Full wwPDB X-ray Structure Validation Report (i)

Jun 24, 2024 – 11:07 PM EDT

PDB ID	:	6ZO7
Title	:	3-Formylrifamycin SV binding to the access pocket of AcrB-G619P L and T protomer
Authors	:	Tam, H.K.; Foong, W.E.; Pos, K.M.
Deposited on	:	2020-07-07
Resolution	:	2.85 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:

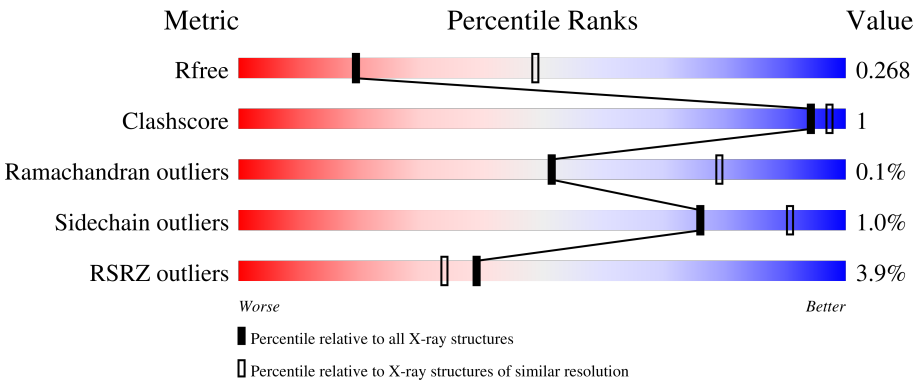
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.85 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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% 94% 5% •
1	B	1057	3% 91% 5% •
1	C	1057	2% 93% 5% •
2	D	169	8% 90% • 9%
2	E	169	23% 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
3	LMT	A	1206	-	-	-	X
3	LMT	B	1204	-	-	-	X

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 26893 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	7937	5105	1313	1475	44	0	1	0
1	B	1023	7794	5018	1286	1447	43	0	1	0
1	C	1034	7858	5058	1296	1460	44	0	0	0

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	619	PRO	GLY	conflict	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	619	PRO	GLY	conflict	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	619	PRO	GLY	conflict	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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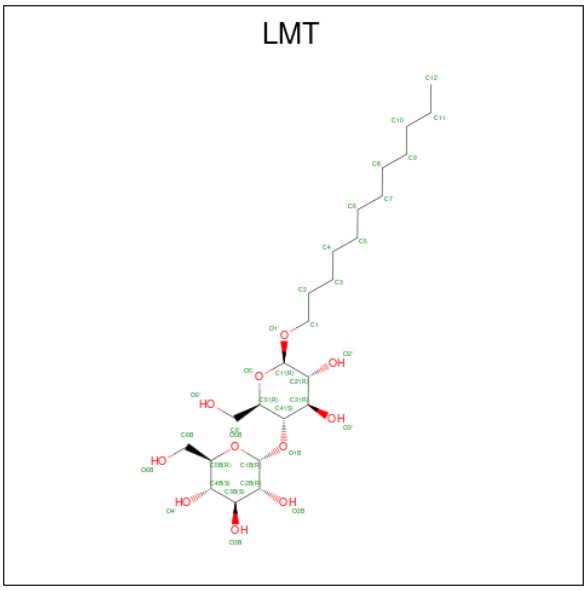
Chain	Residue	Modelled	Actual	Comment	Reference
C	1054	HIS	-	expression tag	UNP P31224
C	1055	HIS	-	expression tag	UNP P31224
C	1056	HIS	-	expression tag	UNP P31224
C	1057	HIS	-	expression tag	UNP P31224

- Molecule 2 is a protein called DARPIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	153	1158	731	202	224	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	A	1	35	24	11	0	0

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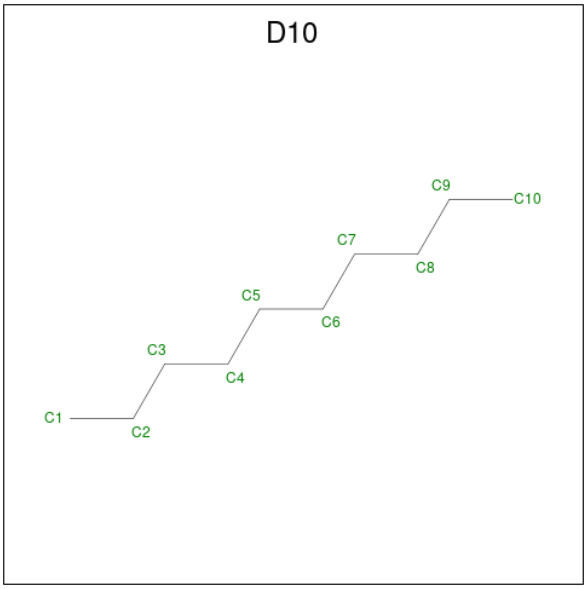
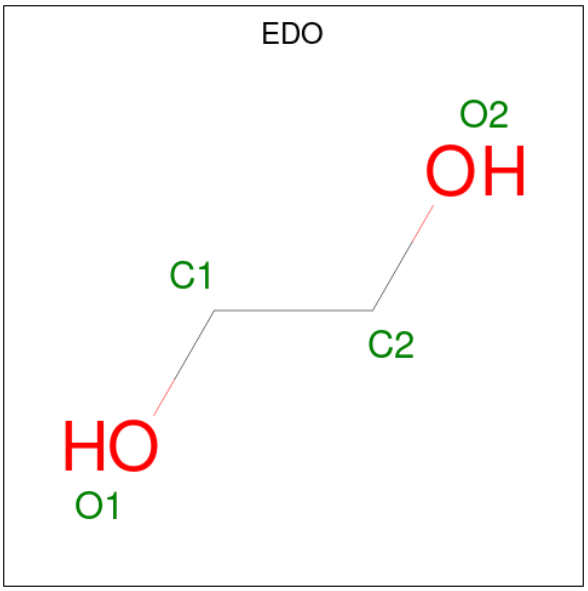
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	B	1	35	24	11	0	0
			Total	C	O		
3	B	1	35	24	11	0	0
			Total	C	O		
3	C	1	35	24	11	0	0
			Total	C	O		
3	C	1	35	24	11	0	0
			Total	C	O		
3	C	1	35	24	11	0	0

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



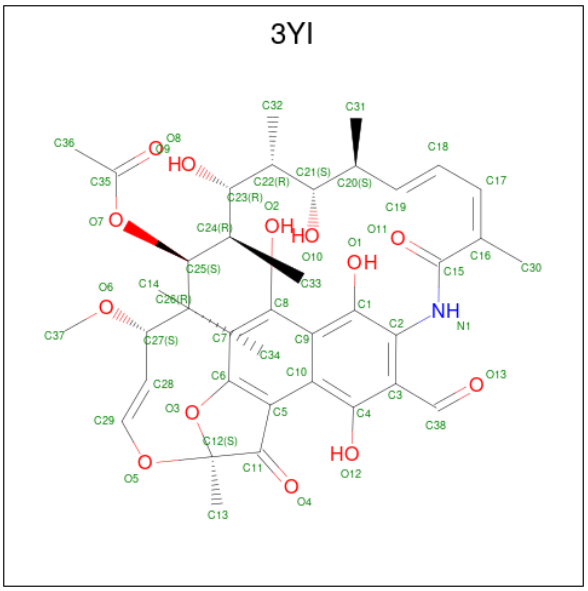
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C		
4	A	1	10	10	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



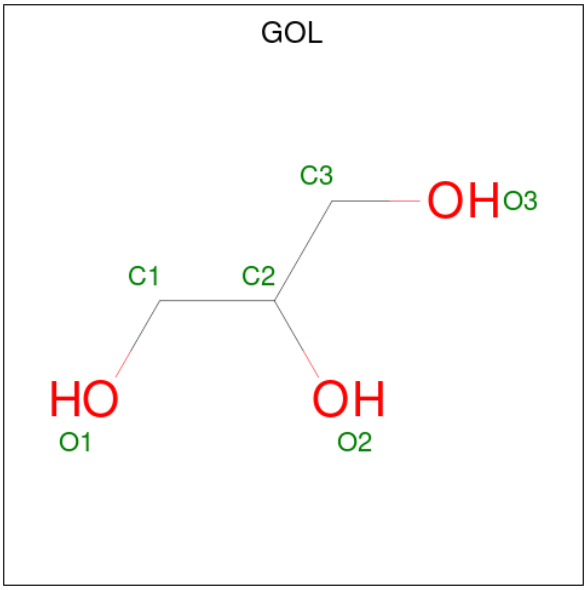
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	4	2	2	0	0
5	A	1	4	2	2	0	0
5	A	1	4	2	2	0	0
5	A	1	4	2	2	0	0
5	B	1	4	2	2	0	0
5	C	1	4	2	2	0	0
5	C	1	4	2	2	0	0
5	E	1	4	2	2	0	0

- Molecule 6 is (2S,12Z,14E,16S,17S,18R,19R,20R,21S,22R,23S,24E)-8-formyl-5,6,9,17,19-pentahydroxy-23-methoxy-2,4,12,16,18,20,22-heptam ethyl-1,11-dioxo-1,2-dihydro-2,7-(epoxypentadeca[1,11,13]trienoimino)naphtho[2,1-b]furan-21-yl acetate (three-letter code: 3YI) (formula: $C_{38}H_{47}NO_{13}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			52	38	1	13		
6	B	1	Total	C	N	O	0	0
			52	38	1	13		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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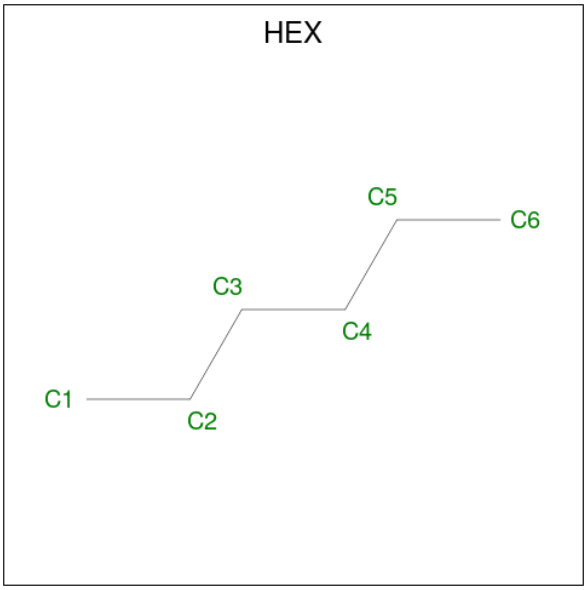
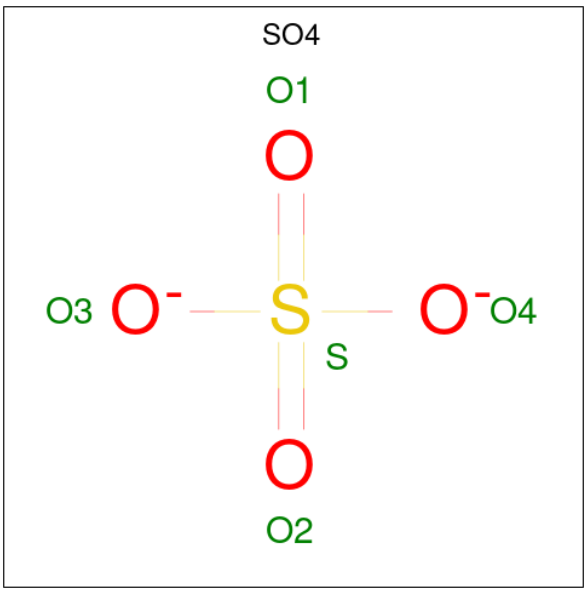
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	E	1	6	3	3	0	0

- Molecule 8 is HEXANE (three-letter code: HEX) (formula: C_6H_{14}).



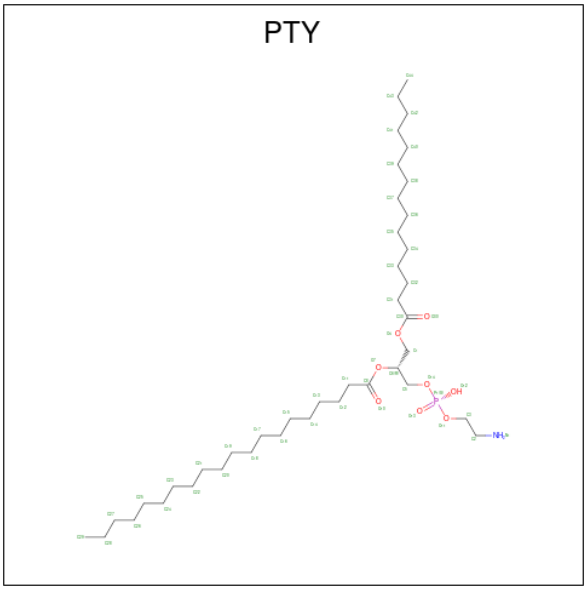
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C		
8	B	1	6	6	0	0

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



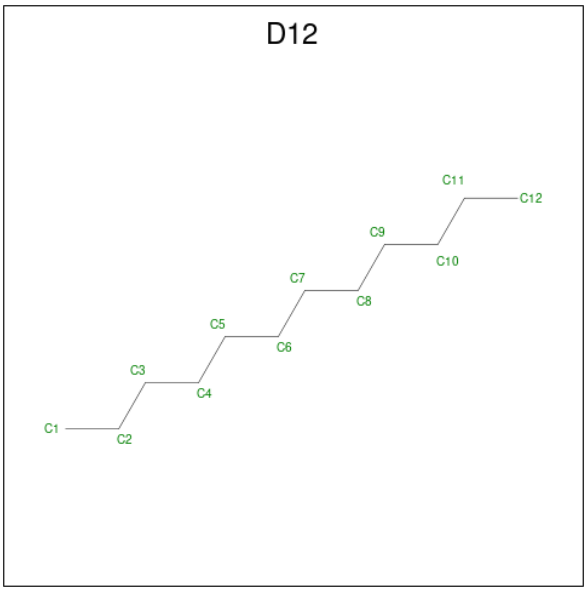
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
9	B	1	5	4	1	0	0

- Molecule 10 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$).



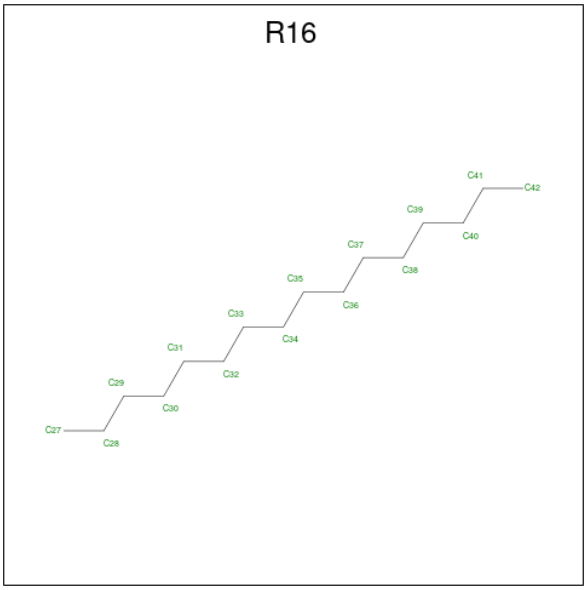
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
10	C	1	50	40	1	8	1	0	0
			Total	C	N	O	P		
10	C	1	50	40	1	8	1	0	0

- Molecule 11 is DODECANE (three-letter code: D12) (formula: $C_{12}H_{26}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	C	1	Total C 12 12	0	0
11	C	1	Total C 12 12	0	0

- Molecule 12 is HEXADECANE (three-letter code: R16) (formula: $C_{16}H_{34}$).

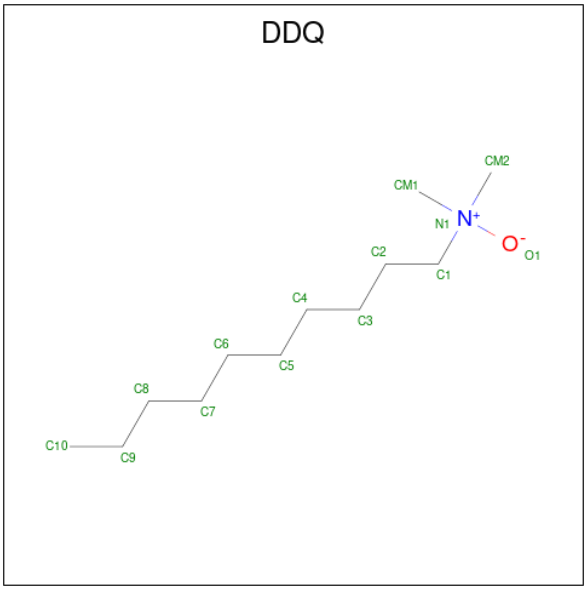


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	C	1	Total C 16 16	0	0

- Molecule 13 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	C	1	Total Cl 1 1	0	0

- Molecule 14 is DECYLAMINE-N,N-DIMETHYL-N-OXIDE (three-letter code: DDQ) (formula: $C_{12}H_{27}NO$).



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

- Molecule 15 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 16 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	108	Total O 111 111	0	3
16	B	89	Total O 90 90	0	1
16	C	82	Total O 83 83	0	1
16	D	5	Total O 5 5	0	0

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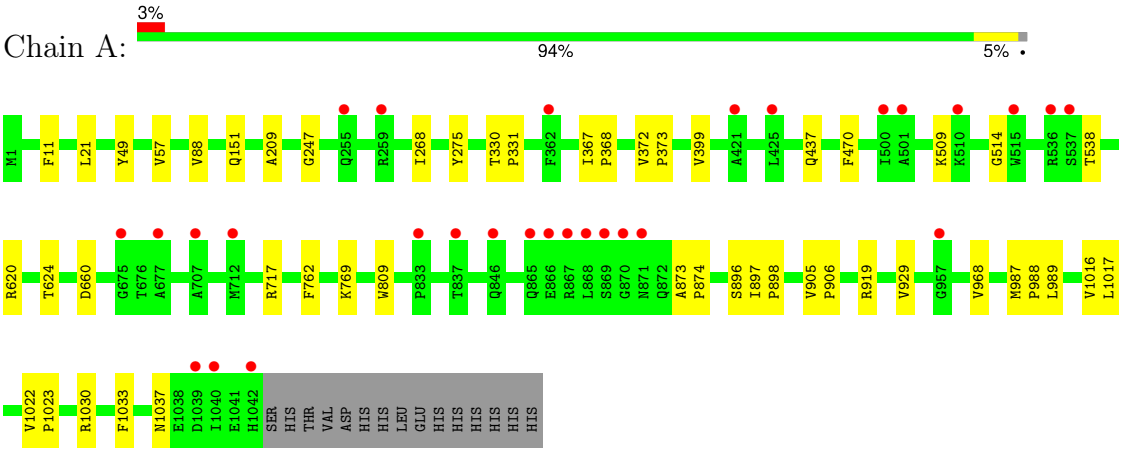
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
16	E	9	9	9	0	0

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.

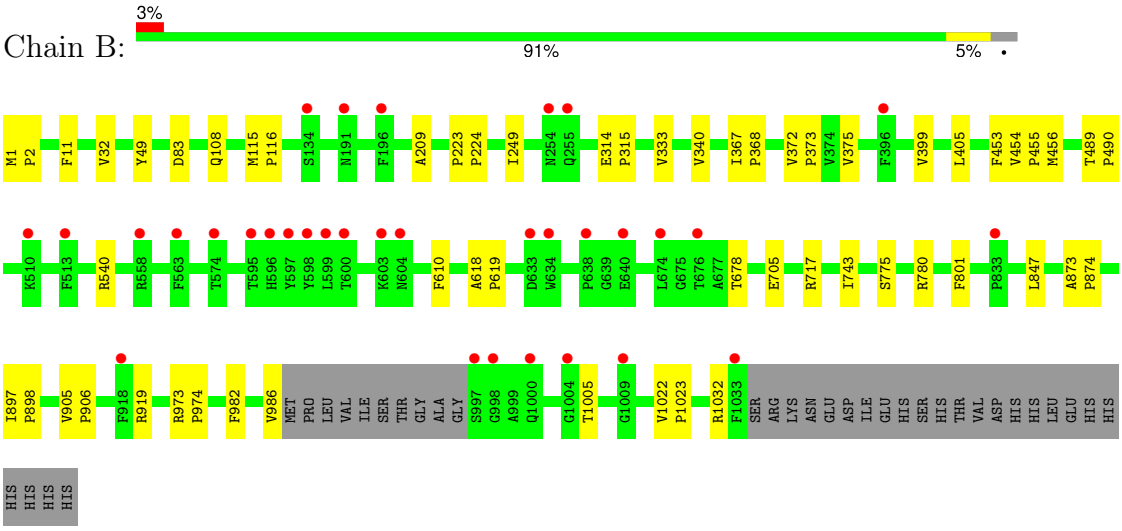
• Molecule 1: Multidrug efflux pump subunit AcrB

Chain A:



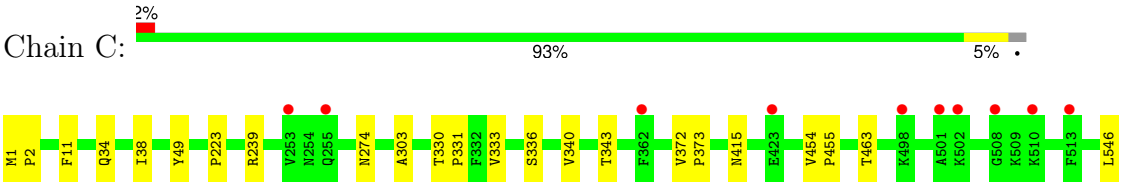
• Molecule 1: Multidrug efflux pump subunit AcrB

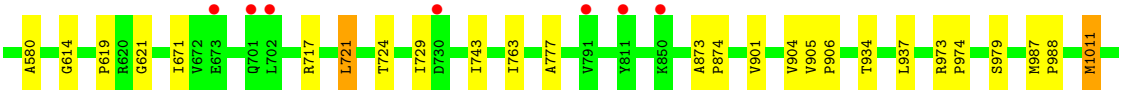
Chain B:

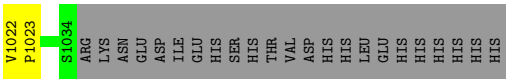


• Molecule 1: Multidrug efflux pump subunit AcrB

Chain C:

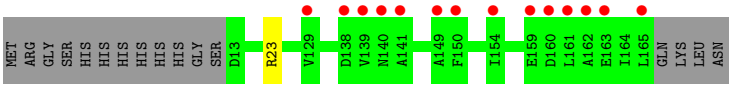






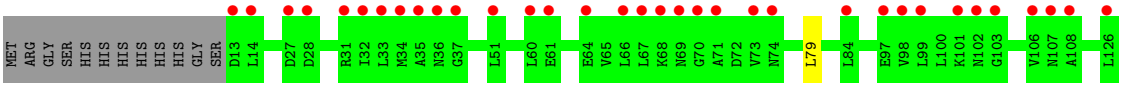
- Molecule 2: DARPIN

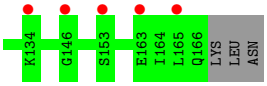
Chain D:



- 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	144.73Å 157.68Å 244.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.86 – 2.85 48.85 – 2.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.86-2.85) 100.0 (48.85-2.85)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.44 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.238 , 0.271 0.239 , 0.268	Depositor DCC
R_{free} test set	6405 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	45.5	Xtriage
Anisotropy	0.916	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 48.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	26893	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.05% 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: D12, 3YI, LMT, CL, DDQ, D10, HEX, EDO, GOL, SO4, R16, NA, PTY

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	0.67	0/8093	0.70	0/10990
1	B	0.67	0/7946	0.70	0/10790
1	C	0.67	0/8009	0.70	0/10878
2	D	0.67	0/1177	0.71	0/1601
2	E	0.68	0/1186	0.71	0/1613
All	All	0.67	0/26411	0.70	0/35872

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	7937	0	8083	25	0
1	B	7794	0	7942	26	0
1	C	7858	0	8010	24	0
2	D	1158	0	1143	0	0
2	E	1167	0	1151	1	0
3	A	175	0	230	0	0
3	B	70	0	92	0	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	10	0	22	0	0
5	A	16	0	24	0	0
5	B	4	0	6	0	0
5	C	8	0	12	0	0
5	E	4	0	6	0	0
6	A	52	0	0	0	0
6	B	52	0	0	1	0
7	B	6	0	8	0	0
7	C	6	0	8	0	0
7	E	6	0	8	0	0
8	B	6	0	14	0	0
9	B	5	0	0	0	0
10	C	100	0	158	0	0
11	C	24	0	52	0	0
12	C	16	0	34	0	0
13	C	1	0	0	0	0
14	C	14	0	27	0	0
15	C	1	0	0	0	0
16	A	111	0	0	0	0
16	B	90	0	0	0	0
16	C	83	0	0	0	0
16	D	5	0	0	0	0
16	E	9	0	0	0	0
All	All	26893	0	27168	72	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 (72) 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:38:ILE:HD11	1:C:671:ILE:HD12	1.81	0.63
1:C:619:PRO:HD2	1:C:721:LEU:HD11	1.85	0.59
1:A:399:VAL:HG11	1:A:989:LEU:HD11	1.84	0.58
1:A:372:VAL:HB	1:A:373:PRO:HD3	1.85	0.57
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.85	0.57
1:A:620:ARG:HB3	1:A:624:THR:HG21	1.87	0.56
1:A:57:VAL:CG1	1:A:88:VAL:HG22	2.35	0.56
1:B:873:ALA:HB3	1:B:874:PRO:HD3	1.88	0.56
1:C:454:VAL:HB	1:C:455:PRO:HD3	1.88	0.56
1:C:372:VAL:HB	1:C:373:PRO:HD3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:580:ALA:HB1	1:C:724:THR:HA	1.90	0.53
1:A:968:VAL:HG11	1:A:1023:PRO:HG3	1.91	0.52
1:B:372:VAL:HB	1:B:373:PRO:HD3	1.92	0.52
1:A:209:ALA:HB1	1:B:743:ILE:HG21	1.92	0.50
1:B:1022:VAL:N	1:B:1023:PRO:HD2	2.27	0.50
1:C:1:MET:HB3	1:C:2:PRO:HD3	1.96	0.48
1:A:762:PHE:CE1	1:A:769:LYS:HB2	2.48	0.48
1:B:982:PHE:HA	1:B:986:VAL:HG12	1.96	0.48
1:C:905:VAL:HB	1:C:906:PRO:HD3	1.95	0.48
1:C:614:GLY:HA2	1:C:621:GLY:O	2.13	0.48
6:B:1206:3YI:O12	6:B:1206:3YI:O4	2.32	0.47
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.97	0.47
1:B:32:VAL:HG12	1:B:333:VAL:HG11	1.96	0.47
1:B:705:GLU:HB3	1:B:847:LEU:HD22	1.97	0.47
1:A:896:SER:HB2	1:A:1033:PHE:CD2	2.50	0.46
1:A:620:ARG:CB	1:A:624:THR:HG21	2.45	0.46
1:A:1016:VAL:HG23	1:A:1017:LEU:HD12	1.98	0.46
1:B:905:VAL:HB	1:B:906:PRO:HD3	1.97	0.45
1:B:314:GLU:HB3	1:B:315:PRO:HD3	1.99	0.45
1:B:209:ALA:HB1	1:C:743:ILE:HD11	1.99	0.45
1:B:489:THR:N	1:B:490:PRO:CD	2.79	0.45
1:C:34:GLN:HB2	1:C:333:VAL:HG13	1.98	0.45
1:C:901:VAL:O	1:C:904:VAL:HG12	2.17	0.45
1:A:809:TRP:CD1	2:E:79:LEU:HD12	2.52	0.44
1:A:987:MET:N	1:A:988:PRO:CD	2.80	0.44
1:B:367:ILE:HB	1:B:368:PRO:HD3	1.99	0.44
1:B:115:MET:N	1:B:116:PRO:CD	2.80	0.44
1:B:897:ILE:N	1:B:898:PRO:CD	2.81	0.44
1:B:375:VAL:HG11	1:B:405:LEU:HD22	2.00	0.43
1:A:897:ILE:N	1:A:898:PRO:CD	2.82	0.43
1:B:453:PHE:O	1:B:456:MET:HG2	2.18	0.43
1:A:470:PHE:CD2	1:A:929:VAL:HG11	2.54	0.43
1:A:330:THR:N	1:A:331:PRO:CD	2.81	0.43
1:C:546:LEU:HD23	1:C:546:LEU:HA	1.91	0.43
1:C:343:THR:HG23	1:C:988:PRO:HB2	2.01	0.43
1:B:618:ALA:HB1	1:B:619:PRO:HD2	2.02	0.42
1:C:873:ALA:N	1:C:874:PRO:CD	2.82	0.42
1:C:979:SER:HA	1:C:1011:MET:HE3	2.01	0.42
1:B:973:ARG:N	1:B:974:PRO:HD2	2.33	0.42
1:C:336:SER:O	1:C:340:VAL:HG23	2.20	0.42
1:A:330:THR:OG1	1:A:331:PRO:HD3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:303:ALA:HB2	1:C:330:THR:HG21	2.02	0.42
1:B:340:VAL:HG22	1:B:399:VAL:HG23	2.02	0.42
1:A:509:LYS:O	1:A:514:GLY:HA3	2.20	0.41
1:A:1022:VAL:N	1:A:1023:PRO:CD	2.83	0.41
1:B:1:MET:HB3	1:B:2:PRO:HD3	2.01	0.41
1:C:987:MET:N	1:C:988:PRO:CD	2.82	0.41
1:B:454:VAL:N	1:B:455:PRO:CD	2.83	0.41
1:C:934:THR:HA	1:C:937:LEU:HD12	2.03	0.41
1:C:239:ARG:HB2	1:C:763:ILE:HG12	2.03	0.41
1:B:897:ILE:N	1:B:898:PRO:HD2	2.36	0.41
1:A:247:GLY:HA2	1:A:268:ILE:CD1	2.51	0.41
1:A:275:TYR:CD1	1:C:223:PRO:HD3	2.55	0.41
1:A:209:ALA:HB1	1:B:743:ILE:CG2	2.51	0.41
1:A:873:ALA:N	1:A:874:PRO:HD2	2.35	0.41
1:B:223:PRO:HA	1:B:224:PRO:HD3	1.99	0.41
1:C:330:THR:OG1	1:C:331:PRO:HD3	2.21	0.41
1:C:1022:VAL:HB	1:C:1023:PRO:HD3	2.02	0.41
1:B:775:SER:HB3	1:B:780:ARG:HD3	2.02	0.40
1:C:973:ARG:N	1:C:974:PRO:HD2	2.36	0.40
1:A:897:ILE:N	1:A:898:PRO:HD2	2.36	0.40
1:B:919:ARG:NH1	1:B:1005:THR:OG1	2.55	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	1041/1057 (98%)	1012 (97%)	27 (3%)	2 (0%)	47 75
1	B	1020/1057 (96%)	988 (97%)	30 (3%)	2 (0%)	47 75
1	C	1032/1057 (98%)	994 (96%)	37 (4%)	1 (0%)	51 79
2	D	151/169 (89%)	145 (96%)	6 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	152/169 (90%)	146 (96%)	6 (4%)	0	100	100
All	All	3396/3509 (97%)	3285 (97%)	106 (3%)	5 (0%)	51	79

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	678	THR
1	A	538	THR
1	A	1037	ASN
1	C	777	ALA
1	B	249	ILE

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	850/864 (98%)	841 (99%)	9 (1%)	73	90
1	B	834/864 (96%)	825 (99%)	9 (1%)	73	90
1	C	841/864 (97%)	832 (99%)	9 (1%)	73	90
2	D	118/132 (89%)	117 (99%)	1 (1%)	81	93
2	E	119/132 (90%)	119 (100%)	0	100	100
All	All	2762/2856 (97%)	2734 (99%)	28 (1%)	76	91

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	PHE
1	A	21	LEU
1	A	49	TYR
1	A	151	GLN
1	A	437	GLN
1	A	660	ASP
1	A	717	ARG

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Mol	Chain	Res	Type
1	A	919	ARG
1	A	1030	ARG
1	B	11	PHE
1	B	49	TYR
1	B	83	ASP
1	B	108	GLN
1	B	540	ARG
1	B	610	PHE
1	B	717	ARG
1	B	801	PHE
1	B	1032	ARG
1	C	11	PHE
1	C	49	TYR
1	C	274	ASN
1	C	415	ASN
1	C	463	THR
1	C	717	ARG
1	C	721	LEU
1	C	729	ILE
1	C	1011	MET
2	D	23	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 34 ligands modelled in this entry, 2 are monoatomic - leaving 32 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	$\#\|Z\| > 2$
8	HEX	B	1203	-	5,5,5	0.12	0	4,4,4	0.10	0
3	LMT	A	1201	-	36,36,36	0.49	1 (2%)	47,47,47	0.65	0
5	EDO	C	1113	-	3,3,3	0.06	0	2,2,2	0.08	0
3	LMT	C	1102	-	36,36,36	0.47	0	47,47,47	0.80	1 (2%)
4	D10	A	1204	-	9,9,9	0.09	0	8,8,8	0.09	0
5	EDO	A	1207	-	3,3,3	0.06	0	2,2,2	0.12	0
3	LMT	A	1203	-	36,36,36	0.47	1 (2%)	47,47,47	0.57	0
5	EDO	A	1205	-	3,3,3	0.07	0	2,2,2	0.08	0
5	EDO	E	202	-	3,3,3	0.06	0	2,2,2	0.13	0
3	LMT	B	1204	-	36,36,36	0.52	0	47,47,47	0.72	1 (2%)
12	R16	C	1107	-	15,15,15	0.08	0	14,14,14	0.07	0
3	LMT	A	1206	-	36,36,36	0.45	0	47,47,47	0.64	0
5	EDO	A	1211	-	3,3,3	0.07	0	2,2,2	0.10	0
3	LMT	C	1105	-	36,36,36	0.49	1 (2%)	47,47,47	0.77	0
11	D12	C	1103	-	11,11,11	0.10	0	10,10,10	0.05	0
7	GOL	C	1110	-	5,5,5	0.09	0	5,5,5	0.29	0
3	LMT	C	1112	-	36,36,36	0.52	1 (2%)	47,47,47	0.82	0
3	LMT	B	1201	-	36,36,36	0.46	0	47,47,47	0.50	0
10	PTY	C	1106	-	49,49,49	0.26	0	52,54,54	0.42	0
14	DDQ	C	1111	-	11,13,13	0.21	0	12,15,15	0.23	0
5	EDO	C	1109	-	3,3,3	0.06	0	2,2,2	0.11	0
11	D12	C	1104	-	11,11,11	0.09	0	10,10,10	0.06	0
5	EDO	A	1208	-	3,3,3	0.06	0	2,2,2	0.12	0
6	3YI	A	1209	-	55,55,55	0.95	2 (3%)	82,83,83	1.46	7 (8%)
6	3YI	B	1206	-	55,55,55	1.27	5 (9%)	82,83,83	1.66	12 (14%)
10	PTY	C	1101	-	49,49,49	0.26	0	52,54,54	0.32	0
9	SO4	B	1207	-	4,4,4	0.34	0	6,6,6	0.08	0
3	LMT	A	1202	-	36,36,36	0.45	0	47,47,47	0.64	0
7	GOL	B	1202	-	5,5,5	0.09	0	5,5,5	0.27	0
3	LMT	A	1210	-	36,36,36	0.52	1 (2%)	47,47,47	0.74	0
7	GOL	E	201	-	5,5,5	0.09	0	5,5,5	0.25	0
5	EDO	B	1205	-	3,3,3	0.07	0	2,2,2	0.13	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	HEX	B	1203	-	-	0/3/3/3	-
3	LMT	A	1201	-	-	13/21/61/61	0/2/2/2
5	EDO	C	1113	-	-	1/1/1/1	-
3	LMT	C	1102	-	-	12/21/61/61	0/2/2/2
4	D10	A	1204	-	-	4/7/7/7	-
5	EDO	A	1207	-	-	1/1/1/1	-
3	LMT	A	1203	-	-	7/21/61/61	0/2/2/2
5	EDO	A	1205	-	-	1/1/1/1	-
5	EDO	E	202	-	-	1/1/1/1	-
3	LMT	B	1204	-	-	11/21/61/61	0/2/2/2
12	R16	C	1107	-	-	5/13/13/13	-
3	LMT	A	1206	-	-	8/21/61/61	0/2/2/2
5	EDO	A	1211	-	-	1/1/1/1	-
3	LMT	C	1105	-	-	11/21/61/61	0/2/2/2
11	D12	C	1103	-	-	2/9/9/9	-
7	GOL	C	1110	-	-	4/4/4/4	-
3	LMT	C	1112	-	-	14/21/61/61	0/2/2/2
3	LMT	B	1201	-	-	8/21/61/61	0/2/2/2
10	PTY	C	1106	-	-	30/53/53/53	-
14	DDQ	C	1111	-	-	4/11/11/11	-
5	EDO	C	1109	-	-	1/1/1/1	-
11	D12	C	1104	-	-	2/9/9/9	-
5	EDO	A	1208	-	-	0/1/1/1	-
6	3YI	A	1209	-	-	13/57/72/72	0/4/4/4
6	3YI	B	1206	-	-	14/57/72/72	0/4/4/4
10	PTY	C	1101	-	-	22/53/53/53	-
3	LMT	A	1202	-	-	9/21/61/61	0/2/2/2
7	GOL	B	1202	-	-	4/4/4/4	-
3	LMT	A	1210	-	-	8/21/61/61	0/2/2/2
7	GOL	E	201	-	-	3/4/4/4	-
5	EDO	B	1205	-	-	1/1/1/1	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1206	3YI	C15-N1	4.55	1.45	1.35
6	A	1209	3YI	C15-N1	4.01	1.43	1.35
6	B	1206	3YI	C2-N1	-3.22	1.37	1.43
6	B	1206	3YI	C22-C23	2.46	1.60	1.54
6	B	1206	3YI	C5-C10	-2.32	1.38	1.42
6	B	1206	3YI	C14-C7	-2.26	1.47	1.51
3	C	1112	LMT	O1'-C1'	2.21	1.43	1.40
6	A	1209	3YI	C14-C7	-2.20	1.47	1.51
3	A	1210	LMT	O1'-C1'	2.14	1.43	1.40
3	A	1201	LMT	O1'-C1'	2.12	1.43	1.40
3	C	1105	LMT	O1'-C1'	2.10	1.43	1.40
3	A	1203	LMT	O1'-C1'	2.01	1.43	1.40

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	1206	3YI	C2-C3-C4	7.19	123.76	119.19
6	A	1209	3YI	C2-C3-C4	6.36	123.23	119.19
6	B	1206	3YI	C4-C3-C38	-4.72	113.35	119.83
6	A	1209	3YI	C4-C3-C38	-4.48	113.69	119.83
6	B	1206	3YI	C17-C16-C15	-3.81	109.61	120.83
6	B	1206	3YI	C30-C16-C15	3.72	124.35	115.22
6	A	1209	3YI	C3-C2-C1	-3.58	118.15	120.68
6	B	1206	3YI	O7-C35-C36	3.45	117.23	111.09
6	B	1206	3YI	C3-C4-C10	-3.18	118.61	121.19
3	C	1102	LMT	C1B-O5B-C5B	3.11	119.80	113.72
6	A	1209	3YI	O7-C35-C36	2.96	116.36	111.09
6	B	1206	3YI	C3-C2-C1	-2.67	118.79	120.68
6	B	1206	3YI	C20-C21-C22	-2.62	109.65	114.97
6	B	1206	3YI	O5-C12-C13	2.54	113.57	106.98
6	A	1209	3YI	C3-C4-C10	-2.54	119.13	121.19
6	B	1206	3YI	O11-C15-C16	2.51	126.10	121.49
6	B	1206	3YI	C5-C10-C4	-2.28	121.87	124.08
3	B	1204	LMT	C2'-C3'-C4'	2.26	114.81	109.68
6	B	1206	3YI	O4-C11-C12	2.21	125.02	120.56
6	A	1209	3YI	O4-C11-C12	2.18	124.95	120.56
6	A	1209	3YI	C20-C21-C22	-2.18	110.56	114.97

There are no chirality outliers.

All (215) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1201	LMT	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
3	C	1105	LMT	C2'-C1'-O1'-C1
3	C	1105	LMT	O5'-C1'-O1'-C1
3	C	1105	LMT	C2-C1-O1'-C1'
3	C	1112	LMT	O5'-C1'-O1'-C1
3	C	1112	LMT	C2-C1-O1'-C1'
6	A	1209	3YI	C26-C27-O6-C37
6	A	1209	3YI	C28-C27-O6-C37
6	B	1206	3YI	C4-C3-C38-O13
6	B	1206	3YI	C26-C27-O6-C37
6	B	1206	3YI	C28-C27-O6-C37
6	B	1206	3YI	C36-C35-O7-C25
6	B	1206	3YI	C34-C26-C27-O6
6	B	1206	3YI	C34-C26-C27-C28
7	B	1202	GOL	C1-C2-C3-O3
7	E	201	GOL	C1-C2-C3-O3
10	C	1101	PTY	C11-C8-O7-C6
10	C	1101	PTY	C3-O11-P1-O12
10	C	1101	PTY	C3-O11-P1-O13
10	C	1101	PTY	C3-O11-P1-O14
10	C	1101	PTY	C5-O14-P1-O11
10	C	1101	PTY	C5-O14-P1-O13
10	C	1106	PTY	C11-C8-O7-C6
10	C	1106	PTY	C3-O11-P1-O12
10	C	1106	PTY	C3-O11-P1-O13
10	C	1106	PTY	C3-O11-P1-O14
10	C	1106	PTY	C5-O14-P1-O13
6	B	1206	3YI	O8-C35-O7-C25
10	C	1106	PTY	O30-C30-O4-C1
3	B	1204	LMT	O5B-C1B-O1B-C4'
10	C	1106	PTY	C31-C30-O4-C1
6	A	1209	3YI	C36-C35-O7-C25
3	C	1112	LMT	O5B-C1B-O1B-C4'
10	C	1101	PTY	O10-C8-O7-C6
3	C	1112	LMT	C2B-C1B-O1B-C4'
10	C	1106	PTY	O10-C8-O7-C6
3	C	1112	LMT	C4B-C5B-C6B-O6B
6	A	1209	3YI	C4-C3-C38-O13
3	C	1112	LMT	O5B-C5B-C6B-O6B
3	A	1202	LMT	O5'-C1'-O1'-C1
3	A	1210	LMT	O5'-C1'-O1'-C1
3	B	1204	LMT	O5'-C5'-C6'-O6'
3	C	1102	LMT	O5B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
10	C	1101	PTY	C31-C30-O4-C1
3	C	1102	LMT	C4B-C5B-C6B-O6B
3	B	1204	LMT	C4'-C5'-C6'-O6'
3	A	1201	LMT	C2'-C1'-O1'-C1
3	A	1202	LMT	C2'-C1'-O1'-C1
3	C	1112	LMT	C2'-C1'-O1'-C1
6	A	1209	3YI	O8-C35-O7-C25
7	E	201	GOL	O2-C2-C3-O3
3	A	1203	LMT	C4B-C5B-C6B-O6B
3	B	1204	LMT	C5-C6-C7-C8
10	C	1101	PTY	O30-C30-O4-C1
10	C	1106	PTY	C30-C31-C32-C33
3	C	1105	LMT	O1'-C1-C2-C3
3	A	1203	LMT	O1'-C1-C2-C3
3	C	1102	LMT	O1'-C1-C2-C3
6	B	1206	3YI	C19-C20-C21-O10
3	A	1203	LMT	O5B-C5B-C6B-O6B
7	B	1202	GOL	O1-C1-C2-C3
7	C	1110	GOL	O1-C1-C2-C3
7	C	1110	GOL	C1-C2-C3-O3
10	C	1106	PTY	C5-C6-O7-C8
3	B	1201	LMT	O1'-C1-C2-C3
12	C	1107	R16	C35-C36-C37-C38
6	B	1206	3YI	C19-C20-C21-C22
14	C	1111	DDQ	C3-C4-C5-C6
10	C	1106	PTY	C14-C15-C16-C17
11	C	1103	D12	C5-C6-C7-C8
3	A	1203	LMT	C4-C5-C6-C7
3	C	1112	LMT	C6-C7-C8-C9
3	C	1102	LMT	C2-C1-O1'-C1'
3	B	1201	LMT	C5-C6-C7-C8
3	C	1105	LMT	C5-C6-C7-C8
14	C	1111	DDQ	C2-C3-C4-C5
10	C	1101	PTY	C11-C12-C13-C14
3	C	1112	LMT	C2-C3-C4-C5
3	A	1210	LMT	C4-C5-C6-C7
5	A	1207	EDO	O1-C1-C2-O2
5	E	202	EDO	O1-C1-C2-O2
3	C	1105	LMT	C7-C8-C9-C10
10	C	1106	PTY	C17-C18-C19-C20
3	A	1206	LMT	O5B-C5B-C6B-O6B
3	C	1112	LMT	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	A	1201	LMT	C4-C5-C6-C7
10	C	1101	PTY	C24-C25-C26-C27
10	C	1101	PTY	C31-C32-C33-C34
3	A	1210	LMT	C1-C2-C3-C4
6	A	1209	3YI	C16-C17-C18-C19
14	C	1111	DDQ	C1-C2-C3-C4
3	A	1201	LMT	C2-C3-C4-C5
3	A	1201	LMT	O1'-C1-C2-C3
10	C	1101	PTY	C17-C18-C19-C20
3	A	1202	LMT	O5'-C5'-C6'-O6'
6	A	1209	3YI	C34-C26-C27-O6
3	C	1112	LMT	O5'-C5'-C6'-O6'
3	A	1201	LMT	C4B-C5B-C6B-O6B
6	B	1206	3YI	C25-C26-C27-O6
6	B	1206	3YI	C25-C26-C27-C28
10	C	1101	PTY	C19-C20-C21-C22
6	A	1209	3YI	O6-C27-C28-C29
6	A	1209	3YI	C26-C27-C28-C29
3	A	1202	LMT	O5B-C5B-C6B-O6B
3	A	1210	LMT	C6-C7-C8-C9
10	C	1106	PTY	O4-C1-C6-C5
3	A	1203	LMT	C2-C3-C4-C5
3	A	1210	LMT	C2-C3-C4-C5
10	C	1106	PTY	C6-C5-O14-P1
3	C	1105	LMT	O5B-C5B-C6B-O6B
3	B	1204	LMT	C1-C2-C3-C4
3	B	1201	LMT	C11-C10-C9-C8
3	C	1112	LMT	C4-C5-C6-C7
10	C	1106	PTY	C26-C27-C28-C29
3	C	1112	LMT	C9-C10-C11-C12
14	C	1111	DDQ	C7-C8-C9-C10
3	B	1204	LMT	C9-C10-C11-C12
3	C	1102	LMT	C9-C10-C11-C12
3	A	1201	LMT	C5-C6-C7-C8
3	C	1105	LMT	C3'-C4'-O1B-C1B
3	A	1206	LMT	C2-C1-O1'-C1'
3	A	1210	LMT	C2-C1-O1'-C1'
3	B	1204	LMT	C2-C1-O1'-C1'
7	B	1202	GOL	O2-C2-C3-O3
7	C	1110	GOL	O2-C2-C3-O3
7	E	201	GOL	O1-C1-C2-O2
10	C	1101	PTY	C6-C5-O14-P1

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Mol	Chain	Res	Type	Atoms
3	A	1210	LMT	C11-C10-C9-C8
10	C	1106	PTY	C21-C22-C23-C24
10	C	1101	PTY	O14-C5-C6-C1
10	C	1101	PTY	C14-C15-C16-C17
6	A	1209	3YI	C18-C19-C20-C31
4	A	1204	D10	C4-C5-C6-C7
5	B	1205	EDO	O1-C1-C2-O2
3	A	1210	LMT	C7-C8-C9-C10
3	A	1206	LMT	O1'-C1-C2-C3
3	C	1105	LMT	C11-C10-C9-C8
3	A	1202	LMT	C2-C3-C4-C5
10	C	1106	PTY	O4-C1-C6-O7
11	C	1104	D12	C4-C5-C6-C7
3	A	1206	LMT	C5-C6-C7-C8
3	C	1102	LMT	C2-C3-C4-C5
3	A	1202	LMT	C3'-C4'-O1B-C1B
7	B	1202	GOL	O1-C1-C2-O2
3	A	1201	LMT	C9-C10-C11-C12
3	C	1105	LMT	C5'-C4'-O1B-C1B
10	C	1106	PTY	C12-C11-C8-O7
10	C	1101	PTY	O14-C5-C6-O7
3	B	1201	LMT	O5'-C1'-O1'-C1
10	C	1101	PTY	C30-C31-C32-C33
10	C	1101	PTY	C2-C3-O11-P1
10	C	1106	PTY	C2-C3-O11-P1
6	B	1206	3YI	C31-C20-C21-C22
3	A	1203	LMT	C9-C10-C11-C12
3	B	1204	LMT	C4-C5-C6-C7
6	A	1209	3YI	C34-C26-C27-C28
3	A	1206	LMT	C1-C2-C3-C4
3	A	1202	LMT	C5'-C4'-O1B-C1B
6	A	1209	3YI	C25-C26-C27-O6
6	A	1209	3YI	C25-C26-C27-C28
3	B	1201	LMT	O5'-C5'-C6'-O6'
10	C	1106	PTY	C12-C13-C14-C15
3	A	1206	LMT	C9-C10-C11-C12
4	A	1204	D10	C5-C6-C7-C8
3	A	1202	LMT	C7-C8-C9-C10
3	A	1203	LMT	C11-C10-C9-C8
3	A	1201	LMT	C3'-C4'-O1B-C1B
3	A	1201	LMT	C5'-C4'-O1B-C1B
3	C	1102	LMT	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
3	C	1102	LMT	C4-C5-C6-C7
10	C	1106	PTY	C39-C40-C41-C42
3	C	1105	LMT	C2-C3-C4-C5
3	C	1102	LMT	O5'-C1'-O1'-C1
3	A	1202	LMT	O1'-C1-C2-C3
12	C	1107	R16	C32-C33-C34-C35
3	B	1201	LMT	C2'-C1'-O1'-C1
3	C	1102	LMT	C2'-C1'-O1'-C1
10	C	1106	PTY	C41-C42-C43-C44
10	C	1106	PTY	C35-C36-C37-C38
3	A	1201	LMT	O5B-C5B-C6B-O6B
11	C	1104	D12	C7-C8-C9-C10
3	C	1102	LMT	C7-C8-C9-C10
5	A	1211	EDO	O1-C1-C2-O2
5	C	1109	EDO	O1-C1-C2-O2
3	C	1112	LMT	C7-C8-C9-C10
3	A	1201	LMT	C1-C2-C3-C4
4	A	1204	D10	C3-C4-C5-C6
6	B	1206	3YI	C18-C19-C20-C31
12	C	1107	R16	C30-C31-C32-C33
12	C	1107	R16	C33-C34-C35-C36
10	C	1101	PTY	C12-C13-C14-C15
3	A	1201	LMT	C3-C4-C5-C6
10	C	1101	PTY	C22-C23-C24-C25
3	B	1204	LMT	C2B-C1B-O1B-C4'
7	C	1110	GOL	O1-C1-C2-O2
3	B	1201	LMT	C3-C4-C5-C6
10	C	1106	PTY	C32-C33-C34-C35
5	A	1205	EDO	O1-C1-C2-O2
5	C	1113	EDO	O1-C1-C2-O2
4	A	1204	D10	C6-C7-C8-C9
3	C	1102	LMT	C1-C2-C3-C4
3	A	1206	LMT	C2'-C1'-O1'-C1
3	B	1204	LMT	C2-C3-C4-C5
3	A	1206	LMT	O5'-C1'-O1'-C1
10	C	1106	PTY	C13-C14-C15-C16
6	B	1206	3YI	C28-C29-O5-C12
3	B	1201	LMT	C4-C5-C6-C7
12	C	1107	R16	C29-C30-C31-C32
11	C	1103	D12	C7-C8-C9-C10
10	C	1106	PTY	C12-C11-C8-O10
10	C	1106	PTY	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
10	C	1106	PTY	C19-C20-C21-C22
10	C	1106	PTY	O4-C30-C31-C32
3	B	1204	LMT	C7-C8-C9-C10
10	C	1106	PTY	C38-C39-C40-C41

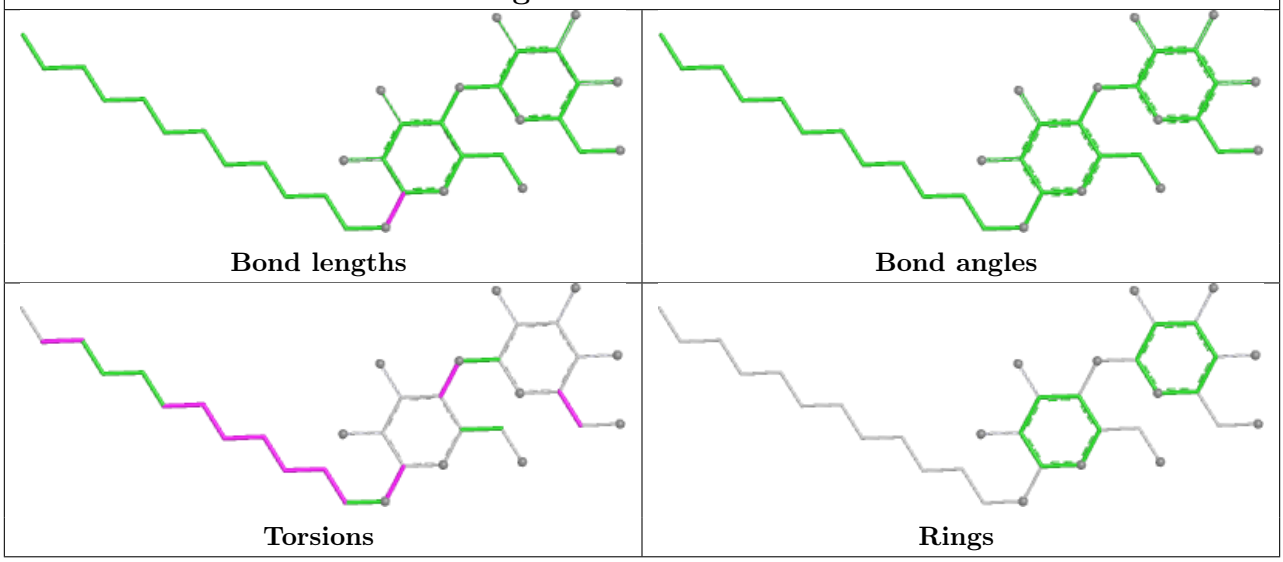
There are no ring outliers.

1 monomer is involved in 1 short contact:

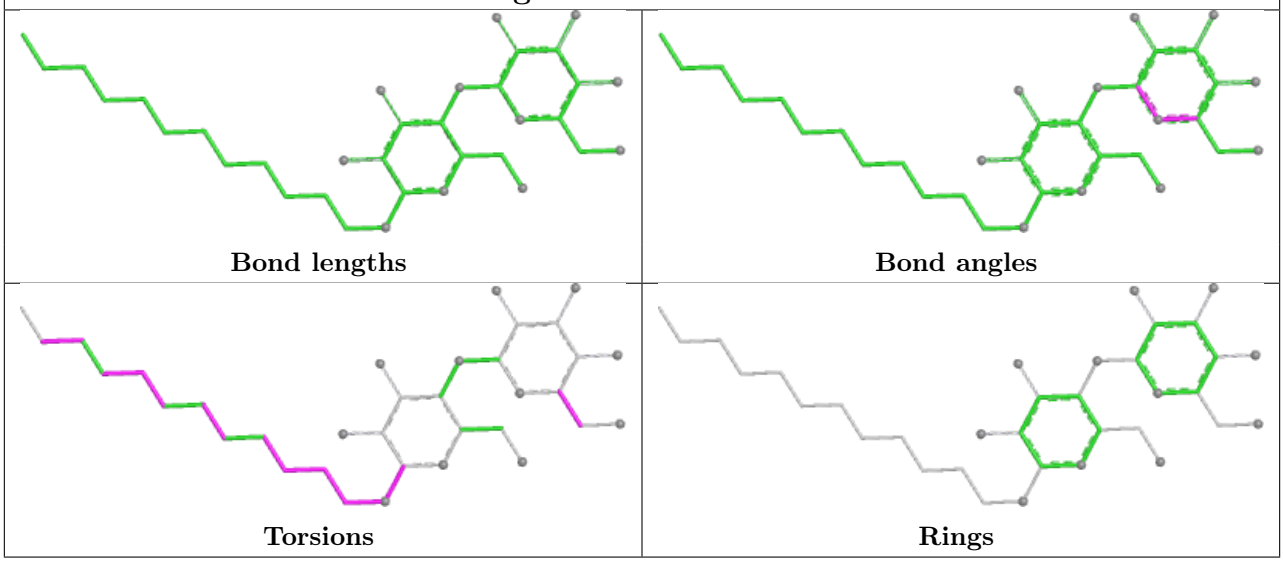
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1206	3YI	1	0

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.

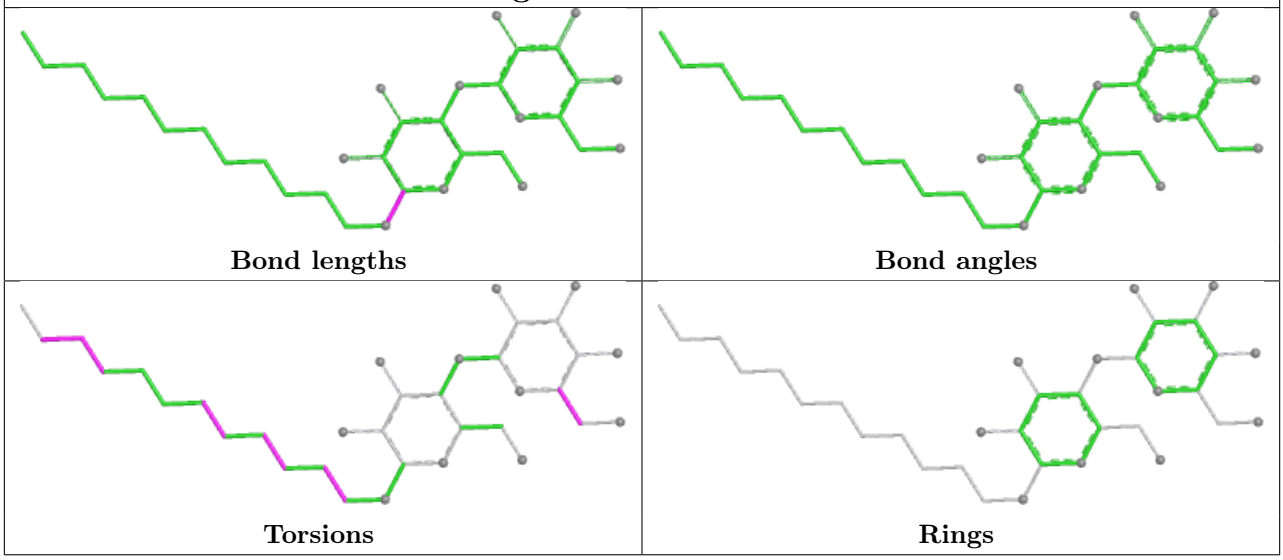
Ligand LMT A 1201



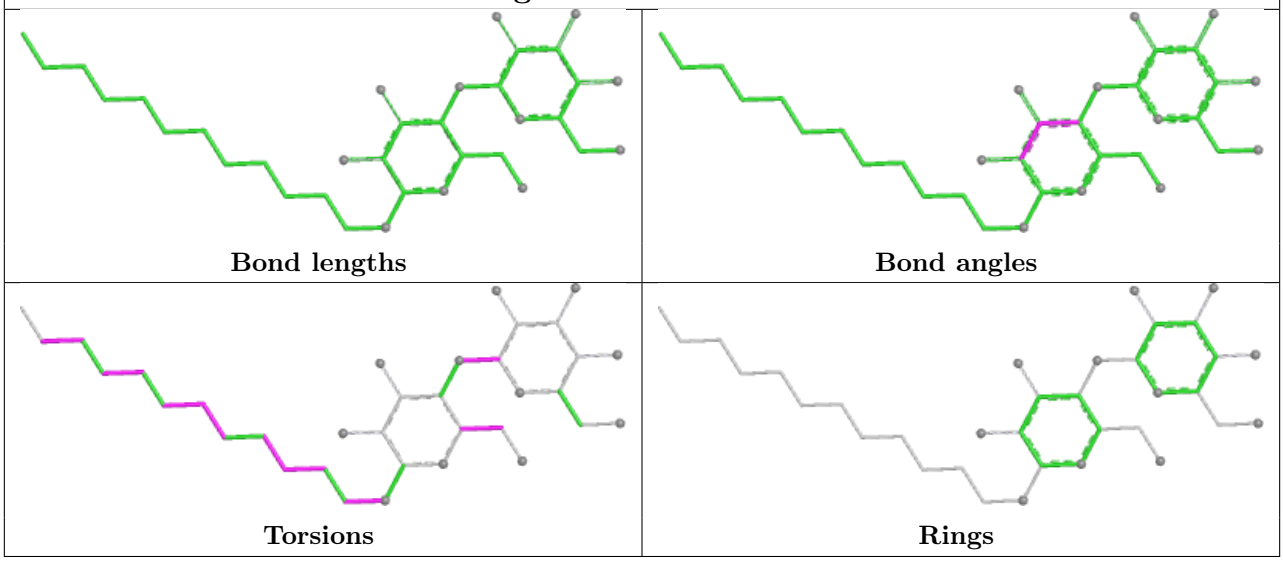
Ligand LMT C 1102



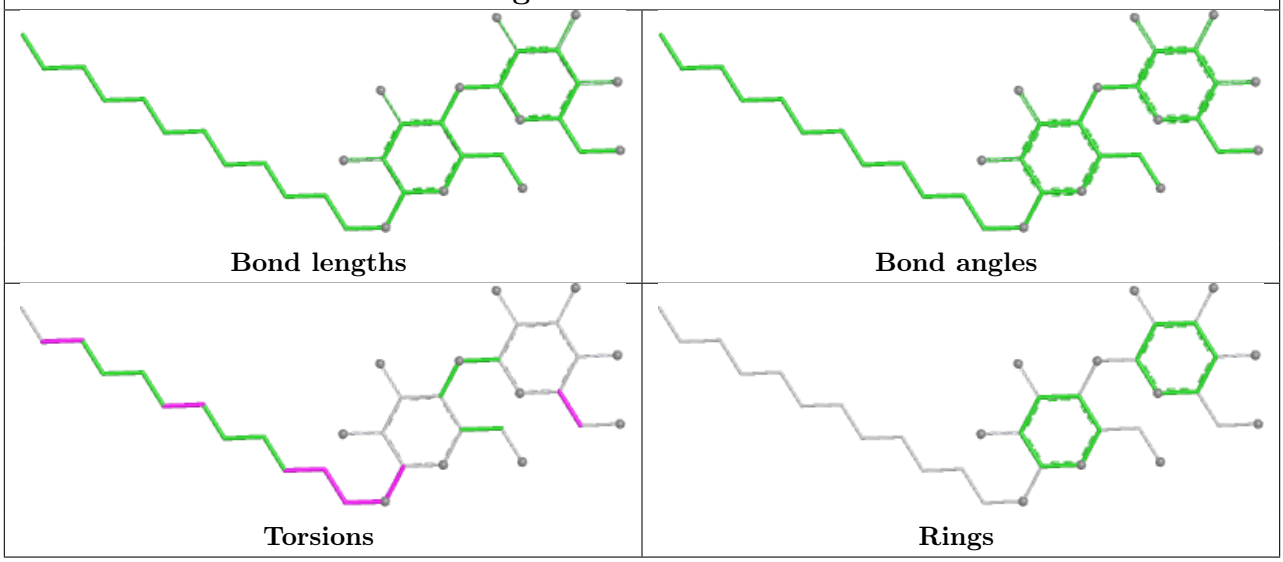
Ligand LMT A 1203



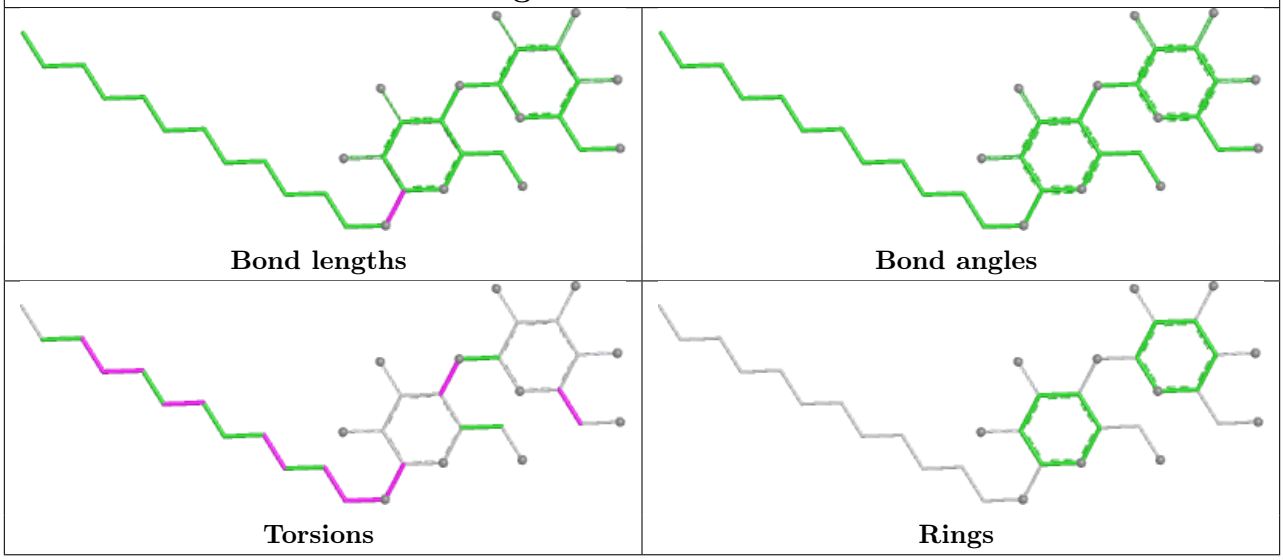
Ligand LMT B 1204



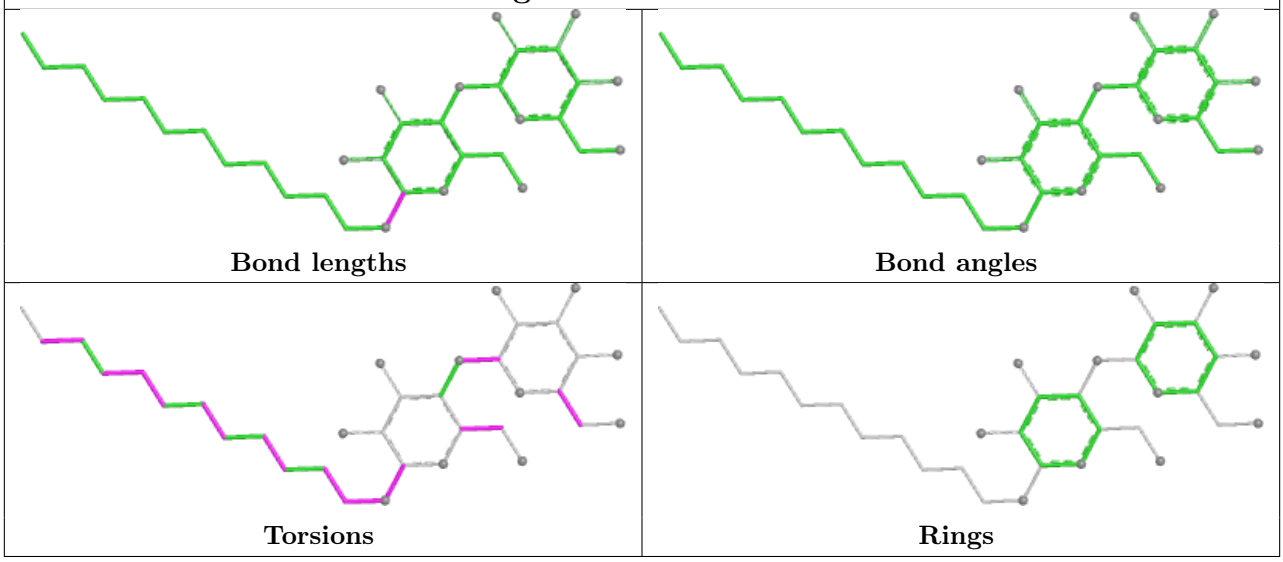
Ligand LMT A 1206

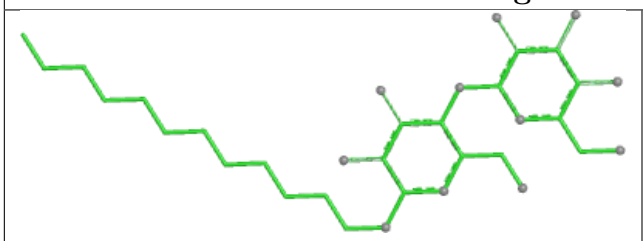
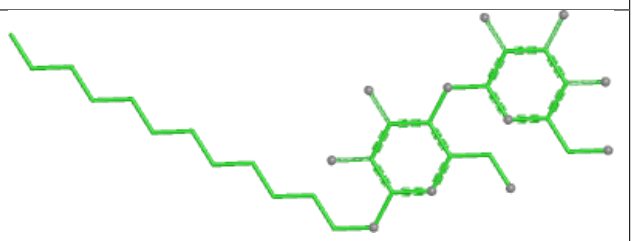
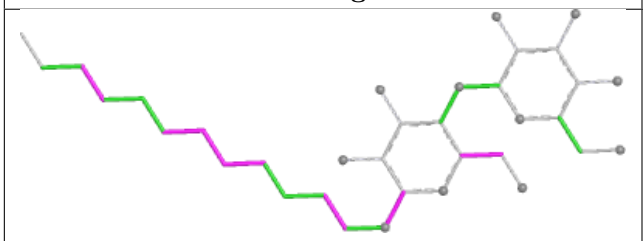
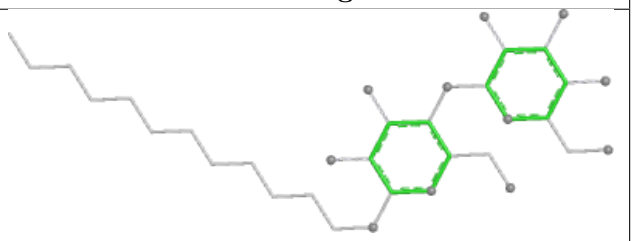


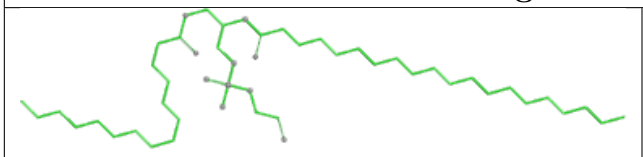
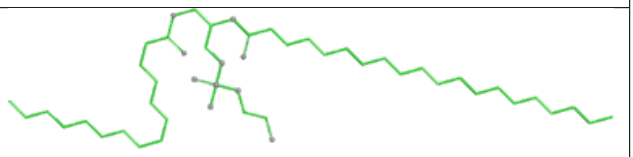
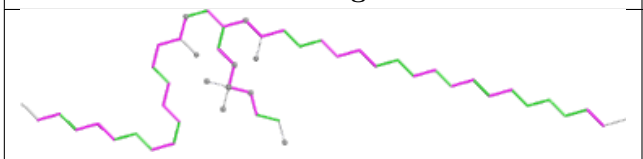
Ligand LMT C 1105



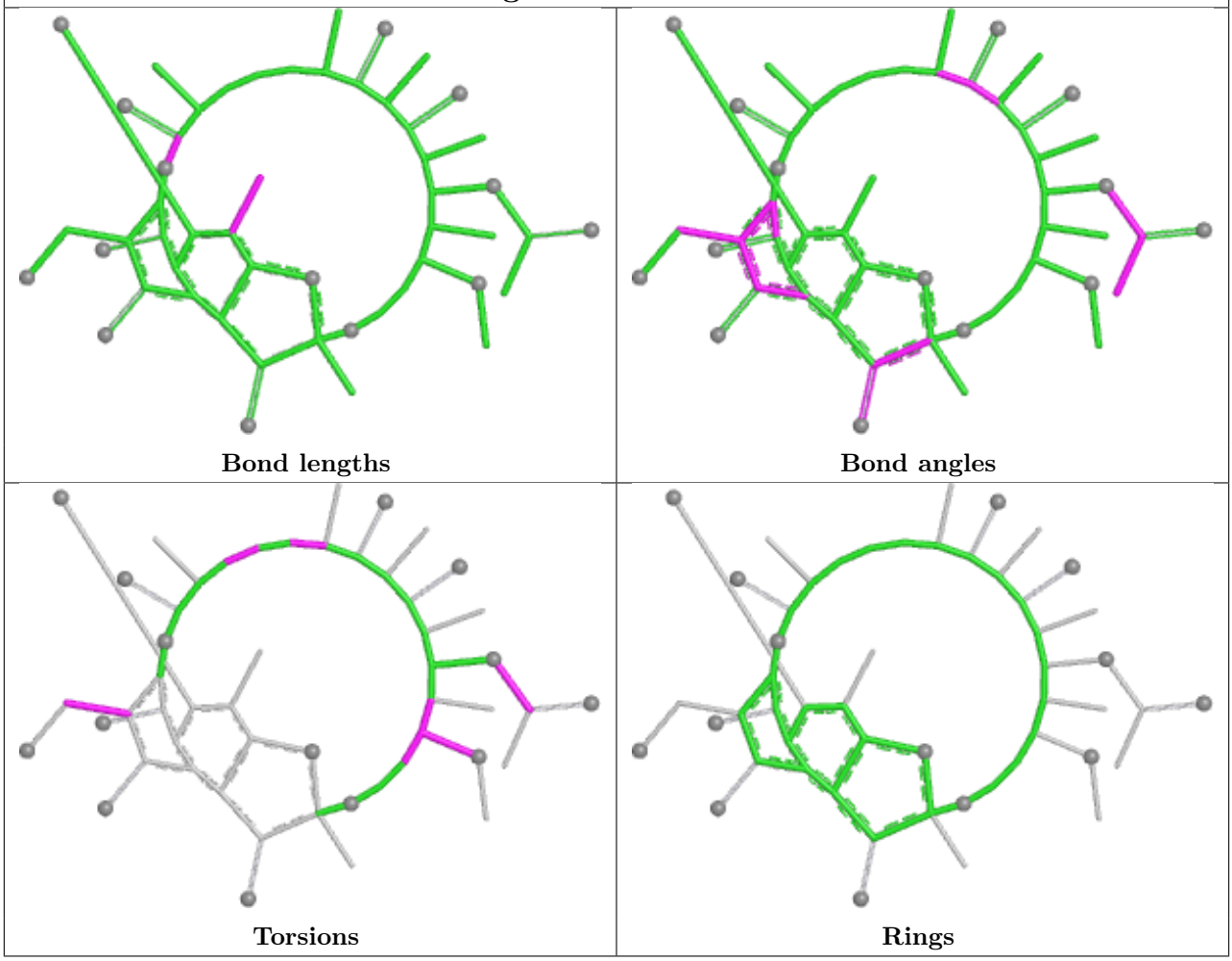
Ligand LMT C 1112



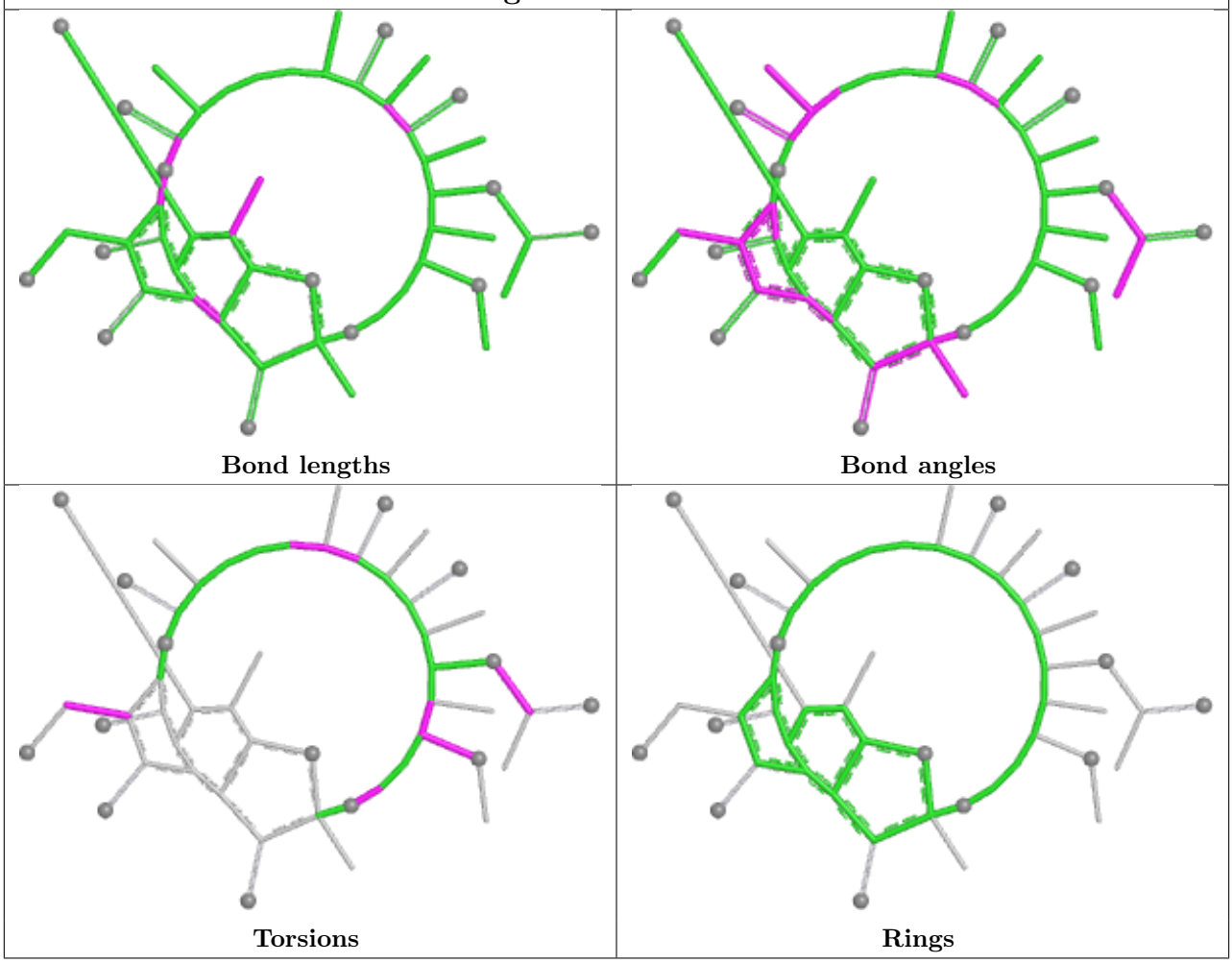
Ligand LMT B 1201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PTY C 1106	
 Bond lengths	 Bond angles
 Torsions	Rings

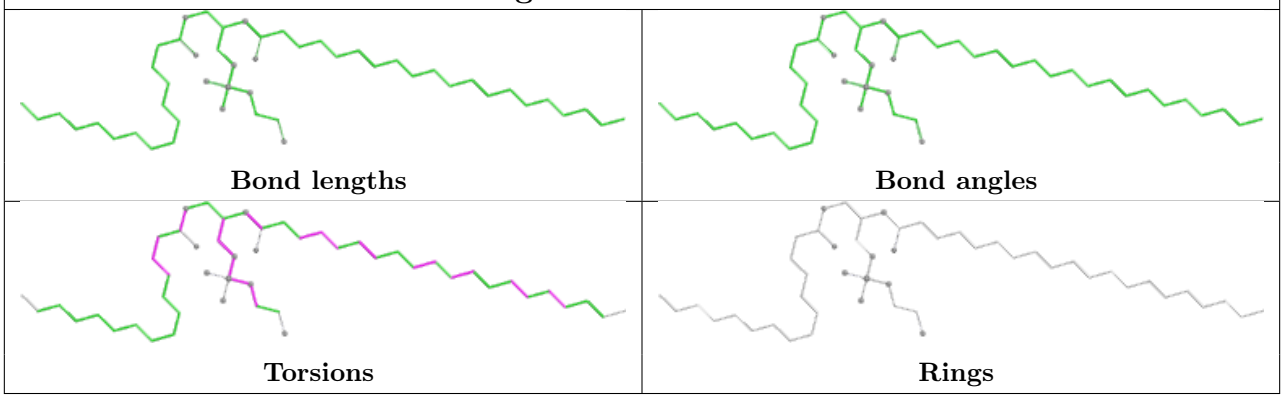
Ligand 3YI A 1209

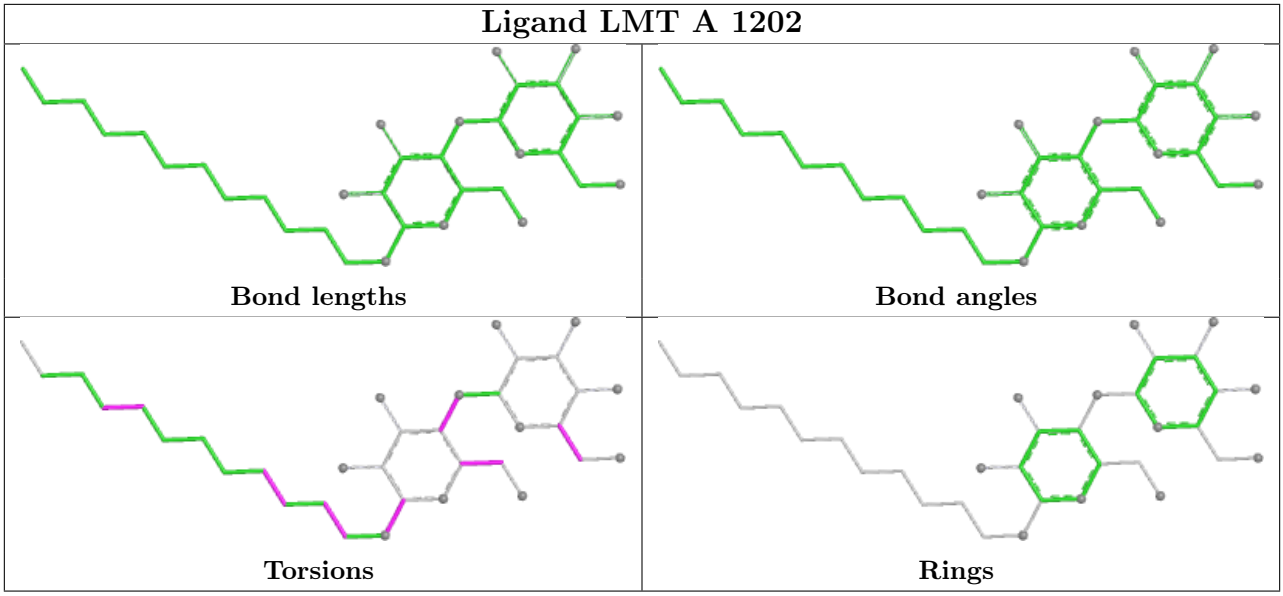


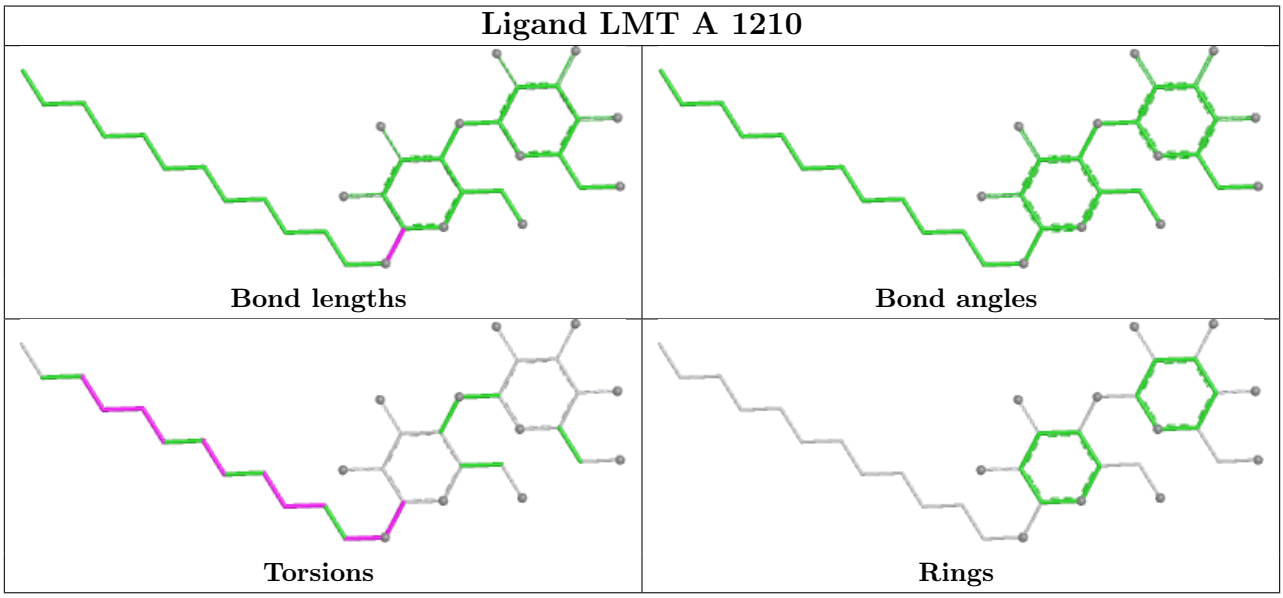
Ligand 3YI B 1206



Ligand PTY C 1101







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%)	0.19	29 (2%)	53	48	33, 55, 89, 103	9 (0%)
1	B	1023/1057 (96%)	0.14	33 (3%)	47	42	36, 54, 80, 116	4 (0%)
1	C	1034/1057 (97%)	0.01	17 (1%)	72	70	36, 49, 67, 84	0
2	D	153/169 (90%)	0.38	14 (9%)	9	6	43, 54, 74, 80	0
2	E	154/169 (91%)	1.23	39 (25%)	0	0	52, 66, 89, 100	0
All	All	3406/3509 (97%)	0.17	132 (3%)	39	34	33, 53, 81, 116	13 (0%)

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	997	SER	6.9
2	E	35	ALA	5.7
2	E	34	MET	5.6
1	A	868	LEU	5.6
2	E	33	LEU	4.7
2	E	36	ASN	4.6
1	A	866	GLU	4.6
1	A	870	GLY	4.6
1	A	869	SER	4.5
1	B	998	GLY	4.4
1	B	1009	GLY	4.3
1	B	676	THR	4.0
2	E	67	LEU	3.9
2	E	70	GLY	3.9
2	E	101	LYS	3.9
1	A	510	LYS	3.8
2	D	163	GLU	3.8
2	E	73	VAL	3.7
2	D	162	ALA	3.7
2	E	74	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
2	E	32	ILE	3.6
1	A	675	GLY	3.5
2	E	107	ASN	3.5
1	A	1042	HIS	3.5
2	E	66	LEU	3.5
2	E	99	LEU	3.5
2	D	165	LEU	3.4
1	B	1004	GLY	3.4
1	B	600	THR	3.4
1	B	1000	GLN	3.4
1	B	604	ASN	3.4
1	A	1039	ASP	3.3
2	D	140	ASN	3.3
1	B	595	THR	3.3
1	A	1040	ILE	3.3
2	D	149	ALA	3.3
1	B	638	PRO	3.3
1	B	134	SER	3.2
2	E	102	ASN	3.2
2	E	134	LYS	3.2
2	D	154	ILE	3.1
1	A	865	GLN	3.1
1	A	515	TRP	3.1
1	B	563	PHE	3.1
1	A	871	ASN	3.1
1	C	253	VAL	3.0
2	E	71	ALA	3.0
1	A	255	GLN	3.0
2	E	51	LEU	2.9
2	E	37	GLY	2.9
1	A	501	ALA	2.9
2	E	68	LYS	2.9
1	A	833	PRO	2.8
1	B	510	LYS	2.8
2	D	160	ASP	2.8
2	D	161	LEU	2.8
2	E	28	ASP	2.8
1	C	501	ALA	2.8
2	E	97	GLU	2.8
2	E	31	ARG	2.8
1	B	599	LEU	2.7
1	A	712	MET	2.7

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Mol	Chain	Res	Type	RSRZ
2	E	64	GLU	2.7
1	A	846	GLN	2.7
2	D	159	GLU	2.7
1	B	574	THR	2.7
1	B	396	PHE	2.6
1	B	634	TRP	2.6
1	C	362	PHE	2.6
2	E	27	ASP	2.6
1	B	674	LEU	2.6
2	E	163	GLU	2.6
1	B	596	HIS	2.6
2	E	98	VAL	2.6
2	D	150	PHE	2.6
1	B	603	LYS	2.6
2	E	84	LEU	2.6
2	E	103	GLY	2.6
1	A	707	ALA	2.6
2	D	139	VAL	2.5
1	C	508	GLY	2.5
1	C	701	GLN	2.5
1	C	513	PHE	2.5
1	A	537	SER	2.5
1	C	255	GLN	2.5
1	B	833	PRO	2.5
1	A	677	ALA	2.4
2	E	61	GLU	2.4
1	B	918	PHE	2.4
2	E	126	LEU	2.4
1	B	191	ASN	2.4
1	A	362	PHE	2.4
1	A	536	ARG	2.4
1	A	867	ARG	2.4
1	B	255	GLN	2.3
2	E	14	LEU	2.3
1	C	502	LYS	2.3
1	B	640	GLU	2.3
1	C	702	LEU	2.3
2	E	108	ALA	2.3
1	C	423	GLU	2.3
1	C	673	GLU	2.3
2	D	141	ALA	2.3
1	B	513	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	811	TYR	2.2
1	C	791	VAL	2.2
1	C	850	LYS	2.2
1	A	421	ALA	2.2
2	E	165	LEU	2.2
2	E	69	ASN	2.2
1	B	558	ARG	2.2
2	E	106	VAL	2.2
1	B	633	ASP	2.2
1	C	510	LYS	2.2
1	A	500	ILE	2.2
2	E	153	SER	2.2
1	B	597	TYR	2.2
1	A	837	THR	2.2
1	B	1033	PHE	2.1
1	C	498	LYS	2.1
2	D	138	ASP	2.1
2	E	60	LEU	2.1
1	A	259	ARG	2.1
1	A	957	GLY	2.1
1	B	254	ASN	2.1
1	C	730	ASP	2.1
1	A	425	LEU	2.1
2	E	13	ASP	2.1
1	B	196	PHE	2.1
2	D	129	VAL	2.0
1	B	598	TYR	2.0
2	E	146	GLY	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,

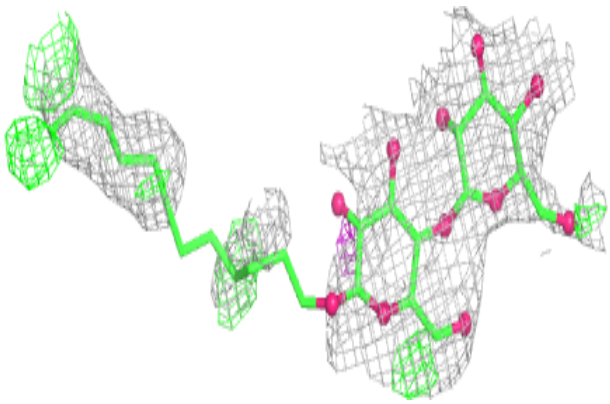
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

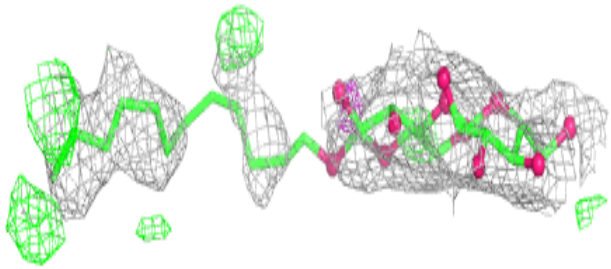
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	LMT	C	1112	35/35	0.59	0.34	95,102,105,107	0
3	LMT	A	1210	35/35	0.66	0.36	77,102,113,113	0
3	LMT	A	1206	35/35	0.68	0.41	77,93,102,103	0
10	PTY	C	1106	50/50	0.69	0.38	83,97,124,126	0
10	PTY	C	1101	50/50	0.74	0.32	76,82,91,93	0
11	D12	C	1104	12/12	0.74	0.33	65,66,67,67	0
5	EDO	E	202	4/4	0.76	0.32	56,57,57,57	0
4	D10	A	1204	10/10	0.76	0.29	65,66,66,66	0
3	LMT	B	1204	35/35	0.77	0.49	101,111,114,114	0
5	EDO	C	1109	4/4	0.78	0.28	57,57,58,58	0
3	LMT	A	1202	35/35	0.79	0.30	71,93,104,104	0
3	LMT	C	1105	35/35	0.80	0.37	87,96,98,98	0
3	LMT	B	1201	35/35	0.80	0.40	96,99,101,102	0
11	D12	C	1103	12/12	0.84	0.29	64,64,64,64	0
12	R16	C	1107	16/16	0.84	0.23	65,68,71,71	0
3	LMT	A	1201	35/35	0.85	0.26	74,84,92,93	0
5	EDO	A	1211	4/4	0.85	0.24	59,60,60,60	0
3	LMT	A	1203	35/35	0.85	0.48	91,92,93,94	0
14	DDQ	C	1111	14/14	0.85	0.22	77,78,79,79	0
7	GOL	E	201	6/6	0.86	0.23	62,62,62,63	0
3	LMT	C	1102	35/35	0.87	0.27	62,66,67,68	0
5	EDO	B	1205	4/4	0.88	0.14	65,65,65,66	0
5	EDO	A	1208	4/4	0.88	0.33	57,58,58,58	0
5	EDO	A	1207	4/4	0.89	0.30	69,69,69,70	0
6	3YI	B	1206	52/52	0.90	0.26	61,63,65,66	0
7	GOL	C	1110	6/6	0.90	0.28	77,77,77,77	0
5	EDO	A	1205	4/4	0.90	0.28	56,56,56,56	0
6	3YI	A	1209	52/52	0.91	0.20	65,68,71,71	0
8	HEX	B	1203	6/6	0.91	0.15	49,50,50,50	0
5	EDO	C	1113	4/4	0.92	0.18	48,49,49,49	0
7	GOL	B	1202	6/6	0.94	0.20	58,58,59,59	0
15	NA	C	1114	1/1	0.94	0.06	34,34,34,34	0
9	SO4	B	1207	5/5	0.96	0.22	82,83,83,84	0
13	CL	C	1108	1/1	0.97	0.24	41,41,41,41	0

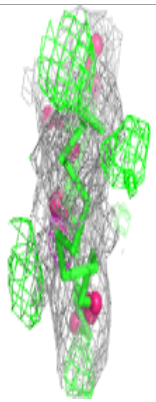
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT C 1112:

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

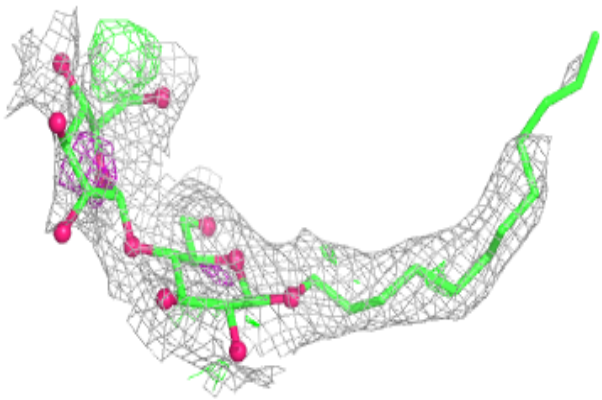


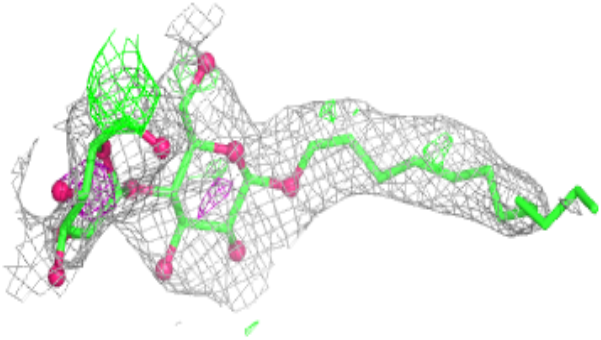


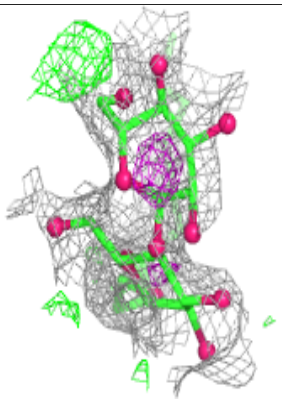


Electron density around LMT A 1210:

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

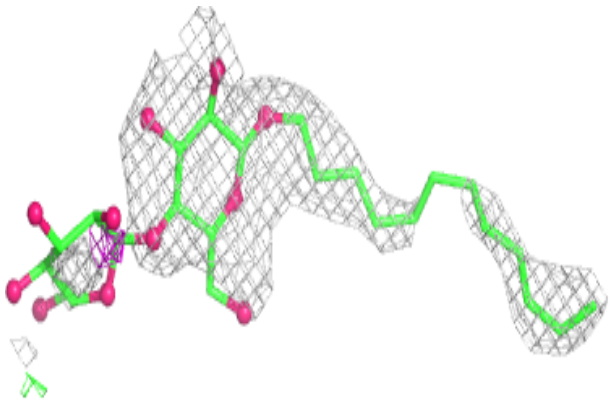


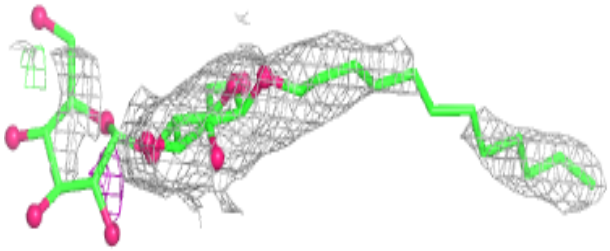


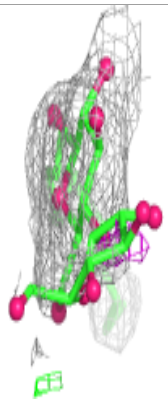


Electron density around LMT A 1206:

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

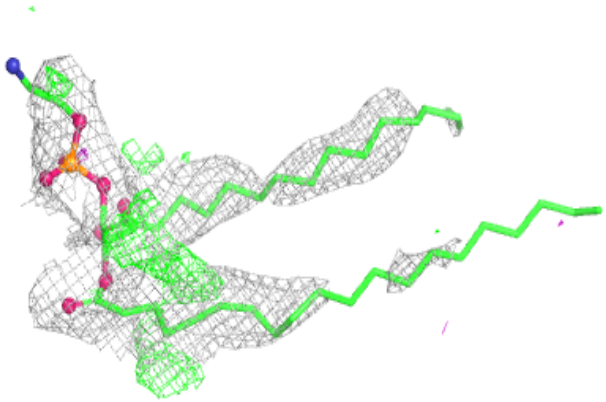


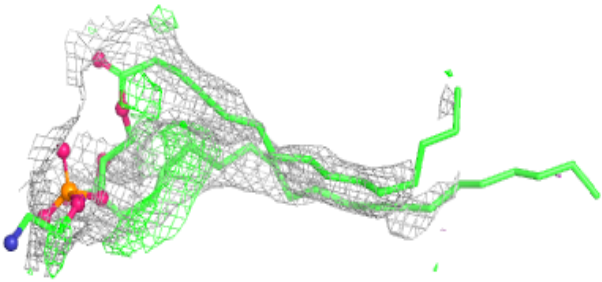


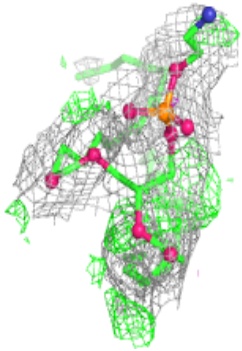


Electron density around PTY C 1106:

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

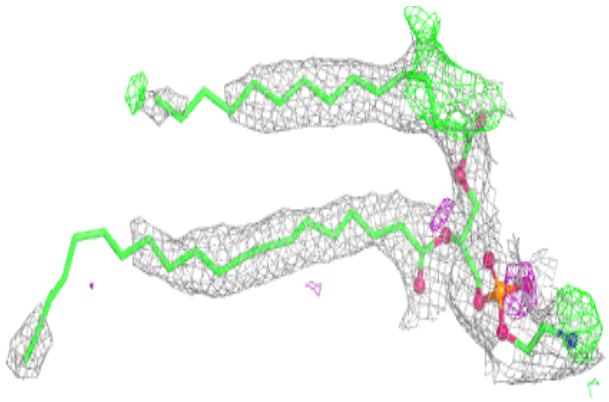


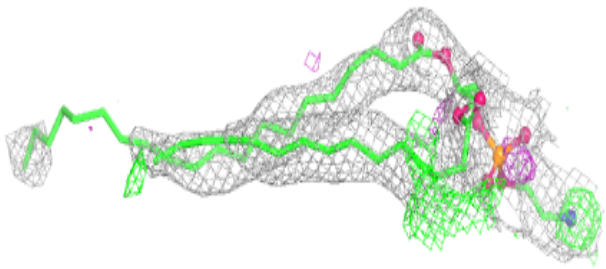


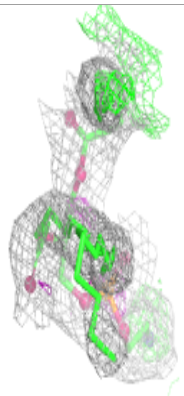


Electron density around PTY C 1101:

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

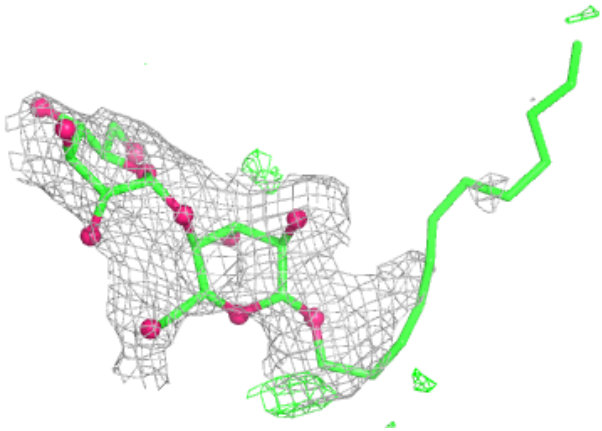


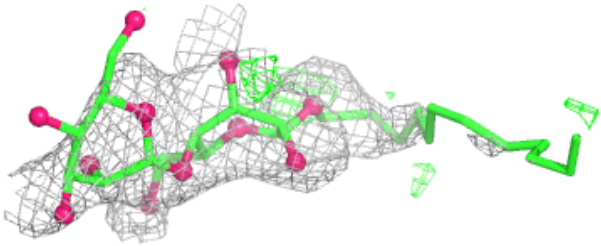


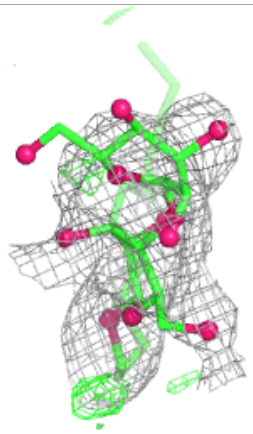


Electron density around LMT B 1204:

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

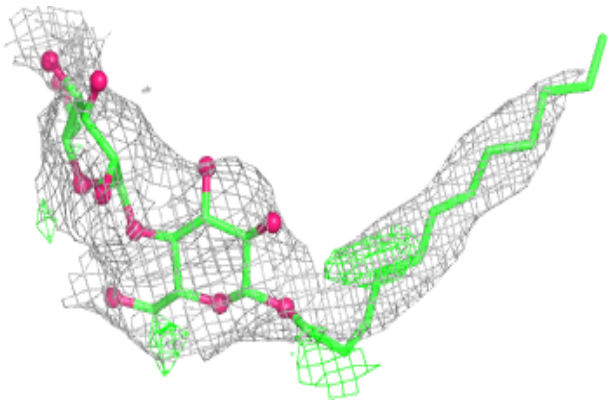


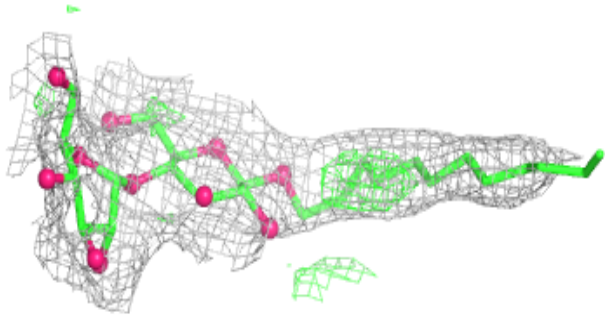


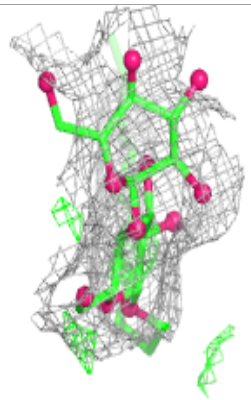


Electron density around LMT A 1202:

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

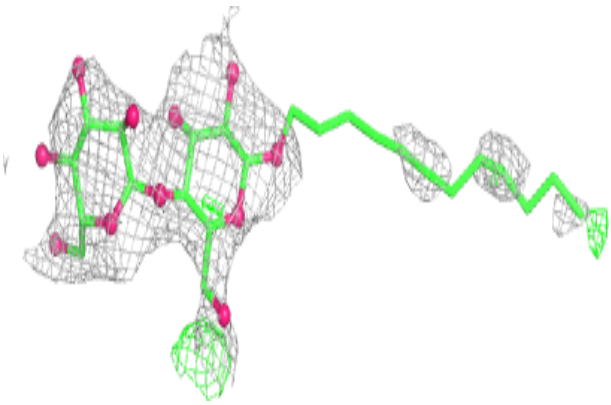


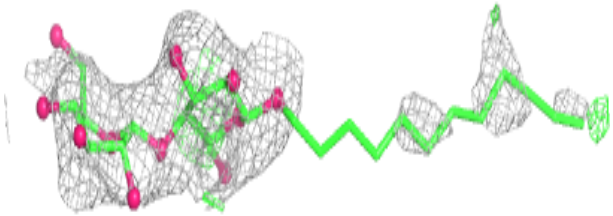


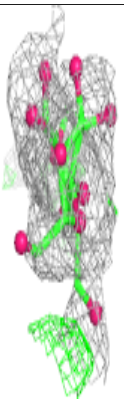


Electron density around LMT C 1105:

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

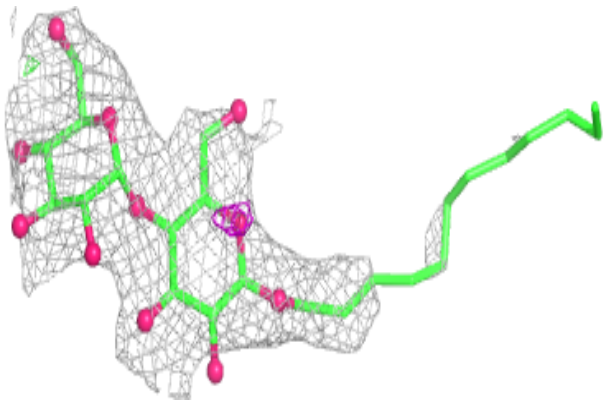


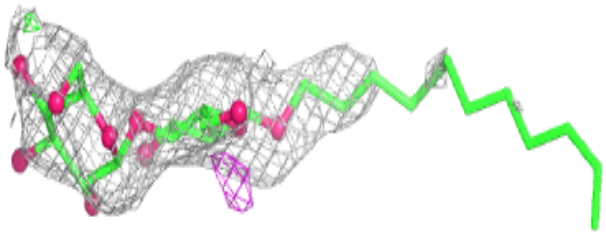


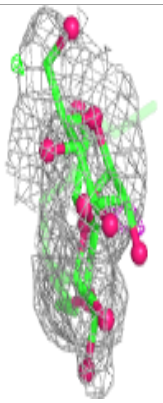


Electron density around LMT B 1201:

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

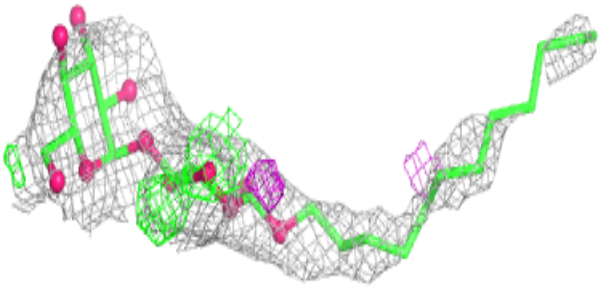


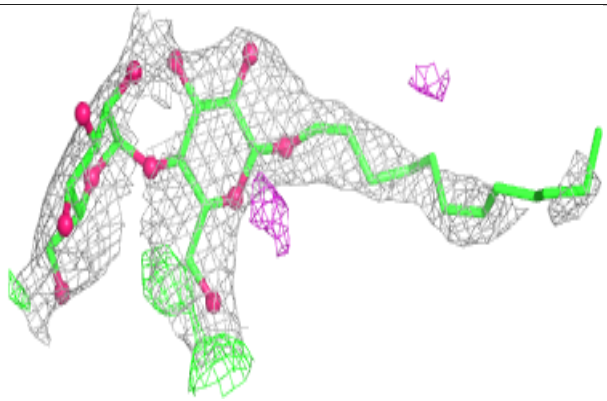


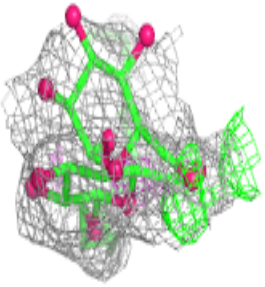


Electron density around LMT A 1201:

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

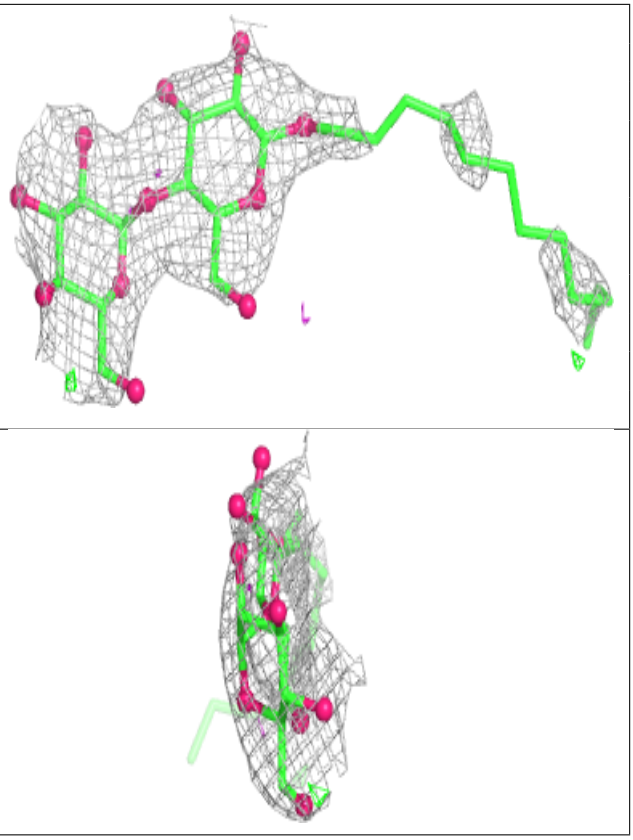






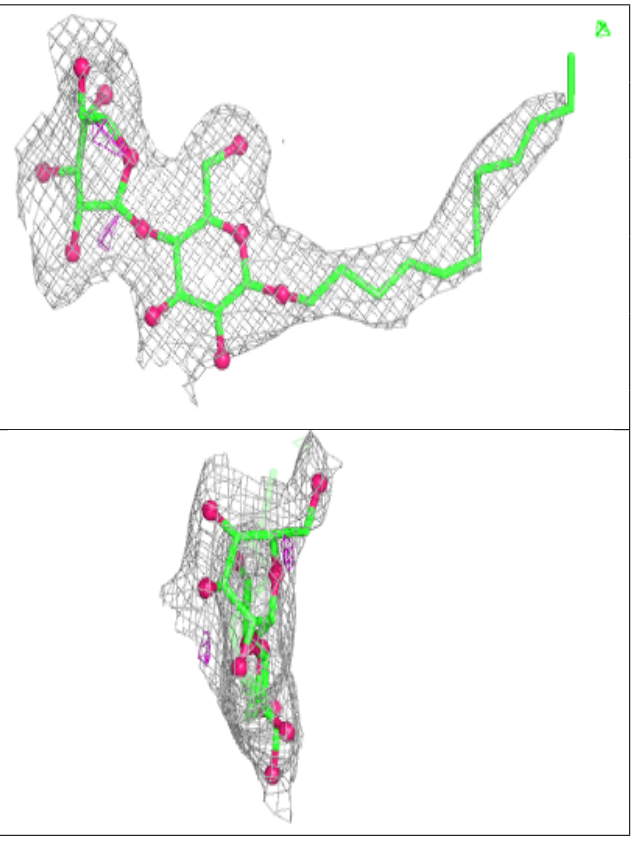
Electron density around LMT A 1203:

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



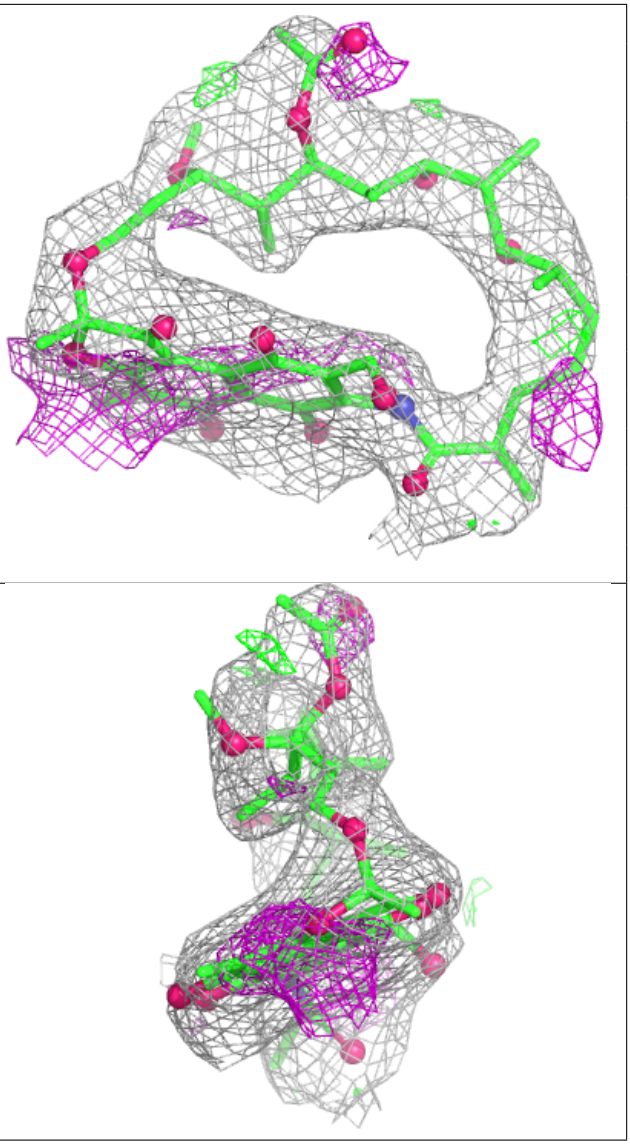
Electron density around LMT C 1102:

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



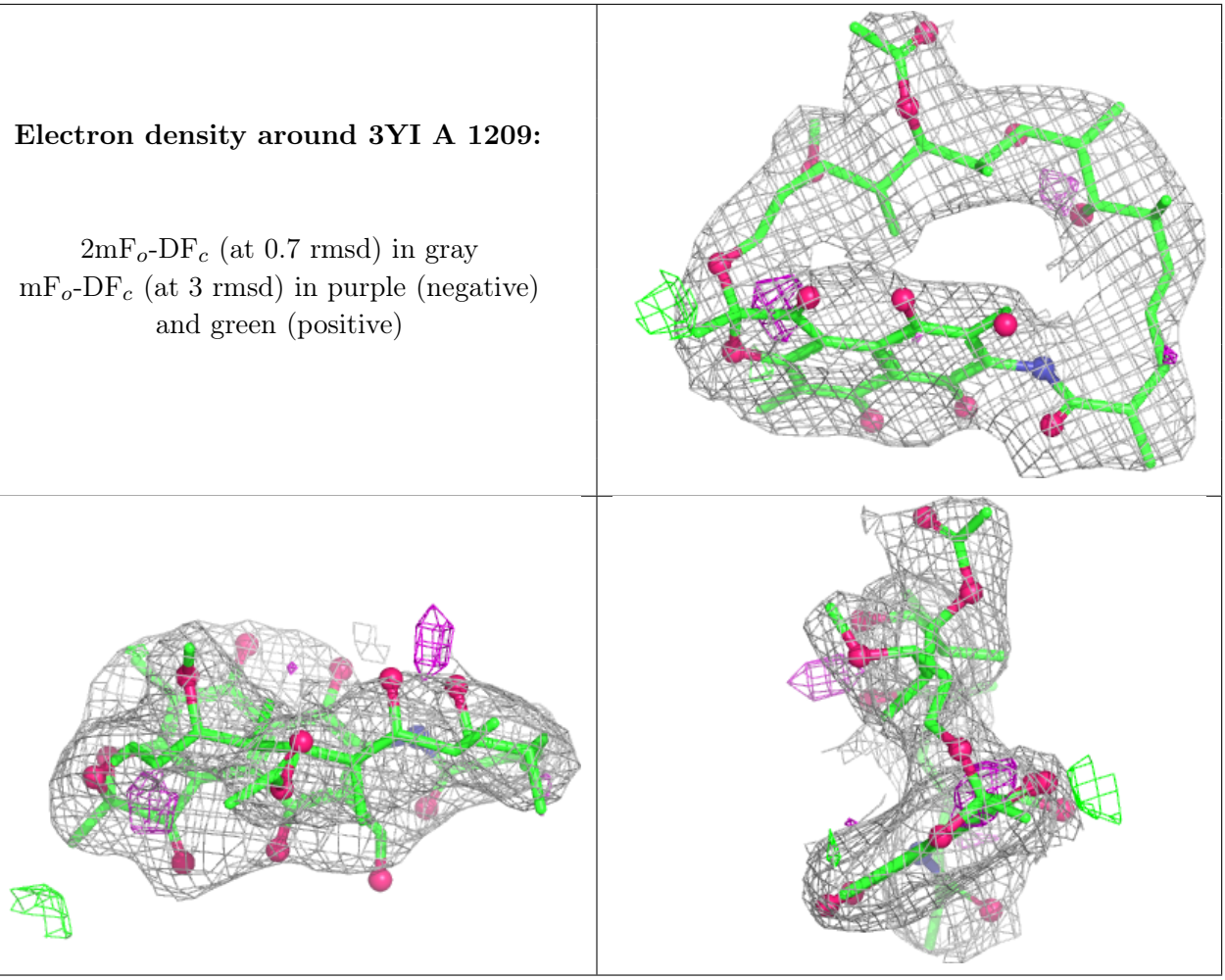
Electron density around 3YI B 1206:

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



Electron density around 3YI A 1209:

$2mF_o$-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.