



wwPDB X-ray Structure Validation Summary Report ⓘ

May 11, 2021 – 10:19 am BST

PDB ID : 6ZOC
Title : Erythromycin binding to the access pocket of AcrB-G616P L protomer and 3-formylrifamycin SV binding to the access pocket of AcrB-G616P T protomer
Authors : Tam, H.K.; Foong, W.E.; Pos, K.M.
Deposited on : 2020-07-07
Resolution : 2.89 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 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

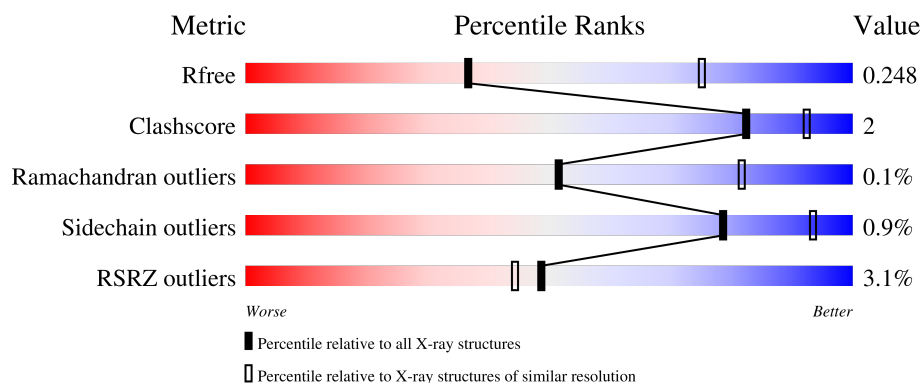
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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> <div>3%</div> <div>90%</div> <div>8%</div> <div>.</div> </div>
1	B	1057	<div> <div>3%</div> <div>91%</div> <div>7%</div> <div>.</div> </div>
1	C	1057	<div> <div>%</div> <div>90%</div> <div>8%</div> <div>.</div> </div>
2	D	169	<div> <div>3%</div> <div>85%</div> <div>7%</div> <div>8%</div> </div>
2	E	169	<div> <div>13%</div> <div>83%</div> <div>8%</div> <div>9%</div> </div>

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 26894 atoms, of which 277 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	1034	Total	C	N	O	S	0	0	0
			7858	5058	1296	1460	44			
1	B	1033	Total	C	N	O	S	0	0	0
			7852	5055	1295	1458	44			
1	C	1034	Total	C	N	O	S	0	0	0
			7858	5058	1296	1460	44			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	616	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	616	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	616	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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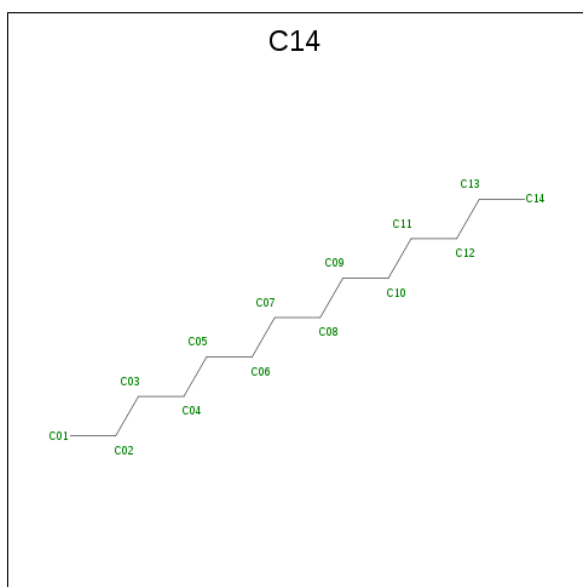
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Chain	Residue	Modelled	Actual	Comment	Reference
C	1054	HIS	-	expression tag	UNP P31224
C	1055	HIS	-	expression tag	UNP P31224
C	1056	HIS	-	expression tag	UNP P31224
C	1057	HIS	-	expression tag	UNP P31224

- Molecule 2 is a protein called DARPIN.

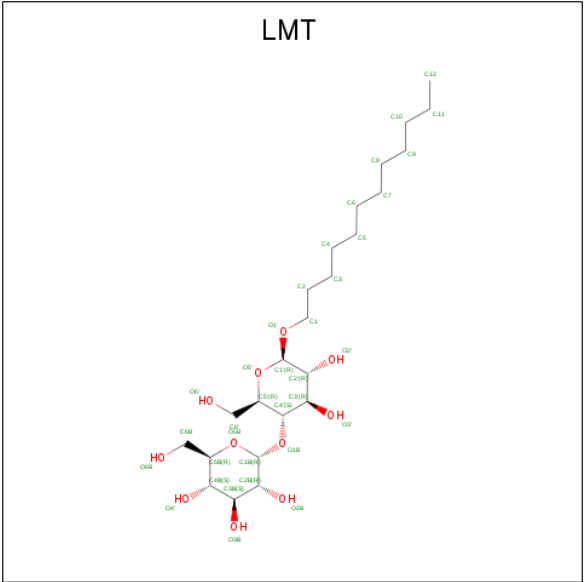
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	155	Total	C	N	O	S	0	0	0
			1168	736	204	227	1			
2	E	154	Total	C	N	O	S	0	0	0
			1167	736	204	226	1			

- Molecule 3 is TETRADECANE (three-letter code: C14) (formula: C₁₄H₃₀).



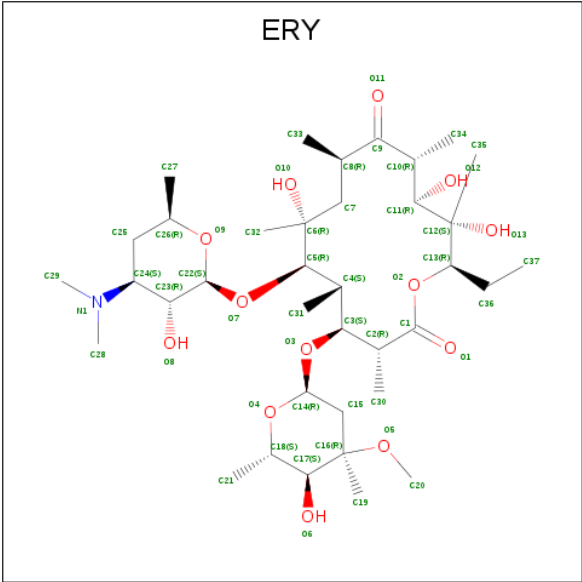
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C H	0	0
			44	14 30		
3	C	1	Total	C	0	0
			14	14		

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



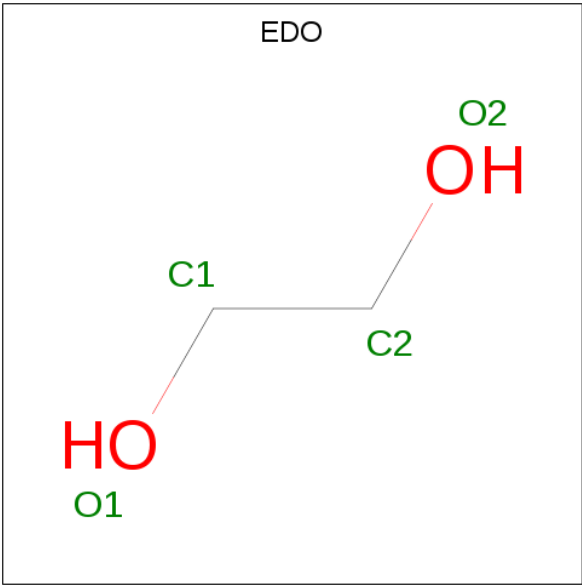
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			35	24	11		
4	B	1	Total	C	O	0	0
			35	24	11		
4	B	1	Total	C	O	0	0
			35	24	11		
4	C	1	Total	C	O	0	0
			35	24	11		
4	C	1	Total	C	O	0	0
			35	24	11		

- Molecule 5 is ERYTHROMYCIN A (three-letter code: ERY) (formula: C₃₇H₆₇NO₁₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			51	37	1	13		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



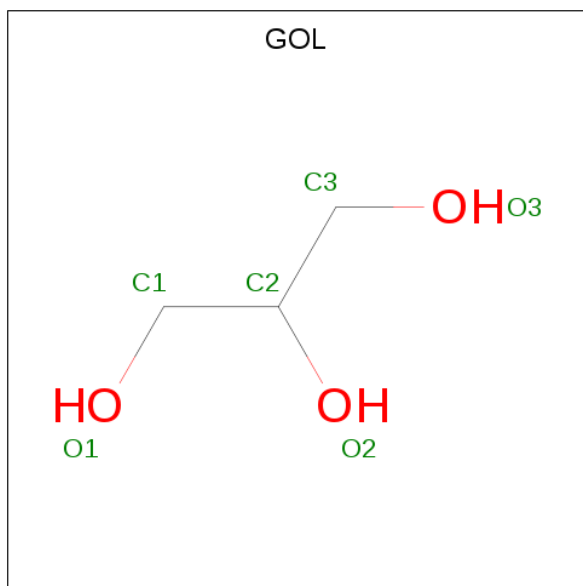
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			10	2	6	2		
6	A	1	Total	C	H	O	0	0
			10	2	6	2		
6	A	1	Total	C	H	O	0	0
			10	2	6	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			10	2	6	2		
6	A	1	Total	C	H	O	0	0
			10	2	6	2		
6	B	1	Total	C	H	O	0	0
			10	2	6	2		
6	C	1	Total	C	H	O	0	0
			10	2	6	2		
6	C	1	Total	C	H	O	0	0
			10	2	6	2		
6	C	1	Total	C	H	O	0	0
			10	2	6	2		
6	C	1	Total	C	H	O	0	0
			10	2	6	2		
6	E	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



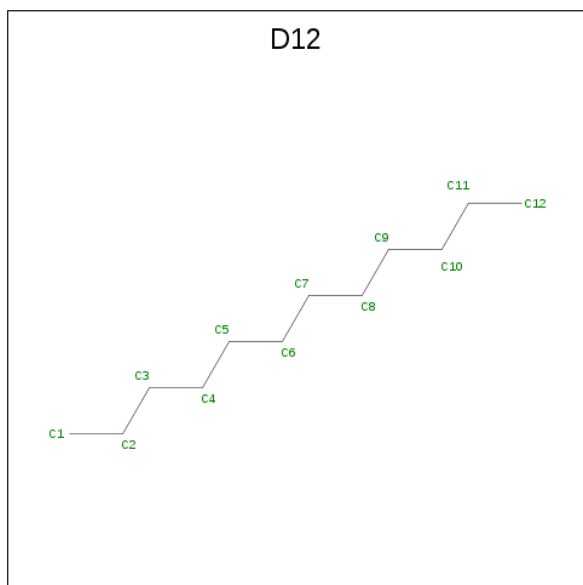
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			14	3	8	3		
7	A	1	Total	C	H	O	0	0
			14	3	8	3		

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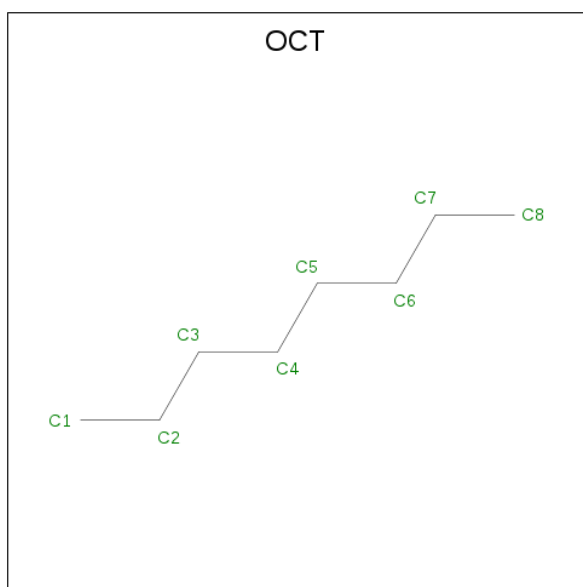
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			14	3	8	3		
7	C	1	Total	C	H	O	0	0
			14	3	8	3		
7	C	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 8 is DODECANE (three-letter code: D12) (formula: $C_{12}H_{26}$).



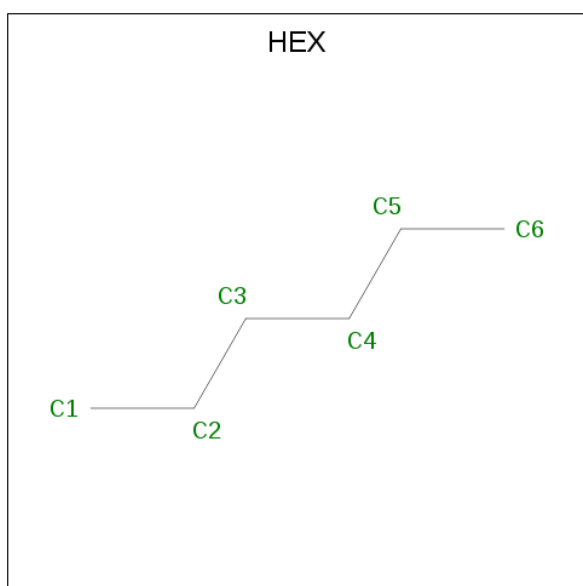
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C		0	0
			12	12			
8	B	1	Total	C	H	0	0
			38	12	26		

- Molecule 9 is N-OCTANE (three-letter code: OCT) (formula: C_8H_{18}).



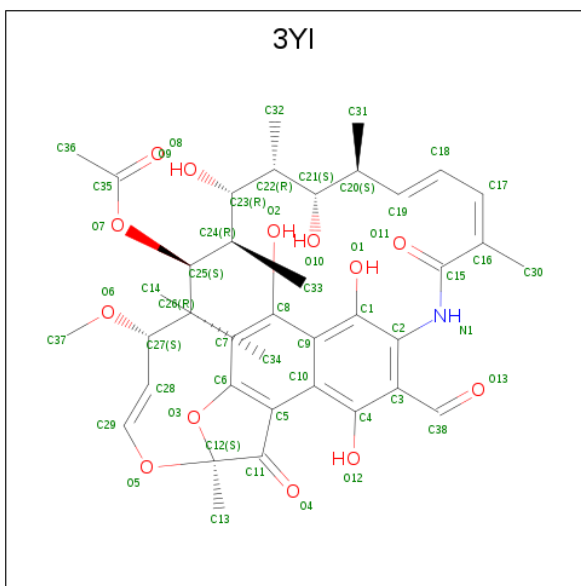
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	H	0	0
			26	8	18		
9	C	1	Total	C	H	0	0
			26	8	18		

- Molecule 10 is HEXANE (three-letter code: HEX) (formula: C₆H₁₄).



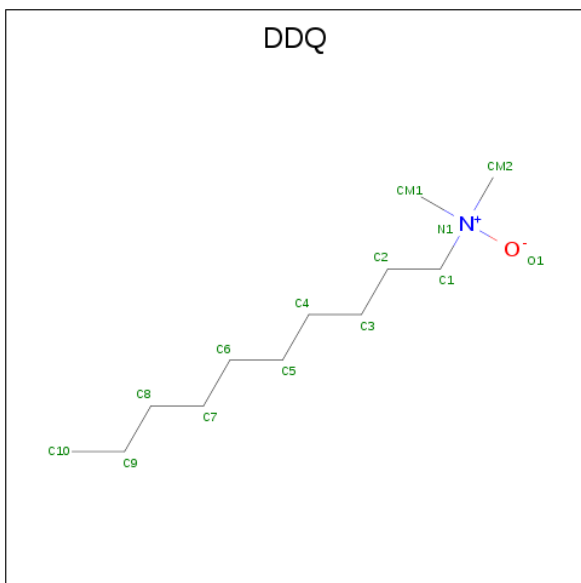
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	H	0	0
			20	6	14		
10	C	1	Total	C	H	0	0
			20	6	14		

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



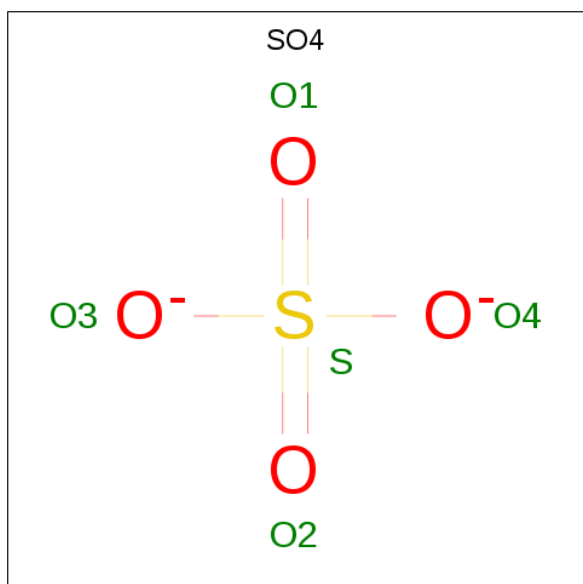
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	N	O	0	0
			52	38	1	13		

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



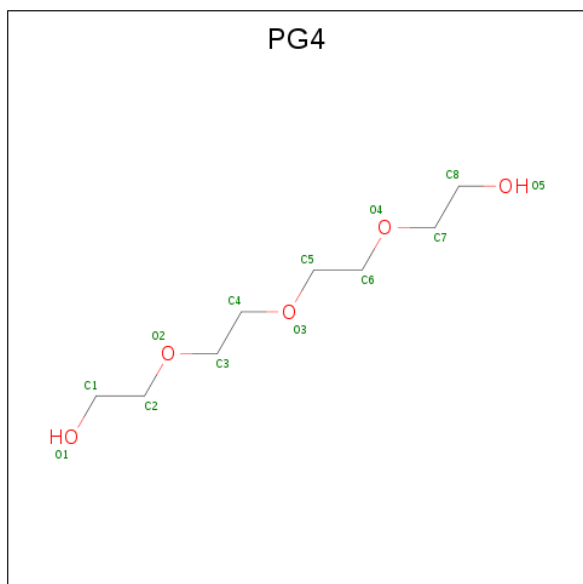
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	B	1	Total	C	H	N	O	0	0
			41	12	27	1	1		

- Molecule 13 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



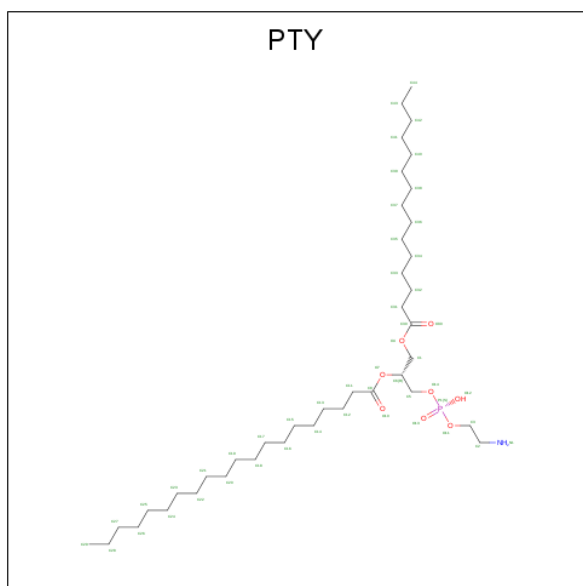
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	B	1	Total	O	S	0	0
			5	4	1		
13	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 14 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	C	1	Total	C	H	O	0	0
			31	8	18	5		

- Molecule 15 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$).



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

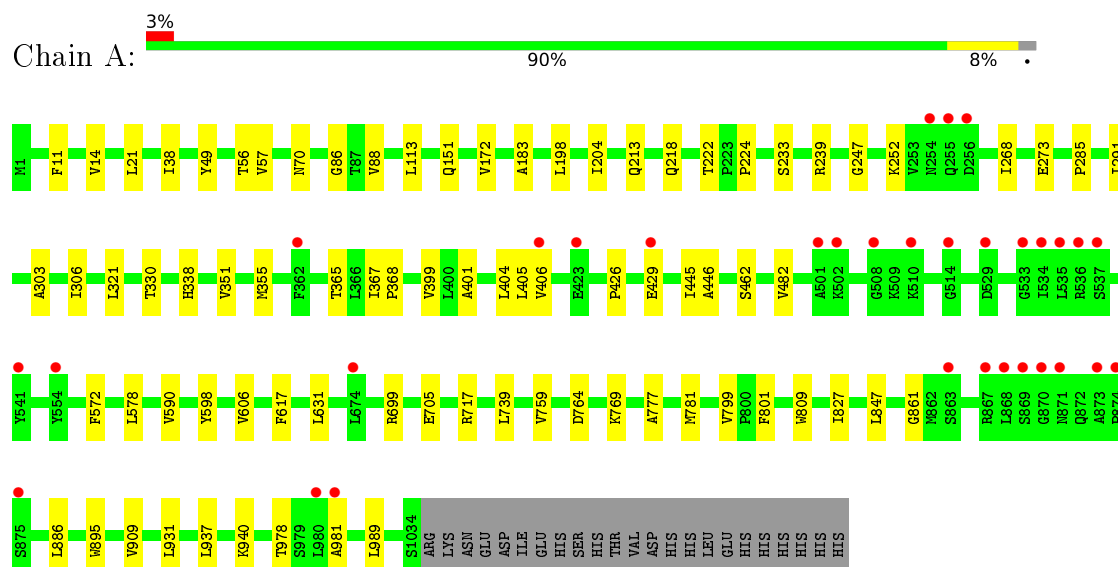
- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	65	Total	O	0	1
			66	66		
16	B	50	Total	O	0	1
			51	51		
16	C	59	Total	O	0	0
			59	59		
16	D	5	Total	O	0	0
			5	5		
16	E	10	Total	O	0	0
			10	10		

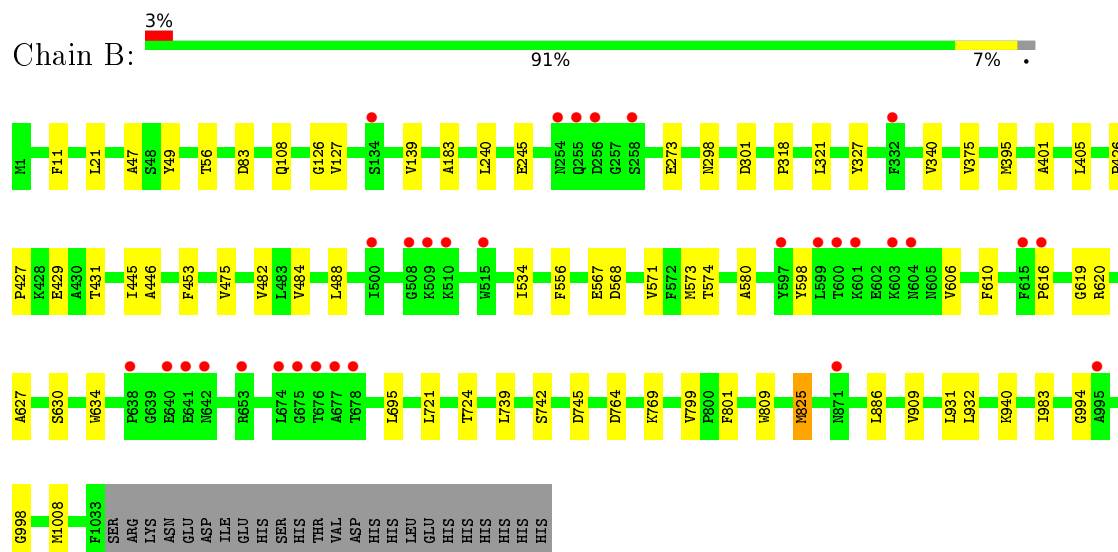
3 Residue-property plots [i](#)

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.

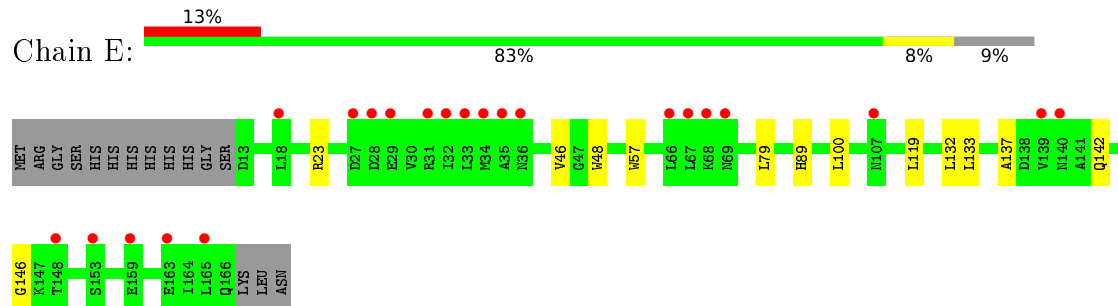
- Molecule 1: Multidrug efflux pump subunit AcrB



- Molecule 1: Multidrug efflux pump subunit AcrB



- Molecule 1: Multidrug efflux pump subunit AcrB



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	145.33Å 161.26Å 244.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.37 – 2.89 49.37 – 2.87	Depositor EDS
% Data completeness (in resolution range)	67.7 (49.37-2.89) 67.7 (49.37-2.87)	Depositor EDS
R_{merge}	0.60	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.86Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.218 , 0.238 0.233 , 0.248	Depositor DCC
R_{free} test set	4399 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	31.7	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 28.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	26894	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.07% 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: 3YI, D12, LMT, OCT, PG4, GOL, SO4, EDO, HEX, C14, ERY, PTY, DDQ

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	0.26	0/8009	0.32	0/10878
1	B	0.25	0/8003	0.31	0/10870
1	C	0.26	0/8009	0.32	0/10878
2	D	0.26	0/1187	0.30	0/1614
2	E	0.26	0/1186	0.29	0/1613
All	All	0.26	0/26394	0.31	0/35853

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	7858	0	8010	45	0
1	B	7852	0	8005	39	0
1	C	7858	0	8010	45	0
2	D	1168	0	1151	7	0
2	E	1167	0	1151	7	0
3	A	14	30	30	0	0
3	C	14	0	30	0	0
4	A	35	0	46	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	70	0	92	1	0
4	C	70	0	92	1	0
5	A	51	0	67	2	0
6	A	20	30	30	0	0
6	B	4	6	6	0	0
6	C	20	30	30	0	0
6	E	4	6	6	0	0
7	A	18	24	24	0	0
7	C	12	16	16	2	0
8	A	12	0	26	1	0
8	B	12	26	26	0	0
9	B	8	18	18	0	0
9	C	8	18	18	0	0
10	B	6	14	14	1	0
10	C	6	14	14	0	0
11	B	52	0	0	0	0
12	B	14	27	27	0	0
13	B	5	0	0	0	0
13	D	5	0	0	0	0
14	C	13	18	18	0	0
15	C	50	0	79	3	0
16	A	66	0	0	0	0
16	B	51	0	0	0	0
16	C	59	0	0	0	0
16	D	5	0	0	0	0
16	E	10	0	0	0	0
All	All	26617	277	27036	133	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 133 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:B:616:PRO:HA	1:B:620:ARG:HB3	1.23	1.14
1:B:809:TRP:CD1	2:D:79:LEU:HD12	2.08	0.89
1:C:895:TRP:HB2	15:C:1113:PTY:HC6	1.56	0.88
1:B:126:GLY:HA3	1:C:116:PRO:HB3	1.68	0.75
1:C:57:VAL:HG21	1:C:86:GLY:HA2	1.76	0.66

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	1032/1057 (98%)	1002 (97%)	29 (3%)	1 (0%)	51	82
1	B	1031/1057 (98%)	1001 (97%)	29 (3%)	1 (0%)	51	82
1	C	1032/1057 (98%)	998 (97%)	34 (3%)	0	100	100
2	D	153/169 (90%)	151 (99%)	2 (1%)	0	100	100
2	E	152/169 (90%)	147 (97%)	5 (3%)	0	100	100
All	All	3400/3509 (97%)	3299 (97%)	99 (3%)	2 (0%)	51	82

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	617	PHE
1	B	994	GLY

5.3.2 Protein sidechains

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	841/864 (97%)	834 (99%)	7 (1%)	81	94
1	B	840/864 (97%)	831 (99%)	9 (1%)	73	92
1	C	841/864 (97%)	834 (99%)	7 (1%)	81	94
2	D	119/132 (90%)	118 (99%)	1 (1%)	81	94
2	E	119/132 (90%)	119 (100%)	0	100	100
All	All	2760/2856 (97%)	2736 (99%)	24 (1%)	78	93

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	801	PHE
1	C	49	TYR
1	C	11	PHE
1	C	219	LEU
1	A	801	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	437	GLN

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](#)

37 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	GOL	A	1206	-	5,5,5	0.03	0	5,5,5	0.11	0
8	D12	A	1210	-	11,11,11	0.24	0	10,10,10	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	HEX	B	1104	-	5,5,5	0.12	0	4,4,4	0.07	0
9	OCT	C	1102	-	7,7,7	0.10	0	6,6,6	0.07	0
9	OCT	B	1103	-	7,7,7	0.11	0	6,6,6	0.07	0
4	LMT	B	1101	-	36,36,36	0.44	0	47,47,47	0.64	1 (2%)
4	LMT	A	1202	-	36,36,36	0.58	1 (2%)	47,47,47	0.99	4 (8%)
10	HEX	C	1114	-	5,5,5	0.14	0	4,4,4	0.08	0
12	DDQ	B	1108	-	10,13,13	2.25	1 (10%)	12,15,15	0.58	0
5	ERY	A	1203	-	53,53,53	0.98	1 (1%)	82,82,82	1.60	15 (18%)
6	EDO	C	1112	-	3,3,3	0.05	0	2,2,2	0.15	0
4	LMT	C	1108	-	36,36,36	0.44	0	47,47,47	0.66	0
6	EDO	A	1205	-	3,3,3	0.06	0	2,2,2	0.16	0
11	3YI	B	1107	-	55,55,55	0.75	2 (3%)	82,83,83	0.44	1 (1%)
13	SO4	D	201	-	4,4,4	0.15	0	6,6,6	0.04	0
15	PTY	C	1113	-	49,49,49	0.94	2 (4%)	52,54,54	1.03	3 (5%)
6	EDO	A	1209	-	3,3,3	0.06	0	2,2,2	0.15	0
7	GOL	C	1105	-	5,5,5	0.09	0	5,5,5	0.14	0
13	SO4	B	1109	-	4,4,4	0.14	0	6,6,6	0.05	0
3	C14	A	1201	-	13,13,13	0.08	0	12,12,12	0.05	0
6	EDO	A	1204	-	3,3,3	0.04	0	2,2,2	0.19	0
6	EDO	C	1110	-	3,3,3	0.06	0	2,2,2	0.15	0
6	EDO	C	1107	-	3,3,3	0.06	0	2,2,2	0.19	0
6	EDO	C	1109	-	3,3,3	0.06	0	2,2,2	0.16	0
6	EDO	B	1102	-	3,3,3	0.05	0	2,2,2	0.16	0
7	GOL	C	1106	-	5,5,5	0.06	0	5,5,5	0.13	0
4	LMT	B	1105	-	36,36,36	0.58	0	47,47,47	1.45	9 (19%)
6	EDO	C	1111	-	3,3,3	0.06	0	2,2,2	0.18	0
4	LMT	C	1101	-	36,36,36	0.43	0	47,47,47	0.65	1 (2%)
6	EDO	A	1212	-	3,3,3	0.06	0	2,2,2	0.19	0
14	PG4	C	1104	-	12,12,12	0.20	0	11,11,11	0.13	0
8	D12	B	1106	-	11,11,11	0.25	0	10,10,10	0.58	0
6	EDO	A	1208	-	3,3,3	0.06	0	2,2,2	0.16	0
6	EDO	E	201	-	3,3,3	0.06	0	2,2,2	0.13	0
7	GOL	A	1211	-	5,5,5	0.06	0	5,5,5	0.17	0
7	GOL	A	1207	-	5,5,5	0.08	0	5,5,5	0.24	0
3	C14	C	1103	-	13,13,13	0.08	0	12,12,12	0.08	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
7	GOL	A	1206	-	-	0/4/4/4	-
8	D12	A	1210	-	-	0/9/9/9	-
10	HEX	B	1104	-	-	0/3/3/3	-
9	OCT	C	1102	-	-	0/5/5/5	-
9	OCT	B	1103	-	-	0/5/5/5	-
4	LMT	B	1101	-	-	6/21/61/61	0/2/2/2
4	LMT	A	1202	-	-	12/21/61/61	0/2/2/2
10	HEX	C	1114	-	-	0/3/3/3	-
12	DDQ	B	1108	-	-	2/11/11/11	-
5	ERY	A	1203	-	-	17/72/107/107	0/3/3/3
6	EDO	C	1112	-	-	0/1/1/1	-
4	LMT	C	1108	-	-	6/21/61/61	0/2/2/2
6	EDO	A	1205	-	-	0/1/1/1	-
11	3YI	B	1107	-	-	6/57/72/72	0/4/4/4
15	PTY	C	1113	-	-	20/53/53/53	-
6	EDO	A	1209	-	-	1/1/1/1	-
7	GOL	C	1105	-	-	0/4/4/4	-
3	C14	A	1201	-	-	4/11/11/11	-
6	EDO	A	1204	-	-	0/1/1/1	-
6	EDO	C	1110	-	-	0/1/1/1	-
6	EDO	C	1107	-	-	0/1/1/1	-
6	EDO	C	1109	-	-	0/1/1/1	-
6	EDO	B	1102	-	-	0/1/1/1	-
7	GOL	C	1106	-	-	1/4/4/4	-
4	LMT	B	1105	-	-	10/21/61/61	0/2/2/2
6	EDO	C	1111	-	-	0/1/1/1	-
4	LMT	C	1101	-	-	6/21/61/61	0/2/2/2
6	EDO	A	1212	-	-	0/1/1/1	-
14	PG4	C	1104	-	-	3/10/10/10	-
8	D12	B	1106	-	-	4/9/9/9	-
6	EDO	A	1208	-	-	0/1/1/1	-
6	EDO	E	201	-	-	0/1/1/1	-
7	GOL	A	1211	-	-	1/4/4/4	-
7	GOL	A	1207	-	-	0/4/4/4	-
3	C14	C	1103	-	-	0/11/11/11	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	1108	DDQ	O1-N1	-7.10	1.25	1.42
5	A	1203	ERY	O2-C1	5.37	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	1113	PTY	O4-C30	4.23	1.45	1.33
15	C	1113	PTY	O7-C8	4.14	1.46	1.34
11	B	1107	3YI	C26-C27	2.32	1.62	1.54

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1203	ERY	O5-C16-C15	-4.82	105.24	112.96
4	B	1105	LMT	C1B-O5B-C5B	4.39	122.31	113.69
15	C	1113	PTY	O7-C8-C11	4.01	120.15	111.50
4	B	1105	LMT	O5B-C5B-C4B	3.85	116.69	109.69
5	A	1203	ERY	O5-C16-C17	3.75	109.36	103.81

There are no chirality outliers.

5 of 99 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1202	LMT	C2'-C1'-O1'-C1
4	A	1202	LMT	O5'-C1'-O1'-C1
5	A	1203	ERY	C35-C12-C13-C36
5	A	1203	ERY	O13-C12-C13-O2
5	A	1203	ERY	O13-C12-C13-C36

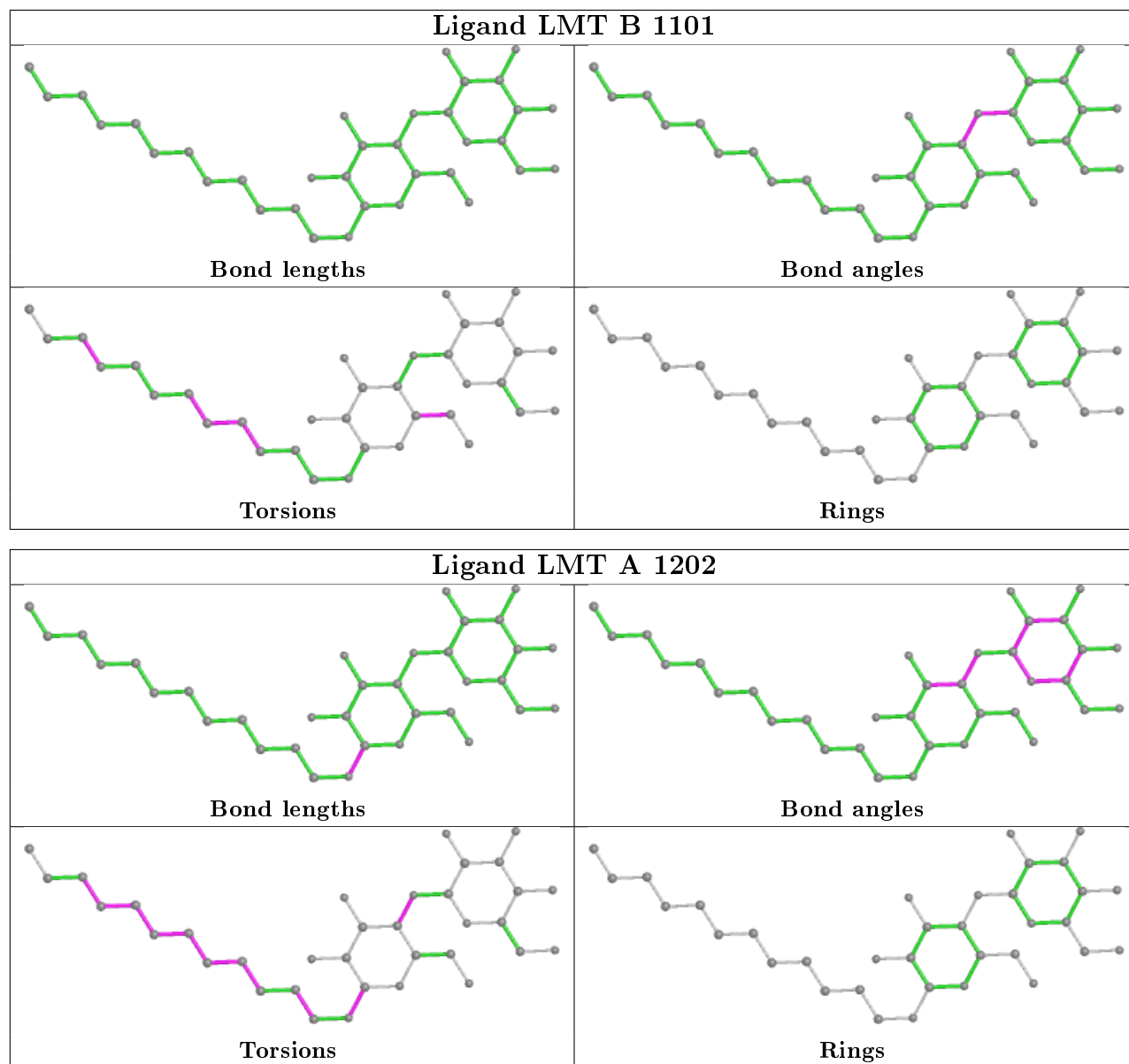
There are no ring outliers.

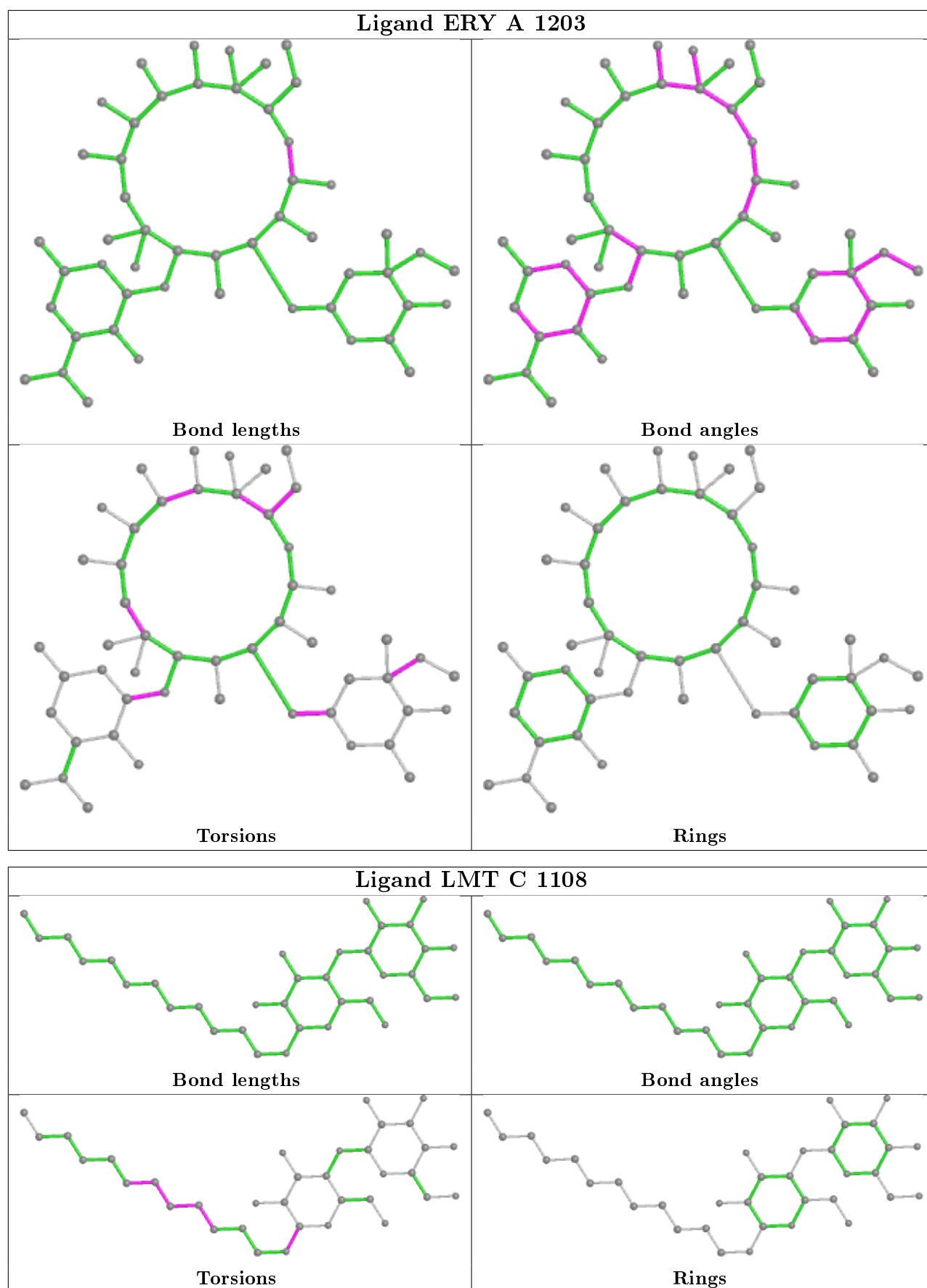
8 monomers are involved in 11 short contacts:

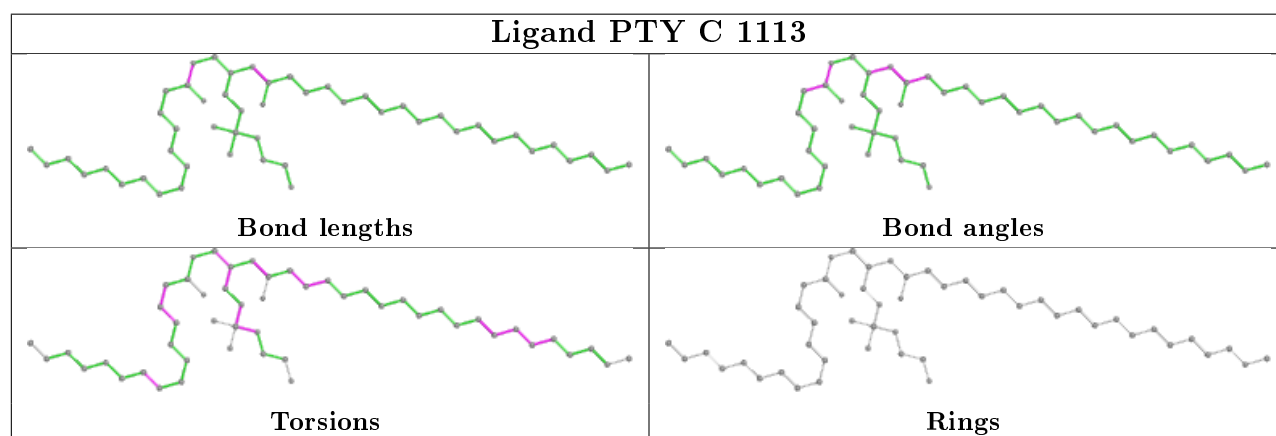
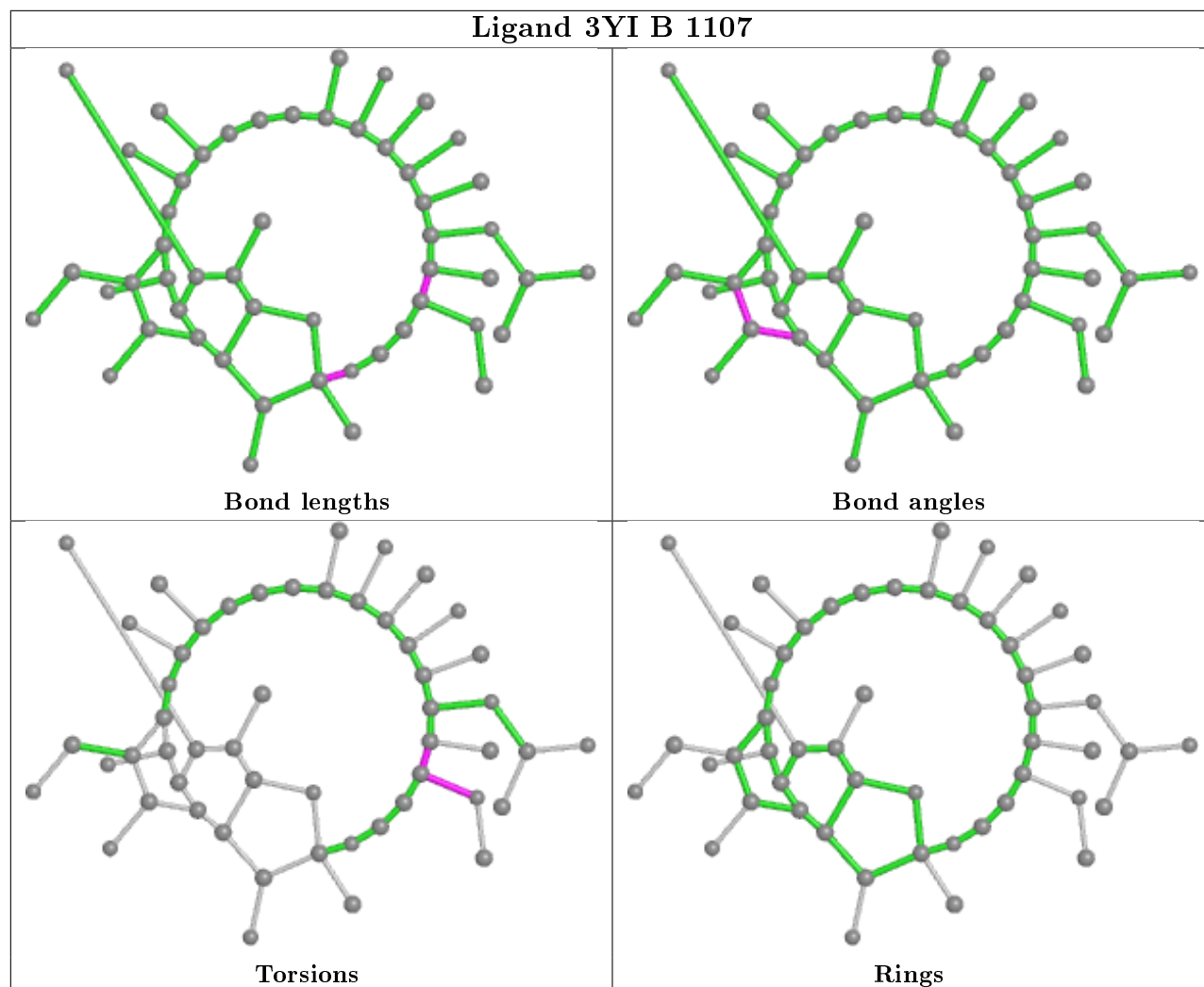
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1210	D12	1	0
10	B	1104	HEX	1	0
4	B	1101	LMT	1	0
5	A	1203	ERY	2	0
4	C	1108	LMT	1	0
15	C	1113	PTY	3	0
7	C	1105	GOL	1	0
7	C	1106	GOL	1	0

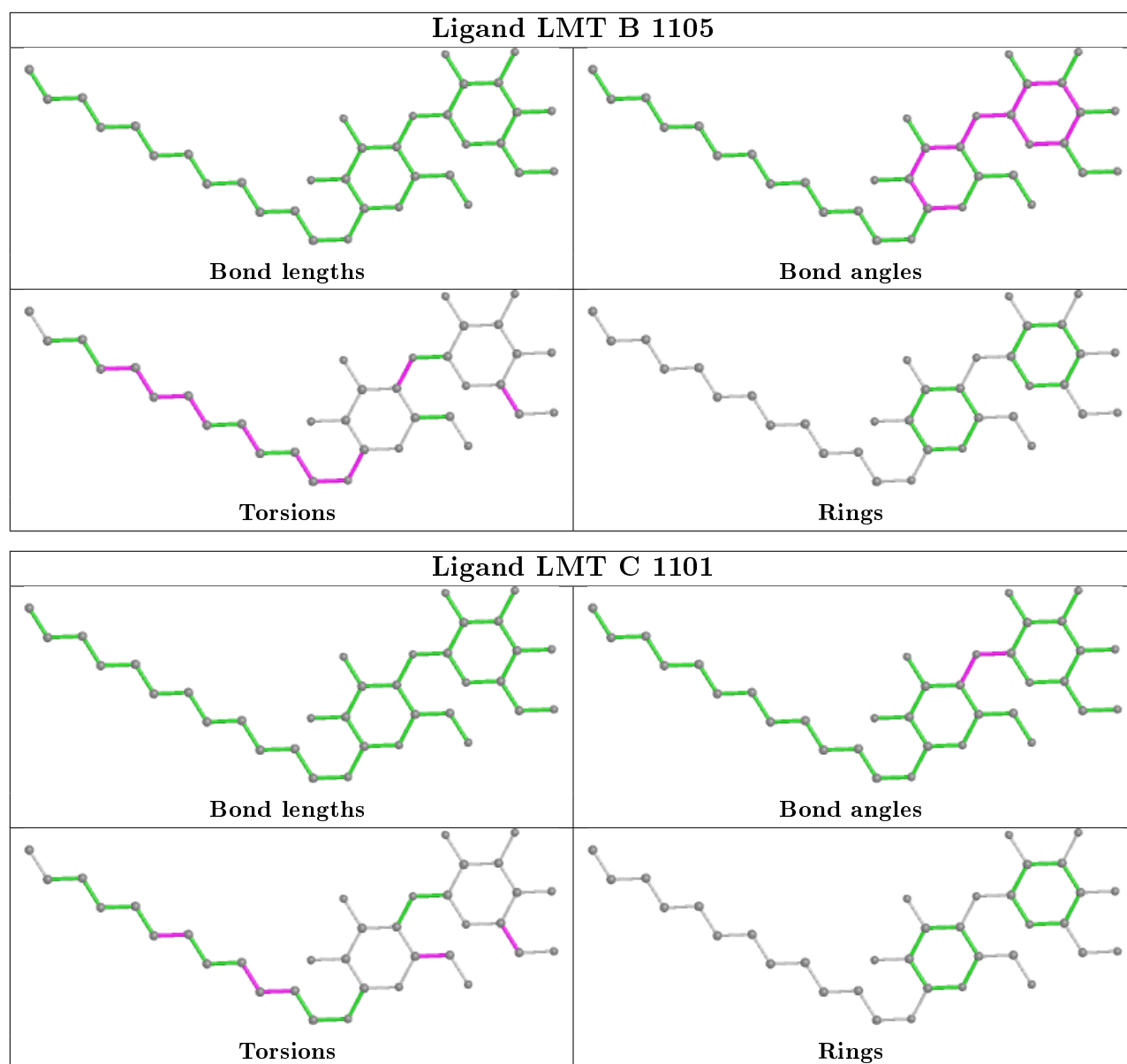
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	1034/1057 (97%)	-0.08	32 (3%)	49	44	10, 35, 73, 94	0
1	B	1033/1057 (97%)	-0.03	31 (3%)	50	45	8, 39, 64, 75	0
1	C	1034/1057 (97%)	-0.16	15 (1%)	73	73	14, 28, 51, 65	8 (0%)
2	D	155/169 (91%)	0.11	5 (3%)	47	43	33, 42, 57, 72	0
2	E	154/169 (91%)	0.85	22 (14%)	2	2	40, 59, 76, 85	0
All	All	3410/3509 (97%)	-0.04	105 (3%)	49	44	8, 36, 65, 94	8 (0%)

The worst 5 of 105 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	616	PRO	6.0
2	E	28	ASP	5.2
1	A	871	ASN	5.0
1	A	873	ALA	4.9
1	A	874	PRO	4.9

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.

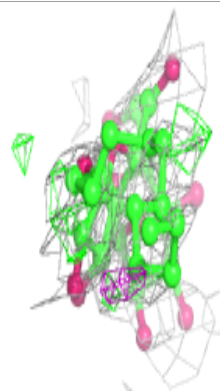
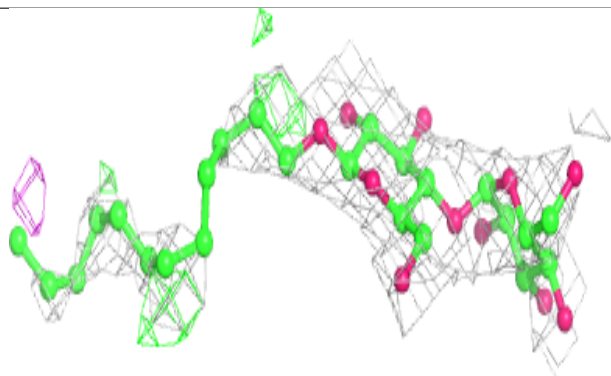
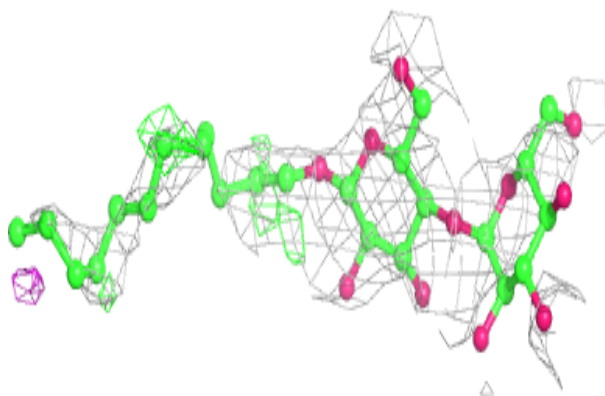
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	LMT	C	1108	35/35	0.67	0.38	128,129,130,130	0
7	GOL	A	1207	6/6	0.73	0.29	62,78,80,80	0
6	EDO	B	1102	4/4	0.81	0.22	37,44,44,44	0
15	PTY	C	1113	50/50	0.81	0.37	73,76,78,78	0
4	LMT	B	1105	35/35	0.83	0.28	72,73,73,73	35
8	D12	B	1106	12/12	0.84	0.27	40,51,54,54	0
4	LMT	B	1101	35/35	0.84	0.32	84,84,84,84	0
6	EDO	C	1111	4/4	0.85	0.40	48,65,66,67	0
6	EDO	A	1212	4/4	0.85	0.26	38,48,49,49	0
9	OCT	C	1102	8/8	0.86	0.28	39,53,56,57	0
13	SO4	B	1109	5/5	0.86	0.23	93,93,93,93	0
4	LMT	A	1202	35/35	0.86	0.21	60,62,63,63	0
5	ERY	A	1203	51/51	0.87	0.27	31,32,32,32	51
10	HEX	B	1104	6/6	0.87	0.18	34,43,44,44	0
14	PG4	C	1104	13/13	0.88	0.27	41,50,53,53	31
7	GOL	A	1211	6/6	0.88	0.22	68,84,85,85	0
6	EDO	A	1205	4/4	0.89	0.18	54,84,86,86	0
4	LMT	C	1101	35/35	0.89	0.26	60,62,63,63	0
11	3YI	B	1107	52/52	0.90	0.25	55,55,55,55	0
3	C14	A	1201	14/14	0.90	0.27	42,53,54,55	0
6	EDO	A	1208	4/4	0.90	0.19	45,56,56,57	0
10	HEX	C	1114	6/6	0.90	0.24	32,45,47,47	0
3	C14	C	1103	14/14	0.91	0.17	25,25,26,26	0
9	OCT	B	1103	8/8	0.92	0.30	27,34,35,36	0
12	DDQ	B	1108	14/14	0.92	0.32	51,66,71,71	0
7	GOL	C	1105	6/6	0.92	0.17	48,57,58,58	0
8	D12	A	1210	12/12	0.92	0.25	18,18,19,19	0
6	EDO	C	1107	4/4	0.92	0.25	44,60,61,61	0
6	EDO	E	201	4/4	0.93	0.22	34,41,46,47	0
7	GOL	A	1206	6/6	0.93	0.17	41,50,51,51	0
6	EDO	A	1204	4/4	0.93	0.19	26,37,38,39	0
6	EDO	C	1112	4/4	0.93	0.17	41,48,48,48	0
7	GOL	C	1106	6/6	0.94	0.27	42,50,50,50	0
13	SO4	D	201	5/5	0.94	0.23	90,90,90,90	0
6	EDO	C	1110	4/4	0.95	0.23	53,65,66,67	0
6	EDO	C	1109	4/4	0.96	0.15	26,29,30,30	0
6	EDO	A	1209	4/4	0.96	0.09	25,28,29,29	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.

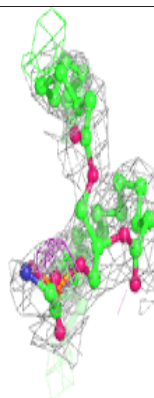
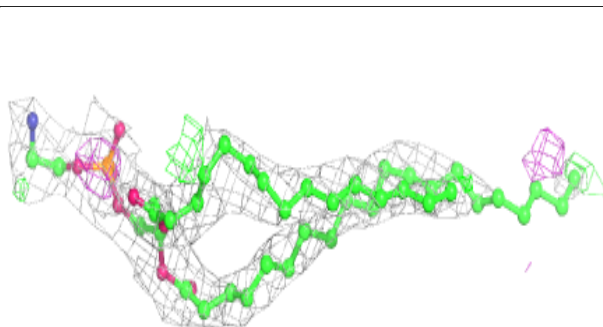
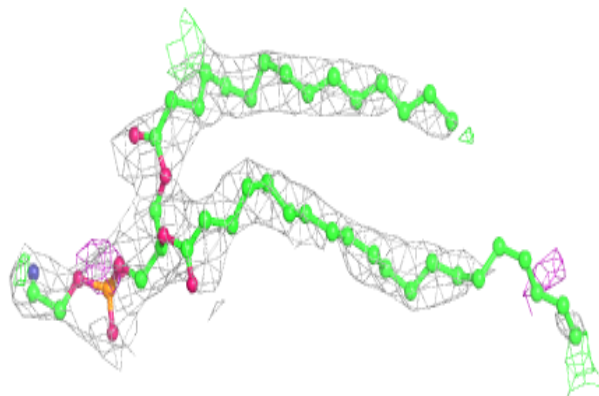
Electron density around LMT C 1108:

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



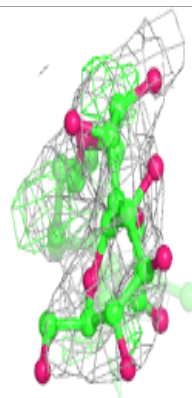
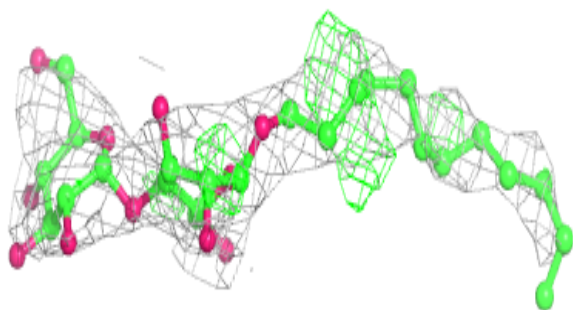
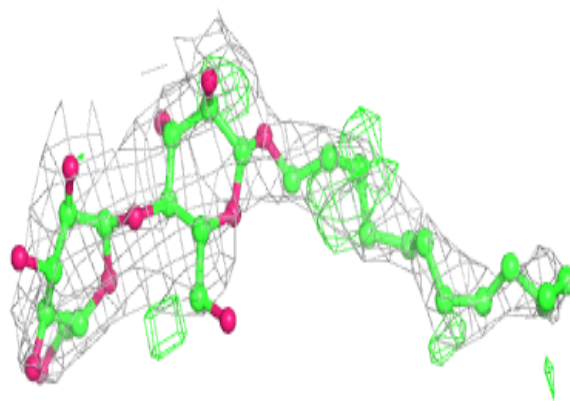
Electron density around PTY C 1113:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

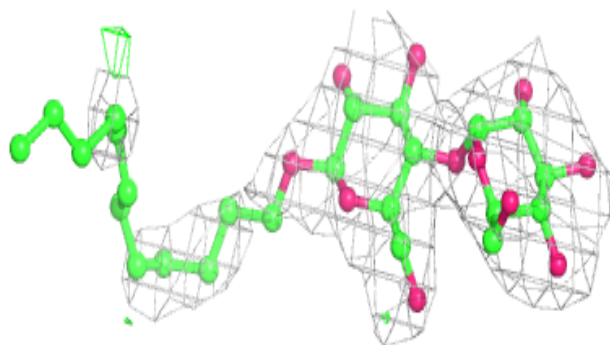
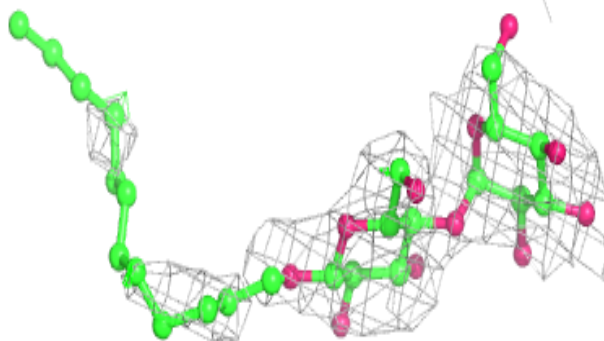


Electron density around LMT B 1105:

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

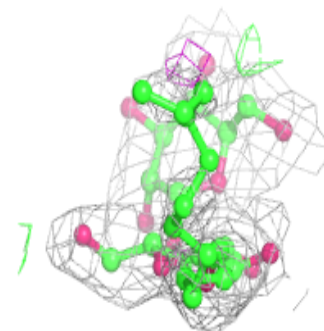
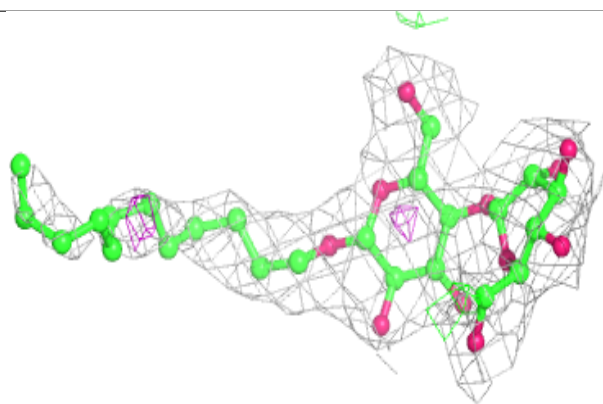
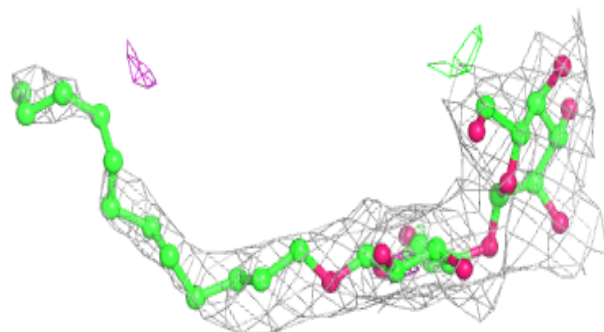
**Electron density around LMT B 1101:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



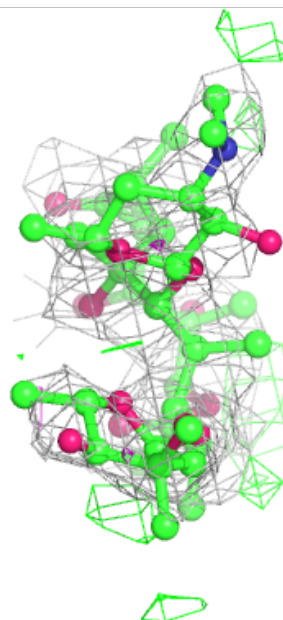
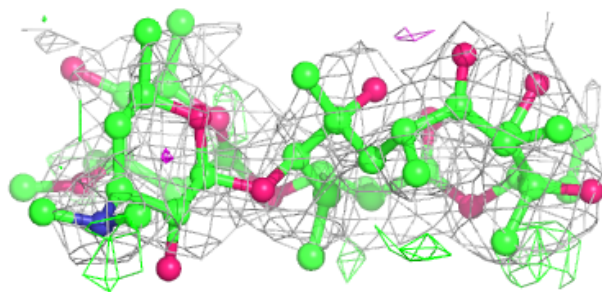
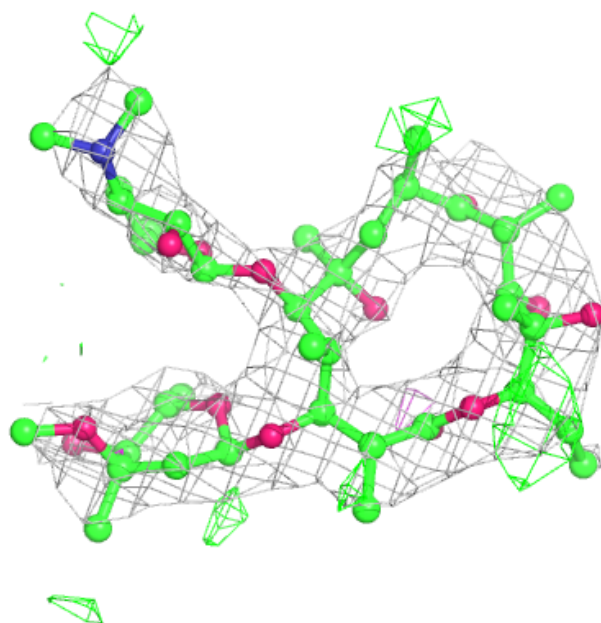
Electron density around LMT A 1202:

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



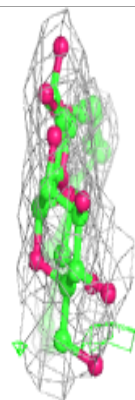
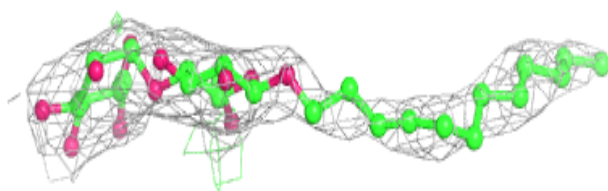
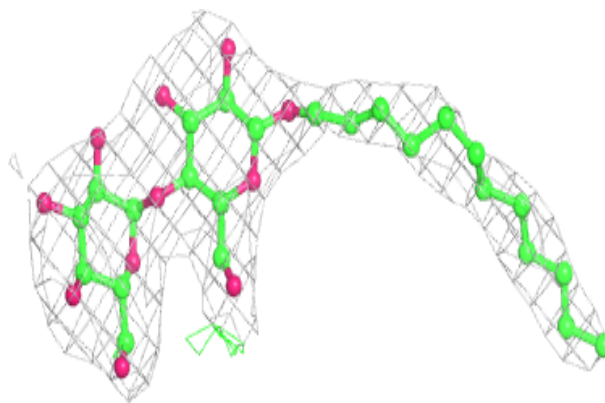
Electron density around ERY A 1203:

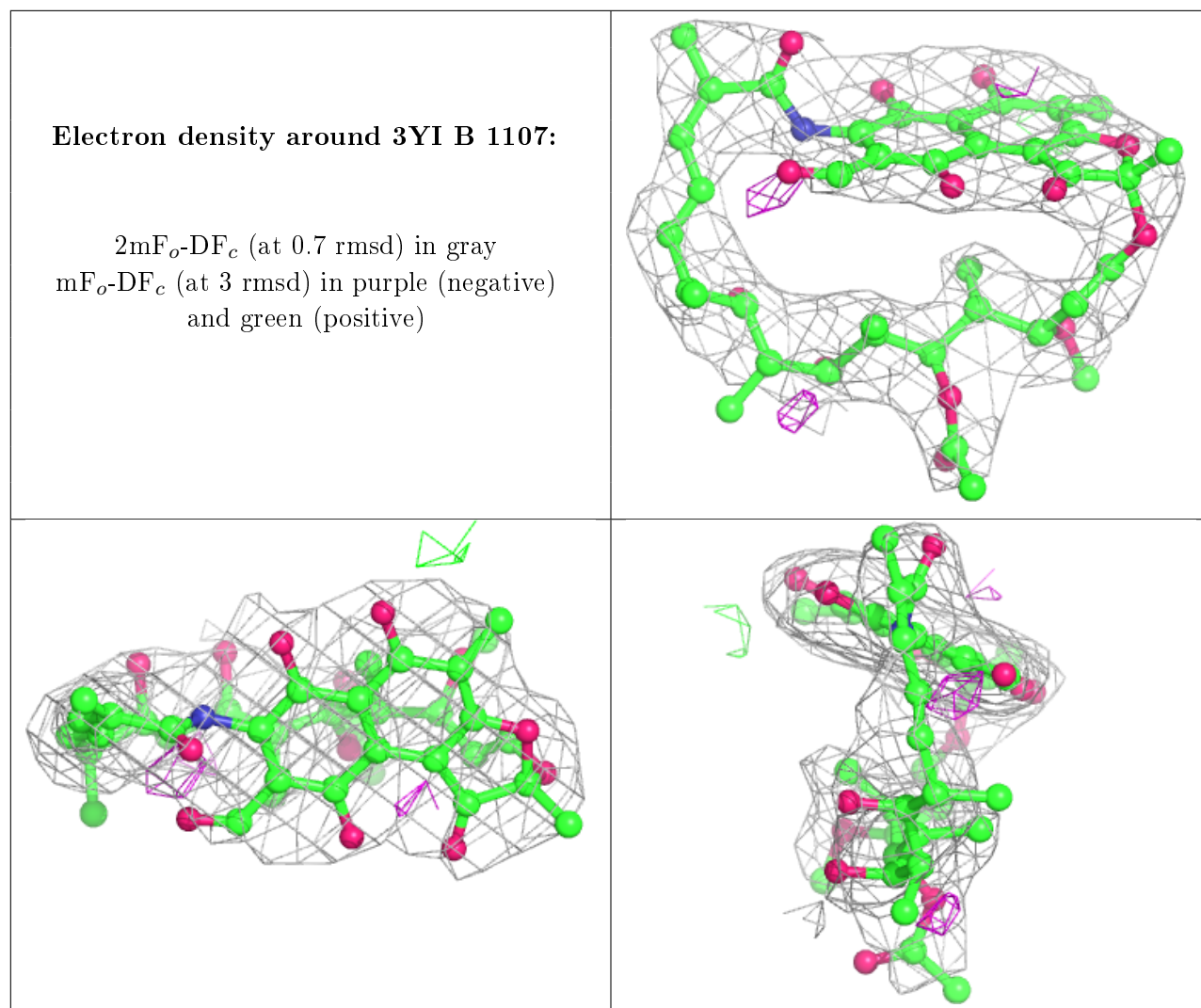
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around LMT C 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.