wwPDB X-ray Structure Validation Summary Report (i)

Nov 5, 2026 – 12:34 pm GMT

PDB ID	:	33WJ / pdb_000033wj
Title	:	Structural and functional evaluation of the classical RND efflux pumps inhibitor PAbN, a systematic study.
Authors	:	Wehbi, H.; Megret, M.; Phan, G.; Broutin, I.
Deposited on	:	2026-08-27
Resolution	:	3.56 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 (i) 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 (i)) were used in the production of this report:

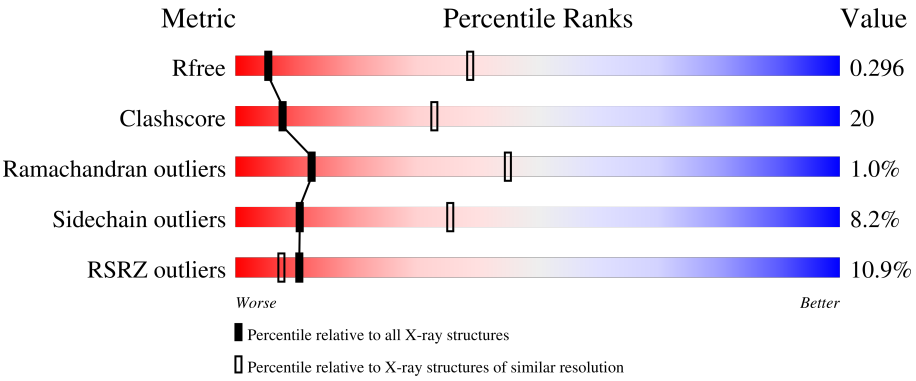
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 3.56 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



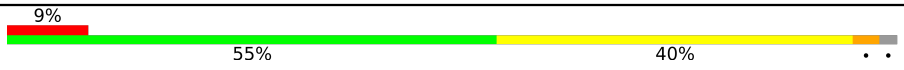
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1410 (3.62-3.50)
Clashscore	190562	1480 (3.62-3.50)
Ramachandran outliers	187476	1440 (3.62-3.50)
Sidechain outliers	187428	1441 (3.62-3.50)
RSRZ outliers	180081	1409 (3.62-3.50)

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 <=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	1056	12% 54% 37%
1	B	1056	11% 56% 38%
1	C	1056	9% 57% 37%
1	D	1056	11% 55% 36%
1	E	1056	11% 57% 37%

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Mol	Chain	Length	Quality of chain
1	F	1056	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 47031 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
1	A	1013	Total	C	N	O	S	6	0	0
			7690	4955	1276	1420	39			
1	B	1030	Total	C	N	O	S	0	0	0
			7812	5027	1299	1446	40			
1	C	1030	Total	C	N	O	S	12	0	0
			7812	5027	1299	1446	40			
1	D	1012	Total	C	N	O	S	6	0	0
			7682	4949	1275	1419	39			
1	E	1030	Total	C	N	O	S	0	0	0
			7812	5027	1299	1446	40			
1	F	1032	Total	C	N	O	S	12	0	0
			7832	5042	1302	1448	40			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	407	ASN	ASP	engineered mutation	UNP P52002
A	1047	LEU	-	expression tag	UNP P52002
A	1048	GLU	-	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
A	1053	HIS	-	expression tag	UNP P52002
A	1054	HIS	-	expression tag	UNP P52002
A	1055	HIS	-	expression tag	UNP P52002
A	1056	HIS	-	expression tag	UNP P52002
B	407	ASN	ASP	engineered mutation	UNP P52002
B	1047	LEU	-	expression tag	UNP P52002
B	1048	GLU	-	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

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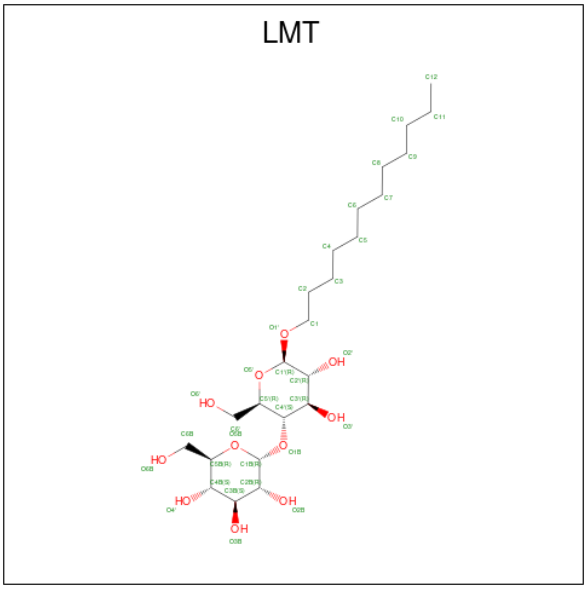
Chain	Residue	Modelled	Actual	Comment	Reference
B	1052	HIS	-	expression tag	UNP P52002
B	1053	HIS	-	expression tag	UNP P52002
B	1054	HIS	-	expression tag	UNP P52002
B	1055	HIS	-	expression tag	UNP P52002
B	1056	HIS	-	expression tag	UNP P52002
C	407	ASN	ASP	engineered mutation	UNP P52002
C	1047	LEU	-	expression tag	UNP P52002
C	1048	GLU	-	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
C	1052	HIS	-	expression tag	UNP P52002
C	1053	HIS	-	expression tag	UNP P52002
C	1054	HIS	-	expression tag	UNP P52002
C	1055	HIS	-	expression tag	UNP P52002
C	1056	HIS	-	expression tag	UNP P52002
D	407	ASN	ASP	engineered mutation	UNP P52002
D	1047	LEU	-	expression tag	UNP P52002
D	1048	GLU	-	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
D	1053	HIS	-	expression tag	UNP P52002
D	1054	HIS	-	expression tag	UNP P52002
D	1055	HIS	-	expression tag	UNP P52002
D	1056	HIS	-	expression tag	UNP P52002
E	407	ASN	ASP	engineered mutation	UNP P52002
E	1047	LEU	-	expression tag	UNP P52002
E	1048	GLU	-	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
E	1053	HIS	-	expression tag	UNP P52002
E	1054	HIS	-	expression tag	UNP P52002
E	1055	HIS	-	expression tag	UNP P52002
E	1056	HIS	-	expression tag	UNP P52002
F	407	ASN	ASP	engineered mutation	UNP P52002
F	1047	LEU	-	expression tag	UNP P52002
F	1048	GLU	-	expression tag	UNP P52002
F	1049	HIS	-	expression tag	UNP P52002

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Chain	Residue	Modelled	Actual	Comment	Reference
F	1050	HIS	-	expression tag	UNP P52002
F	1051	HIS	-	expression tag	UNP P52002
F	1052	HIS	-	expression tag	UNP P52002
F	1053	HIS	-	expression tag	UNP P52002
F	1054	HIS	-	expression tag	UNP P52002
F	1055	HIS	-	expression tag	UNP P52002
F	1056	HIS	-	expression tag	UNP P52002

- Molecule 2 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).



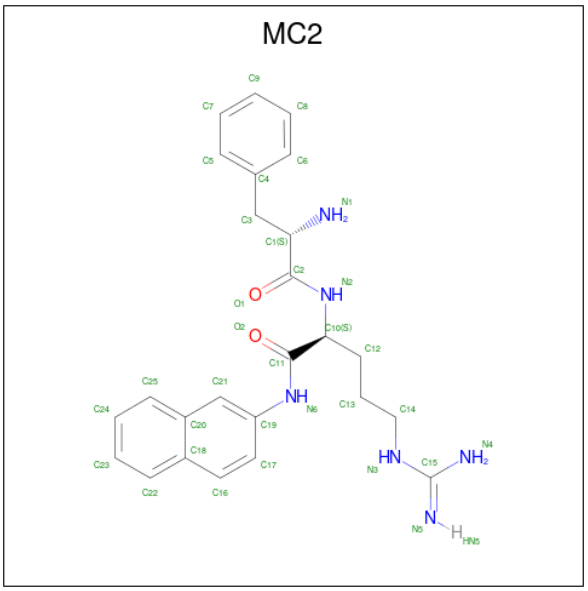
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 35 24 11	0	0
2	A	1	Total C O 35 24 11	0	0
2	B	1	Total C O 35 24 11	0	0
2	B	1	Total C O 35 24 11	0	0
2	B	1	Total C O 35 24 11	0	0
2	B	1	Total C O 35 24 11	0	0
2	D	1	Total C O 35 24 11	0	0

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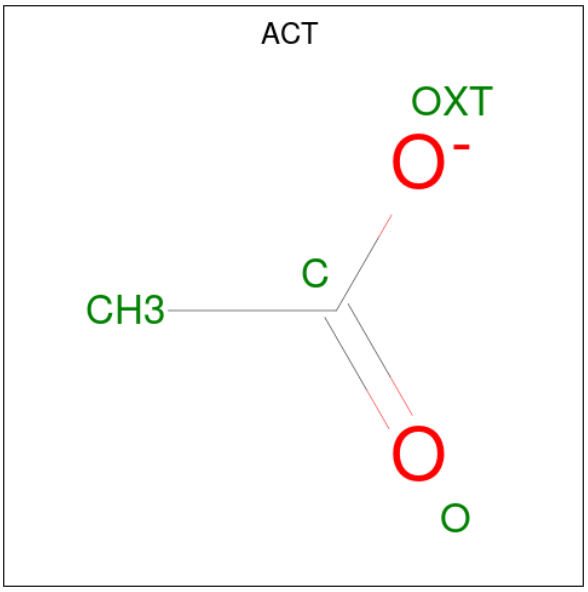
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total C O 35 24 11	0	0
2	E	1	Total C O 35 24 11	0	0
2	E	1	Total C O 35 24 11	0	0

- Molecule 3 is N2-(L-PHENYLALANYL)-N1-(NAPHTHALENYL)-L-ARIGNINAMIDE (CCD ID: MC2) (formula: $C_{25}H_{30}N_6O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C N O 33 25 6 2	0	0

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0

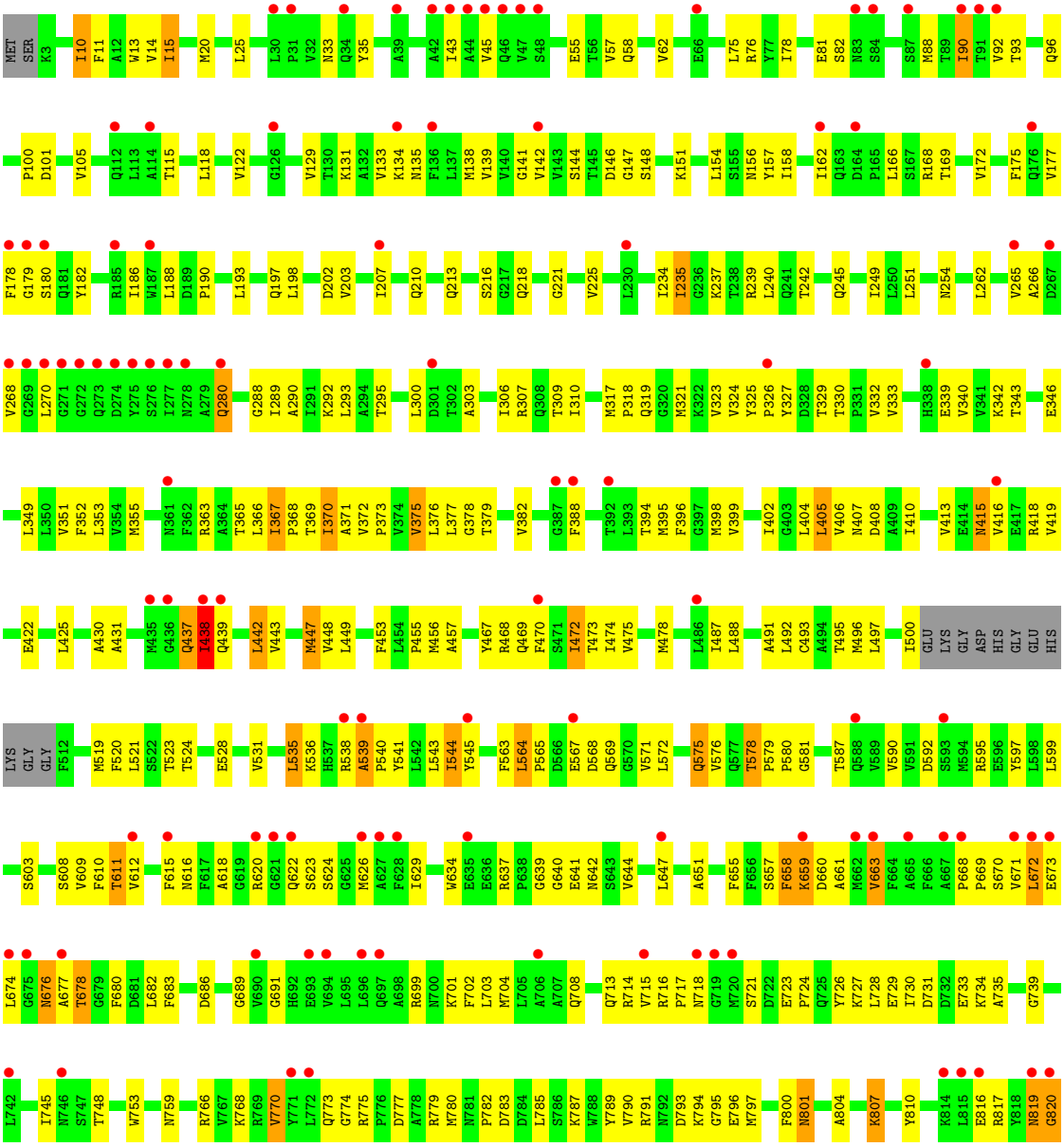
3 Residue-property plots (i)

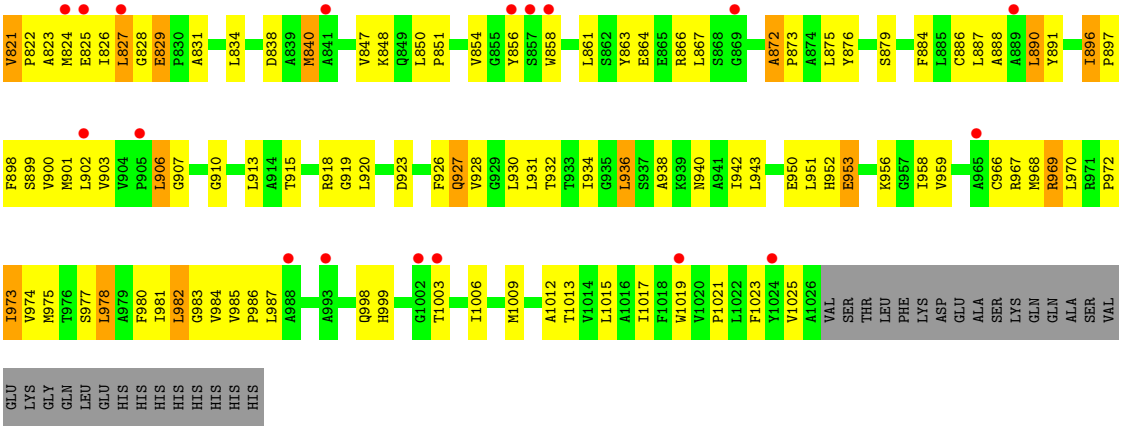
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

Chain A:



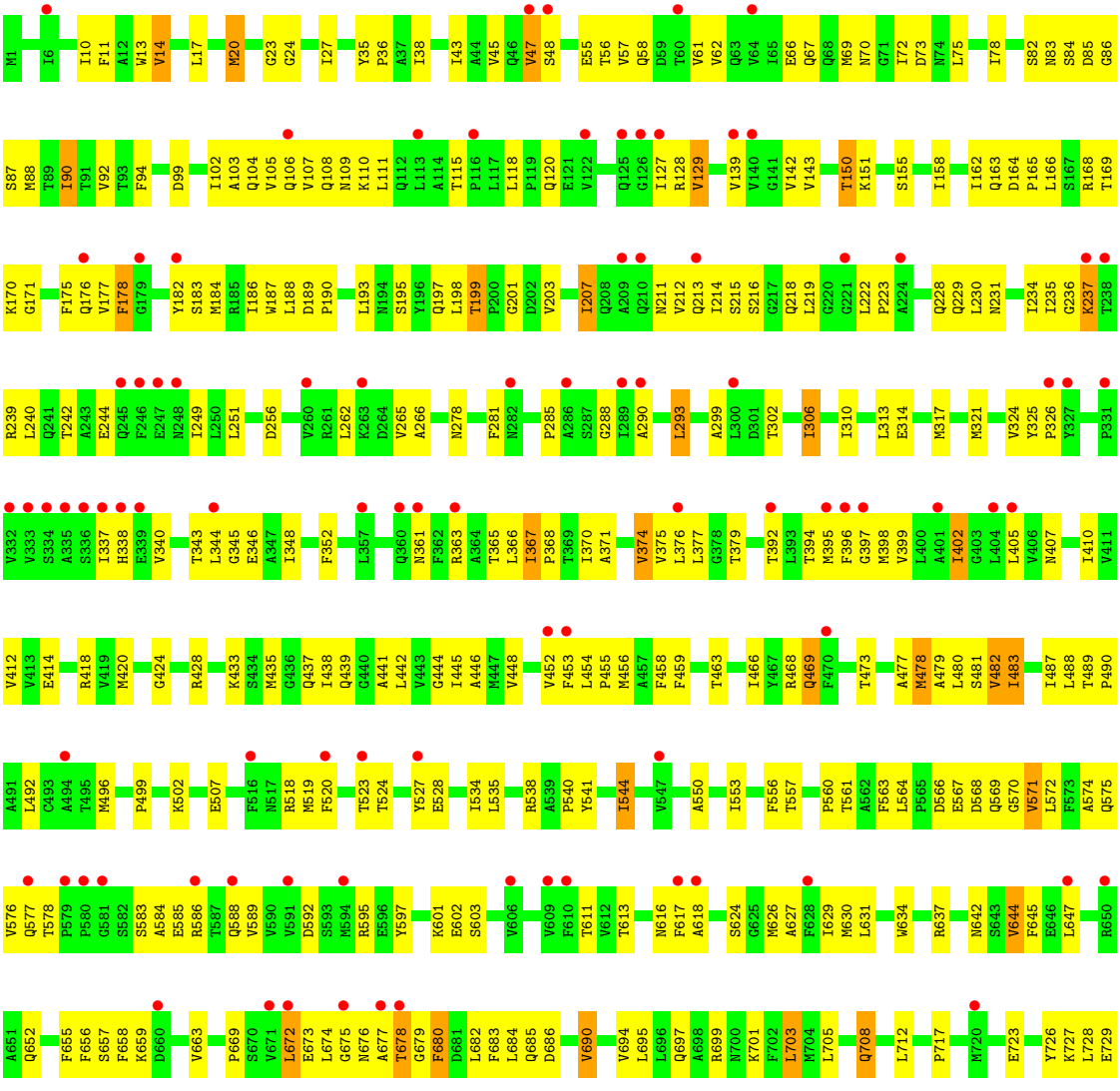


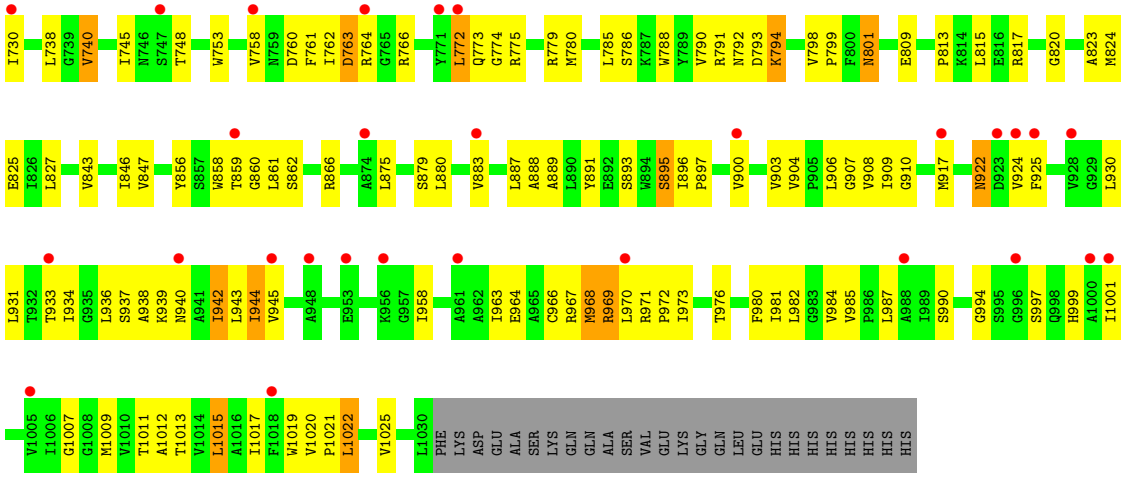


• Molecule 1: Multidrug resistance protein MexB

Chain B:



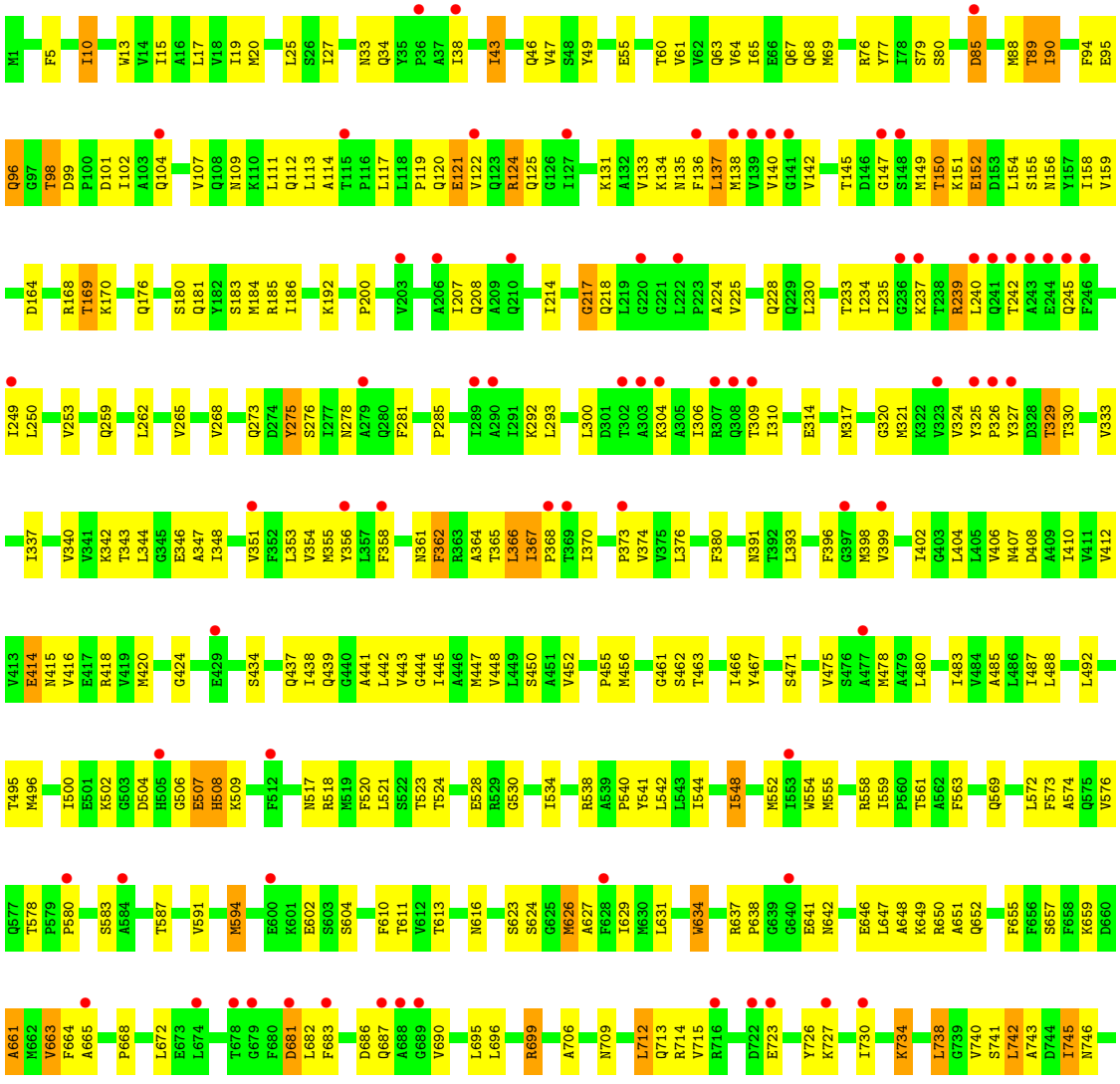


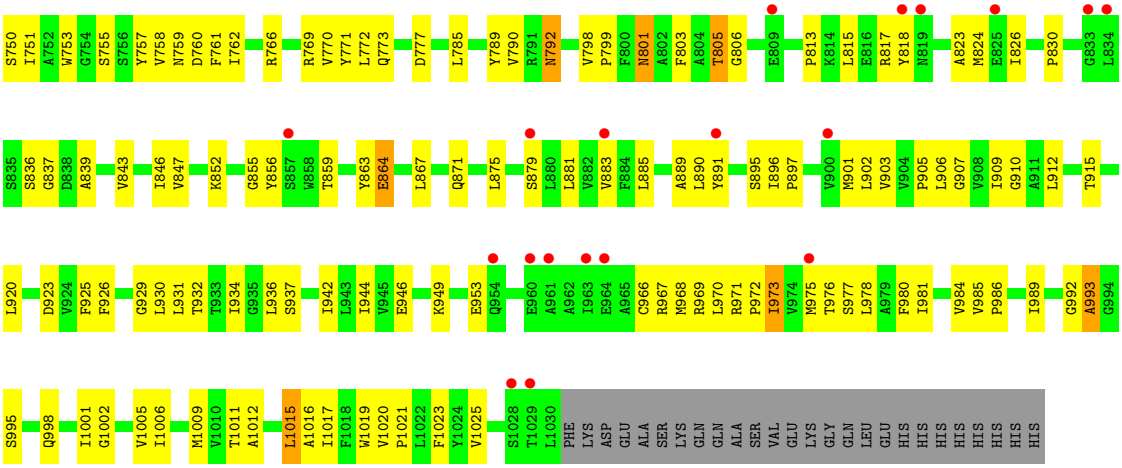


• Molecule 1: Multidrug resistance protein MexB

Chain C:



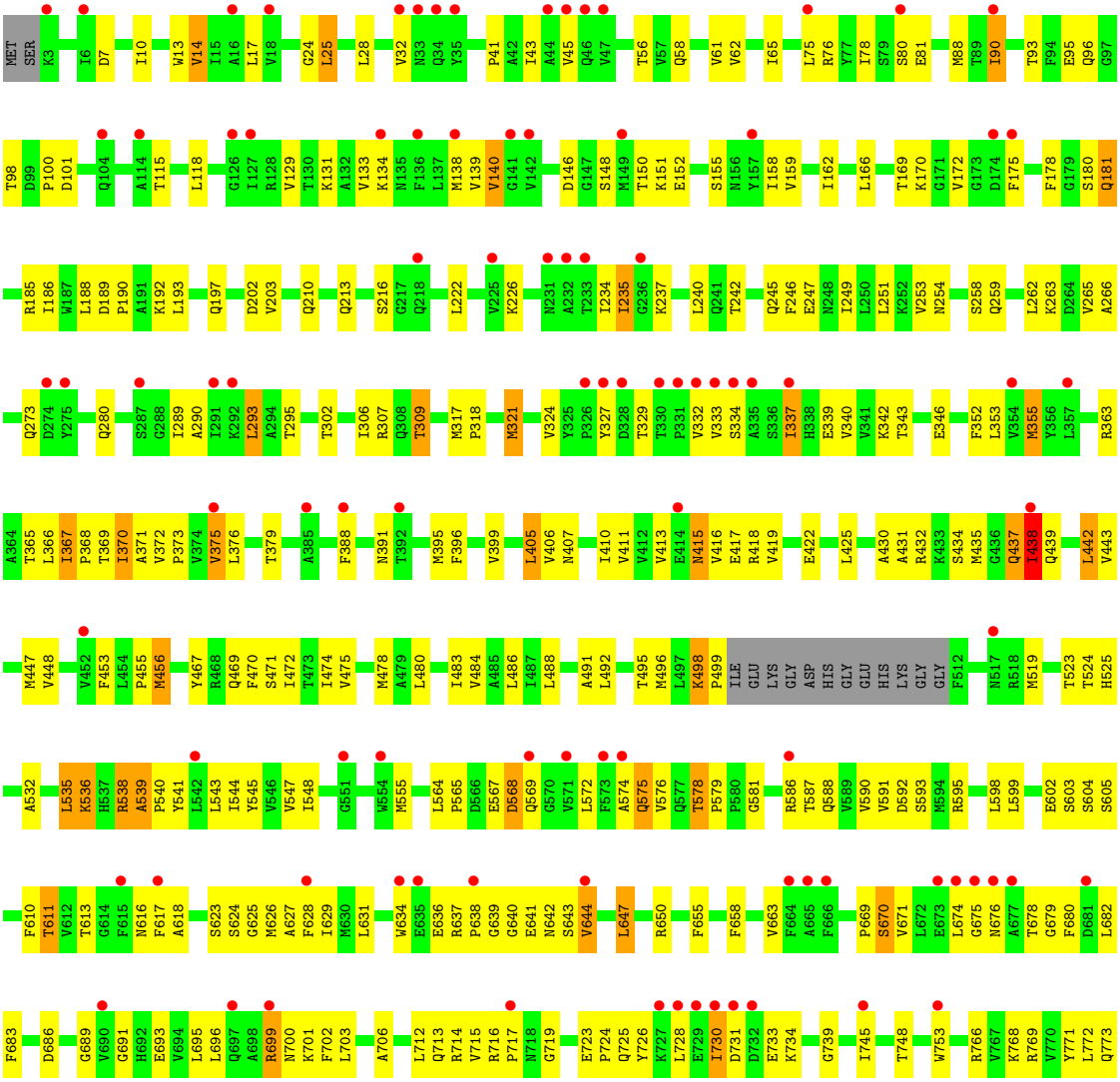


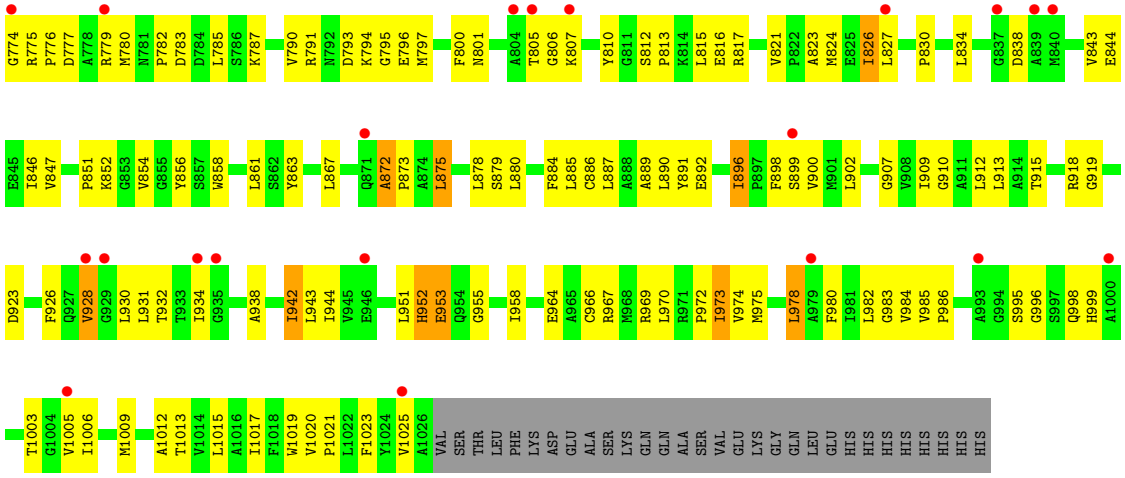


• Molecule 1: Multidrug resistance protein MexB

Chain D:



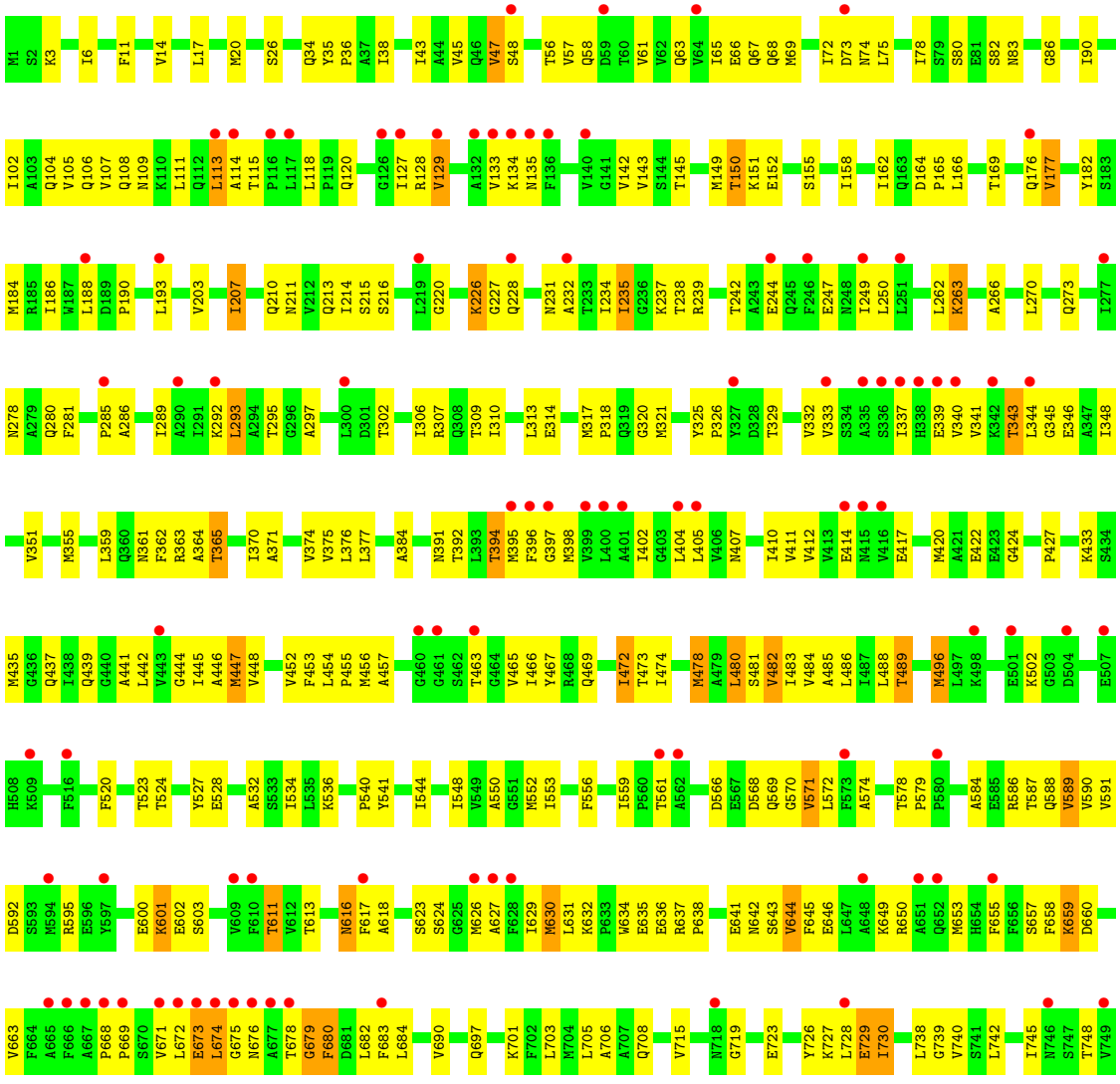


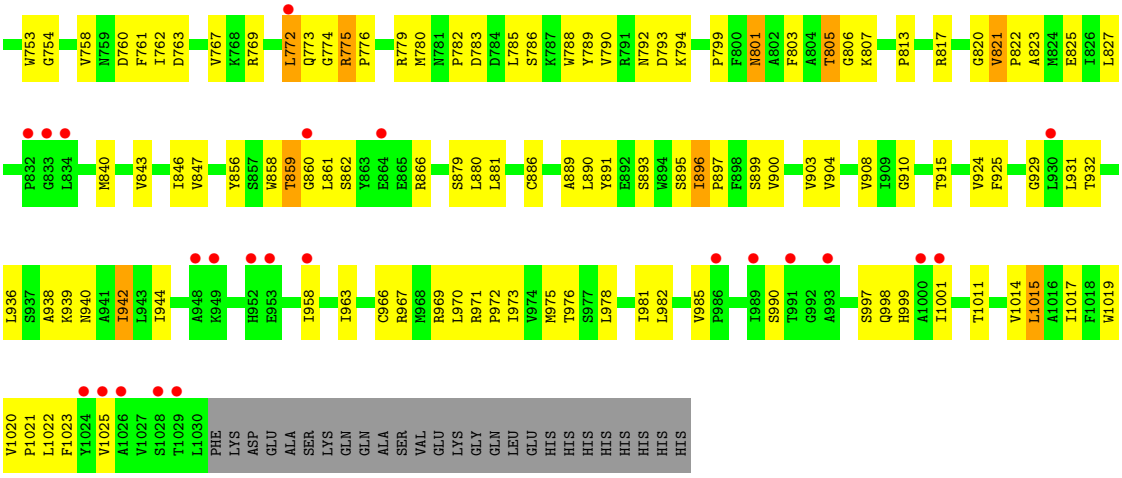


• Molecule 1: Multidrug resistance protein MexB

Chain E:



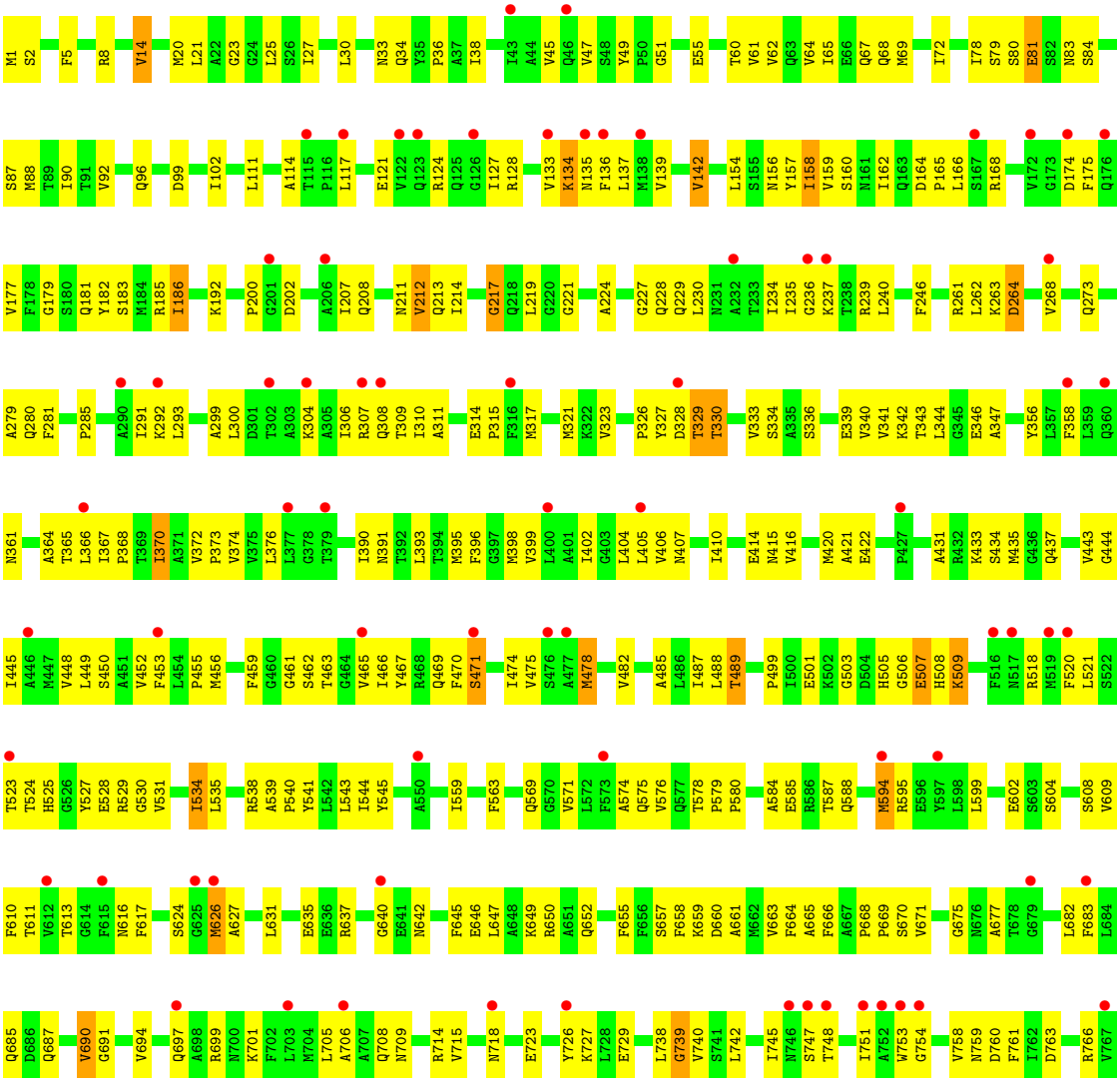


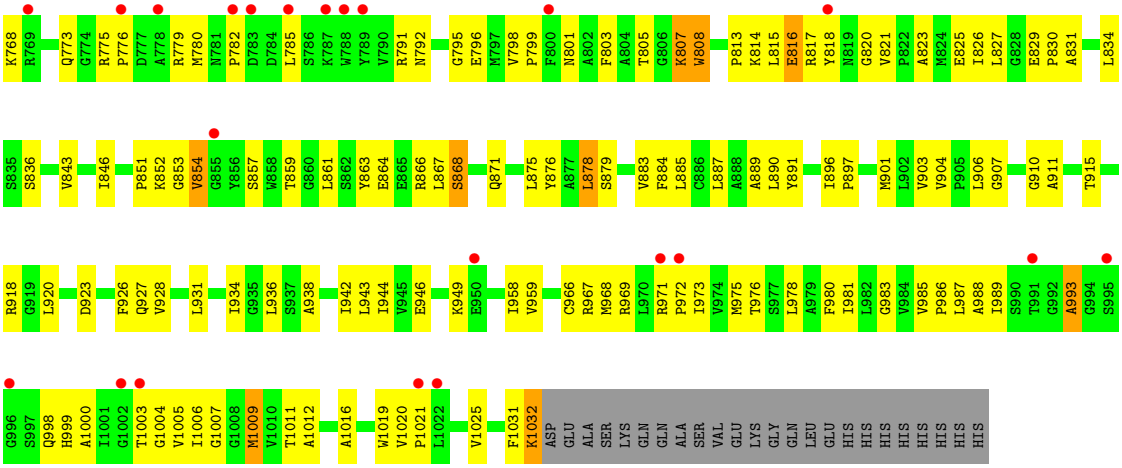


• Molecule 1: Multidrug resistance protein MexB

Chain F:






K768 R769 Q773 G774 R775 P776 D777 A778 R779 M780 N781 P782 D783 D784 L785 S786 K787 W788 Y789 V790 R791 N792 G795 E796 M797 V798 P799 F800 N801 A802 F803 A804 T805 G806 K807 W808 P813 K814 L815 E816 R817 Y818 N819 G820 V821 P822 A823 M824 E825 I826 L827 G828 E829 P830 A831 L834
S835 S836 V843 I846 P851 K852 G853 V854 G855 Y856 S857 W858 T859 G860 L861 S862 Y863 E864 E865 R866 L867 S868 Q871 L875 Y876 A877 L878 S879 V883 F884 L885 C886 L887 A888 A889 L890 Y891 I896 P897 M901 L902 V903 V904 P905 L906 G907 G910 A911 T915
R918 G919 L920 D923 F926 Q927 V928 L931 I934 G935 L936 S937 A938 I942 L943 I944 V945 E946 K949 E950 I958 V959 C966 R967 M968 R969 L970 R971 P972 I973 V974 M975 T976 S977 L978 A979 F980 I981 L982 G983 V984 V985 P986 L987 A988 I989 S990 T991 G992 A993 G994 S995
G996 S997 Q998 H999 A1000 I1001 G1002 T1003 G1004 V1005 I1006 G1007 G1008 M1009 V1010 T1011 A1012 A1016 W1019 V1020 P1021 L1022 V1025 F1031 K1032 ASP GLU ALA SER LYS GLN GLN ALA SER VAL GLU LYS GLY GLN LEU GLU HIS HIS HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	125.93Å 135.71Å 153.21Å 86.19° 69.11° 87.56°	Depositor
Resolution (Å)	45.81 – 3.56 45.81 – 3.56	Depositor EDS
% Data completeness (in resolution range)	92.5 (45.81-3.56) 92.7 (45.81-3.56)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.23 (at 3.07Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.285 , 0.297 0.279 , 0.296	Depositor DCC
R_{free} test set	1711 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å^2)	109.6	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 65.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	47031	wwPDB-VP
Average B, all atoms (Å^2)	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.89% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: LMT, ACT, MC2

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	0/7846	0.61	1/10666 (0.0%)
1	B	0.26	0/7971	0.59	0/10833
1	C	0.25	0/7971	0.59	0/10833
1	D	0.24	0/7838	0.60	0/10655
1	E	0.25	0/7971	0.60	1/10833 (0.0%)
1	F	0.26	0/7992	0.58	0/10860
All	All	0.26	0/47589	0.59	2/64680 (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 (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	820	GLY	N-CA-C	-5.65	108.25	115.42
1	E	602	GLU	N-CA-C	-5.02	106.90	112.57

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	678	THR	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	7690	0	7828	336	0
1	B	7812	0	7946	329	0
1	C	7812	0	7946	311	0
1	D	7682	0	7817	320	0
1	E	7812	0	7946	310	0
1	F	7832	0	7968	360	0
2	A	70	0	92	5	0
2	B	140	0	184	7	0
2	D	70	0	92	8	0
2	E	70	0	92	6	0
3	B	33	0	29	3	0
4	C	4	0	3	0	0
4	F	4	0	3	0	0
All	All	47031	0	47946	1885	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 20.

The worst 5 of 1885 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:F:414:GLU:HG2	1:F:972:PRO:HG3	1.41	1.01
1:B:617:PHE:HB3	3:B:1101:MC2:H17	1.46	0.97
1:E:446:ALA:HB2	1:E:482:VAL:HG21	1.53	0.90
1:F:738:LEU:HB2	1:F:803:PHE:HZ	1.36	0.88
1:A:135:ASN:HA	1:A:674:LEU:HG	1.55	0.88

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	1009/1056 (96%)	951 (94%)	46 (5%)	12 (1%)	10 42
1	B	1028/1056 (97%)	987 (96%)	34 (3%)	7 (1%)	18 51
1	C	1028/1056 (97%)	980 (95%)	39 (4%)	9 (1%)	14 47
1	D	1008/1056 (96%)	954 (95%)	37 (4%)	17 (2%)	7 35
1	E	1028/1056 (97%)	987 (96%)	35 (3%)	6 (1%)	21 54
1	F	1030/1056 (98%)	981 (95%)	38 (4%)	11 (1%)	11 43
All	All	6131/6336 (97%)	5840 (95%)	229 (4%)	62 (1%)	12 45

5 of 62 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	438	ILE
1	A	640	GLY
1	A	658	PHE
1	A	795	GLY
1	A	872	ALA

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	828/864 (96%)	752 (91%)	76 (9%)	8 32
1	B	841/864 (97%)	763 (91%)	78 (9%)	8 32
1	C	841/864 (97%)	774 (92%)	67 (8%)	11 36
1	D	827/864 (96%)	756 (91%)	71 (9%)	10 34
1	E	841/864 (97%)	764 (91%)	77 (9%)	8 32
1	F	843/864 (98%)	798 (95%)	45 (5%)	20 47
All	All	5021/5184 (97%)	4607 (92%)	414 (8%)	10 35

5 of 414 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	251	LEU
1	D	964	GLU
1	F	626	MET
1	D	337	ILE
1	D	599	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	161	ASN
1	F	391	ASN
1	D	577	GLN
1	F	229	GLN
1	F	759	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

13 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	1101	-	36,36,36	1.14	2 (5%)	47,47,47	0.96	1 (2%)
3	MC2	B	1101	-	35,35,35	1.81	6 (17%)	45,46,46	1.91	9 (20%)
2	LMT	E	1101	-	36,36,36	1.19	2 (5%)	47,47,47	0.89	1 (2%)
4	ACT	F	1101	-	3,3,3	0.93	0	3,3,3	0.80	0
2	LMT	B	1102	-	36,36,36	1.17	2 (5%)	47,47,47	0.90	0
2	LMT	B	1104	-	36,36,36	1.22	3 (8%)	47,47,47	1.22	4 (8%)
2	LMT	B	1105	-	36,36,36	1.13	2 (5%)	47,47,47	0.89	1 (2%)
2	LMT	A	1102	-	36,36,36	1.14	2 (5%)	47,47,47	0.83	1 (2%)
4	ACT	C	1101	-	3,3,3	0.92	0	3,3,3	0.87	0
2	LMT	E	1102	-	36,36,36	1.14	2 (5%)	47,47,47	0.89	1 (2%)
2	LMT	B	1103	-	36,36,36	1.12	2 (5%)	47,47,47	1.03	1 (2%)
2	LMT	D	1102	-	36,36,36	1.13	2 (5%)	47,47,47	1.06	2 (4%)
2	LMT	A	1101	-	36,36,36	1.23	3 (8%)	47,47,47	1.27	7 (14%)

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	1101	-	-	9/21/61/61	0/2/2/2
3	MC2	B	1101	-	-	10/27/27/27	0/3/3/3
2	LMT	E	1101	-	-	14/21/61/61	0/2/2/2
2	LMT	B	1102	-	-	13/21/61/61	0/2/2/2
2	LMT	B	1104	-	-	7/21/61/61	0/2/2/2
2	LMT	B	1105	-	-	8/21/61/61	0/2/2/2
2	LMT	A	1102	-	-	9/21/61/61	0/2/2/2
2	LMT	E	1102	-	-	13/21/61/61	0/2/2/2
2	LMT	B	1103	-	-	14/21/61/61	0/2/2/2
2	LMT	D	1102	-	-	13/21/61/61	0/2/2/2
2	LMT	A	1101	-	-	15/21/61/61	0/2/2/2

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1101	MC2	C15-N3	5.95	1.45	1.33
3	B	1101	MC2	C2-N2	5.11	1.45	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1101	MC2	C11-N6	4.27	1.45	1.35
2	A	1101	LMT	O5'-C1'	3.87	1.51	1.41
2	B	1104	LMT	O5B-C1B	3.71	1.51	1.41

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1101	MC2	C17-C19-N6	-5.61	101.54	120.40
3	B	1101	MC2	C19-N6-C11	5.33	140.17	127.40
2	B	1104	LMT	O5B-C5B-C4B	4.29	117.48	109.69
3	B	1101	MC2	C13-C12-C10	-3.81	102.17	113.92
3	B	1101	MC2	C12-C10-C11	3.80	119.06	110.20

There are no chirality outliers.

5 of 125 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	LMT	C2'-C1'-O1'-C1
2	A	1101	LMT	O5'-C1'-O1'-C1
2	B	1102	LMT	C2-C1-O1'-C1'
2	B	1105	LMT	O5'-C1'-O1'-C1
2	D	1101	LMT	C2-C1-O1'-C1'

There are no ring outliers.

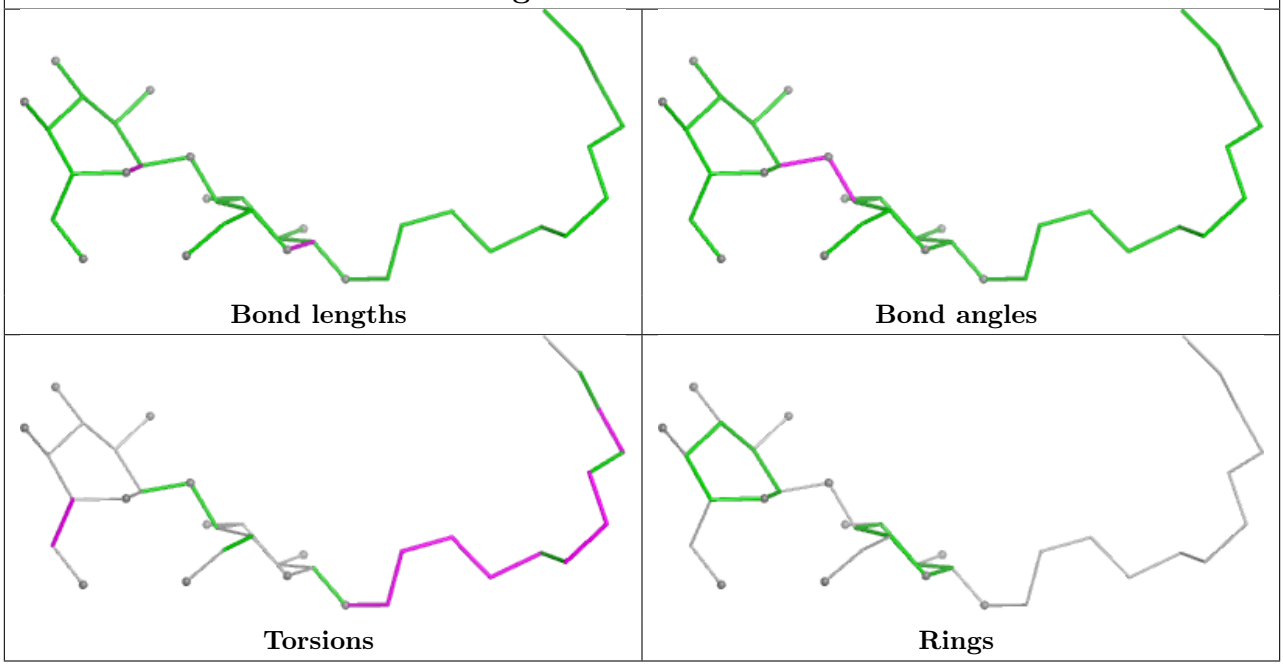
10 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1101	LMT	7	0
3	B	1101	MC2	3	0
2	E	1101	LMT	4	0
2	B	1102	LMT	1	0
2	B	1105	LMT	1	0
2	A	1102	LMT	4	0
2	E	1102	LMT	2	0
2	B	1103	LMT	5	0
2	D	1102	LMT	1	0
2	A	1101	LMT	1	0

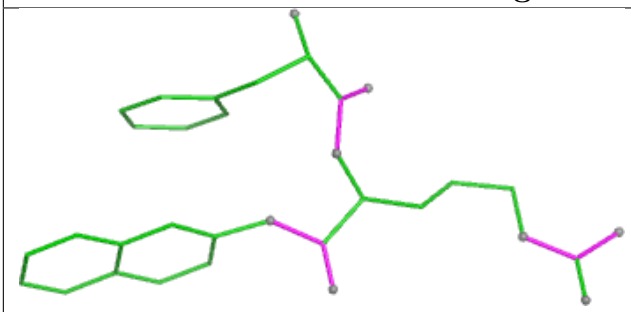
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 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.

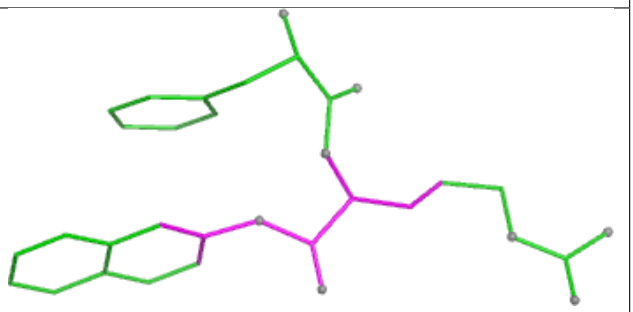
Ligand LMT D 1101



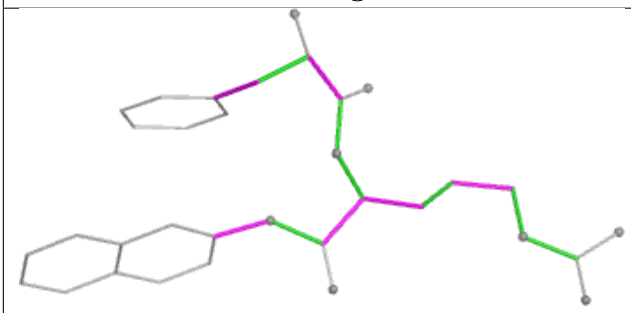
Ligand MC2 B 1101



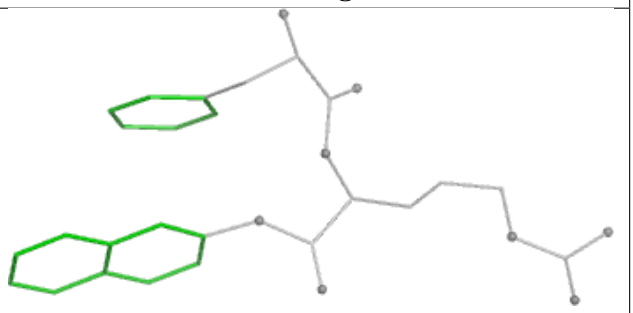
Bond lengths



Bond angles

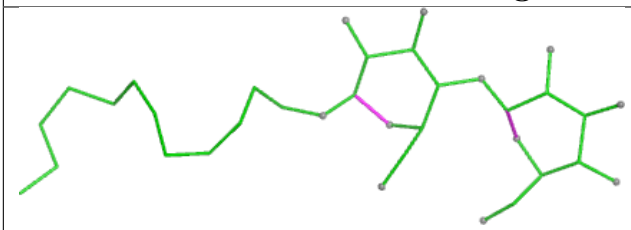


Torsions

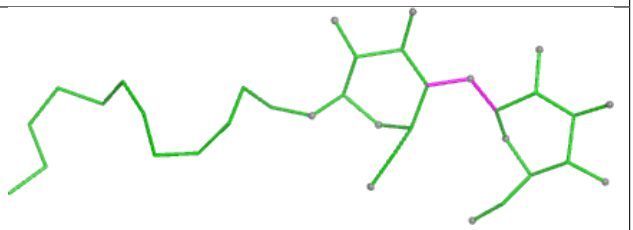


Rings

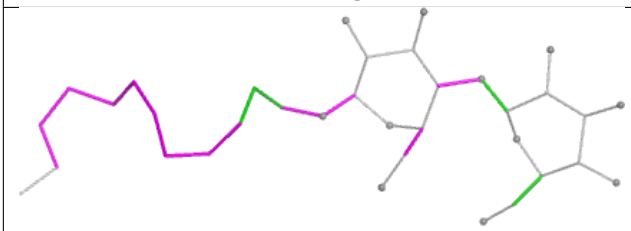
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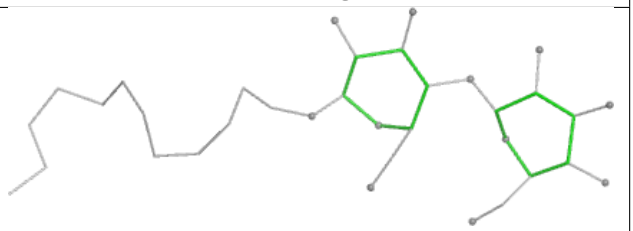
Bond lengths



Bond angles

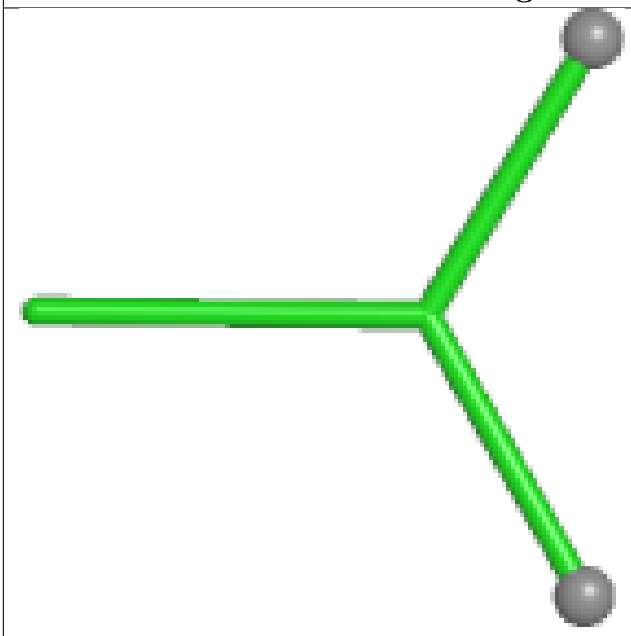


Torsions

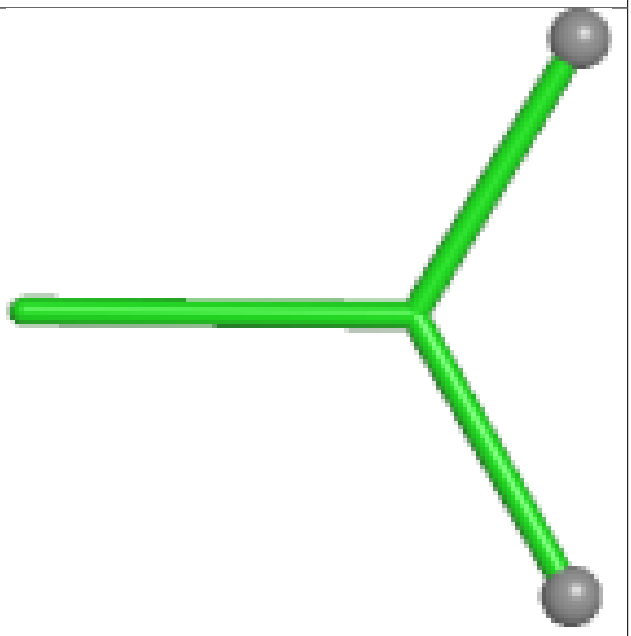


Rings

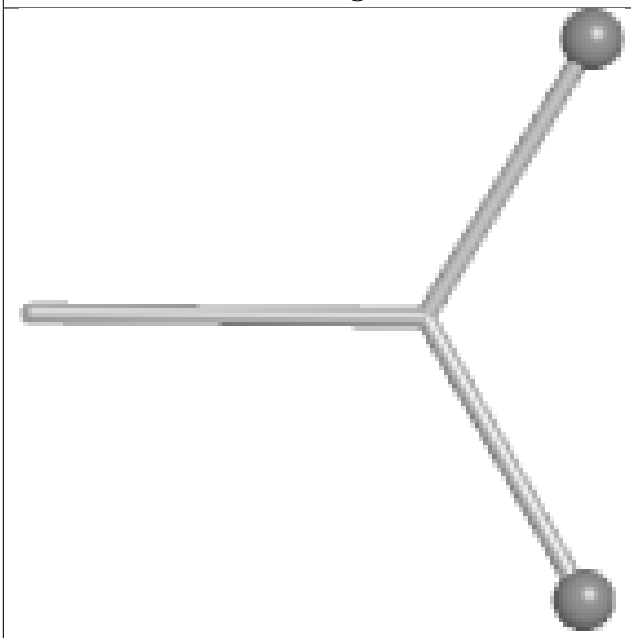
Ligand ACT F 1101



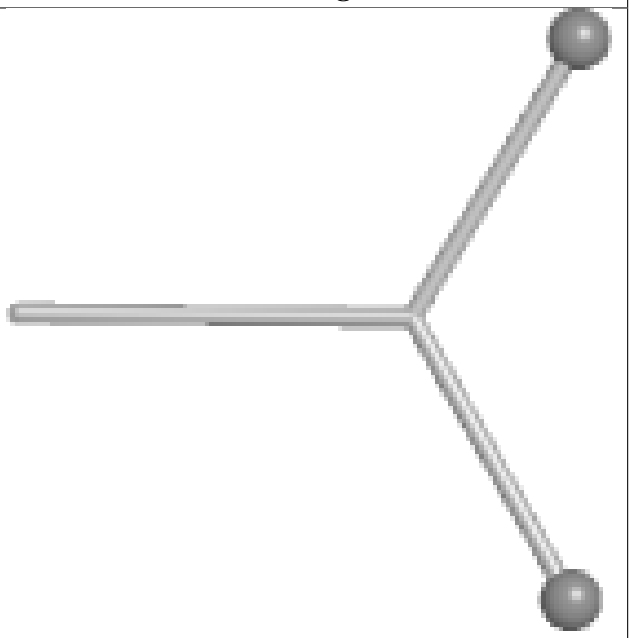
Bond lengths



Bond angles

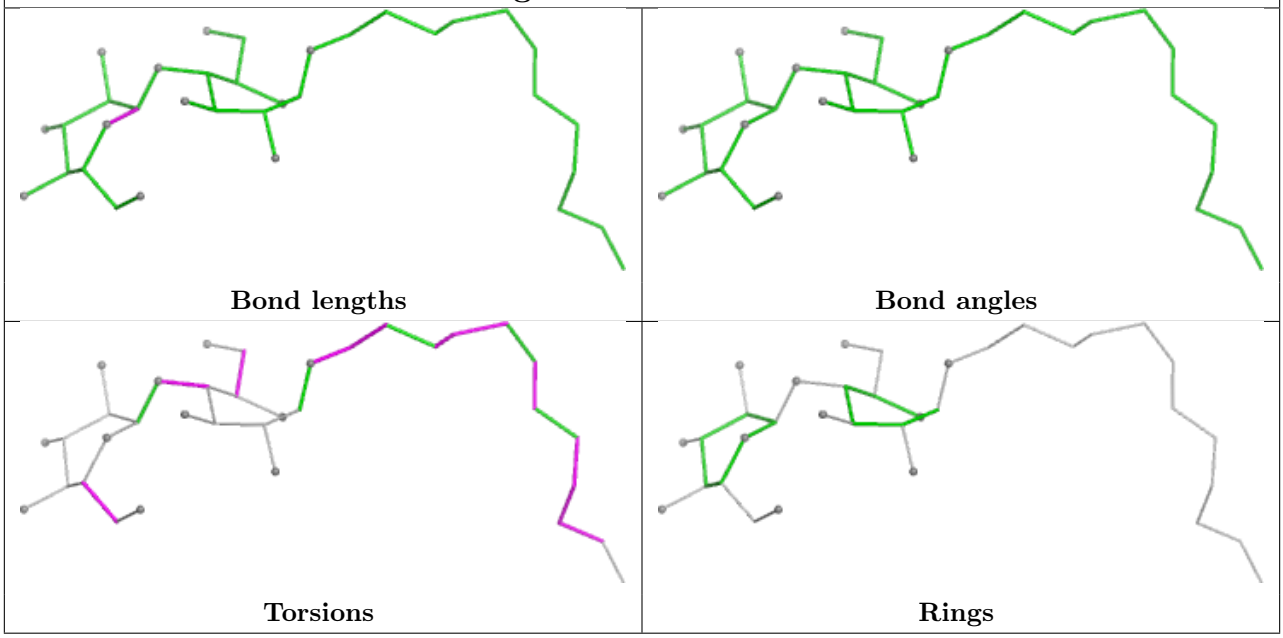


Torsions

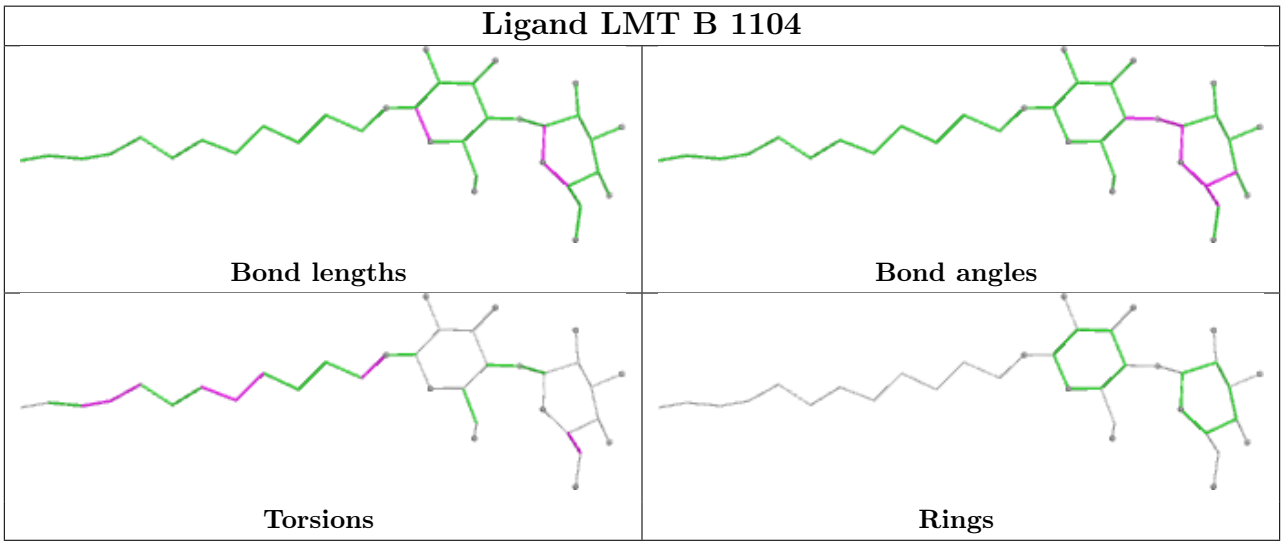


Rings

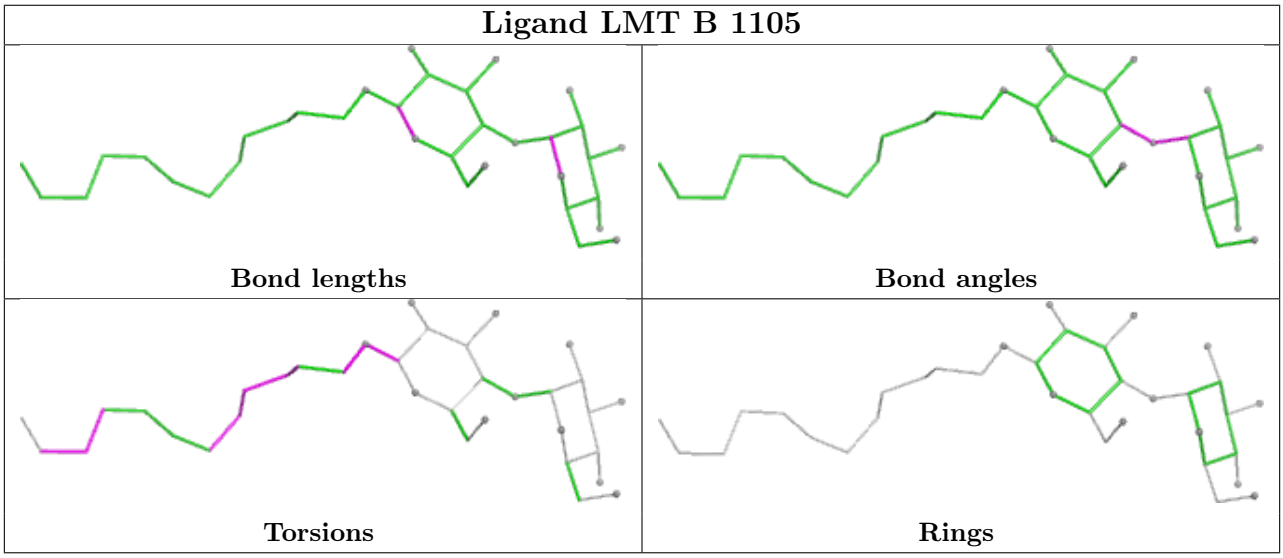
Ligand LMT B 1102



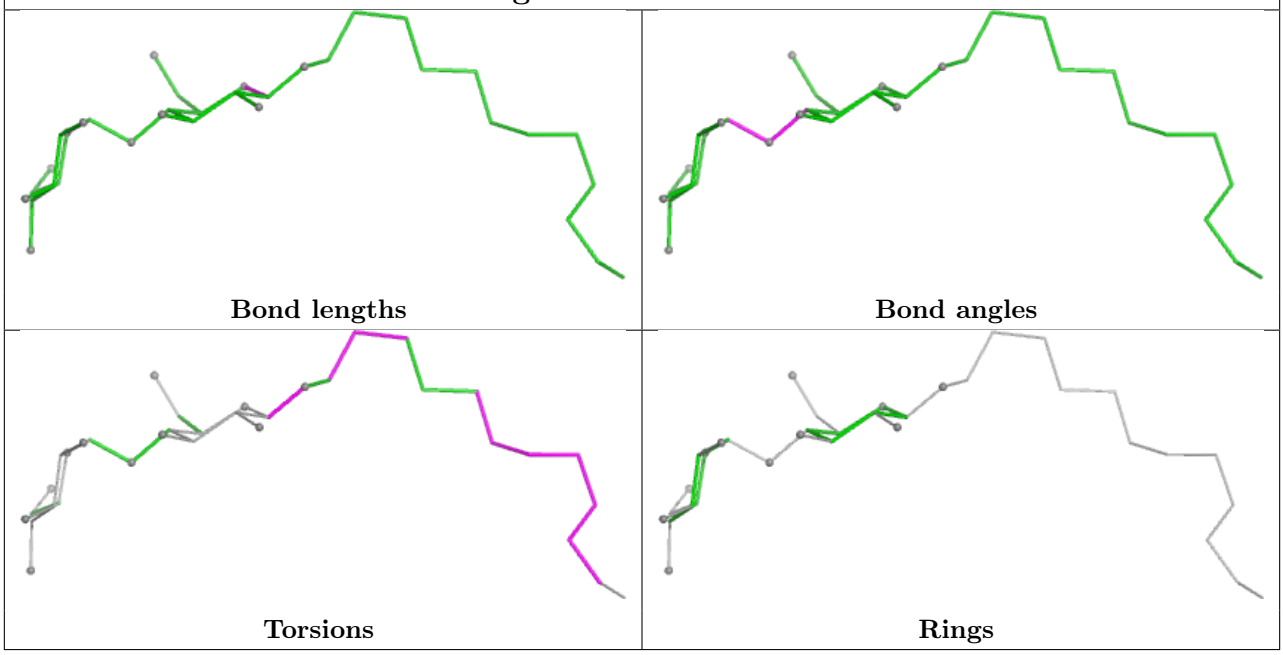
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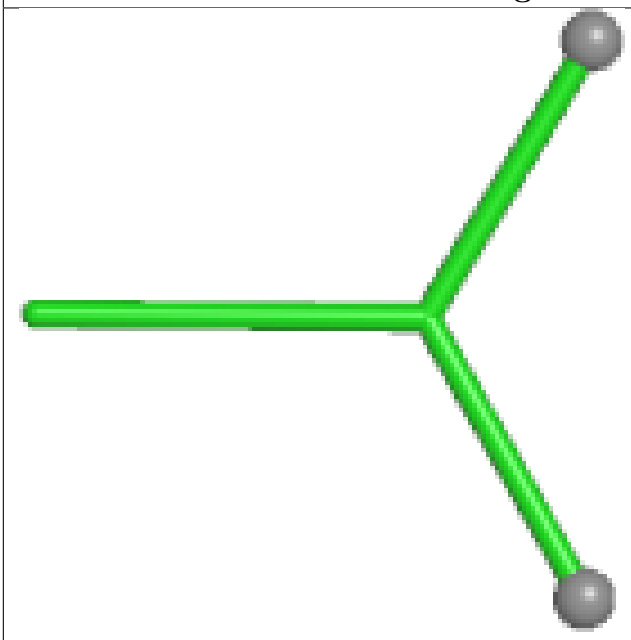
Ligand LMT B 1105



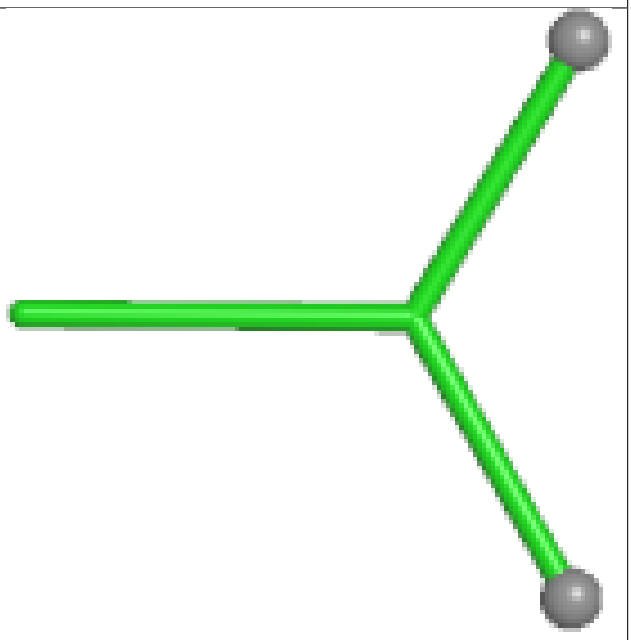
Ligand LMT A 1102



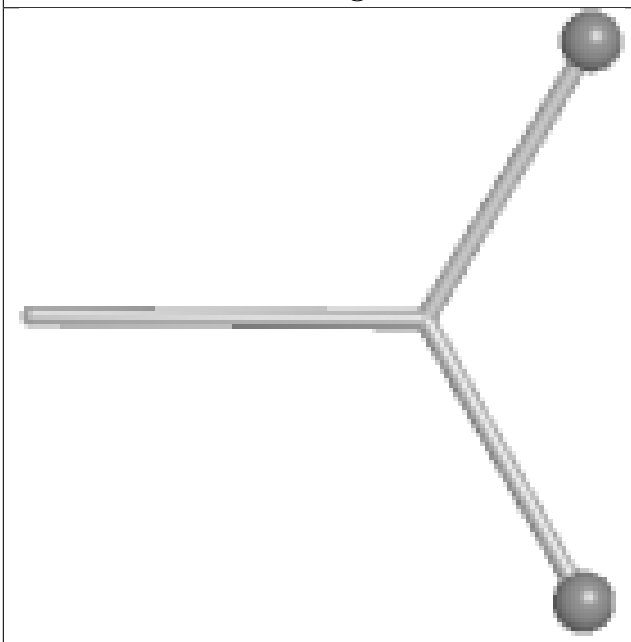
Ligand ACT C 1101



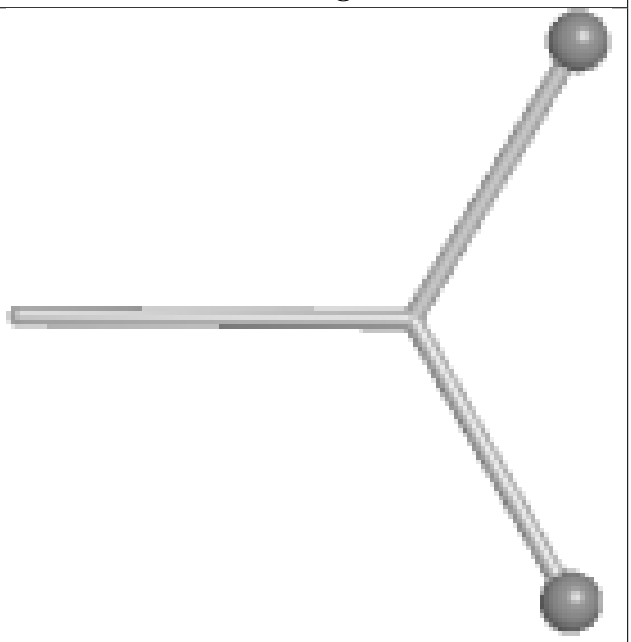
Bond lengths



Bond angles

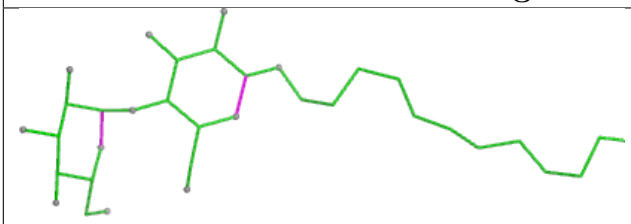


Torsions

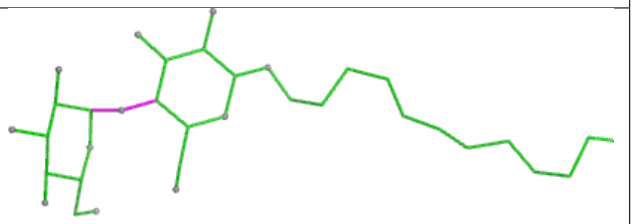


Rings

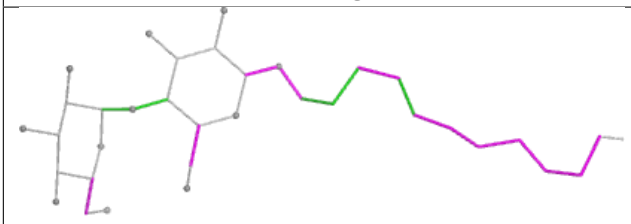
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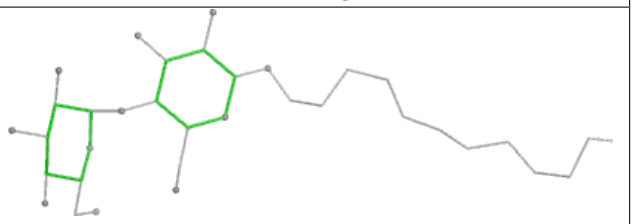
Bond lengths



Bond angles

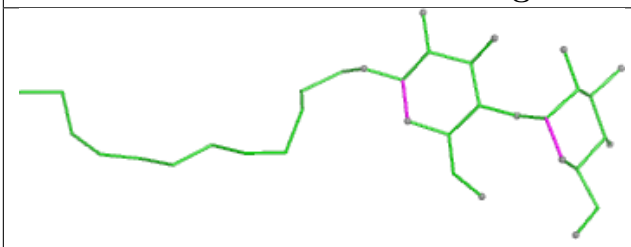


Torsions

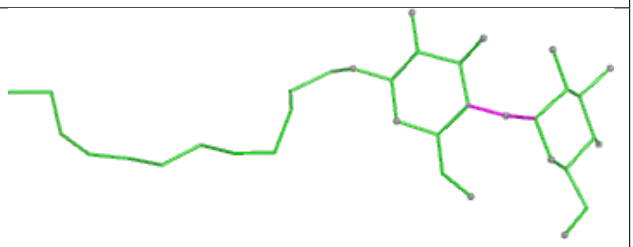


Rings

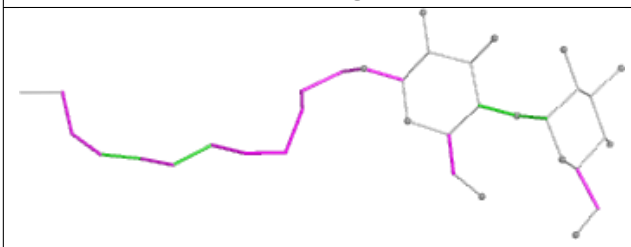
Ligand LMT B 1103



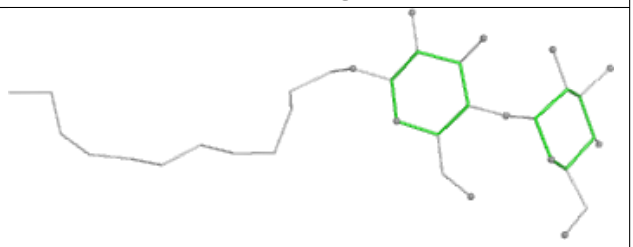
Bond lengths



Bond angles

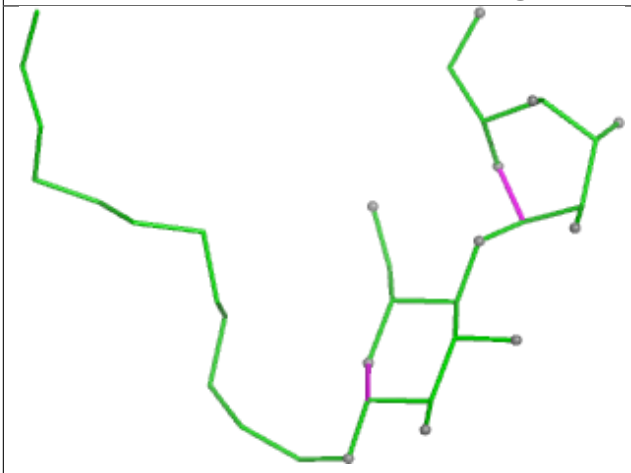


Torsions

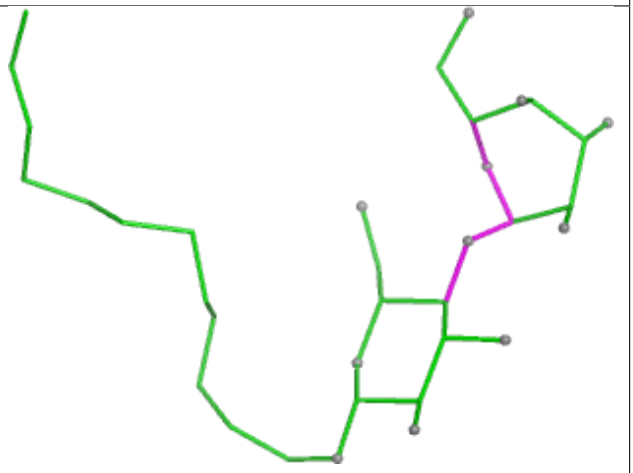


Rings

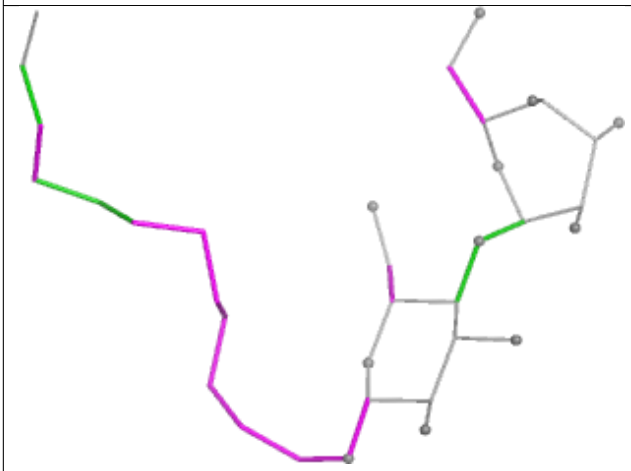
Ligand LMT D 1102



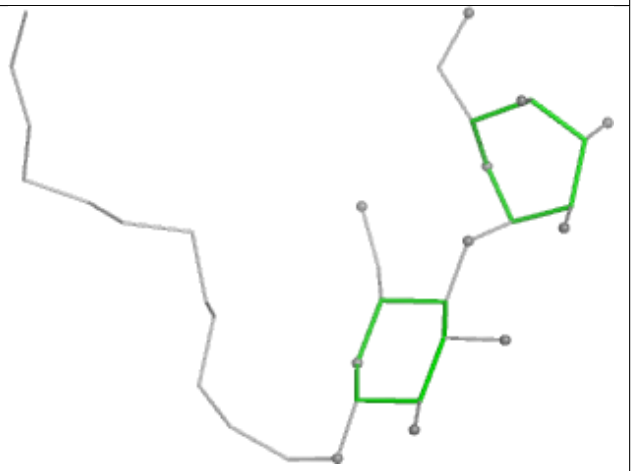
Bond lengths



Bond angles

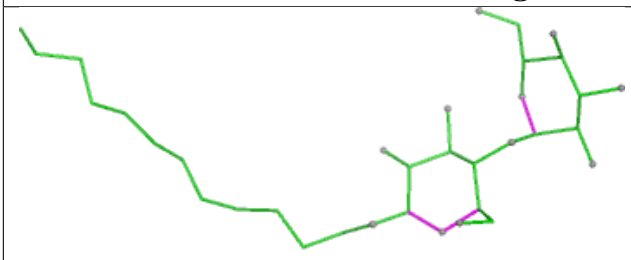


Torsions

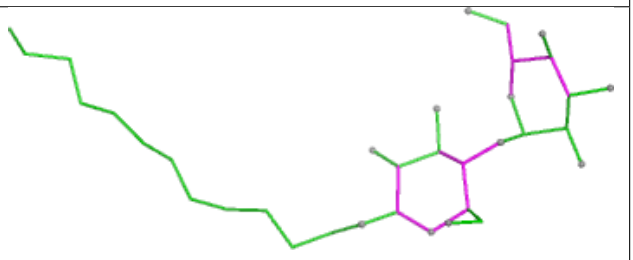


Rings

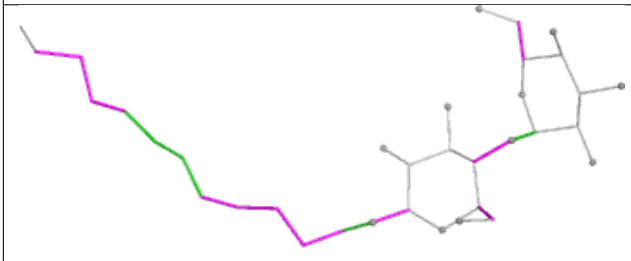
Ligand LMT A 1101



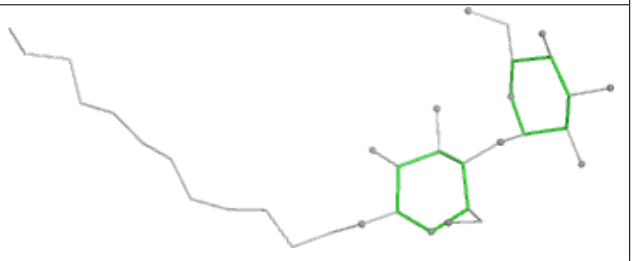
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	1012/1056 (95%)	0.83	127 (12%) 8 6	84, 117, 146, 168	0
1	B	1030/1056 (97%)	0.83	120 (11%) 9 7	78, 115, 160, 194	0
1	C	1028/1056 (97%)	0.67	93 (9%) 15 10	88, 132, 186, 229	0
1	D	1011/1056 (95%)	0.87	116 (11%) 9 7	87, 123, 159, 192	0
1	E	1030/1056 (97%)	0.80	120 (11%) 9 7	85, 123, 170, 189	0
1	F	1030/1056 (97%)	0.72	94 (9%) 15 9	87, 128, 181, 224	0
All	All	6141/6336 (96%)	0.79	670 (10%) 10 7	78, 123, 170, 229	0

The worst 5 of 670 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	675	GLY	10.7
1	D	676	ASN	10.5
1	B	126	GLY	10.3
1	A	44	ALA	10.2
1	D	728	LEU	10.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands (i)

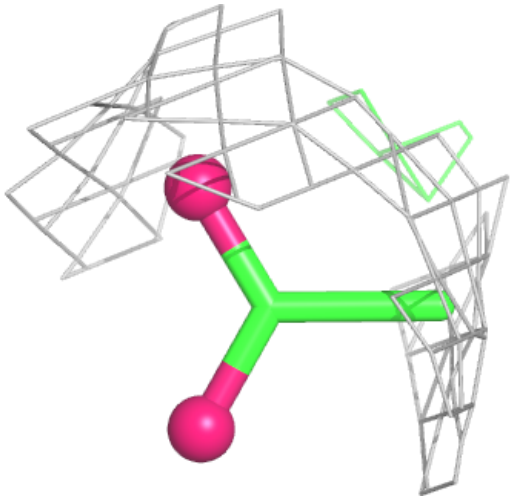
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

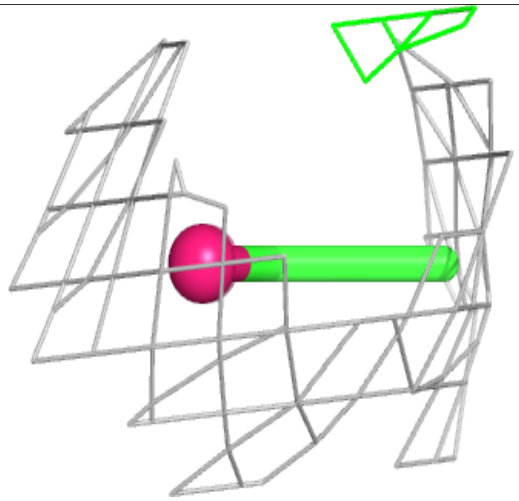
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ACT	F	1101	4/4	0.36	0.30	130,130,131,131	0
4	ACT	C	1101	4/4	0.50	0.21	112,112,112,112	0
2	LMT	B	1102	35/35	0.56	0.19	120,123,128,129	0
3	MC2	B	1101	33/33	0.56	0.27	137,138,139,139	0
2	LMT	B	1103	35/35	0.71	0.30	122,135,152,160	0
2	LMT	D	1102	35/35	0.75	0.17	98,104,120,123	0
2	LMT	B	1104	35/35	0.76	0.14	106,115,128,132	0
2	LMT	E	1101	35/35	0.79	0.18	107,126,138,143	0
2	LMT	A	1101	35/35	0.79	0.17	102,116,141,146	0
2	LMT	E	1102	35/35	0.81	0.14	103,120,131,140	0
2	LMT	D	1101	35/35	0.84	0.12	112,127,148,154	0
2	LMT	A	1102	35/35	0.85	0.15	102,119,134,138	0
2	LMT	B	1105	35/35	0.88	0.11	98,104,109,113	0

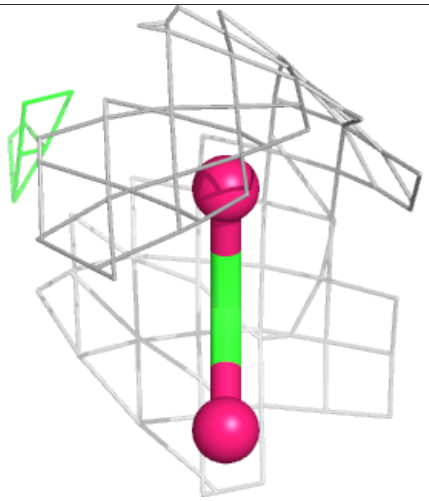
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACT F 1101:

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

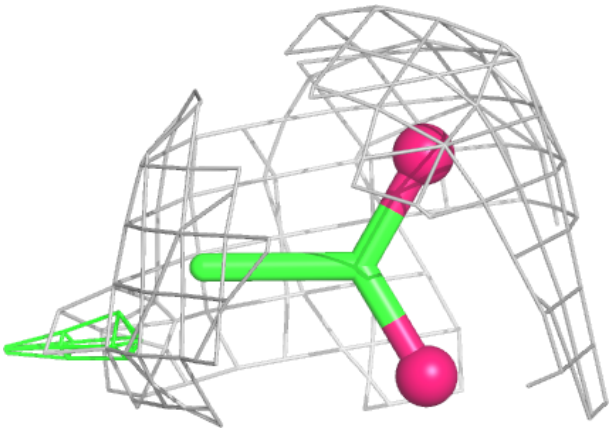


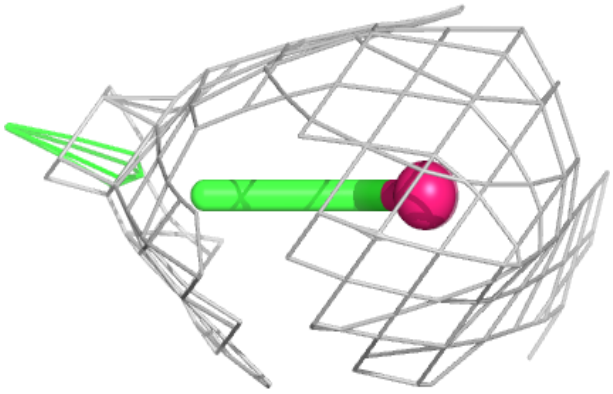


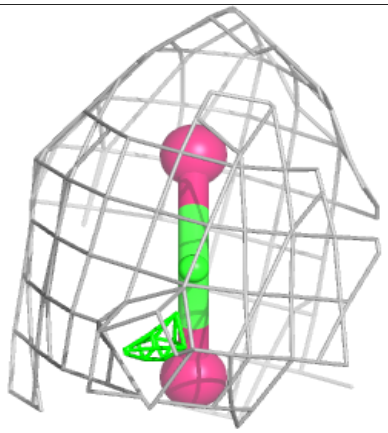


Electron density around ACT C 1101:

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

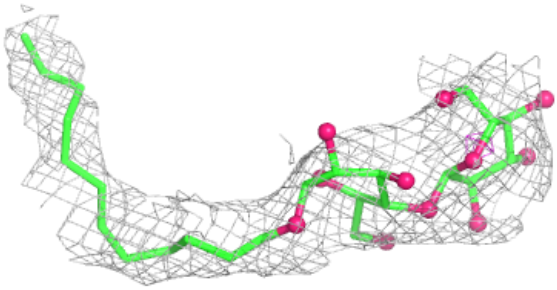


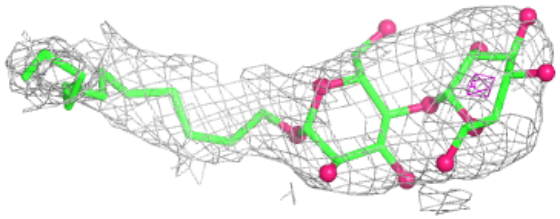


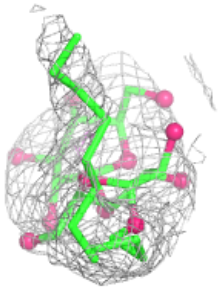


Electron density around LMT B 1102:

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

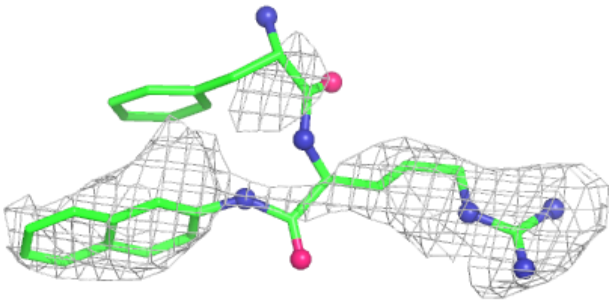


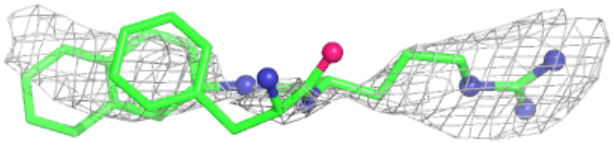


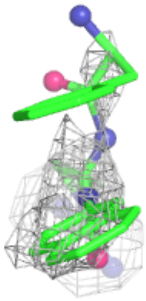


Electron density around MC2 B 1101:

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

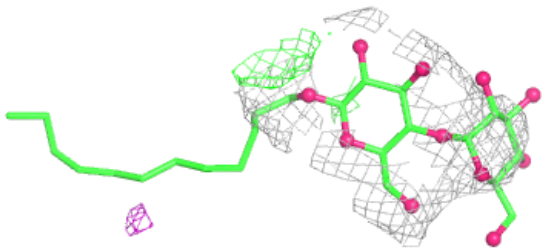


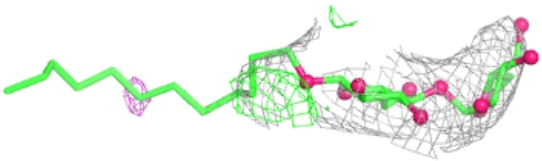




Electron density around LMT B 1103:

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

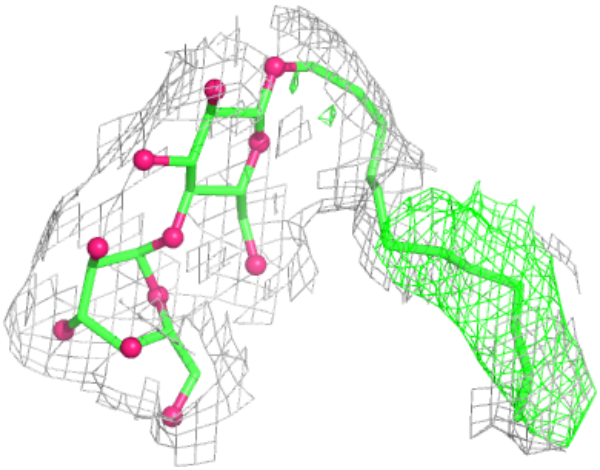


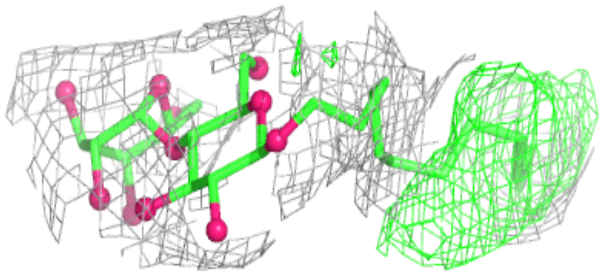


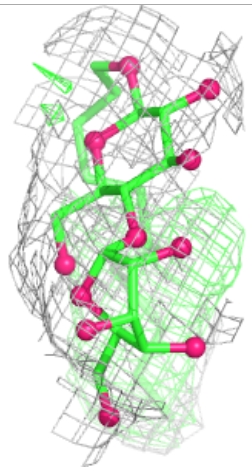


Electron density around LMT D 1102:

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

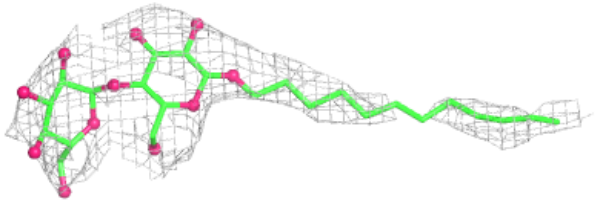


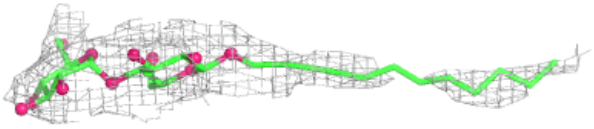


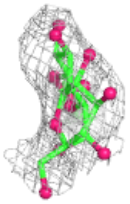


Electron density around LMT B 1104:

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

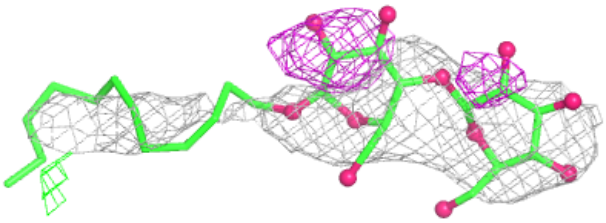


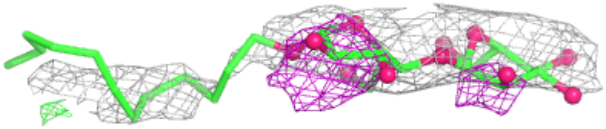


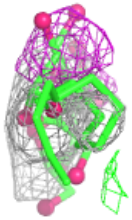


Electron density around LMT E 1101:

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

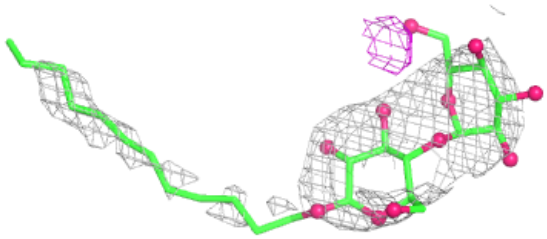


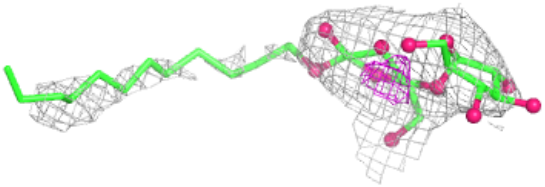




Electron density around LMT A 1101:

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

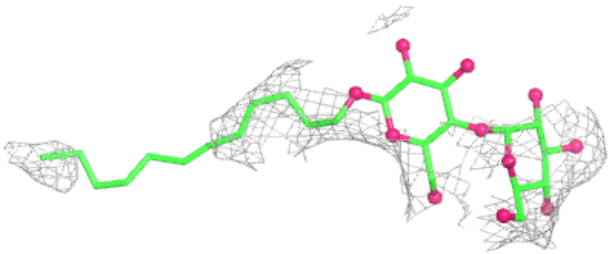


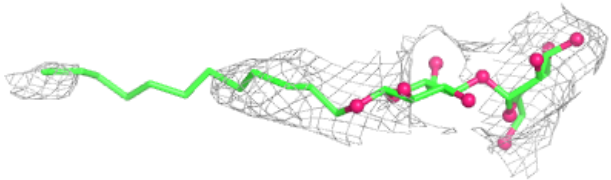


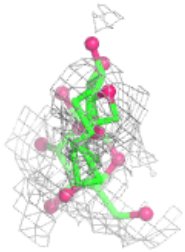


Electron density around LMT E 1102:

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

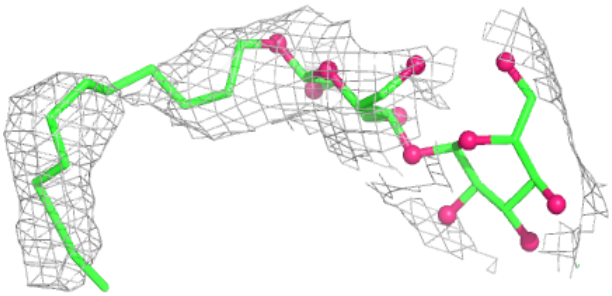


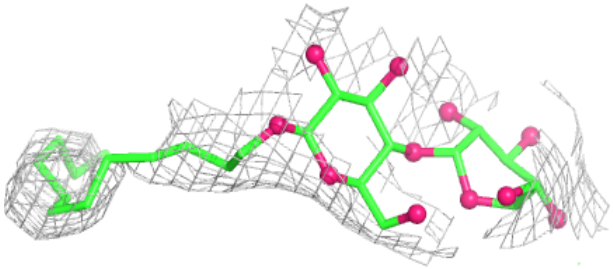




Electron density around LMT D 1101:

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

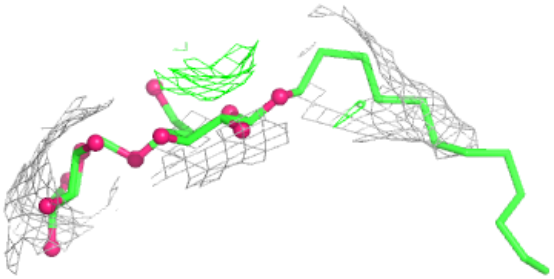


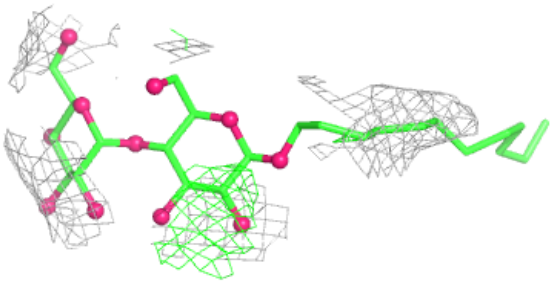


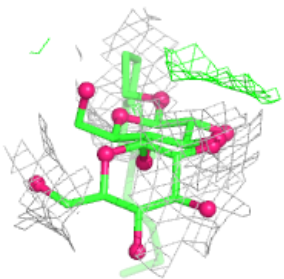


Electron density around LMT A 1102:

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

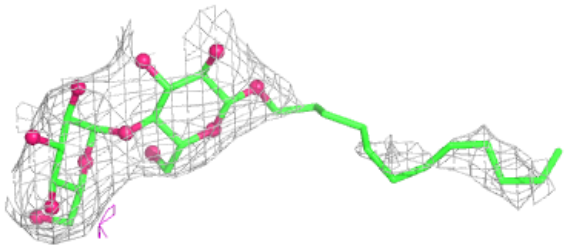


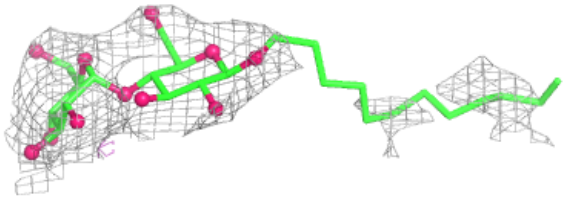


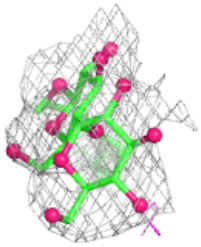


Electron density around LMT B 1105:

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







6.5 Other polymers

There are no such residues in this entry.