



Full wwPDB X-ray Structure Validation Report ⓘ

May 11, 2021 – 10:22 am BST

PDB ID : 6ZO9
Title : Binding of two rifabutins to the access pocket of AcrB-G621P T protomer
Authors : Tam, H.K.; Foong, W.E.; Pos, K.M.
Deposited on : 2020-07-07
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.18
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) : 2.18

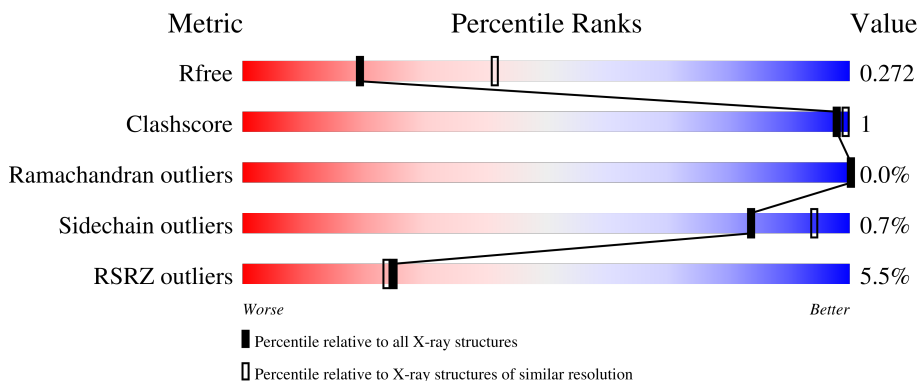
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 95%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">95%</p>
1	B	1057	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 94%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">94%</p>
1	C	1057	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 96%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">96%</p>
2	D	169	<div style="display: flex; align-items: center;"> <div style="width: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 92%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">92%</p>
2	E	169	<div style="display: flex; align-items: center;"> <div style="width: 27%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 91%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">91%</p>

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
4	LMT	C	1107	-	-	-	X
6	GOL	C	1112	-	-	-	X

2 Entry composition i

There are 16 unique types of molecules in this entry. The entry contains 26945 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	7959	5119	1319	1477	44	0	4	0
1	B	1034	7858	5058	1296	1460	44	0	0	0
1	C	1035	7892	5082	1303	1462	45	0	3	0

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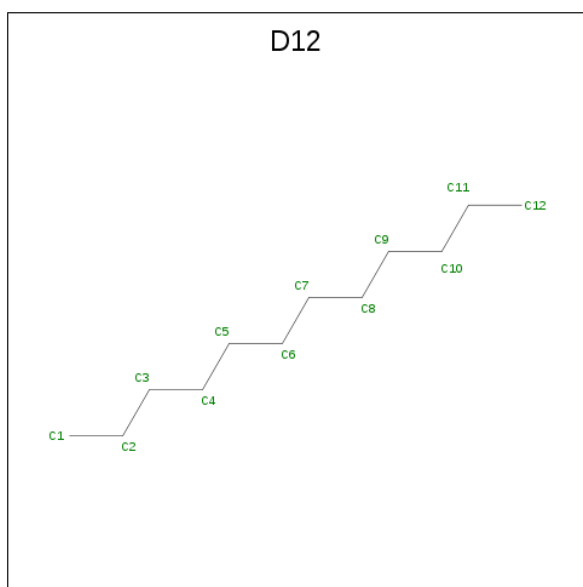
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Chain	Residue	Modelled	Actual	Comment	Reference
C	1054	HIS	-	expression tag	UNP P31224
C	1055	HIS	-	expression tag	UNP P31224
C	1056	HIS	-	expression tag	UNP P31224
C	1057	HIS	-	expression tag	UNP P31224

- Molecule 2 is a protein called DARPIN.

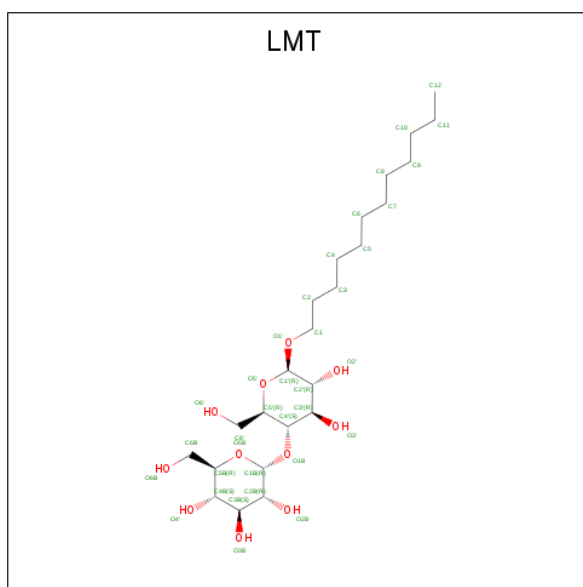
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	156	1177	741	206	229	1	0	0	0
2	E	154	1167	736	204	226	1	0	0	0

- Molecule 3 is DODECANE (three-letter code: D12) (formula: C₁₂H₂₆).



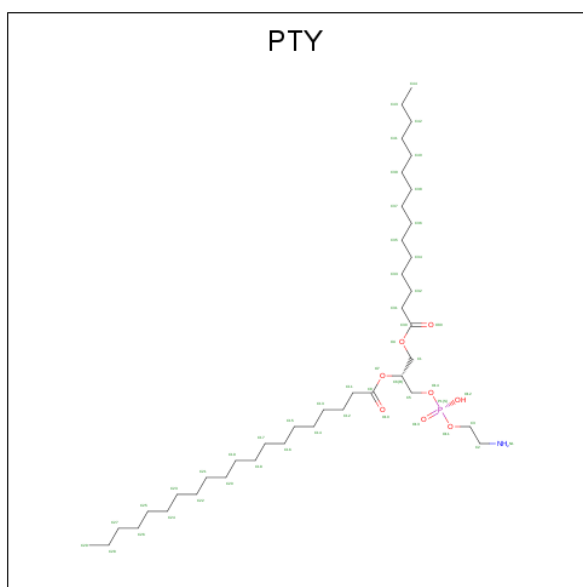
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C	0	0
			12	12		
3	C	1	Total	C	0	0
			12	12		
3	C	1	Total	C	0	0
			12	12		

- Molecule 4 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



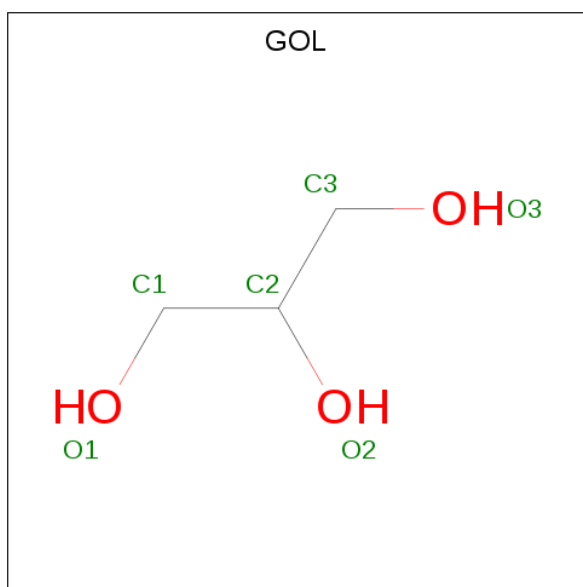
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			35	24	11		
4	A	1	Total	C	O	0	0
			35	24	11		
4	A	1	Total	C	O	0	0
			35	24	11		
4	B	1	Total	C	O	0	0
			35	24	11		
4	C	1	Total	C	O	0	0
			35	24	11		
4	C	1	Total	C	O	0	0
			35	24	11		

- Molecule 5 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$).



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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



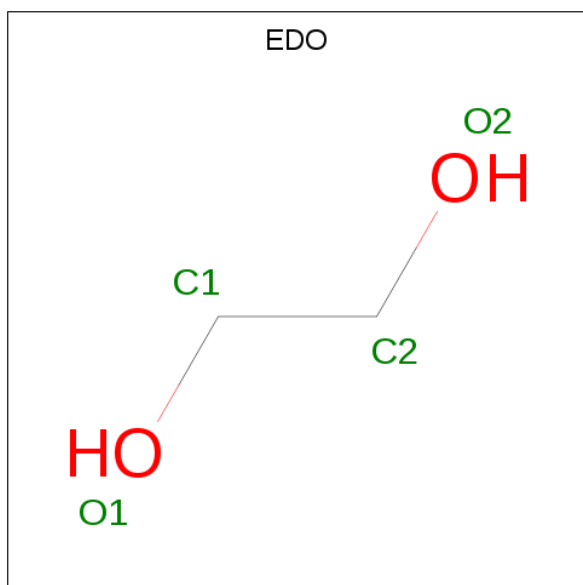
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	Total 6	C 3	O 3	0	0

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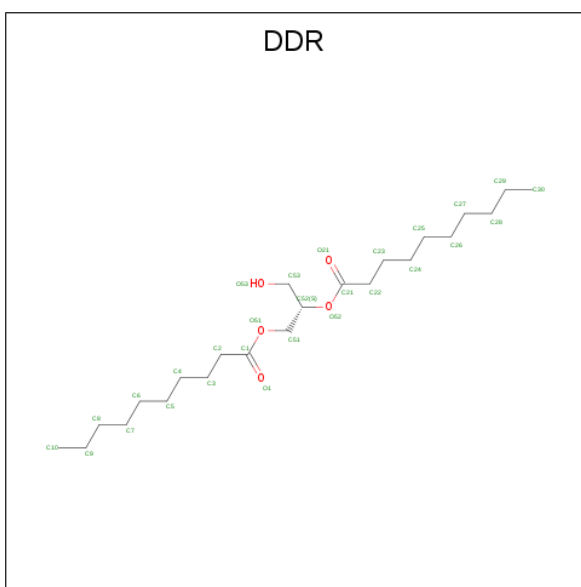
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



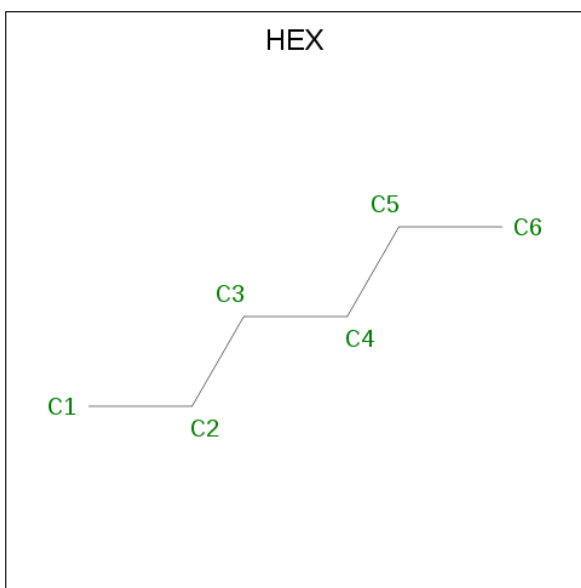
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is (2S)-3-hydroxypropane-1,2-diyl didecanoate (three-letter code: DDR) (formula: C₂₃H₄₄O₅).



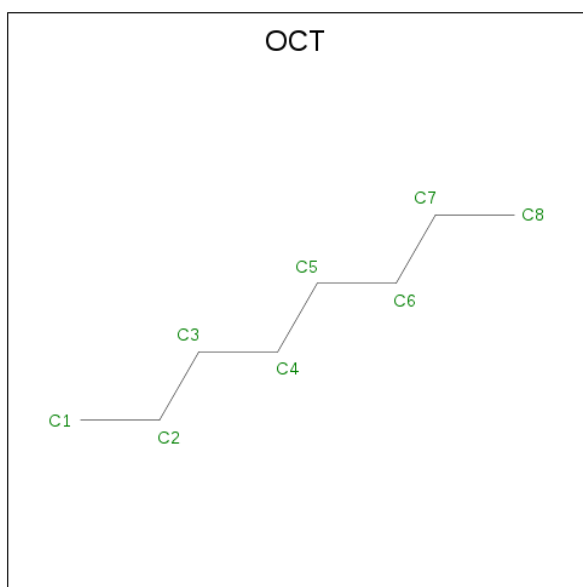
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	C O	0	0
			28	23 5		

- Molecule 9 is HEXANE (three-letter code: HEX) (formula: C₆H₁₄).



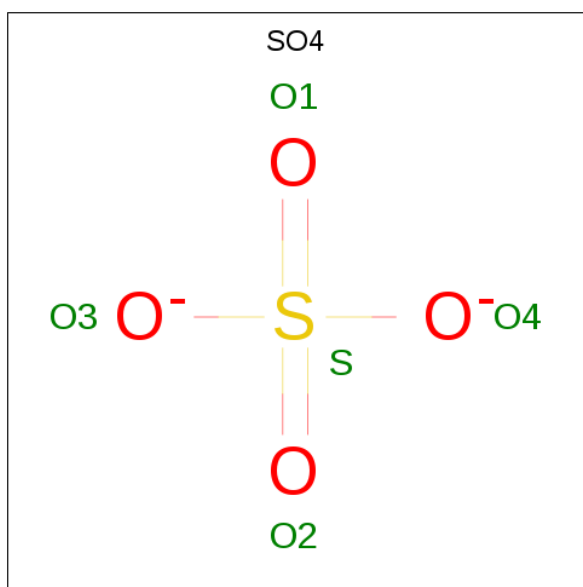
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	C	0	0
			6	6		
9	C	1	Total	C	0	0
			6	6		

- Molecule 10 is N-OCTANE (three-letter code: OCT) (formula: C₈H₁₈).



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

- Molecule 11 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



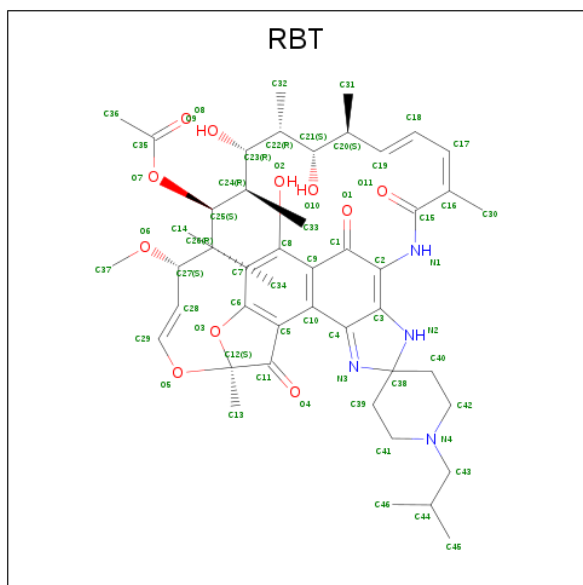
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	1	Total O S 5 4 1	0	0

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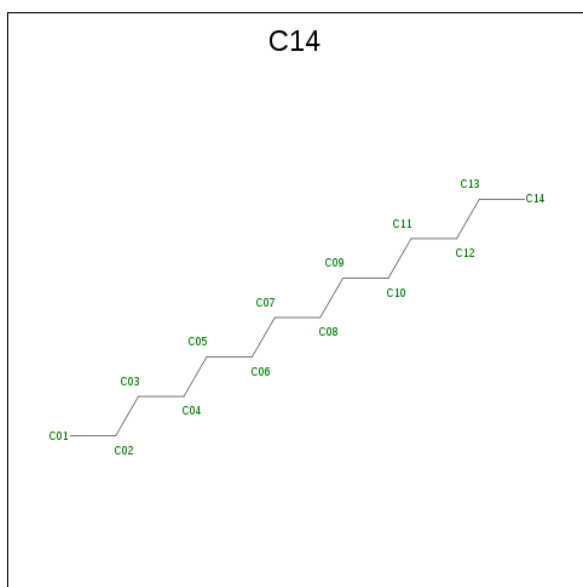
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 12 is RIFABUTIN (three-letter code: RBT) (formula: $C_{46}H_{62}N_4O_{11}$) (labeled as "Ligand of Interest" by depositor).



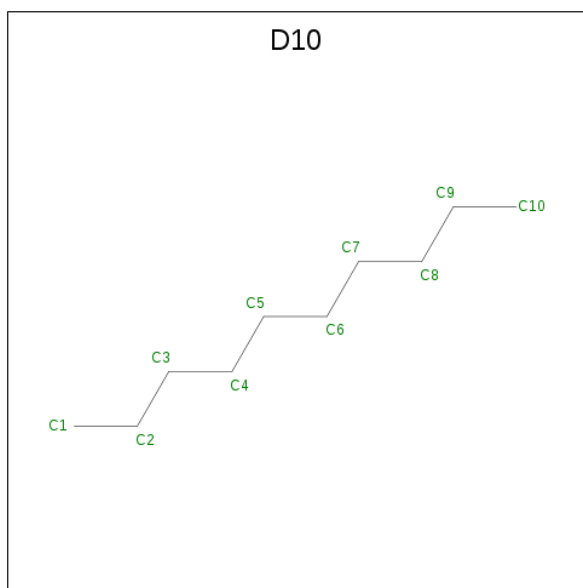
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	B	1	Total	C	N	O	0	0
			61	46	4	11		
12	B	1	Total	C	N	O	0	0
			61	46	4	11		

- Molecule 13 is TETRADECANE (three-letter code: C14) (formula: $C_{14}H_{30}$).



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

- Molecule 14 is DECANE (three-letter code: D10) (formula: C₁₀H₂₂).



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

- Molecule 15 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

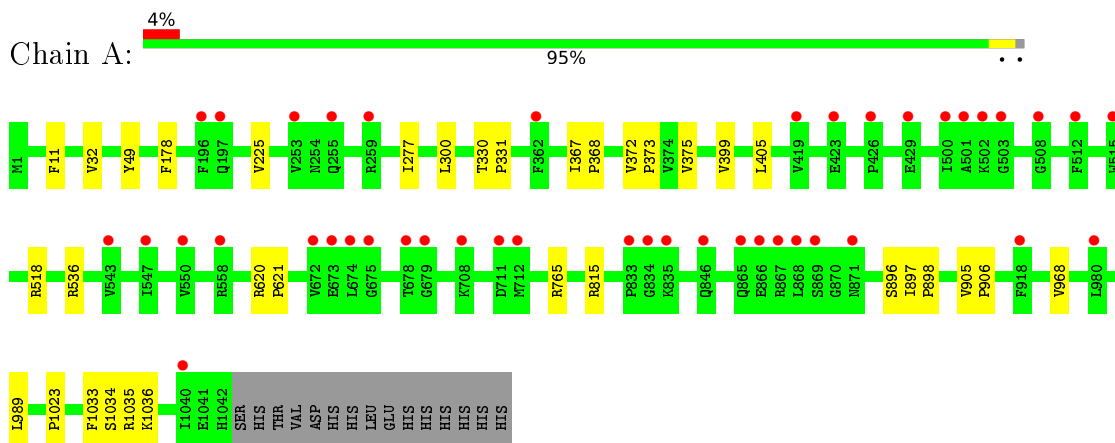
- Molecule 16 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	76	Total O 76 76	0	0
16	B	54	Total O 54 54	0	0
16	C	86	Total O 86 86	0	0
16	D	5	Total O 5 5	0	0
16	E	10	Total O 10 10	0	0

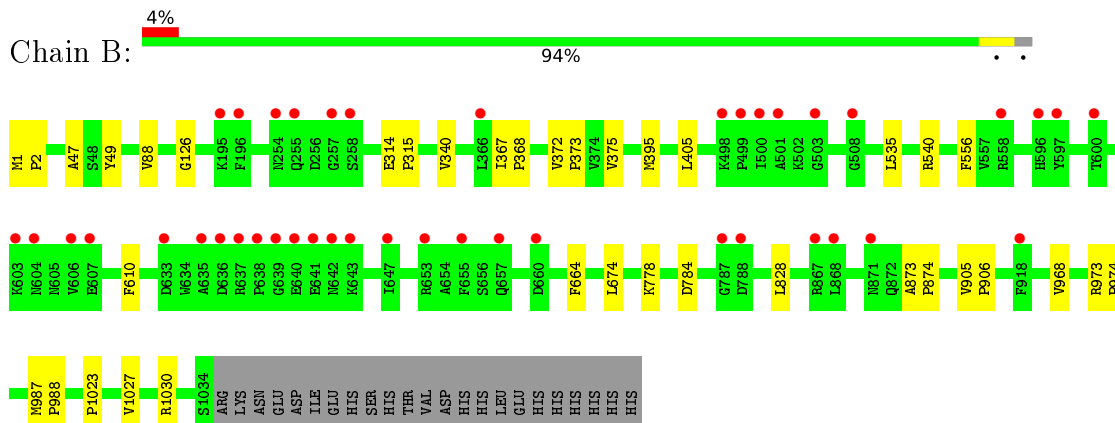
3 Residue-property plots

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.

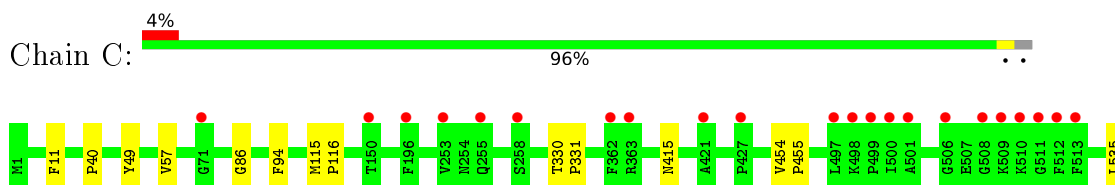
- Molecule 1: Multidrug efflux pump subunit AcrB

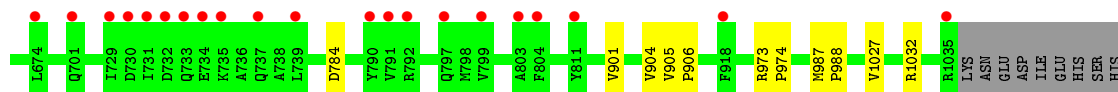


- Molecule 1: Multidrug efflux pump subunit AcrB



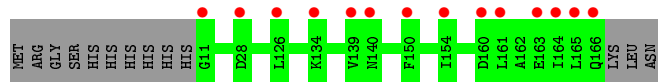
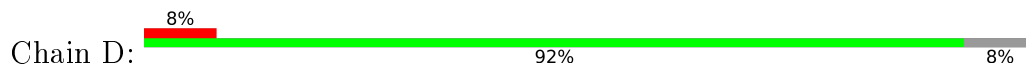
- Molecule 1: Multidrug efflux pump subunit AcrB



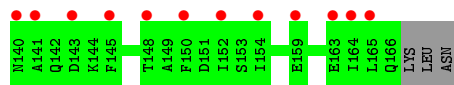
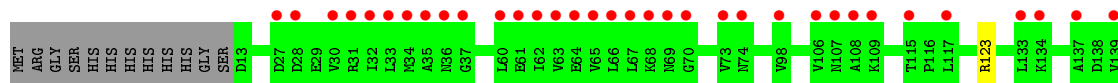


THR VAL ASP HIS HIS LEU GLU HIS HIS HIS HIS HIS HIS HIS

● Molecule 2: DARPIN



● Molecule 2: DARPIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	147.16Å 160.52Å 244.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.05 – 2.70 49.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.05-2.70) 100.0 (49.00-2.70)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.69Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.241 , 0.274 0.243 , 0.272	Depositor DCC
R_{free} test set	7750 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	51.4	Xtrriage
Anisotropy	0.576	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 33.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	26945	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.13% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, C14, CL, HEX, EDO, PTY, D12, RBT, OCT, D10, DDR, GOL, LMT

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	0/8124	0.69	0/11030
1	B	0.67	0/8009	0.69	0/10878
1	C	0.67	0/8051	0.69	0/10933
2	D	0.68	0/1196	0.69	0/1626
2	E	0.68	0/1186	0.69	0/1613
All	All	0.67	0/26566	0.69	0/36080

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	7959	0	8115	14	0
1	B	7858	0	8010	17	0
1	C	7892	0	8047	11	0
2	D	1177	0	1159	0	0
2	E	1167	0	1151	0	0
3	A	12	0	26	0	0
3	C	24	0	52	0	0
4	A	105	0	138	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	35	0	46	0	0
4	C	70	0	92	0	0
5	A	50	0	79	0	0
5	C	100	0	158	0	0
6	A	6	0	8	0	0
6	B	6	0	8	0	0
6	C	6	0	8	0	0
7	A	4	0	6	0	0
7	B	12	0	18	0	0
8	B	28	0	44	0	0
9	B	6	0	14	0	0
9	C	6	0	14	0	0
10	B	16	0	36	0	0
10	C	8	0	18	0	0
11	B	5	0	0	0	0
11	C	5	0	0	0	0
12	B	122	0	122	2	0
13	C	14	0	30	0	0
14	C	20	0	44	0	0
15	C	1	0	0	0	0
16	A	76	0	0	0	0
16	B	54	0	0	0	0
16	C	86	0	0	0	0
16	D	5	0	0	0	0
16	E	10	0	0	0	0
All	All	26945	0	27443	40	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 (40) 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:A:375:VAL:HG11	1:A:405:LEU:HD22	1.85	0.58
1:B:873:ALA:HB3	1:B:874:PRO:HD3	1.87	0.57
1:B:968:VAL:HG11	1:B:1023:PRO:HG3	1.88	0.56
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.93	0.51
1:B:126:GLY:HA3	1:C:116:PRO:HB3	1.93	0.50
1:A:968:VAL:HG11	1:A:1023:PRO:HG3	1.93	0.49
1:A:896:SER:HB2	1:A:1033:PHE:CD2	2.48	0.48
1:C:115:MET:N	1:C:116:PRO:HD2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:VAL:HB	1:A:373:PRO:HD3	1.94	0.48
1:C:57:VAL:HG21	1:C:86:GLY:HA2	1.95	0.48
1:A:178:PHE:HA	1:A:277:ILE:HG21	1.96	0.48
1:B:340:VAL:HG21	1:B:395:MET:HB3	1.97	0.47
1:C:987:MET:N	1:C:988:PRO:HD2	2.30	0.47
1:C:901:VAL:O	1:C:904:VAL:HG12	2.16	0.46
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.98	0.46
1:C:454:VAL:HB	1:C:455:PRO:HD3	1.97	0.46
1:A:897:ILE:N	1:A:898:PRO:CD	2.80	0.45
1:B:367:ILE:HB	1:B:368:PRO:HD3	1.98	0.45
1:A:330:THR:N	1:A:331:PRO:CD	2.80	0.45
1:C:535:LEU:HD22	1:C:1027:VAL:HG21	1.98	0.45
1:A:399:VAL:HG11	1:A:989:LEU:HD11	1.99	0.44
1:B:372:VAL:HB	1:B:373:PRO:HD3	1.99	0.44
1:B:375:VAL:HG11	1:B:405:LEU:HD22	1.99	0.43
1:C:905:VAL:HB	1:C:906:PRO:HD3	2.00	0.43
1:A:225:VAL:HG11	1:B:778:LYS:HA	2.00	0.42
1:B:828:LEU:HD22	12:B:1111:RBT:H19	2.00	0.42
1:B:674:LEU:O	12:B:1112:RBT:H422	2.20	0.42
1:C:330:THR:N	1:C:331:PRO:CD	2.83	0.42
1:A:620:ARG:N	1:A:621:PRO:CD	2.82	0.42
1:A:32:VAL:HB	1:A:300:LEU:HD12	2.01	0.42
1:A:1033:PHE:O	1:A:1035:ARG:HG3	2.20	0.42
1:B:535:LEU:HD22	1:B:1027:VAL:HG21	2.01	0.42
1:B:905:VAL:HB	1:B:906:PRO:HD3	2.01	0.42
1:B:47:ALA:HB3	1:B:88:VAL:CG1	2.50	0.41
1:B:987:MET:N	1:B:988:PRO:CD	2.84	0.41
1:B:973:ARG:N	1:B:974:PRO:HD2	2.35	0.40
1:B:314:GLU:HB2	1:B:315:PRO:HD3	2.04	0.40
1:B:1:MET:HB3	1:B:2:PRO:HD3	2.04	0.40
1:C:40:PRO:HB2	1:C:94:PHE:O	2.21	0.40
1:C:973:ARG:N	1:C:974:PRO:HD2	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1044/1057 (99%)	1014 (97%)	29 (3%)	1 (0%)	51	78
1	B	1032/1057 (98%)	1006 (98%)	26 (2%)	0	100	100
1	C	1036/1057 (98%)	1000 (96%)	36 (4%)	0	100	100
2	D	154/169 (91%)	152 (99%)	2 (1%)	0	100	100
2	E	152/169 (90%)	147 (97%)	5 (3%)	0	100	100
All	All	3418/3509 (97%)	3319 (97%)	98 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1034	SER

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	853/864 (99%)	846 (99%)	7 (1%)	81	93
1	B	841/864 (97%)	834 (99%)	7 (1%)	81	93
1	C	845/864 (98%)	840 (99%)	5 (1%)	86	95
2	D	120/132 (91%)	120 (100%)	0	100	100
2	E	119/132 (90%)	118 (99%)	1 (1%)	81	93
All	All	2778/2856 (97%)	2758 (99%)	20 (1%)	84	94

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	PHE
1	A	49	TYR
1	A	518	ARG

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Mol	Chain	Res	Type
1	A	536	ARG
1	A	765	ARG
1	A	815	ARG
1	A	1036	LYS
1	B	49	TYR
1	B	540	ARG
1	B	556	PHE
1	B	610	PHE
1	B	664	PHE
1	B	784	ASP
1	B	1030	ARG
1	C	11	PHE
1	C	49	TYR
1	C	415	ASN
1	C	784	ASP
1	C	1032	ARG
2	E	123	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 33 ligands modelled in this entry, 1 is 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
5	PTY	C	1109	-	49,49,49	0.26	0	52,54,54	0.36	0
4	LMT	C	1106	-	36,36,36	0.44	0	47,47,47	0.56	0
13	C14	C	1101	-	13,13,13	0.09	0	12,12,12	0.06	0
7	EDO	B	1110	-	3,3,3	0.07	0	2,2,2	0.18	0
10	OCT	C	1111	-	7,7,7	0.11	0	6,6,6	0.07	0
4	LMT	B	1101	-	36,36,36	0.43	0	47,47,47	0.51	0
11	SO4	B	1107	-	4,4,4	0.39	0	6,6,6	0.05	0
3	D12	C	1104	-	11,11,11	0.09	0	10,10,10	0.07	0
4	LMT	A	1102	-	36,36,36	0.45	0	47,47,47	0.60	0
4	LMT	C	1107	-	36,36,36	0.47	0	47,47,47	0.63	0
12	RBT	B	1112	-	61,66,66	0.70	2 (3%)	86,101,101	1.20	5 (5%)
14	D10	C	1103	-	9,9,9	0.10	0	8,8,8	0.06	0
10	OCT	B	1105	-	7,7,7	0.11	0	6,6,6	0.07	0
10	OCT	B	1104	-	7,7,7	0.11	0	6,6,6	0.06	0
11	SO4	C	1113	-	4,4,4	0.39	0	6,6,6	0.04	0
9	HEX	B	1103	-	5,5,5	0.14	0	4,4,4	0.11	0
5	PTY	A	1105	-	49,49,49	0.26	0	52,54,54	0.31	0
12	RBT	B	1111	-	61,66,66	0.62	2 (3%)	86,101,101	0.97	6 (6%)
7	EDO	B	1109	-	3,3,3	0.06	0	2,2,2	0.17	0
9	HEX	C	1110	-	5,5,5	0.13	0	4,4,4	0.09	0
7	EDO	B	1108	-	3,3,3	0.05	0	2,2,2	0.18	0
14	D10	C	1102	-	9,9,9	0.10	0	8,8,8	0.08	0
5	PTY	C	1108	-	49,49,49	0.26	0	52,54,54	0.31	0
6	GOL	B	1106	-	5,5,5	0.09	0	5,5,5	0.26	0
4	LMT	A	1104	-	36,36,36	0.46	0	47,47,47	0.60	0
3	D12	C	1105	-	11,11,11	0.09	0	10,10,10	0.09	0
6	GOL	C	1112	-	5,5,5	0.09	0	5,5,5	0.27	0
3	D12	A	1101	-	11,11,11	0.09	0	10,10,10	0.06	0
8	DDR	B	1102	-	27,27,27	0.24	0	29,29,29	0.25	0
7	EDO	A	1107	-	3,3,3	0.06	0	2,2,2	0.18	0
6	GOL	A	1106	-	5,5,5	0.10	0	5,5,5	0.26	0
4	LMT	A	1103	-	36,36,36	0.49	1 (2%)	47,47,47	0.68	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
5	PTY	C	1109	-	-	21/53/53/53	-
4	LMT	C	1106	-	-	10/21/61/61	0/2/2/2
13	C14	C	1101	-	-	0/11/11/11	-
7	EDO	B	1110	-	-	1/1/1/1	-
10	OCT	C	1111	-	-	1/5/5/5	-
4	LMT	B	1101	-	-	6/21/61/61	0/2/2/2
3	D12	C	1104	-	-	1/9/9/9	-
4	LMT	A	1102	-	-	10/21/61/61	0/2/2/2
4	LMT	C	1107	-	-	9/21/61/61	0/2/2/2
12	RBT	B	1112	-	-	22/59/116/116	1/5/6/6
14	D10	C	1103	-	-	1/7/7/7	-
10	OCT	B	1105	-	-	2/5/5/5	-
10	OCT	B	1104	-	-	1/5/5/5	-
9	HEX	B	1103	-	-	1/3/3/3	-
5	PTY	A	1105	-	-	22/53/53/53	-
12	RBT	B	1111	-	-	16/59/116/116	1/5/6/6
7	EDO	B	1109	-	-	0/1/1/1	-
9	HEX	C	1110	-	-	0/3/3/3	-
7	EDO	B	1108	-	-	1/1/1/1	-
14	D10	C	1102	-	-	2/7/7/7	-
5	PTY	C	1108	-	-	22/53/53/53	-
6	GOL	B	1106	-	-	0/4/4/4	-
4	LMT	A	1104	-	-	6/21/61/61	0/2/2/2
3	D12	C	1105	-	-	4/9/9/9	-
6	GOL	C	1112	-	-	3/4/4/4	-
3	D12	A	1101	-	-	2/9/9/9	-
8	DDR	B	1102	-	-	16/29/29/29	-
7	EDO	A	1107	-	-	1/1/1/1	-
6	GOL	A	1106	-	-	2/4/4/4	-
4	LMT	A	1103	-	-	12/21/61/61	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	1112	RBT	C2-C1	-3.18	1.40	1.50
12	B	1111	RBT	C2-C1	-2.82	1.41	1.50
12	B	1112	RBT	C3-C4	-2.59	1.39	1.48
12	B	1111	RBT	C3-C4	-2.23	1.40	1.48
4	A	1103	LMT	O1'-C1'	2.01	1.43	1.40

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	1112	RBT	C3-C2-C1	-4.75	117.00	121.44
12	B	1112	RBT	C2-C3-N2	4.72	136.76	127.95
12	B	1112	RBT	C10-C4-C3	-3.68	119.87	123.42
12	B	1111	RBT	C5-C6-C7	-3.57	122.52	125.33
12	B	1111	RBT	C2-C3-N2	3.41	134.32	127.95
12	B	1112	RBT	C5-C6-C7	-3.34	122.71	125.33
12	B	1111	RBT	C3-C2-C1	-3.04	118.60	121.44
12	B	1111	RBT	C39-C38-N3	-2.66	109.01	111.42
12	B	1112	RBT	C1-C2-N1	2.41	120.92	115.28
12	B	1111	RBT	C25-O7-C35	2.07	120.92	117.72
12	B	1111	RBT	C10-C4-C3	-2.05	121.44	123.42

There are no chirality outliers.

All (195) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1102	LMT	C2'-C1'-O1'-C1
4	A	1102	LMT	O5'-C1'-O1'-C1
4	A	1103	LMT	C2-C1-O1'-C1'
4	C	1106	LMT	C2-C1-O1'-C1'
4	C	1107	LMT	C2'-C1'-O1'-C1
4	C	1107	LMT	O5'-C1'-O1'-C1
5	A	1105	PTY	N1-C2-C3-O11
5	C	1108	PTY	N1-C2-C3-O11
5	C	1108	PTY	C11-C8-O7-C6
5	C	1109	PTY	N1-C2-C3-O11
5	C	1109	PTY	C3-O11-P1-O13
5	C	1109	PTY	C3-O11-P1-O14
5	C	1109	PTY	C5-O14-P1-O11
12	B	1111	RBT	C16-C15-N1-C2
12	B	1111	RBT	O11-C15-N1-C2
12	B	1111	RBT	C15-C16-C17-C18
12	B	1111	RBT	C30-C16-C17-C18
12	B	1111	RBT	C36-C35-O7-C25
12	B	1111	RBT	O8-C35-O7-C25
12	B	1112	RBT	C16-C15-N1-C2
12	B	1112	RBT	O11-C15-N1-C2
4	C	1107	LMT	O5B-C1B-O1B-C4'
5	A	1105	PTY	O10-C8-O7-C6
5	C	1108	PTY	O10-C8-O7-C6
4	C	1107	LMT	C2B-C1B-O1B-C4'

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Mol	Chain	Res	Type	Atoms
5	A	1105	PTY	C11-C8-O7-C6
12	B	1112	RBT	N4-C43-C44-C46
8	B	1102	DDR	C2-C1-O51-C51
4	A	1102	LMT	O5'-C5'-C6'-O6'
12	B	1112	RBT	N4-C43-C44-C45
4	A	1103	LMT	O5B-C5B-C6B-O6B
4	C	1107	LMT	O5'-C5'-C6'-O6'
12	B	1112	RBT	C20-C21-C22-C23
4	A	1102	LMT	C4'-C5'-C6'-O6'
4	C	1106	LMT	C4'-C5'-C6'-O6'
8	B	1102	DDR	O1-C1-O51-C51
5	C	1108	PTY	C31-C30-O4-C1
5	C	1109	PTY	C31-C30-O4-C1
4	A	1104	LMT	O5'-C5'-C6'-O6'
4	A	1103	LMT	C5'-C4'-O1B-C1B
4	C	1106	LMT	O5'-C5'-C6'-O6'
4	B	1101	LMT	C4'-C5'-C6'-O6'
6	A	1106	GOL	O2-C2-C3-O3
12	B	1111	RBT	C17-C18-C19-C20
5	C	1109	PTY	O30-C30-O4-C1
5	C	1108	PTY	O30-C30-O4-C1
12	B	1111	RBT	N4-C43-C44-C45
4	A	1103	LMT	C4B-C5B-C6B-O6B
4	A	1104	LMT	C4'-C5'-C6'-O6'
4	C	1107	LMT	C4'-C5'-C6'-O6'
5	C	1109	PTY	C11-C8-O7-C6
8	B	1102	DDR	C22-C21-O52-C52
5	C	1108	PTY	C5-O14-P1-O11
5	C	1109	PTY	O10-C8-O7-C6
8	B	1102	DDR	O21-C21-O52-C52
12	B	1111	RBT	N4-C43-C44-C46
3	C	1104	D12	C7-C8-C9-C10
8	B	1102	DDR	C21-C22-C23-C24
5	A	1105	PTY	C11-C12-C13-C14
4	A	1103	LMT	C3-C4-C5-C6
4	C	1106	LMT	O1'-C1-C2-C3
4	C	1107	LMT	C3-C4-C5-C6
5	A	1105	PTY	C37-C38-C39-C40
4	A	1102	LMT	C4B-C5B-C6B-O6B
12	B	1112	RBT	O10-C21-C22-C32
4	B	1101	LMT	C3-C4-C5-C6
6	A	1106	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
6	C	1112	GOL	C1-C2-C3-O3
5	C	1108	PTY	C21-C22-C23-C24
4	A	1104	LMT	C5-C6-C7-C8
5	A	1105	PTY	C16-C17-C18-C19
4	B	1101	LMT	O5B-C5B-C6B-O6B
8	B	1102	DDR	C22-C23-C24-C25
12	B	1111	RBT	C28-C27-O6-C37
5	C	1109	PTY	C24-C25-C26-C27
5	A	1105	PTY	C19-C20-C21-C22
4	B	1101	LMT	O5'-C5'-C6'-O6'
4	C	1107	LMT	O5B-C5B-C6B-O6B
5	C	1109	PTY	C19-C20-C21-C22
5	A	1105	PTY	C36-C37-C38-C39
10	C	1111	OCT	C4-C5-C6-C7
4	A	1104	LMT	C3-C4-C5-C6
5	A	1105	PTY	C31-C30-O4-C1
12	B	1112	RBT	C15-C16-C17-C18
8	B	1102	DDR	C26-C27-C28-C29
4	A	1104	LMT	C1-C2-C3-C4
12	B	1112	RBT	C34-C26-C27-C28
12	B	1112	RBT	C34-C26-C27-O6
12	B	1112	RBT	C25-C26-C27-O6
5	A	1105	PTY	O30-C30-O4-C1
5	C	1108	PTY	C6-C5-O14-P1
5	C	1109	PTY	O14-C5-C6-C1
4	A	1104	LMT	O5B-C5B-C6B-O6B
8	B	1102	DDR	C3-C4-C5-C6
4	A	1103	LMT	C3'-C4'-O1B-C1B
10	B	1105	OCT	C3-C4-C5-C6
4	C	1106	LMT	O5B-C5B-C6B-O6B
12	B	1112	RBT	C30-C16-C17-C18
4	A	1103	LMT	C5-C6-C7-C8
7	A	1107	EDO	O1-C1-C2-O2
12	B	1112	RBT	O10-C21-C22-C23
5	A	1105	PTY	C25-C26-C27-C28
14	C	1103	D10	C6-C7-C8-C9
12	B	1111	RBT	C44-C43-N4-C42
5	A	1105	PTY	C21-C22-C23-C24
12	B	1112	RBT	C20-C21-C22-C32
4	C	1107	LMT	C11-C10-C9-C8
8	B	1102	DDR	O51-C51-C52-C53
5	C	1108	PTY	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
5	C	1109	PTY	C8-C11-C12-C13
3	A	1101	D12	C11-C10-C9-C8
4	B	1101	LMT	C11-C10-C9-C8
14	C	1102	D10	C3-C4-C5-C6
12	B	1111	RBT	C16-C17-C18-C19
4	A	1102	LMT	C11-C10-C9-C8
4	C	1106	LMT	C3-C4-C5-C6
7	B	1110	EDO	O1-C1-C2-O2
4	A	1102	LMT	C9-C10-C11-C12
5	A	1105	PTY	C34-C35-C36-C37
8	B	1102	DDR	C2-C3-C4-C5
5	C	1109	PTY	C18-C19-C20-C21
5	C	1109	PTY	C11-C12-C13-C14
12	B	1111	RBT	C24-C25-O7-C35
5	C	1108	PTY	O4-C1-C6-C5
5	C	1109	PTY	O14-C5-C6-O7
5	A	1105	PTY	C31-C32-C33-C34
8	B	1102	DDR	O51-C51-C52-O52
4	A	1103	LMT	C9-C10-C11-C12
4	B	1101	LMT	C9-C10-C11-C12
4	A	1103	LMT	C11-C10-C9-C8
5	A	1105	PTY	C5-O14-P1-O11
4	A	1103	LMT	O1'-C1-C2-C3
10	B	1105	OCT	C2-C3-C4-C5
5	C	1108	PTY	C5-O14-P1-O13
5	C	1109	PTY	C5-O14-P1-O12
12	B	1111	RBT	C44-C43-N4-C41
12	B	1112	RBT	C11-C12-O5-C29
12	B	1112	RBT	C13-C12-O5-C29
12	B	1112	RBT	O3-C12-O5-C29
3	C	1105	D12	C2-C3-C4-C5
12	B	1111	RBT	C26-C25-O7-C35
12	B	1112	RBT	C1-C2-N1-C15
5	C	1108	PTY	O4-C1-C6-O7
4	A	1102	LMT	O5B-C5B-C6B-O6B
4	A	1102	LMT	C6-C7-C8-C9
5	C	1108	PTY	C31-C32-C33-C34
5	A	1105	PTY	C3-O11-P1-O14
12	B	1112	RBT	O11-C15-C16-C30
5	C	1108	PTY	C32-C33-C34-C35
6	C	1112	GOL	O2-C2-C3-O3
8	B	1102	DDR	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
3	C	1105	D12	C1-C2-C3-C4
4	C	1106	LMT	C11-C10-C9-C8
4	C	1106	LMT	C7-C8-C9-C10
5	C	1108	PTY	C22-C23-C24-C25
5	A	1105	PTY	O4-C1-C6-O7
5	C	1108	PTY	C39-C40-C41-C42
5	C	1108	PTY	C36-C37-C38-C39
12	B	1112	RBT	C28-C29-O5-C12
3	C	1105	D12	C11-C10-C9-C8
5	C	1108	PTY	C24-C25-C26-C27
4	A	1103	LMT	C7-C8-C9-C10
5	A	1105	PTY	C35-C36-C37-C38
12	B	1112	RBT	N1-C15-C16-C30
5	A	1105	PTY	O4-C30-C31-C32
6	C	1112	GOL	O1-C1-C2-C3
9	B	1103	HEX	C2-C3-C4-C5
14	C	1102	D10	C7-C8-C9-C10
12	B	1112	RBT	O11-C15-C16-C17
3	A	1101	D12	C7-C8-C9-C10
5	C	1108	PTY	O4-C30-C31-C32
4	C	1106	LMT	C4-C5-C6-C7
8	B	1102	DDR	C5-C6-C7-C8
7	B	1108	EDO	O1-C1-C2-O2
4	A	1103	LMT	C2-C3-C4-C5
4	A	1102	LMT	C3-C4-C5-C6
5	C	1109	PTY	C34-C35-C36-C37
5	A	1105	PTY	C12-C11-C8-O7
5	C	1109	PTY	O4-C30-C31-C32
3	C	1105	D12	C3-C4-C5-C6
5	C	1109	PTY	C21-C22-C23-C24
12	B	1111	RBT	C28-C29-O5-C12
5	C	1109	PTY	C12-C11-C8-O7
5	C	1108	PTY	C13-C14-C15-C16
5	C	1108	PTY	C38-C39-C40-C41
5	C	1108	PTY	O30-C30-C31-C32
12	B	1112	RBT	C17-C18-C19-C20
5	C	1109	PTY	C12-C13-C14-C15
8	B	1102	DDR	C7-C8-C9-C10
5	A	1105	PTY	C3-O11-P1-O13
5	A	1105	PTY	C12-C11-C8-O10
4	C	1106	LMT	C6-C7-C8-C9
10	B	1104	OCT	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
8	B	1102	DDR	O52-C21-C22-C23
8	B	1102	DDR	O21-C21-C22-C23

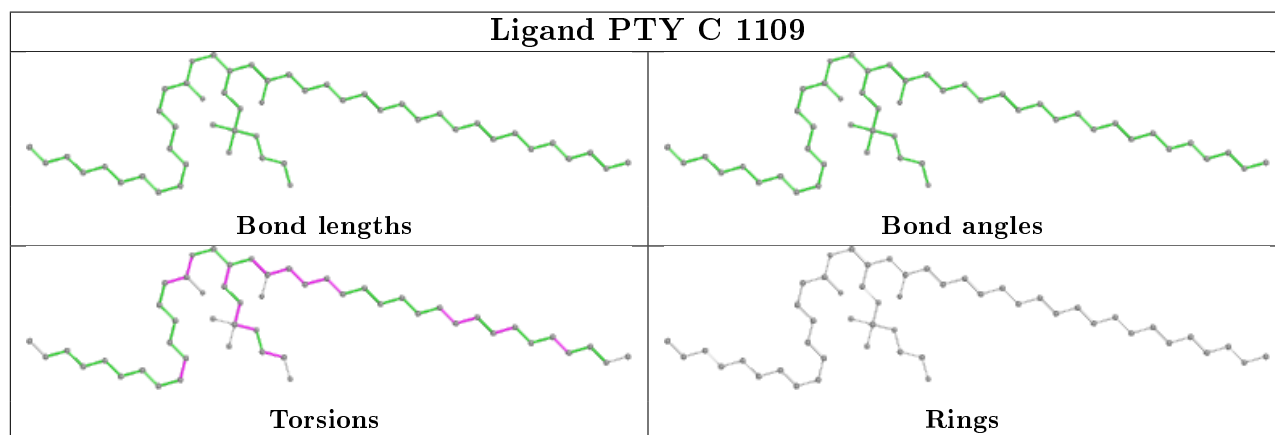
All (2) ring outliers are listed below:

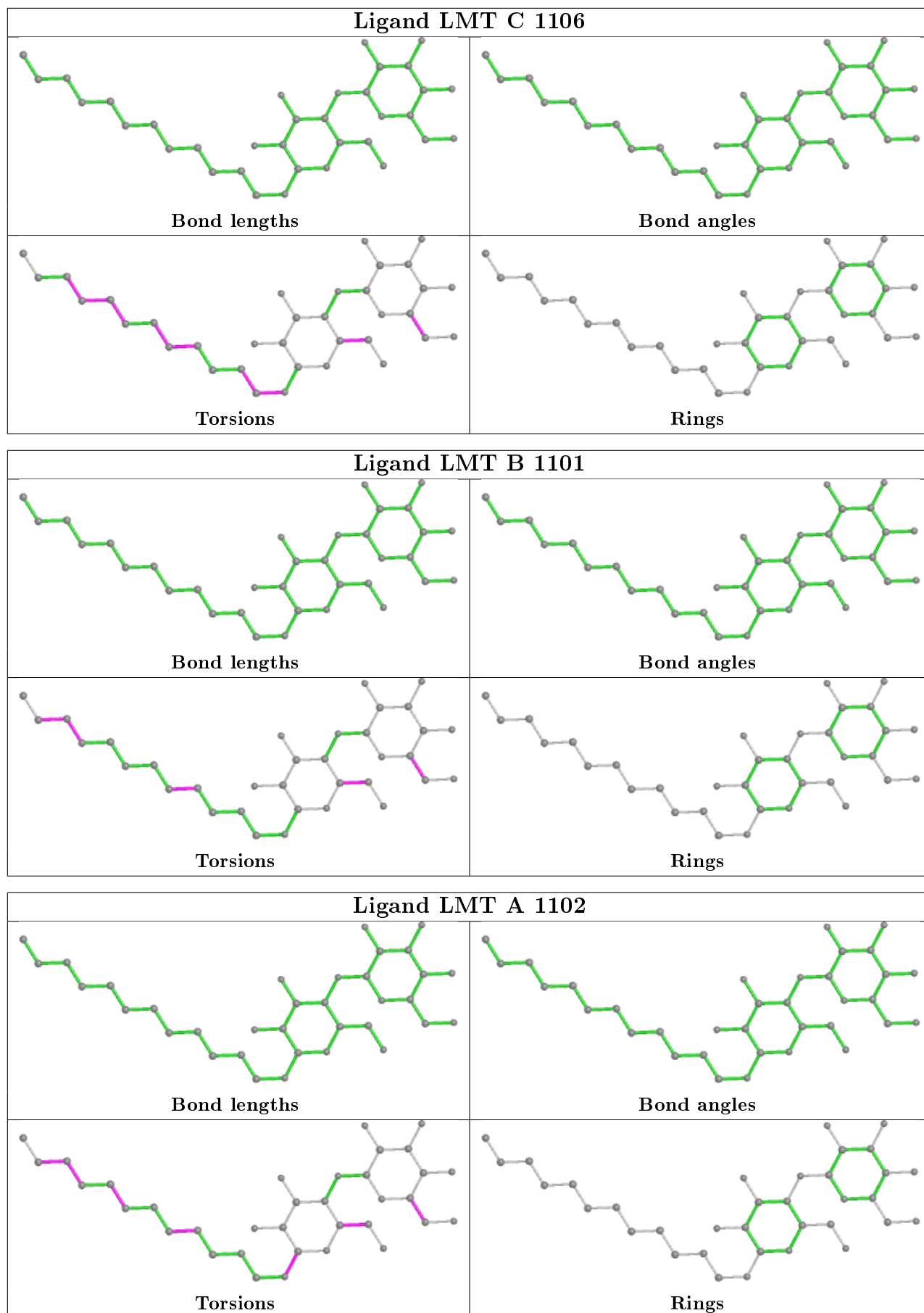
Mol	Chain	Res	Type	Atoms
12	B	1112	RBT	C38-C39-C40-C41-C42-N4
12	B	1111	RBT	C38-C39-C40-C41-C42-N4

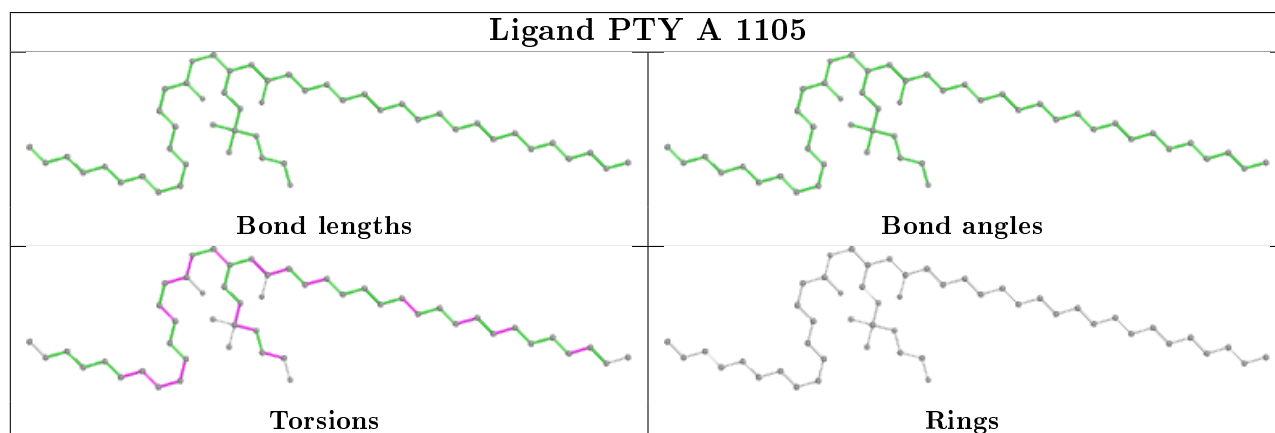
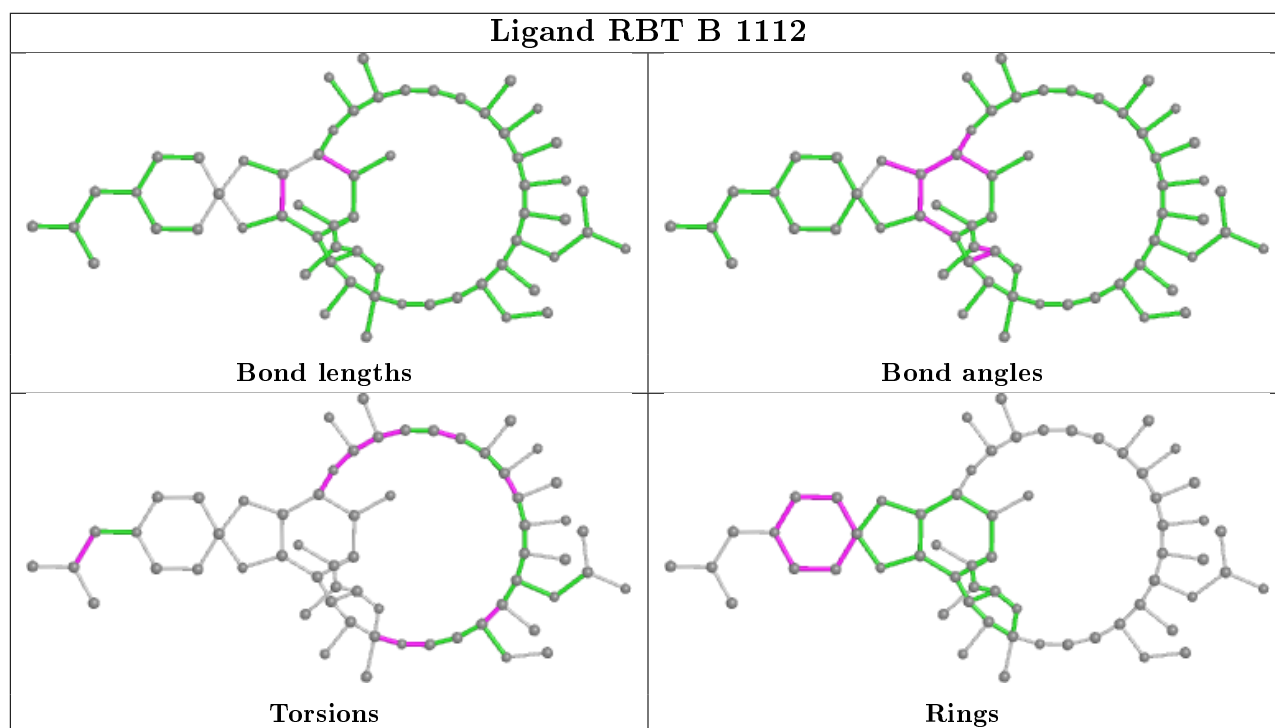
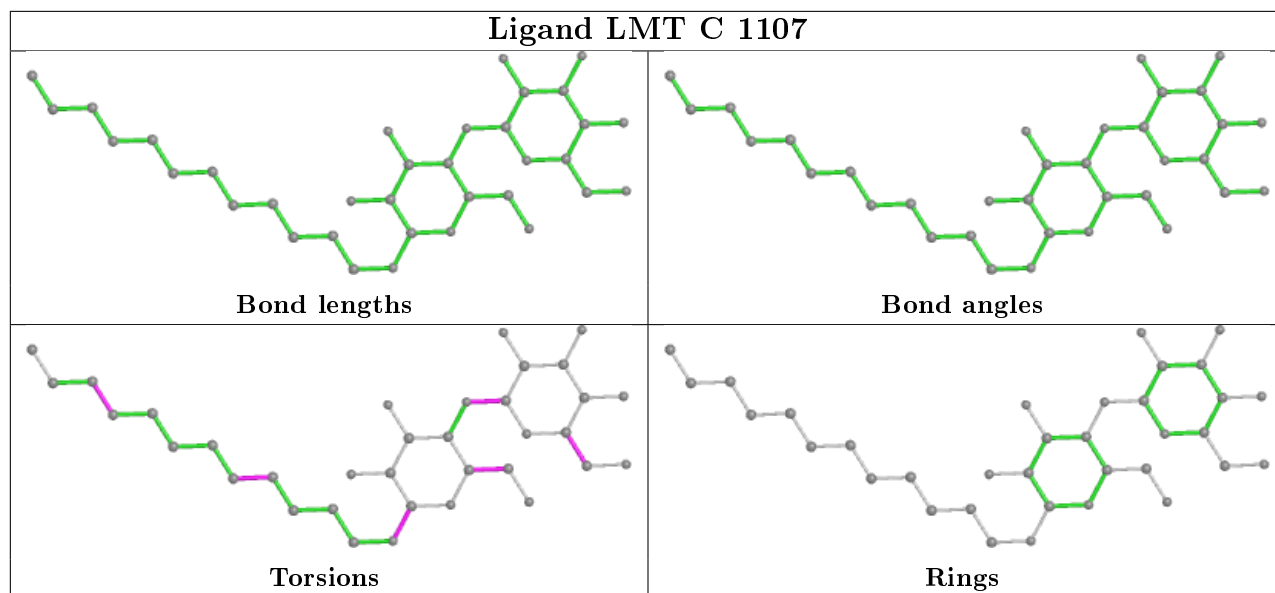
2 monomers are involved in 2 short contacts:

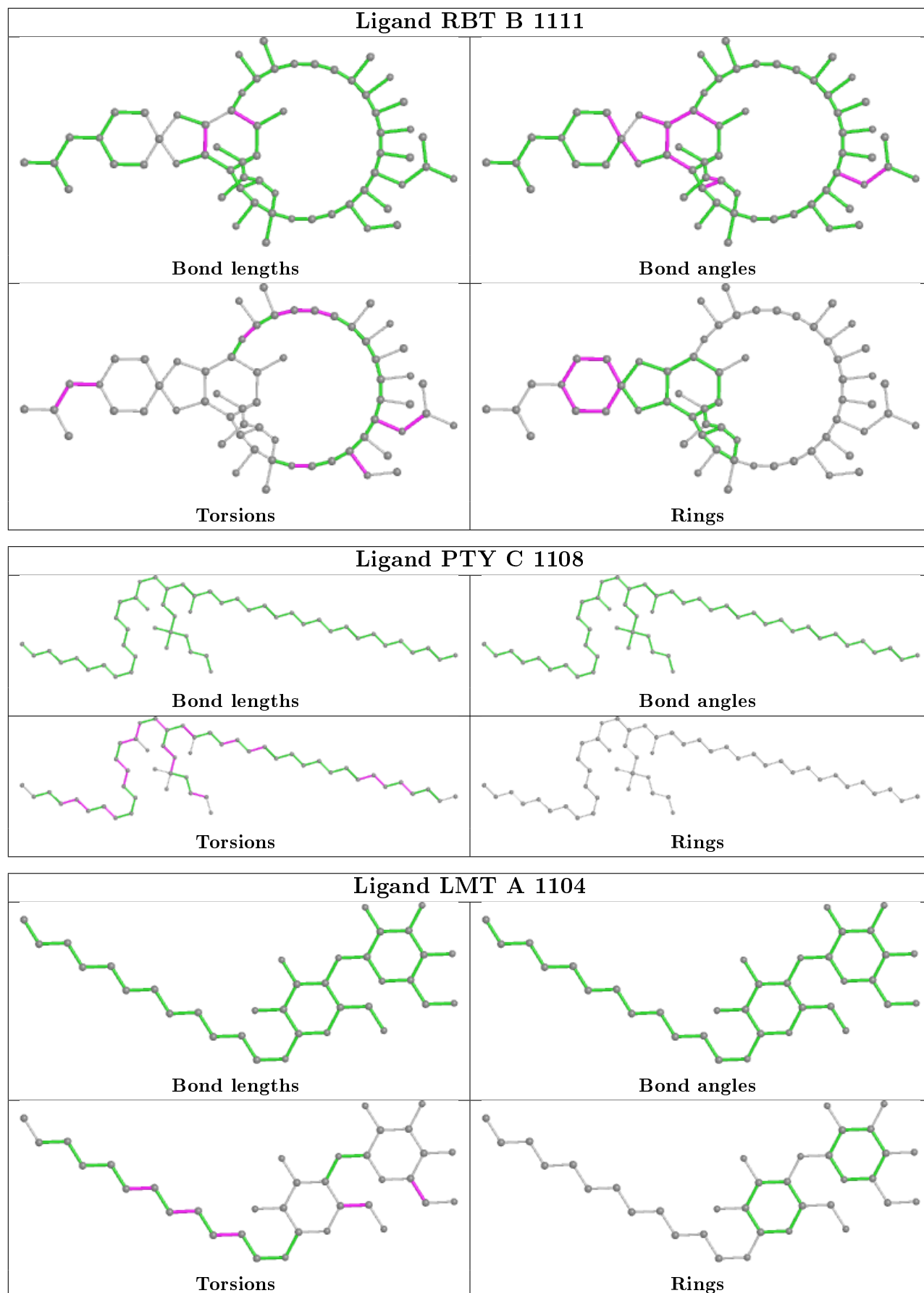
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	B	1112	RBT	1	0
12	B	1111	RBT	1	0

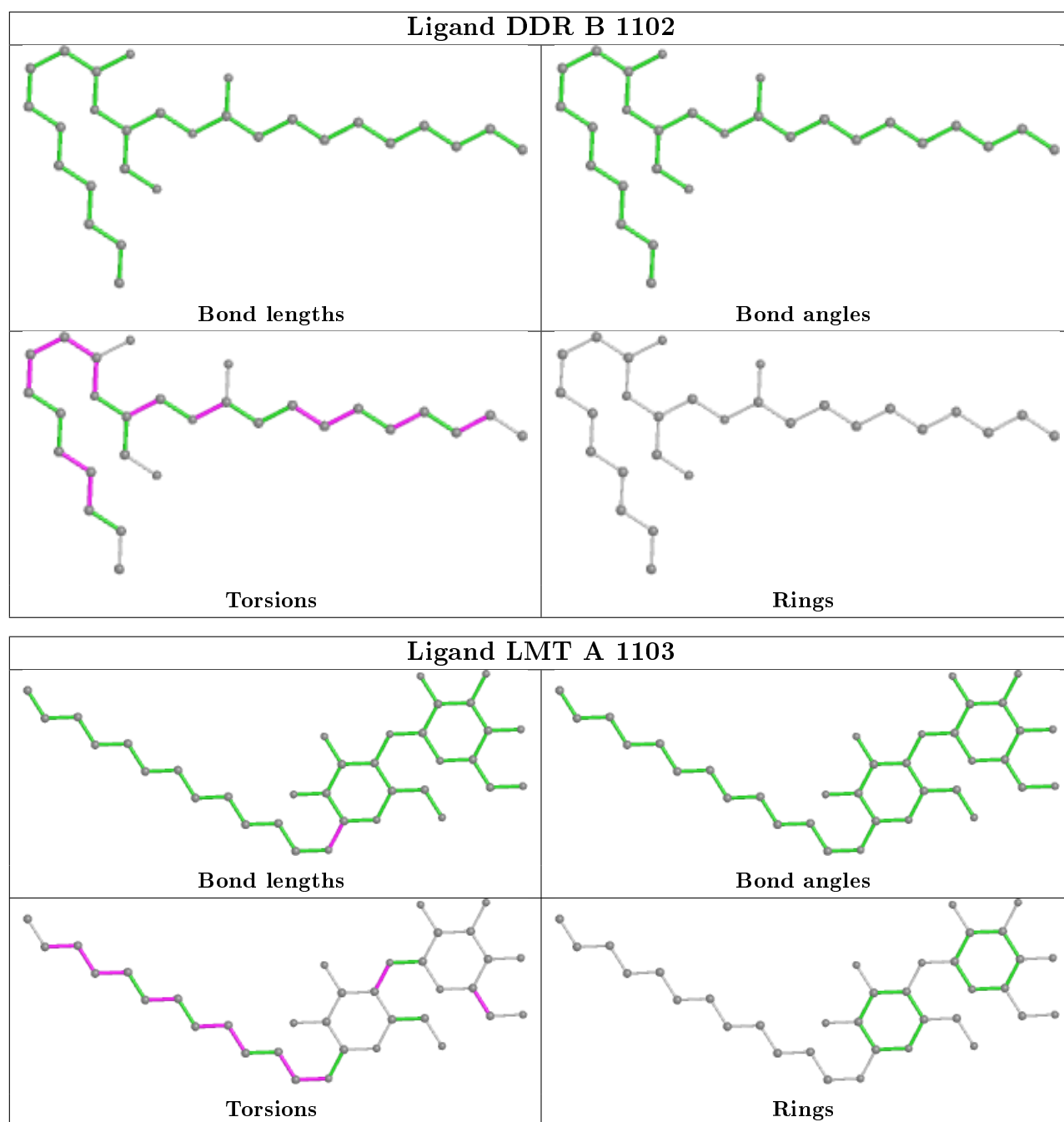
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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%)	0.23	43 (4%) 37 36	34, 61, 92, 113	12 (1%)
1	B	1034/1057 (97%)	0.15	42 (4%) 37 36	34, 57, 78, 96	0
1	C	1035/1057 (97%)	0.16	43 (4%) 36 35	36, 50, 73, 100	0
2	D	156/169 (92%)	0.56	14 (8%) 9 7	49, 60, 80, 93	0
2	E	154/169 (91%)	1.37	46 (29%) 0 0	61, 77, 100, 106	0
All	All	3421/3509 (97%)	0.25	188 (5%) 25 24	34, 57, 87, 113	12 (0%)

All (188) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	510	LYS	6.2
2	E	32	ILE	5.8
2	E	31	ARG	5.4
2	E	28	ASP	5.2
2	E	165	LEU	5.1
2	E	66	LEU	5.0
2	E	35	ALA	5.0
1	A	865	GLN	4.9
2	E	33	LEU	4.8
1	A	866	GLU	4.6
2	E	36	ASN	4.5
1	C	732	ASP	4.4
1	A	918	PHE	4.3
1	A	673	GLU	4.0
2	E	106	VAL	4.0
1	A	834	GLY	3.9
2	E	107	ASN	3.9
1	C	739	LEU	3.9
1	A	547	ILE	3.9
2	D	165	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	603	LYS	3.8
1	B	657	GLN	3.8
2	E	34	MET	3.8
1	C	497	LEU	3.8
1	C	511	GLY	3.8
2	E	139	VAL	3.8
2	E	150	PHE	3.8
1	B	642	ASN	3.7
1	A	543	VAL	3.7
1	B	638	PRO	3.7
1	A	674	LEU	3.7
2	E	117	LEU	3.7
2	E	62	ILE	3.7
1	A	869	SER	3.7
1	C	363	ARG	3.7
1	A	675	GLY	3.7
2	E	140	ASN	3.6
1	B	606	VAL	3.6
2	E	27	ASP	3.5
2	E	141	ALA	3.5
1	C	506	GLY	3.5
2	E	163	GLU	3.5
1	A	503	GLY	3.4
1	C	730	ASP	3.4
2	D	11	GLY	3.4
1	C	499	PRO	3.4
1	C	811	TYR	3.4
1	C	253	VAL	3.4
1	C	362	PHE	3.3
2	E	115	THR	3.3
1	B	501	ALA	3.3
1	A	712	MET	3.3
2	D	163	GLU	3.3
1	A	362	PHE	3.3
2	E	68	LYS	3.2
1	C	731	ILE	3.2
1	A	1040	ILE	3.2
2	D	150	PHE	3.2
2	D	126	LEU	3.2
1	B	257	GLY	3.2
2	D	134	LYS	3.2
2	E	109	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	604	ASN	3.1
1	C	421	ALA	3.1
1	B	868	LEU	3.1
1	B	655	PHE	3.1
1	B	508	GLY	3.1
1	C	513	PHE	3.1
1	C	737	GLN	3.1
1	B	641	GLU	3.0
1	B	633	ASP	3.0
1	A	835	LYS	3.0
2	E	60	LEU	3.0
1	C	71	GLY	3.0
1	C	918	PHE	3.0
1	A	678	THR	2.9
1	A	501	ALA	2.9
1	C	508	GLY	2.9
2	E	61	GLU	2.9
2	E	137	ALA	2.9
2	E	133	LEU	2.9
1	A	867	ARG	2.9
2	E	74	ASN	2.8
1	B	636	ASP	2.8
1	B	653	ARG	2.8
1	A	429	GLU	2.8
2	E	67	LEU	2.8
1	C	799	VAL	2.8
1	A	833	PRO	2.7
1	A	550	VAL	2.7
2	E	30	VAL	2.7
2	E	148	THR	2.7
1	A	711	ASP	2.7
2	E	69	ASN	2.7
1	B	498	LYS	2.7
2	E	134	LYS	2.7
2	E	145	PHE	2.7
2	E	152	ILE	2.7
1	A	871	ASN	2.7
1	A	196	PHE	2.6
1	C	498	LYS	2.6
1	B	366	LEU	2.6
1	B	635	ALA	2.6
1	C	803	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	139	VAL	2.6
2	D	28	ASP	2.6
1	A	512	PHE	2.6
1	B	639	GLY	2.6
2	E	64	GLU	2.6
1	A	708	LYS	2.6
2	E	154	ILE	2.6
1	C	804	PHE	2.5
1	C	735	LYS	2.5
1	A	508	GLY	2.5
2	D	154	ILE	2.5
2	E	98	VAL	2.5
1	B	647	ILE	2.5
2	D	161	LEU	2.5
2	D	166	GLN	2.5
1	C	500	ILE	2.4
1	B	255	GLN	2.4
1	B	195	LYS	2.4
2	E	108	ALA	2.4
1	A	423	GLU	2.4
1	C	701	GLN	2.4
1	A	259	ARG	2.4
1	C	258	SER	2.4
1	B	640	GLU	2.4
1	A	255	GLN	2.4
1	B	500	ILE	2.4
2	D	164	ILE	2.4
1	C	196	PHE	2.4
2	E	159	GLU	2.4
1	C	733	GLN	2.4
1	B	788	ASP	2.4
1	A	419	VAL	2.4
1	C	790	TYR	2.3
1	C	150	THR	2.3
1	B	637	ARG	2.3
1	A	515	TRP	2.3
2	E	37	GLY	2.3
2	E	73	VAL	2.3
2	D	140	ASN	2.3
1	B	600	THR	2.3
1	B	660	ASP	2.3
1	C	427	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	846	GLN	2.3
2	E	70	GLY	2.2
1	A	868	LEU	2.2
1	C	512	PHE	2.2
1	A	672	VAL	2.2
1	C	797	GLN	2.2
2	E	65	VAL	2.2
2	D	160	ASP	2.2
1	B	787	GLY	2.2
1	A	253	VAL	2.2
1	B	254	ASN	2.2
1	B	503	GLY	2.2
1	A	500	ILE	2.2
1	A	679	GLY	2.2
1	B	597	TYR	2.2
1	A	426	PRO	2.2
1	B	499	PRO	2.2
1	C	255	GLN	2.1
1	C	501	ALA	2.1
1	A	980	LEU	2.1
1	B	643	LYS	2.1
1	C	729	ILE	2.1
1	C	791	VAL	2.1
1	C	734	GLU	2.1
1	B	871	ASN	2.1
1	B	196	PHE	2.1
1	B	258	SER	2.1
1	C	792	ARG	2.1
1	B	867	ARG	2.1
1	A	197	GLN	2.1
2	E	164	ILE	2.1
1	C	1035	ARG	2.1
2	E	63	VAL	2.0
1	B	918	PHE	2.0
1	B	596	HIS	2.0
1	A	558	ARG	2.0
1	A	502	LYS	2.0
1	B	607	GLU	2.0
1	C	509	LYS	2.0
2	E	143	ASP	2.0
1	B	558	ARG	2.0
1	C	674	LEU	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.

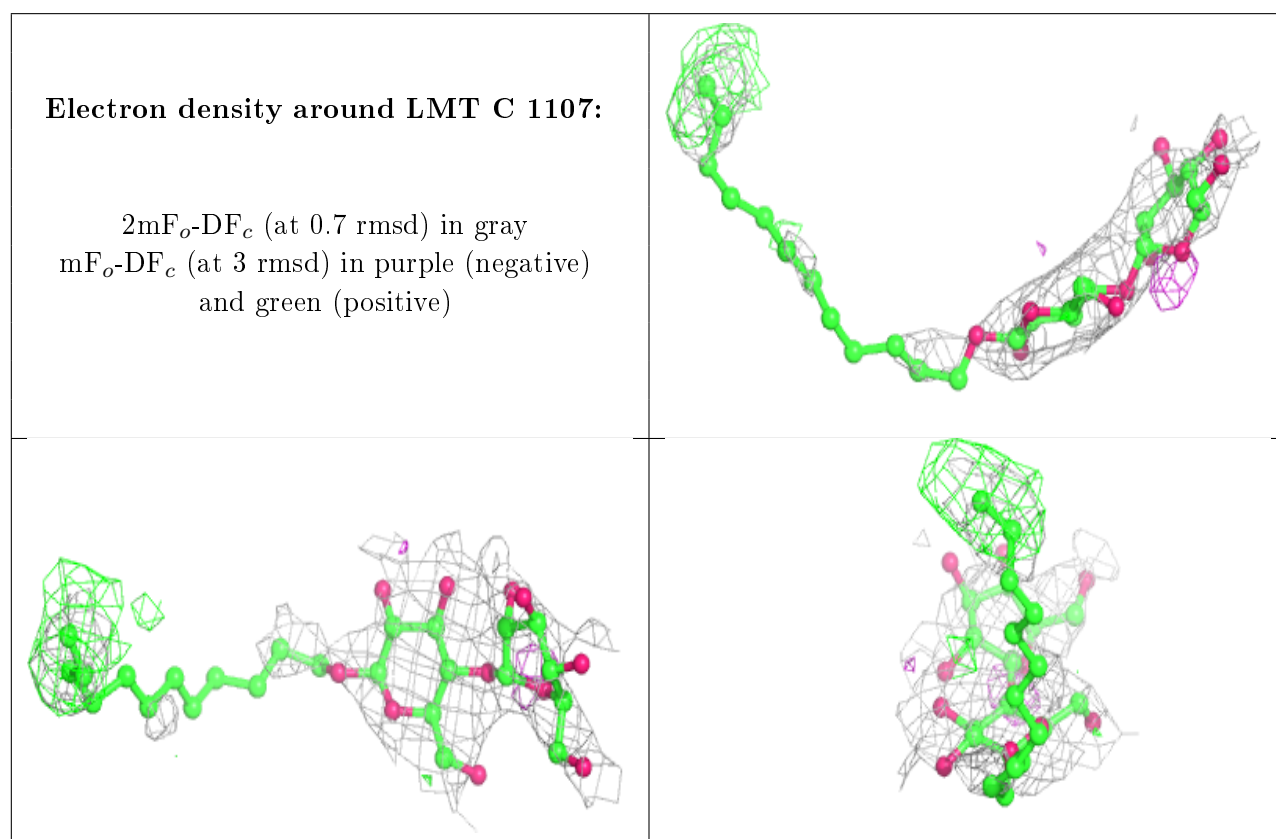
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	LMT	C	1107	35/35	0.64	0.45	104,110,112,112	0
5	PTY	A	1105	50/50	0.64	0.36	91,115,127,130	0
3	D12	A	1101	12/12	0.67	0.26	83,85,87,87	0
5	PTY	C	1108	50/50	0.69	0.34	88,95,100,101	0
6	GOL	C	1112	6/6	0.69	0.41	79,80,80,80	0
9	HEX	B	1103	6/6	0.72	0.26	62,63,63,63	0
10	OCT	C	1111	8/8	0.74	0.36	67,67,68,68	0
14	D10	C	1103	10/10	0.74	0.23	76,77,80,80	0
5	PTY	C	1109	50/50	0.75	0.32	93,109,126,128	0
3	D12	C	1105	12/12	0.77	0.26	72,75,76,76	0
9	HEX	C	1110	6/6	0.77	0.20	64,64,64,65	0
7	EDO	B	1109	4/4	0.78	0.31	90,91,91,91	0
10	OCT	B	1104	8/8	0.79	0.26	74,75,75,75	0
3	D12	C	1104	12/12	0.79	0.27	63,65,67,67	0
6	GOL	A	1106	6/6	0.79	0.24	72,72,72,72	0
13	C14	C	1101	14/14	0.80	0.29	70,71,71,71	0
7	EDO	B	1110	4/4	0.81	0.33	85,85,85,85	0
10	OCT	B	1105	8/8	0.83	0.32	74,74,74,74	0
4	LMT	A	1102	35/35	0.83	0.26	81,93,101,101	0
7	EDO	A	1107	4/4	0.83	0.32	70,70,71,71	0
8	DDR	B	1102	28/28	0.83	0.31	77,84,94,95	0
4	LMT	A	1103	35/35	0.84	0.21	71,83,94,95	0
14	D10	C	1102	10/10	0.85	0.35	69,71,73,73	0
12	RBT	B	1111	61/61	0.87	0.23	72,76,79,80	0
7	EDO	B	1108	4/4	0.88	0.20	54,54,54,54	0
4	LMT	B	1101	35/35	0.88	0.27	76,80,92,93	0
12	RBT	B	1112	61/61	0.88	0.20	79,81,83,85	0

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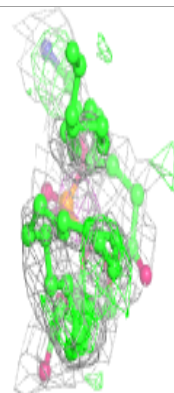
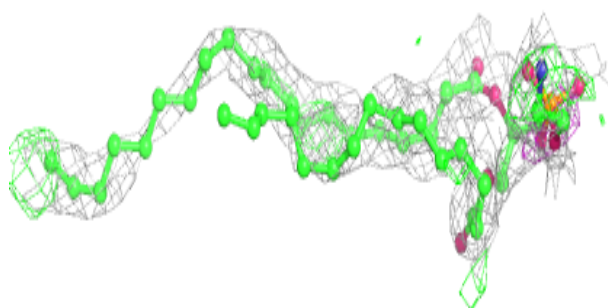
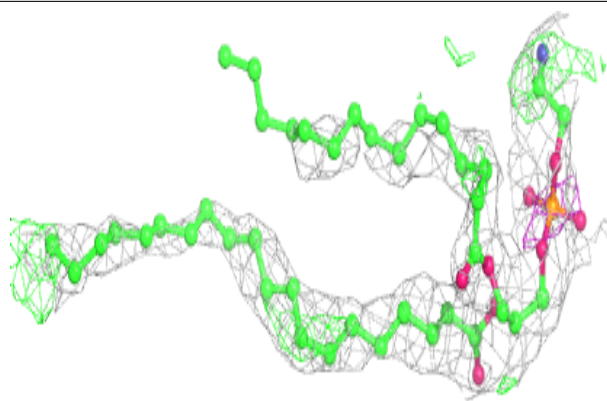
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	LMT	A	1104	35/35	0.90	0.34	91,96,102,102	0
6	GOL	B	1106	6/6	0.91	0.17	70,71,71,72	0
4	LMT	C	1106	35/35	0.92	0.22	61,66,74,75	0
11	SO4	C	1113	5/5	0.93	0.15	85,85,85,86	0
15	CL	C	1114	1/1	0.93	0.15	63,63,63,63	0
11	SO4	B	1107	5/5	0.97	0.09	81,81,81,81	0

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

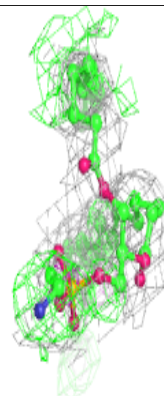
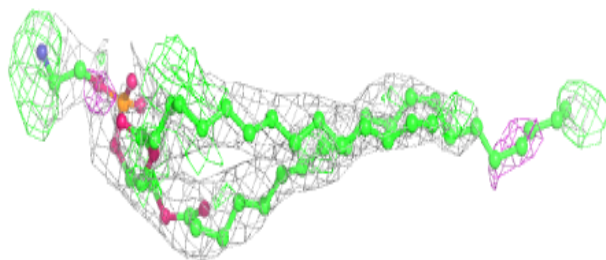
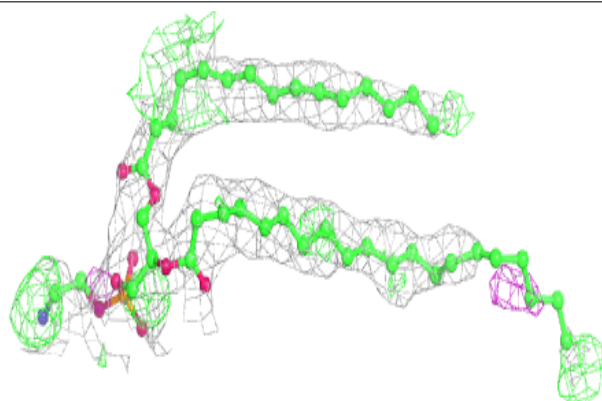


Electron density around PTY A 1105:

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

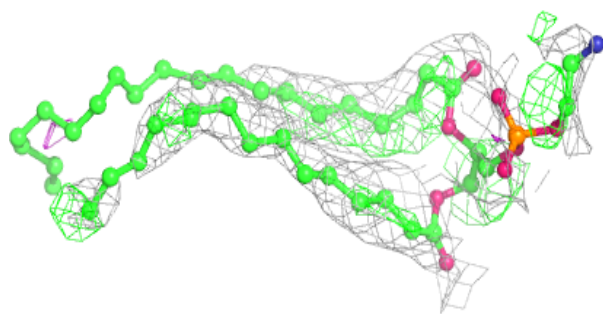
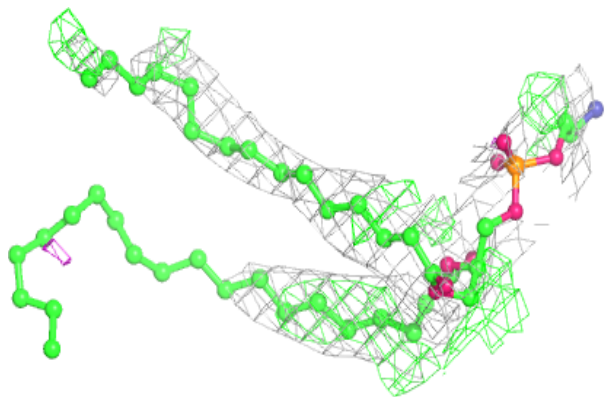
**Electron density around PTY C 1108:**

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

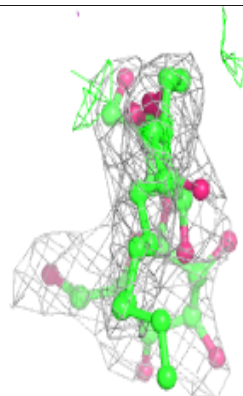
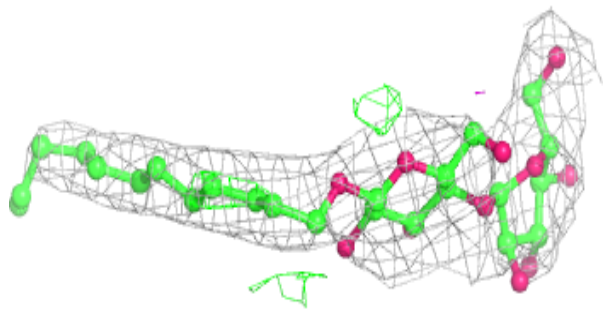
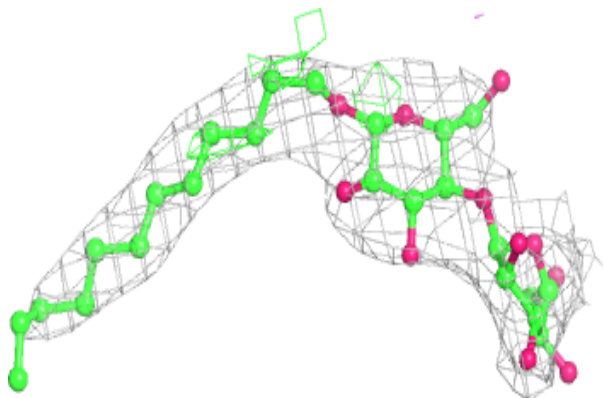


Electron density around PTY C 1109:

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

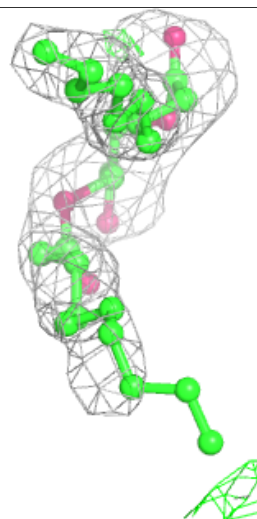
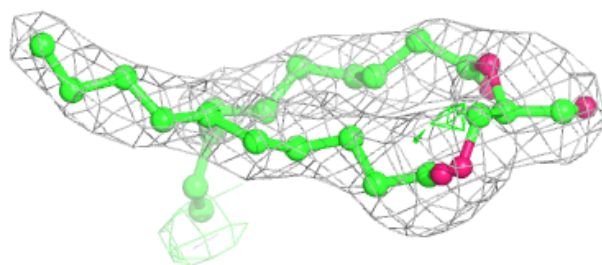
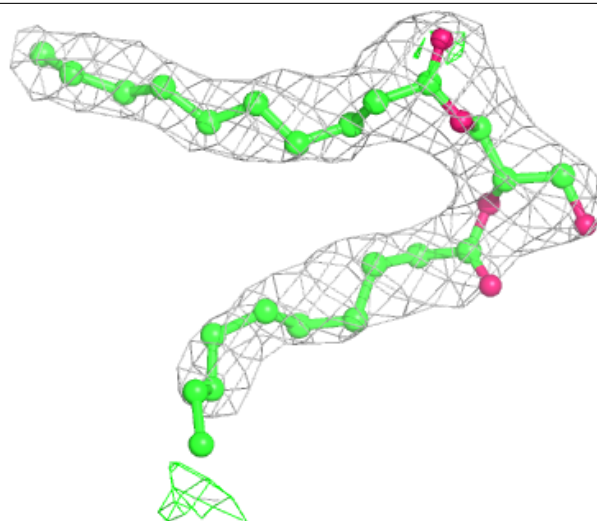
**Electron density around LMT A 1102:**

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



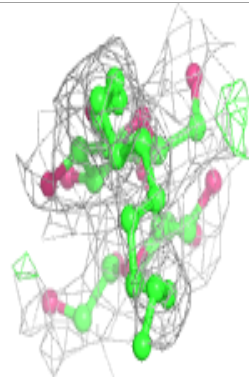
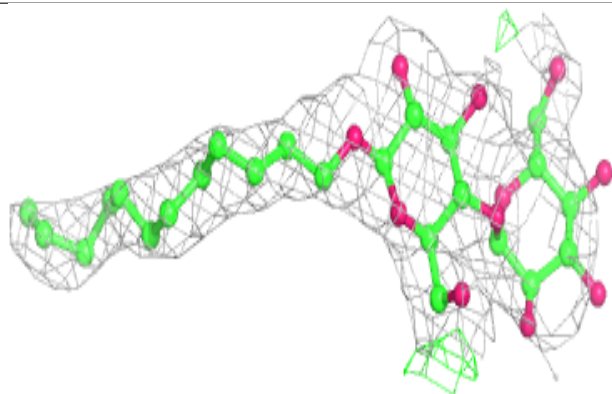
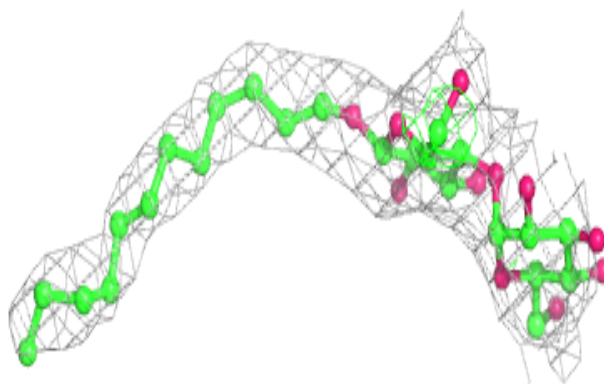
Electron density around DDR B 1102:

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



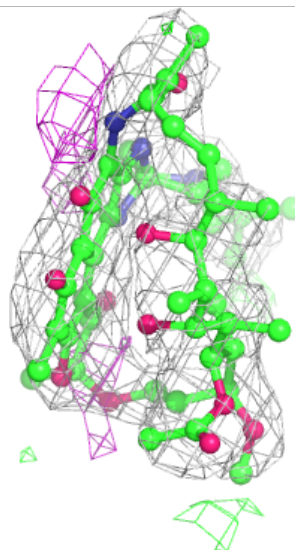
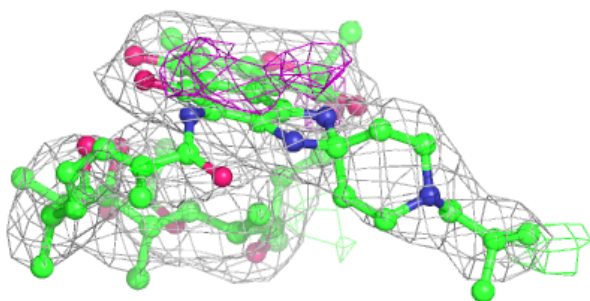
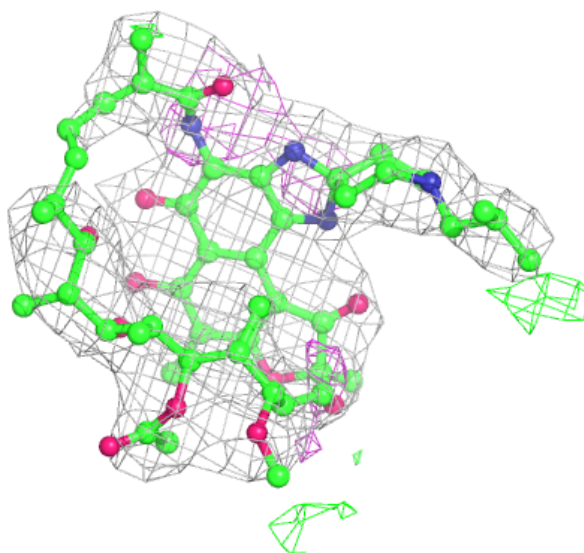
Electron density around LMT A 1103:

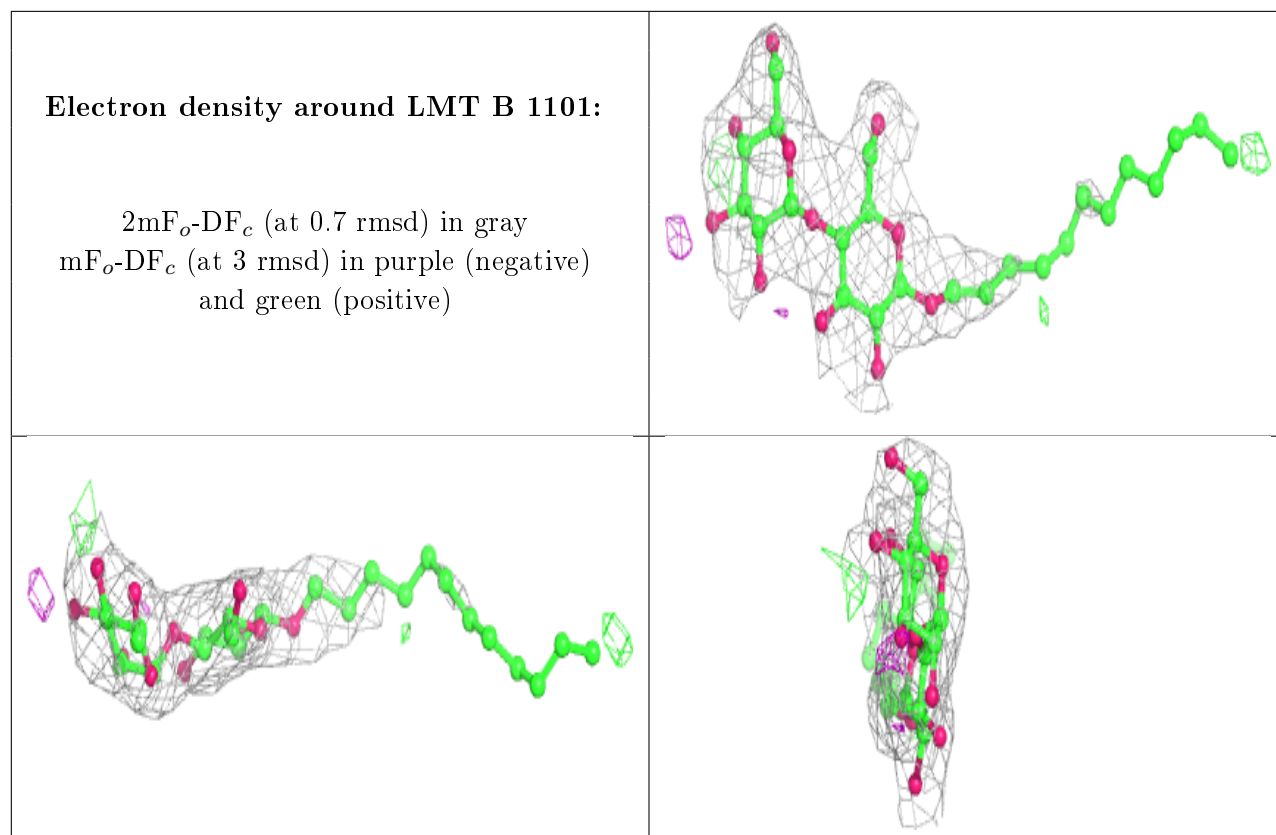
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around RBT B 1111:

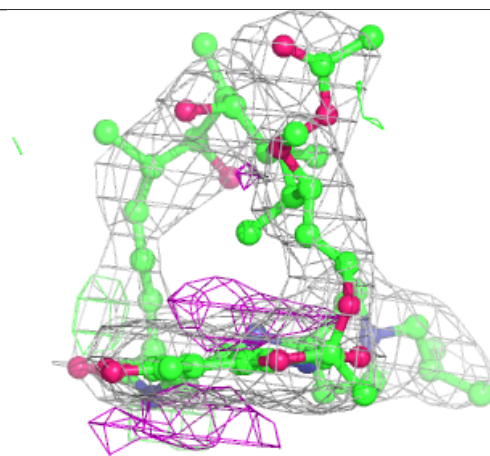
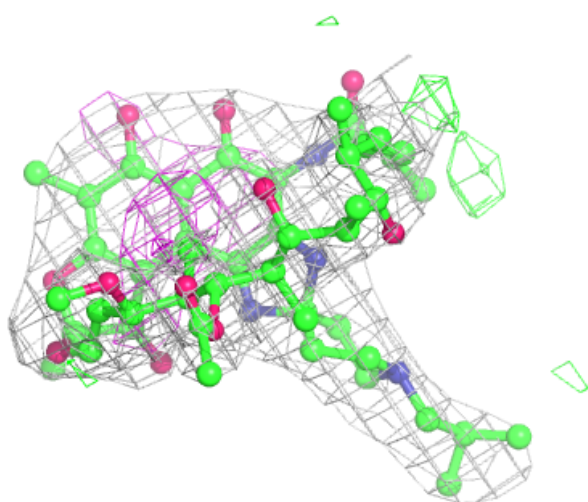
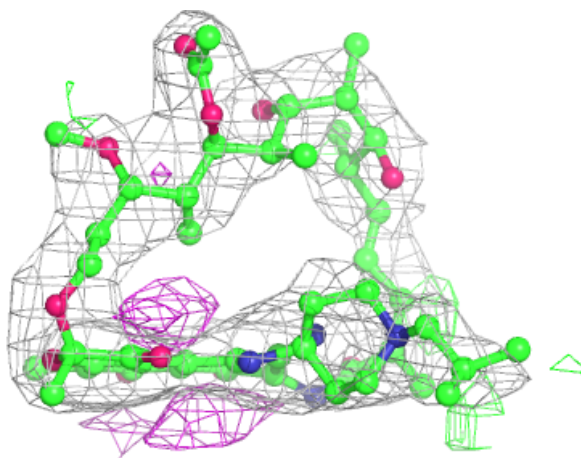
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





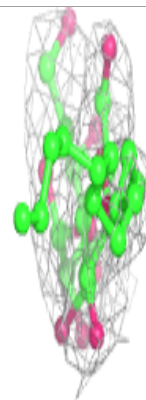
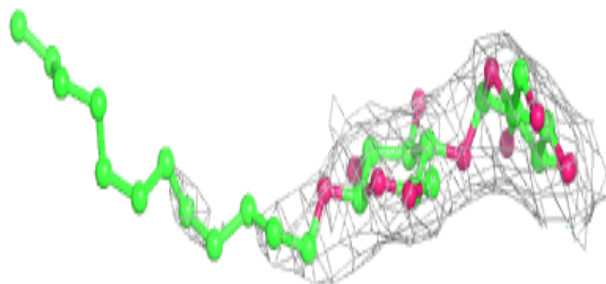
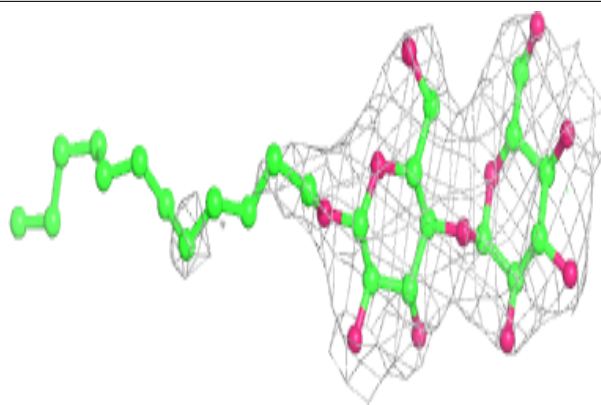
Electron density around RBT B 1112:

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

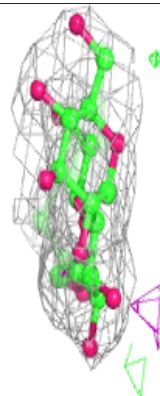
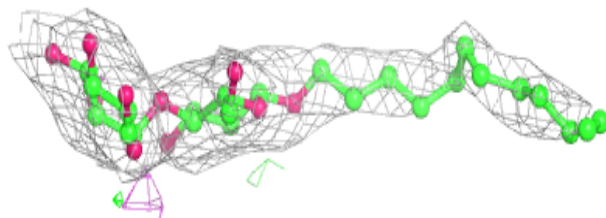
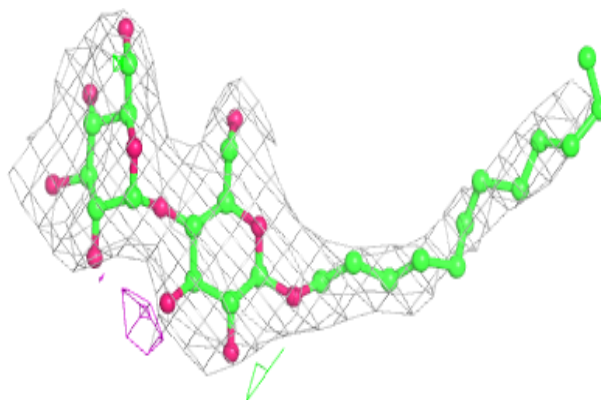


Electron density around LMT A 1104:

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

**Electron density around LMT C 1106:**

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



6.5 Other polymers

There are no such residues in this entry.