



wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 06:50 pm BST

PDB ID : 3W9I
Title : Structural basis for the inhibition of bacterial multidrug exporters
Authors : Sakurai, K.; Nakashima, R.; Hayashi, K.; Yamaguchi, A.
Deposited on : 2013-04-04
Resolution : 2.71 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 : 2.11
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) : 2.11

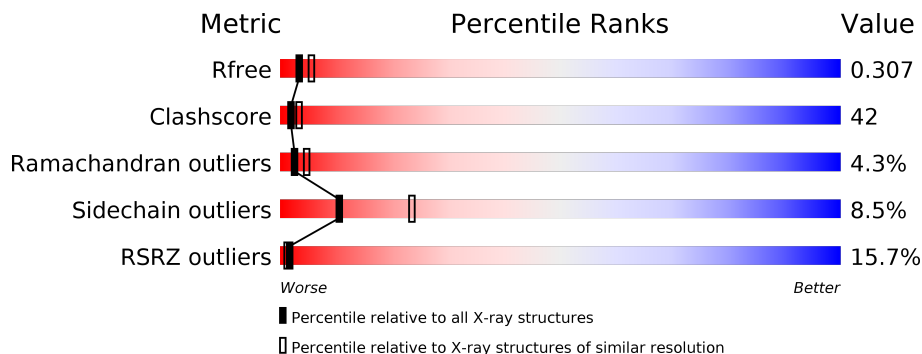
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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 on 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	1046	
1	B	1046	
1	C	1046	
1	D	1046	
1	E	1046	
1	F	1046	

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
2	LMT	B	2002	-	-	-	X
2	LMT	C	2001	-	-	-	X
2	LMT	D	2001	-	-	-	X
2	LMT	E	2001	-	-	X	-
2	LMT	E	2002	-	-	X	-

2 Entry composition [i](#)

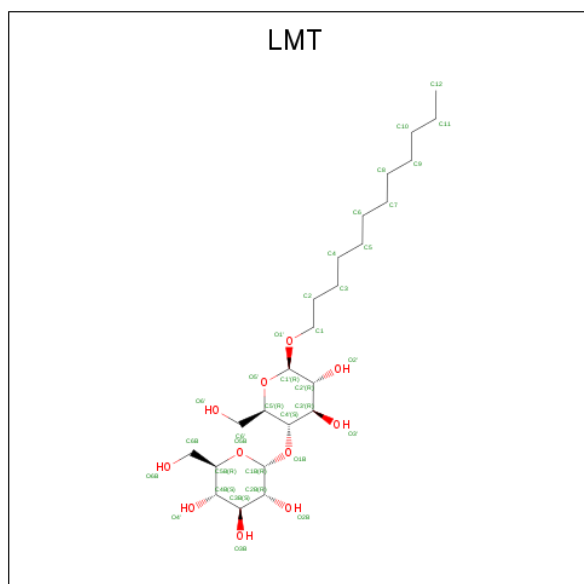
There are 3 unique types of molecules in this entry. The entry contains 47305 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 resistance protein MexB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1017	Total 7718	C 4972	N 1279	O 1427	S 40	0	0	0
1	B	1030	Total 7812	C 5027	N 1298	O 1447	S 40	0	0	0
1	C	1030	Total 7812	C 5027	N 1298	O 1447	S 40	0	0	0
1	D	1020	Total 7744	C 4990	N 1283	O 1431	S 40	0	0	0
1	E	1030	Total 7812	C 5027	N 1298	O 1447	S 40	0	0	0
1	F	1033	Total 7840	C 5046	N 1302	O 1452	S 40	0	0	0

- Molecule 2 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			35	24	11		
2	A	1	Total	C	O	0	0
			35	24	11		
2	B	1	Total	C	O	0	0
			35	24	11		
2	B	1	Total	C	O	0	0
			35	24	11		
2	B	1	Total	C	O	0	0
			35	24	11		
2	B	1	Total	C	O	0	0
			35	24	11		
2	C	1	Total	C	O	0	0
			35	24	11		
2	C	1	Total	C	O	0	0
			35	24	11		
2	D	1	Total	C	O	0	0
			35	24	11		
2	D	1	Total	C	O	0	0
			35	24	11		
2	D	1	Total	C	O	0	0
			35	24	11		
2	E	1	Total	C	O	0	0
			35	24	11		
2	E	1	Total	C	O	0	0
			35	24	11		
2	E	1	Total	C	O	0	0
			35	24	11		
2	F	1	Total	C	O	0	0
			35	24	11		
2	F	1	Total	C	O	0	0
			35	24	11		

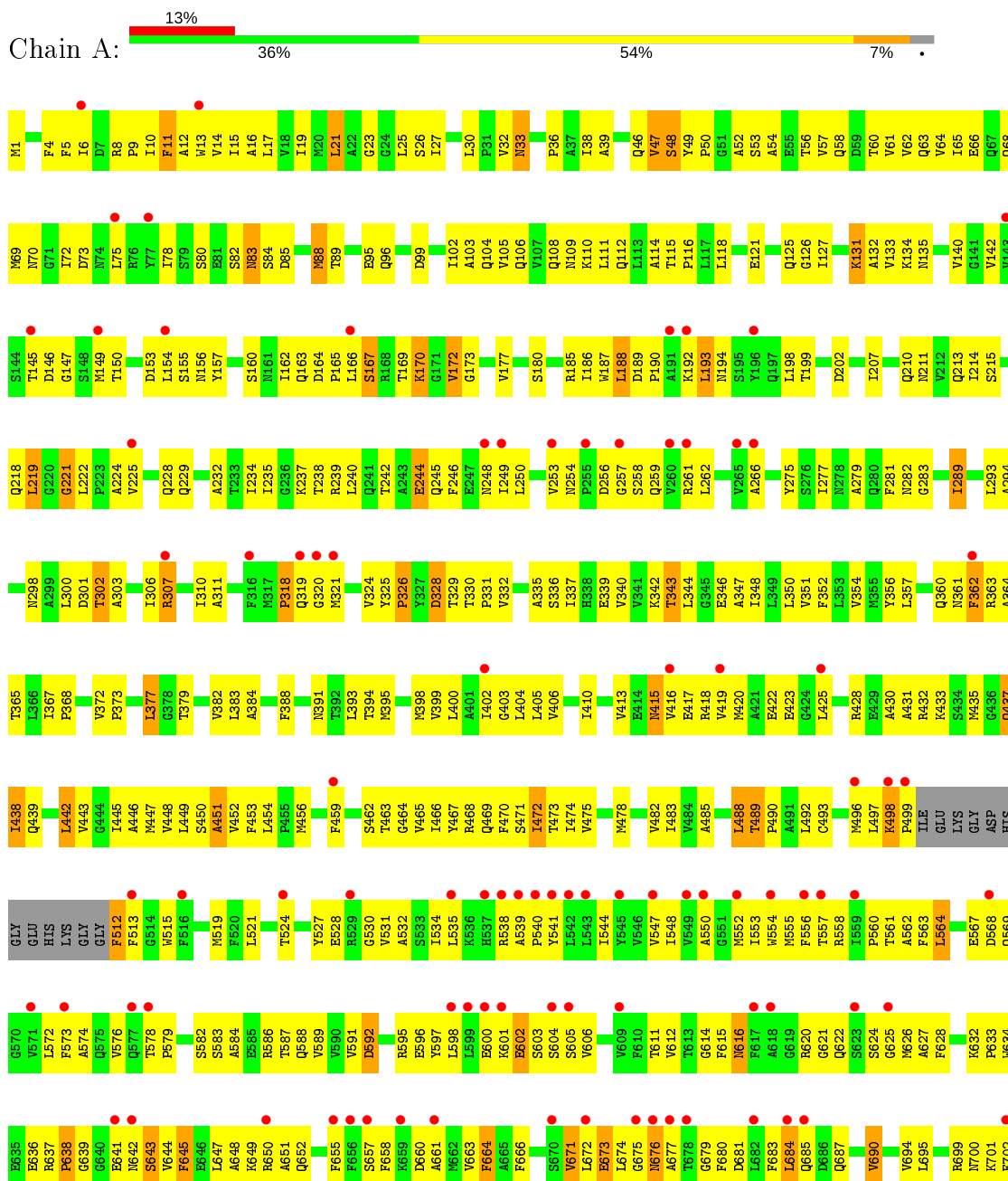
- Molecule 3 is water.

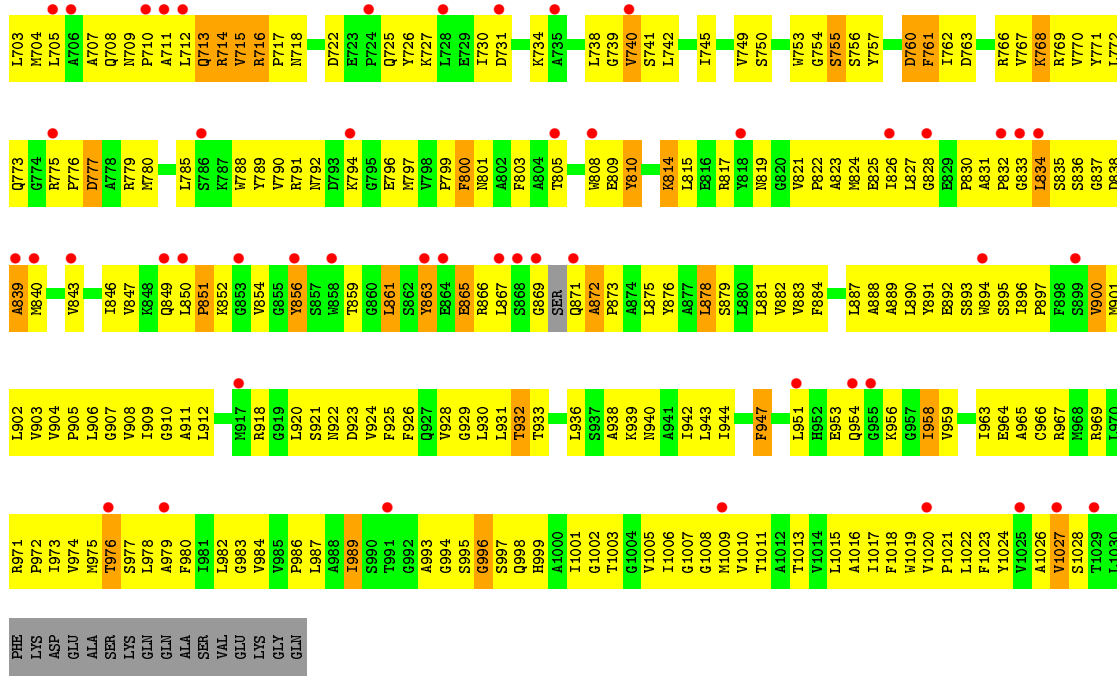
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O	0	0
			1	1		
3	B	3	Total	O	0	0
			3	3		
3	C	1	Total	O	0	0
			1	1		
3	D	2	Total	O	0	0
			2	2		

3 Residue-property plots

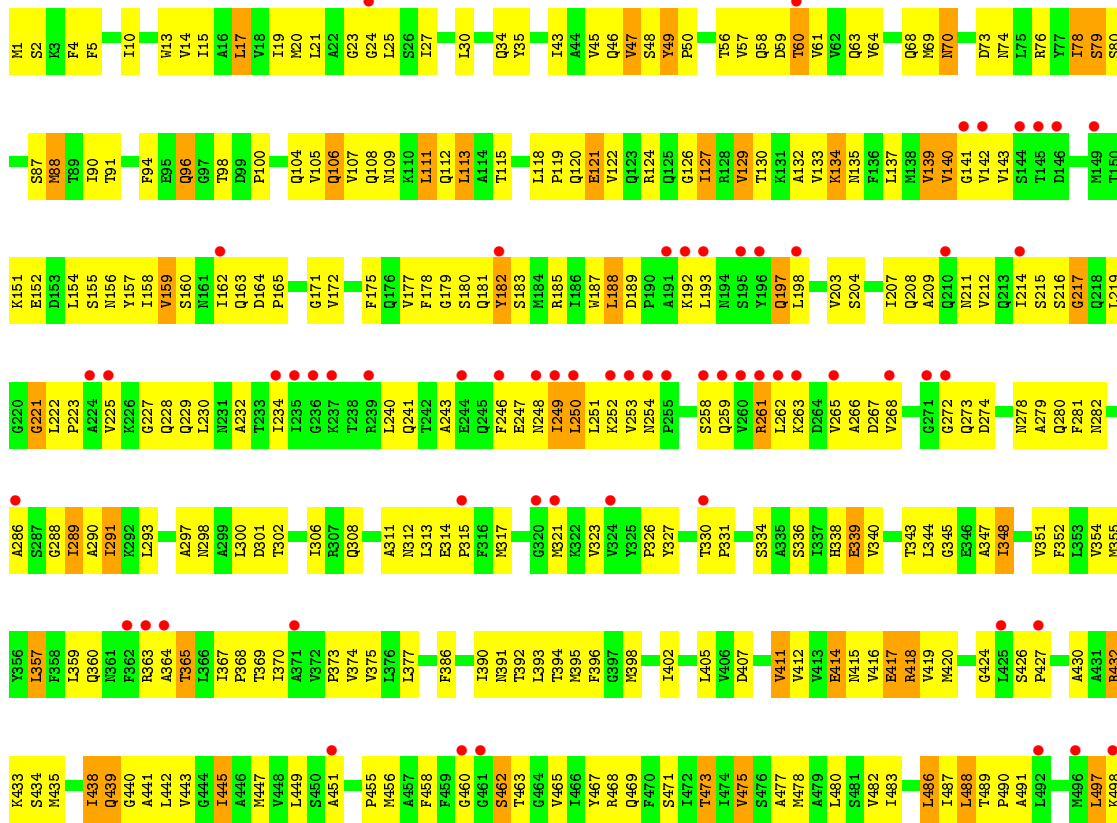
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

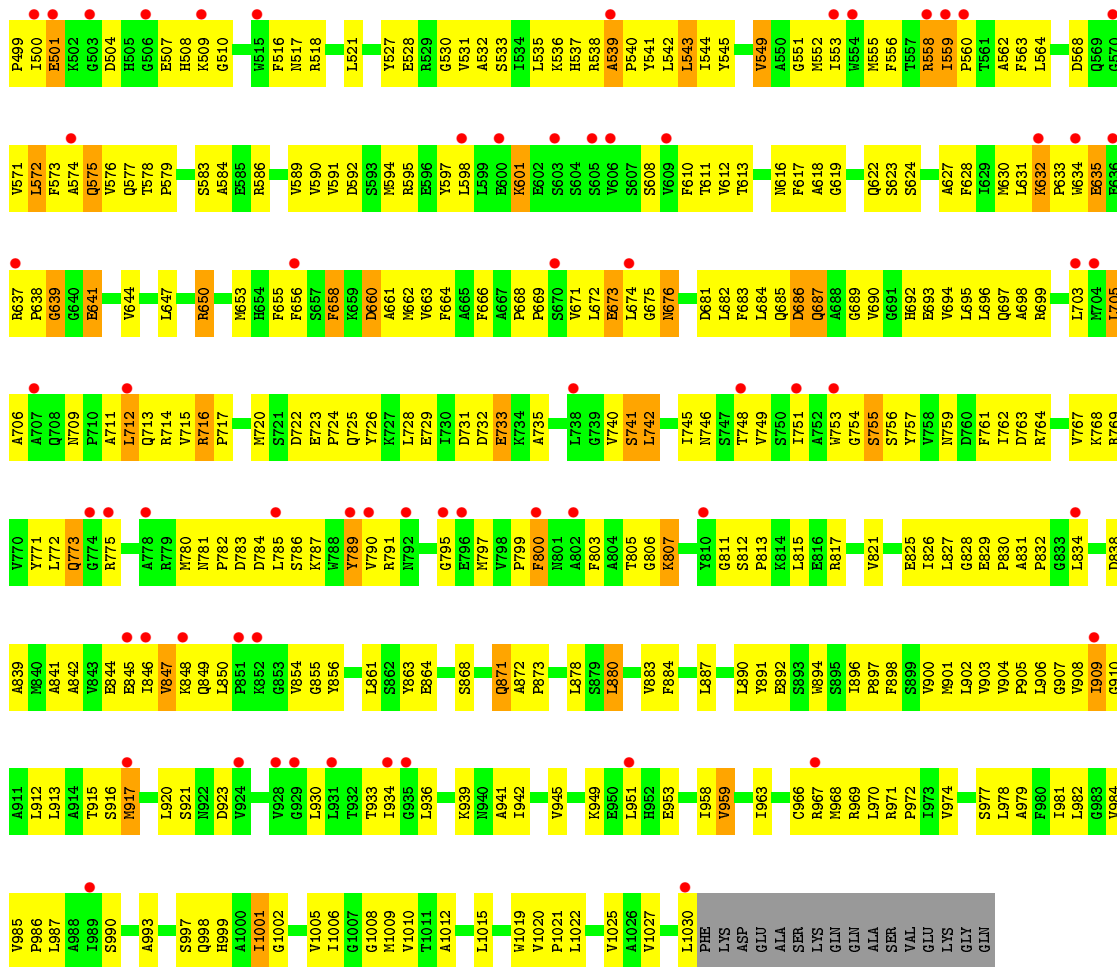
- Molecule 1: Multidrug resistance protein MexB



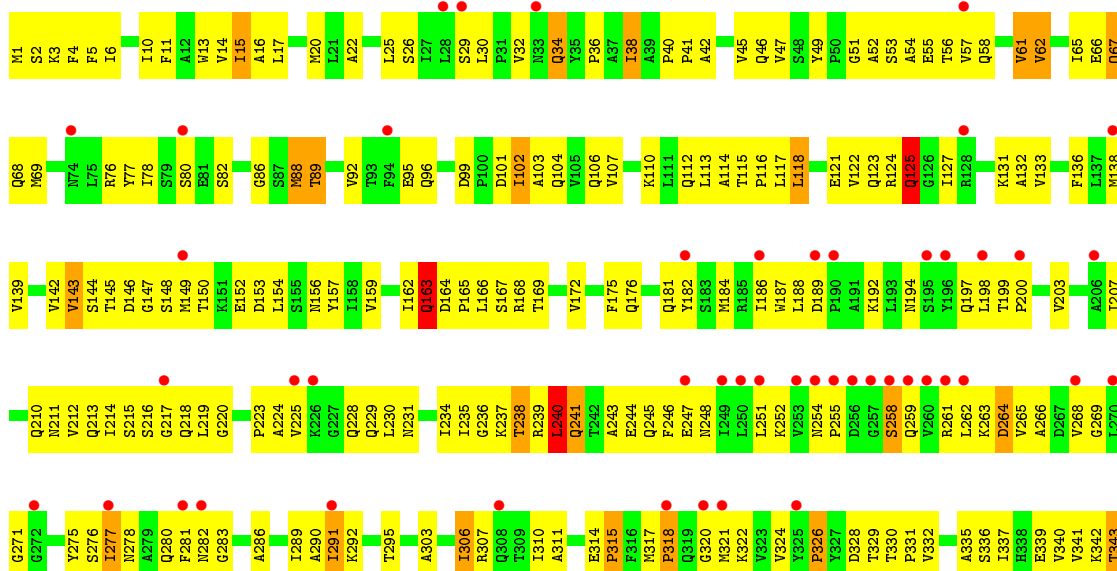


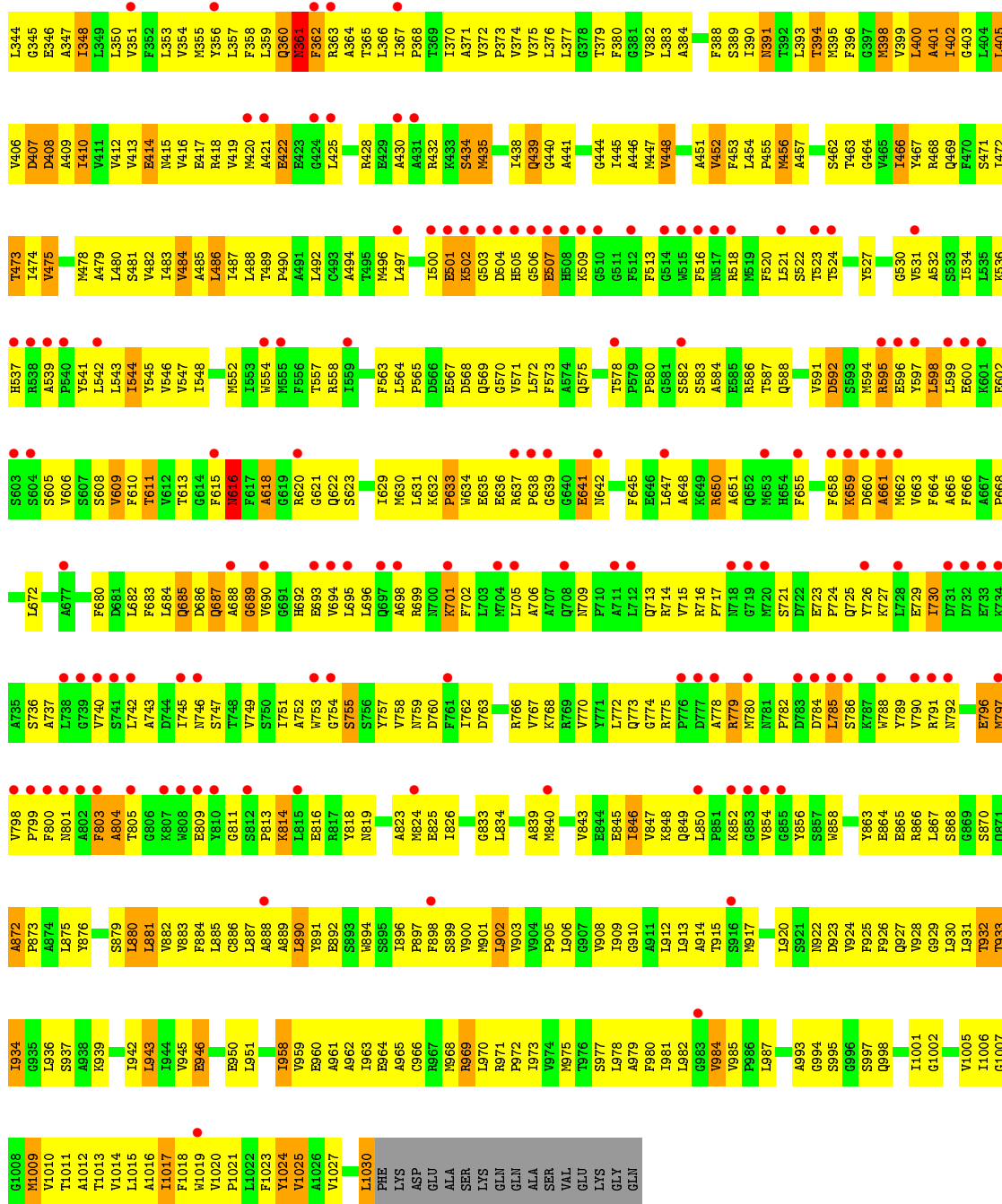
● Molecule 1: Multidrug resistance protein MexB



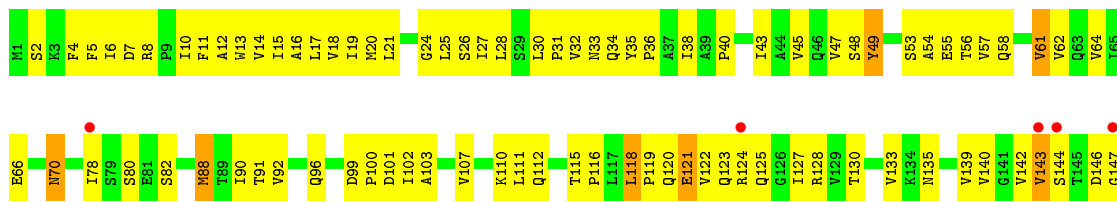


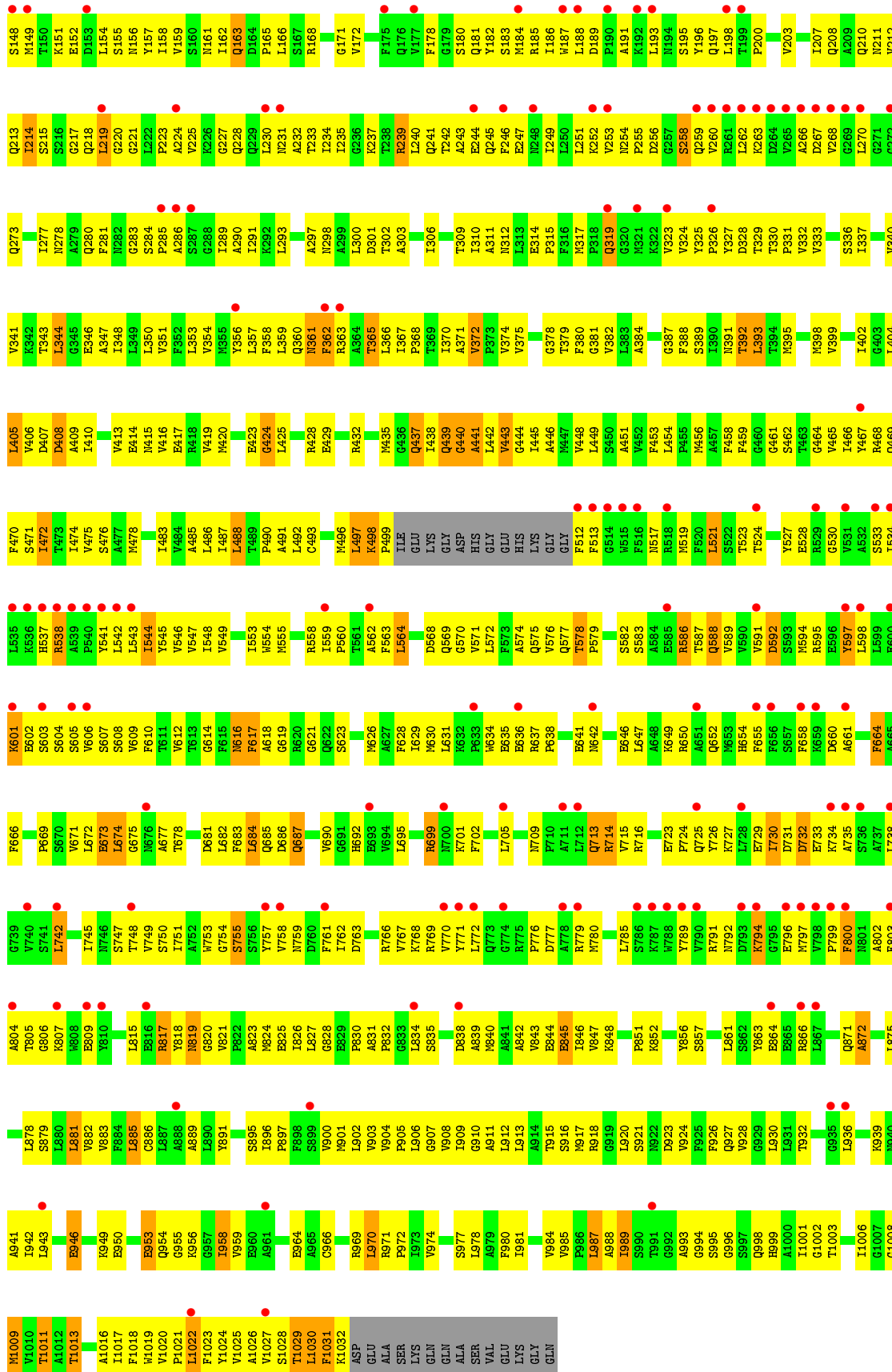
● Molecule 1: Multidrug resistance protein MexB

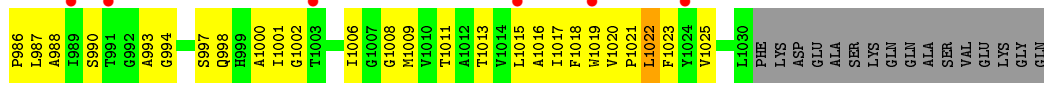
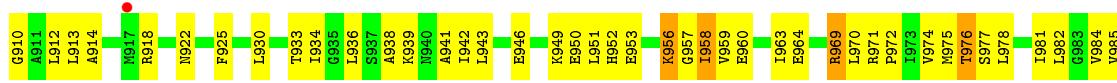




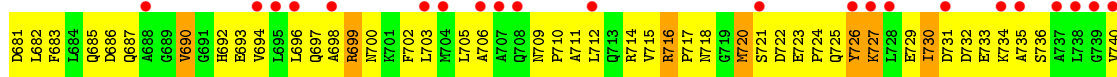
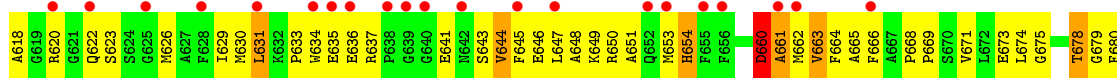
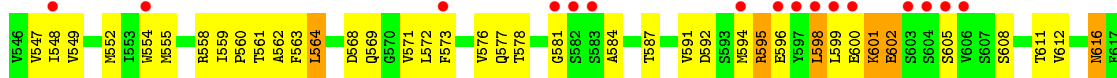
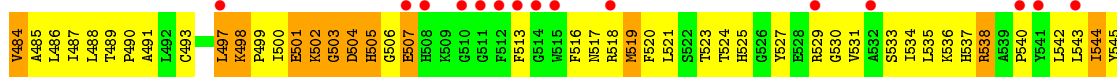
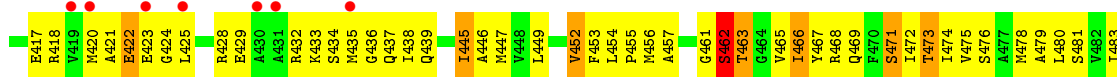
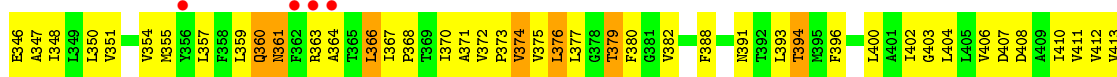
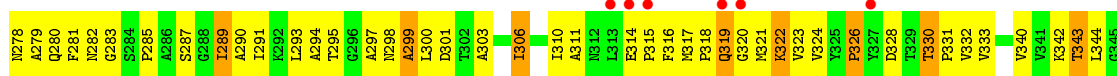
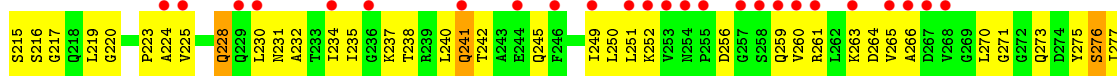
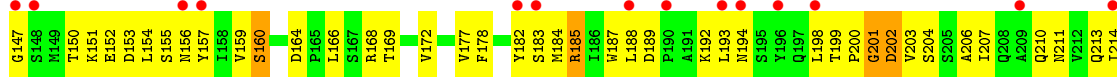
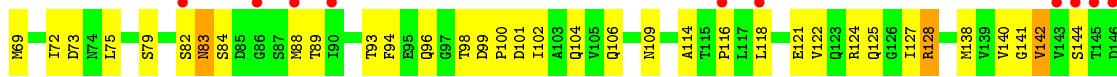
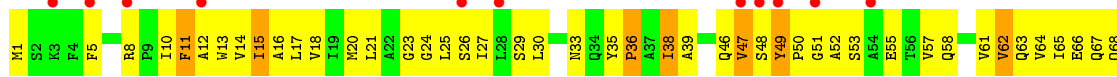
● Molecule 1: Multidrug resistance protein MexB







• Molecule 1: Multidrug resistance protein MexB



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	124.81Å 133.98Å 150.47Å 87.14° 69.49° 88.54°	Depositor
Resolution (Å)	48.33 – 2.71 48.33 – 2.71	Depositor EDS
% Data completeness (in resolution range)	97.0 (48.33-2.71) 97.0 (48.33-2.71)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.12 (at 2.73Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.282 , 0.315 0.278 , 0.307	Depositor DCC
R_{free} test set	12079 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	69.8	Xtrriage
Anisotropy	0.385	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 81.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtrriage
Estimated twinning fraction	0.000 for -h,k,-l	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	47305	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% 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:
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	0.48	0/7873	0.65	0/10701
1	B	0.53	0/7971	0.70	2/10833 (0.0%)
1	C	0.45	0/7971	0.62	1/10833 (0.0%)
1	D	0.45	0/7901	0.63	0/10739
1	E	0.41	0/7971	0.59	0/10833
1	F	0.44	0/8000	0.61	0/10871
All	All	0.46	0/47687	0.63	3/64810 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	686	ASP	CB-CG-OD2	5.92	123.63	118.30
1	C	401	ALA	CB-CA-C	-5.41	101.99	110.10
1	B	432	ARG	NE-CZ-NH2	-5.34	117.63	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	675	GLY	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7718	0	7858	683	0
1	B	7812	0	7944	628	0
1	C	7812	0	7944	758	0
1	D	7744	0	7886	710	0
1	E	7812	0	7944	626	0
1	F	7840	0	7970	668	0
2	A	70	0	92	12	0
2	B	140	0	184	28	0
2	C	70	0	92	18	0
2	D	105	0	138	14	0
2	E	105	0	138	33	0
2	F	70	0	92	8	0
3	A	1	0	0	1	0
3	B	3	0	0	0	0
3	C	1	0	0	0	0
3	D	2	0	0	0	0
All	All	47305	0	48282	3970	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 42.

The worst 5 of 3970 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:E:142:VAL:HG21	1:E:158:ILE:HD11	1.33	1.10
1:D:454:LEU:CD1	2:D:2001:LMT:H101	1.82	1.09
1:E:435:MET:O	1:E:439:GLN:HB2	1.53	1.09
1:A:343:THR:HG21	1:A:998:GLN:HE22	1.16	1.08
1:B:359:LEU:HD22	1:B:417:GLU:HG2	1.34	1.07

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	1011/1046 (97%)	834 (82%)	139 (14%)	38 (4%)	3	6
1	B	1028/1046 (98%)	878 (85%)	123 (12%)	27 (3%)	5	12
1	C	1028/1046 (98%)	814 (79%)	161 (16%)	53 (5%)	2	3
1	D	1016/1046 (97%)	815 (80%)	156 (15%)	45 (4%)	2	4
1	E	1028/1046 (98%)	839 (82%)	147 (14%)	42 (4%)	3	5
1	F	1031/1046 (99%)	837 (81%)	133 (13%)	61 (6%)	1	2
All	All	6142/6276 (98%)	5017 (82%)	859 (14%)	266 (4%)	2	5

5 of 266 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	326	PRO
1	A	603	SER
1	A	673	GLU
1	A	714	ARG
1	A	740	VAL

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	832/854 (97%)	759 (91%)	73 (9%)	10	22
1	B	841/854 (98%)	762 (91%)	79 (9%)	8	19
1	C	841/854 (98%)	762 (91%)	79 (9%)	8	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	835/854 (98%)	766 (92%)	69 (8%)	11	25
1	E	841/854 (98%)	784 (93%)	57 (7%)	16	35
1	F	844/854 (99%)	771 (91%)	73 (9%)	10	23
All	All	5034/5124 (98%)	4604 (92%)	430 (8%)	10	23

5 of 430 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	486	LEU
1	D	163	GLN
1	F	486	LEU
1	C	595	ARG
1	C	902	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 206 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	616	ASN
1	D	231	ASN
1	F	437	GLN
1	C	708	GLN
1	D	63	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 carbohydrates in this entry.

5.6 Ligand geometry

16 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
2	LMT	B	2002	-	36,36,36	0.77	1 (2%)	47,47,47	1.75	11 (23%)
2	LMT	D	2002	-	36,36,36	0.65	1 (2%)	47,47,47	1.34	4 (8%)
2	LMT	A	1102	-	36,36,36	0.68	1 (2%)	47,47,47	1.62	11 (23%)
2	LMT	F	2002	-	36,36,36	0.84	1 (2%)	47,47,47	1.34	5 (10%)
2	LMT	D	2001	-	36,36,36	0.94	2 (5%)	47,47,47	1.45	7 (14%)
2	LMT	B	2001	-	36,36,36	0.47	0	47,47,47	1.30	4 (8%)
2	LMT	E	2003	-	36,36,36	0.75	1 (2%)	47,47,47	1.49	5 (10%)
2	LMT	F	2001	-	36,36,36	0.82	1 (2%)	47,47,47	1.98	15 (31%)
2	LMT	E	2001	-	36,36,36	0.69	1 (2%)	47,47,47	1.10	3 (6%)
2	LMT	B	2003	-	36,36,36	0.82	1 (2%)	47,47,47	1.58	10 (21%)
2	LMT	B	2004	-	36,36,36	0.48	0	47,47,47	1.01	3 (6%)
2	LMT	C	2001	-	36,36,36	0.75	1 (2%)	47,47,47	1.24	5 (10%)
2	LMT	E	2002	-	36,36,36	0.96	1 (2%)	47,47,47	1.45	9 (19%)
2	LMT	C	2002	-	36,36,36	0.70	1 (2%)	47,47,47	1.29	5 (10%)
2	LMT	D	2003	-	36,36,36	0.79	1 (2%)	47,47,47	1.36	6 (12%)
2	LMT	A	1101	-	36,36,36	0.84	1 (2%)	47,47,47	1.72	14 (29%)

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
2	LMT	B	2002	-	-	12/21/61/61	0/2/2/2
2	LMT	D	2002	-	-	9/21/61/61	0/2/2/2
2	LMT	A	1102	-	-	11/21/61/61	0/2/2/2
2	LMT	F	2002	-	-	12/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LMT	D	2001	-	-	16/21/61/61	0/2/2/2
2	LMT	B	2001	-	-	5/21/61/61	0/2/2/2
2	LMT	E	2003	-	-	14/21/61/61	0/2/2/2
2	LMT	F	2001	-	-	12/21/61/61	0/2/2/2
2	LMT	E	2001	-	-	9/21/61/61	0/2/2/2
2	LMT	B	2003	-	-	8/21/61/61	0/2/2/2
2	LMT	B	2004	-	-	9/21/61/61	0/2/2/2
2	LMT	C	2001	-	-	14/21/61/61	0/2/2/2
2	LMT	E	2002	-	-	5/21/61/61	0/2/2/2
2	LMT	C	2002	-	-	14/21/61/61	0/2/2/2
2	LMT	D	2003	-	-	7/21/61/61	0/2/2/2
2	LMT	A	1101	-	-	13/21/61/61	0/2/2/2

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2001	LMT	O1'-C1'	3.21	1.45	1.40
2	E	2002	LMT	O1'-C1'	3.20	1.45	1.40
2	D	2003	LMT	O1'-C1'	3.20	1.45	1.40
2	D	2001	LMT	O1'-C1'	3.11	1.45	1.40
2	B	2003	LMT	O1'-C1'	3.01	1.45	1.40

The worst 5 of 117 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2003	LMT	C1B-O5B-C5B	5.82	125.11	113.69
2	E	2003	LMT	C1B-O5B-C5B	5.04	123.58	113.69
2	F	2001	LMT	C3'-C4'-C5'	-4.96	99.55	110.93
2	B	2002	LMT	O5B-C5B-C4B	4.64	118.12	109.69
2	F	2001	LMT	C1-O1'-C1'	4.59	121.45	113.84

There are no chirality outliers.

5 of 170 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2002	LMT	C2'-C1'-O1'-C1
2	B	2002	LMT	O5'-C1'-O1'-C1
2	F	2002	LMT	C2'-C1'-O1'-C1
2	F	2002	LMT	O5'-C1'-O1'-C1

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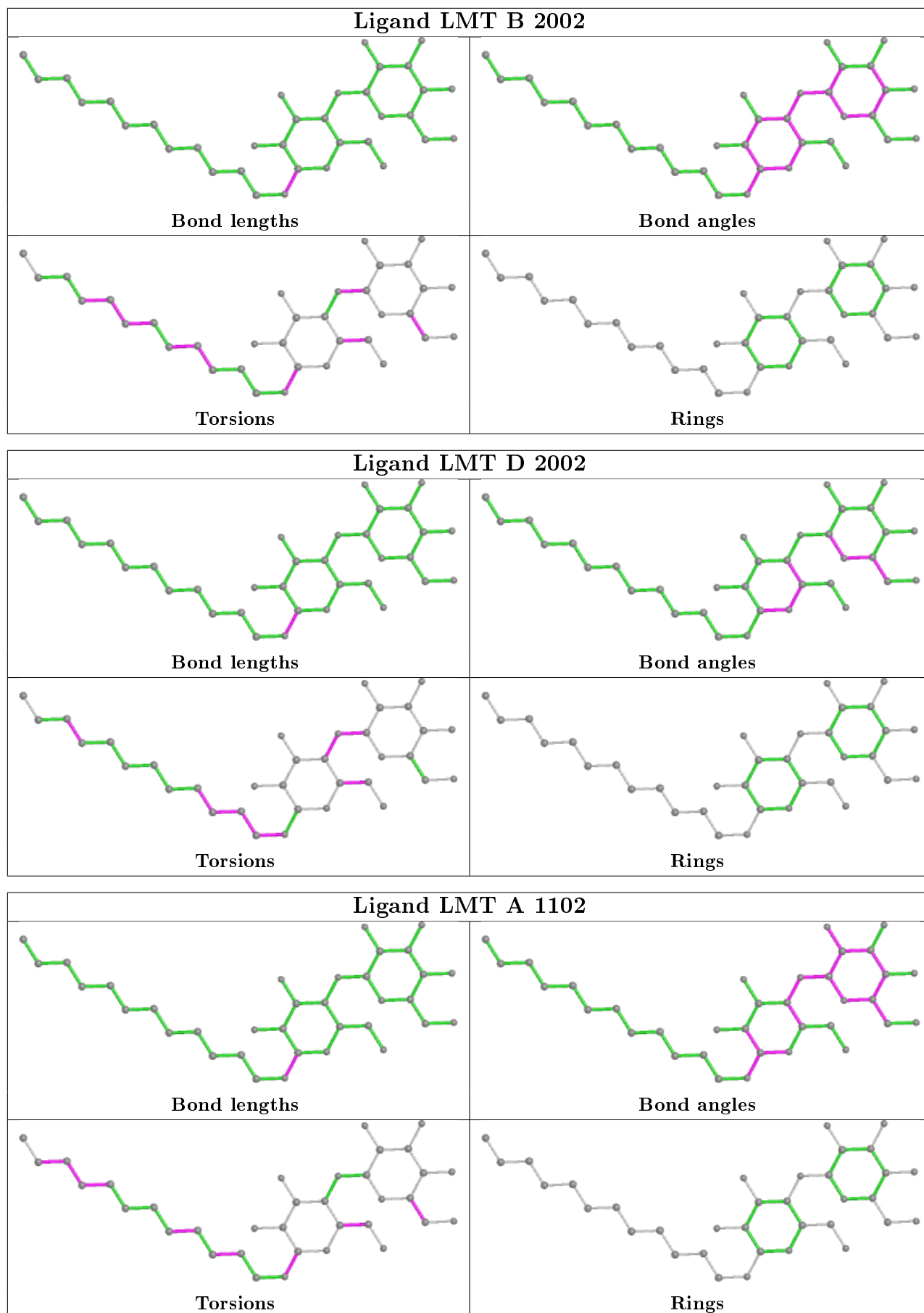
Mol	Chain	Res	Type	Atoms
2	D	2001	LMT	C2'-C1'-O1'-C1

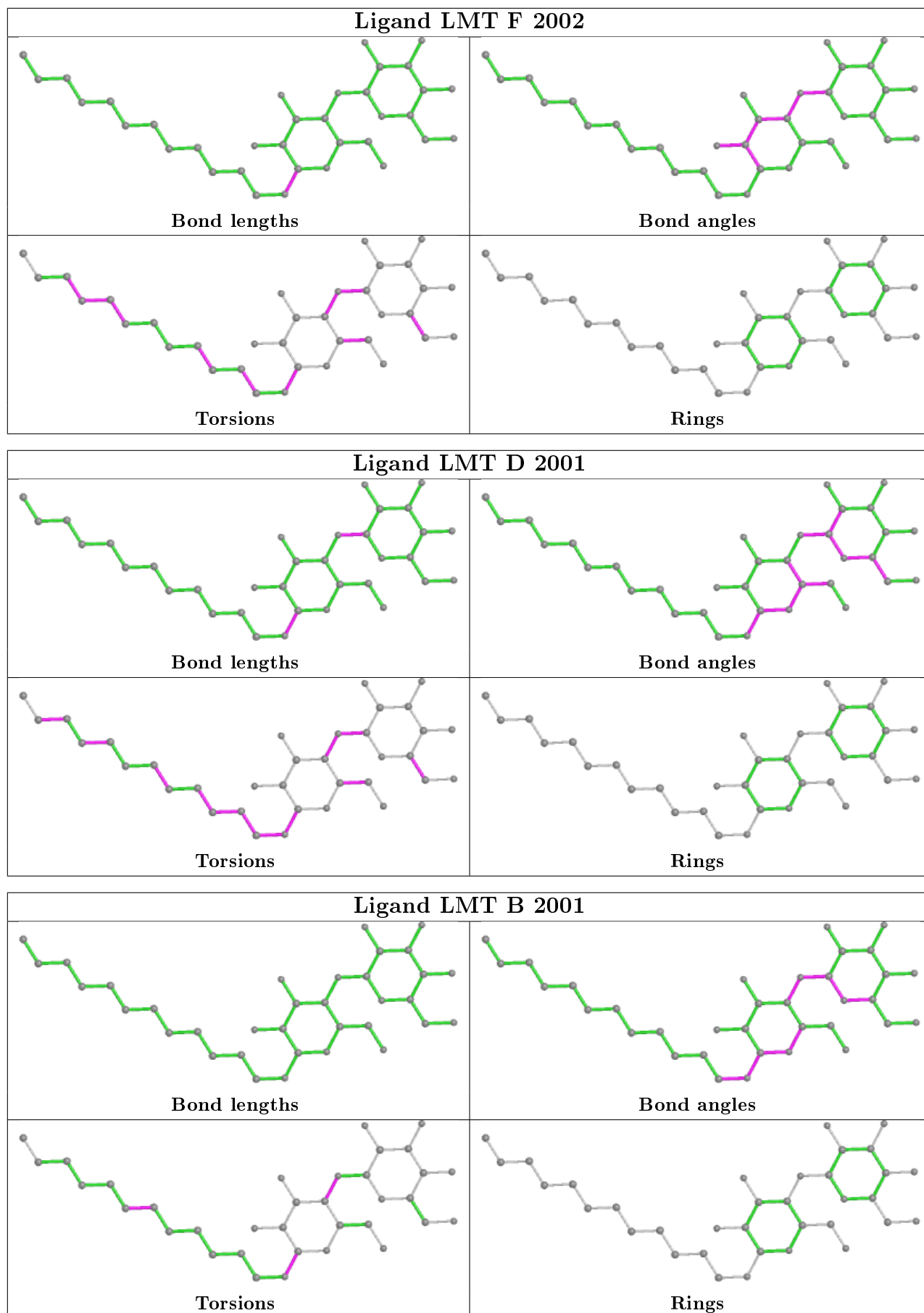
There are no ring outliers.

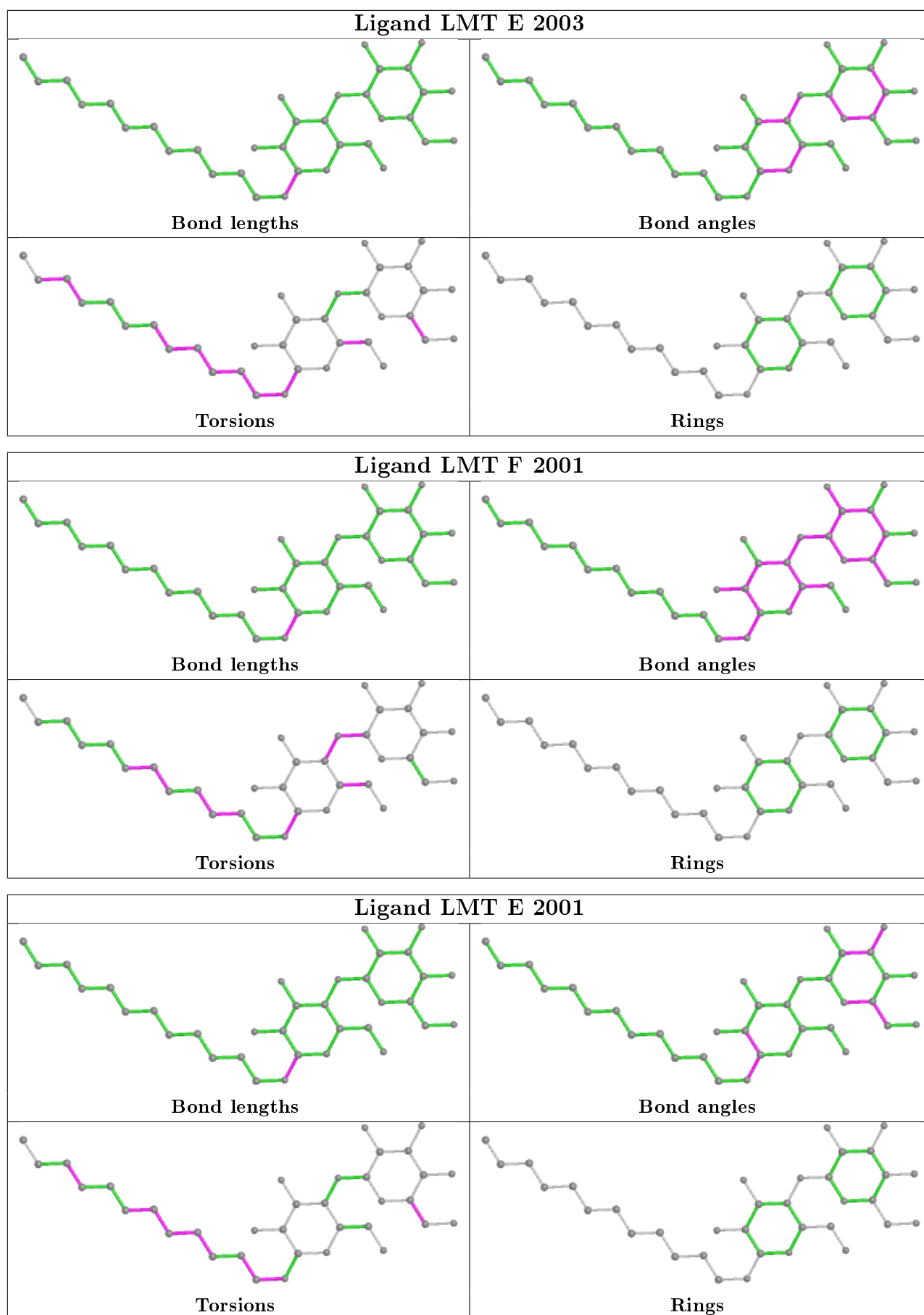
15 monomers are involved in 113 short contacts:

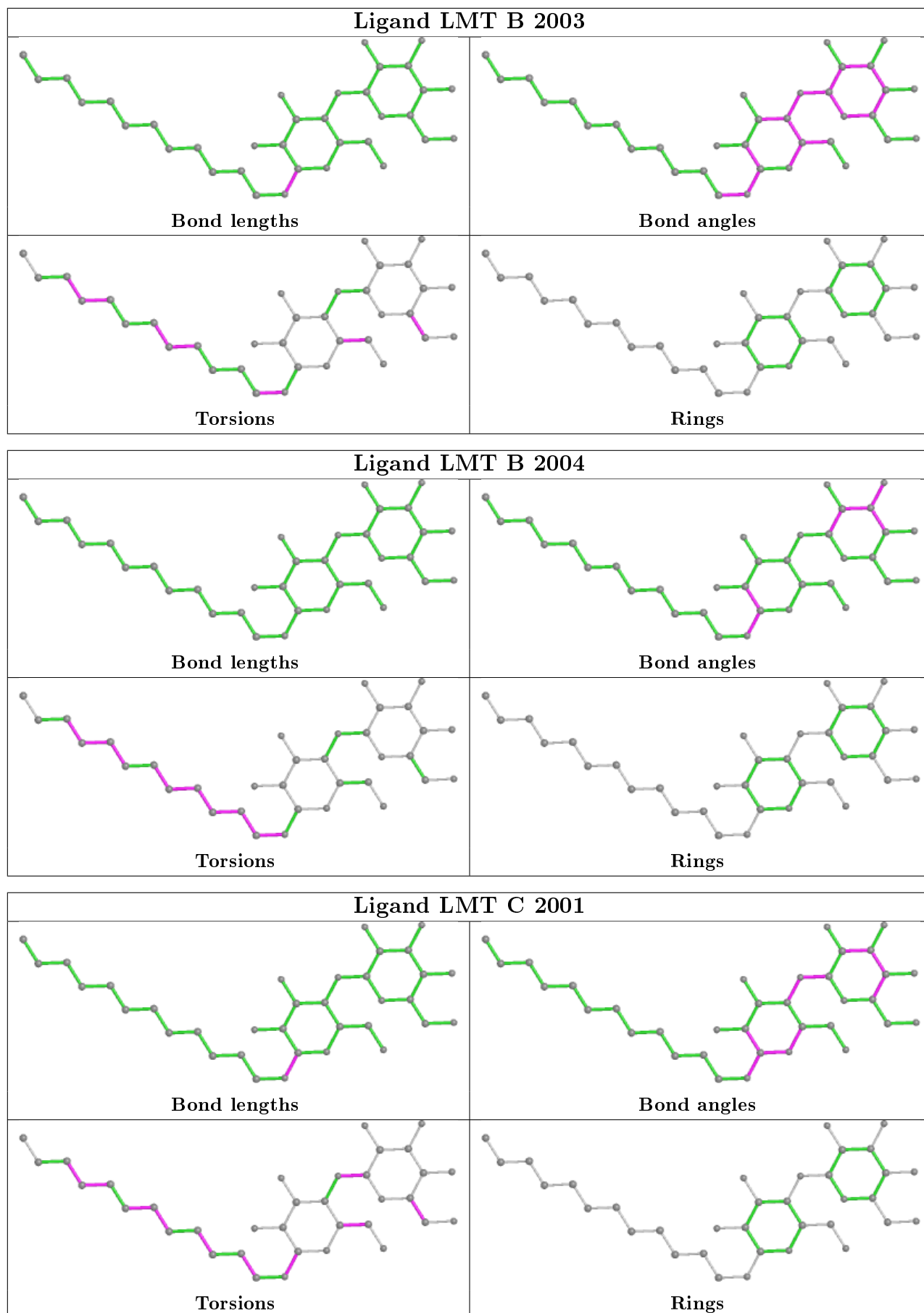
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2002	LMT	1	0
2	D	2002	LMT	3	0
2	A	1102	LMT	6	0
2	F	2002	LMT	2	0
2	D	2001	LMT	9	0
2	B	2001	LMT	18	0
2	F	2001	LMT	6	0
2	E	2001	LMT	21	0
2	B	2003	LMT	5	0
2	B	2004	LMT	4	0
2	C	2001	LMT	4	0
2	E	2002	LMT	23	0
2	C	2002	LMT	14	0
2	D	2003	LMT	2	0
2	A	1101	LMT	6	0

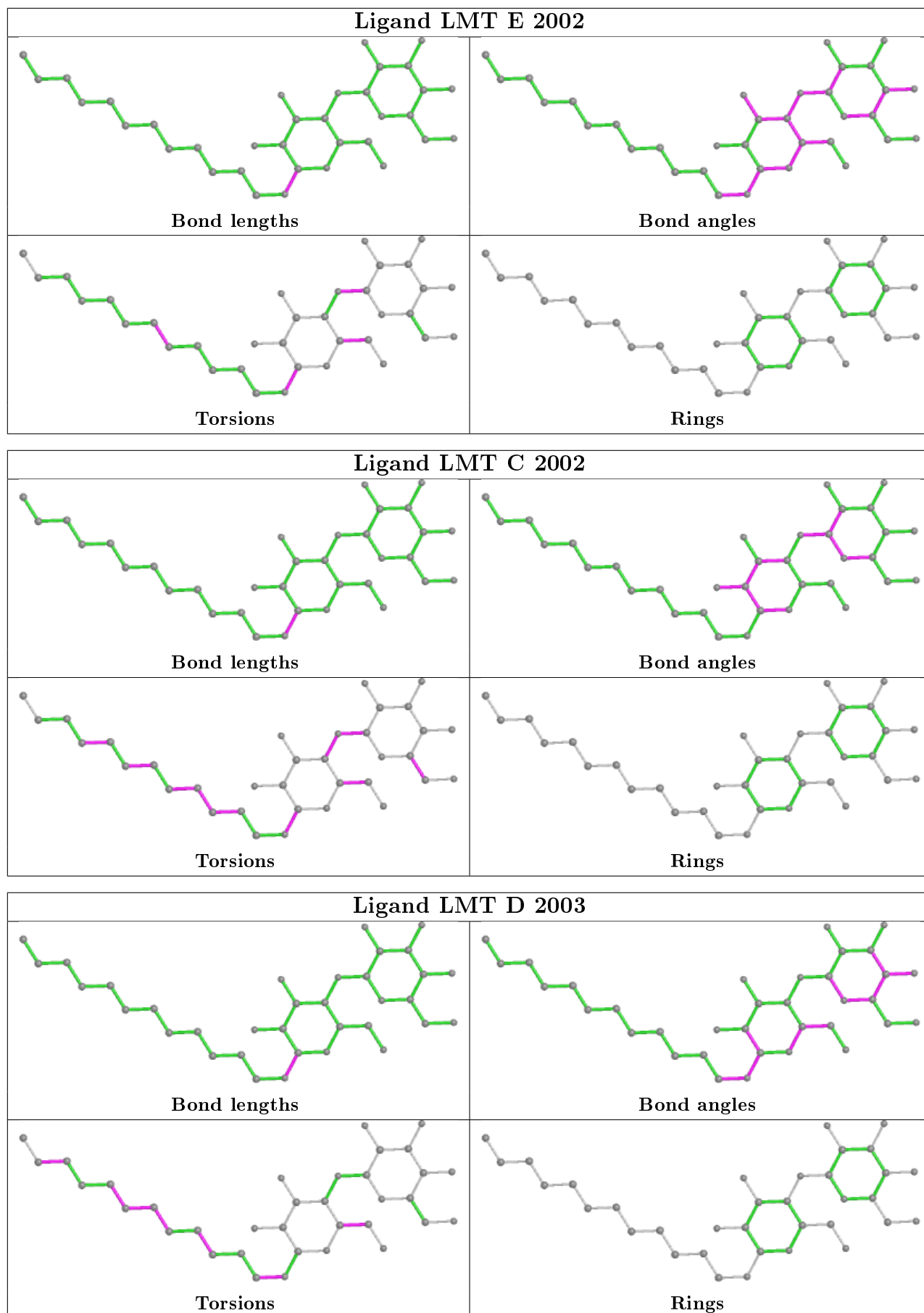
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

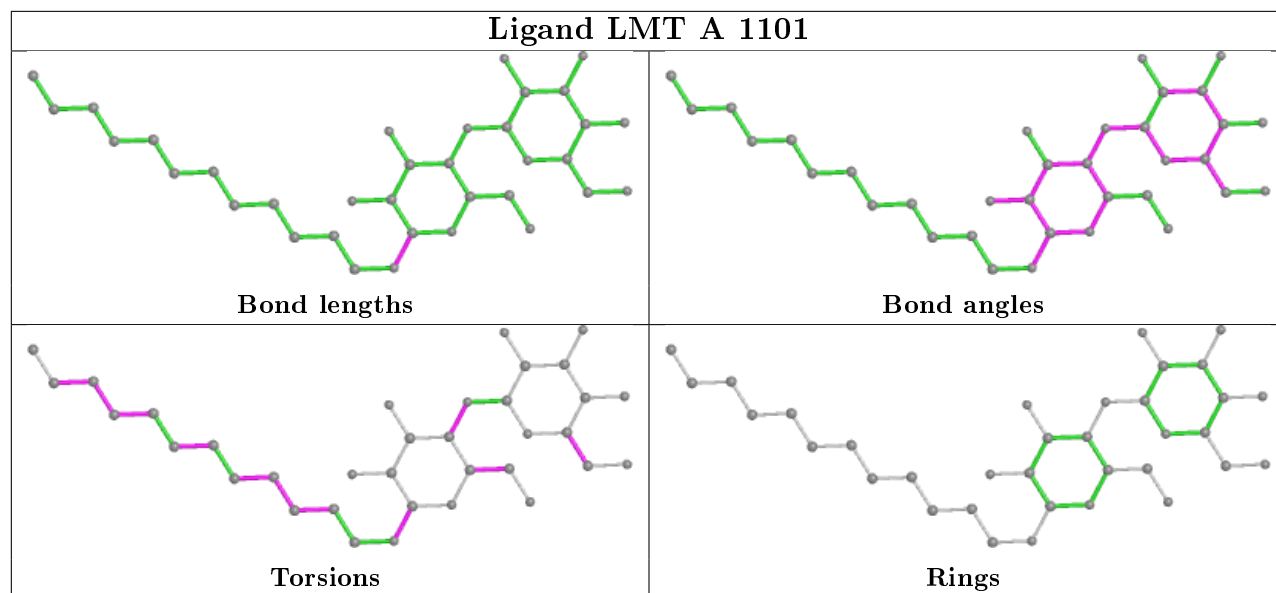












5.7 Other polymers [i](#)

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	1017/1046 (97%)	0.90	140 (13%) 2 2	32, 75, 118, 160	0
1	B	1030/1046 (98%)	0.87	127 (12%) 4 3	29, 69, 112, 139	0
1	C	1030/1046 (98%)	1.03	184 (17%) 1 1	38, 77, 131, 172	0
1	D	1020/1046 (97%)	0.88	147 (14%) 2 1	29, 77, 121, 165	0
1	E	1030/1046 (98%)	0.94	171 (16%) 1 1	37, 83, 126, 159	0
1	F	1033/1046 (98%)	1.07	199 (19%) 1 0	39, 78, 132, 178	0
All	All	6160/6276 (98%)	0.95	968 (15%) 2 1	29, 76, 125, 178	0

The worst 5 of 968 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	742	LEU	14.4
1	C	738	LEU	11.7
1	E	599	LEU	10.1
1	B	253	VAL	9.9
1	E	774	GLY	9.8

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 carbohydrates in this entry.

6.4 Ligands

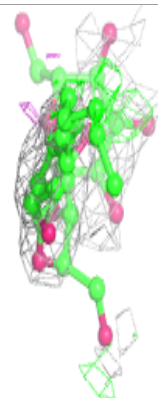
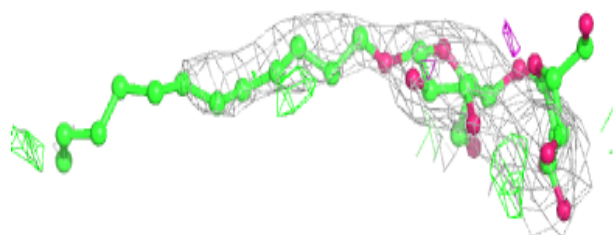
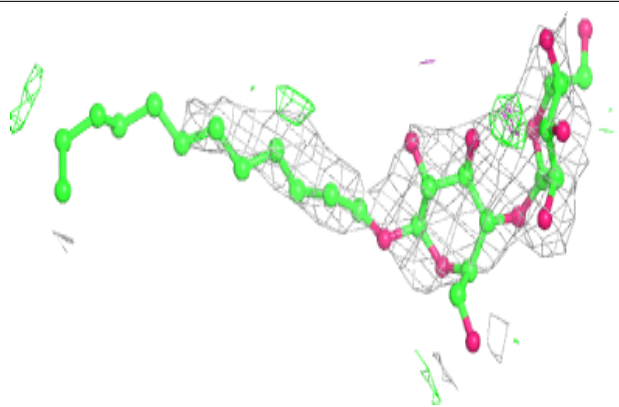
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	LMT	D	2001	35/35	0.62	0.55	47,65,79,89	35
2	LMT	B	2002	35/35	0.64	0.41	63,106,135,137	0
2	LMT	B	2001	35/35	0.65	0.36	75,97,124,139	0
2	LMT	F	2002	35/35	0.66	0.39	76,118,147,148	0
2	LMT	E	2003	35/35	0.66	0.36	67,94,108,124	0
2	LMT	F	2001	35/35	0.69	0.38	82,104,126,139	0
2	LMT	C	2002	35/35	0.69	0.36	80,105,146,151	0
2	LMT	E	2002	35/35	0.71	0.38	67,106,124,132	0
2	LMT	D	2002	35/35	0.72	0.35	69,111,137,144	0
2	LMT	A	1102	35/35	0.74	0.39	64,90,115,120	0
2	LMT	C	2001	35/35	0.75	0.43	43,66,94,103	0
2	LMT	D	2003	35/35	0.75	0.40	70,98,134,144	0
2	LMT	A	1101	35/35	0.80	0.37	60,86,132,142	0
2	LMT	B	2003	35/35	0.82	0.25	71,82,104,111	0
2	LMT	B	2004	35/35	0.85	0.33	62,69,78,84	0
2	LMT	E	2001	35/35	0.85	0.43	67,74,100,103	0

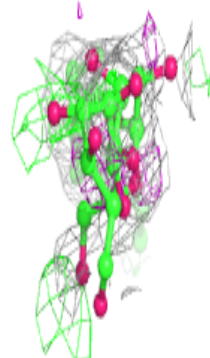
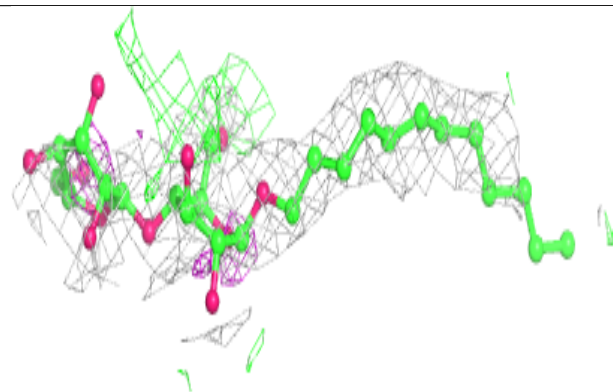
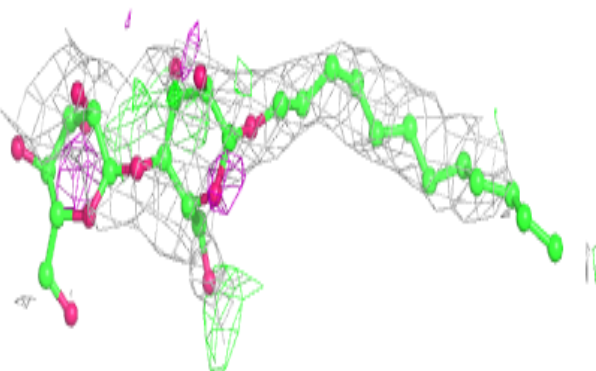
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT D 2001:

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

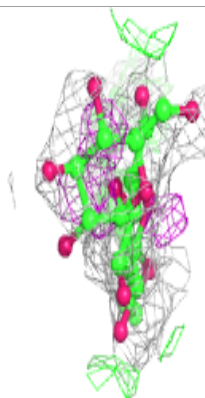
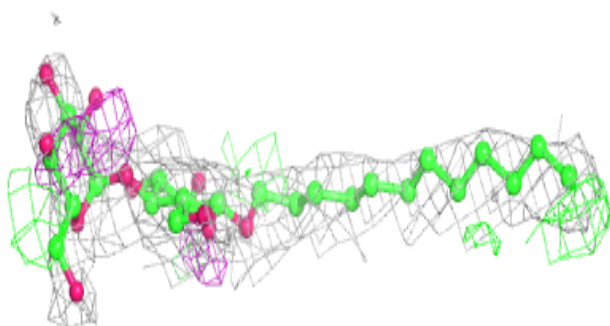
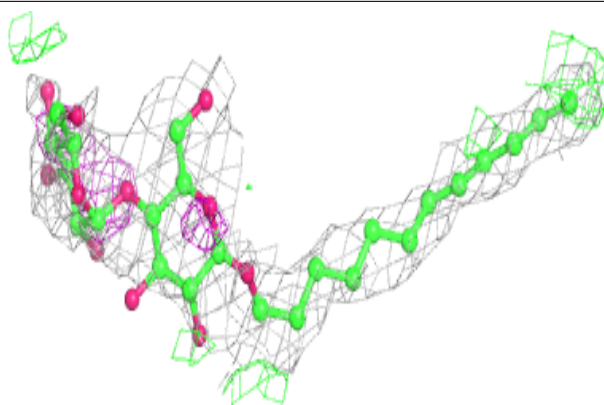
**Electron density around LMT B 2002:**

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

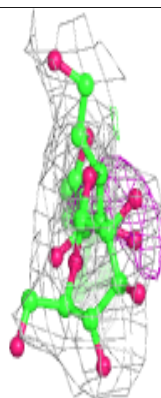
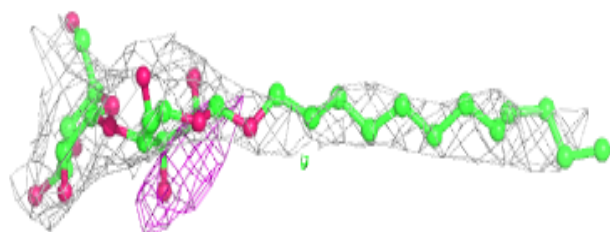
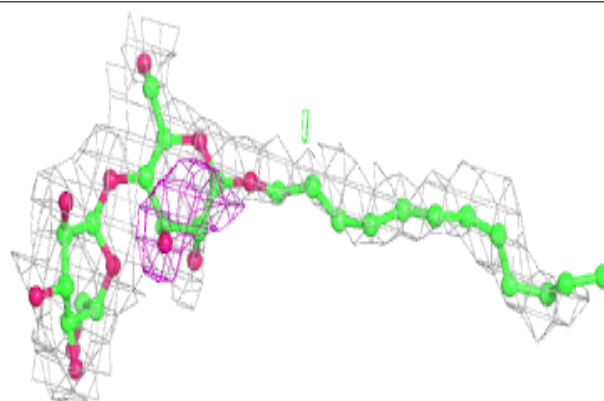


Electron density around LMT B 2001:

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

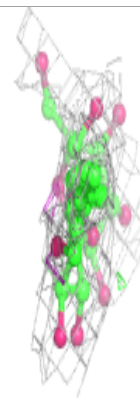
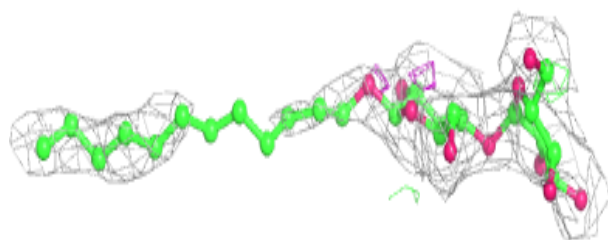
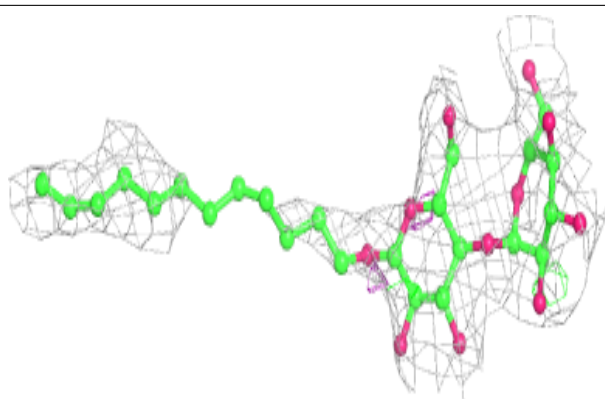
**Electron density around LMT F 2002:**

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

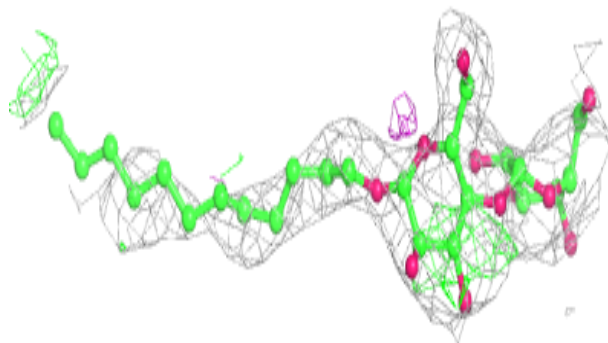
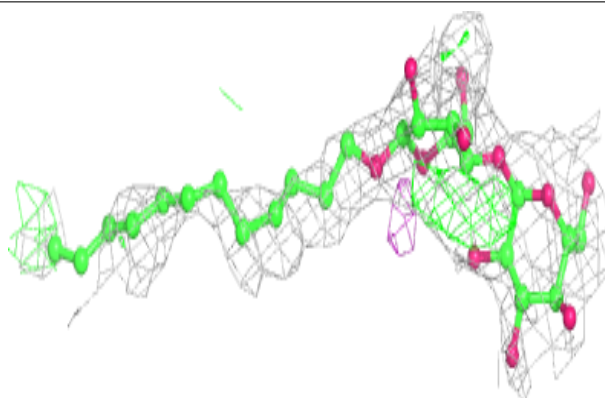


Electron density around LMT E 2003:

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

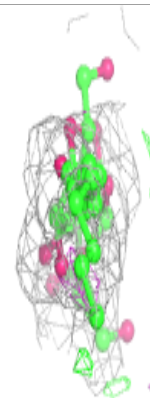
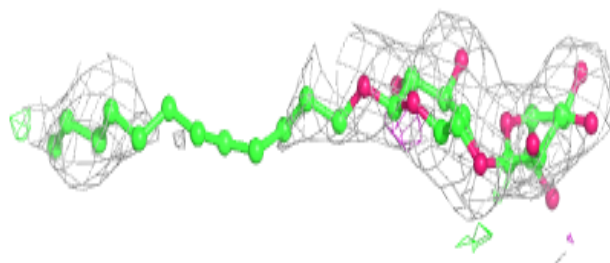
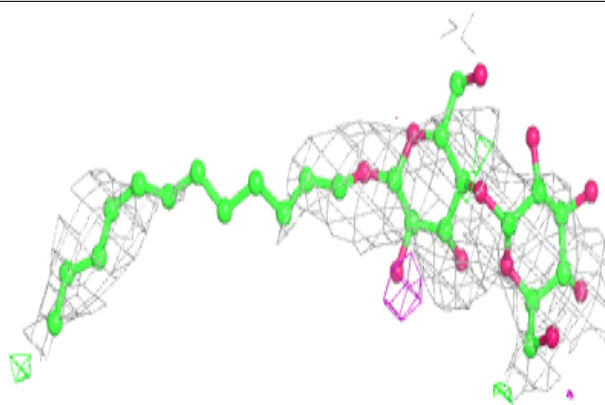
**Electron density around LMT F 2001:**

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

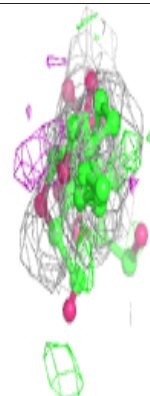
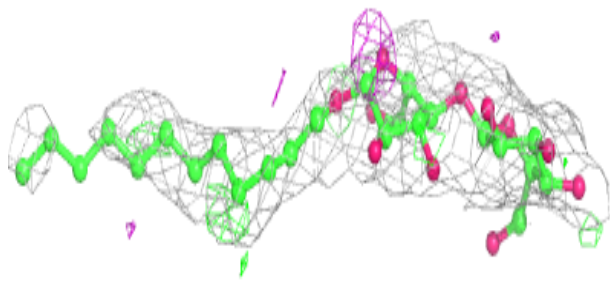
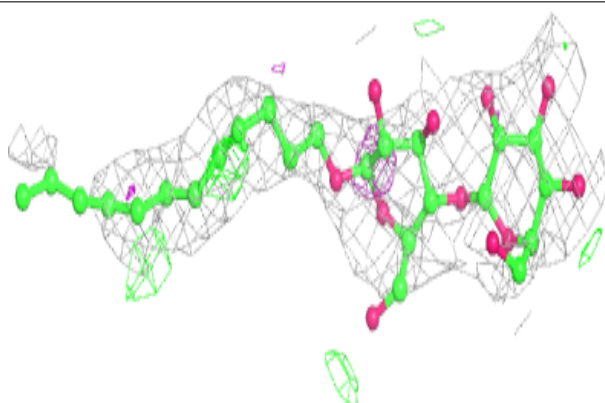


Electron density around LMT C 2002:

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

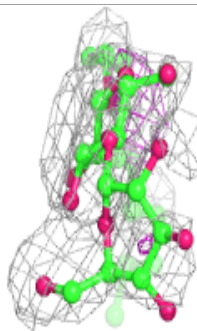
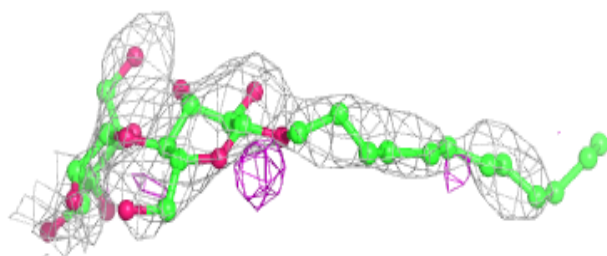
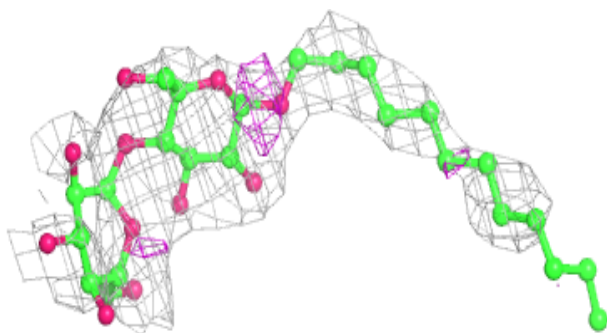
**Electron density around LMT E 2002:**

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

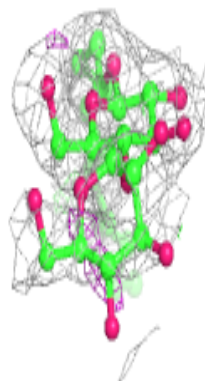
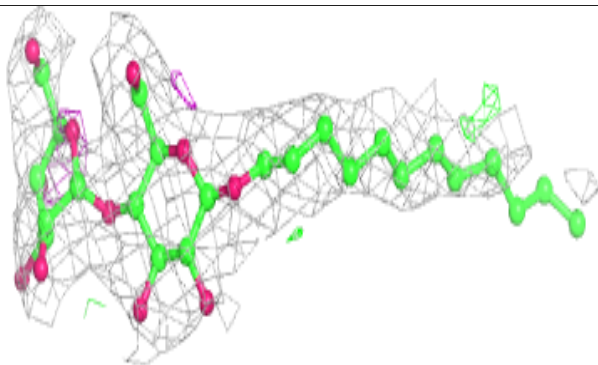
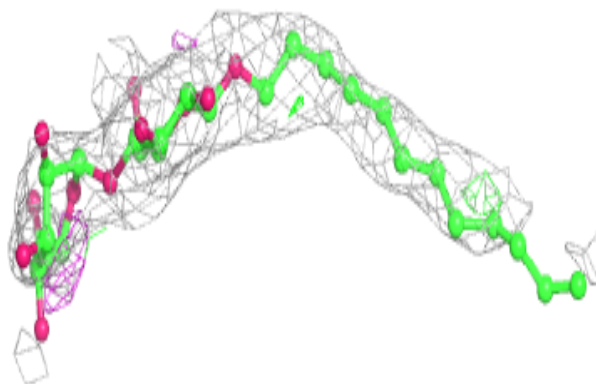


Electron density around LMT D 2002:

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

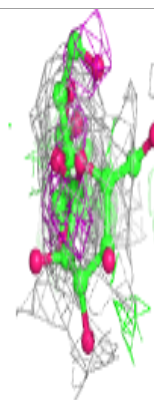
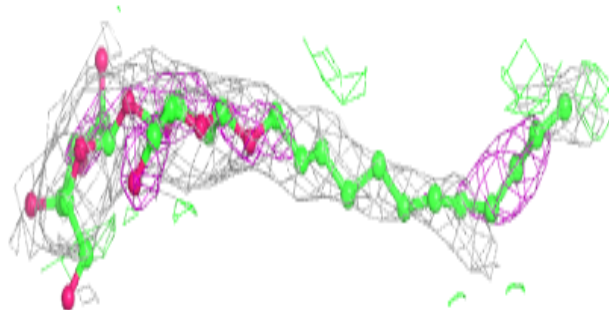
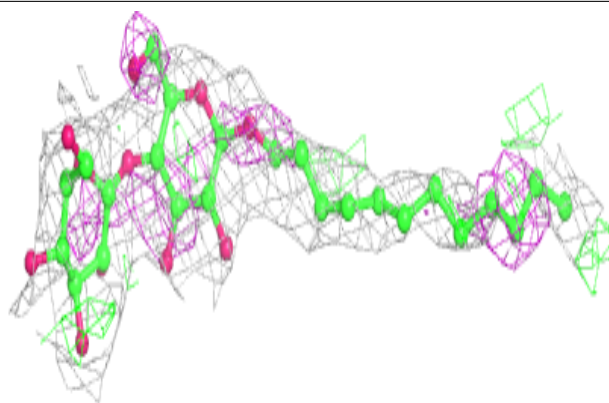
**Electron density around LMT A 1102:**

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

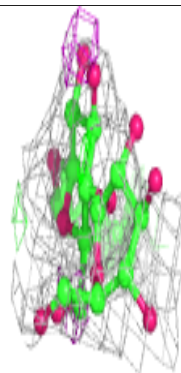
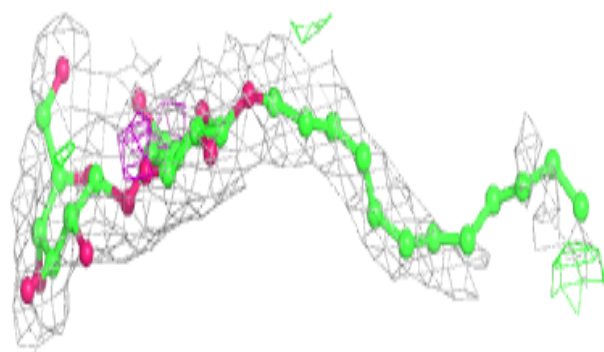
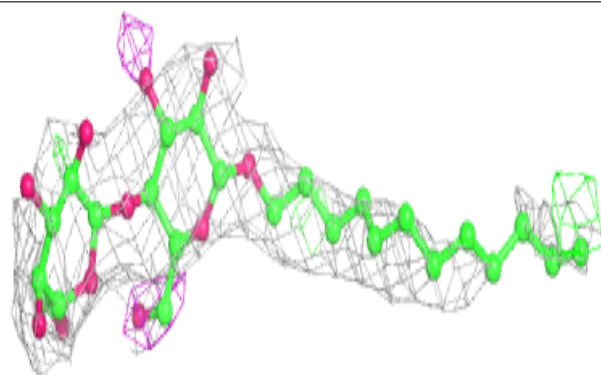


Electron density around LMT C 2001:

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

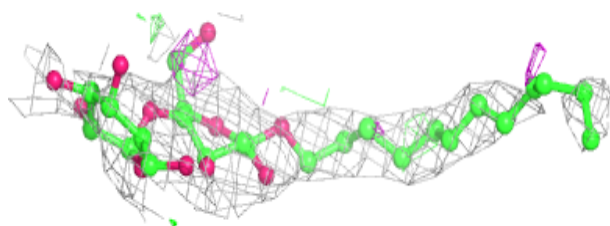
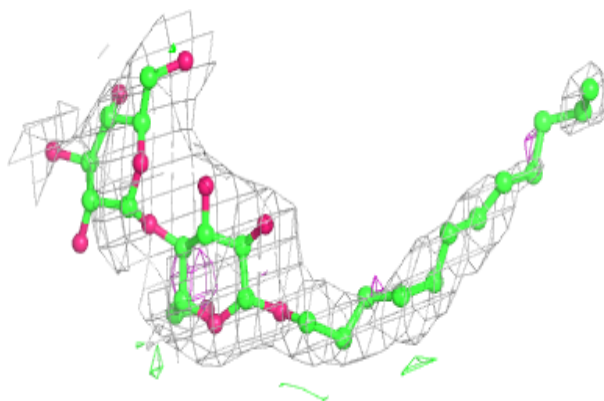
**Electron density around LMT D 2003:**

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

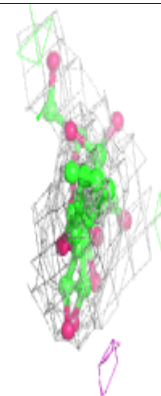
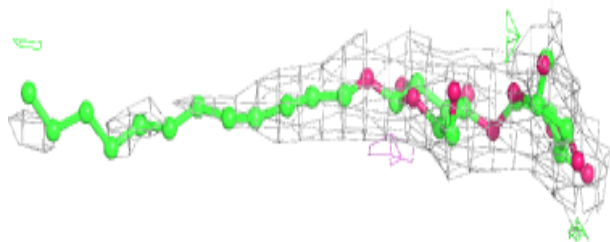
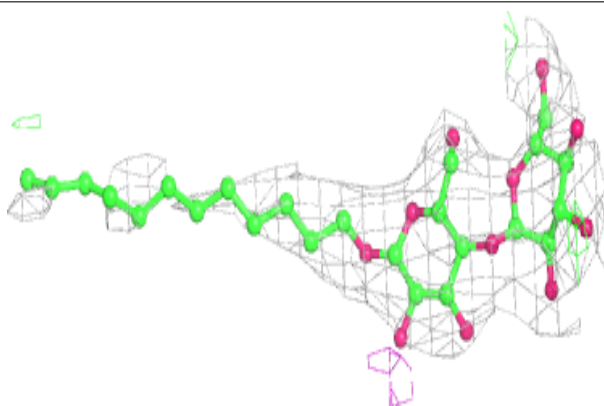


Electron density around LMT A 1101:

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

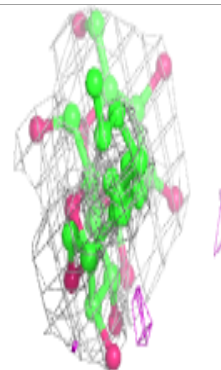
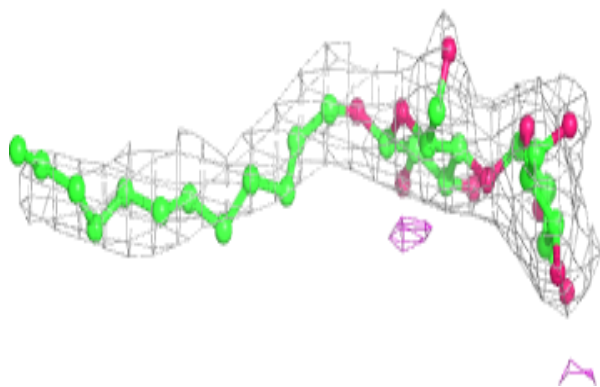
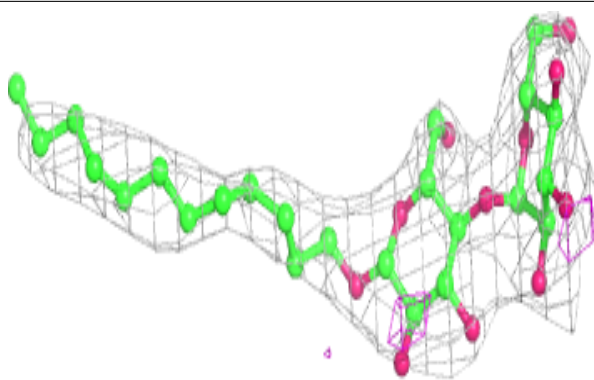
**Electron density around LMT B 2003:**

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

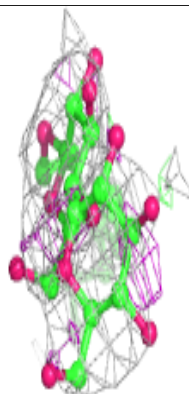
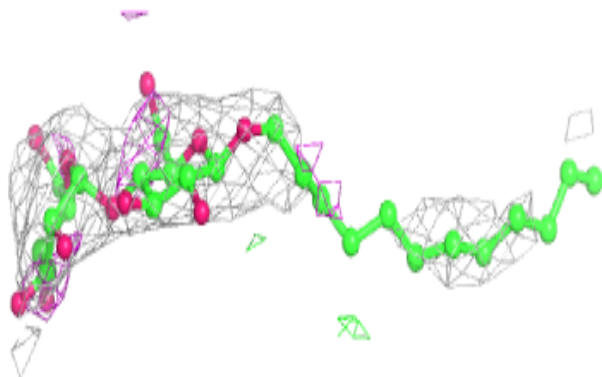
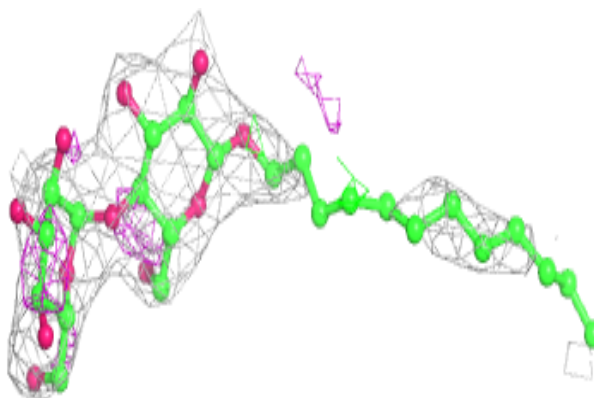


Electron density around LMT B 2004:

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

**Electron density around LMT E 2001:**

$2mF_o-DF_c$ (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.