



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 12, 2024 – 05:06 PM EDT

PDB ID : 3W9J
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 : 3.15 Å(reported)

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

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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 : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 2.36.2
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) : 2.36.2

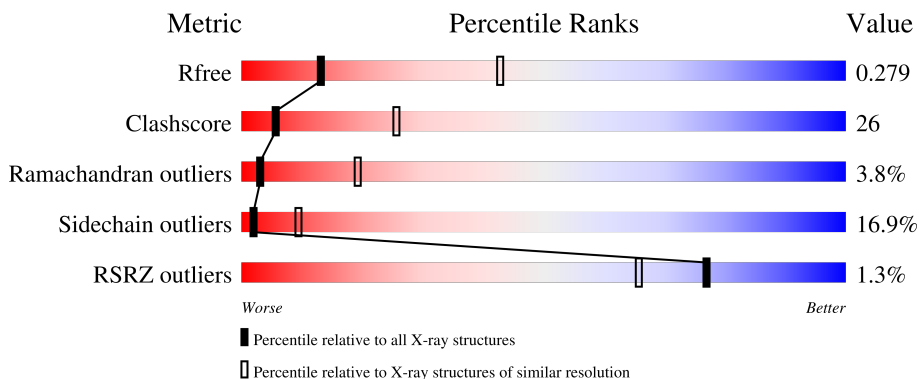
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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	1052	
1	B	1052	
1	C	1052	
1	D	1052	
1	E	1052	

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Mol	Chain	Length	Quality of chain
1	F	1052	 <p>A horizontal bar chart showing the quality of chain. The bar is divided into three segments: a green segment representing 48%, a yellow segment representing 39%, and an orange/red segment representing 11%. A small red square is at the beginning of the bar, and a small black dot is at the end.</p>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LMT	D	2001	-	-	-	X

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 47358 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	1018	7724	4975	1280	1429	40	0	0	0
1	B	1030	7812	5027	1298	1447	40	0	0	0
1	C	1030	7812	5027	1298	1447	40	0	0	0
1	D	1019	7735	4984	1281	1430	40	0	0	0
1	E	1030	7812	5027	1298	1447	40	0	0	0
1	F	1033	7840	5046	1302	1452	40	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

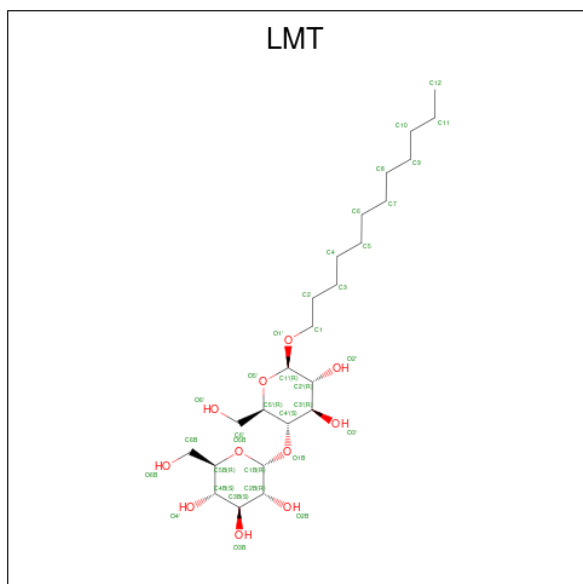
Chain	Residue	Modelled	Actual	Comment	Reference
A	1047	HIS	-	expression tag	UNP P52002
A	1048	HIS	-	expression tag	UNP P52002
A	1049	HIS	-	expression tag	UNP P52002
A	1050	HIS	-	expression tag	UNP P52002
A	1051	HIS	-	expression tag	UNP P52002
A	1052	HIS	-	expression tag	UNP P52002
B	1047	HIS	-	expression tag	UNP P52002
B	1048	HIS	-	expression tag	UNP P52002
B	1049	HIS	-	expression tag	UNP P52002
B	1050	HIS	-	expression tag	UNP P52002
B	1051	HIS	-	expression tag	UNP P52002
B	1052	HIS	-	expression tag	UNP P52002
C	1047	HIS	-	expression tag	UNP P52002
C	1048	HIS	-	expression tag	UNP P52002
C	1049	HIS	-	expression tag	UNP P52002
C	1050	HIS	-	expression tag	UNP P52002
C	1051	HIS	-	expression tag	UNP P52002

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1052	HIS	-	expression tag	UNP P52002
D	1047	HIS	-	expression tag	UNP P52002
D	1048	HIS	-	expression tag	UNP P52002
D	1049	HIS	-	expression tag	UNP P52002
D	1050	HIS	-	expression tag	UNP P52002
D	1051	HIS	-	expression tag	UNP P52002
D	1052	HIS	-	expression tag	UNP P52002
E	1047	HIS	-	expression tag	UNP P52002
E	1048	HIS	-	expression tag	UNP P52002
E	1049	HIS	-	expression tag	UNP P52002
E	1050	HIS	-	expression tag	UNP P52002
E	1051	HIS	-	expression tag	UNP P52002
E	1052	HIS	-	expression tag	UNP P52002
F	1047	HIS	-	expression tag	UNP P52002
F	1048	HIS	-	expression tag	UNP P52002
F	1049	HIS	-	expression tag	UNP P52002
F	1050	HIS	-	expression tag	UNP P52002
F	1051	HIS	-	expression tag	UNP P52002
F	1052	HIS	-	expression tag	UNP P52002

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



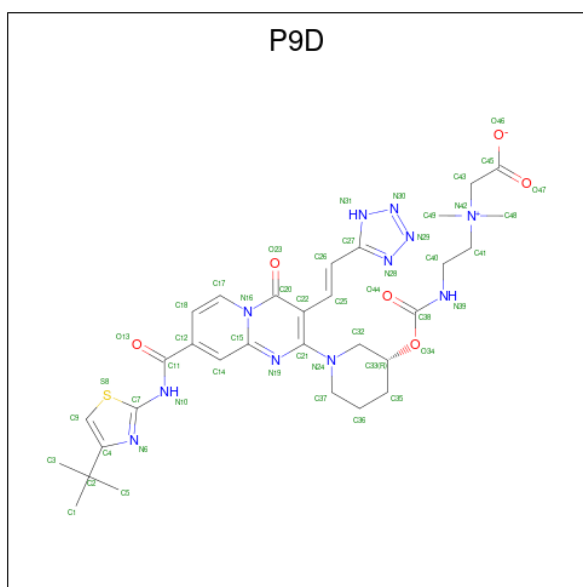
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	C O	0	0
			35	24 11		

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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	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 [{2-[(3R)-1-{8-[4-tert-butyl-1,3-thiazol-2-yl]carbamoyl}-4-oxo-3-(E)-2-(1H-tetrazol-5-yl)ethenyl]-4H-pyrido[1,2-a]pyrimidin-2-yl}piperidin-3-yl]oxy}carbonyl]amino]ethyl} (dimethyl)ammonio]acetate (three-letter code: P9D) (formula: C₃₁H₃₉N₁₁O₆S).

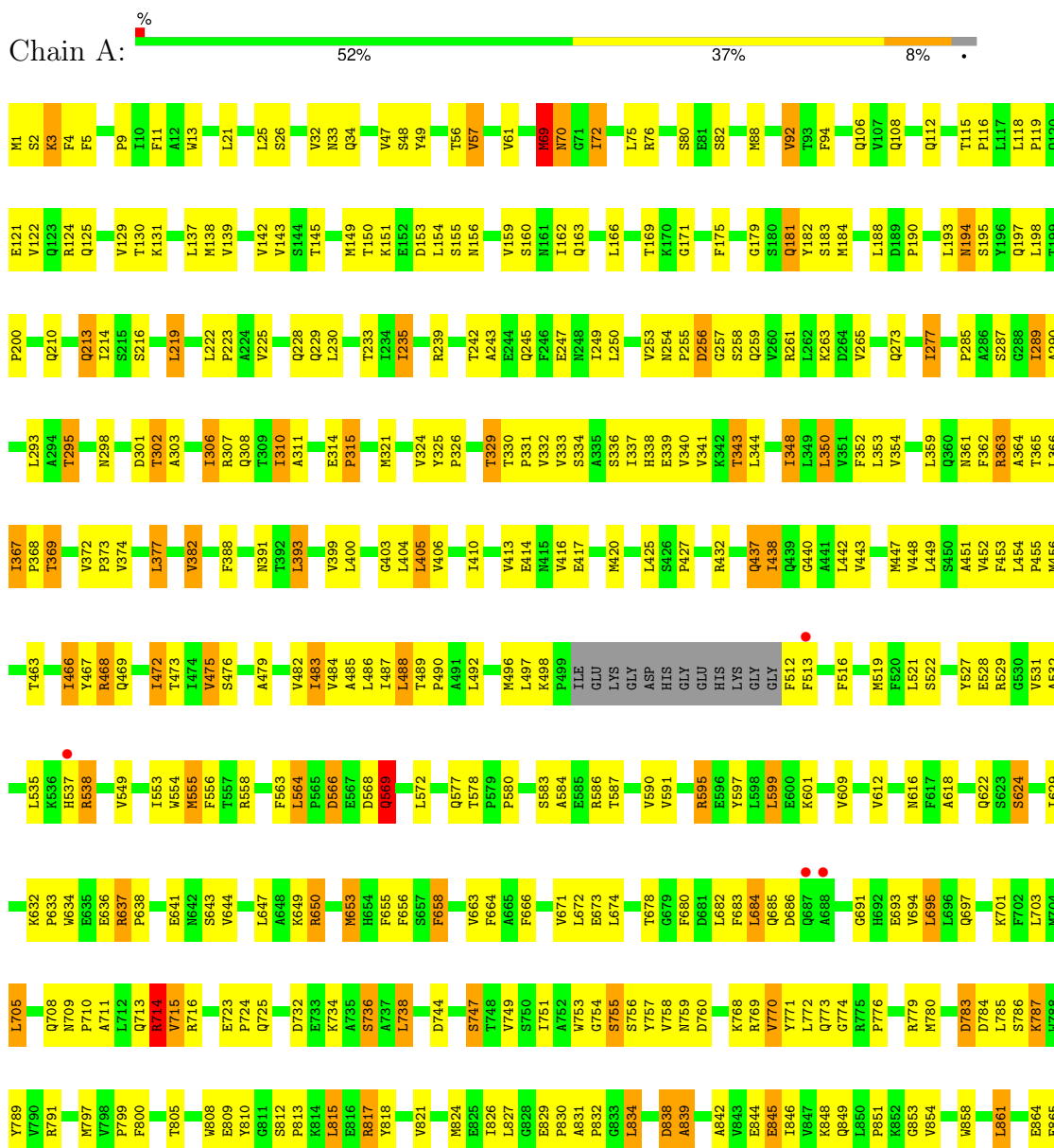


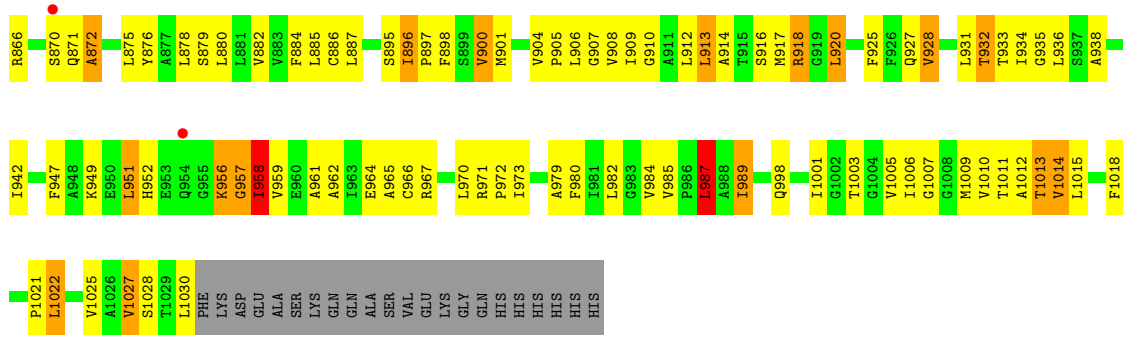
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			S
3	B	1	49	31	11	6	1	0	0
3	E	1	49	31	11	6	1	0	0

3 Residue-property plots

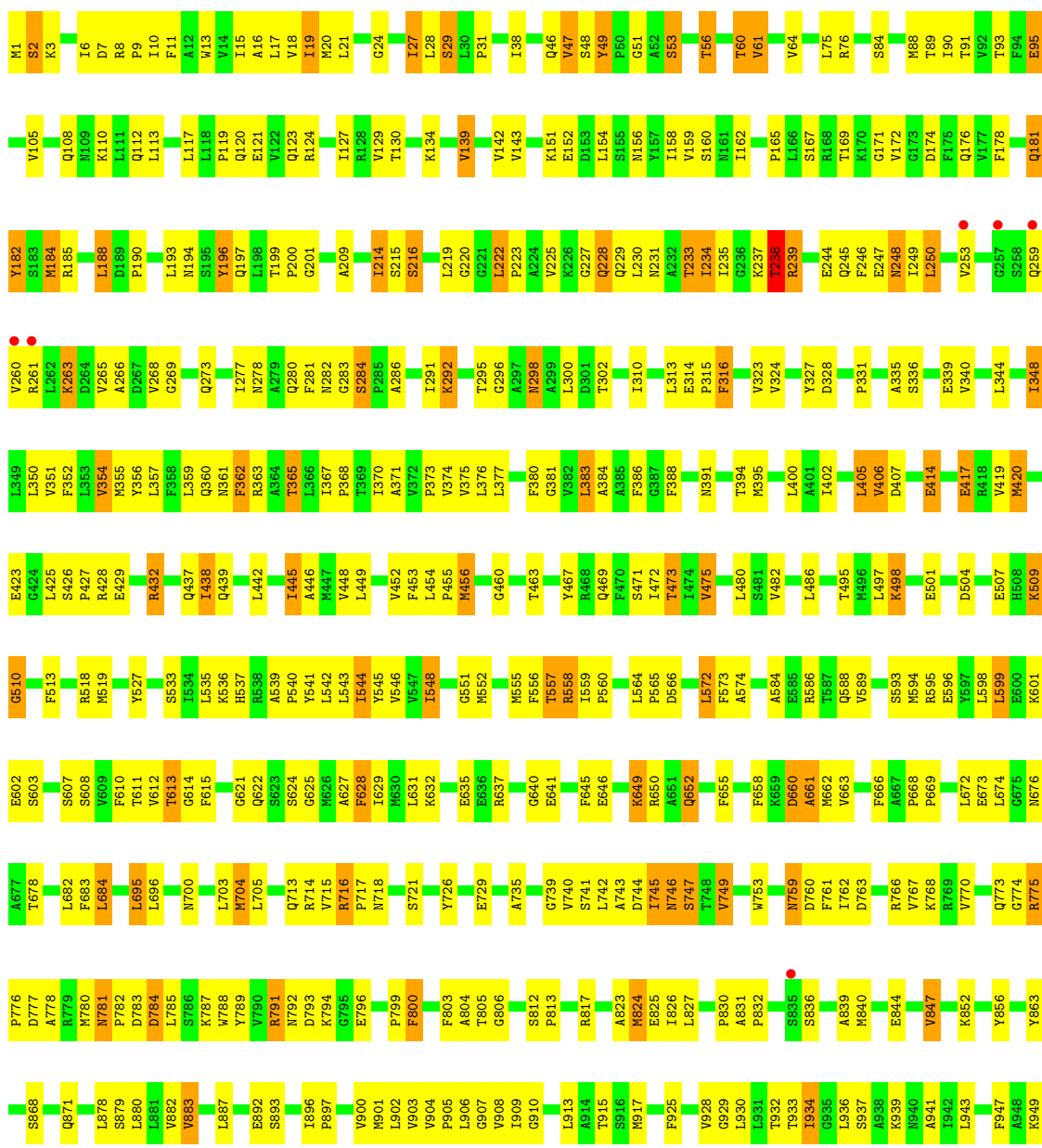
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

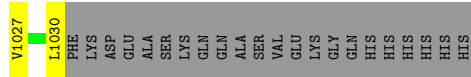
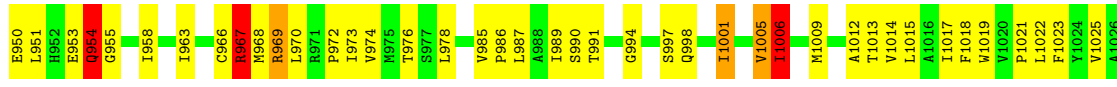
- Molecule 1: Multidrug resistance protein MexB



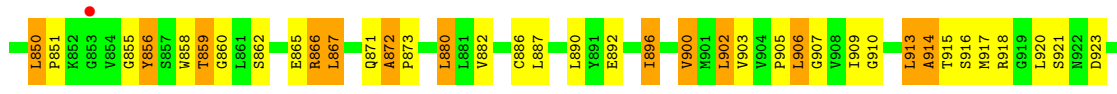
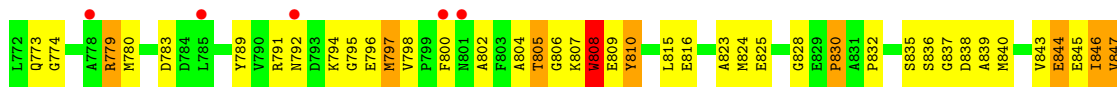
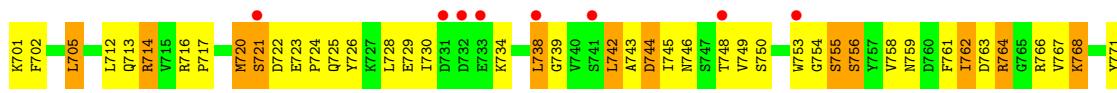
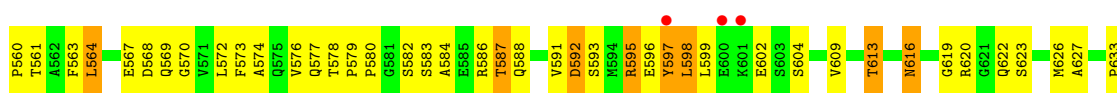
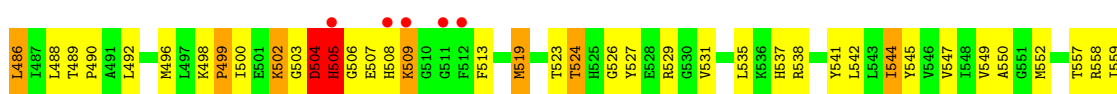
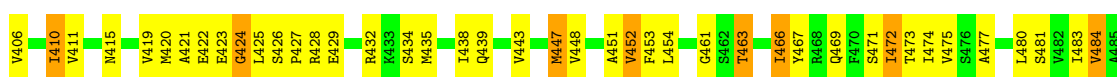
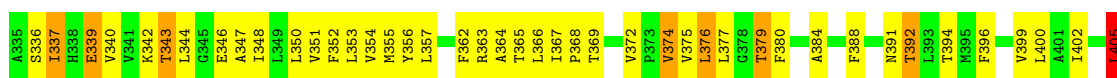
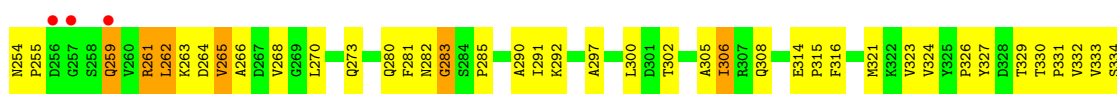
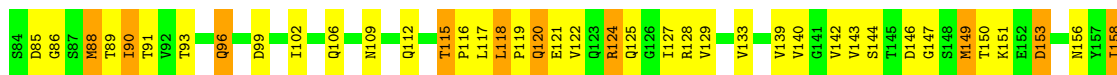
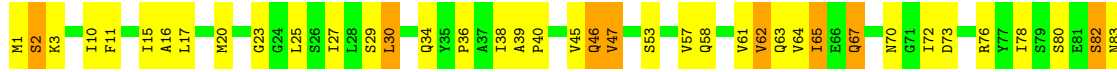


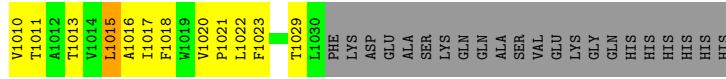
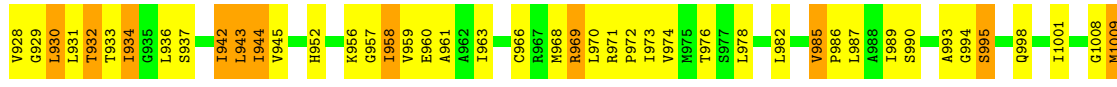
● Molecule 1: Multidrug resistance protein MexB



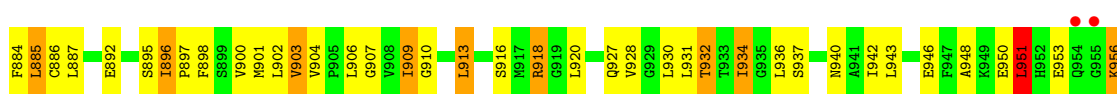
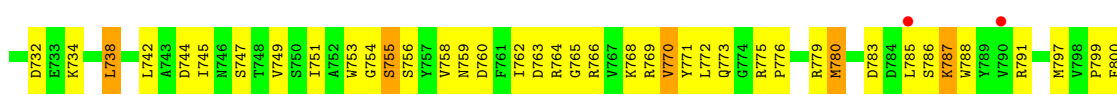
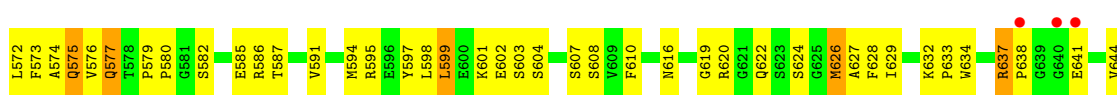
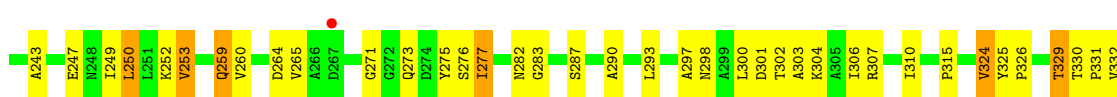
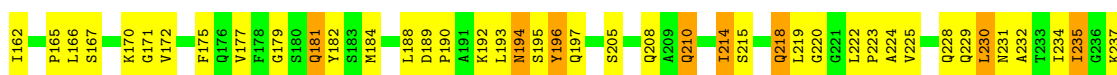
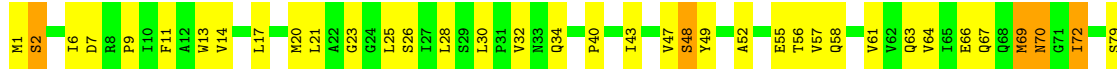


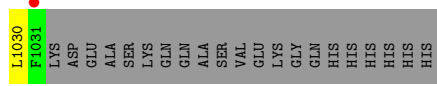
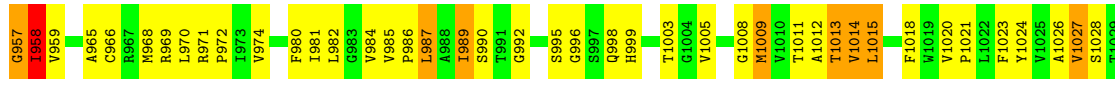
• Molecule 1: Multidrug resistance protein MexB



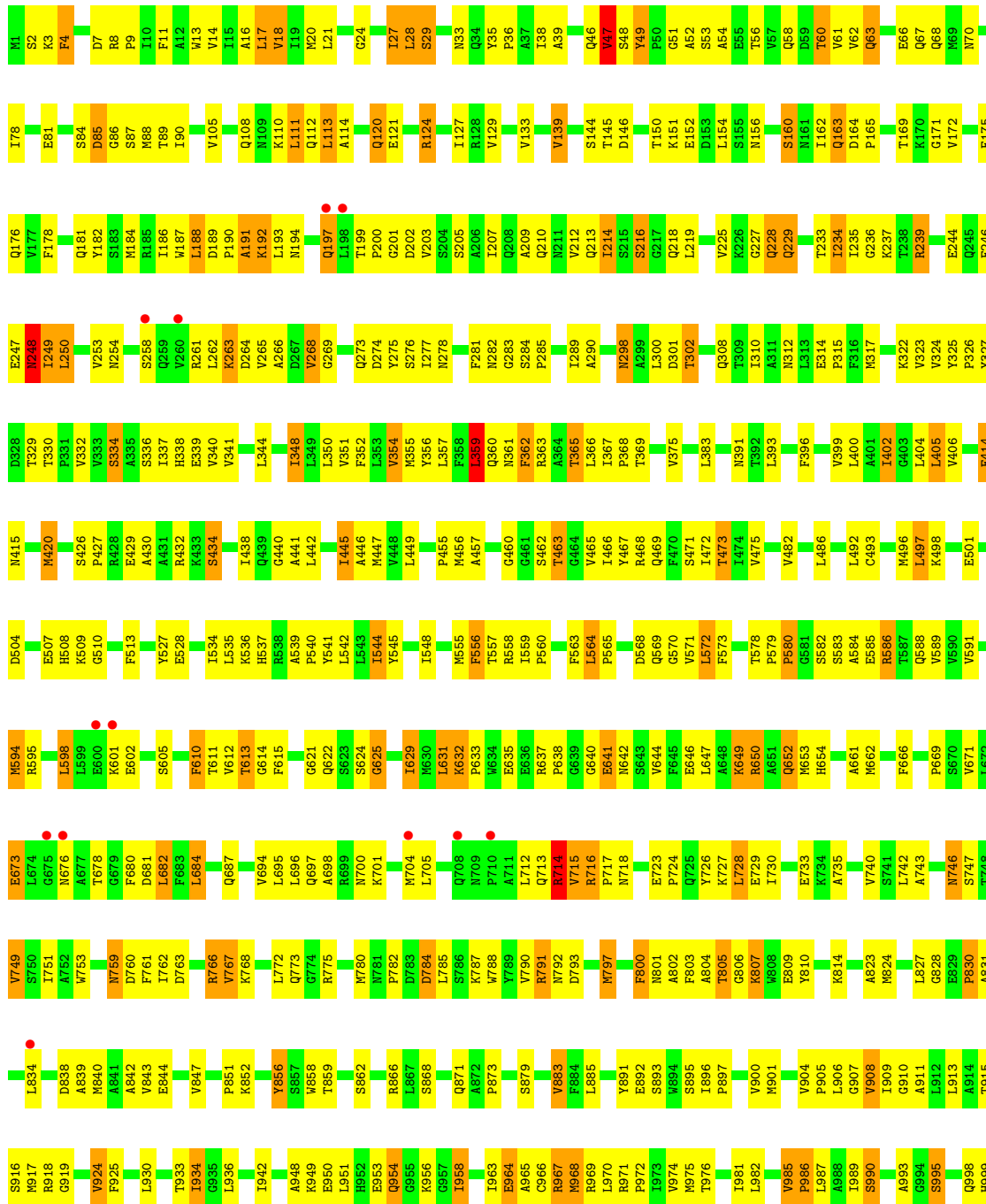


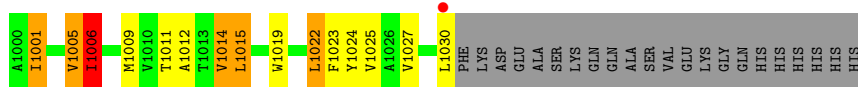
● Molecule 1: Multidrug resistance protein MexB



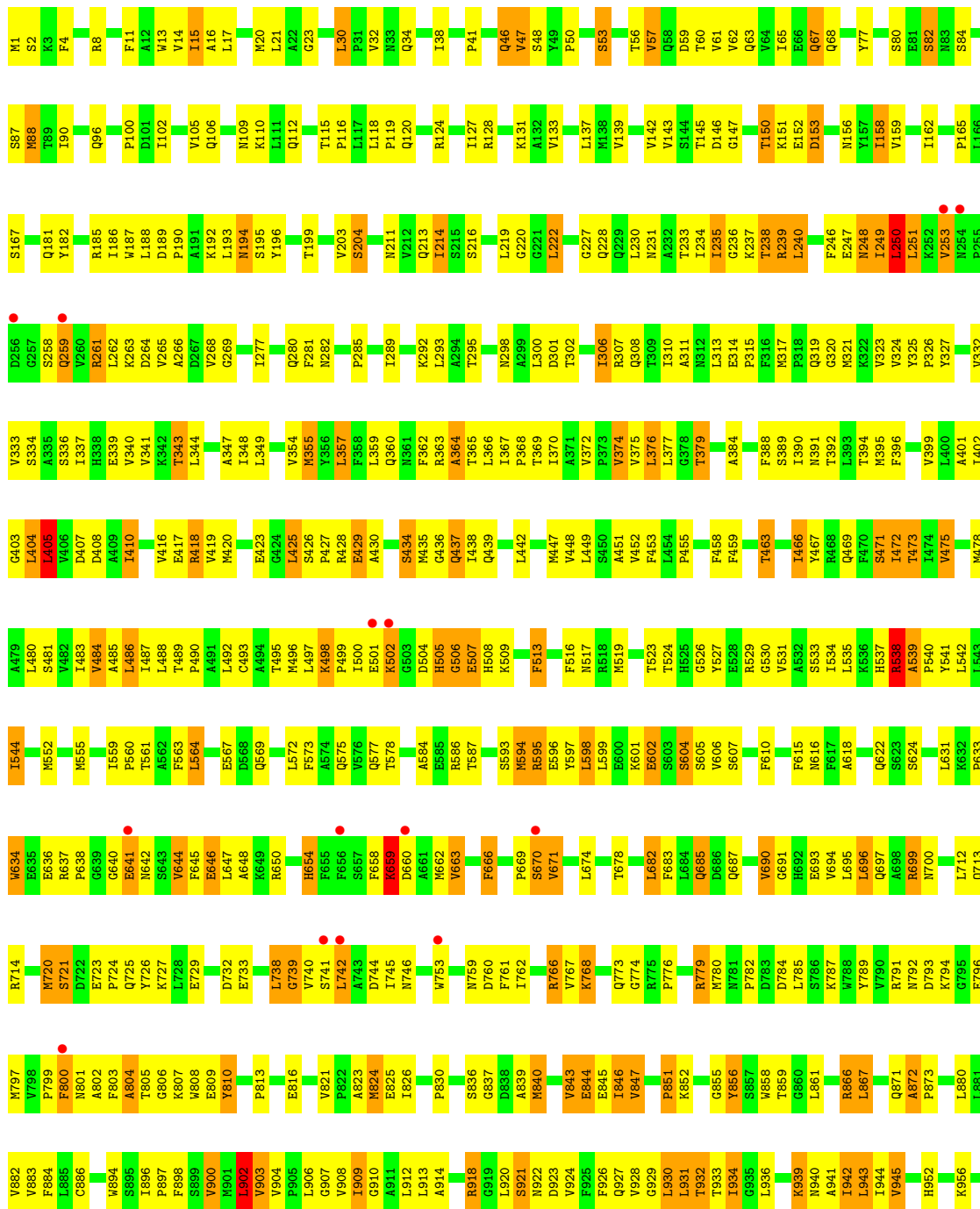


• Molecule 1: Multidrug resistance protein MexB





• Molecule 1: Multidrug resistance protein MexB



V959	GLU
I963	LYS
C966	GLY
R969	GLN
L970	HIS
R971	HIS
P972	HIS
I973	HIS
L978	HIS
L982	HIS
V985	HIS
P986	HIS
L987	HIS
A988	HIS
I989	HIS
S990	HIS
T991	HIS
G992	HIS
A993	HIS
G996	HIS
S997	HIS
Q998	HIS
I1006	HIS
G1007	HIS
G1008	HIS
M1009	HIS
V1010	HIS
T1011	HIS
L1015	HIS
F1018	HIS
W1019	HIS
V1020	HIS
P1021	HIS
L1022	HIS
F1023	HIS
Y1024	HIS
V1025	HIS
L1030	HIS
D1033	GLU
	ALA
	SER
	LYS
	GLN
	GLN
	ALA
	SER
	VAL

GLU
LYS
GLY
GLN
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	126.20Å 137.03Å 152.28Å 85.75° 68.93° 87.39°	Depositor
Resolution (Å)	42.19 – 3.15 42.19 – 3.15	Depositor EDS
% Data completeness (in resolution range)	97.3 (42.19-3.15) 97.4 (42.19-3.15)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 3.12Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.202 , 0.279 0.202 , 0.279	Depositor DCC
R_{free} test set	7980 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	80.1	Xtrriage
Anisotropy	0.052	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 59.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	47358	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: P9D, 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	0.55	0/7880	0.81	4/10712 (0.0%)
1	B	0.54	0/7971	0.79	0/10833
1	C	0.51	0/7971	0.78	3/10833 (0.0%)
1	D	0.52	0/7892	0.79	6/10728 (0.1%)
1	E	0.53	0/7971	0.79	3/10833 (0.0%)
1	F	0.53	0/8000	0.80	6/10871 (0.1%)
All	All	0.53	0/47685	0.79	22/64810 (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
1	D	0	2
All	All	0	3

There are no bond length outliers.

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	405	LEU	CA-CB-CG	8.26	134.30	115.30
1	D	705	LEU	CA-CB-CG	7.54	132.64	115.30
1	E	359	LEU	CA-CB-CG	7.48	132.51	115.30
1	D	405	LEU	CA-CB-CG	7.38	132.28	115.30
1	A	393	LEU	CA-CB-CG	-7.24	98.65	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	951	LEU	Peptide
1	D	691	GLY	Peptide
1	D	951	LEU	Peptide

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	7724	0	7864	375	0
1	B	7812	0	7944	395	0
1	C	7812	0	7944	484	0
1	D	7735	0	7873	417	0
1	E	7812	0	7944	421	0
1	F	7840	0	7970	439	0
2	A	105	0	138	6	0
2	B	105	0	138	5	0
2	C	35	0	46	6	0
2	D	105	0	138	5	0
2	E	105	0	138	10	0
2	F	70	0	92	7	0
3	B	49	0	39	8	0
3	E	49	0	39	8	0
All	All	47358	0	48307	2452	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 26.

The worst 5 of 2452 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:D:780:MET:CE	1:F:220:GLY:HA2	1.75	1.17
1:E:958:ILE:HD12	1:E:958:ILE:H	1.11	1.10
1:F:239:ARG:HG2	1:F:239:ARG:HH11	1.11	1.10
1:B:469:GLN:O	1:B:473:THR:HG22	1.52	1.10
1:C:239:ARG:HG2	1:C:239:ARG:HH11	0.96	1.09

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	1014/1052 (96%)	861 (85%)	122 (12%)	31 (3%)	4	23
1	B	1028/1052 (98%)	874 (85%)	127 (12%)	27 (3%)	5	28
1	C	1028/1052 (98%)	844 (82%)	129 (12%)	55 (5%)	2	12
1	D	1015/1052 (96%)	846 (83%)	130 (13%)	39 (4%)	3	19
1	E	1028/1052 (98%)	865 (84%)	127 (12%)	36 (4%)	3	21
1	F	1031/1052 (98%)	862 (84%)	125 (12%)	44 (4%)	2	17
All	All	6144/6312 (97%)	5152 (84%)	760 (12%)	232 (4%)	3	19

5 of 232 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	69	MET
1	A	70	ASN
1	A	498	LYS
1	A	673	GLU
1	A	714	ARG

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	833/860 (97%)	696 (84%)	137 (16%)	2	10
1	B	841/860 (98%)	703 (84%)	138 (16%)	2	10
1	C	841/860 (98%)	699 (83%)	142 (17%)	2	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	834/860 (97%)	696 (84%)	138 (16%)	2	10
1	E	841/860 (98%)	697 (83%)	144 (17%)	2	9
1	F	844/860 (98%)	693 (82%)	151 (18%)	2	8
All	All	5034/5160 (98%)	4184 (83%)	850 (17%)	2	9

5 of 850 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	350	LEU
1	E	111	LEU
1	F	693	GLU
1	D	414	GLU
1	D	348	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 167 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	120	GLN
1	F	176	GLN
1	E	248	ASN
1	E	652	GLN
1	F	415	ASN

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

17 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	D	2002	-	36,36,36	0.66	1 (2%)	47,47,47	1.35	4 (8%)
2	LMT	A	2001	-	36,36,36	0.76	1 (2%)	47,47,47	1.25	5 (10%)
3	P9D	B	2001	-	49,53,53	1.95	12 (24%)	52,77,77	2.15	14 (26%)
2	LMT	F	2001	-	36,36,36	0.82	1 (2%)	47,47,47	2.00	13 (27%)
2	LMT	B	2002	-	36,36,36	0.77	1 (2%)	47,47,47	1.77	11 (23%)
2	LMT	A	2003	-	36,36,36	0.69	1 (2%)	47,47,47	1.64	11 (23%)
2	LMT	C	2001	-	36,36,36	0.71	1 (2%)	47,47,47	1.32	5 (10%)
2	LMT	D	2003	-	36,36,36	0.81	1 (2%)	47,47,47	1.38	6 (12%)
2	LMT	E	2002	-	36,36,36	0.97	1 (2%)	47,47,47	1.47	9 (19%)
2	LMT	B	2004	-	36,36,36	0.48	0	47,47,47	1.02	3 (6%)
2	LMT	B	2003	-	36,36,36	0.83	1 (2%)	47,47,47	1.61	10 (21%)
2	LMT	E	2003	-	36,36,36	0.76	1 (2%)	47,47,47	1.51	5 (10%)
2	LMT	D	2001	-	36,36,36	0.94	2 (5%)	47,47,47	1.47	7 (14%)
2	LMT	F	2002	-	36,36,36	0.85	1 (2%)	47,47,47	1.36	5 (10%)
2	LMT	E	2004	-	36,36,36	0.69	1 (2%)	47,47,47	1.11	3 (6%)
2	LMT	A	2002	-	36,36,36	0.85	1 (2%)	47,47,47	1.74	15 (31%)
3	P9D	E	2001	-	49,53,53	2.01	9 (18%)	52,77,77	1.71	8 (15%)

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	D	2002	-	-	9/21/61/61	0/2/2/2
2	LMT	A	2001	-	-	14/21/61/61	0/2/2/2
3	P9D	B	2001	-	-	19/35/49/49	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LMT	F	2001	-	-	12/21/61/61	0/2/2/2
2	LMT	B	2002	-	-	12/21/61/61	0/2/2/2
2	LMT	A	2003	-	-	11/21/61/61	0/2/2/2
2	LMT	C	2001	-	-	14/21/61/61	0/2/2/2
2	LMT	D	2003	-	-	7/21/61/61	0/2/2/2
2	LMT	E	2002	-	-	10/21/61/61	0/2/2/2
2	LMT	B	2004	-	-	9/21/61/61	0/2/2/2
2	LMT	B	2003	-	-	8/21/61/61	0/2/2/2
2	LMT	E	2003	-	-	14/21/61/61	0/2/2/2
2	LMT	D	2001	-	-	16/21/61/61	0/2/2/2
2	LMT	F	2002	-	-	12/21/61/61	0/2/2/2
2	LMT	E	2004	-	-	10/21/61/61	0/2/2/2
2	LMT	A	2002	-	-	13/21/61/61	0/2/2/2
3	P9D	E	2001	-	-	18/35/49/49	1/5/5/5

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2001	P9D	O34-C38	6.54	1.46	1.35
3	B	2001	P9D	N30-N29	5.50	1.41	1.32
3	B	2001	P9D	O34-C38	5.48	1.44	1.35
3	E	2001	P9D	N30-N29	4.95	1.40	1.32
3	E	2001	P9D	N31-N30	4.38	1.41	1.35

The worst 5 of 134 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2001	P9D	C9-C4-C2	-6.65	120.64	129.11
2	B	2003	LMT	C1B-O5B-C5B	5.84	125.12	113.72
3	E	2001	P9D	C9-C4-C2	-5.63	121.94	129.11
3	B	2001	P9D	N28-C27-N31	5.55	117.45	111.45
2	F	2001	LMT	C3'-C4'-C5'	-5.13	99.55	110.93

There are no chirality outliers.

5 of 208 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2001	LMT	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
2	A	2002	LMT	C3'-C4'-O1B-C1B
2	B	2004	LMT	C2-C1-O1'-C1'
2	D	2001	LMT	C2'-C1'-O1'-C1
2	D	2001	LMT	O5'-C1'-O1'-C1

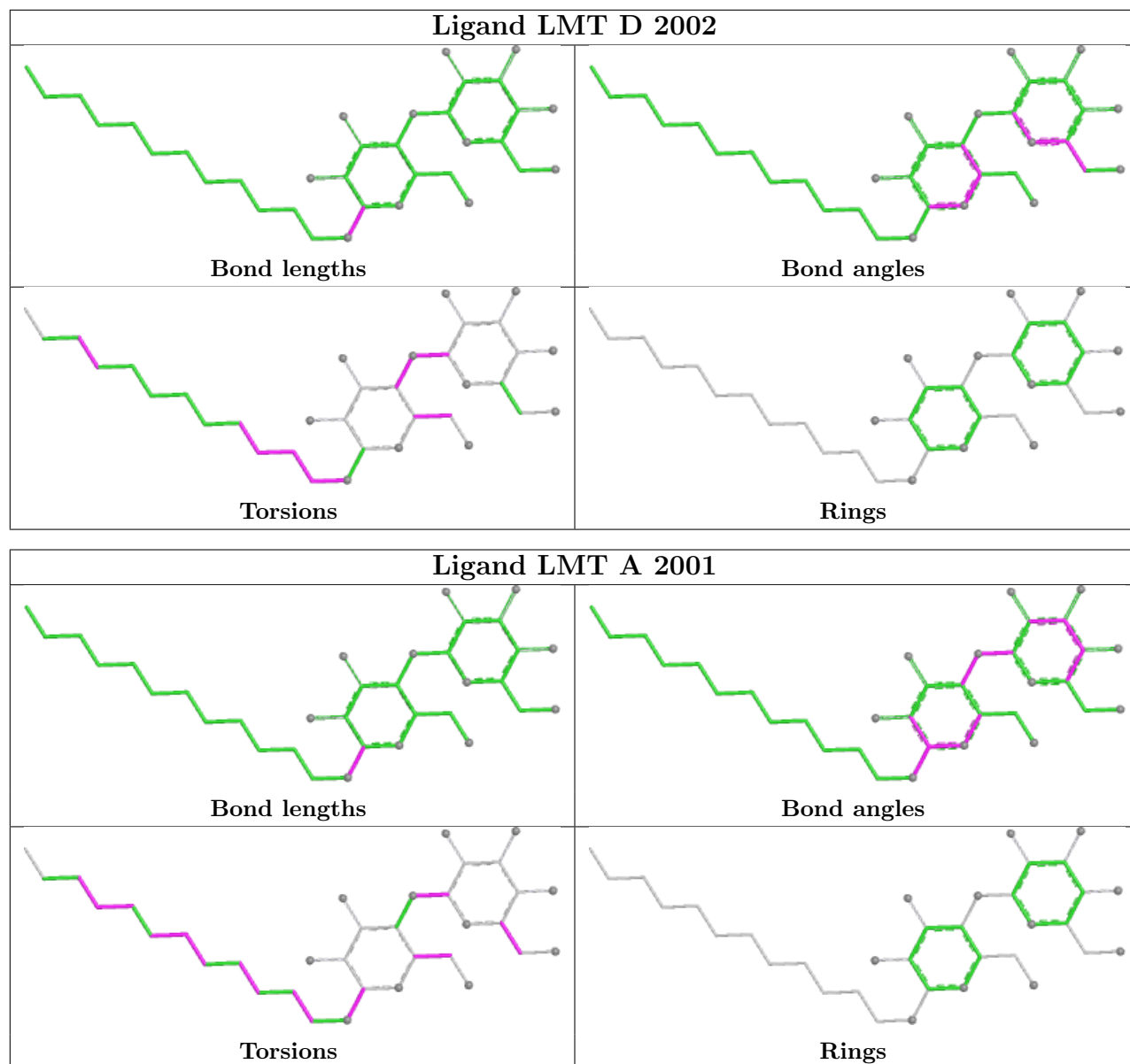
All (1) ring outliers are listed below:

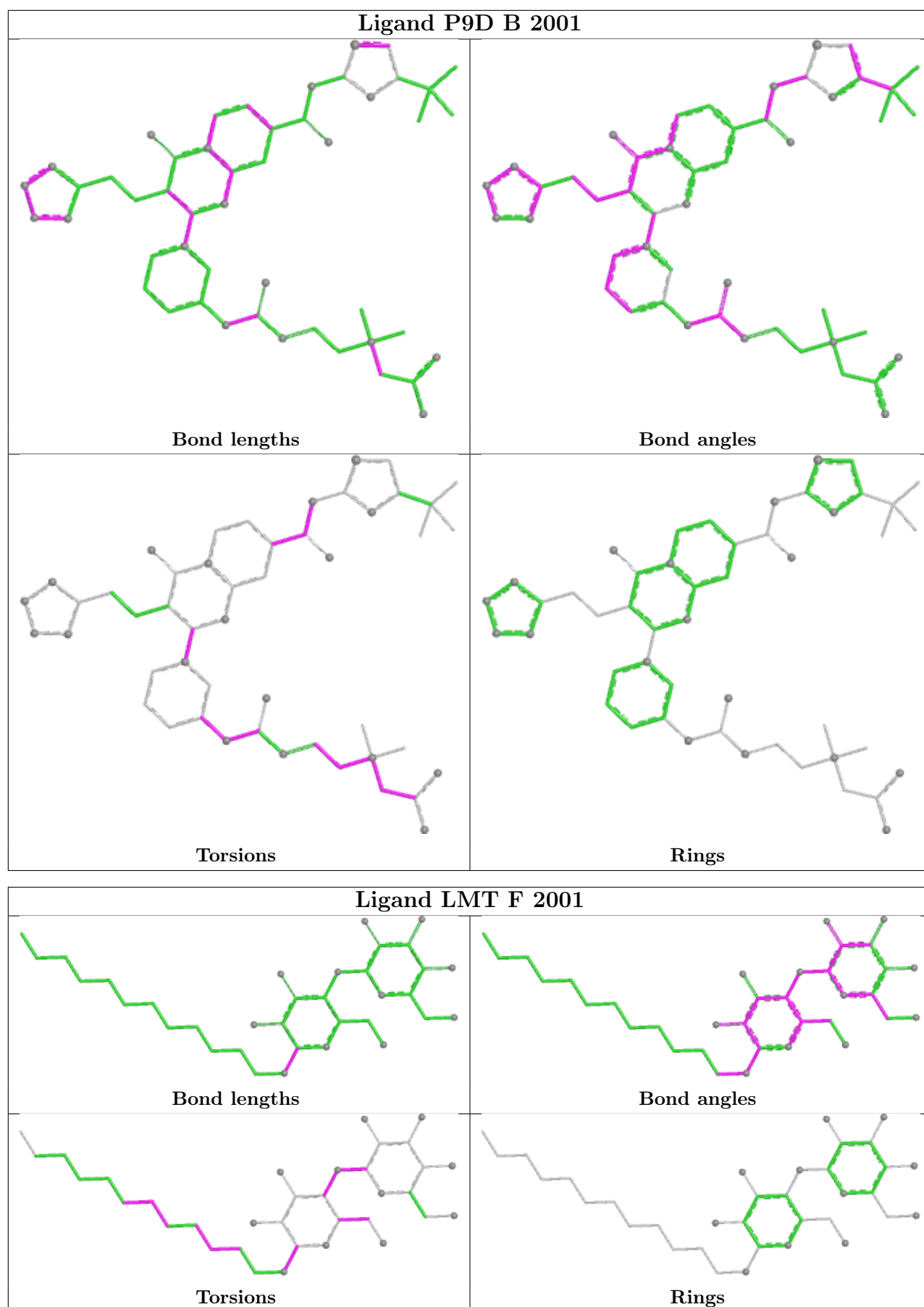
Mol	Chain	Res	Type	Atoms
3	E	2001	P9D	C32-C33-C35-C36-C37-N24

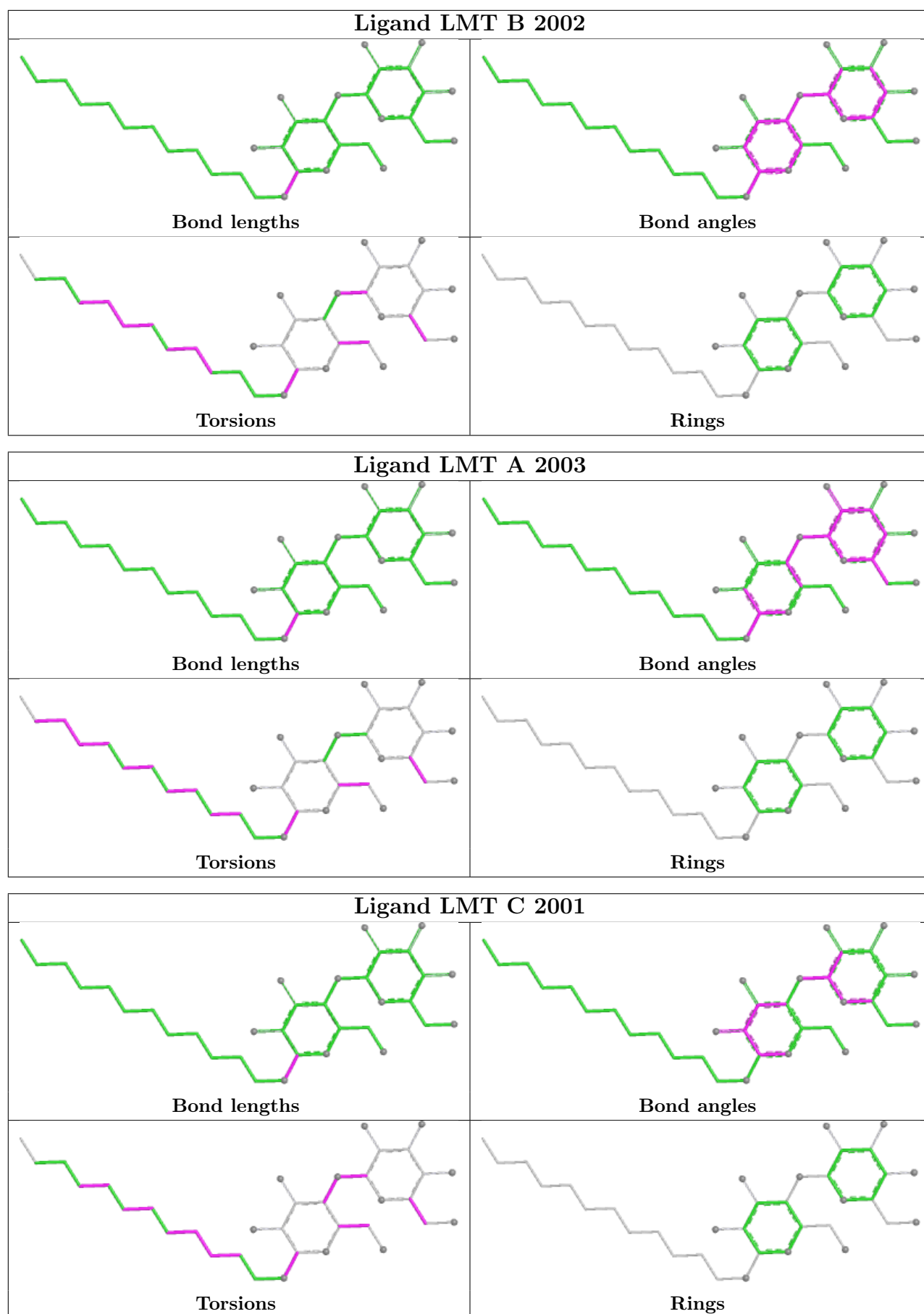
16 monomers are involved in 55 short contacts:

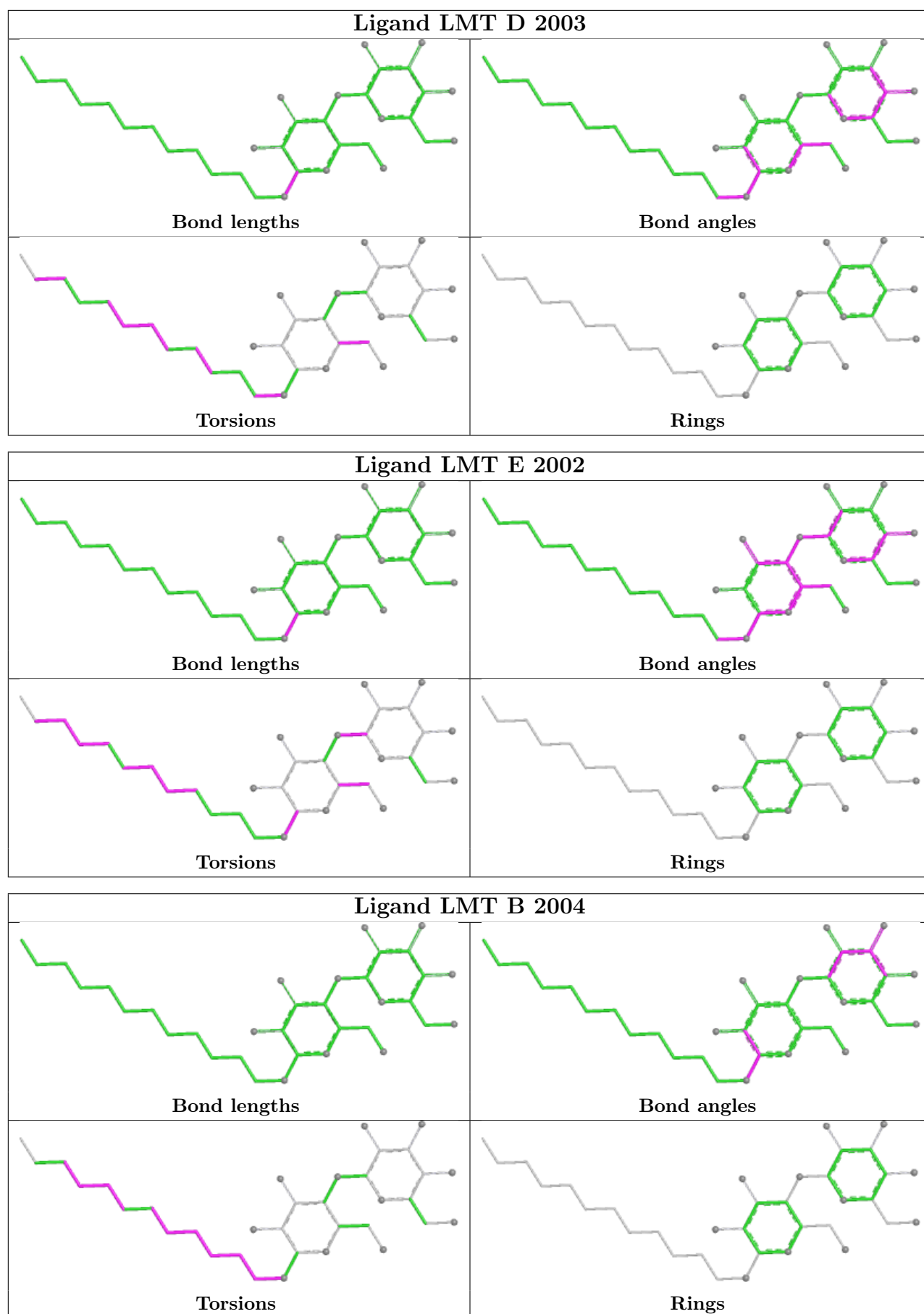
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2002	LMT	1	0
2	A	2001	LMT	2	0
3	B	2001	P9D	8	0
2	F	2001	LMT	4	0
2	B	2002	LMT	2	0
2	A	2003	LMT	2	0
2	C	2001	LMT	6	0
2	D	2003	LMT	2	0
2	E	2002	LMT	9	0
2	B	2004	LMT	1	0
2	B	2003	LMT	2	0
2	E	2003	LMT	1	0
2	D	2001	LMT	2	0
2	F	2002	LMT	3	0
2	A	2002	LMT	2	0
3	E	2001	P9D	8	0

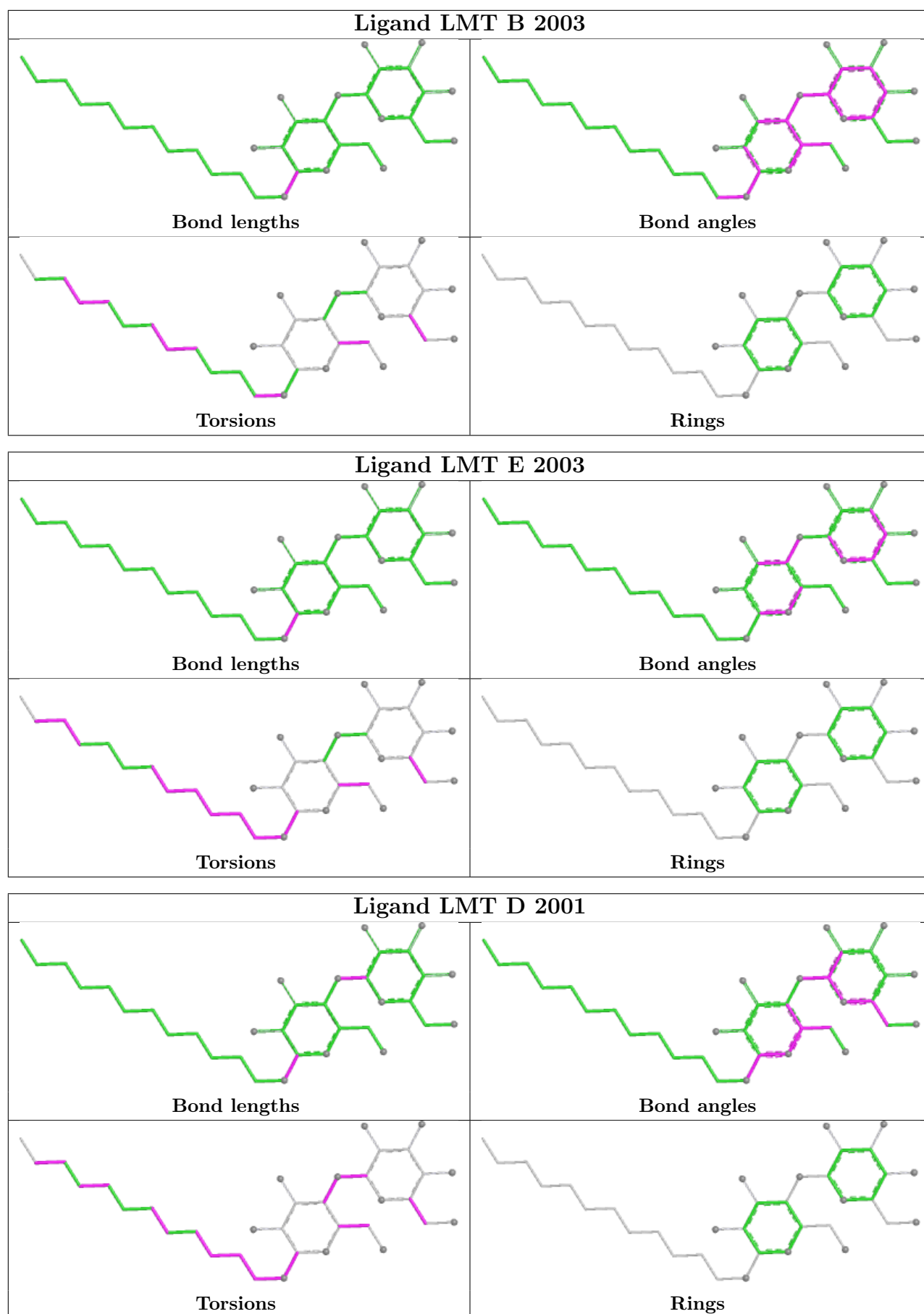
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

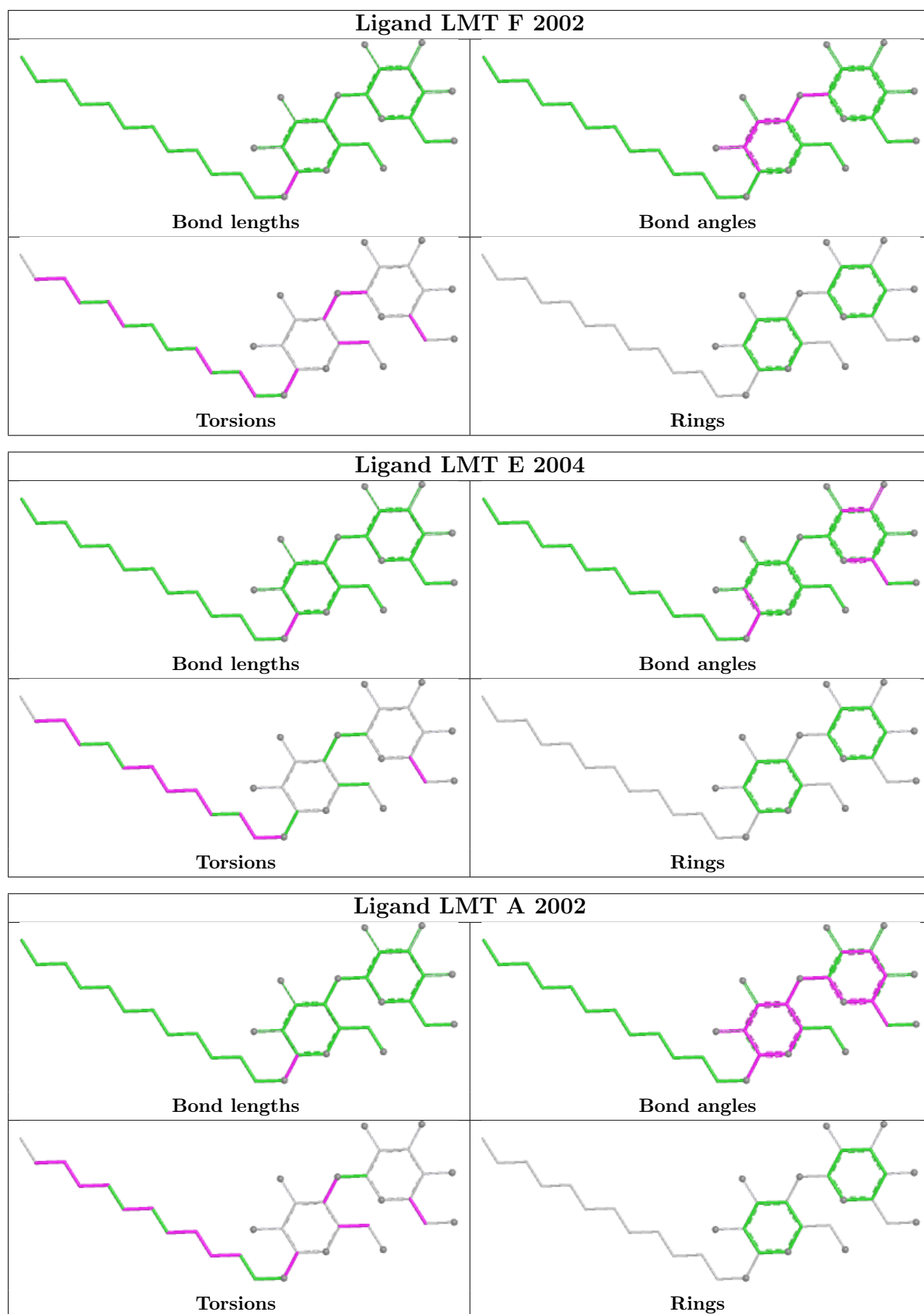


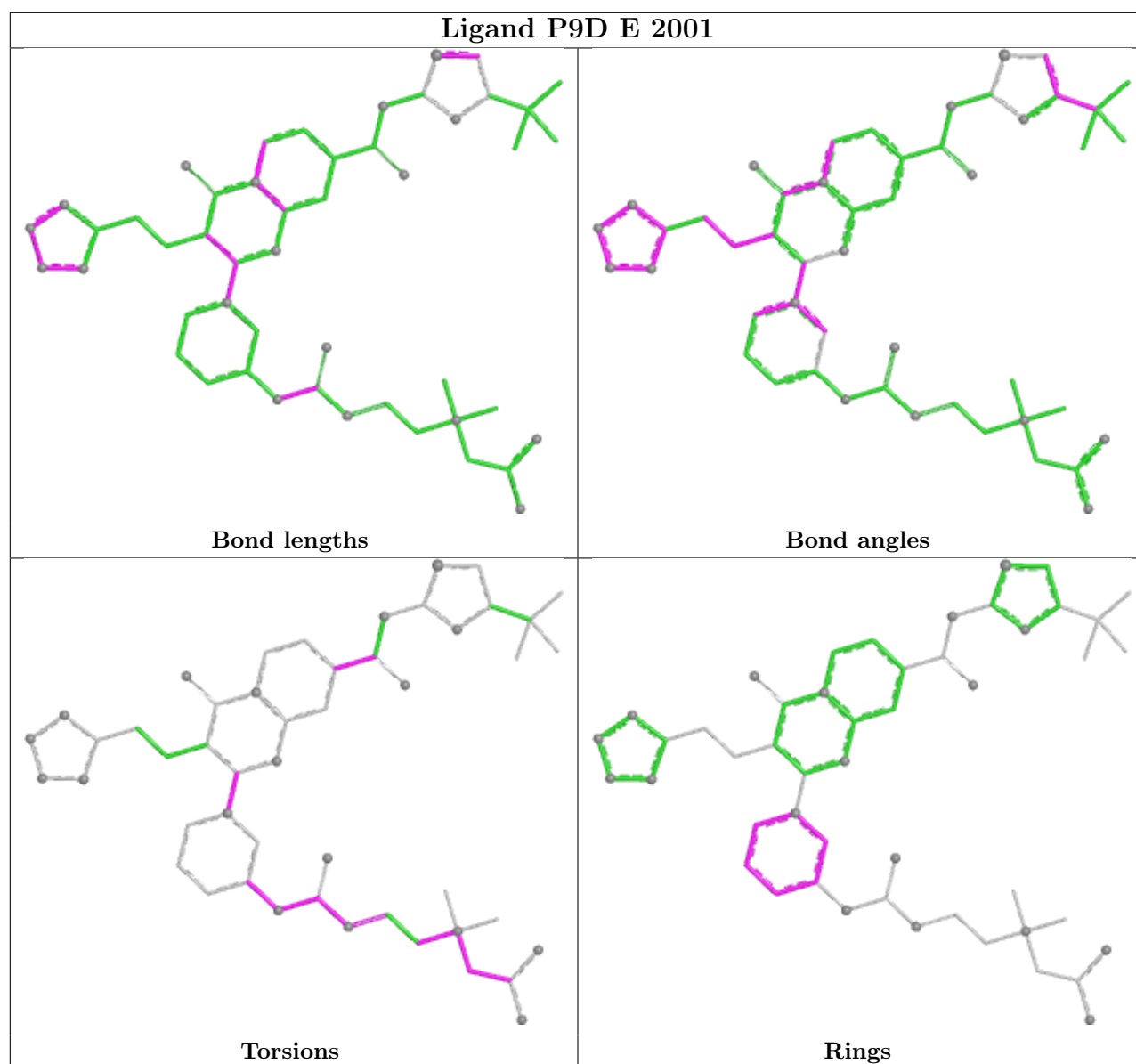












5.7 Other polymers [i](#)

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	1018/1052 (96%)	-0.36	6 (0%) 89 84	39, 75, 112, 164	0
1	B	1030/1052 (97%)	-0.40	6 (0%) 89 84	40, 73, 113, 152	0
1	C	1030/1052 (97%)	-0.23	28 (2%) 54 38	43, 87, 143, 201	0
1	D	1019/1052 (96%)	-0.37	11 (1%) 80 70	47, 78, 117, 160	0
1	E	1030/1052 (97%)	-0.28	13 (1%) 77 66	46, 78, 124, 162	0
1	F	1033/1052 (98%)	-0.26	15 (1%) 73 61	45, 79, 129, 264	0
All	All	6160/6312 (97%)	-0.32	79 (1%) 77 66	39, 78, 124, 264	0

The worst 5 of 79 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	253	VAL	5.6
1	F	259	GLN	4.8
1	F	742	LEU	4.3
1	C	600	GLU	4.0
1	C	256	ASP	3.8

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 monosaccharides in this entry.

6.4 Ligands

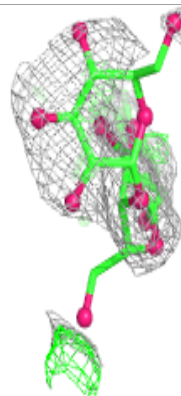
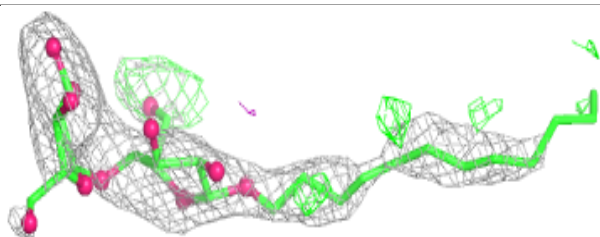
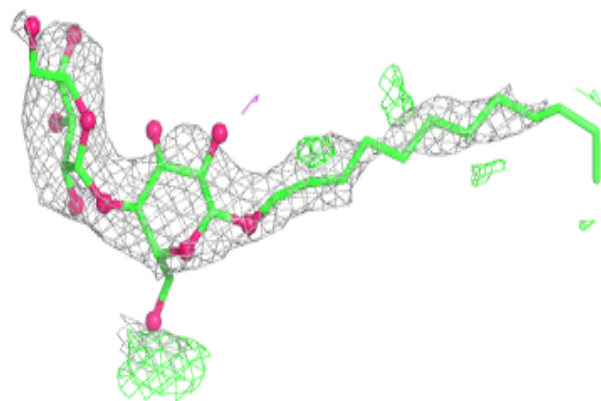
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	0.79	0.44	47,65,79,89	35
2	LMT	F	2001	35/35	0.84	0.28	82,104,126,139	0
2	LMT	A	2001	35/35	0.85	0.34	43,66,94,103	35
2	LMT	F	2002	35/35	0.85	0.34	76,118,147,148	0
2	LMT	C	2001	35/35	0.88	0.34	80,105,146,151	0
2	LMT	E	2002	35/35	0.90	0.25	67,106,124,132	0
2	LMT	E	2003	35/35	0.90	0.38	67,94,108,124	0
2	LMT	B	2002	35/35	0.90	0.23	63,106,135,137	0
2	LMT	D	2003	35/35	0.90	0.25	70,98,134,144	0
2	LMT	A	2002	35/35	0.91	0.26	60,86,132,142	0
2	LMT	A	2003	35/35	0.91	0.23	64,90,115,120	0
2	LMT	D	2002	35/35	0.93	0.31	69,111,137,144	0
2	LMT	B	2003	35/35	0.93	0.28	71,82,104,111	0
3	P9D	E	2001	49/49	0.93	0.27	60,78,108,123	0
3	P9D	B	2001	49/49	0.94	0.24	53,71,85,108	0
2	LMT	B	2004	35/35	0.94	0.23	62,69,78,84	0
2	LMT	E	2004	35/35	0.95	0.32	67,74,100,103	0

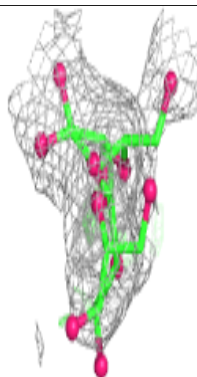
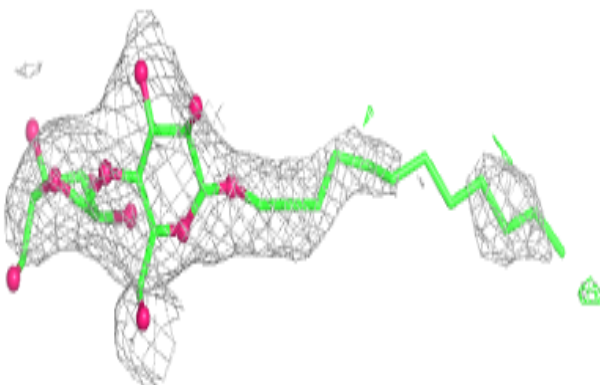
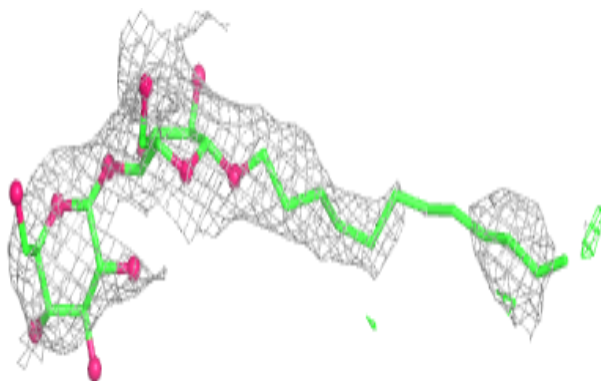
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

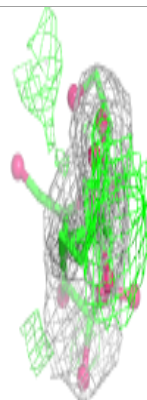
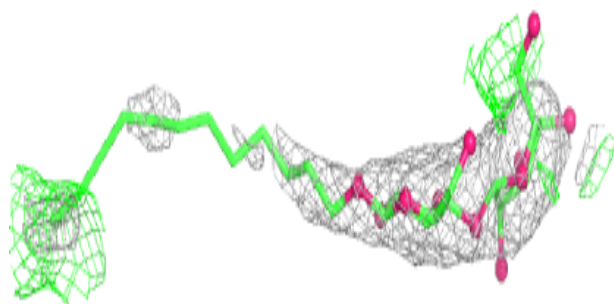
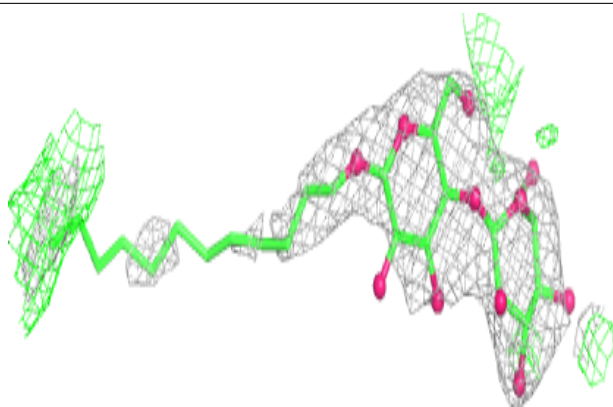
**Electron density around LMT F 2001:**

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

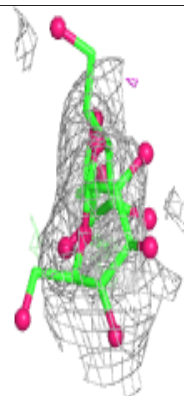
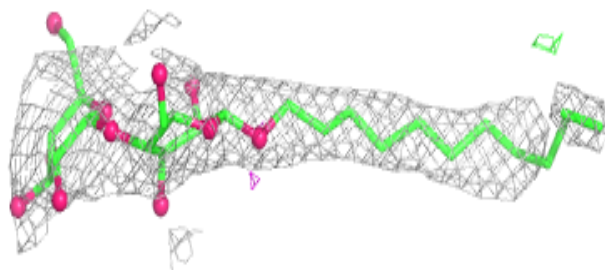
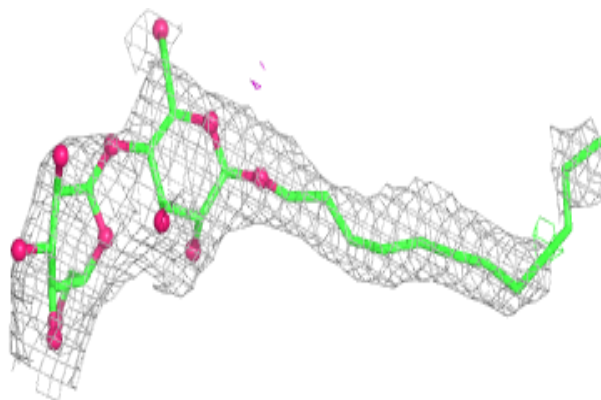


Electron density around LMT A 2001:

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

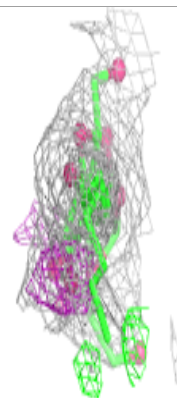
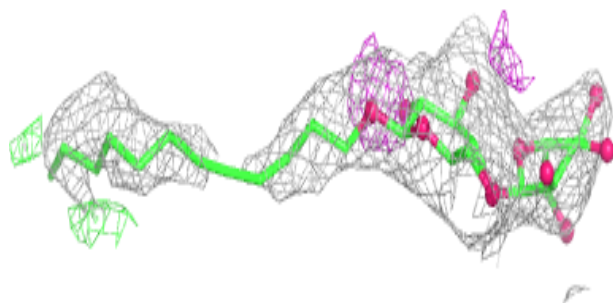
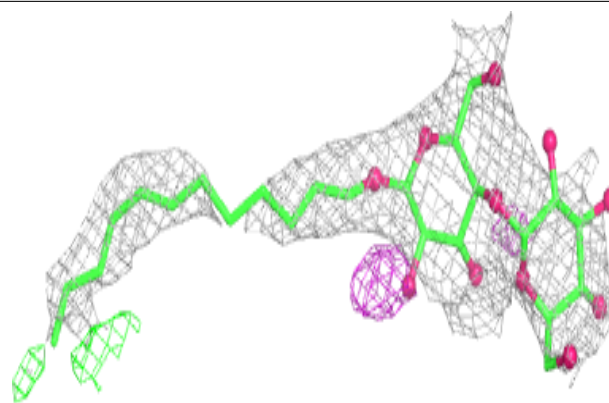
**Electron density around LMT F 2002:**

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

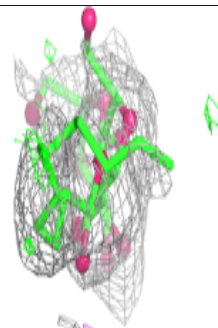
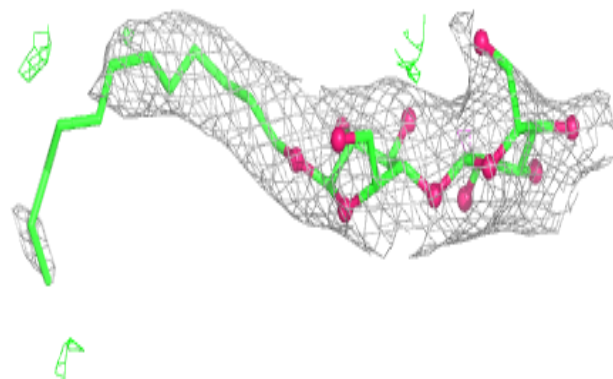
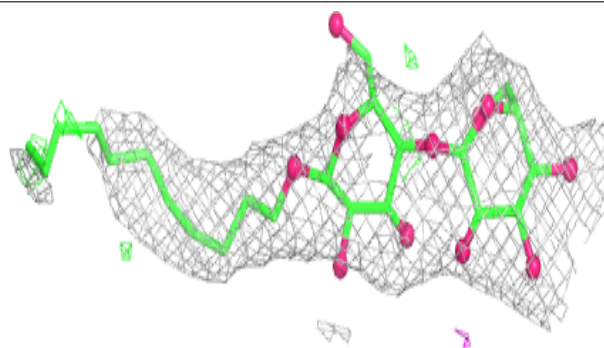


Electron density around LMT C 2001:

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

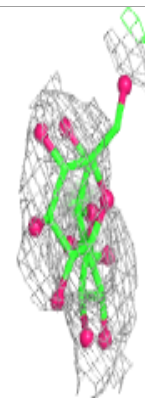
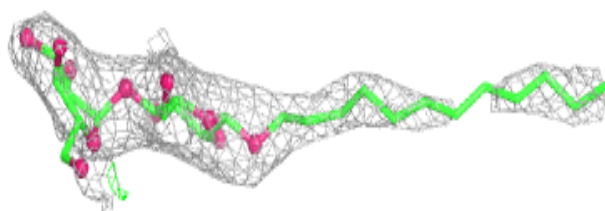
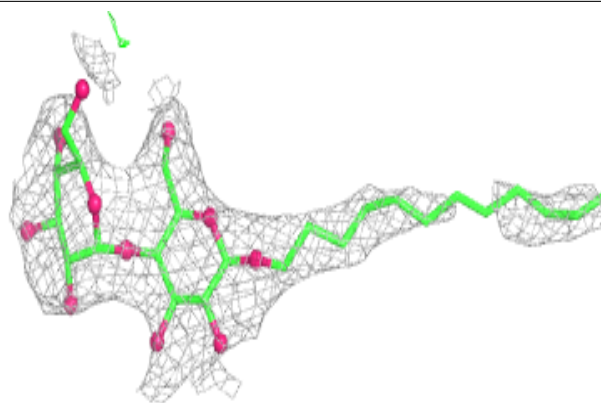
**Electron density around LMT E 2002:**

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

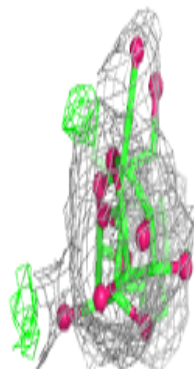
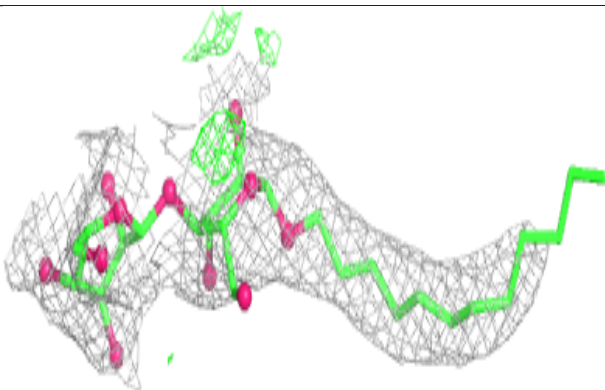
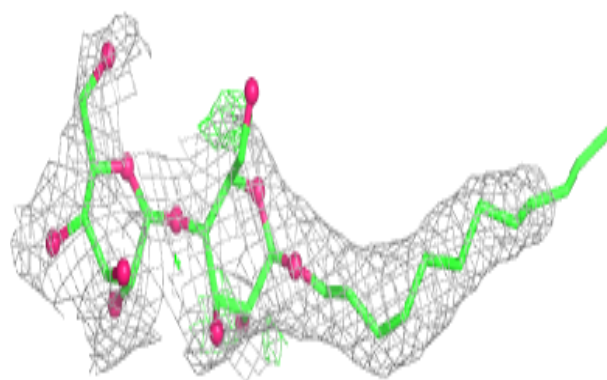


Electron density around LMT E 2003:

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

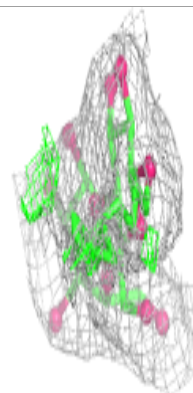
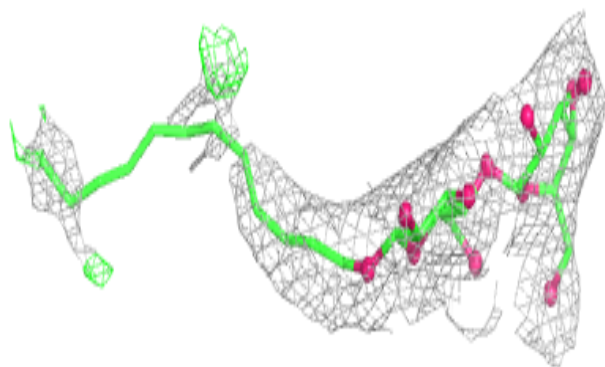
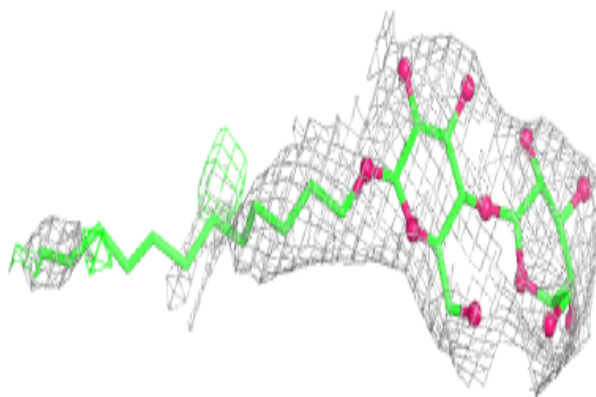
**Electron density around LMT B 2002:**

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

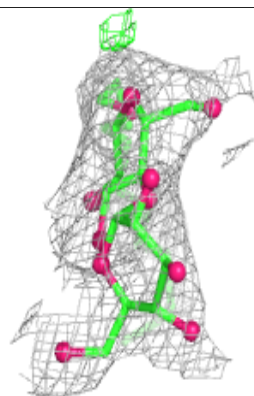
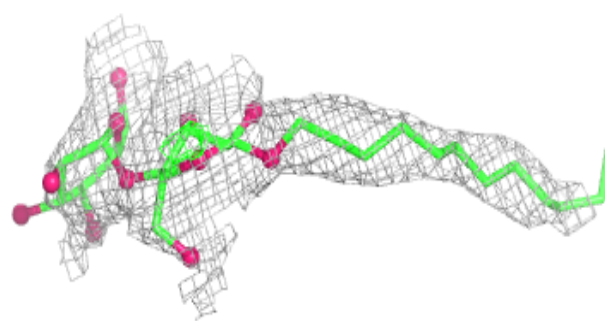
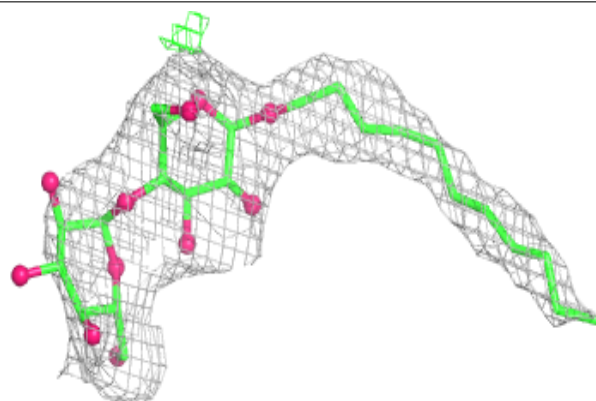


Electron density around LMT D 2003:

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

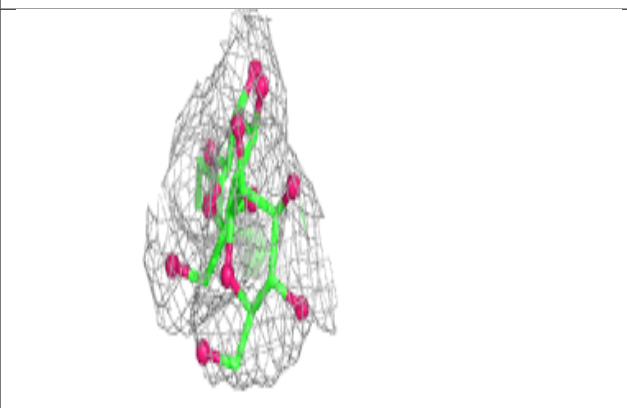
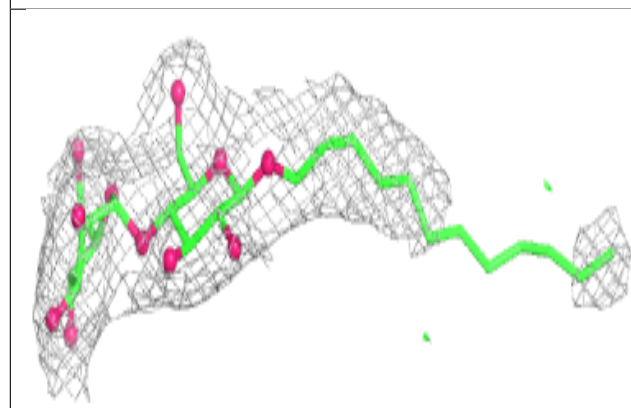
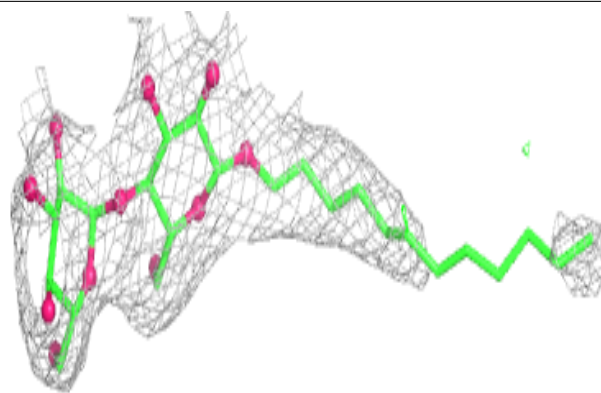
**Electron density around LMT A 2002:**

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

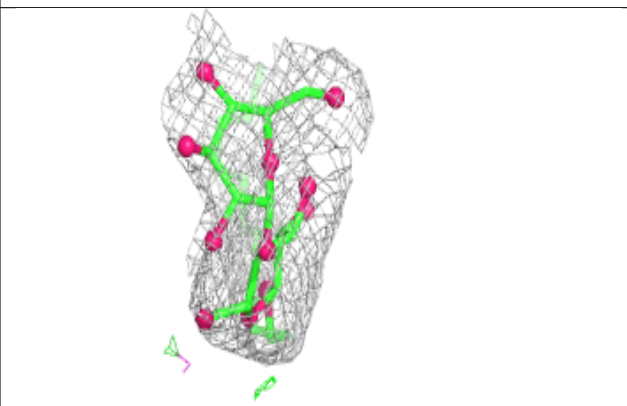
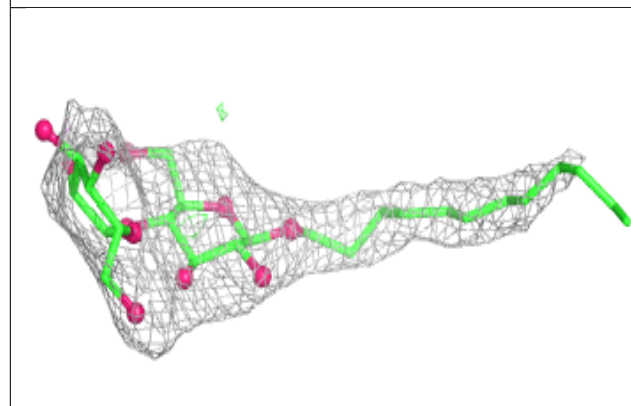
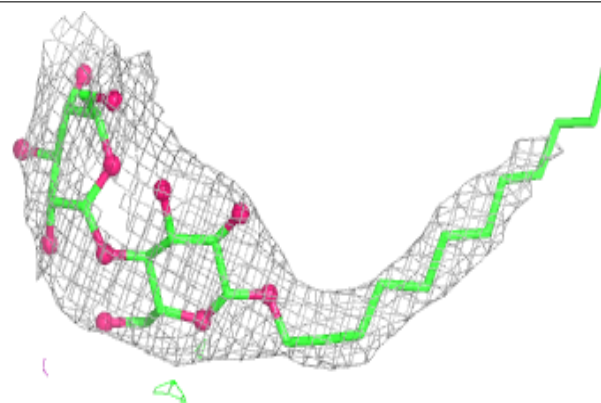


Electron density around LMT A 2003:

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

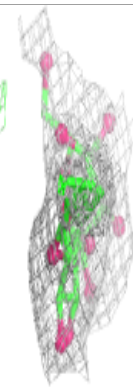
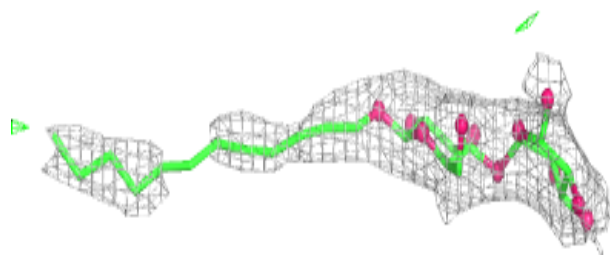
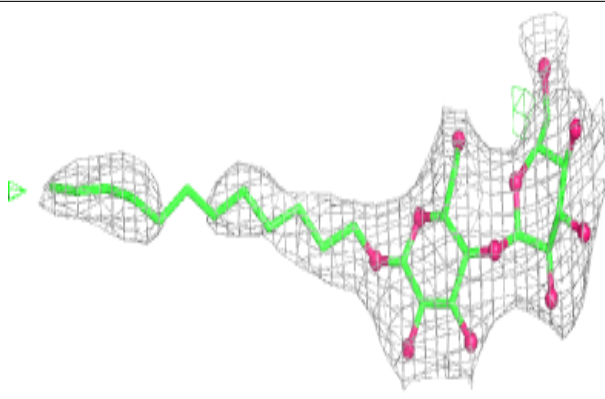
**Electron density around LMT D 2002:**

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

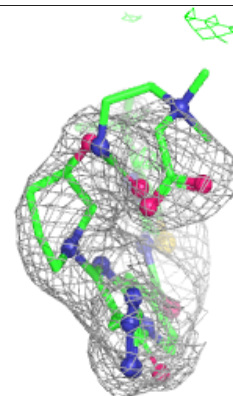
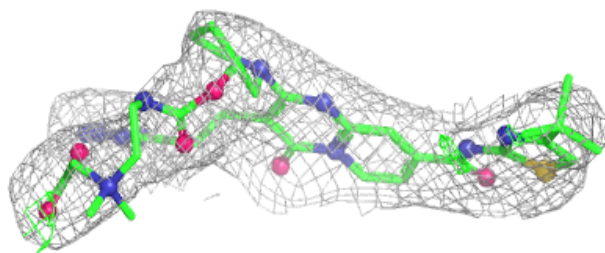
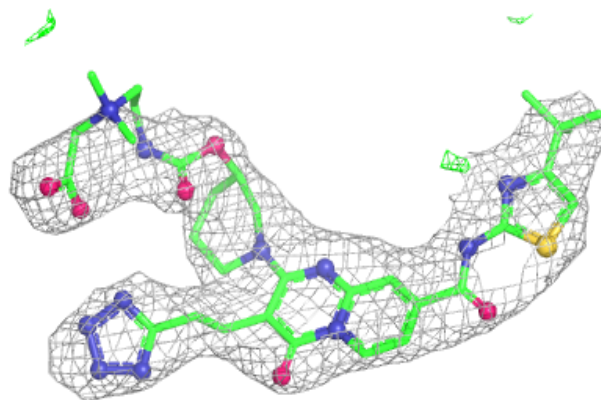


Electron density around LMT B 2003:

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

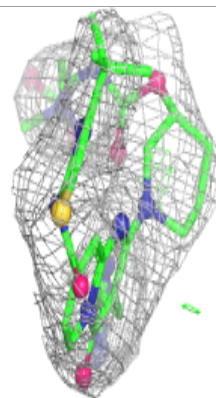
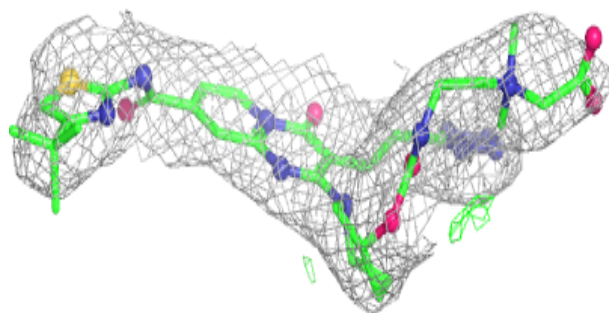
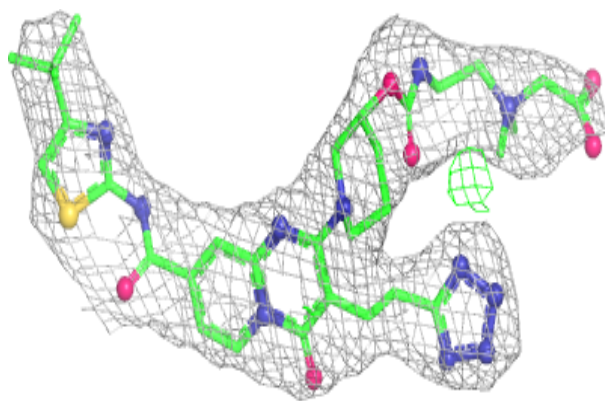
**Electron density around P9D E 2001:**

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

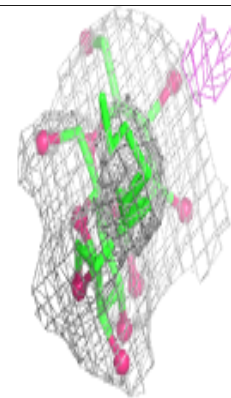
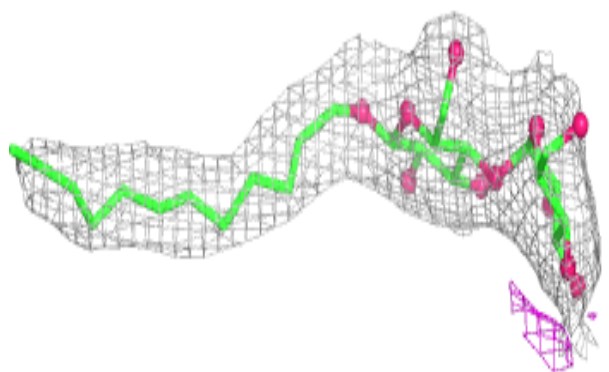
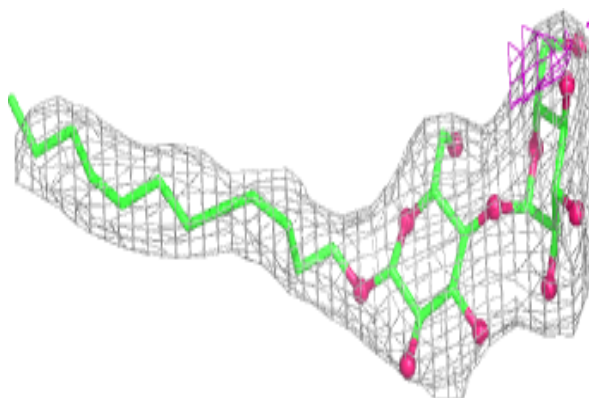


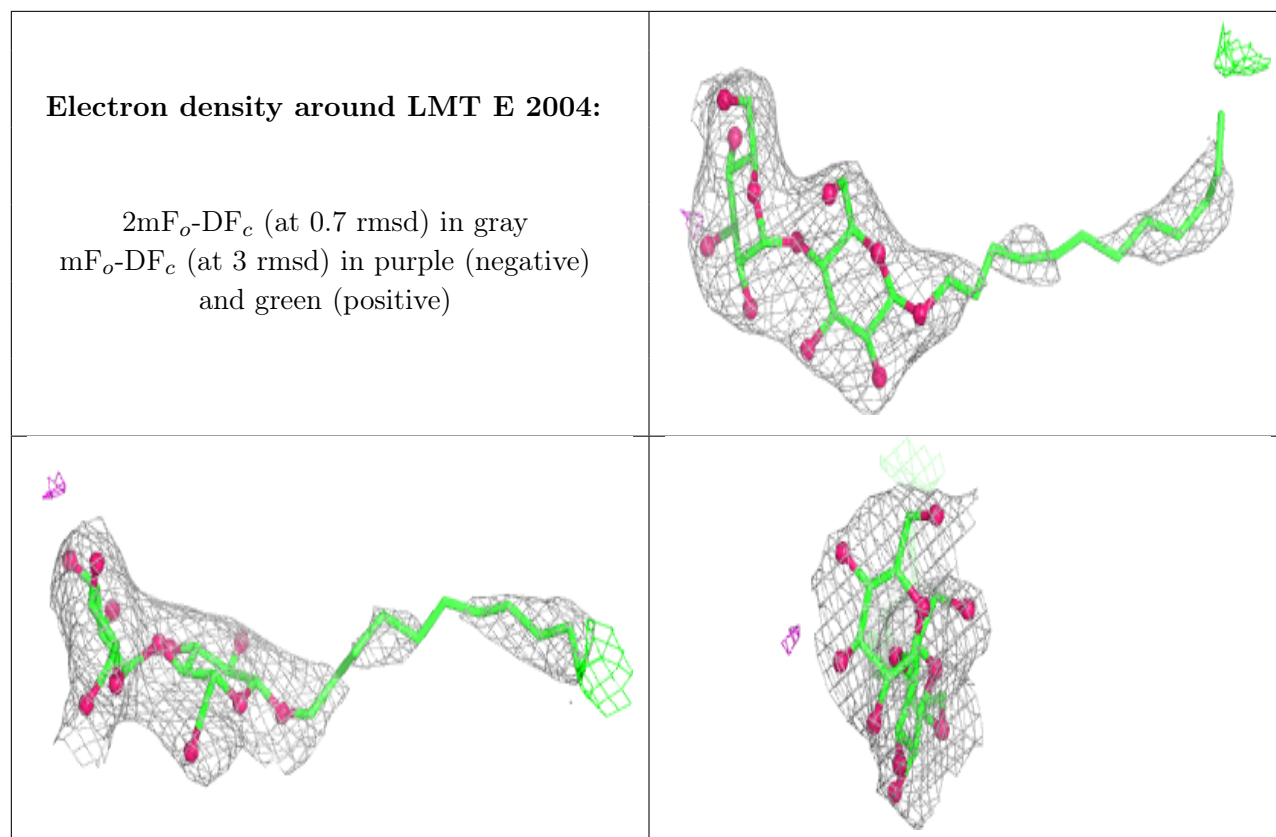
Electron density around P9D B 2001:

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

**Electron density around LMT 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.