



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:43 PM UTC

PDB ID : 5JMN / pdb_00005jmn
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 types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

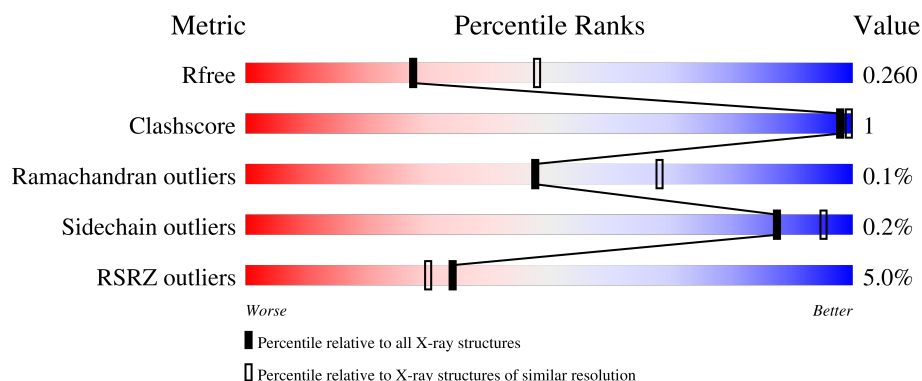
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1057	7% 95% ..
1	B	1057	6% 96% ..
1	C	1057	2% 96% ..
2	D	169	2% 93% 7%
2	E	169	6% 90% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	OCT	B	1109	-	-	-	X

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

Continued on next page...

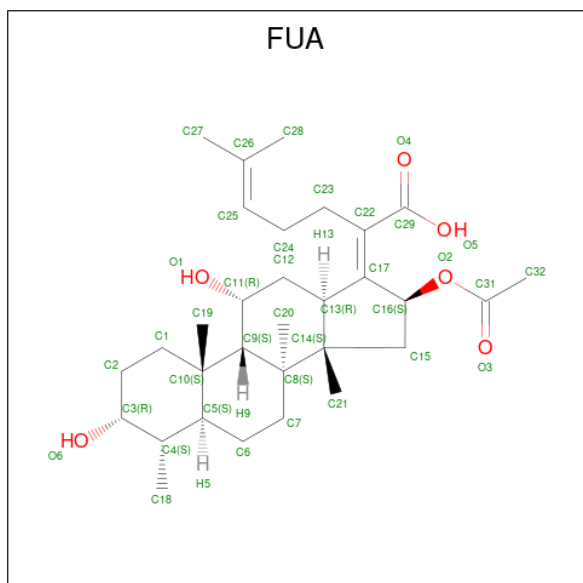
Continued from previous page...

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

- Molecule 2 is a protein called DARPin.

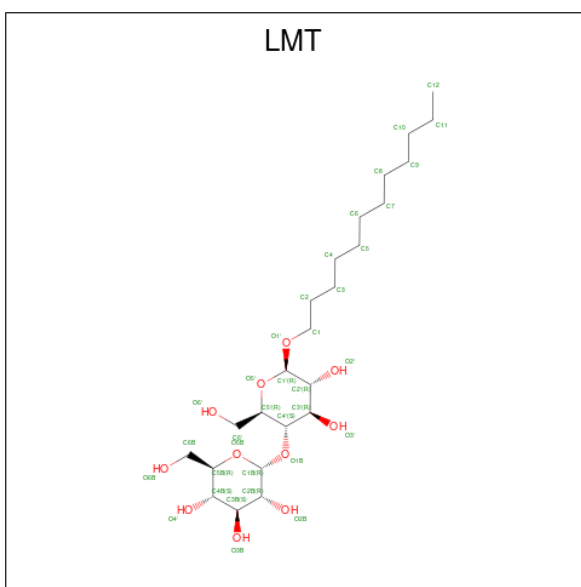
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	158	Total	C	N	O	S	0	0	0
			1194	753	209	231	1			
2	E	154	Total	C	N	O	S	0	1	0
			1173	740	204	228	1			

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



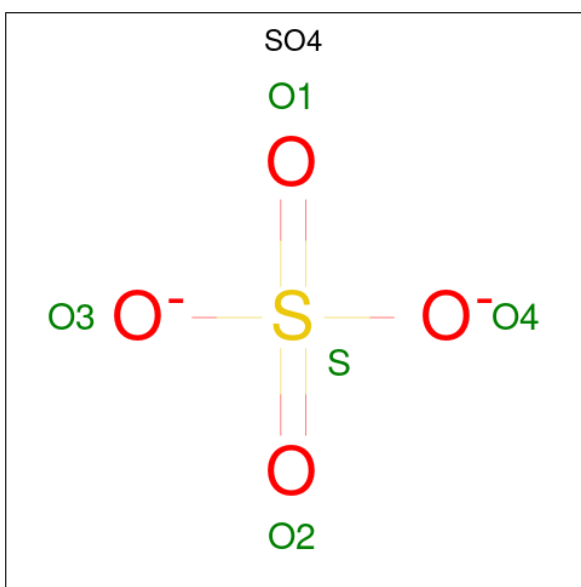
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			37	31	6		
3	B	1	Total	C	O	0	0
			37	31	6		
3	C	1	Total	C	O	0	0
			37	31	6		

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



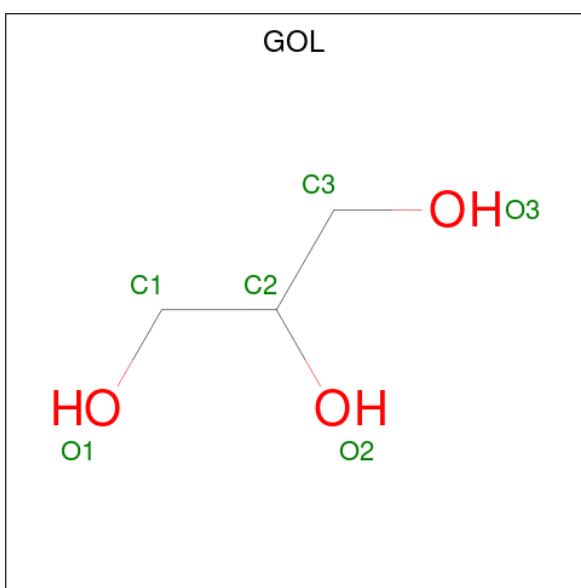
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 35	C 24	O 11	0	0
4	A	1	Total 35	C 24	O 11	0	0
4	A	1	Total 35	C 24	O 11	0	0
4	B	1	Total 35	C 24	O 11	0	0
4	B	1	Total 35	C 24	O 11	0	0
4	B	1	Total 35	C 24	O 11	0	0
4	C	1	Total 35	C 24	O 11	0	0
4	C	1	Total 35	C 24	O 11	0	0
4	C	1	Total 35	C 24	O 11	0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

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



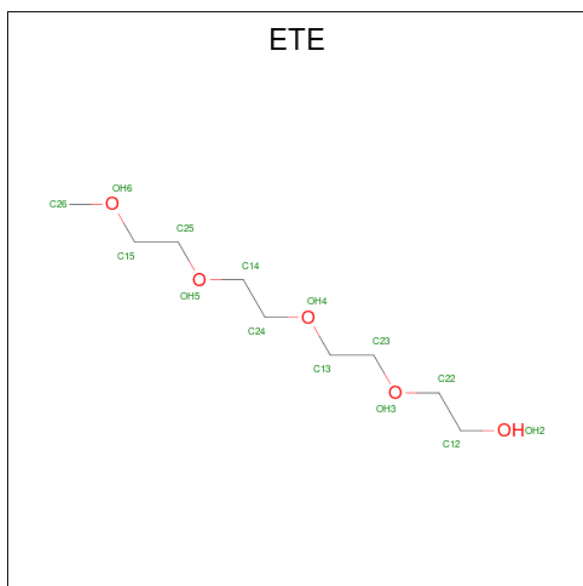
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

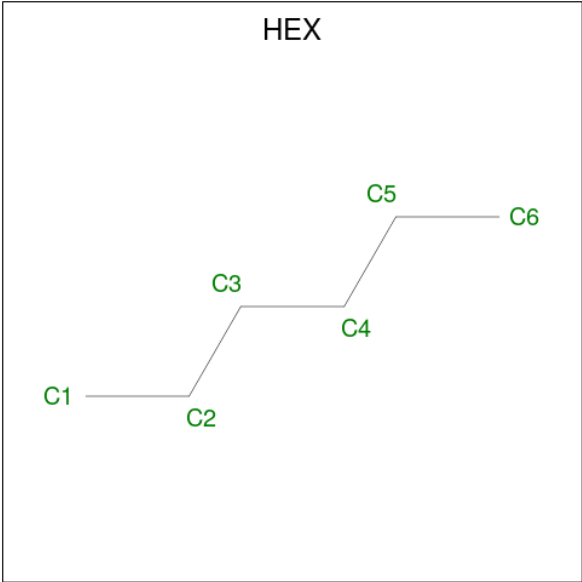
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		
6	E	1	Total	C	O	0	0
			6	3	3		
6	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is 2-{2-[2-2-(METHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (CCD ID: ETE) (formula: C₉H₂₀O₅).



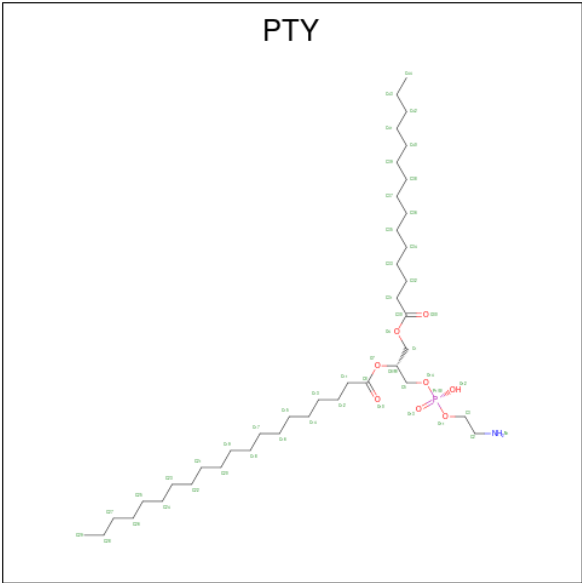
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			14	9	5		
7	A	1	Total	C	O	0	0
			14	9	5		
7	C	1	Total	C	O	0	0
			14	9	5		

- Molecule 8 is HEXANE (CCD ID: HEX) (formula: C₆H₁₄).



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

- Molecule 9 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: C₄₀H₈₀NO₈P).



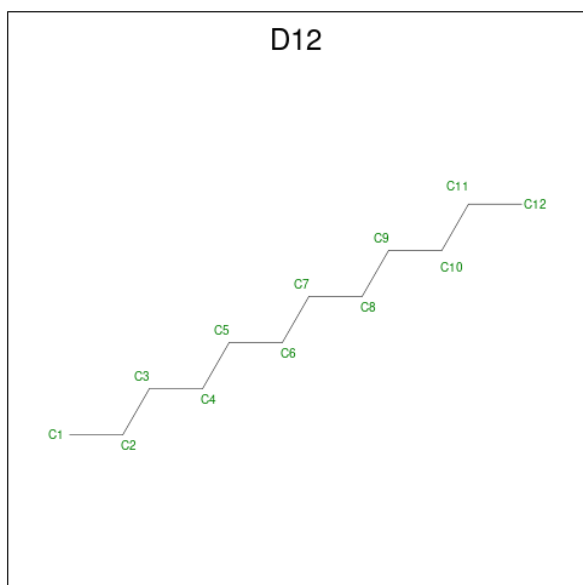
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	P	0	0
			50	40	1	8	1		
9	C	1	Total	C	N	O	P	0	0
			50	40	1	8	1		

Continued on next page...

Continued from previous page...

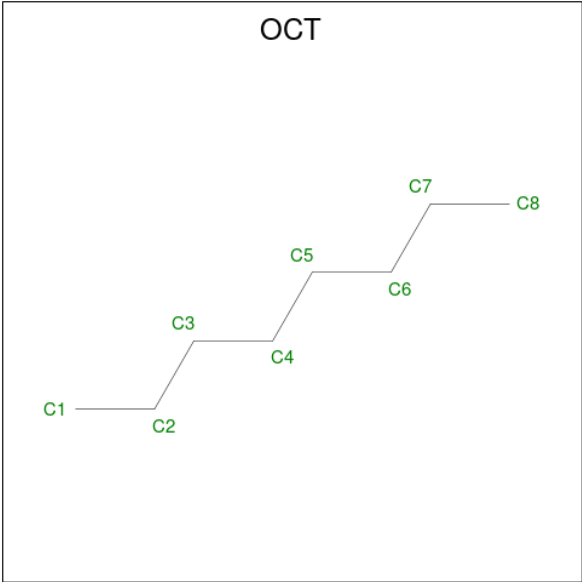
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	C	1	Total	C	N	O	P	0	0
			50	40	1	8	1		
9	C	1	Total	C	N	O	P	0	0
			50	40	1	8	1		

- Molecule 10 is DODECANE (CCD ID: D12) (formula: $C_{12}H_{26}$).



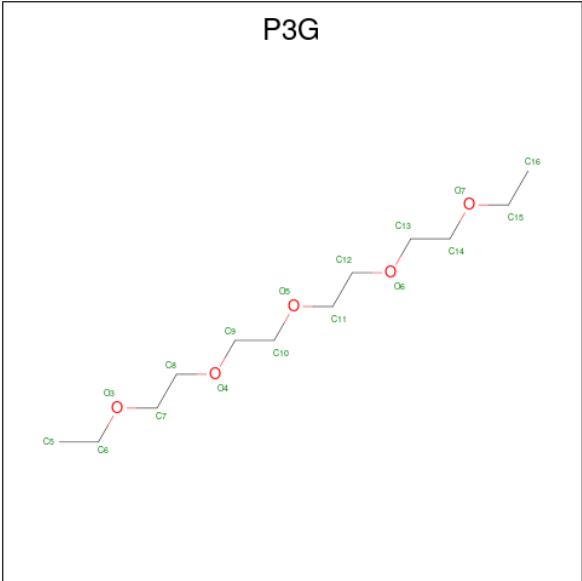
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	1	Total	C	0	0
			12	12		
10	C	1	Total	C	0	0
			12	12		
10	C	1	Total	C	0	0
			12	12		
10	C	1	Total	C	0	0
			12	12		

- Molecule 11 is N-OCTANE (CCD ID: OCT) (formula: C_8H_{18}).



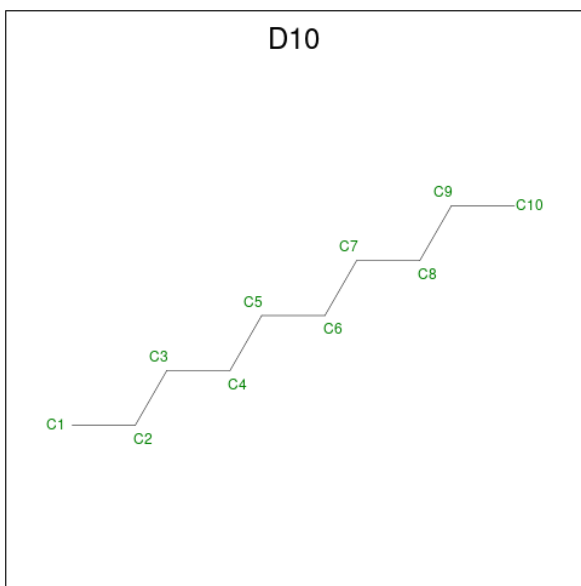
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	B	1	Total	C	0	0
			8	8		
11	C	1	Total	C	0	0
			8	8		

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



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

- Molecule 13 is DECANE (CCD ID: D10) (formula: $C_{10}H_{22}$).

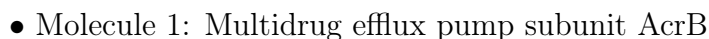
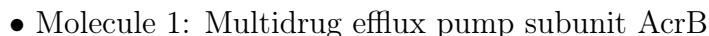


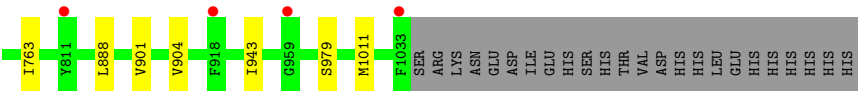
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	B	1	Total C 10 10	0	0
13	B	1	Total C 10 10	0	0

- Molecule 14 is water.

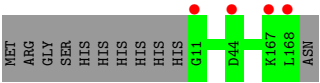
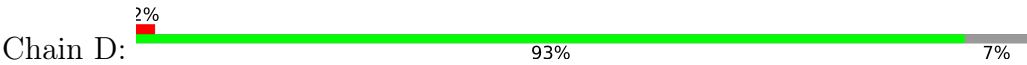
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	265	Total O 265 265	0	0
14	B	223	Total O 223 223	0	0
14	C	271	Total O 271 271	0	0
14	D	28	Total O 28 28	0	0
14	E	28	Total O 28 28	0	0

- Molecule 1: Multidrug efflux pump subunit AcrB

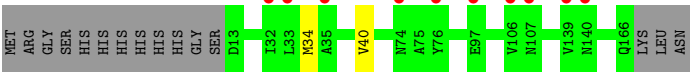
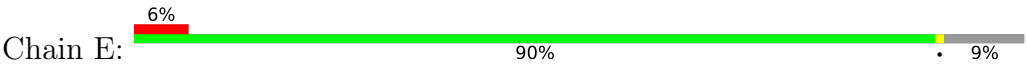




● Molecule 2: DARPin



● Molecule 2: DARPin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	145.65Å 163.25Å 246.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.15 – 2.50 49.15 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.15-2.50) 99.9 (49.15-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 , 34.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, FUA, SO4, P3G, OCT, ETE, D12, D10, LMT, PTY, HEX

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	0.55	0/8033	0.81	0/10907
1	B	0.55	1/8005 (0.0%)	0.82	0/10871
1	C	0.54	0/8008	0.80	0/10875
2	D	0.52	0/1213	0.78	0/1648
2	E	0.56	0/1195	0.79	0/1625
All	All	0.54	1/26454 (0.0%)	0.81	0/35926

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	905	VAL	CA-CB	5.19	1.56	1.54

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7874	0	8034	16	0
1	B	7855	0	8006	8	0
1	C	7855	0	8007	12	0
2	D	1194	0	1183	0	0
2	E	1173	0	1157	1	0

Continued on next page...

Continued from previous page...

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	36	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 (36) 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:A:456:MET:HE1	1:A:929:VAL:HG12	1.83	0.58
1:C:57:VAL:HG21	1:C:86:GLY:HA2	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:901:VAL:O	1:C:904:VAL:HG12	2.06	0.56
1:B:375:VAL:HG11	1:B:405:LEU:HD22	1.88	0.54
1:C:979:SER:HA	1:C:1011:MET:HE3	1.89	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:B:380:PHE:CE1	1:B:395:MET:HE1	2.50	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:A:987:MET:SD	1:A:1008:MET:HE1	2.56	0.45
1:C:572:PHE:HE2	1:C:631:LEU:HD21	1.83	0.44
1:A:56:THR:HG23	1:C:213:GLN:HG3	1.99	0.44
1:B:344:LEU:CD2	1:B:402:ILE:HD13	2.48	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

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1035/1057 (98%)	1011 (98%)	23 (2%)	1 (0%)	48	68
1	B	1032/1057 (98%)	1011 (98%)	20 (2%)	1 (0%)	48	68
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%)	48	68

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	843/863 (98%)	839 (100%)	4 (0%)	81	92
1	B	840/863 (97%)	838 (100%)	2 (0%)	87	95
1	C	840/863 (97%)	839 (100%)	1 (0%)	88	96
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%)	2758 (100%)	7 (0%)	87	94

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	630	SER
1	A	649[B]	MET
1	A	649[C]	MET
1	A	801	PHE
1	B	88	VAL
1	B	361	ASN
1	C	110	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	125	GLN
1	A	361	ASN
1	A	871	ASN
1	A	923	ASN
1	B	81	ASN
1	B	112	GLN
1	B	213	GLN
1	B	218	GLN
1	B	231	ASN
1	B	584	GLN
1	B	865	GLN
1	B	923	ASN
1	B	1001	ASN
1	C	151	GLN
1	C	231	ASN
1	C	361	ASN
1	C	577	GLN
1	C	584	GLN
1	C	604	ASN
1	C	605	ASN
1	C	642	ASN
2	D	69	ASN
2	D	92	HIS
2	D	155	ASN
2	E	122	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 oligosaccharides 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$
4	LMT	B	1102	-	36,36,36	0.51	1 (2%)	47,47,47	0.64	1 (2%)
11	OCT	C	1116	-	7,7,7	0.28	0	6,6,6	0.42	0
3	FUA	C	1101	-	39,40,40	1.12	1 (2%)	50,64,64	1.55	8 (16%)
5	SO4	C	1106	-	4,4,4	0.43	0	6,6,6	0.10	0
6	GOL	E	201	-	5,5,5	0.31	0	5,5,5	0.22	0
8	HEX	C	1117	-	5,5,5	0.26	0	4,4,4	0.31	0
4	LMT	A	1102	-	36,36,36	0.51	1 (2%)	47,47,47	0.67	0
4	LMT	B	1104	-	36,36,36	0.53	1 (2%)	47,47,47	0.96	1 (2%)
6	GOL	C	1108	-	5,5,5	0.37	0	5,5,5	0.24	0
6	GOL	B	1105	-	5,5,5	0.34	0	5,5,5	0.31	0
12	P3G	B	1110	-	16,16,16	0.52	0	15,15,15	0.24	0
13	D10	B	1111	-	9,9,9	0.28	0	8,8,8	0.45	0
5	SO4	A	1105	-	4,4,4	0.42	0	6,6,6	0.19	0
4	LMT	A	1104	-	36,36,36	0.50	0	47,47,47	0.68	0
9	PTY	B	1107	-	49,49,49	0.98	2 (4%)	52,54,54	0.92	2 (3%)
11	OCT	B	1109	-	7,7,7	0.26	0	6,6,6	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GOL	B	1106	-	5,5,5	0.36	0	5,5,5	0.26	0
4	LMT	C	1105	-	36,36,36	0.58	1 (2%)	47,47,47	0.91	1 (2%)
6	GOL	A	1106	-	5,5,5	0.36	0	5,5,5	0.27	0
7	ETE	A	1107	-	13,13,13	0.51	0	12,12,12	0.14	0
10	D12	B	1108	-	11,11,11	0.30	0	10,10,10	0.42	0
10	D12	C	1114	-	11,11,11	0.26	0	10,10,10	0.50	0
4	LMT	C	1104	-	36,36,36	0.50	0	47,47,47	0.61	0
9	PTY	C	1111	-	49,49,49	1.00	2 (4%)	52,54,54	0.93	3 (5%)
3	FUA	B	1101	-	39,40,40	1.05	1 (2%)	50,64,64	1.48	6 (12%)
6	GOL	C	1107	-	5,5,5	0.26	0	5,5,5	0.15	0
9	PTY	C	1109	-	49,49,49	1.00	2 (4%)	52,54,54	0.96	2 (3%)
10	D12	C	1112	-	11,11,11	0.29	0	10,10,10	0.42	0
4	LMT	C	1102	-	36,36,36	0.52	1 (2%)	47,47,47	0.67	0
4	LMT	C	1103	-	36,36,36	0.50	1 (2%)	47,47,47	0.63	0
13	D10	B	1112	-	9,9,9	0.29	0	8,8,8	0.40	0
6	GOL	E	202	-	5,5,5	0.25	0	5,5,5	0.28	0
7	ETE	C	1115	-	13,13,13	0.52	0	12,12,12	0.22	0
3	FUA	A	1101	-	39,40,40	1.07	1 (2%)	50,64,64	1.52	8 (16%)
4	LMT	B	1103	-	36,36,36	0.58	1 (2%)	47,47,47	0.82	0
6	GOL	D	201	-	5,5,5	0.35	0	5,5,5	0.25	0
9	PTY	C	1110	-	49,49,49	0.96	2 (4%)	52,54,54	0.97	2 (3%)
10	D12	C	1113	-	11,11,11	0.29	0	10,10,10	0.41	0
7	ETE	A	1108	-	13,13,13	0.53	0	12,12,12	0.18	0
8	HEX	A	1109	-	5,5,5	0.28	0	4,4,4	0.27	0
4	LMT	A	1103	-	36,36,36	0.51	0	47,47,47	0.87	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
4	LMT	B	1102	-	-	5/21/61/61	0/2/2/2
11	OCT	C	1116	-	-	1/5/5/5	-
3	FUA	C	1101	-	-	4/16/92/92	0/4/4/4
6	GOL	E	201	-	-	2/4/4/4	-
8	HEX	C	1117	-	-	0/3/3/3	-
4	LMT	A	1102	-	-	6/21/61/61	0/2/2/2
4	LMT	B	1104	-	-	8/21/61/61	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	C	1108	-	-	2/4/4/4	-
6	GOL	B	1105	-	-	1/4/4/4	-
12	P3G	B	1110	-	-	4/14/14/14	-
13	D10	B	1111	-	-	1/7/7/7	-
4	LMT	A	1104	-	-	8/21/61/61	0/2/2/2
9	PTY	B	1107	-	-	21/53/53/53	-
11	OCT	B	1109	-	-	2/5/5/5	-
6	GOL	B	1106	-	-	0/4/4/4	-
4	LMT	C	1105	-	-	11/21/61/61	0/2/2/2
6	GOL	A	1106	-	-	2/4/4/4	-
7	ETE	A	1107	-	-	4/11/11/11	-
10	D12	B	1108	-	-	2/9/9/9	-
10	D12	C	1114	-	-	2/9/9/9	-
4	LMT	C	1104	-	-	2/21/61/61	0/2/2/2
9	PTY	C	1111	-	-	24/53/53/53	-
3	FUA	B	1101	-	-	4/16/92/92	0/4/4/4
6	GOL	C	1107	-	-	2/4/4/4	-
9	PTY	C	1109	-	-	17/53/53/53	-
10	D12	C	1112	-	-	3/9/9/9	-
4	LMT	C	1102	-	-	12/21/61/61	0/2/2/2
4	LMT	C	1103	-	-	10/21/61/61	0/2/2/2
13	D10	B	1112	-	-	2/7/7/7	-
6	GOL	E	202	-	-	0/4/4/4	-
7	ETE	C	1115	-	-	6/11/11/11	-
3	FUA	A	1101	-	-	8/16/92/92	0/4/4/4
4	LMT	B	1103	-	-	10/21/61/61	0/2/2/2
6	GOL	D	201	-	-	2/4/4/4	-
9	PTY	C	1110	-	-	31/53/53/53	-
10	D12	C	1113	-	-	3/9/9/9	-
7	ETE	A	1108	-	-	6/11/11/11	-
8	HEX	A	1109	-	-	1/3/3/3	-
4	LMT	A	1103	-	-	9/21/61/61	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	5.18	1.46	1.35
3	B	1101	FUA	O2-C31	5.09	1.46	1.35
3	A	1101	FUA	O2-C31	5.08	1.46	1.35
9	C	1111	PTY	O4-C30	4.66	1.46	1.33
9	C	1109	PTY	O7-C8	4.50	1.47	1.34
9	B	1107	PTY	O4-C30	4.43	1.46	1.33
9	C	1109	PTY	O4-C30	4.42	1.46	1.33
9	B	1107	PTY	O7-C8	4.40	1.46	1.34
9	C	1110	PTY	O4-C30	4.33	1.46	1.33
9	C	1110	PTY	O7-C8	4.21	1.46	1.34
9	C	1111	PTY	O7-C8	4.19	1.46	1.34
4	B	1103	LMT	O1'-C1'	2.39	1.44	1.40
4	C	1105	LMT	O1'-C1'	2.36	1.44	1.40
4	C	1102	LMT	O1'-C1'	2.15	1.43	1.40
4	A	1102	LMT	O1'-C1'	2.10	1.43	1.40
4	B	1104	LMT	O1'-C1'	2.07	1.43	1.40
4	B	1102	LMT	O1'-C1'	2.07	1.43	1.40
4	C	1103	LMT	O1'-C1'	2.06	1.43	1.40

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1101	FUA	O2-C31-C32	5.05	120.10	111.09
3	A	1101	FUA	O2-C31-C32	4.85	119.73	111.09
3	C	1101	FUA	O2-C31-C32	4.32	118.80	111.09
9	C	1110	PTY	O7-C8-C11	4.17	120.50	111.48
9	C	1109	PTY	O7-C8-C11	4.02	120.17	111.48
9	C	1111	PTY	O7-C8-C11	3.85	119.81	111.48
9	B	1107	PTY	O7-C8-C11	3.66	119.41	111.48
3	B	1101	FUA	C19-C10-C9	-3.49	104.55	113.19
3	A	1101	FUA	C1-C10-C9	3.21	116.38	109.16
3	A	1101	FUA	C1-C2-C3	3.17	117.54	111.59
3	A	1101	FUA	C19-C10-C9	-3.15	105.39	113.19
3	C	1101	FUA	C19-C10-C9	-3.13	105.43	113.19
3	C	1101	FUA	C7-C8-C14	3.08	113.44	110.78
9	C	1109	PTY	O4-C30-C31	2.76	120.24	111.83
9	B	1107	PTY	O4-C30-C31	2.75	120.21	111.83
9	C	1110	PTY	O4-C30-C31	2.75	120.21	111.83
3	C	1101	FUA	C20-C8-C7	-2.69	103.41	107.83
9	C	1111	PTY	O4-C30-C31	2.59	119.74	111.83
3	B	1101	FUA	O2-C31-O3	-2.56	118.05	122.99
4	C	1105	LMT	C1'-C2'-C3'	2.56	115.39	110.01
3	B	1101	FUA	C5-C10-C9	2.56	114.20	108.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	1111	PTY	O7-C8-O10	-2.49	117.87	123.70
3	C	1101	FUA	C13-C12-C11	2.47	115.48	111.90
4	B	1104	LMT	O1'-C1'-C2'	2.45	112.00	108.27
3	A	1101	FUA	O2-C31-O3	-2.45	118.27	122.99
3	C	1101	FUA	C1-C10-C9	2.32	114.36	109.16
3	C	1101	FUA	C6-C5-C4	-2.24	110.78	114.27
3	B	1101	FUA	C1-C10-C9	2.24	114.19	109.16
3	A	1101	FUA	C28-C26-C27	2.12	119.47	114.59
3	C	1101	FUA	C5-C10-C9	2.11	113.14	108.19
3	A	1101	FUA	C7-C6-C5	-2.10	109.56	113.14
4	B	1102	LMT	O5'-C5'-C6'	2.07	111.58	106.44
4	A	1103	LMT	C1-O1'-C1'	2.07	117.21	113.68
3	A	1101	FUA	C20-C8-C7	-2.06	104.45	107.83
3	B	1101	FUA	C7-C8-C14	2.01	112.52	110.78

There are no chirality outliers.

All (238) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1101	FUA	C23-C22-C29-O4
3	A	1101	FUA	C23-C22-C29-O5
3	A	1101	FUA	C32-C31-O2-C16
3	A	1101	FUA	O3-C31-O2-C16
3	B	1101	FUA	C23-C22-C29-O4
3	B	1101	FUA	C23-C22-C29-O5
3	B	1101	FUA	C32-C31-O2-C16
3	C	1101	FUA	C23-C22-C29-O4
3	C	1101	FUA	C23-C22-C29-O5
4	A	1104	LMT	C2-C1-O1'-C1'
4	B	1103	LMT	O5'-C1'-O1'-C1
4	B	1103	LMT	C2-C1-O1'-C1'
4	B	1104	LMT	O5'-C1'-O1'-C1
4	C	1105	LMT	O5'-C1'-O1'-C1
4	C	1105	LMT	C2-C1-O1'-C1'
9	B	1107	PTY	N1-C2-C3-O11
9	C	1110	PTY	C11-C8-O7-C6
9	C	1110	PTY	C3-O11-P1-O13
9	C	1110	PTY	C3-O11-P1-O14
9	C	1111	PTY	C11-C8-O7-C6
9	C	1111	PTY	C3-O11-P1-O12
9	C	1111	PTY	C3-O11-P1-O14
9	C	1111	PTY	C5-O14-P1-O11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	C	1111	PTY	C5-O14-P1-O12
9	C	1111	PTY	C5-O14-P1-O13
3	B	1101	FUA	O3-C31-O2-C16
3	C	1101	FUA	C32-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'
9	C	1110	PTY	C31-C30-O4-C1
4	C	1102	LMT	O5'-C5'-C6'-O6'
4	B	1102	LMT	O5'-C5'-C6'-O6'
4	B	1103	LMT	C4'-C5'-C6'-O6'
4	C	1105	LMT	O5'-C5'-C6'-O6'
12	B	1110	P3G	O5-C10-C9-O4
9	C	1110	PTY	O30-C30-O4-C1
4	A	1103	LMT	O5'-C1'-O1'-C1
4	B	1104	LMT	O5'-C5'-C6'-O6'
9	C	1109	PTY	C11-C8-O7-C6
3	C	1101	FUA	O3-C31-O2-C16
4	C	1103	LMT	C4'-C5'-C6'-O6'
4	B	1104	LMT	C4'-C5'-C6'-O6'
4	A	1103	LMT	C2'-C1'-O1'-C1
4	B	1103	LMT	C2'-C1'-O1'-C1
4	B	1102	LMT	C4'-C5'-C6'-O6'
9	B	1107	PTY	O14-C5-C6-O7
7	A	1107	ETE	OH6-C15-C25-OH5
7	A	1107	ETE	OH5-C14-C24-OH4
9	B	1107	PTY	C31-C30-O4-C1
7	A	1108	ETE	OH4-C13-C23-OH3
4	C	1102	LMT	C4'-C5'-C6'-O6'
7	A	1107	ETE	OH4-C13-C23-OH3
9	B	1107	PTY	C30-C31-C32-C33
9	C	1109	PTY	O10-C8-O7-C6
7	A	1108	ETE	OH5-C14-C24-OH4
7	C	1115	ETE	OH6-C15-C25-OH5
9	C	1109	PTY	C30-C31-C32-C33
4	C	1102	LMT	O5B-C1B-O1B-C4'
9	B	1107	PTY	O30-C30-O4-C1
4	C	1102	LMT	C2B-C1B-O1B-C4'
7	A	1108	ETE	OH6-C15-C25-OH5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	C	1102	LMT	C2'-C1'-O1'-C1
4	C	1105	LMT	C2'-C1'-O1'-C1
6	A	1106	GOL	O1-C1-C2-C3
6	C	1107	GOL	O1-C1-C2-C3
6	C	1108	GOL	O1-C1-C2-C3
6	D	201	GOL	O1-C1-C2-C3
6	E	201	GOL	O1-C1-C2-C3
7	C	1115	ETE	OH4-C13-C23-OH3
4	C	1102	LMT	O5'-C1'-O1'-C1
4	B	1103	LMT	O5B-C5B-C6B-O6B
4	B	1103	LMT	C3-C4-C5-C6
4	C	1105	LMT	C5-C6-C7-C8
4	B	1103	LMT	O1'-C1-C2-C3
9	C	1110	PTY	C25-C26-C27-C28
6	C	1108	GOL	O1-C1-C2-O2
6	E	201	GOL	O1-C1-C2-O2
4	A	1102	LMT	C4B-C5B-C6B-O6B
13	B	1112	D10	C6-C7-C8-C9
10	B	1108	D12	C7-C8-C9-C10
4	C	1105	LMT	C4'-C5'-C6'-O6'
12	B	1110	P3G	O3-C7-C8-O4
4	C	1103	LMT	C7-C8-C9-C10
4	B	1104	LMT	C11-C10-C9-C8
9	C	1109	PTY	C24-C25-C26-C27
9	C	1109	PTY	C31-C30-O4-C1
4	A	1103	LMT	C2-C3-C4-C5
9	B	1107	PTY	C20-C21-C22-C23
9	C	1111	PTY	C36-C37-C38-C39
9	B	1107	PTY	C34-C35-C36-C37
4	A	1102	LMT	O1'-C1-C2-C3
4	B	1102	LMT	C7-C8-C9-C10
4	A	1102	LMT	C1-C2-C3-C4
13	B	1112	D10	C4-C5-C6-C7
3	A	1101	FUA	C29-C22-C23-C24
4	A	1104	LMT	O5B-C5B-C6B-O6B
9	C	1111	PTY	C12-C13-C14-C15
9	B	1107	PTY	C11-C8-O7-C6
9	C	1109	PTY	O30-C30-O4-C1
9	B	1107	PTY	O10-C8-O7-C6
4	A	1104	LMT	C7-C8-C9-C10
4	A	1103	LMT	C4B-C5B-C6B-O6B
9	C	1109	PTY	C20-C21-C22-C23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	C	1110	PTY	C15-C16-C17-C18
9	B	1107	PTY	C11-C12-C13-C14
9	C	1109	PTY	C36-C37-C38-C39
4	B	1103	LMT	C7-C8-C9-C10
9	B	1107	PTY	C37-C38-C39-C40
9	B	1107	PTY	C15-C16-C17-C18
10	C	1112	D12	C3-C4-C5-C6
9	C	1109	PTY	C35-C36-C37-C38
4	A	1103	LMT	C3-C4-C5-C6
9	C	1111	PTY	C35-C36-C37-C38
9	B	1107	PTY	C24-C25-C26-C27
10	C	1113	D12	C3-C4-C5-C6
6	A	1106	GOL	O1-C1-C2-O2
4	C	1105	LMT	C2-C3-C4-C5
9	B	1107	PTY	O14-C5-C6-C1
9	C	1110	PTY	C18-C19-C20-C21
4	A	1102	LMT	C3-C4-C5-C6
9	C	1110	PTY	C22-C23-C24-C25
4	C	1103	LMT	O5B-C5B-C6B-O6B
3	A	1101	FUA	C17-C22-C23-C24
9	C	1109	PTY	C21-C22-C23-C24
10	B	1108	D12	C5-C6-C7-C8
4	C	1104	LMT	C2-C3-C4-C5
9	C	1110	PTY	C40-C41-C42-C43
12	B	1110	P3G	O6-C13-C14-O7
9	B	1107	PTY	C13-C14-C15-C16
9	C	1111	PTY	C21-C22-C23-C24
10	C	1113	D12	C1-C2-C3-C4
4	C	1103	LMT	C5-C6-C7-C8
4	A	1103	LMT	C2-C1-O1'-C1'
4	C	1102	LMT	C2-C1-O1'-C1'
6	C	1107	GOL	O1-C1-C2-O2
9	C	1111	PTY	C20-C21-C22-C23
4	A	1104	LMT	C4-C5-C6-C7
11	C	1116	OCT	C1-C2-C3-C4
9	C	1111	PTY	C31-C32-C33-C34
4	A	1102	LMT	O5B-C5B-C6B-O6B
4	B	1102	LMT	C9-C10-C11-C12
4	B	1104	LMT	C3-C4-C5-C6
9	C	1111	PTY	C37-C38-C39-C40
4	C	1102	LMT	C1-C2-C3-C4
10	C	1113	D12	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	C	1109	PTY	C38-C39-C40-C41
9	C	1109	PTY	C8-C11-C12-C13
4	B	1104	LMT	C2'-C1'-O1'-C1
4	C	1105	LMT	C9-C10-C11-C12
4	C	1102	LMT	C6-C7-C8-C9
4	C	1104	LMT	C6-C7-C8-C9
4	A	1103	LMT	O5B-C5B-C6B-O6B
9	C	1110	PTY	C35-C36-C37-C38
10	C	1114	D12	C2-C3-C4-C5
7	C	1115	ETE	C15-C25-OH5-C14
9	C	1110	PTY	O14-C5-C6-C1
8	A	1109	HEX	C2-C3-C4-C5
12	B	1110	P3G	C11-C12-O6-C13
9	C	1110	PTY	C16-C17-C18-C19
4	A	1103	LMT	C9-C10-C11-C12
9	C	1110	PTY	C38-C39-C40-C41
9	C	1110	PTY	C2-C3-O11-P1
9	C	1111	PTY	C18-C19-C20-C21
4	C	1103	LMT	O1'-C1-C2-C3
9	C	1109	PTY	C33-C34-C35-C36
7	C	1115	ETE	C23-C13-OH4-C24
9	C	1110	PTY	C33-C34-C35-C36
9	C	1110	PTY	C14-C15-C16-C17
9	C	1110	PTY	O14-C5-C6-O7
4	A	1103	LMT	C5-C6-C7-C8
4	C	1105	LMT	C11-C10-C9-C8
9	C	1111	PTY	O4-C1-C6-O7
9	C	1111	PTY	O4-C1-C6-C5
9	B	1107	PTY	C26-C27-C28-C29
4	B	1104	LMT	C5-C6-C7-C8
9	C	1111	PTY	C11-C12-C13-C14
4	A	1104	LMT	O1'-C1-C2-C3
3	A	1101	FUA	C17-C22-C29-O4
3	A	1101	FUA	C17-C22-C29-O5
9	C	1110	PTY	C3-O11-P1-O12
9	C	1110	PTY	C5-O14-P1-O13
9	C	1111	PTY	N1-C2-C3-O11
4	A	1102	LMT	O5'-C5'-C6'-O6'
9	C	1110	PTY	C6-C5-O14-P1
7	C	1115	ETE	OH2-C12-C22-OH3
4	C	1102	LMT	C5-C6-C7-C8
9	B	1107	PTY	C33-C34-C35-C36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	C	1102	LMT	C4-C5-C6-C7
4	B	1102	LMT	C5-C6-C7-C8
10	C	1112	D12	C6-C7-C8-C9
4	A	1104	LMT	C3-C4-C5-C6
4	C	1103	LMT	C2-C3-C4-C5
9	C	1110	PTY	C11-C12-C13-C14
9	C	1111	PTY	C32-C33-C34-C35
10	C	1112	D12	C5-C6-C7-C8
10	C	1114	D12	C3-C4-C5-C6
9	C	1111	PTY	C15-C16-C17-C18
7	A	1107	ETE	C12-C22-OH3-C23
9	C	1109	PTY	O4-C1-C6-O7
4	C	1103	LMT	C1-C2-C3-C4
11	B	1109	OCT	C4-C5-C6-C7
7	A	1108	ETE	C15-C25-OH5-C14
6	B	1105	GOL	O1-C1-C2-C3
9	C	1111	PTY	C33-C34-C35-C36
9	C	1110	PTY	C32-C33-C34-C35
9	C	1109	PTY	C17-C18-C19-C20
6	D	201	GOL	O1-C1-C2-O2
11	B	1109	OCT	C1-C2-C3-C4
4	B	1104	LMT	C1-C2-C3-C4
4	C	1102	LMT	C9-C10-C11-C12
9	C	1109	PTY	C6-C5-O14-P1
7	A	1108	ETE	C23-C13-OH4-C24
4	C	1103	LMT	C2-C1-O1'-C1'
9	C	1110	PTY	C39-C40-C41-C42
9	C	1109	PTY	C23-C24-C25-C26
9	C	1111	PTY	C24-C25-C26-C27
7	A	1108	ETE	C24-C14-OH5-C25
13	B	1111	D10	C2-C3-C4-C5
9	B	1107	PTY	O4-C30-C31-C32
4	B	1103	LMT	C6-C7-C8-C9
4	C	1103	LMT	C9-C10-C11-C12
9	C	1110	PTY	C12-C11-C8-O7
9	C	1110	PTY	O4-C30-C31-C32
7	C	1115	ETE	OH5-C14-C24-OH4
4	A	1104	LMT	O5B-C1B-O1B-C4'
9	C	1111	PTY	C17-C18-C19-C20
9	C	1110	PTY	C17-C18-C19-C20
9	B	1107	PTY	O30-C30-C31-C32
9	C	1110	PTY	O30-C30-C31-C32

Continued on next page...

Continued from previous page...

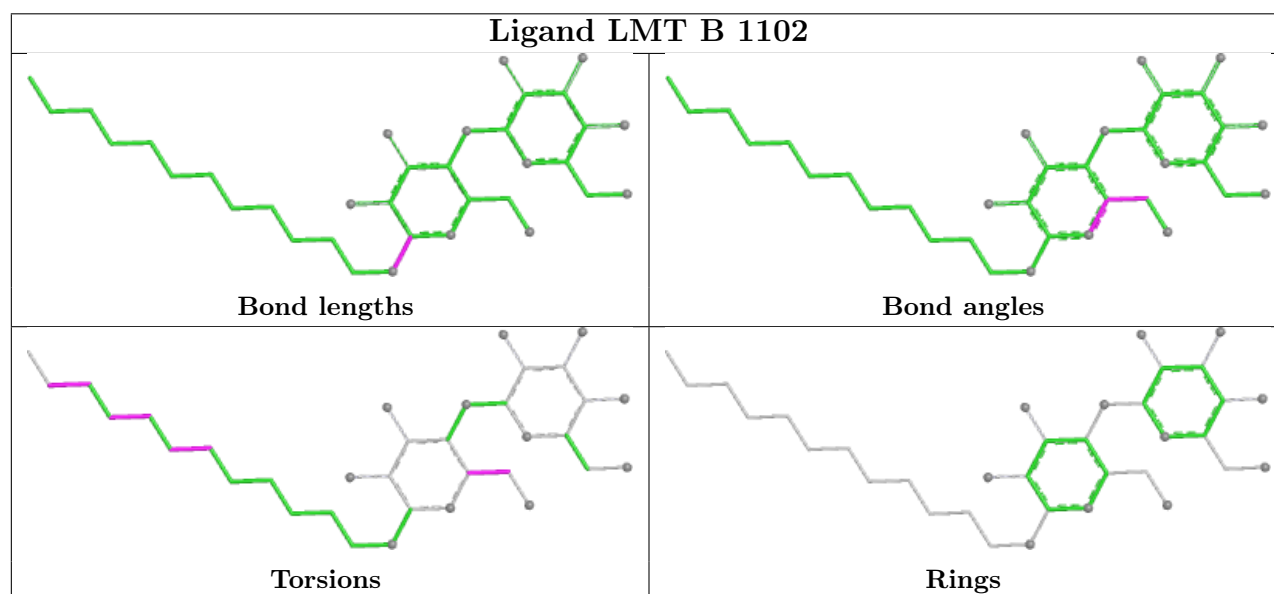
Mol	Chain	Res	Type	Atoms
9	C	1110	PTY	C12-C11-C8-O10
9	B	1107	PTY	C12-C11-C8-O7
4	A	1104	LMT	C2B-C1B-O1B-C4'
9	C	1110	PTY	C26-C27-C28-C29
9	B	1107	PTY	C17-C18-C19-C20

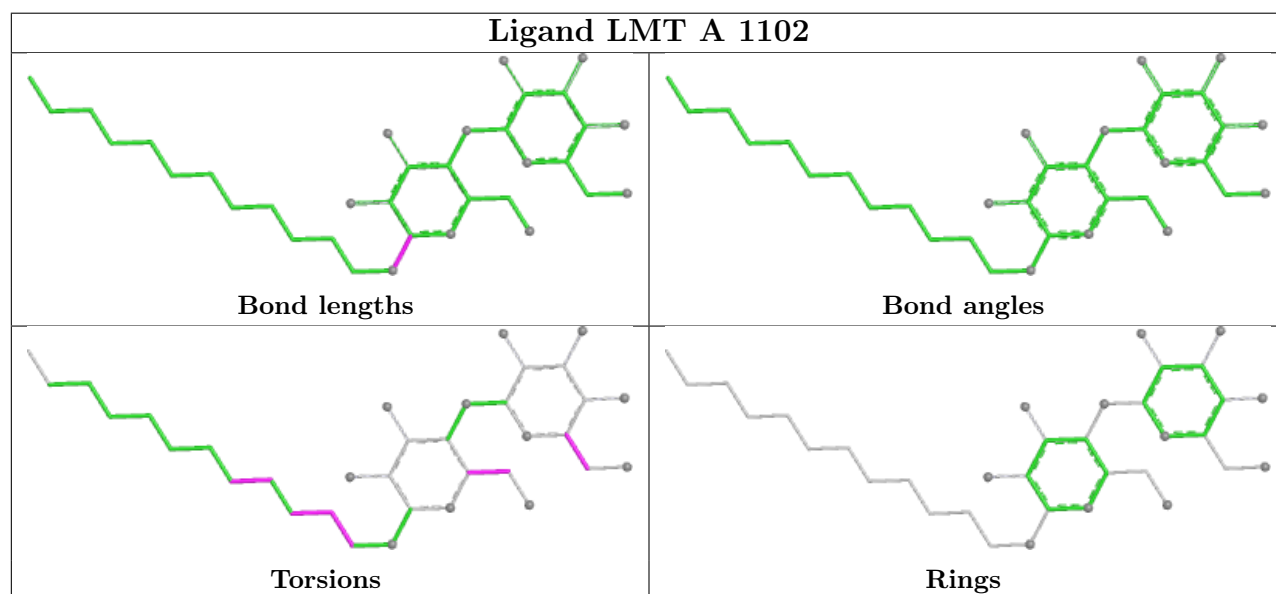
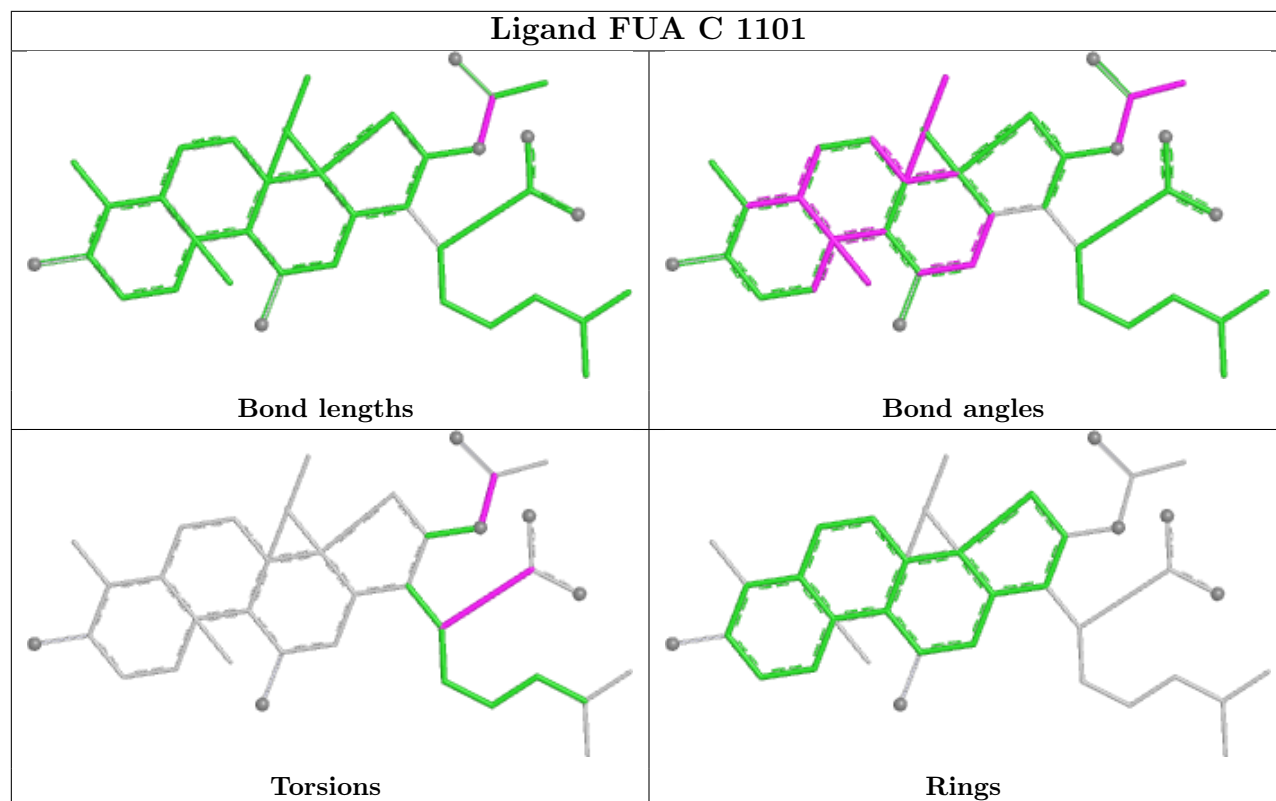
There are no ring outliers.

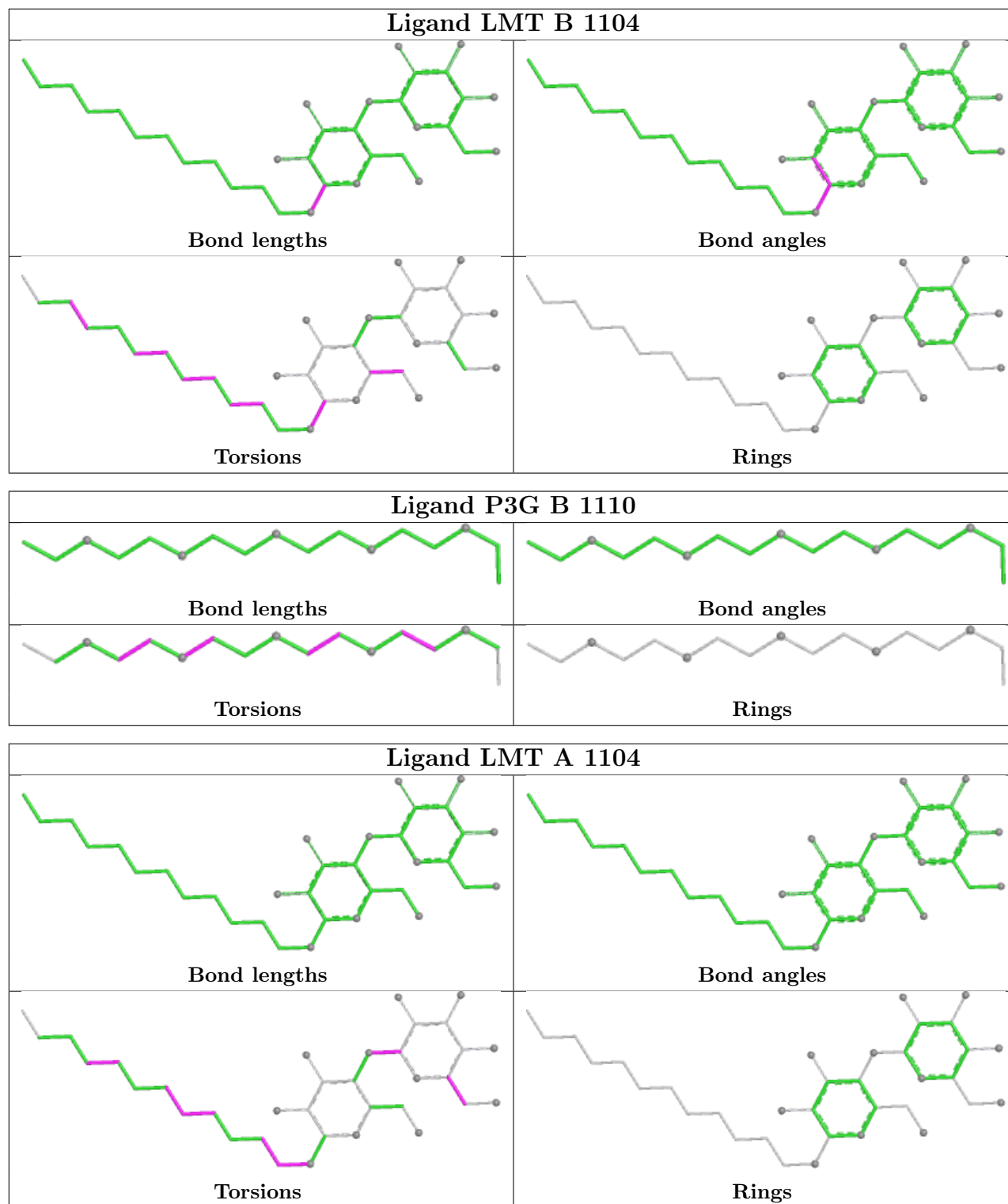
3 monomers are involved in 4 short contacts:

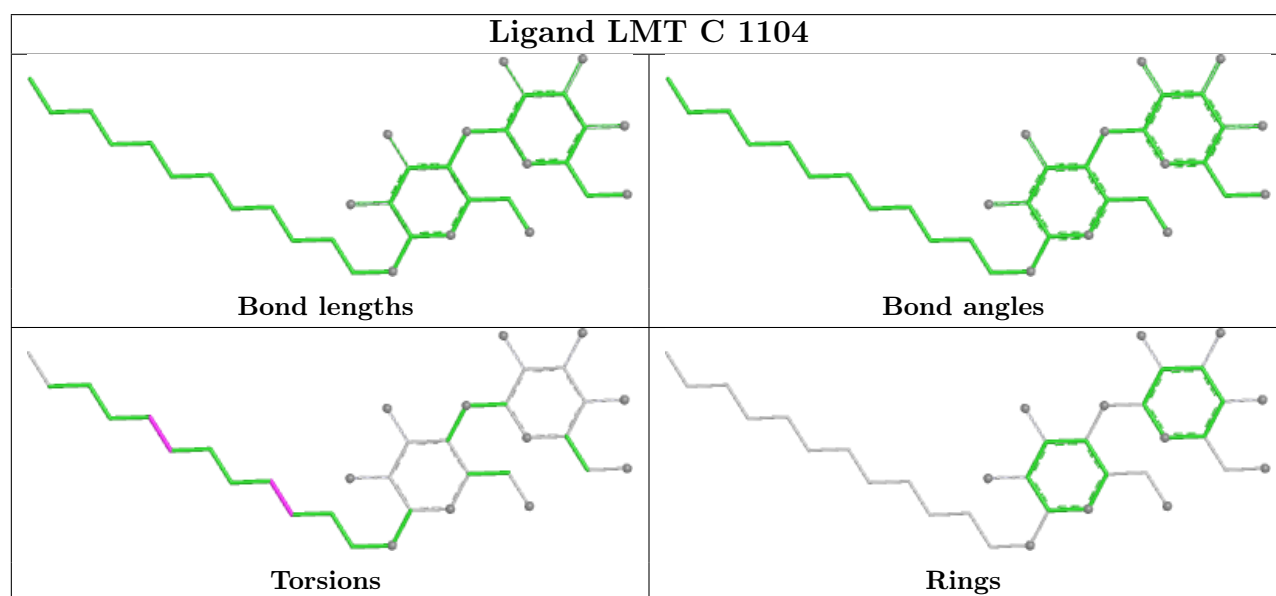
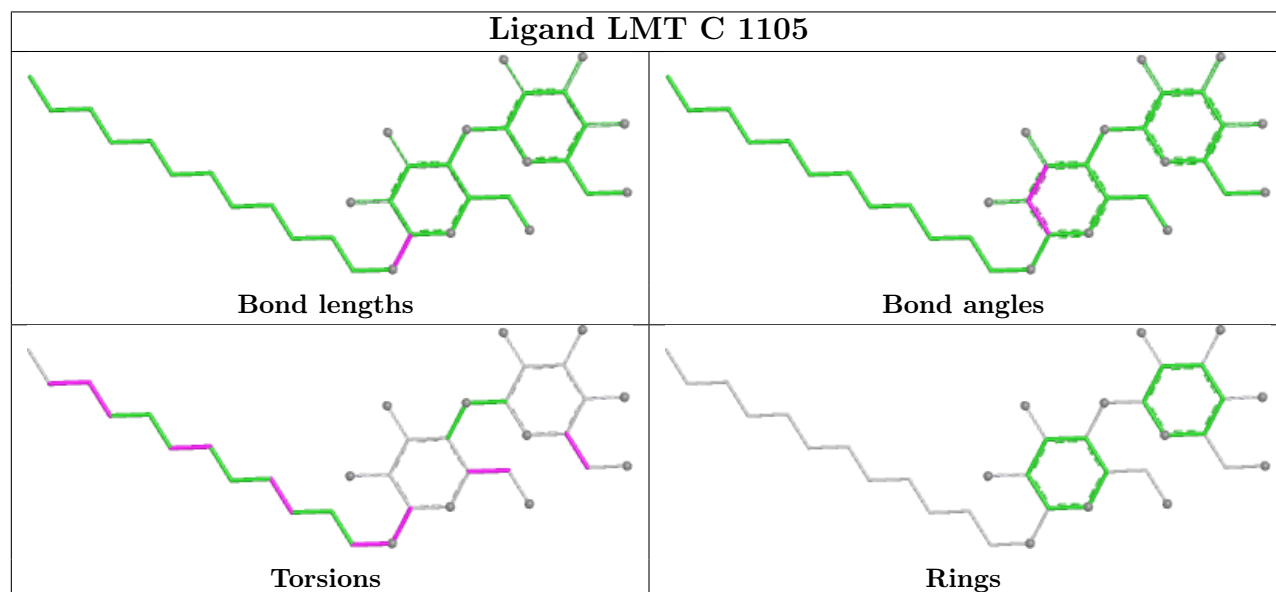
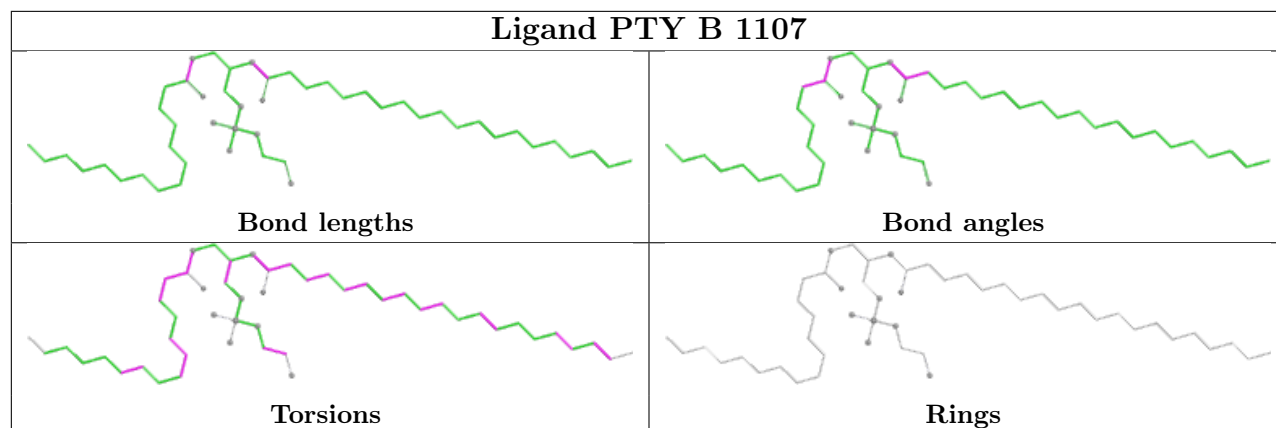
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1101	FUA	1	0
3	B	1101	FUA	2	0
3	A	1101	FUA	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

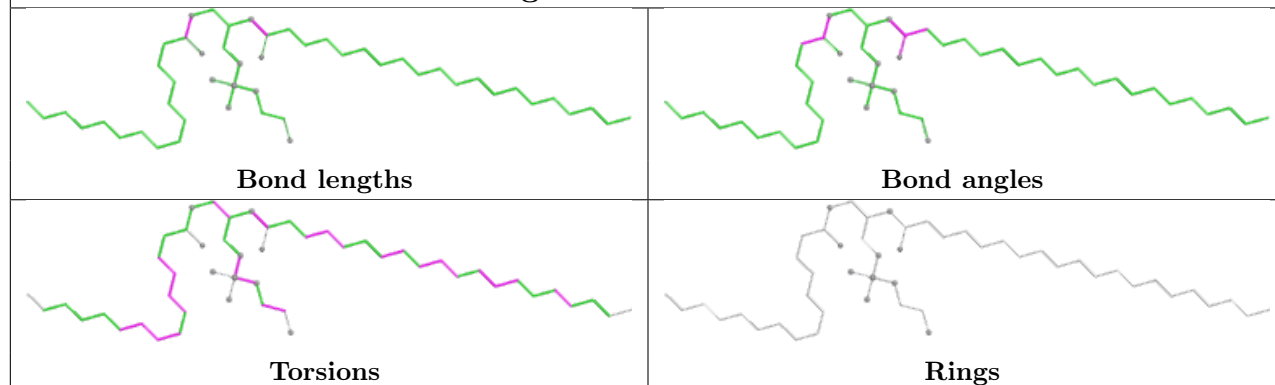




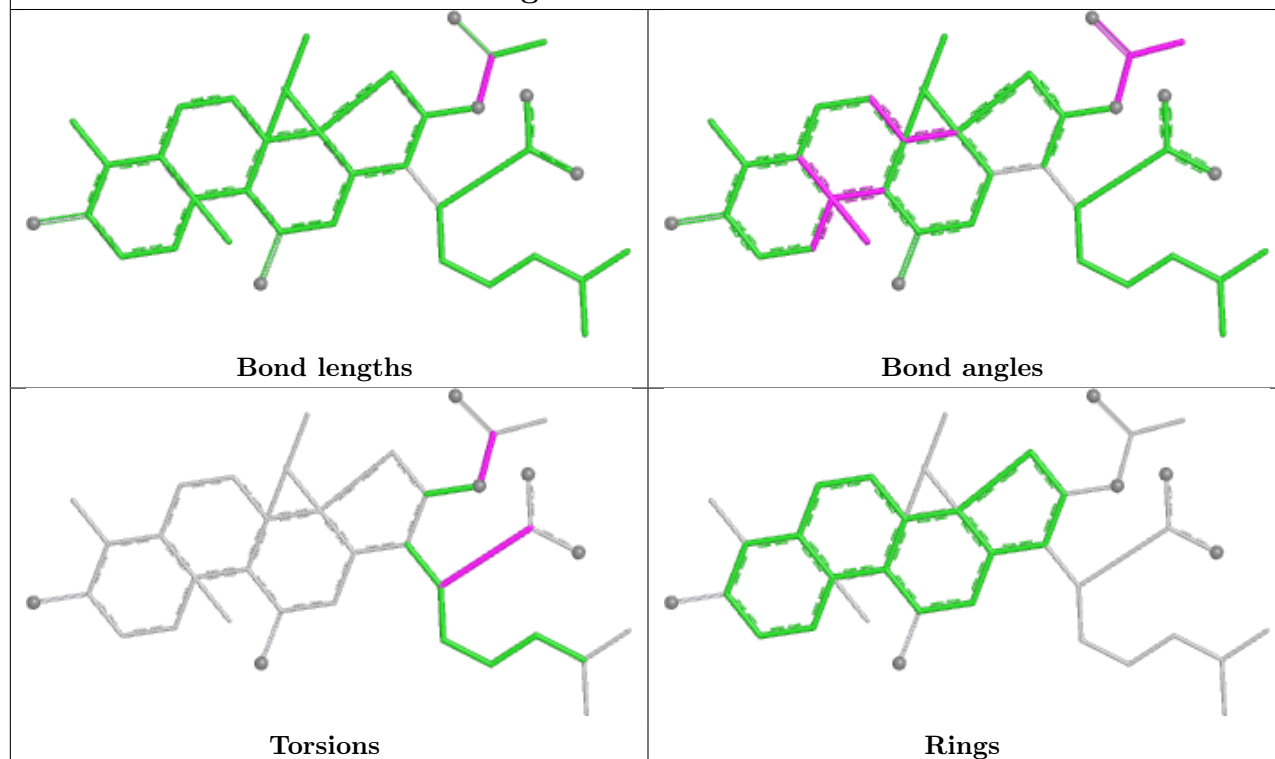




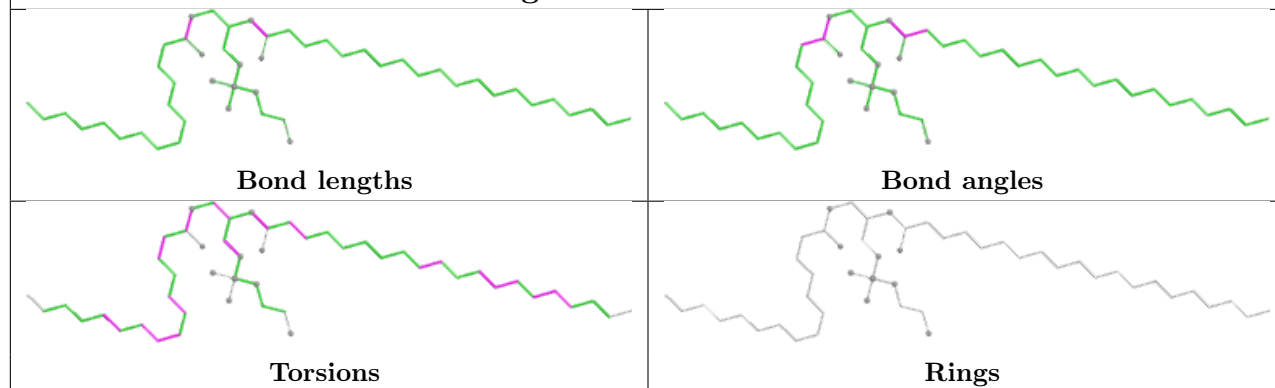
Ligand PTY C 1111

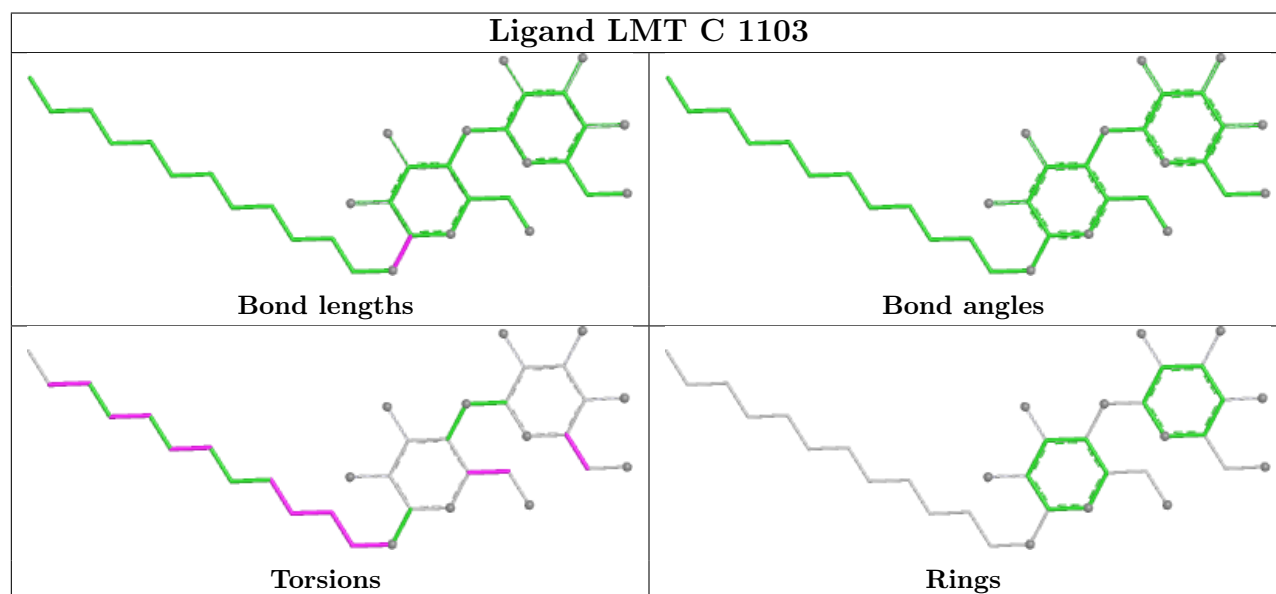
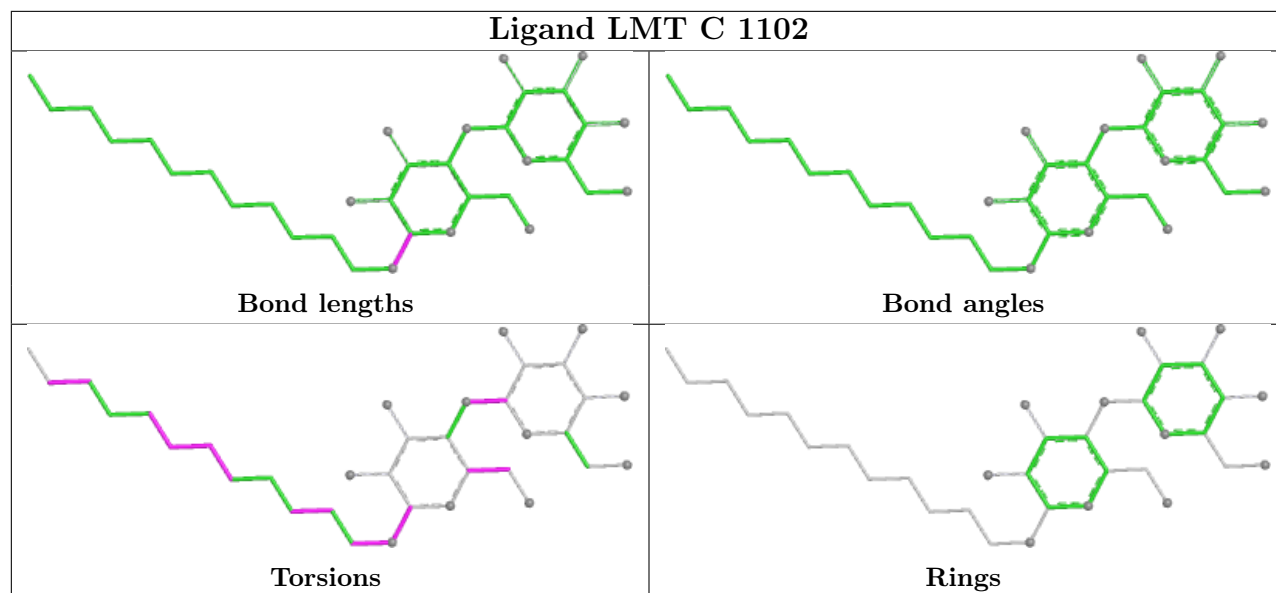


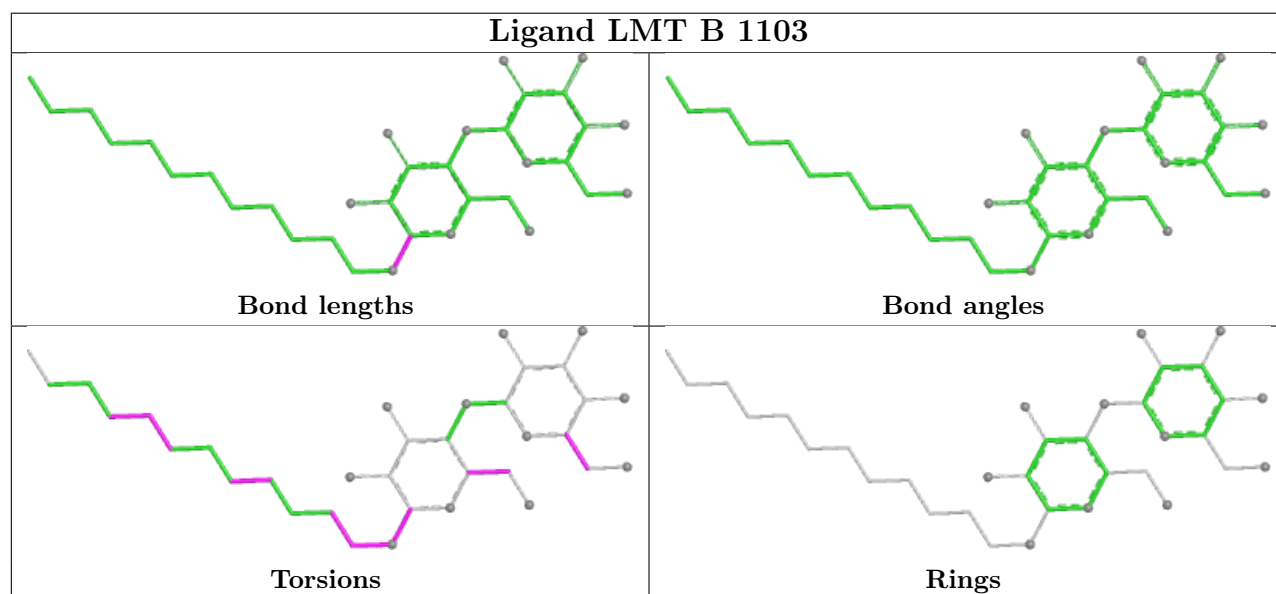
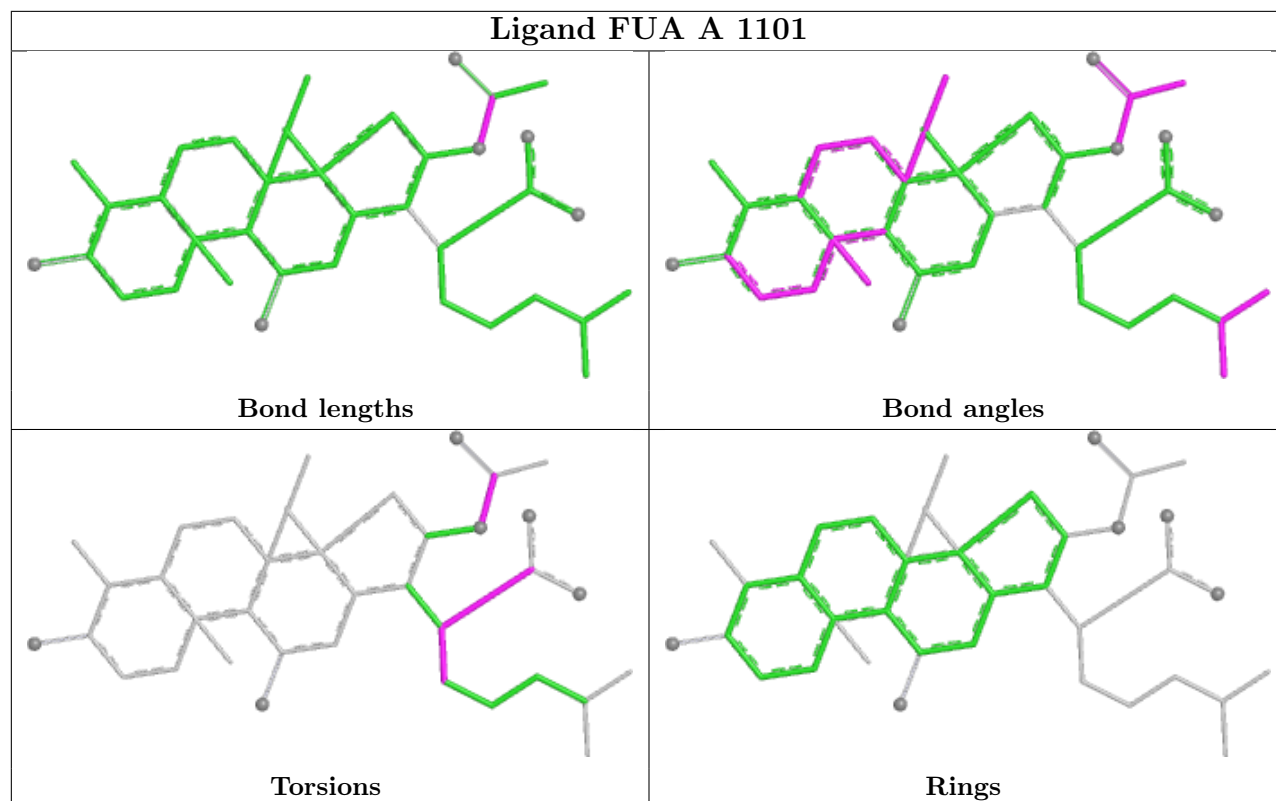
Ligand FUA B 1101

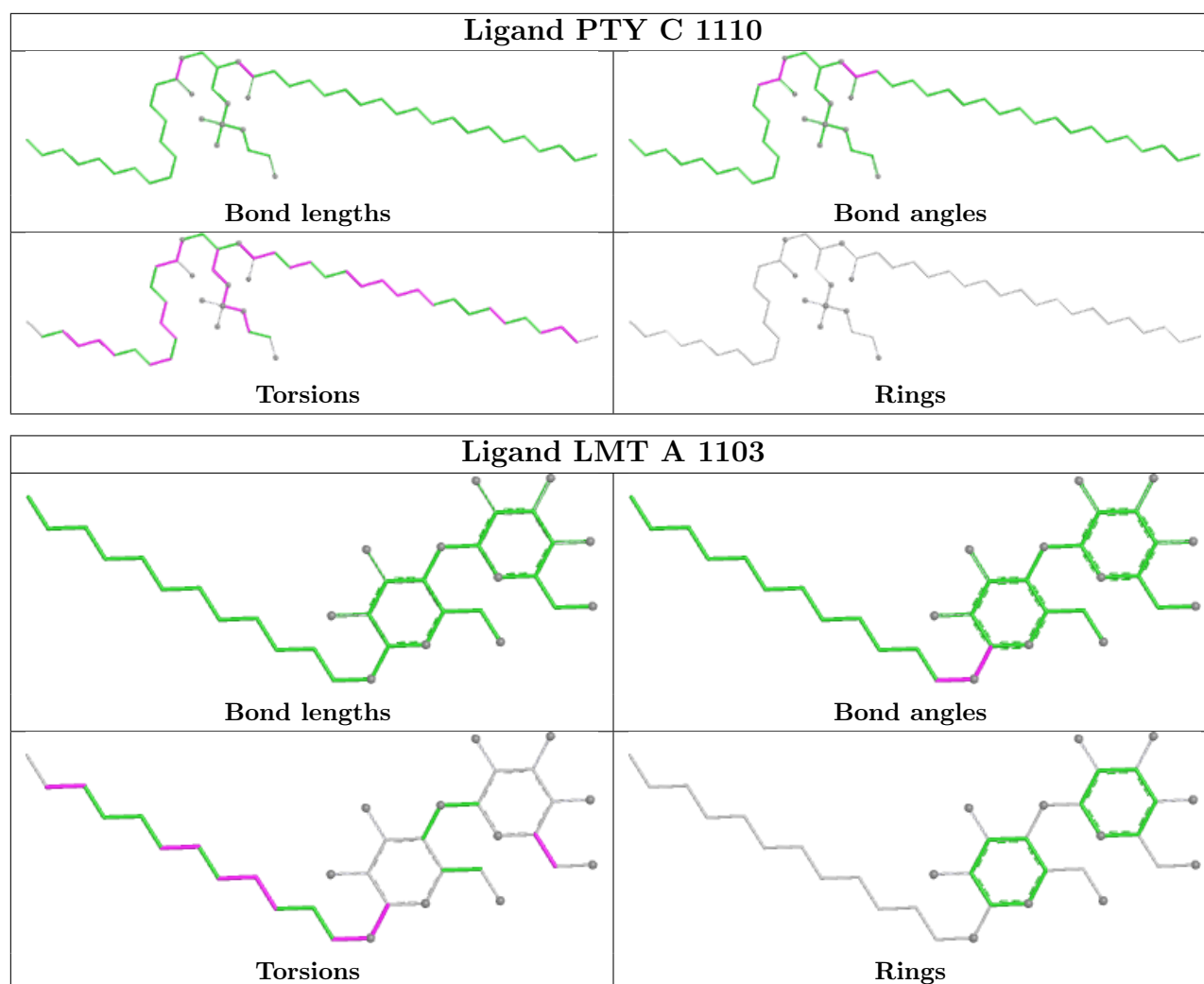


Ligand PTY C 1109









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, 95th 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%)	0.51	72 (6%)	22	20	25, 63, 115, 150	3 (0%)
1	B	1034/1057 (97%)	0.47	63 (6%)	27	23	33, 60, 91, 125	0
1	C	1033/1057 (97%)	0.21	23 (2%)	62	58	34, 52, 85, 110	1 (0%)
2	D	158/169 (93%)	0.45	4 (2%)	58	54	48, 60, 90, 134	0
2	E	154/169 (91%)	0.83	10 (6%)	25	22	44, 71, 100, 112	1 (0%)
All	All	3413/3509 (97%)	0.42	172 (5%)	34	30	25, 58, 100, 150	5 (0%)

All (172) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	868	LEU	6.7
2	D	168	LEU	6.1
1	B	134	SER	5.8
1	A	668	LEU	5.5
1	B	675	GLY	4.9
1	B	676	THR	4.8
1	A	510	LYS	4.7
1	B	618	ALA	4.7
1	A	674	LEU	4.5
1	A	617	PHE	4.4
1	A	961	ILE	4.4
1	B	672	VAL	4.4
1	A	678	THR	4.3
1	C	671	ILE	4.2
1	A	670	ALA	4.2
1	B	634	TRP	4.1
1	A	672	VAL	4.0
1	B	575	MET	3.9
1	B	662	MET	3.9
1	A	676	THR	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	618	ALA	3.8
1	B	97	GLY	3.8
1	B	868	LEU	3.6
1	B	987	MET	3.6
1	A	980	LEU	3.5
1	B	508	GLY	3.5
1	B	673	GLU	3.4
1	A	956	GLU	3.4
1	B	332	PHE	3.3
1	B	617	PHE	3.3
1	A	502	LYS	3.3
1	B	674	LEU	3.3
1	C	670	ALA	3.3
1	B	38	ILE	3.3
1	A	955	LYS	3.3
1	C	918	PHE	3.3
1	B	133	SER	3.2
1	C	497	LEU	3.2
1	B	362	PHE	3.2
1	A	543	VAL	3.2
1	B	867	ARG	3.2
1	A	677	ALA	3.1
1	B	561	SER	3.1
1	C	620	ARG	3.1
1	A	499	PRO	3.0
1	B	593	GLU	3.0
1	A	361	ASN	3.0
1	A	402	ILE	3.0
1	B	577	GLN	3.0
1	B	670	ALA	3.0
1	B	677	ALA	3.0
1	B	669	PRO	3.0
1	A	501	ALA	2.9
1	A	500	ILE	2.9
2	E	33	LEU	2.9
1	B	628	PHE	2.9
1	B	918	PHE	2.9
1	A	431	THR	2.8
2	D	44	ASP	2.8
1	A	509	LYS	2.8
1	A	957	GLY	2.8
1	A	675	GLY	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	870	GLY	2.8
2	E	32	ILE	2.8
1	A	498	LYS	2.8
1	B	556	PHE	2.8
1	B	619	GLY	2.8
2	E	74	ASN	2.8
1	A	406	VAL	2.8
1	A	364	ALA	2.8
1	B	563	PHE	2.8
1	C	362	PHE	2.8
1	C	811	TYR	2.7
1	B	28	LEU	2.7
1	A	423	GLU	2.7
1	B	498	LYS	2.7
1	A	544	LEU	2.6
1	A	538	THR	2.6
1	B	655	PHE	2.6
1	A	441	ALA	2.6
1	A	362	PHE	2.6
1	B	666	PHE	2.5
1	B	135	SER	2.5
1	C	502	LYS	2.5
1	A	960	LEU	2.5
1	B	664	PHE	2.5
1	A	123	GLN	2.5
1	C	619	GLY	2.5
1	B	873	ALA	2.5
1	B	1034	SER	2.5
2	E	97[A]	GLU	2.5
1	A	1028	VAL	2.5
1	B	132	SER	2.5
1	B	337	ILE	2.4
1	A	952	LEU	2.4
1	A	1022	VAL	2.4
2	E	139	VAL	2.4
1	A	620	ARG	2.4
1	B	557	VAL	2.4
1	B	871	ASN	2.4
1	A	865	GLN	2.4
1	A	944	LEU	2.4
1	A	512	PHE	2.4
1	C	617	PHE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	1015	THR	2.4
1	C	71	GLY	2.4
1	C	124	GLN	2.4
1	A	618	ALA	2.4
2	E	35	ALA	2.4
1	B	660	ASP	2.3
1	C	1033	PHE	2.3
1	A	895	TRP	2.3
1	A	1034	SER	2.3
1	B	29	LYS	2.3
1	B	366	LEU	2.3
1	A	968	VAL	2.3
1	A	871	ASN	2.3
1	B	854	GLY	2.3
1	A	547	ILE	2.3
1	B	659	LYS	2.3
1	A	11	PHE	2.3
1	A	918	PHE	2.3
1	A	418	ARG	2.3
1	A	981	ALA	2.2
1	A	524	THR	2.2
1	B	37	THR	2.2
1	B	463	THR	2.2
1	B	936	GLY	2.2
1	B	279	ALA	2.2
2	E	140	ASN	2.2
1	B	284	GLN	2.2
1	B	569	GLN	2.2
1	C	675	GLY	2.2
1	C	425	LEU	2.2
1	A	963	ALA	2.2
2	D	167	LYS	2.2
1	B	478	MET	2.2
1	A	25	LEU	2.2
1	A	877	TYR	2.2
1	B	1006	GLY	2.2
2	D	11	GLY	2.2
1	C	2	PRO	2.2
1	C	428	LYS	2.2
1	C	421	ALA	2.1
1	A	425	LEU	2.1
1	A	495	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	984	LEU	2.1
1	A	541	TYR	2.1
1	B	991	ILE	2.1
1	A	426	PRO	2.1
1	B	459	PHE	2.1
1	A	575	MET	2.1
1	B	509	LYS	2.1
1	A	649[B]	MET	2.1
1	A	1012	VAL	2.1
2	E	106	VAL	2.1
1	A	995	ALA	2.1
1	A	497	LEU	2.1
1	B	620	ARG	2.1
2	E	76	TYR	2.1
1	B	627	ALA	2.1
1	C	959	GLY	2.1
1	C	500	ILE	2.0
1	A	869	SER	2.0
1	A	526	HIS	2.0
1	A	120	GLN	2.0
1	C	672	VAL	2.0
1	B	831	ALA	2.0
1	A	619	GLY	2.0
2	E	107	ASN	2.0
1	A	991	ILE	2.0
1	C	134	SER	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 oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

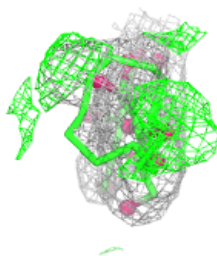
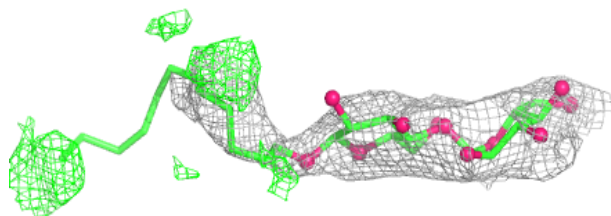
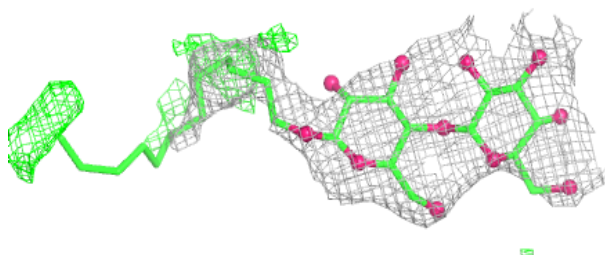
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	LMT	C	1105	35/35	0.53	0.23	122,130,133,134	0
7	ETE	A	1107	14/14	0.68	0.22	111,115,122,122	0
4	LMT	B	1103	35/35	0.73	0.19	114,125,131,133	0
12	P3G	B	1110	17/17	0.74	0.26	109,120,121,121	0
11	OCT	B	1109	8/8	0.75	0.45	93,94,96,97	0
3	FUA	C	1101	37/37	0.75	0.27	122,147,159,162	0
7	ETE	A	1108	14/14	0.76	0.19	95,98,100,100	0
10	D12	C	1114	12/12	0.77	0.39	89,92,94,95	0
4	LMT	C	1102	35/35	0.77	0.23	114,142,153,155	0
9	PTY	C	1111	50/50	0.77	0.27	79,97,115,120	0
3	FUA	A	1101	37/37	0.79	0.24	122,146,149,149	0
11	OCT	C	1116	8/8	0.79	0.40	89,91,93,94	0
7	ETE	C	1115	14/14	0.79	0.23	91,97,99,99	0
8	HEX	A	1109	6/6	0.80	0.28	68,70,71,72	0
9	PTY	C	1109	50/50	0.81	0.28	76,111,132,138	0
4	LMT	B	1102	35/35	0.81	0.20	93,101,111,111	0
6	GOL	D	201	6/6	0.82	0.20	67,70,70,72	0
5	SO4	A	1105	5/5	0.83	0.17	86,90,92,92	0
6	GOL	C	1108	6/6	0.83	0.23	68,71,71,72	0
9	PTY	C	1110	50/50	0.83	0.28	88,118,139,144	0
4	LMT	A	1104	35/35	0.83	0.19	84,121,151,152	0
6	GOL	B	1105	6/6	0.84	0.23	67,68,72,74	0
9	PTY	B	1107	50/50	0.84	0.22	92,107,159,165	0
6	GOL	A	1106	6/6	0.84	0.19	80,82,82,85	0
4	LMT	A	1102	35/35	0.85	0.20	96,115,129,133	0
4	LMT	B	1104	35/35	0.86	0.17	86,95,102,102	0
4	LMT	A	1103	35/35	0.86	0.16	80,107,132,133	0
8	HEX	C	1117	6/6	0.87	0.29	82,84,84,84	0
10	D12	B	1108	12/12	0.87	0.24	71,74,75,75	0
4	LMT	C	1104	35/35	0.87	0.18	98,132,157,157	0
13	D10	B	1111	10/10	0.87	0.31	88,92,94,95	0
10	D12	C	1113	12/12	0.88	0.31	84,89,90,90	0
3	FUA	B	1101	37/37	0.88	0.17	94,96,103,105	0
6	GOL	B	1106	6/6	0.88	0.19	62,66,68,68	0
10	D12	C	1112	12/12	0.89	0.21	68,72,75,76	0
6	GOL	E	201	6/6	0.90	0.18	72,74,76,77	0
13	D10	B	1112	10/10	0.90	0.24	81,83,83,84	0
6	GOL	E	202	6/6	0.91	0.12	64,65,66,67	0
4	LMT	C	1103	35/35	0.92	0.14	73,81,91,92	0
5	SO4	C	1106	5/5	0.93	0.15	76,76,77,78	0
6	GOL	C	1107	6/6	0.95	0.10	43,44,45,45	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

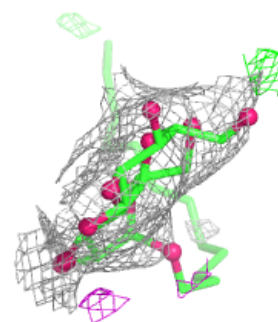
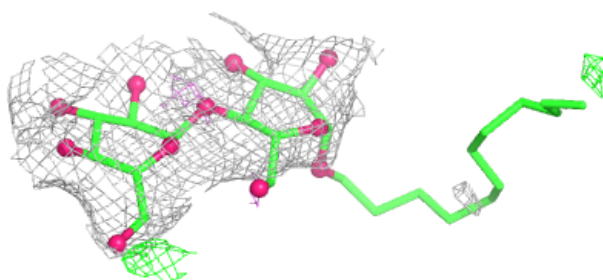
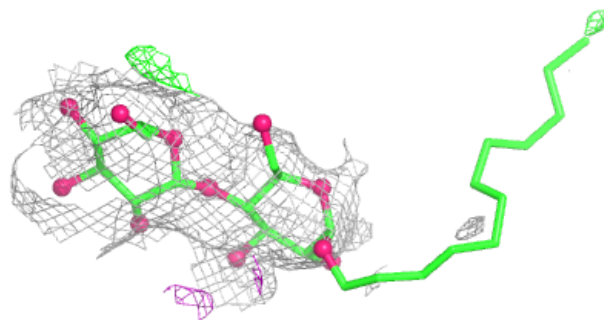
Electron density around LMT C 1105:

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

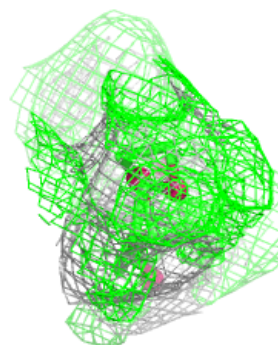
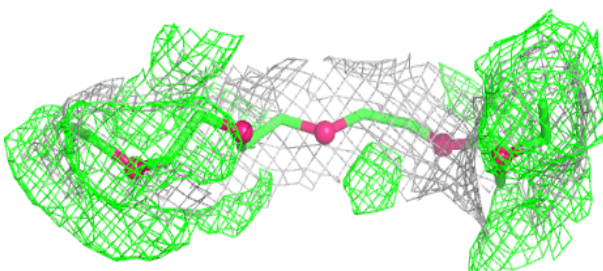
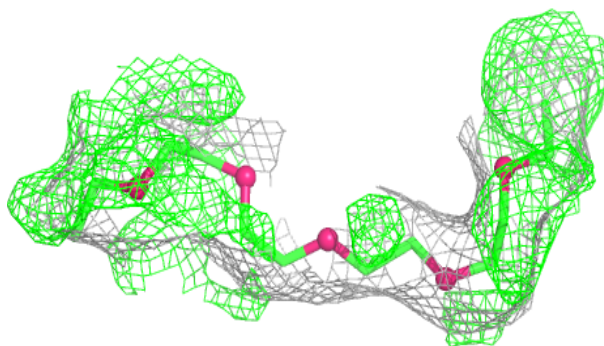


Electron density around LMT B 1103:

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

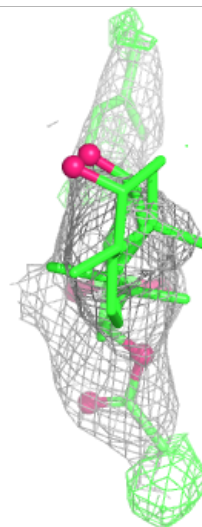
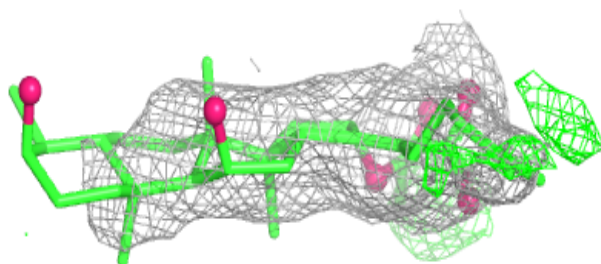
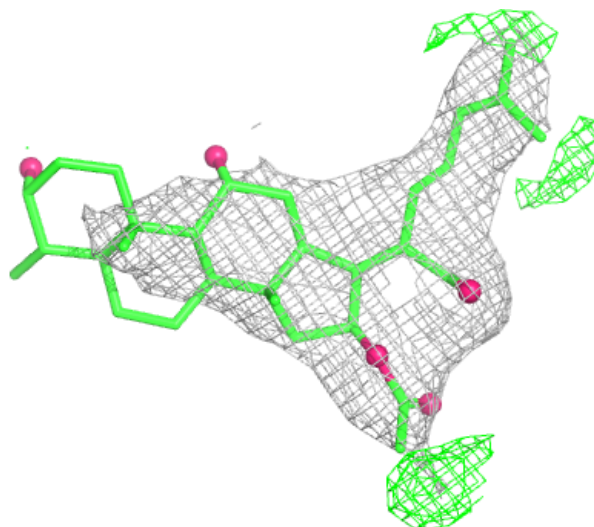
**Electron density around P3G B 1110:**

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



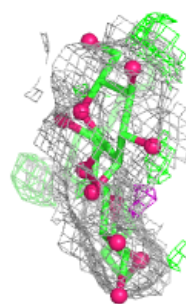
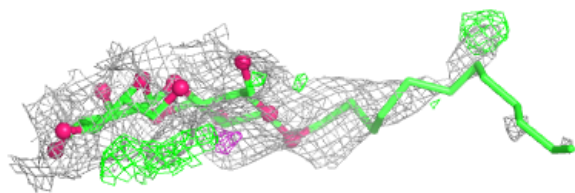
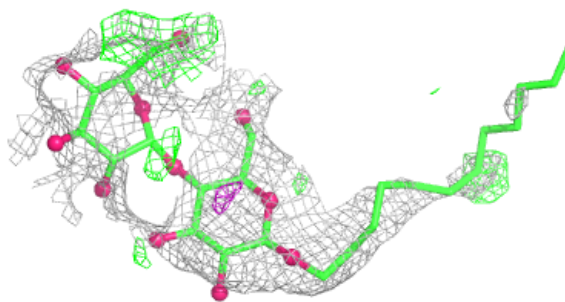
Electron density around FUA C 1101:

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

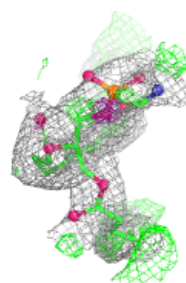
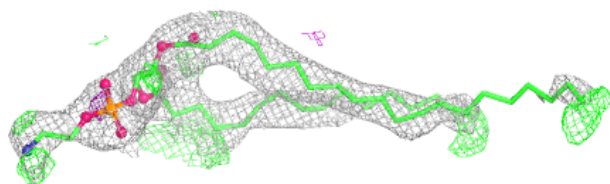
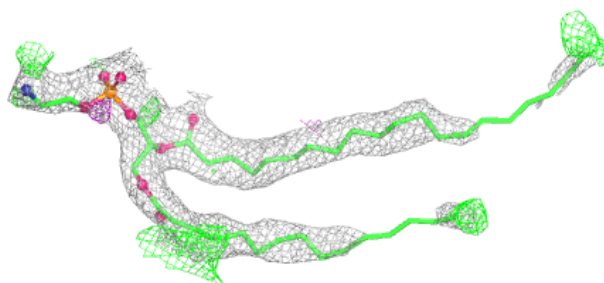


Electron density around LMT C 1102:

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

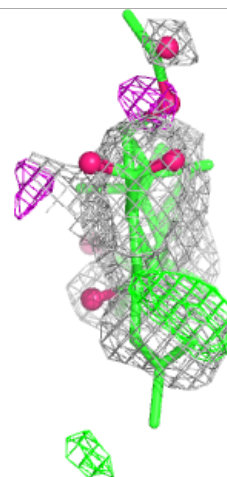
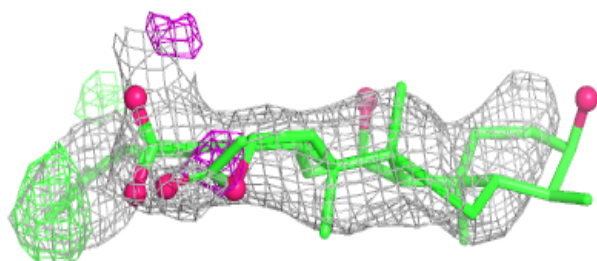
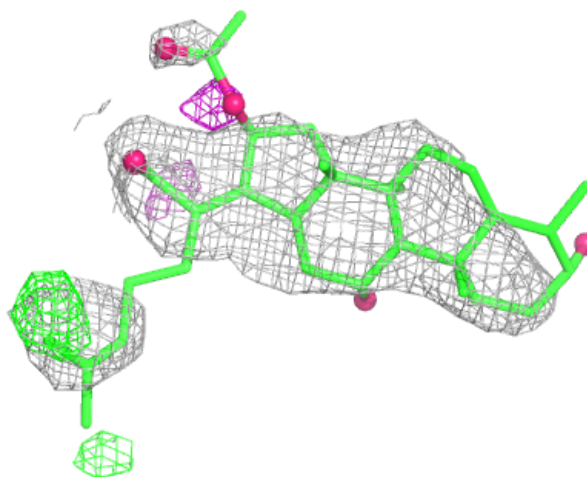
**Electron density around PTY C 1111:**

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



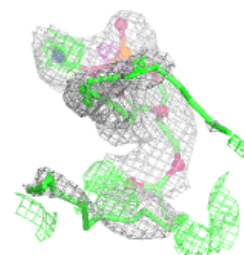
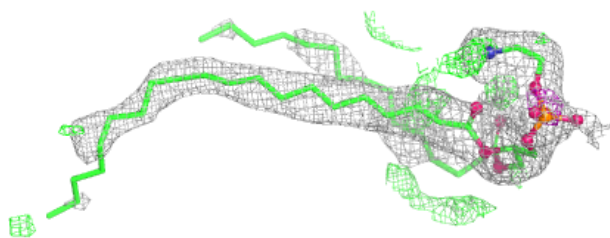
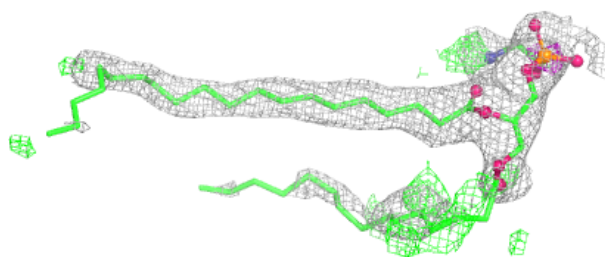
Electron density around FUA A 1101:

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

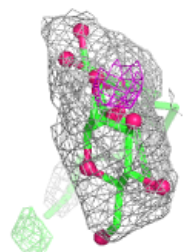
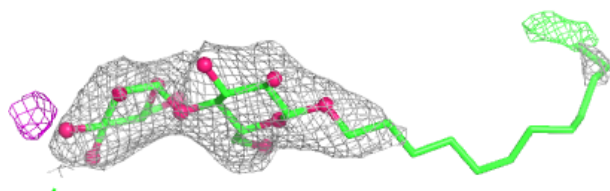
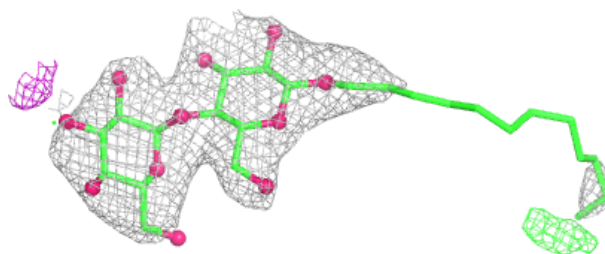


Electron density around PTY C 1109:

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

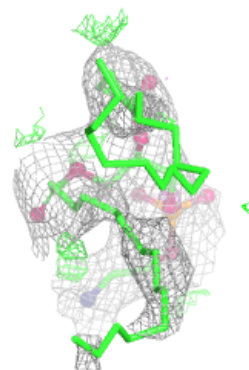
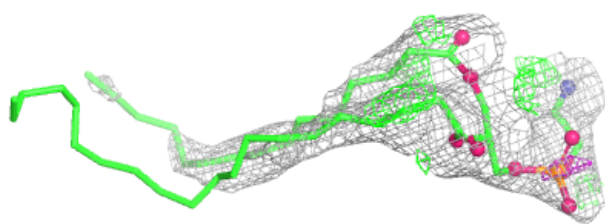
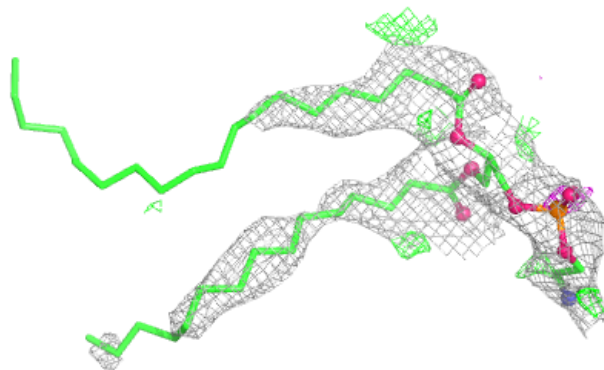
**Electron density around LMT B 1102:**

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

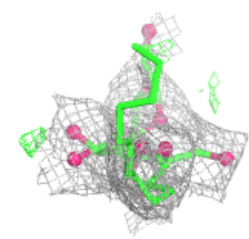
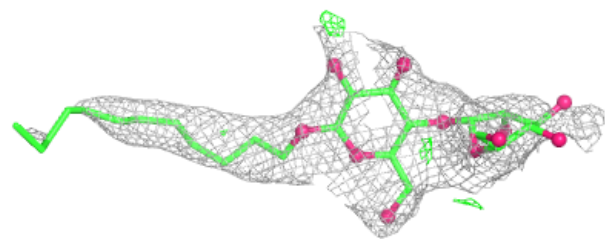
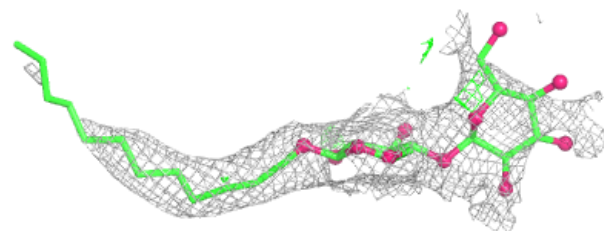


Electron density around PTY C 1110:

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

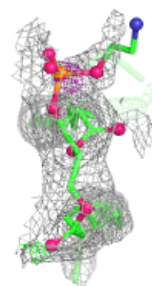
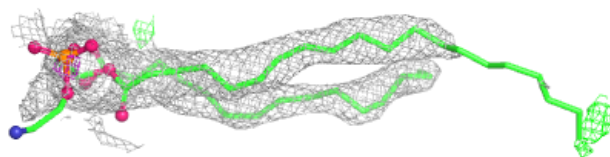
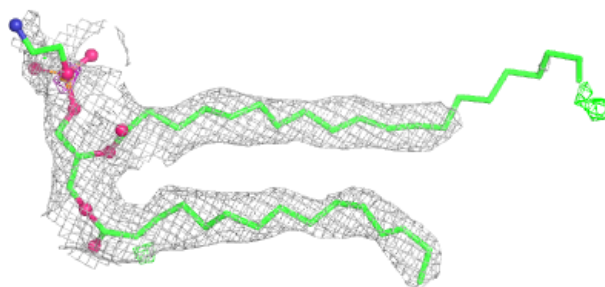
**Electron density around LMT A 1104:**

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

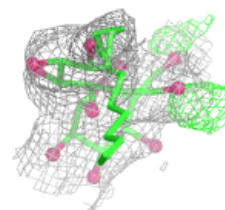
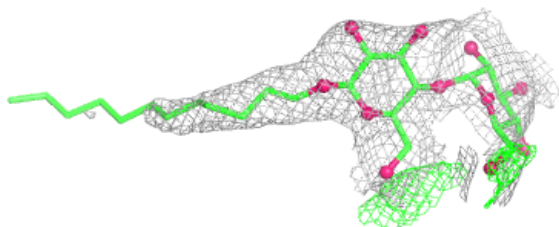
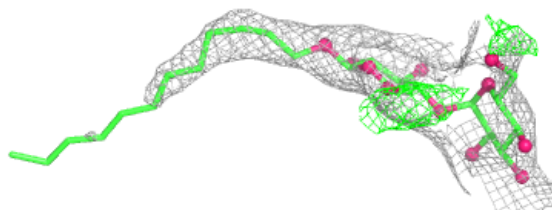


Electron density around PTY B 1107:

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

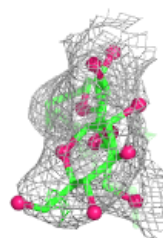
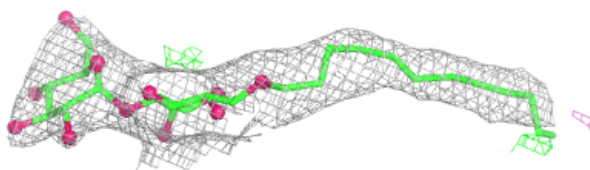
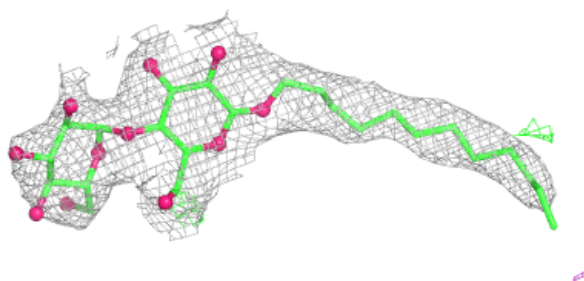
**Electron density around LMT A 1102:**

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

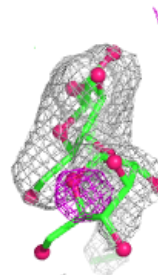
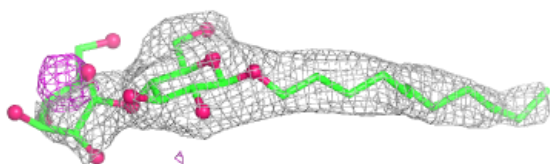
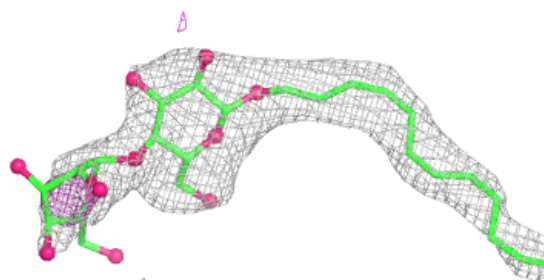


Electron density around LMT B 1104:

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

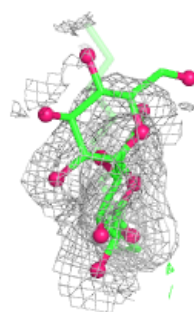
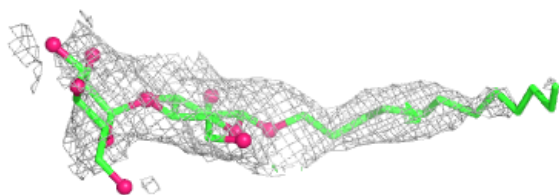
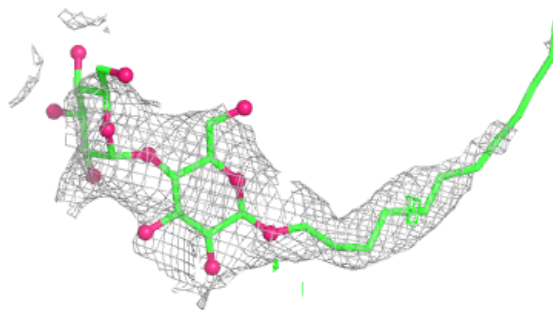
**Electron density around LMT A 1103:**

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

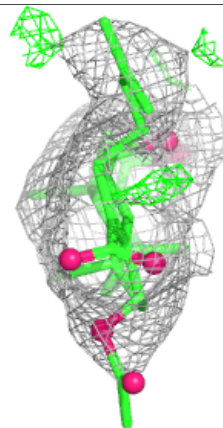
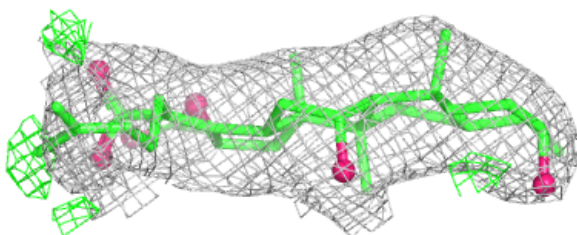
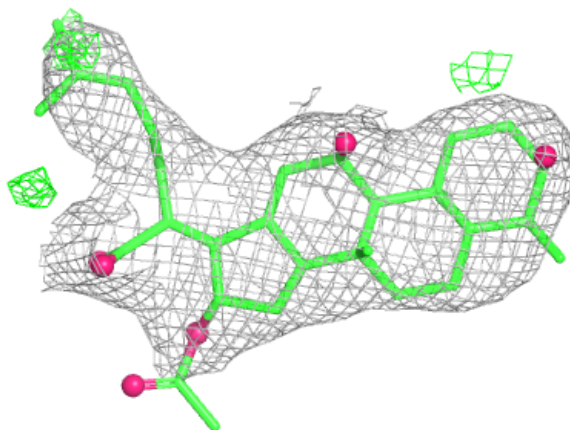


Electron density around LMT C 1104:

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

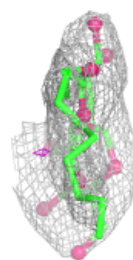
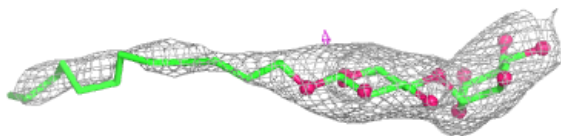
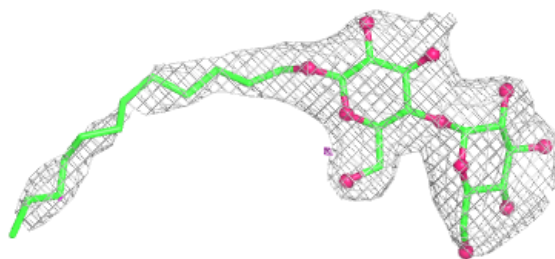
**Electron density around FUA B 1101:**

$2mF_o-DF_c$ (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.