Full wwPDB X-ray Structure Validation 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 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 (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:

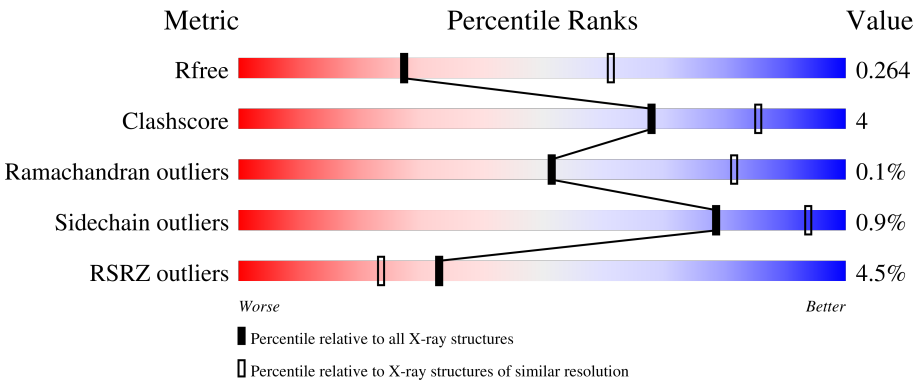
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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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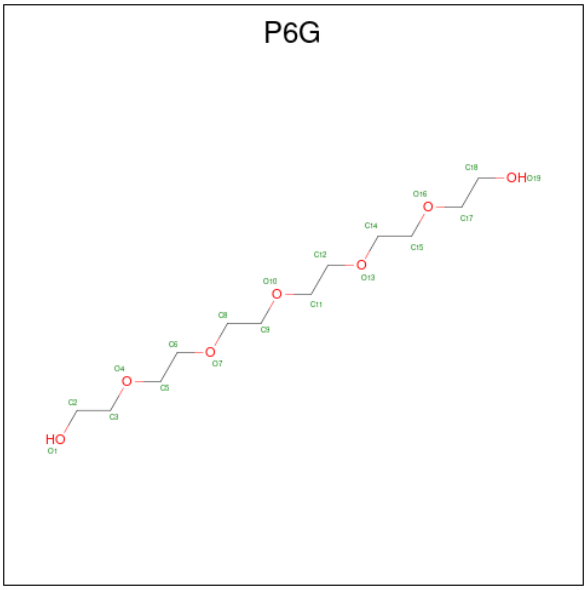
Chain	Residue	Modelled	Actual	Comment	Reference
C	1054	HIS	-	expression tag	UNP P31224
C	1055	HIS	-	expression tag	UNP P31224
C	1056	HIS	-	expression tag	UNP P31224
C	1057	HIS	-	expression tag	UNP P31224

- Molecule 2 is a protein called DARPin.

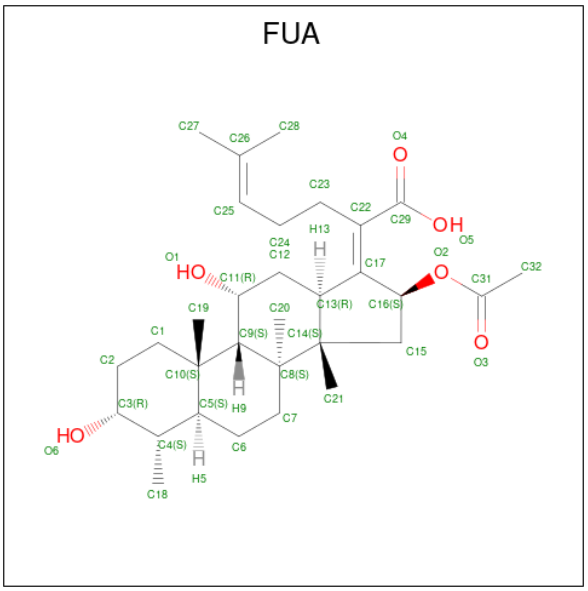
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	156	1177	741	206	229	1	0	0	0
			Total	C	N	O	S			
2	E	154	1167	736	204	226	1	0	0	0

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



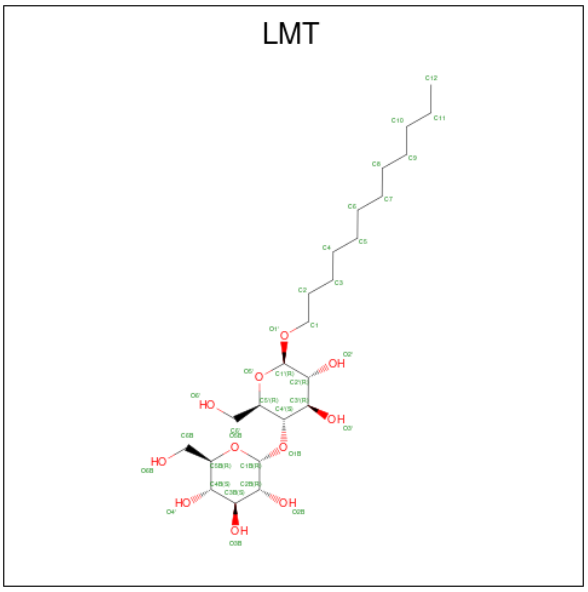
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	19	12	7	0	0

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



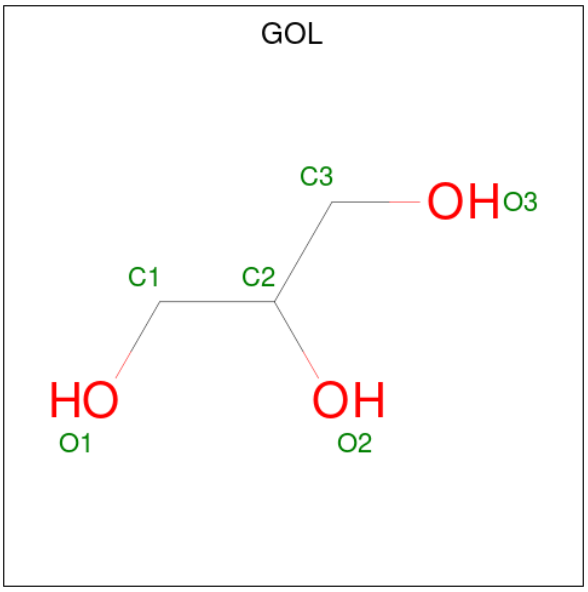
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	37	31	6	0	0
			Total	C	O		
4	B	1	37	31	6	0	0
			Total	C	O		
4	C	1	37	31	6	0	0

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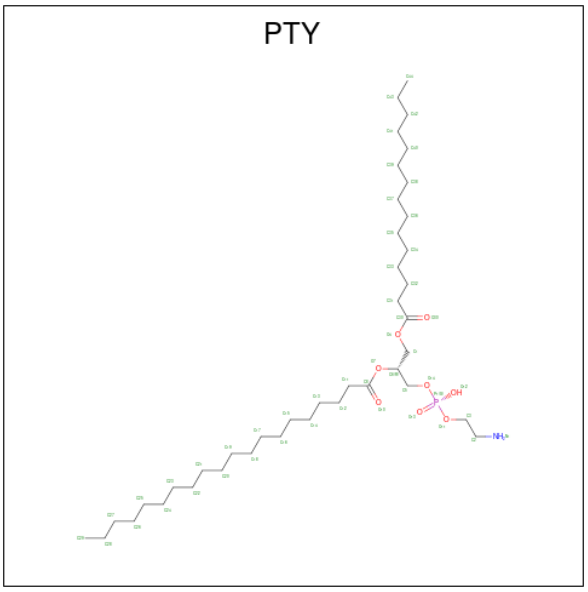
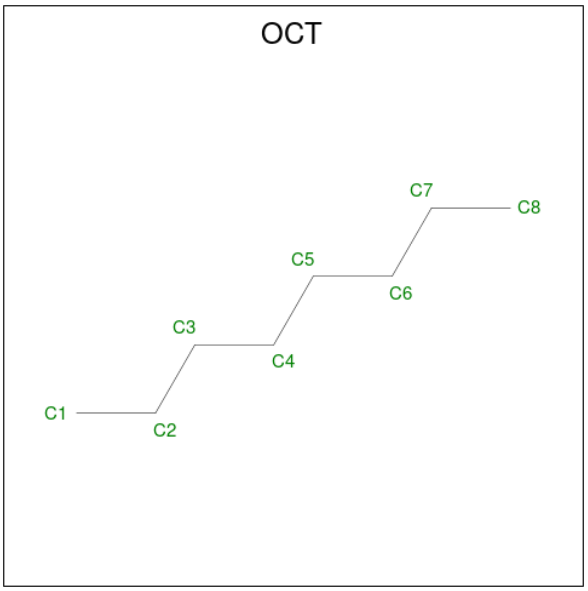
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	E	1	6	3	3	0	0
			Total	C	O		
6	E	1	6	3	3	0	0

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



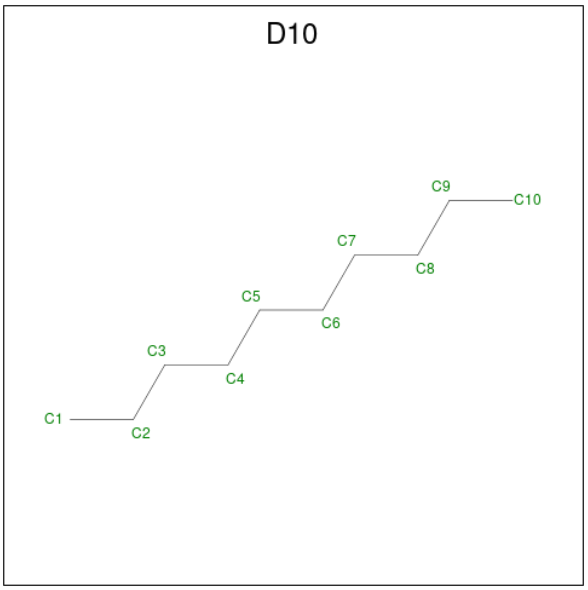
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
7	B	1	50	40	1	8	1	0	0
			Total	C	N	O	P		
7	C	1	50	40	1	8	1	0	0
			Total	C	N	O	P		
7	C	1	50	40	1	8	1	0	0
			Total	C	N	O	P		
7	C	1	50	40	1	8	1	0	0

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



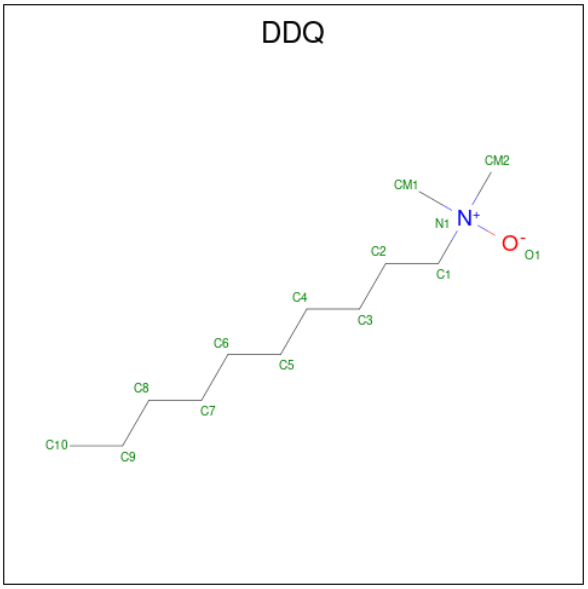
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C 8 8	0	0
8	B	1	Total C 8 8	0	0
8	C	1	Total C 8 8	0	0
8	C	1	Total C 8 8	0	0
8	C	1	Total C 8 8	0	0

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



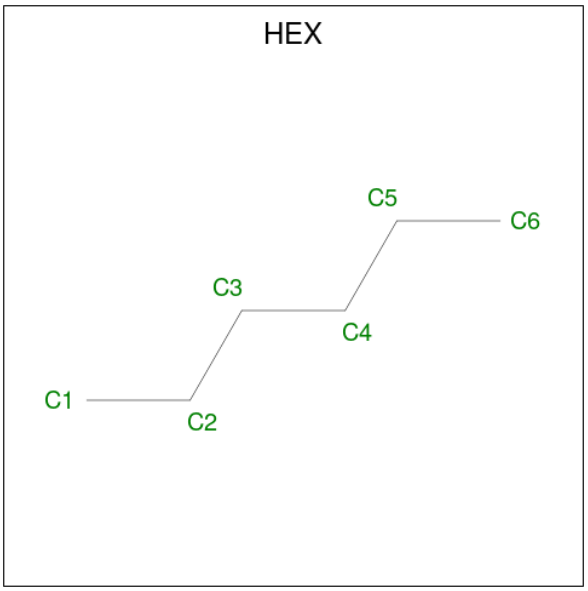
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C 10 10	0	0
9	B	1	Total C 10 10	0	0
9	B	1	Total C 10 10	0	0
9	B	1	Total C 10 10	0	0
9	C	1	Total C 10 10	0	0

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



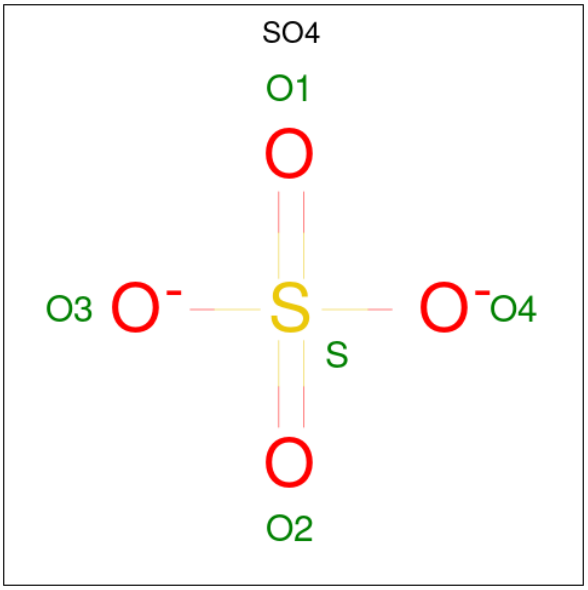
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total C N O 14 12 1 1	0	0
10	C	1	Total C N O 14 12 1 1	0	0

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



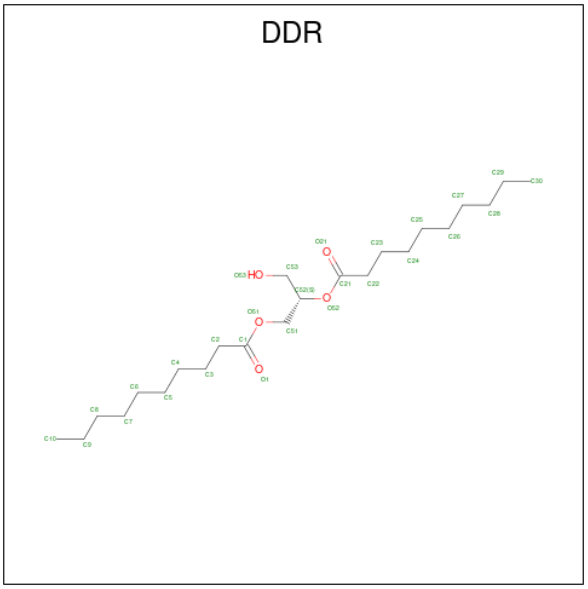
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	1	Total C 6 6	0	0
11	C	1	Total C 6 6	0	0

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



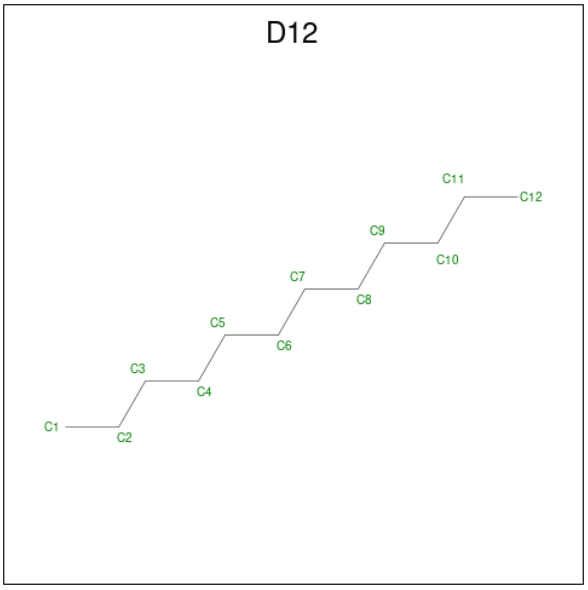
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	B	1	Total O S 5 4 1	0	0
12	C	1	Total O S 5 4 1	0	0

- 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.

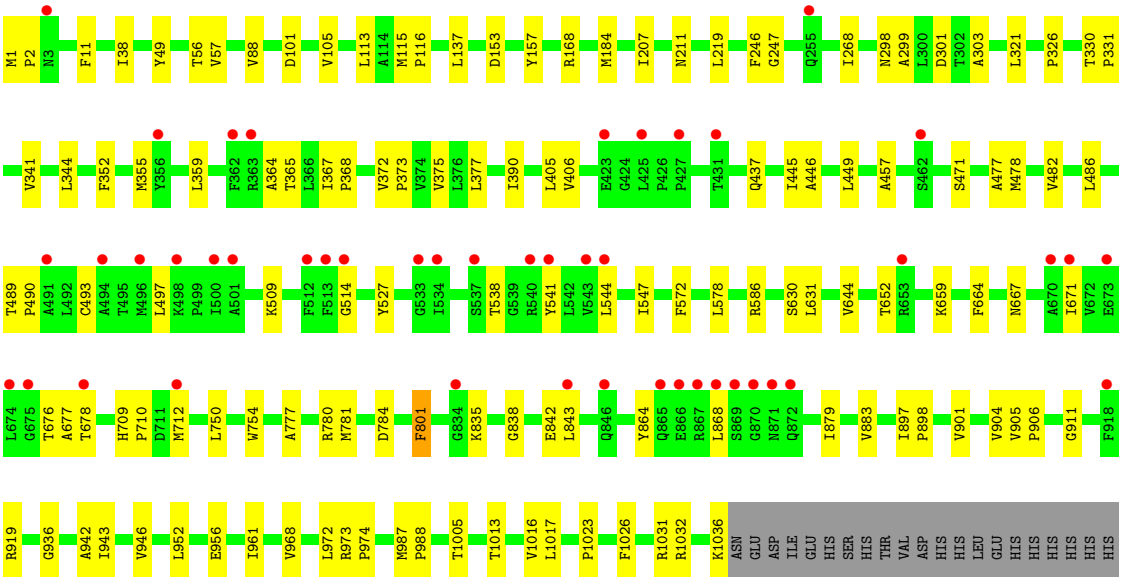
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
15	A	79	79	79	0	0
			Total	O		
15	B	76	76	76	0	0
			Total	O		
15	C	105	105	105	0	0
			Total	O		
15	D	18	18	18	0	0
			Total	O		
15	E	7	7	7	0	0

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.

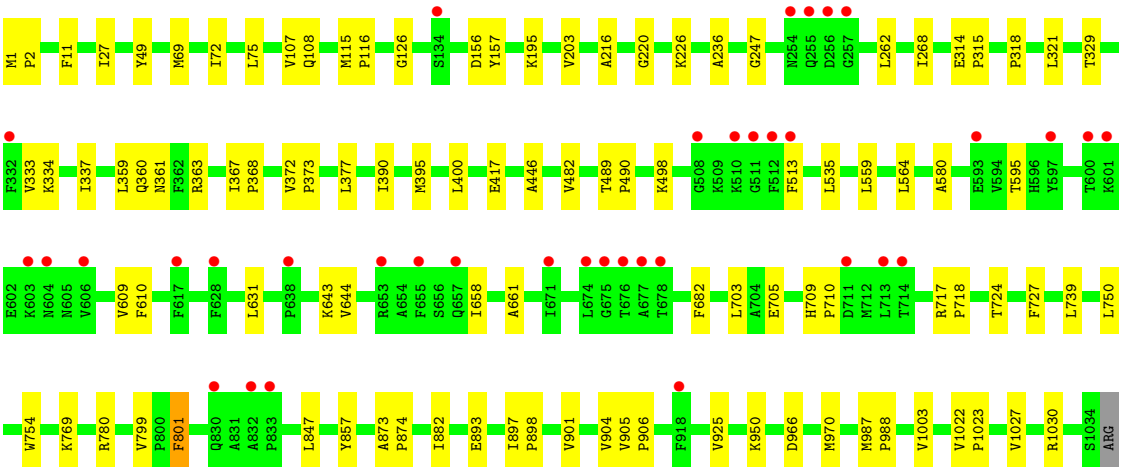
• Molecule 1: Multidrug efflux pump subunit AcrB

Chain A:



• Molecule 1: Multidrug efflux pump subunit AcrB

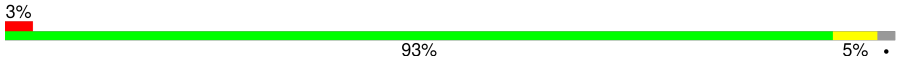
Chain B:



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.

All (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
1:C:901:VAL:O	1:C:904:VAL:HG12	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:1105:PTY:H282	10:B:1113:DDQ:H102	1.71	0.72
1:C:904:VAL:HG23	1:C:907:LEU:HD12	1.71	0.71
7:B:1105:PTY:H172	7:B:1105:PTY:H402	1.73	0.71
4:B:1101:FUA:H202	4:B:1101:FUA:H5	1.74	0.69
4:C:1101:FUA:H122	4:C:1101:FUA:H231	1.75	0.68
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.76	0.68
1:A:493:CYS:O	1:A:497:LEU:HB2	1.94	0.67
1:A:355:MET:HB2	1:A:365:THR:HG23	1.77	0.65
1:A:968:VAL:HG11	1:A:1023:PRO:HG3	1.77	0.65
7:C:1106:PTY:H322	7:C:1106:PTY:C1	2.27	0.65
1:B:535:LEU:HD22	1:B:1027:VAL:HG21	1.79	0.64
1:B:901:VAL:O	1:B:904:VAL:HG12	1.97	0.64
7:B:1105:PTY:H331	7:B:1105:PTY:HC11	1.81	0.63
1:B:247:GLY:HA2	1:B:268:ILE:CD1	2.29	0.63
1:A:375:VAL:HG11	1:A:405:LEU:HD22	1.81	0.62
1:A:446:ALA:HB2	1:A:482:VAL:HG21	1.80	0.62
1:A:372:VAL:HG21	1:A:406:VAL:HG22	1.81	0.62
1:C:671:ILE:HD11	1:C:674:LEU:HD12	1.83	0.61
1:A:247:GLY:HA2	1:A:268:ILE:CD1	2.31	0.60
1:C:445:ILE:HD11	1:C:944:LEU:HD21	1.82	0.60
1:A:527:TYR:CD2	1:A:972:LEU:HD22	2.38	0.59
2:D:91:GLY:HA2	2:D:128:ILE:CD1	2.33	0.59
4:C:1101:FUA:H272	4:C:1101:FUA:H232	1.85	0.58
1:A:113:LEU:HD11	1:C:128:SER:HB3	1.86	0.58
1:B:400:LEU:HD21	1:B:1003:VAL:HG13	1.86	0.58
1:A:919:ARG:HD3	1:A:1005:THR:HG21	1.85	0.58
1:B:580:ALA:HB1	1:B:724:THR:HG22	1.86	0.58
1:A:942:ALA:O	1:A:946:VAL:HG23	2.03	0.57
1:A:219:LEU:HD23	1:B:754:TRP:CZ3	2.39	0.56
1:A:897:ILE:N	1:A:898:PRO:HD2	2.19	0.56
1:B:1:MET:HB3	1:B:2:PRO:HD3	1.85	0.56
2:D:91:GLY:HA2	2:D:128:ILE:HD12	1.87	0.56
1:A:572:PHE:HE2	1:A:631:LEU:HD21	1.71	0.55
1:C:35:TYR:HB3	1:C:36:PRO:HD2	1.88	0.55
1:B:334:LYS:HG3	4:B:1101:FUA:H281	1.87	0.55
2:E:20:GLU:HG2	6:E:201:GOL:H11	1.87	0.55
1:A:541:TYR:HA	1:A:544:LEU:HD12	1.89	0.54
2:E:14:LEU:HD23	2:E:38:ALA:HA	1.90	0.54
1:A:101:ASP:O	1:A:105:VAL:HG23	2.09	0.53
1:B:446:ALA:HB2	1:B:482:VAL:HG21	1.90	0.53
1:A:709:HIS:N	1:A:710:PRO:HD3	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:LEU:CD2	1:B:1003:VAL:HG13	2.40	0.52
1:B:705:GLU:HB3	1:B:847:LEU:HD22	1.92	0.52
1:A:676:THR:O	1:A:678:THR:N	2.43	0.52
1:A:879:ILE:O	1:A:883:VAL:HG23	2.09	0.52
1:A:652:THR:HG23	1:A:664:PHE:CB	2.39	0.52
1:C:987:MET:HB3	1:C:988:PRO:HD3	1.92	0.52
1:B:367:ILE:HB	1:B:368:PRO:HD3	1.91	0.51
1:C:32:VAL:HG12	1:C:337:ILE:HD13	1.92	0.51
1:B:882:ILE:HG23	9:B:1111:D10:H91	1.92	0.51
1:B:372:VAL:HB	1:B:373:PRO:HD3	1.92	0.51
1:A:372:VAL:HB	1:A:373:PRO:HD3	1.93	0.51
1:B:337:ILE:HG21	4:B:1101:FUA:H272	1.92	0.51
1:A:457:ALA:HB2	1:A:471:SER:CB	2.41	0.50
1:A:489:THR:HB	1:A:490:PRO:HD3	1.93	0.50
1:A:115:MET:HB2	1:A:116:PRO:HD3	1.94	0.50
1:A:355:MET:CB	1:A:365:THR:HG23	2.42	0.50
1:B:682:PHE:CZ	1:B:857:TYR:HB2	2.47	0.50
1:A:57:VAL:CG1	1:A:88:VAL:HG22	2.41	0.50
1:A:879:ILE:HD13	1:C:25:LEU:HD11	1.94	0.50
1:C:303:ALA:HB2	1:C:330:THR:HG21	1.92	0.50
1:A:57:VAL:HG12	1:A:88:VAL:HG22	1.92	0.50
1:A:644:VAL:CG1	1:A:667:ASN:HB2	2.42	0.50
1:C:671:ILE:HD11	1:C:674:LEU:CD1	2.41	0.50
4:A:1102:FUA:H202	4:A:1102:FUA:C5	2.34	0.50
1:A:341:VAL:O	1:A:344:LEU:HB2	2.12	0.49
1:B:966:ASP:O	1:B:970:MET:HG3	2.11	0.49
1:A:390:ILE:HG21	5:A:1104:LMT:H32	1.94	0.49
1:B:220:GLY:HA2	1:C:781:MET:SD	2.52	0.49
1:B:390:ILE:HD13	5:B:1103:LMT:H31	1.95	0.49
1:A:341:VAL:HG12	4:A:1102:FUA:H323	1.95	0.49
1:C:873:ALA:HB3	1:C:874:PRO:HD3	1.95	0.49
1:A:509:LYS:O	1:A:514:GLY:HA3	2.13	0.48
1:C:448:VAL:HG11	1:C:943:ILE:HD11	1.95	0.48
2:E:91:GLY:HA2	2:E:128:ILE:HD12	1.95	0.48
1:A:879:ILE:CD1	1:C:25:LEU:HD11	2.43	0.48
1:B:905:VAL:HB	1:B:906:PRO:HD3	1.94	0.48
1:A:987:MET:HB3	1:A:988:PRO:HD3	1.95	0.48
1:B:897:ILE:HD13	1:B:950:LYS:HD2	1.96	0.48
1:A:352:PHE:CD1	1:A:365:THR:HG22	2.49	0.48
1:A:375:VAL:HG11	1:A:405:LEU:CD2	2.42	0.48
1:A:1016:VAL:HG23	1:A:1017:LEU:HD12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1008:MET:O	1:C:1012:VAL:HG23	2.14	0.48
1:A:712:MET:SD	1:A:835:LYS:HD2	2.54	0.48
1:C:57:VAL:HG21	1:C:86:GLY:HA2	1.96	0.48
1:A:56:THR:HG23	1:C:213:GLN:HG3	1.95	0.47
4:B:1101:FUA:C12	4:B:1101:FUA:C23	2.90	0.47
1:B:873:ALA:HB3	1:B:874:PRO:HD3	1.97	0.47
1:C:330:THR:N	1:C:331:PRO:CD	2.77	0.47
1:C:367:ILE:HB	1:C:368:PRO:HD3	1.96	0.47
2:D:46:VAL:HG23	2:D:48:TRP:CD1	2.49	0.47
1:A:973:ARG:N	1:A:974:PRO:HD2	2.29	0.47
7:B:1105:PTY:H361	7:C:1104:PTY:H371	1.95	0.47
7:B:1105:PTY:H112	7:B:1105:PTY:HC12	1.96	0.46
1:A:968:VAL:HG11	1:A:1023:PRO:CG	2.44	0.46
1:B:157:TYR:CE2	1:B:318:PRO:HD3	2.51	0.46
7:C:1106:PTY:H171	7:C:1106:PTY:H352	1.97	0.46
1:A:298:ASN:HB3	1:A:301:ASP:HB2	1.98	0.46
1:A:330:THR:N	1:A:331:PRO:CD	2.79	0.46
1:B:359:LEU:HD13	1:B:417:GLU:HG3	1.98	0.45
1:B:595:THR:HG23	1:B:609:VAL:HB	1.98	0.45
1:B:703:LEU:HD11	1:B:718:PRO:HD3	1.97	0.45
7:C:1106:PTY:C1	7:C:1106:PTY:C32	2.92	0.45
1:B:156:ASP:OD1	1:B:769:LYS:NZ	2.49	0.45
1:B:1022:VAL:N	1:B:1023:PRO:HD2	2.31	0.45
1:A:946:VAL:HG13	1:A:1026:PHE:CE1	2.52	0.45
1:B:360:GLN:HG2	1:B:513:PHE:CD2	2.50	0.45
1:B:658:ILE:HG22	1:B:661:ALA:HB3	1.99	0.45
1:A:184:MET:HG2	1:A:246:PHE:CD2	2.51	0.45
1:A:864:TYR:O	1:A:868:LEU:HD13	2.17	0.45
1:A:961:ILE:HD11	1:A:1031:ARG:NH2	2.31	0.45
6:A:1107:GOL:H31	1:B:75:LEU:HD23	1.99	0.45
2:E:133:LEU:HD21	2:E:139:VAL:HG12	1.99	0.45
1:C:671:ILE:HD11	1:C:674:LEU:CG	2.46	0.45
4:C:1101:FUA:H202	4:C:1101:FUA:C5	2.40	0.45
1:C:10:ILE:O	1:C:14:VAL:HG23	2.17	0.45
2:E:82:THR:O	2:E:85:HIS:HB2	2.17	0.45
2:E:23:ARG:HG3	2:E:57:TRP:CD1	2.52	0.45
1:A:207:ILE:O	1:A:211:ASN:HB3	2.18	0.44
1:A:482:VAL:O	1:A:486:LEU:HG	2.17	0.44
1:A:712:MET:HG2	1:A:843:LEU:HD22	1.98	0.44
1:A:901:VAL:O	1:A:904:VAL:HG22	2.17	0.44
1:B:27:ILE:CD1	1:B:377:LEU:HD22	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:631:LEU:HD11	1:B:644:VAL:HG22	1.98	0.44
1:B:750:LEU:HB2	1:B:801:PHE:CZ	2.52	0.44
1:B:897:ILE:N	1:B:898:PRO:HD2	2.31	0.44
1:A:838:GLY:O	1:A:842:GLU:HG3	2.17	0.44
1:A:330:THR:OG1	1:A:331:PRO:HD3	2.17	0.44
2:E:91:GLY:HA2	2:E:128:ILE:CD1	2.48	0.44
4:A:1102:FUA:O4	4:A:1102:FUA:H242	2.17	0.44
1:C:359:LEU:HG	1:C:977:MET:CE	2.48	0.44
1:A:219:LEU:HD11	1:B:727:PHE:CG	2.53	0.43
1:B:395:MET:HA	1:B:395:MET:CE	2.47	0.43
1:A:1:MET:HB2	1:A:2:PRO:HD3	2.00	0.43
1:A:184:MET:HG2	1:A:246:PHE:CE2	2.53	0.43
1:B:489:THR:OG1	1:B:490:PRO:HD3	2.18	0.43
1:A:449:LEU:HB3	1:A:478:MET:SD	2.58	0.43
1:B:754:TRP:CH2	1:B:780:ARG:HA	2.53	0.43
7:B:1105:PTY:P1	7:B:1105:PTY:H311	2.57	0.43
4:A:1102:FUA:C5	4:A:1102:FUA:C20	2.96	0.43
1:C:705:GLU:HB3	1:C:847:LEU:HD22	2.01	0.43
1:C:915:ALA:HA	5:C:1103:LMT:H92	2.01	0.43
1:A:952:LEU:O	1:A:956:GLU:HB2	2.18	0.43
4:A:1102:FUA:O1	4:A:1102:FUA:H12	2.19	0.43
1:B:72:ILE:HD13	1:B:107:VAL:HG22	2.00	0.43
1:B:216:ALA:HB2	1:B:236:ALA:HB2	2.00	0.43
1:C:454:VAL:HB	1:C:455:PRO:HD3	2.00	0.43
1:C:904:VAL:HG11	1:C:942:ALA:HB2	2.01	0.43
4:C:1101:FUA:H232	4:C:1101:FUA:C27	2.47	0.43
2:E:108:ALA:O	2:E:116:PRO:HD3	2.19	0.43
1:A:644:VAL:HG12	1:A:667:ASN:HB2	2.01	0.42
7:C:1106:PTY:O14	7:C:1106:PTY:HC21	2.18	0.42
1:A:911:GLY:CA	1:A:1013:THR:HG21	2.49	0.42
1:B:893:GLU:O	1:B:893:GLU:HG3	2.19	0.42
1:C:671:ILE:HD11	1:C:674:LEU:HG	2.00	0.42
1:B:897:ILE:N	1:B:898:PRO:CD	2.82	0.42
1:A:359:LEU:HD13	1:A:364:ALA:HB1	2.02	0.42
1:C:736:ALA:HB1	1:C:741:VAL:HG23	2.00	0.42
1:A:754:TRP:CZ3	1:A:780:ARG:HA	2.54	0.42
1:B:709:HIS:N	1:B:710:PRO:HD3	2.34	0.42
1:B:126:GLY:HA3	1:C:116:PRO:HB3	2.02	0.42
1:B:987:MET:N	1:B:988:PRO:CD	2.82	0.42
7:B:1105:PTY:HC11	7:B:1105:PTY:C33	2.49	0.42
1:B:739:LEU:HD13	1:B:799:VAL:HG11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:LEU:O	1:A:547:ILE:HB	2.20	0.41
1:A:968:VAL:CG1	1:A:1023:PRO:HG3	2.48	0.41
1:A:754:TRP:HZ3	1:C:219:LEU:HD23	1.85	0.41
4:A:1102:FUA:H122	4:A:1102:FUA:C23	2.50	0.41
1:B:363:ARG:HD2	1:B:498:LYS:HE3	2.02	0.41
1:A:38:ILE:HD11	1:A:671:ILE:HD13	2.02	0.41
1:A:137:LEU:HD11	1:A:299:ALA:HB1	2.02	0.41
1:B:314:GLU:HB2	1:B:315:PRO:HD3	2.02	0.41
1:A:445:ILE:CG1	1:A:943:ILE:HG21	2.51	0.41
1:B:329:THR:O	1:B:333:VAL:HG23	2.20	0.41
1:A:377:LEU:HD23	1:A:377:LEU:HA	1.96	0.41
1:A:445:ILE:HG12	1:A:943:ILE:HG21	2.03	0.41
1:B:203:VAL:HG13	1:B:262:LEU:CD1	2.51	0.41
1:A:405:LEU:HD21	1:A:477:ALA:HB1	2.02	0.41
2:D:100:LEU:HD11	2:D:132:LEU:HD23	2.03	0.41
1:A:449:LEU:HD21	1:A:936:GLY:CA	2.51	0.41
1:B:559:LEU:HD12	1:B:559:LEU:HA	1.94	0.41
1:C:904:VAL:HG13	1:C:938:SER:HB3	2.02	0.41
1:A:578:LEU:HD23	1:A:586:ARG:HE	1.85	0.41
1:A:777:ALA:O	1:A:781:MET:HG2	2.21	0.41
1:A:168:ARG:HG2	1:B:69:MET:O	2.21	0.40
1:B:115:MET:HB2	1:B:116:PRO:HD3	2.03	0.40
1:B:318:PRO:HD2	1:B:321:LEU:HD22	2.03	0.40
1:A:905:VAL:N	1:A:906:PRO:CD	2.84	0.40
1:A:1016:VAL:HG23	1:A:1017:LEU:CD1	2.51	0.40
1:C:905:VAL:HB	1:C:906:PRO:HD3	2.03	0.40
1:A:157:TYR:CD2	1:A:321:LEU:HD21	2.56	0.40
1:A:326:PRO:O	1:A:630:SER:HB2	2.20	0.40
1:A:750:LEU:HB2	1:A:801:PHE:CZ	2.56	0.40
1:B:564:LEU:HD23	1:B:925:VAL:HG22	2.04	0.40
1:B:643:LYS:HA	1:B:643:LYS:HD3	1.82	0.40
7:B:1105:PTY:H382	7:C:1104:PTY:H391	2.02	0.40
1:A:946:VAL:HG13	1:A:1026:PHE:CD1	2.56	0.40
4:B:1101:FUA:H202	4:B:1101:FUA:C5	2.45	0.40
4:C:1101:FUA:H231	4:C:1101:FUA:C12	2.47	0.40
1:A:303:ALA:HB2	1:A:330:THR:HG21	2.04	0.40
1:C:115:MET:N	1:C:116:PRO:HD2	2.36	0.40
1:C:947:GLU:OE2	7:C:1106:PTY:N1	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1035/1057 (98%)	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
2	E	119/132 (90%)	118 (99%)	1 (1%)	81	94
All	All	2760/2850 (97%)	2736 (99%)	24 (1%)	78	94

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	PHE
1	A	49	TYR
1	A	153	ASP
1	A	437	GLN
1	A	659	LYS
1	A	784	ASP
1	A	801	PHE
1	A	1032	ARG
1	A	1036	LYS
1	B	11	PHE
1	B	49	TYR
1	B	108	GLN
1	B	195	LYS
1	B	226	LYS
1	B	361	ASN
1	B	610	PHE
1	B	717	ARG
1	B	801	PHE
1	B	1030	ARG
1	C	11	PHE
1	C	49	TYR
1	C	671	ILE
1	C	717	ARG
2	E	34	MET

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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
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
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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	-

All (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
13	B	1116	DDR	O51-C1	4.35	1.46	1.33
13	B	1116	DDR	O52-C21	4.07	1.45	1.34
10	B	1113	DDQ	C1-N1	-3.24	1.48	1.51
10	C	1112	DDQ	C1-N1	-3.21	1.48	1.51
4	A	1102	FUA	O5-C29	-2.64	1.23	1.30
4	C	1101	FUA	O5-C29	-2.58	1.23	1.30
4	B	1101	FUA	O5-C29	-2.56	1.23	1.30
5	C	1103	LMT	O1'-C1'	2.22	1.43	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1102	FUA	C9-C11	2.03	1.57	1.54

All (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
13	B	1116	DDR	O51-C1-C2	2.73	120.17	111.83
5	C	1103	LMT	O5'-C5'-C4'	2.71	115.32	109.72
5	C	1103	LMT	C3'-C4'-C5'	2.56	116.61	110.93
5	C	1103	LMT	O5'-C1'-C2'	-2.52	105.20	110.37
4	C	1101	FUA	C6-C5-C10	2.50	114.66	111.66
13	B	1116	DDR	C52-O52-C21	-2.50	111.82	117.80
5	A	1104	LMT	C1B-O1B-C4'	-2.34	112.43	117.98
5	B	1104	LMT	C3'-C4'-C5'	2.21	115.83	110.93
4	A	1102	FUA	C24-C23-C22	2.17	117.34	112.72
4	C	1101	FUA	O2-C16-C17	2.17	114.66	108.30
4	C	1101	FUA	C18-C4-C5	2.15	116.43	112.95
4	B	1101	FUA	C7-C8-C14	2.14	112.63	110.78
4	B	1101	FUA	C14-C8-C9	-2.10	105.60	109.30
5	C	1103	LMT	C1B-C2B-C3B	2.07	114.36	110.01
5	A	1103	LMT	C1B-O1B-C4'	-2.00	113.24	117.98

There are no chirality outliers.

All (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
4	B	1101	FUA	O3-C31-O2-C16
4	C	1101	FUA	C23-C22-C29-O4
4	C	1101	FUA	C23-C22-C29-O5
4	C	1101	FUA	C23-C24-C25-C26
5	B	1102	LMT	C2'-C1'-O1'-C1
5	B	1102	LMT	O5'-C1'-O1'-C1
5	B	1103	LMT	C2-C1-O1'-C1'

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Mol	Chain	Res	Type	Atoms
7	B	1105	PTY	C11-C8-O7-C6
7	B	1105	PTY	C3-O11-P1-O12
7	B	1105	PTY	C3-O11-P1-O14
7	C	1104	PTY	O4-C1-C6-O7
7	C	1104	PTY	C3-O11-P1-O12
7	C	1104	PTY	C3-O11-P1-O14
7	C	1105	PTY	C11-C8-O7-C6
7	C	1105	PTY	C3-O11-P1-O13
7	C	1105	PTY	C3-O11-P1-O14
7	C	1105	PTY	C5-O14-P1-O11
7	C	1106	PTY	N1-C2-C3-O11
7	C	1106	PTY	C2-C3-O11-P1
7	C	1106	PTY	C11-C8-O7-C6
7	C	1106	PTY	C3-O11-P1-O13
7	C	1106	PTY	C3-O11-P1-O14
7	C	1106	PTY	C5-O14-P1-O11
4	A	1102	FUA	C32-C31-O2-C16
7	B	1105	PTY	C31-C30-O4-C1
7	B	1105	PTY	O30-C30-O4-C1
7	C	1106	PTY	O30-C30-O4-C1
7	B	1105	PTY	O10-C8-O7-C6
7	C	1105	PTY	O10-C8-O7-C6
7	C	1106	PTY	C31-C30-O4-C1
4	A	1102	FUA	O3-C31-O2-C16
7	C	1106	PTY	O10-C8-O7-C6
5	A	1105	LMT	O5B-C5B-C6B-O6B
5	C	1103	LMT	O5'-C5'-C6'-O6'
5	C	1103	LMT	C4'-C5'-C6'-O6'
4	A	1102	FUA	C22-C23-C24-C25
4	C	1101	FUA	C22-C23-C24-C25
3	A	1101	P6G	O4-C5-C6-O7
5	B	1103	LMT	O5'-C1'-O1'-C1
5	C	1102	LMT	O5'-C1'-O1'-C1
5	B	1103	LMT	O5'-C5'-C6'-O6'
5	A	1103	LMT	O5B-C5B-C6B-O6B
5	A	1103	LMT	C4B-C5B-C6B-O6B
3	A	1101	P6G	O7-C8-C9-O10
5	C	1103	LMT	C4B-C5B-C6B-O6B
5	C	1102	LMT	C2'-C1'-O1'-C1
5	B	1103	LMT	C4'-C5'-C6'-O6'
7	C	1105	PTY	C31-C30-O4-C1
13	B	1116	DDR	C2-C1-O51-C51

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Mol	Chain	Res	Type	Atoms
5	C	1103	LMT	O5B-C5B-C6B-O6B
3	A	1101	P6G	O13-C14-C15-O16
3	A	1101	P6G	O16-C17-C18-O19
5	A	1105	LMT	C4B-C5B-C6B-O6B
7	C	1105	PTY	C8-C11-C12-C13
5	C	1103	LMT	O5'-C1'-O1'-C1
7	B	1105	PTY	C24-C25-C26-C27
13	B	1116	DDR	C22-C21-O52-C52
7	C	1105	PTY	O30-C30-O4-C1
7	C	1106	PTY	C8-C11-C12-C13
13	B	1116	DDR	O21-C21-O52-C52
5	A	1105	LMT	O1'-C1-C2-C3
13	B	1116	DDR	O1-C1-O51-C51
5	C	1103	LMT	C2'-C1'-O1'-C1
7	B	1105	PTY	C26-C27-C28-C29
6	A	1107	GOL	O1-C1-C2-C3
6	B	1106	GOL	C1-C2-C3-O3
6	E	202	GOL	C1-C2-C3-O3
5	C	1102	LMT	C6-C7-C8-C9
9	B	1109	D10	C6-C7-C8-C9
7	C	1104	PTY	C32-C33-C34-C35
7	C	1106	PTY	C18-C19-C20-C21
7	C	1104	PTY	C18-C19-C20-C21
6	A	1107	GOL	O1-C1-C2-O2
6	B	1106	GOL	O2-C2-C3-O3
5	C	1103	LMT	C3-C4-C5-C6
5	A	1105	LMT	C3-C4-C5-C6
7	C	1104	PTY	C35-C36-C37-C38
5	A	1104	LMT	C6-C7-C8-C9
5	A	1103	LMT	C1-C2-C3-C4
5	C	1102	LMT	C7-C8-C9-C10
7	C	1104	PTY	C13-C14-C15-C16
7	C	1106	PTY	C12-C13-C14-C15
5	B	1103	LMT	C1-C2-C3-C4
5	A	1103	LMT	O5'-C5'-C6'-O6'
5	B	1103	LMT	C5-C6-C7-C8
9	B	1109	D10	C3-C4-C5-C6
3	A	1101	P6G	O10-C11-C12-O13
5	C	1103	LMT	C2-C3-C4-C5
7	C	1106	PTY	C11-C12-C13-C14
7	B	1105	PTY	C35-C36-C37-C38
7	B	1105	PTY	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
8	C	1110	OCT	C2-C3-C4-C5
5	B	1104	LMT	O5B-C1B-O1B-C4'
8	C	1109	OCT	C4-C5-C6-C7
5	A	1104	LMT	C4-C5-C6-C7
5	B	1104	LMT	C5-C6-C7-C8
7	C	1104	PTY	C31-C32-C33-C34
7	C	1105	PTY	C32-C33-C34-C35
4	A	1102	FUA	C29-C22-C23-C24
5	B	1104	LMT	C4-C5-C6-C7
7	C	1104	PTY	C38-C39-C40-C41
7	C	1106	PTY	C17-C18-C19-C20
13	B	1116	DDR	C1-C2-C3-C4
7	C	1105	PTY	C22-C23-C24-C25
5	A	1103	LMT	C2-C3-C4-C5
7	B	1105	PTY	C19-C20-C21-C22
10	C	1112	DDQ	C6-C7-C8-C9
13	B	1116	DDR	C23-C24-C25-C26
8	B	1107	OCT	C3-C4-C5-C6
7	B	1105	PTY	C34-C35-C36-C37
7	C	1105	PTY	C39-C40-C41-C42
9	C	1111	D10	C2-C3-C4-C5
5	B	1102	LMT	C6-C7-C8-C9
7	C	1106	PTY	C25-C26-C27-C28
9	B	1110	D10	C6-C7-C8-C9
5	B	1102	LMT	C5-C6-C7-C8
7	C	1104	PTY	C11-C8-O7-C6
5	C	1102	LMT	C1-C2-C3-C4
5	B	1104	LMT	C7-C8-C9-C10
7	B	1105	PTY	C20-C21-C22-C23
5	B	1102	LMT	C2-C3-C4-C5
7	C	1106	PTY	C33-C34-C35-C36
7	C	1106	PTY	C20-C21-C22-C23
10	C	1112	DDQ	C7-C8-C9-C10
8	C	1108	OCT	C3-C4-C5-C6
9	B	1109	D10	C2-C3-C4-C5
11	C	1113	HEX	C2-C3-C4-C5
5	A	1105	LMT	C5-C6-C7-C8
7	C	1105	PTY	C18-C19-C20-C21
5	B	1103	LMT	O5B-C5B-C6B-O6B
7	C	1104	PTY	C12-C13-C14-C15
7	C	1106	PTY	C23-C24-C25-C26
5	B	1103	LMT	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
5	A	1105	LMT	C11-C10-C9-C8
7	B	1105	PTY	C31-C32-C33-C34
14	B	1117	D12	C7-C8-C9-C10
7	B	1105	PTY	O14-C5-C6-C1
7	C	1104	PTY	O10-C8-O7-C6
7	C	1104	PTY	C40-C41-C42-C43
7	C	1105	PTY	C24-C25-C26-C27
10	C	1112	DDQ	C4-C5-C6-C7
7	C	1104	PTY	O4-C1-C6-C5
5	A	1103	LMT	C4-C5-C6-C7
4	A	1102	FUA	C17-C22-C23-C24
7	B	1105	PTY	C17-C18-C19-C20
7	C	1106	PTY	C21-C22-C23-C24
7	C	1104	PTY	C15-C16-C17-C18
7	C	1106	PTY	C5-C6-O7-C8
7	C	1105	PTY	C25-C26-C27-C28
13	B	1116	DDR	C22-C23-C24-C25
8	C	1109	OCT	C1-C2-C3-C4
5	B	1102	LMT	O5B-C5B-C6B-O6B
7	C	1106	PTY	C38-C39-C40-C41
9	B	1111	D10	C7-C8-C9-C10
5	C	1103	LMT	C5-C6-C7-C8
13	B	1116	DDR	C27-C28-C29-C30
7	C	1105	PTY	C11-C12-C13-C14
5	B	1102	LMT	C9-C10-C11-C12
9	B	1111	D10	C1-C2-C3-C4
5	A	1103	LMT	C3-C4-C5-C6
7	C	1104	PTY	C26-C27-C28-C29
5	A	1103	LMT	C7-C8-C9-C10
13	B	1116	DDR	C7-C8-C9-C10
13	B	1116	DDR	C24-C25-C26-C27
5	C	1102	LMT	C2-C1-O1'-C1'
5	C	1103	LMT	C2-C1-O1'-C1'
14	B	1117	D12	C6-C7-C8-C9
7	C	1105	PTY	C6-C5-O14-P1
7	C	1106	PTY	C6-C5-O14-P1
8	C	1110	OCT	C1-C2-C3-C4
5	A	1105	LMT	C1-C2-C3-C4
10	B	1113	DDQ	C7-C8-C9-C10
7	C	1105	PTY	O14-C5-C6-C1
9	B	1112	D10	C4-C5-C6-C7
7	C	1106	PTY	O4-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
9	B	1110	D10	C7-C8-C9-C10
9	C	1111	D10	C1-C2-C3-C4
5	C	1102	LMT	C9-C10-C11-C12
7	C	1106	PTY	C41-C42-C43-C44
7	B	1105	PTY	C21-C22-C23-C24
8	C	1110	OCT	C4-C5-C6-C7
13	B	1116	DDR	C51-C52-C53-O53
7	C	1104	PTY	C33-C34-C35-C36
7	B	1105	PTY	O14-C5-C6-O7
7	C	1105	PTY	O14-C5-C6-O7
7	B	1105	PTY	C33-C34-C35-C36
7	C	1104	PTY	C20-C21-C22-C23
7	C	1106	PTY	C19-C20-C21-C22
5	A	1104	LMT	C2-C3-C4-C5
8	C	1108	OCT	C2-C3-C4-C5
5	A	1105	LMT	O5'-C5'-C6'-O6'
3	A	1101	P6G	C8-C9-O10-C11
13	B	1116	DDR	C3-C4-C5-C6
14	B	1117	D12	C1-C2-C3-C4
7	C	1104	PTY	C23-C24-C25-C26
5	B	1103	LMT	C2-C3-C4-C5
10	B	1113	DDQ	C6-C7-C8-C9
7	B	1105	PTY	C25-C26-C27-C28
7	C	1105	PTY	C20-C21-C22-C23
3	A	1101	P6G	O1-C2-C3-O4
7	C	1104	PTY	C34-C35-C36-C37
5	A	1103	LMT	C11-C10-C9-C8
8	C	1110	OCT	C5-C6-C7-C8
5	A	1105	LMT	C9-C10-C11-C12
7	B	1105	PTY	C32-C33-C34-C35
7	C	1106	PTY	C24-C25-C26-C27
7	B	1105	PTY	C11-C12-C13-C14
7	B	1105	PTY	C8-C11-C12-C13
8	C	1108	OCT	C1-C2-C3-C4
3	A	1101	P6G	C15-C14-O13-C12
7	C	1105	PTY	C21-C22-C23-C24
7	C	1105	PTY	C26-C27-C28-C29
5	B	1104	LMT	C3-C4-C5-C6
5	A	1103	LMT	C5-C6-C7-C8
7	C	1105	PTY	C40-C41-C42-C43
9	B	1110	D10	C3-C4-C5-C6
13	B	1116	DDR	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
5	C	1103	LMT	C7-C8-C9-C10
9	B	1112	D10	C3-C4-C5-C6
5	A	1104	LMT	C4B-C5B-C6B-O6B
7	C	1106	PTY	C31-C32-C33-C34
3	A	1101	P6G	C14-C15-O16-C17
7	B	1105	PTY	C38-C39-C40-C41
7	B	1105	PTY	C3-O11-P1-O13
7	B	1105	PTY	C5-O14-P1-O13
7	C	1105	PTY	C3-O11-P1-O12
7	C	1105	PTY	C5-O14-P1-O13
7	C	1106	PTY	C5-O14-P1-O13
6	E	202	GOL	O2-C2-C3-O3
7	B	1105	PTY	C41-C42-C43-C44
7	C	1106	PTY	C16-C17-C18-C19
7	C	1104	PTY	C24-C25-C26-C27
5	B	1103	LMT	O1'-C1-C2-C3
5	B	1102	LMT	O1'-C1-C2-C3
9	B	1110	D10	C2-C3-C4-C5
7	C	1106	PTY	C15-C16-C17-C18
5	A	1105	LMT	C2-C3-C4-C5
14	B	1117	D12	C9-C10-C11-C12
5	A	1105	LMT	C4-C5-C6-C7
5	B	1103	LMT	C3'-C4'-O1B-C1B
7	C	1105	PTY	C16-C17-C18-C19
5	B	1102	LMT	O5'-C5'-C6'-O6'
5	B	1104	LMT	C1-C2-C3-C4
7	C	1106	PTY	C35-C36-C37-C38
13	B	1116	DDR	O52-C52-C53-O53
9	B	1111	D10	C5-C6-C7-C8
5	B	1103	LMT	C5'-C4'-O1B-C1B
6	C	1107	GOL	O1-C1-C2-O2
8	B	1107	OCT	C1-C2-C3-C4
14	B	1117	D12	C4-C5-C6-C7
7	B	1105	PTY	C12-C13-C14-C15
5	B	1103	LMT	C6-C7-C8-C9
7	C	1104	PTY	C21-C22-C23-C24
7	C	1106	PTY	O30-C30-C31-C32
8	B	1107	OCT	C4-C5-C6-C7
13	B	1116	DDR	C26-C27-C28-C29
9	B	1110	D10	C5-C6-C7-C8
13	B	1116	DDR	O52-C21-C22-C23
5	C	1102	LMT	C4B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
9	B	1111	D10	C4-C5-C6-C7
9	B	1111	D10	C2-C3-C4-C5
13	B	1116	DDR	C25-C26-C27-C28
4	C	1101	FUA	C17-C16-O2-C31
4	B	1101	FUA	C29-C22-C23-C24
5	A	1103	LMT	C4'-C5'-C6'-O6'
7	C	1104	PTY	C25-C26-C27-C28
8	B	1107	OCT	C2-C3-C4-C5
3	A	1101	P6G	C5-C6-O7-C8
8	B	1108	OCT	C5-C6-C7-C8
7	B	1105	PTY	C36-C37-C38-C39
5	A	1103	LMT	O5B-C1B-O1B-C4'
7	B	1105	PTY	C16-C17-C18-C19
13	B	1116	DDR	O21-C21-C22-C23
7	C	1106	PTY	C13-C14-C15-C16
3	A	1101	P6G	C2-C3-O4-C5
3	A	1101	P6G	C6-C5-O4-C3

There are no ring outliers.

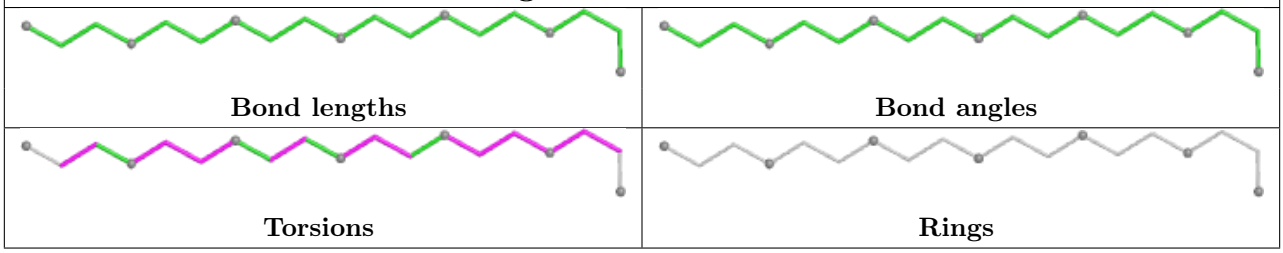
13 monomers are involved in 40 short contacts:

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

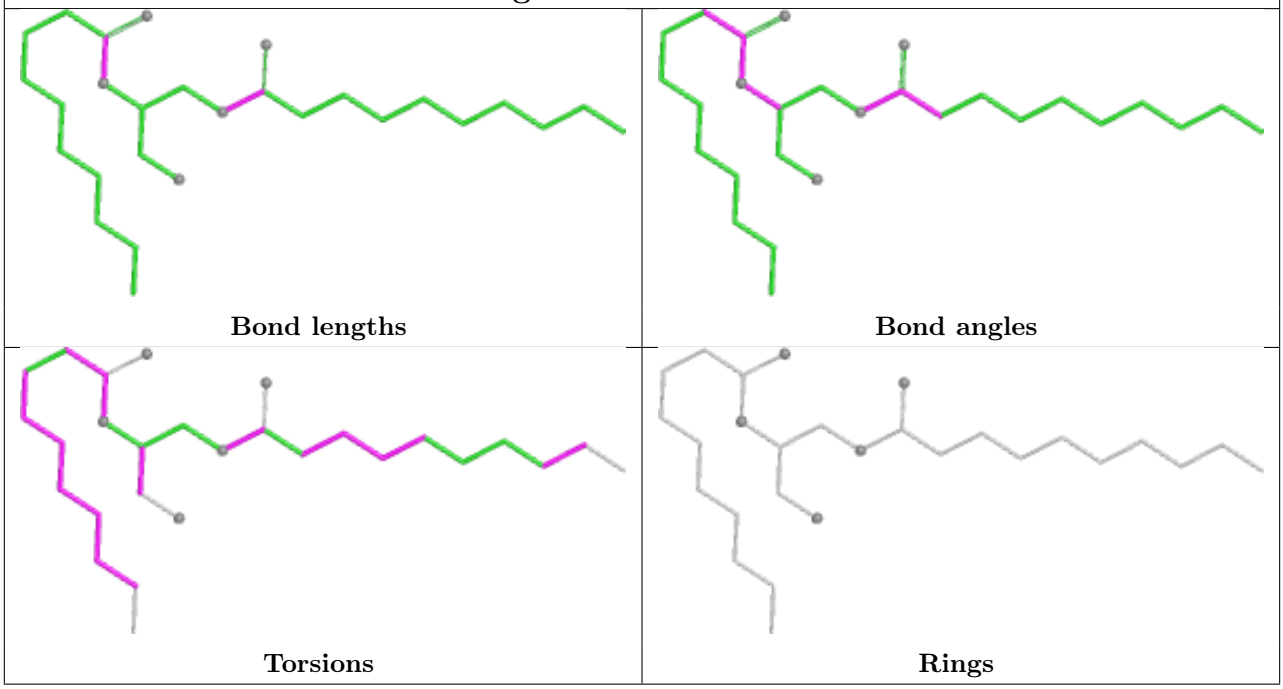
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

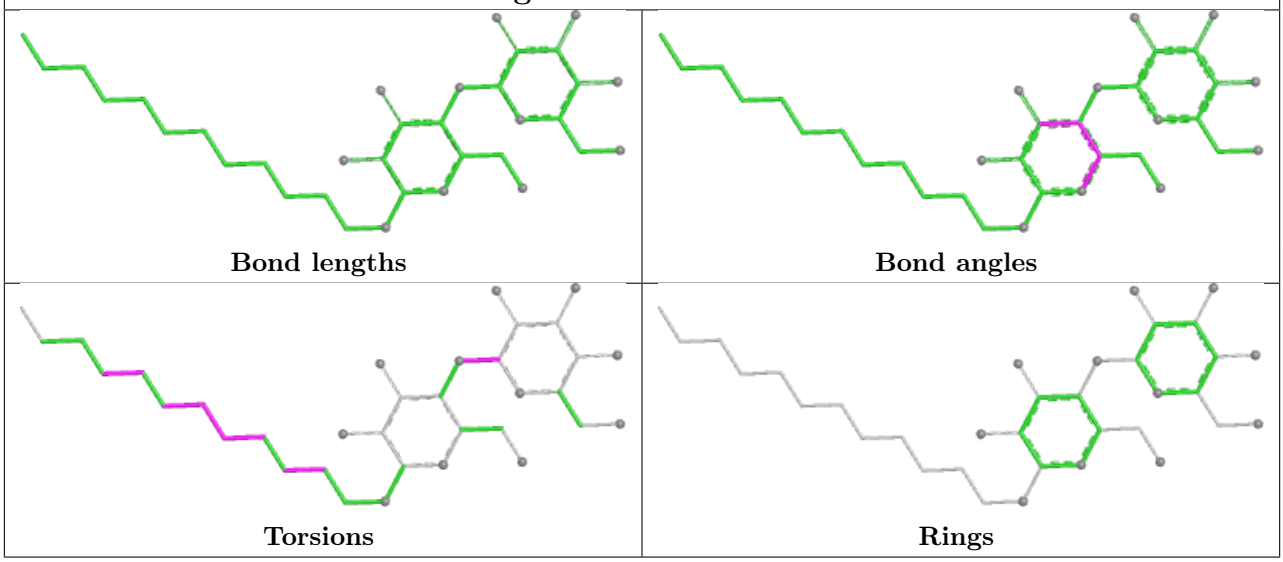
Ligand P6G A 1101



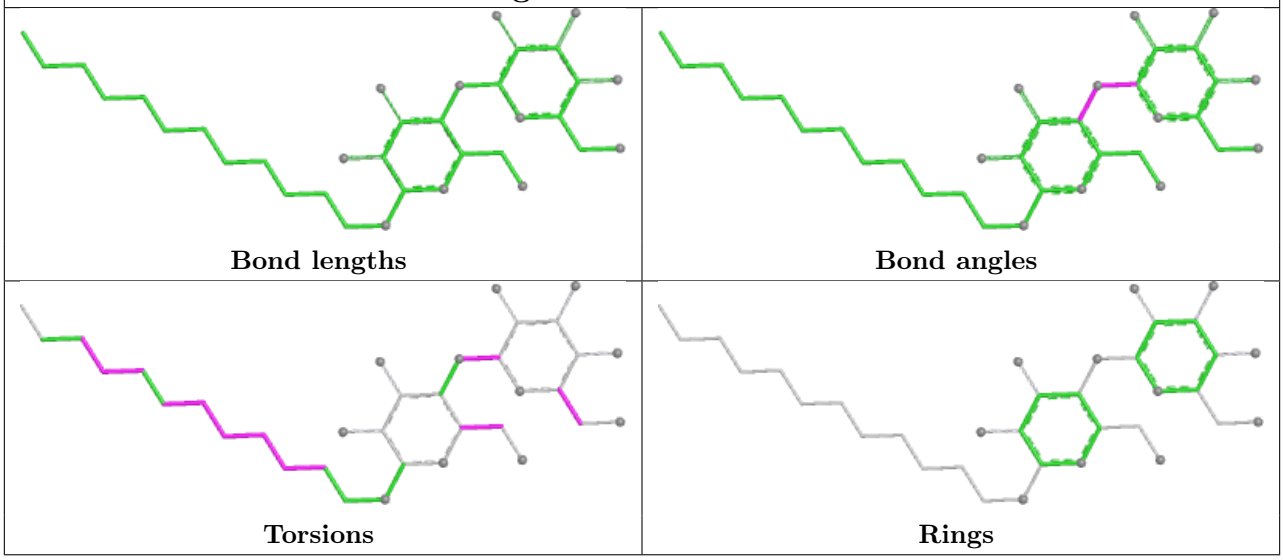
Ligand DDR B 1116



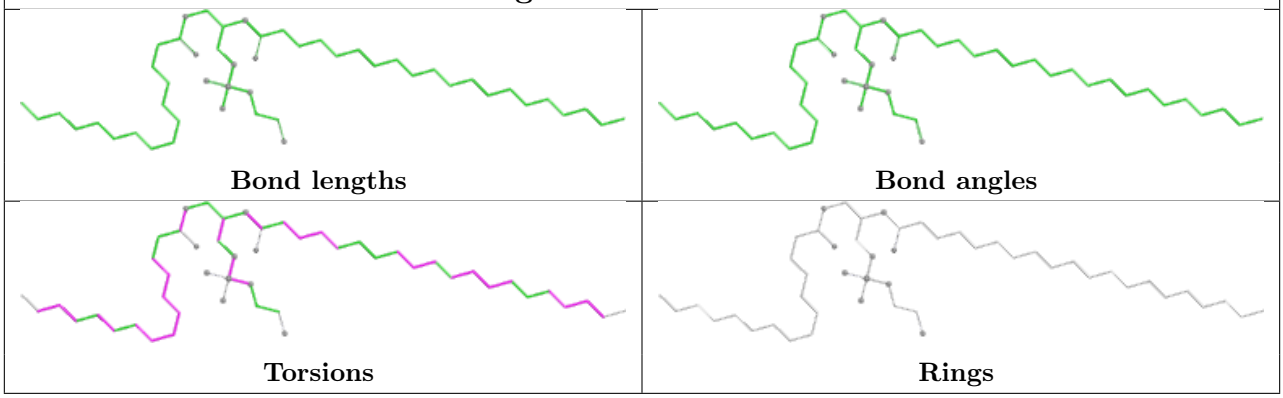
Ligand LMT B 1104



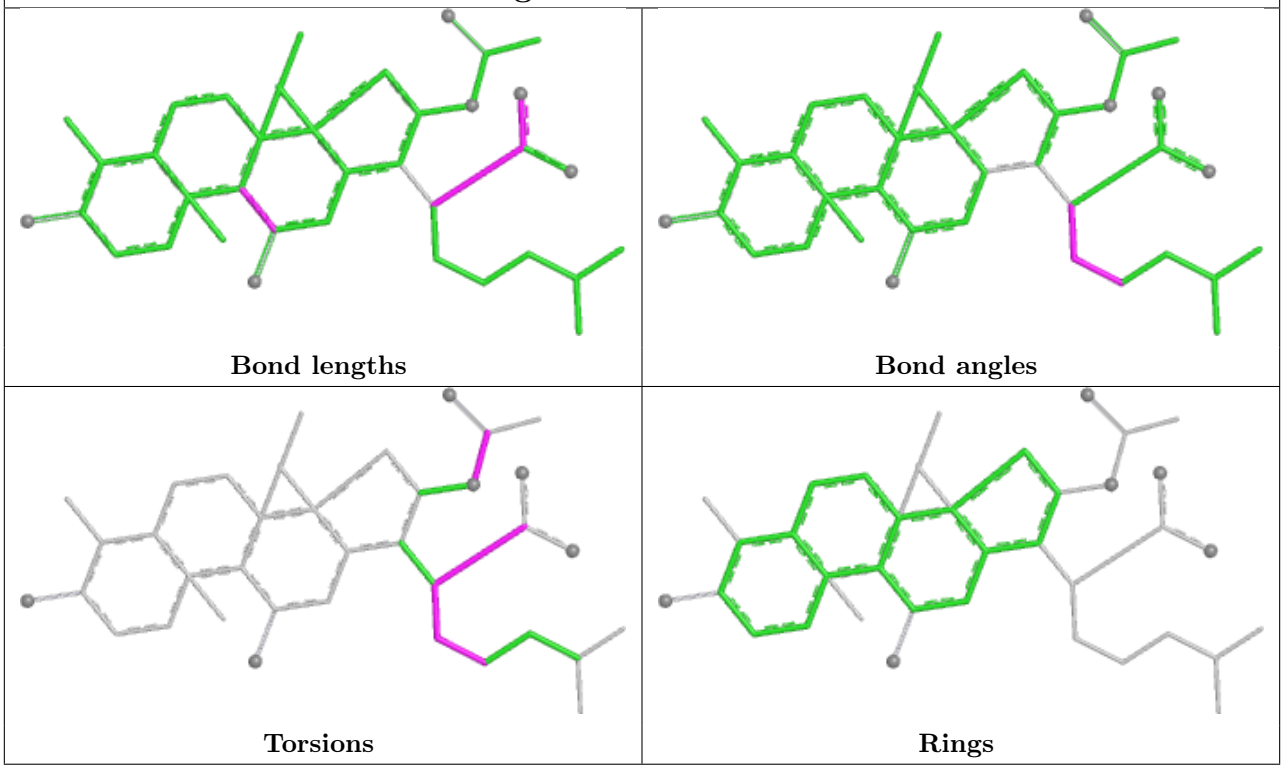
Ligand LMT A 1103



Ligand PTY B 1105



Ligand FUA A 1102



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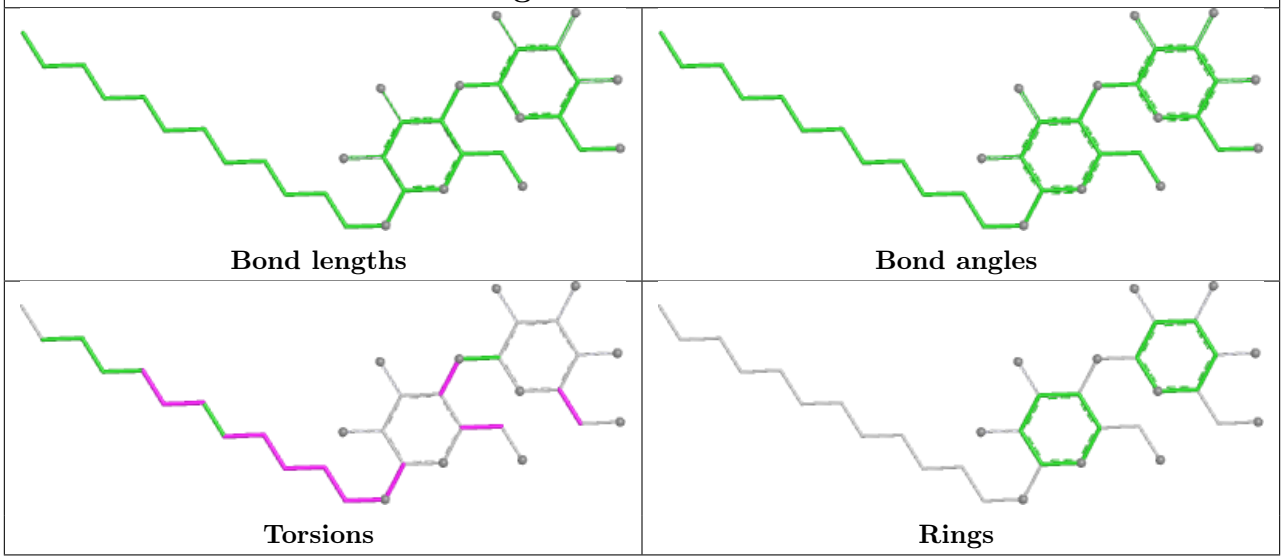
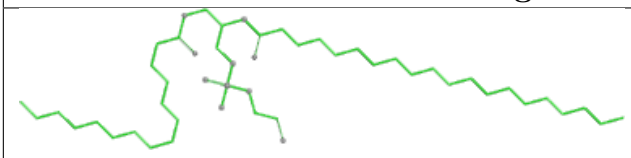
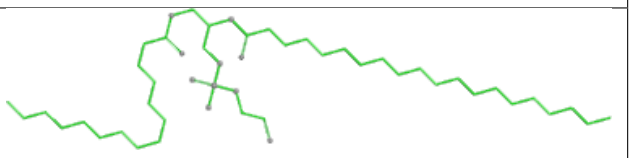


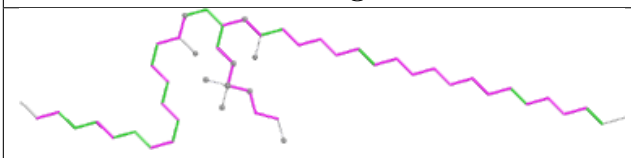
Ligand PTY C 1106



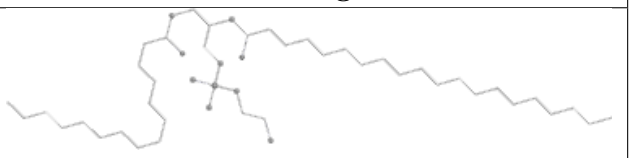
Bond lengths



Bond angles

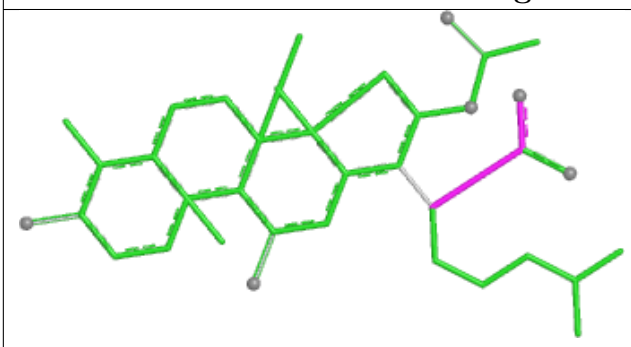


Torsions

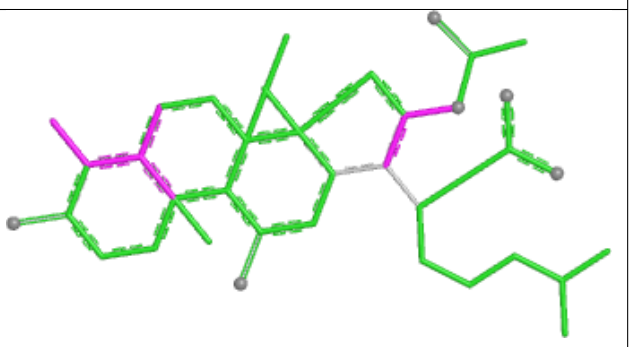


Rings

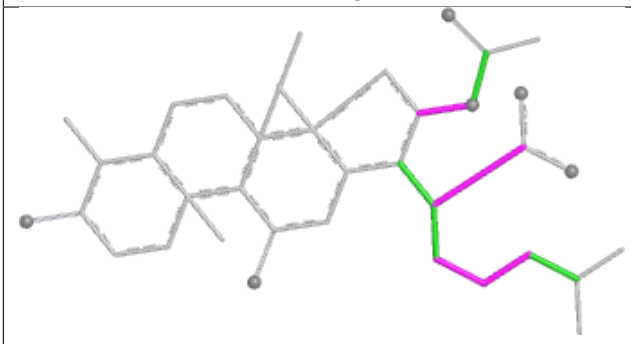
Ligand FUA C 1101



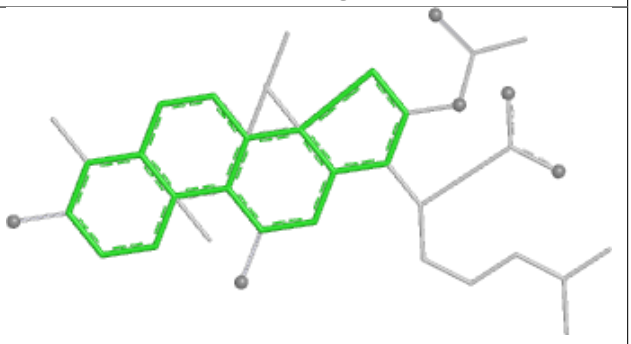
Bond lengths



Bond angles

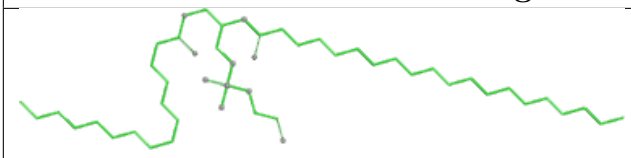


Torsions

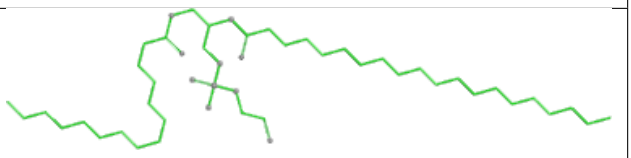


Rings

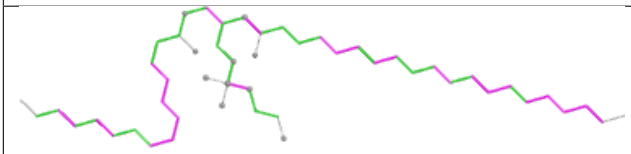
Ligand PTY C 1104



Bond lengths



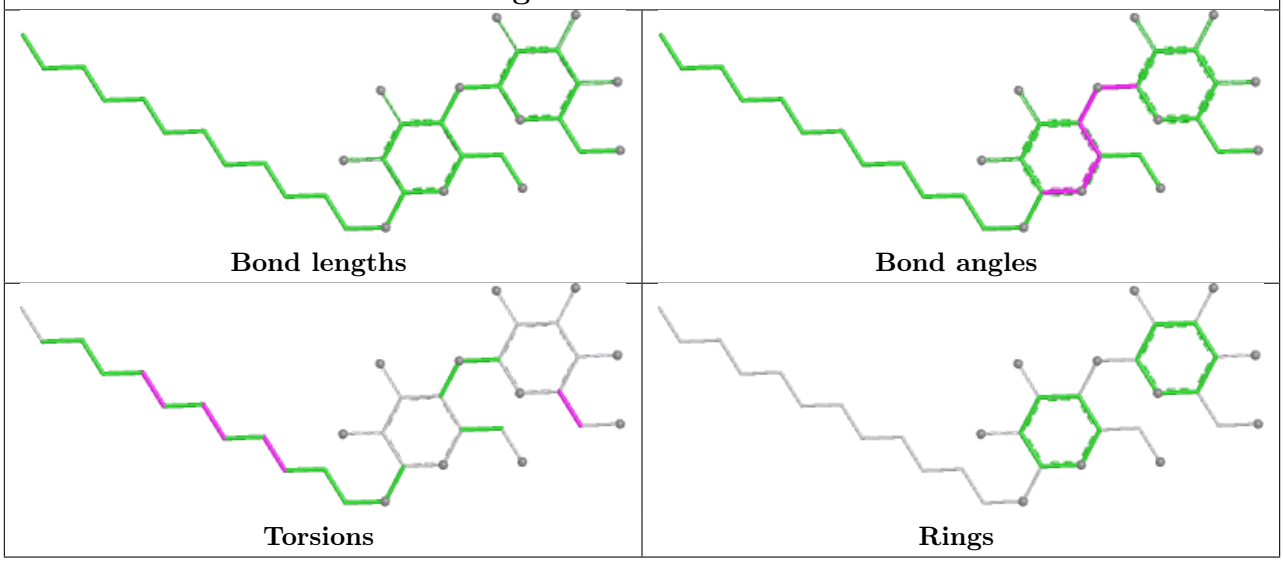
Bond angles



Torsions

Rings

Ligand LMT A 1104



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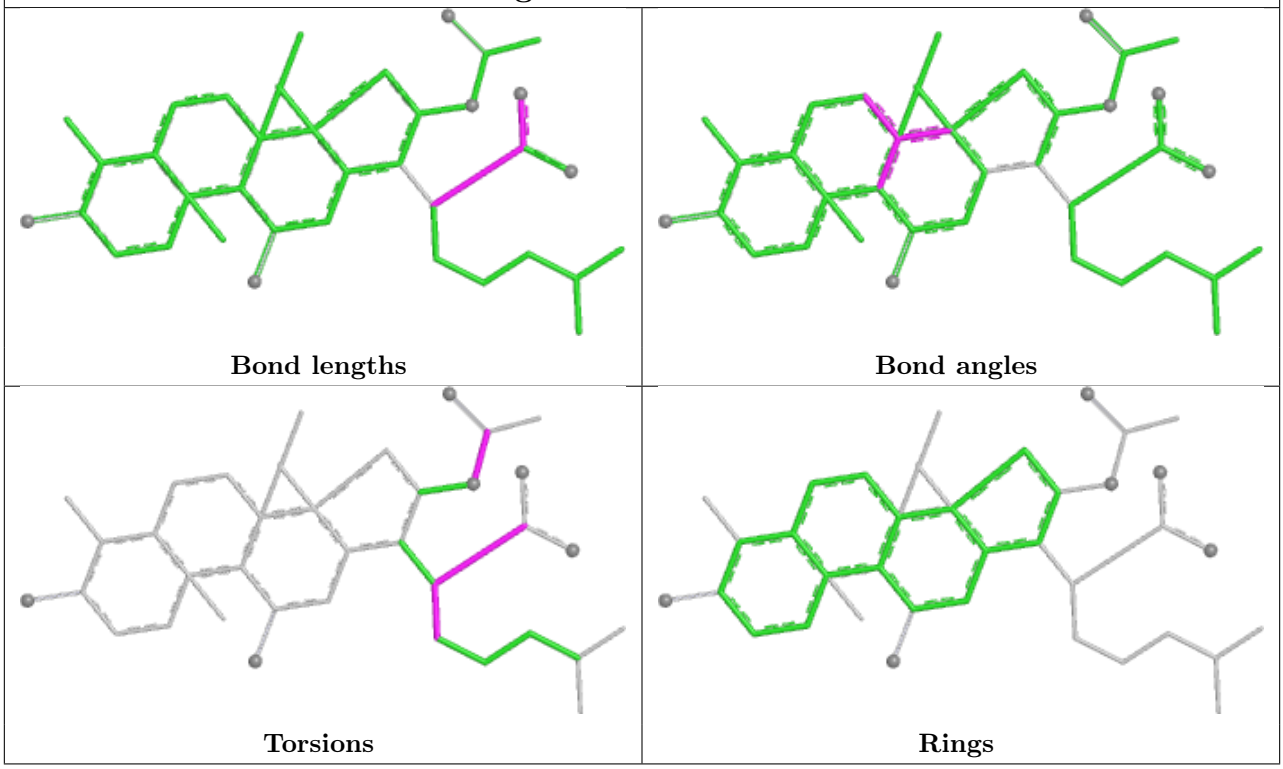

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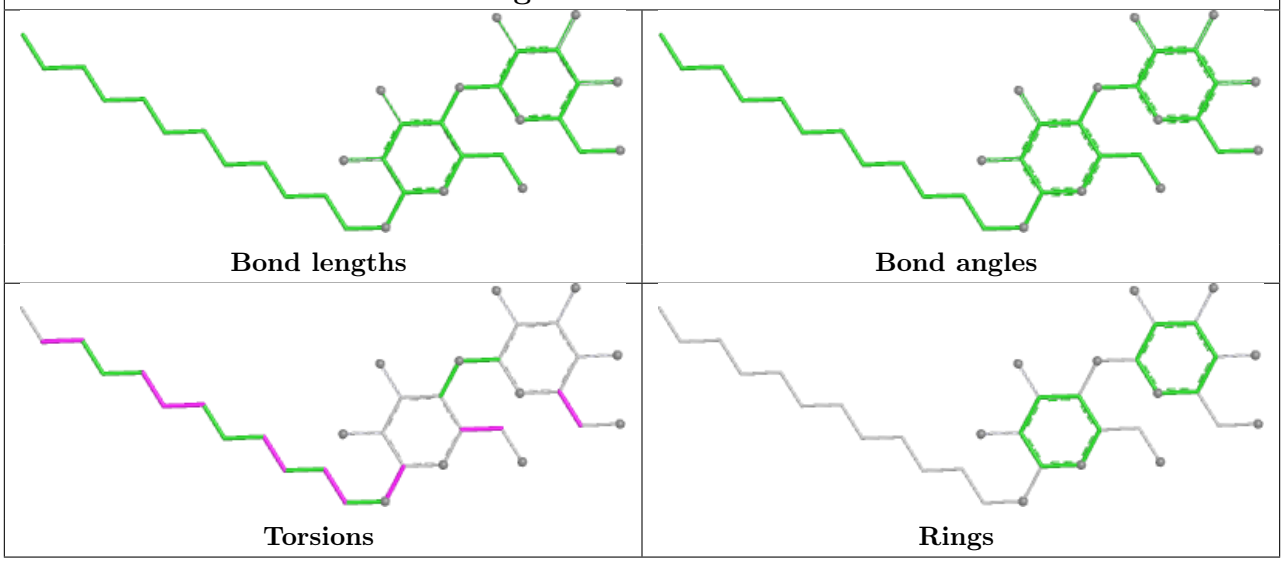
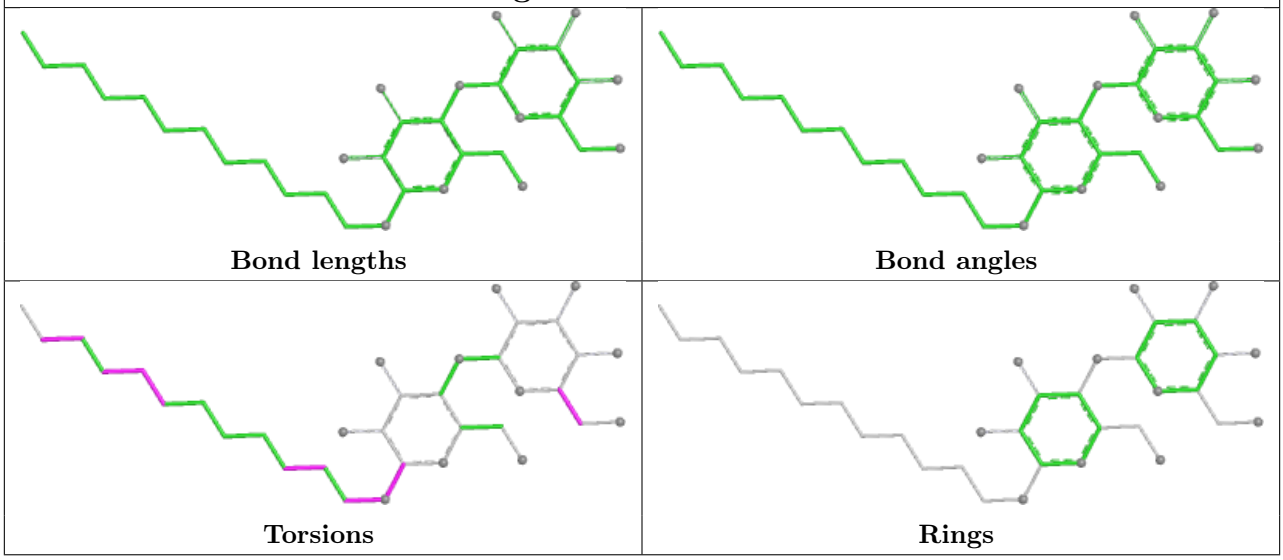
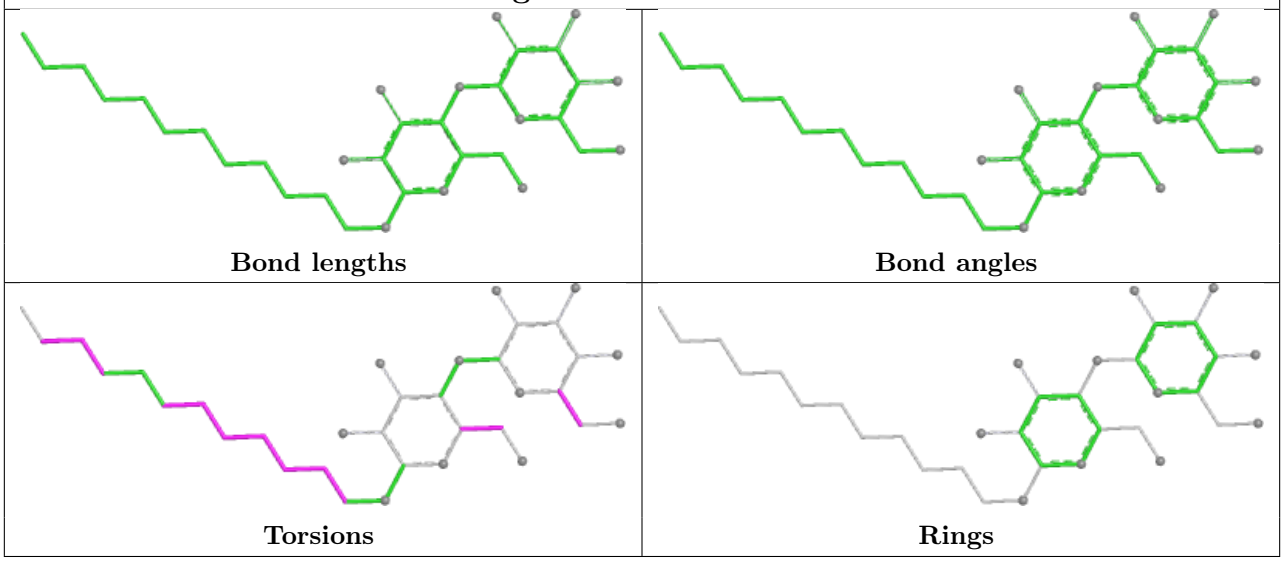
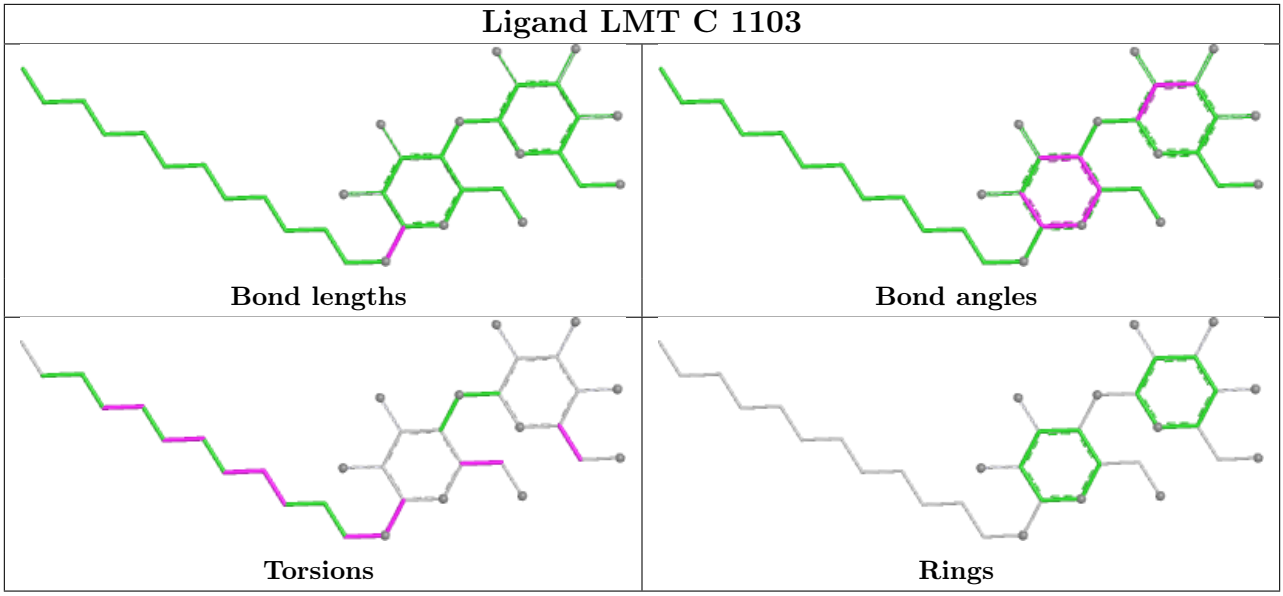


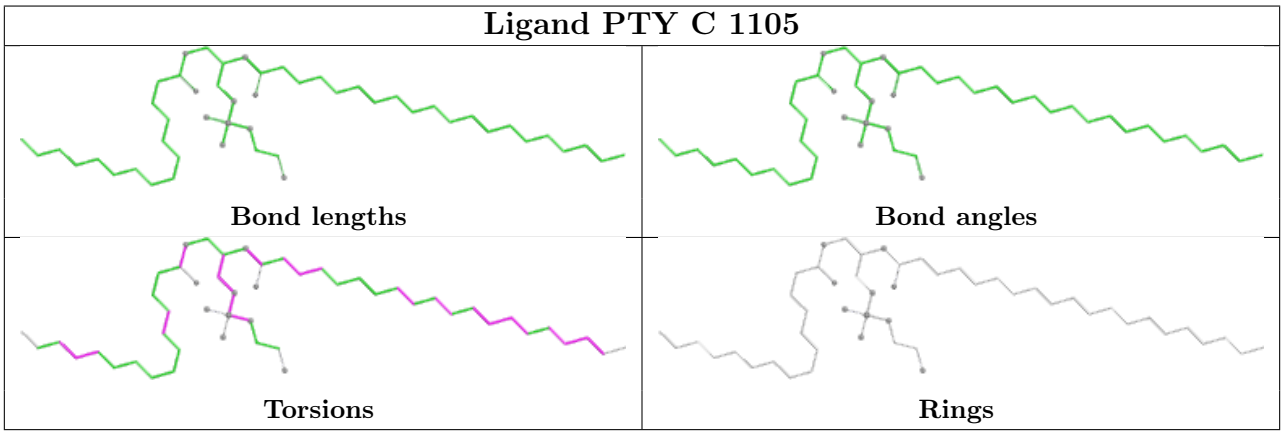
Ligand LMT C 1102



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%)

All (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
1	A	423	GLU	5.1
1	C	508	GLY	5.0
1	A	673	GLU	4.9
1	B	714	THR	4.8
1	B	833	PRO	4.7
2	E	34	MET	4.4
1	C	496	MET	4.1
1	A	712	MET	3.9
1	A	870	GLY	3.8
1	A	500	ILE	3.8
2	E	33	LEU	3.7
2	D	161	LEU	3.7
2	E	66	LEU	3.7
2	E	28	ASP	3.7
1	B	603	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	597	TYR	3.6
2	E	32	ILE	3.6
1	A	834	GLY	3.6
2	D	165	LEU	3.6
1	C	730	ASP	3.6
2	E	67	LEU	3.5
2	D	150	PHE	3.5
1	A	869	SER	3.4
1	C	500	ILE	3.4
2	E	68	LYS	3.4
2	E	143	ASP	3.4
2	E	36	ASN	3.4
1	B	657	GLN	3.4
1	B	677	ALA	3.4
1	B	604	ASN	3.3
1	B	671	ILE	3.3
1	C	361	ASN	3.3
1	B	134	SER	3.3
2	E	126	LEU	3.3
1	A	427	PRO	3.2
1	A	501	ALA	3.2
2	E	163	GLU	3.2
1	A	871	ASN	3.2
2	E	69	ASN	3.2
1	B	617	PHE	3.2
1	A	512	PHE	3.1
1	A	362	PHE	3.1
1	A	533	GLY	3.1
2	E	99	LEU	3.1
1	C	803	ALA	3.0
2	D	153	SER	3.0
2	E	146	GLY	3.0
1	C	804	PHE	3.0
1	B	510	LYS	3.0
1	A	356	TYR	3.0
1	C	811	TYR	3.0
1	A	537	SER	2.9
1	C	512	PHE	2.9
1	A	867	ARG	2.9
1	C	362	PHE	2.9
1	A	431	THR	2.8
1	A	678	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	711	ASP	2.8
2	E	27	ASP	2.8
1	B	255	GLN	2.8
2	E	30	VAL	2.8
2	E	139	VAL	2.8
2	D	141	ALA	2.8
1	A	674	LEU	2.8
1	A	868	LEU	2.8
2	E	106	VAL	2.8
1	A	255	GLN	2.8
1	A	872	GLN	2.8
2	E	140	ASN	2.8
1	C	1034	SER	2.8
1	A	363	ARG	2.8
1	B	508	GLY	2.8
2	E	165	LEU	2.8
2	E	130	GLU	2.7
2	E	141	ALA	2.7
1	B	600	THR	2.6
1	B	676	THR	2.6
2	D	140	ASN	2.6
2	E	107	ASN	2.6
1	A	496	MET	2.6
1	C	363	ARG	2.6
1	B	832	ALA	2.6
1	C	513	PHE	2.6
1	A	425	LEU	2.6
1	B	256	ASP	2.6
1	A	670	ALA	2.6
1	A	498	LYS	2.6
1	A	918	PHE	2.6
1	B	653	ARG	2.6
2	E	29	GLU	2.5
1	C	425	LEU	2.5
1	A	543	VAL	2.5
1	A	866	GLU	2.5
1	A	534	ILE	2.4
1	C	426	PRO	2.4
1	C	253	VAL	2.4
1	A	846	GLN	2.4
1	C	705	GLU	2.4
1	C	918	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	497	LEU	2.4
2	D	126	LEU	2.4
2	D	163	GLU	2.4
1	A	544	LEU	2.4
1	B	675	GLY	2.4
1	A	3	ASN	2.4
1	B	593	GLU	2.4
1	B	601	LYS	2.4
1	A	494	ALA	2.4
1	B	628	PHE	2.4
2	E	97	GLU	2.4
1	A	671	ILE	2.4
1	B	606	VAL	2.3
1	B	674	LEU	2.3
1	B	918	PHE	2.3
1	C	701	GLN	2.3
2	E	37	GLY	2.3
1	A	843	LEU	2.3
2	E	62	ILE	2.3
1	C	702	LEU	2.3
2	E	150	PHE	2.3
1	B	257	GLY	2.3
1	A	513	PHE	2.2
1	C	558	ARG	2.2
1	A	491	ALA	2.2
1	C	515	TRP	2.2
1	A	462	SER	2.2
1	C	806	SER	2.2
2	E	93	LEU	2.2
1	A	541	TYR	2.2
1	C	698	ALA	2.2
1	A	540	ARG	2.2
1	A	865	GLN	2.2
1	B	713	LEU	2.2
1	A	514	GLY	2.1
1	B	512	PHE	2.1
1	B	513	PHE	2.1
1	B	254	ASN	2.1
1	B	655	PHE	2.1
2	D	166	GLN	2.1
1	A	653	ARG	2.1
1	B	638	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	511	GLY	2.1
2	E	87	ALA	2.0
2	E	109	LYS	2.0
1	B	332	PHE	2.0
1	B	830	GLN	2.0
1	C	733	GLN	2.0
1	C	850	LYS	2.0
1	C	511	GLY	2.0
2	D	149	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

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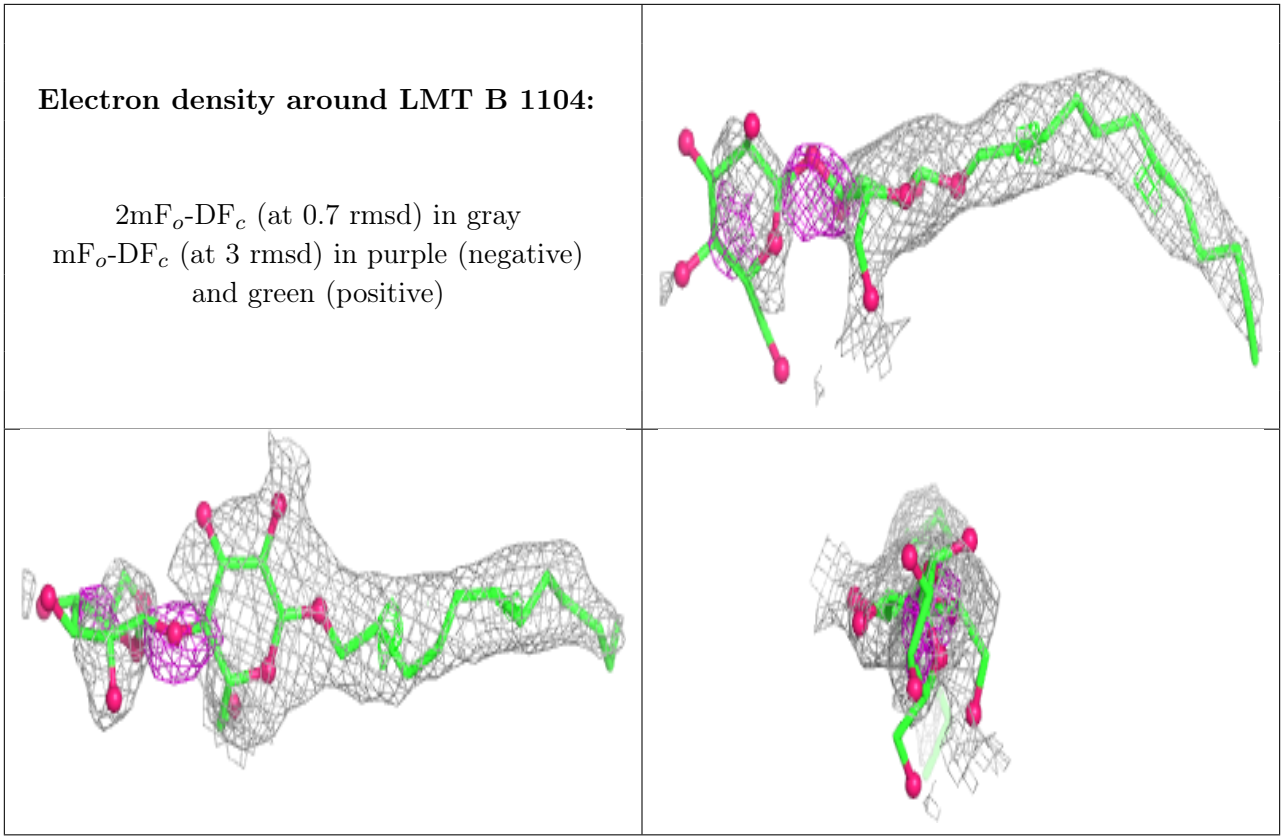
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	FUA	C	1101	37/37	0.81	0.46	90,94,96,96	37
5	LMT	A	1103	35/35	0.81	0.35	93,104,109,109	0
8	OCT	C	1110	8/8	0.81	0.32	80,81,81,81	0
10	DDQ	C	1112	14/14	0.82	0.28	83,83,84,84	0
9	D10	B	1109	10/10	0.82	0.33	69,70,70,70	0
8	OCT	B	1107	8/8	0.82	0.22	88,90,90,90	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.

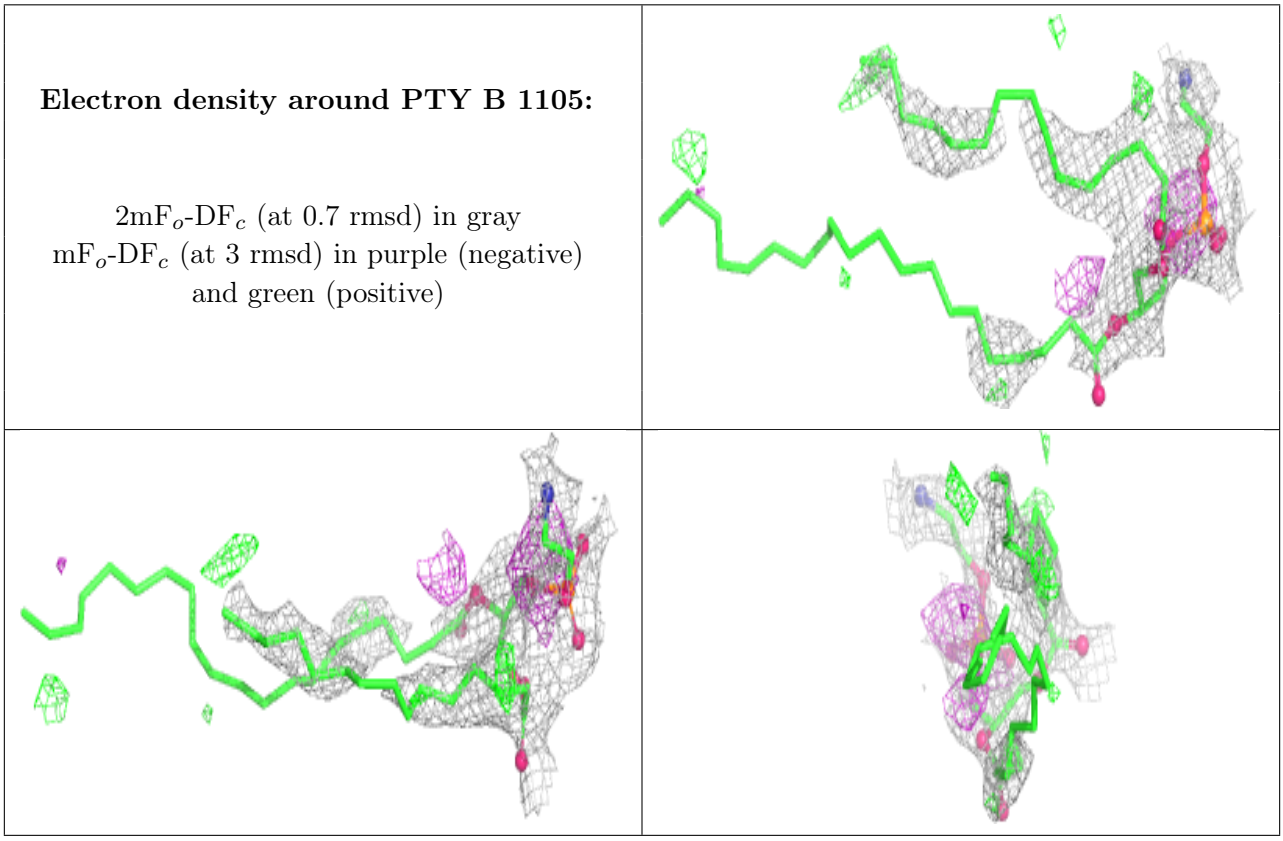
Electron density around LMT B 1104:

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



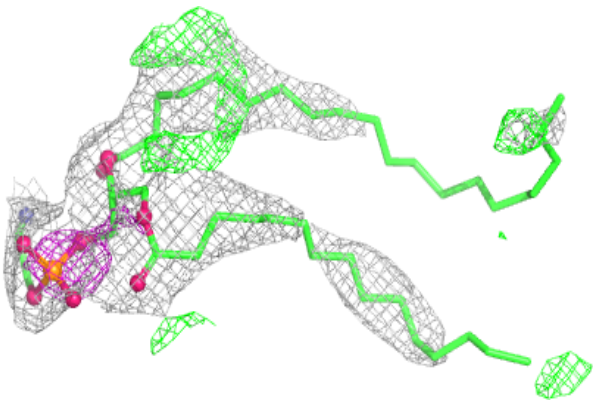
Electron density around PTY B 1105:

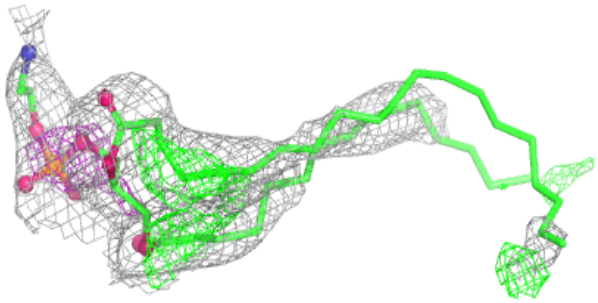
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

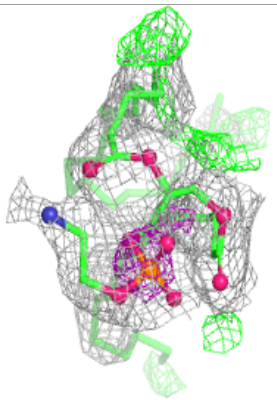


Electron density around PTY C 1106:

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

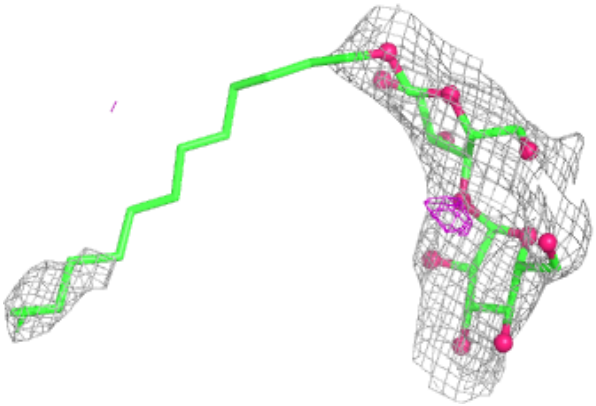


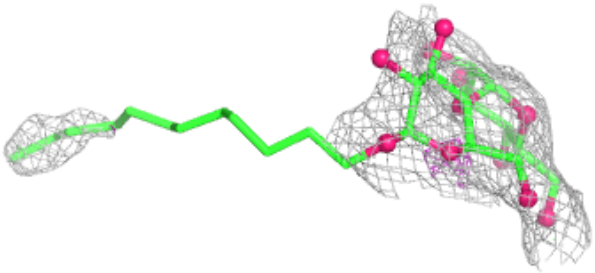


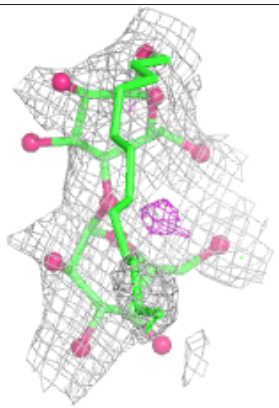


Electron density around LMT C 1103:

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

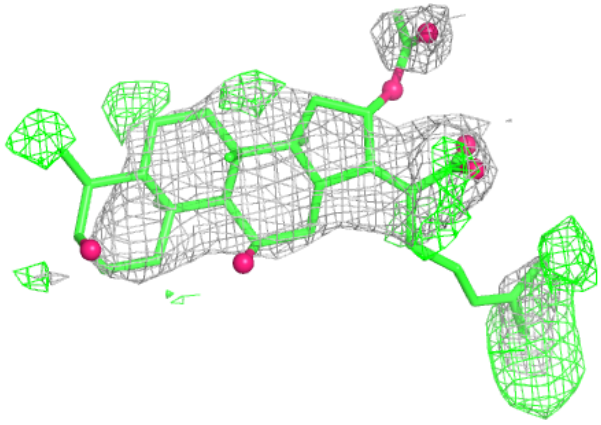


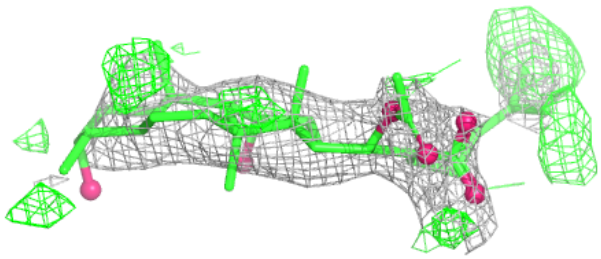


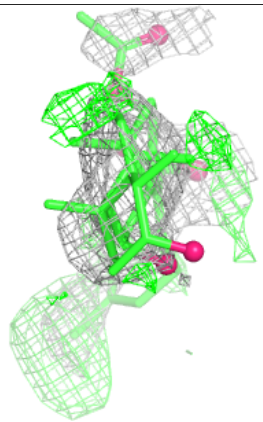


Electron density around FUA A 1102:

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

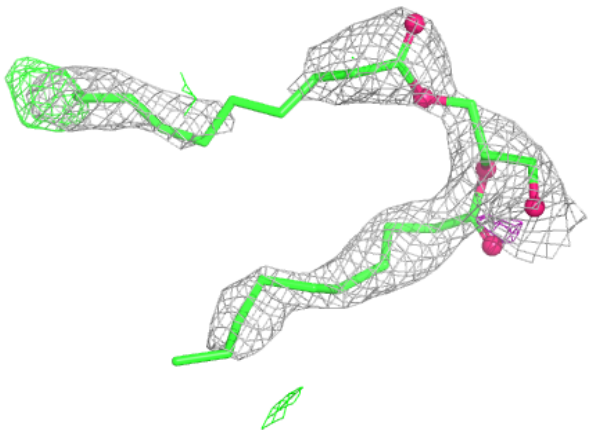


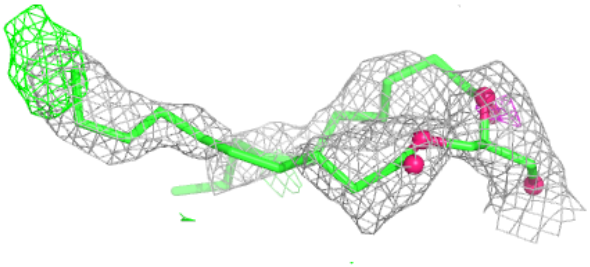


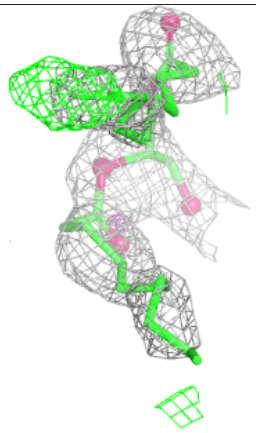


Electron density around DDR B 1116:

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

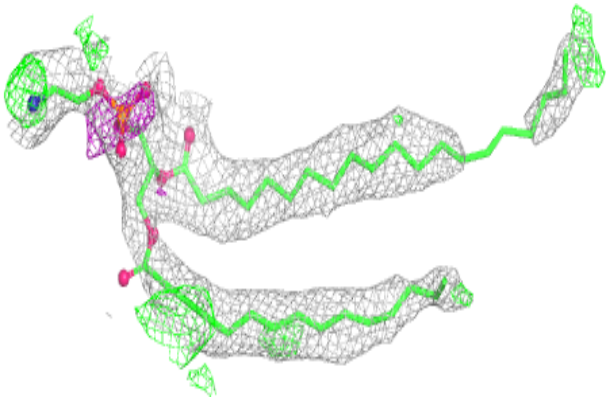


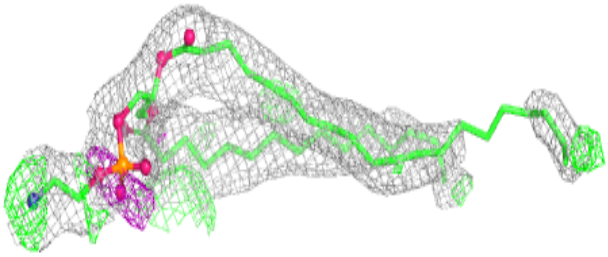


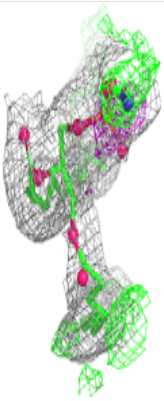


Electron density around PTY C 1105:

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

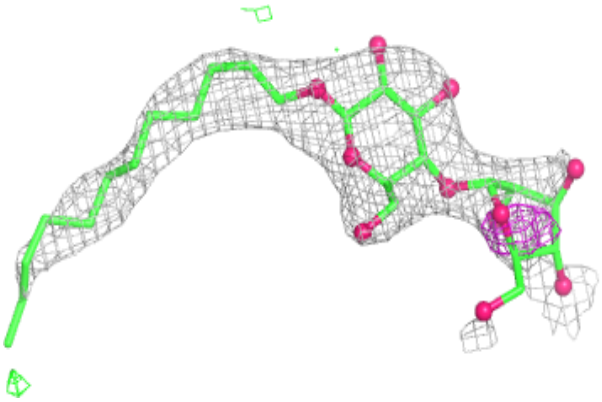


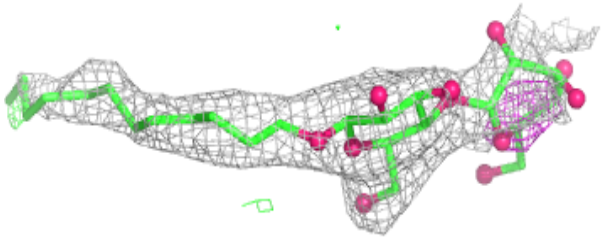


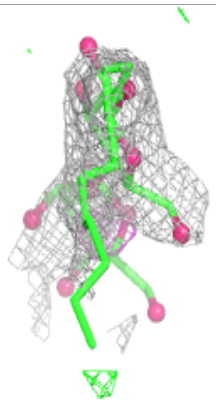


Electron density around LMT A 1104:

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

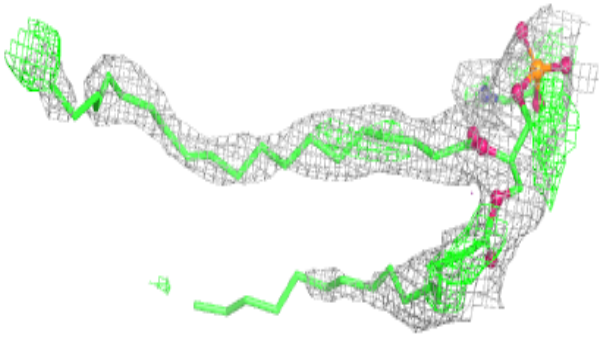


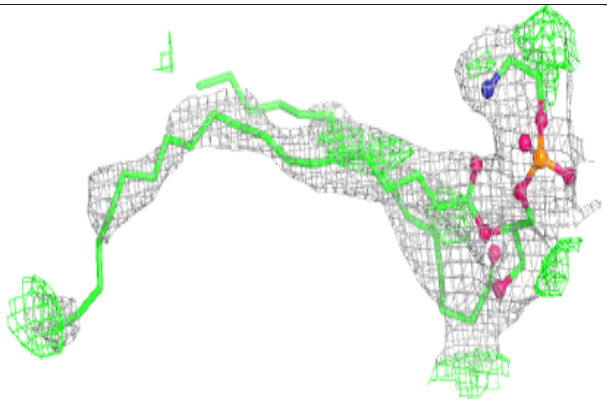


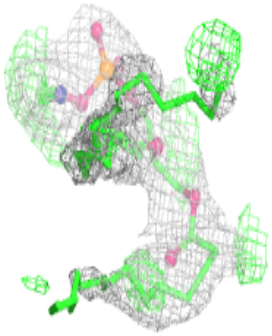


Electron density around PTY C 1104:

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

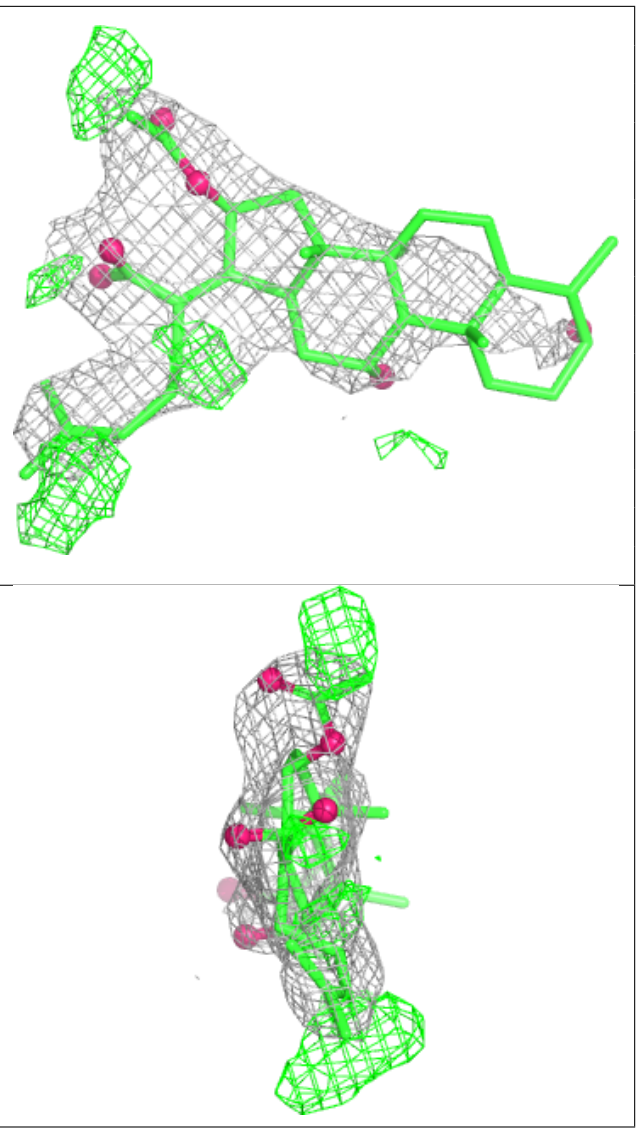






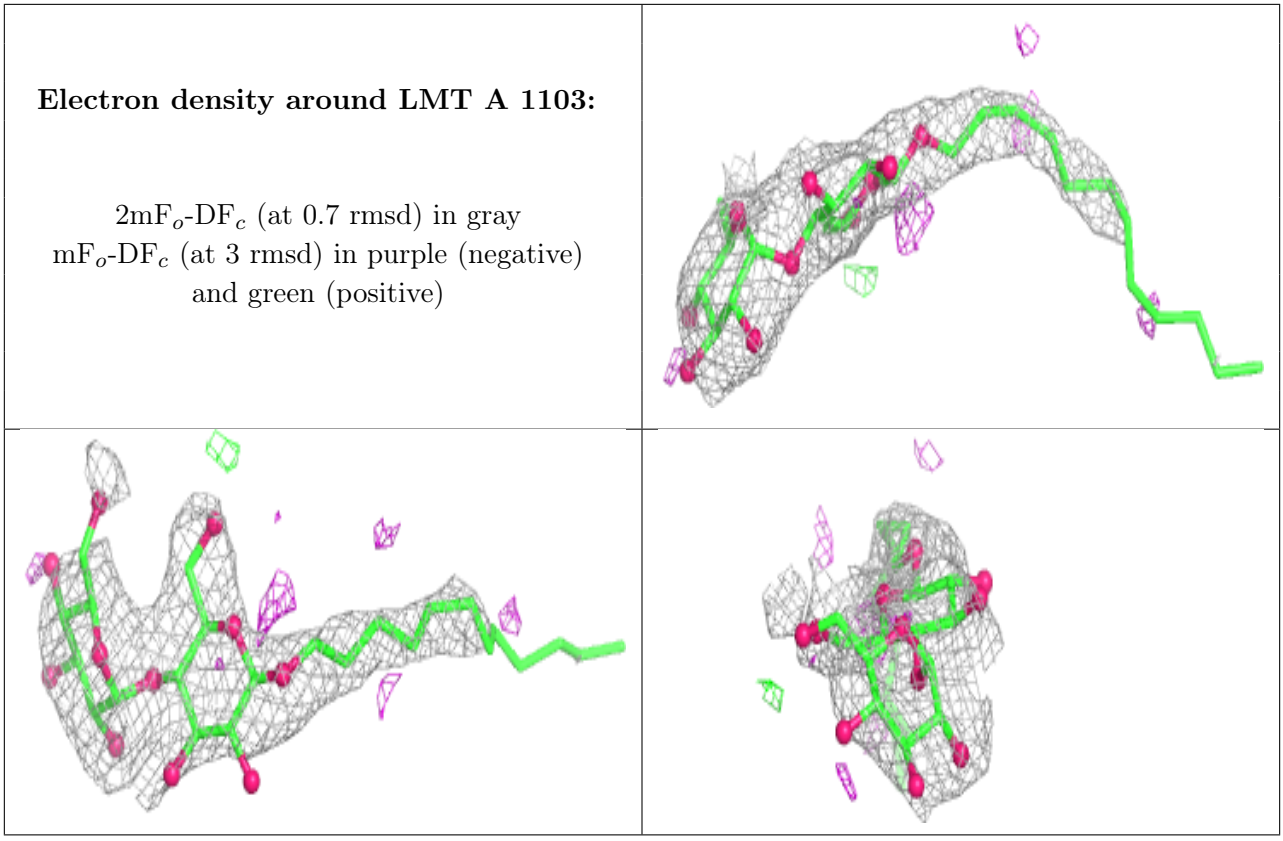
Electron density around FUA C 1101:

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



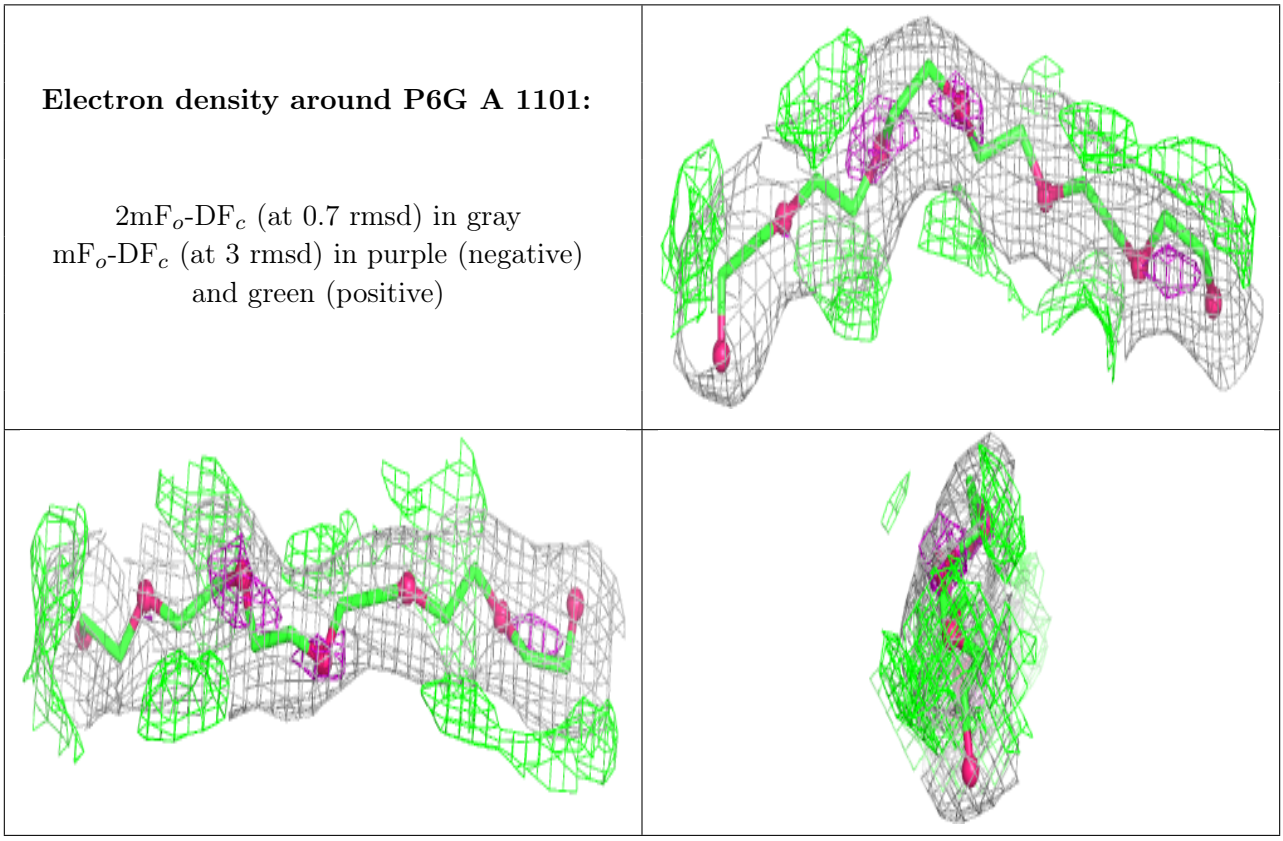
Electron density around LMT A 1103:

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



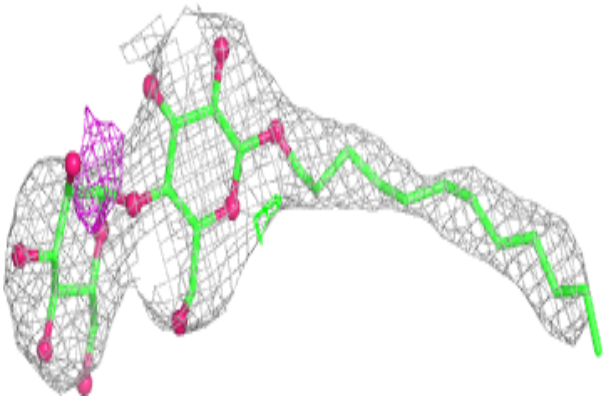
Electron density around P6G A 1101:

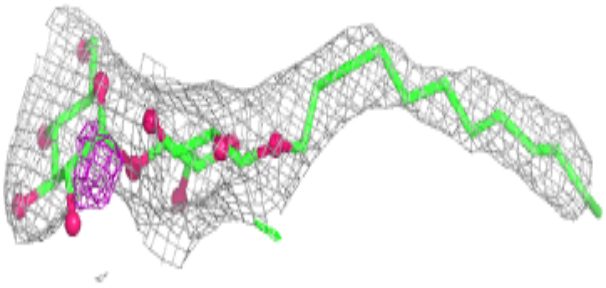
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

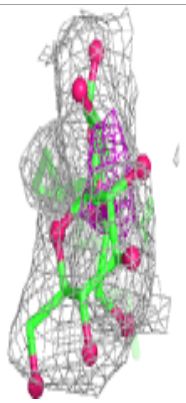


Electron density around LMT B 1103:

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

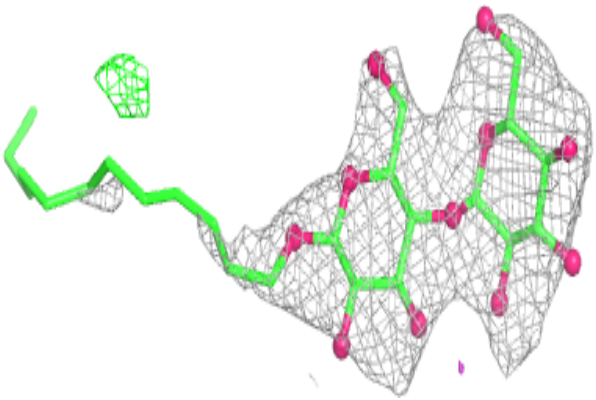


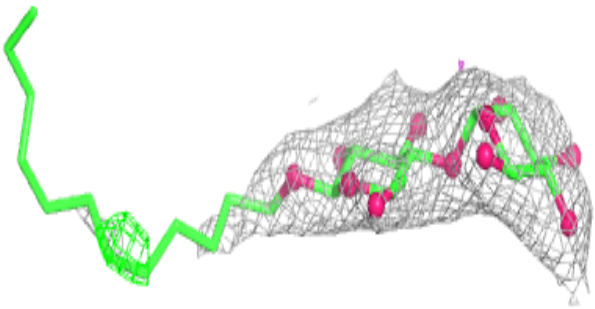


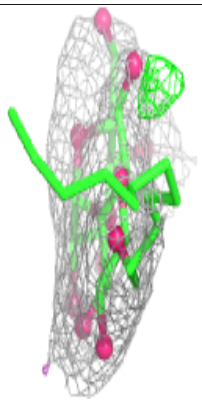


Electron density around LMT B 1102:

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

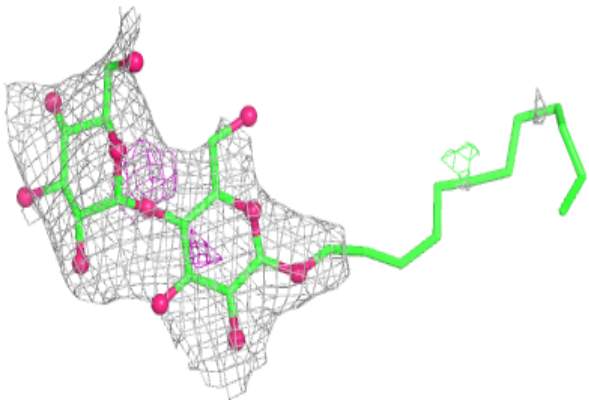


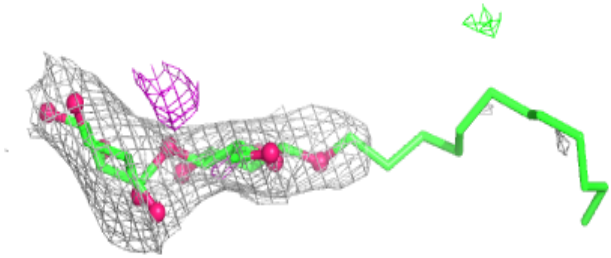


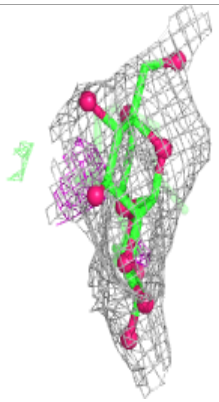


Electron density around LMT A 1105:

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

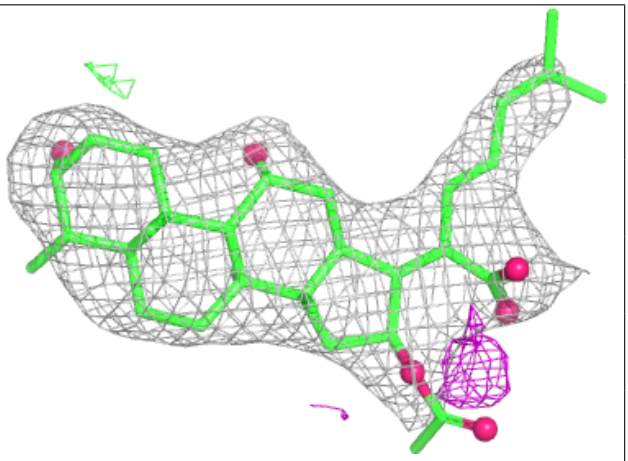


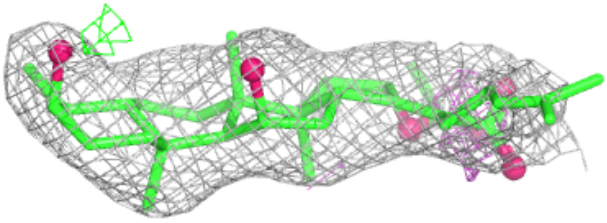


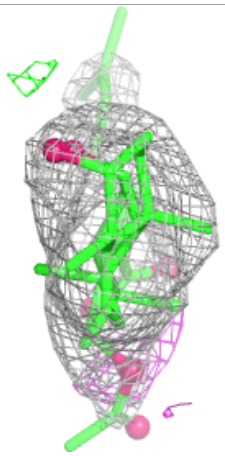


Electron density around FUA B 1101:

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

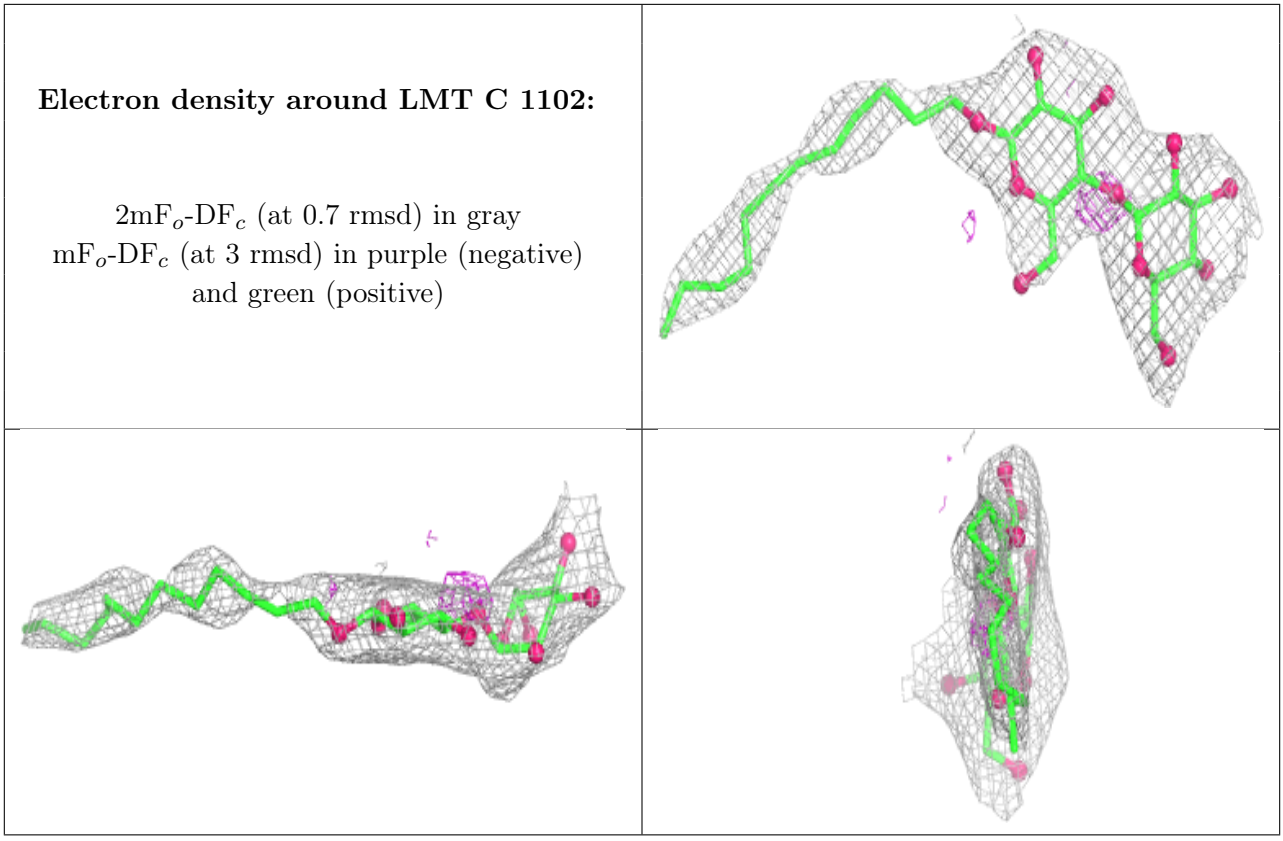






Electron density around LMT C 1102:

$2mF_o$-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.