



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 05:25 PM UTC

PDB ID : 6ZO9 / pdb_00006zo9
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 wwPDB X-ray Structure Validation Summary 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

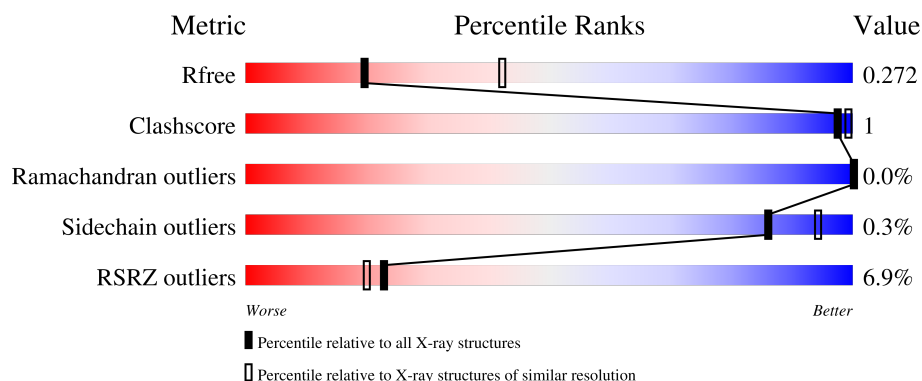
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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	10% 96%
1	B	1057	5% 94%
1	C	1057	4% 96%
2	D	169	% 92% 8%
2	E	169	20% 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
9	HEX	C	1110	-	-	-	X

2 Entry composition

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
1	A	1042	Total	C	N	O	S	0	4	0
			7959	5119	1319	1477	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
			7892	5082	1303	1462	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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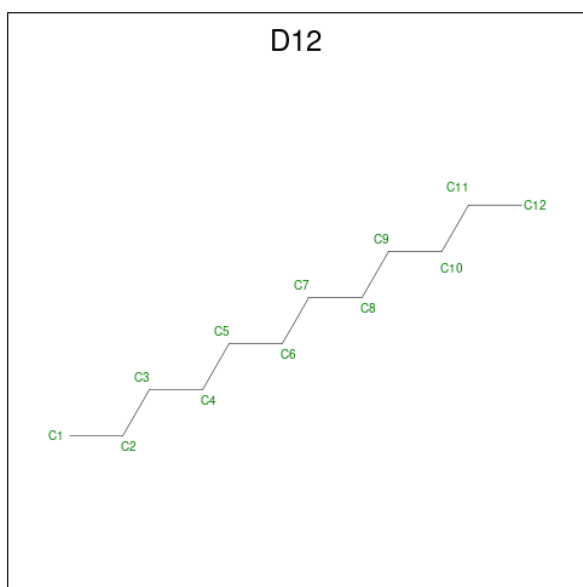
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Chain	Residue	Modelled	Actual	Comment	Reference
C	1054	HIS	-	expression tag	UNP P31224
C	1055	HIS	-	expression tag	UNP P31224
C	1056	HIS	-	expression tag	UNP P31224
C	1057	HIS	-	expression tag	UNP P31224

- Molecule 2 is a protein called DARPIN.

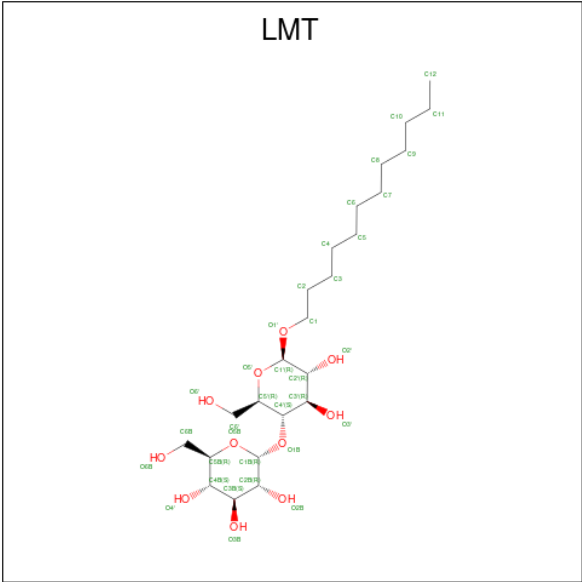
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	156	Total	C	N	O	S	0	0	0
			1177	741	206	229	1			
2	E	154	Total	C	N	O	S	0	0	0
			1167	736	204	226	1			

- Molecule 3 is DODECANE (CCD ID: D12) (formula: C₁₂H₂₆).



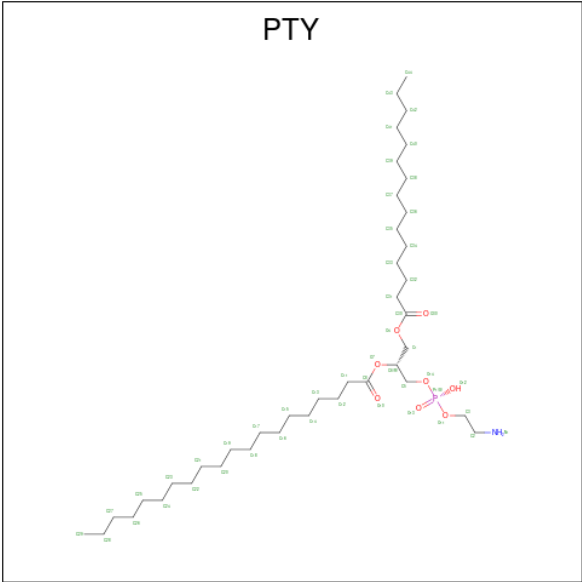
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C	0	0
			12	12		
3	C	1	Total	C	0	0
			12	12		
3	C	1	Total	C	0	0
			12	12		

- Molecule 4 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



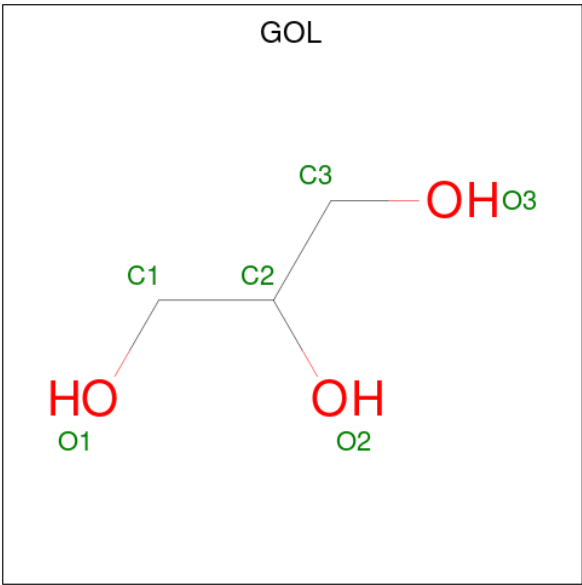
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			35	24	11		
4	A	1	Total	C	O	0	0
			35	24	11		
4	A	1	Total	C	O	0	0
			35	24	11		
4	B	1	Total	C	O	0	0
			35	24	11		
4	C	1	Total	C	O	0	0
			35	24	11		
4	C	1	Total	C	O	0	0
			35	24	11		

- Molecule 5 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: C₄₀H₈₀NO₈P).



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

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



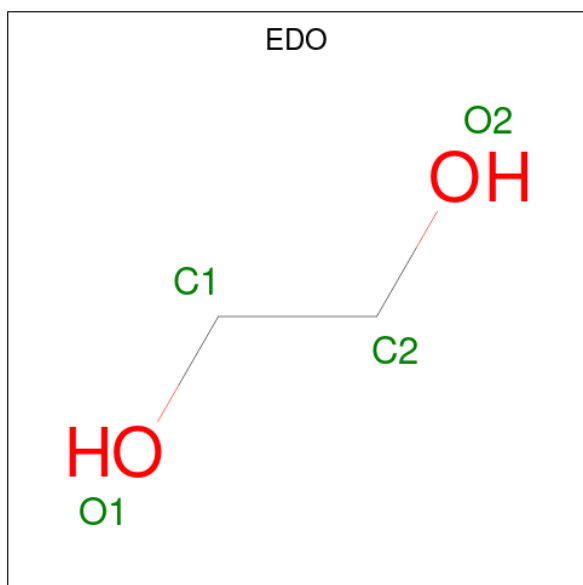
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		

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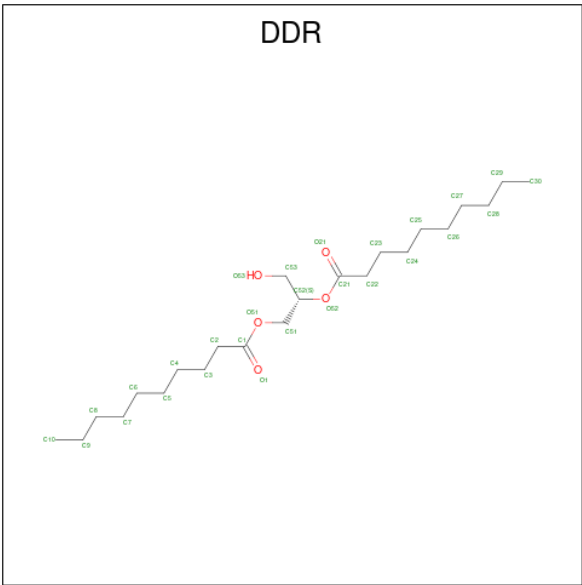
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



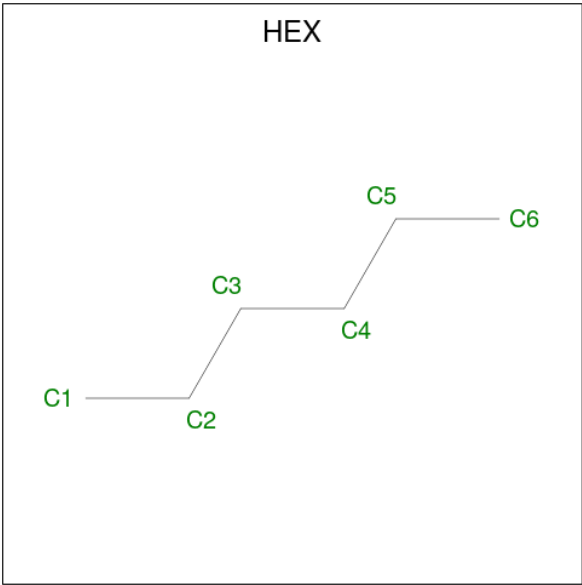
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is (2S)-3-hydroxypropane-1,2-diyl didecanoate (CCD ID: DDR) (formula: $C_{23}H_{44}O_5$).



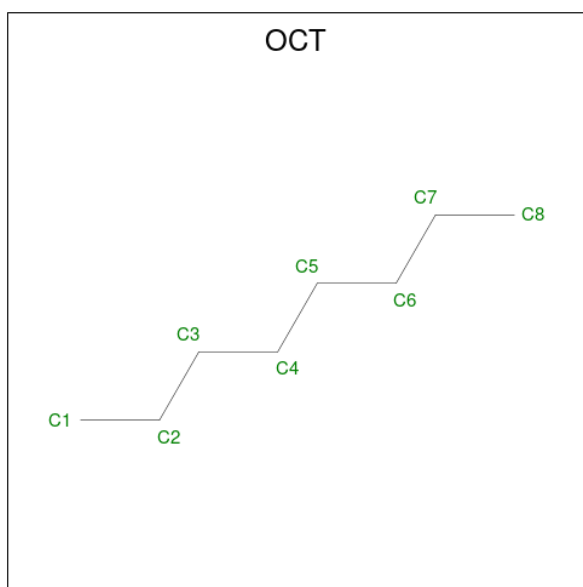
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	C O	0	0
			28	23 5		

- Molecule 9 is HEXANE (CCD ID: HEX) (formula: C₆H₁₄).



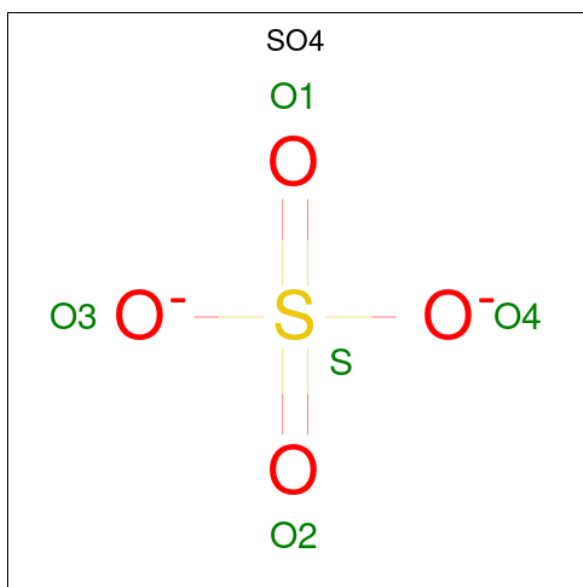
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	C	0	0
			6	6		
9	C	1	Total	C	0	0
			6	6		

- Molecule 10 is N-OCTANE (CCD ID: OCT) (formula: C₈H₁₈).



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

- Molecule 11 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



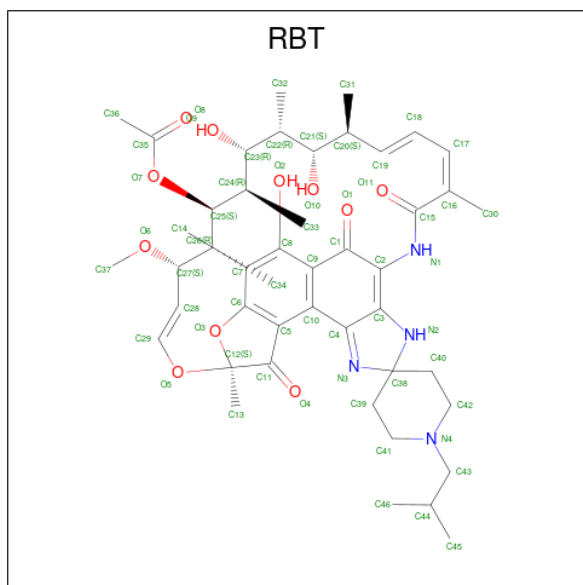
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	O	S	0	0
			5	4	1		

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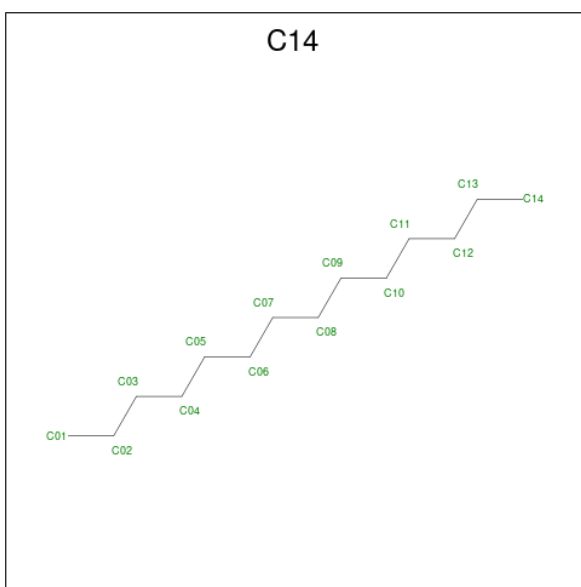
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	C	1	Total	O	S	0	0
			5	4	1		

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



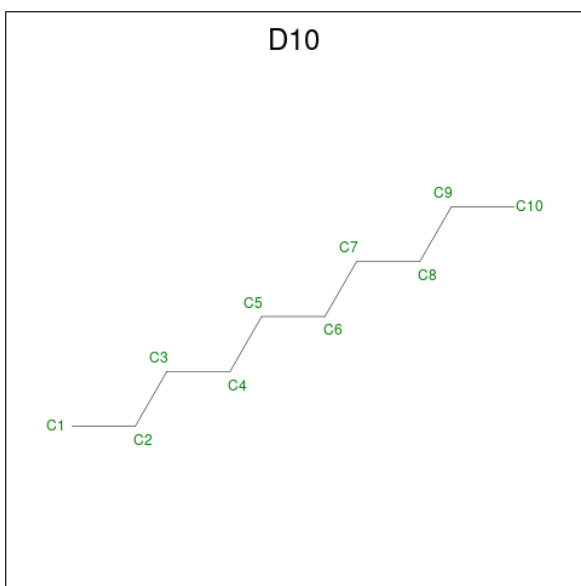
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	B	1	Total	C	N	O	0	0
			61	46	4	11		
12	B	1	Total	C	N	O	0	0
			61	46	4	11		

- Molecule 13 is TETRADECANE (CCD ID: 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 (CCD ID: 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 (CCD ID: CL) (formula: Cl).

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

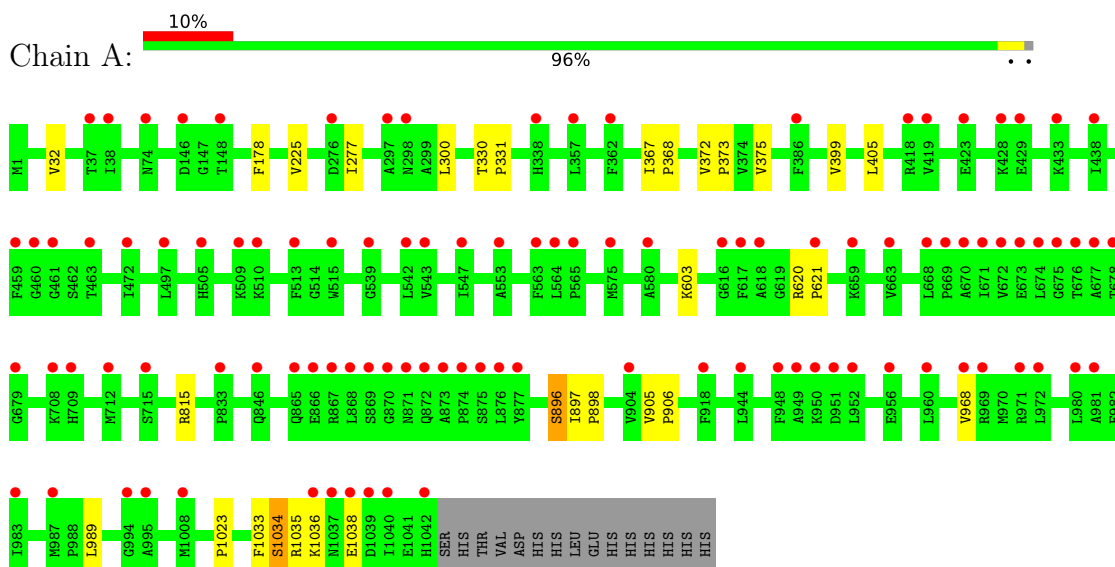
- Molecule 16 is water.

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

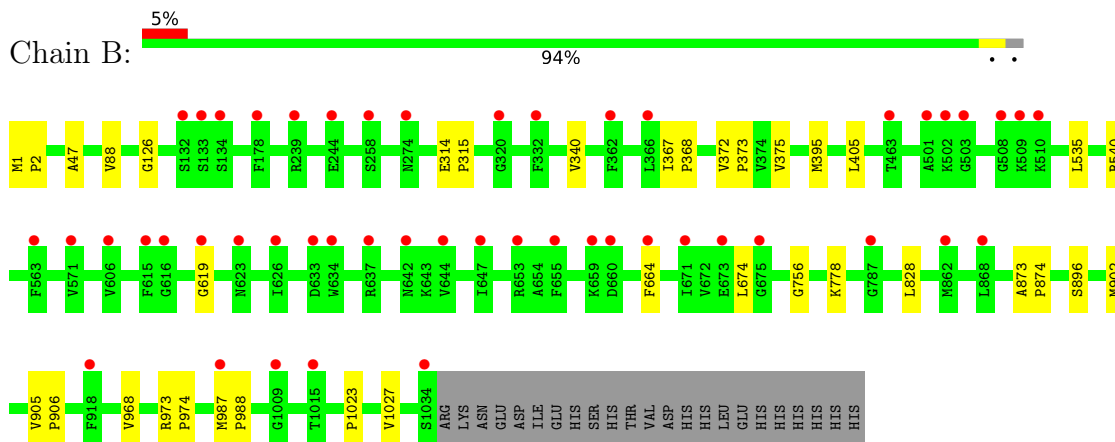
3 Residue-property plots [i](#)

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

• Molecule 1: Multidrug efflux pump subunit AcrB

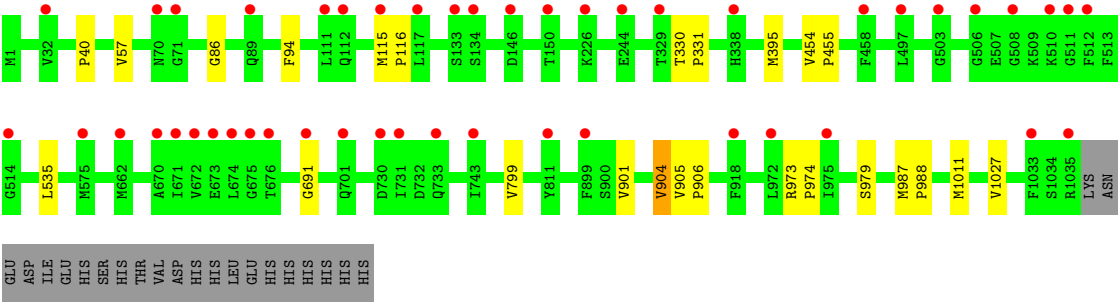


• Molecule 1: Multidrug efflux pump subunit AcrB

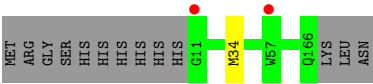
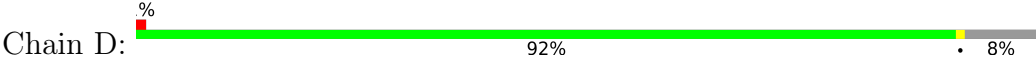


• Molecule 1: Multidrug efflux pump subunit AcrB

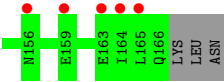
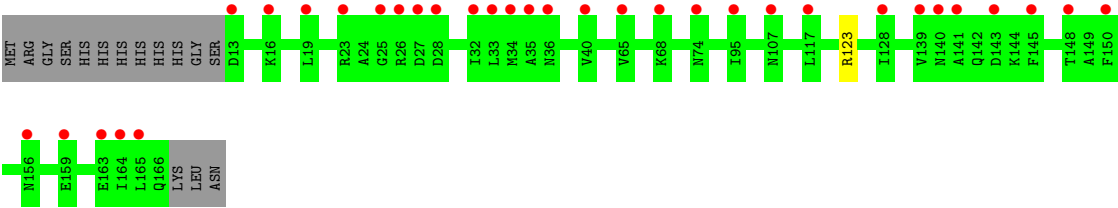
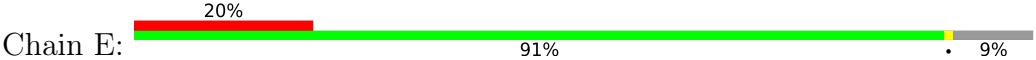




● Molecule 2: DARPIN



● 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 49.05 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.05-2.70) 100.0 (49.05-2.70)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.69Å)	Xtriage
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 (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	51.4	Xtriage
Anisotropy	0.576	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 29.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	26945	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage'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: HEX, EDO, CL, PTY, SO4, GOL, LMT, D12, DDR, OCT, C14, RBT, D10

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	1.03	0/8124	1.55	2/11030 (0.0%)
1	B	1.04	0/8009	1.55	4/10878 (0.0%)
1	C	1.04	1/8051 (0.0%)	1.54	3/10933 (0.0%)
2	D	1.04	0/1196	1.57	0/1626
2	E	1.04	0/1186	1.56	0/1613
All	All	1.04	1/26566 (0.0%)	1.55	9/36080 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	799	VAL	N-CA	5.19	1.49	1.45

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	896	SER	CA-C-N	7.29	124.83	120.24
1	A	896	SER	C-N-CA	7.29	124.83	120.24
1	B	896	SER	CA-C-N	7.18	124.76	120.24
1	B	896	SER	C-N-CA	7.18	124.76	120.24
1	B	756	GLY	CA-C-O	-6.12	118.01	122.23

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	15	0
1	B	7858	0	8010	18	0
1	C	7892	0	8047	13	0
2	D	1177	0	1159	1	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
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	1	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	45	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.

The worst 5 of 45 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:C:979:SER:HA	1:C:1011:MET:HE3	1.91	0.52
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.93	0.51

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%)	48	73
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%)	849 (100%)	4 (0%)	81	92
1	B	841/864 (97%)	839 (100%)	2 (0%)	87	95
1	C	845/864 (98%)	845 (100%)	0	100	100
2	D	120/132 (91%)	120 (100%)	0	100	100
2	E	119/132 (90%)	118 (99%)	1 (1%)	73	88
All	All	2778/2856 (97%)	2771 (100%)	7 (0%)	86	94

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1038	GLU
1	B	540	ARG
2	E	123	ARG
1	B	664	PHE
1	A	1036	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1001	ASN
2	D	125	HIS
2	E	125	HIS
2	E	59	HIS
1	B	737	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	$\# Z > 2$
9	HEX	B	1103	-	5,5,5	0.12	0	4,4,4	0.12	0
5	PTY	C	1108	-	49,49,49	0.27	0	52,54,54	0.31	0
13	C14	C	1101	-	13,13,13	0.10	0	12,12,12	0.05	0
3	D12	A	1101	-	11,11,11	0.09	0	10,10,10	0.06	0
4	LMT	A	1102	-	36,36,36	0.45	0	47,47,47	0.62	0
4	LMT	C	1107	-	36,36,36	0.47	1 (2%)	47,47,47	0.64	0
6	GOL	A	1106	-	5,5,5	0.09	0	5,5,5	0.25	0
4	LMT	C	1106	-	36,36,36	0.44	0	47,47,47	0.56	0
3	D12	C	1105	-	11,11,11	0.09	0	10,10,10	0.09	0
4	LMT	A	1103	-	36,36,36	0.49	1 (2%)	47,47,47	0.69	1 (2%)
7	EDO	B	1110	-	3,3,3	0.07	0	2,2,2	0.11	0
12	RBT	B	1112	-	61,66,66	0.65	1 (1%)	87,101,101	1.17	5 (5%)
5	PTY	C	1109	-	49,49,49	0.26	0	52,54,54	0.36	0
6	GOL	C	1112	-	5,5,5	0.09	0	5,5,5	0.26	0
8	DDR	B	1102	-	27,27,27	0.23	0	29,29,29	0.25	0
7	EDO	B	1109	-	3,3,3	0.06	0	2,2,2	0.10	0
3	D12	C	1104	-	11,11,11	0.09	0	10,10,10	0.07	0
6	GOL	B	1106	-	5,5,5	0.09	0	5,5,5	0.25	0
10	OCT	B	1104	-	7,7,7	0.11	0	6,6,6	0.06	0
4	LMT	A	1104	-	36,36,36	0.47	0	47,47,47	0.61	0
14	D10	C	1102	-	9,9,9	0.11	0	8,8,8	0.08	0
7	EDO	B	1108	-	3,3,3	0.06	0	2,2,2	0.11	0
12	RBT	B	1111	-	61,66,66	0.60	1 (1%)	87,101,101	0.99	7 (8%)
14	D10	C	1103	-	9,9,9	0.10	0	8,8,8	0.06	0
10	OCT	B	1105	-	7,7,7	0.10	0	6,6,6	0.08	0
11	SO4	B	1107	-	4,4,4	0.34	0	6,6,6	0.07	0
9	HEX	C	1110	-	5,5,5	0.12	0	4,4,4	0.10	0
7	EDO	A	1107	-	3,3,3	0.06	0	2,2,2	0.11	0
11	SO4	C	1113	-	4,4,4	0.34	0	6,6,6	0.07	0
10	OCT	C	1111	-	7,7,7	0.10	0	6,6,6	0.08	0
5	PTY	A	1105	-	49,49,49	0.26	0	52,54,54	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	LMT	B	1101	-	36,36,36	0.44	0	47,47,47	0.52	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
9	HEX	B	1103	-	-	1/3/3/3	-
5	PTY	C	1108	-	-	22/53/53/53	-
13	C14	C	1101	-	-	0/11/11/11	-
3	D12	A	1101	-	-	2/9/9/9	-
4	LMT	A	1102	-	-	10/21/61/61	0/2/2/2
4	LMT	C	1107	-	-	9/21/61/61	0/2/2/2
6	GOL	A	1106	-	-	2/4/4/4	-
4	LMT	C	1106	-	-	10/21/61/61	0/2/2/2
3	D12	C	1105	-	-	4/9/9/9	-
4	LMT	A	1103	-	-	12/21/61/61	0/2/2/2
7	EDO	B	1110	-	-	1/1/1/1	-
12	RBT	B	1112	-	-	23/59/116/116	1/5/6/6
5	PTY	C	1109	-	-	20/53/53/53	-
6	GOL	C	1112	-	-	3/4/4/4	-
8	DDR	B	1102	-	-	15/29/29/29	-
7	EDO	B	1109	-	-	0/1/1/1	-
3	D12	C	1104	-	-	1/9/9/9	-
6	GOL	B	1106	-	-	0/4/4/4	-
10	OCT	B	1104	-	-	1/5/5/5	-
4	LMT	A	1104	-	-	6/21/61/61	0/2/2/2
14	D10	C	1102	-	-	2/7/7/7	-
7	EDO	B	1108	-	-	1/1/1/1	-
12	RBT	B	1111	-	-	17/59/116/116	1/5/6/6
14	D10	C	1103	-	-	1/7/7/7	-
10	OCT	B	1105	-	-	2/5/5/5	-
9	HEX	C	1110	-	-	0/3/3/3	-
7	EDO	A	1107	-	-	1/1/1/1	-
10	OCT	C	1111	-	-	1/5/5/5	-
5	PTY	A	1105	-	-	21/53/53/53	-
4	LMT	B	1101	-	-	6/21/61/61	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	1112	RBT	C2-C1	-2.91	1.40	1.49
12	B	1111	RBT	C2-C1	-2.57	1.41	1.49
4	A	1103	LMT	O1'-C1'	2.05	1.43	1.40
4	C	1107	LMT	O1'-C1'	2.01	1.43	1.40

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	1112	RBT	C2-C3-N2	4.65	136.76	127.61
12	B	1112	RBT	C10-C4-C3	-3.68	119.87	123.42
12	B	1111	RBT	C5-C6-C7	-3.64	122.52	125.40
12	B	1112	RBT	C3-C2-C1	-3.46	117.00	121.19
12	B	1111	RBT	C2-C3-N2	3.41	134.32	127.61

There are no chirality outliers.

5 of 194 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1102	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	1108	PTY	C5-O14-P1-O11

All (2) ring outliers are listed below:

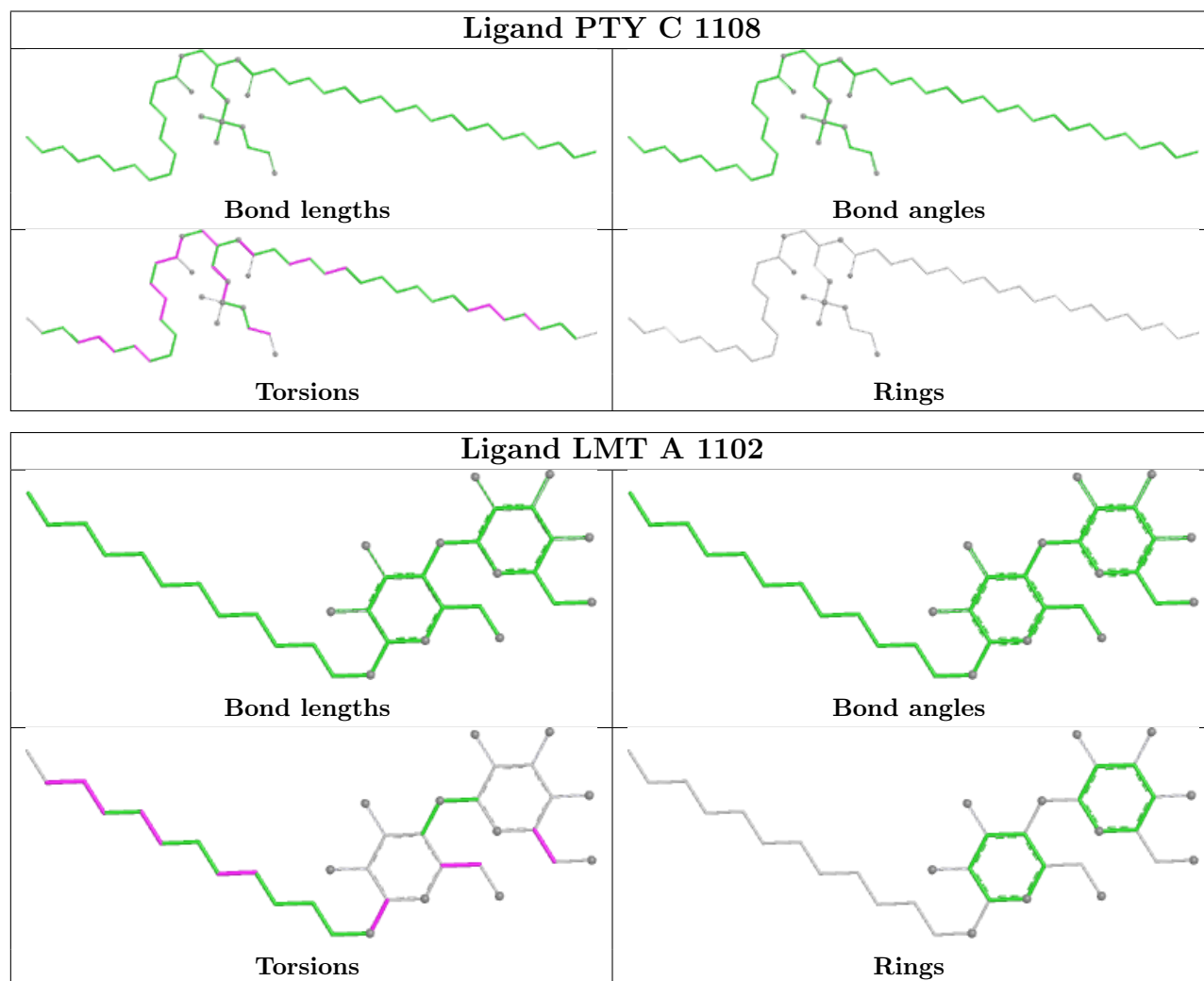
Mol	Chain	Res	Type	Atoms
12	B	1112	RBT	C38-C39-C40-C41-C42-N4
12	B	1111	RBT	C38-C39-C40-C41-C42-N4

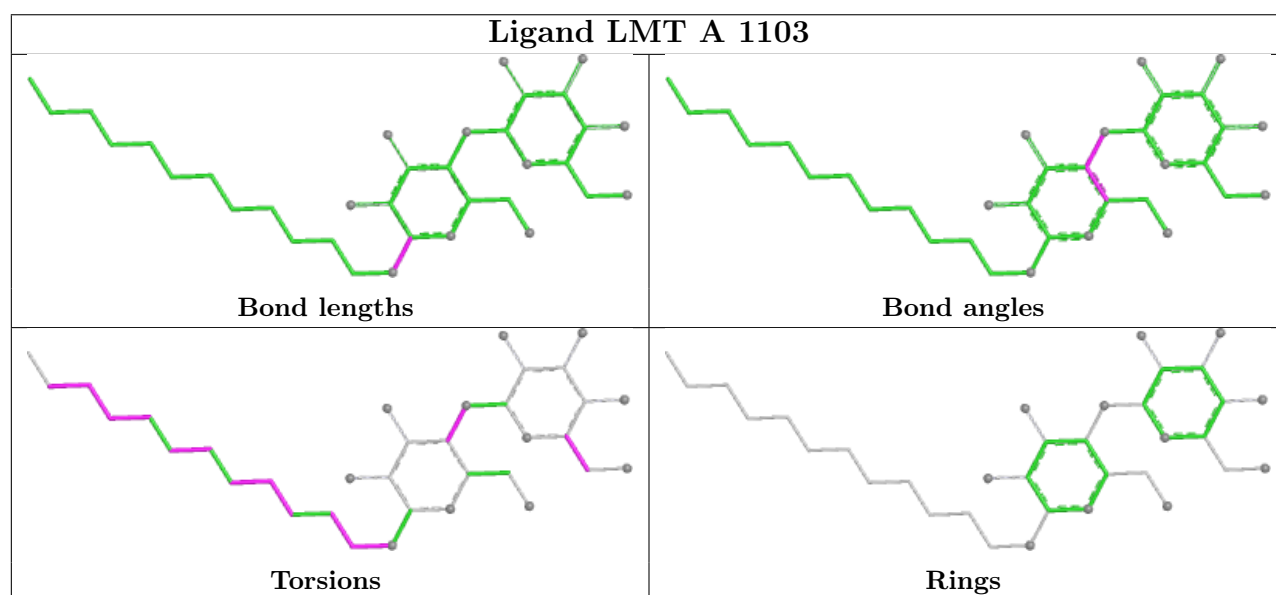
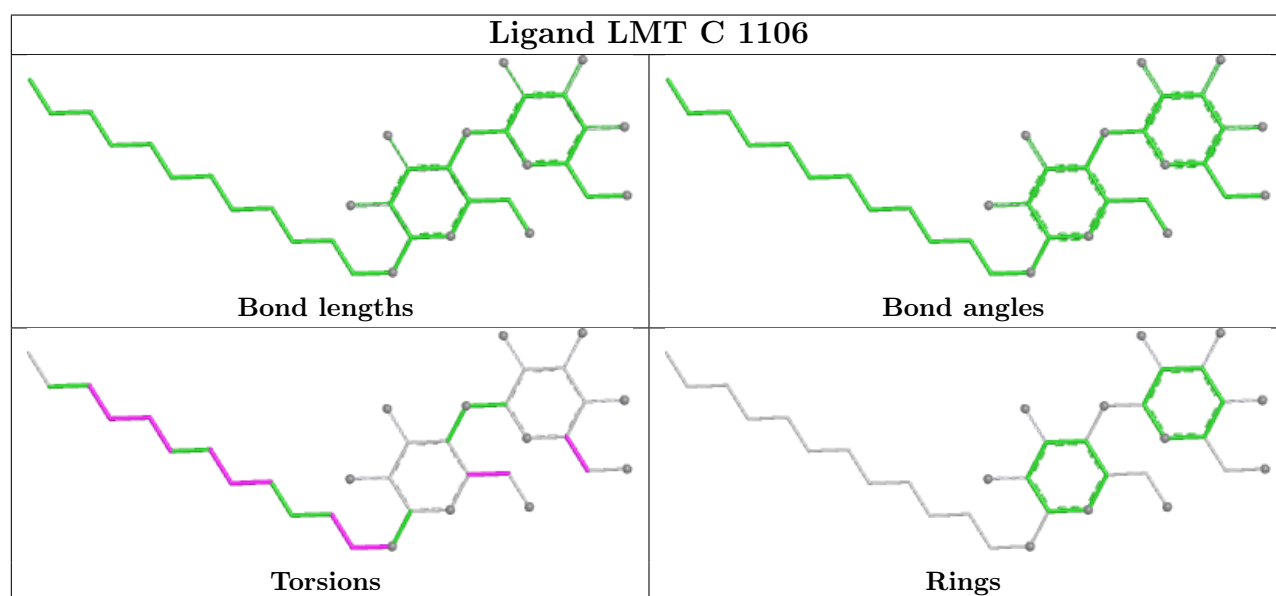
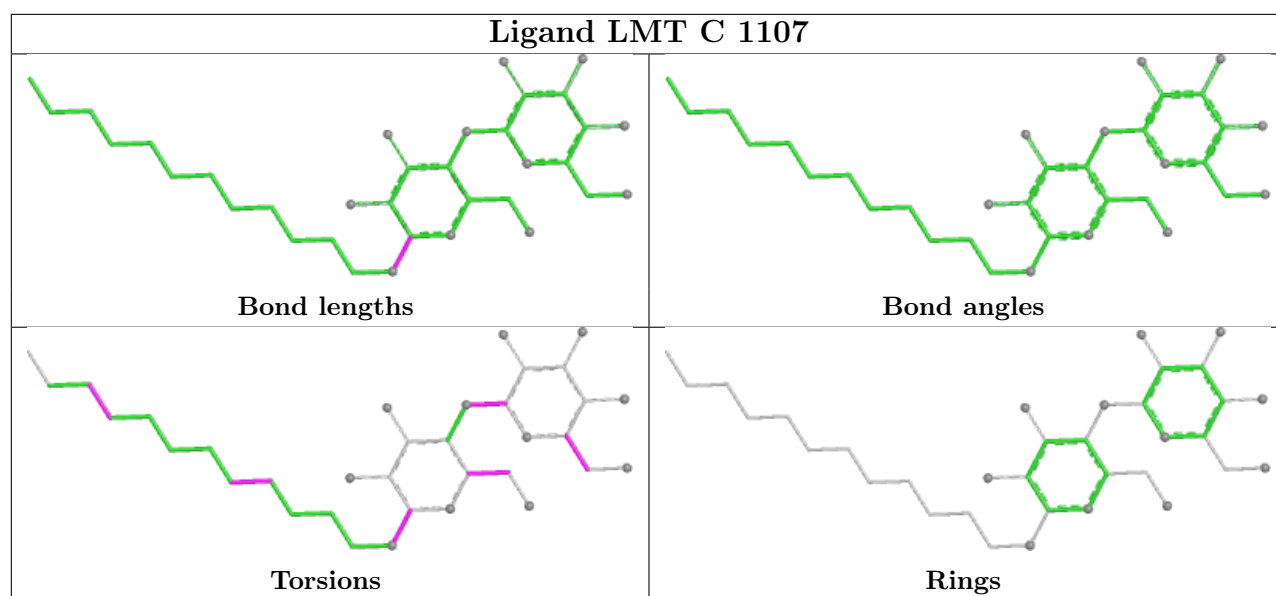
3 monomers are involved in 3 short contacts:

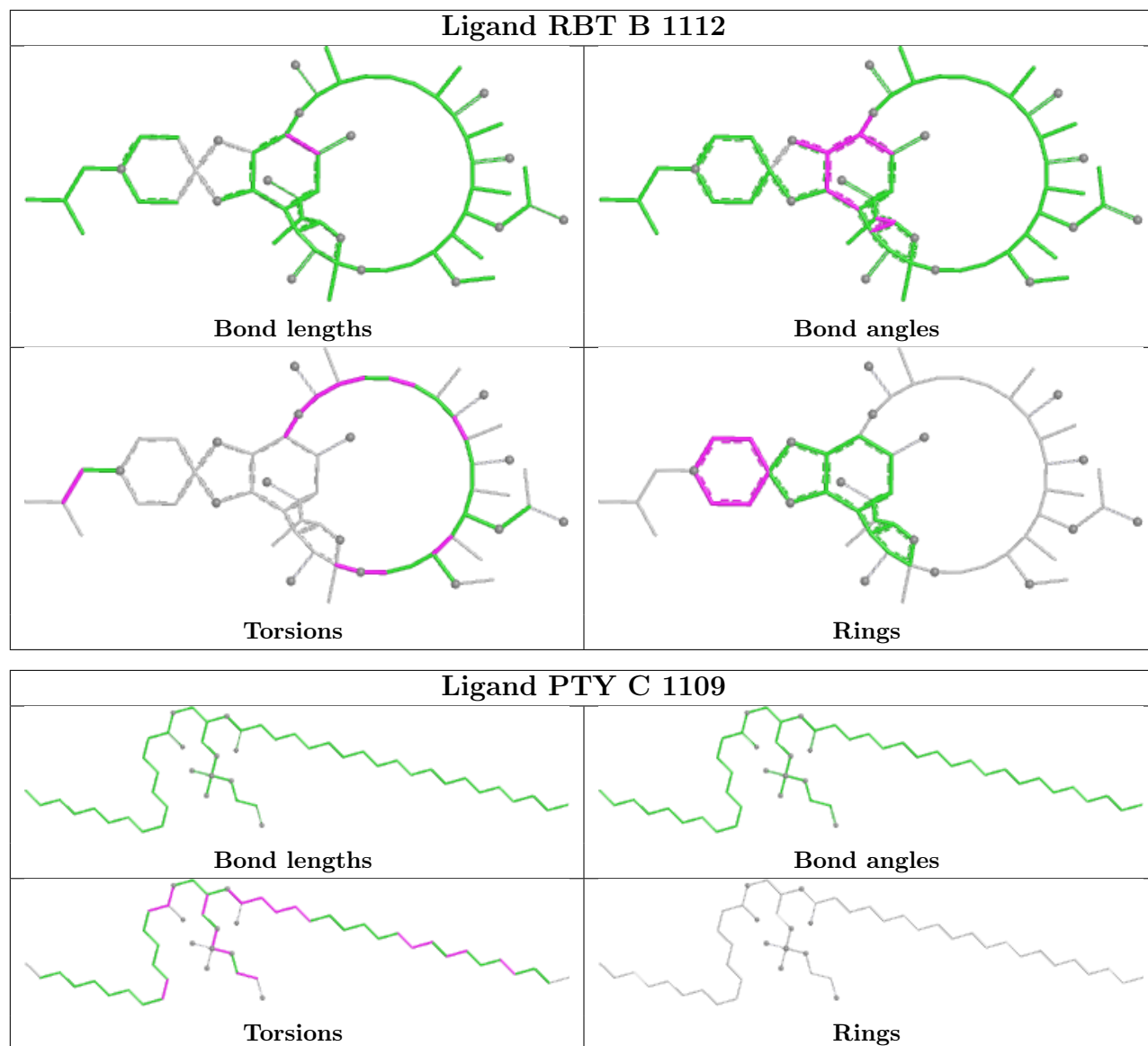
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	B	1112	RBT	1	0
12	B	1111	RBT	1	0
10	B	1105	OCT	1	0

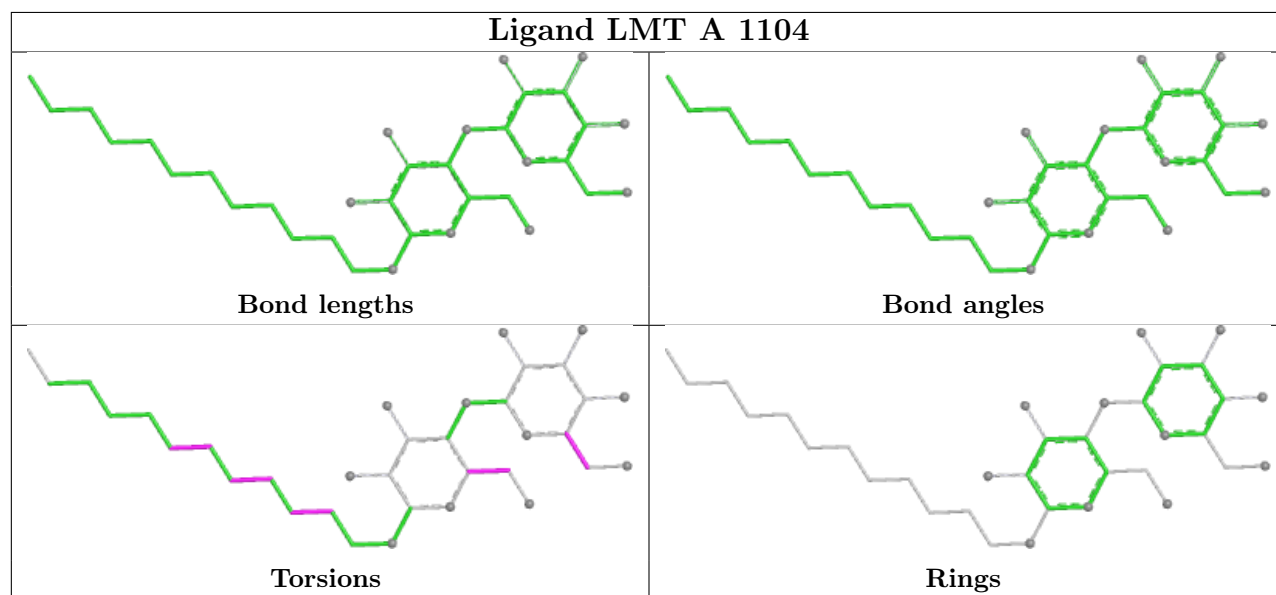
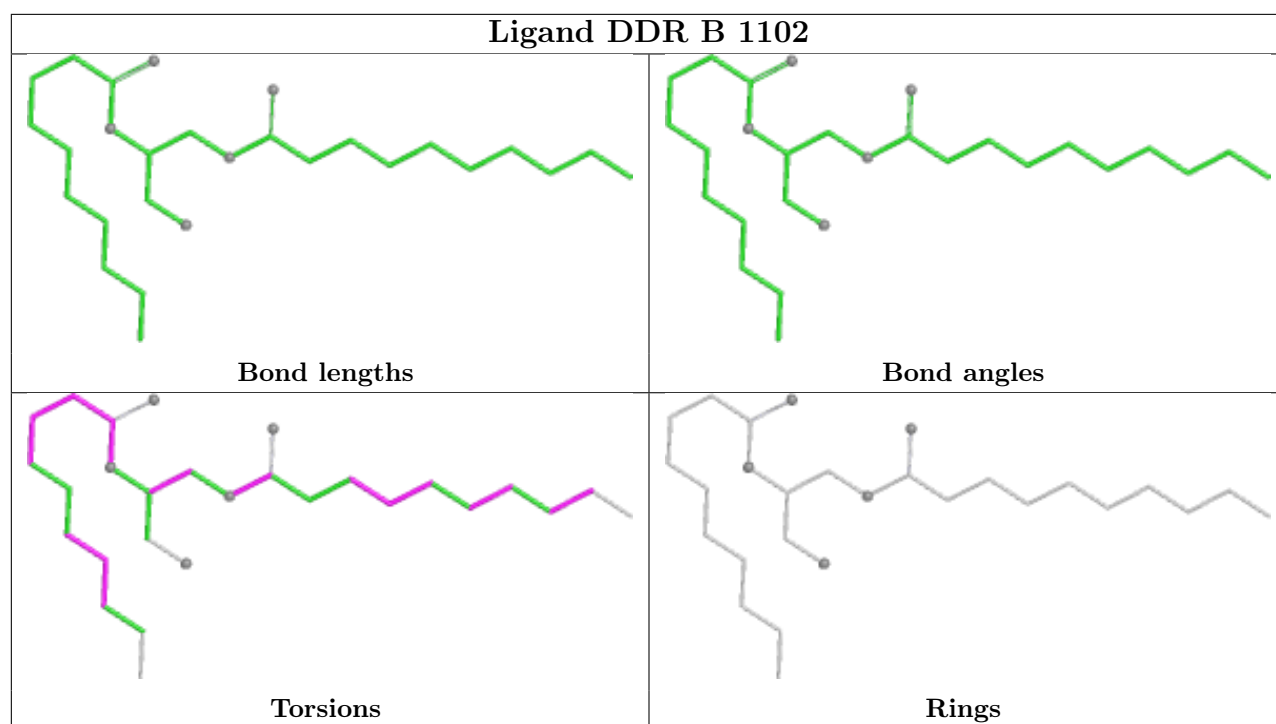
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

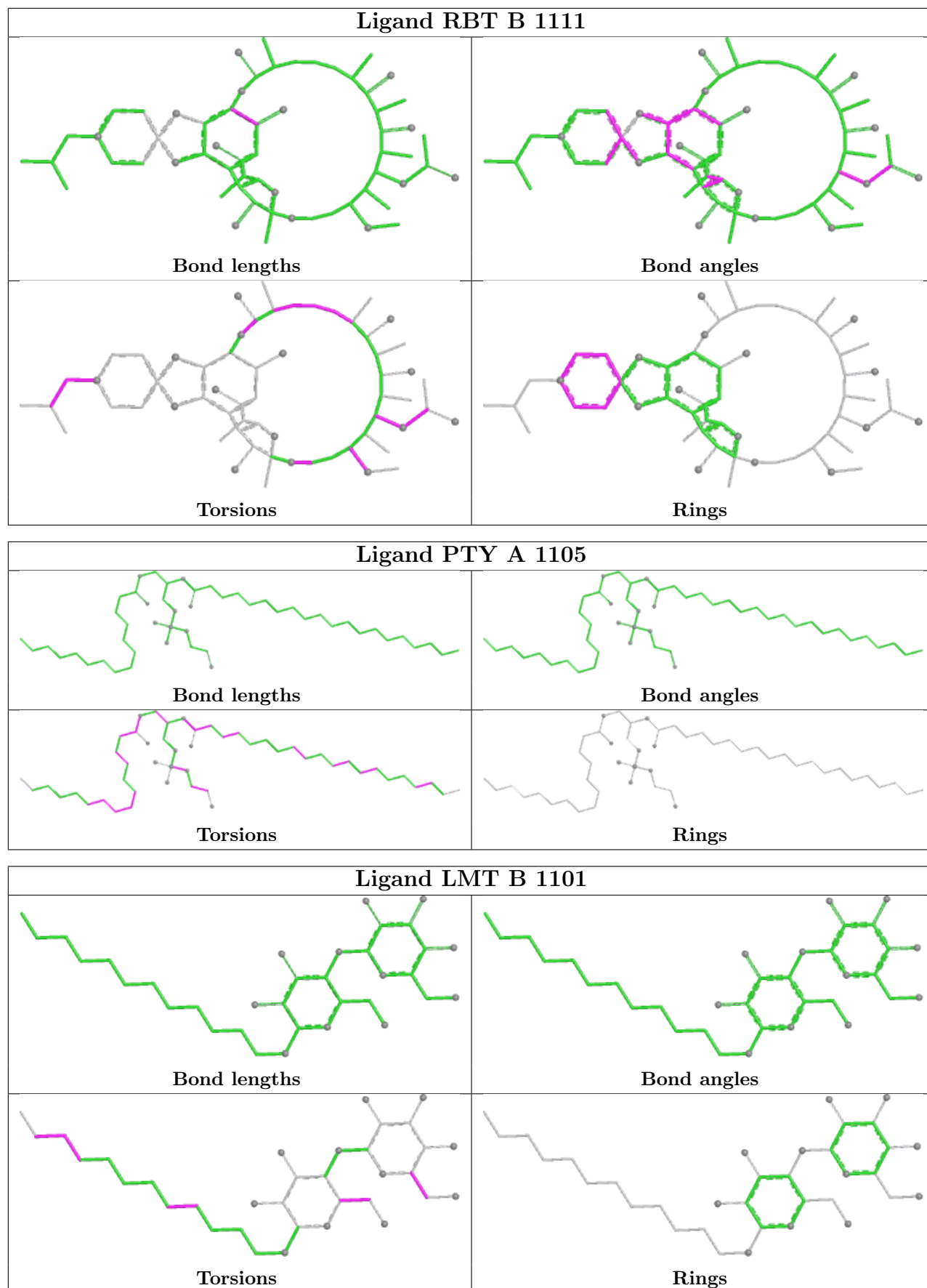
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1042/1057 (98%)	0.84	104 (9%) 12 10	27, 61, 91, 111	16 (1%)
1	B	1034/1057 (97%)	0.62	49 (4%) 36 33	34, 57, 78, 96	0
1	C	1035/1057 (97%)	0.49	47 (4%) 38 34	26, 50, 73, 100	3 (0%)
2	D	156/169 (92%)	0.70	2 (1%) 75 73	49, 60, 80, 93	0
2	E	154/169 (91%)	1.42	33 (21%) 2 2	61, 77, 100, 106	0
All	All	3421/3509 (97%)	0.69	235 (6%) 23 20	26, 57, 87, 111	19 (0%)

The worst 5 of 235 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	674	LEU	9.6
1	A	868	LEU	6.7
1	A	672	VAL	6.2
1	A	673	GLU	6.0
1	A	670	ALA	5.5

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,

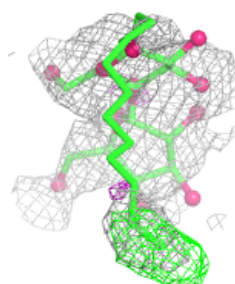
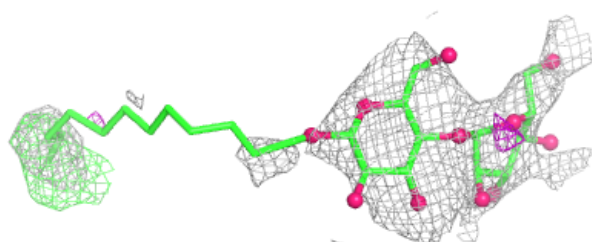
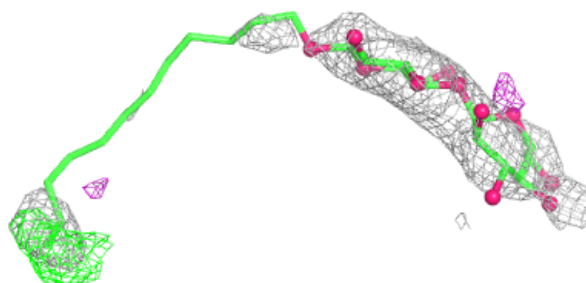
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	HEX	B	1103	6/6	0.57	0.35	62,63,63,63	0
10	OCT	C	1111	8/8	0.64	0.40	67,67,68,68	0
4	LMT	C	1107	35/35	0.65	0.26	104,110,112,112	0
6	GOL	C	1112	6/6	0.70	0.35	79,80,80,80	0
9	HEX	C	1110	6/6	0.72	0.40	64,64,64,65	0
7	EDO	B	1109	4/4	0.72	0.33	90,91,91,91	0
7	EDO	B	1110	4/4	0.73	0.25	85,85,85,85	0
13	C14	C	1101	14/14	0.73	0.33	70,71,71,71	0
10	OCT	B	1104	8/8	0.76	0.35	74,75,75,75	0
5	PTY	C	1108	50/50	0.76	0.33	88,95,100,101	0
3	D12	C	1104	12/12	0.76	0.31	63,65,67,67	0
6	GOL	A	1106	6/6	0.77	0.23	72,72,72,72	0
5	PTY	A	1105	50/50	0.78	0.31	91,115,127,130	0
4	LMT	A	1104	35/35	0.79	0.18	91,96,102,102	0
3	D12	C	1105	12/12	0.79	0.34	72,75,76,76	0
5	PTY	C	1109	50/50	0.79	0.32	93,109,126,128	0
7	EDO	A	1107	4/4	0.80	0.20	70,70,71,71	0
14	D10	C	1103	10/10	0.81	0.31	76,77,80,80	0
4	LMT	A	1103	35/35	0.82	0.17	71,83,94,95	0
12	RBT	B	1111	61/61	0.82	0.19	72,76,79,80	0
12	RBT	B	1112	61/61	0.82	0.22	79,81,83,85	0
3	D12	A	1101	12/12	0.82	0.33	83,85,87,87	0
4	LMT	B	1101	35/35	0.82	0.20	76,80,92,93	0
10	OCT	B	1105	8/8	0.83	0.27	74,74,74,74	0
4	LMT	A	1102	35/35	0.83	0.18	81,93,101,101	0
7	EDO	B	1108	4/4	0.85	0.19	54,54,54,54	0
8	DDR	B	1102	28/28	0.88	0.23	77,84,94,95	0
11	SO4	C	1113	5/5	0.88	0.17	85,85,85,86	0
4	LMT	C	1106	35/35	0.91	0.14	61,66,74,75	0
11	SO4	B	1107	5/5	0.92	0.10	81,81,81,81	0
14	D10	C	1102	10/10	0.92	0.21	69,71,73,73	0
6	GOL	B	1106	6/6	0.92	0.16	70,71,71,72	0
15	CL	C	1114	1/1	0.97	0.14	63,63,63,63	0

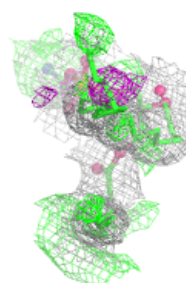
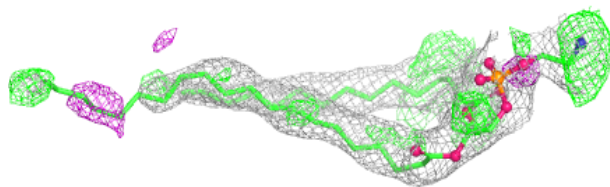
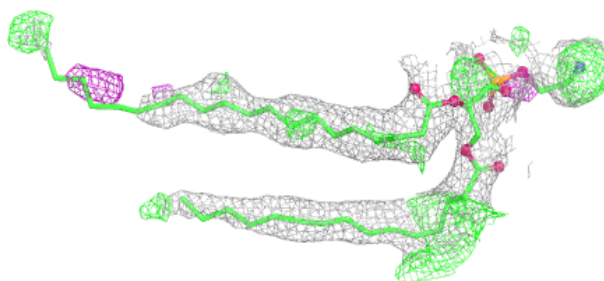
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT C 1107:

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

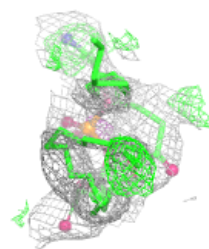
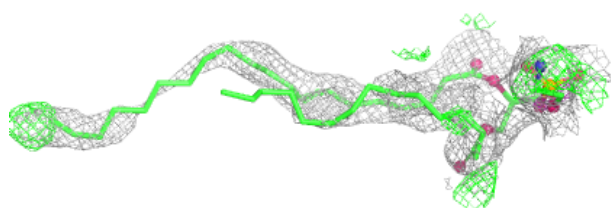
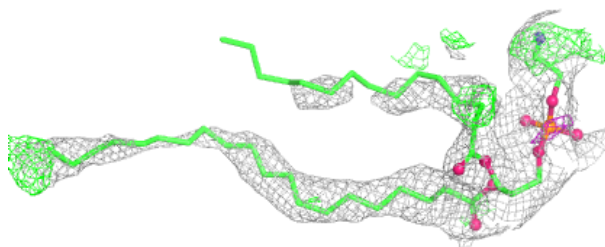
**Electron density around PTY C 1108:**

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

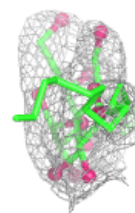
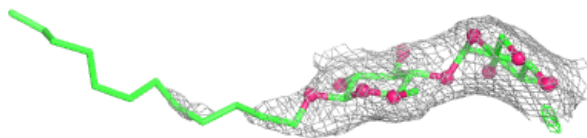
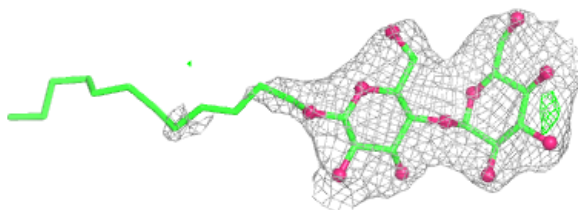


Electron density around PTY A 1105:

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

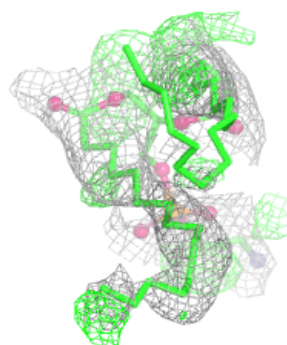
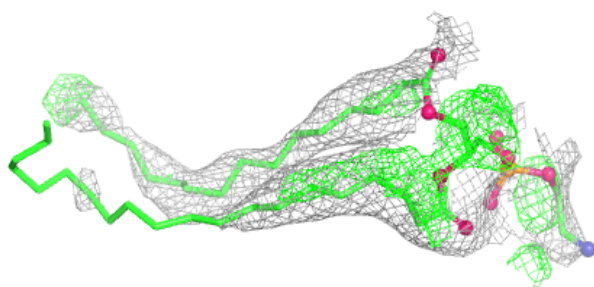
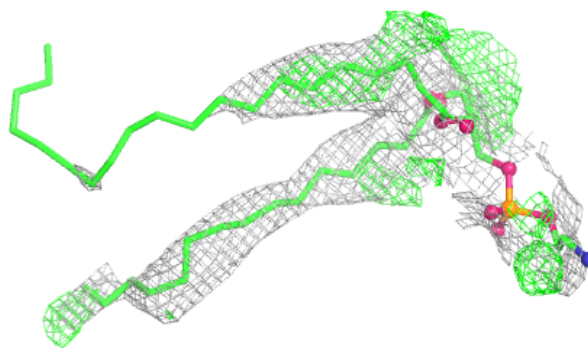
**Electron density around LMT A 1104:**

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

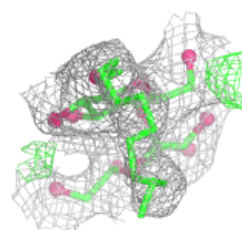
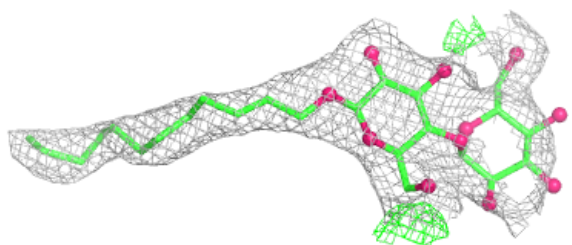
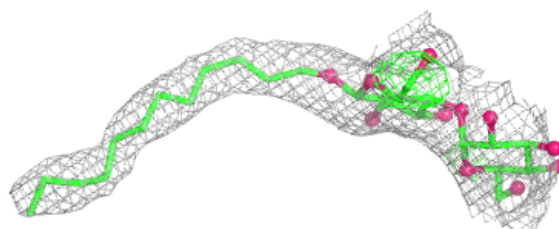


Electron density around PTY C 1109:

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

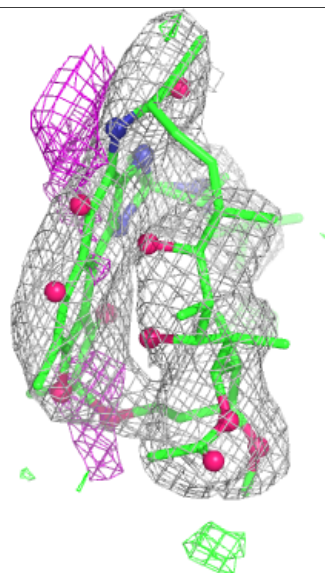
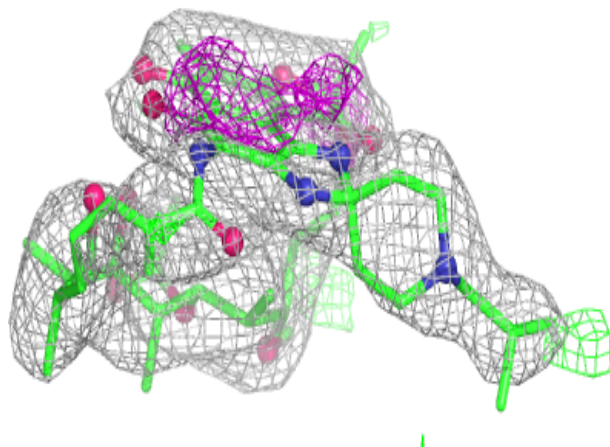
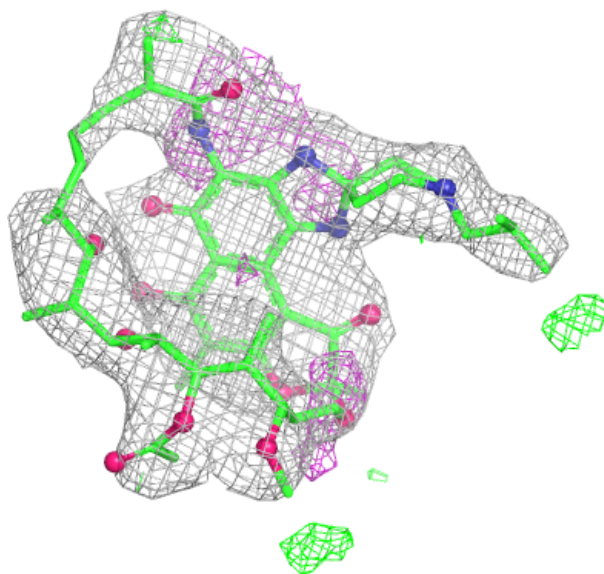
**Electron density around LMT A 1103:**

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



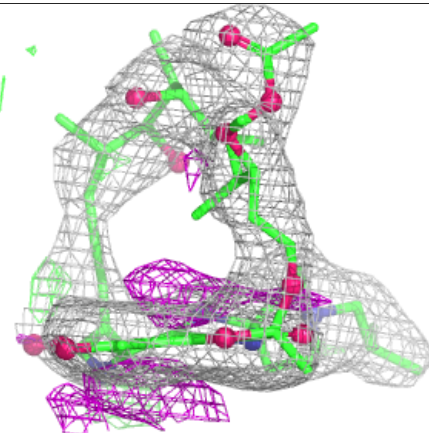
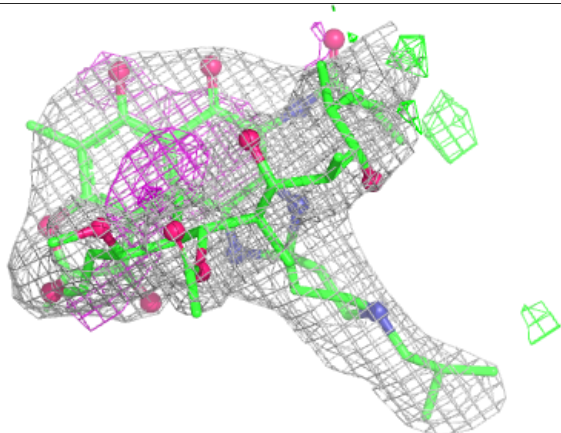
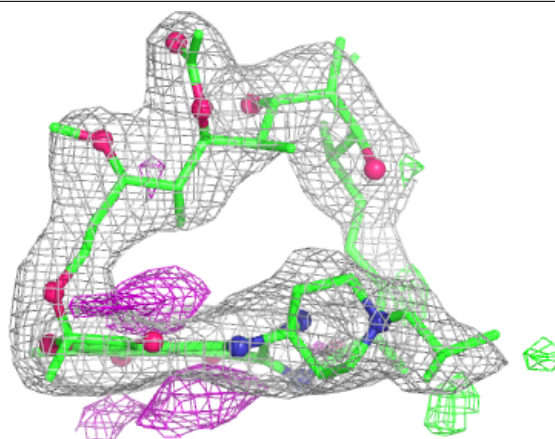
Electron density around RBT B 1111:

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

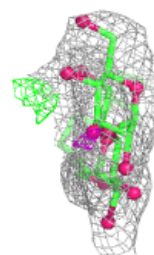
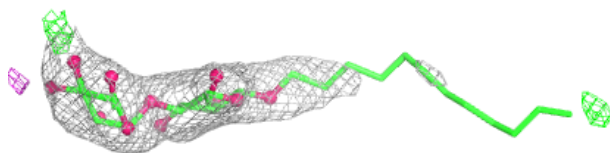
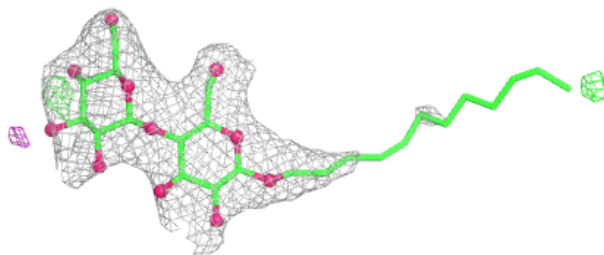


Electron density around RBT B 1112:

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

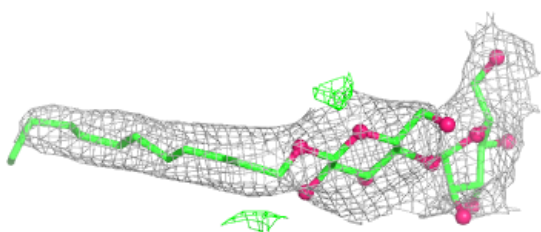
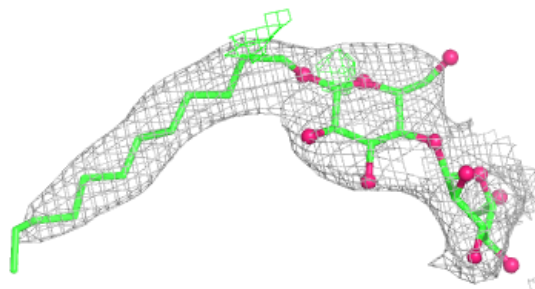
**Electron density around LMT B 1101:**

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



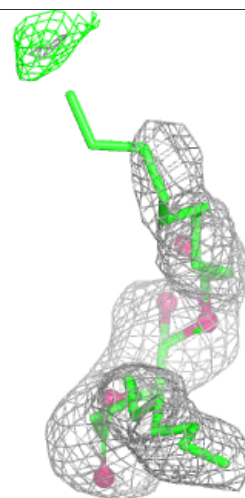
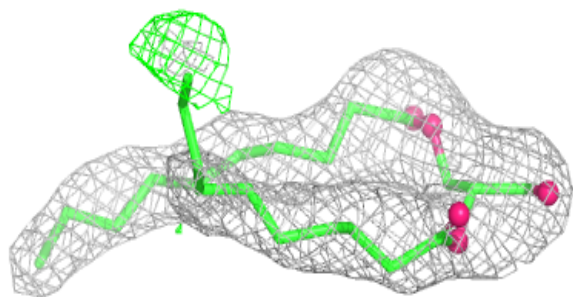
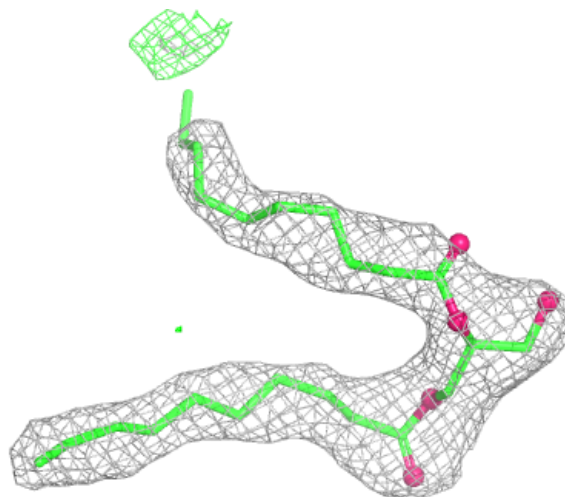
Electron density around LMT A 1102:

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



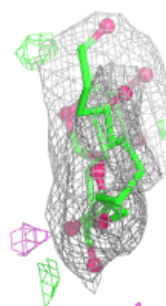
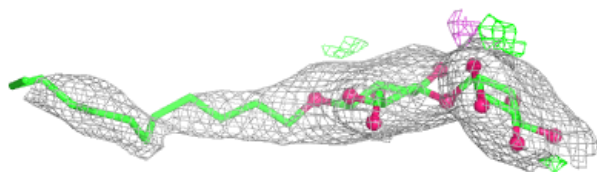
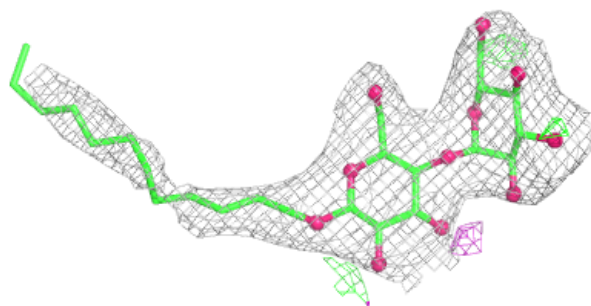
Electron density around DDR B 1102:

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



Electron density around LMT 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.