



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:55 PM UTC

PDB ID : 6ZO8 / pdb_00006zo8
Title : Minocycline binding to the deep binding pocket of AcrB-G621P
Authors : Tam, H.K.; Foong, W.E.; Pos, K.M.
Deposited on : 2020-07-07
Resolution : 2.50 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

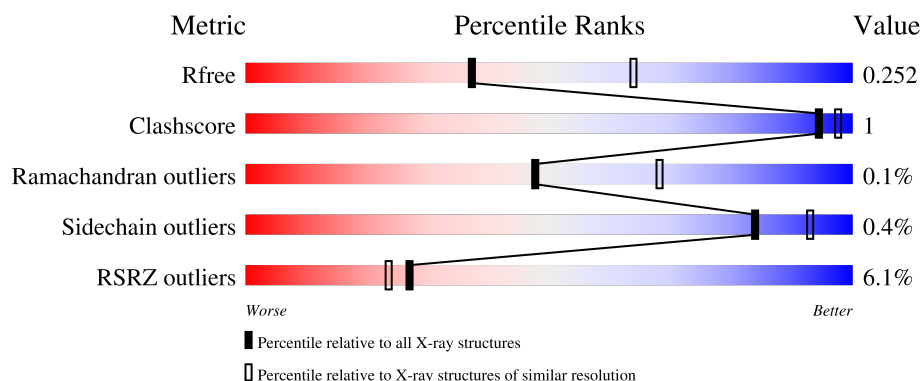
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 $\leq 5\%$. 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	10% 94% ..
1	B	1057	4% 93% ..
1	C	1057	3% 93% 5% .
2	D	169	5% 92% 8%
2	E	169	7% 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
14	HEX	C	1124	-	-	-	X

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 27356 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	0	0
			7930	5100	1311	1475	44			
1	B	1034	Total	C	N	O	S	0	0	0
			7858	5058	1296	1460	44			
1	C	1035	Total	C	N	O	S	0	3	0
			7885	5075	1302	1463	45			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	621	PRO	GLY	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	621	PRO	GLY	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	621	PRO	GLY	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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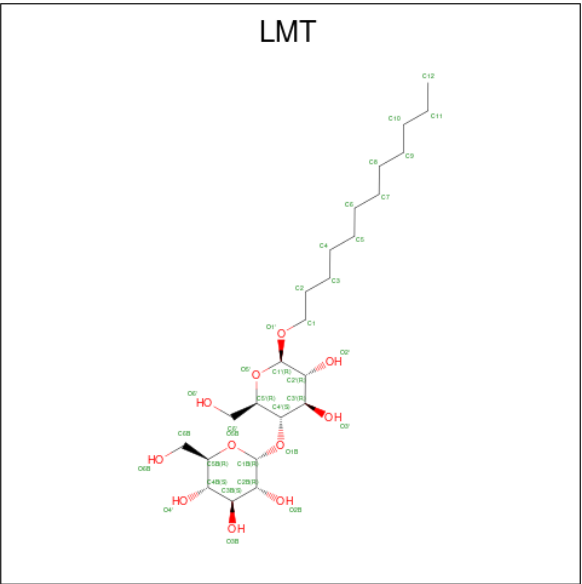
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Chain	Residue	Modelled	Actual	Comment	Reference
C	1054	HIS	-	expression tag	UNP P31224
C	1055	HIS	-	expression tag	UNP P31224
C	1056	HIS	-	expression tag	UNP P31224
C	1057	HIS	-	expression tag	UNP P31224

- Molecule 2 is a protein called DARPIN.

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

- Molecule 3 is DODECYL-BETA-D-MALTOSE (CCD ID: 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	A	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	0	0
			35	24	11		
3	C	1	Total	C	O	0	0
			35	24	11		
3	C	1	Total	C	O	0	0
			35	24	11		
3	C	1	Total	C	O	0	0
			35	24	11		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



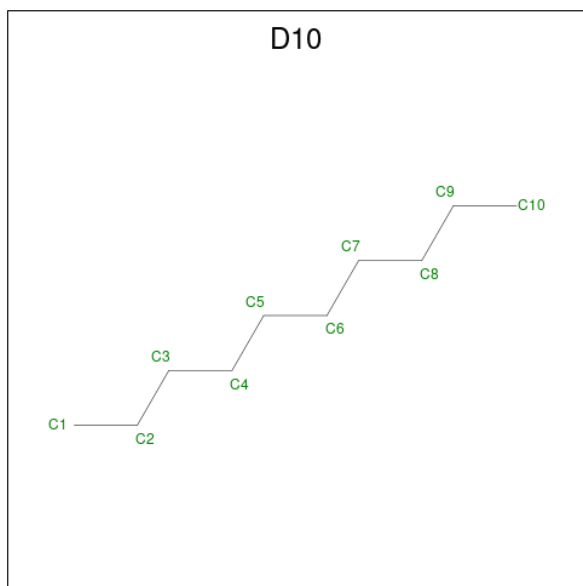
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 5 is DECANE (CCD ID: D10) (formula: C₁₀H₂₂).



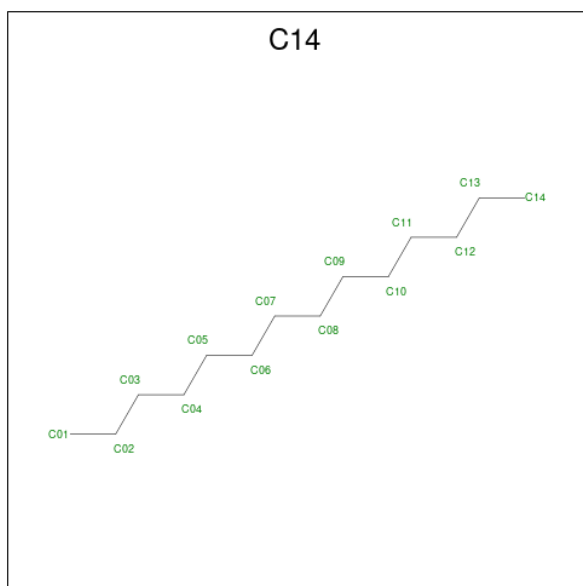
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C 10 10	0	0
5	A	1	Total C 10 10	0	0

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

- Molecule 6 is TETRADECANE (CCD ID: C14) (formula: C₁₄H₃₀).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C 14 14	0	0
6	C	1	Total C 14 14	0	0

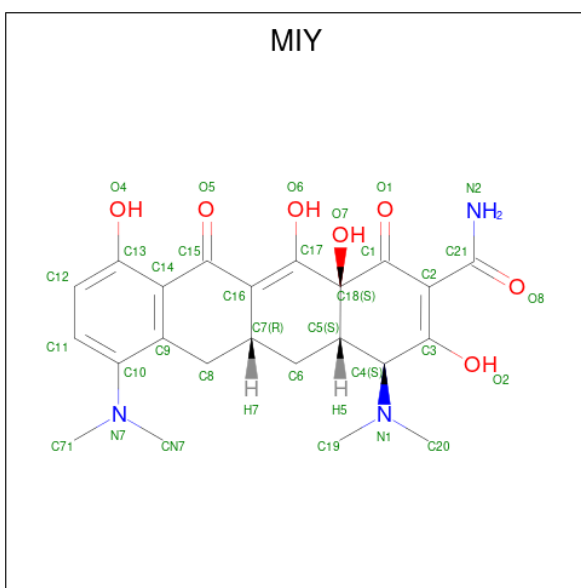
- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

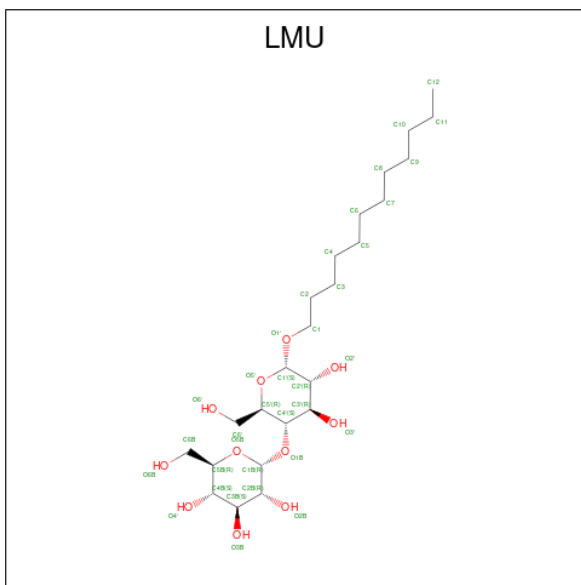
- Molecule 8 is (4S,4AS,5AR,12AS)-4,7-BIS(DIMETHYLAMINO)-3,10,12,12A-TETRAHYDROXY-1,11-DIOXO-1,4,4A,5,5A,6,11,12A-OCTAHYDROTETRACENE-2-CARBOXAMIDE (CCD ID: MIY) (formula: C₂₃H₂₇N₃O₇) (labeled as "Ligand of Interest")

by depositor).



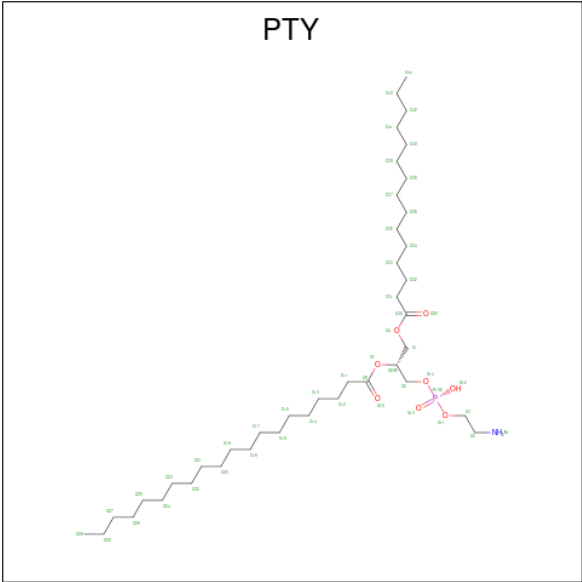
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	N	O	0	0
			33	23	3	7		

- Molecule 9 is DODECYL-ALPHA-D-MALTOSE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$).



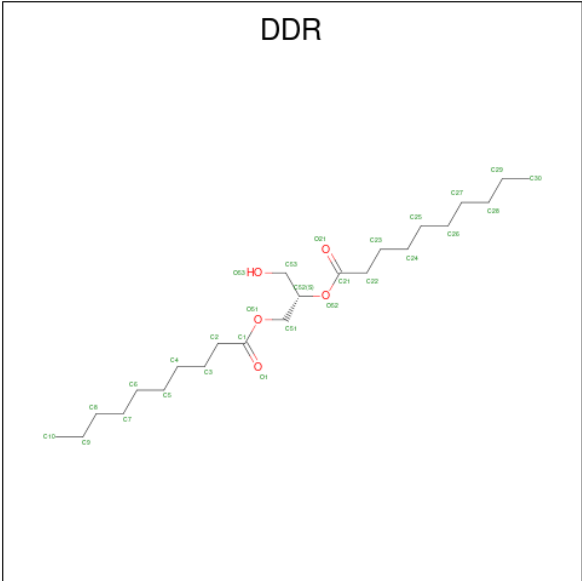
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			35	24	11		

- Molecule 10 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: $C_{40}H_{80}NO_8P$).



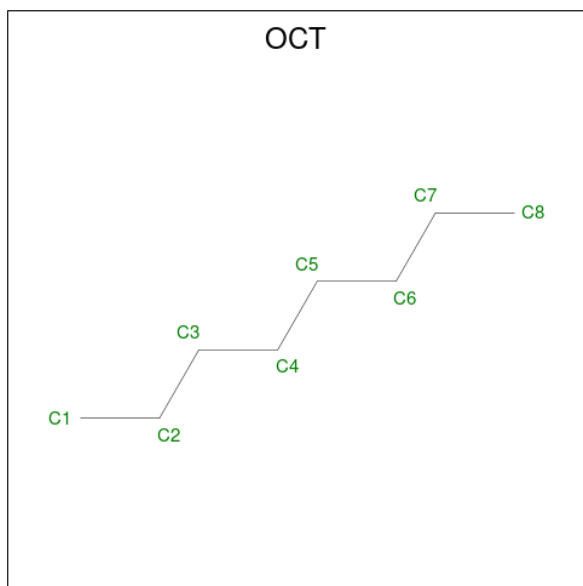
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	P	0	0
			50	40	1	8	1		
10	C	1	Total	C	N	O	P	0	0
			50	40	1	8	1		

- Molecule 11 is (2S)-3-hydroxypropane-1,2-diyl didecanoate (CCD ID: DDR) (formula: C₂₃H₄₄O₅).



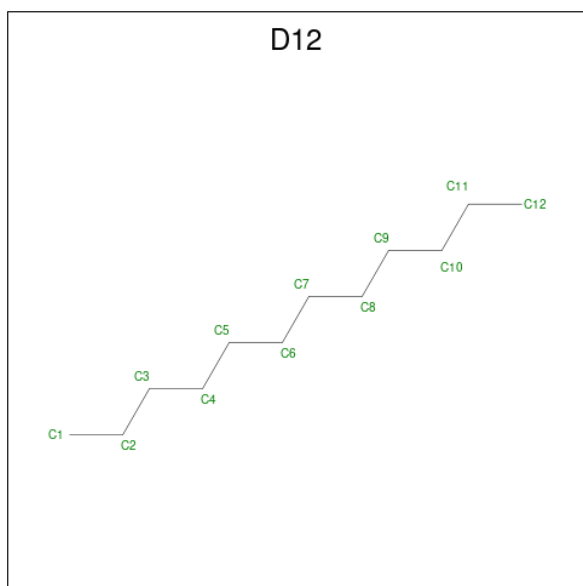
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	C	O	0	0
			28	23	5		

- Molecule 12 is N-OCTANE (CCD ID: OCT) (formula: C_8H_{18}).



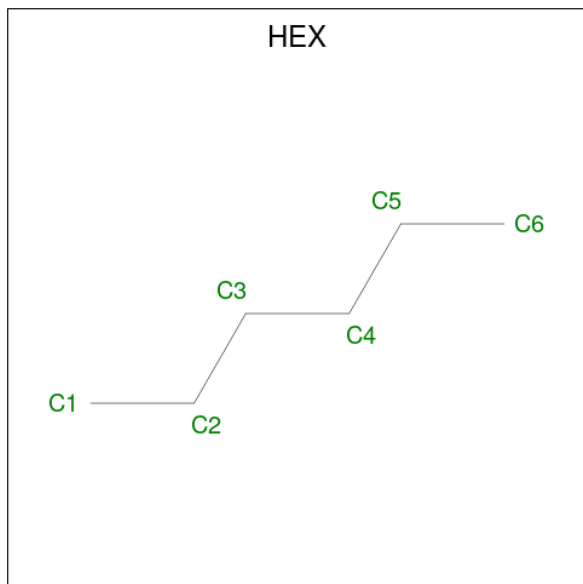
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	B	1	Total C 8 8	0	0
12	C	1	Total C 8 8	0	0
12	C	1	Total C 8 8	0	0

- Molecule 13 is DODECANE (CCD ID: D12) (formula: $C_{12}H_{26}$).



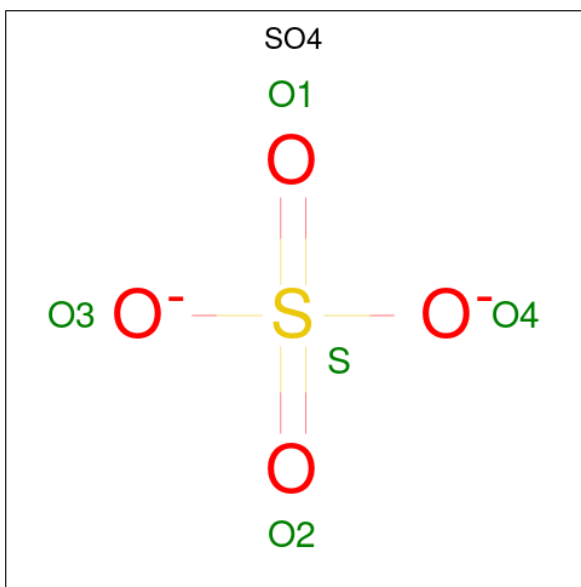
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	B	1	Total C 12 12	0	0
13	C	1	Total C 12 12	0	0
13	C	1	Total C 12 12	0	0

- Molecule 14 is HEXANE (CCD ID: HEX) (formula: C₆H₁₄).



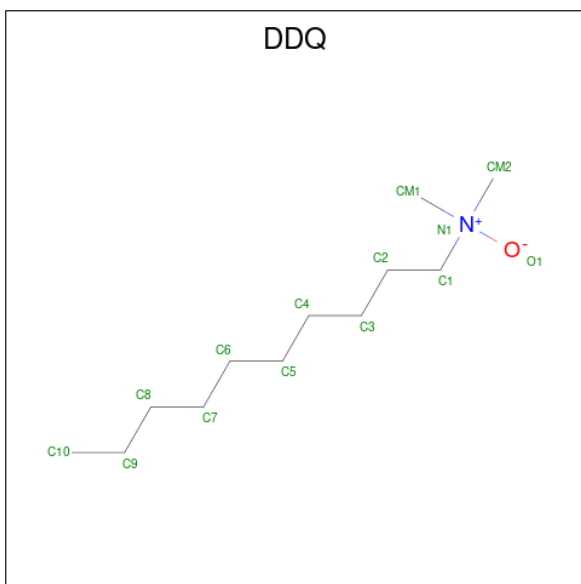
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	B	1	Total C 6 6	0	0
14	C	1	Total C 6 6	0	0
14	C	1	Total C 6 6	0	0

- Molecule 15 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 16 is DECYLAMINE-N,N-DIMETHYL-N-OXIDE (CCD ID: DDQ) (formula: C₁₂H₂₇NO).



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

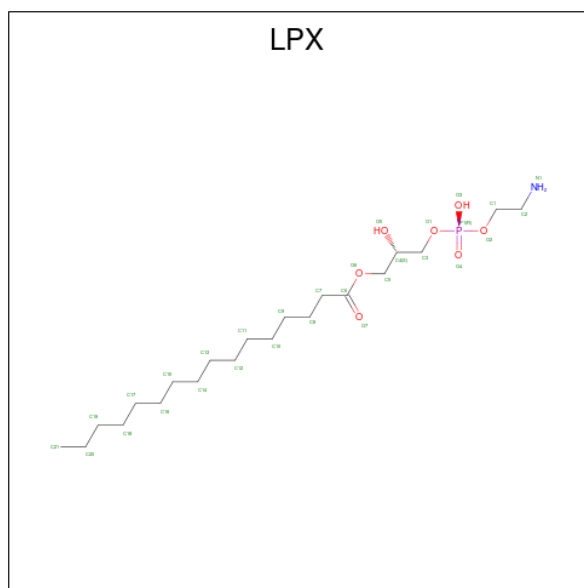
- Molecule 17 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	B	1	Total	Na	0	0
			1	1		

- Molecule 18 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	B	1	Total	Cl	0	0
			1	1		

- Molecule 19 is (2S)-3-{[(R)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-hydroxypropyl hexadecanoate (CCD ID: LPX) (formula: C₂₁H₄₄NO₇P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	C	1	Total	C	N	O	P	0	0
			30	21	1	7	1		
19	C	1	Total	C	N	O	P	0	0
			30	21	1	7	1		

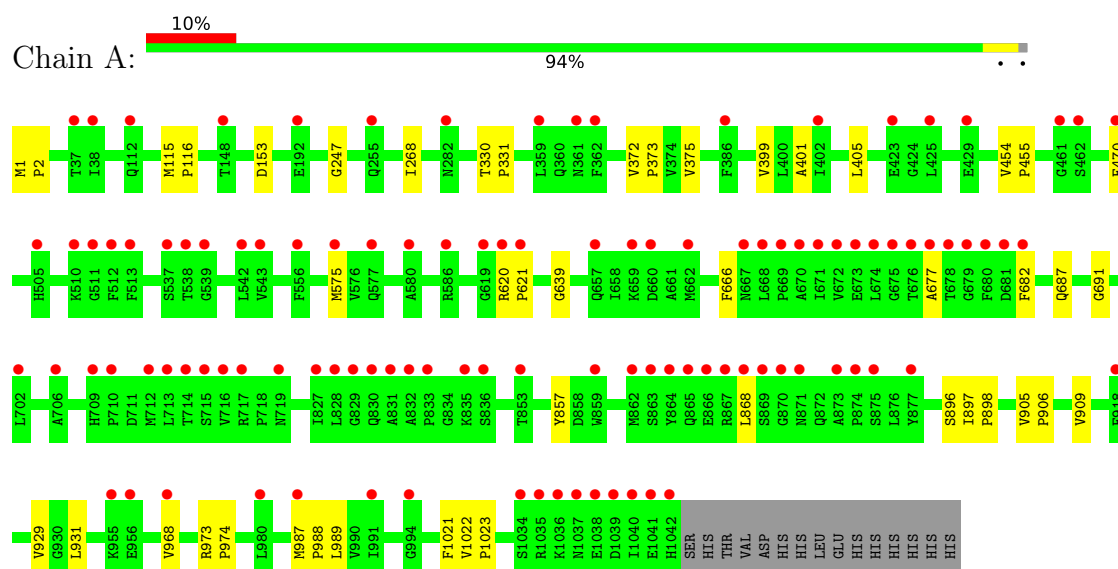
- Molecule 20 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	105	Total 107	O 107	0	2
20	B	137	Total 139	O 139	0	2
20	C	140	Total 141	O 141	0	1
20	D	28	Total 28	O 28	0	0
20	E	2	Total 2	O 2	0	0

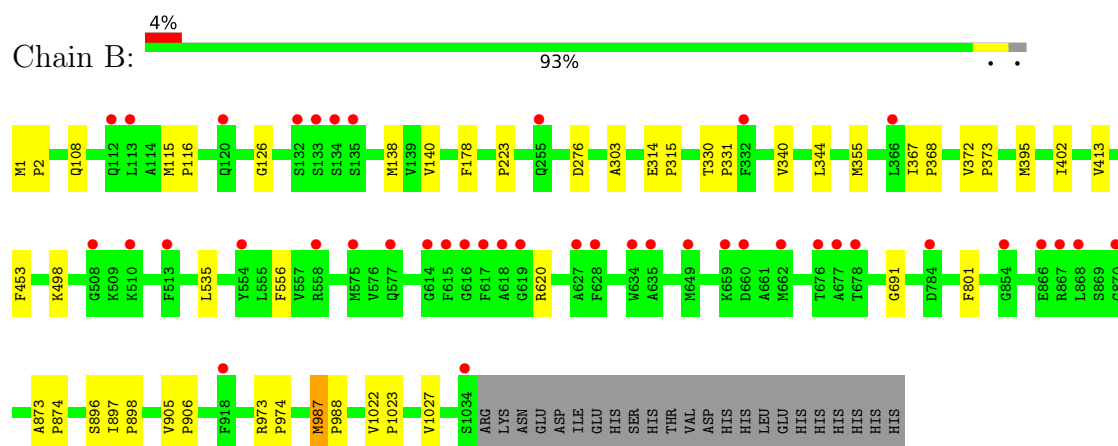
3 Residue-property plots

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



• Molecule 1: Multidrug efflux pump subunit AcrB



• Molecule 1: Multidrug efflux pump subunit AcrB



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	146.41Å 161.62Å 245.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.87 – 2.50 48.87 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.87-2.50) 100.0 (48.87-2.50)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0232	Depositor
R, R_{free}	0.219 , 0.249 0.223 , 0.252	Depositor DCC
R_{free} test set	9946 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	50.4	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 33.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	27356	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.01% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: LPX, D10, LMU, DDR, CL, NA, DDQ, MIY, C14, D12, LMT, SO4, OCT, HEX, GOL, PTY, EDO

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	1.02	0/8082	1.54	6/10975 (0.1%)
1	B	1.02	0/8009	1.53	5/10878 (0.0%)
1	C	1.01	0/8045	1.51	0/10925
2	D	1.03	0/1196	1.55	0/1626
2	E	1.03	0/1186	1.59	0/1613
All	All	1.02	0/26518	1.53	11/36017 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	896	SER	CA-C-N	7.61	125.04	120.24
1	A	896	SER	C-N-CA	7.61	125.04	120.24
1	B	896	SER	CA-C-N	6.74	124.49	120.24
1	B	896	SER	C-N-CA	6.74	124.49	120.24
1	A	639	GLY	CA-C-O	-5.70	118.30	122.23
1	A	1021	PHE	CA-C-N	5.55	123.74	120.24
1	A	1021	PHE	C-N-CA	5.55	123.74	120.24
1	A	691	GLY	CA-C-O	-5.42	118.55	122.45
1	B	691	GLY	CA-C-O	-5.17	118.44	122.52
1	B	453	PHE	CA-C-N	5.02	123.41	120.24
1	B	453	PHE	C-N-CA	5.02	123.41	120.24

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	7930	0	8076	21	0
1	B	7858	0	8010	25	0
1	C	7885	0	8046	26	0
2	D	1177	0	1159	0	0
2	E	1167	0	1151	0	0
3	A	175	0	230	0	0
3	B	35	0	46	0	0
3	C	105	0	138	0	0
4	A	12	0	16	0	0
4	B	30	0	40	0	0
4	C	54	0	72	0	0
5	A	20	0	44	0	0
5	B	20	0	44	0	0
5	C	30	0	66	1	0
6	A	14	0	30	0	0
6	C	14	0	30	0	0
7	A	8	0	12	0	0
7	B	16	0	24	0	0
7	C	8	0	12	0	0
7	D	12	0	18	0	0
7	E	4	0	6	0	0
8	B	33	0	24	1	0
9	B	35	0	46	0	0
10	B	50	0	79	0	0
10	C	50	0	79	1	0
11	B	28	0	44	0	0
12	B	8	0	18	0	0
12	C	16	0	36	0	0
13	B	12	0	26	0	0
13	C	24	0	52	0	0
14	B	6	0	14	0	0
14	C	12	0	28	0	0
15	B	5	0	0	0	0
15	C	10	0	0	0	0
16	B	14	0	27	0	0
17	B	1	0	0	0	0
18	B	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	C	60	0	86	3	0
20	A	107	0	0	0	0
20	B	139	0	0	0	0
20	C	141	0	0	0	0
20	D	28	0	0	0	0
20	E	2	0	0	0	0
All	All	27356	0	27829	73	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 (73) 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:57:VAL:HG21	1:C:86:GLY:HA2	1.69	0.75
1:A:375:VAL:HG11	1:A:405:LEU:HD22	1.79	0.65
1:C:979:SER:HA	1:C:1011:MET:HE3	1.81	0.62
1:A:968:VAL:HG11	1:A:1023:PRO:HG3	1.81	0.61
1:B:498:LYS:NZ	18:B:1123:CL:CL	2.74	0.58
1:B:535:LEU:HD22	1:B:1027:VAL:HG21	1.89	0.55
1:C:671:ILE:HG13	1:C:671:ILE:O	2.05	0.54
1:C:111:LEU:HD22	1:C:129:VAL:CG2	2.38	0.53
1:A:247:GLY:HA2	1:A:268:ILE:CD1	2.39	0.52
5:C:1116:D10:H102	19:C:1122:LPX:H7	1.90	0.52
1:A:372:VAL:HB	1:A:373:PRO:HD3	1.92	0.52
1:B:1022:VAL:N	1:B:1023:PRO:HD2	2.26	0.51
1:C:151:GLN:NE2	1:C:279:ALA:O	2.44	0.51
10:C:1104:PTY:H162	10:C:1104:PTY:H331	1.95	0.48
1:C:314:GLU:N	1:C:315:PRO:HD2	2.29	0.48
1:A:575:MET:HG2	1:A:666:PHE:CE1	2.50	0.47
1:B:873:ALA:HB3	1:B:874:PRO:HD3	1.97	0.47
1:C:901:VAL:O	1:C:904:VAL:HG12	2.14	0.47
1:C:53:ASP:O	1:C:57:VAL:HG23	2.14	0.47
1:A:973:ARG:HB3	1:A:974:PRO:HD3	1.98	0.46
1:C:1:MET:HB3	1:C:2:PRO:HD3	1.98	0.46
1:C:336:SER:O	1:C:340:VAL:HG23	2.16	0.46
1:B:108:GLN:OE1	1:C:112[B]:GLN:HG3	2.16	0.46
1:B:897:ILE:N	1:B:898:PRO:CD	2.79	0.46
1:B:897:ILE:N	1:B:898:PRO:HD2	2.32	0.45
1:B:126:GLY:HA3	1:C:116:PRO:CB	2.46	0.45
1:C:463:THR:HG22	1:C:467:TYR:CZ	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:448:VAL:HG11	1:C:943:ILE:HD11	1.99	0.45
1:B:303:ALA:HB2	1:B:330:THR:HG21	1.99	0.45
1:B:314:GLU:HB2	1:B:315:PRO:HD3	1.99	0.45
1:B:340:VAL:HG21	1:B:395:MET:HB3	1.97	0.45
1:C:303:ALA:HB2	1:C:330:THR:HG21	1.99	0.45
1:A:909:VAL:HA	1:A:931:LEU:HD11	1.99	0.44
1:C:904:VAL:HG13	1:C:938:SER:HB3	1.99	0.44
19:C:1123:LPX:C8	19:C:1123:LPX:H14	2.47	0.44
1:B:223:PRO:HD3	1:C:275:TYR:CD1	2.52	0.44
1:C:330:THR:N	1:C:331:PRO:CD	2.80	0.44
1:B:344:LEU:HD23	1:B:402:ILE:HD11	2.00	0.44
1:C:892:TYR:O	1:C:893:GLU:C	2.60	0.44
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.99	0.44
1:B:355:MET:HE1	1:B:413:VAL:HG11	2.00	0.44
1:B:1:MET:HB3	1:B:2:PRO:HD3	1.99	0.43
1:B:138:MET:HE2	1:B:140:VAL:CG2	2.49	0.43
1:B:367:ILE:HB	1:B:368:PRO:HD3	2.00	0.43
1:C:454:VAL:HB	1:C:455:PRO:HD3	1.99	0.43
1:A:399:VAL:HG11	1:A:989:LEU:HD11	2.00	0.43
1:C:980:LEU:HG	1:C:984:LEU:HD13	2.00	0.43
1:A:401:ALA:O	1:A:405:LEU:HG	2.19	0.43
1:A:620:ARG:N	1:A:621:PRO:CD	2.82	0.42
1:A:897:ILE:N	1:A:898:PRO:CD	2.82	0.42
19:C:1123:LPX:H14	19:C:1123:LPX:H8	2.01	0.42
1:C:40:PRO:HB2	1:C:94:PHE:O	2.19	0.42
1:B:372:VAL:HB	1:B:373:PRO:HD3	2.00	0.42
1:A:330:THR:N	1:A:331:PRO:CD	2.82	0.42
1:C:905:VAL:HB	1:C:906:PRO:HD3	2.02	0.42
1:A:1022:VAL:N	1:A:1023:PRO:CD	2.83	0.42
1:A:454:VAL:N	1:A:455:PRO:CD	2.83	0.42
1:C:343:THR:HG23	1:C:988:PRO:HB2	2.02	0.42
1:B:973:ARG:N	1:B:974:PRO:HD2	2.35	0.42
1:A:115:MET:HB2	1:A:116:PRO:HD3	2.02	0.41
1:C:209:ALA:O	1:C:237:GLN:NE2	2.53	0.41
1:A:1:MET:HB3	1:A:2:PRO:HD3	2.03	0.41
1:A:987:MET:N	1:A:988:PRO:CD	2.84	0.41
1:A:470:PHE:CD2	1:A:929:VAL:HG11	2.56	0.41
1:A:682:PHE:CZ	1:A:857:TYR:HB2	2.56	0.41
1:B:178:PHE:CE1	8:B:1101:MIY:H713	2.56	0.41
1:B:987:MET:N	1:B:988:PRO:CD	2.84	0.41
1:C:57:VAL:CG2	1:C:86:GLY:HA2	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:905:VAL:HB	1:B:906:PRO:HD3	2.03	0.41
1:B:276:ASP:OD2	1:B:620:ARG:NH1	2.54	0.40
1:B:330:THR:N	1:B:331:PRO:CD	2.84	0.40
1:B:115:MET:N	1:B:116:PRO:CD	2.84	0.40
1:A:575:MET:HG2	1:A:666:PHE:HE1	1.86	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	1040/1057 (98%)	1013 (97%)	25 (2%)	2 (0%)	43	63
1	B	1032/1057 (98%)	1011 (98%)	21 (2%)	0	100	100
1	C	1036/1057 (98%)	1008 (97%)	28 (3%)	0	100	100
2	D	154/169 (91%)	151 (98%)	3 (2%)	0	100	100
2	E	152/169 (90%)	151 (99%)	1 (1%)	0	100	100
All	All	3414/3509 (97%)	3334 (98%)	78 (2%)	2 (0%)	48	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	868	LEU
1	A	677	ALA

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	849/864 (98%)	847 (100%)	2 (0%)	87	95
1	B	841/864 (97%)	838 (100%)	3 (0%)	84	93
1	C	845/864 (98%)	839 (99%)	6 (1%)	76	89
2	D	120/132 (91%)	120 (100%)	0	100	100
2	E	119/132 (90%)	119 (100%)	0	100	100
All	All	2774/2856 (97%)	2763 (100%)	11 (0%)	84	93

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	153	ASP
1	A	687	GLN
1	B	556	PHE
1	B	801	PHE
1	B	987	MET
1	C	81	ASN
1	C	176	GLN
1	C	558	ARG
1	C	662[A]	MET
1	C	662[B]	MET
1	C	795	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	A	194	ASN
1	A	237	GLN
1	A	361	ASN
1	A	605	ASN
1	A	865	GLN
1	A	1001	ASN
1	A	1042	HIS
1	B	58	GLN
1	B	218	GLN
1	B	231	ASN
1	B	747	ASN

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Mol	Chain	Res	Type
1	C	34	GLN
1	C	58	GLN
1	C	74	ASN
1	C	81	ASN
1	C	89	GLN
1	C	197	GLN
1	C	231	ASN
1	C	505	HIS
1	C	526	HIS
1	C	1001	ASN
2	D	59	HIS
2	D	92	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 68 ligands modelled in this entry, 2 are monoatomic - leaving 66 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	GOL	B	1107	-	5,5,5	0.10	0	5,5,5	0.27	0
4	GOL	C	1107	-	5,5,5	0.10	0	5,5,5	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	OCT	C	1118	-	7,7,7	0.10	0	6,6,6	0.07	0
9	LMU	B	1102	-	36,36,36	0.50	1 (2%)	47,47,47	0.87	1 (2%)
7	EDO	A	1112	-	3,3,3	0.07	0	2,2,2	0.17	0
3	LMT	A	1104	-	36,36,36	0.54	1 (2%)	47,47,47	0.87	2 (4%)
15	SO4	C	1129	-	4,4,4	0.34	0	6,6,6	0.08	0
4	GOL	C	1106	-	5,5,5	0.08	0	5,5,5	0.28	0
5	D10	A	1109	-	9,9,9	0.10	0	8,8,8	0.15	0
12	OCT	B	1113	-	7,7,7	0.11	0	6,6,6	0.08	0
7	EDO	B	1118	-	3,3,3	0.06	0	2,2,2	0.14	0
4	GOL	C	1110	-	5,5,5	0.10	0	5,5,5	0.29	0
4	GOL	B	1108	-	5,5,5	0.08	0	5,5,5	0.25	0
7	EDO	B	1119	-	3,3,3	0.07	0	2,2,2	0.12	0
4	GOL	C	1111	-	5,5,5	0.09	0	5,5,5	0.27	0
4	GOL	B	1109	-	5,5,5	0.09	0	5,5,5	0.25	0
14	HEX	B	1115	-	5,5,5	0.12	0	4,4,4	0.10	0
19	LPX	C	1123	-	29,29,29	0.30	0	31,33,33	0.35	0
3	LMT	C	1103	-	36,36,36	0.53	1 (2%)	47,47,47	0.90	2 (4%)
6	C14	A	1110	-	13,13,13	0.08	0	12,12,12	0.13	0
7	EDO	B	1117	-	3,3,3	0.05	0	2,2,2	0.09	0
4	GOL	C	1112	-	5,5,5	0.09	0	5,5,5	0.30	0
4	GOL	A	1107	-	5,5,5	0.08	0	5,5,5	0.24	0
4	GOL	A	1106	-	5,5,5	0.09	0	5,5,5	0.27	0
4	GOL	B	1110	-	5,5,5	0.10	0	5,5,5	0.31	0
4	GOL	C	1109	-	5,5,5	0.09	0	5,5,5	0.26	0
5	D10	B	1111	-	9,9,9	0.09	0	8,8,8	0.06	0
11	DDR	B	1105	-	27,27,27	1.24	2 (7%)	29,29,29	1.25	2 (6%)
13	D12	C	1120	-	11,11,11	0.25	0	10,10,10	0.50	0
7	EDO	B	1116	-	3,3,3	0.07	0	2,2,2	0.08	0
14	HEX	C	1125	-	5,5,5	0.13	0	4,4,4	0.09	0
4	GOL	C	1105	-	5,5,5	0.10	0	5,5,5	0.28	0
13	D12	C	1121	-	11,11,11	0.28	0	10,10,10	0.46	0
10	PTY	C	1104	-	49,49,49	0.26	0	52,54,54	0.37	0
7	EDO	C	1127	-	3,3,3	0.05	0	2,2,2	0.09	0
7	EDO	E	201	-	3,3,3	0.06	0	2,2,2	0.09	0
8	MIY	B	1101	-	36,36,36	1.05	2 (5%)	42,58,58	1.03	2 (4%)
15	SO4	B	1120	-	4,4,4	0.34	0	6,6,6	0.08	0
15	SO4	C	1128	-	4,4,4	0.35	0	6,6,6	0.06	0
14	HEX	C	1124	-	5,5,5	0.12	0	4,4,4	0.10	0
6	C14	C	1119	-	13,13,13	0.08	0	12,12,12	0.08	0
3	LMT	A	1101	-	36,36,36	0.48	0	47,47,47	0.73	0
3	LMT	B	1103	-	36,36,36	0.48	1 (2%)	47,47,47	0.54	0
3	LMT	A	1103	-	36,36,36	0.46	0	47,47,47	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	B	1106	-	5,5,5	0.08	0	5,5,5	0.19	0
7	EDO	D	201	-	3,3,3	0.08	0	2,2,2	0.08	0
7	EDO	D	202	-	3,3,3	0.07	0	2,2,2	0.11	0
7	EDO	D	203	-	3,3,3	0.07	0	2,2,2	0.14	0
4	GOL	C	1113	-	5,5,5	0.08	0	5,5,5	0.27	0
5	D10	B	1112	-	9,9,9	0.08	0	8,8,8	0.07	0
10	PTY	B	1104	-	49,49,49	0.26	0	52,54,54	0.33	0
13	D12	B	1114	-	11,11,11	0.27	0	10,10,10	0.48	0
5	D10	C	1114	-	9,9,9	0.09	0	8,8,8	0.06	0
3	LMT	A	1102	-	36,36,36	0.52	1 (2%)	47,47,47	0.78	2 (4%)
5	D10	A	1108	-	9,9,9	0.10	0	8,8,8	0.10	0
4	GOL	C	1108	-	5,5,5	0.10	0	5,5,5	0.28	0
5	D10	C	1115	-	9,9,9	0.09	0	8,8,8	0.06	0
16	DDQ	B	1121	-	11,13,13	2.23	2 (18%)	12,15,15	0.51	0
3	LMT	A	1105	-	36,36,36	0.56	1 (2%)	47,47,47	0.70	1 (2%)
7	EDO	C	1126	-	3,3,3	0.06	0	2,2,2	0.16	0
3	LMT	C	1102	-	36,36,36	0.59	1 (2%)	47,47,47	1.10	3 (6%)
7	EDO	A	1111	-	3,3,3	0.07	0	2,2,2	0.09	0
19	LPX	C	1122	-	29,29,29	0.29	0	31,33,33	0.36	0
5	D10	C	1116	-	9,9,9	0.09	0	8,8,8	0.08	0
12	OCT	C	1117	-	7,7,7	0.11	0	6,6,6	0.08	0
3	LMT	C	1101	-	36,36,36	0.46	0	47,47,47	0.56	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	GOL	B	1107	-	-	4/4/4/4	-
4	GOL	C	1107	-	-	2/4/4/4	-
12	OCT	C	1118	-	-	1/5/5/5	-
9	LMU	B	1102	-	-	9/21/61/61	0/2/2/2
7	EDO	A	1112	-	-	1/1/1/1	-
3	LMT	A	1104	-	-	14/21/61/61	0/2/2/2
4	GOL	C	1106	-	-	0/4/4/4	-
5	D10	A	1109	-	-	2/7/7/7	-
12	OCT	B	1113	-	-	0/5/5/5	-
7	EDO	B	1118	-	-	0/1/1/1	-
4	GOL	C	1110	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	B	1108	-	-	2/4/4/4	-
7	EDO	B	1119	-	-	1/1/1/1	-
4	GOL	C	1111	-	-	4/4/4/4	-
4	GOL	B	1109	-	-	2/4/4/4	-
14	HEX	B	1115	-	-	0/3/3/3	-
19	LPX	C	1123	-	-	19/31/31/31	-
3	LMT	C	1103	-	-	13/21/61/61	0/2/2/2
6	C14	A	1110	-	-	6/11/11/11	-
7	EDO	B	1117	-	-	1/1/1/1	-
4	GOL	C	1112	-	-	2/4/4/4	-
4	GOL	A	1107	-	-	0/4/4/4	-
4	GOL	A	1106	-	-	2/4/4/4	-
4	GOL	B	1110	-	-	2/4/4/4	-
4	GOL	C	1109	-	-	2/4/4/4	-
5	D10	B	1111	-	-	3/7/7/7	-
11	DDR	B	1105	-	-	13/29/29/29	-
13	D12	C	1120	-	-	2/9/9/9	-
7	EDO	B	1116	-	-	0/1/1/1	-
14	HEX	C	1125	-	-	1/3/3/3	-
4	GOL	C	1105	-	-	2/4/4/4	-
13	D12	C	1121	-	-	3/9/9/9	-
10	PTY	C	1104	-	-	34/53/53/53	-
7	EDO	C	1127	-	-	1/1/1/1	-
7	EDO	E	201	-	-	1/1/1/1	-
8	MIY	B	1101	-	-	0/12/70/70	0/4/4/4
14	HEX	C	1124	-	-	1/3/3/3	-
6	C14	C	1119	-	-	2/11/11/11	-
3	LMT	A	1101	-	-	11/21/61/61	0/2/2/2
3	LMT	B	1103	-	-	6/21/61/61	0/2/2/2
3	LMT	A	1103	-	-	11/21/61/61	0/2/2/2
4	GOL	B	1106	-	-	2/4/4/4	-
7	EDO	D	201	-	-	1/1/1/1	-
7	EDO	D	202	-	-	1/1/1/1	-
7	EDO	D	203	-	-	1/1/1/1	-
4	GOL	C	1113	-	-	0/4/4/4	-
5	D10	B	1112	-	-	2/7/7/7	-
10	PTY	B	1104	-	-	21/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	D12	B	1114	-	-	1/9/9/9	-
5	D10	C	1114	-	-	2/7/7/7	-
3	LMT	A	1102	-	-	12/21/61/61	0/2/2/2
5	D10	A	1108	-	-	4/7/7/7	-
4	GOL	C	1108	-	-	1/4/4/4	-
5	D10	C	1115	-	-	2/7/7/7	-
16	DDQ	B	1121	-	-	3/11/11/11	-
3	LMT	A	1105	-	-	15/21/61/61	0/2/2/2
7	EDO	C	1126	-	-	1/1/1/1	-
3	LMT	C	1102	-	-	15/21/61/61	0/2/2/2
7	EDO	A	1111	-	-	1/1/1/1	-
19	LPX	C	1122	-	-	13/31/31/31	-
5	D10	C	1116	-	-	4/7/7/7	-
12	OCT	C	1117	-	-	0/5/5/5	-
3	LMT	C	1101	-	-	7/21/61/61	0/2/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	1121	DDQ	O1-N1	-6.77	1.25	1.42
8	B	1101	MIY	C21-N2	4.99	1.47	1.33
11	B	1105	DDR	O52-C21	4.30	1.46	1.34
11	B	1105	DDR	O51-C1	4.23	1.45	1.33
16	B	1121	DDQ	C1-N1	-2.85	1.48	1.51
3	C	1102	LMT	O1'-C1'	2.55	1.44	1.40
3	A	1105	LMT	O1'-C1'	2.30	1.44	1.40
3	C	1103	LMT	O1'-C1'	2.29	1.44	1.40
8	B	1101	MIY	O5-C15	2.27	1.28	1.23
3	A	1104	LMT	O1'-C1'	2.18	1.43	1.40
9	B	1102	LMU	O1'-C1'	2.03	1.43	1.40
3	A	1102	LMT	O1'-C1'	2.02	1.43	1.40
3	B	1103	LMT	O1'-C1'	2.00	1.43	1.40

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	1105	DDR	O52-C21-C22	4.26	120.69	111.48
3	C	1102	LMT	C1-O1'-C1'	2.93	118.68	113.68
3	A	1104	LMT	C2'-C3'-C4'	2.88	116.21	109.68
11	B	1105	DDR	O51-C1-C2	2.84	120.49	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1102	LMT	O1'-C1'-C2'	2.76	112.47	108.27
3	C	1103	LMT	O1'-C1'-C2'	2.57	112.18	108.27
3	C	1102	LMT	C1'-O5'-C5'	2.57	118.74	113.72
3	A	1102	LMT	C1B-C2B-C3B	2.46	115.18	110.01
3	A	1104	LMT	C1'-C2'-C3'	2.44	115.14	110.01
8	B	1101	MIY	C18-C5-C4	2.43	114.96	111.64
9	B	1102	LMU	C1'-C2'-C3'	2.33	114.90	110.01
3	A	1102	LMT	O1B-C4'-C3'	2.27	112.99	107.23
3	A	1105	LMT	C1'-O5'-C5'	2.17	117.97	113.72
3	C	1103	LMT	C2'-C3'-C4'	2.14	114.53	109.68
8	B	1101	MIY	O7-C18-C17	-2.08	106.82	110.14

There are no chirality outliers.

All (291) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1105	LMT	C2'-C1'-O1'-C1
3	A	1105	LMT	O5'-C1'-O1'-C1
3	C	1102	LMT	O5'-C1'-O1'-C1
3	C	1103	LMT	O5'-C1'-O1'-C1
4	A	1106	GOL	C1-C2-C3-O3
4	B	1107	GOL	C1-C2-C3-O3
4	C	1107	GOL	O1-C1-C2-C3
4	C	1110	GOL	C1-C2-C3-O3
4	C	1111	GOL	O1-C1-C2-C3
4	C	1112	GOL	O1-C1-C2-C3
10	B	1104	PTY	C11-C8-O7-C6
10	B	1104	PTY	C3-O11-P1-O12
10	B	1104	PTY	C5-O14-P1-O11
10	B	1104	PTY	C5-O14-P1-O13
10	C	1104	PTY	N1-C2-C3-O11
10	C	1104	PTY	O14-C5-C6-O7
10	C	1104	PTY	C11-C8-O7-C6
10	C	1104	PTY	C5-O14-P1-O11
10	C	1104	PTY	C5-O14-P1-O13
19	C	1122	LPX	C3-O1-P1-O2
19	C	1122	LPX	C3-O1-P1-O4
19	C	1122	LPX	C1-O2-P1-O1
19	C	1122	LPX	C1-O2-P1-O3
19	C	1122	LPX	C1-O2-P1-O4
19	C	1123	LPX	O5-C4-C5-O6
19	C	1123	LPX	C3-O1-P1-O3

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Mol	Chain	Res	Type	Atoms
19	C	1123	LPX	C1-O2-P1-O1
19	C	1123	LPX	C1-O2-P1-O3
19	C	1123	LPX	C1-O2-P1-O4
19	C	1123	LPX	O2-C1-C2-N1
3	A	1104	LMT	O5B-C1B-O1B-C4'
3	A	1105	LMT	O5B-C1B-O1B-C4'
10	C	1104	PTY	O30-C30-O4-C1
19	C	1123	LPX	O7-C6-O6-C5
3	C	1102	LMT	O5B-C1B-O1B-C4'
10	B	1104	PTY	O10-C8-O7-C6
10	C	1104	PTY	O10-C8-O7-C6
10	C	1104	PTY	C31-C30-O4-C1
19	C	1123	LPX	C7-C6-O6-C5
3	A	1102	LMT	C3'-C4'-O1B-C1B
3	B	1103	LMT	O5'-C5'-C6'-O6'
3	C	1102	LMT	C3'-C4'-O1B-C1B
11	B	1105	DDR	C2-C1-O51-C51
11	B	1105	DDR	C22-C21-O52-C52
3	A	1105	LMT	O5'-C5'-C6'-O6'
11	B	1105	DDR	O1-C1-O51-C51
11	B	1105	DDR	O21-C21-O52-C52
3	A	1104	LMT	C4B-C5B-C6B-O6B
3	B	1103	LMT	C4'-C5'-C6'-O6'
3	A	1101	LMT	O5'-C1'-O1'-C1
3	A	1102	LMT	O5'-C1'-O1'-C1
3	A	1104	LMT	O5'-C1'-O1'-C1
3	C	1101	LMT	C4'-C5'-C6'-O6'
3	A	1103	LMT	O5B-C5B-C6B-O6B
3	C	1102	LMT	O5'-C5'-C6'-O6'
9	B	1102	LMU	O5'-C5'-C6'-O6'
10	B	1104	PTY	C31-C30-O4-C1
9	B	1102	LMU	O5B-C5B-C6B-O6B
3	A	1101	LMT	C2'-C1'-O1'-C1
3	A	1102	LMT	C2'-C1'-O1'-C1
3	A	1104	LMT	C2'-C1'-O1'-C1
3	C	1102	LMT	C4'-C5'-C6'-O6'
3	A	1104	LMT	O5B-C5B-C6B-O6B
3	C	1101	LMT	O5'-C5'-C6'-O6'
9	B	1102	LMU	C4'-C5'-C6'-O6'
4	A	1106	GOL	O2-C2-C3-O3
4	B	1108	GOL	O1-C1-C2-O2
4	B	1109	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	C	1110	GOL	O2-C2-C3-O3
4	C	1111	GOL	O2-C2-C3-O3
3	A	1103	LMT	O1'-C1-C2-C3
10	C	1104	PTY	C30-C31-C32-C33
10	B	1104	PTY	O30-C30-O4-C1
3	C	1103	LMT	O5B-C5B-C6B-O6B
9	B	1102	LMU	O1'-C1-C2-C3
10	C	1104	PTY	C8-C11-C12-C13
3	C	1103	LMT	O1'-C1-C2-C3
3	A	1102	LMT	O5'-C5'-C6'-O6'
19	C	1122	LPX	C7-C6-O6-C5
3	A	1104	LMT	O1'-C1-C2-C3
3	C	1102	LMT	C5'-C4'-O1B-C1B
3	A	1103	LMT	C4B-C5B-C6B-O6B
19	C	1123	LPX	C3-C4-C5-O6
4	B	1106	GOL	O1-C1-C2-C3
4	B	1107	GOL	O1-C1-C2-C3
4	B	1108	GOL	O1-C1-C2-C3
4	B	1109	GOL	O1-C1-C2-C3
4	B	1110	GOL	C1-C2-C3-O3
4	C	1105	GOL	O1-C1-C2-C3
4	C	1109	GOL	O1-C1-C2-C3
4	C	1111	GOL	C1-C2-C3-O3
3	C	1103	LMT	C2-C3-C4-C5
3	A	1103	LMT	C5-C6-C7-C8
3	A	1104	LMT	C6-C7-C8-C9
3	B	1103	LMT	C5-C6-C7-C8
3	C	1102	LMT	C2-C3-C4-C5
10	C	1104	PTY	C16-C17-C18-C19
3	C	1103	LMT	C11-C10-C9-C8
19	C	1122	LPX	O7-C6-O6-C5
3	C	1103	LMT	C2-C1-O1'-C1'
4	B	1107	GOL	O1-C1-C2-O2
4	B	1110	GOL	O2-C2-C3-O3
4	C	1107	GOL	O1-C1-C2-O2
4	C	1109	GOL	O1-C1-C2-O2
4	C	1111	GOL	O1-C1-C2-O2
19	C	1122	LPX	C12-C13-C14-C15
3	B	1103	LMT	C6-C7-C8-C9
10	C	1104	PTY	C31-C32-C33-C34
19	C	1123	LPX	C14-C15-C16-C17
10	C	1104	PTY	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
10	C	1104	PTY	C39-C40-C41-C42
3	A	1102	LMT	C3-C4-C5-C6
3	A	1103	LMT	C2-C3-C4-C5
10	C	1104	PTY	C20-C21-C22-C23
13	C	1120	D12	C7-C8-C9-C10
5	C	1116	D10	C3-C4-C5-C6
7	B	1119	EDO	O1-C1-C2-O2
7	D	202	EDO	O1-C1-C2-O2
7	E	201	EDO	O1-C1-C2-O2
10	C	1104	PTY	C24-C25-C26-C27
10	B	1104	PTY	C32-C33-C34-C35
3	A	1105	LMT	C4-C5-C6-C7
10	B	1104	PTY	C12-C13-C14-C15
3	C	1103	LMT	C5-C6-C7-C8
3	C	1101	LMT	C5-C6-C7-C8
13	B	1114	D12	C2-C3-C4-C5
3	A	1105	LMT	C5-C6-C7-C8
3	A	1105	LMT	C4'-C5'-C6'-O6'
3	C	1101	LMT	C11-C10-C9-C8
19	C	1123	LPX	C9-C10-C11-C12
10	C	1104	PTY	C12-C13-C14-C15
3	A	1101	LMT	C11-C10-C9-C8
3	A	1101	LMT	C1-C2-C3-C4
3	A	1103	LMT	C1-C2-C3-C4
3	A	1105	LMT	C2-C3-C4-C5
10	B	1104	PTY	C39-C40-C41-C42
3	A	1103	LMT	C7-C8-C9-C10
19	C	1122	LPX	C11-C12-C13-C14
12	C	1118	OCT	C3-C4-C5-C6
10	C	1104	PTY	C32-C33-C34-C35
4	C	1112	GOL	O1-C1-C2-O2
19	C	1123	LPX	C10-C11-C12-C13
10	B	1104	PTY	C34-C35-C36-C37
3	A	1105	LMT	C4B-C5B-C6B-O6B
19	C	1123	LPX	C11-C12-C13-C14
3	B	1103	LMT	C7-C8-C9-C10
10	C	1104	PTY	C15-C16-C17-C18
3	C	1102	LMT	C2'-C1'-O1'-C1
6	A	1110	C14	C03-C04-C05-C06
19	C	1122	LPX	C16-C17-C18-C19
3	C	1102	LMT	O5B-C5B-C6B-O6B
7	C	1126	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
7	D	201	EDO	O1-C1-C2-O2
6	A	1110	C14	C05-C06-C07-C08
3	C	1102	LMT	C7-C8-C9-C10
10	B	1104	PTY	C35-C36-C37-C38
3	A	1101	LMT	O5B-C5B-C6B-O6B
3	C	1103	LMT	O5'-C5'-C6'-O6'
11	B	1105	DDR	C2-C3-C4-C5
10	C	1104	PTY	C33-C34-C35-C36
10	C	1104	PTY	C37-C38-C39-C40
13	C	1120	D12	C5-C6-C7-C8
9	B	1102	LMU	C4-C5-C6-C7
10	B	1104	PTY	C30-C31-C32-C33
11	B	1105	DDR	C4-C5-C6-C7
5	A	1109	D10	C6-C7-C8-C9
16	B	1121	DDQ	C4-C5-C6-C7
3	A	1101	LMT	C3-C4-C5-C6
10	B	1104	PTY	C16-C17-C18-C19
10	C	1104	PTY	C21-C22-C23-C24
11	B	1105	DDR	O51-C51-C52-O52
3	C	1102	LMT	O1'-C1-C2-C3
10	C	1104	PTY	C25-C26-C27-C28
3	A	1102	LMT	C5-C6-C7-C8
6	A	1110	C14	C06-C07-C08-C09
10	B	1104	PTY	C26-C27-C28-C29
19	C	1122	LPX	C11-C10-C9-C8
3	A	1102	LMT	C9-C10-C11-C12
10	C	1104	PTY	C41-C42-C43-C44
3	A	1104	LMT	C3-C4-C5-C6
3	C	1102	LMT	C11-C10-C9-C8
3	C	1102	LMT	C2-C1-O1'-C1'
4	C	1105	GOL	O1-C1-C2-O2
4	C	1108	GOL	O2-C2-C3-O3
14	C	1124	HEX	C2-C3-C4-C5
3	C	1103	LMT	C2'-C1'-O1'-C1
13	C	1121	D12	C4-C5-C6-C7
10	C	1104	PTY	C26-C27-C28-C29
10	B	1104	PTY	C17-C18-C19-C20
13	C	1121	D12	C6-C7-C8-C9
3	A	1102	LMT	C7-C8-C9-C10
11	B	1105	DDR	C5-C6-C7-C8
3	C	1101	LMT	C1-C2-C3-C4
9	B	1102	LMU	C4B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
5	A	1108	D10	C6-C7-C8-C9
7	D	203	EDO	O1-C1-C2-O2
10	C	1104	PTY	C14-C15-C16-C17
5	C	1114	D10	C4-C5-C6-C7
5	C	1115	D10	C4-C5-C6-C7
16	B	1121	DDQ	C5-C6-C7-C8
5	B	1111	D10	C4-C5-C6-C7
3	C	1103	LMT	C4-C5-C6-C7
3	A	1103	LMT	C3-C4-C5-C6
3	C	1102	LMT	C5-C6-C7-C8
4	B	1107	GOL	O2-C2-C3-O3
3	A	1104	LMT	C3'-C4'-O1B-C1B
7	A	1111	EDO	O1-C1-C2-O2
6	A	1110	C14	C07-C08-C09-C10
10	C	1104	PTY	O4-C1-C6-O7
3	C	1101	LMT	C9-C10-C11-C12
5	A	1108	D10	C1-C2-C3-C4
3	A	1102	LMT	C2-C3-C4-C5
5	C	1116	D10	C2-C3-C4-C5
3	A	1104	LMT	C5'-C4'-O1B-C1B
19	C	1123	LPX	C11-C10-C9-C8
3	B	1103	LMT	C3-C4-C5-C6
3	A	1102	LMT	C5'-C4'-O1B-C1B
10	C	1104	PTY	O14-C5-C6-C1
3	C	1103	LMT	C7-C8-C9-C10
3	A	1102	LMT	C4'-C5'-C6'-O6'
3	A	1103	LMT	C9-C10-C11-C12
5	C	1116	D10	C1-C2-C3-C4
3	A	1102	LMT	C4-C5-C6-C7
11	B	1105	DDR	C25-C26-C27-C28
5	C	1114	D10	C1-C2-C3-C4
3	A	1105	LMT	O1'-C1-C2-C3
19	C	1122	LPX	C18-C19-C20-C21
3	A	1104	LMT	C2B-C1B-O1B-C4'
10	B	1104	PTY	C3-O11-P1-O14
19	C	1123	LPX	C3-O1-P1-O2
19	C	1123	LPX	C3-O1-P1-O4
3	A	1101	LMT	C5'-C4'-O1B-C1B
5	C	1116	D10	C4-C5-C6-C7
3	A	1101	LMT	C3'-C4'-O1B-C1B
16	B	1121	DDQ	C1-C2-C3-C4
19	C	1123	LPX	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
3	A	1103	LMT	C4-C5-C6-C7
10	B	1104	PTY	O14-C5-C6-C1
3	A	1105	LMT	C7-C8-C9-C10
3	A	1105	LMT	C2B-C1B-O1B-C4'
11	B	1105	DDR	O51-C51-C52-C53
10	B	1104	PTY	C19-C20-C21-C22
7	B	1117	EDO	O1-C1-C2-O2
3	A	1101	LMT	C2-C3-C4-C5
9	B	1102	LMU	C5-C6-C7-C8
3	A	1103	LMT	C2-C1-O1'-C1'
3	A	1104	LMT	C2-C1-O1'-C1'
9	B	1102	LMU	C2-C1-O1'-C1'
3	C	1102	LMT	C4-C5-C6-C7
9	B	1102	LMU	C7-C8-C9-C10
6	C	1119	C14	C06-C07-C08-C09
10	C	1104	PTY	C22-C23-C24-C25
10	C	1104	PTY	C11-C12-C13-C14
19	C	1123	LPX	C7-C8-C9-C10
3	A	1101	LMT	C4-C5-C6-C7
10	C	1104	PTY	C19-C20-C21-C22
4	B	1106	GOL	O1-C1-C2-O2
6	C	1119	C14	C02-C03-C04-C05
6	A	1110	C14	C02-C03-C04-C05
3	A	1105	LMT	C9-C10-C11-C12
19	C	1123	LPX	C18-C19-C20-C21
3	A	1104	LMT	C5-C6-C7-C8
5	B	1112	D10	C2-C3-C4-C5
11	B	1105	DDR	C24-C25-C26-C27
3	C	1101	LMT	C2-C3-C4-C5
5	C	1115	D10	C3-C4-C5-C6
7	A	1112	EDO	O1-C1-C2-O2
5	B	1111	D10	C2-C3-C4-C5
6	A	1110	C14	C04-C05-C06-C07
3	C	1103	LMT	C6-C7-C8-C9
10	C	1104	PTY	C23-C24-C25-C26
14	C	1125	HEX	C2-C3-C4-C5
7	C	1127	EDO	O1-C1-C2-O2
19	C	1122	LPX	C15-C16-C17-C18
5	A	1109	D10	C5-C6-C7-C8
10	C	1104	PTY	C18-C19-C20-C21
5	A	1108	D10	C7-C8-C9-C10
3	A	1105	LMT	C2-C1-O1'-C1'

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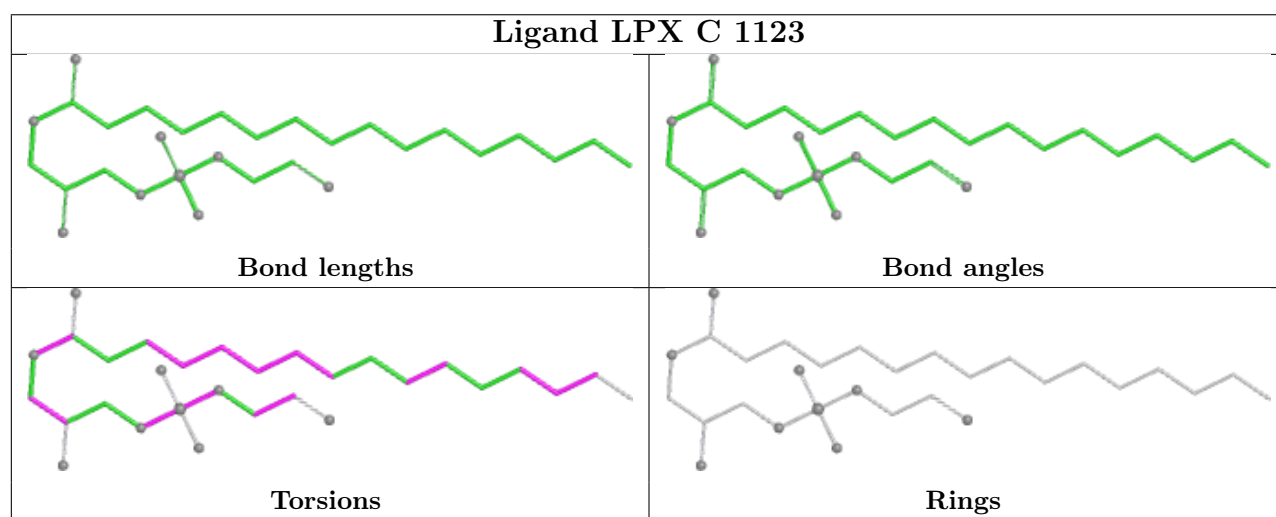
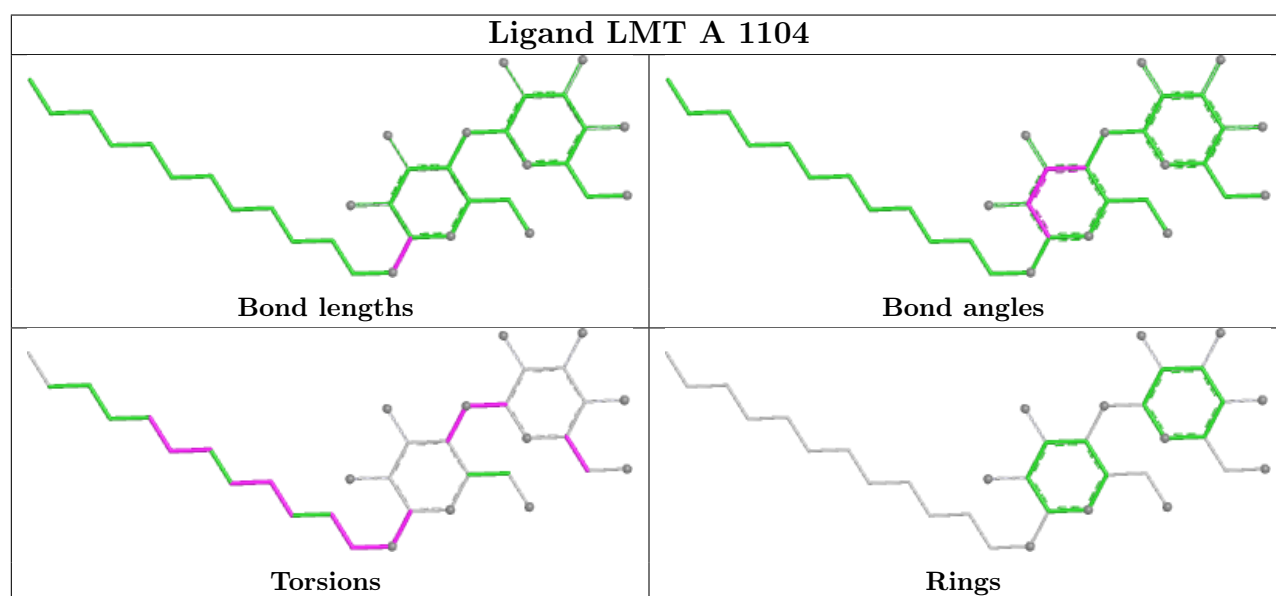
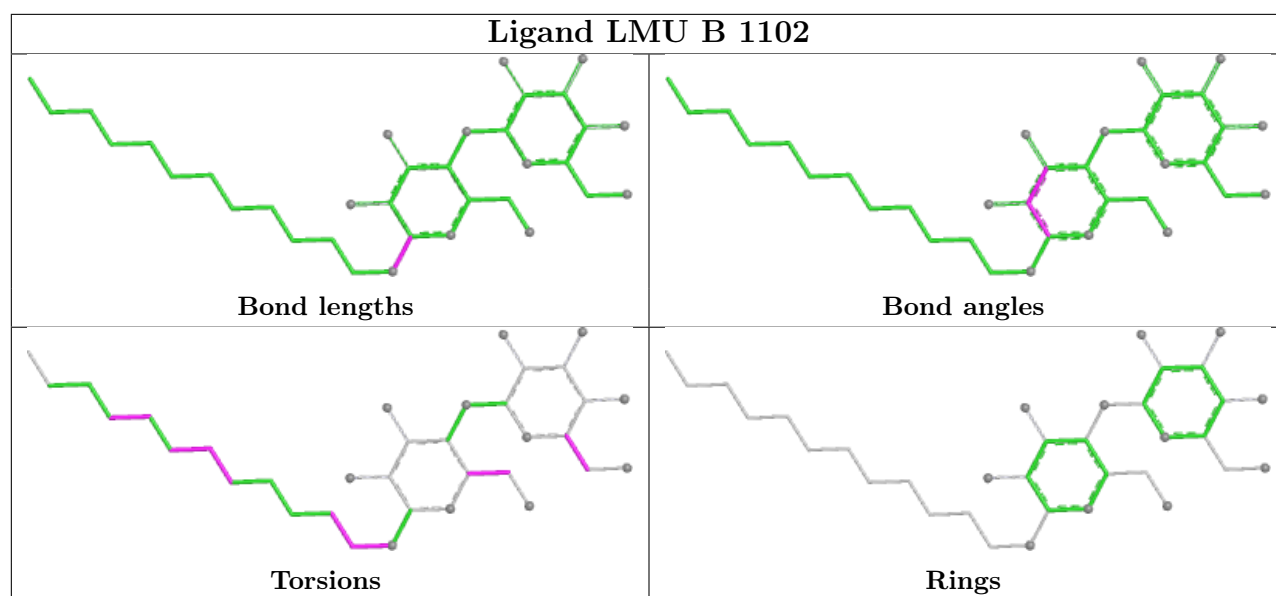
Mol	Chain	Res	Type	Atoms
10	C	1104	PTY	O4-C1-C6-C5
5	B	1111	D10	C6-C7-C8-C9
13	C	1121	D12	C7-C8-C9-C10
5	A	1108	D10	C3-C4-C5-C6
3	A	1104	LMT	C2-C3-C4-C5
3	A	1101	LMT	C5-C6-C7-C8
3	C	1103	LMT	C3'-C4'-O1B-C1B
10	B	1104	PTY	C8-C11-C12-C13
11	B	1105	DDR	O51-C1-C2-C3
10	B	1104	PTY	C37-C38-C39-C40
5	B	1112	D10	C3-C4-C5-C6
3	A	1105	LMT	O5B-C5B-C6B-O6B
11	B	1105	DDR	O52-C21-C22-C23

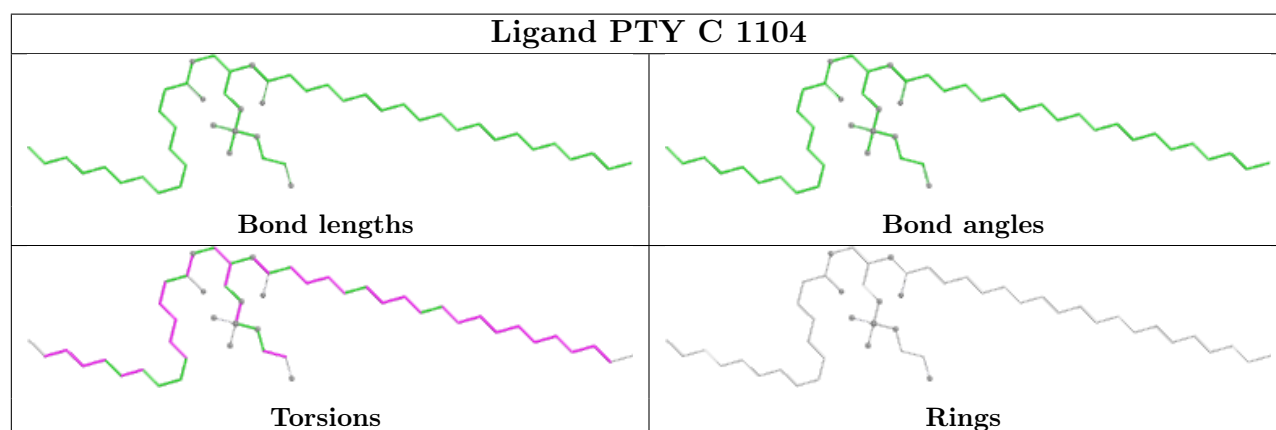
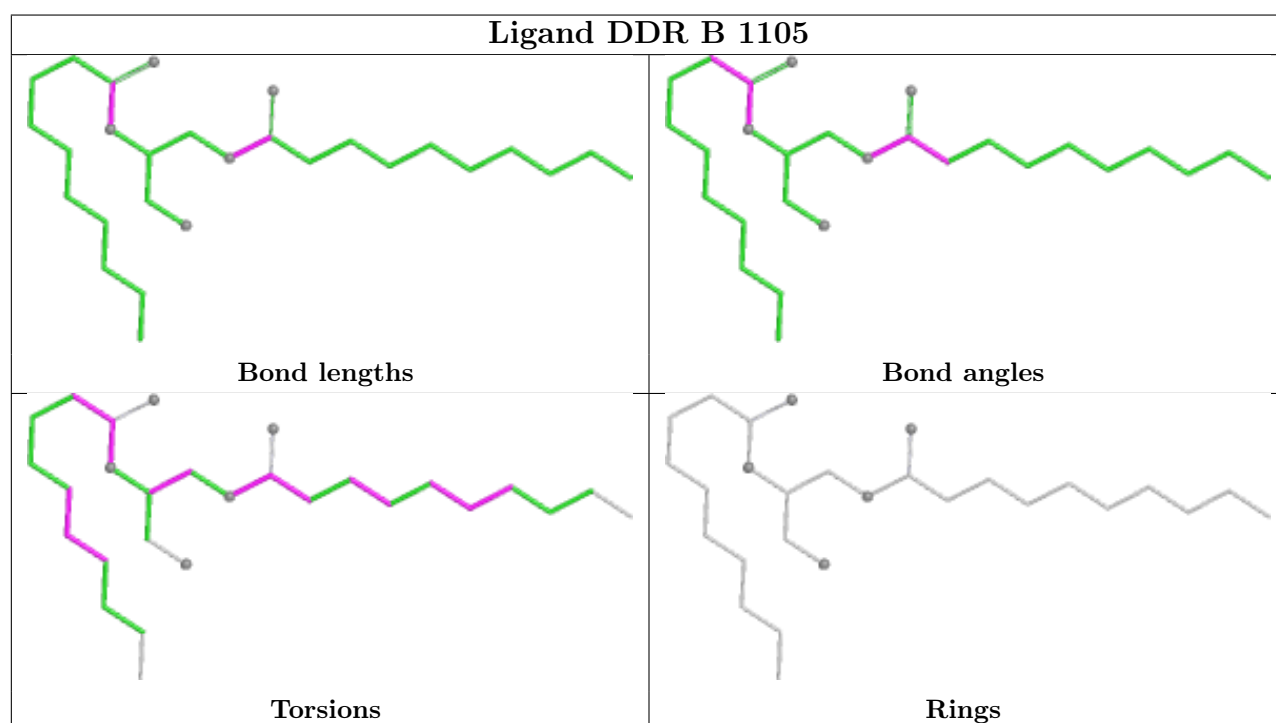
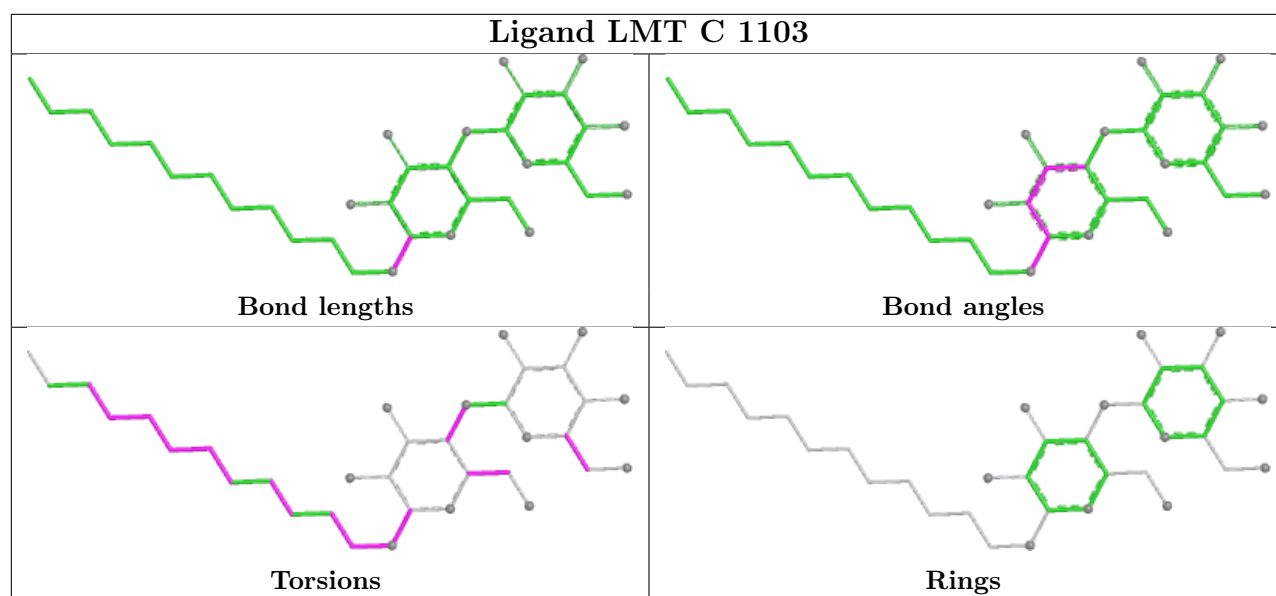
There are no ring outliers.

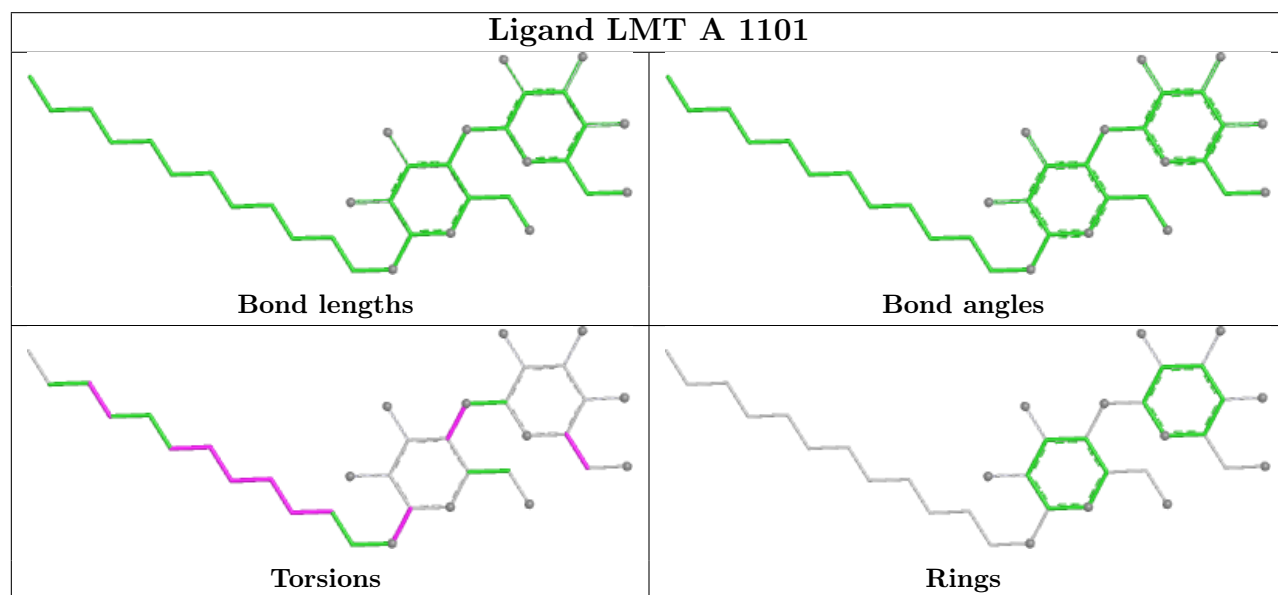
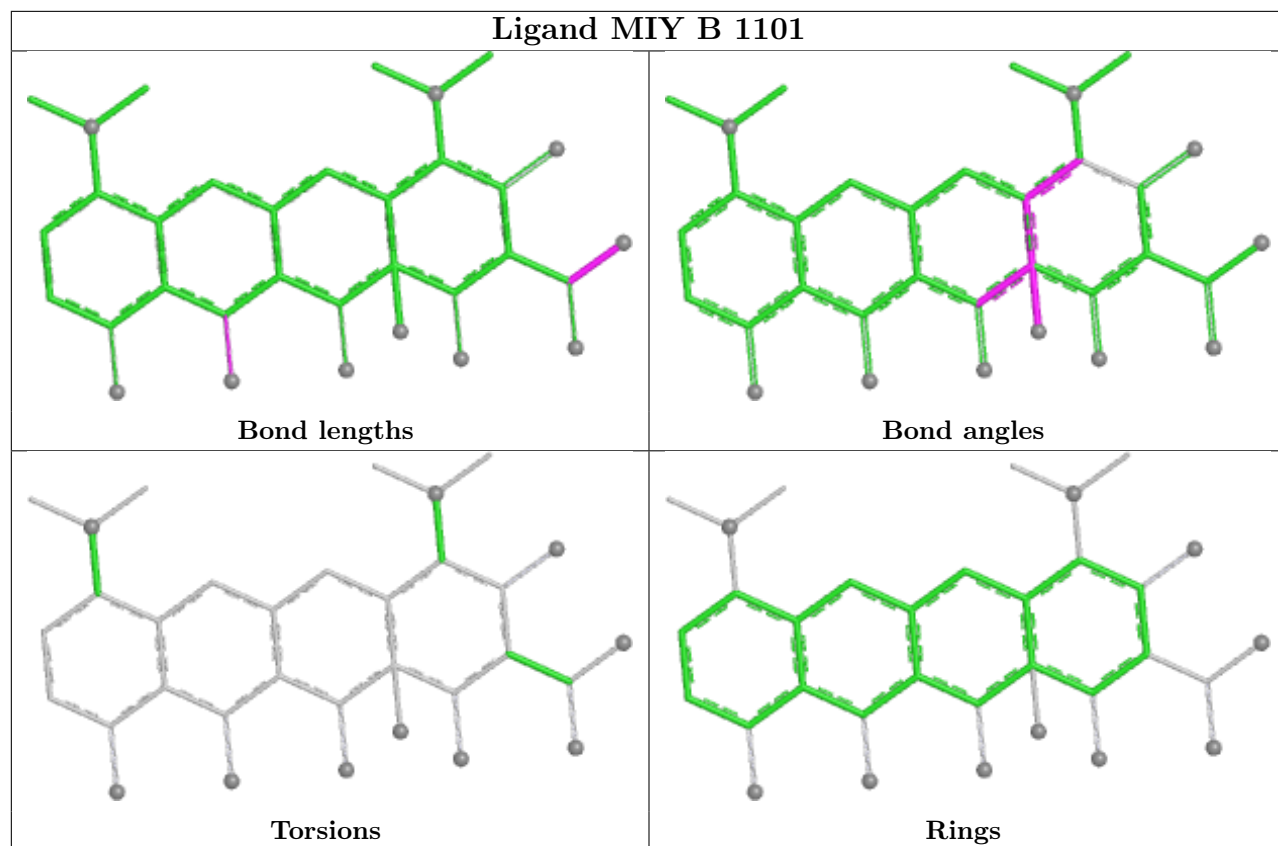
5 monomers are involved in 5 short contacts:

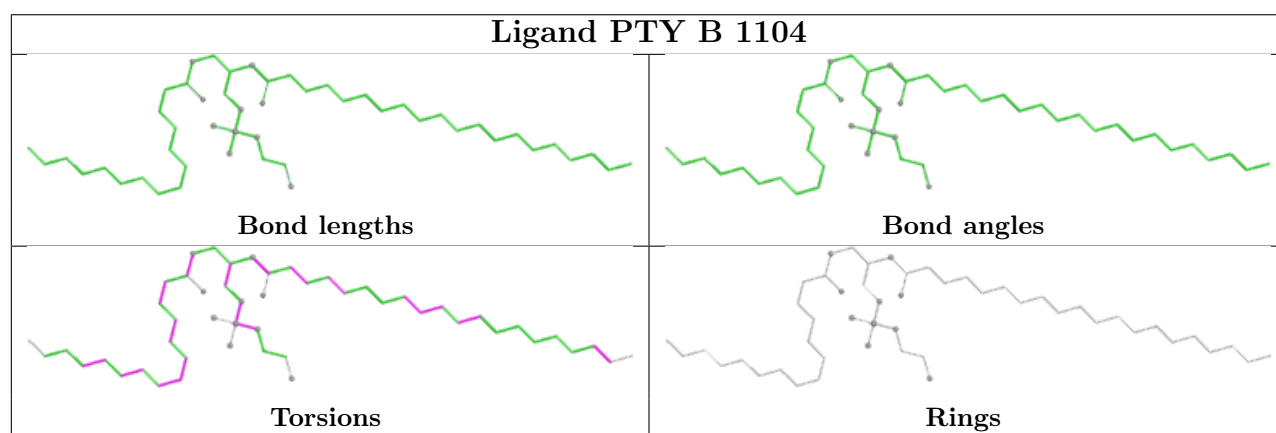
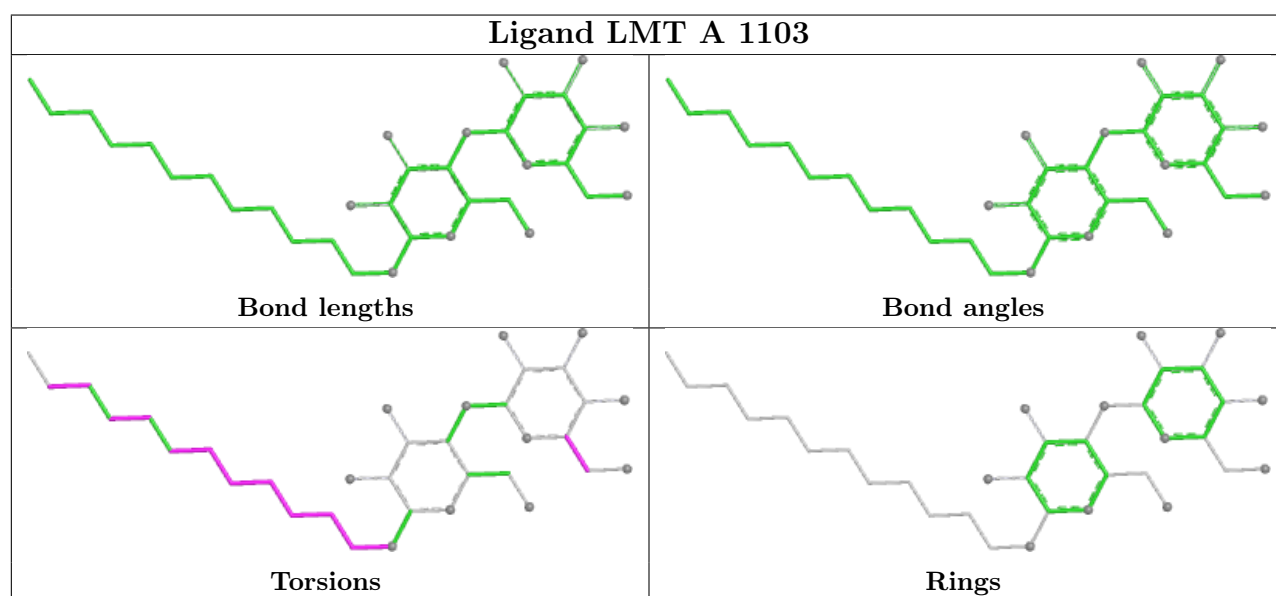
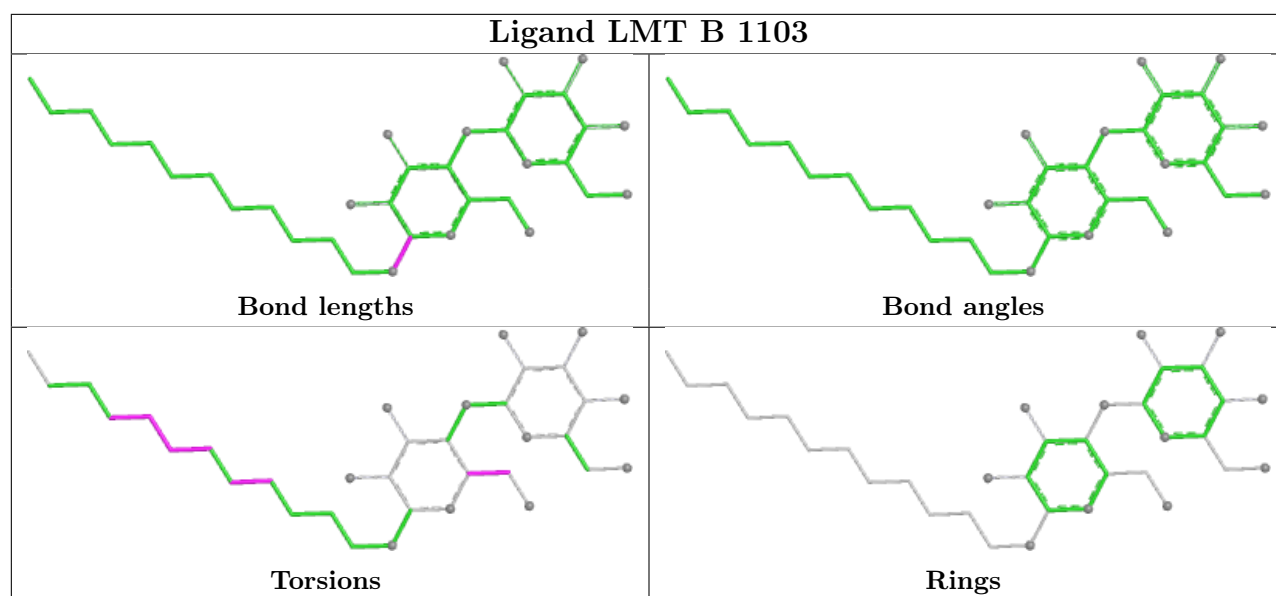
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	C	1123	LPX	2	0
10	C	1104	PTY	1	0
8	B	1101	MIY	1	0
19	C	1122	LPX	1	0
5	C	1116	D10	1	0

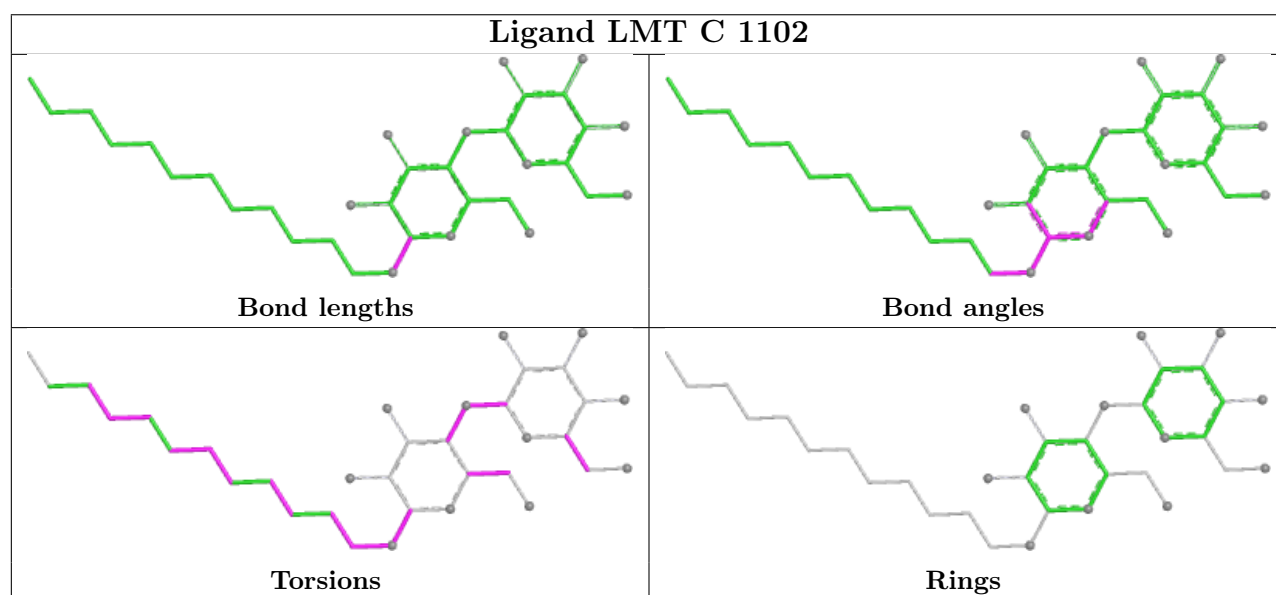
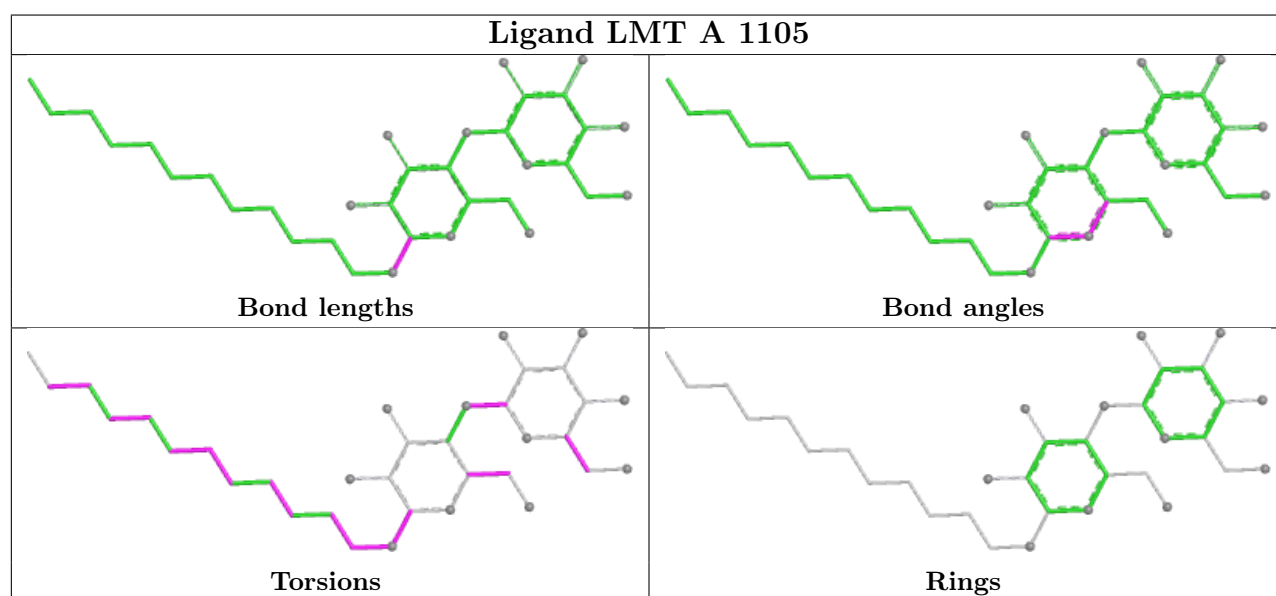
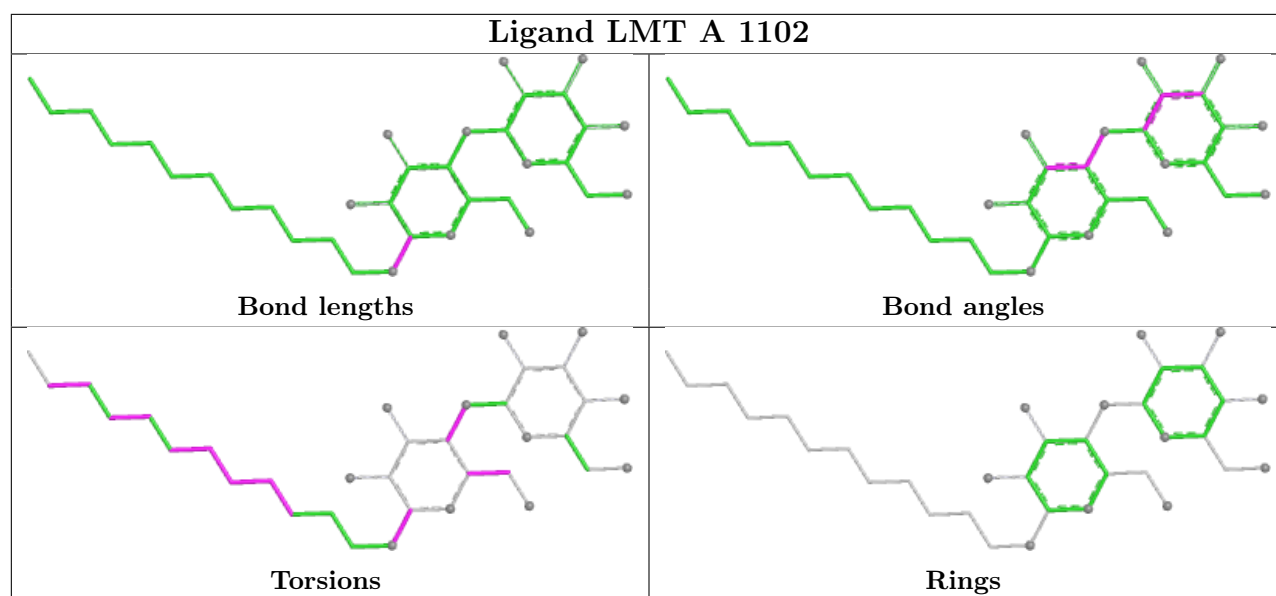
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

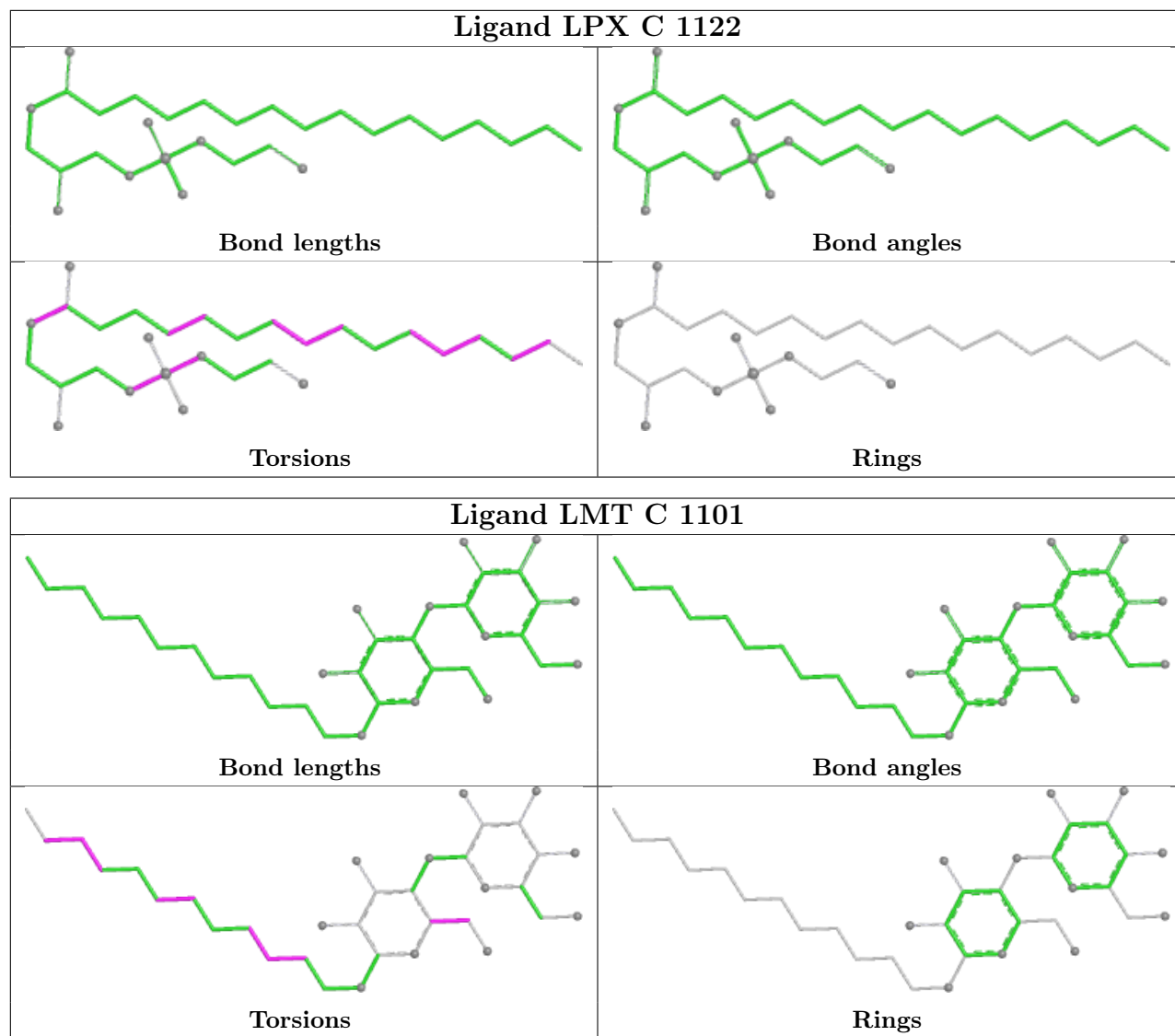












5.7 Other polymers [i](#)

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

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, 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%)	0.67	109 (10%) 11 10	31, 57, 90, 140	5 (0%)
1	B	1034/1057 (97%)	0.38	42 (4%) 41 37	33, 50, 72, 95	0
1	C	1035/1057 (97%)	0.26	36 (3%) 47 42	28, 46, 66, 100	3 (0%)
2	D	156/169 (92%)	0.48	9 (5%) 29 25	42, 53, 78, 97	0
2	E	154/169 (91%)	0.84	12 (7%) 19 17	51, 68, 93, 100	0
All	All	3421/3509 (97%)	0.46	208 (6%) 27 23	28, 51, 82, 140	8 (0%)

All (208) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	868	LEU	9.1
1	A	672	VAL	8.1
1	A	678	THR	7.3
1	A	677	ALA	7.2
1	A	670	ALA	6.8
1	A	676	THR	6.6
1	A	1040	ILE	6.6
1	A	867	ARG	6.2
1	A	674	LEU	6.2
1	A	869	SER	5.7
1	C	671	ILE	5.6
1	A	673	GLU	5.2
1	A	362	PHE	5.1
1	B	617	PHE	4.9
1	B	616	GLY	4.9
1	B	618	ALA	4.6
1	A	679	GLY	4.5
1	C	670	ALA	4.5
1	B	134	SER	4.5
1	A	1042	HIS	4.4

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Mol	Chain	Res	Type	RSRZ
1	C	1032	ARG	4.3
1	C	362	PHE	4.3
1	A	668	LEU	4.3
1	C	673	GLU	4.2
1	A	510	LYS	4.0
1	C	672	VAL	4.0
1	A	1038	GLU	3.9
1	A	956	GLU	3.9
1	C	674	LEU	3.9
1	A	866	GLU	3.9
1	A	918	PHE	3.8
1	A	829	GLY	3.7
1	B	676	THR	3.6
1	A	828	LEU	3.6
1	A	662	MET	3.6
1	A	1035	ARG	3.6
1	A	148	THR	3.6
1	A	675	GLY	3.6
1	A	423	GLU	3.5
1	A	1037	ASN	3.5
1	A	831	ALA	3.5
1	A	955	LYS	3.5
1	B	866	GLU	3.5
1	C	675	GLY	3.4
1	B	615	PHE	3.4
1	C	112[A]	GLN	3.4
1	B	868	LEU	3.4
1	A	671	ILE	3.4
1	B	677	ALA	3.3
1	A	827	ILE	3.3
1	B	1034	SER	3.3
1	A	680	PHE	3.3
1	B	660	ASP	3.3
1	A	580	ALA	3.3
1	A	112	GLN	3.2
1	C	918	PHE	3.2
1	A	681	ASP	3.2
1	A	429	GLU	3.2
1	A	877	TYR	3.2
1	B	508	GLY	3.2
1	C	124	GLN	3.2
1	A	716	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	870	GLY	3.2
1	A	715	SER	3.1
1	C	134	SER	3.1
1	C	811	TYR	3.1
1	A	862	MET	3.1
1	A	833	PRO	3.1
1	C	70[A]	ASN	3.0
1	B	112	GLN	3.0
1	A	539	GLY	3.0
1	B	619	GLY	3.0
1	A	1039	ASP	2.9
1	B	332	PHE	2.9
1	C	120	GLN	2.9
1	A	620	ARG	2.9
1	B	635	ALA	2.9
1	B	133	SER	2.9
2	D	166	GLN	2.9
1	B	659	LYS	2.8
2	E	165	LEU	2.8
1	A	669	PRO	2.7
1	B	678	THR	2.7
2	E	164	ILE	2.7
1	C	116	PRO	2.7
1	A	538	THR	2.7
1	C	691	GLY	2.7
1	B	662	MET	2.7
1	A	714	THR	2.7
1	C	1035	ARG	2.7
1	B	577	GLN	2.7
1	C	743	ILE	2.7
1	A	712	MET	2.7
1	A	513	PHE	2.6
1	A	682	PHE	2.6
1	B	558	ARG	2.6
1	B	649	MET	2.6
1	B	132	SER	2.6
1	A	255	GLN	2.6
1	B	784	ASP	2.6
1	B	867	ARG	2.6
1	A	987	MET	2.6
1	B	918	PHE	2.6
1	A	830	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	510	LYS	2.6
1	A	511	GLY	2.6
2	E	143	ASP	2.6
1	A	1036	LYS	2.6
1	B	870	GLY	2.5
1	C	497	LEU	2.5
1	C	361	ASN	2.5
1	A	863	SER	2.5
1	C	508	GLY	2.5
1	C	834	GLY	2.5
1	C	693	GLU	2.5
1	C	510	LYS	2.5
1	A	537	SER	2.5
1	B	634	TRP	2.5
1	A	470	PHE	2.5
1	A	865	GLN	2.5
1	C	89	GLN	2.5
1	A	543	VAL	2.5
1	A	709	HIS	2.5
2	D	61	GLU	2.5
1	A	575	MET	2.5
1	A	864	TYR	2.4
1	A	706	ALA	2.4
1	A	621	PRO	2.4
1	B	575	MET	2.4
1	C	659	LYS	2.4
2	D	28	ASP	2.4
1	A	871	ASN	2.4
1	A	875	SER	2.4
1	A	425	LEU	2.4
1	A	702	LEU	2.4
1	A	37	THR	2.3
1	C	676	THR	2.3
2	D	11	GLY	2.3
1	C	29	LYS	2.3
1	A	719	ASN	2.3
2	E	35	ALA	2.3
1	A	717	ARG	2.3
1	B	854	GLY	2.3
1	B	120	GLN	2.3
1	A	660	ASP	2.3
1	A	968	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	361	ASN	2.3
1	A	836	SER	2.3
1	A	859	TRP	2.3
1	A	1034	SER	2.3
1	B	135	SER	2.3
1	B	255	GLN	2.3
1	A	359	LEU	2.3
1	C	498	LYS	2.3
1	B	628	PHE	2.3
2	D	55	ALA	2.2
1	A	505	HIS	2.2
1	A	577	GLN	2.2
1	A	619	GLY	2.2
1	B	614	GLY	2.2
1	A	713	LEU	2.2
1	C	133	SER	2.2
2	E	14	LEU	2.2
2	E	13	ASP	2.2
1	A	657	GLN	2.2
1	A	853	THR	2.2
1	B	513	PHE	2.2
2	E	145	PHE	2.2
1	A	710	PRO	2.2
1	B	627	ALA	2.2
1	B	113	LEU	2.2
1	A	991	ILE	2.2
1	A	386	PHE	2.2
1	A	512	PHE	2.2
1	A	659	LYS	2.2
2	D	36	ASN	2.2
1	A	402	ILE	2.2
2	D	164	ILE	2.2
2	D	159	GLU	2.2
1	C	1033	PHE	2.2
2	E	40	VAL	2.1
2	D	150	PHE	2.1
1	A	873	ALA	2.1
1	A	542	LEU	2.1
2	E	146	GLY	2.1
1	A	835	LYS	2.1
1	C	519	MET	2.1
1	C	899	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	166	GLN	2.1
1	A	980	LEU	2.1
1	A	586	ARG	2.1
1	C	255	GLN	2.1
1	A	282	ASN	2.1
1	A	667	ASN	2.1
1	A	874	PRO	2.1
1	B	366	LEU	2.0
1	A	192	GLU	2.0
1	A	1041	GLU	2.0
1	A	38	ILE	2.0
1	C	575	MET	2.0
1	A	556	PHE	2.0
2	E	139	VAL	2.0
1	A	832	ALA	2.0
1	A	461	GLY	2.0
1	A	994	GLY	2.0
1	A	462	SER	2.0
1	B	554	TYR	2.0
2	E	135	TYR	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 oligosaccharides 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
7	EDO	D	201	4/4	0.60	0.29	78,80,80,81	0
7	EDO	A	1112	4/4	0.67	0.40	79,80,81,82	0
3	LMT	A	1105	35/35	0.68	0.28	112,128,134,134	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	LMT	C	1103	35/35	0.70	0.24	97,117,123,123	0
7	EDO	C	1126	4/4	0.72	0.32	70,72,72,72	0
14	HEX	C	1124	6/6	0.72	0.42	69,69,70,70	0
5	D10	B	1111	10/10	0.73	0.35	82,85,86,87	0
14	HEX	B	1115	6/6	0.73	0.38	70,73,74,75	0
6	C14	A	1110	14/14	0.73	0.32	67,72,77,77	0
5	D10	A	1109	10/10	0.74	0.35	79,81,85,85	0
4	GOL	B	1110	6/6	0.74	0.20	91,92,93,94	0
3	LMT	A	1104	35/35	0.75	0.23	88,123,129,130	0
10	PTY	B	1104	50/50	0.75	0.28	73,109,143,147	0
4	GOL	C	1107	6/6	0.76	0.28	91,92,93,93	0
3	LMT	C	1102	35/35	0.76	0.25	97,125,136,138	0
15	SO4	B	1120	5/5	0.76	0.20	118,118,119,120	0
4	GOL	C	1111	6/6	0.77	0.18	79,80,81,82	0
5	D10	A	1108	10/10	0.78	0.31	76,76,77,77	0
5	D10	C	1116	10/10	0.78	0.36	72,74,79,80	0
14	HEX	C	1125	6/6	0.79	0.34	72,74,75,75	0
10	PTY	C	1104	50/50	0.79	0.30	85,101,116,118	0
6	C14	C	1119	14/14	0.80	0.26	69,70,72,72	0
5	D10	C	1114	10/10	0.80	0.31	80,81,82,82	0
12	OCT	C	1117	8/8	0.80	0.39	86,89,90,90	0
13	D12	C	1120	12/12	0.80	0.28	69,72,80,80	0
16	DDQ	B	1121	14/14	0.80	0.36	86,101,121,121	0
19	LPX	C	1122	30/30	0.80	0.26	79,87,98,103	0
7	EDO	C	1127	4/4	0.81	0.35	80,80,80,80	0
4	GOL	B	1107	6/6	0.81	0.28	80,83,84,85	0
13	D12	C	1121	12/12	0.81	0.28	68,69,71,71	0
19	LPX	C	1123	30/30	0.81	0.24	72,80,92,93	0
3	LMT	A	1102	35/35	0.82	0.21	68,91,112,114	0
12	OCT	B	1113	8/8	0.82	0.32	72,74,77,78	0
4	GOL	C	1112	6/6	0.82	0.18	84,85,85,85	0
3	LMT	A	1101	35/35	0.83	0.17	66,89,110,111	0
7	EDO	B	1117	4/4	0.84	0.31	71,72,72,73	0
7	EDO	B	1119	4/4	0.84	0.18	69,69,70,71	0
7	EDO	D	203	4/4	0.84	0.18	62,63,63,63	0
7	EDO	A	1111	4/4	0.84	0.21	64,64,64,65	0
4	GOL	C	1113	6/6	0.85	0.22	78,80,81,81	0
4	GOL	C	1108	6/6	0.85	0.25	95,96,97,98	0
4	GOL	A	1106	6/6	0.85	0.18	56,60,61,61	0
17	NA	B	1122	1/1	0.85	0.43	67,67,67,67	0
3	LMT	A	1103	35/35	0.85	0.17	89,92,104,106	0
5	D10	B	1112	10/10	0.85	0.29	71,72,73,73	0

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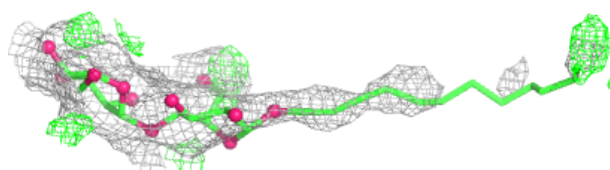
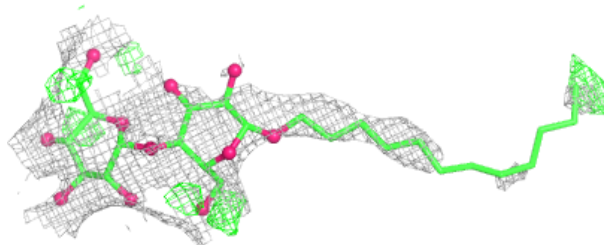
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	LMU	B	1102	35/35	0.87	0.18	76,89,92,93	0
8	MIY	B	1101	33/33	0.88	0.13	64,66,67,68	0
13	D12	B	1114	12/12	0.88	0.21	69,71,71,72	0
4	GOL	C	1106	6/6	0.88	0.16	61,65,65,66	0
5	D10	C	1115	10/10	0.88	0.26	63,66,71,72	0
7	EDO	B	1118	4/4	0.88	0.17	62,62,63,63	0
3	LMT	B	1103	35/35	0.88	0.18	65,71,101,102	0
4	GOL	B	1109	6/6	0.89	0.20	73,74,76,78	0
7	EDO	E	201	4/4	0.89	0.23	68,69,69,70	0
7	EDO	D	202	4/4	0.89	0.22	64,65,65,65	0
15	SO4	C	1129	5/5	0.89	0.08	89,91,92,93	0
4	GOL	C	1110	6/6	0.90	0.16	63,64,64,65	0
7	EDO	B	1116	4/4	0.90	0.24	59,59,60,60	0
12	OCT	C	1118	8/8	0.90	0.19	63,64,64,65	0
4	GOL	C	1109	6/6	0.90	0.19	70,72,73,73	0
11	DDR	B	1105	28/28	0.90	0.21	72,86,91,91	0
15	SO4	C	1128	5/5	0.91	0.14	79,80,80,82	0
4	GOL	B	1108	6/6	0.92	0.16	64,66,68,69	0
3	LMT	C	1101	35/35	0.93	0.13	61,65,88,89	0
4	GOL	A	1107	6/6	0.93	0.14	62,64,66,67	0
4	GOL	B	1106	6/6	0.93	0.11	52,53,54,55	0
4	GOL	C	1105	6/6	0.94	0.11	44,46,48,49	0
18	CL	B	1123	1/1	0.94	0.12	57,57,57,57	0

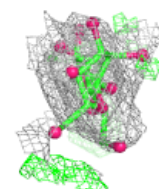
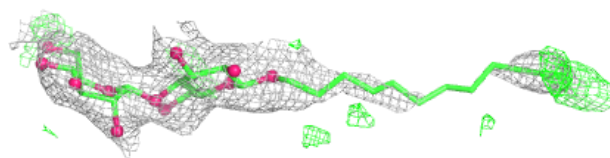
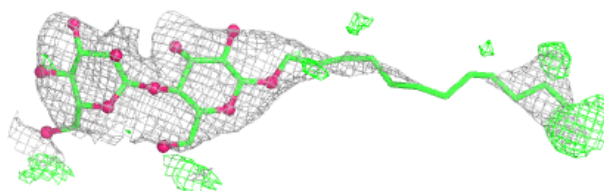
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT A 1105:

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

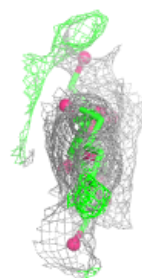
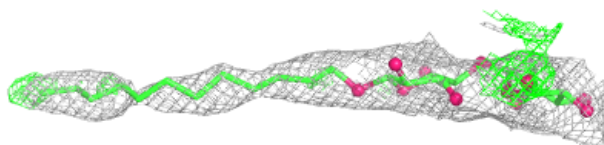
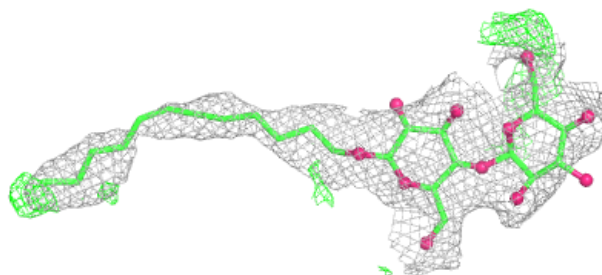
**Electron density around LMT C 1103:**

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

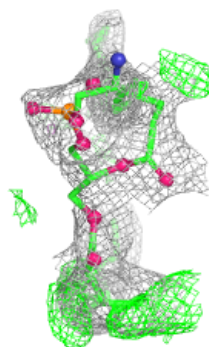
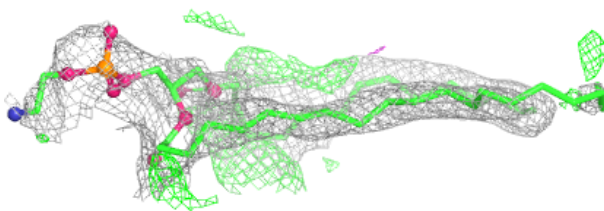
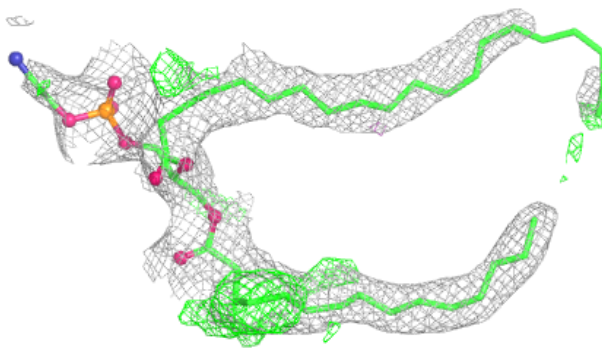


Electron density around LMT A 1104:

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

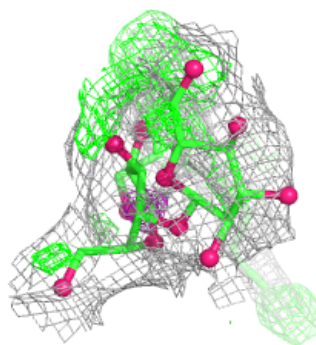
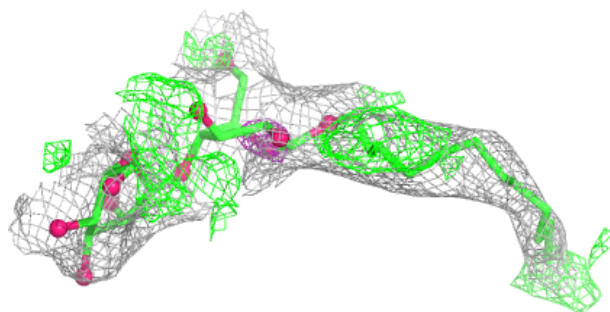
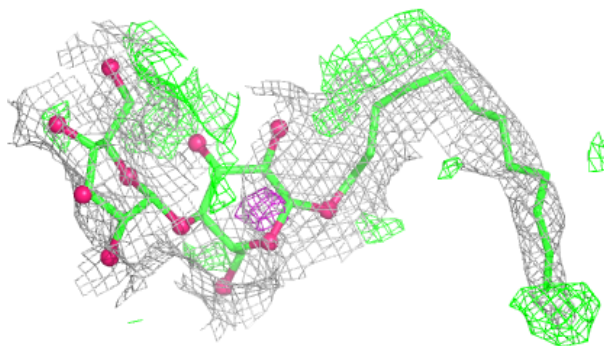
**Electron density around PTY B 1104:**

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

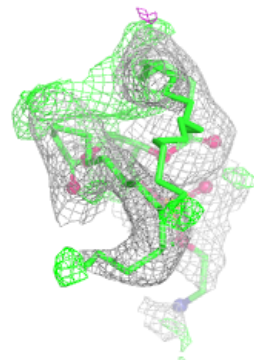
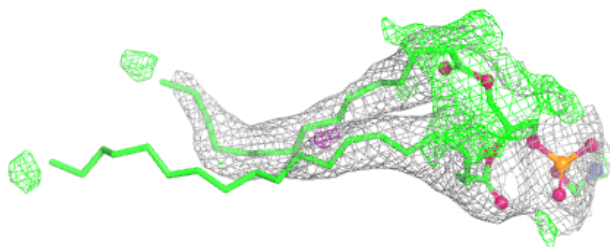
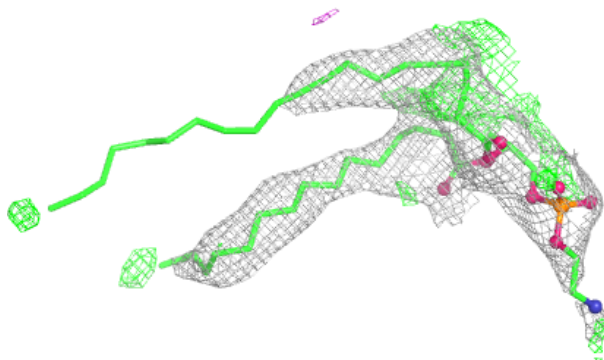


Electron density around LMT C 1102:

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

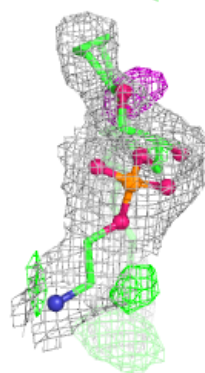
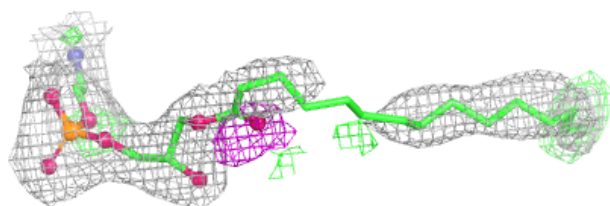
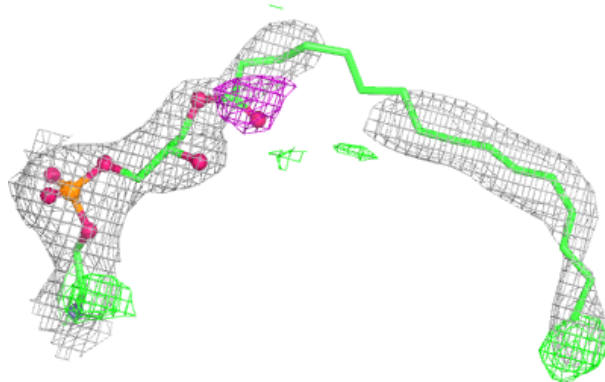
**Electron density around PTY C 1104:**

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

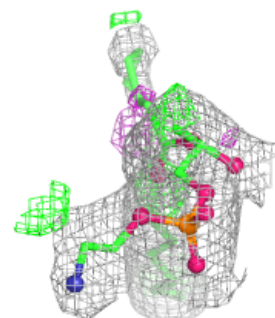
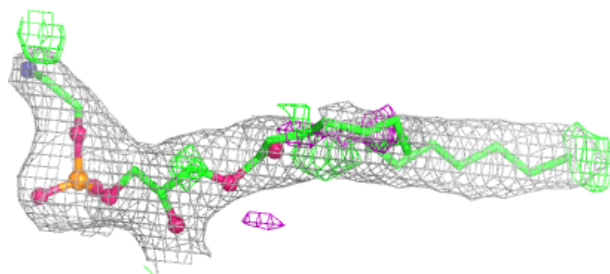
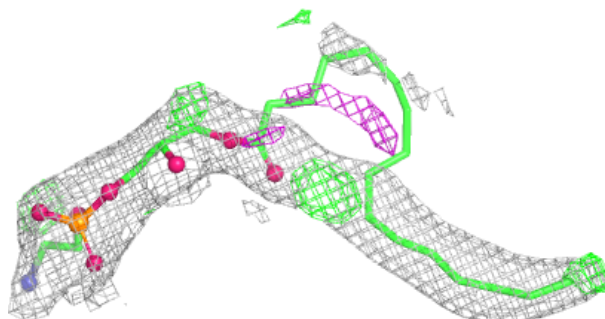


Electron density around LPX C 1122:

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

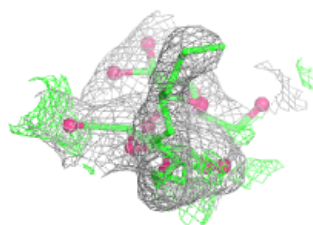
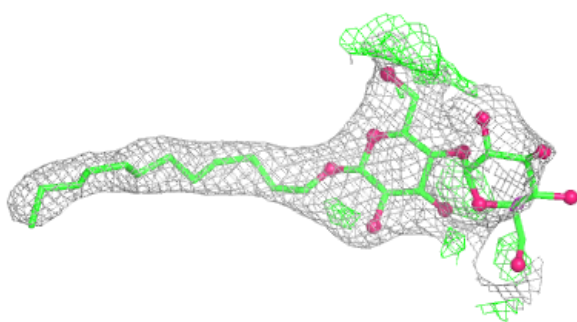
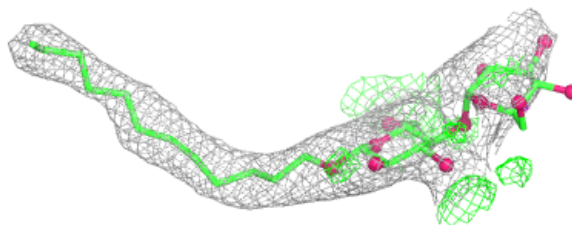
**Electron density around LPX C 1123:**

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

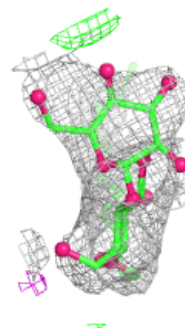
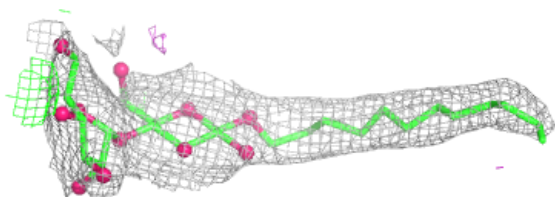
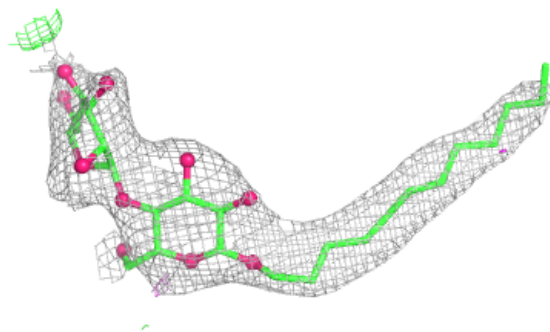


Electron density around LMT A 1102:

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

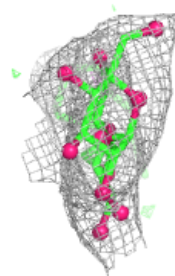
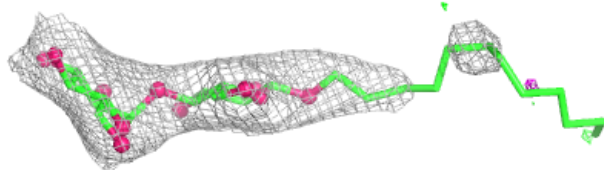
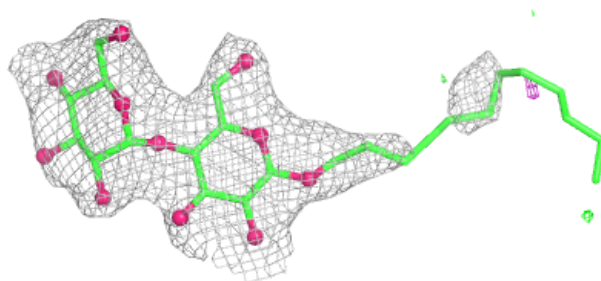
**Electron density around LMT A 1101:**

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

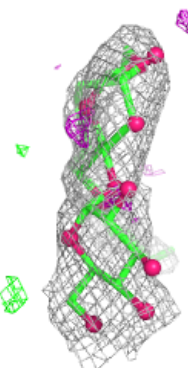
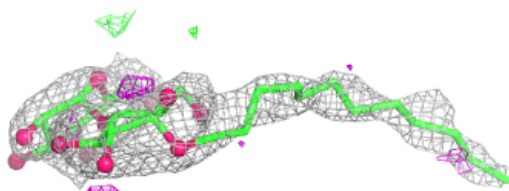
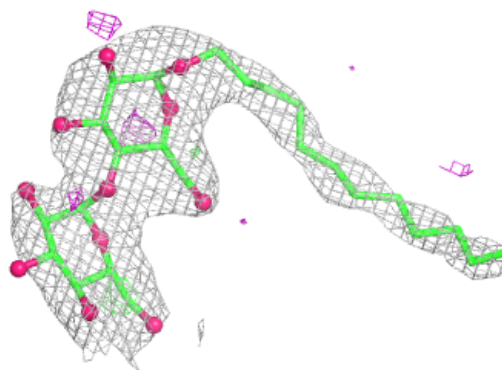


Electron density around LMT A 1103:

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

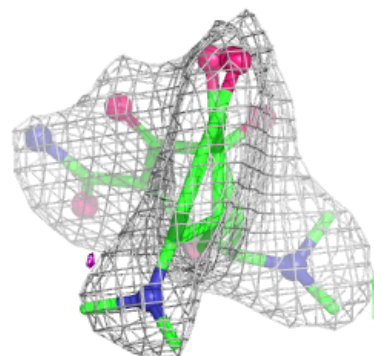
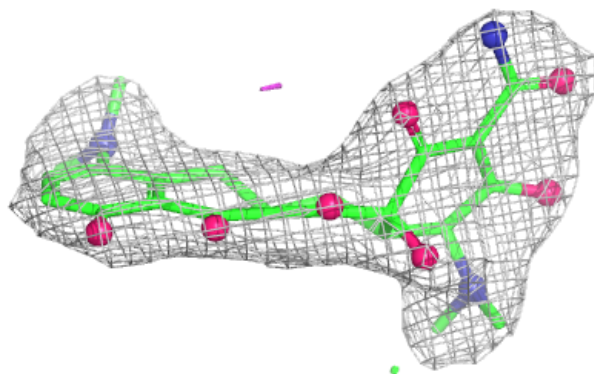
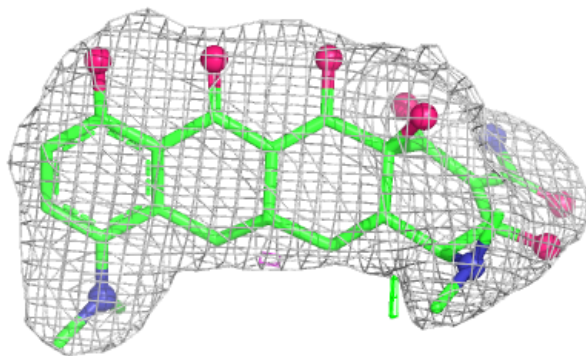
**Electron density around LMU B 1102:**

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

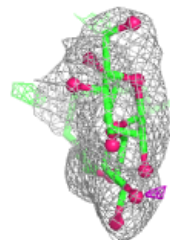
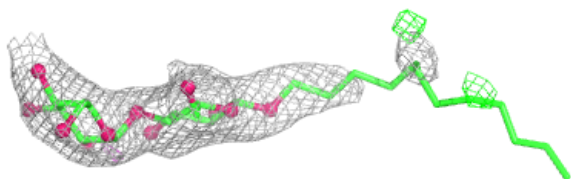
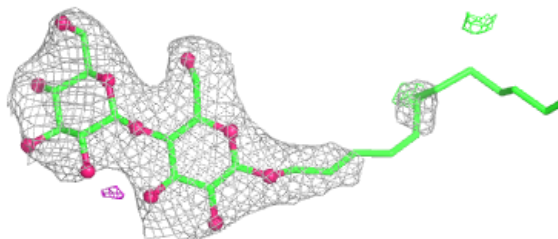


Electron density around MIY B 1101:

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

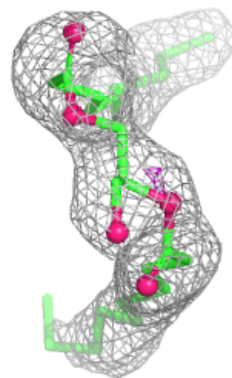
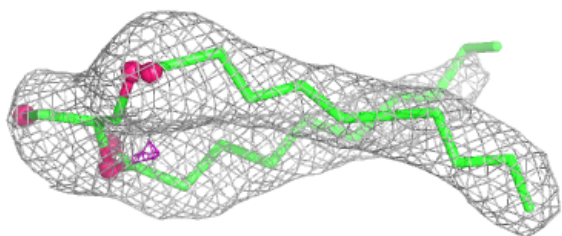
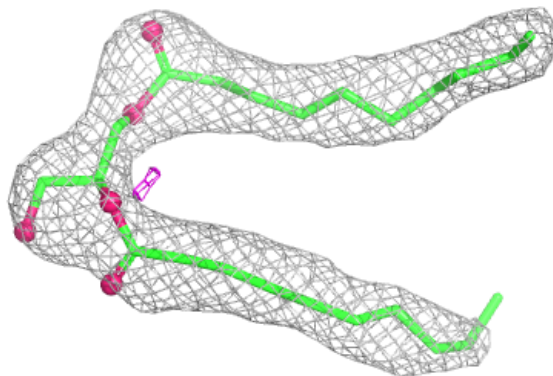
**Electron density around LMT B 1103:**

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

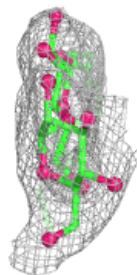
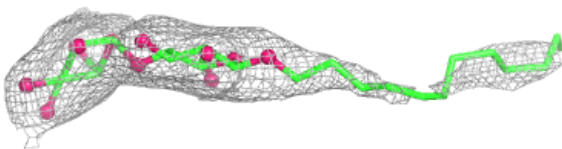
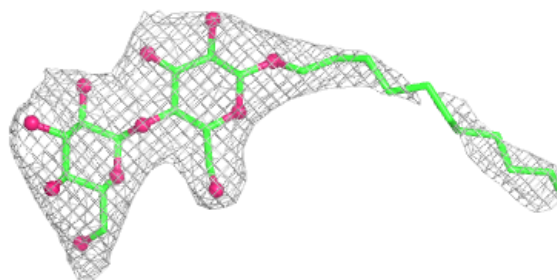


Electron density around DDR B 1105:

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

**Electron density around LMT C 1101:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.