Full wwPDB X-ray Structure Validation Report (i)

Jun 23, 2024 – 07:37 PM EDT

PDB ID	:	6Q4P
Title	:	Fusidic acid bound AcrB_N298A
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:

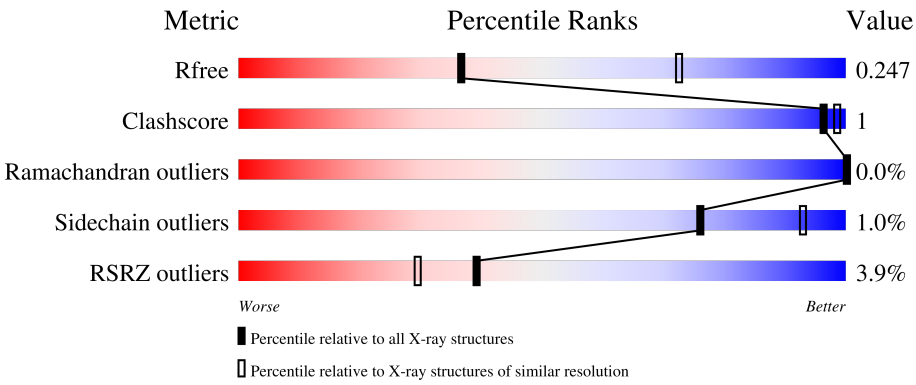
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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	3% 95%
1	B	1057	3% 94%
1	C	1057	2% 95%
2	D	169	8% 92% 8%
2	E	169	22% 90% 9%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	D10	B	1116	-	-	-	X
3	LMT	C	1103	-	-	-	X
4	D12	B	1106	-	-	-	X
5	DDQ	A	1106	-	-	-	X
8	FUA	B	1104	-	-	-	X

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 27306 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	1042	7942	5108	1312	1478	44	0	3	0
1	B	1034	7861	5060	1295	1462	44	0	2	0
1	C	1034	7877	5073	1300	1460	44	0	3	0

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	298	ALA	ASN	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	298	ALA	ASN	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	298	ALA	ASN	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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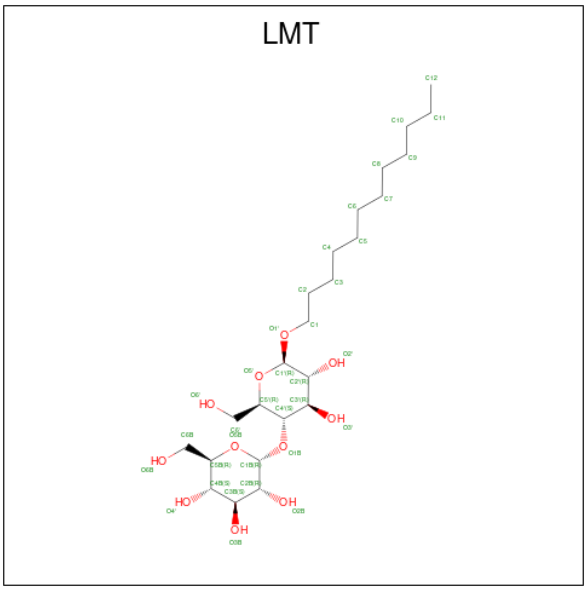
Chain	Residue	Modelled	Actual	Comment	Reference
C	1054	HIS	-	expression tag	UNP P31224
C	1055	HIS	-	expression tag	UNP P31224
C	1056	HIS	-	expression tag	UNP P31224
C	1057	HIS	-	expression tag	UNP P31224

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



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

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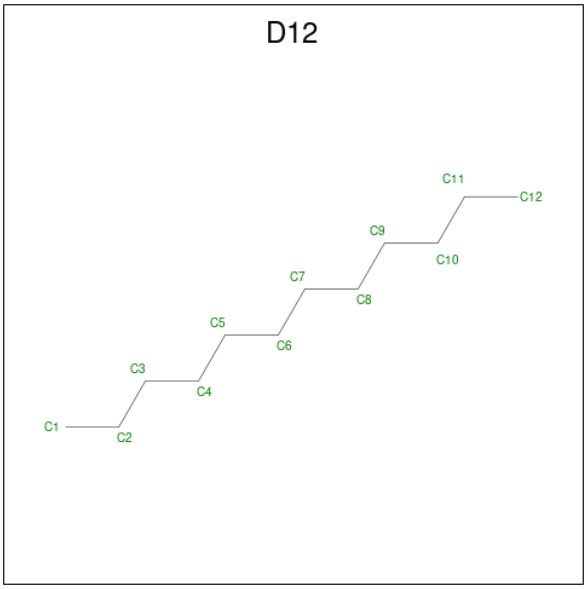
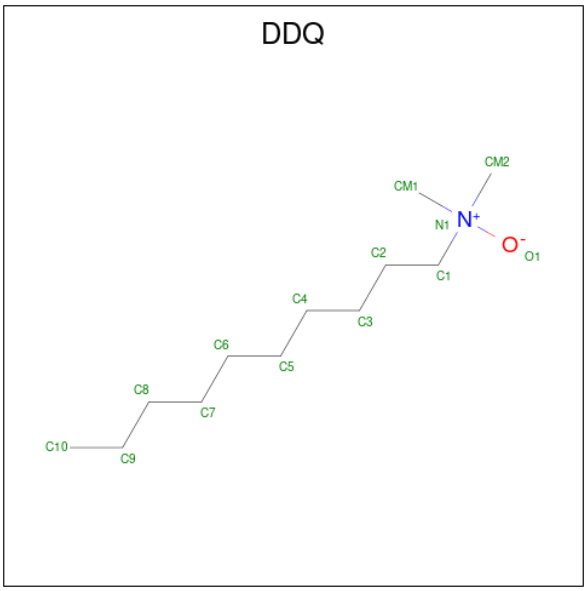
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	B	1	35	24	11	0	0
			Total	C	O		
3	B	1	35	24	11	0	0
			Total	C	O		
3	C	1	35	24	11	0	0
			Total	C	O		
3	C	1	35	24	11	0	0
			Total	C	O		
3	C	1	35	24	11	0	0

- Molecule 4 is DODECANE (three-letter code: D12) (formula: $C_{12}H_{26}$).



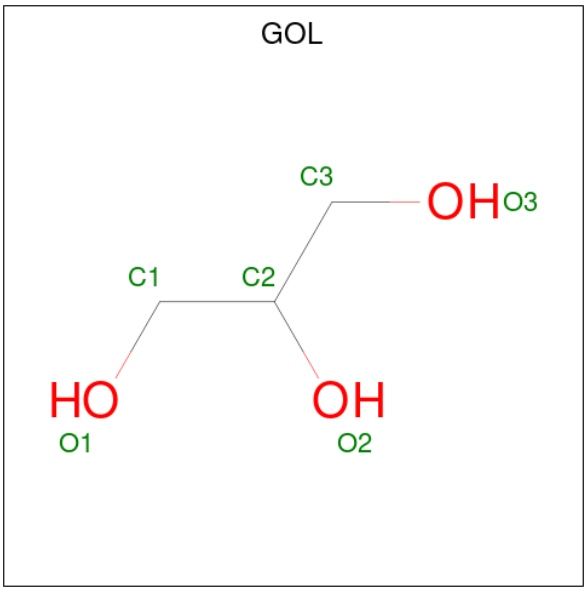
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C		
4	A	1	12	12	0	0
			Total	C		
4	B	1	12	12	0	0
			Total	C		
4	C	1	12	12	0	0

- Molecule 5 is DECYLAMINE-N,N-DIMETHYL-N-OXIDE (three-letter code: DDQ) (formula: $C_{12}H_{27}NO$).



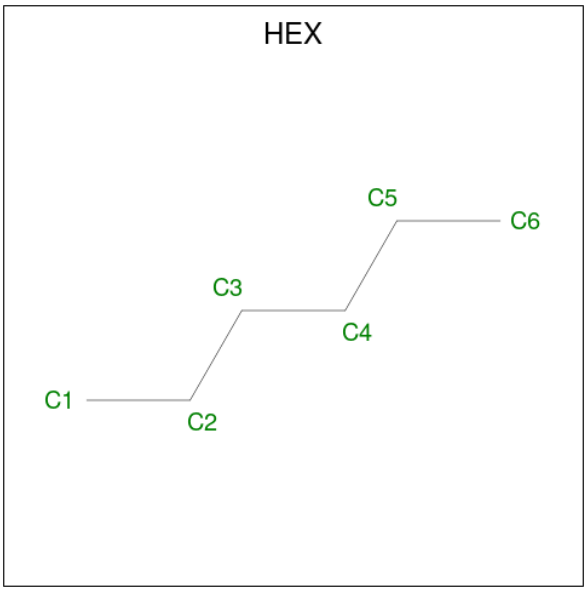
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	14	12	1	1	0	0
			Total	C	N	O		
5	B	1	14	12	1	1	0	0
			Total	C	N	O		
5	B	1	14	12	1	1	0	0
			Total	C	N	O		
5	C	1	14	12	1	1	0	0
			Total	C	N	O		
5	C	1	14	12	1	1	0	0
			Total	C	N	O		
5	C	1	14	12	1	1	0	0

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



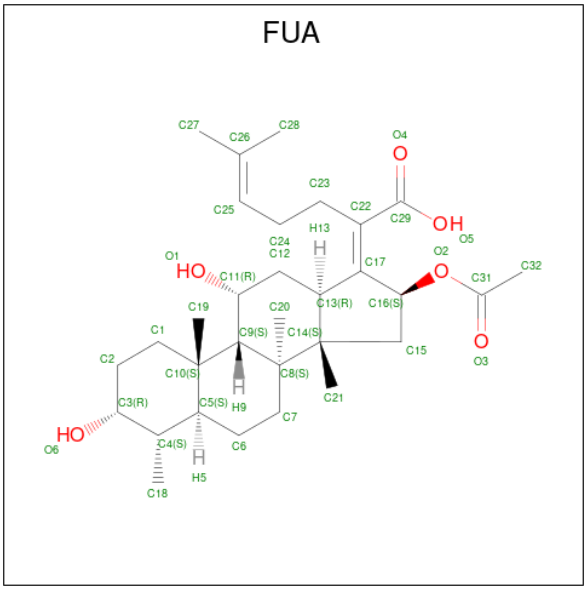
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	6	3	3	0	0
			Total	C	O		
6	A	1	6	3	3	0	0
			Total	C	O		
6	A	1	6	3	3	0	0
			Total	C	O		
6	B	1	6	3	3	0	0
			Total	C	O		
6	C	1	6	3	3	0	0
			Total	C	O		
6	E	1	6	3	3	0	0

- Molecule 7 is HEXANE (three-letter code: HEX) (formula: C_6H_{14}).



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

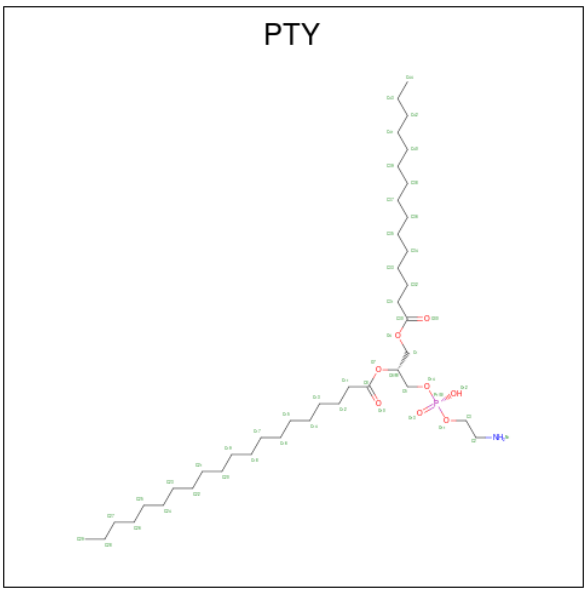
- Molecule 8 is FUSIDIC ACID (three-letter code: FUA) (formula: $C_{31}H_{48}O_6$).



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

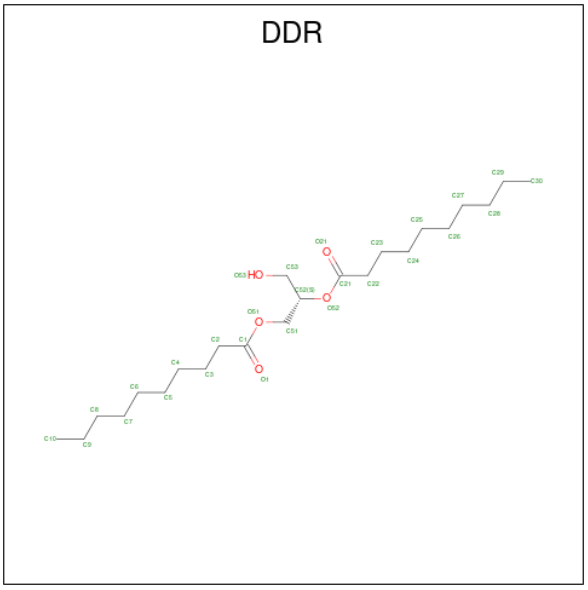
- Molecule 9 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula:

$C_{40}H_{80}NO_8P$).



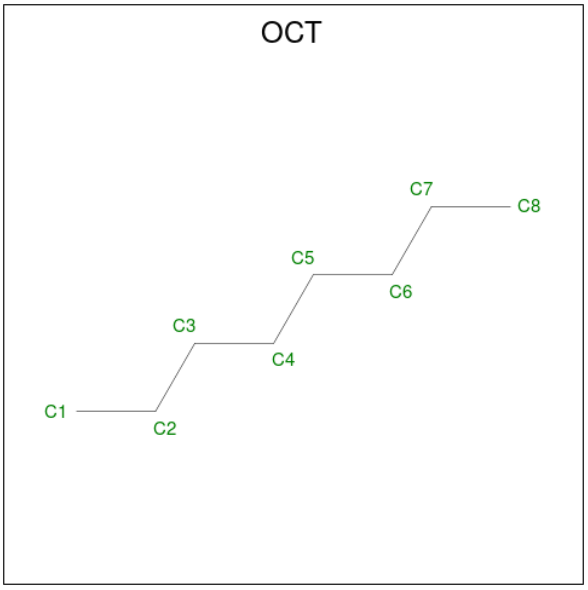
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
9	B	1	50	40	1	8	1	0	0
			Total	C	N	O	P		
9	C	1	50	40	1	8	1	0	0

- Molecule 10 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		
10	B	1	28	23	5	0	0

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

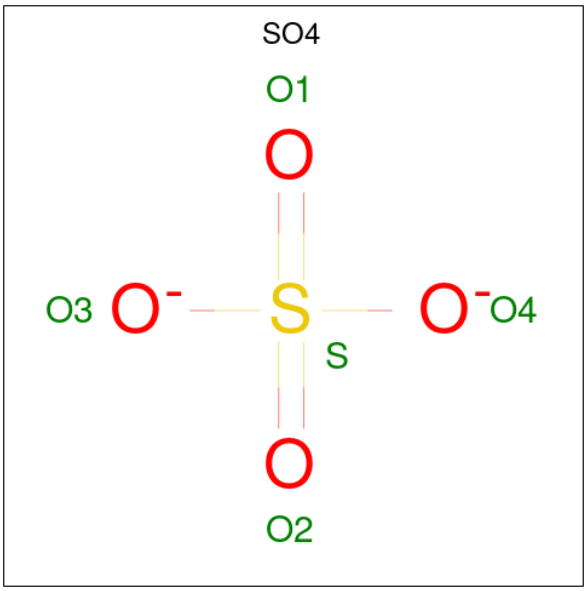


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C			
11	B	1	8	8		0	0
			Total	C			
11	B	1	8	8		0	0
			Total	C			
11	C	1	8	8		0	0

- Molecule 12 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

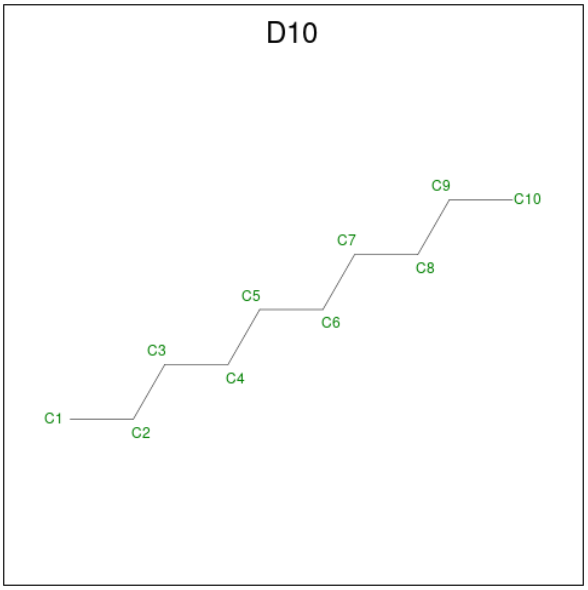
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Cl			
12	B	1	1	1		0	0
			Total	Cl			
12	C	4	4	4		0	0

- Molecule 13 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



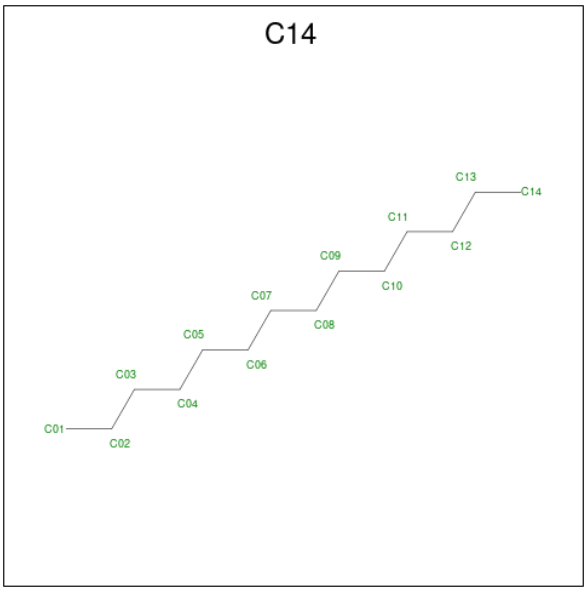
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	B	1	Total O S 5 4 1	0	0
13	B	1	Total O S 5 4 1	0	0

- Molecule 14 is DECANE (three-letter code: D10) (formula: $C_{10}H_{22}$).



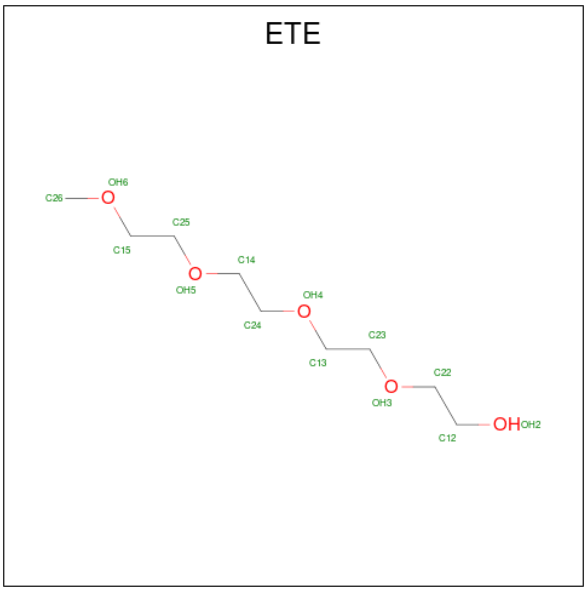
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	B	1	Total C 10 10	0	0

- Molecule 15 is TETRADECANE (three-letter code: C14) (formula: $C_{14}H_{30}$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C		
15	C	1	14	14	0	0

- Molecule 16 is 2-{2-[2-2-(METHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (three-letter code: ETE) (formula: $C_9H_{20}O_5$).



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

- Molecule 17 is water.

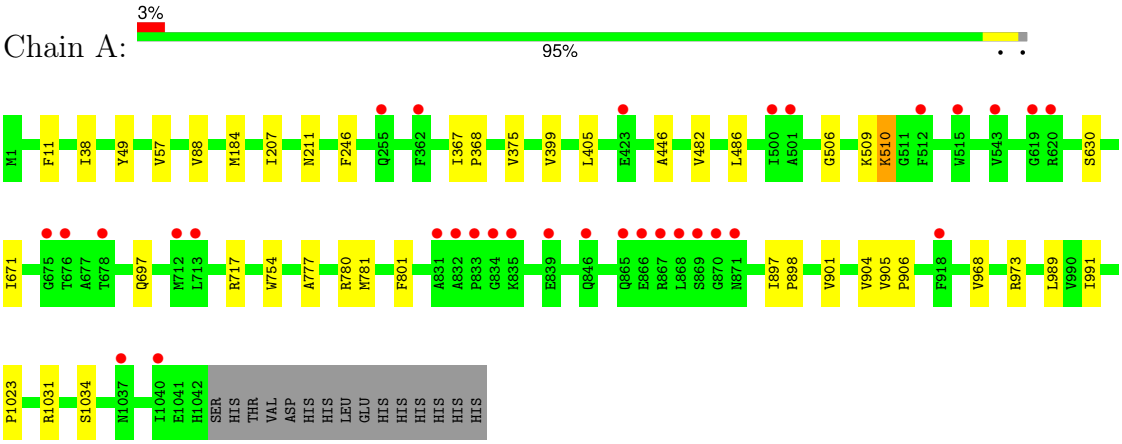
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
17	A	158	158	158	0	0
			Total	O		
17	B	132	132	132	0	0
			Total	O		
17	C	192	192	192	0	0
			Total	O		
17	D	26	26	26	0	0
			Total	O		
17	E	14	14	14	0	0

3 Residue-property plots (i)

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

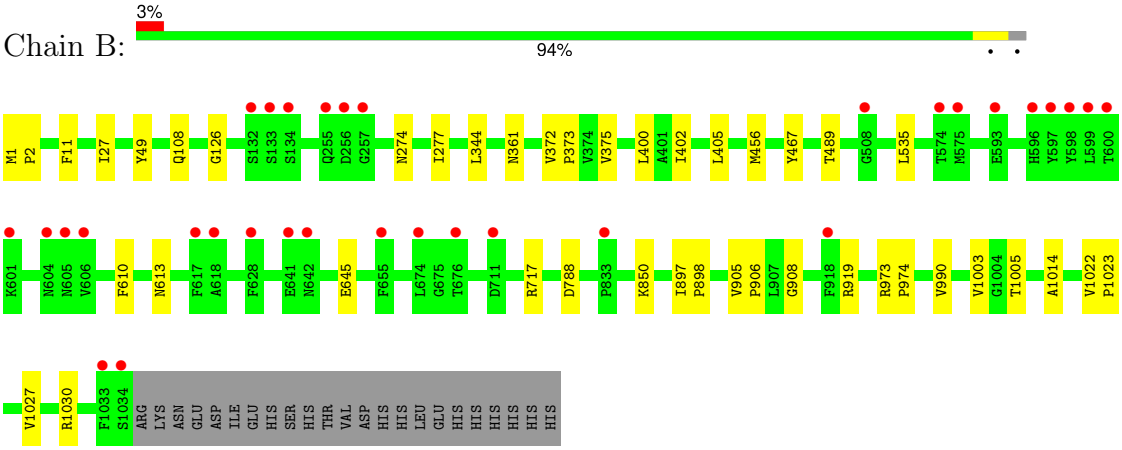
• Molecule 1: Multidrug efflux pump subunit AcrB

Chain A:



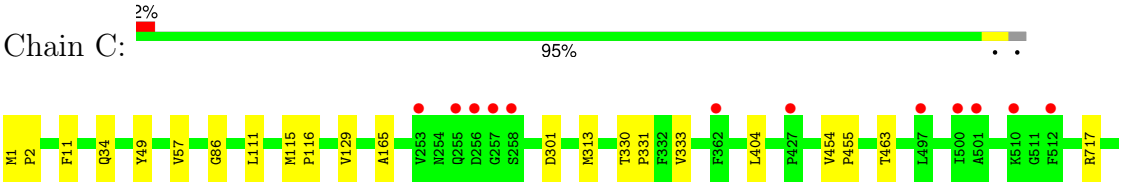
• Molecule 1: Multidrug efflux pump subunit AcrB

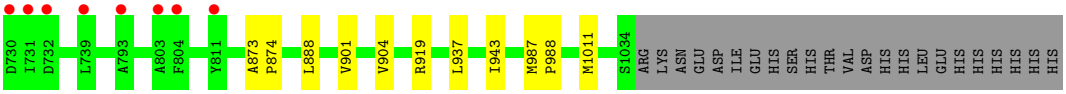
Chain B:



• Molecule 1: Multidrug efflux pump subunit AcrB

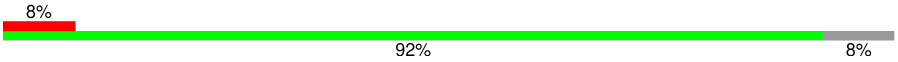
Chain C:

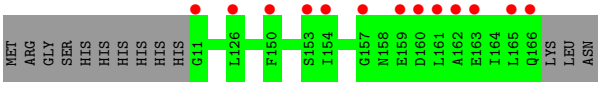




- Molecule 2: DARPin

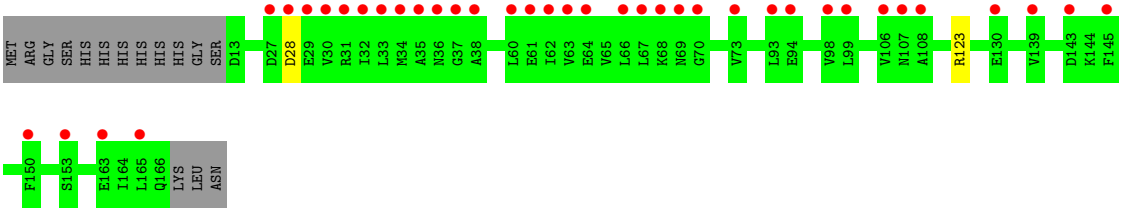
Chain D:





- Molecule 2: DARPin

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	146.22Å 162.63Å 245.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.76 – 2.80 49.71 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.76-2.80) 100.0 (49.71-2.80)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.55 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.211 , 0.247 0.214 , 0.247	Depositor DCC
R_{free} test set	7127 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	58.4	Xtriage
Anisotropy	0.478	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 40.2	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	0.92	EDS
Total number of atoms	27306	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.06% 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: OCT, CL, LMT, D12, DDR, DDQ, ETE, C14, D10, GOL, SO4, PTY, HEX, FUA

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	0/8102	0.70	0/11000
1	B	0.66	0/8017	0.70	0/10887
1	C	0.66	0/8034	0.70	0/10908
2	D	0.67	0/1196	0.70	0/1626
2	E	0.68	0/1186	0.70	0/1613
All	All	0.66	0/26535	0.70	0/36034

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	7942	0	8093	19	0
1	B	7861	0	8016	19	0
1	C	7877	0	8039	16	0
2	D	1177	0	1159	0	0
2	E	1167	0	1151	0	0
3	A	140	0	184	0	0
3	B	105	0	138	1	0
3	C	105	0	138	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	12	0	26	0	0
4	B	12	0	26	0	0
4	C	12	0	26	0	0
5	A	14	0	27	0	0
5	B	28	0	54	0	0
5	C	42	0	81	0	0
6	A	18	0	24	0	0
6	B	6	0	8	0	0
6	C	6	0	8	0	0
6	E	6	0	8	0	0
7	A	6	0	14	0	0
7	C	6	0	14	0	0
8	B	37	0	47	4	0
9	B	50	0	79	0	0
9	C	50	0	79	0	0
10	B	28	0	44	0	0
11	B	16	0	36	0	0
11	C	8	0	18	0	0
12	B	1	0	0	0	0
12	C	4	0	0	0	0
13	B	10	0	0	0	0
14	B	10	0	22	0	0
15	C	14	0	30	0	0
16	C	14	0	20	0	0
17	A	158	0	0	0	0
17	B	132	0	0	0	0
17	C	192	0	0	0	0
17	D	26	0	0	0	0
17	E	14	0	0	0	0
All	All	27306	0	27609	56	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (56) 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)
8:B:1104:FUA:H202	8:B:1104:FUA:H5	1.66	0.77
1:A:968:VAL:HG11	1:A:1023:PRO:HG3	1.76	0.68
1:A:697[B]:GLN:HA	1:A:697[B]:GLN:OE1	1.95	0.67
1:B:990:VAL:HG13	1:B:1005:THR:HG22	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:919:ARG:HD2	1:B:1005:THR:HG21	1.85	0.57
1:C:901:VAL:O	1:C:904:VAL:HG12	2.05	0.56
1:B:375:VAL:HG11	1:B:405:LEU:HD22	1.90	0.54
1:C:57:VAL:HG21	1:C:86:GLY:HA2	1.90	0.53
1:A:375:VAL:HG11	1:A:405:LEU:HD22	1.89	0.52
1:A:57:VAL:CG1	1:A:88:VAL:HG22	2.40	0.52
1:B:535:LEU:HD22	1:B:1027:VAL:HG21	1.93	0.51
1:B:897:ILE:N	1:B:898:PRO:HD2	2.26	0.51
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.92	0.49
1:C:34:GLN:HB2	1:C:333:VAL:HG13	1.94	0.49
1:B:126:GLY:HA3	1:C:116:PRO:CB	2.43	0.48
1:B:1:MET:HB3	1:B:2:PRO:HD3	1.96	0.48
1:C:111:LEU:HD22	1:C:129:VAL:CG2	2.44	0.47
1:A:506:GLY:HA2	1:A:509:LYS:HE3	1.96	0.47
8:B:1104:FUA:H232	8:B:1104:FUA:C12	2.43	0.47
8:B:1104:FUA:H202	8:B:1104:FUA:C5	2.42	0.47
1:C:987:MET:N	1:C:988:PRO:HD2	2.30	0.47
1:A:207:ILE:O	1:A:211:ASN:HB3	2.16	0.46
1:A:38:ILE:HD11	1:A:671:ILE:HG21	1.98	0.46
1:A:184:MET:HG2	1:A:246:PHE:CD2	2.50	0.46
1:B:400:LEU:HD21	1:B:1003:VAL:HG13	1.98	0.45
1:A:510:LYS:C	1:A:510:LYS:HD3	2.37	0.45
1:A:897:ILE:N	1:A:898:PRO:CD	2.80	0.45
1:A:57:VAL:HG12	1:A:88:VAL:HG22	1.99	0.44
1:A:777:ALA:O	1:A:781:MET:HG2	2.18	0.44
1:B:344:LEU:CD2	1:B:402:ILE:HD13	2.48	0.44
1:B:908:GLY:HA2	1:B:1014:ALA:HB2	1.99	0.44
1:B:277:ILE:HA	1:B:613:ASN:O	2.17	0.43
1:A:482:VAL:O	1:A:486:LEU:HG	2.18	0.43
1:B:456:MET:HG2	1:B:467:TYR:HB3	2.01	0.43
1:A:754:TRP:CZ3	1:A:780:ARG:HA	2.54	0.43
1:A:905:VAL:HB	1:A:906:PRO:HD3	2.00	0.43
1:C:1:MET:HB3	1:C:2:PRO:HD3	2.01	0.42
1:B:1022:VAL:N	1:B:1023:PRO:HD2	2.34	0.42
1:C:454:VAL:HB	1:C:455:PRO:HD3	2.02	0.42
1:C:404:LEU:HD21	1:C:937:LEU:CD2	2.50	0.42
1:A:399:VAL:HG11	1:A:989:LEU:HD11	2.01	0.42
1:A:446:ALA:HB2	1:A:482:VAL:HG21	2.02	0.42
1:B:850:LYS:HD3	1:B:850:LYS:HA	1.93	0.42
1:C:873:ALA:HB3	1:C:874:PRO:HD3	2.02	0.42
1:C:165:ALA:HB3	1:C:313:MET:HE1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:901:VAL:O	1:A:904:VAL:HG22	2.20	0.41
1:B:372:VAL:HB	1:B:373:PRO:HD3	2.01	0.41
1:C:330:THR:N	1:C:331:PRO:CD	2.84	0.41
1:C:115:MET:N	1:C:116:PRO:HD2	2.35	0.41
1:C:404:LEU:HD21	1:C:937:LEU:HD21	2.03	0.41
1:C:888:LEU:HD21	1:C:943:ILE:HD11	2.03	0.41
1:B:27:ILE:HD13	8:B:1104:FUA:H193	2.02	0.41
1:B:126:GLY:HA3	1:C:116:PRO:HB3	2.03	0.40
1:B:905:VAL:HB	1:B:906:PRO:HD3	2.03	0.40
3:B:1103:LMT:H6B	3:B:1103:LMT:H3O2	1.69	0.40
1:B:973:ARG:N	1:B:974:PRO:HD2	2.36	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	1043/1057 (99%)	1019 (98%)	23 (2%)	1 (0%)	51 81
1	B	1034/1057 (98%)	1007 (97%)	27 (3%)	0	100 100
1	C	1035/1057 (98%)	1012 (98%)	23 (2%)	0	100 100
2	D	154/169 (91%)	153 (99%)	1 (1%)	0	100 100
2	E	152/169 (90%)	152 (100%)	0	0	100 100
All	All	3418/3509 (97%)	3343 (98%)	74 (2%)	1 (0%)	100 100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1034	SER

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	850/862 (99%)	841 (99%)	9 (1%)	73	92
1	B	841/862 (98%)	830 (99%)	11 (1%)	69	91
1	C	842/862 (98%)	835 (99%)	7 (1%)	81	94
2	D	120/132 (91%)	120 (100%)	0	100	100
2	E	119/132 (90%)	117 (98%)	2 (2%)	60	87
All	All	2772/2850 (97%)	2743 (99%)	29 (1%)	76	93

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	PHE
1	A	49	TYR
1	A	510	LYS
1	A	630	SER
1	A	717	ARG
1	A	801	PHE
1	A	973	ARG
1	A	991	ILE
1	A	1031	ARG
1	B	11	PHE
1	B	49	TYR
1	B	108	GLN
1	B	274	ASN
1	B	361	ASN
1	B	489	THR
1	B	610	PHE
1	B	645	GLU
1	B	717	ARG
1	B	788	ASP
1	B	1030	ARG
1	C	11	PHE
1	C	49	TYR
1	C	301	ASP

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Mol	Chain	Res	Type
1	C	463	THR
1	C	717	ARG
1	C	919	ARG
1	C	1011	MET
2	E	28	ASP
2	E	123	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	361	ASN
1	C	255	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)

Of 44 ligands modelled in this entry, 5 are monoatomic - leaving 39 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	D12	A	1105	-	11,11,11	0.27	0	10,10,10	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	GOL	C	1115	-	5,5,5	0.09	0	5,5,5	0.31	0
5	DDQ	B	1108	-	11,13,13	2.20	2 (18%)	12,15,15	0.52	0
6	GOL	A	1109	-	5,5,5	0.10	0	5,5,5	0.29	0
6	GOL	E	201	-	5,5,5	0.09	0	5,5,5	0.26	0
5	DDQ	A	1106	-	11,13,13	2.18	2 (18%)	12,15,15	0.51	0
11	OCT	C	1110	-	7,7,7	0.10	0	6,6,6	0.10	0
3	LMT	A	1101	-	36,36,36	0.50	1 (2%)	47,47,47	0.69	0
14	D10	B	1116	-	9,9,9	0.11	0	8,8,8	0.10	0
9	PTY	C	1104	-	49,49,49	0.26	0	52,54,54	0.31	0
3	LMT	C	1101	-	36,36,36	0.50	1 (2%)	47,47,47	0.66	1 (2%)
3	LMT	B	1102	-	36,36,36	0.50	1 (2%)	47,47,47	0.73	1 (2%)
5	DDQ	C	1109	-	11,13,13	2.24	2 (18%)	12,15,15	0.41	0
3	LMT	C	1102	-	36,36,36	0.55	1 (2%)	47,47,47	0.84	1 (2%)
3	LMT	B	1101	-	36,36,36	0.49	1 (2%)	47,47,47	0.68	0
4	D12	C	1105	-	11,11,11	0.30	0	10,10,10	0.41	0
5	DDQ	C	1107	-	11,13,13	2.28	2 (18%)	12,15,15	0.31	0
3	LMT	C	1103	-	36,36,36	0.54	1 (2%)	47,47,47	0.82	1 (2%)
15	C14	C	1106	-	13,13,13	0.08	0	12,12,12	0.09	0
8	FUA	B	1104	-	39,40,40	1.59	2 (5%)	50,64,64	1.11	5 (10%)
6	GOL	A	1108	-	5,5,5	0.10	0	5,5,5	0.28	0
5	DDQ	B	1109	-	11,13,13	2.25	2 (18%)	12,15,15	0.46	0
3	LMT	A	1103	-	36,36,36	0.50	1 (2%)	47,47,47	0.72	0
9	PTY	B	1105	-	49,49,49	0.27	0	52,54,54	0.35	0
7	HEX	C	1117	-	5,5,5	0.13	0	4,4,4	0.12	0
11	OCT	B	1110	-	7,7,7	0.10	0	6,6,6	0.12	0
3	LMT	A	1104	-	36,36,36	0.49	1 (2%)	47,47,47	0.54	0
11	OCT	B	1111	-	7,7,7	0.11	0	6,6,6	0.08	0
10	DDR	B	1107	-	27,27,27	1.25	2 (7%)	29,29,29	1.14	2 (6%)
5	DDQ	C	1108	-	11,13,13	2.26	2 (18%)	12,15,15	0.49	0
3	LMT	B	1103	-	36,36,36	0.51	1 (2%)	47,47,47	0.78	0
6	GOL	A	1107	-	5,5,5	0.10	0	5,5,5	0.27	0
16	ETE	C	1116	-	13,13,13	0.21	0	12,12,12	0.12	0
7	HEX	A	1110	-	5,5,5	0.12	0	4,4,4	0.13	0
13	SO4	B	1113	-	4,4,4	0.34	0	6,6,6	0.07	0
6	GOL	B	1115	-	5,5,5	0.09	0	5,5,5	0.24	0
4	D12	B	1106	-	11,11,11	0.29	0	10,10,10	0.45	0
3	LMT	A	1102	-	36,36,36	0.49	1 (2%)	47,47,47	0.62	0
13	SO4	B	1114	-	4,4,4	0.34	0	6,6,6	0.08	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
4	D12	A	1105	-	-	2/9/9/9	-
6	GOL	C	1115	-	-	4/4/4/4	-
5	DDQ	B	1108	-	-	2/11/11/11	-
6	GOL	A	1109	-	-	0/4/4/4	-
6	GOL	E	201	-	-	1/4/4/4	-
5	DDQ	A	1106	-	-	3/11/11/11	-
11	OCT	C	1110	-	-	2/5/5/5	-
3	LMT	A	1101	-	-	12/21/61/61	0/2/2/2
14	D10	B	1116	-	-	3/7/7/7	-
9	PTY	C	1104	-	-	21/53/53/53	-
3	LMT	C	1101	-	-	11/21/61/61	0/2/2/2
3	LMT	B	1102	-	-	7/21/61/61	0/2/2/2
5	DDQ	C	1109	-	-	2/11/11/11	-
3	LMT	C	1102	-	-	9/21/61/61	0/2/2/2
3	LMT	B	1101	-	-	8/21/61/61	0/2/2/2
4	D12	C	1105	-	-	6/9/9/9	-
5	DDQ	C	1107	-	-	4/11/11/11	-
3	LMT	C	1103	-	-	10/21/61/61	0/2/2/2
15	C14	C	1106	-	-	4/11/11/11	-
8	FUA	B	1104	-	-	5/16/92/92	0/4/4/4
6	GOL	A	1108	-	-	2/4/4/4	-
5	DDQ	B	1109	-	-	2/11/11/11	-
3	LMT	A	1103	-	-	13/21/61/61	0/2/2/2
9	PTY	B	1105	-	-	25/53/53/53	-
7	HEX	C	1117	-	-	1/3/3/3	-
11	OCT	B	1110	-	-	0/5/5/5	-
3	LMT	A	1104	-	-	6/21/61/61	0/2/2/2
11	OCT	B	1111	-	-	2/5/5/5	-
10	DDR	B	1107	-	-	16/29/29/29	-
5	DDQ	C	1108	-	-	2/11/11/11	-
3	LMT	B	1103	-	-	10/21/61/61	0/2/2/2
6	GOL	A	1107	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	HEX	A	1110	-	-	1/3/3/3	-
6	GOL	B	1115	-	-	1/4/4/4	-
4	D12	B	1106	-	-	2/9/9/9	-
3	LMT	A	1102	-	-	7/21/61/61	0/2/2/2
16	ETE	C	1116	-	-	5/11/11/11	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	1104	FUA	C29-C22	-9.04	1.35	1.47
5	C	1109	DDQ	O1-N1	-6.85	1.25	1.42
5	C	1108	DDQ	O1-N1	-6.82	1.25	1.42
5	C	1107	DDQ	O1-N1	-6.80	1.25	1.42
5	B	1108	DDQ	O1-N1	-6.76	1.25	1.42
5	B	1109	DDQ	O1-N1	-6.76	1.25	1.42
5	A	1106	DDQ	O1-N1	-6.71	1.25	1.42
10	B	1107	DDR	O52-C21	4.36	1.46	1.34
10	B	1107	DDR	O51-C1	4.27	1.45	1.33
5	C	1107	DDQ	C1-N1	-3.16	1.48	1.51
5	C	1108	DDQ	C1-N1	-3.00	1.48	1.51
5	B	1109	DDQ	C1-N1	-3.00	1.48	1.51
5	C	1109	DDQ	C1-N1	-2.76	1.48	1.51
8	B	1104	FUA	O5-C29	-2.61	1.23	1.30
5	A	1106	DDQ	C1-N1	-2.57	1.48	1.51
5	B	1108	DDQ	C1-N1	-2.54	1.48	1.51
3	C	1102	LMT	O1'-C1'	2.32	1.44	1.40
3	C	1101	LMT	O1'-C1'	2.24	1.43	1.40
3	A	1101	LMT	O1'-C1'	2.20	1.43	1.40
3	C	1103	LMT	O1'-C1'	2.18	1.43	1.40
3	A	1102	LMT	O1'-C1'	2.13	1.43	1.40
3	B	1101	LMT	O1'-C1'	2.12	1.43	1.40
3	B	1102	LMT	O1'-C1'	2.09	1.43	1.40
3	B	1103	LMT	O1'-C1'	2.09	1.43	1.40
3	A	1103	LMT	O1'-C1'	2.05	1.43	1.40
3	A	1104	LMT	O1'-C1'	2.04	1.43	1.40

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	1107	DDR	O52-C21-C22	4.01	120.16	111.48
8	B	1104	FUA	O2-C16-C17	3.17	117.57	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	1104	FUA	C6-C5-C10	2.96	115.20	111.66
10	B	1107	DDR	O51-C1-C2	2.56	119.63	111.83
3	C	1102	LMT	C1B-O5B-C5B	2.42	118.44	113.72
3	C	1101	LMT	C1-O1'-C1'	2.29	117.59	113.68
3	C	1103	LMT	C1B-O5B-C5B	2.27	118.15	113.72
8	B	1104	FUA	O2-C16-C15	-2.23	105.49	110.81
8	B	1104	FUA	C10-C5-C4	-2.22	110.51	113.20
3	B	1102	LMT	C1'-O5'-C5'	2.14	117.89	113.72
8	B	1104	FUA	C1-C10-C5	-2.10	105.03	107.77

There are no chirality outliers.

All (213) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1103	LMT	O5'-C1'-O1'-C1
3	C	1101	LMT	C2'-C1'-O1'-C1
3	C	1102	LMT	C2'-C1'-O1'-C1
3	C	1102	LMT	O5'-C1'-O1'-C1
5	A	1106	DDQ	C2-C1-N1-CM1
5	B	1108	DDQ	N1-C1-C2-C3
6	A	1107	GOL	O1-C1-C2-C3
6	C	1115	GOL	C1-C2-C3-O3
8	B	1104	FUA	C23-C22-C29-O4
8	B	1104	FUA	C23-C22-C29-O5
8	B	1104	FUA	C32-C31-O2-C16
8	B	1104	FUA	O3-C31-O2-C16
9	B	1105	PTY	N1-C2-C3-O11
9	B	1105	PTY	C11-C8-O7-C6
9	B	1105	PTY	C5-O14-P1-O11
9	B	1105	PTY	C5-O14-P1-O12
9	B	1105	PTY	C5-O14-P1-O13
9	C	1104	PTY	C11-C8-O7-C6
9	C	1104	PTY	C3-O11-P1-O12
9	C	1104	PTY	C3-O11-P1-O14
10	B	1107	DDR	O52-C52-C53-O53
10	B	1107	DDR	C51-C52-C53-O53
3	C	1103	LMT	O5B-C1B-O1B-C4'
9	B	1105	PTY	O10-C8-O7-C6
9	C	1104	PTY	O10-C8-O7-C6
3	C	1103	LMT	C2B-C1B-O1B-C4'
9	B	1105	PTY	C31-C30-O4-C1
3	B	1103	LMT	O5B-C1B-O1B-C4'

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Mol	Chain	Res	Type	Atoms
9	B	1105	PTY	O30-C30-O4-C1
3	A	1101	LMT	O5B-C5B-C6B-O6B
3	C	1102	LMT	O5B-C5B-C6B-O6B
3	B	1102	LMT	O5'-C5'-C6'-O6'
8	B	1104	FUA	C22-C23-C24-C25
3	A	1102	LMT	O5'-C1'-O1'-C1
3	B	1103	LMT	O5'-C1'-O1'-C1
3	C	1101	LMT	O5'-C1'-O1'-C1
3	A	1103	LMT	O5B-C5B-C6B-O6B
3	B	1101	LMT	O5'-C5'-C6'-O6'
3	A	1102	LMT	C2'-C1'-O1'-C1
3	A	1103	LMT	C2'-C1'-O1'-C1
3	B	1103	LMT	C2'-C1'-O1'-C1
3	A	1101	LMT	O5'-C5'-C6'-O6'
9	B	1105	PTY	C30-C31-C32-C33
3	C	1101	LMT	O5'-C5'-C6'-O6'
3	A	1103	LMT	C4B-C5B-C6B-O6B
6	A	1108	GOL	O2-C2-C3-O3
6	C	1115	GOL	O2-C2-C3-O3
3	B	1101	LMT	O5B-C5B-C6B-O6B
16	C	1116	ETE	OH2-C12-C22-OH3
3	C	1102	LMT	C4B-C5B-C6B-O6B
3	C	1102	LMT	C4'-C5'-C6'-O6'
3	C	1103	LMT	C4B-C5B-C6B-O6B
3	A	1101	LMT	O5'-C1'-O1'-C1
3	A	1101	LMT	C4B-C5B-C6B-O6B
3	A	1103	LMT	O5'-C5'-C6'-O6'
3	B	1101	LMT	C4'-C5'-C6'-O6'
3	A	1103	LMT	O1'-C1-C2-C3
6	A	1108	GOL	C1-C2-C3-O3
6	B	1115	GOL	O1-C1-C2-C3
6	C	1115	GOL	O1-C1-C2-C3
3	B	1102	LMT	C4'-C5'-C6'-O6'
16	C	1116	ETE	OH5-C14-C24-OH4
3	B	1103	LMT	C5'-C4'-O1B-C1B
3	A	1102	LMT	C1-C2-C3-C4
3	B	1102	LMT	C11-C10-C9-C8
9	C	1104	PTY	C11-C12-C13-C14
3	A	1103	LMT	C2-C1-O1'-C1'
3	C	1101	LMT	C2-C1-O1'-C1'
3	C	1102	LMT	C2-C1-O1'-C1'
6	A	1107	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
9	B	1105	PTY	C13-C14-C15-C16
10	B	1107	DDR	C22-C23-C24-C25
3	A	1104	LMT	C2-C3-C4-C5
9	C	1104	PTY	C32-C33-C34-C35
3	C	1101	LMT	C7-C8-C9-C10
3	C	1102	LMT	O1'-C1-C2-C3
3	A	1101	LMT	C2-C3-C4-C5
3	A	1102	LMT	C4-C5-C6-C7
5	C	1107	DDQ	C4-C5-C6-C7
5	C	1108	DDQ	C2-C3-C4-C5
3	B	1103	LMT	C3'-C4'-O1B-C1B
10	B	1107	DDR	C22-C21-O52-C52
10	B	1107	DDR	C24-C25-C26-C27
3	C	1101	LMT	O1'-C1-C2-C3
5	C	1109	DDQ	C3-C4-C5-C6
10	B	1107	DDR	C4-C5-C6-C7
3	B	1101	LMT	C3-C4-C5-C6
5	B	1108	DDQ	C1-C2-C3-C4
3	B	1103	LMT	C5-C6-C7-C8
3	C	1102	LMT	O5'-C5'-C6'-O6'
9	B	1105	PTY	C14-C15-C16-C17
3	A	1101	LMT	C4'-C5'-C6'-O6'
3	A	1101	LMT	C7-C8-C9-C10
3	C	1101	LMT	C5-C6-C7-C8
5	C	1107	DDQ	C6-C7-C8-C9
3	C	1101	LMT	C4'-C5'-C6'-O6'
9	C	1104	PTY	C35-C36-C37-C38
9	C	1104	PTY	C21-C22-C23-C24
3	A	1102	LMT	O1'-C1-C2-C3
3	C	1103	LMT	O5'-C5'-C6'-O6'
10	B	1107	DDR	O21-C21-O52-C52
9	B	1105	PTY	C19-C20-C21-C22
4	A	1105	D12	C11-C10-C9-C8
3	B	1102	LMT	O5B-C5B-C6B-O6B
4	C	1105	D12	C6-C7-C8-C9
3	B	1102	LMT	O1'-C1-C2-C3
3	C	1101	LMT	O5B-C5B-C6B-O6B
10	B	1107	DDR	C2-C1-O51-C51
9	C	1104	PTY	C20-C21-C22-C23
3	B	1103	LMT	O5'-C5'-C6'-O6'
11	B	1111	OCT	C4-C5-C6-C7
14	B	1116	D10	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
9	B	1105	PTY	C23-C24-C25-C26
3	A	1103	LMT	C4-C5-C6-C7
9	B	1105	PTY	C38-C39-C40-C41
4	C	1105	D12	C1-C2-C3-C4
3	A	1104	LMT	O1'-C1-C2-C3
5	B	1109	DDQ	C3-C4-C5-C6
3	A	1101	LMT	C2-C1-O1'-C1'
3	B	1102	LMT	C2-C1-O1'-C1'
6	E	201	GOL	O2-C2-C3-O3
4	C	1105	D12	C9-C10-C11-C12
15	C	1106	C14	C05-C06-C07-C08
3	C	1102	LMT	C9-C10-C11-C12
9	B	1105	PTY	O4-C1-C6-C5
10	B	1107	DDR	O51-C51-C52-C53
9	C	1104	PTY	C38-C39-C40-C41
3	C	1103	LMT	C11-C10-C9-C8
10	B	1107	DDR	C5-C6-C7-C8
3	C	1103	LMT	O5B-C5B-C6B-O6B
10	B	1107	DDR	O1-C1-O51-C51
5	B	1109	DDQ	C1-C2-C3-C4
9	B	1105	PTY	C41-C42-C43-C44
3	B	1103	LMT	C9-C10-C11-C12
15	C	1106	C14	C10-C11-C12-C13
11	C	1110	OCT	C3-C4-C5-C6
5	C	1108	DDQ	C4-C5-C6-C7
14	B	1116	D10	C1-C2-C3-C4
3	A	1103	LMT	C3-C4-C5-C6
3	B	1102	LMT	C5-C6-C7-C8
9	B	1105	PTY	C11-C12-C13-C14
3	A	1103	LMT	C2-C3-C4-C5
3	B	1101	LMT	C7-C8-C9-C10
9	B	1105	PTY	C2-C3-O11-P1
9	B	1105	PTY	O4-C1-C6-O7
3	C	1101	LMT	C2-C3-C4-C5
4	B	1106	D12	C3-C4-C5-C6
4	B	1106	D12	C2-C3-C4-C5
5	A	1106	DDQ	C2-C1-N1-CM2
3	A	1101	LMT	C1-C2-C3-C4
3	C	1103	LMT	C2-C3-C4-C5
3	A	1104	LMT	C6-C7-C8-C9
11	C	1110	OCT	C1-C2-C3-C4
4	C	1105	D12	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
10	B	1107	DDR	O51-C51-C52-O52
3	C	1103	LMT	C4-C5-C6-C7
3	C	1103	LMT	C5-C6-C7-C8
9	B	1105	PTY	C39-C40-C41-C42
4	C	1105	D12	C5-C6-C7-C8
3	A	1104	LMT	C9-C10-C11-C12
6	C	1115	GOL	O1-C1-C2-O2
5	A	1106	DDQ	C6-C7-C8-C9
3	B	1101	LMT	C9-C10-C11-C12
3	A	1103	LMT	C4'-C5'-C6'-O6'
3	A	1104	LMT	C7-C8-C9-C10
5	C	1107	DDQ	C1-C2-C3-C4
9	C	1104	PTY	C30-C31-C32-C33
3	B	1103	LMT	C2-C1-O1'-C1'
9	C	1104	PTY	C12-C13-C14-C15
5	C	1107	DDQ	C2-C3-C4-C5
9	B	1105	PTY	C37-C38-C39-C40
4	C	1105	D12	C11-C10-C9-C8
3	A	1101	LMT	C5-C6-C7-C8
5	C	1109	DDQ	C6-C7-C8-C9
3	C	1103	LMT	O1'-C1-C2-C3
3	B	1103	LMT	C2-C3-C4-C5
3	A	1101	LMT	C4-C5-C6-C7
9	C	1104	PTY	C24-C25-C26-C27
9	C	1104	PTY	C41-C42-C43-C44
3	B	1101	LMT	C6-C7-C8-C9
3	A	1104	LMT	C5-C6-C7-C8
16	C	1116	ETE	C24-C14-OH5-C25
10	B	1107	DDR	C25-C26-C27-C28
3	A	1102	LMT	C7-C8-C9-C10
9	C	1104	PTY	O4-C1-C6-C5
3	B	1101	LMT	C4B-C5B-C6B-O6B
16	C	1116	ETE	C23-C13-OH4-C24
9	C	1104	PTY	C18-C19-C20-C21
3	C	1101	LMT	C6-C7-C8-C9
3	A	1103	LMT	C5-C6-C7-C8
16	C	1116	ETE	C25-C15-OH6-C26
3	A	1103	LMT	C7-C8-C9-C10
9	B	1105	PTY	C17-C18-C19-C20
7	A	1110	HEX	C3-C4-C5-C6
4	A	1105	D12	C2-C3-C4-C5
7	C	1117	HEX	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
11	B	1111	OCT	C2-C3-C4-C5
9	B	1105	PTY	C12-C13-C14-C15
3	A	1102	LMT	C4'-C5'-C6'-O6'
10	B	1107	DDR	O52-C21-C22-C23
9	C	1104	PTY	C17-C18-C19-C20
9	C	1104	PTY	O14-C5-C6-C1
9	B	1105	PTY	O4-C30-C31-C32
14	B	1116	D10	C6-C7-C8-C9
15	C	1106	C14	C02-C03-C04-C05
9	C	1104	PTY	O4-C30-C31-C32
9	C	1104	PTY	O14-C5-C6-O7
10	B	1107	DDR	O51-C1-C2-C3
15	C	1106	C14	C03-C04-C05-C06
10	B	1107	DDR	O21-C21-C22-C23
9	B	1105	PTY	O30-C30-C31-C32
9	C	1104	PTY	O30-C30-C31-C32
3	A	1101	LMT	C3-C4-C5-C6

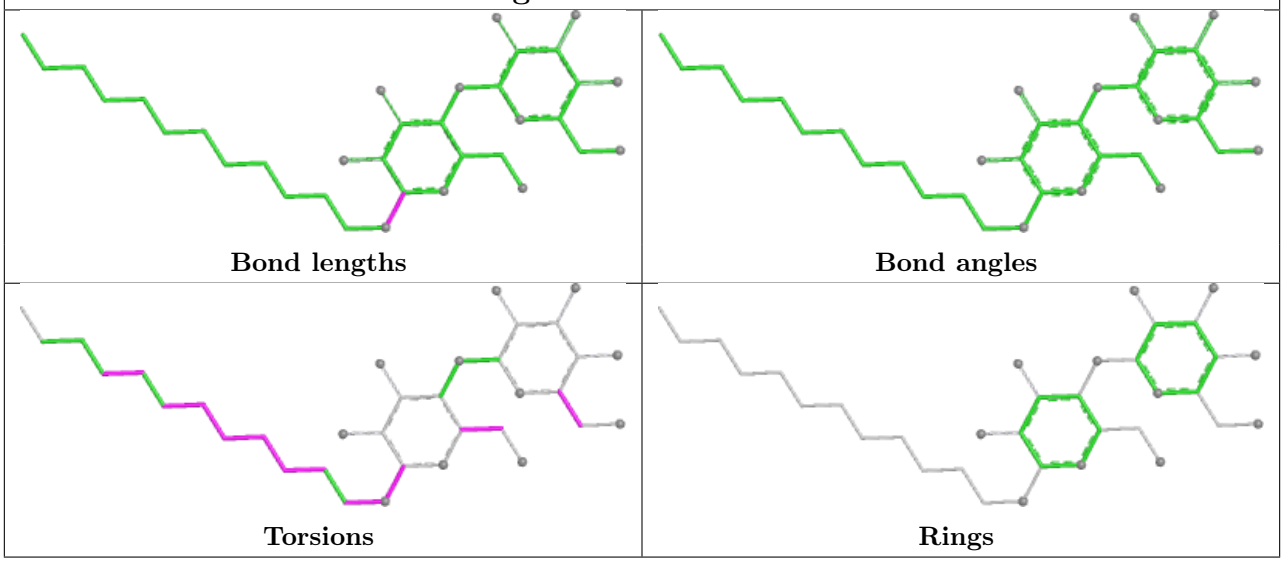
There are no ring outliers.

2 monomers are involved in 5 short contacts:

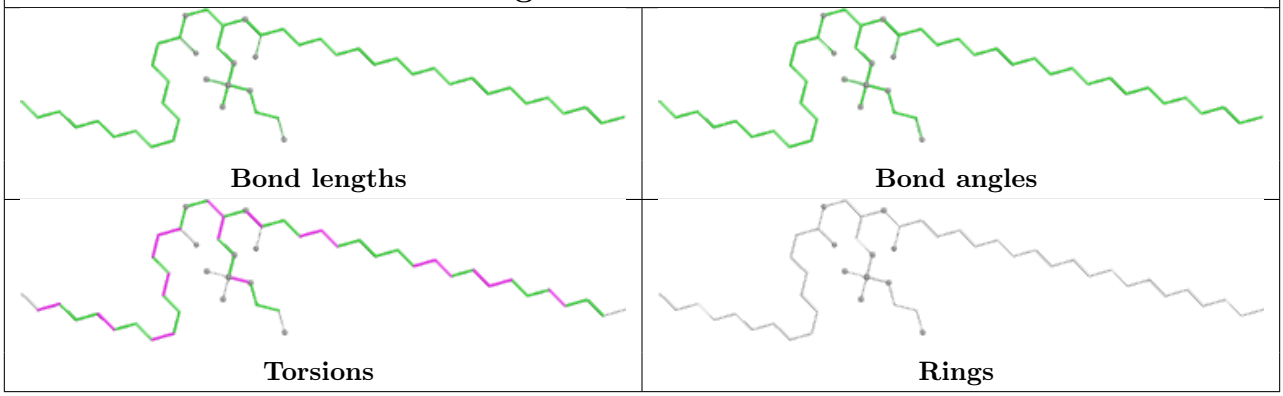
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	1104	FUA	4	0
3	B	1103	LMT	1	0

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.

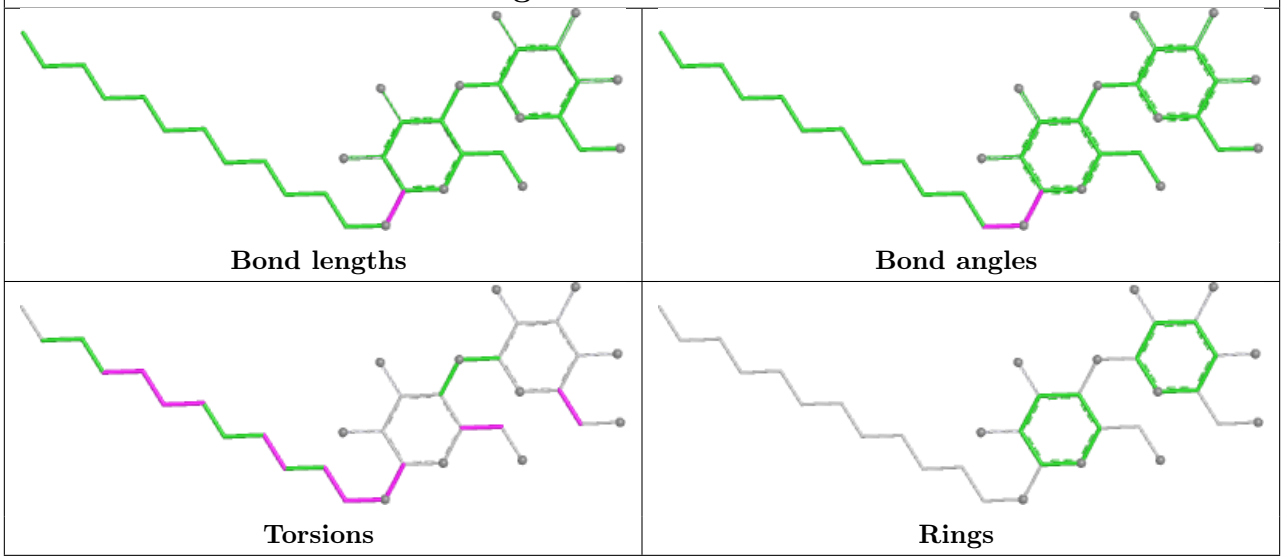
Ligand LMT A 1101



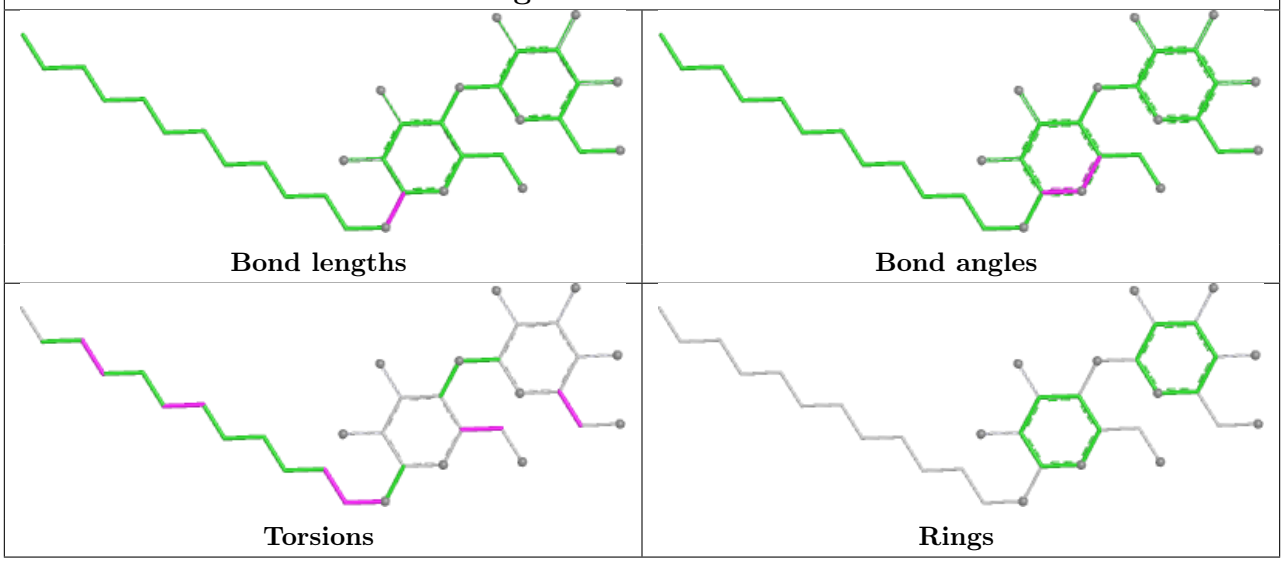
Ligand PTY C 1104



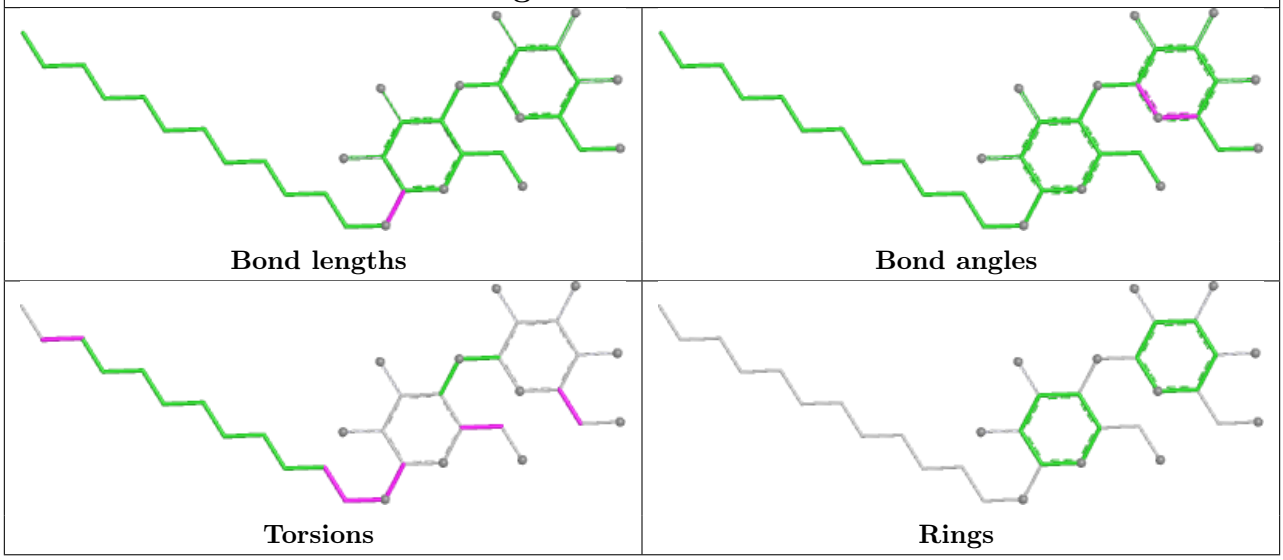
Ligand LMT C 1101



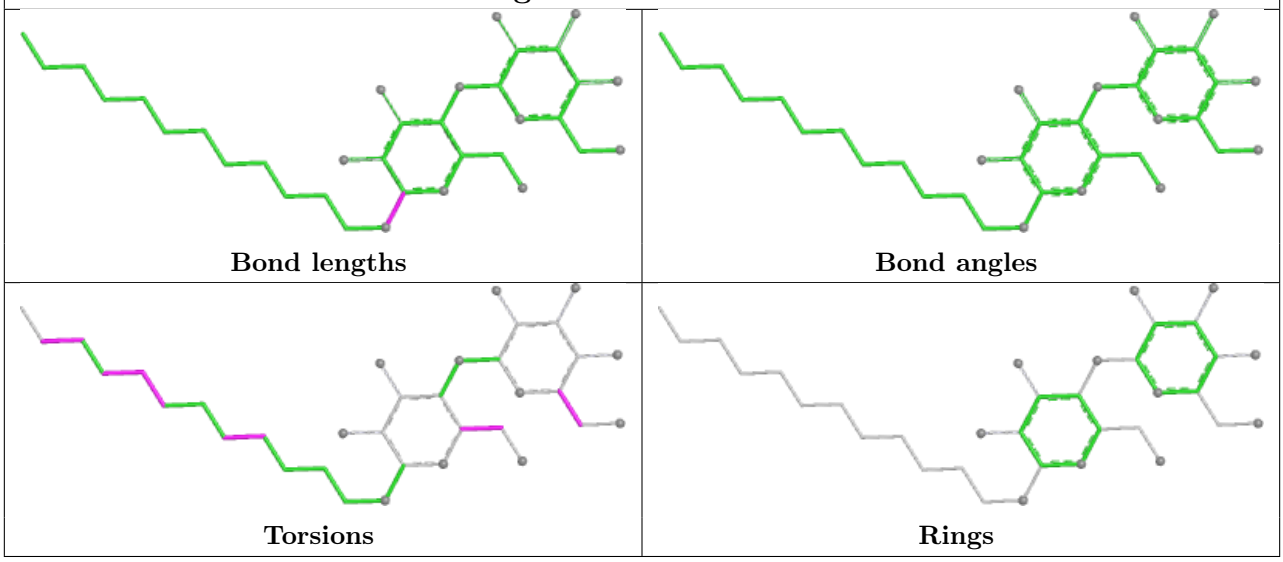
Ligand LMT B 1102



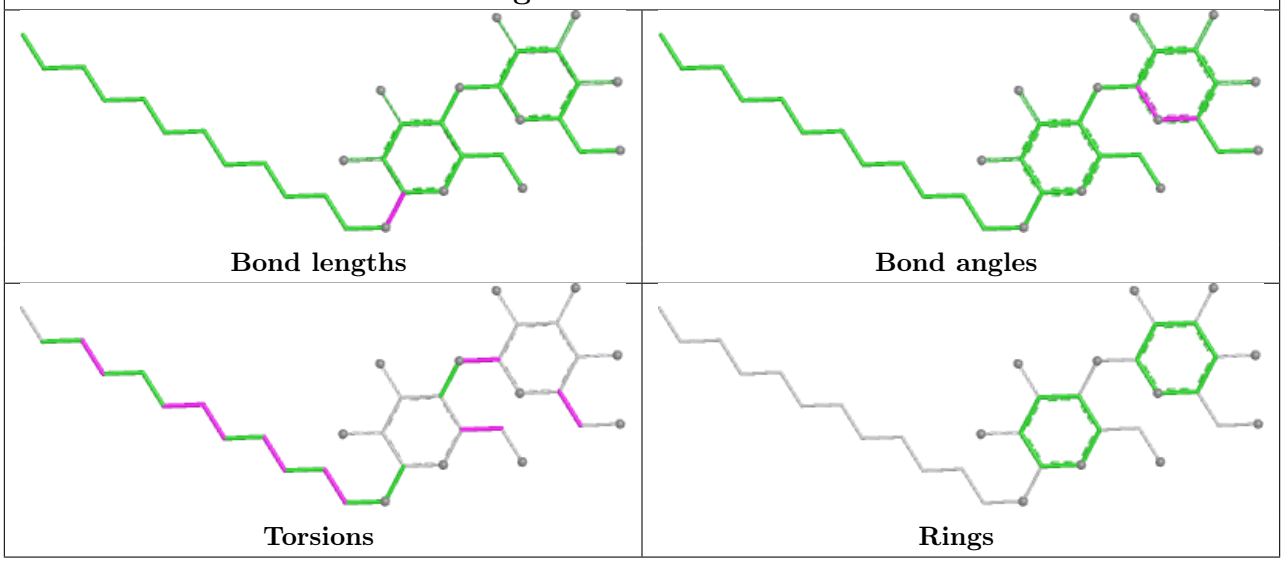
Ligand LMT C 1102



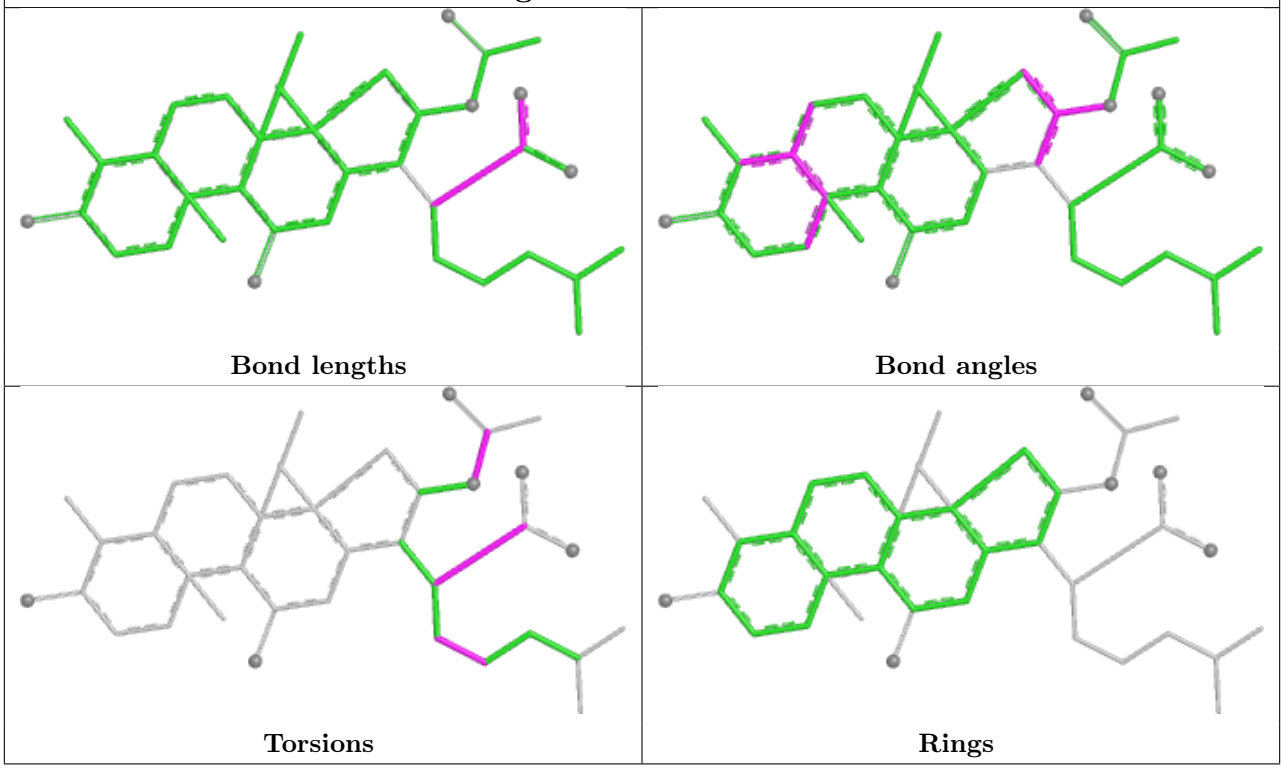
Ligand LMT B 1101



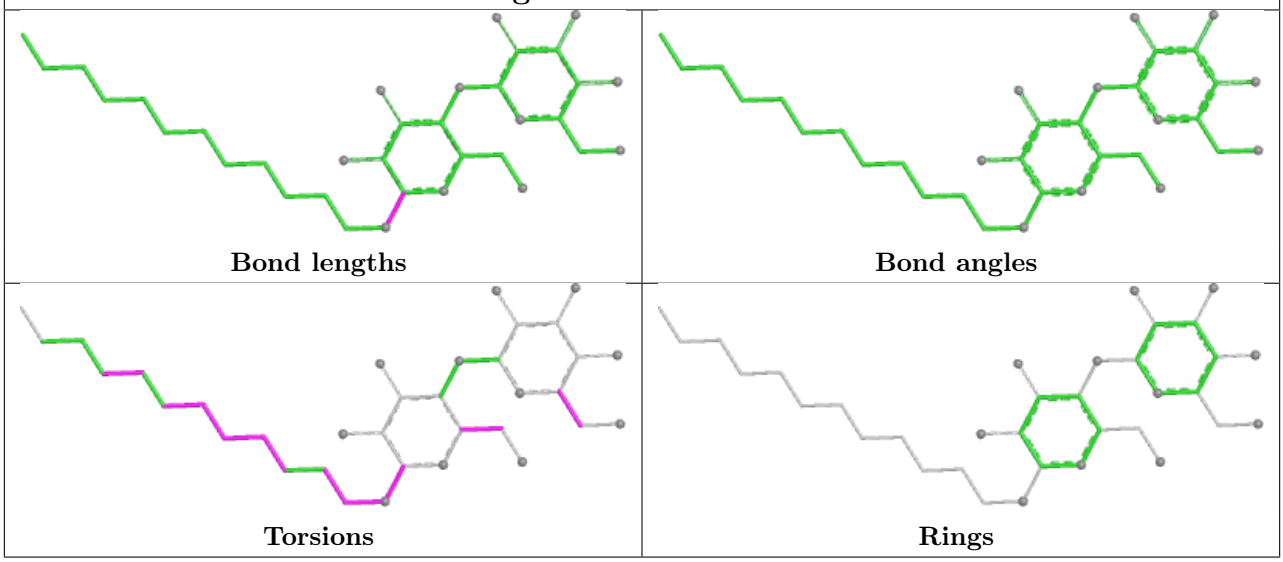
Ligand LMT C 1103



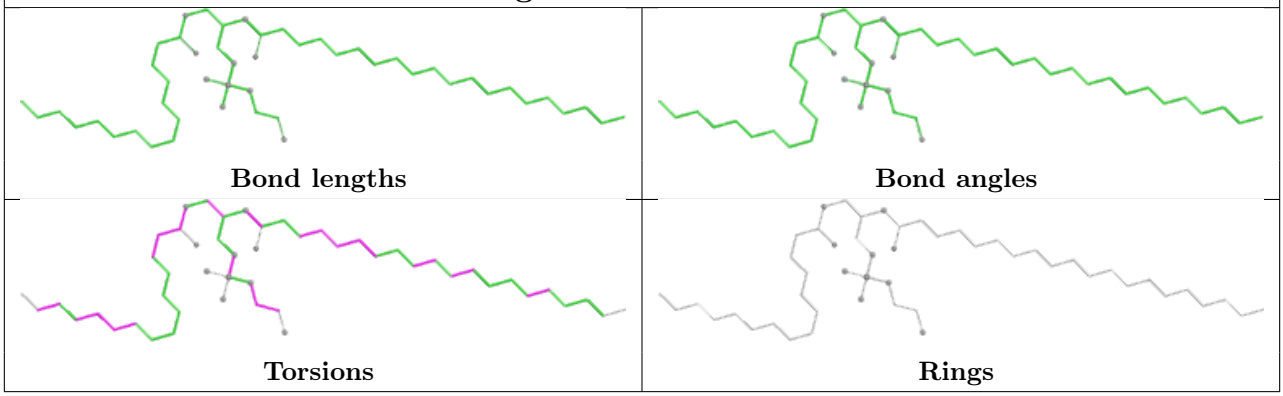
Ligand FUA B 1104



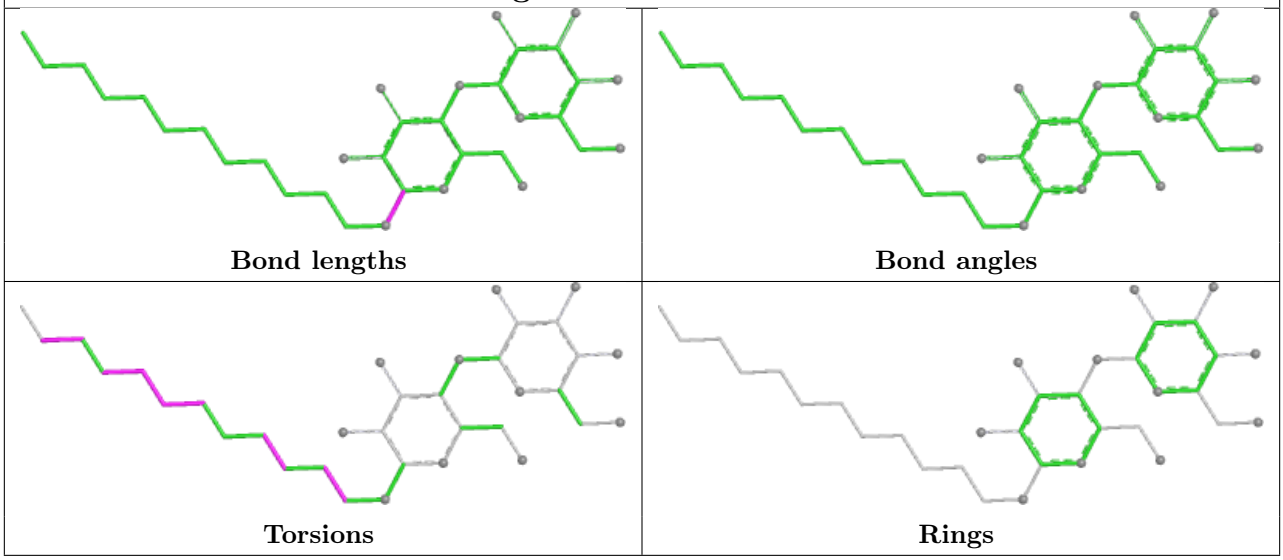
Ligand LMT A 1103



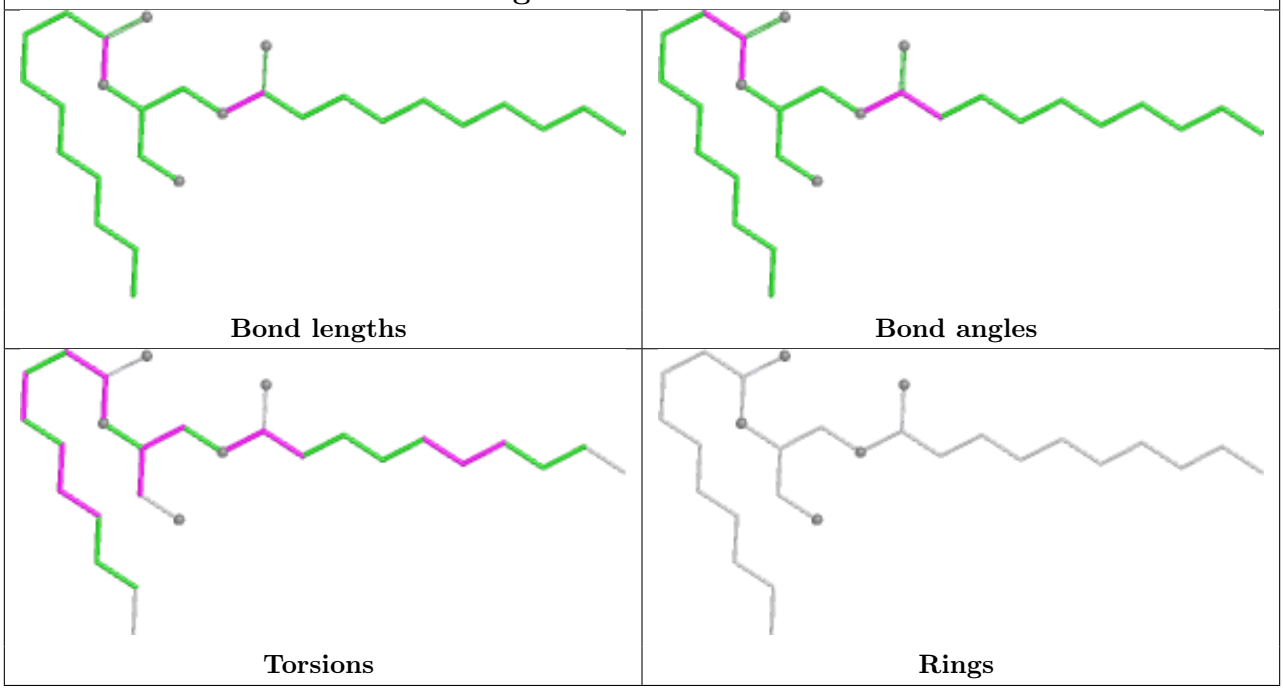
Ligand PTY B 1105



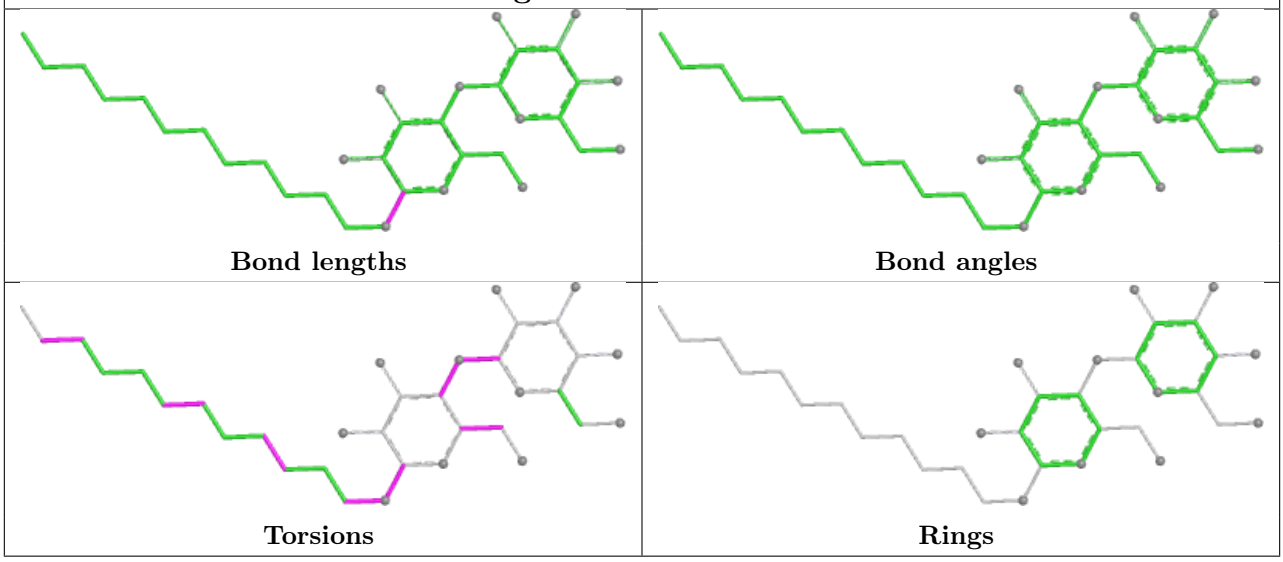
Ligand LMT A 1104

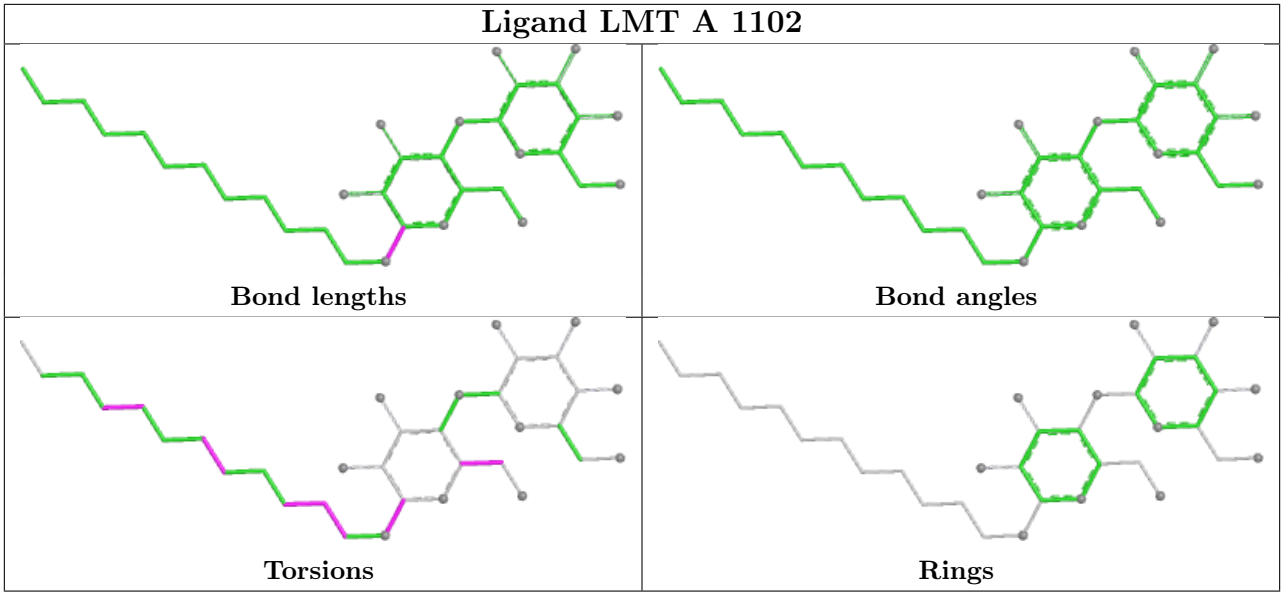


Ligand DDR B 1107



Ligand LMT B 1103





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	1042/1057 (98%)	0.07	32 (3%)	49	39	34, 63, 102, 140	0
1	B	1034/1057 (97%)	-0.00	32 (3%)	49	39	34, 62, 90, 106	0
1	C	1034/1057 (97%)	-0.07	20 (1%)	66	59	36, 53, 77, 104	0
2	D	156/169 (92%)	0.30	13 (8%)	11	6	50, 62, 95, 116	0
2	E	154/169 (91%)	1.08	38 (24%)	0	0	53, 73, 100, 106	0
All	All	3420/3509 (97%)	0.06	135 (3%)	39	29	34, 59, 93, 140	0

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	35	ALA	5.7
2	E	34	MET	5.1
2	D	166	GLN	4.9
2	E	31	ARG	4.7
1	A	868	LEU	4.5
1	B	600	THR	4.4
1	C	253	VAL	4.3
2	E	67	LEU	4.2
1	A	1037	ASN	4.2
1	A	675	GLY	4.1
1	A	869	SER	4.1
1	A	866	GLU	4.0
2	D	160	ASP	3.9
2	E	66	LEU	3.9
2	E	33	LEU	3.9
2	E	32	ILE	3.8
1	B	604	ASN	3.8
1	B	918	PHE	3.8
2	E	38	ALA	3.7
2	E	99	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
2	E	36	ASN	3.7
2	D	159	GLU	3.7
2	E	106	VAL	3.6
1	A	867	ARG	3.5
2	E	107	ASN	3.4
1	A	712	MET	3.4
2	E	163	GLU	3.4
1	A	833	PRO	3.3
2	E	28	ASP	3.3
1	A	501	ALA	3.3
1	C	730	ASP	3.3
1	A	871	ASN	3.3
2	D	165	LEU	3.3
1	A	362	PHE	3.3
2	E	69	ASN	3.2
2	E	68	LYS	3.2
2	D	150	PHE	3.2
1	C	811	TYR	3.2
1	C	255	GLN	3.2
1	B	134	SER	3.1
1	B	711	ASP	3.1
1	B	597	TYR	3.1
1	A	870	GLY	3.1
2	D	153	SER	3.1
1	B	255	GLN	3.1
1	C	256	ASP	3.0
2	E	61	GLU	3.0
1	C	510	LYS	3.0
2	D	163	GLU	3.0
1	A	515	TRP	2.9
2	E	73	VAL	2.9
1	C	501	ALA	2.9
1	B	655	PHE	2.9
1	B	606	VAL	2.8
1	B	598	TYR	2.8
1	B	601	LYS	2.8
2	E	64	GLU	2.8
2	D	161	LEU	2.8
2	D	154	ILE	2.8
1	A	865	GLN	2.7
1	C	803	ALA	2.7
2	E	37	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
2	E	30	VAL	2.7
1	B	676	THR	2.7
2	E	62	ILE	2.7
2	E	94	GLU	2.7
2	E	70	GLY	2.7
1	C	497	LEU	2.6
2	D	162	ALA	2.6
1	C	500	ILE	2.6
1	A	619	GLY	2.6
1	A	1040	ILE	2.6
1	A	846	GLN	2.5
1	B	508	GLY	2.5
1	B	132	SER	2.5
1	B	642	ASN	2.5
1	A	678	THR	2.5
1	B	574	THR	2.5
1	A	839	GLU	2.5
2	E	139	VAL	2.5
1	A	918	PHE	2.4
1	B	833	PRO	2.4
1	B	575	MET	2.4
1	C	362	PHE	2.4
2	E	130	GLU	2.4
1	B	605	ASN	2.4
1	A	832	ALA	2.4
2	E	63	VAL	2.4
2	E	145	PHE	2.4
1	C	793	ALA	2.4
1	B	641	GLU	2.4
1	B	674	LEU	2.3
1	B	1034	SER	2.3
2	E	27	ASP	2.3
1	C	427	PRO	2.3
1	A	831	ALA	2.3
1	A	512	PHE	2.3
2	E	98	VAL	2.2
1	B	257	GLY	2.2
2	E	29	GLU	2.2
1	A	835	LYS	2.2
1	C	739	LEU	2.2
1	B	596	HIS	2.2
2	E	150	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	676	THR	2.2
2	E	143	ASP	2.2
2	D	157	GLY	2.1
1	B	256	ASP	2.1
2	E	60	LEU	2.1
1	B	618	ALA	2.1
1	A	620	ARG	2.1
2	E	165	LEU	2.1
1	A	543	VAL	2.1
2	D	126	LEU	2.1
1	B	617	PHE	2.1
2	E	93	LEU	2.1
1	C	258	SER	2.1
1	C	732	ASP	2.1
2	E	108	ALA	2.1
1	B	599	LEU	2.1
1	C	804	PHE	2.1
1	A	500	ILE	2.1
1	A	834	GLY	2.1
1	A	713	LEU	2.1
1	A	423	GLU	2.1
1	B	593	GLU	2.1
2	D	11	GLY	2.0
1	B	133	SER	2.0
2	E	153	SER	2.0
1	B	1033	PHE	2.0
1	C	512	PHE	2.0
1	A	255	GLN	2.0
1	C	731	ILE	2.0
1	C	257	GLY	2.0
1	B	628	PHE	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
14	D10	B	1116	10/10	0.66	0.52	89,92,96,96	0
5	DDQ	A	1106	14/14	0.67	0.52	95,104,118,119	0
8	FUA	B	1104	37/37	0.71	0.58	125,130,132,134	37
9	PTY	C	1104	50/50	0.72	0.32	88,97,127,133	0
5	DDQ	C	1109	14/14	0.73	0.40	112,115,118,118	0
16	ETE	C	1116	14/14	0.74	0.24	102,104,107,108	0
3	LMT	B	1103	35/35	0.75	0.26	103,138,153,154	0
3	LMT	C	1103	35/35	0.75	0.42	100,111,120,120	0
5	DDQ	B	1109	14/14	0.76	0.26	92,104,116,117	0
3	LMT	B	1102	35/35	0.76	0.31	110,127,138,139	0
3	LMT	A	1101	35/35	0.76	0.27	90,113,133,134	0
11	OCT	B	1111	8/8	0.77	0.28	76,78,79,80	0
4	D12	B	1106	12/12	0.77	0.45	76,79,80,80	0
7	HEX	A	1110	6/6	0.77	0.31	90,91,91,91	0
11	OCT	B	1110	8/8	0.78	0.26	77,79,81,81	0
15	C14	C	1106	14/14	0.80	0.22	72,79,82,82	0
3	LMT	C	1102	35/35	0.80	0.26	72,114,138,139	0
3	LMT	A	1102	35/35	0.81	0.27	85,99,121,123	0
7	HEX	C	1117	6/6	0.81	0.35	74,76,77,77	0
3	LMT	A	1103	35/35	0.81	0.31	85,124,129,130	0
5	DDQ	B	1108	14/14	0.82	0.28	74,80,96,96	0
9	PTY	B	1105	50/50	0.83	0.30	95,118,136,139	0
4	D12	A	1105	12/12	0.85	0.25	91,94,95,95	0
5	DDQ	C	1108	14/14	0.85	0.27	90,94,99,99	0
11	OCT	C	1110	8/8	0.85	0.26	68,70,71,71	0
6	GOL	A	1108	6/6	0.86	0.36	80,83,84,84	0
6	GOL	E	201	6/6	0.87	0.23	77,77,78,78	0
3	LMT	A	1104	35/35	0.87	0.33	91,100,110,111	0
4	D12	C	1105	12/12	0.87	0.23	69,70,71,71	0
5	DDQ	C	1107	14/14	0.89	0.28	89,91,94,94	0
3	LMT	B	1101	35/35	0.89	0.33	87,98,115,116	0
6	GOL	C	1115	6/6	0.89	0.31	54,55,55,56	0
12	CL	C	1112	1/1	0.90	0.23	74,74,74,74	0
10	DDR	B	1107	28/28	0.90	0.28	86,96,104,106	0
6	GOL	A	1107	6/6	0.91	0.21	71,73,74,74	0
6	GOL	A	1109	6/6	0.91	0.30	68,71,74,75	0
12	CL	C	1114	1/1	0.91	0.13	67,67,67,67	0

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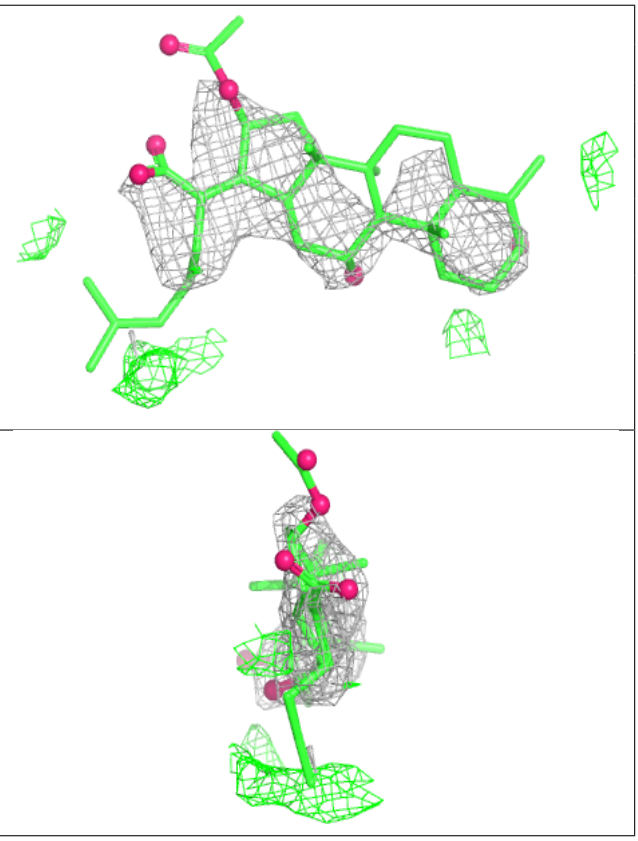
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	GOL	B	1115	6/6	0.93	0.24	75,76,76,76	0
3	LMT	C	1101	35/35	0.94	0.25	65,71,88,89	0
12	CL	C	1113	1/1	0.95	0.35	57,57,57,57	0
13	SO4	B	1114	5/5	0.96	0.17	87,87,89,89	0
12	CL	B	1112	1/1	0.96	0.11	62,62,62,62	0
13	SO4	B	1113	5/5	0.97	0.12	79,80,81,83	0
12	CL	C	1111	1/1	0.99	0.31	44,44,44,44	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.

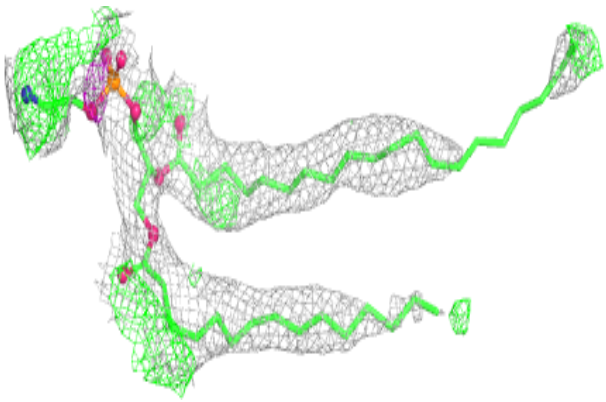
Electron density around FUA B 1104:

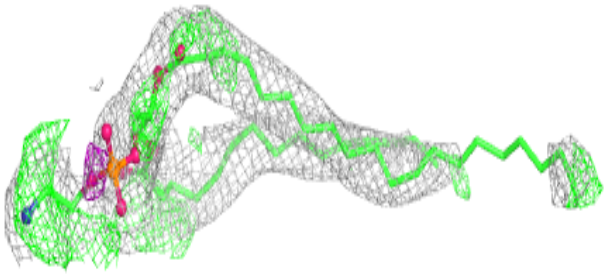
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

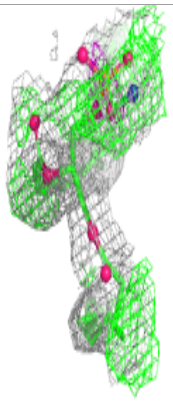


Electron density around PTY C 1104:

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

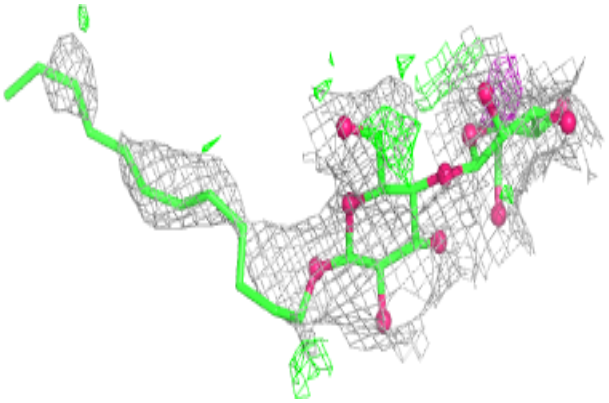


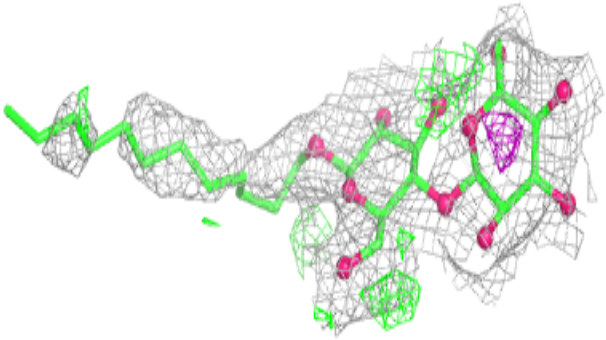


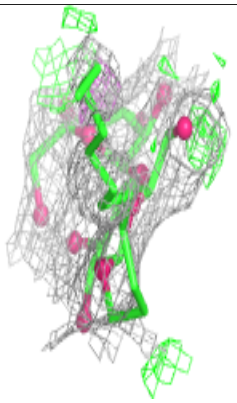


Electron density around LMT B 1103:

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

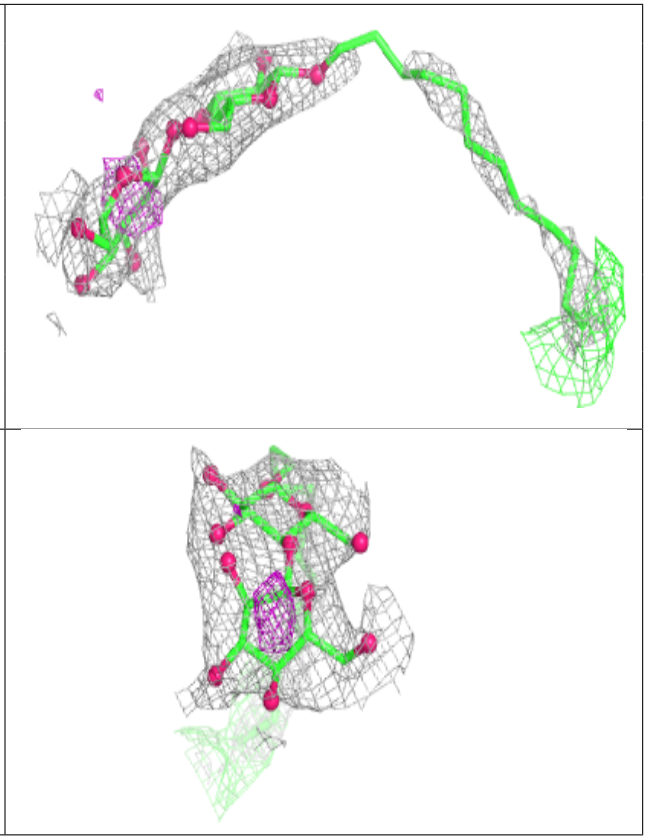






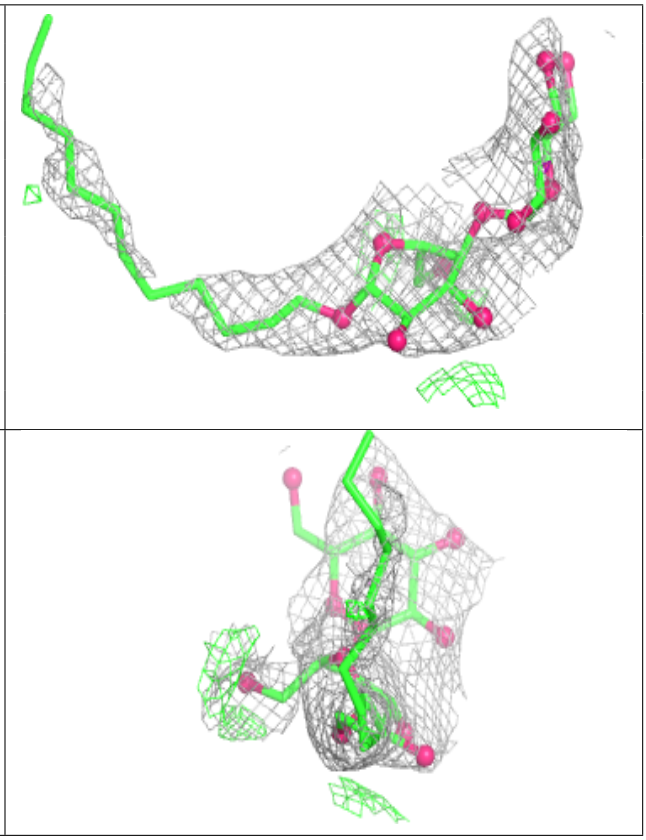
Electron density around LMT C 1103:

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



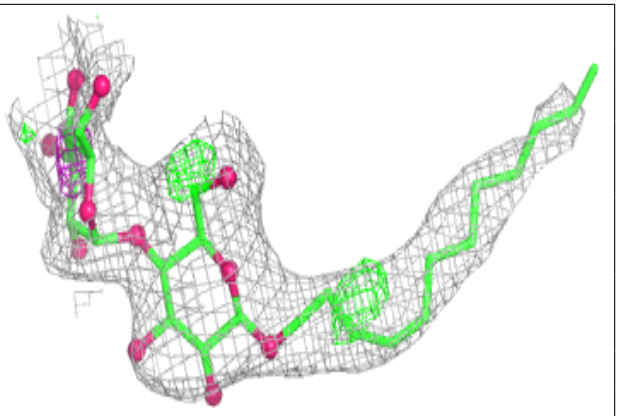
Electron density around LMT B 1102:

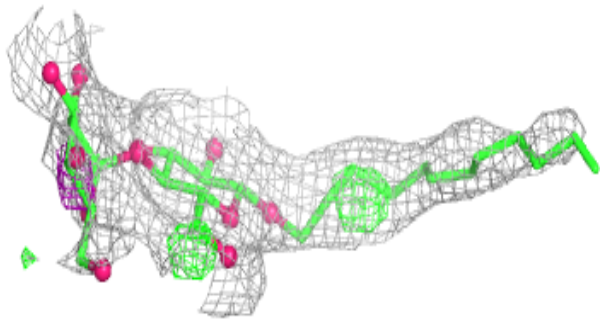
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

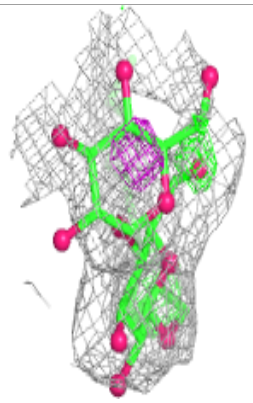


Electron density around LMT A 1101:

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

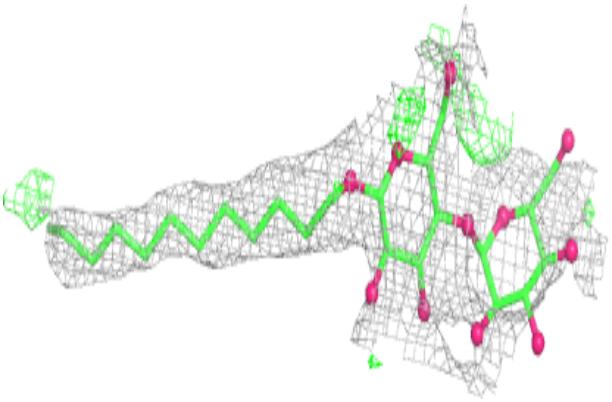


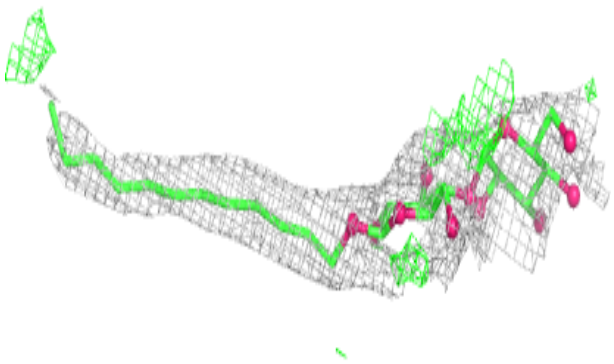


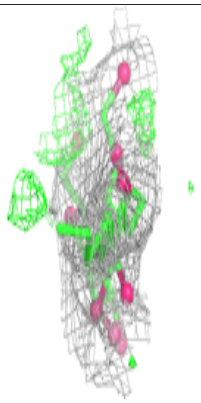


Electron density around LMT C 1102:

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

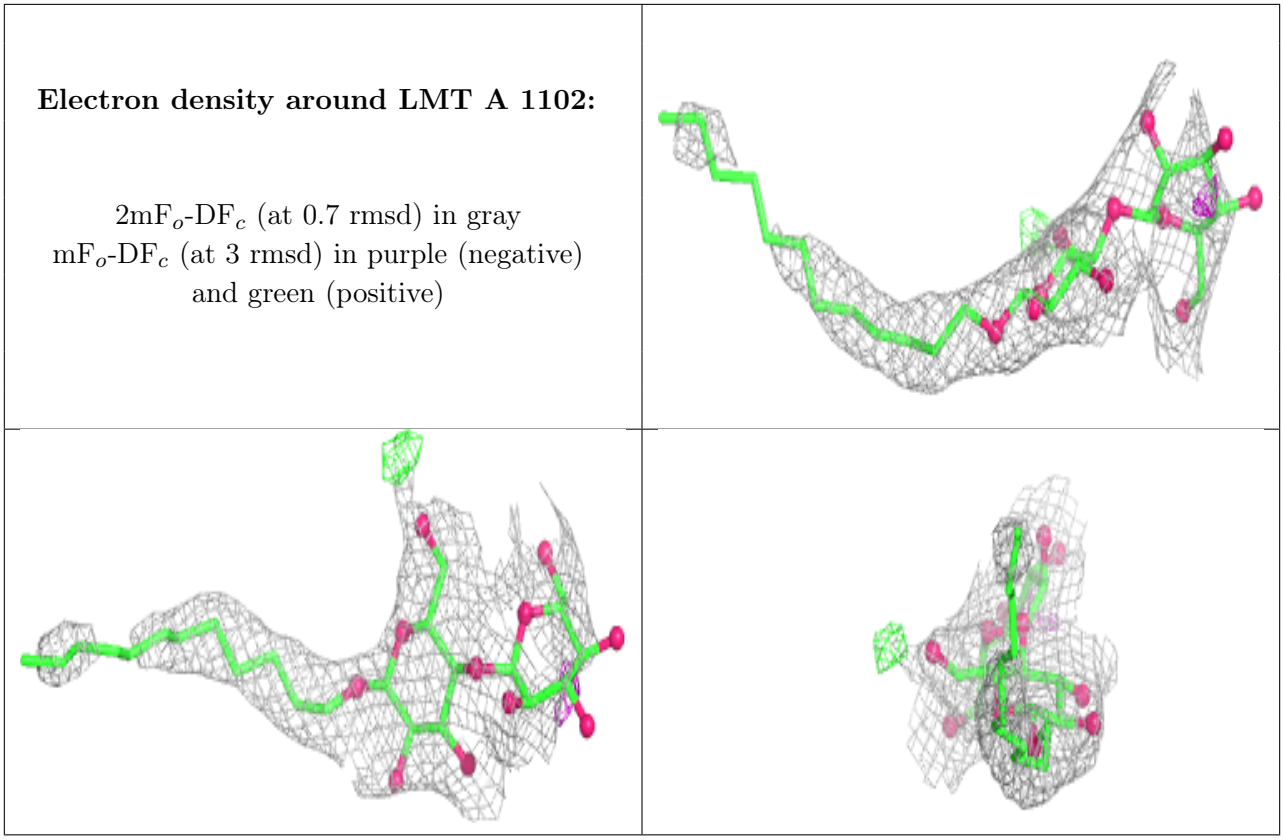






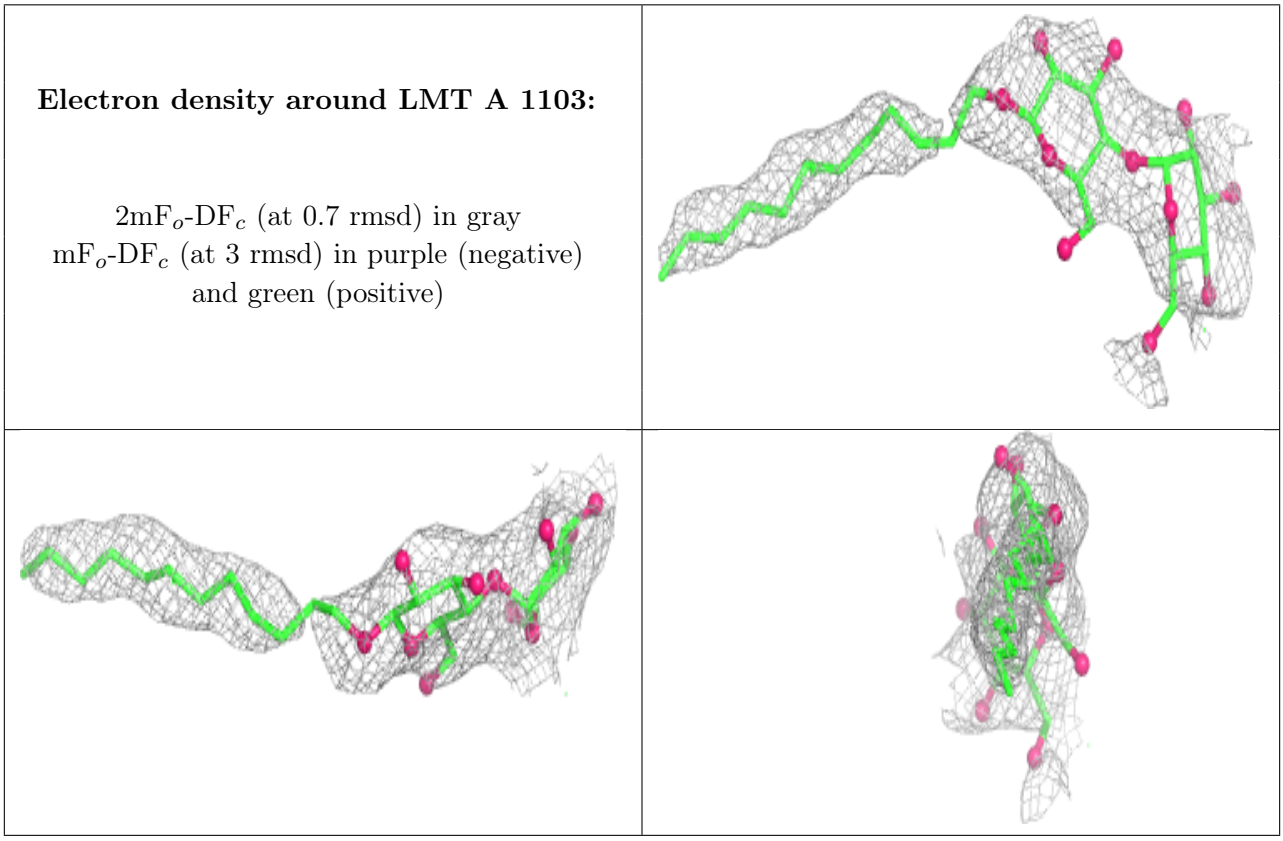
Electron density around LMT A 1102:

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



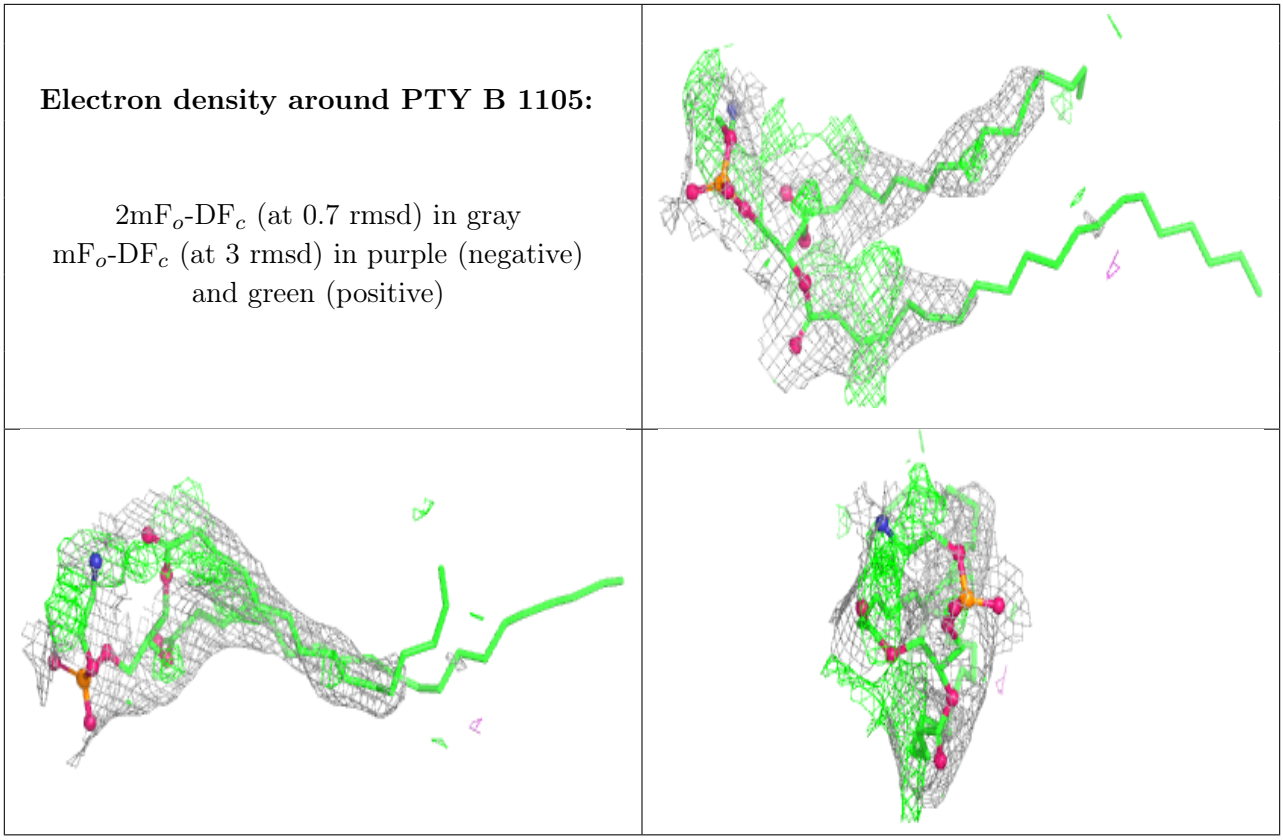
Electron density around LMT A 1103:

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



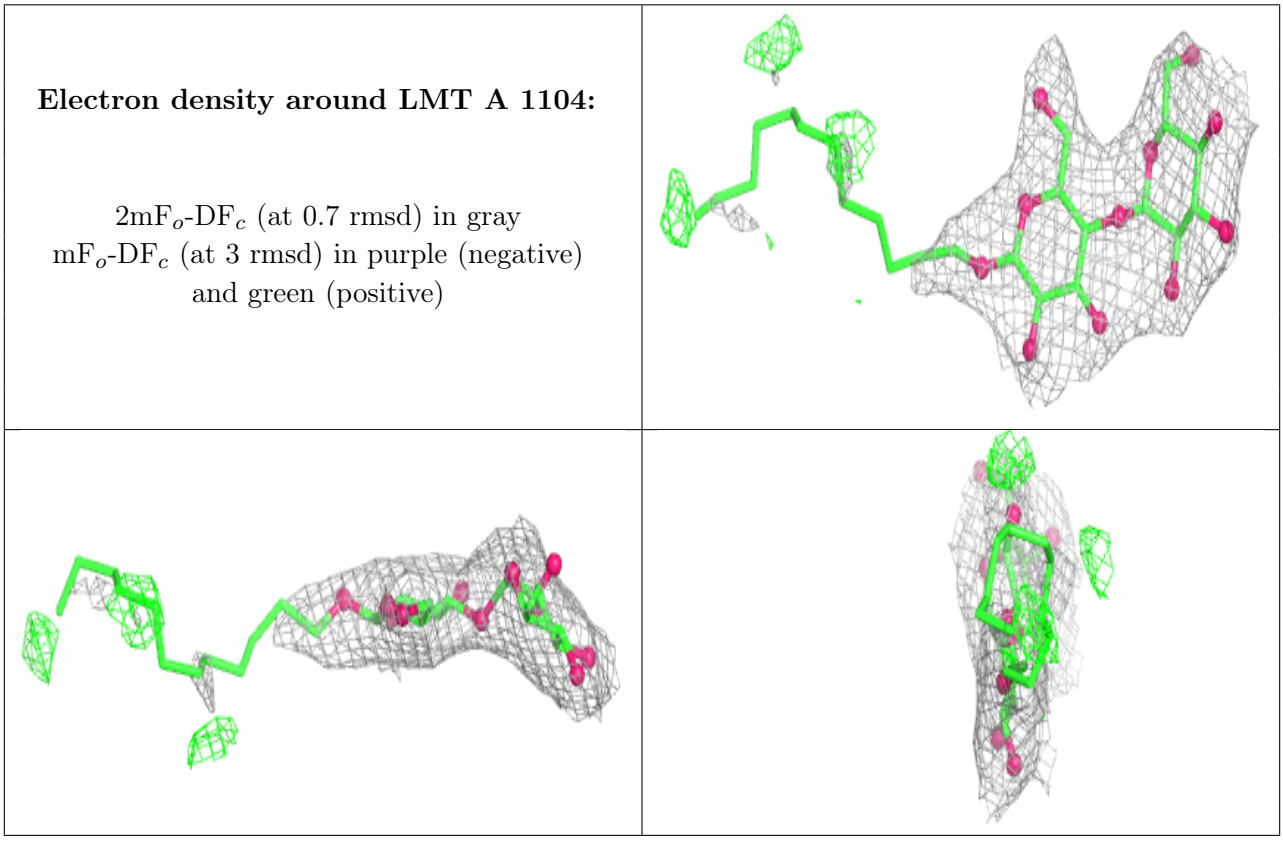
Electron density around PTY B 1105:

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



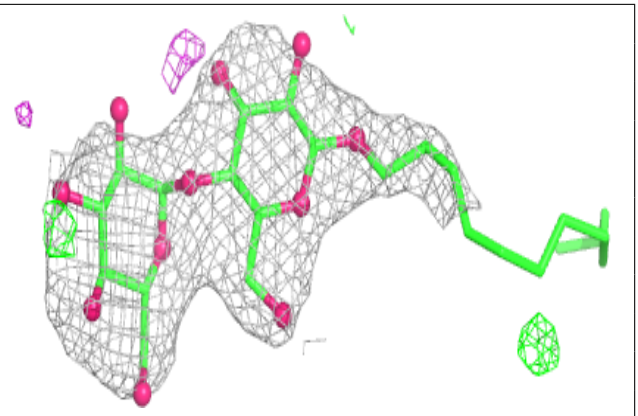
Electron density around LMT A 1104:

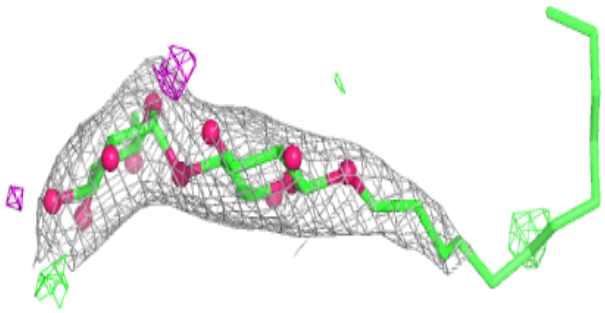
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

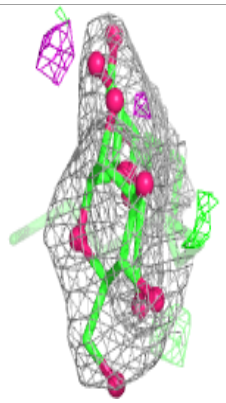


Electron density around LMT B 1101:

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

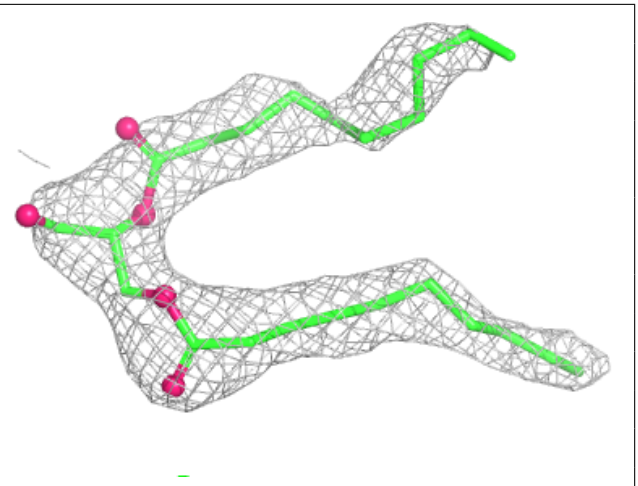


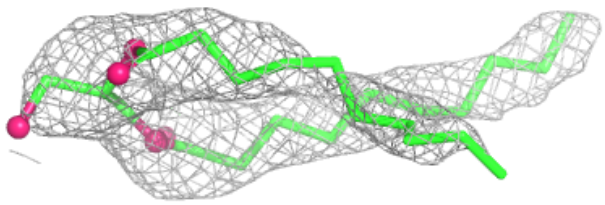


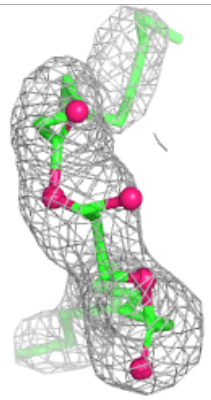


Electron density around DDR B 1107:

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

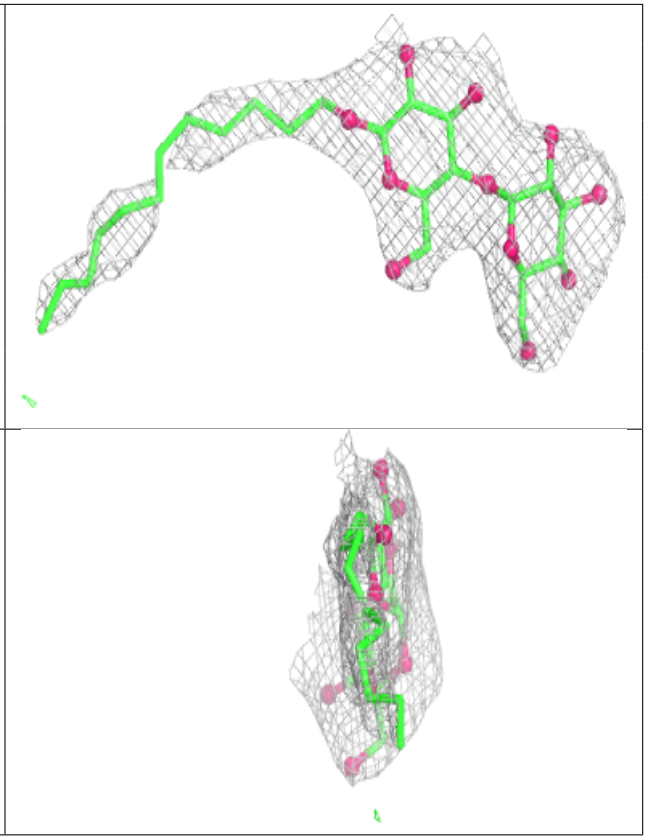






Electron density around LMT C 1101:

$2mF_o$-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.