Full wwPDB X-ray Structure Validation Report ⓘ

Sep 19, 2020 – 09:39 AM BST

PDB ID	:	6Q4O
Title	:	Fusidic acid bound AcrB_I27A
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 ⓘ symbol.

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

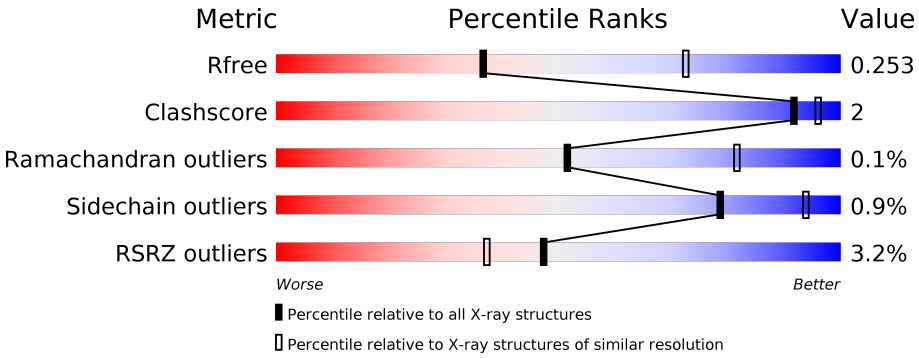
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

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

Mol	Chain	Length	Quality of chain
1	A	1057	3% 92% 7%
1	B	1057	2% 94%
1	C	1057	% 93% 5%
2	D	169	10% 92% 8%
2	E	169	12% 91% 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
12	PTY	C	1119	-	-	-	X
3	LMT	A	1101	-	-	-	X
3	LMT	A	1103	-	-	-	X
5	DDQ	A	1107	-	-	-	X
5	DDQ	A	1109	-	-	-	X
7	HEX	B	1117	-	-	-	X
7	HEX	C	1114	-	-	-	X

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 27628 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1042	Total	C	N	O	S	0	4	0
			7952	5115	1314	1479	44			
1	B	1034	Total	C	N	O	S	0	1	0
			7860	5060	1296	1460	44			
1	C	1035	Total	C	N	O	S	0	1	0
			7871	5063	1303	1461	44			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	ALA	ILE	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	27	ALA	ILE	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	27	ALA	ILE	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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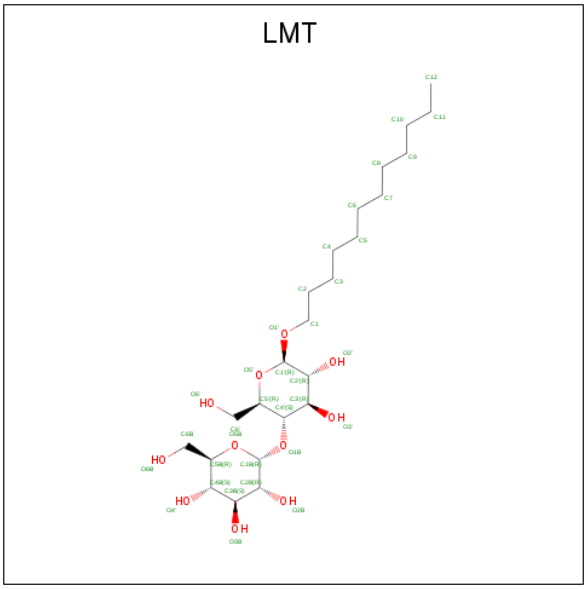
Chain	Residue	Modelled	Actual	Comment	Reference
C	1054	HIS	-	expression tag	UNP P31224
C	1055	HIS	-	expression tag	UNP P31224
C	1056	HIS	-	expression tag	UNP P31224
C	1057	HIS	-	expression tag	UNP P31224

- Molecule 2 is a protein called DARPIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	156	Total	C	N	O	S	0	0	0
			1182	745	207	229	1			
2	E	154	Total	C	N	O	S	0	0	0
			1167	736	204	226	1			

- Molecule 3 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



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

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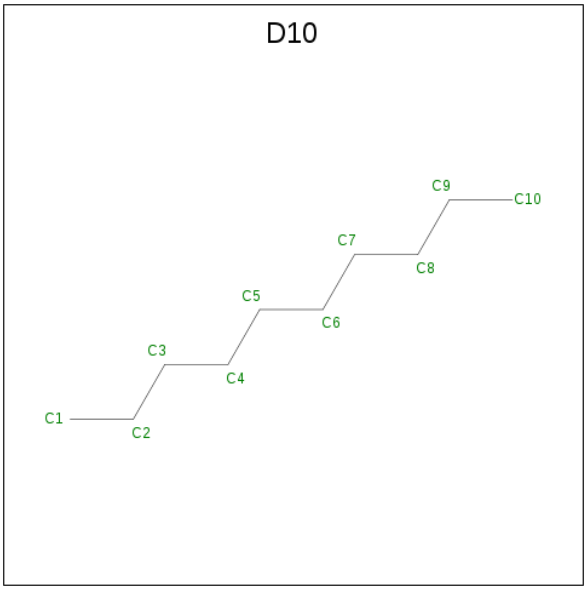
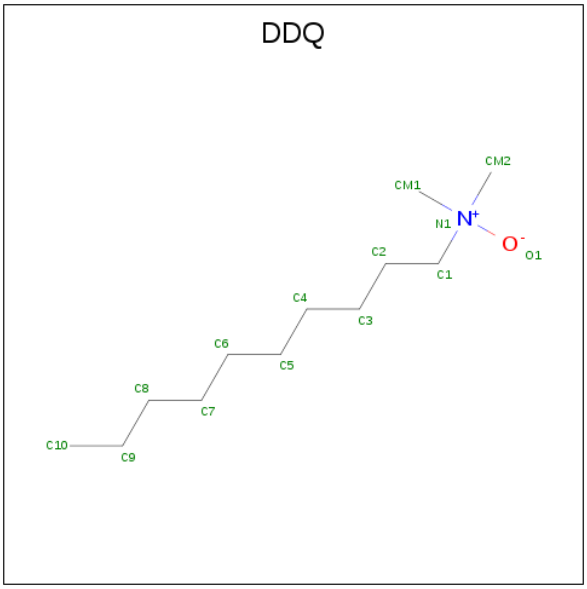
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 35 24 11	0	0
3	C	1	Total C O 35 24 11	0	0
3	C	1	Total C O 35 24 11	0	0

- Molecule 4 is DECANE (three-letter code: D10) (formula: $C_{10}H_{22}$).



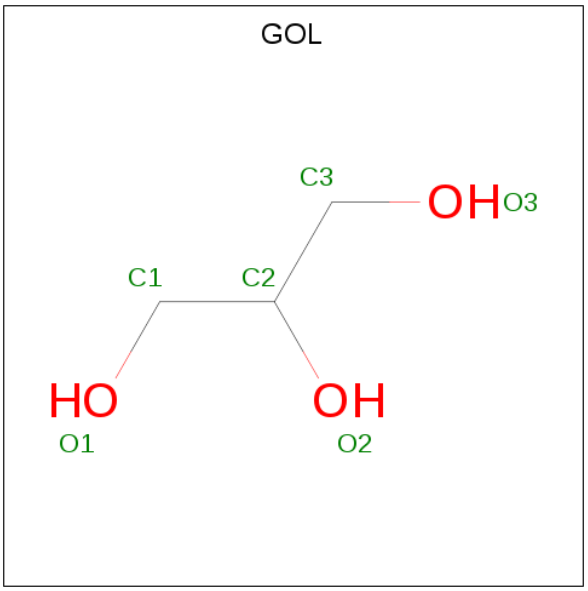
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C 10 10	0	0
4	A	1	Total C 10 10	0	0
4	B	1	Total C 10 10	0	0
4	B	1	Total C 10 10	0	0
4	B	1	Total C 10 10	0	0
4	C	1	Total C 10 10	0	0
4	C	1	Total C 10 10	0	0
4	C	1	Total C 10 10	0	0

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



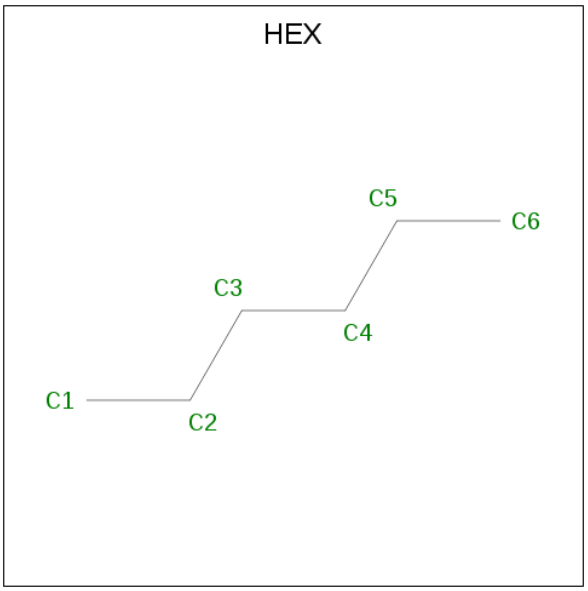
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 14 12 1 1	0	0
5	A	1	Total C N O 14 12 1 1	0	0
5	A	1	Total C N O 14 12 1 1	0	0
5	B	1	Total C N O 14 12 1 1	0	0
5	B	1	Total C N O 14 12 1 1	0	0
5	B	1	Total C N O 14 12 1 1	0	0
5	B	1	Total C N O 14 12 1 1	0	0
5	C	1	Total C N O 14 12 1 1	0	0
5	C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

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



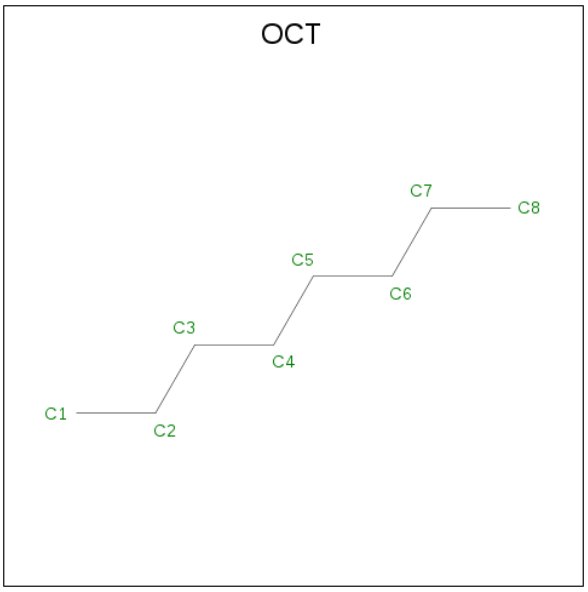
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	C	1	Total C O 6 3 3	0	0
6	C	1	Total C O 6 3 3	0	0
6	C	1	Total C O 6 3 3	0	0
6	C	1	Total C O 6 3 3	0	0
6	D	1	Total C O 6 3 3	0	0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

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



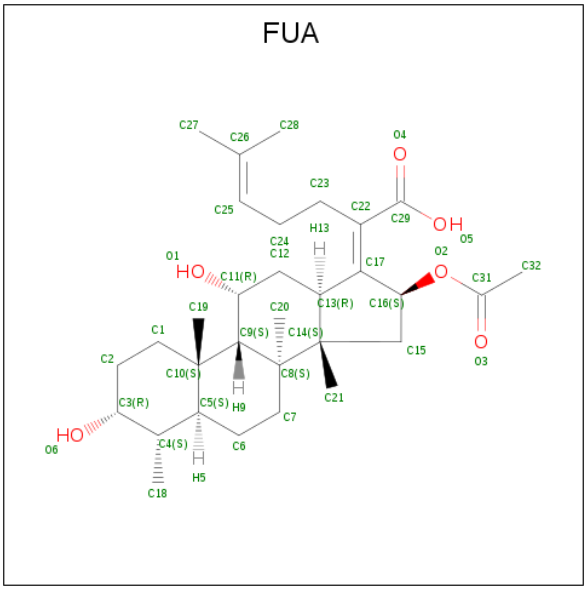
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C 6 6	0	0
7	B	1	Total C 6 6	0	0
7	B	1	Total C 6 6	0	0
7	B	1	Total C 6 6	0	0
7	B	1	Total C 6 6	0	0
7	C	1	Total C 6 6	0	0
7	C	1	Total C 6 6	0	0
7	C	1	Total C 6 6	0	0
7	C	1	Total C 6 6	0	0

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



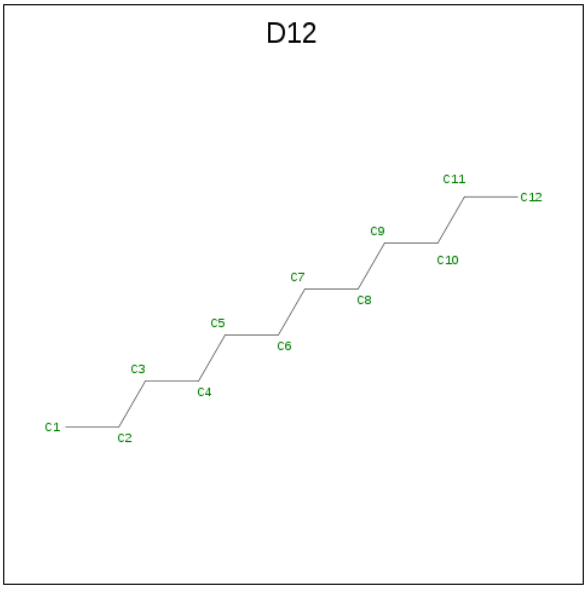
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C 8 8	0	0
8	A	1	Total C 8 8	0	0
8	B	1	Total C 8 8	0	0
8	B	1	Total C 8 8	0	0

- Molecule 9 is FUSIDIC ACID (three-letter code: FUA) (formula: $C_{31}H_{48}O_6$) (labeled as "Ligand of Interest" by author).



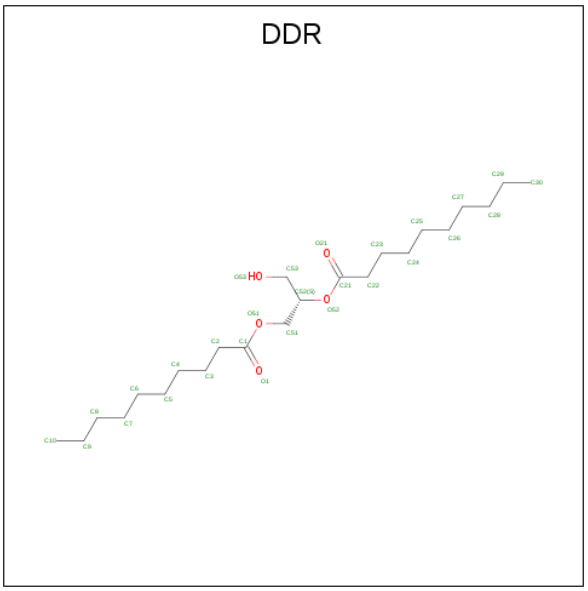
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C O 37 31 6	0	0

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



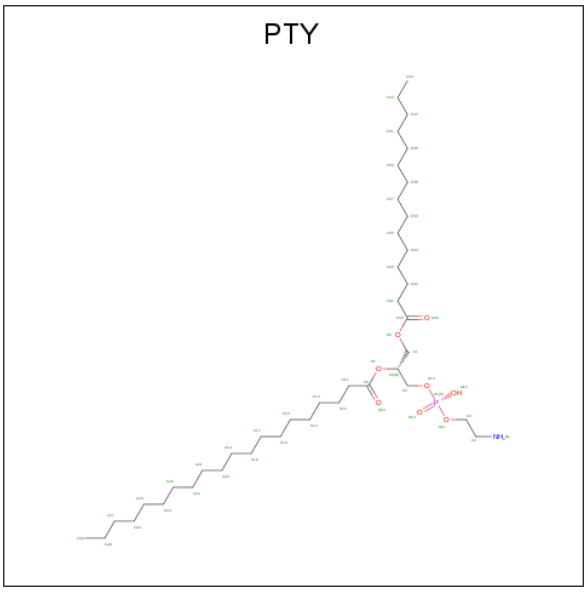
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total C 12 12	0	0
10	C	1	Total C 12 12	0	0
10	C	1	Total C 12 12	0	0
10	C	1	Total C 12 12	0	0

- Molecule 11 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
11	B	1	Total	C	O	0	0
			28	23	5		

- Molecule 12 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$).



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

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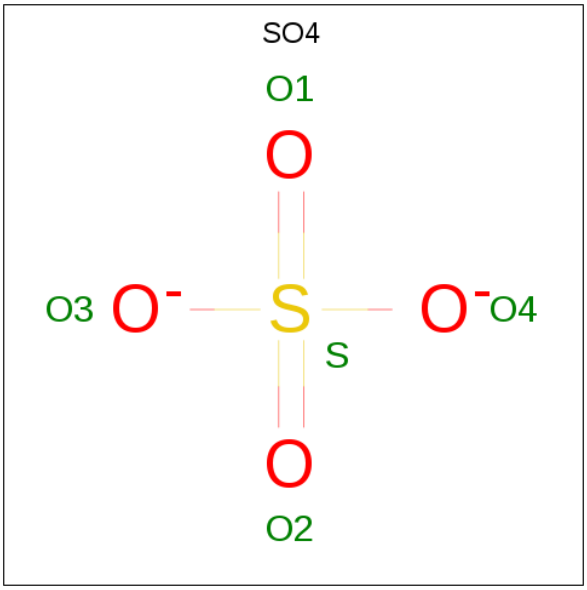
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	C	1	Total	C	N	O	P	0	0
			50	40	1	8	1		
12	C	1	Total	C	N	O	P	0	0
			50	40	1	8	1		

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



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

- Molecule 14 is water.

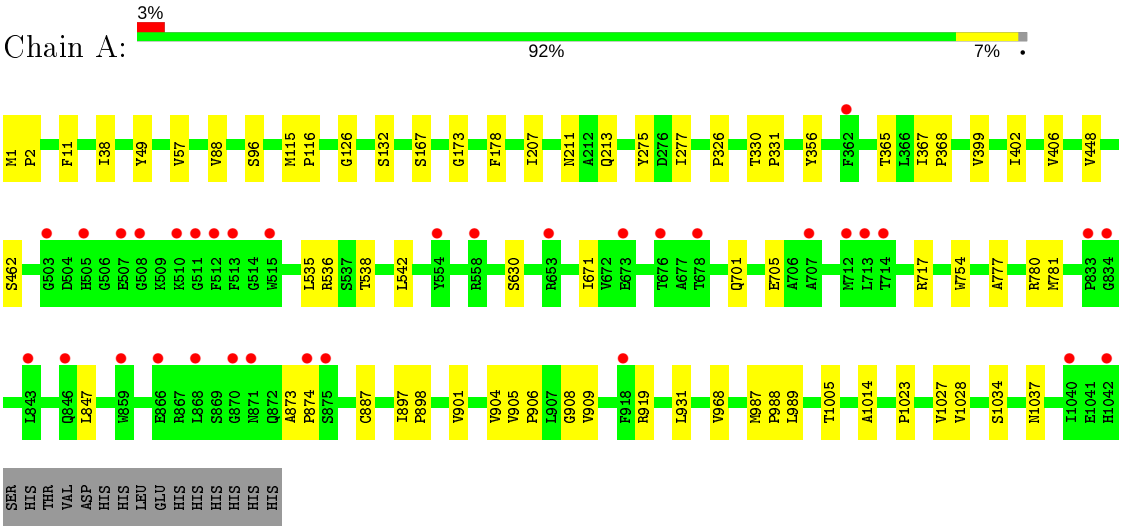
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	197	Total	O	0	0
			197	197		
14	B	173	Total	O	0	0
			173	173		
14	C	227	Total	O	0	0
			227	227		
14	D	34	Total	O	0	0
			34	34		
14	E	9	Total	O	0	0
			9	9		

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.

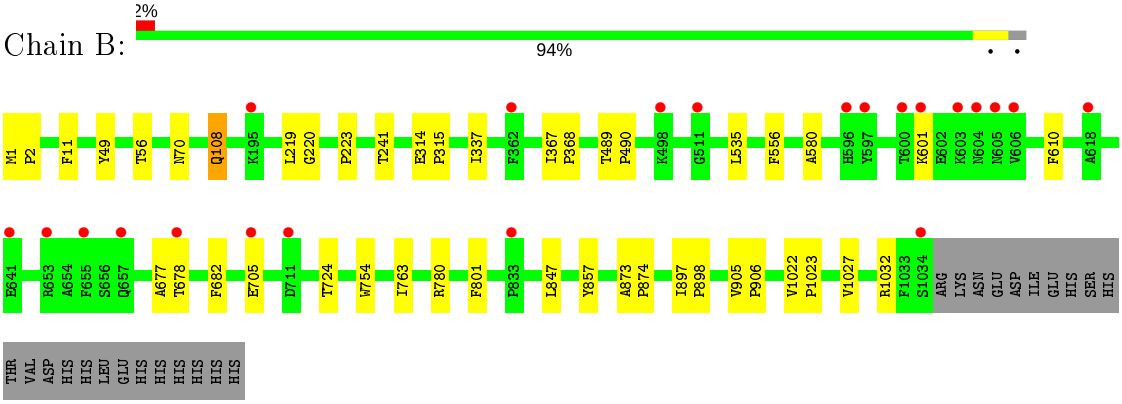
- Molecule 1: Multidrug efflux pump subunit AcrB

Chain A:



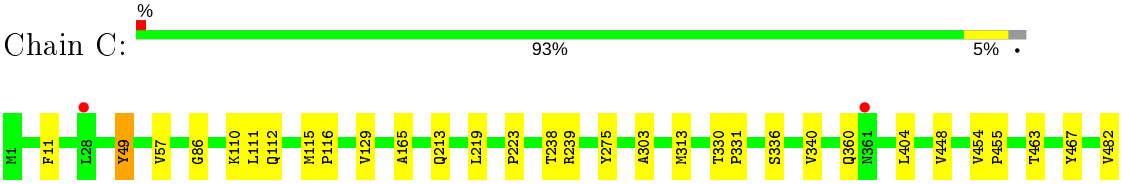
- Molecule 1: Multidrug efflux pump subunit AcrB

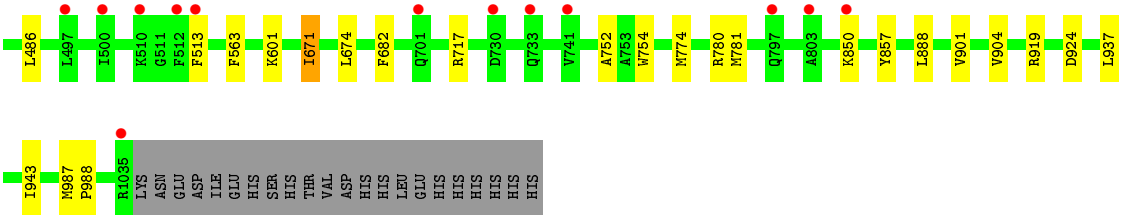
Chain B:



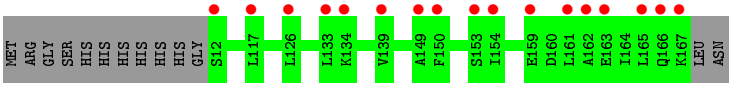
- Molecule 1: Multidrug efflux pump subunit AcrB

Chain C:

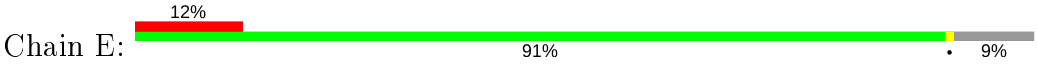


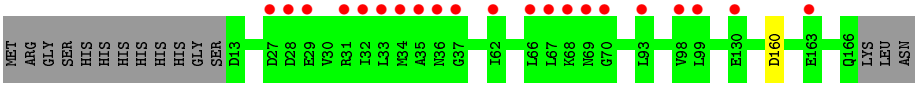


- Molecule 2: DARPIN



- Molecule 2: DARPIN





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	145.20Å 162.57Å 243.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.52 – 2.80 47.47 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.8 (47.52-2.80) 98.8 (47.47-2.80)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.212 , 0.256 0.213 , 0.253	Depositor DCC
R_{free} test set	6961 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	45.4	Xtriage
Anisotropy	0.383	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 42.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	27628	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, D10, D12, DDR, DDQ, HEX, SO4, PTY, FUA, LMT, 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	0.65	0/8116	0.71	0/11018
1	B	0.65	0/8014	0.70	0/10883
1	C	0.65	0/8024	0.70	0/10895
2	D	0.67	0/1201	0.70	0/1632
2	E	0.67	0/1186	0.70	0/1613
All	All	0.65	0/26541	0.70	0/36041

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

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	7952	0	8100	36	0
1	B	7860	0	8009	23	0
1	C	7871	0	8026	33	0
2	D	1182	0	1169	0	0
2	E	1167	0	1151	0	0
3	A	140	0	184	0	0
3	B	70	0	92	1	0
3	C	70	0	92	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	20	0	44	0	0
4	B	30	0	66	0	0
4	C	30	0	66	0	0
5	A	42	0	81	0	0
5	B	56	0	108	0	0
5	C	28	0	54	0	0
6	A	12	0	16	0	0
6	B	18	0	24	0	0
6	C	24	0	32	0	0
6	D	6	0	8	0	0
6	E	6	0	8	0	0
7	A	6	0	14	0	0
7	B	24	0	56	0	0
7	C	24	0	56	0	0
8	A	16	0	36	0	0
8	B	16	0	36	1	0
9	B	37	0	47	6	0
10	B	12	0	26	0	0
10	C	36	0	78	0	0
11	B	28	0	44	0	0
12	C	200	0	316	2	0
13	C	5	0	0	0	0
14	A	197	0	0	0	0
14	B	173	0	0	0	0
14	C	227	0	0	0	0
14	D	34	0	0	0	0
14	E	9	0	0	0	0
All	All	27628	0	28039	90	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 2.

All (90) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:671:ILE:HD11	1:C:674:LEU:HD12	1.64	0.80
9:B:1101:FUA:H202	9:B:1101:FUA:H5	1.66	0.76
1:A:968:VAL:HG11	1:A:1023:PRO:HG3	1.68	0.75
1:C:360:GLN:HG2	1:C:513:PHE:CG	2.32	0.65
1:C:57:VAL:HG21	1:C:86:GLY:HA2	1.80	0.64
9:B:1101:FUA:H232	9:B:1101:FUA:C12	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:754:TRP:CZ3	1:C:219:LEU:HD23	2.37	0.58
1:A:57:VAL:CG1	1:A:88:VAL:HG22	2.34	0.57
1:C:360:GLN:HG2	1:C:513:PHE:CD1	2.39	0.57
1:A:754:TRP:HZ3	1:C:219:LEU:HD23	1.70	0.57
1:C:901:VAL:O	1:C:904:VAL:HG12	2.05	0.56
1:B:337:ILE:HG21	9:B:1101:FUA:H282	1.88	0.56
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.88	0.56
1:B:897:ILE:N	1:B:898:PRO:HD2	2.22	0.55
9:B:1101:FUA:H232	9:B:1101:FUA:H122	1.89	0.55
1:B:108:GLN:HG3	1:C:112:GLN:HG3	1.87	0.55
1:C:671:ILE:HG12	1:C:671:ILE:O	2.07	0.54
1:C:111:LEU:HD22	1:C:129:VAL:CG2	2.38	0.53
1:B:220:GLY:HA2	1:C:781:MET:SD	2.49	0.53
1:A:38:ILE:HD11	1:A:671:ILE:HG21	1.90	0.53
1:A:873:ALA:HB3	1:A:874:PRO:HD3	1.91	0.52
1:B:682:PHE:CZ	1:B:857:TYR:HB2	2.44	0.52
1:C:563:PHE:O	1:C:924:ASP:HB2	2.08	0.52
1:C:448:VAL:HG11	1:C:943:ILE:HD11	1.93	0.51
1:C:336:SER:O	1:C:340:VAL:HG23	2.11	0.50
1:A:330:THR:OG1	1:A:331:PRO:HD3	2.12	0.50
12:C:1116:PTY:H341	12:C:1116:PTY:HC12	1.94	0.49
1:C:671:ILE:CG1	1:C:671:ILE:O	2.60	0.49
1:C:330:THR:N	1:C:331:PRO:CD	2.76	0.48
1:B:1022:VAL:N	1:B:1023:PRO:HD2	2.29	0.48
1:A:987:MET:N	1:A:988:PRO:HD2	2.29	0.48
1:B:873:ALA:HB3	1:B:874:PRO:HD3	1.96	0.47
1:A:178:PHE:HA	1:A:277:ILE:HG21	1.94	0.47
1:B:905:VAL:HB	1:B:906:PRO:HD3	1.96	0.47
1:A:399:VAL:HG11	1:A:989:LEU:HD11	1.95	0.47
1:B:535:LEU:HD22	1:B:1027:VAL:HG21	1.97	0.47
1:B:580:ALA:HB1	1:B:724:THR:HG22	1.96	0.47
8:B:1119:OCT:H83	12:C:1116:PTY:H401	1.97	0.47
1:B:1:MET:HB3	1:B:2:PRO:HD3	1.97	0.46
1:A:1:MET:HB3	1:A:2:PRO:HD3	1.97	0.46
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.97	0.46
1:A:777:ALA:O	1:A:781:MET:HG2	2.16	0.46
1:A:897:ILE:N	1:A:898:PRO:HD2	2.29	0.46
1:A:908:GLY:HA2	1:A:1014:ALA:HB2	1.97	0.46
1:A:57:VAL:HG12	1:A:88:VAL:HG22	1.97	0.46
1:C:213:GLN:HE22	1:C:238:THR:HG22	1.81	0.46
1:B:223:PRO:HD3	1:C:275:TYR:CD1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:705:GLU:HB3	1:A:847:LEU:HD22	1.98	0.45
1:C:888:LEU:HD21	1:C:943:ILE:HD11	1.98	0.45
1:C:463:THR:HG22	1:C:467:TYR:CZ	2.52	0.44
1:A:132:SER:HB3	1:A:173:GLY:HA3	1.99	0.44
1:B:219:LEU:HD23	1:C:754:TRP:CZ3	2.51	0.44
9:B:1101:FUA:H202	9:B:1101:FUA:C5	2.41	0.44
1:A:919:ARG:HD3	1:A:1005:THR:HG21	2.00	0.44
1:A:326:PRO:O	1:A:630:SER:HB2	2.17	0.44
1:B:677:ALA:O	1:B:678:THR:OG1	2.31	0.44
1:C:404:LEU:HD21	1:C:937:LEU:CD2	2.48	0.43
1:B:489:THR:OG1	1:B:490:PRO:HD3	2.18	0.43
1:A:754:TRP:CZ3	1:A:780:ARG:HA	2.54	0.43
1:B:754:TRP:CZ3	1:B:780:ARG:HA	2.54	0.42
1:C:165:ALA:HB3	1:C:313:MET:CE	2.49	0.42
1:A:356:TYR:HA	1:A:365:THR:HG21	2.01	0.42
1:A:38:ILE:HD12	1:A:462:SER:HB3	2.01	0.42
1:C:49:TYR:HB3	1:C:57:VAL:HG22	2.01	0.42
1:C:987:MET:HB3	1:C:988:PRO:HD3	2.01	0.42
1:A:167:SER:HB3	1:B:70:ASN:HB3	2.01	0.42
1:A:538:THR:O	1:A:542:LEU:HG	2.19	0.42
1:B:754:TRP:CH2	1:B:780:ARG:HA	2.54	0.42
1:B:705:GLU:HB3	1:B:847:LEU:HD22	2.02	0.42
1:A:901:VAL:O	1:A:904:VAL:HG22	2.20	0.42
1:C:454:VAL:HB	1:C:455:PRO:HD3	2.02	0.42
1:A:402:ILE:O	1:A:406:VAL:HG22	2.19	0.41
1:A:275:TYR:CD1	1:C:223:PRO:HD3	2.55	0.41
1:B:314:GLU:N	1:B:315:PRO:HD2	2.35	0.41
1:C:682:PHE:CZ	1:C:857:TYR:HB2	2.55	0.41
9:B:1101:FUA:H25	3:B:1102:LMT:H22	2.02	0.41
1:C:754:TRP:CH2	1:C:780:ARG:HA	2.55	0.41
1:A:542:LEU:HD21	1:A:1028:VAL:HG21	2.02	0.41
1:C:752:ALA:O	1:C:774:MET:HA	2.21	0.41
1:A:115:MET:N	1:A:116:PRO:HD2	2.34	0.41
1:A:909:VAL:HG22	1:A:931:LEU:HD11	2.01	0.41
1:A:213:GLN:HG3	1:B:56:THR:HG23	2.03	0.41
1:A:207:ILE:O	1:A:211:ASN:HB3	2.21	0.41
1:C:303:ALA:HB2	1:C:330:THR:HG21	2.03	0.41
1:B:367:ILE:HB	1:B:368:PRO:HD3	2.02	0.41
1:B:241:THR:HA	1:B:763:ILE:O	2.21	0.41
1:C:482:VAL:O	1:C:486:LEU:HG	2.21	0.40
1:A:535:LEU:HD22	1:A:1027:VAL:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:VAL:HG22	1:A:887:CYS:HB3	2.03	0.40
1:C:115:MET:N	1:C:116: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	1044/1057 (99%)	1014 (97%)	27 (3%)	3 (0%)	41 72
1	B	1033/1057 (98%)	1012 (98%)	21 (2%)	0	100 100
1	C	1034/1057 (98%)	1014 (98%)	20 (2%)	0	100 100
2	D	154/169 (91%)	152 (99%)	2 (1%)	0	100 100
2	E	152/169 (90%)	150 (99%)	2 (1%)	0	100 100
All	All	3417/3509 (97%)	3342 (98%)	72 (2%)	3 (0%)	51 81

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1034	SER
1	A	126	GLY
1	A	1037	ASN

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	851/862 (99%)	845 (99%)	6 (1%)	84 95
1	B	840/862 (97%)	832 (99%)	8 (1%)	76 93
1	C	841/862 (98%)	832 (99%)	9 (1%)	73 92
2	D	121/132 (92%)	121 (100%)	0	100 100
2	E	119/132 (90%)	118 (99%)	1 (1%)	81 94
All	All	2772/2850 (97%)	2748 (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	96	SER
1	A	536	ARG
1	A	701	GLN
1	A	717	ARG
1	B	11	PHE
1	B	49	TYR
1	B	108	GLN
1	B	556	PHE
1	B	601	LYS
1	B	610	PHE
1	B	801	PHE
1	B	1032	ARG
1	C	11	PHE
1	C	49	TYR
1	C	110	LYS
1	C	239	ARG
1	C	601	LYS
1	C	671	ILE
1	C	717	ARG
1	C	850	LYS
1	C	919	ARG
2	E	160	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	604	ASN
1	A	747	ASN

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Mol	Chain	Res	Type
1	A	1000	GLN
1	B	439	GLN
1	B	1000	GLN
1	C	124	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

60 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	D10	C	1104	-	9,9,9	0.11	0	8,8,8	0.07	0
4	D10	B	1106	-	9,9,9	0.11	0	8,8,8	0.05	0
5	DDQ	C	1106	-	10,13,13	2.24	1 (10%)	12,15,15	0.38	0
7	HEX	C	1115	-	5,5,5	0.15	0	4,4,4	0.10	0
6	GOL	D	201	-	5,5,5	0.11	0	5,5,5	0.29	0
5	DDQ	B	1108	-	10,13,13	2.29	1 (10%)	12,15,15	0.45	0
6	GOL	E	201	-	5,5,5	0.09	0	5,5,5	0.25	0
8	OCT	A	1114	-	7,7,7	0.13	0	6,6,6	0.07	0
10	D12	B	1120	-	11,11,11	0.30	0	10,10,10	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	DDQ	C	1107	-	10,13,13	2.29	1 (10%)	12,15,15	0.45	0
5	DDQ	A	1107	-	10,13,13	2.25	1 (10%)	12,15,15	0.50	0
5	DDQ	A	1109	-	10,13,13	2.32	1 (10%)	12,15,15	0.43	0
5	DDQ	B	1110	-	10,13,13	2.27	1 (10%)	12,15,15	0.55	0
6	GOL	A	1111	-	5,5,5	0.09	0	5,5,5	0.27	0
3	LMT	A	1104	-	36,36,36	0.49	0	47,47,47	0.65	0
13	SO4	C	1123	-	4,4,4	0.38	0	6,6,6	0.05	0
6	GOL	C	1109	-	5,5,5	0.10	0	5,5,5	0.31	0
4	D10	C	1105	-	9,9,9	0.11	0	8,8,8	0.11	0
4	D10	A	1105	-	9,9,9	0.09	0	8,8,8	0.08	0
6	GOL	B	1113	-	5,5,5	0.11	0	5,5,5	0.31	0
11	DDR	B	1121	-	27,27,27	1.24	2 (7%)	29,29,29	1.23	2 (6%)
12	PTY	C	1116	-	49,49,49	0.27	0	52,54,54	0.32	0
7	HEX	A	1112	-	5,5,5	0.14	0	4,4,4	0.08	0
4	D10	A	1106	-	9,9,9	0.11	0	8,8,8	0.06	0
3	LMT	C	1101	-	36,36,36	0.48	1 (2%)	47,47,47	0.70	0
5	DDQ	A	1108	-	10,13,13	2.27	1 (10%)	12,15,15	0.54	0
3	LMT	C	1102	-	36,36,36	0.63	1 (2%)	47,47,47	1.17	7 (14%)
8	OCT	A	1113	-	7,7,7	0.13	0	6,6,6	0.08	0
6	GOL	B	1111	-	5,5,5	0.09	0	5,5,5	0.24	0
4	D10	C	1103	-	9,9,9	0.11	0	8,8,8	0.06	0
6	GOL	C	1111	-	5,5,5	0.08	0	5,5,5	0.25	0
7	HEX	B	1116	-	5,5,5	0.15	0	4,4,4	0.09	0
10	D12	C	1122	-	11,11,11	0.27	0	10,10,10	0.46	0
8	OCT	B	1119	-	7,7,7	0.11	0	6,6,6	0.09	0
7	HEX	B	1117	-	5,5,5	0.15	0	4,4,4	0.11	0
3	LMT	B	1103	-	36,36,36	0.47	0	47,47,47	0.61	0
4	D10	B	1104	-	9,9,9	0.12	0	8,8,8	0.07	0
6	GOL	A	1110	-	5,5,5	0.11	0	5,5,5	0.29	0
6	GOL	C	1110	-	5,5,5	0.10	0	5,5,5	0.31	0
6	GOL	B	1112	-	5,5,5	0.09	0	5,5,5	0.27	0
5	DDQ	B	1109	-	10,13,13	2.28	1 (10%)	12,15,15	0.43	0
5	DDQ	B	1107	-	10,13,13	2.27	1 (10%)	12,15,15	0.39	0
12	PTY	C	1119	-	49,49,49	0.27	0	52,54,54	0.34	0
7	HEX	C	1112	-	5,5,5	0.14	0	4,4,4	0.08	0
3	LMT	B	1102	-	36,36,36	0.45	0	47,47,47	0.68	0
7	HEX	C	1114	-	5,5,5	0.15	0	4,4,4	0.10	0
9	FUA	B	1101	-	36,40,40	0.47	0	46,64,64	0.89	2 (4%)
12	PTY	C	1117	-	49,49,49	0.27	0	52,54,54	0.36	0
3	LMT	A	1103	-	36,36,36	0.55	0	47,47,47	1.06	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	D12	C	1120	-	11,11,11	0.31	0	10,10,10	0.39	0
4	D10	B	1105	-	9,9,9	0.12	0	8,8,8	0.08	0
7	HEX	C	1113	-	5,5,5	0.14	0	4,4,4	0.08	0
8	OCT	B	1118	-	7,7,7	0.11	0	6,6,6	0.05	0
7	HEX	B	1114	-	5,5,5	0.15	0	4,4,4	0.07	0
7	HEX	B	1115	-	5,5,5	0.15	0	4,4,4	0.10	0
6	GOL	C	1108	-	5,5,5	0.08	0	5,5,5	0.25	0
3	LMT	A	1101	-	36,36,36	0.47	0	47,47,47	0.58	0
12	PTY	C	1118	-	49,49,49	0.27	0	52,54,54	0.32	0
3	LMT	A	1102	-	36,36,36	0.52	1 (2%)	47,47,47	0.72	0
10	D12	C	1121	-	11,11,11	0.29	0	10,10,10	0.46	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	D10	C	1104	-	-	3/7/7/7	-
4	D10	B	1106	-	-	2/7/7/7	-
5	DDQ	C	1106	-	-	2/11/11/11	-
7	HEX	C	1115	-	-	0/3/3/3	-
6	GOL	D	201	-	-	4/4/4/4	-
5	DDQ	B	1108	-	-	3/11/11/11	-
6	GOL	E	201	-	-	0/4/4/4	-
8	OCT	A	1114	-	-	0/5/5/5	-
10	D12	B	1120	-	-	3/9/9/9	-
5	DDQ	C	1107	-	-	6/11/11/11	-
5	DDQ	A	1107	-	-	3/11/11/11	-
5	DDQ	A	1109	-	-	1/11/11/11	-
5	DDQ	B	1110	-	-	5/11/11/11	-
6	GOL	A	1111	-	-	1/4/4/4	-
3	LMT	A	1104	-	-	10/21/61/61	0/2/2/2
7	HEX	C	1114	-	-	0/3/3/3	-
6	GOL	C	1109	-	-	2/4/4/4	-
4	D10	C	1105	-	-	4/7/7/7	-
4	D10	A	1105	-	-	0/7/7/7	-
6	GOL	B	1113	-	-	2/4/4/4	-
11	DDR	B	1121	-	-	17/29/29/29	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	PTY	C	1116	-	-	31/53/53/53	-
7	HEX	A	1112	-	-	1/3/3/3	-
4	D10	A	1106	-	-	3/7/7/7	-
3	LMT	C	1101	-	-	10/21/61/61	0/2/2/2
5	DDQ	A	1108	-	-	1/11/11/11	-
3	LMT	C	1102	-	-	8/21/61/61	0/2/2/2
8	OCT	A	1113	-	-	0/5/5/5	-
6	GOL	B	1111	-	-	0/4/4/4	-
4	D10	C	1103	-	-	2/7/7/7	-
6	GOL	C	1111	-	-	0/4/4/4	-
7	HEX	B	1116	-	-	0/3/3/3	-
10	D12	C	1122	-	-	3/9/9/9	-
8	OCT	B	1119	-	-	4/5/5/5	-
7	HEX	B	1117	-	-	1/3/3/3	-
3	LMT	B	1103	-	-	5/21/61/61	0/2/2/2
4	D10	B	1104	-	-	1/7/7/7	-
6	GOL	A	1110	-	-	0/4/4/4	-
6	GOL	C	1110	-	-	2/4/4/4	-
6	GOL	B	1112	-	-	0/4/4/4	-
5	DDQ	B	1109	-	-	1/11/11/11	-
5	DDQ	B	1107	-	-	5/11/11/11	-
12	PTY	C	1119	-	-	19/53/53/53	-
7	HEX	C	1112	-	-	1/3/3/3	-
3	LMT	B	1102	-	-	6/21/61/61	0/2/2/2
9	FUA	B	1101	-	-	3/11/92/92	0/4/4/4
12	PTY	C	1117	-	-	24/53/53/53	-
3	LMT	A	1103	-	-	10/21/61/61	0/2/2/2
10	D12	C	1120	-	-	2/9/9/9	-
4	D10	B	1105	-	-	2/7/7/7	-
7	HEX	C	1113	-	-	0/3/3/3	-
8	OCT	B	1118	-	-	2/5/5/5	-
7	HEX	B	1114	-	-	0/3/3/3	-
7	HEX	B	1115	-	-	0/3/3/3	-
6	GOL	C	1108	-	-	1/4/4/4	-
3	LMT	A	1101	-	-	10/21/61/61	0/2/2/2
12	PTY	C	1118	-	-	29/53/53/53	-
3	LMT	A	1102	-	-	14/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	D12	C	1121	-	-	3/9/9/9	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1109	DDQ	O1-N1	-7.27	1.25	1.42
5	C	1107	DDQ	O1-N1	-7.20	1.25	1.42
5	B	1108	DDQ	O1-N1	-7.17	1.25	1.42
5	B	1109	DDQ	O1-N1	-7.14	1.25	1.42
5	A	1108	DDQ	O1-N1	-7.14	1.25	1.42
5	B	1110	DDQ	O1-N1	-7.13	1.25	1.42
5	B	1107	DDQ	O1-N1	-7.10	1.25	1.42
5	A	1107	DDQ	O1-N1	-7.08	1.25	1.42
5	C	1106	DDQ	O1-N1	-7.01	1.25	1.42
11	B	1121	DDR	O52-C21	4.32	1.46	1.34
11	B	1121	DDR	O51-C1	4.21	1.45	1.33
3	C	1102	LMT	O1'-C1'	2.37	1.44	1.40
3	A	1102	LMT	O1'-C1'	2.06	1.43	1.40
3	C	1101	LMT	O1'-C1'	2.01	1.43	1.40

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	B	1121	DDR	O52-C21-C22	4.33	120.84	111.50
3	A	1103	LMT	O1B-C4'-C3'	3.32	116.11	107.28
3	C	1102	LMT	C1B-O5B-C5B	3.19	119.95	113.69
3	C	1102	LMT	O5'-C1'-C2'	-2.78	104.47	110.35
3	C	1102	LMT	O5B-C1B-C2B	2.75	116.17	110.35
11	B	1121	DDR	O51-C1-C2	2.68	120.32	111.91
3	C	1102	LMT	C1B-C2B-C3B	2.57	115.34	110.00
3	A	1103	LMT	C1B-C2B-C3B	2.48	115.17	110.00
9	B	1101	FUA	C7-C8-C14	2.21	112.77	110.77
9	B	1101	FUA	O2-C16-C17	2.12	114.83	108.43
3	A	1103	LMT	C4B-C3B-C2B	2.11	114.50	110.82
3	C	1102	LMT	C3'-C4'-C5'	2.10	115.75	110.93
3	C	1102	LMT	O1'-C1'-C2'	2.10	111.58	108.30
3	C	1102	LMT	O5'-C5'-C4'	2.07	114.11	109.75
3	A	1103	LMT	C1B-O1B-C4'	2.03	122.99	117.96
3	A	1103	LMT	C1-O1'-C1'	2.02	117.19	113.84

There are no chirality outliers.

All (272) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	201	GOL	O1-C1-C2-O2
6	D	201	GOL	O1-C1-C2-C3
5	C	1107	DDQ	C2-C1-N1-CM2
5	A	1107	DDQ	N1-C1-C2-C3
6	C	1109	GOL	O1-C1-C2-C3
12	C	1116	PTY	C5-O14-P1-O12
3	C	1101	LMT	C2'-C1'-O1'-C1
3	C	1101	LMT	O5'-C1'-O1'-C1
3	C	1102	LMT	C2'-C1'-O1'-C1
3	C	1102	LMT	O5'-C1'-O1'-C1
6	C	1110	GOL	C1-C2-C3-O3
5	B	1107	DDQ	C2-C1-N1-CM2
12	C	1119	PTY	N1-C2-C3-O11
12	C	1119	PTY	C11-C8-O7-C6
12	C	1119	PTY	C3-O11-P1-O13
9	B	1101	FUA	O3-C31-O2-C16
12	C	1117	PTY	N1-C2-C3-O11
12	C	1117	PTY	C11-C8-O7-C6
12	C	1117	PTY	C3-O11-P1-O12
12	C	1117	PTY	C5-O14-P1-O11
12	C	1117	PTY	C5-O14-P1-O13
12	C	1118	PTY	C3-O11-P1-O12
12	C	1118	PTY	C3-O11-P1-O13
12	C	1118	PTY	C3-O11-P1-O14
12	C	1118	PTY	C5-O14-P1-O11
12	C	1118	PTY	C5-O14-P1-O12
12	C	1118	PTY	C5-O14-P1-O13
3	A	1102	LMT	C2'-C1'-O1'-C1
3	A	1102	LMT	O5'-C1'-O1'-C1
9	B	1101	FUA	C32-C31-O2-C16
3	A	1103	LMT	C3'-C4'-O1B-C1B
12	C	1119	PTY	O10-C8-O7-C6
12	C	1117	PTY	O10-C8-O7-C6
3	C	1102	LMT	O5'-C5'-C6'-O6'
12	C	1116	PTY	C25-C26-C27-C28
12	C	1116	PTY	C31-C30-O4-C1
12	C	1116	PTY	O30-C30-O4-C1
3	A	1104	LMT	O5B-C5B-C6B-O6B
3	C	1101	LMT	O5'-C5'-C6'-O6'
11	B	1121	DDR	C22-C21-O52-C52
3	A	1103	LMT	O5'-C5'-C6'-O6'
3	A	1103	LMT	C2B-C1B-O1B-C4'

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Mol	Chain	Res	Type	Atoms
3	B	1103	LMT	O5'-C5'-C6'-O6'
3	A	1101	LMT	O5B-C5B-C6B-O6B
3	A	1102	LMT	O5B-C5B-C6B-O6B
3	C	1102	LMT	C4'-C5'-C6'-O6'
12	C	1116	PTY	C6-C5-O14-P1
3	A	1102	LMT	C5'-C4'-O1B-C1B
3	A	1101	LMT	O5'-C5'-C6'-O6'
3	A	1104	LMT	C4B-C5B-C6B-O6B
3	C	1101	LMT	C4'-C5'-C6'-O6'
11	B	1121	DDR	O21-C21-O52-C52
3	A	1103	LMT	O5B-C1B-O1B-C4'
3	A	1102	LMT	O5'-C5'-C6'-O6'
3	A	1103	LMT	C4'-C5'-C6'-O6'
3	A	1102	LMT	C4B-C5B-C6B-O6B
12	C	1117	PTY	C8-C11-C12-C13
3	A	1101	LMT	C4'-C5'-C6'-O6'
3	B	1103	LMT	C4'-C5'-C6'-O6'
12	C	1118	PTY	C31-C30-O4-C1
3	B	1103	LMT	O5B-C5B-C6B-O6B
3	A	1102	LMT	C4'-C5'-C6'-O6'
12	C	1116	PTY	C3-O11-P1-O14
12	C	1119	PTY	C5-O14-P1-O11
12	C	1117	PTY	C3-O11-P1-O14
12	C	1119	PTY	C31-C30-O4-C1
12	C	1118	PTY	O10-C8-O7-C6
3	A	1102	LMT	O1'-C1-C2-C3
3	C	1102	LMT	C3-C4-C5-C6
12	C	1118	PTY	C11-C8-O7-C6
12	C	1116	PTY	C21-C22-C23-C24
12	C	1116	PTY	C34-C35-C36-C37
12	C	1116	PTY	C19-C20-C21-C22
12	C	1116	PTY	C23-C24-C25-C26
8	B	1119	OCT	C4-C5-C6-C7
3	A	1103	LMT	C3-C4-C5-C6
12	C	1118	PTY	C13-C14-C15-C16
12	C	1118	PTY	O30-C30-O4-C1
12	C	1119	PTY	O30-C30-O4-C1
7	A	1112	HEX	C2-C3-C4-C5
10	C	1122	D12	C2-C3-C4-C5
5	C	1106	DDQ	C4-C5-C6-C7
12	C	1116	PTY	C24-C25-C26-C27
6	D	201	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
6	A	1111	GOL	O1-C1-C2-C3
6	B	1113	GOL	O1-C1-C2-C3
5	B	1108	DDQ	C3-C4-C5-C6
12	C	1117	PTY	C32-C33-C34-C35
8	B	1118	OCT	C2-C3-C4-C5
3	A	1104	LMT	C3-C4-C5-C6
12	C	1116	PTY	C13-C14-C15-C16
11	B	1121	DDR	C22-C23-C24-C25
11	B	1121	DDR	C21-C22-C23-C24
3	A	1104	LMT	C11-C10-C9-C8
3	C	1101	LMT	C1-C2-C3-C4
12	C	1116	PTY	C35-C36-C37-C38
12	C	1119	PTY	O4-C1-C6-C5
12	C	1119	PTY	C14-C15-C16-C17
6	C	1109	GOL	O1-C1-C2-O2
6	B	1113	GOL	O1-C1-C2-O2
11	B	1121	DDR	C3-C4-C5-C6
12	C	1117	PTY	C18-C19-C20-C21
5	C	1107	DDQ	C1-C2-C3-C4
3	C	1102	LMT	C2-C3-C4-C5
4	C	1104	D10	C5-C6-C7-C8
12	C	1116	PTY	C16-C17-C18-C19
12	C	1118	PTY	C25-C26-C27-C28
11	B	1121	DDR	C4-C5-C6-C7
11	B	1121	DDR	C2-C1-O51-C51
12	C	1117	PTY	C31-C30-O4-C1
11	B	1121	DDR	C25-C26-C27-C28
5	A	1108	DDQ	C1-C2-C3-C4
10	C	1120	D12	C4-C5-C6-C7
12	C	1118	PTY	C31-C32-C33-C34
3	B	1103	LMT	C4-C5-C6-C7
3	A	1101	LMT	C11-C10-C9-C8
12	C	1118	PTY	C15-C16-C17-C18
4	C	1105	D10	C4-C5-C6-C7
3	A	1103	LMT	C6-C7-C8-C9
3	A	1101	LMT	O1'-C1-C2-C3
12	C	1118	PTY	C33-C34-C35-C36
3	B	1102	LMT	C7-C8-C9-C10
3	A	1101	LMT	C3-C4-C5-C6
12	C	1116	PTY	C5-O14-P1-O11
12	C	1116	PTY	C18-C19-C20-C21
12	C	1118	PTY	O14-C5-C6-C1

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Mol	Chain	Res	Type	Atoms
12	C	1117	PTY	C24-C25-C26-C27
12	C	1118	PTY	C23-C24-C25-C26
12	C	1116	PTY	C36-C37-C38-C39
10	C	1122	D12	C11-C10-C9-C8
3	A	1101	LMT	C2-C3-C4-C5
11	B	1121	DDR	O1-C1-O51-C51
5	B	1110	DDQ	C1-C2-C3-C4
10	C	1121	D12	C7-C8-C9-C10
10	B	1120	D12	C11-C10-C9-C8
12	C	1118	PTY	C22-C23-C24-C25
3	A	1103	LMT	O5B-C5B-C6B-O6B
3	A	1102	LMT	C1-C2-C3-C4
11	B	1121	DDR	C7-C8-C9-C10
12	C	1119	PTY	C26-C27-C28-C29
12	C	1116	PTY	C22-C23-C24-C25
3	C	1101	LMT	O5B-C5B-C6B-O6B
12	C	1117	PTY	O30-C30-O4-C1
5	B	1107	DDQ	C1-C2-C3-C4
11	B	1121	DDR	C2-C3-C4-C5
3	A	1101	LMT	C7-C8-C9-C10
6	C	1110	GOL	O2-C2-C3-O3
4	C	1105	D10	C6-C7-C8-C9
5	B	1109	DDQ	C2-C3-C4-C5
3	A	1101	LMT	C5-C6-C7-C8
4	A	1106	D10	C1-C2-C3-C4
5	C	1107	DDQ	C6-C7-C8-C9
3	A	1103	LMT	O1'-C1-C2-C3
3	A	1102	LMT	C3'-C4'-O1B-C1B
5	B	1108	DDQ	C2-C3-C4-C5
5	C	1106	DDQ	N1-C1-C2-C3
5	B	1110	DDQ	C6-C7-C8-C9
12	C	1116	PTY	C31-C32-C33-C34
10	B	1120	D12	C3-C4-C5-C6
5	B	1110	DDQ	C3-C4-C5-C6
3	C	1102	LMT	C2-C1-O1'-C1'
3	B	1102	LMT	C2-C1-O1'-C1'
4	C	1104	D10	C1-C2-C3-C4
12	C	1118	PTY	C19-C20-C21-C22
3	A	1104	LMT	C4-C5-C6-C7
11	B	1121	DDR	O51-C51-C52-C53
12	C	1116	PTY	O4-C1-C6-C5
12	C	1116	PTY	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
12	C	1116	PTY	C15-C16-C17-C18
5	A	1107	DDQ	C3-C4-C5-C6
3	A	1101	LMT	C4B-C5B-C6B-O6B
6	D	201	GOL	O2-C2-C3-O3
12	C	1118	PTY	O14-C5-C6-O7
10	C	1122	D12	C7-C8-C9-C10
12	C	1117	PTY	C22-C23-C24-C25
11	B	1121	DDR	O51-C51-C52-O52
12	C	1116	PTY	O4-C1-C6-O7
12	C	1117	PTY	C39-C40-C41-C42
3	A	1102	LMT	C5-C6-C7-C8
12	C	1116	PTY	C40-C41-C42-C43
12	C	1119	PTY	C6-C5-O14-P1
12	C	1117	PTY	C38-C39-C40-C41
12	C	1117	PTY	C40-C41-C42-C43
12	C	1116	PTY	C41-C42-C43-C44
12	C	1118	PTY	C41-C42-C43-C44
3	B	1103	LMT	C3-C4-C5-C6
4	C	1103	D10	C5-C6-C7-C8
3	A	1104	LMT	C5-C6-C7-C8
3	A	1104	LMT	C1-C2-C3-C4
5	C	1107	DDQ	C2-C1-N1-CM1
5	B	1107	DDQ	C2-C1-N1-CM1
12	C	1119	PTY	C36-C37-C38-C39
3	C	1101	LMT	C6-C7-C8-C9
11	B	1121	DDR	C24-C25-C26-C27
3	B	1102	LMT	C2-C3-C4-C5
12	C	1117	PTY	C11-C12-C13-C14
3	A	1104	LMT	O1'-C1-C2-C3
8	B	1119	OCT	C2-C3-C4-C5
12	C	1118	PTY	C39-C40-C41-C42
12	C	1119	PTY	C39-C40-C41-C42
12	C	1119	PTY	C31-C32-C33-C34
4	B	1106	D10	C1-C2-C3-C4
12	C	1118	PTY	C6-C5-O14-P1
12	C	1116	PTY	C3-O11-P1-O13
12	C	1116	PTY	C5-O14-P1-O13
12	C	1119	PTY	C5-O14-P1-O13
12	C	1117	PTY	O14-C5-C6-C1
3	C	1102	LMT	C7-C8-C9-C10
5	B	1107	DDQ	C2-C1-N1-O1
12	C	1117	PTY	O14-C5-C6-O7

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Mol	Chain	Res	Type	Atoms
3	A	1103	LMT	C2-C3-C4-C5
12	C	1118	PTY	C38-C39-C40-C41
12	C	1116	PTY	C39-C40-C41-C42
12	C	1119	PTY	O4-C1-C6-O7
3	A	1102	LMT	C9-C10-C11-C12
4	B	1104	D10	C6-C7-C8-C9
5	C	1107	DDQ	C4-C5-C6-C7
12	C	1117	PTY	C20-C21-C22-C23
12	C	1118	PTY	C14-C15-C16-C17
5	B	1110	DDQ	C5-C6-C7-C8
10	C	1120	D12	C3-C4-C5-C6
3	C	1101	LMT	C2-C3-C4-C5
12	C	1119	PTY	C23-C24-C25-C26
4	C	1105	D10	C5-C6-C7-C8
5	B	1107	DDQ	C5-C6-C7-C8
4	C	1105	D10	C3-C4-C5-C6
5	A	1107	DDQ	C5-C6-C7-C8
12	C	1118	PTY	C21-C22-C23-C24
12	C	1118	PTY	C18-C19-C20-C21
12	C	1119	PTY	C12-C11-C8-O7
3	B	1102	LMT	C11-C10-C9-C8
4	B	1106	D10	C3-C4-C5-C6
12	C	1117	PTY	C37-C38-C39-C40
4	B	1105	D10	C3-C4-C5-C6
4	A	1106	D10	C6-C7-C8-C9
11	B	1121	DDR	C5-C6-C7-C8
3	A	1102	LMT	C6-C7-C8-C9
10	C	1121	D12	C1-C2-C3-C4
12	C	1116	PTY	O10-C8-O7-C6
3	C	1101	LMT	C4-C5-C6-C7
4	B	1105	D10	C7-C8-C9-C10
8	B	1119	OCT	C5-C6-C7-C8
10	B	1120	D12	C4-C5-C6-C7
5	B	1108	DDQ	C4-C5-C6-C7
4	C	1103	D10	C2-C3-C4-C5
4	C	1104	D10	C4-C5-C6-C7
11	B	1121	DDR	O52-C21-C22-C23
7	B	1117	HEX	C3-C4-C5-C6
12	C	1118	PTY	C8-C11-C12-C13
4	A	1106	D10	C5-C6-C7-C8
3	B	1102	LMT	C5'-C4'-O1B-C1B
12	C	1119	PTY	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
12	C	1117	PTY	C21-C22-C23-C24
5	A	1109	DDQ	C7-C8-C9-C10
12	C	1116	PTY	C32-C33-C34-C35
5	C	1107	DDQ	C3-C4-C5-C6
3	B	1102	LMT	C3'-C4'-O1B-C1B
8	B	1118	OCT	C5-C6-C7-C8
3	A	1104	LMT	C9-C10-C11-C12
8	B	1119	OCT	C1-C2-C3-C4
12	C	1116	PTY	C11-C8-O7-C6
3	A	1104	LMT	C2-C3-C4-C5
11	B	1121	DDR	O21-C21-C22-C23
6	C	1108	GOL	O1-C1-C2-C3
10	C	1121	D12	C6-C7-C8-C9
7	C	1112	HEX	C2-C3-C4-C5
12	C	1117	PTY	C12-C13-C14-C15
5	B	1110	DDQ	C2-C1-N1-O1
3	C	1101	LMT	C9-C10-C11-C12
3	A	1102	LMT	C4-C5-C6-C7
9	B	1101	FUA	C17-C16-O2-C31
12	C	1118	PTY	O4-C30-C31-C32

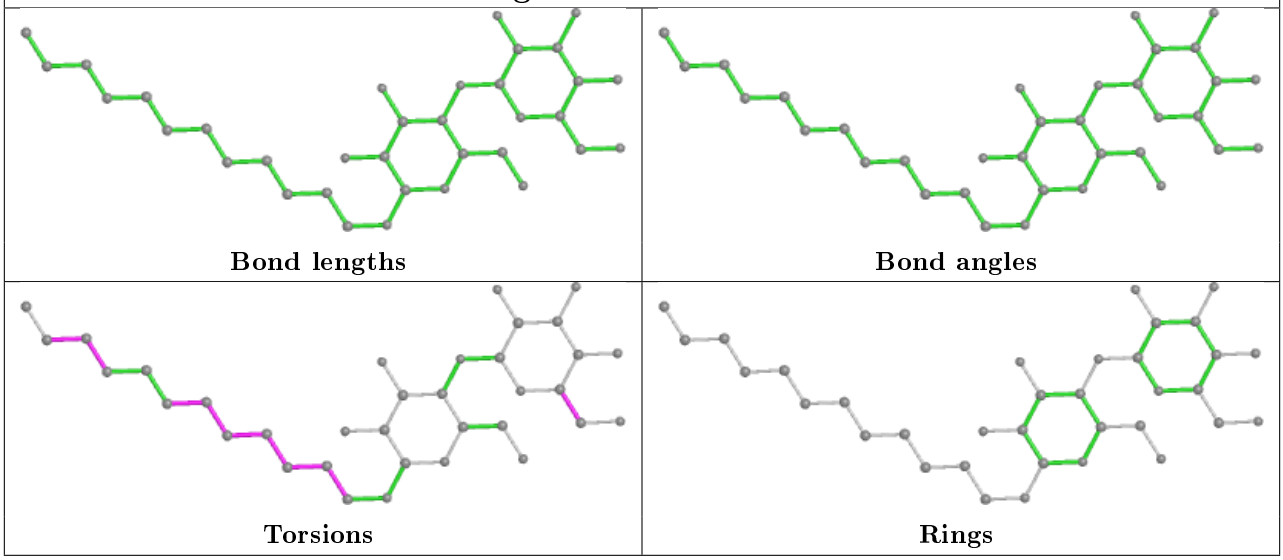
There are no ring outliers.

4 monomers are involved in 8 short contacts:

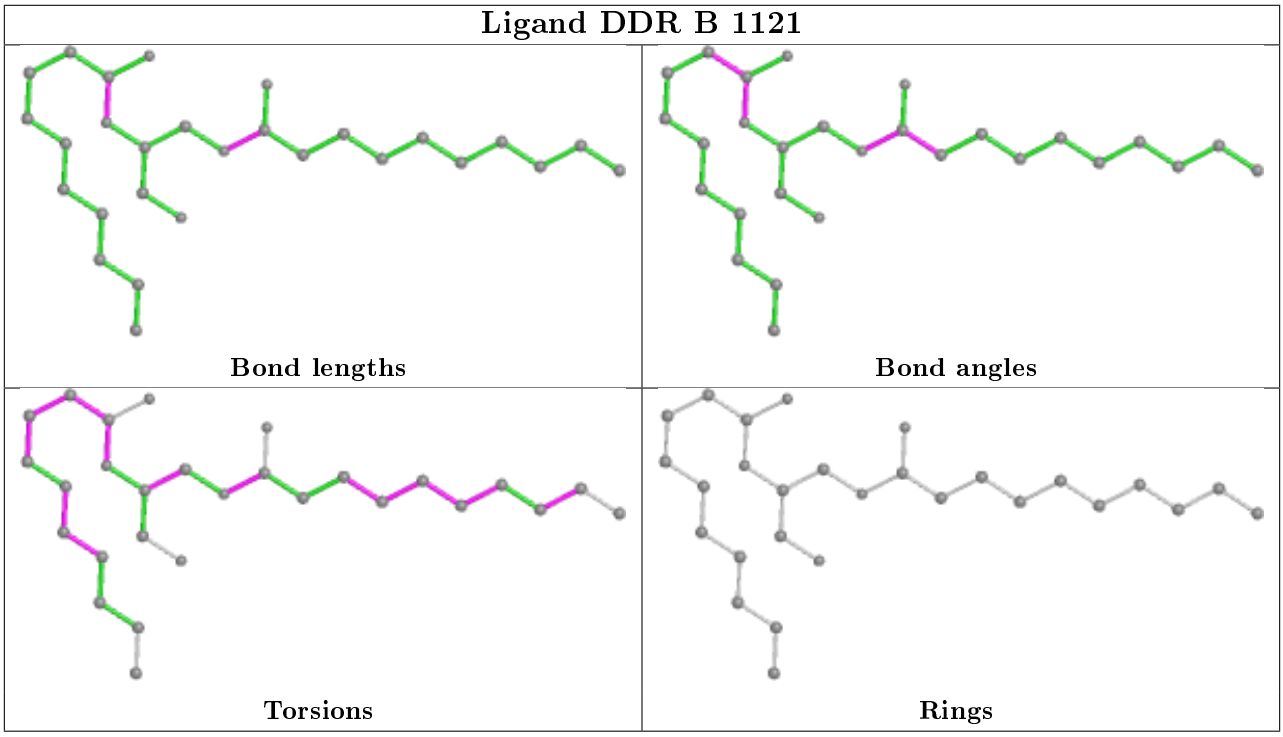
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	C	1116	PTY	2	0
8	B	1119	OCT	1	0
3	B	1102	LMT	1	0
9	B	1101	FUA	6	0

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.

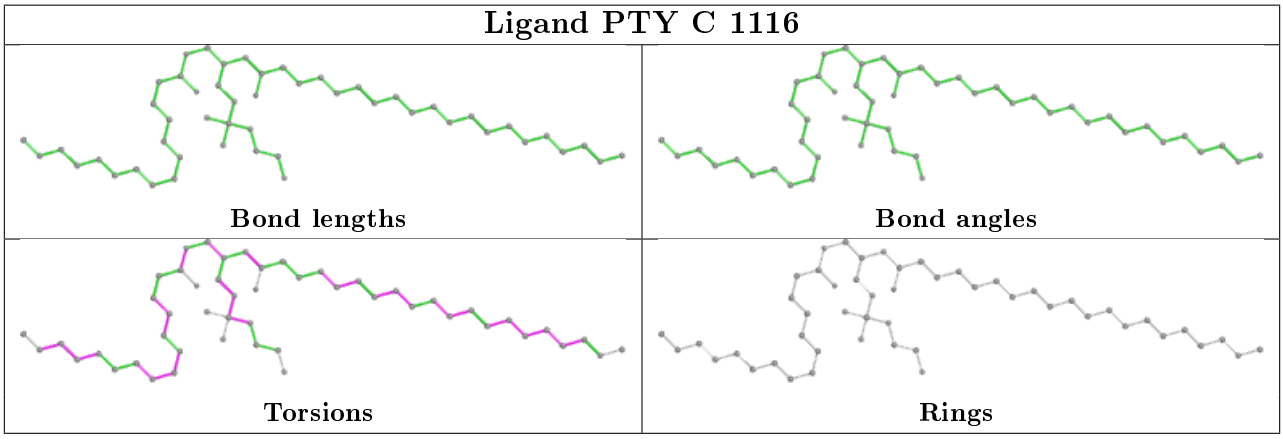
Ligand LMT A 1104



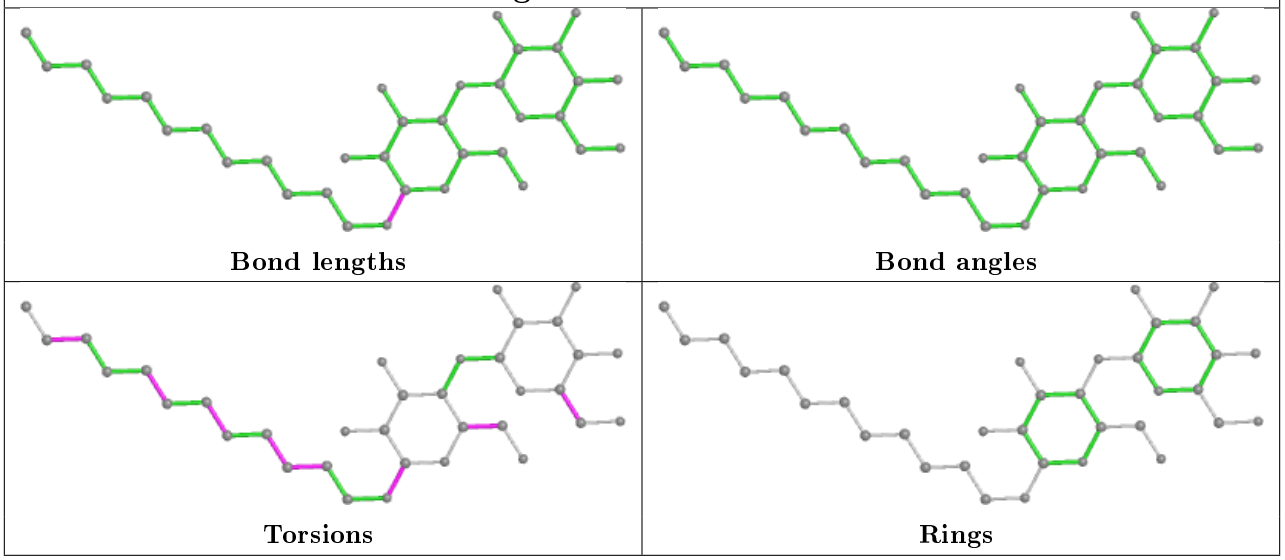
Ligand DDR B 1121



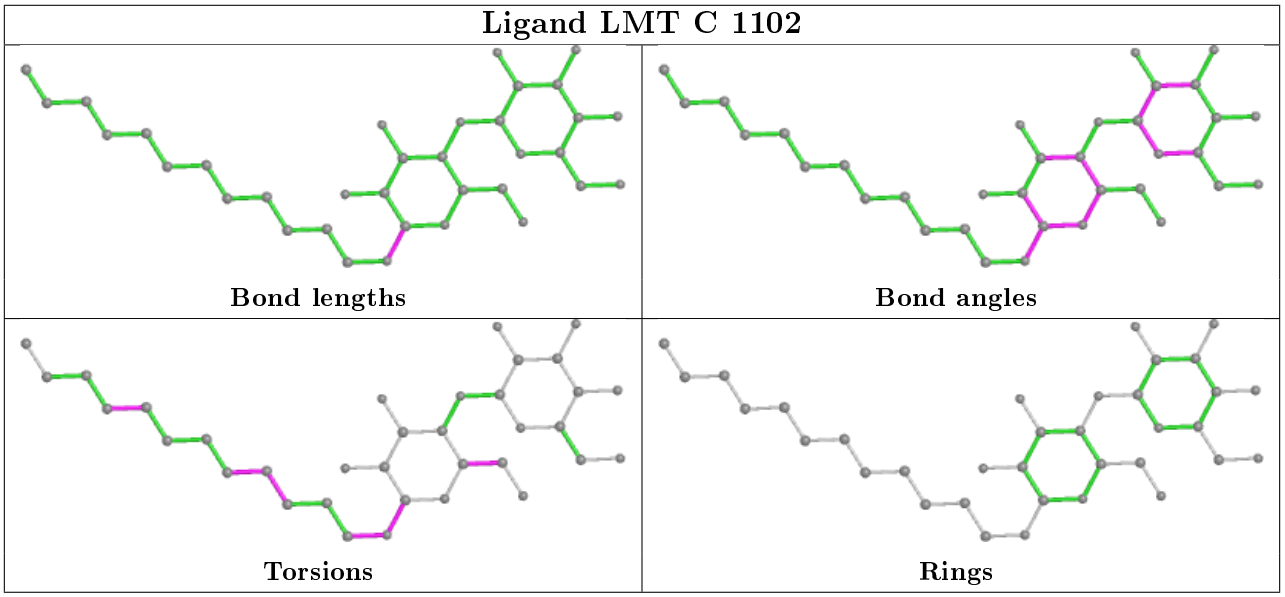
Ligand PTY C 1116



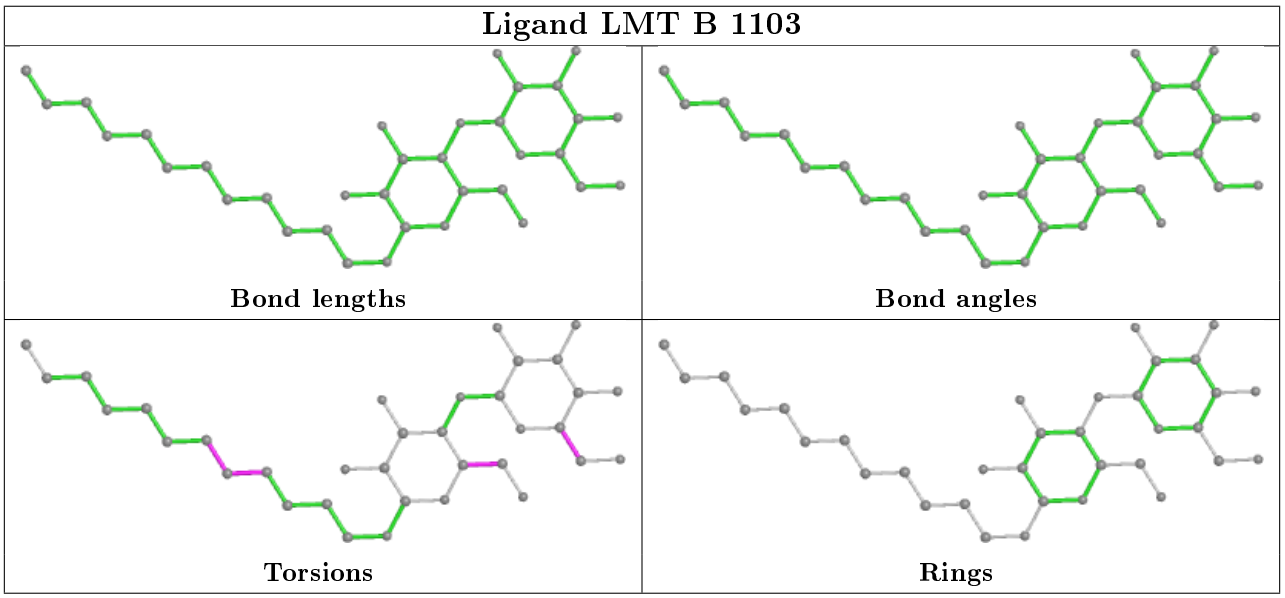
Ligand LMT C 1101



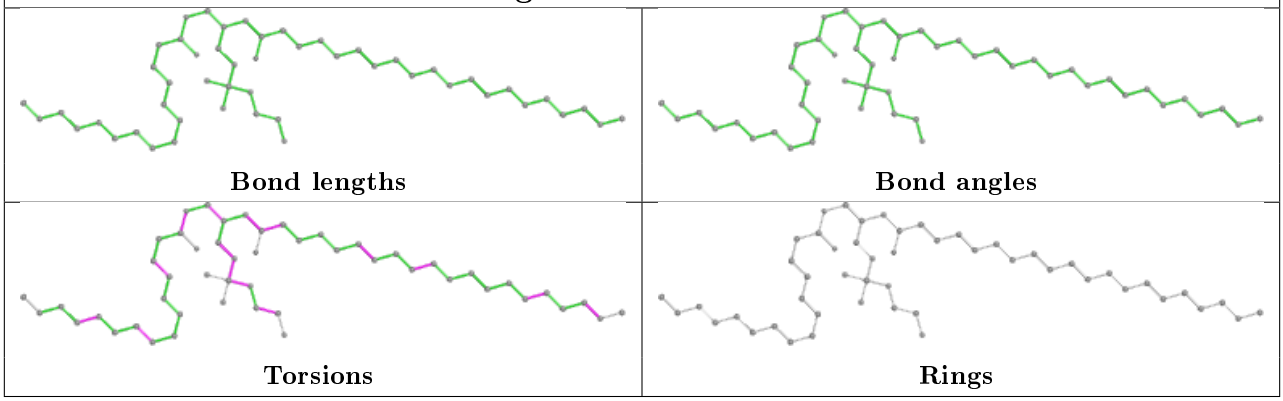
Ligand LMT C 1102



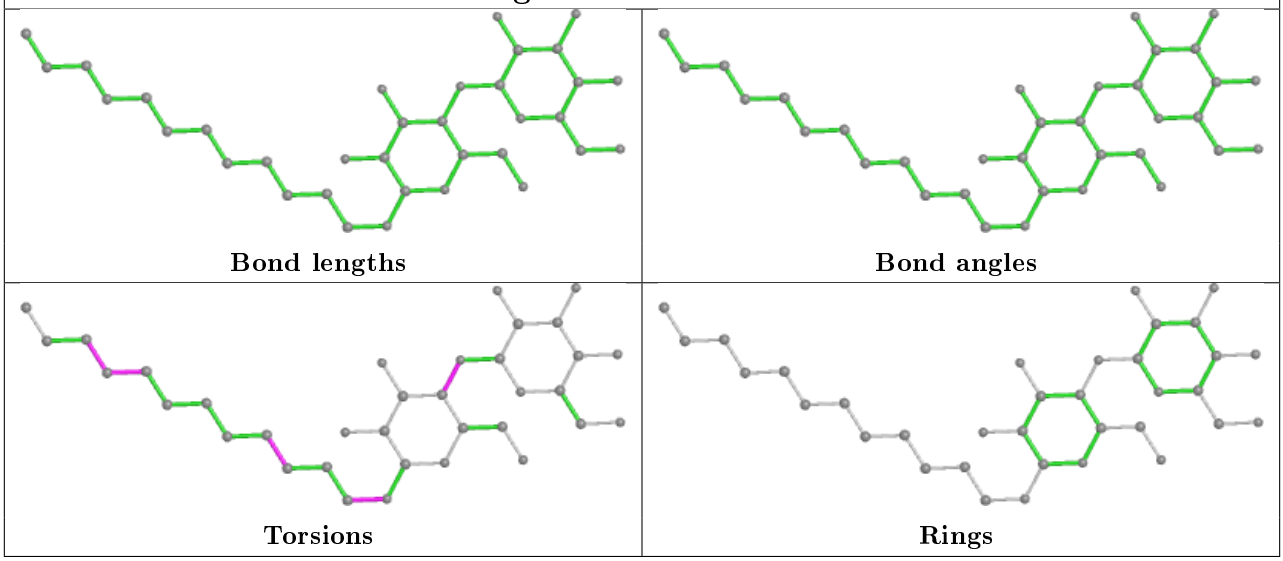
Ligand LMT B 1103



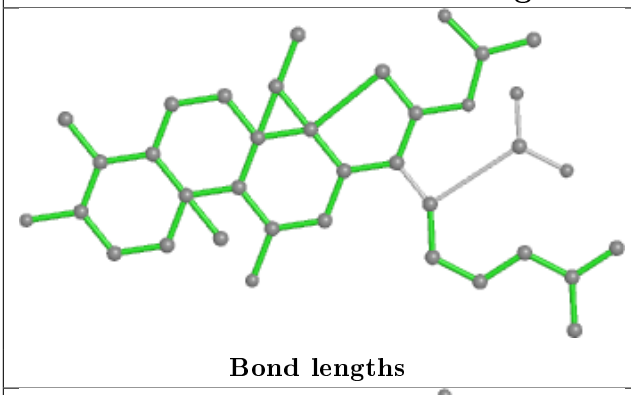
Ligand PTY C 1119



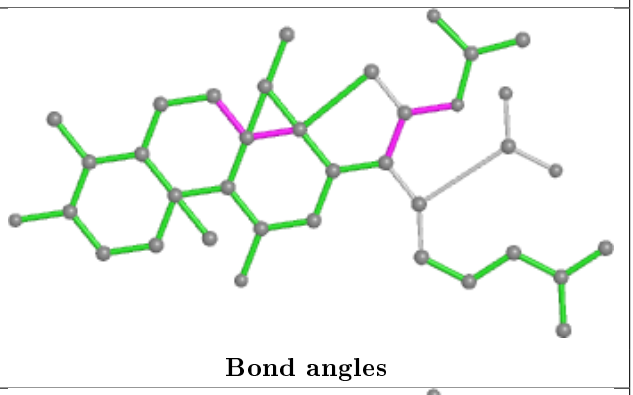
Ligand LMT B 1102



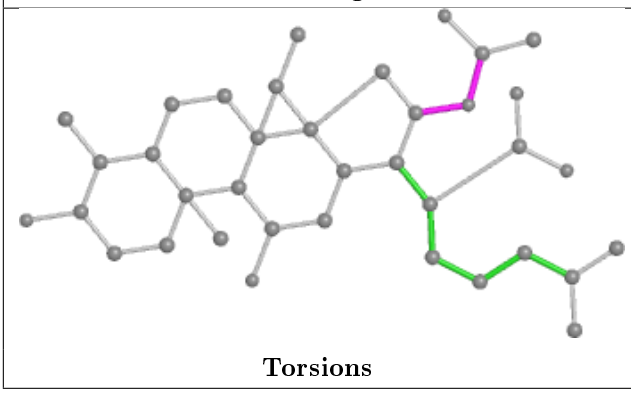
Ligand FUA B 1101



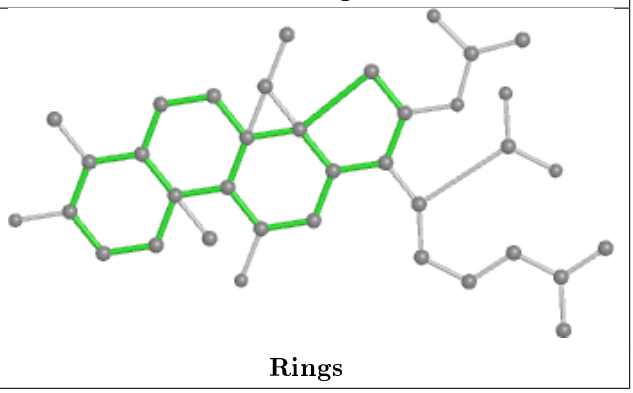
Bond lengths



Bond angles

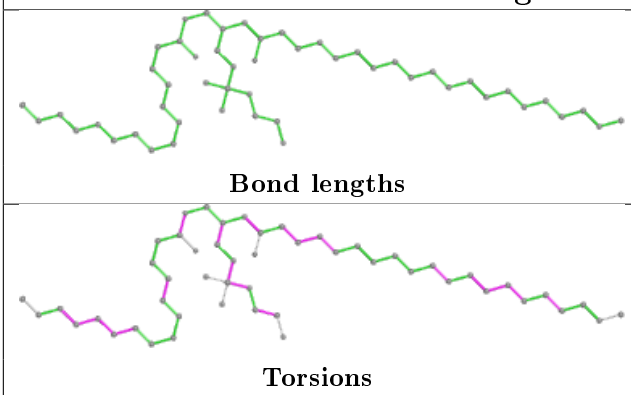


Torsions

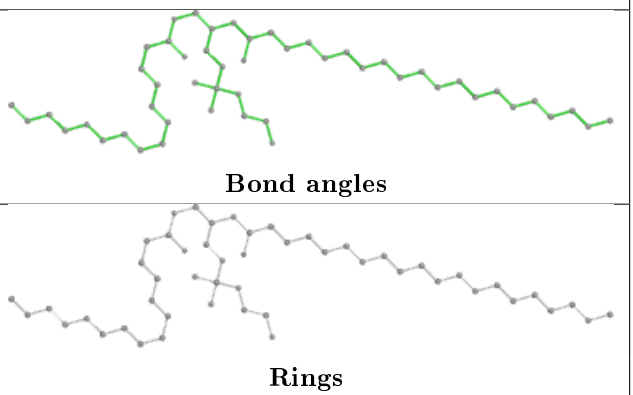


Rings

Ligand PTY C 1117



Bond lengths

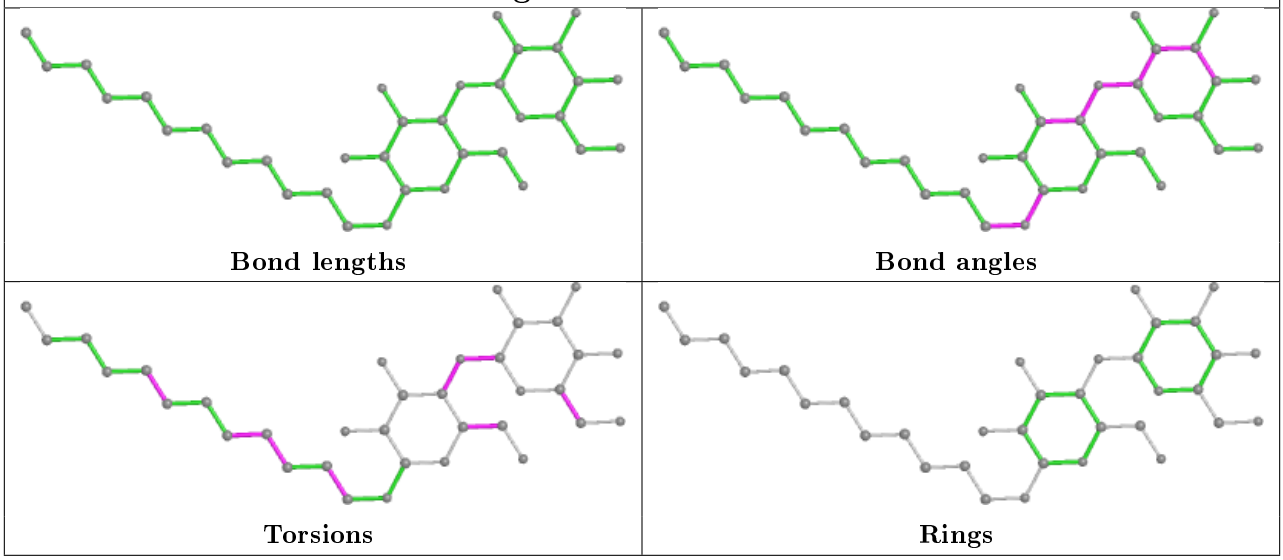


Bond angles

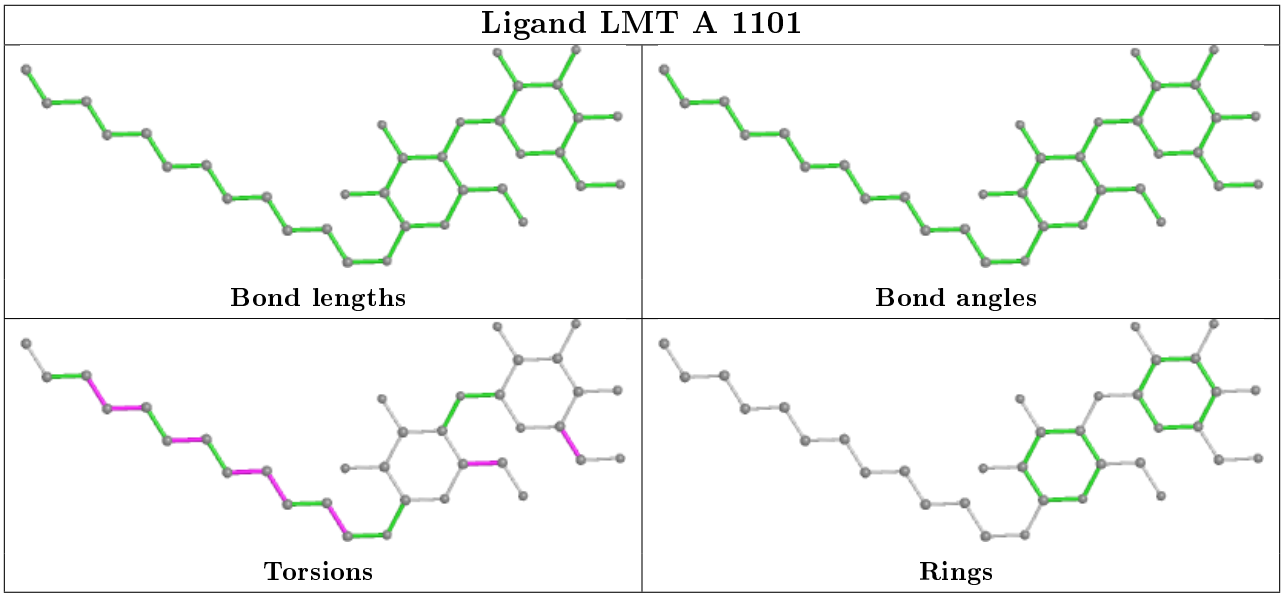
Torsions

Rings

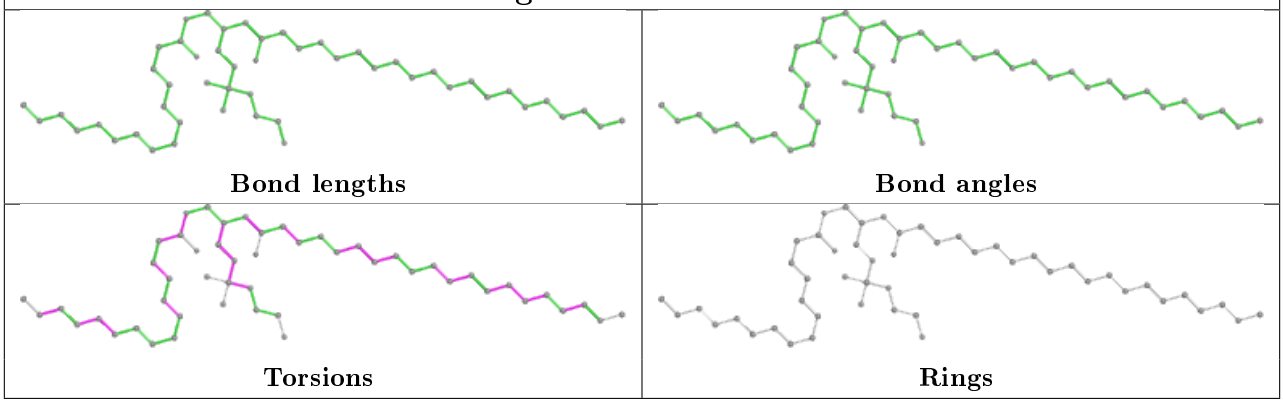
Ligand LMT A 1103



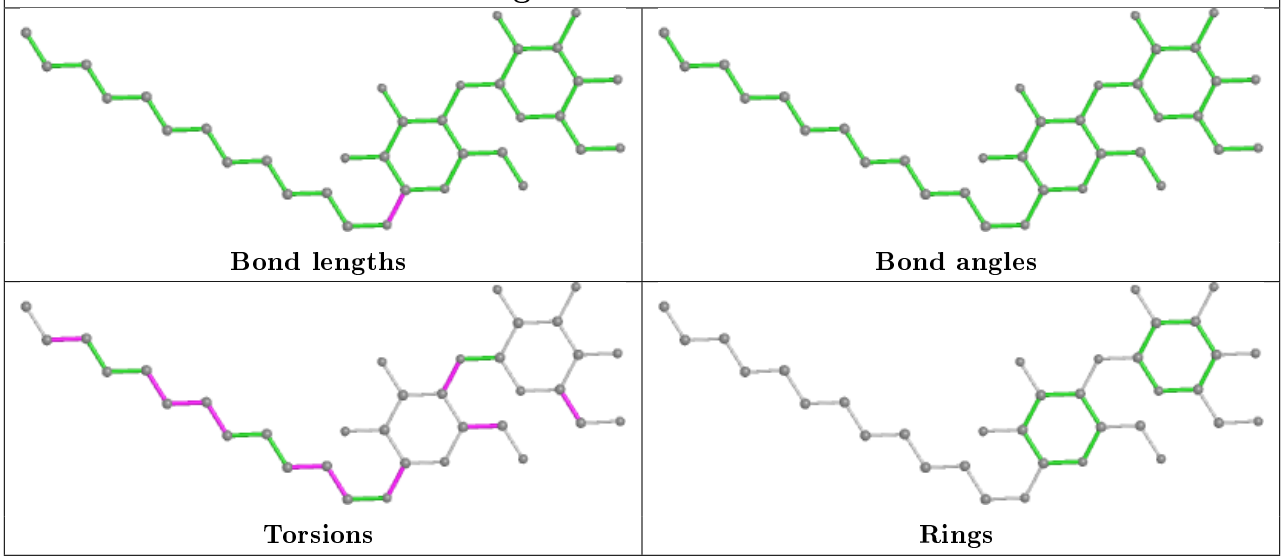
Ligand LMT A 1101



Ligand PTY C 1118



Ligand LMT A 1102



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1042/1057 (98%)	-0.05	34 (3%) 46 36	26, 50, 87, 138	0
1	B	1034/1057 (97%)	-0.15	22 (2%) 63 54	27, 47, 73, 92	0
1	C	1035/1057 (97%)	-0.16	15 (1%) 75 70	28, 42, 66, 100	0
2	D	156/169 (92%)	0.26	17 (10%) 5 3	39, 48, 80, 105	0
2	E	154/169 (91%)	0.78	21 (13%) 3 1	42, 63, 88, 98	0
All	All	3421/3509 (97%)	-0.06	109 (3%) 47 37	26, 47, 79, 138	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	871	ASN	4.9
1	A	874	PRO	4.6
1	A	676	THR	4.6
2	E	32	ILE	4.5
1	B	600	THR	4.3
2	E	31	ARG	4.1
1	B	604	ASN	4.0
2	D	165	LEU	3.9
2	E	33	LEU	3.9
1	A	846	GLN	3.8
1	A	510	LYS	3.8
1	B	678	THR	3.8
1	A	714	THR	3.7
1	B	601	LYS	3.7
1	C	1035	ARG	3.7
1	B	603	LYS	3.6
2	E	34	MET	3.6
2	E	35	ALA	3.6
1	B	597	TYR	3.5
1	A	834	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	868	LEU	3.5
1	A	712	MET	3.5
1	C	500	ILE	3.5
1	B	657	GLN	3.4
1	A	503	GLY	3.3
2	D	166	GLN	3.2
2	D	159	GLU	3.2
2	E	66	LEU	3.2
1	C	803	ALA	3.1
1	A	1040	ILE	3.1
2	D	150	PHE	3.1
1	C	497	LEU	3.1
1	C	361	ASN	3.0
2	D	161	LEU	3.0
1	A	512	PHE	3.0
1	A	515	TRP	3.0
1	C	730	ASP	3.0
1	A	866	GLU	2.8
1	A	513	PHE	2.8
1	B	606	VAL	2.8
1	A	673	GLU	2.8
2	E	27	ASP	2.8
1	C	510	LYS	2.8
1	B	1034	SER	2.8
2	D	162	ALA	2.8
2	E	36	ASN	2.7
2	E	29	GLU	2.7
1	B	498	LYS	2.7
2	D	134	LYS	2.7
2	D	167	LYS	2.7
2	D	149	ALA	2.7
2	D	153	SER	2.6
1	A	713	LEU	2.6
1	B	833	PRO	2.6
2	E	67	LEU	2.6
1	A	362	PHE	2.6
1	A	875	SER	2.6
1	A	653	ARG	2.6
2	E	69	ASN	2.5
1	A	558	ARG	2.5
1	A	918	PHE	2.5
1	A	707	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	508	GLY	2.5
1	B	655	PHE	2.5
1	A	1042	HIS	2.4
2	D	163	GLU	2.4
1	B	596	HIS	2.4
2	E	28	ASP	2.4
1	B	618	ALA	2.4
1	B	195	LYS	2.4
2	E	99	LEU	2.4
1	B	605	ASN	2.3
1	A	554	TYR	2.3
2	D	126	LEU	2.3
1	B	641	GLU	2.3
1	A	870	GLY	2.3
2	D	154	ILE	2.3
1	C	28	LEU	2.2
1	B	362	PHE	2.2
1	B	711	ASP	2.2
2	E	68	LYS	2.2
2	E	163	GLU	2.2
1	C	733	GLN	2.2
1	A	507	GLU	2.2
2	E	130	GLU	2.2
2	E	93	LEU	2.2
1	A	833	PRO	2.2
1	B	705	GLU	2.2
1	C	741	VAL	2.2
1	C	512	PHE	2.1
1	B	511	GLY	2.1
2	D	117	LEU	2.1
1	C	701	GLN	2.1
2	E	62	ILE	2.1
2	D	133	LEU	2.1
2	D	12	SER	2.1
2	D	139	VAL	2.1
1	A	843	LEU	2.1
1	C	850	LYS	2.1
2	E	37	GLY	2.1
1	A	678	THR	2.1
1	A	505	HIS	2.1
1	C	513	PHE	2.1
1	A	511	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	70	GLY	2.0
1	C	797	GLN	2.0
1	B	653	ARG	2.0
1	A	859	TRP	2.0
2	E	98	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	PTY	C	1119	50/50	0.59	0.51	99,115,144,151	0
5	DDQ	A	1108	14/14	0.62	0.32	104,113,120,121	0
3	LMT	A	1103	35/35	0.62	0.41	78,110,135,135	0
4	D10	C	1105	10/10	0.67	0.32	76,80,83,83	0
12	PTY	C	1118	50/50	0.67	0.37	88,112,129,132	0
3	LMT	A	1101	35/35	0.68	0.46	80,107,125,126	0
5	DDQ	A	1109	14/14	0.68	0.55	97,100,100,100	0
12	PTY	C	1117	50/50	0.70	0.32	73,84,97,102	0
5	DDQ	B	1110	14/14	0.71	0.37	99,103,114,114	0
3	LMT	C	1102	35/35	0.72	0.39	74,91,104,106	0
12	PTY	C	1116	50/50	0.74	0.30	65,95,115,125	0
7	HEX	C	1114	6/6	0.74	0.42	69,72,73,73	0
5	DDQ	A	1107	14/14	0.76	0.52	92,102,112,112	0
10	D12	C	1120	12/12	0.76	0.23	62,69,74,74	0
7	HEX	C	1112	6/6	0.77	0.29	72,73,74,74	0
7	HEX	B	1115	6/6	0.77	0.31	63,65,66,66	0
7	HEX	B	1117	6/6	0.78	0.43	69,69,70,70	0
7	HEX	B	1116	6/6	0.80	0.30	63,64,65,65	0

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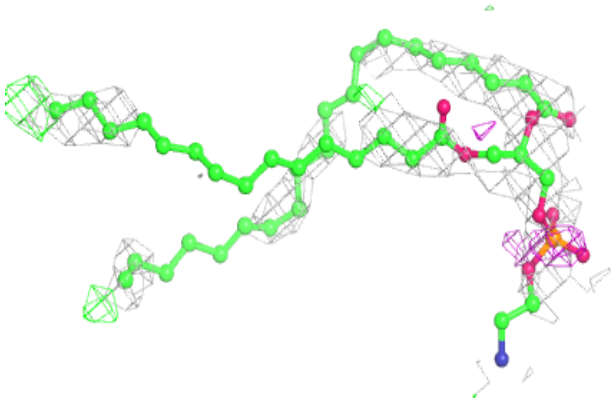
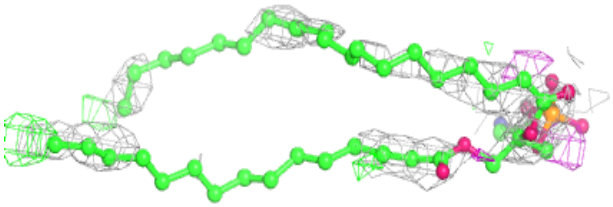
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	OCT	B	1118	8/8	0.81	0.48	69,71,72,72	0
4	D10	A	1105	10/10	0.81	0.43	71,74,74,75	0
10	D12	C	1122	12/12	0.81	0.39	78,79,81,81	0
8	OCT	B	1119	8/8	0.81	0.34	83,85,86,86	0
8	OCT	A	1113	8/8	0.82	0.30	73,75,76,76	0
5	DDQ	B	1108	14/14	0.82	0.37	82,87,92,93	0
6	GOL	B	1113	6/6	0.82	0.33	69,70,71,72	0
6	GOL	D	201	6/6	0.82	0.44	63,65,66,68	0
5	DDQ	B	1109	14/14	0.83	0.28	78,90,102,105	0
5	DDQ	B	1107	14/14	0.83	0.25	70,76,92,93	0
6	GOL	C	1111	6/6	0.83	0.26	71,73,74,74	0
3	LMT	A	1102	35/35	0.83	0.23	64,81,98,99	0
4	D10	A	1106	10/10	0.84	0.32	61,63,64,64	0
6	GOL	B	1111	6/6	0.84	0.31	61,63,64,65	0
10	D12	C	1121	12/12	0.84	0.27	58,67,69,69	0
5	DDQ	C	1106	14/14	0.85	0.36	76,78,81,82	0
8	OCT	A	1114	8/8	0.85	0.31	65,66,67,67	0
7	HEX	B	1114	6/6	0.85	0.26	67,67,68,68	0
10	D12	B	1120	12/12	0.85	0.35	69,70,70,71	0
11	DDR	B	1121	28/28	0.86	0.34	75,88,99,101	0
4	D10	C	1103	10/10	0.88	0.32	68,69,69,70	0
7	HEX	C	1115	6/6	0.88	0.29	57,58,59,59	0
3	LMT	A	1104	35/35	0.88	0.35	79,91,102,103	0
7	HEX	C	1113	6/6	0.89	0.32	74,75,75,75	0
6	GOL	C	1109	6/6	0.89	0.20	58,60,62,62	0
7	HEX	A	1112	6/6	0.89	0.21	79,80,81,82	0
4	D10	B	1105	10/10	0.90	0.36	63,65,68,68	0
6	GOL	A	1110	6/6	0.90	0.29	63,63,64,64	0
4	D10	C	1104	10/10	0.90	0.29	57,61,63,63	0
6	GOL	A	1111	6/6	0.90	0.18	72,73,73,74	0
6	GOL	E	201	6/6	0.90	0.19	61,62,63,64	0
5	DDQ	C	1107	14/14	0.91	0.24	82,86,90,91	0
6	GOL	C	1110	6/6	0.91	0.25	65,67,67,68	0
6	GOL	B	1112	6/6	0.91	0.21	52,54,56,59	0
3	LMT	B	1103	35/35	0.91	0.30	61,68,89,90	0
4	D10	B	1104	10/10	0.91	0.29	60,62,62,63	0
3	LMT	B	1102	35/35	0.92	0.21	64,67,69,71	0
9	FUA	B	1101	37/37	0.93	0.22	64,66,71,72	0
4	D10	B	1106	10/10	0.93	0.18	56,56,57,57	0
3	LMT	C	1101	35/35	0.94	0.25	52,60,76,76	0
13	SO4	C	1123	5/5	0.95	0.13	67,67,67,68	0
6	GOL	C	1108	6/6	0.96	0.14	37,39,39,40	0

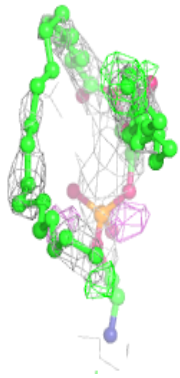
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PTY C 1119:

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

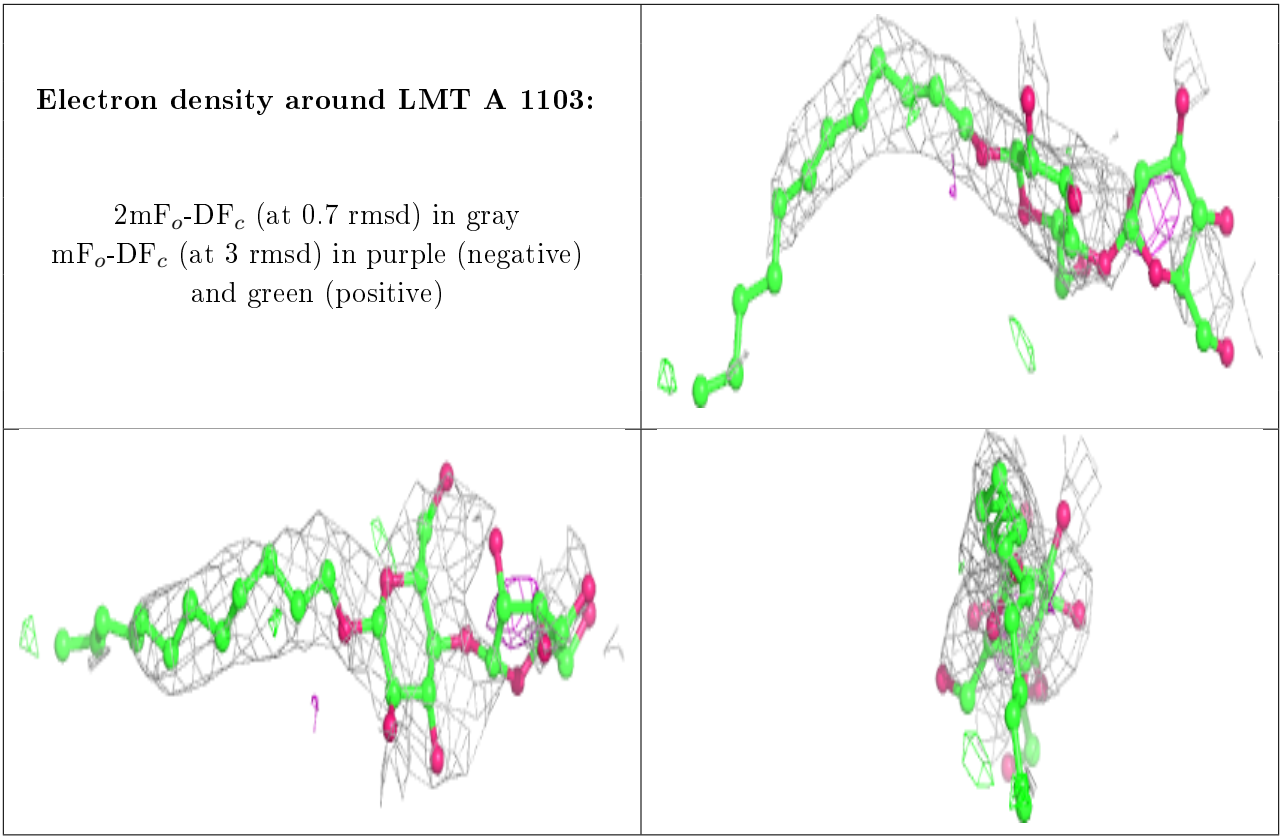






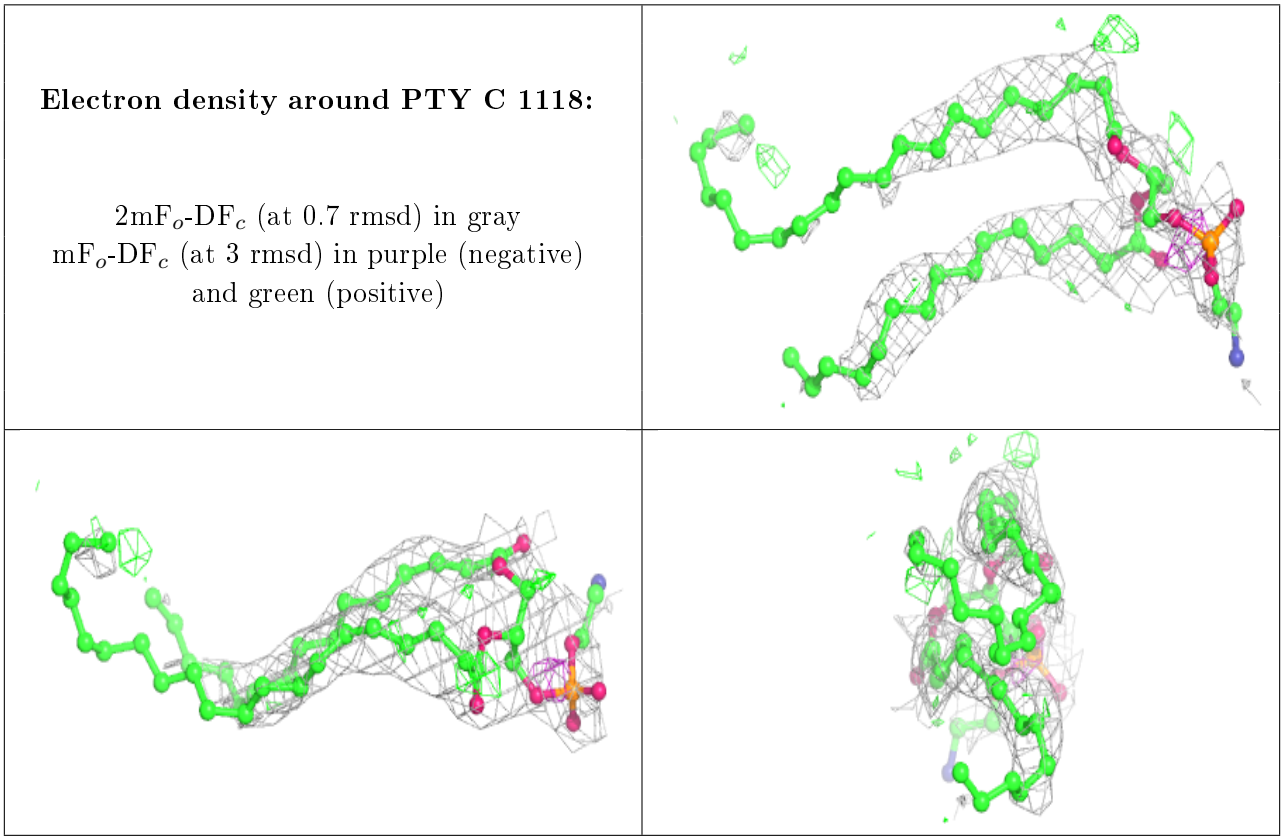
Electron density around LMT A 1103:

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



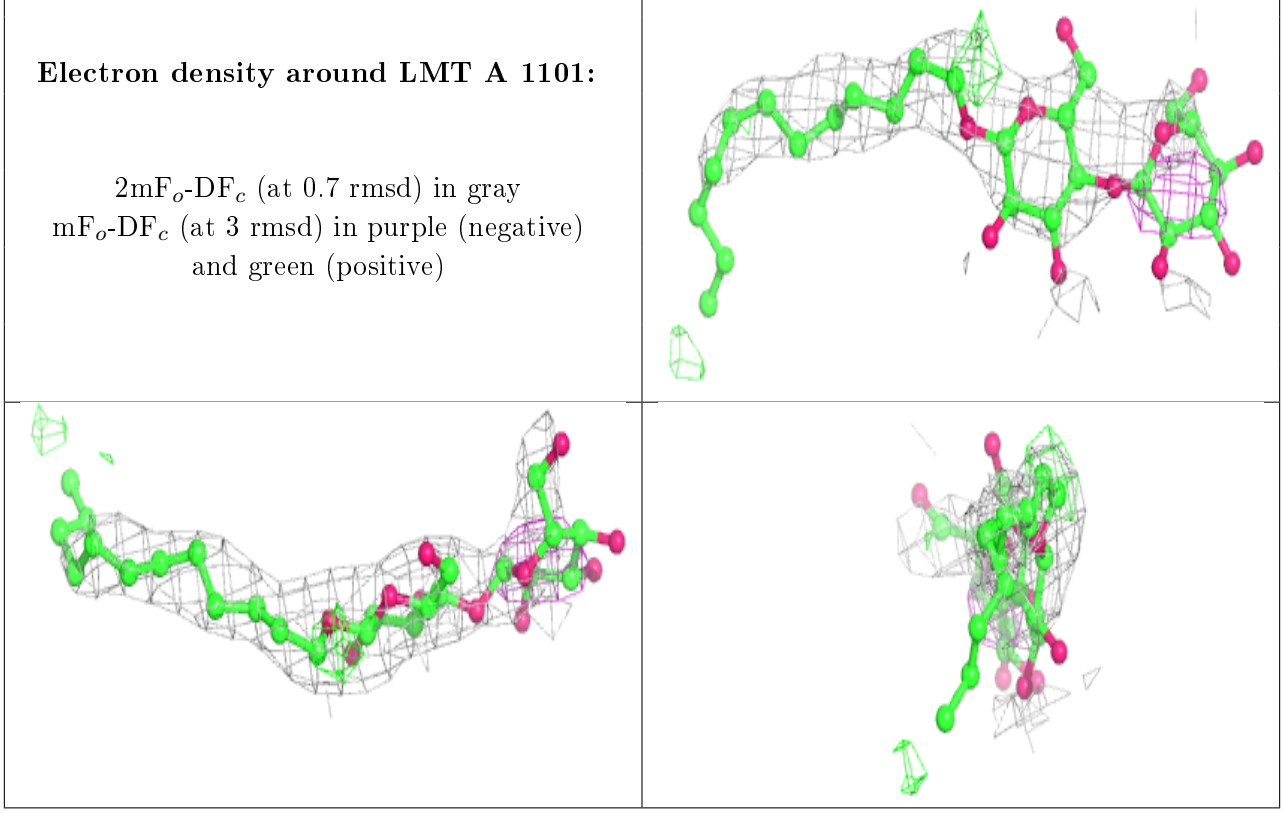
Electron density around PTY C 1118:

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



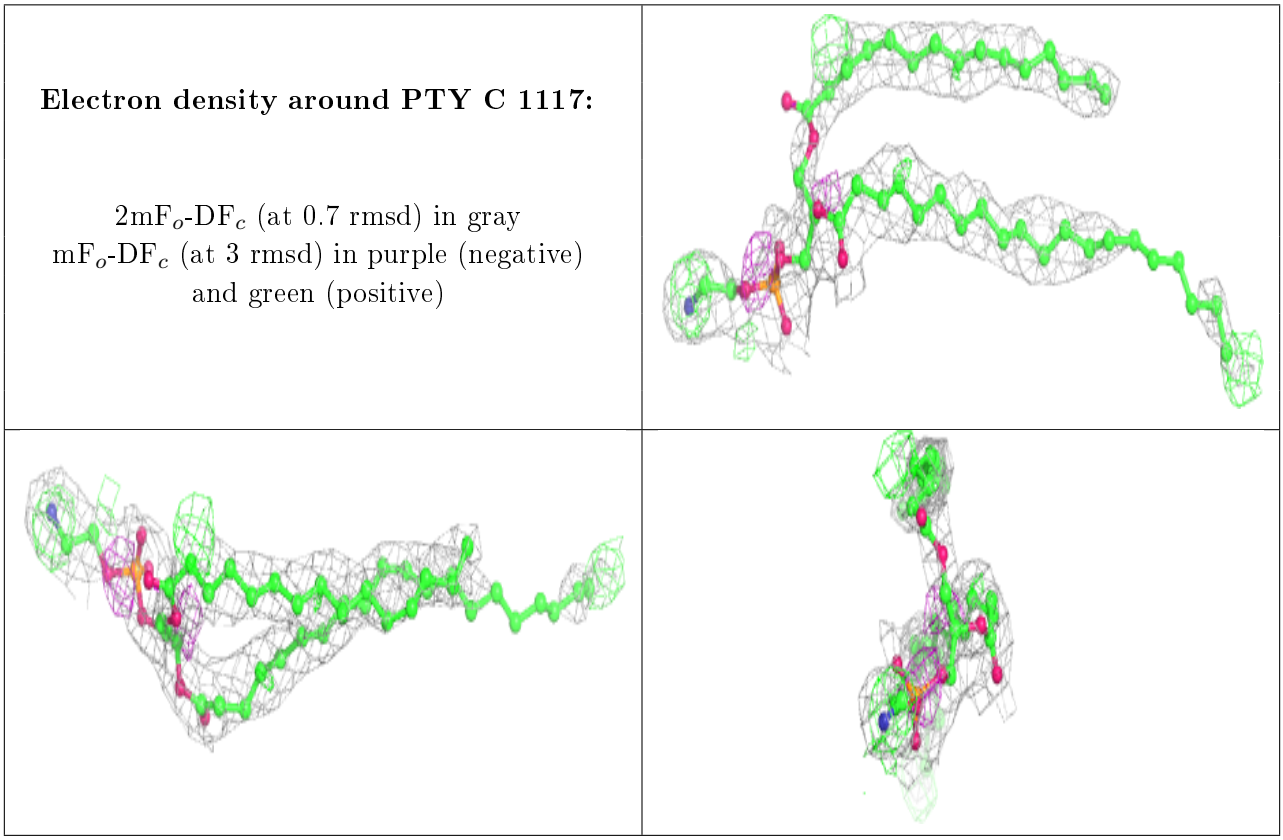
Electron density around LMT A 1101:

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



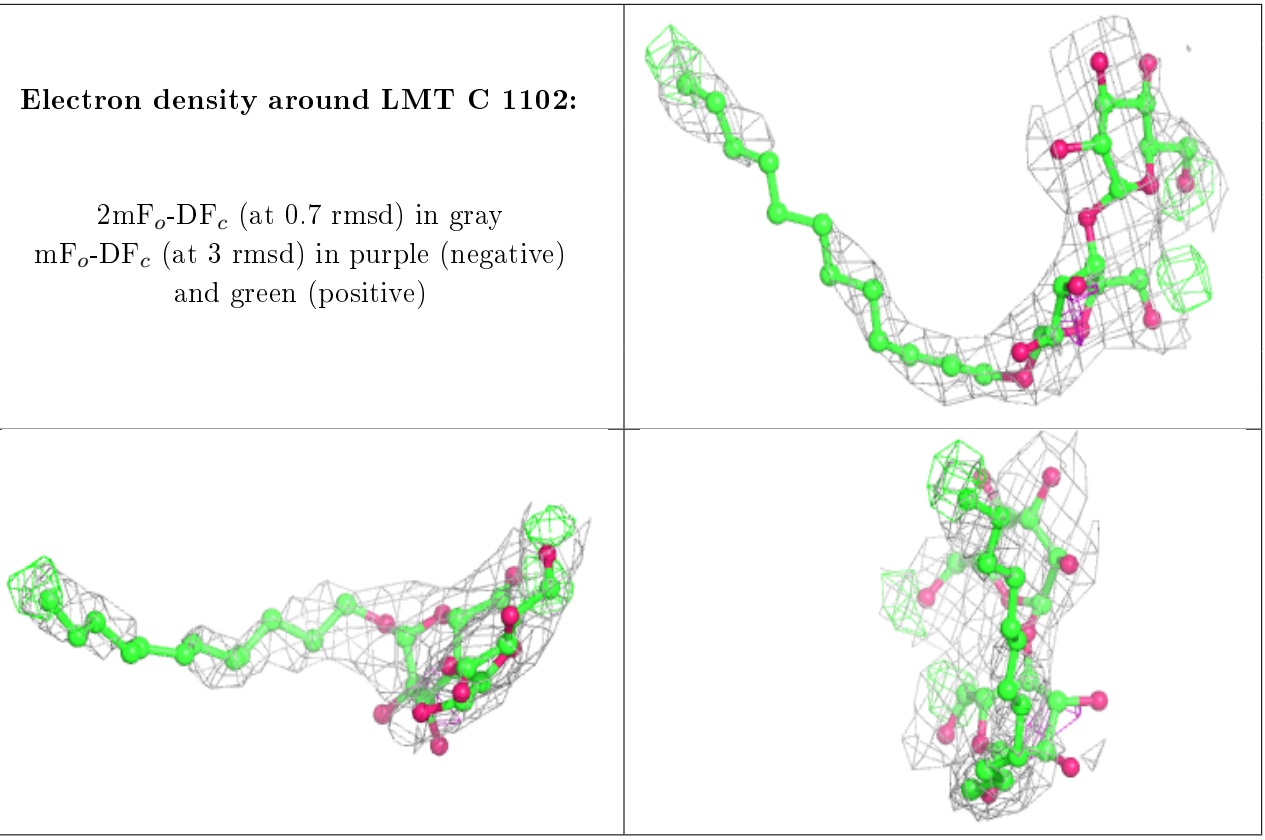
Electron density around PTY C 1117:

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



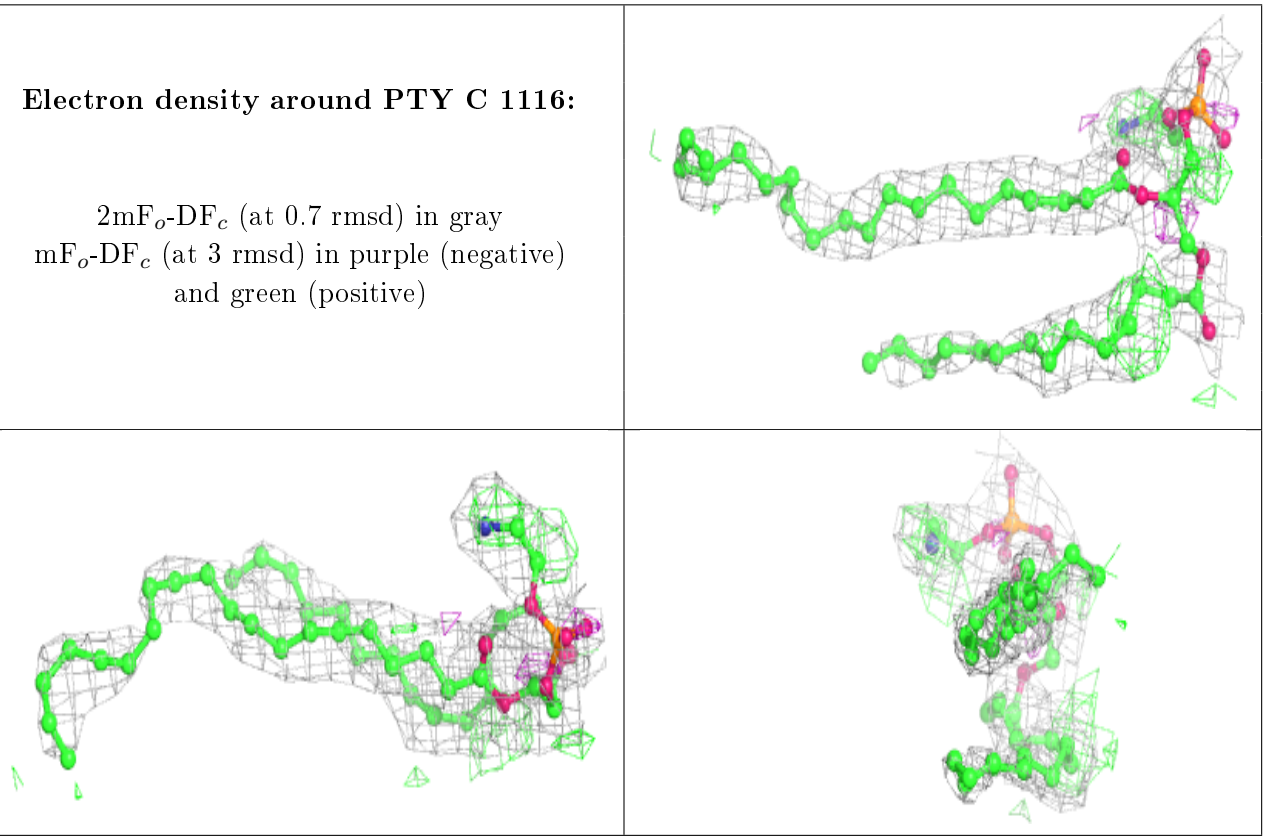
Electron density around LMT C 1102:

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



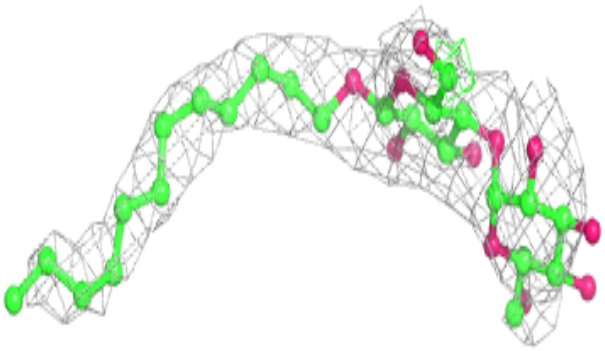
Electron density around PTY C 1116:

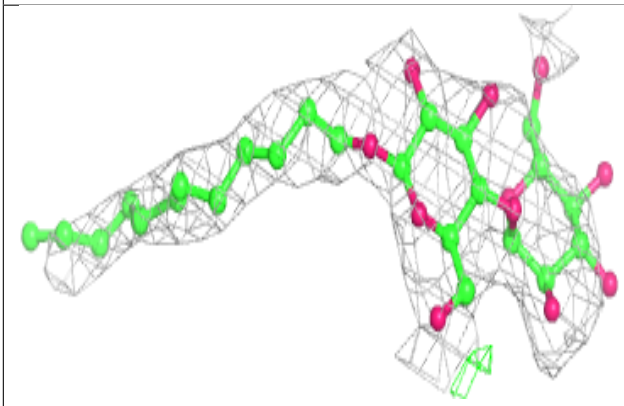
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

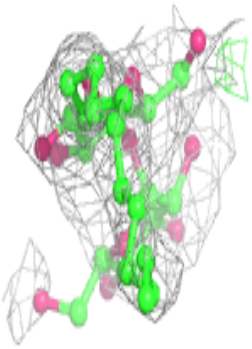


Electron density around LMT A 1102:

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

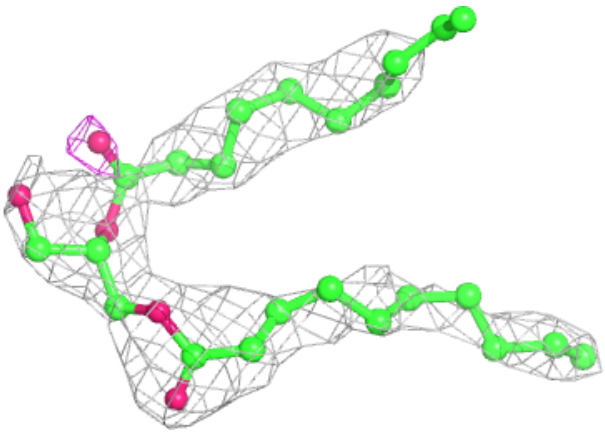


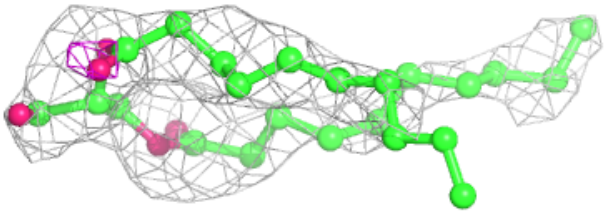


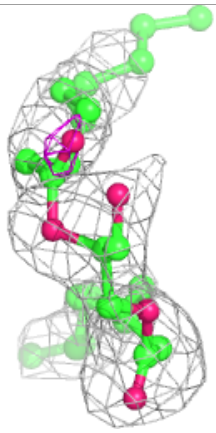


Electron density around DDR B 1121:

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

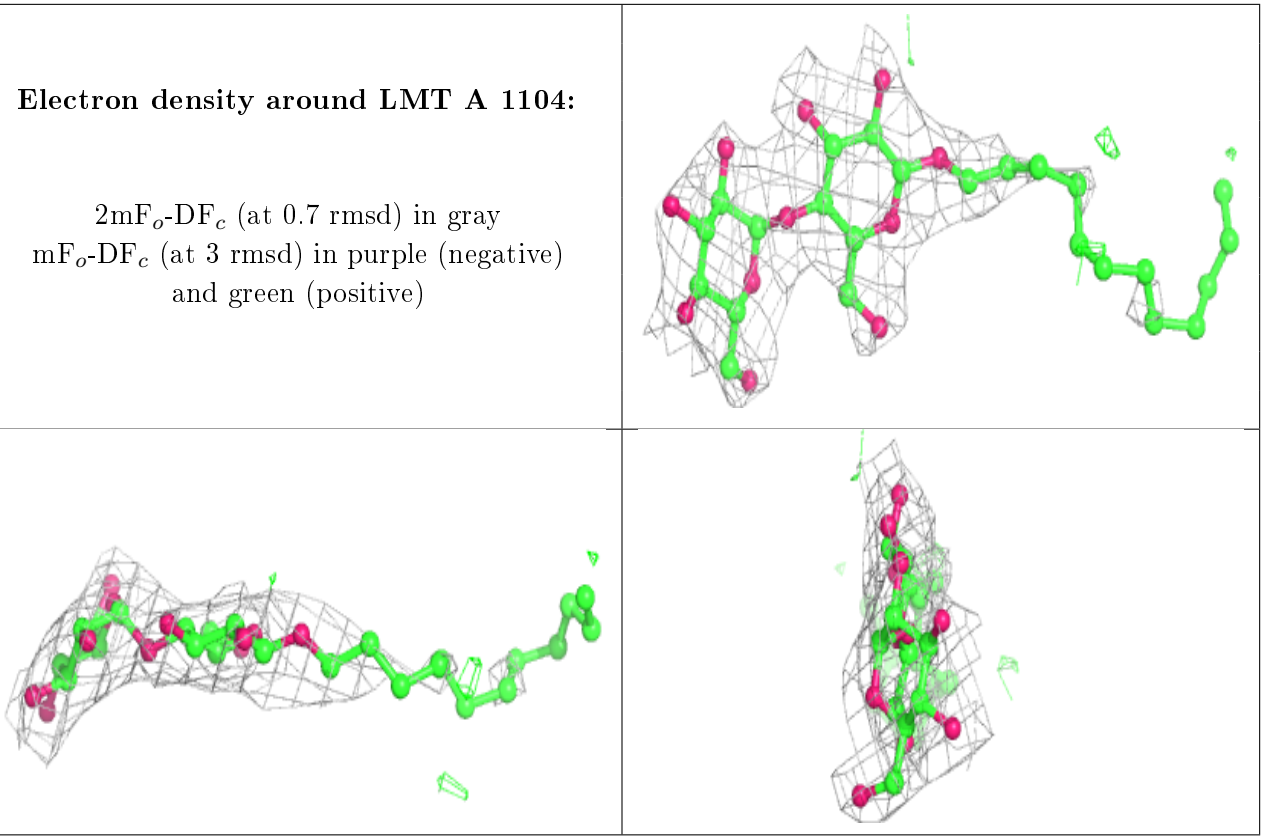






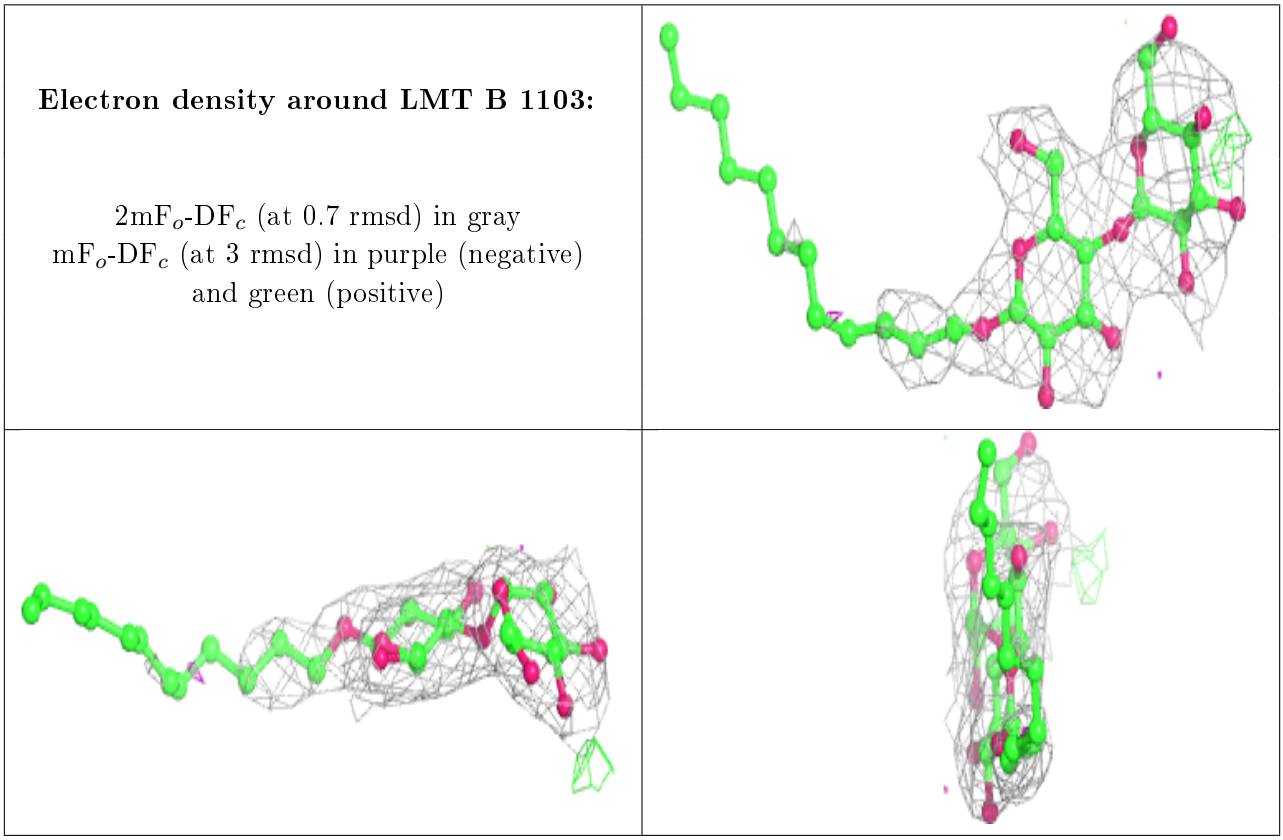
Electron density around LMT A 1104:

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



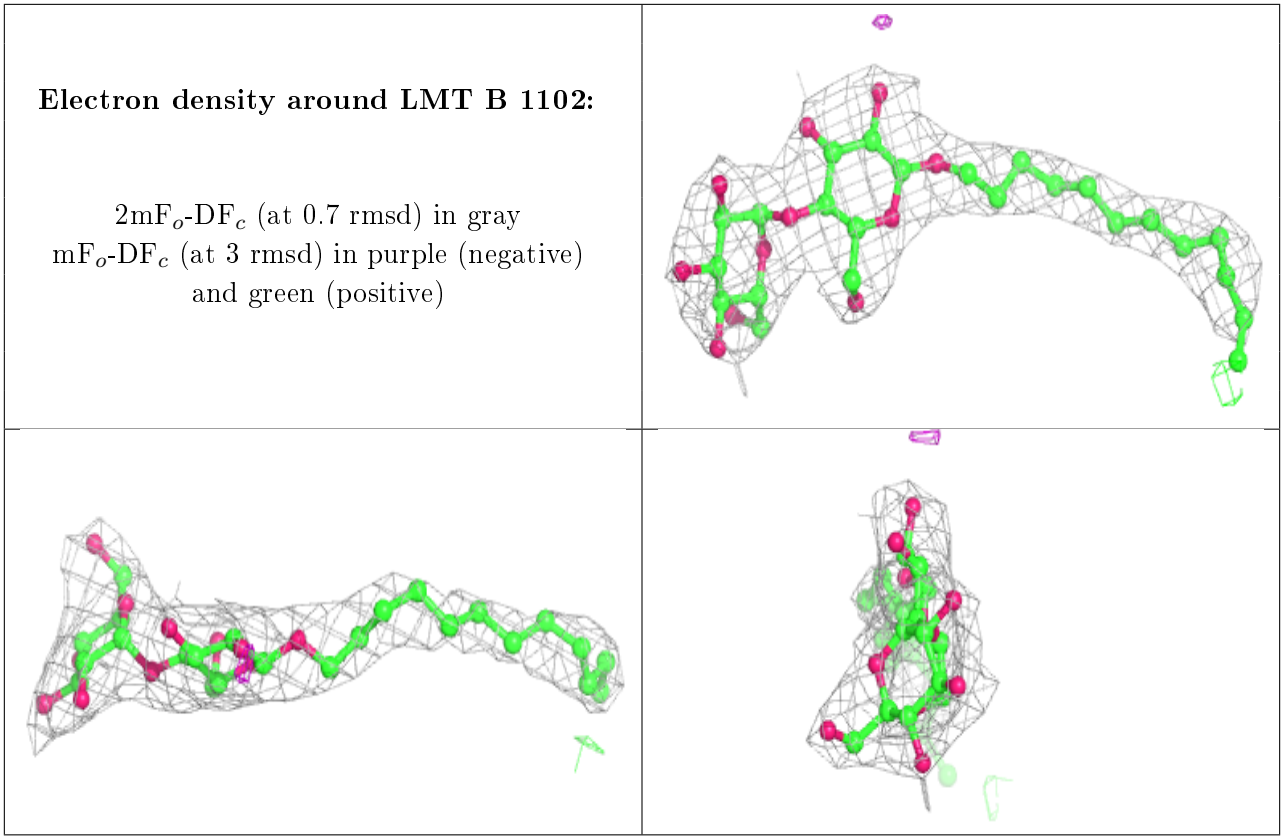
Electron density around LMT B 1103:

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



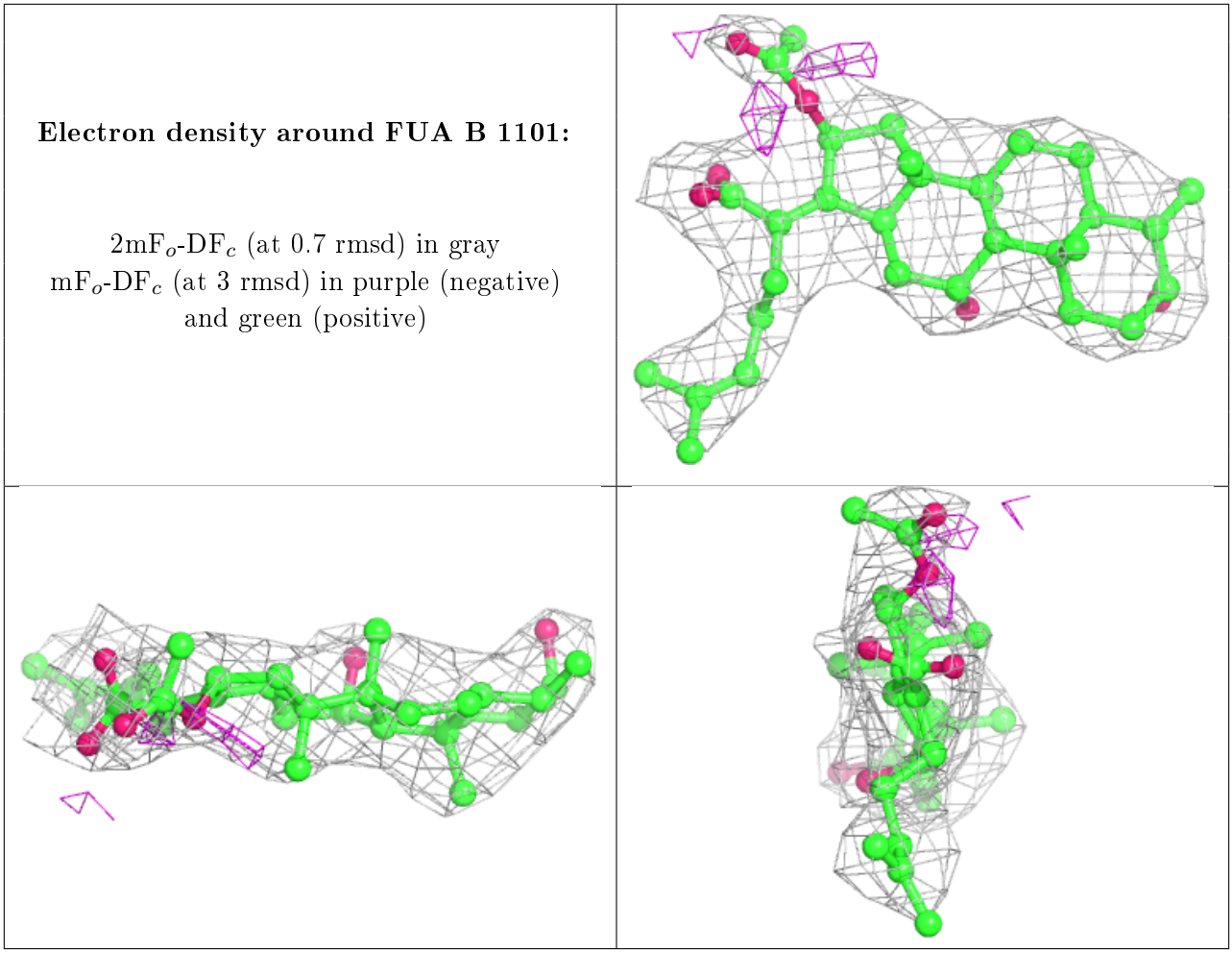
Electron density around LMT B 1102:

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



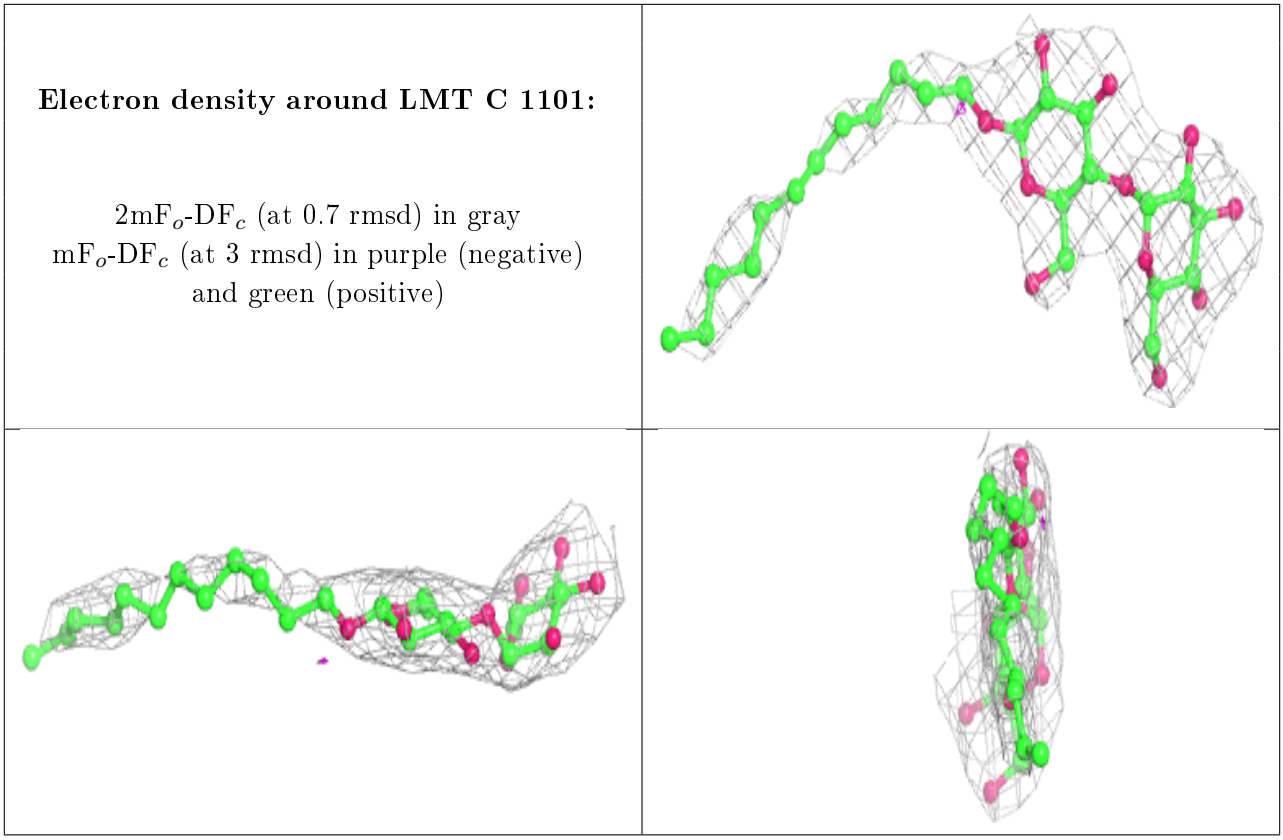
Electron density around FUA B 1101:

$2mF_o$-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 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

There are no such residues in this entry.