wwPDB X-ray Structure Validation Summary Report (i)

Jun 23, 2024 – 07:16 PM EDT

PDB ID	:	6Q4N
Title	:	Fusidic acid bound AcrB_V340A
Authors	:	Tam, H.K.; Pos, K.M.
Deposited on	:	2018-12-06
Resolution	:	2.80 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

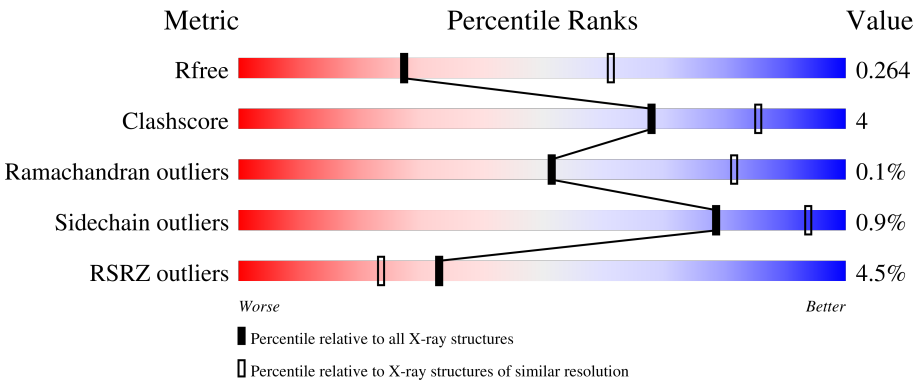
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1057	4% 86% 12% •
1	B	1057	4% 88% 10% •
1	C	1057	3% 93% 5% •
2	D	169	7% 89% • 8%
2	E	169	20% 83% 8% 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
13	DDR	B	1116	-	-	-	X
5	LMT	B	1104	-	-	-	X
5	LMT	C	1103	-	-	-	X
7	PTY	B	1105	-	-	-	X

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 27045 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1036	7879	5069	1302	1464	44	0	1	0
1	B	1034	7853	5053	1296	1460	44	0	0	0
1	C	1034	7858	5056	1297	1461	44	0	1	0

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	340	ALA	VAL	engineered mutation	UNP P31224
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	340	ALA	VAL	engineered mutation	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	340	ALA	VAL	engineered mutation	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

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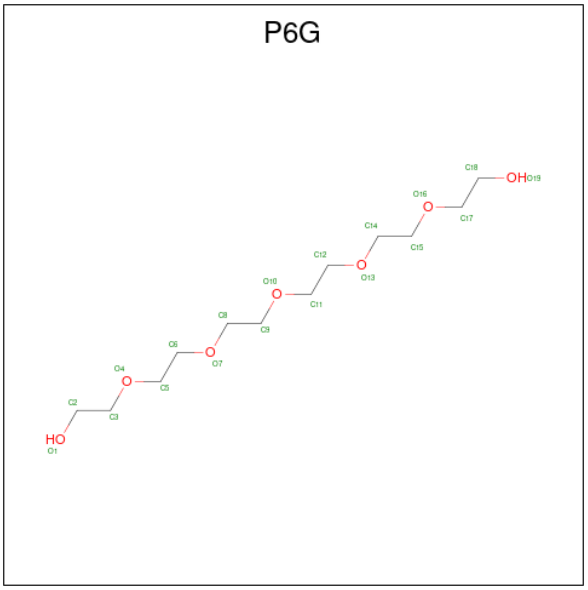
Chain	Residue	Modelled	Actual	Comment	Reference
C	1054	HIS	-	expression tag	UNP P31224
C	1055	HIS	-	expression tag	UNP P31224
C	1056	HIS	-	expression tag	UNP P31224
C	1057	HIS	-	expression tag	UNP P31224

- Molecule 2 is a protein called DARPin.

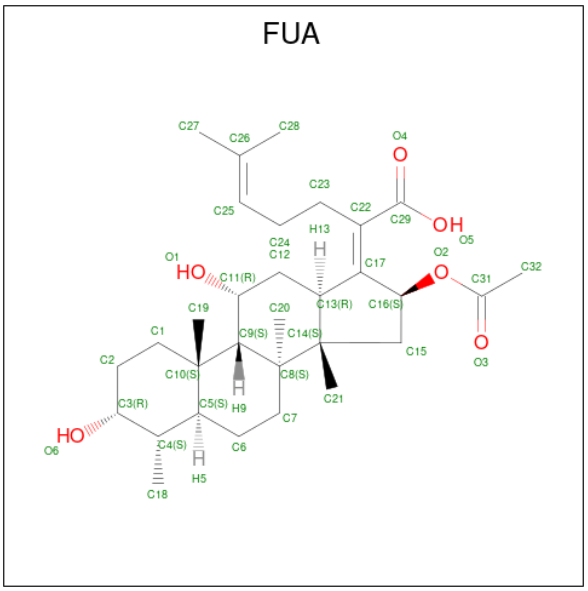
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	156	1177	741	206	229	1	0	0	0
			Total	C	N	O	S			
2	E	154	1167	736	204	226	1	0	0	0

- Molecule 3 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$).



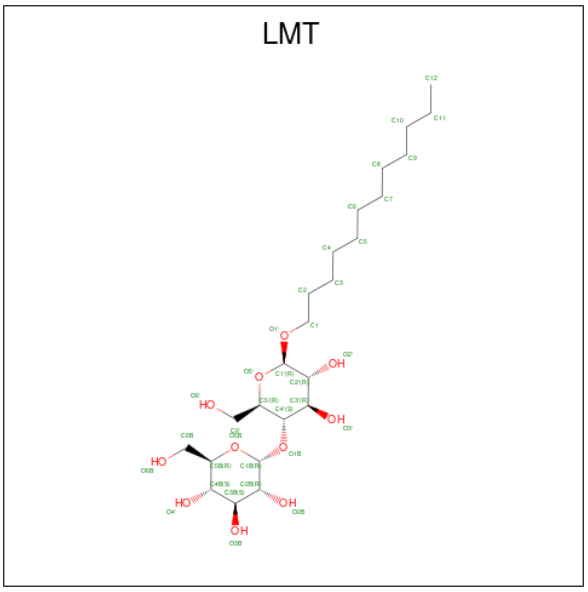
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	19	12	7	0	0

- Molecule 4 is FUSIDIC ACID (three-letter code: FUA) (formula: $C_{31}H_{48}O_6$) (labeled as "Ligand of Interest" by depositor).



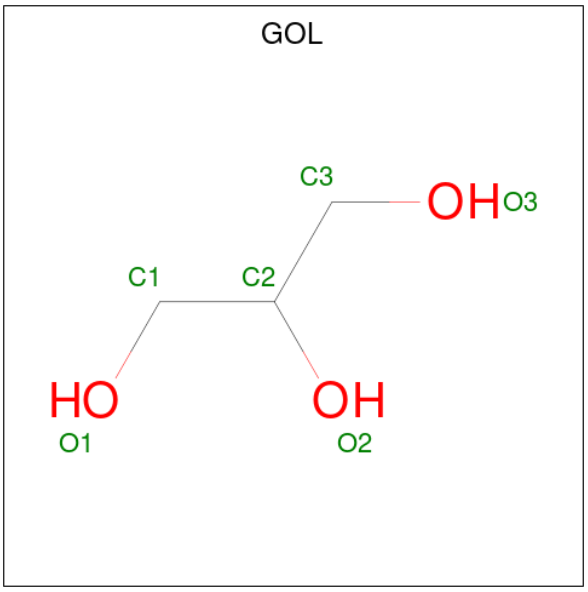
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	37	31	6	0	0
			Total	C	O		
4	B	1	37	31	6	0	0
			Total	C	O		
4	C	1	37	31	6	0	0

- Molecule 5 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



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

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



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

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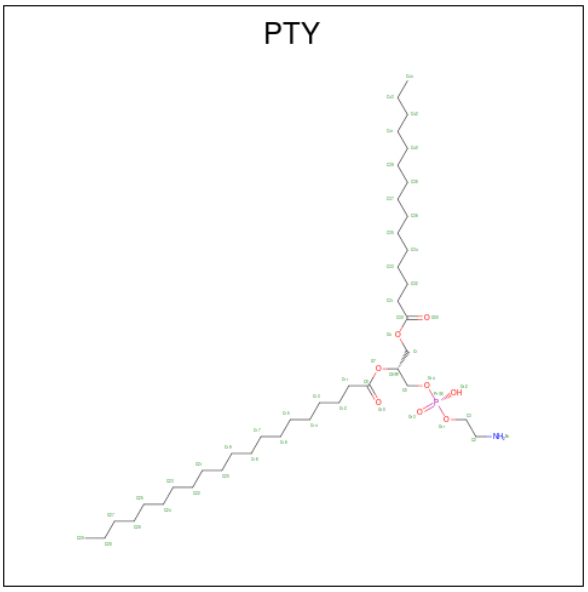
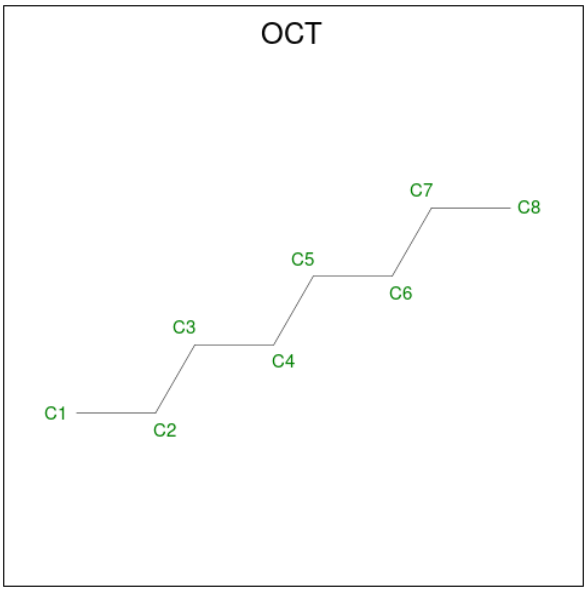
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	E	1	6	3	3	0	0
			Total	C	O		
6	E	1	6	3	3	0	0

- Molecule 7 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$).



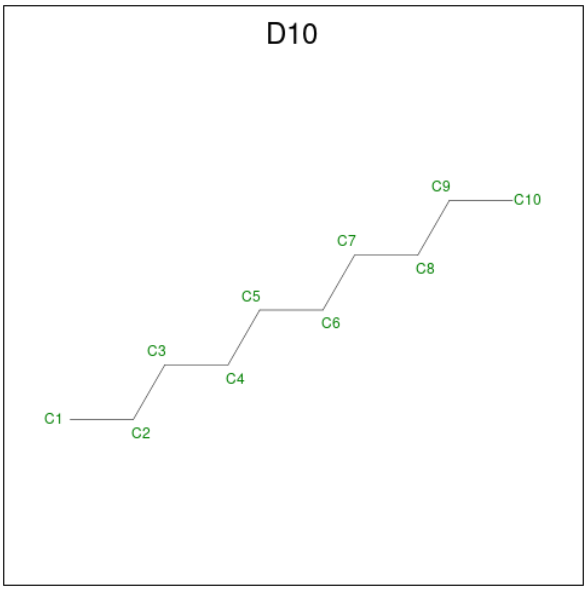
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
7	B	1	50	40	1	8	1	0	0
			Total	C	N	O	P		
7	C	1	50	40	1	8	1	0	0
			Total	C	N	O	P		
7	C	1	50	40	1	8	1	0	0
			Total	C	N	O	P		
7	C	1	50	40	1	8	1	0	0

- Molecule 8 is N-OCTANE (three-letter code: OCT) (formula: C_8H_{18}).



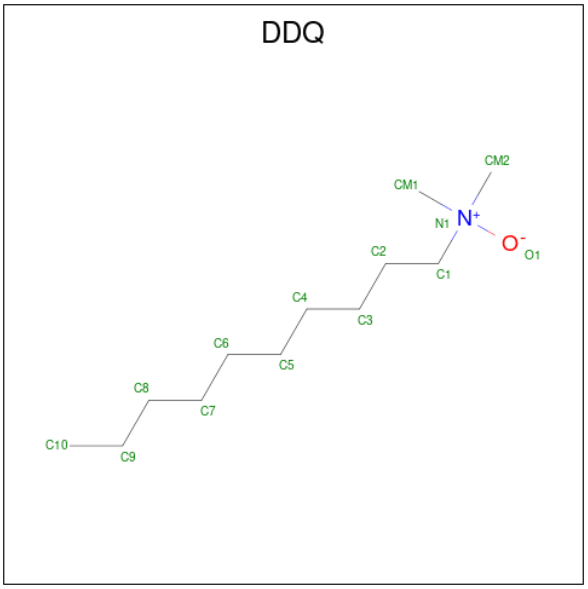
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C 8 8	0	0
8	B	1	Total C 8 8	0	0
8	C	1	Total C 8 8	0	0
8	C	1	Total C 8 8	0	0
8	C	1	Total C 8 8	0	0

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



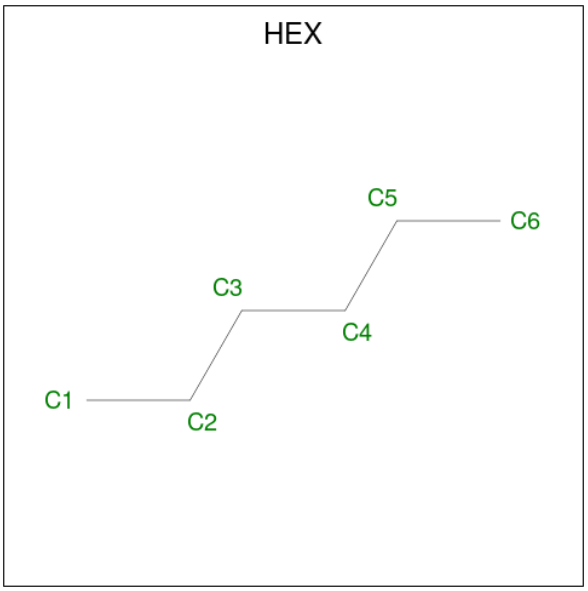
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C		
9	B	1	10	10	0	0
			Total	C		
9	B	1	10	10	0	0
			Total	C		
9	B	1	10	10	0	0
			Total	C		
9	B	1	10	10	0	0
			Total	C		
9	C	1	10	10	0	0

- Molecule 10 is DECYLAMINE-N,N-DIMETHYL-N-OXIDE (three-letter code: DDQ) (formula: $C_{12}H_{27}NO$).



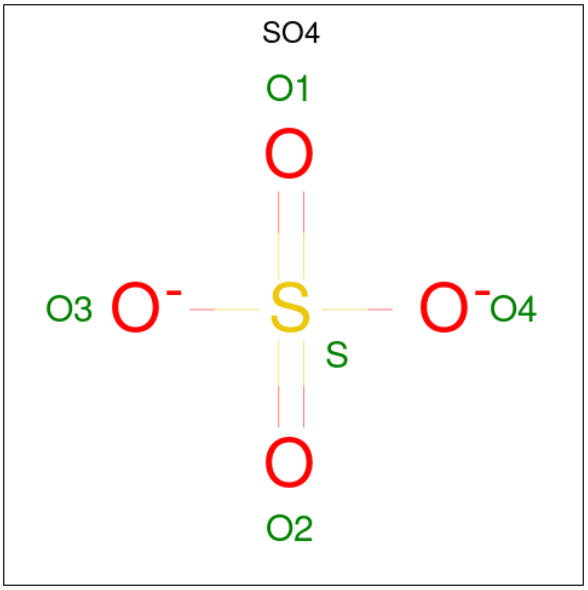
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
10	B	1	14	12	1	1	0	0
			Total	C	N	O		
10	C	1	14	12	1	1	0	0

- Molecule 11 is HEXANE (three-letter code: HEX) (formula: C_6H_{14}).



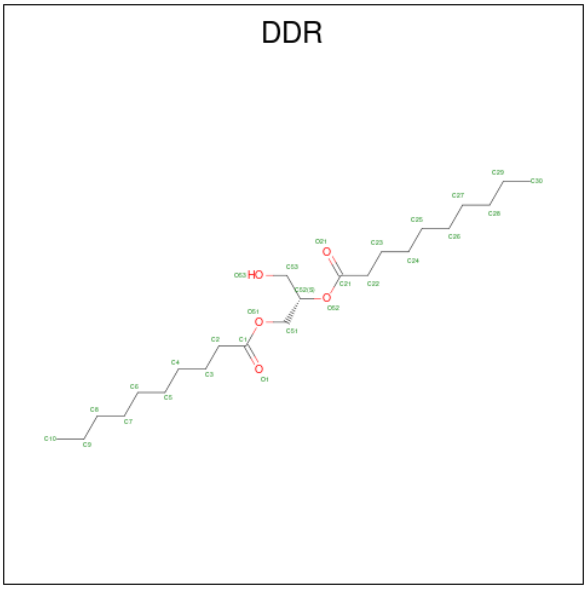
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	1	Total C 6 6	0	0
11	C	1	Total C 6 6	0	0

- Molecule 12 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



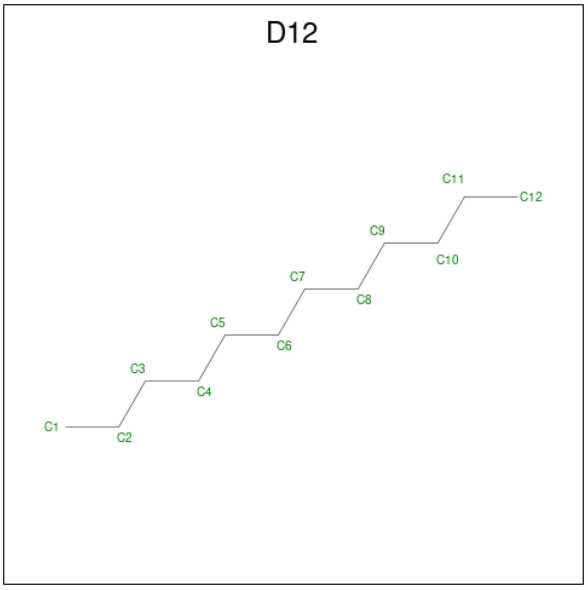
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	B	1	Total O S 5 4 1	0	0
12	C	1	Total O S 5 4 1	0	0

- Molecule 13 is (2S)-3-hydroxypropane-1,2-diyl didecanoate (three-letter code: DDR) (formula: $C_{23}H_{44}O_5$).



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

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



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

- Molecule 15 is water.

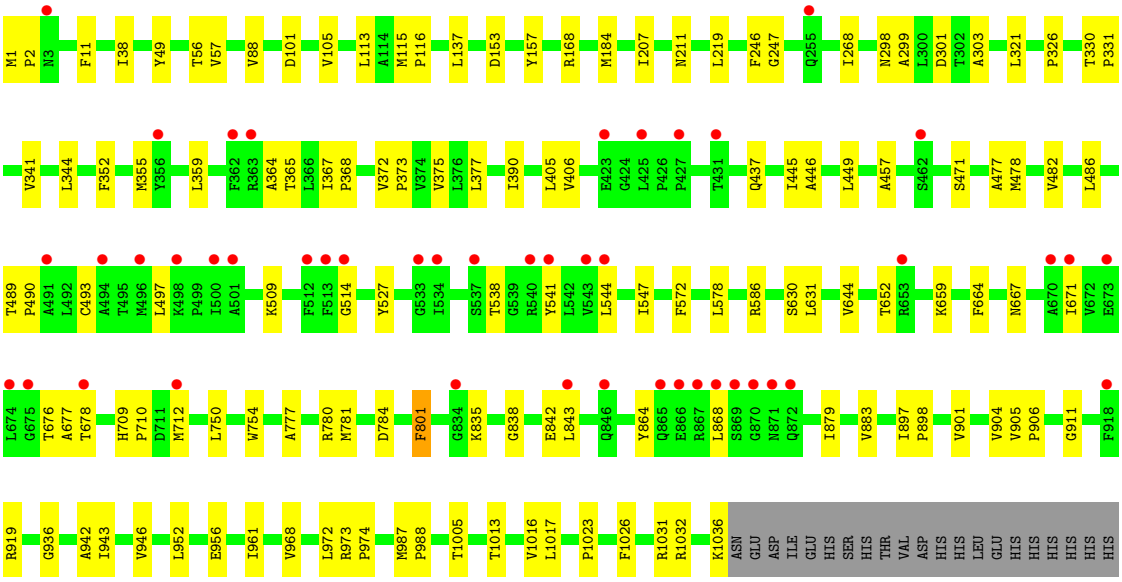
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
15	A	79	79	79	0	0
			Total	O		
15	B	76	76	76	0	0
			Total	O		
15	C	105	105	105	0	0
			Total	O		
15	D	18	18	18	0	0
			Total	O		
15	E	7	7	7	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

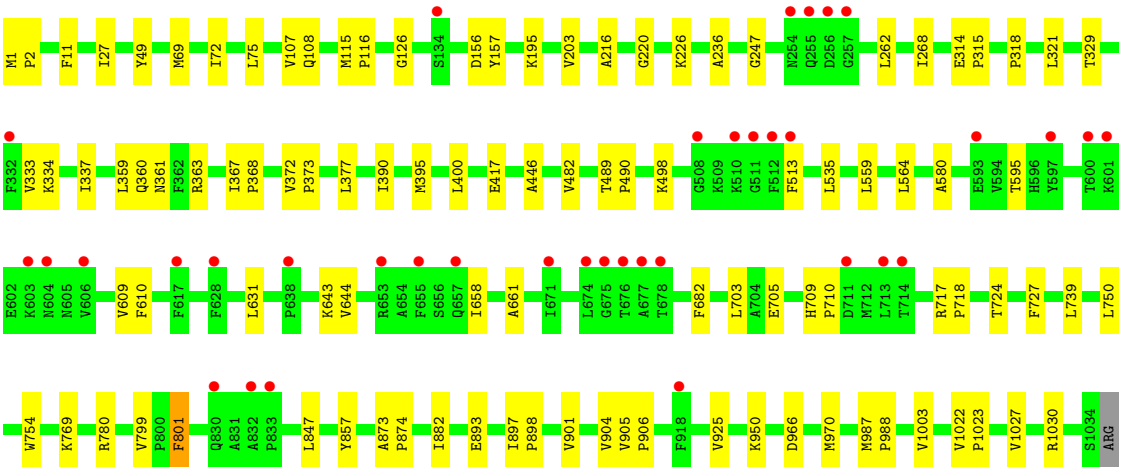
• Molecule 1: Multidrug efflux pump subunit AcrB

Chain A:



• Molecule 1: Multidrug efflux pump subunit AcrB

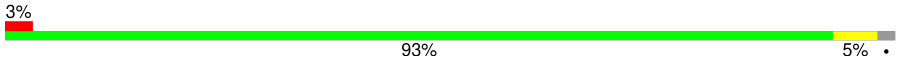
Chain B:



LYS ASN GLU ASP ILE GLU HIS SER HIS THR VAL ASP HIS HIS LEU GLU HIS HIS HIS HIS HIS HIS

- Molecule 1: Multidrug efflux pump subunit AcrB

Chain C:



M1 I10 F11 V14 L25 V32 Y35 P36 Y49 V57 G86 M115 P116 S128 Q213 L219 V253 A303 T330 P331 I337 L359 Q360 N361 F362 R363 I367 P368 L425 P426 I445 V448 V454 P455 M496 L497

I500 G508 G511 F512 F513 G514 W515 R558 I671 L674 A698 Q701 L702 E705 R717 D730 Q733 A736 V741 M781 A803 F804 S805 S806 Y811 L847 K850 A873 P874 V901 V904 V905 P906 L907 A915 F918

S938 A942 I943 L944 E947 M977 M987 P988 M1008 V1012 S1034 ARG LYS ASN GLU ASP ILE GLU HIS SER HIS THR VAL ASP HIS HIS LEU GLU HIS HIS HIS HIS HIS HIS

- Molecule 2: DARPin

Chain D:

MET ARG GLY SER HIS HIS HIS HIS HIS HIS G11 V46 G47 W48 G91 L100 L126 E127 I128 L132 N140 A141 A149 F150 S153 L161 A162 E163 I164 L165 Q166 LYS LEU ASN

- Molecule 2: DARPin

Chain E:

MET ARG GLY SER HIS HIS HIS HIS HIS HIS GLY SER D13 L14 E20 R23 D27 D28 E29 V30 R31 I32 L33 M34 A35 N36 G37 A38 W57 I62 L66 L67 K68 N69 T82 H85 L86 A87 G91 H92 L93 E97 V98 L99 V106 N107 A108 K109

P116 L126 E127 I128 V129 E130 L133 V139 N140 A141 Q142 D143 G146 F150 E163 I164 L165 Q166 LYS LEU ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	145.21Å 162.99Å 245.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.09 – 2.80 49.04 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.09-2.80) 100.0 (49.04-2.80)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.54 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.233 , 0.265 0.234 , 0.264	Depositor DCC
R_{free} test set	7105 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	56.4	Xtriage
Anisotropy	0.537	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 44.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	27045	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.95% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: P6G, D12, PTY, DDR, SO4, LMT, FUA, HEX, DDQ, GOL, D10, 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	0.66	0/8032	0.72	0/10905
1	B	0.66	0/8003	0.71	0/10868
1	C	0.66	0/8011	0.70	0/10879
2	D	0.67	0/1196	0.71	0/1626
2	E	0.67	0/1186	0.71	0/1613
All	All	0.66	0/26428	0.71	0/35891

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7879	0	8034	84	0
1	B	7853	0	8002	57	0
1	C	7858	0	8008	35	0
2	D	1177	0	1159	4	0
2	E	1167	0	1151	8	0
3	A	19	0	26	0	0
4	A	37	0	47	7	0
4	B	37	0	47	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	37	0	47	6	0
5	A	105	0	138	1	0
5	B	105	0	138	1	0
5	C	70	0	92	1	0
6	A	12	0	16	1	0
6	B	6	0	8	0	0
6	C	6	0	8	0	0
6	E	12	0	16	1	0
7	B	50	0	79	8	0
7	C	150	0	237	8	0
8	B	16	0	36	0	0
8	C	24	0	54	0	0
9	B	40	0	88	1	0
9	C	10	0	22	0	0
10	B	14	0	27	1	0
10	C	14	0	27	0	0
11	B	6	0	14	0	0
11	C	6	0	14	0	0
12	B	5	0	0	0	0
12	C	5	0	0	0	0
13	B	28	0	44	0	0
14	B	12	0	26	0	0
15	A	79	0	0	0	0
15	B	76	0	0	0	0
15	C	105	0	0	0	0
15	D	18	0	0	0	0
15	E	7	0	0	0	0
All	All	27045	0	27605	208	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 4.

The worst 5 of 208 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)
4:B:1101:FUA:H122	4:B:1101:FUA:H232	1.54	0.89
4:A:1102:FUA:H202	4:A:1102:FUA:H5	1.54	0.88
4:C:1101:FUA:H202	4:C:1101:FUA:H5	1.62	0.81
7:C:1106:PTY:HC11	7:C:1106:PTY:H322	1.63	0.79
4:B:1101:FUA:H232	4:B:1101:FUA:C12	2.13	0.78

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%)	997 (96%)	36 (4%)	2 (0%)	47 78
1	B	1032/1057 (98%)	1008 (98%)	24 (2%)	0	100 100
1	C	1033/1057 (98%)	1010 (98%)	23 (2%)	0	100 100
2	D	154/169 (91%)	152 (99%)	2 (1%)	0	100 100
2	E	152/169 (90%)	148 (97%)	4 (3%)	0	100 100
All	All	3406/3509 (97%)	3315 (97%)	89 (3%)	2 (0%)	51 81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	677	ALA
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	842/862 (98%)	833 (99%)	9 (1%)	73 92
1	B	839/862 (97%)	829 (99%)	10 (1%)	71 92
1	C	840/862 (97%)	836 (100%)	4 (0%)	88 96
2	D	120/132 (91%)	120 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	E	119/132 (90%)	118 (99%)	1 (1%)	81 94
All	All	2760/2850 (97%)	2736 (99%)	24 (1%)	78 94

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	361	ASN
1	B	801	PHE
1	B	717	ARG
1	B	1030	ARG
1	A	801	PHE

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

Mol	Chain	Res	Type
1	B	846	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

40 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	$\#\|Z\| > 2$
8	OCT	C	1109	-	7,7,7	0.10	0	6,6,6	0.07	0
3	P6G	A	1101	-	18,18,18	0.51	0	17,17,17	0.20	0
6	GOL	A	1107	-	5,5,5	0.09	0	5,5,5	0.28	0
9	D10	B	1109	-	9,9,9	0.09	0	8,8,8	0.09	0
13	DDR	B	1116	-	27,27,27	1.23	2 (7%)	29,29,29	1.18	3 (10%)
5	LMT	B	1104	-	36,36,36	0.43	0	47,47,47	0.94	2 (4%)
5	LMT	A	1103	-	36,36,36	0.41	0	47,47,47	0.71	1 (2%)
7	PTY	B	1105	-	49,49,49	0.30	0	52,54,54	0.38	0
10	DDQ	C	1112	-	11,13,13	2.28	2 (18%)	12,15,15	0.51	0
6	GOL	E	202	-	5,5,5	0.09	0	5,5,5	0.26	0
9	D10	C	1111	-	9,9,9	0.11	0	8,8,8	0.05	0
4	FUA	A	1102	-	39,40,40	1.67	3 (7%)	50,64,64	0.88	1 (2%)
5	LMT	B	1103	-	36,36,36	0.47	0	47,47,47	0.68	0
7	PTY	C	1106	-	49,49,49	0.28	0	52,54,54	0.46	0
8	OCT	C	1110	-	7,7,7	0.10	0	6,6,6	0.11	0
9	D10	B	1110	-	9,9,9	0.11	0	8,8,8	0.14	0
4	FUA	C	1101	-	39,40,40	1.67	2 (5%)	50,64,64	1.03	4 (8%)
14	D12	B	1117	-	11,11,11	0.21	0	10,10,10	0.55	0
11	HEX	C	1113	-	5,5,5	0.13	0	4,4,4	0.07	0
6	GOL	C	1107	-	5,5,5	0.09	0	5,5,5	0.26	0
7	PTY	C	1104	-	49,49,49	0.27	0	52,54,54	0.38	0
8	OCT	B	1108	-	7,7,7	0.11	0	6,6,6	0.17	0
5	LMT	A	1104	-	36,36,36	0.39	0	47,47,47	1.04	3 (6%)
9	D10	B	1111	-	9,9,9	0.14	0	8,8,8	0.13	0
4	FUA	B	1101	-	39,40,40	1.70	2 (5%)	50,64,64	0.94	2 (4%)
8	OCT	B	1107	-	7,7,7	0.09	0	6,6,6	0.11	0
5	LMT	B	1102	-	36,36,36	0.43	0	47,47,47	0.61	0
5	LMT	C	1102	-	36,36,36	0.40	0	47,47,47	0.55	0
5	LMT	A	1105	-	36,36,36	0.43	0	47,47,47	0.57	0
12	SO4	B	1115	-	4,4,4	0.34	0	6,6,6	0.07	0
10	DDQ	B	1113	-	11,13,13	2.28	2 (18%)	12,15,15	0.55	0
6	GOL	A	1106	-	5,5,5	0.09	0	5,5,5	0.24	0
9	D10	B	1112	-	9,9,9	0.12	0	8,8,8	0.07	0
6	GOL	B	1106	-	5,5,5	0.09	0	5,5,5	0.26	0
5	LMT	C	1103	-	36,36,36	0.54	1 (2%)	47,47,47	1.01	4 (8%)
7	PTY	C	1105	-	49,49,49	0.30	0	52,54,54	0.33	0
8	OCT	C	1108	-	7,7,7	0.10	0	6,6,6	0.09	0
6	GOL	E	201	-	5,5,5	0.09	0	5,5,5	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	SO4	C	1114	-	4,4,4	0.34	0	6,6,6	0.08	0
11	HEX	B	1114	-	5,5,5	0.13	0	4,4,4	0.11	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	OCT	C	1109	-	-	2/5/5/5	-
3	P6G	A	1101	-	-	12/16/16/16	-
6	GOL	A	1107	-	-	2/4/4/4	-
9	D10	B	1109	-	-	3/7/7/7	-
13	DDR	B	1116	-	-	18/29/29/29	-
5	LMT	B	1104	-	-	6/21/61/61	0/2/2/2
5	LMT	A	1103	-	-	12/21/61/61	0/2/2/2
7	PTY	B	1105	-	-	30/53/53/53	-
10	DDQ	C	1112	-	-	3/11/11/11	-
6	GOL	E	202	-	-	2/4/4/4	-
9	D10	C	1111	-	-	2/7/7/7	-
4	FUA	A	1102	-	-	7/16/92/92	0/4/4/4
5	LMT	B	1103	-	-	13/21/61/61	0/2/2/2
7	PTY	C	1106	-	-	33/53/53/53	-
8	OCT	C	1110	-	-	4/5/5/5	-
9	D10	B	1110	-	-	5/7/7/7	-
4	FUA	C	1101	-	-	5/16/92/92	0/4/4/4
14	D12	B	1117	-	-	5/9/9/9	-
11	HEX	C	1113	-	-	1/3/3/3	-
6	GOL	C	1107	-	-	1/4/4/4	-
7	PTY	C	1104	-	-	23/53/53/53	-
8	OCT	B	1108	-	-	1/5/5/5	-
5	LMT	A	1104	-	-	4/21/61/61	0/2/2/2
9	D10	B	1111	-	-	5/7/7/7	-
4	FUA	B	1101	-	-	5/16/92/92	0/4/4/4
8	OCT	B	1107	-	-	4/5/5/5	-
5	LMT	B	1102	-	-	9/21/61/61	0/2/2/2
5	LMT	C	1102	-	-	8/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	LMT	A	1105	-	-	11/21/61/61	0/2/2/2
10	DDQ	B	1113	-	-	2/11/11/11	-
6	GOL	A	1106	-	-	0/4/4/4	-
9	D10	B	1112	-	-	2/7/7/7	-
6	GOL	B	1106	-	-	2/4/4/4	-
5	LMT	C	1103	-	-	11/21/61/61	0/2/2/2
7	PTY	C	1105	-	-	25/53/53/53	-
8	OCT	C	1108	-	-	3/5/5/5	-
6	GOL	E	201	-	-	0/4/4/4	-
11	HEX	B	1114	-	-	0/3/3/3	-

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1101	FUA	C29-C22	-9.96	1.33	1.47
4	C	1101	FUA	C29-C22	-9.71	1.34	1.47
4	A	1102	FUA	C29-C22	-9.51	1.34	1.47
10	B	1113	DDQ	O1-N1	-6.80	1.25	1.42
10	C	1112	DDQ	O1-N1	-6.77	1.25	1.42

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	B	1116	DDR	O52-C21-C22	3.56	119.17	111.48
5	A	1104	LMT	O5'-C5'-C4'	3.11	116.15	109.72
5	B	1104	LMT	O5'-C5'-C4'	3.10	116.14	109.72
4	C	1101	FUA	C10-C5-C4	-3.05	109.50	113.20
5	A	1104	LMT	C1'-O5'-C5'	2.87	119.32	113.72

There are no chirality outliers.

5 of 281 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1102	FUA	C23-C22-C29-O4
4	A	1102	FUA	C23-C22-C29-O5
4	B	1101	FUA	C23-C22-C29-O4
4	B	1101	FUA	C23-C22-C29-O5
4	B	1101	FUA	C32-C31-O2-C16

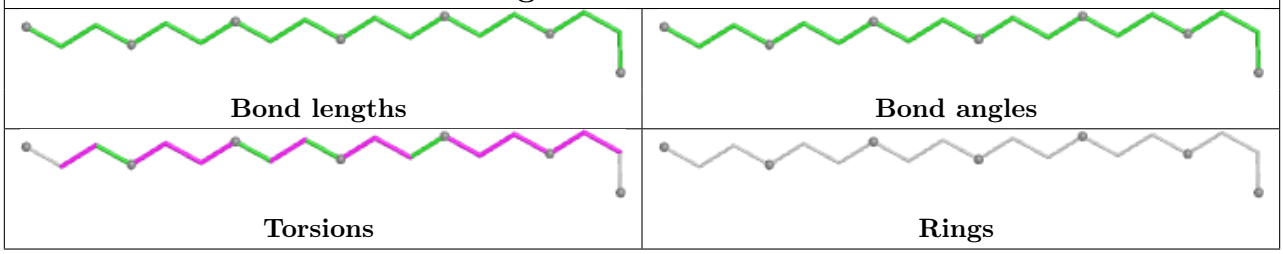
There are no ring outliers.

13 monomers are involved in 40 short contacts:

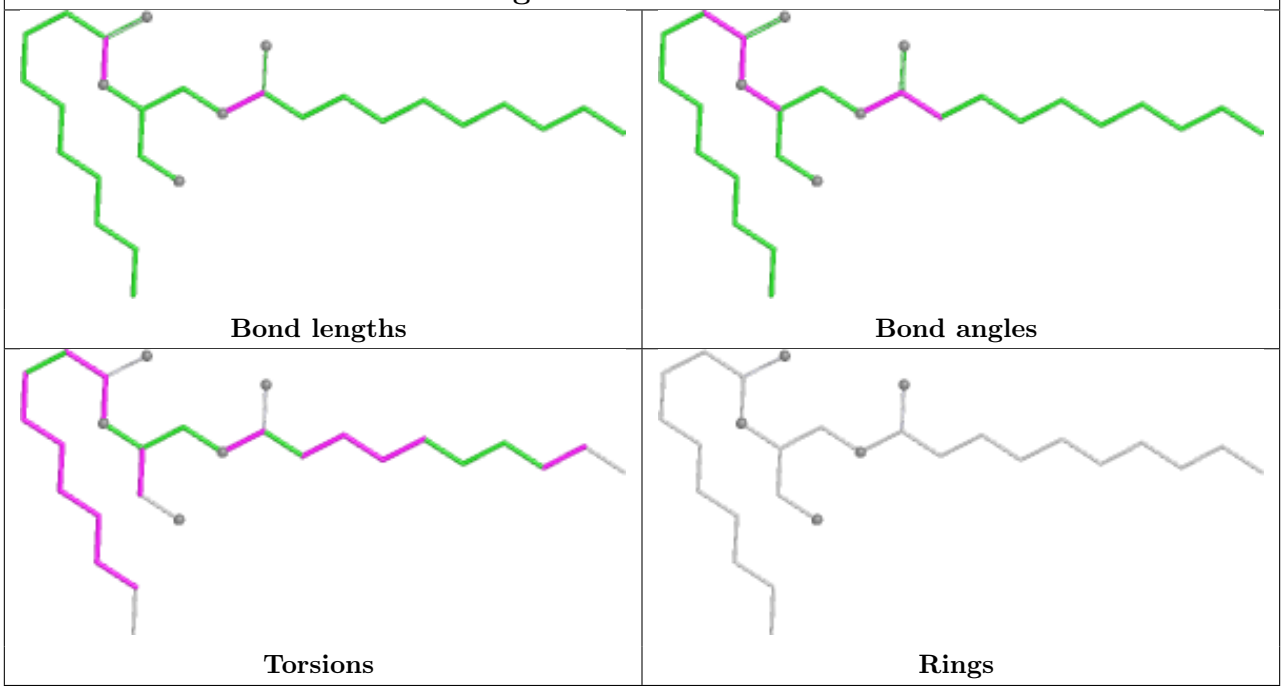
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1107	GOL	1	0
7	B	1105	PTY	8	0
4	A	1102	FUA	7	0
5	B	1103	LMT	1	0
7	C	1106	PTY	6	0
4	C	1101	FUA	6	0
7	C	1104	PTY	2	0
5	A	1104	LMT	1	0
9	B	1111	D10	1	0
4	B	1101	FUA	7	0
10	B	1113	DDQ	1	0
5	C	1103	LMT	1	0
6	E	201	GOL	1	0

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 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.

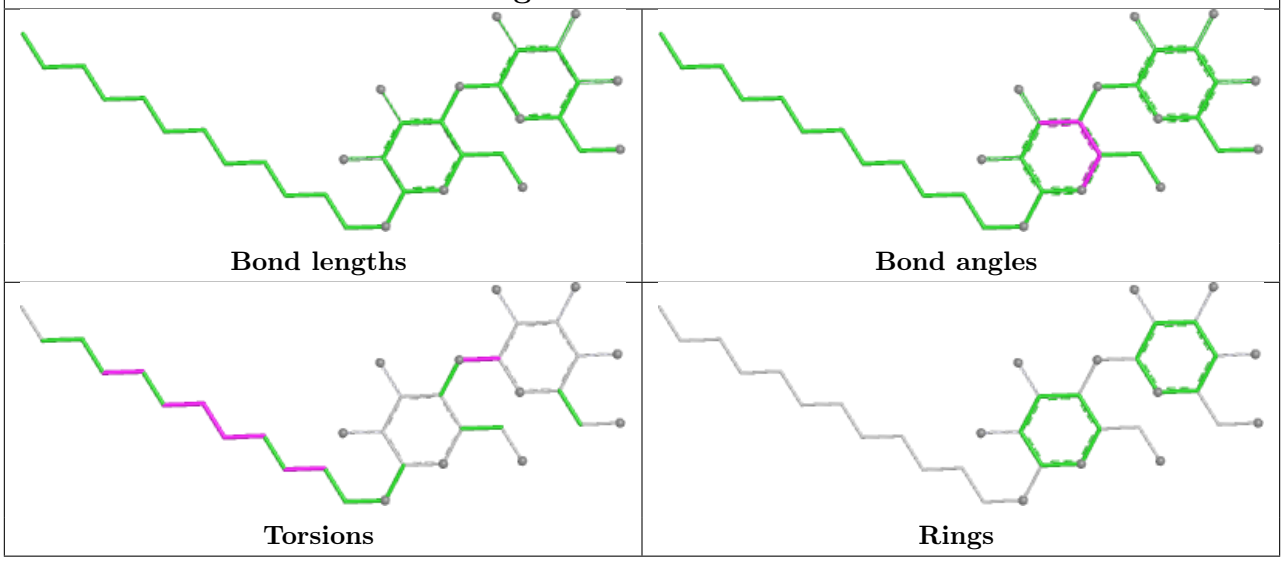
Ligand P6G A 1101



Ligand DDR B 1116



Ligand LMT B 1104



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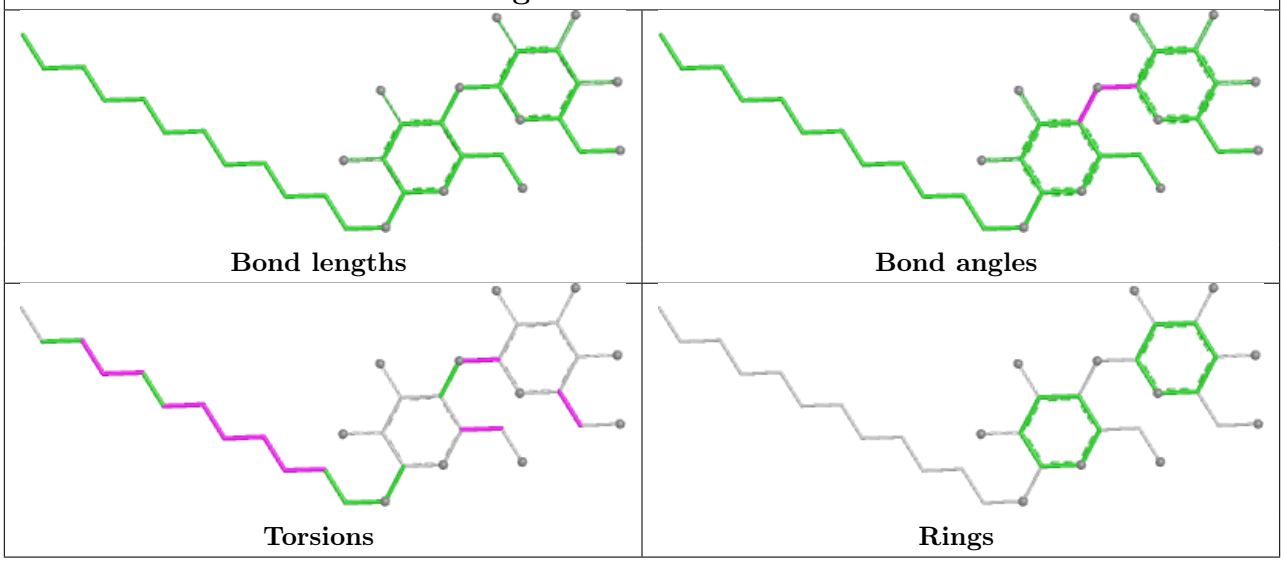

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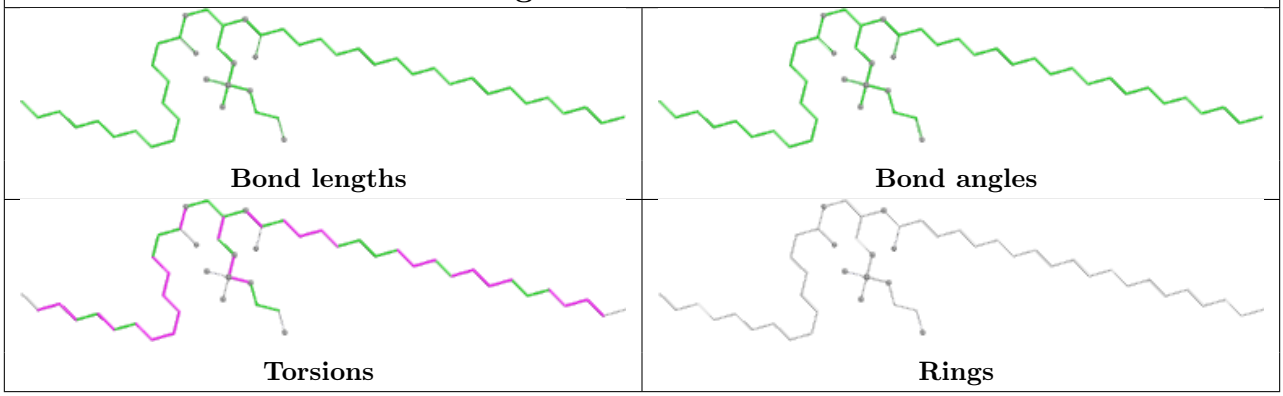

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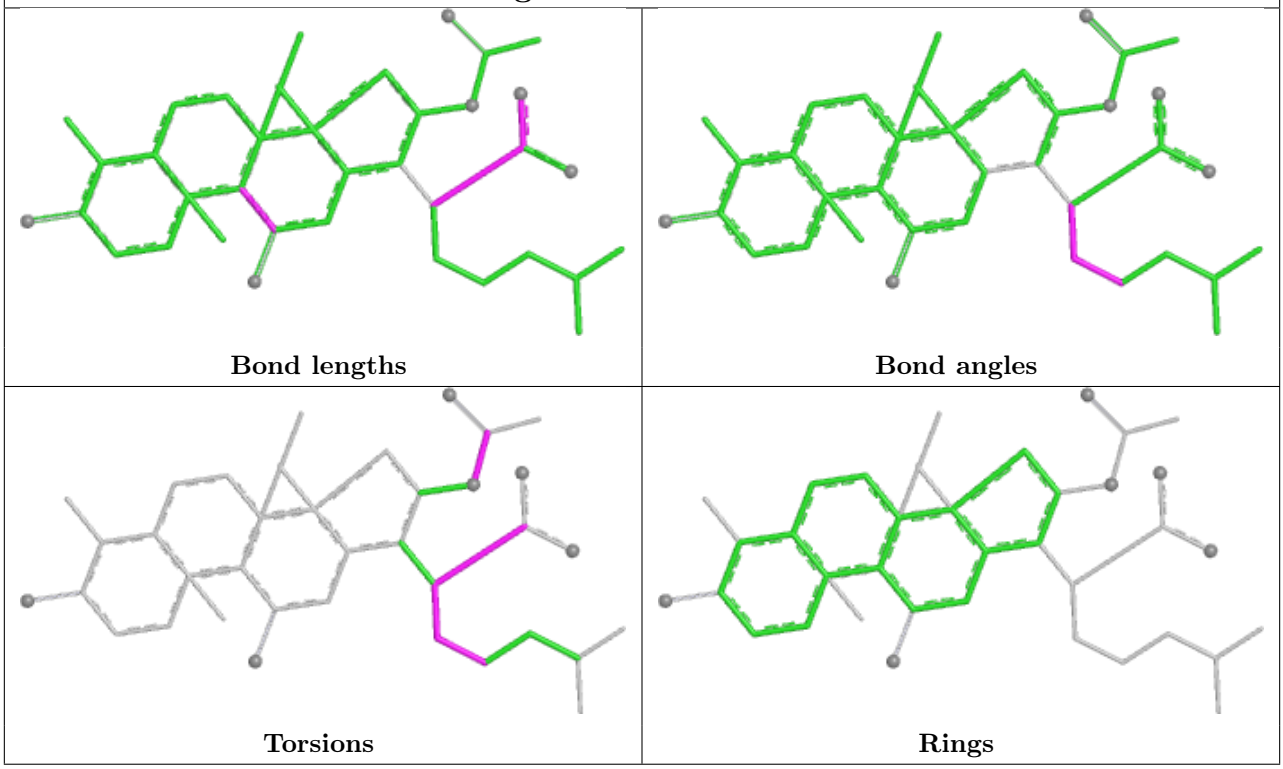

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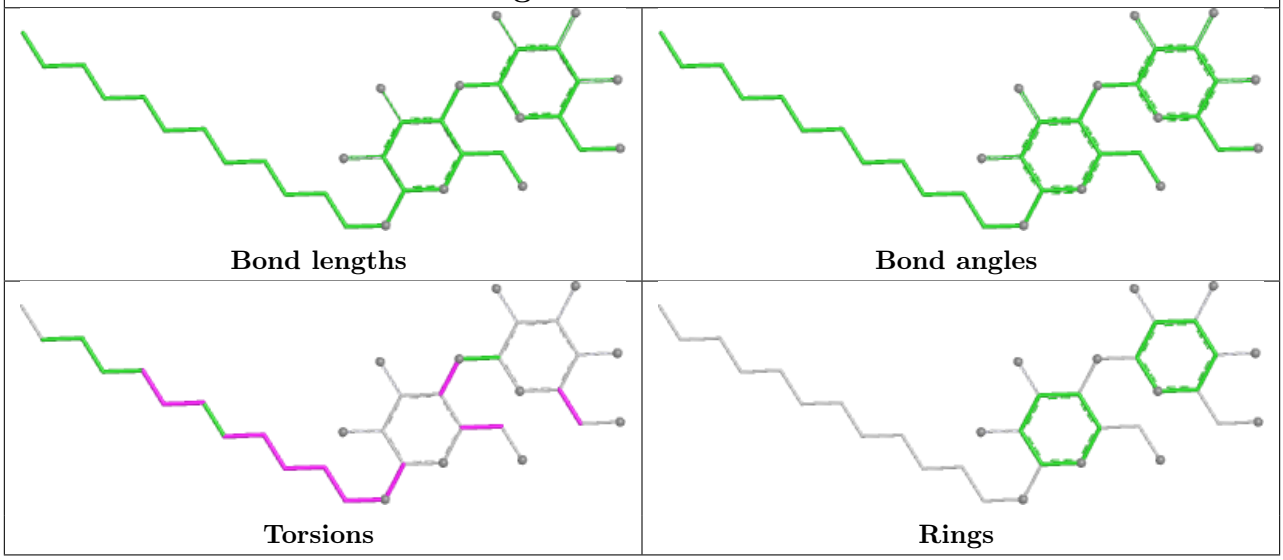

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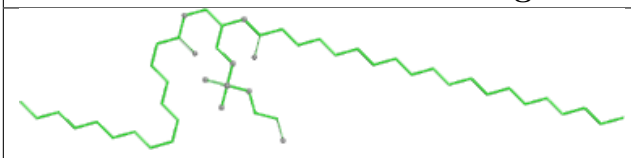
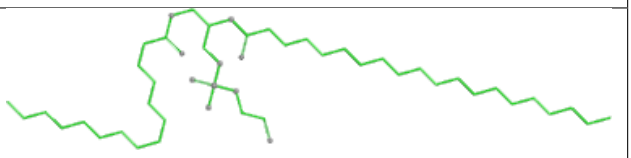
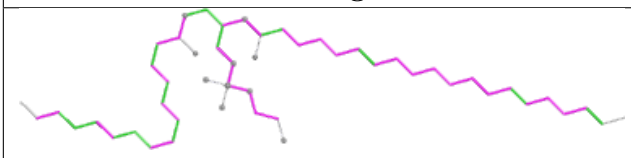


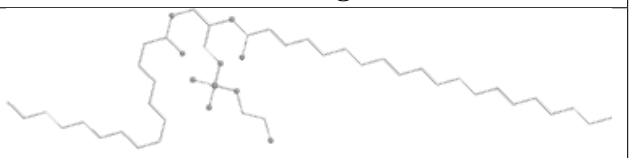
Bond lengths



Bond angles

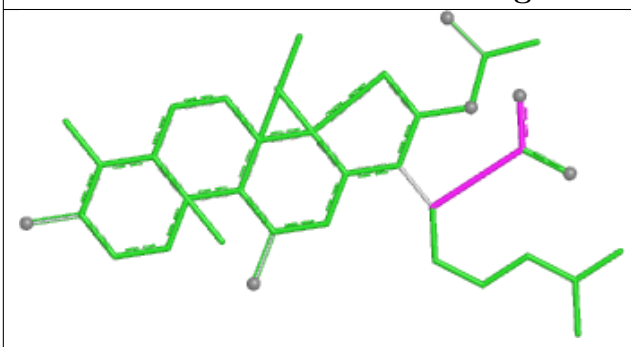


Torsions



Rings

Ligand FUA C 1101



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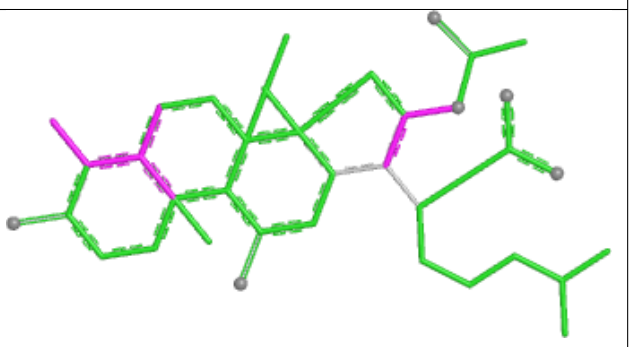
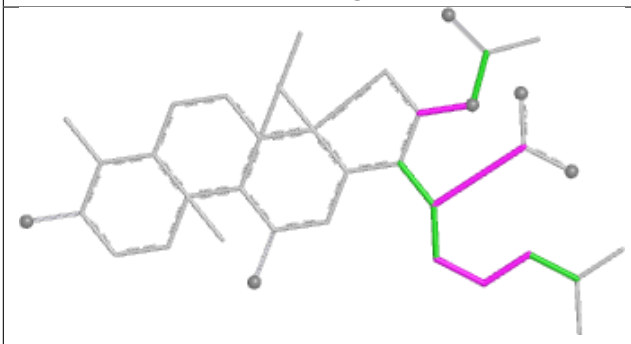
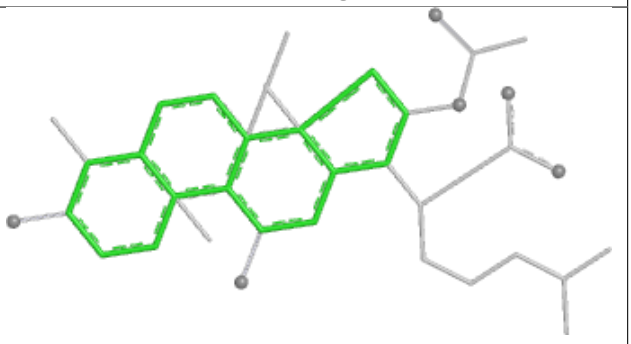


Bond angles

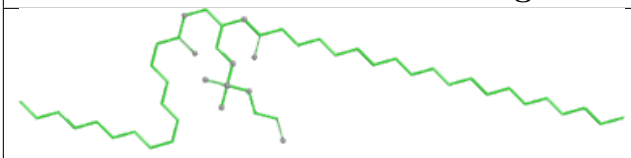


Torsions

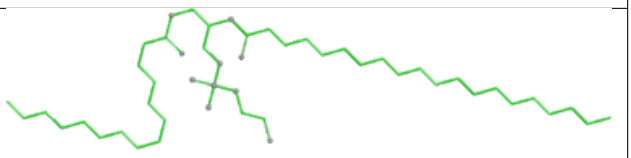


Rings

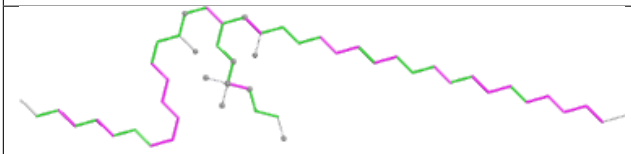
Ligand PTY C 1104



Bond lengths



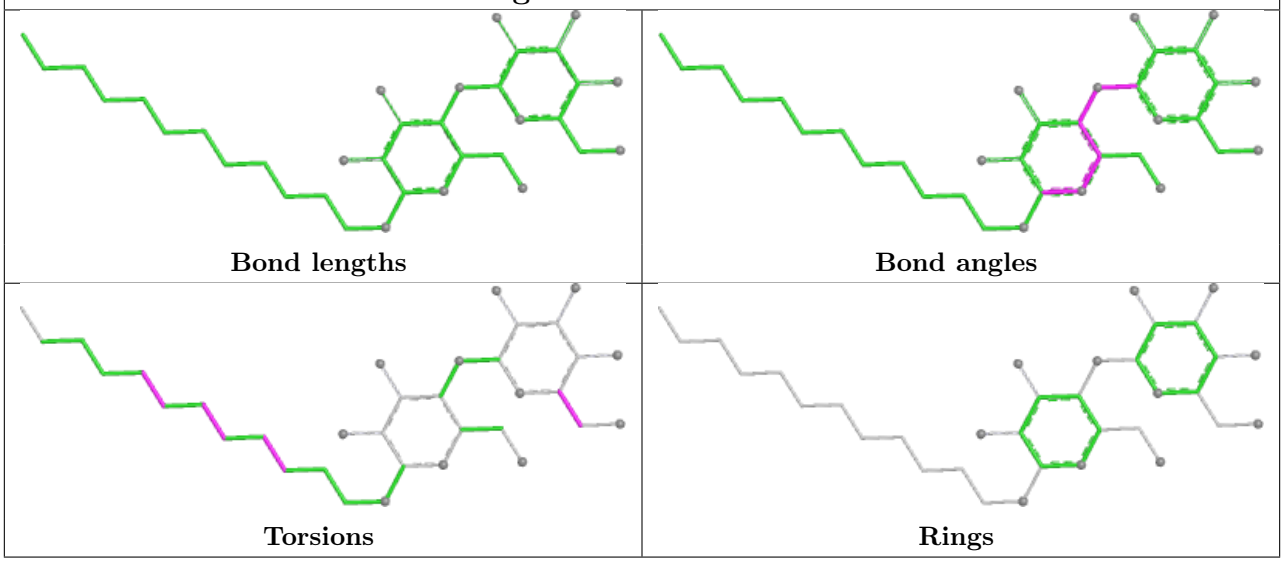
Bond angles



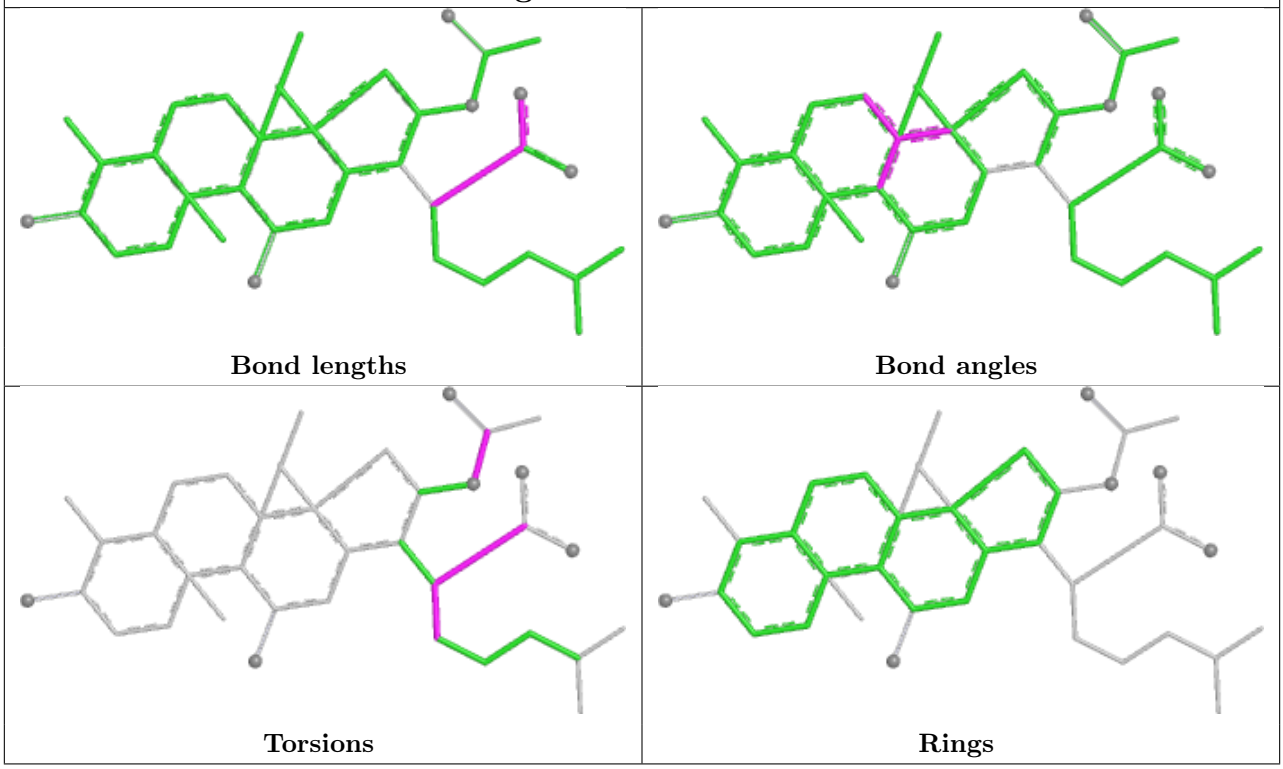
Torsions

Rings

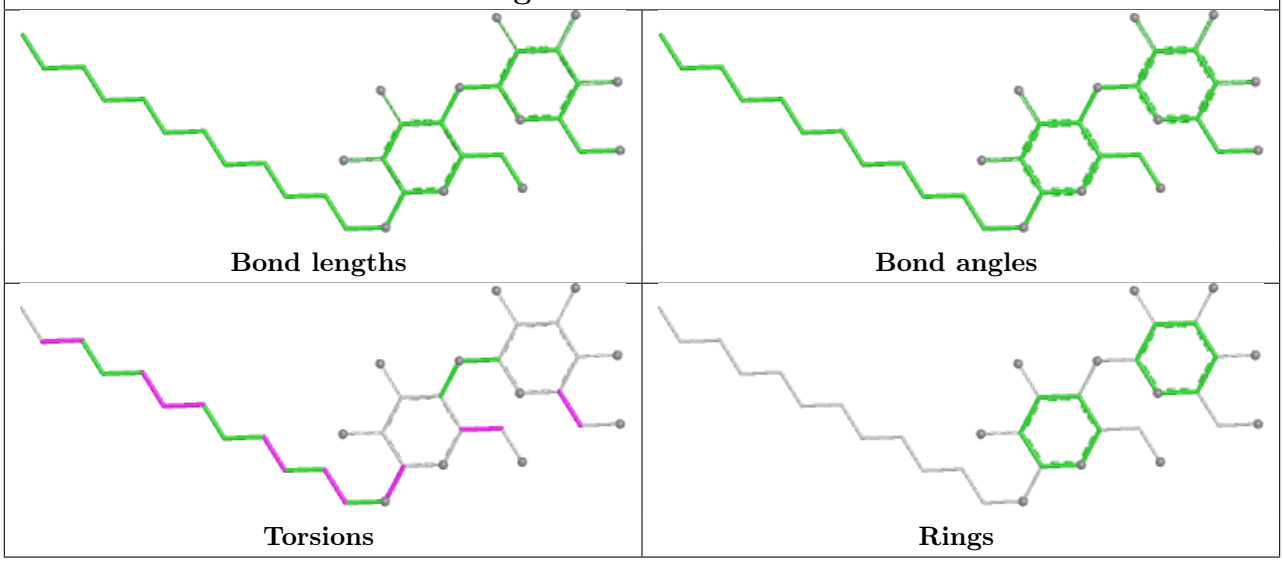
Ligand LMT A 1104



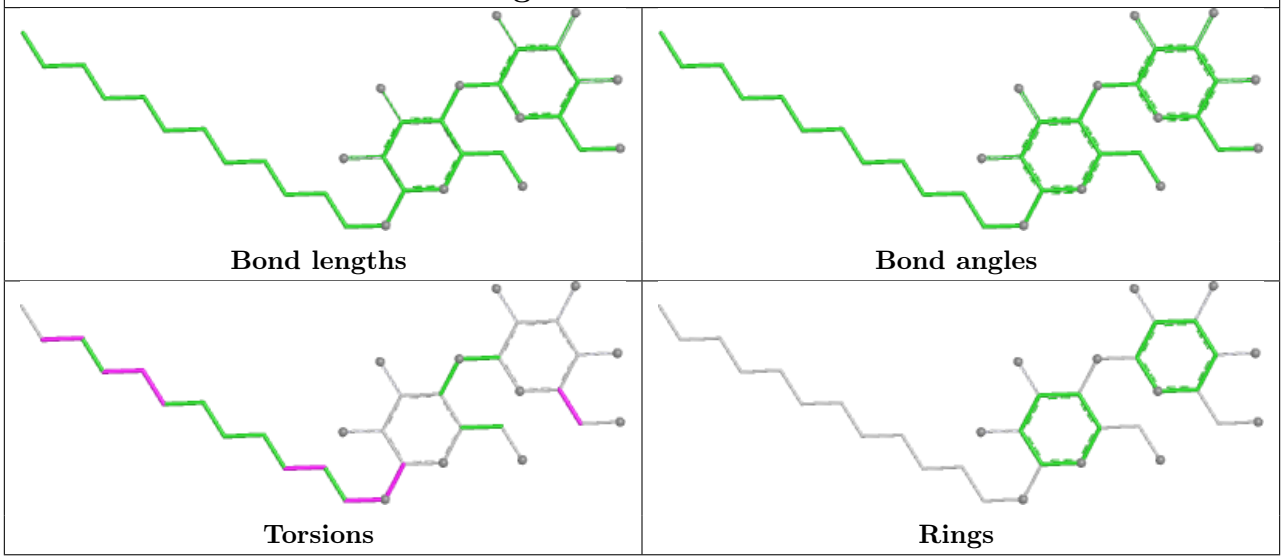
Ligand FUA B 1101



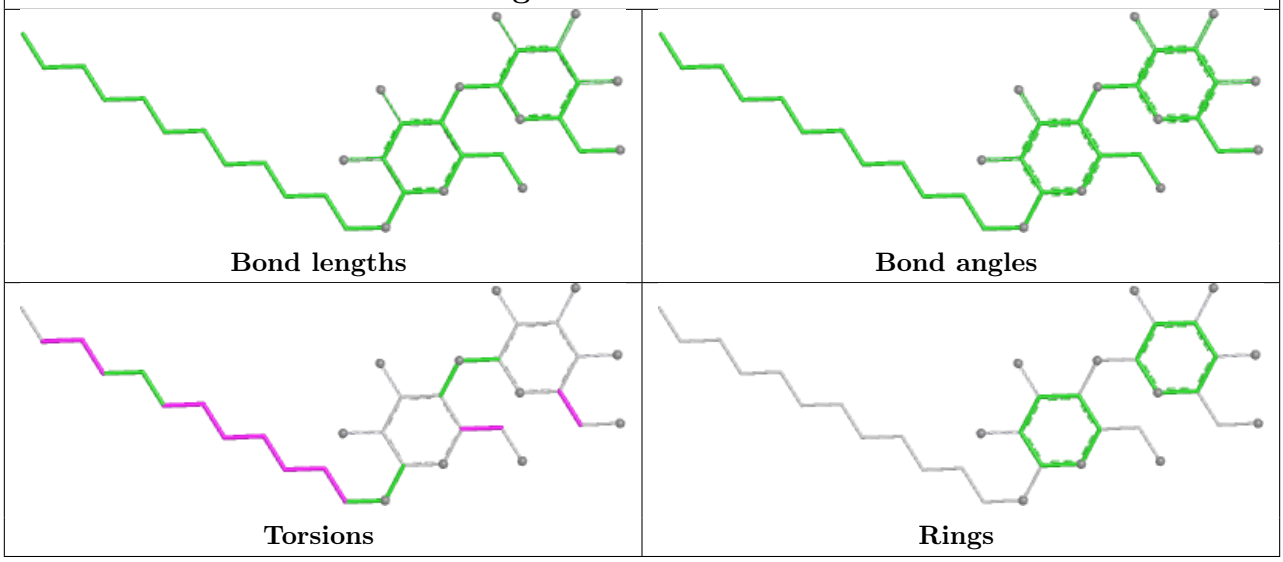
Ligand LMT B 1102

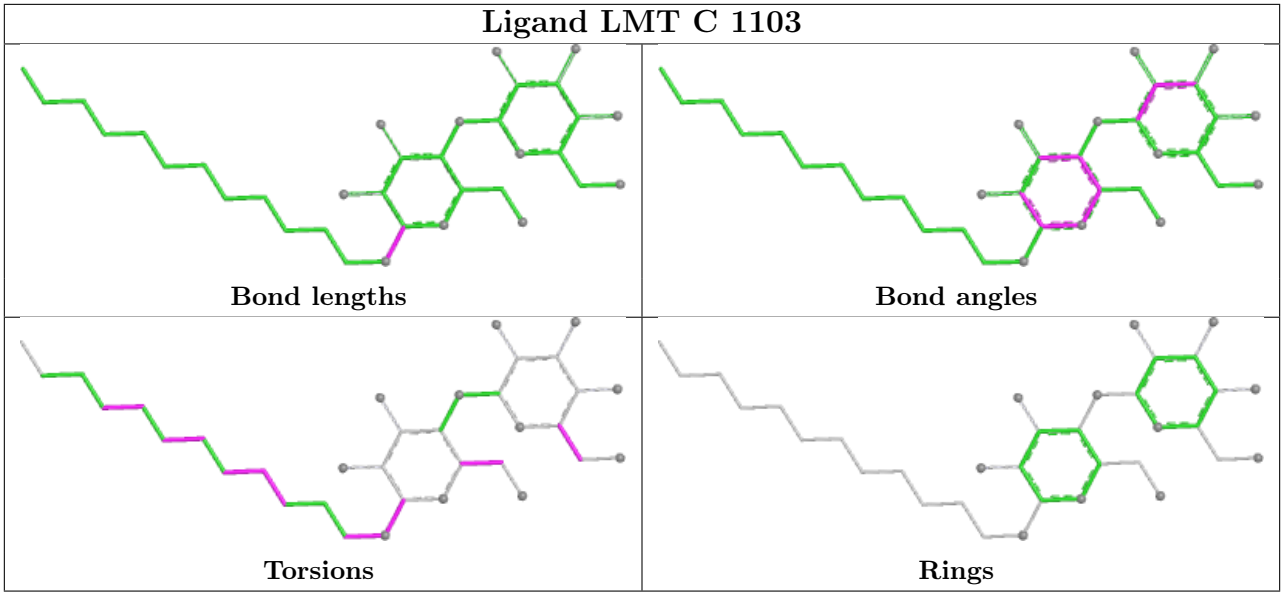


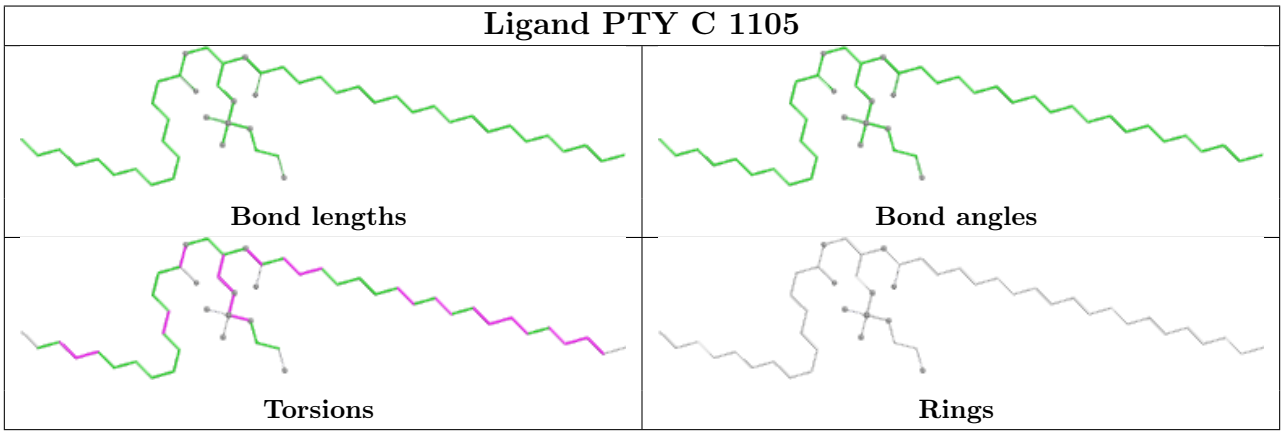
Ligand LMT C 1102



Ligand LMT A 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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1036/1057 (98%)	0.21	46 (4%)	34	24	40, 69, 105, 127	1 (0%)
1	B	1034/1057 (97%)	0.09	37 (3%)	42	32	40, 62, 86, 103	1 (0%)
1	C	1034/1057 (97%)	0.15	28 (2%)	54	44	42, 55, 79, 94	0
2	D	156/169 (92%)	0.46	11 (7%)	16	9	51, 62, 81, 98	0
2	E	154/169 (91%)	1.09	33 (21%)	0	0	60, 75, 98, 104	0
All	All	3414/3509 (97%)	0.21	155 (4%)	33	23	40, 61, 94, 127	2 (0%)

The worst 5 of 155 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	35	ALA	8.3
1	B	678	THR	6.6
2	D	11	GLY	6.4
1	A	675	GLY	6.1
2	E	31	ARG	5.2

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,

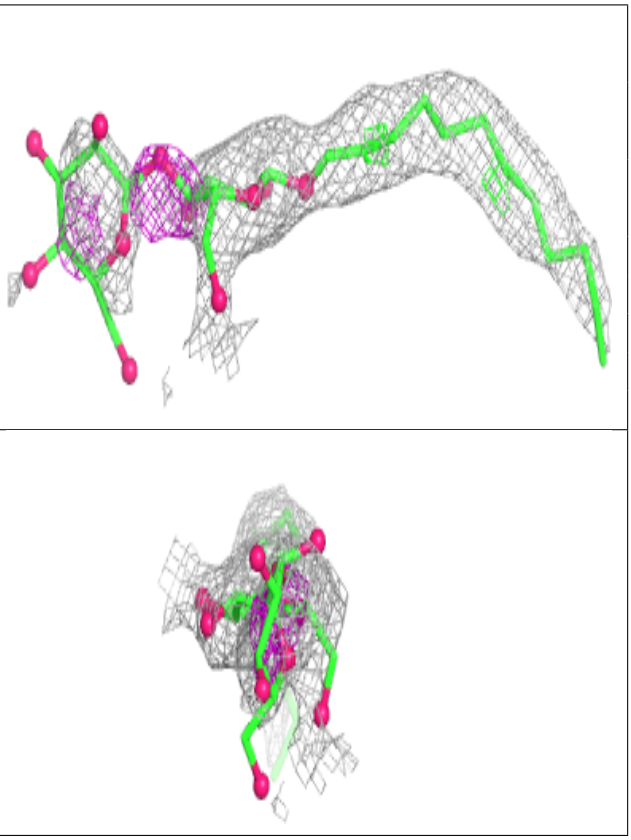
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

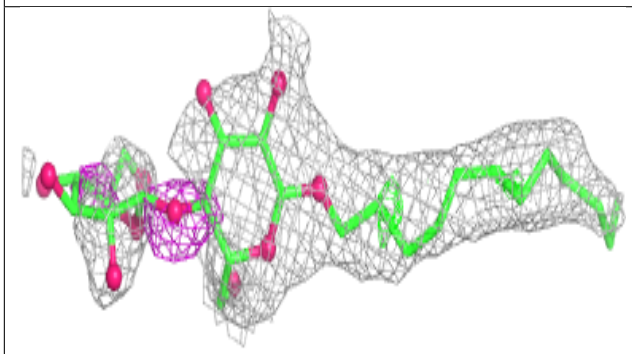
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	LMT	B	1104	35/35	0.56	0.42	91,114,123,123	0
8	OCT	C	1108	8/8	0.69	0.32	67,68,68,68	0
7	PTY	B	1105	50/50	0.70	0.44	106,123,136,137	0
7	PTY	C	1106	50/50	0.72	0.37	96,112,125,127	0
5	LMT	C	1103	35/35	0.73	0.45	93,112,114,114	0
4	FUA	A	1102	37/37	0.74	0.39	98,100,100,100	37
13	DDR	B	1116	28/28	0.74	0.41	95,104,105,107	0
7	PTY	C	1105	50/50	0.75	0.28	83,88,97,99	0
6	GOL	A	1106	6/6	0.76	0.34	70,71,71,72	0
10	DDQ	B	1113	14/14	0.76	0.29	97,102,107,107	0
5	LMT	A	1104	35/35	0.76	0.39	104,117,129,130	0
8	OCT	C	1109	8/8	0.77	0.30	78,79,80,80	0
7	PTY	C	1104	50/50	0.79	0.31	91,112,121,123	0
11	HEX	B	1114	6/6	0.80	0.41	64,64,64,64	0
4	FUA	C	1101	37/37	0.81	0.46	90,94,96,96	37
5	LMT	A	1103	35/35	0.81	0.35	93,104,109,109	0
8	OCT	C	1110	8/8	0.81	0.32	80,81,81,81	0
10	DDQ	C	1112	14/14	0.82	0.28	83,83,84,84	0
9	D10	B	1109	10/10	0.82	0.33	69,70,70,70	0
8	OCT	B	1107	8/8	0.82	0.22	88,90,90,90	0
14	D12	B	1117	12/12	0.82	0.26	85,86,87,87	0
3	P6G	A	1101	19/19	0.85	0.26	45,46,47,47	0
5	LMT	B	1103	35/35	0.85	0.27	84,89,90,91	0
8	OCT	B	1108	8/8	0.85	0.34	85,86,86,86	0
5	LMT	B	1102	35/35	0.86	0.33	83,89,94,94	0
6	GOL	A	1107	6/6	0.86	0.26	69,70,70,70	0
6	GOL	B	1106	6/6	0.86	0.29	81,82,83,83	0
9	D10	B	1111	10/10	0.88	0.29	71,71,72,72	0
5	LMT	A	1105	35/35	0.88	0.42	107,112,116,116	0
4	FUA	B	1101	37/37	0.89	0.28	79,81,84,84	0
9	D10	B	1110	10/10	0.89	0.23	73,74,74,74	0
6	GOL	C	1107	6/6	0.90	0.27	52,53,53,54	0
6	GOL	E	202	6/6	0.90	0.18	85,85,86,86	0
9	D10	C	1111	10/10	0.90	0.37	73,74,74,74	0
5	LMT	C	1102	35/35	0.90	0.29	72,74,76,76	0
9	D10	B	1112	10/10	0.91	0.20	73,74,74,74	0
11	HEX	C	1113	6/6	0.92	0.43	33,33,33,33	0
6	GOL	E	201	6/6	0.93	0.18	72,72,73,73	0
12	SO4	B	1115	5/5	0.97	0.12	82,83,83,83	0
12	SO4	C	1114	5/5	0.97	0.10	74,74,75,75	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around LMT B 1104:

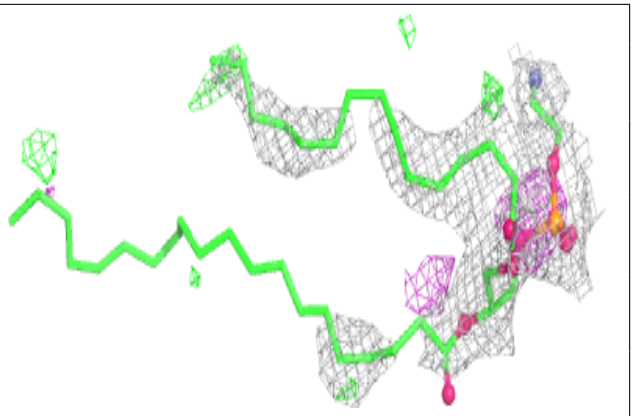
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

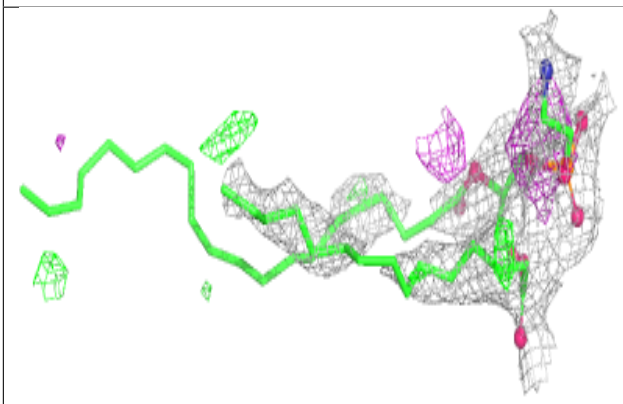




Electron density around PTY B 1105:

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





Electron density around PTY C 1106:

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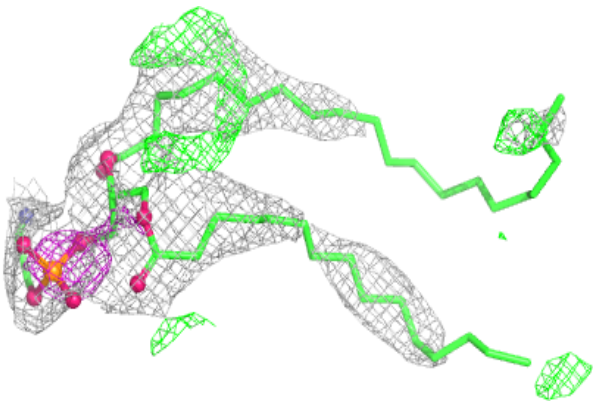
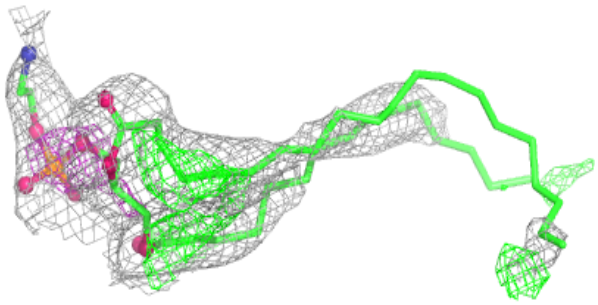
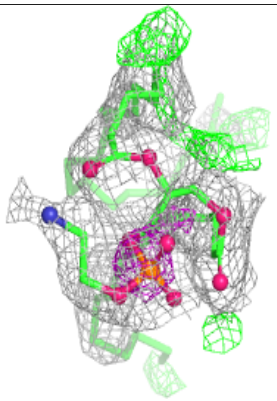
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

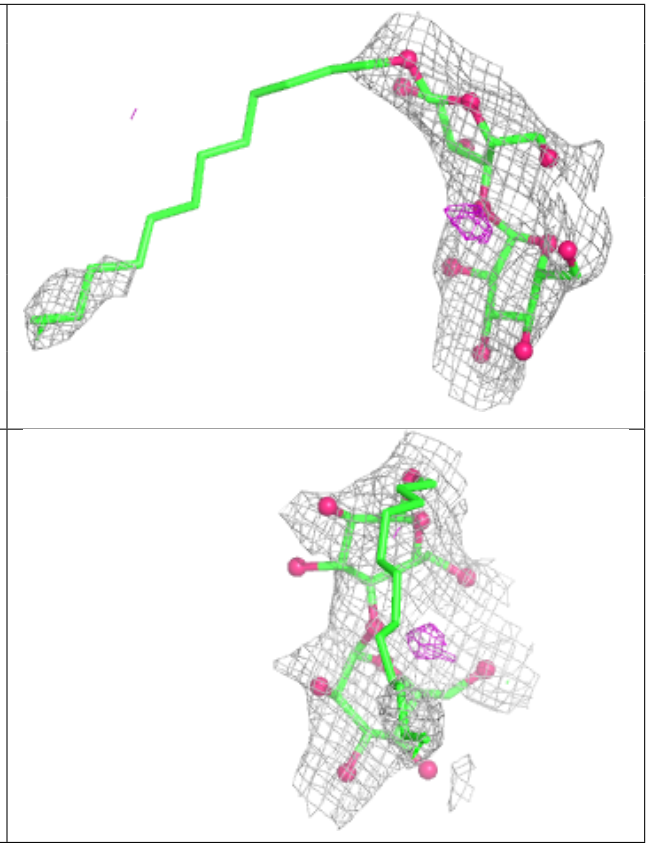






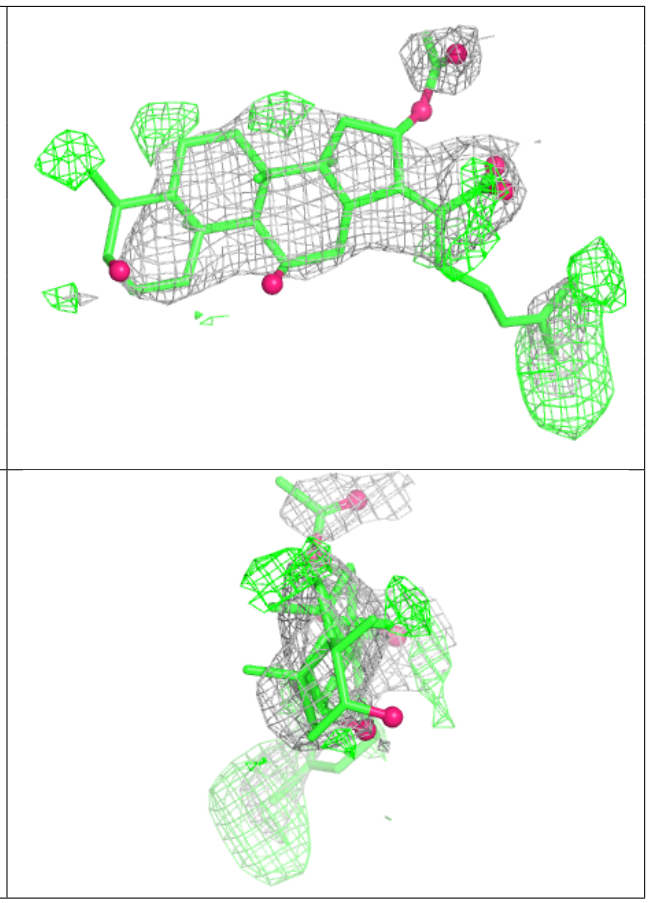
Electron density around LMT C 1103:

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



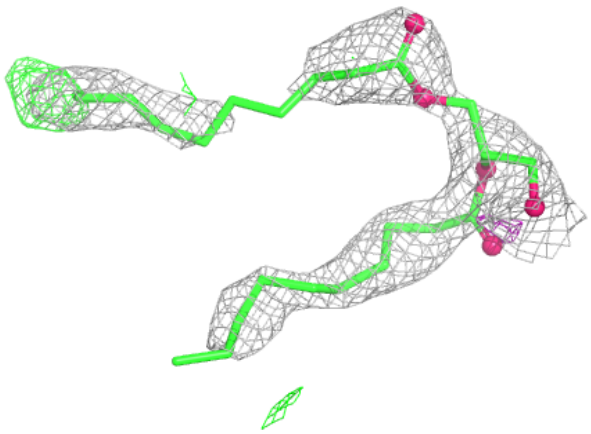
Electron density around FUA A 1102:

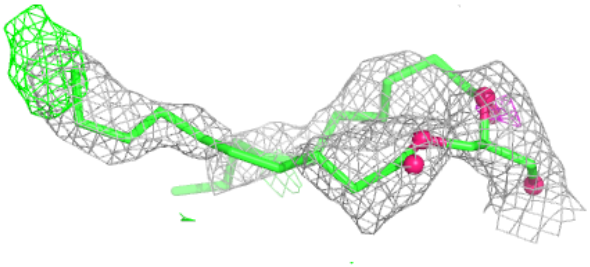
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

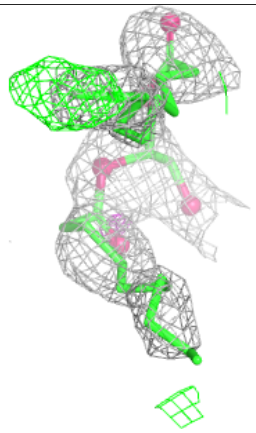


Electron density around DDR B 1116:

$2mF_o$-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 1105:

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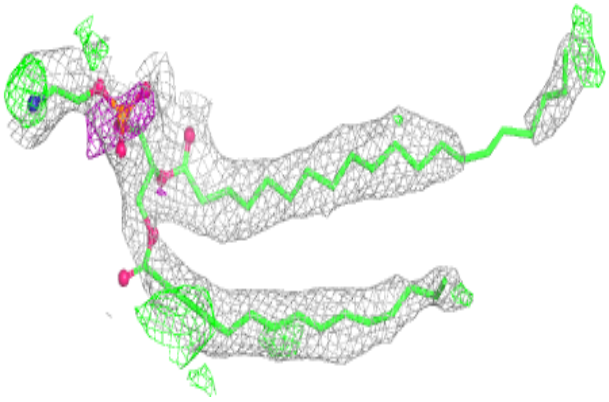
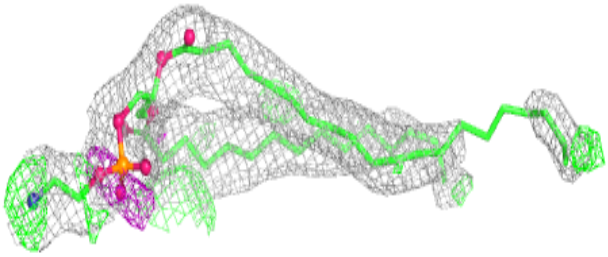
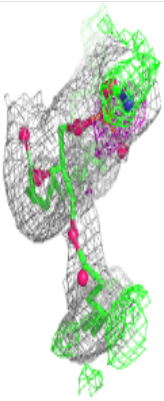
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around LMT A 1104:

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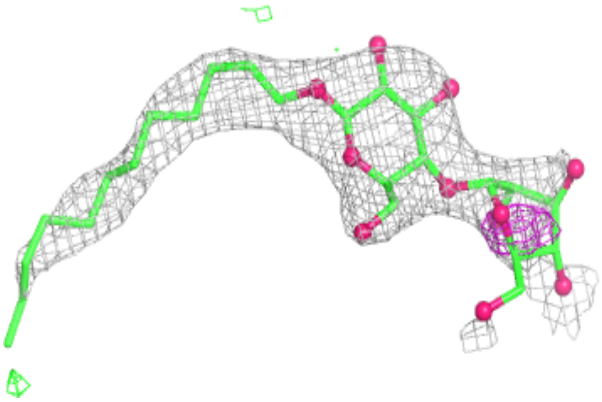
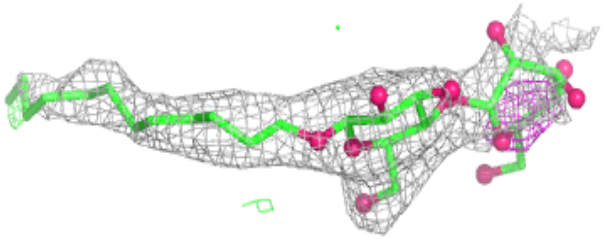
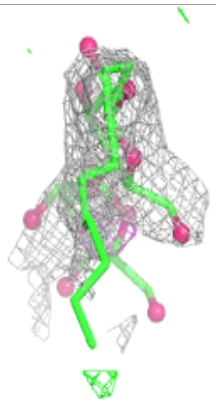
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

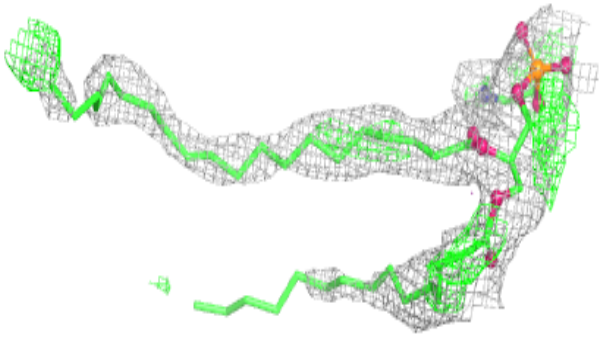


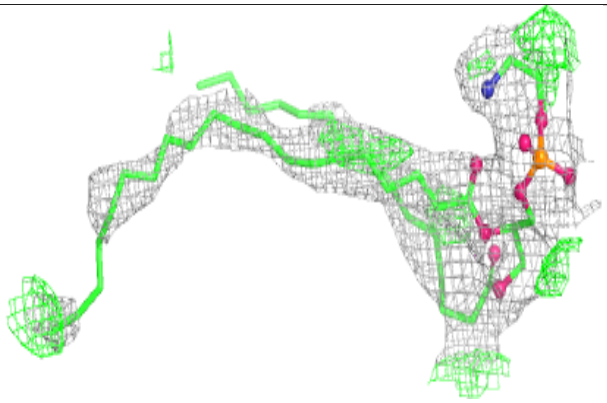


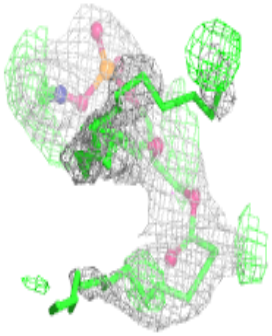


Electron density around PTY C 1104:

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

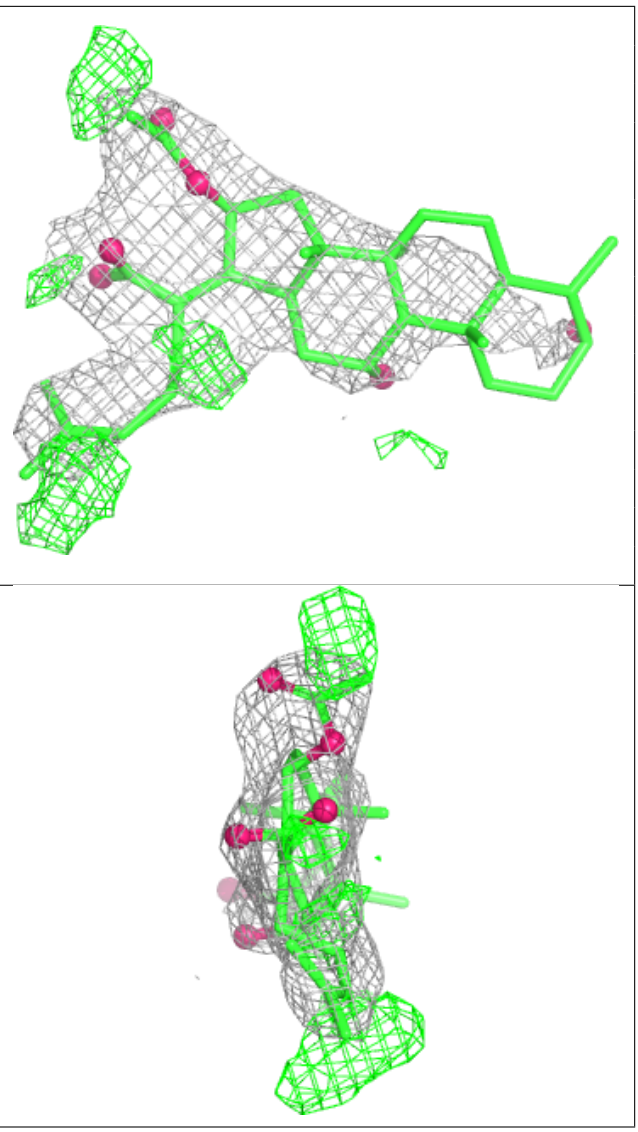






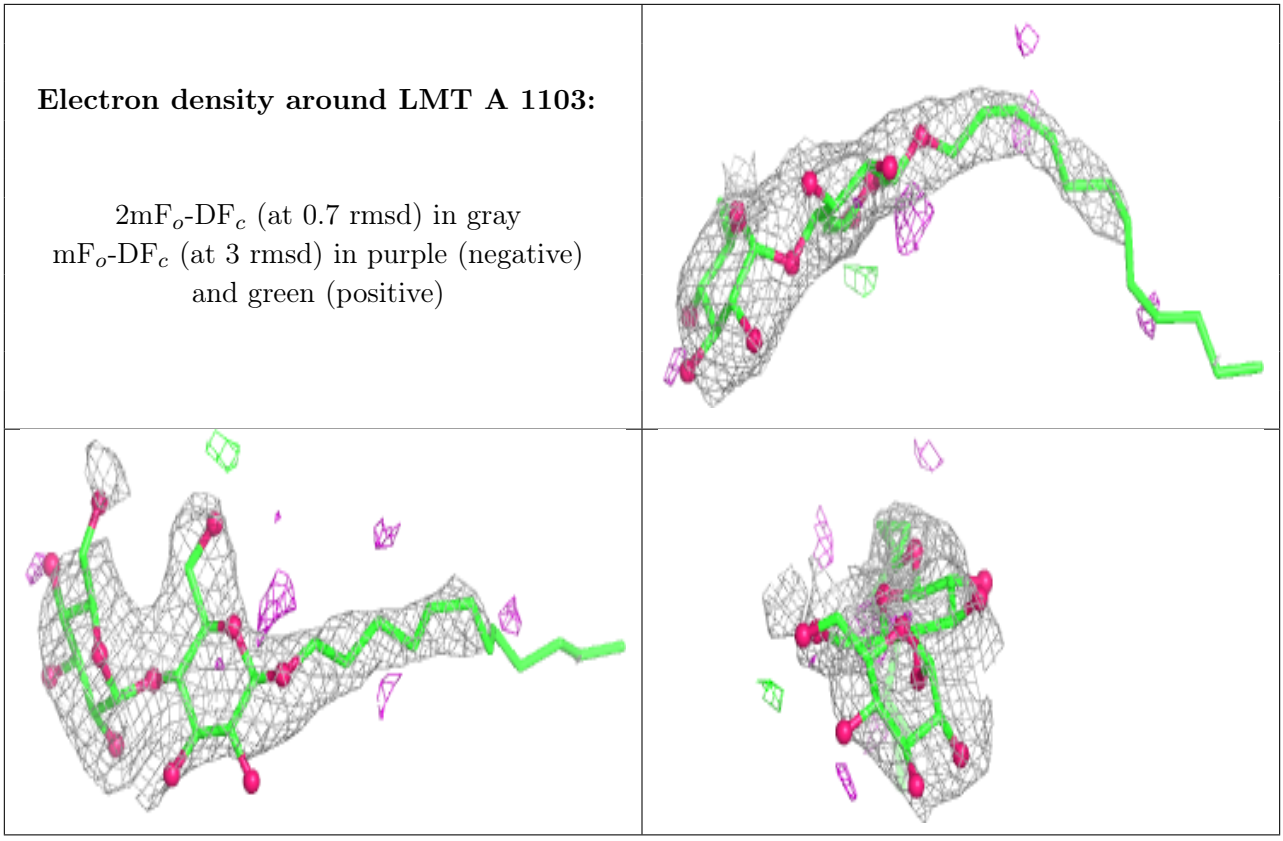
Electron density around FUA C 1101:

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



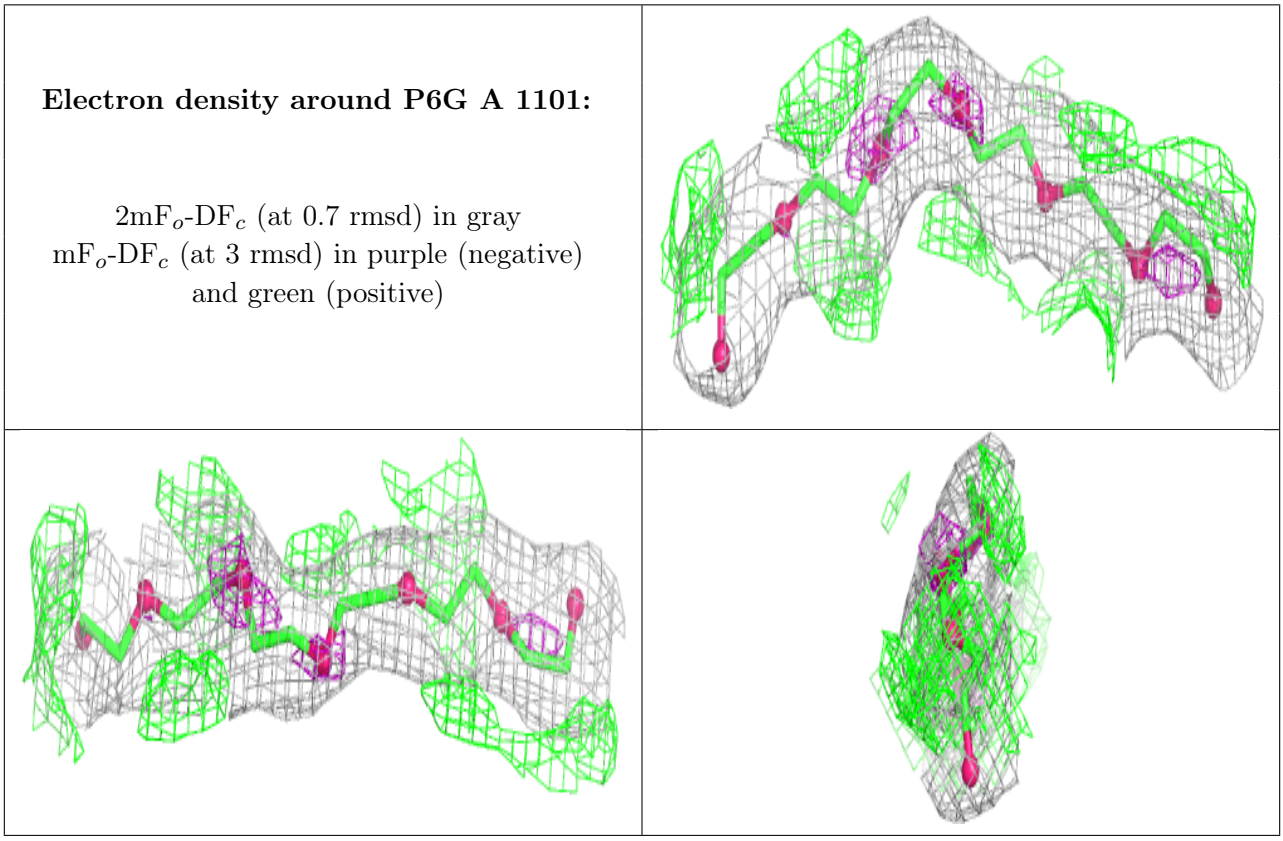
Electron density around LMT A 1103:

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



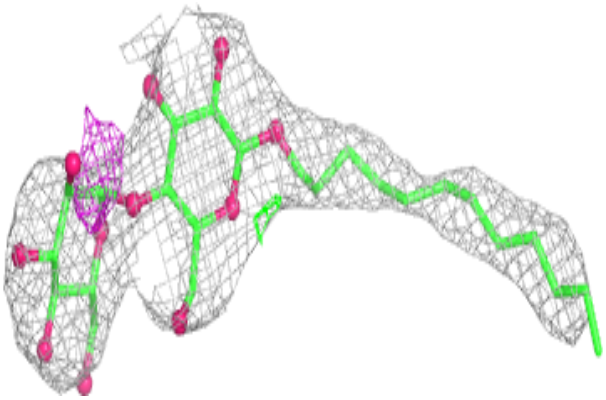
Electron density around P6G A 1101:

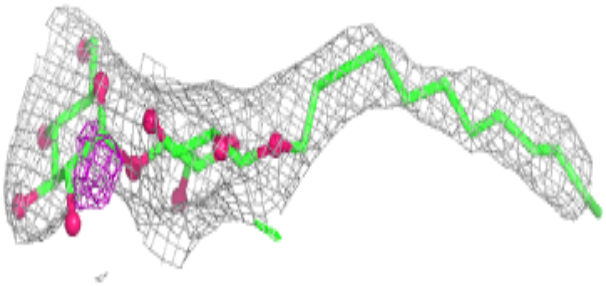
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

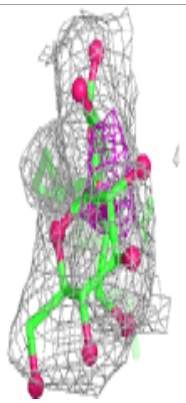


Electron density around LMT B 1103:

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

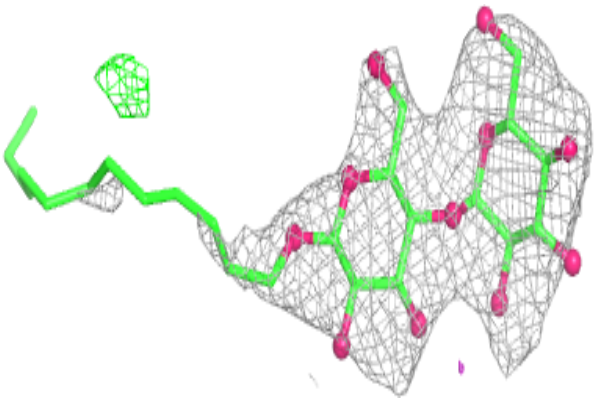


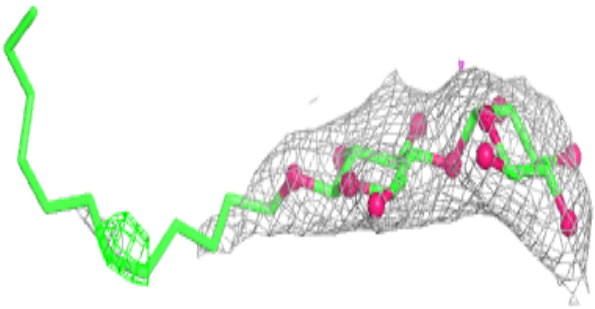


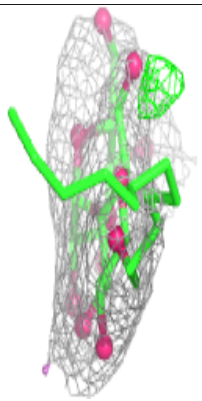


Electron density around LMT B 1102:

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

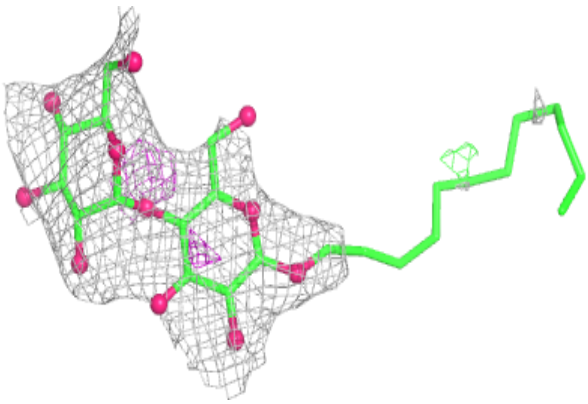


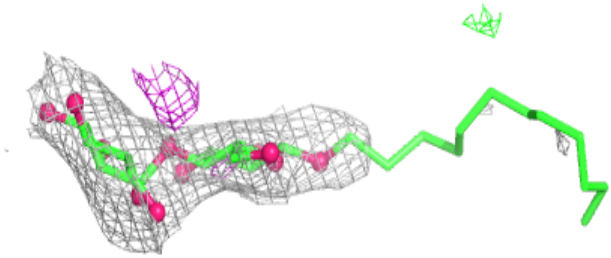


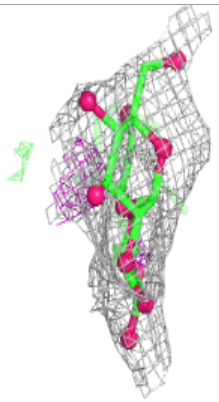


Electron density around LMT A 1105:

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

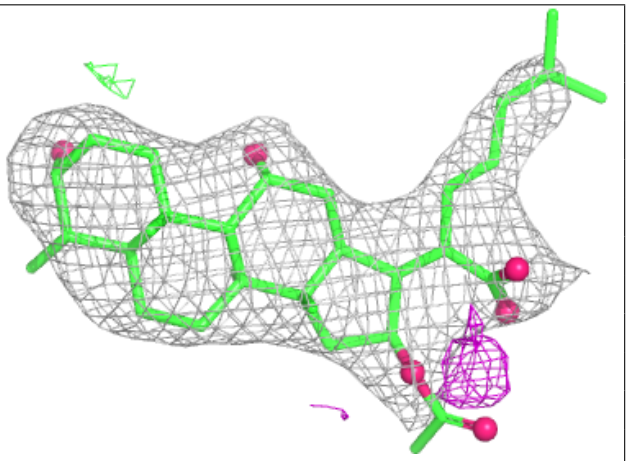


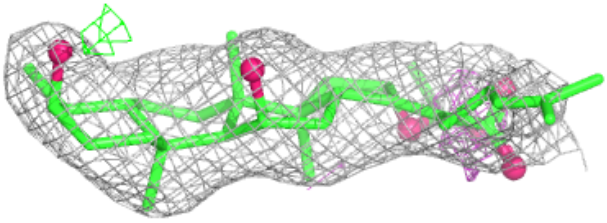


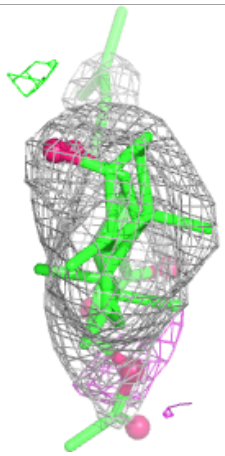


Electron density around FUA B 1101:

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

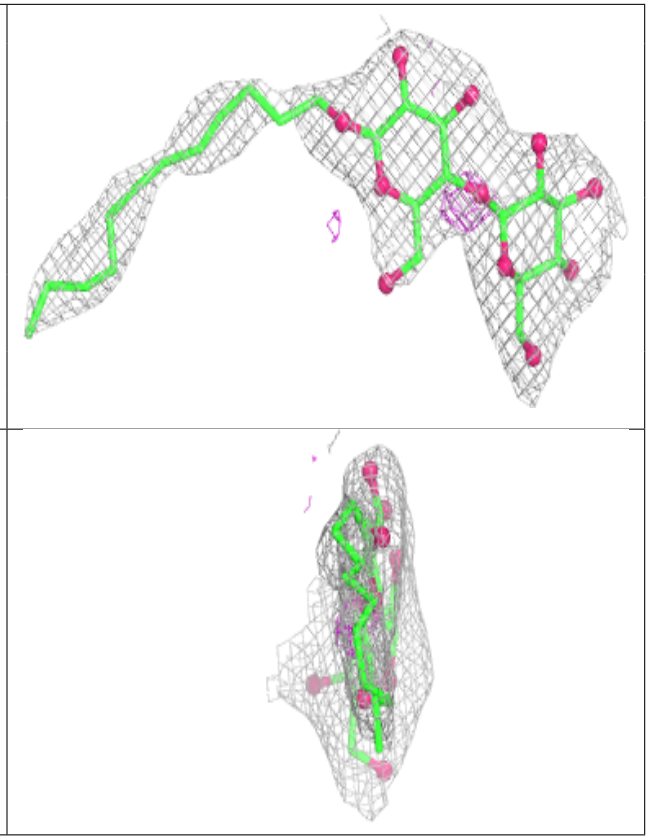






Electron density around LMT C 1102:

$2mF_o$-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.