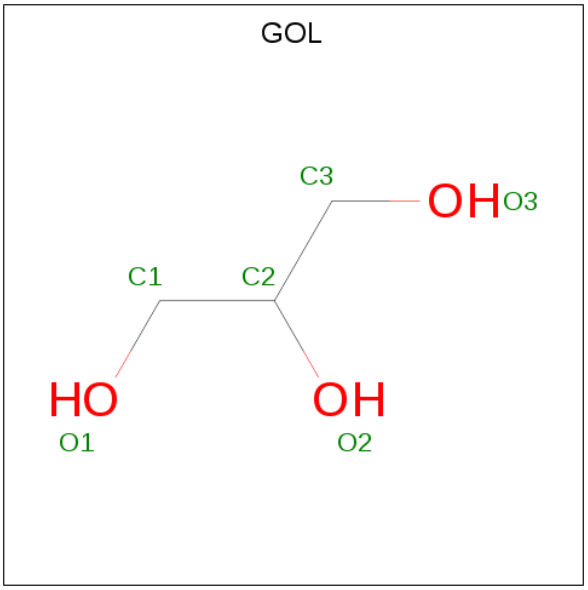
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 35 24 11	0	0
4	A	1	Total C O 35 24 11	0	0
4	A	1	Total C O 35 24 11	0	0
4	B	1	Total C O 35 24 11	0	0
4	B	1	Total C O 35 24 11	0	0
4	B	1	Total C O 35 24 11	0	0
4	C	1	Total C O 35 24 11	0	0
4	C	1	Total C O 35 24 11	0	0
4	C	1	Total C O 35 24 11	0	0
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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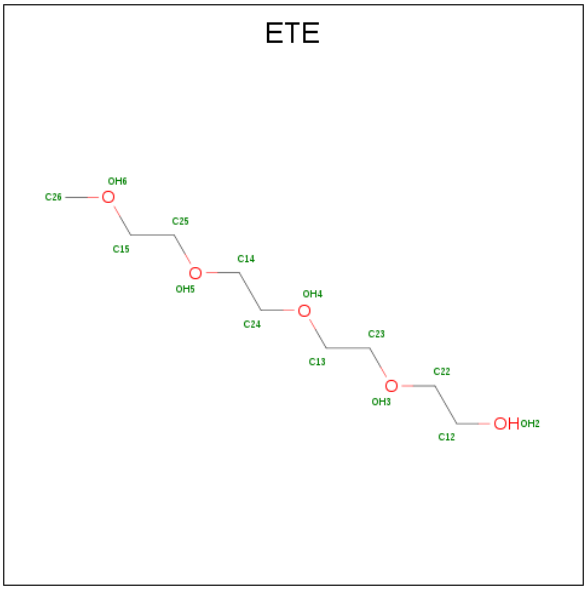
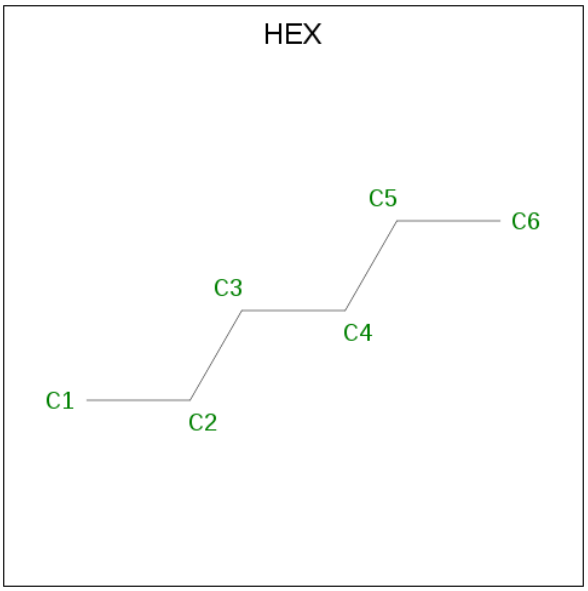
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 6 3 3	0	0
6	C	1	Total C O 6 3 3	0	0
6	C	1	Total C O 6 3 3	0	0
6	D	1	Total C O 6 3 3	0	0
6	E	1	Total C O 6 3 3	0	0
6	E	1	Total C O 6 3 3	0	0

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



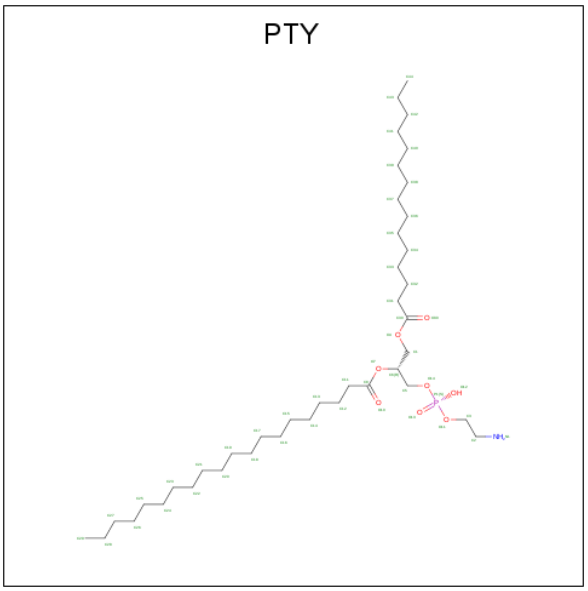
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 14 9 5	0	0
7	A	1	Total C O 14 9 5	0	0
7	C	1	Total C O 14 9 5	0	0

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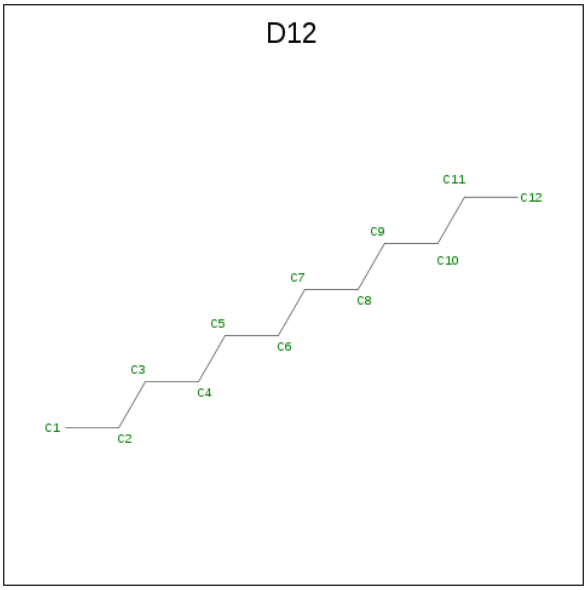
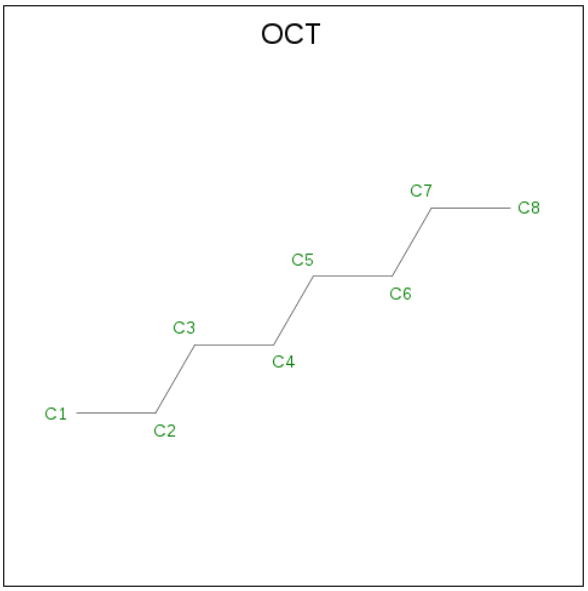
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	C	1	Total	C	N	O	P	0	0
			50	40	1	8	1		
9	C	1	Total	C	N	O	P	0	0
			50	40	1	8	1		
9	C	1	Total	C	N	O	P	0	0
			50	40	1	8	1		

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



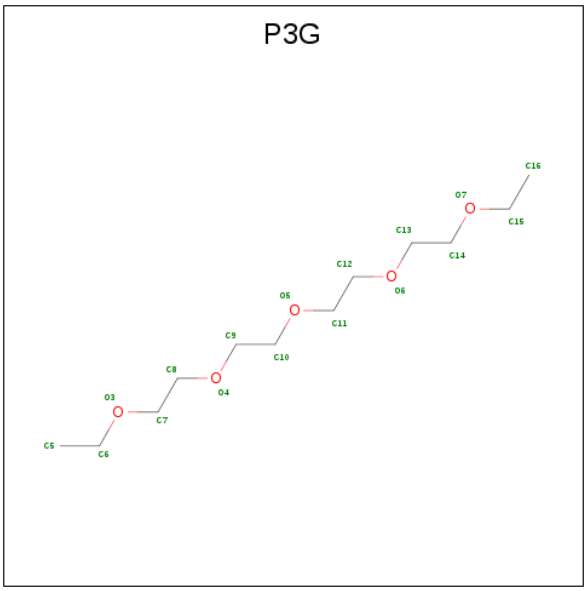
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	1	Total	C	0	0
			12	12		
10	C	1	Total	C	0	0
			12	12		
10	C	1	Total	C	0	0
			12	12		
10	C	1	Total	C	0	0
			12	12		

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



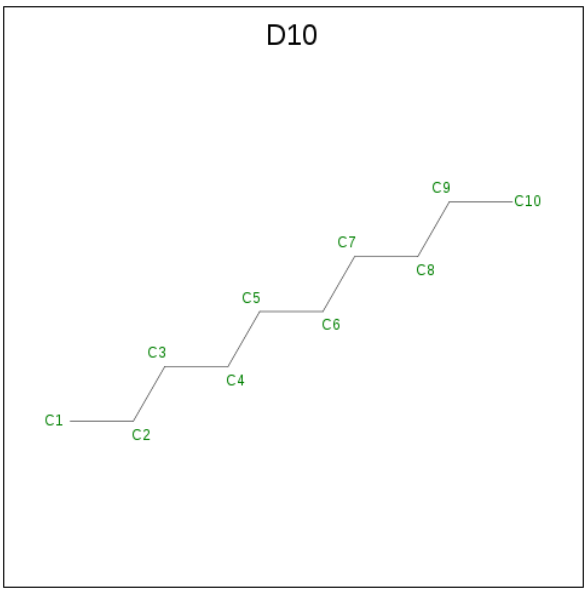
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	1	Total C 8 8	0	0
11	C	1	Total C 8 8	0	0

- 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

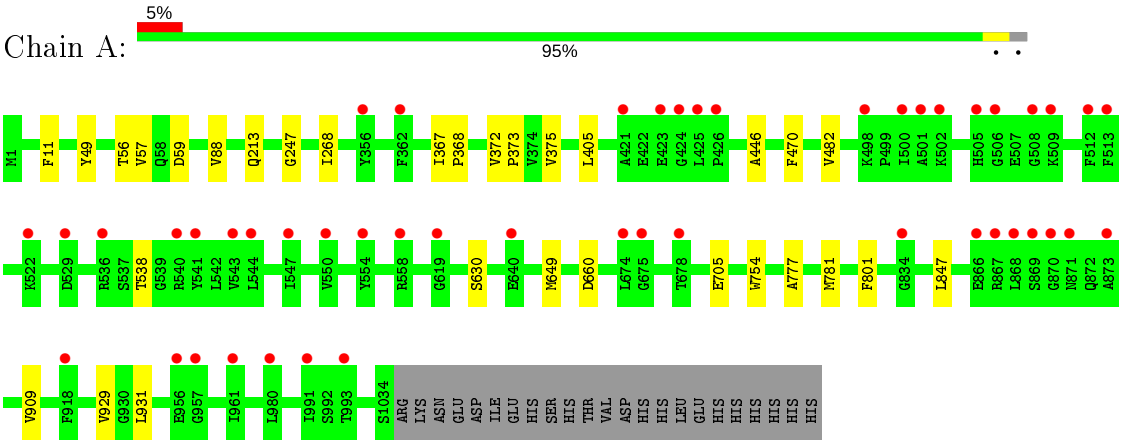
- Molecule 14 is water.

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

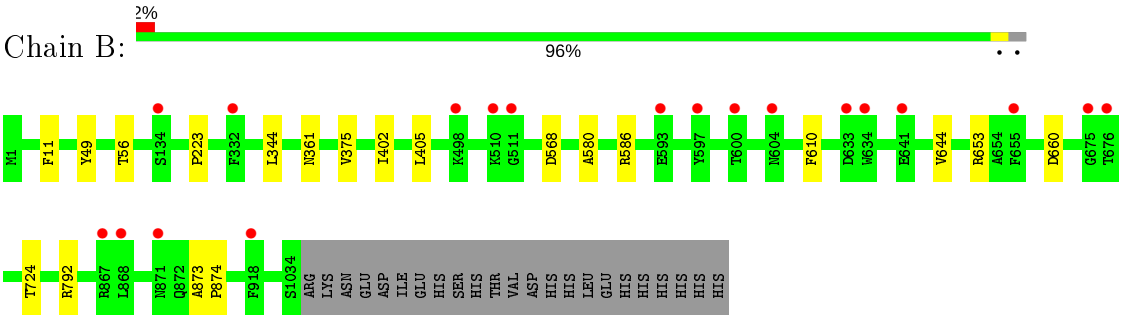
3 Residue-property plots (i)

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.

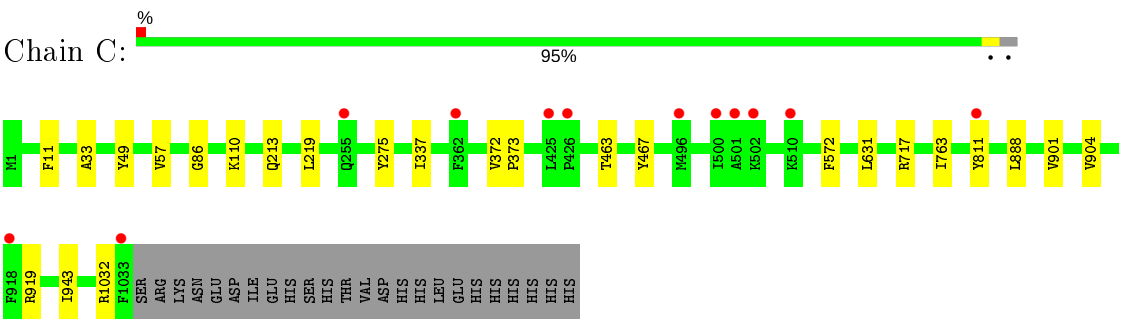
• Molecule 1: Multidrug efflux pump subunit AcrB



• Molecule 1: Multidrug efflux pump subunit AcrB

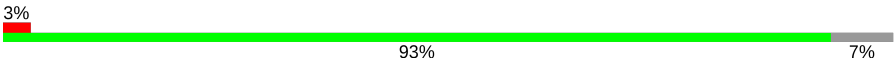


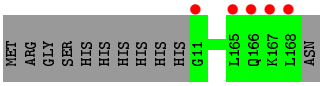
• Molecule 1: Multidrug efflux pump subunit AcrB



• Molecule 2: DARPin

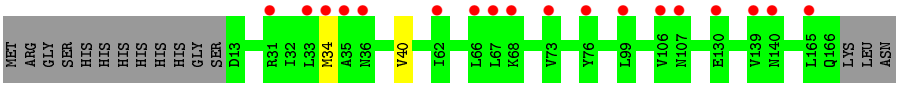
Chain D:





- 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	145.65Å 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.

All (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
3:A:1101:FUA:O4	14:A:1201:HOH:O	2.19	0.53
1:B:580:ALA:HB1	1:B:724:THR:HG22	1.91	0.53
1:A:57:VAL:CG1	1:A:88:VAL:HG22	2.41	0.50
1:C:888:LEU:HD21	1:C:943:ILE:HD11	1.93	0.49
3:C:1101:FUA:H5	3:C:1101:FUA:H202	1.96	0.47
1:A:909:VAL:HG22	1:A:931:LEU:HD11	1.97	0.47
1:A:446:ALA:HB2	1:A:482:VAL:HG21	1.97	0.46
1:A:59:ASP:HB3	1:C:763:ILE:HD11	1.98	0.45
1:A:247:GLY:HA2	1:A:268:ILE:CD1	2.47	0.45
1:C:572:PHE:HE2	1:C:631:LEU:HD21	1.83	0.44
1:B:344:LEU:CD2	1:B:402:ILE:HD13	2.48	0.44
1:A:56:THR:HG23	1:C:213:GLN:HG3	1.99	0.44
1:A:470:PHE:CD2	1:A:929:VAL:HG11	2.52	0.44
1:B:873:ALA:HB3	1:B:874:PRO:HD3	2.00	0.43
1:C:463:THR:HG22	1:C:467:TYR:CZ	2.54	0.43
1:A:705:GLU:HB3	1:A:847:LEU:HD22	2.01	0.42
1:C:33:ALA:O	1:C:337:ILE:HD11	2.19	0.42
1:C:372:VAL:HB	1:C:373:PRO:HD3	2.00	0.42
1:A:367:ILE:HB	1:A:368:PRO:HD3	2.01	0.42
1:A:754:TRP:HZ3	1:C:219:LEU:HD23	1.85	0.42
1:A:213:GLN:HG3	1:B:56:THR:HG23	2.02	0.42
1:B:223:PRO:HD3	1:C:275:TYR:CD1	2.55	0.42
1:B:568:ASP:OD2	1:B:644:VAL:HG23	2.20	0.41
1:A:372:VAL:HB	1:A:373:PRO:HD3	2.03	0.41
1:A:777:ALA:O	1:A:781:MET:HG2	2.21	0.41
3:B:1101:FUA:H202	3:B:1101:FUA:C5	2.52	0.40
2:E:34:MET:SD	2:E:40:VAL:HG12	2.62	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	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

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	PHE
1	A	49	TYR
1	A	630	SER
1	A	649[B]	MET
1	A	649[C]	MET
1	A	660	ASP

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Mol	Chain	Res	Type
1	A	801	PHE
1	B	11	PHE
1	B	49	TYR
1	B	361	ASN
1	B	586	ARG
1	B	610	PHE
1	B	653	ARG
1	C	11	PHE
1	C	49	TYR
1	C	110	LYS
1	C	717	ARG
1	C	811	TYR
1	C	919	ARG
1	C	1032	ARG

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

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

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
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
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	-
9	PTY	C	1109	-	-	19/53/53/53	-
4	LMT	C	1102	-	-	12/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

All (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
9	B	1107	PTY	O4-C30	4.42	1.46	1.33
9	C	1109	PTY	O4-C30	4.41	1.46	1.33
9	B	1107	PTY	O7-C8	4.40	1.46	1.34
9	C	1110	PTY	O4-C30	4.32	1.46	1.33
9	C	1110	PTY	O7-C8	4.20	1.46	1.34
9	C	1111	PTY	O7-C8	4.19	1.46	1.34
4	B	1103	LMT	O1'-C1'	2.34	1.44	1.40
4	C	1105	LMT	O1'-C1'	2.31	1.44	1.40
4	C	1102	LMT	O1'-C1'	2.10	1.43	1.40
4	A	1102	LMT	O1'-C1'	2.05	1.43	1.40
4	B	1104	LMT	O1'-C1'	2.03	1.43	1.40
4	B	1102	LMT	O1'-C1'	2.03	1.43	1.40
4	C	1103	LMT	O1'-C1'	2.02	1.43	1.40

All (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
9	C	1111	PTY	O7-C8-C11	3.85	119.81	111.50
9	B	1107	PTY	O7-C8-C11	3.67	119.41	111.50
3	B	1101	FUA	C19-C10-C9	-3.54	104.55	113.09
3	A	1101	FUA	C19-C10-C9	-3.19	105.39	113.09
3	C	1101	FUA	C19-C10-C9	-3.18	105.43	113.09
3	A	1101	FUA	C1-C10-C9	3.07	116.38	109.13
3	A	1101	FUA	C1-C2-C3	3.00	117.54	111.72
3	C	1101	FUA	C7-C8-C14	2.95	113.44	110.77
9	C	1109	PTY	O4-C30-C31	2.66	120.24	111.91
9	B	1107	PTY	O4-C30-C31	2.65	120.21	111.91
9	C	1110	PTY	O4-C30-C31	2.64	120.21	111.91
3	C	1101	FUA	C20-C8-C7	-2.60	103.41	107.84
4	C	1105	LMT	C1'-C2'-C3'	2.59	115.39	110.00
3	B	1101	FUA	C5-C10-C9	2.59	114.20	108.09
3	C	1101	FUA	C13-C12-C11	2.56	115.48	111.90
9	C	1111	PTY	O4-C30-C31	2.50	119.74	111.91
3	B	1101	FUA	O2-C31-O3	-2.47	118.05	122.96
9	C	1111	PTY	O7-C8-O10	-2.41	117.87	123.70
4	B	1104	LMT	O1'-C1'-C2'	2.37	112.00	108.30
3	A	1101	FUA	O2-C31-O3	-2.36	118.27	122.96
3	C	1101	FUA	C6-C5-C4	-2.25	110.78	114.32
3	C	1101	FUA	C1-C10-C9	2.22	114.36	109.13
3	A	1101	FUA	C28-C26-C27	2.20	119.47	114.60
3	B	1101	FUA	C1-C10-C9	2.15	114.19	109.13
3	C	1101	FUA	C5-C10-C9	2.14	113.14	108.09
4	B	1102	LMT	O5'-C5'-C6'	2.07	111.58	106.44
3	A	1101	FUA	C7-C6-C5	-2.05	109.56	113.11
4	A	1103	LMT	C1-O1'-C1'	2.03	117.21	113.84

There are no chirality outliers.

All (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'

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Mol	Chain	Res	Type	Atoms
9	C	1111	PTY	C11-C8-O7-C6
9	C	1111	PTY	C3-O11-P1-O12
9	C	1111	PTY	C5-O14-P1-O12
9	C	1111	PTY	C5-O14-P1-O13
3	A	1101	FUA	C17-C22-C23-C24
3	A	1101	FUA	C29-C22-C23-C24
3	A	1101	FUA	C32-C31-O2-C16
3	A	1101	FUA	O3-C31-O2-C16
4	A	1103	LMT	C2'-C1'-O1'-C1
4	A	1103	LMT	O5'-C1'-O1'-C1
3	B	1101	FUA	C32-C31-O2-C16
4	A	1104	LMT	C2-C1-O1'-C1'
9	B	1107	PTY	N1-C2-C3-O11
4	C	1105	LMT	O5'-C1'-O1'-C1
4	C	1105	LMT	C2-C1-O1'-C1'
3	C	1101	FUA	C32-C31-O2-C16
3	B	1101	FUA	O3-C31-O2-C16
4	C	1105	LMT	C4B-C5B-C6B-O6B
9	C	1110	PTY	O10-C8-O7-C6
9	C	1111	PTY	O10-C8-O7-C6
4	B	1103	LMT	O5'-C5'-C6'-O6'
4	C	1105	LMT	O5B-C5B-C6B-O6B
4	C	1103	LMT	O5'-C5'-C6'-O6'
4	C	1102	LMT	O5'-C5'-C6'-O6'
9	C	1110	PTY	C31-C30-O4-C1
4	B	1102	LMT	O5'-C5'-C6'-O6'
4	C	1105	LMT	O5'-C5'-C6'-O6'
4	B	1103	LMT	C4'-C5'-C6'-O6'
12	B	1110	P3G	O5-C10-C9-O4
4	B	1104	LMT	O5'-C5'-C6'-O6'
9	C	1110	PTY	O30-C30-O4-C1
3	C	1101	FUA	O3-C31-O2-C16
4	C	1103	LMT	C4'-C5'-C6'-O6'
9	C	1109	PTY	C11-C8-O7-C6
4	B	1102	LMT	C4'-C5'-C6'-O6'
4	B	1104	LMT	C4'-C5'-C6'-O6'
7	A	1107	ETE	OH6-C15-C25-OH5
9	B	1107	PTY	O14-C5-C6-O7
7	A	1107	ETE	OH5-C14-C24-OH4
4	B	1103	LMT	C2'-C1'-O1'-C1
4	C	1105	LMT	C2'-C1'-O1'-C1
9	B	1107	PTY	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
4	C	1102	LMT	O5B-C1B-O1B-C4'
4	C	1102	LMT	C2B-C1B-O1B-C4'
7	A	1108	ETE	OH4-C13-C23-OH3
7	C	1115	ETE	OH6-C15-C25-OH5
7	A	1108	ETE	OH5-C14-C24-OH4
9	B	1107	PTY	C31-C30-O4-C1
7	A	1107	ETE	OH4-C13-C23-OH3
7	A	1108	ETE	OH6-C15-C25-OH5
9	C	1109	PTY	C30-C31-C32-C33
9	C	1109	PTY	O10-C8-O7-C6
4	C	1102	LMT	C4'-C5'-C6'-O6'
9	B	1107	PTY	O30-C30-O4-C1
9	C	1110	PTY	C3-O11-P1-O14
9	C	1111	PTY	C3-O11-P1-O14
9	C	1111	PTY	C5-O14-P1-O11
4	B	1103	LMT	C3-C4-C5-C6
4	C	1105	LMT	C5-C6-C7-C8
9	C	1110	PTY	C25-C26-C27-C28
10	B	1108	D12	C7-C8-C9-C10
4	A	1102	LMT	C4B-C5B-C6B-O6B
4	A	1103	LMT	C2-C3-C4-C5
4	C	1102	LMT	C2'-C1'-O1'-C1
7	C	1115	ETE	OH4-C13-C23-OH3
13	B	1112	D10	C6-C7-C8-C9
4	B	1104	LMT	C11-C10-C9-C8
4	B	1103	LMT	O1'-C1-C2-C3
4	B	1103	LMT	O5B-C5B-C6B-O6B
4	C	1103	LMT	C7-C8-C9-C10
9	C	1109	PTY	C24-C25-C26-C27
13	B	1112	D10	C4-C5-C6-C7
6	C	1108	GOL	O1-C1-C2-C3
6	C	1107	GOL	O1-C1-C2-C3
6	D	201	GOL	O1-C1-C2-C3
6	E	201	GOL	O1-C1-C2-C3
6	A	1106	GOL	O1-C1-C2-C3
9	C	1111	PTY	C36-C37-C38-C39
4	C	1102	LMT	O5'-C1'-O1'-C1
9	C	1111	PTY	C12-C13-C14-C15
9	B	1107	PTY	C20-C21-C22-C23
9	B	1107	PTY	C34-C35-C36-C37
4	A	1103	LMT	C2-C1-O1'-C1'
12	B	1110	P3G	O3-C7-C8-O4

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Mol	Chain	Res	Type	Atoms
9	B	1107	PTY	C11-C12-C13-C14
4	C	1105	LMT	C4'-C5'-C6'-O6'
4	B	1102	LMT	C7-C8-C9-C10
9	B	1107	PTY	C15-C16-C17-C18
6	C	1108	GOL	O1-C1-C2-O2
6	E	201	GOL	O1-C1-C2-O2
10	C	1112	D12	C3-C4-C5-C6
4	B	1103	LMT	C7-C8-C9-C10
9	B	1107	PTY	C37-C38-C39-C40
4	A	1102	LMT	O1'-C1-C2-C3
4	A	1104	LMT	C7-C8-C9-C10
9	B	1107	PTY	C24-C25-C26-C27
10	C	1113	D12	C3-C4-C5-C6
4	A	1103	LMT	C4B-C5B-C6B-O6B
4	C	1105	LMT	C2-C3-C4-C5
9	C	1109	PTY	C31-C30-O4-C1
4	A	1102	LMT	C1-C2-C3-C4
4	A	1104	LMT	O5B-C5B-C6B-O6B
9	C	1110	PTY	C15-C16-C17-C18
9	C	1110	PTY	C18-C19-C20-C21
9	C	1109	PTY	C20-C21-C22-C23
9	B	1107	PTY	O10-C8-O7-C6
4	A	1102	LMT	C3-C4-C5-C6
9	C	1109	PTY	C36-C37-C38-C39
9	B	1107	PTY	C11-C8-O7-C6
9	C	1111	PTY	C35-C36-C37-C38
4	A	1103	LMT	C3-C4-C5-C6
9	C	1109	PTY	C35-C36-C37-C38
9	C	1109	PTY	O30-C30-O4-C1
9	C	1109	PTY	C21-C22-C23-C24
9	C	1110	PTY	C22-C23-C24-C25
9	B	1107	PTY	O14-C5-C6-C1
4	C	1104	LMT	C2-C3-C4-C5
9	C	1110	PTY	C40-C41-C42-C43
6	A	1106	GOL	O1-C1-C2-O2
10	B	1108	D12	C5-C6-C7-C8
4	C	1103	LMT	O5B-C5B-C6B-O6B
10	C	1113	D12	C1-C2-C3-C4
4	C	1103	LMT	C5-C6-C7-C8
9	C	1111	PTY	C20-C21-C22-C23
4	A	1104	LMT	C4-C5-C6-C7
4	B	1104	LMT	C2'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
11	C	1116	OCT	C1-C2-C3-C4
9	C	1111	PTY	C21-C22-C23-C24
9	B	1107	PTY	C13-C14-C15-C16
12	B	1110	P3G	O6-C13-C14-O7
9	C	1111	PTY	C31-C32-C33-C34
4	B	1104	LMT	C3-C4-C5-C6
9	C	1109	PTY	C8-C11-C12-C13
4	B	1102	LMT	C9-C10-C11-C12
4	C	1103	LMT	C2-C1-O1'-C1'
4	C	1102	LMT	C2-C1-O1'-C1'
9	C	1111	PTY	C37-C38-C39-C40
10	C	1113	D12	C7-C8-C9-C10
4	A	1102	LMT	O5B-C5B-C6B-O6B
9	C	1109	PTY	C38-C39-C40-C41
6	C	1107	GOL	O1-C1-C2-O2
4	C	1102	LMT	C1-C2-C3-C4
4	C	1104	LMT	C6-C7-C8-C9
9	C	1110	PTY	C35-C36-C37-C38
4	C	1102	LMT	C6-C7-C8-C9
10	C	1114	D12	C2-C3-C4-C5
8	A	1109	HEX	C2-C3-C4-C5
4	C	1105	LMT	C9-C10-C11-C12
9	C	1110	PTY	O14-C5-C6-C1
9	C	1110	PTY	C16-C17-C18-C19
4	A	1103	LMT	O5B-C5B-C6B-O6B
7	C	1115	ETE	C15-C25-OH5-C14
9	C	1110	PTY	C38-C39-C40-C41
9	C	1111	PTY	C18-C19-C20-C21
4	A	1103	LMT	C9-C10-C11-C12
12	B	1110	P3G	C11-C12-O6-C13
4	C	1103	LMT	O1'-C1-C2-C3
9	C	1109	PTY	C33-C34-C35-C36
9	C	1109	PTY	C3-O11-P1-O14
9	C	1110	PTY	C6-C5-O14-P1
9	C	1110	PTY	C14-C15-C16-C17
9	C	1110	PTY	C33-C34-C35-C36
9	C	1110	PTY	C3-O11-P1-O12
4	A	1103	LMT	C5-C6-C7-C8
9	C	1110	PTY	C2-C3-O11-P1
4	C	1105	LMT	C11-C10-C9-C8
9	C	1110	PTY	O14-C5-C6-O7
4	B	1104	LMT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
9	C	1111	PTY	C11-C12-C13-C14
7	C	1115	ETE	C23-C13-OH4-C24
9	B	1107	PTY	C26-C27-C28-C29
9	C	1111	PTY	O4-C1-C6-C5
9	C	1111	PTY	O4-C1-C6-O7
4	A	1102	LMT	O5'-C5'-C6'-O6'
9	B	1107	PTY	C33-C34-C35-C36
4	C	1102	LMT	C5-C6-C7-C8
4	C	1102	LMT	C4-C5-C6-C7
4	A	1104	LMT	O1'-C1-C2-C3
4	B	1102	LMT	C5-C6-C7-C8
10	C	1112	D12	C6-C7-C8-C9
4	C	1103	LMT	C2-C3-C4-C5
4	A	1104	LMT	C3-C4-C5-C6
9	C	1110	PTY	C11-C12-C13-C14
10	C	1112	D12	C5-C6-C7-C8
10	C	1114	D12	C3-C4-C5-C6
9	C	1111	PTY	C15-C16-C17-C18
9	C	1111	PTY	C32-C33-C34-C35
7	C	1115	ETE	OH2-C12-C22-OH3
9	C	1110	PTY	C5-O14-P1-O11
9	B	1107	PTY	C3-O11-P1-O14
9	C	1109	PTY	C6-C5-O14-P1
11	B	1109	OCT	C4-C5-C6-C7
7	A	1108	ETE	C15-C25-OH5-C14
9	C	1111	PTY	N1-C2-C3-O11
4	C	1103	LMT	C1-C2-C3-C4
9	C	1111	PTY	C33-C34-C35-C36
7	A	1107	ETE	C12-C22-OH3-C23
9	C	1109	PTY	O4-C1-C6-O7
9	C	1110	PTY	C32-C33-C34-C35
9	C	1109	PTY	C17-C18-C19-C20
11	B	1109	OCT	C1-C2-C3-C4
4	B	1104	LMT	C1-C2-C3-C4
4	C	1102	LMT	C9-C10-C11-C12
7	A	1108	ETE	C23-C13-OH4-C24
9	C	1110	PTY	C39-C40-C41-C42
6	B	1105	GOL	O1-C1-C2-C3
9	C	1109	PTY	C23-C24-C25-C26
9	C	1111	PTY	C24-C25-C26-C27
6	D	201	GOL	O1-C1-C2-O2
7	A	1108	ETE	C24-C14-OH5-C25

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Mol	Chain	Res	Type	Atoms
9	B	1107	PTY	O4-C30-C31-C32
9	C	1110	PTY	C12-C11-C8-O7
9	C	1110	PTY	O4-C30-C31-C32
13	B	1111	D10	C2-C3-C4-C5
4	C	1103	LMT	C9-C10-C11-C12
4	B	1103	LMT	C6-C7-C8-C9
7	C	1115	ETE	OH5-C14-C24-OH4
9	B	1107	PTY	O30-C30-C31-C32
9	C	1110	PTY	O30-C30-C31-C32
9	C	1111	PTY	C17-C18-C19-C20
9	C	1110	PTY	C12-C11-C8-O10
9	C	1110	PTY	C17-C18-C19-C20
9	C	1110	PTY	C5-O14-P1-O13
9	B	1107	PTY	C12-C11-C8-O7
9	B	1107	PTY	C2-C3-O11-P1
9	C	1110	PTY	C26-C27-C28-C29
9	B	1107	PTY	C17-C18-C19-C20
4	B	1104	LMT	C2-C1-O1'-C1'
9	B	1107	PTY	C12-C11-C8-O10
10	C	1114	D12	C4-C5-C6-C7
9	C	1109	PTY	C39-C40-C41-C42

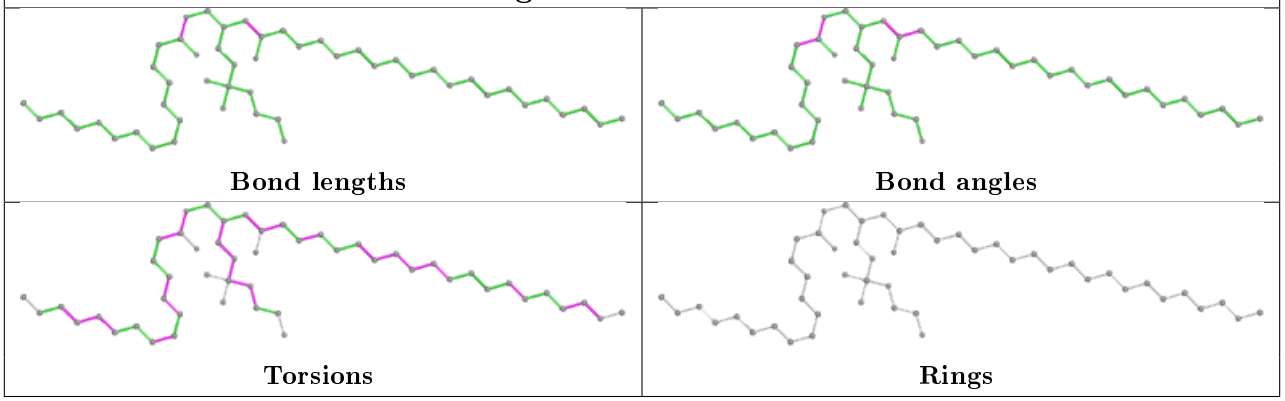
There are no ring outliers.

3 monomers are involved in 4 short contacts:

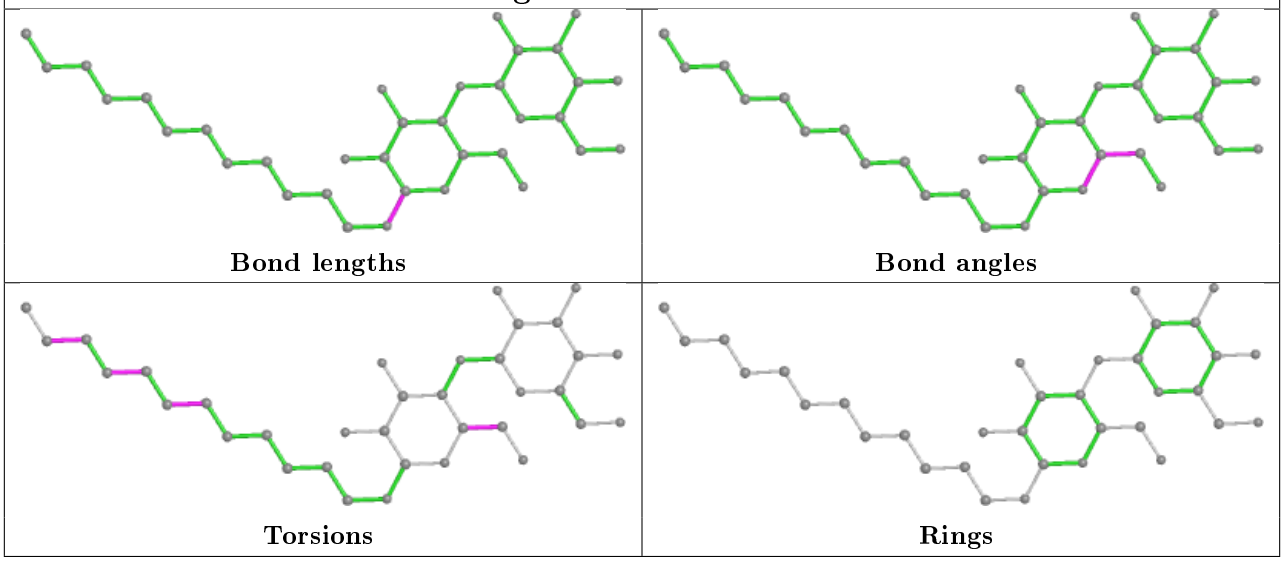
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1101	FUA	1	0
3	A	1101	FUA	1	0
3	B	1101	FUA	2	0

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.

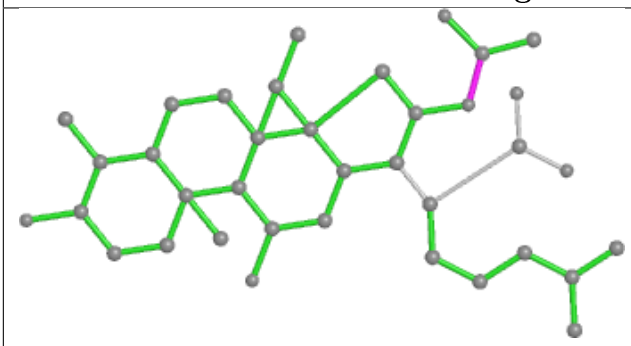
Ligand PTY C 1110



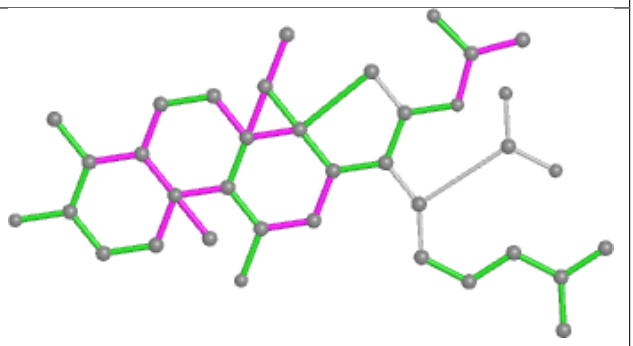
Ligand LMT B 1102



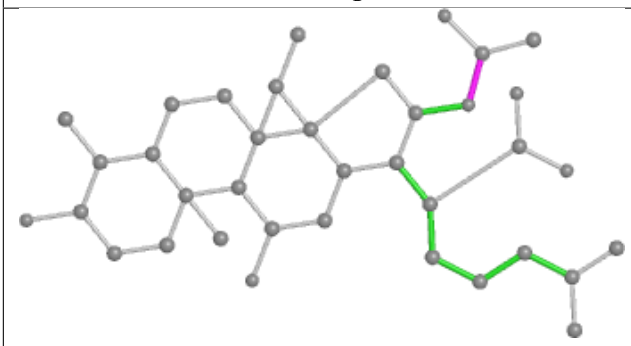
Ligand FUA C 1101



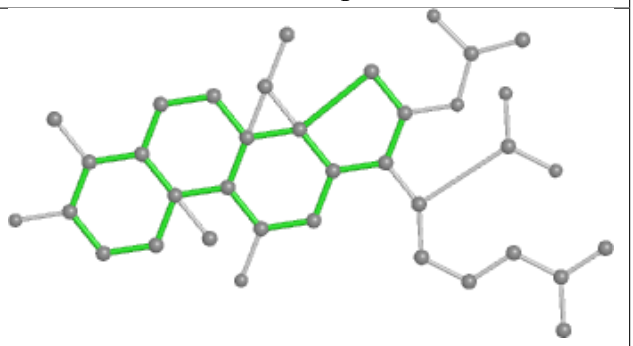
Bond lengths



Bond angles

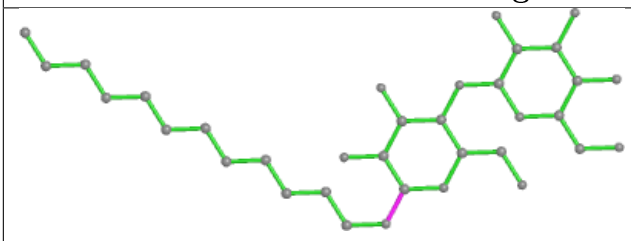


Torsions

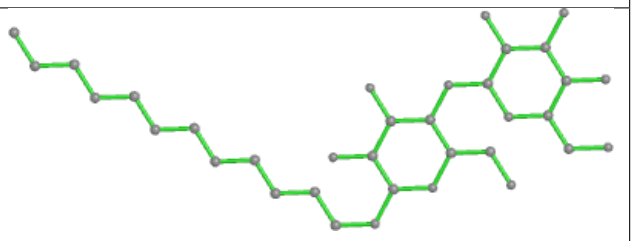


Rings

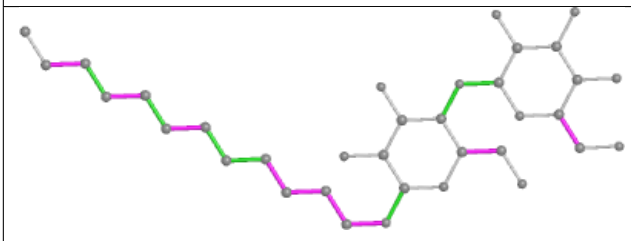
Ligand LMT C 1103



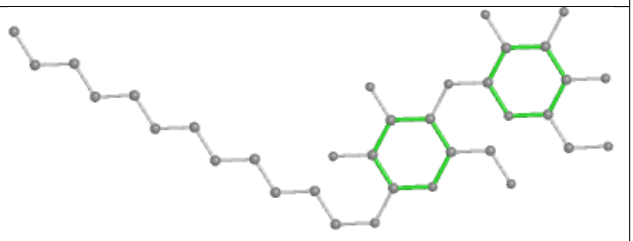
Bond lengths



Bond angles

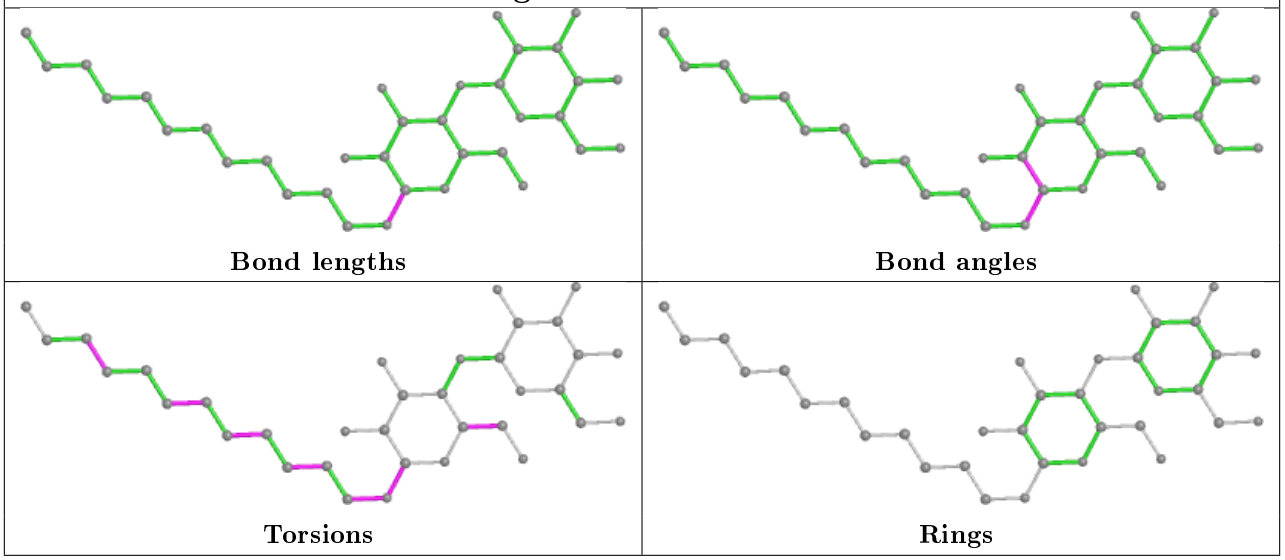


Torsions

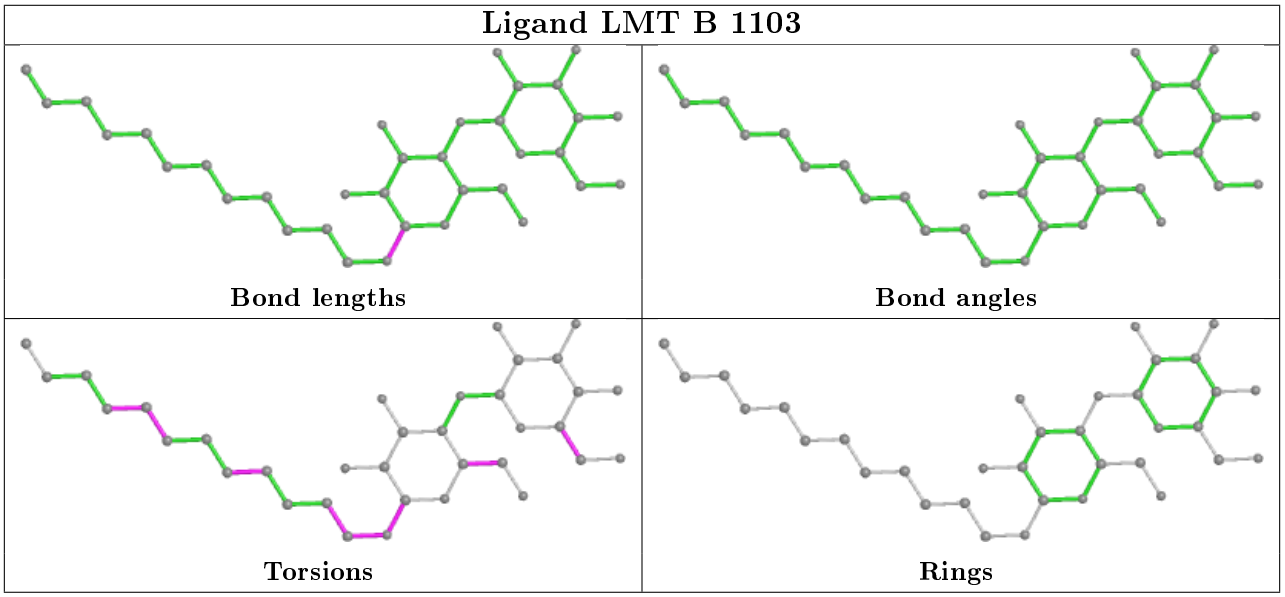


Rings

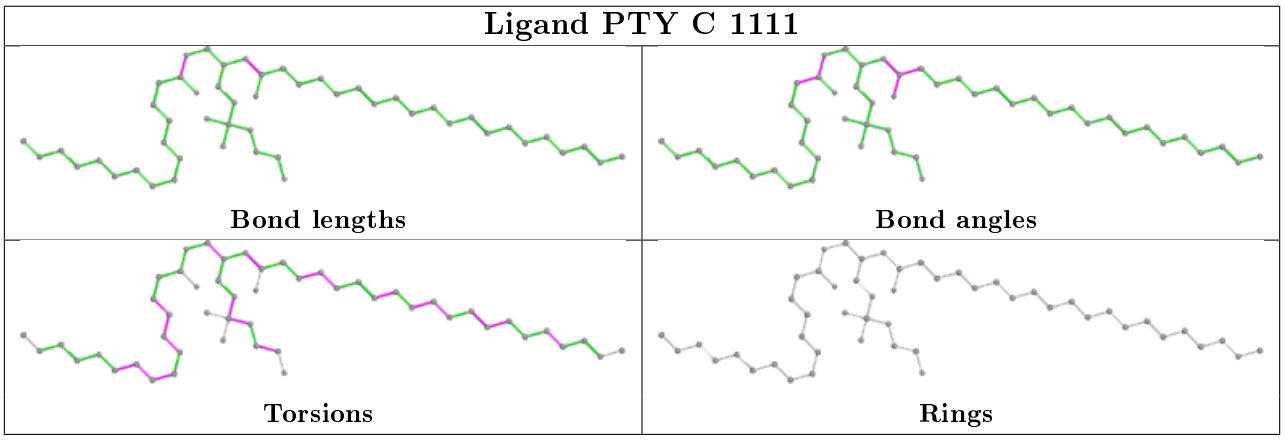
Ligand LMT B 1104



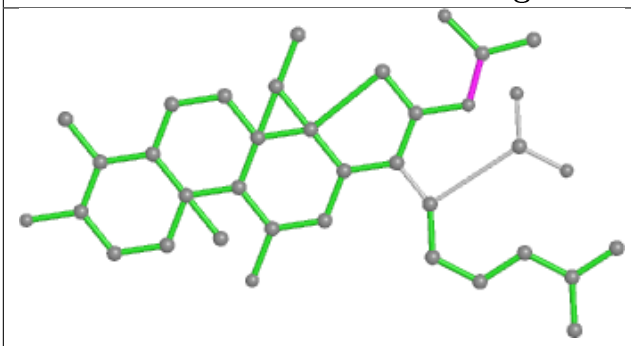
Ligand LMT B 1103



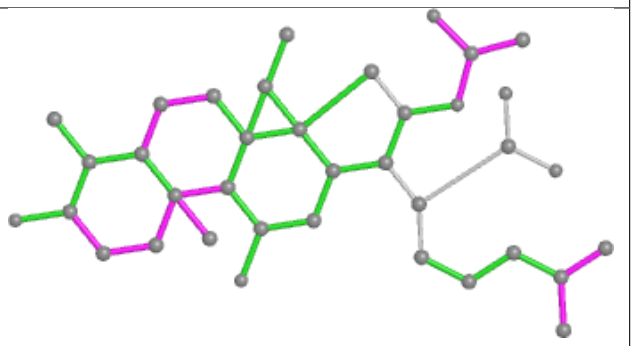
Ligand PTY C 1111



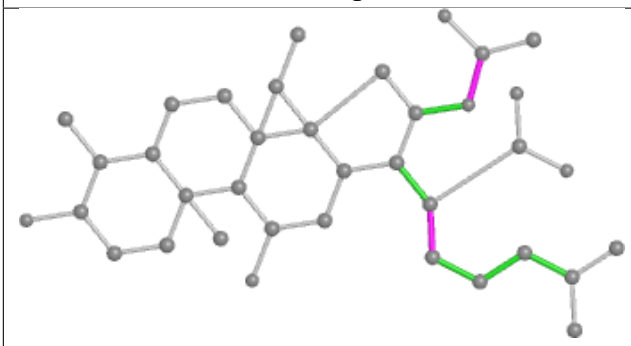
Ligand FUA A 1101



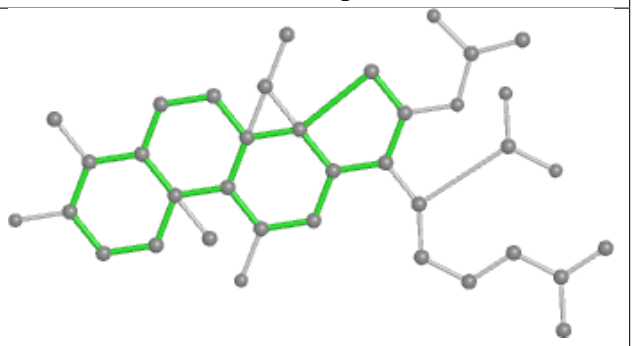
Bond lengths



Bond angles

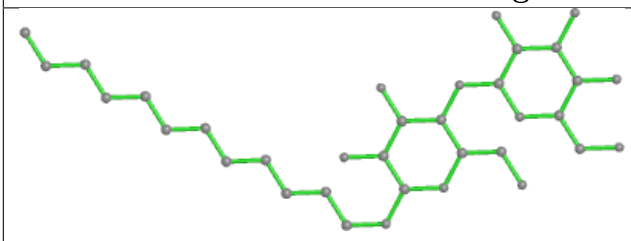


Torsions

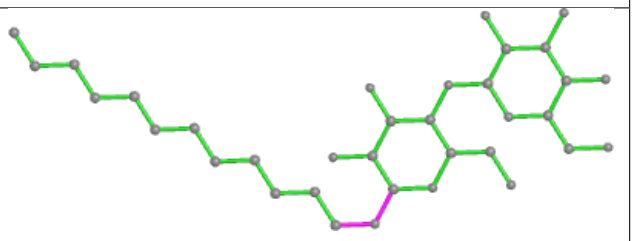


Rings

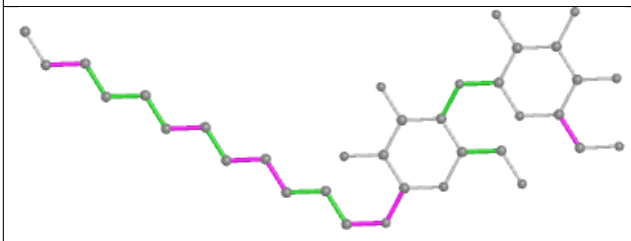
Ligand LMT A 1103



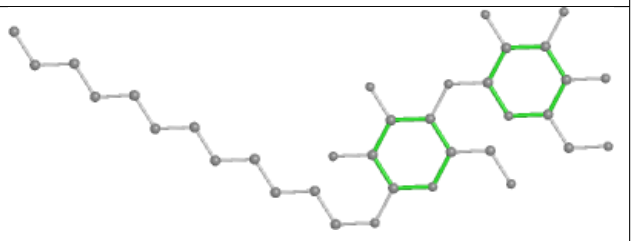
Bond lengths



Bond angles

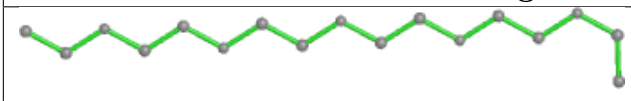


Torsions

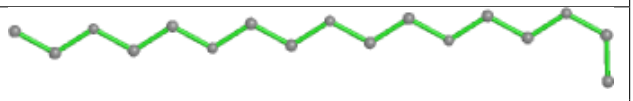


Rings

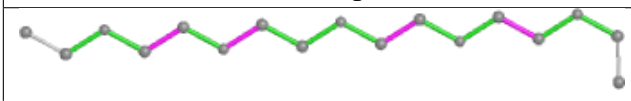
Ligand P3G B 1110



Bond lengths



Bond angles



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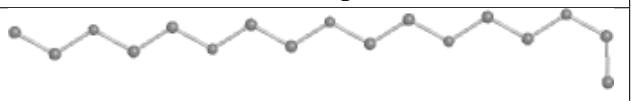
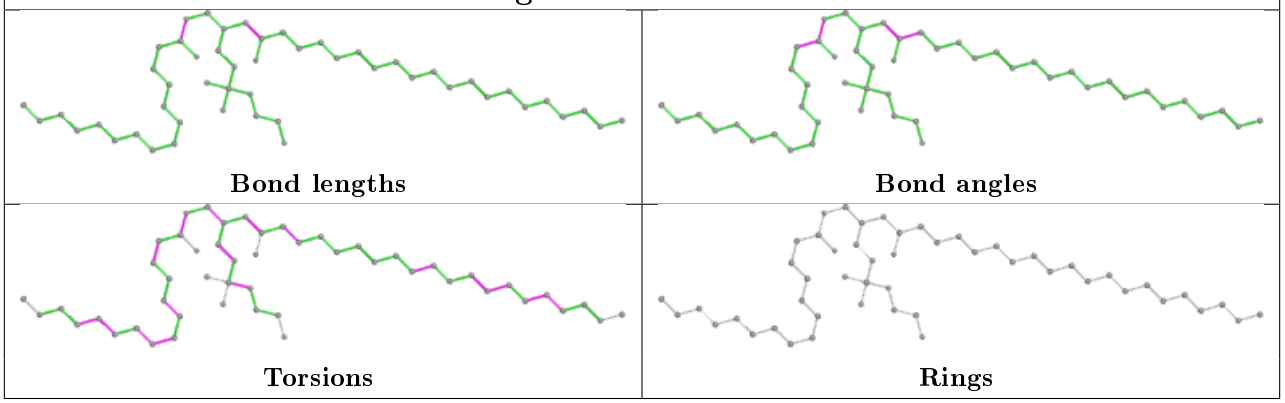


Rings

Ligand PTY C 1109



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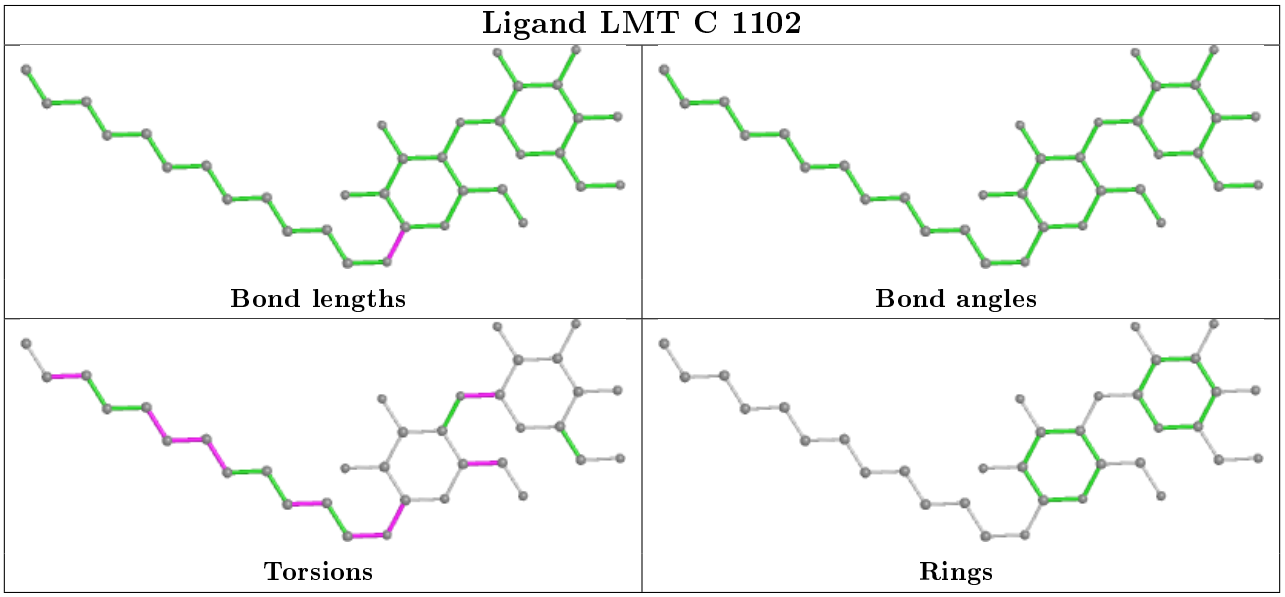

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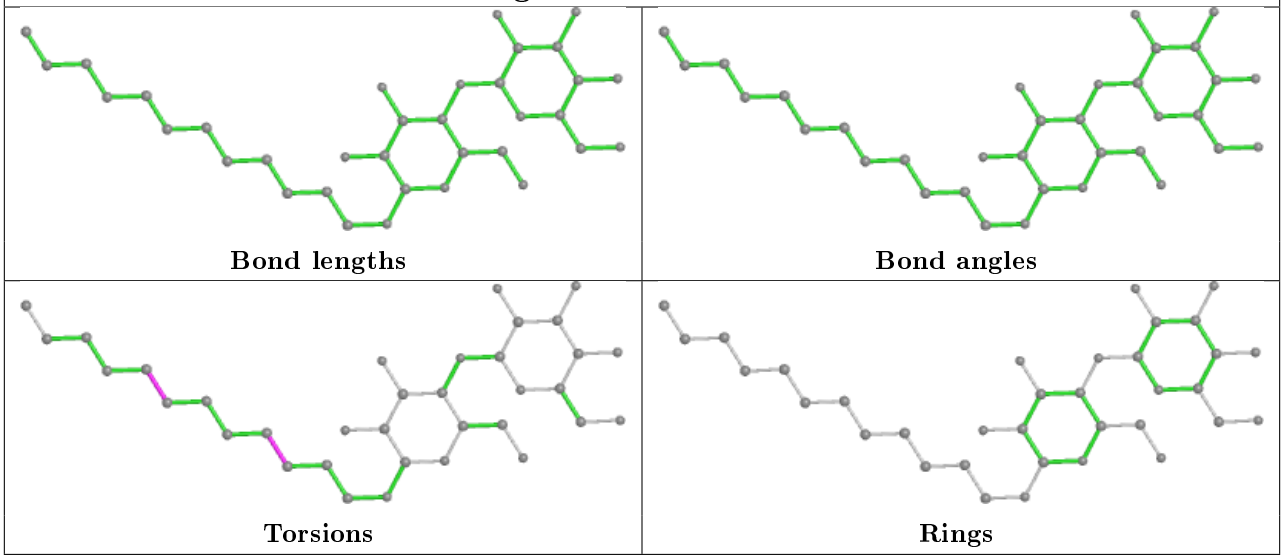
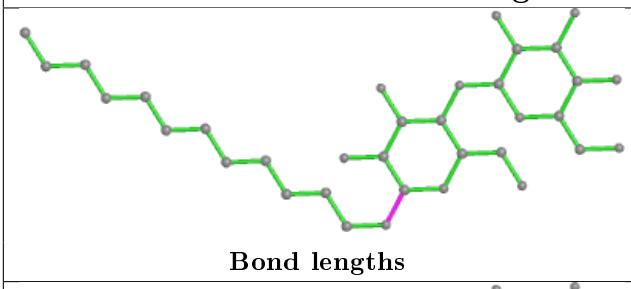
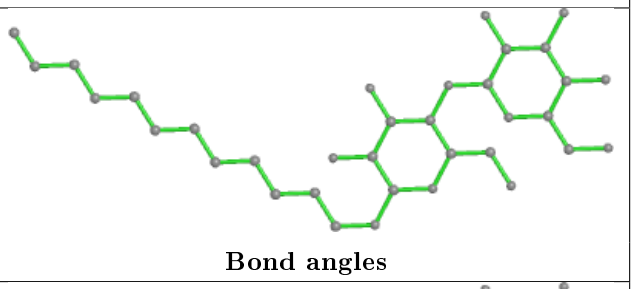


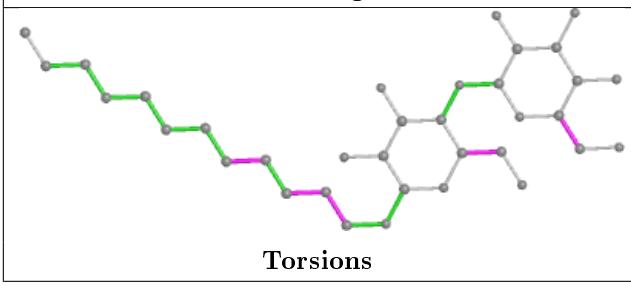
Ligand LMT A 1102



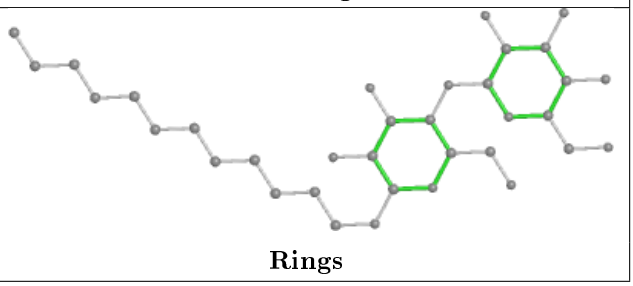
Bond lengths



Bond angles

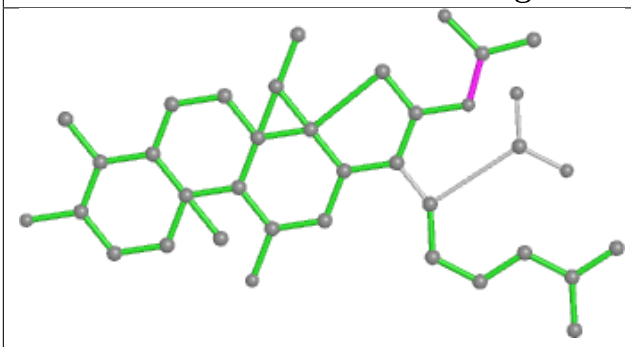


Torsions

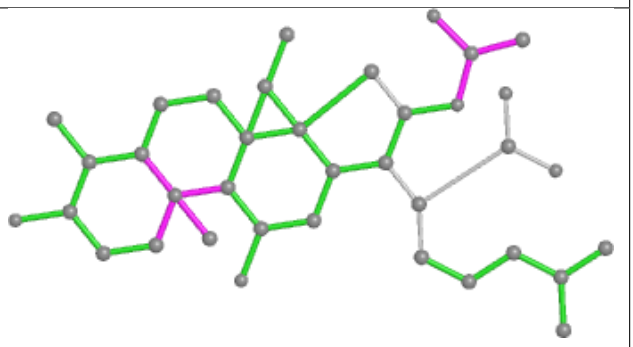


Rings

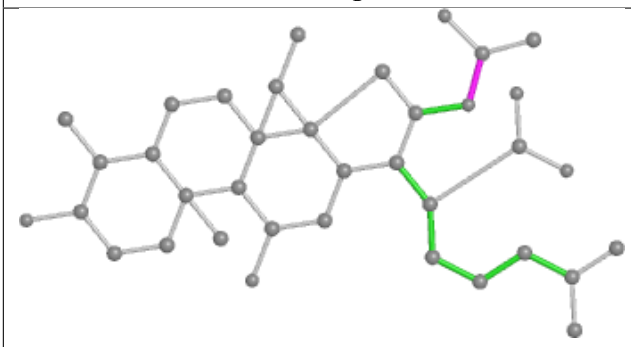
Ligand FUA B 1101



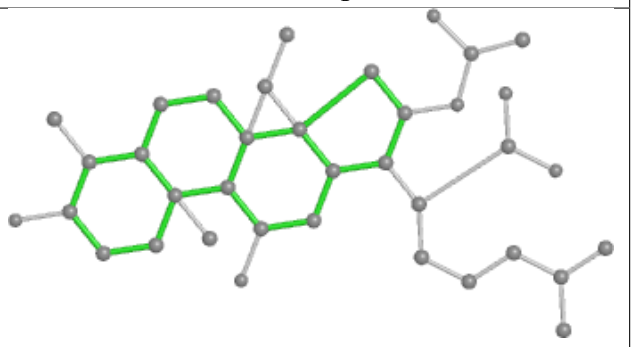
Bond lengths



Bond angles

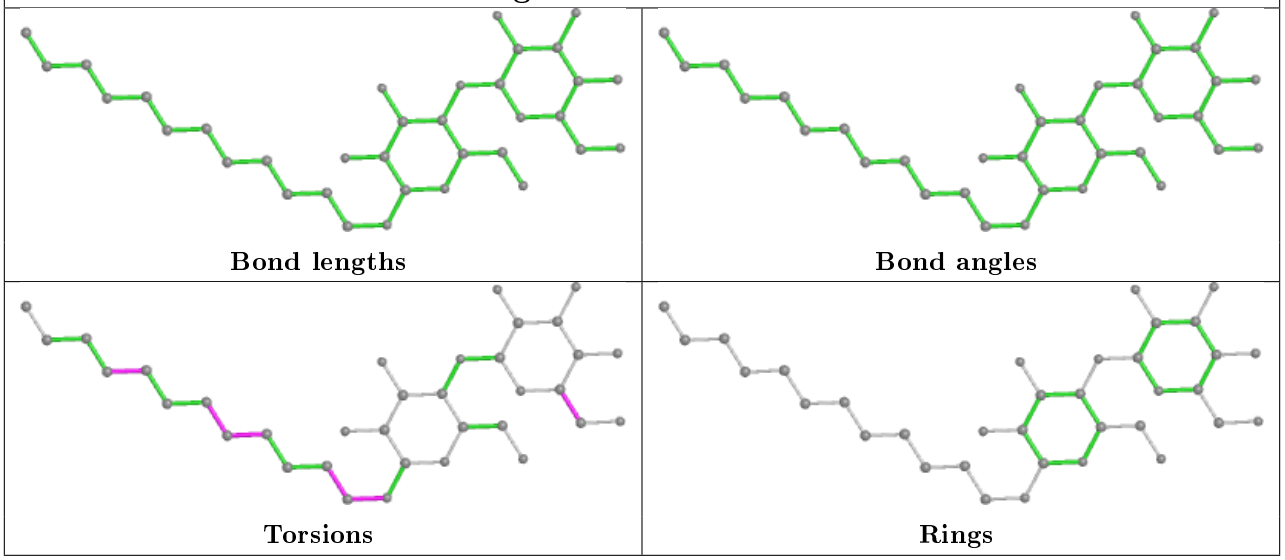


Torsions

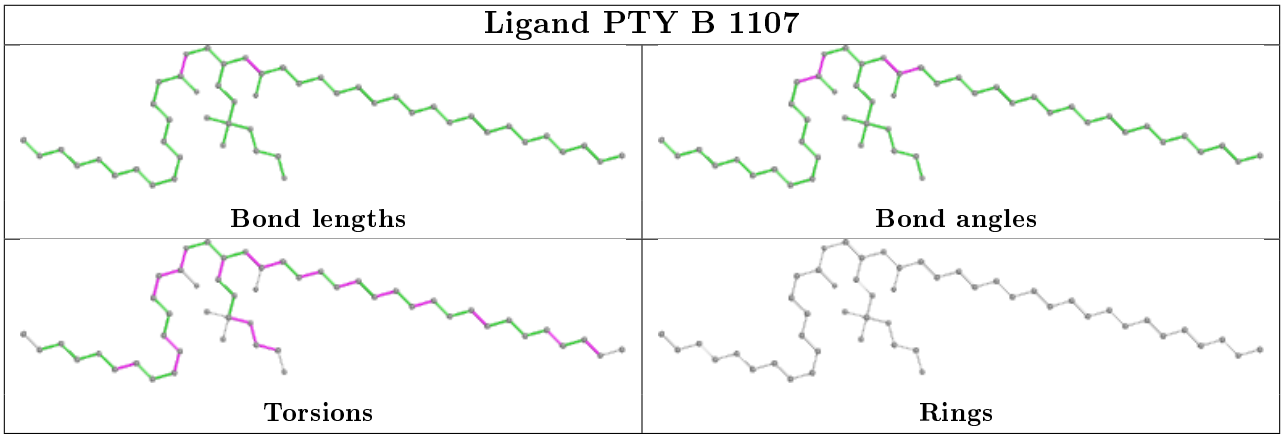


Rings

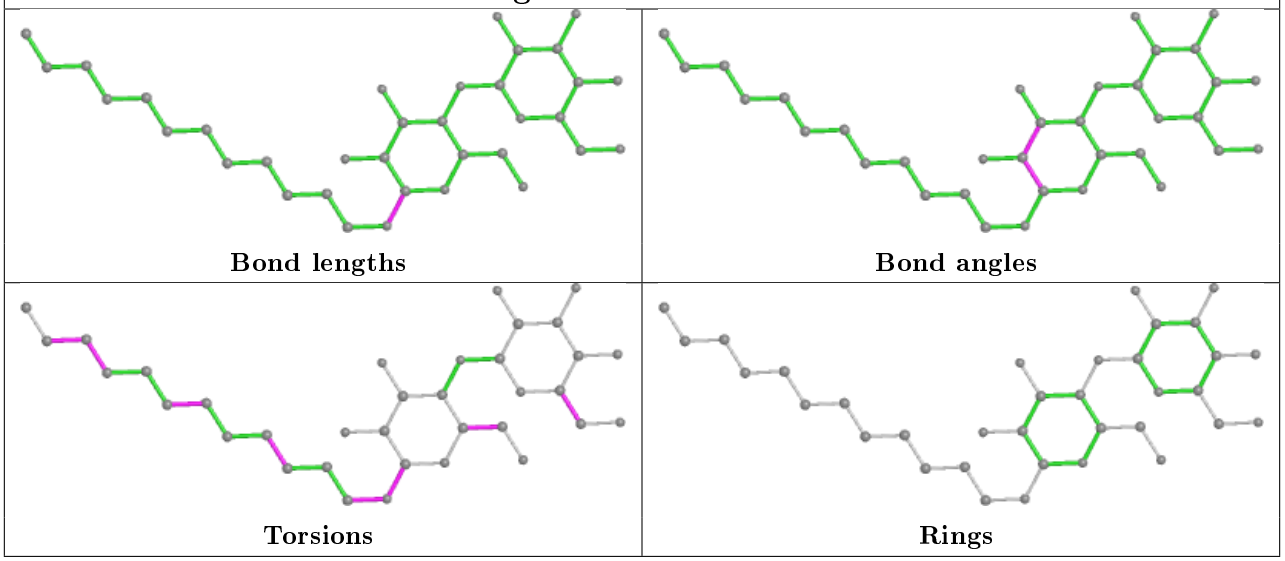
Ligand LMT A 1104



Ligand PTY B 1107



Ligand LMT C 1105



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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

All (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
2	E	35	ALA	5.8
1	A	543	VAL	5.5
2	E	66	LEU	5.4
1	A	870	GLY	5.3
2	D	11	GLY	5.3
1	B	634	TRP	4.4
1	A	508	GLY	4.3
1	A	501	ALA	4.3
1	A	675	GLY	4.3
1	A	512	PHE	4.1
2	E	31	ARG	4.0
1	C	510	LYS	4.0
1	A	869	SER	3.9
2	D	166	GLN	3.8
1	C	502	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	134	SER	3.6
1	C	362	PHE	3.5
1	A	678	THR	3.4
1	A	540	ARG	3.2
1	A	500	ILE	3.2
1	A	957	GLY	3.1
2	E	139	VAL	3.1
1	A	356	TYR	3.0
2	E	99	LEU	3.0
1	A	866	GLU	2.9
2	E	34	MET	2.9
1	A	513	PHE	2.9
1	A	547	ILE	2.9
2	E	106	VAL	2.9
1	C	426	PRO	2.9
1	B	867	ARG	2.9
1	A	918	PHE	2.8
1	B	655	PHE	2.8
1	A	424	GLY	2.8
1	A	640	GLU	2.8
1	A	421	ALA	2.8
1	A	544	LEU	2.8
2	D	167	LYS	2.7
2	E	33	LEU	2.7
1	B	600	THR	2.7
2	E	68	LYS	2.7
2	E	67	LEU	2.7
1	B	641	GLU	2.7
1	A	423	GLU	2.7
1	B	593	GLU	2.7
1	B	498	LYS	2.7
1	A	991	ILE	2.6
1	C	255	GLN	2.6
1	A	956	GLU	2.6
1	C	500	ILE	2.6
1	A	541	TYR	2.5
1	A	980	LEU	2.5
2	E	130	GLU	2.5
1	B	510	LYS	2.5
1	B	511	GLY	2.5
1	C	918	PHE	2.5
1	A	873	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	498	LYS	2.5
1	B	332	PHE	2.5
1	A	529	ASP	2.5
1	A	506	GLY	2.4
1	C	501	ALA	2.4
2	D	165	LEU	2.4
1	A	961	ILE	2.4
1	A	505	HIS	2.4
1	B	675	GLY	2.3
1	A	522	LYS	2.3
1	A	867	ARG	2.3
1	B	918	PHE	2.3
1	C	811	TYR	2.3
1	B	871	ASN	2.3
1	A	674	LEU	2.3
1	B	676	THR	2.2
1	A	619	GLY	2.2
2	E	165	LEU	2.2
1	C	496	MET	2.2
2	E	140	ASN	2.2
1	A	426	PRO	2.2
2	E	62	ILE	2.1
1	C	1033	PHE	2.1
1	B	633	ASP	2.1
2	E	73	VAL	2.1
1	A	362	PHE	2.1
1	C	425	LEU	2.1
1	A	550	VAL	2.1
1	B	597	TYR	2.1
1	A	554	TYR	2.1
1	A	993	THR	2.0
1	A	834	GLY	2.0
1	A	509	LYS	2.0
1	A	536	ARG	2.0
1	B	604	ASN	2.0
2	E	36	ASN	2.0
2	E	107	ASN	2.0
1	A	558	ARG	2.0
1	A	425	LEU	2.0
2	E	76	TYR	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
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

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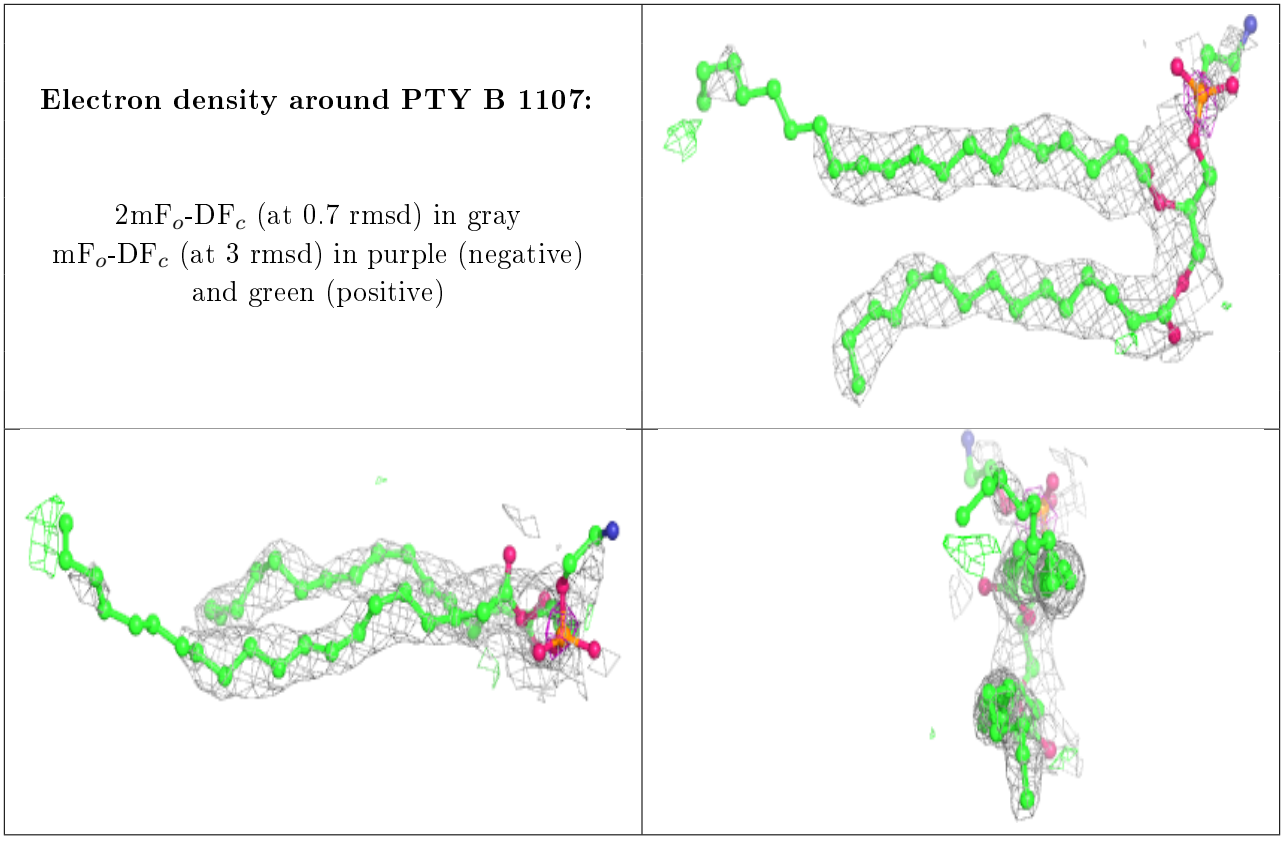
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
13	D10	B	1112	10/10	0.84	0.18	81,83,83,84	0
6	GOL	D	201	6/6	0.84	0.18	67,70,70,72	0
10	D12	B	1108	12/12	0.84	0.17	71,74,75,75	0
6	GOL	B	1106	6/6	0.86	0.17	62,66,68,68	0
6	GOL	B	1105	6/6	0.87	0.25	67,68,72,74	0
6	GOL	A	1106	6/6	0.88	0.15	80,82,82,85	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.

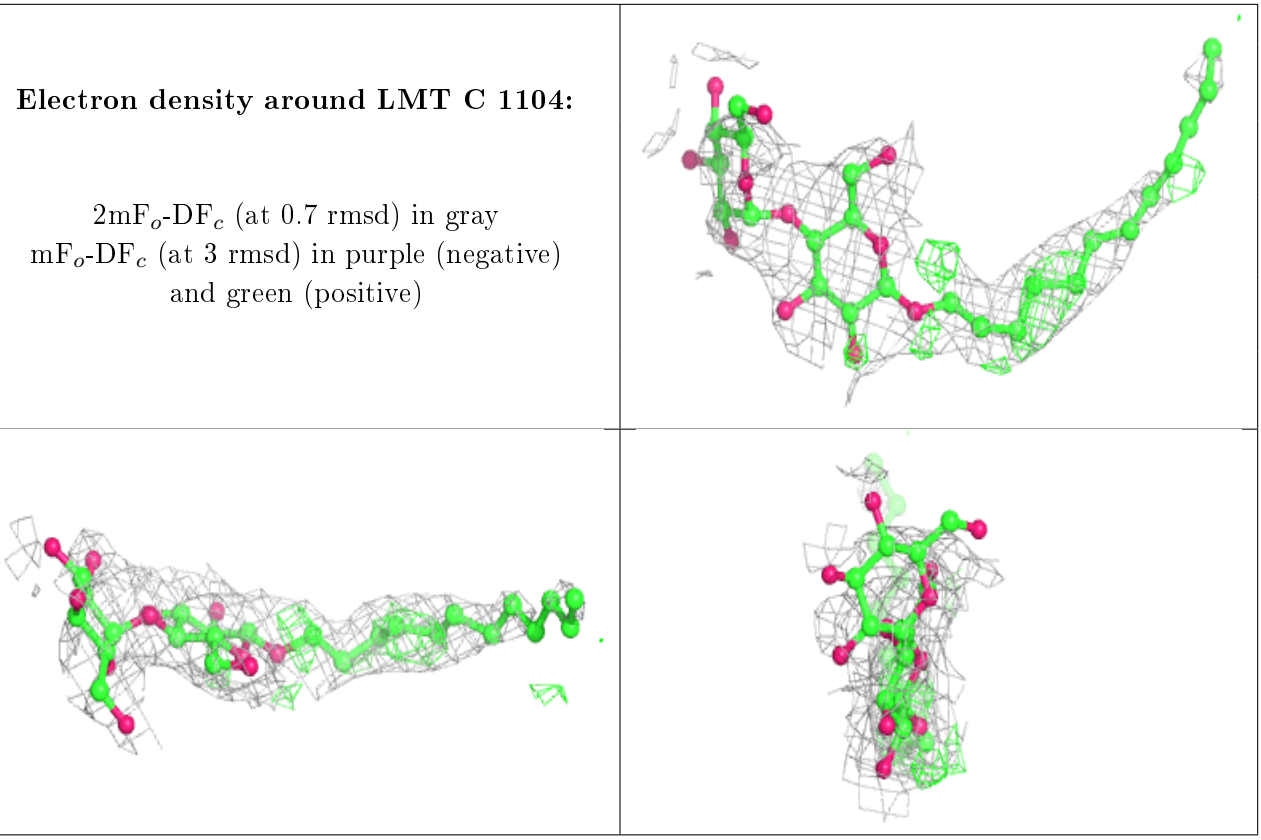
Electron density around PTY B 1107:

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



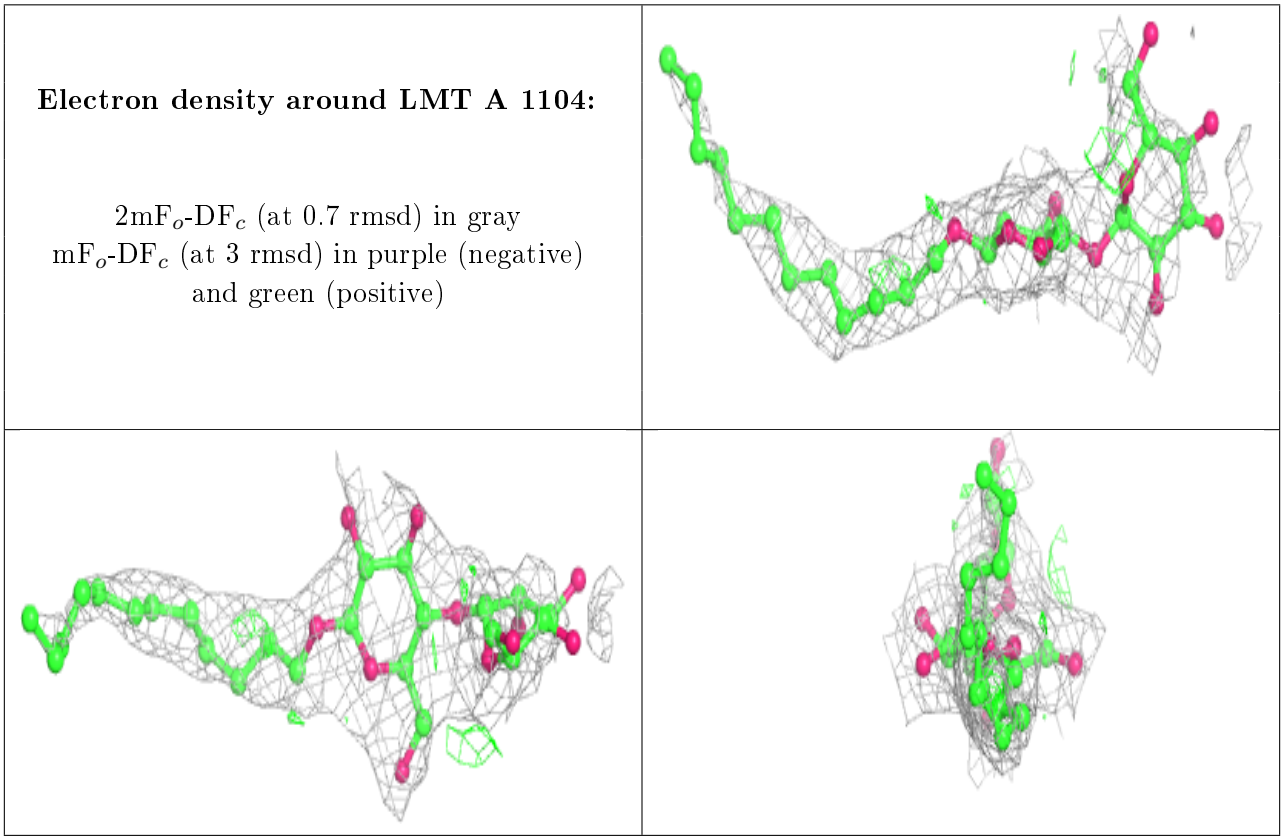
Electron density around LMT C 1104:

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



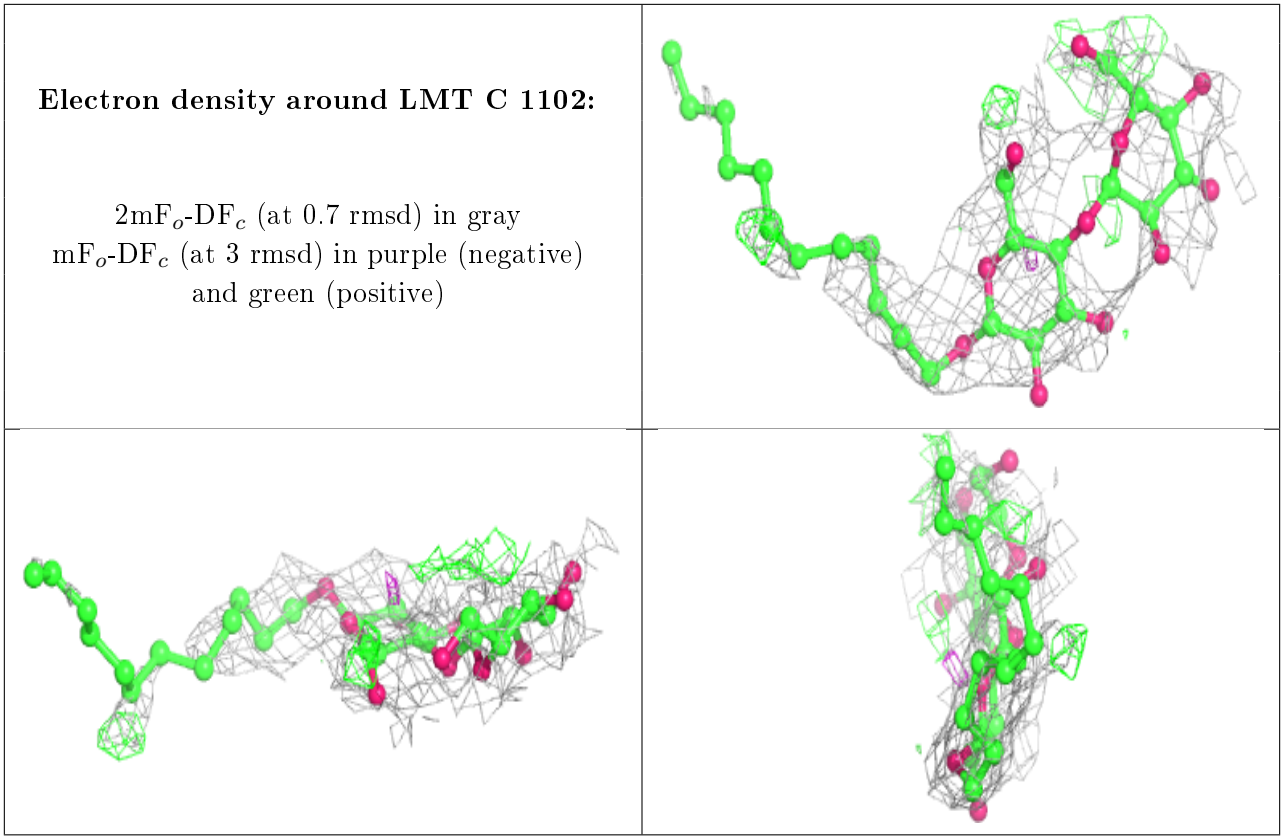
Electron density around LMT A 1104:

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



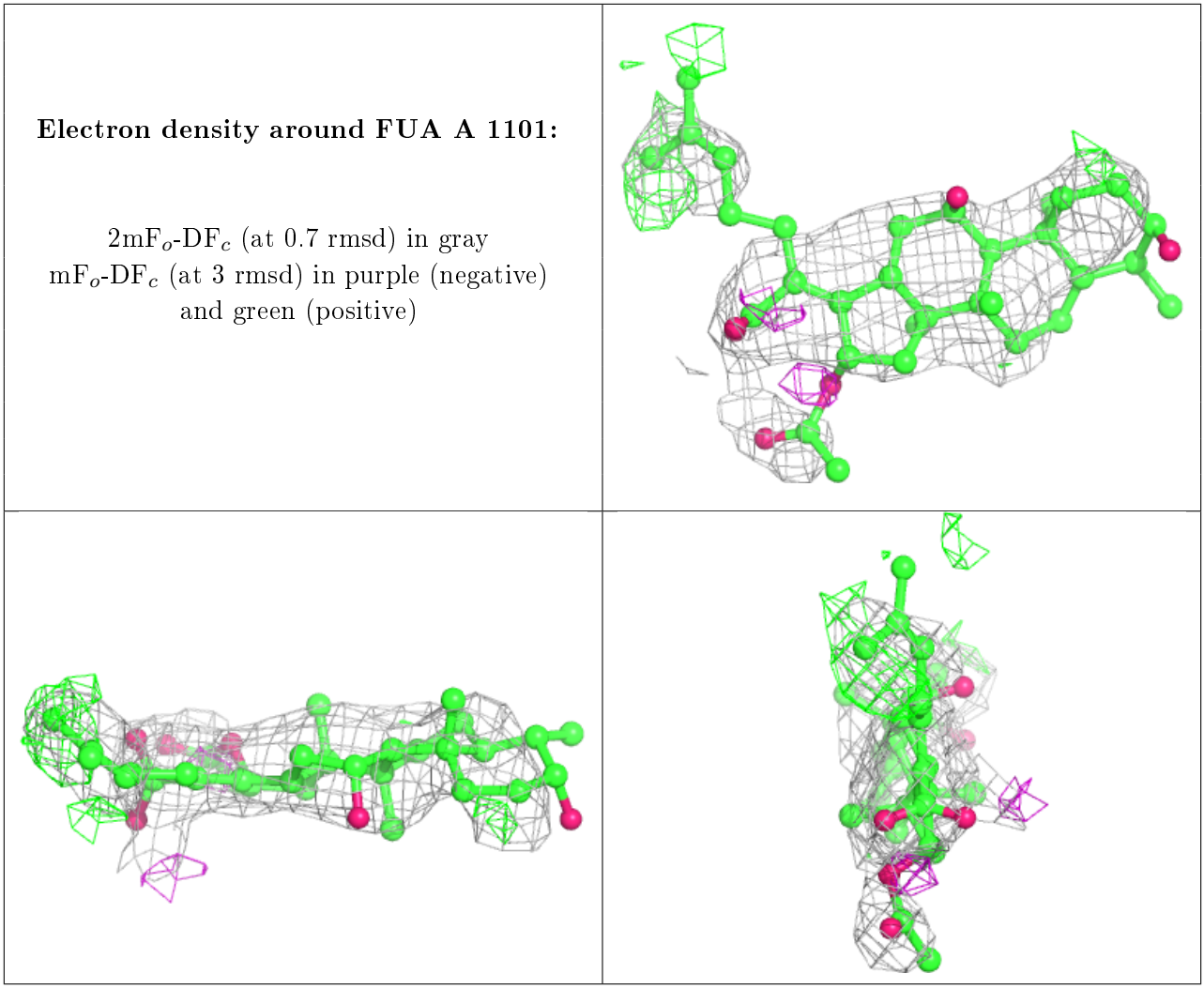
Electron density around LMT C 1102:

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



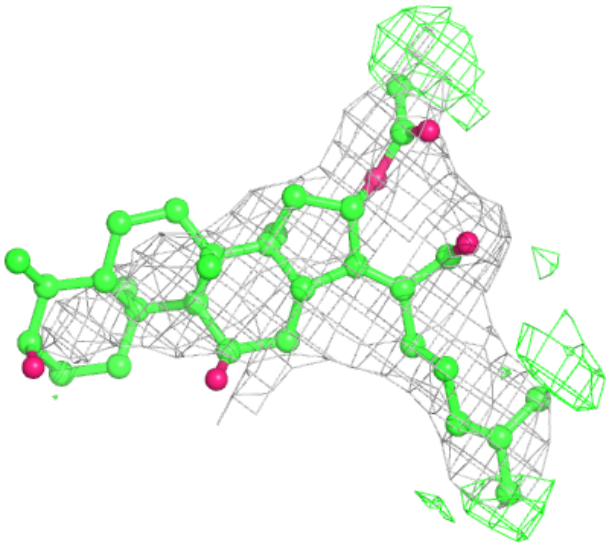
Electron density around FUA A 1101:

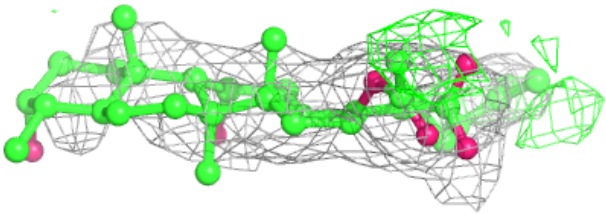
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

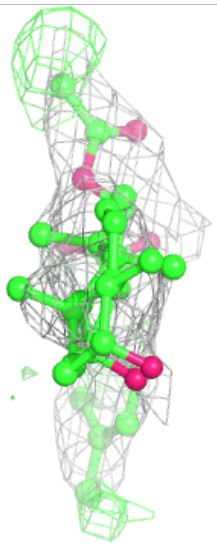


Electron density around FUA C 1101:

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

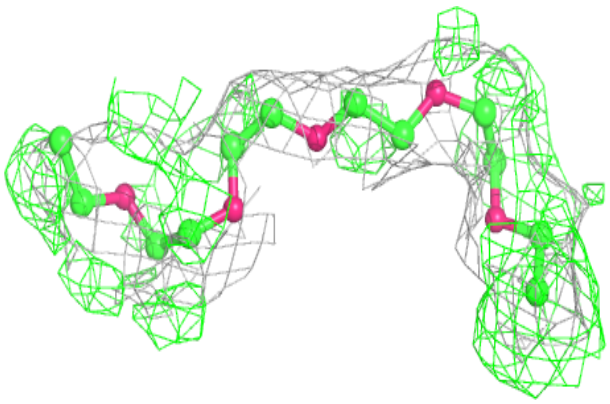


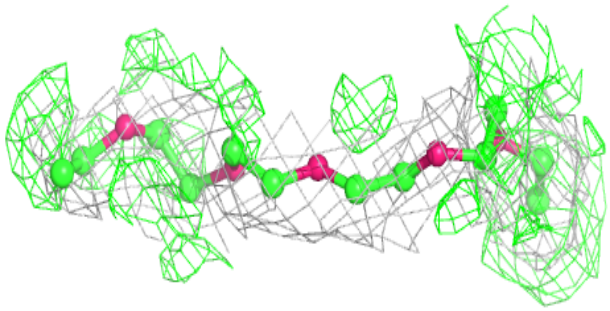


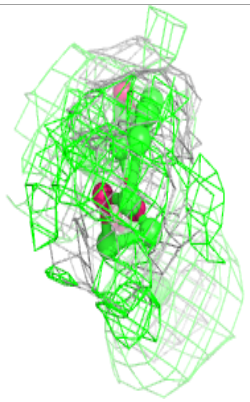


Electron density around P3G B 1110:

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

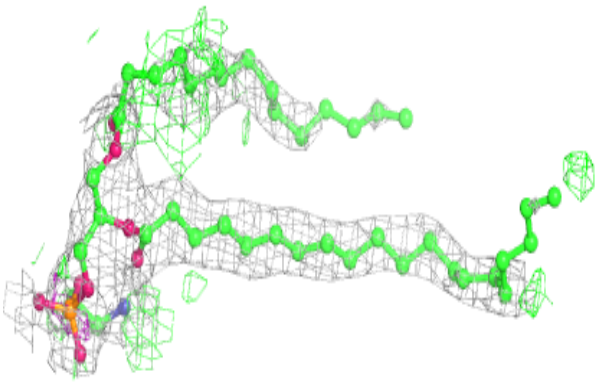


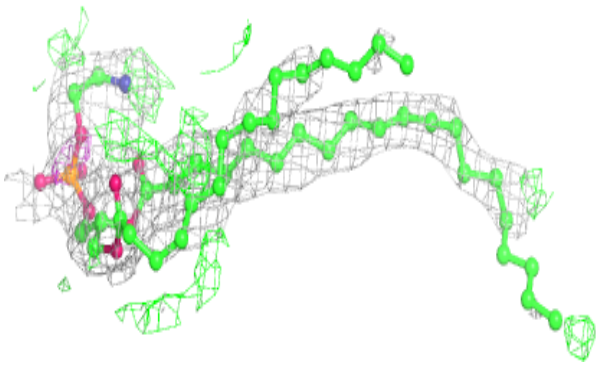


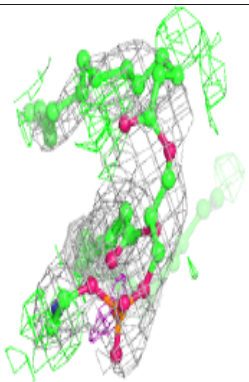


Electron density around PTY C 1109:

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

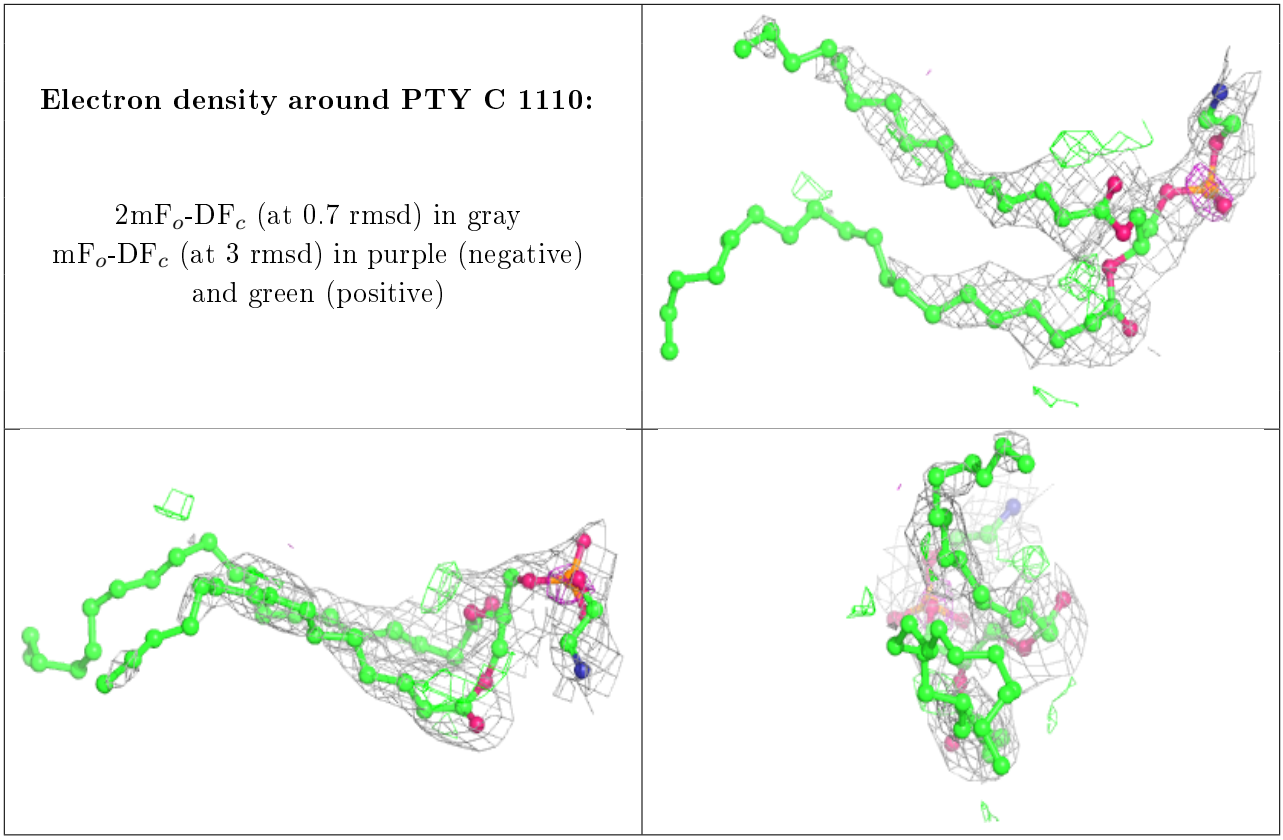






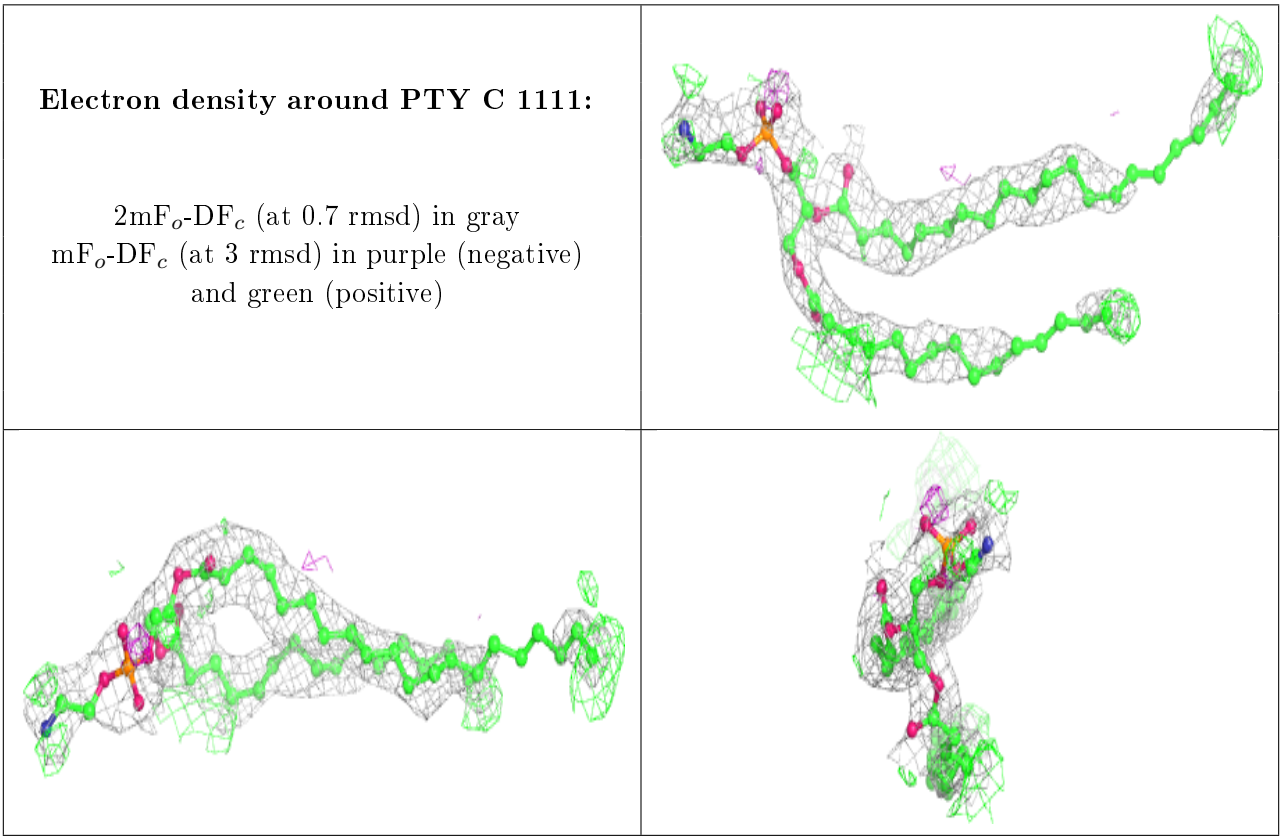
Electron density around PTY C 1110:

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



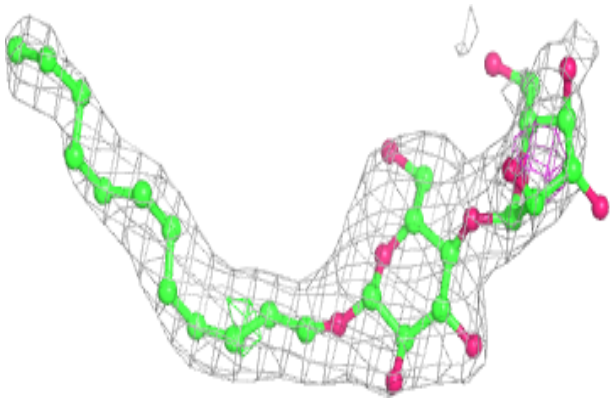
Electron density around PTY C 1111:

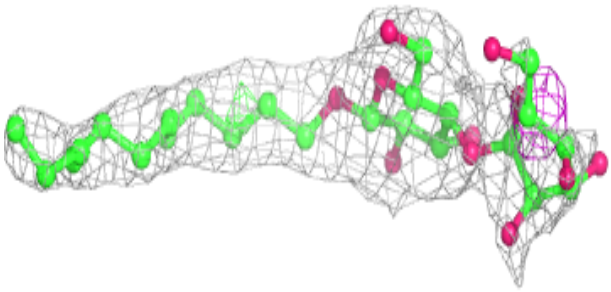
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

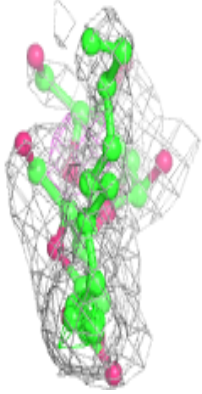


Electron density around LMT A 1103:

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

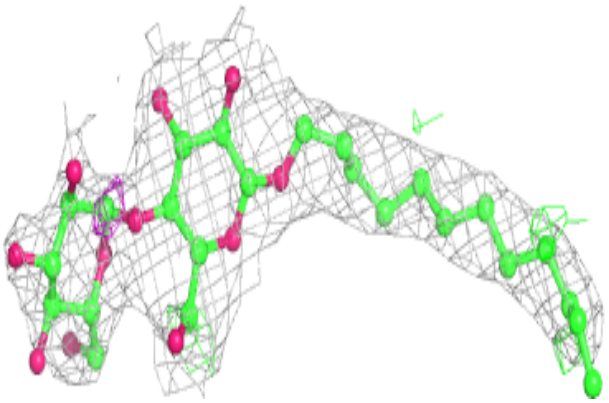


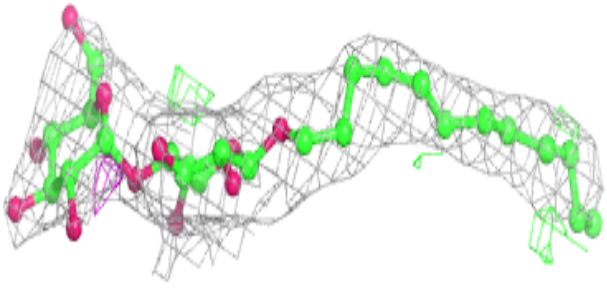


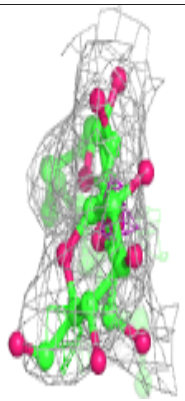


Electron density around LMT B 1104:

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

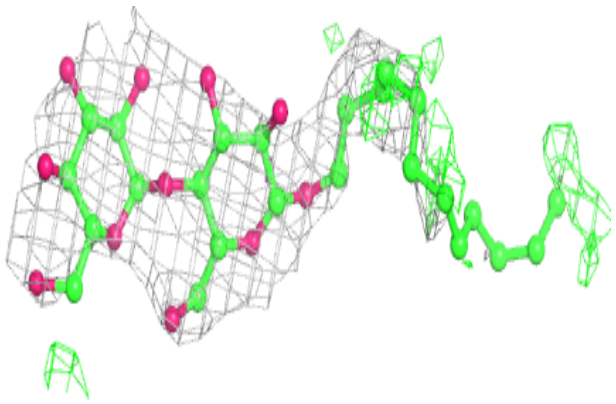


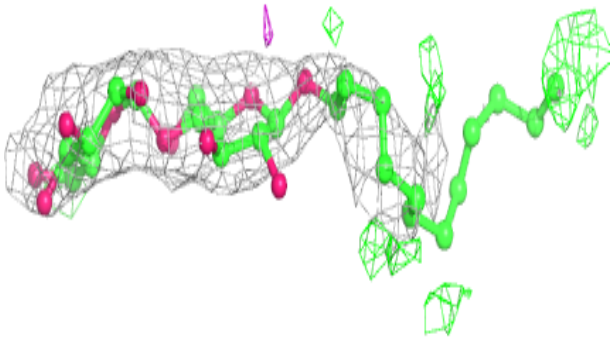


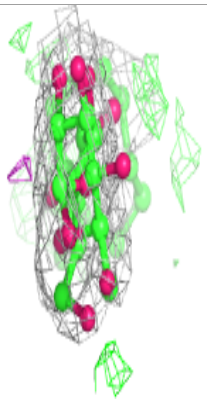


Electron density around LMT C 1105:

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

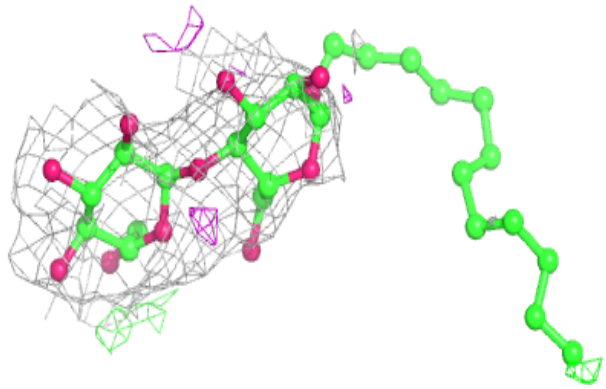


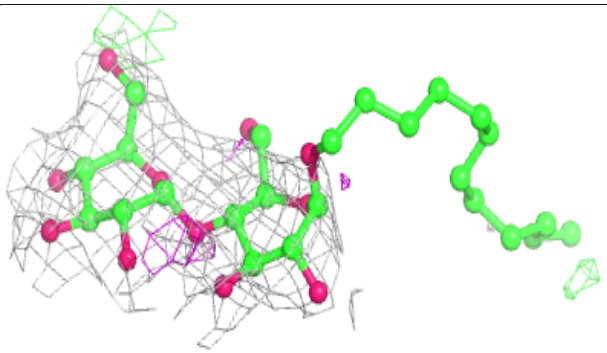


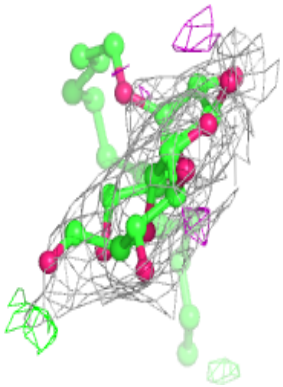


Electron density around LMT B 1103:

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

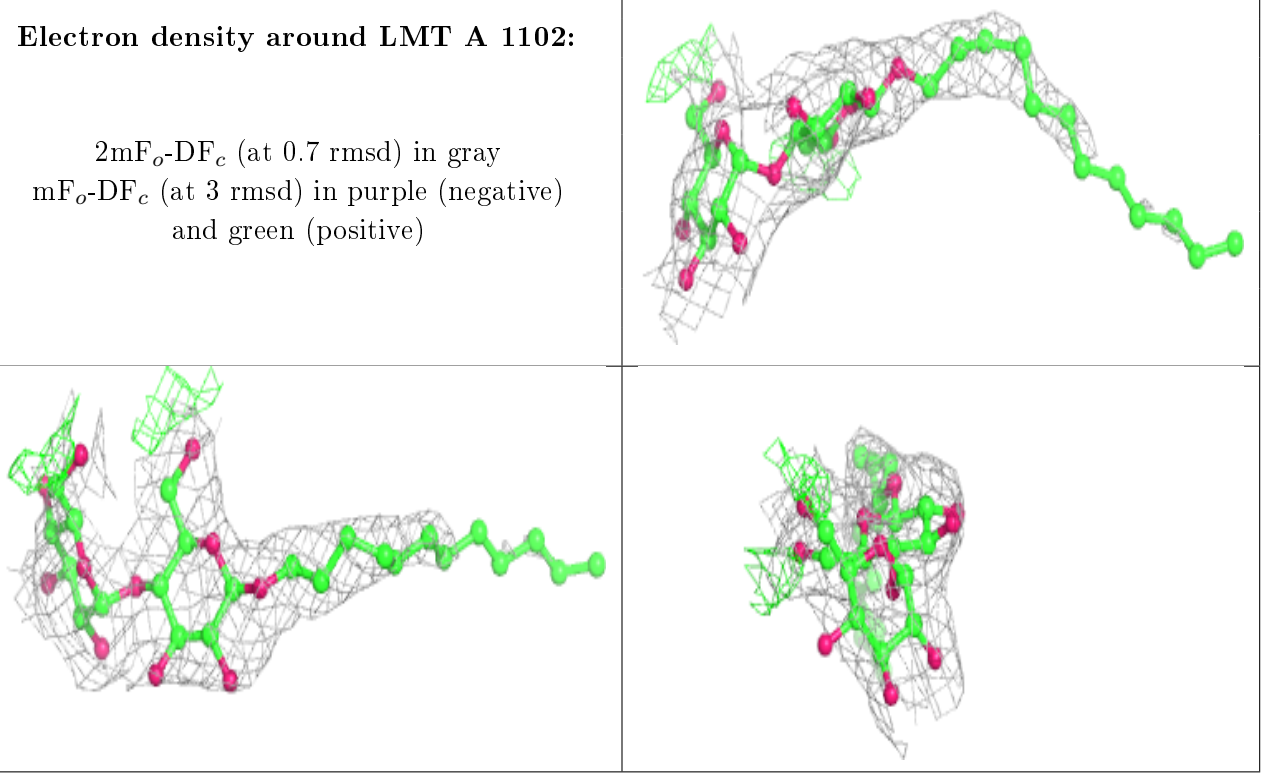






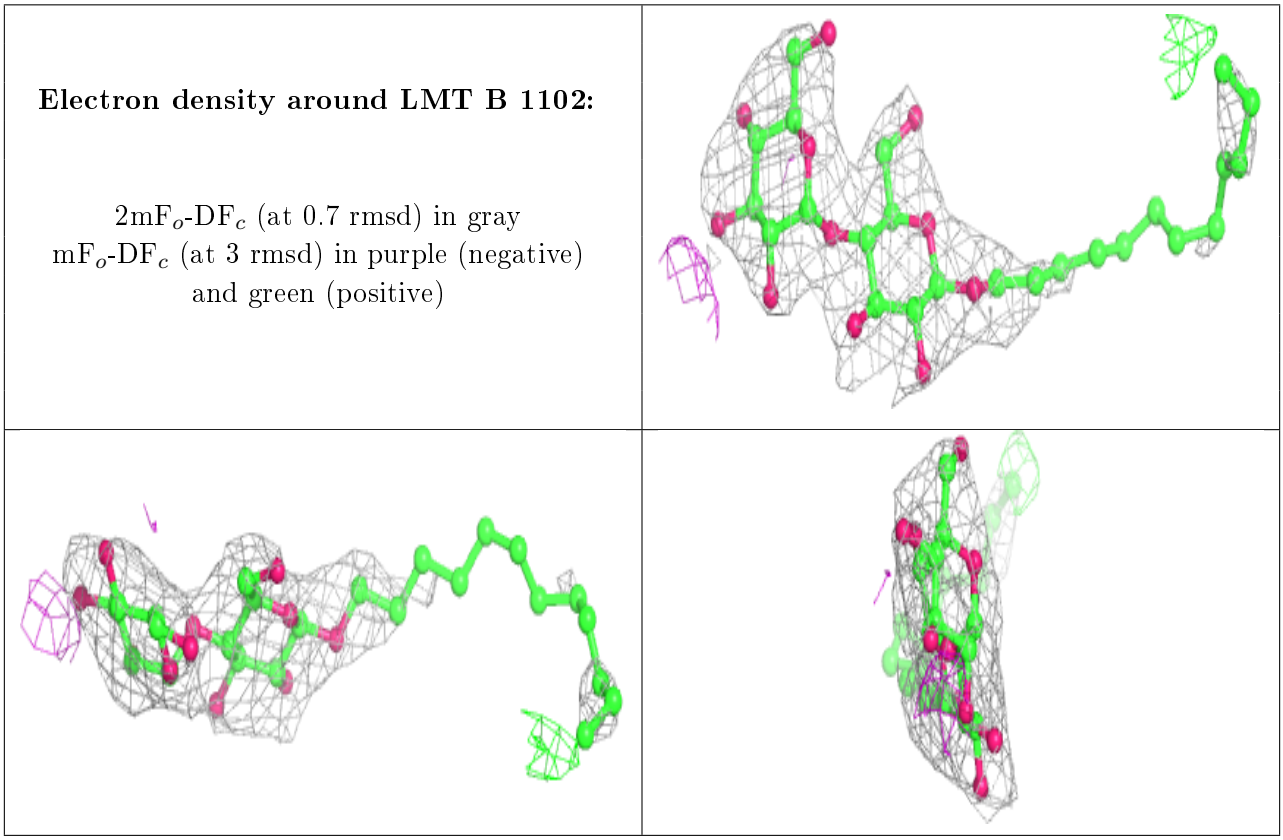
Electron density around LMT A 1102:

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



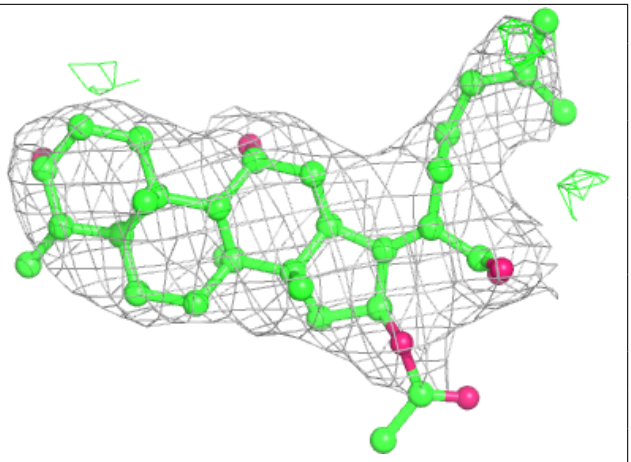
Electron density around LMT B 1102:

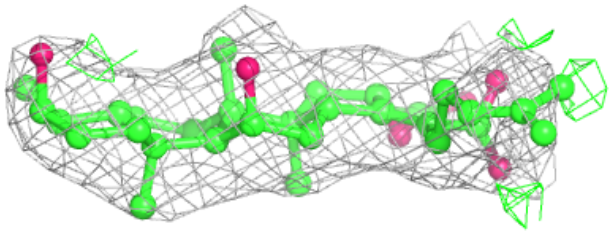
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

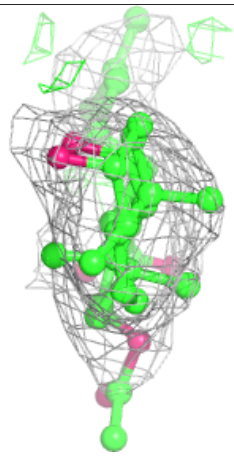


Electron density around FUA B 1101:

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

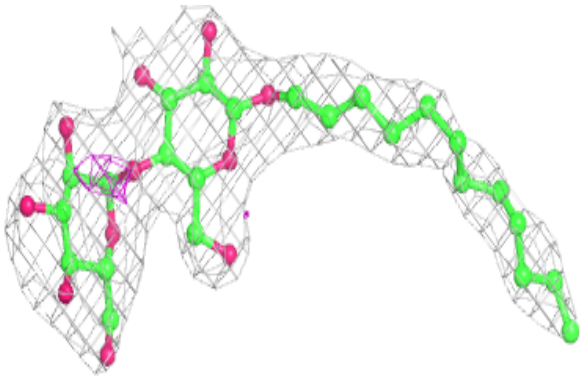


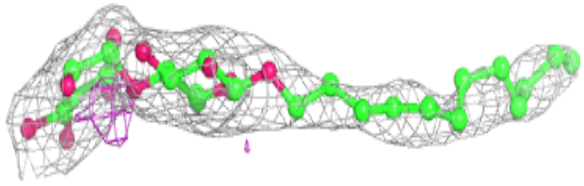


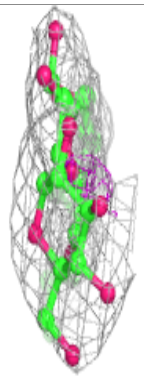


Electron density around LMT C 1103:

$2mF_o$-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.