wwPDB X-ray Structure Validation Summary Report (i)

Dec 3, 2023 – 12:31 pm GMT

PDB ID	:	2V50
Title	:	The Missing Part of the Bacterial MexAB-OprM System: Structural determination of the Multidrug Exporter MexB
Authors	:	Sennhauser, G.; Bukowska, M.A.; Gruetter, M.G.
Deposited on	:	2008-10-01
Resolution	:	3.00 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:

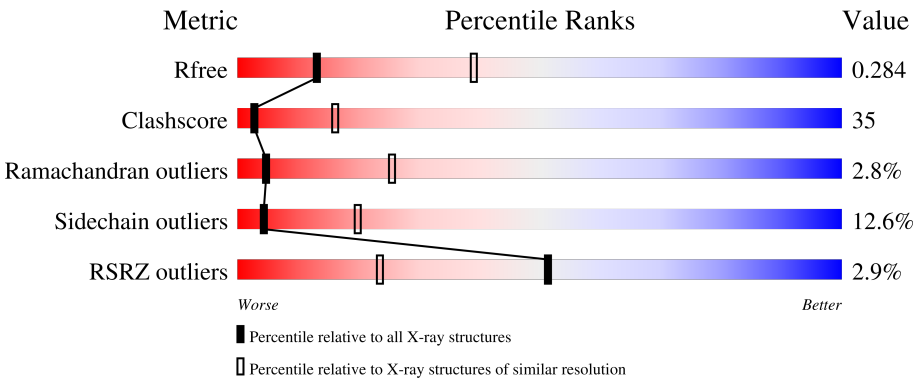
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	1052	.% 37% 46% 12% • •
1	B	1052	2% 46% 44% 8% •
1	C	1052	4% 46% 45% 7% •
1	D	1052	2% 38% 46% 11% • 5%
1	E	1052	4% 44% 44% 8% •

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Mol	Chain	Length	Quality of chain
1	F	1052	4% 46% 45% 7%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LMT	B	2033	-	-	-	X

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 46628 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	1005	7634	4920	1265	1410	39	6	0	0
1	B	1030	7812	5027	1298	1447	40	0	0	0
1	C	1030	7812	5027	1298	1447	40	12	0	0
1	D	998	7582	4888	1255	1399	40	0	0	0
1	E	1012	7696	4956	1279	1421	40	0	0	0
1	F	1030	7812	5027	1298	1447	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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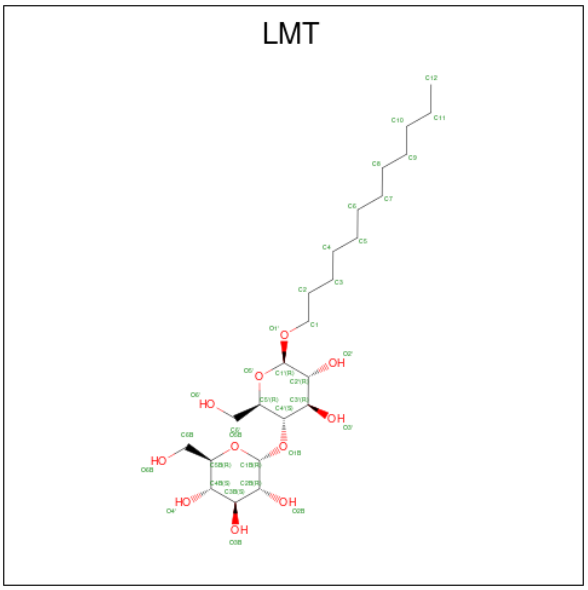
Chain	Residue	Modelled	Actual	Comment	Reference
C	1052	HIS	-	expression tag	UNP P52002
D	1047	HIS	-	expression tag	UNP P52002
D	1048	HIS	-	expression tag	UNP P52002
D	1049	HIS	-	expression tag	UNP P52002
D	1050	HIS	-	expression tag	UNP P52002
D	1051	HIS	-	expression tag	UNP P52002
D	1052	HIS	-	expression 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-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



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

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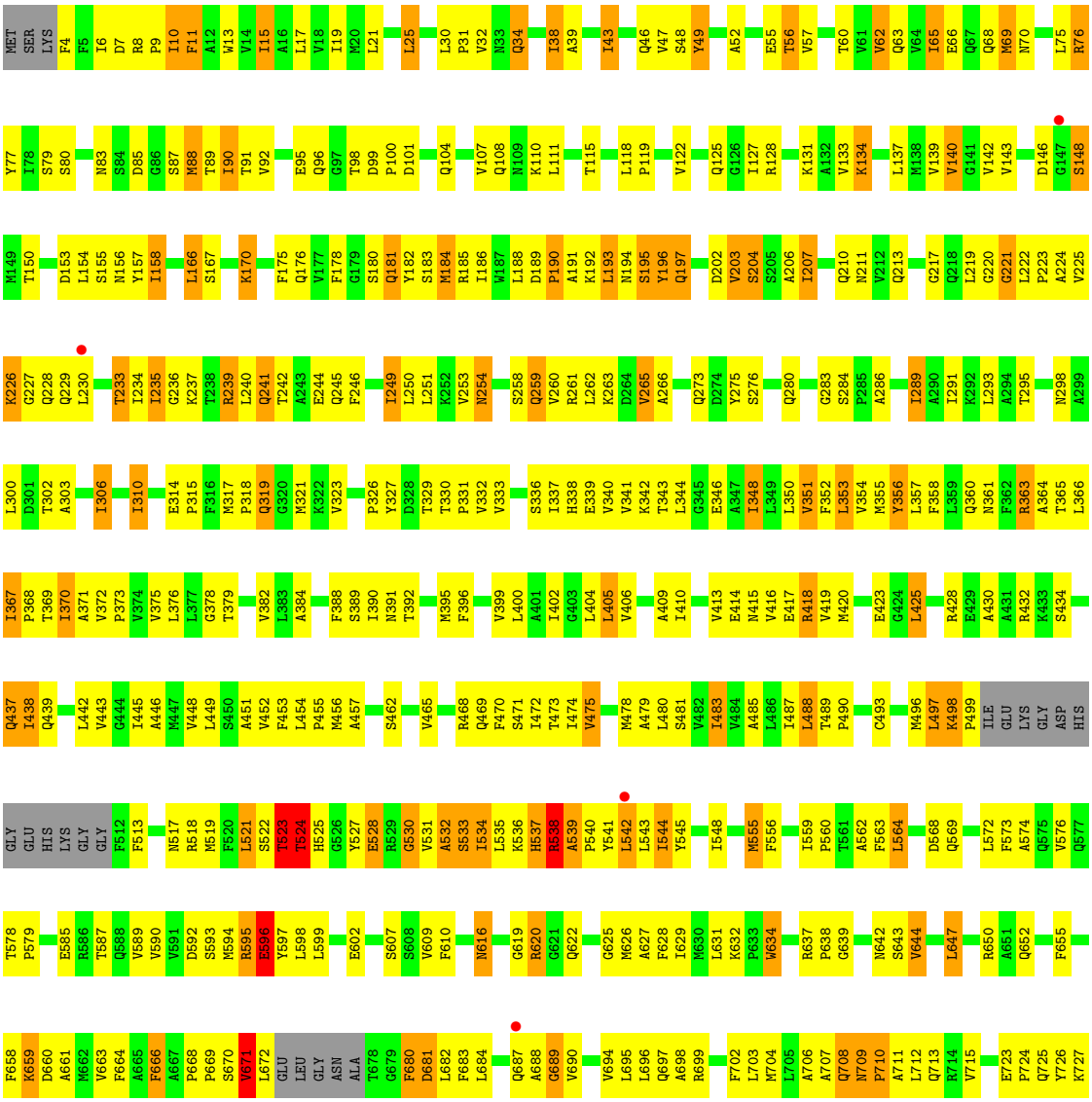
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	B	1	35	24	11	0	0
			Total	C	O		
2	B	1	35	24	11	0	0
			Total	C	O		
2	B	1	35	24	11	0	0
			Total	C	O		
2	D	1	35	24	11	0	0
			Total	C	O		
2	E	1	35	24	11	0	0
			Total	C	O		
2	E	1	35	24	11	0	0
			Total	C	O		
2	E	1	35	24	11	0	0

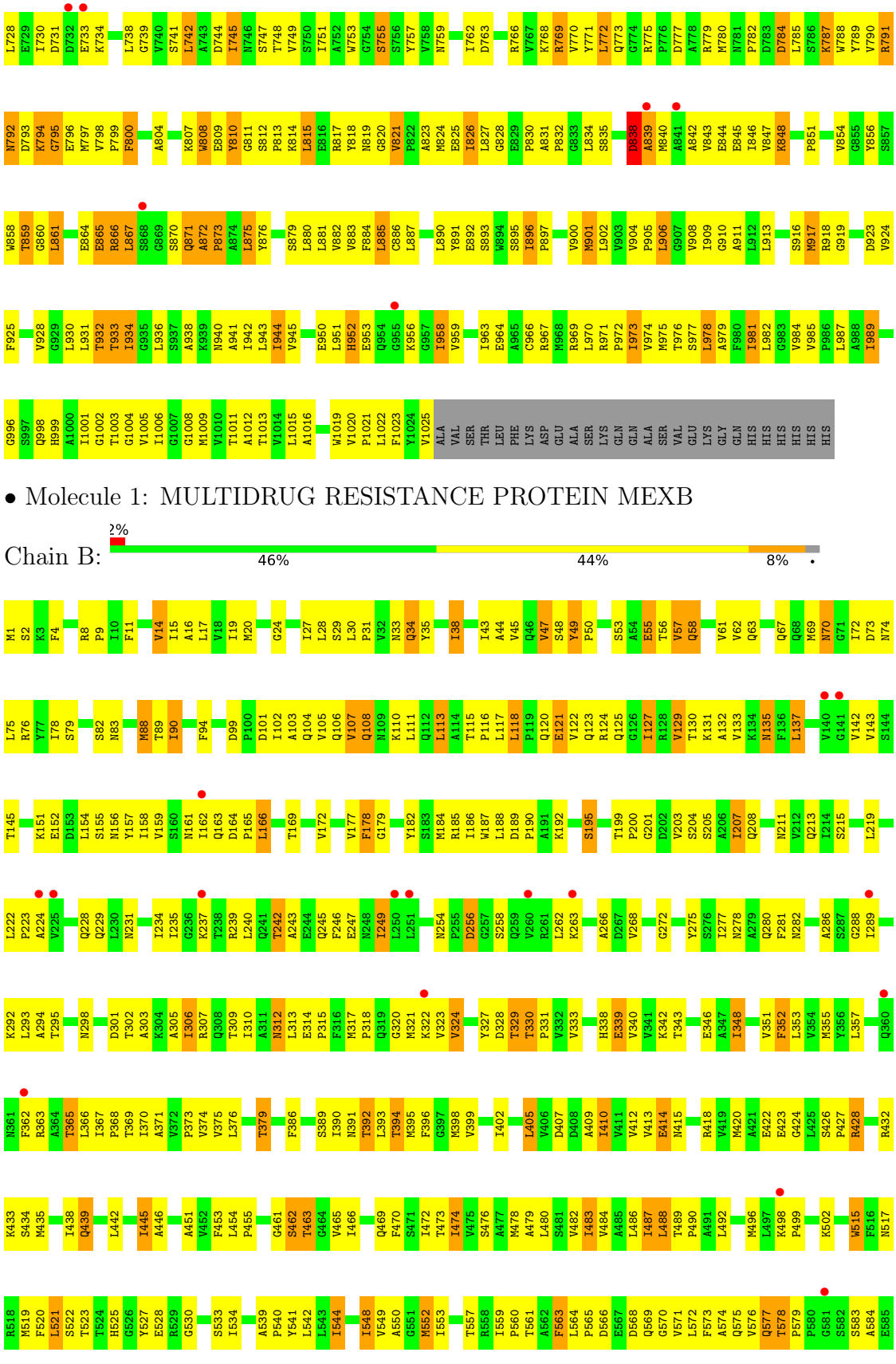
3 Residue-property plots (i)

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

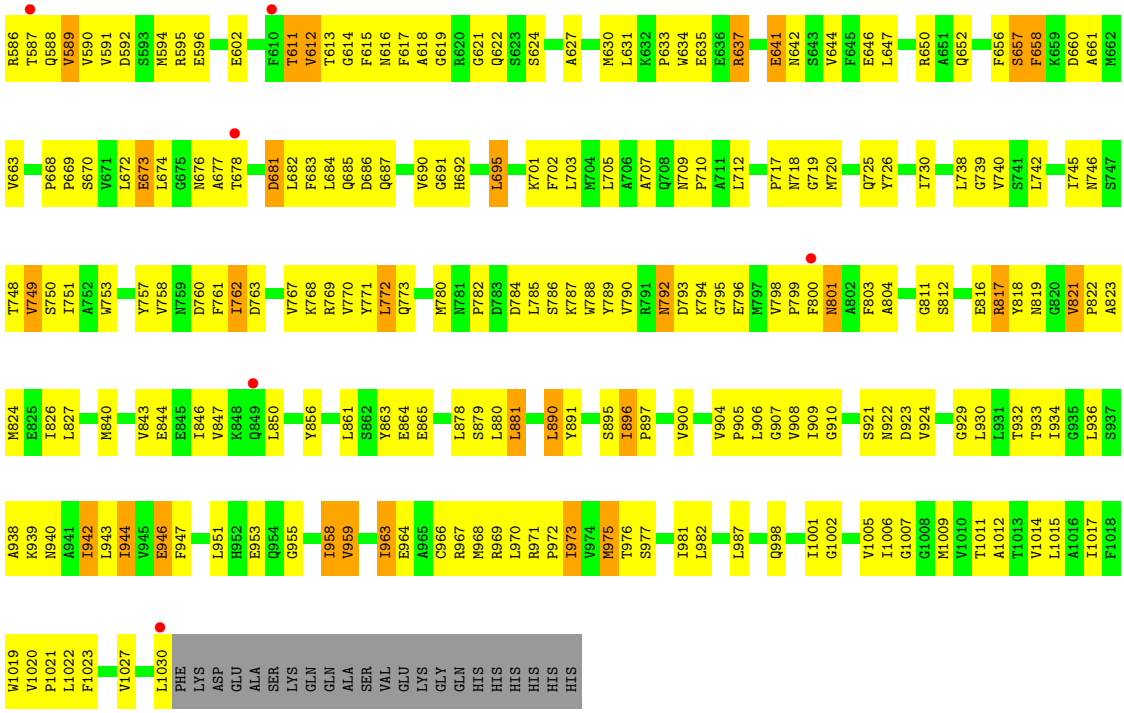
Chain A:





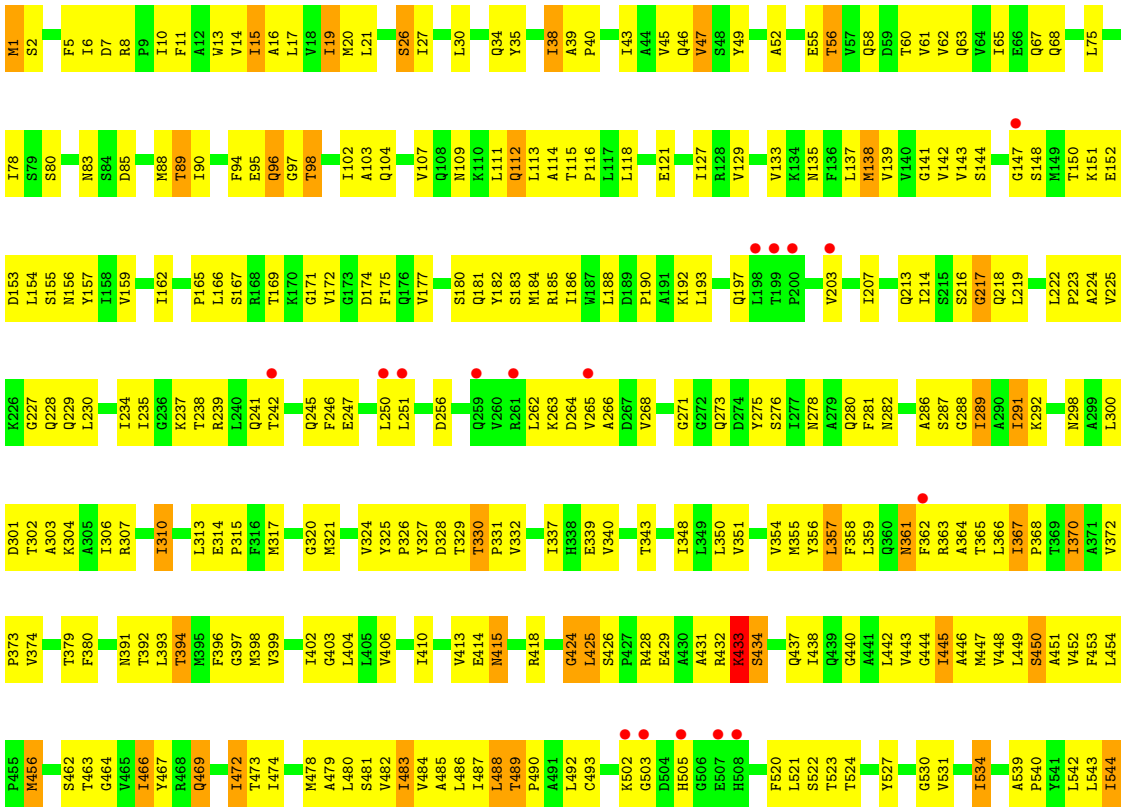
• Molecule 1: MULTIDRUG RESISTANCE PROTEIN MEXB

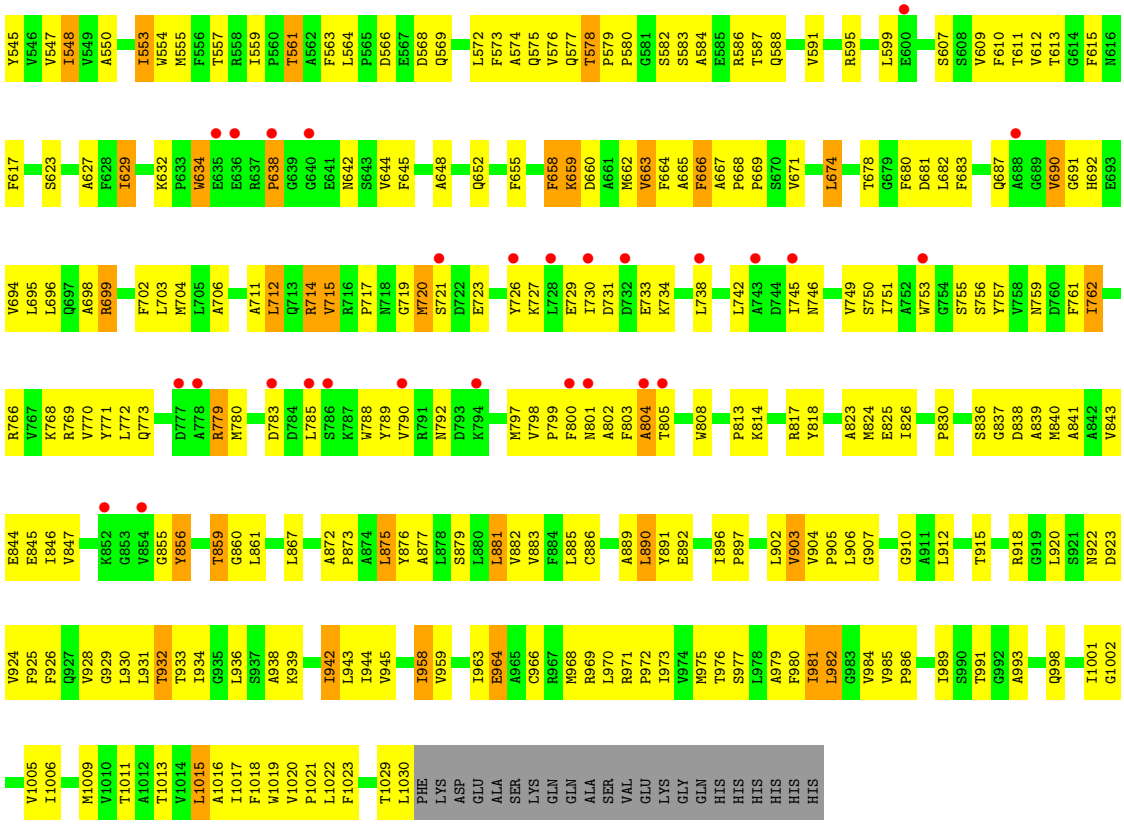
Chain B: 2% 46% 44% 8%



• Molecule 1: MULTIDRUG RESISTANCE PROTEIN MEXB

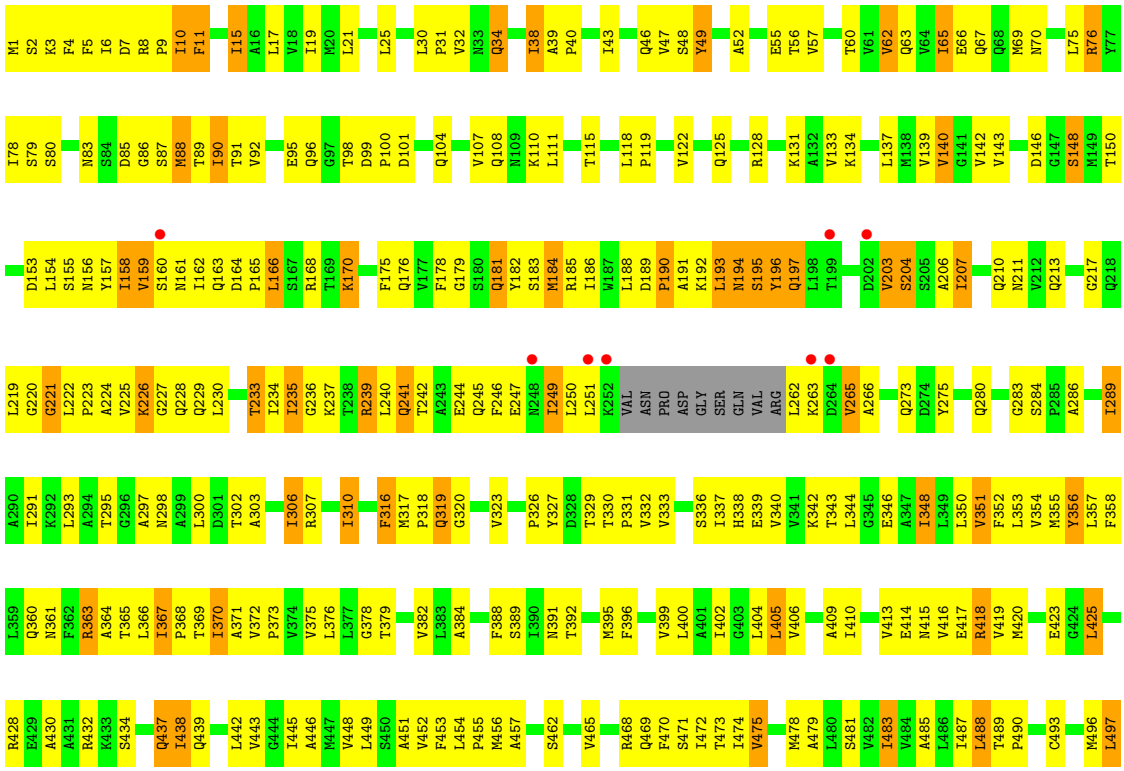
Chain C: 4% 46% 45% 7%





• Molecule 1: MULTIDRUG RESISTANCE PROTEIN MEXB

Chain D:



K498 P499 ILE GLU LYS GLY ASP HIS GLY GLU HIS LYS GLY GLY F512 F513 N517 R518 M519 F520 L521 S522 T523 T524 H525 G526 Y527 E528 R529 G530 V531 A532 S533 I534 L535 K536 H537 R538 A539 P540 Y541 L542 L543 I544 Y545 I548 M555 F556 A562 F563 L564 D568 Q569 G570 V571

L572 F573 A574 Q576 V576 Q577 T578 P579 P580 G581 S582 S583 A584 E585 R586 T587 Q588 V589 V590 V591 D592 S593 S594 R595 E596 L599 E600 K601 E602 S603 S604 S607 S608 V609 F610 T611 N616 R620 G621 Q622 G625 M626 A627 F628 I629 M630 L631 K632 P633 W634 E635 E636 R637 P638 G639

N642 S643 V644 L647 R650 A651 Q652 F655 F658 K659 D660 A661 M662 V663 F664 A665 F666 A667 P668 P669 SER VAL LEU GLU LEU GLY N676 F680 D681 L682 F683 L684 A688 G689 V690 V694 L695 L696 Q697 A698 R699 N700 K701 F702 L703 M704 L705 Q708 L712 Q713

R714 V715 E723 P724 Q725 Y726 K727 L728 E729 I730 D731 D732 E733 K734 L738 G739 V740 S741 L742 A743 D744 T745 N746 S747 T748 V749 S750 I751 A752 W753 G754 S755 S756 Y757 V758 N759 I762 D763 R766 V767 K768 R769 V770 Y771 L772 Q773 G774 R775 P776 D777 A778 R779 M780 N781 P782 D783

D784 L785 S786 K787 W788 Y789 V790 R791 W792 D793 K794 M797 V798 P799 F800 A804 T805 G806 K807 W808 E809 Y810 G811 S812 P813 K814 L815 E816 R817 Y818 N819 G820 A823 M824 E825 I826 L827 G828 E829 P830 A831 P832 S835 D838 A839 M840 A841 A842 V843 E844 E845 I846 V847 K848 Q849

L850 P851 V854 G855 Y856 S857 W858 T859 G860 L861 E864 E865 R866 L867 S870 Q871 A872 P873 A874 L875 Y876 S879 L880 L881 V882 V883 F884 L885 C886 L887 L890 Y891 E892 S893 W894 S895 I896 P897 V900 M901 L902 W903 V904 P905 L906 G907 V908 I909 G910 A911 L912 L913 S916

M917 R918 D923 V928 G929 L930 L931 T932 T933 I934 G935 L936 S937 A938 K939 N940 A941 I942 L943 I944 V945 E950 L951 H952 E953 K956 G957 I958 V959 I963 E964 A965 C966 R967 H968 R969 L970 R971 P972 I973 V974 M975 T976 S977 L978 A979 F980 I981 L982 G983 V984 V985 P986 L987

G996 S997 Q998 H999 A1000 I1001 G1002 T1003 G1004 V1005 I1006 G1007 G1008 M1009 A1012 T1013 V1014 L1015 A1016 W1019 V1020 P1021 L1022 F1023 Y1024 V1025 ALA VAL SER THR LEU PHE LYS ASP GLU ALA SER LYS GLN GLN ALA SER VAL GLU LYS GLY GLN HIS HIS HIS HIS HIS HIS

- Molecule 1: MULTIDRUG RESISTANCE PROTEIN MEXB

Chain E: 4% 44% 44% 8%

M1 S2 K3 F4 R8 P9 I10 F11 V14 I15 A16 L17 V18 I19 M20 G24 I27 L28 S29 L30 P31 V32 N33 Q34 Y35 I38 I43 A44 V45 Q46 V47 S48 Y49 S53 A54 E55 T56 V57 Q58 V61 V62 Q63 Q67 Q68 M69 N70 G71 I72 D73 N74 L75

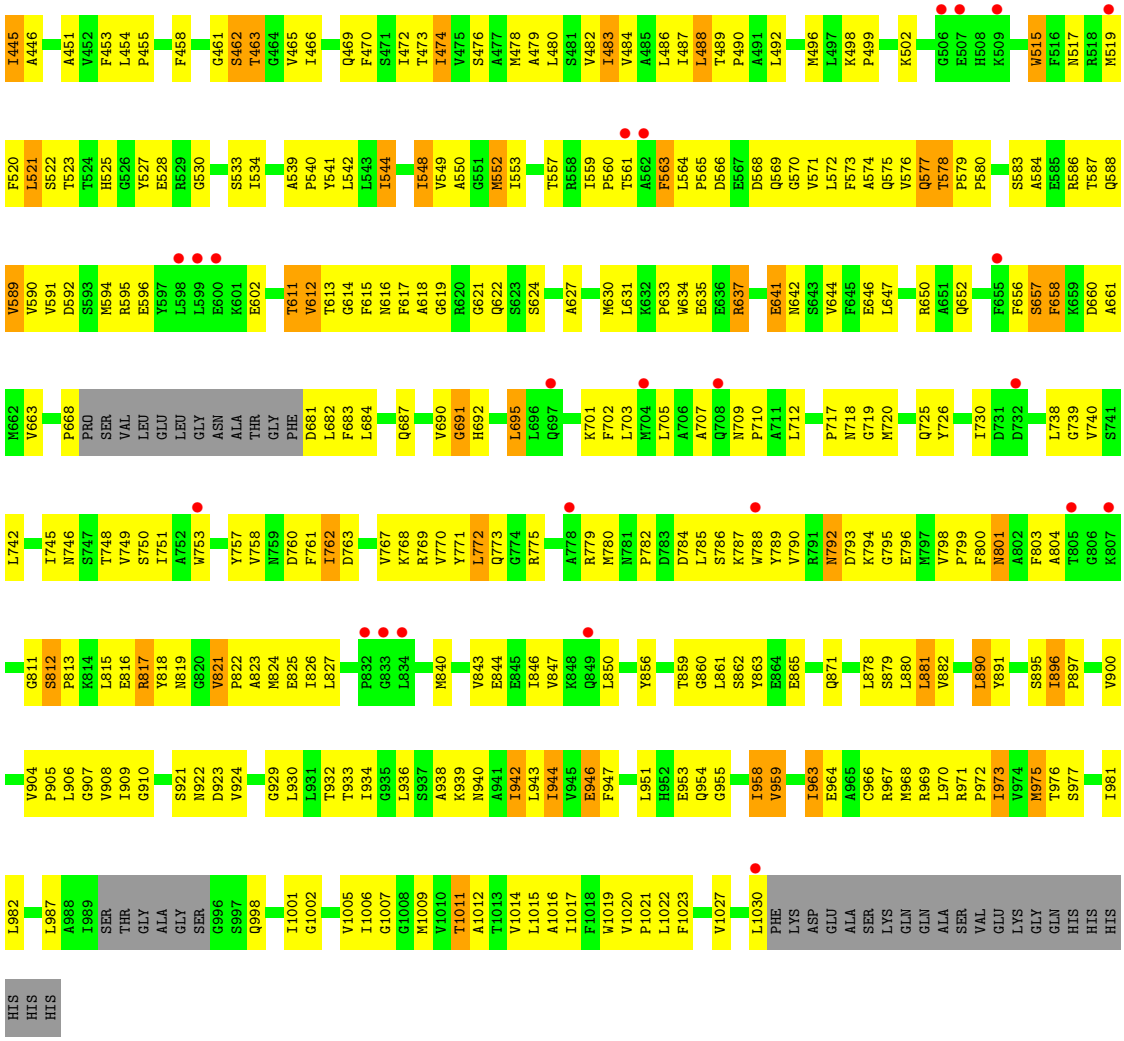
R76 Y77 I78 S79 S82 N83 S84 D85 M88 T89 I90 F94 D99 P100 D101 I102 A103 Q104 V105 Q106 V107 Q108 N109 K110 L111 Q112 L113 A114 T115 P116 L117 L118 P119 Q120 E121 V122 Q123 R124 Q125 G126 I127 R128 V129 T130 K131 A132 V133 K134 N135 F136 L137 V142 V143 S144 T145

K151 E152 D153 L154 S155 N156 Y157 I158 V159 S160 N161 I162 Q163 D164 P165 L166 T169 V172 V177 F178 Y182 S183 M184 R185 I186 W187 L188 D189 P190 A191 K192 S195 T199 P200 G201 D202 V203 S204 I207 Q208 N211 V212 Q213 I214 S215 L219 A224 Q228

Q229 L230 N231 A232 T233 I234 I235 G236 K237 T238 R239 L240 Q241 T242 A243 E244 Q245 F246 E247 N248 I249 L250 L251 K252 V253 N254 P255 D256 G257 S258 Q259 V260 R261 L262 K263 D264 V265 A266 D267 V268 G271 G272 I277 N278 A279 Q280 F281 N282 A286 S287 G288 I289 K292 L293 A294 T295

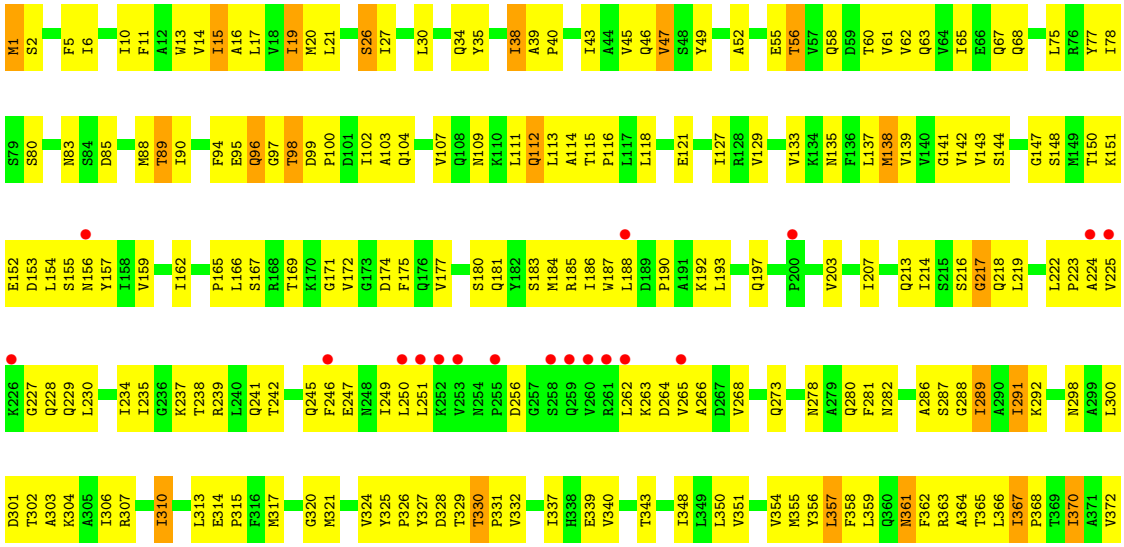
N298 D301 T302 A303 K304 A305 I306 R307 Q308 T309 I310 A311 N312 L313 E314 P315 F316 M317 P318 Q319 G320 M321 K322 V323 V324 Y327 D328 T329 T330 P331 V332 V333 H338 E339 V340 V341 K342 T343 E346 A347 I348 V351 F352 L353 V354 M355 Y356 L357 F362 R363 A364 T365 L366

I367 P368 T369 I370 A371 V374 V375 L376 T379 S389 I390 N391 T392 L393 T394 N395 F396 G397 M398 V399 I402 L405 V406 D407 D408 A409 I410 V411 V412 V413 E414 N415 R418 V419 M420 A421 E422 E423 G424 L425 S426 P427 R428 R432 K433 S434 M435 I438 Q439 L442



• Molecule 1: MULTIDRUG RESISTANCE PROTEIN MEXB

Chain F: 4% 46% 45% 7%



P373 V374 T379 F380 N391 T392 L393 T394 M395 F396 G397 M398 V399 I402 G403 L404 L405 V406 D407 D408 A409 I410 V413 E414 M415 R418 G424 L425 S426 P427 R428 E429 K433 S434 Q437 I438 Q439 G440 A441 L442 V443 G444 I445 A446 M447 V448 L449 S450 A451 V452 F453 L454
P455 M456 S462 T463 G464 V465 I466 Y467 R468 Q469 I472 T473 I474 M478 A479 L480 S481 V482 I483 V484 A485 L486 I487 L488 T489 P490 A491 L492 C493 K502 G503 D504 H505 G506 E507 F520 L521 S522 T523 T524 H525 G526 Y527 G530 V531 I534 A539 P540 Y541 L542 L543 I544
Y545 I548 V549 A550 I553 W554 M555 F556 T557 R558 I559 P560 T561 A562 F563 L564 P565 D566 E567 D568 Q569 L572 F573 A574 Q575 V576 Q577 T578 P579 P580 G581 S582 S583 A584 E585 R586 T587 Q588 V591 R595 L599 E600 K601 S607 S608 V609 F610 T611 V612 T613 G614 F615 N616
F617 S623 M626 A627 F628 I629 K632 P633 W634 P638 G639 G640 E641 N642 S643 V644 F645 A648 Q652 F655 F658 K659 D660 A661 M662 V663 F664 A665 F666 A667 P668 P669 S670 V671 L674 T678 G679 F680 D681 L682 F683 Q687 V690 G691 H692 E693 V694 L695
L696 Q697 A698 R699 F702 L703 M704 L705 A706 N709 P710 A711 L712 Q713 R714 V715 R716 P717 N718 G719 M720 S721 D722 E723 P724 Q725 Y726 E729 I730 D731 D732 E733 K734 L738 L742 A743 D744 I745 N746 S747 T748 V749 S750 I751 A752 W753 G754 S755 S756 Y757 V758 N759 D760 F761 I762
R766 V767 K768 R769 V770 Y771 L772 Q773 R779 M780 D783 D784 L785 W788 Y789 V790 R791 N792 D793 K794 G795 E796 W797 V798 P799 F800 N801 A802 F803 A804 T805 W808 S812 P813 K814 R817 Y818 A823 M824 E825 I826 P830 G837 D838 A839 M840 A841 A842 V843
I846 V847 G855 Y856 T859 G860 L867 A872 P873 A874 L875 Y876 A877 L878 S879 L880 L881 V882 V883 F884 L885 C886 A889 L890 Y891 E892 I896 P897 L902 V903 V904 P905 L906 G907 G910 A911 L912 T915 L920 S921 N922 D923 V924 F925 F926 Q927 V928 G929 L930 L931
T932 T933 I934 G935 L936 S937 A938 K939 I942 L943 I944 V945 E946 I958 V959 I963 E964 A965 C966 R967 M968 R969 L970 R971 P972 I973 V974 M975 T976 S977 L978 A979 F980 I981 L982 G983 V984 V985 P986 I989 S990 T991 G992 A993 Q998 I1001 G1002 V1005 I1006 M1009 V1010 T1011
A1012 T1013 V1014 L1015 A1016 I1017 F1018 W1019 V1020 P1021 L1022 F1023 T1029 L1030 PHE LYS ASP GLU ALA SER LYS GLN GLN ALA SER VAL GLU LYS GLY GLN 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	125.05Å 134.58Å 151.02Å 86.99° 69.70° 88.16°	Depositor
Resolution (Å)	49.76 – 3.00 49.76 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.3 (49.76-3.00) 96.3 (49.76-3.00)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.13 (at 3.01Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.242 , 0.287 0.241 , 0.284	Depositor DCC
R_{free} test set	3539 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å^2)	88.4	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 66.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	46628	wwPDB-VP
Average B, all atoms (Å^2)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: LMT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.30	0/7789	0.50	0/10588
1	B	0.30	0/7971	0.46	0/10833
1	C	0.27	0/7971	0.45	0/10833
1	D	0.30	0/7735	0.50	0/10510
1	E	0.29	0/7851	0.47	0/10666
1	F	0.28	0/7971	0.45	0/10833
All	All	0.29	0/47288	0.47	0/64263

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7634	0	7765	689	0
1	B	7812	0	7944	541	0
1	C	7812	0	7944	509	0
1	D	7582	0	7716	665	0
1	E	7696	0	7832	528	0
1	F	7812	0	7944	509	0
2	A	35	0	46	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	105	0	138	17	0
2	D	35	0	46	5	0
2	E	105	0	138	22	0
All	All	46628	0	47513	3338	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 35.

The worst 5 of 3338 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ARG:HG2	1:A:76:ARG:HH11	1.09	1.13
1:B:43:ILE:HG21	1:B:107:VAL:HG11	1.30	1.12
1:A:375:VAL:HG21	1:A:405:LEU:HG	1.33	1.11
1:C:699:ARG:HG3	1:C:699:ARG:HH11	1.09	1.10
1:F:699:ARG:HH11	1:F:699:ARG:HG3	1.08	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	999/1052 (95%)	830 (83%)	123 (12%)	46 (5%)	2 14
1	B	1028/1052 (98%)	863 (84%)	147 (14%)	18 (2%)	8 37
1	C	1028/1052 (98%)	859 (84%)	143 (14%)	26 (2%)	5 28
1	D	990/1052 (94%)	820 (83%)	132 (13%)	38 (4%)	3 18
1	E	1006/1052 (96%)	847 (84%)	141 (14%)	18 (2%)	8 37
1	F	1028/1052 (98%)	866 (84%)	136 (13%)	26 (2%)	5 28
All	All	6079/6312 (96%)	5085 (84%)	822 (14%)	172 (3%)	5 25

5 of 172 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	VAL
1	A	134	LYS
1	A	203	VAL
1	A	204	SER
1	A	498	LYS

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	823/860 (96%)	697 (85%)	126 (15%)	2	13
1	B	841/860 (98%)	736 (88%)	105 (12%)	4	20
1	C	841/860 (98%)	755 (90%)	86 (10%)	7	28
1	D	816/860 (95%)	695 (85%)	121 (15%)	3	14
1	E	829/860 (96%)	727 (88%)	102 (12%)	4	21
1	F	841/860 (98%)	751 (89%)	90 (11%)	6	26
All	All	4991/5160 (97%)	4361 (87%)	630 (13%)	4	20

5 of 630 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	135	ASN
1	F	367	ILE
1	E	324	VAL
1	E	133	VAL
1	E	801	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 158 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	67	GLN
1	F	67	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	156	ASN
1	E	312	ASN
1	F	437	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	LMT	B	2032	-	36,36,36	0.76	1 (2%)	47,47,47	2.01	9 (19%)
2	LMT	D	2026	-	36,36,36	0.71	1 (2%)	47,47,47	1.76	8 (17%)
2	LMT	A	2026	-	36,36,36	0.57	0	47,47,47	1.44	6 (12%)
2	LMT	E	2031	-	36,36,36	0.89	1 (2%)	47,47,47	1.81	9 (19%)
2	LMT	B	2033	-	36,36,36	1.19	3 (8%)	47,47,47	3.63	19 (40%)
2	LMT	E	2033	-	36,36,36	1.11	4 (11%)	47,47,47	3.55	18 (38%)
2	LMT	E	2032	-	36,36,36	0.62	1 (2%)	47,47,47	1.40	5 (10%)
2	LMT	B	2031	-	36,36,36	0.97	1 (2%)	47,47,47	1.42	9 (19%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LMT	B	2032	-	-	0/21/61/61	0/2/2/2
2	LMT	D	2026	-	-	4/21/61/61	0/2/2/2
2	LMT	A	2026	-	-	6/21/61/61	0/2/2/2
2	LMT	E	2031	-	-	1/21/61/61	0/2/2/2
2	LMT	B	2033	-	-	7/21/61/61	0/2/2/2
2	LMT	E	2033	-	-	7/21/61/61	0/2/2/2
2	LMT	E	2032	-	-	5/21/61/61	0/2/2/2
2	LMT	B	2031	-	-	1/21/61/61	0/2/2/2

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2033	LMT	O1'-C1'	4.28	1.47	1.40
2	E	2033	LMT	O1'-C1'	3.77	1.46	1.40
2	B	2032	LMT	O1'-C1'	3.68	1.46	1.40
2	B	2031	LMT	O1'-C1'	3.41	1.46	1.40
2	E	2031	LMT	O1'-C1'	3.16	1.45	1.40

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2033	LMT	C1-O1'-C1'	14.36	137.65	113.84
2	E	2033	LMT	C1-O1'-C1'	13.64	136.47	113.84
2	B	2033	LMT	C1B-O1B-C4'	-10.03	93.14	117.96
2	E	2033	LMT	C1B-O1B-C4'	-9.66	94.06	117.96
2	B	2033	LMT	C3'-C4'-C5'	-7.90	92.81	110.93

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2026	LMT	O5'-C1'-O1'-C1
2	B	2033	LMT	O5'-C1'-O1'-C1
2	B	2033	LMT	C2-C1-O1'-C1'
2	D	2026	LMT	C2'-C1'-O1'-C1
2	D	2026	LMT	O5'-C1'-O1'-C1

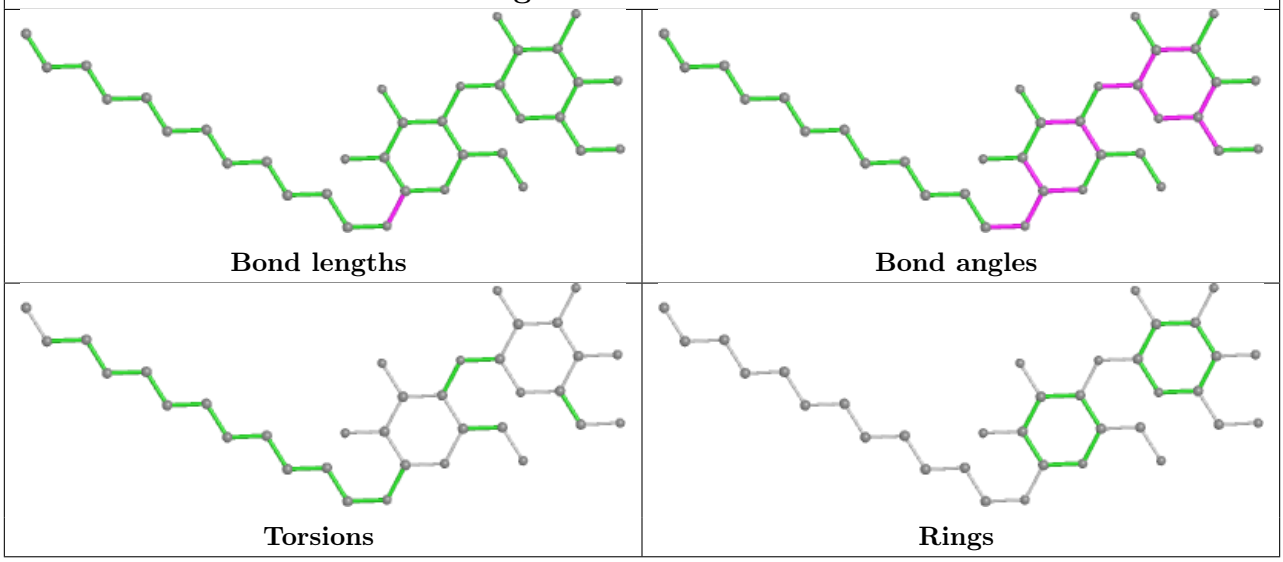
There are no ring outliers.

8 monomers are involved in 54 short contacts:

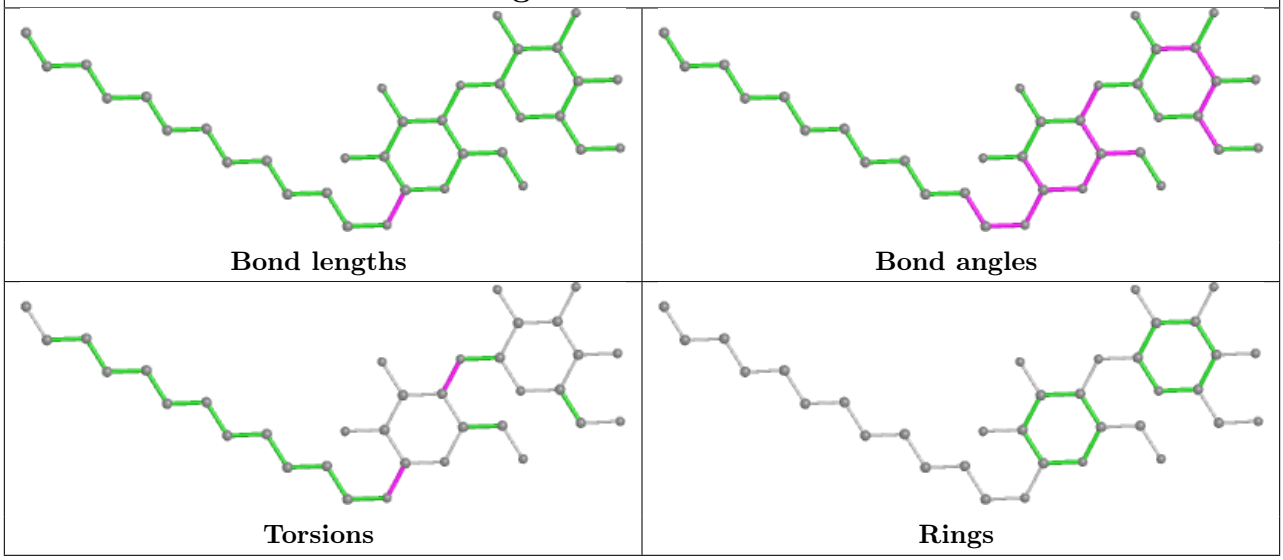
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2032	LMT	4	0
2	D	2026	LMT	5	0
2	A	2026	LMT	10	0
2	E	2031	LMT	4	0
2	B	2033	LMT	8	0
2	E	2033	LMT	10	0
2	E	2032	LMT	8	0
2	B	2031	LMT	5	0

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.

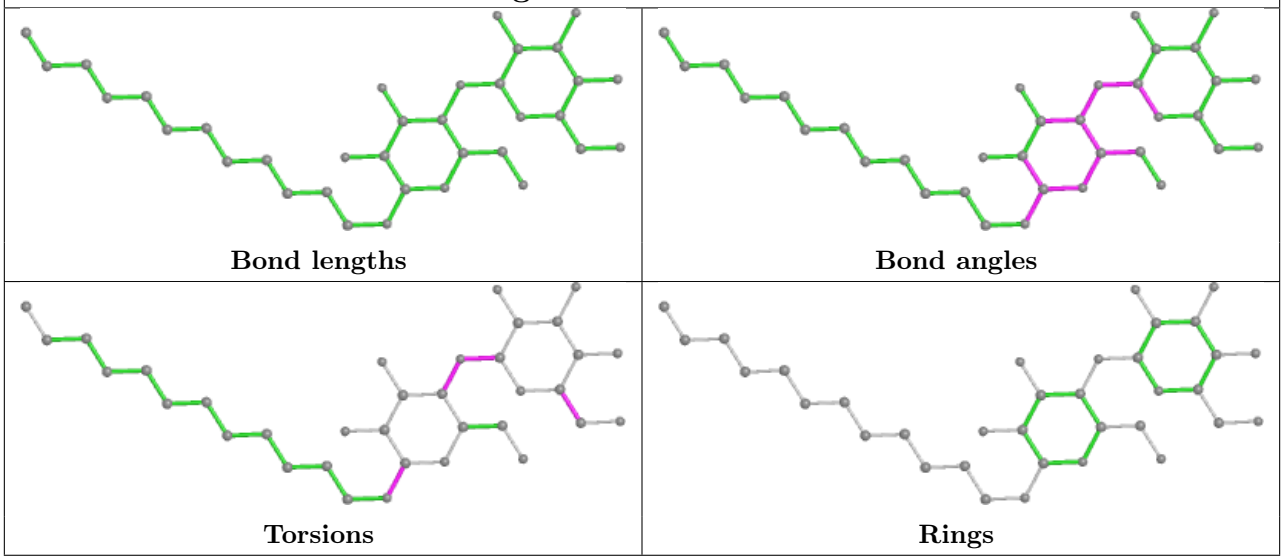
Ligand LMT B 2032



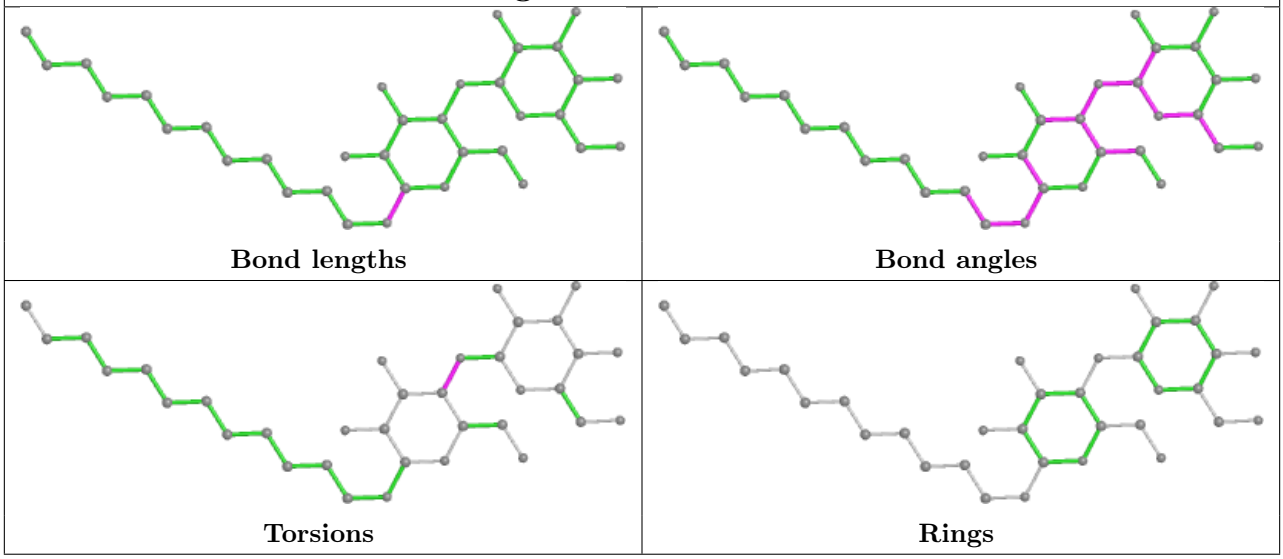
Ligand LMT D 2026



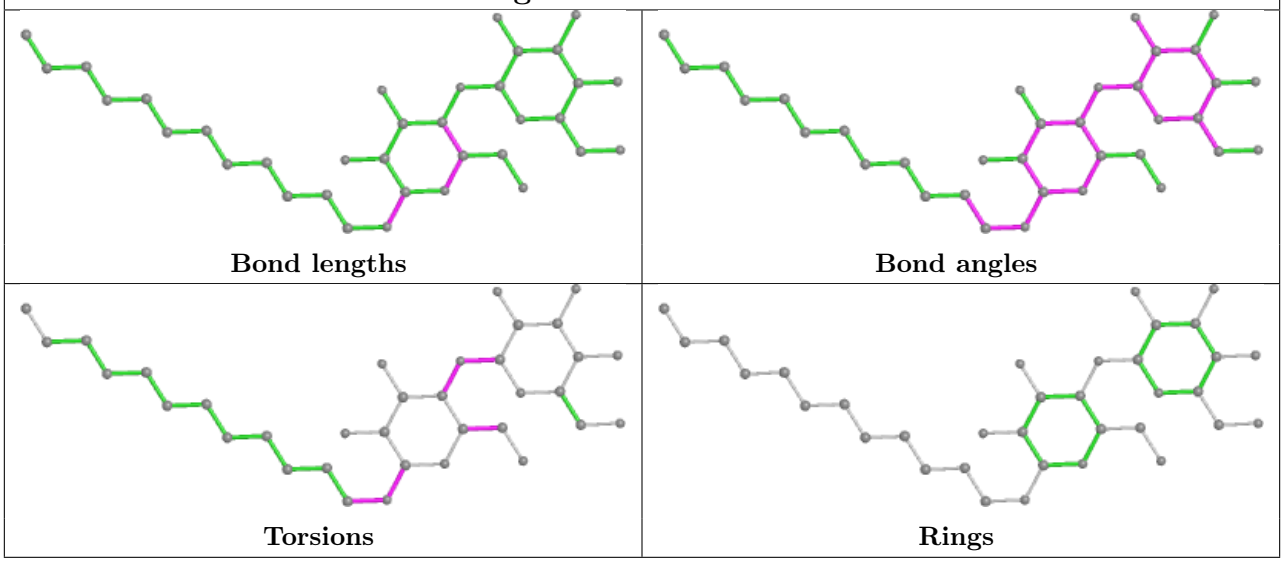
Ligand LMT A 2026



Ligand LMT E 2031



Ligand LMT B 2033



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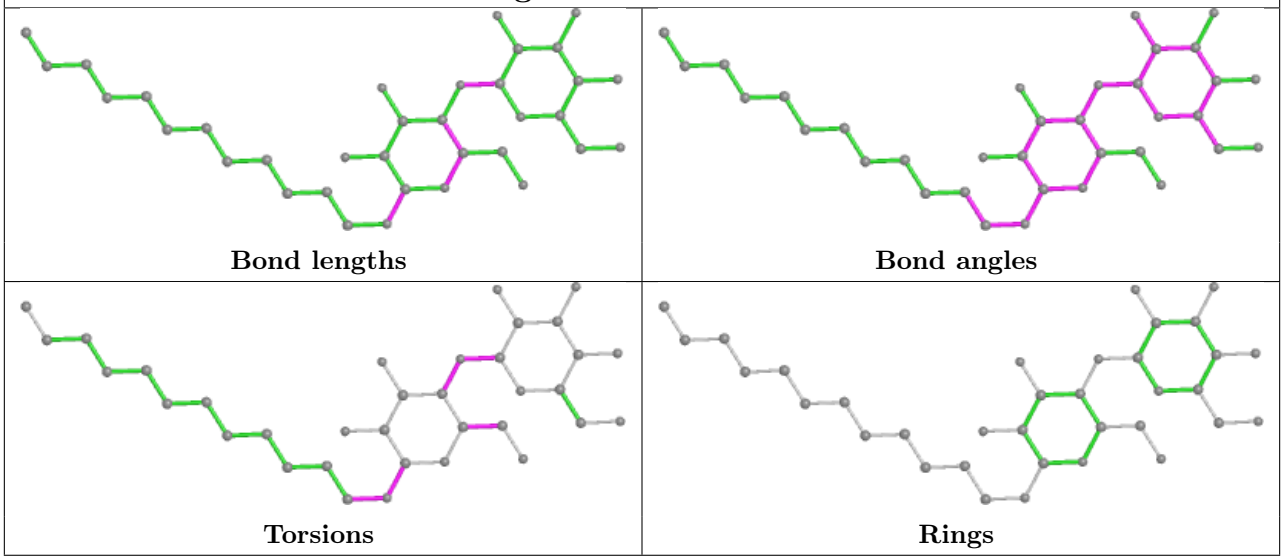
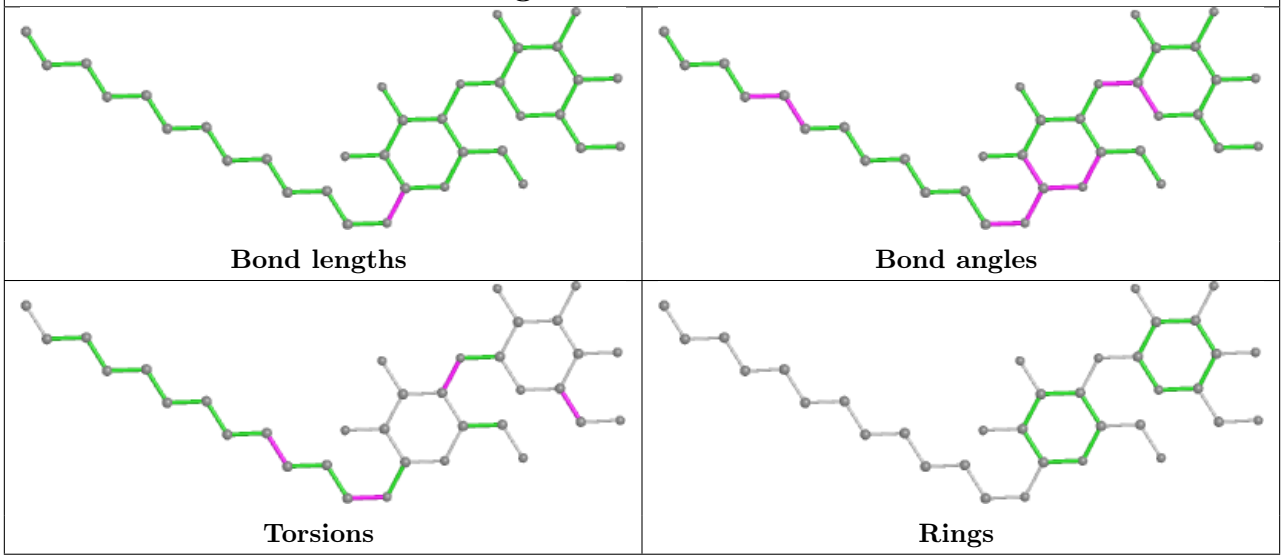
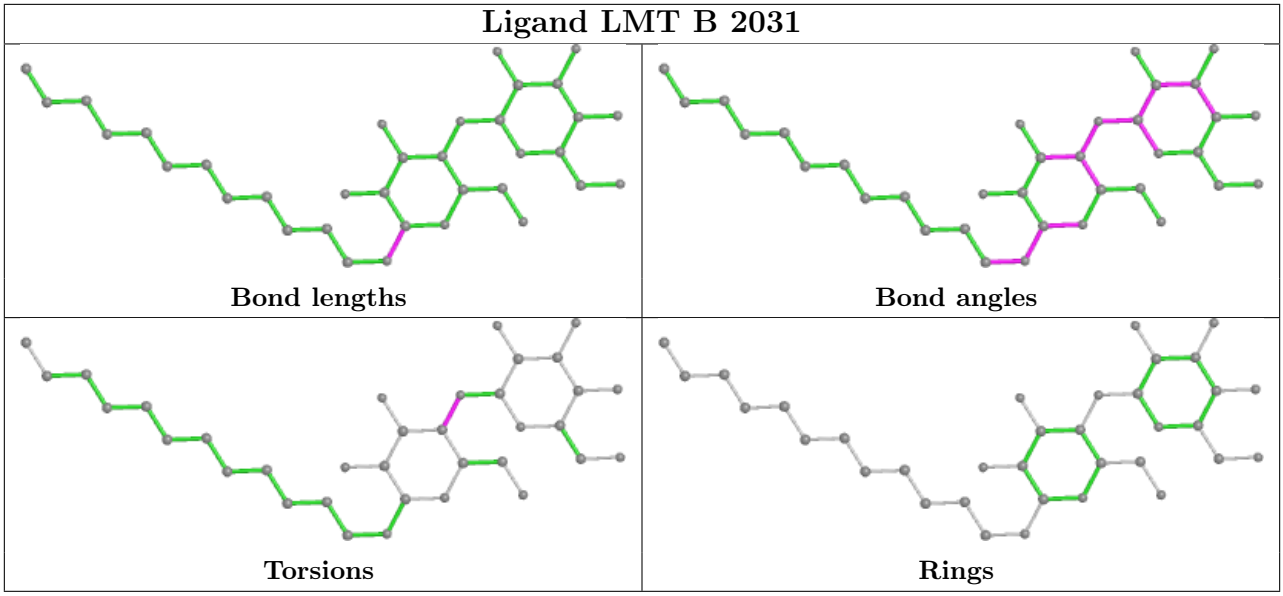


Ligand LMT E 2032





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	1004/1052 (95%)	-0.24	10 (0%)	82	59	54, 91, 132, 178	0
1	B	1030/1052 (97%)	-0.13	22 (2%)	63	34	53, 91, 143, 188	0
1	C	1028/1052 (97%)	-0.07	45 (4%)	34	13	58, 101, 178, 238	0
1	D	998/1052 (94%)	-0.28	19 (1%)	66	37	58, 91, 134, 179	0
1	E	1012/1052 (96%)	-0.15	38 (3%)	40	16	55, 93, 143, 189	0
1	F	1030/1052 (97%)	-0.09	46 (4%)	33	12	59, 100, 177, 238	0
All	All	6102/6312 (96%)	-0.16	180 (2%)	51	23	53, 94, 153, 238	0

The worst 5 of 180 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	803	PHE	7.4
1	E	260	VAL	6.6
1	E	251	LEU	6.0
1	C	778	ALA	6.0
1	F	753	TRP	5.3

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

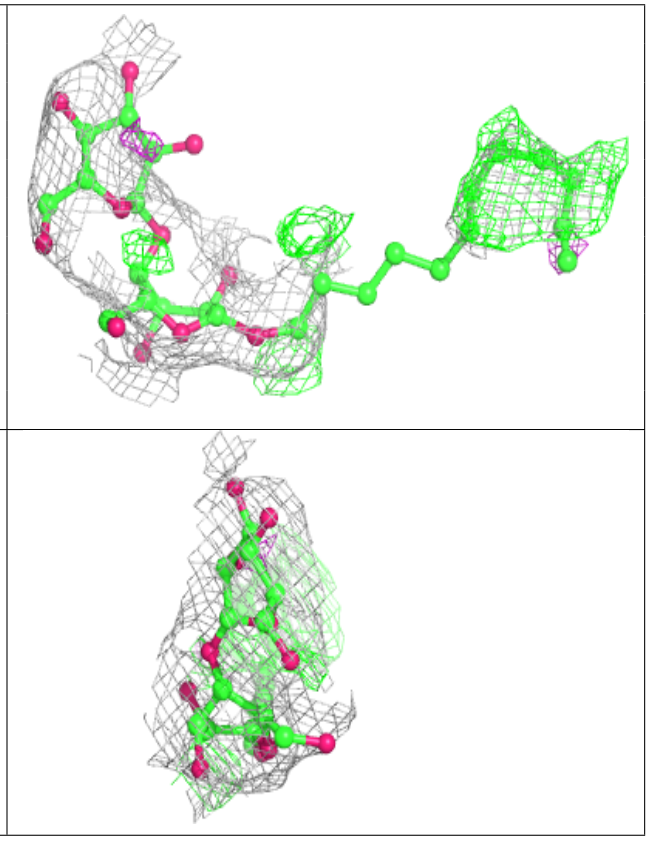
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	LMT	B	2033	35/35	0.72	0.42	100,155,176,183	0
2	LMT	E	2033	35/35	0.76	0.33	111,146,174,179	0
2	LMT	E	2031	35/35	0.85	0.23	72,95,121,130	0
2	LMT	B	2031	35/35	0.90	0.20	59,82,109,114	0
2	LMT	A	2026	35/35	0.90	0.21	80,110,145,173	0
2	LMT	D	2026	35/35	0.91	0.16	75,113,140,142	0
2	LMT	E	2032	35/35	0.93	0.23	66,90,115,128	0
2	LMT	B	2032	35/35	0.93	0.25	52,70,157,169	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.

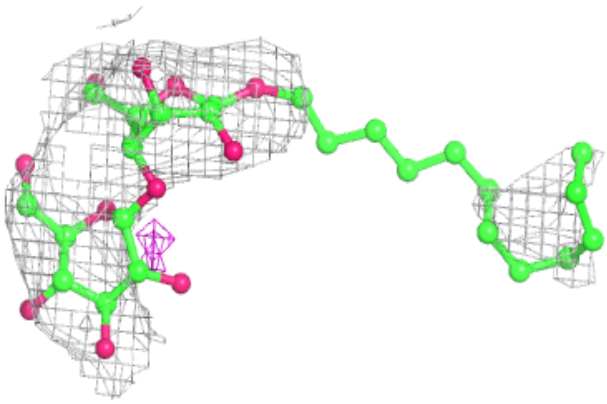
Electron density around LMT B 2033:

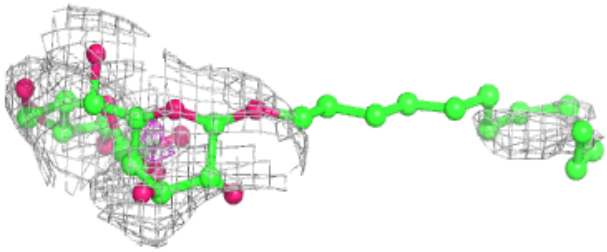
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

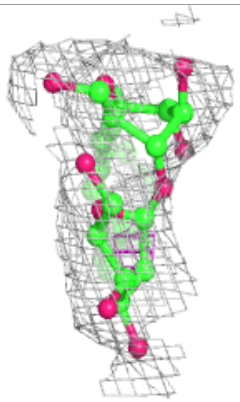


Electron density around LMT E 2033:

$2mF_o$-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 2031:

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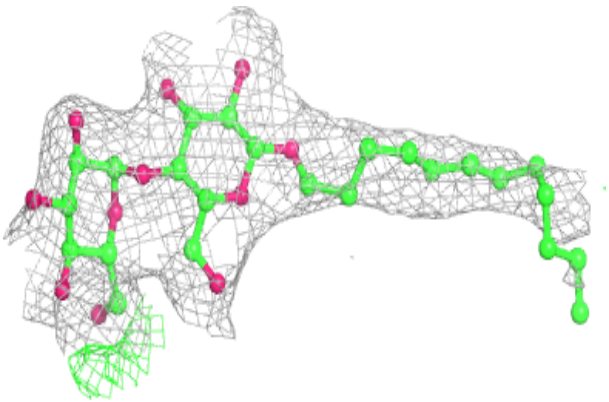
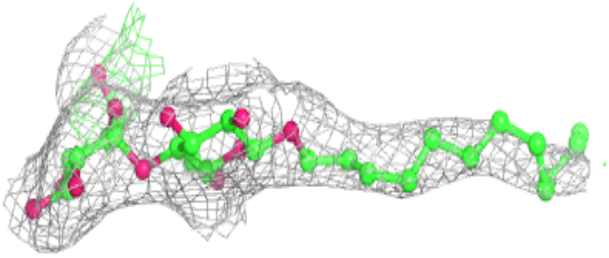
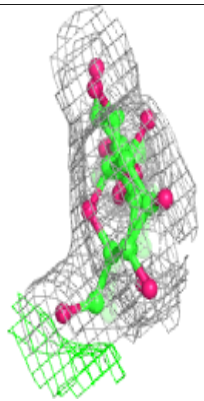
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

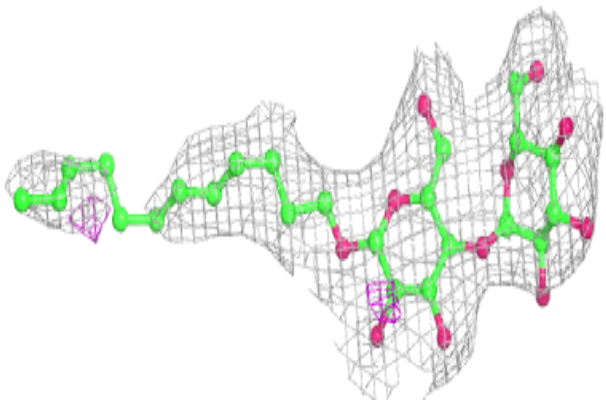


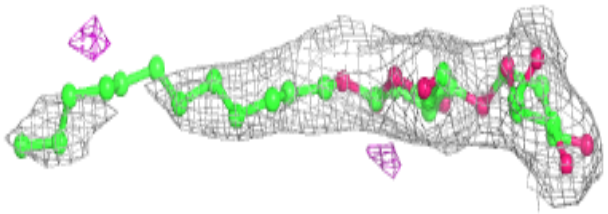


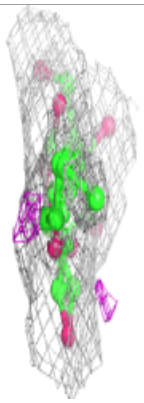


Electron density around LMT B 2031:

$2mF_o$-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 2026:

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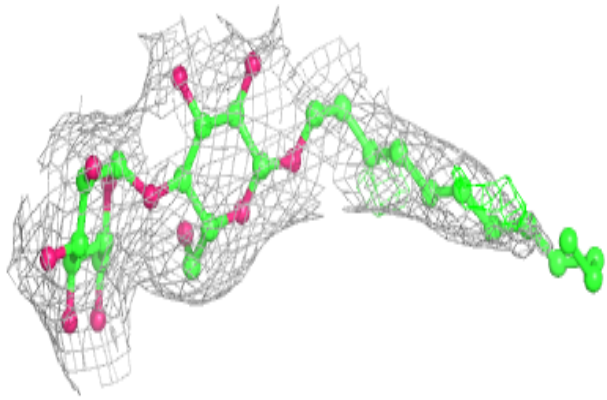
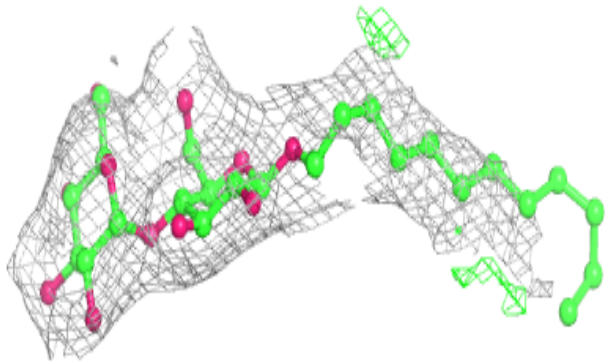
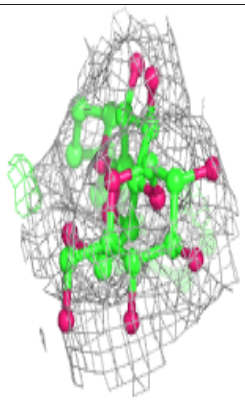
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around LMT D 2026:

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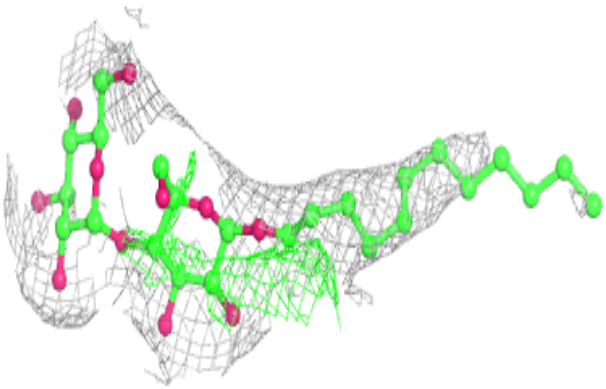
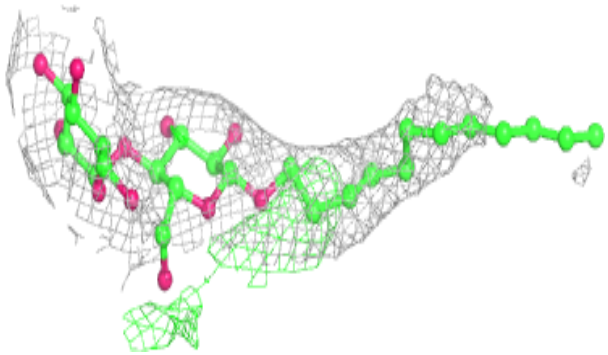
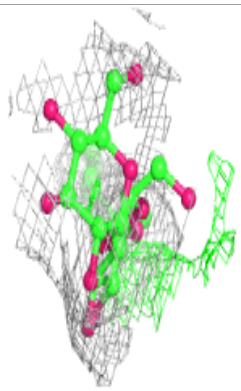
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

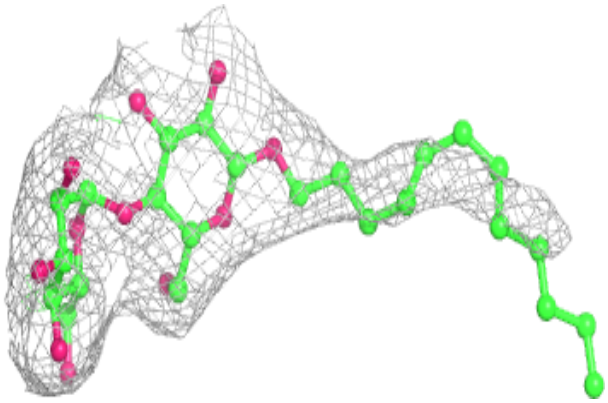


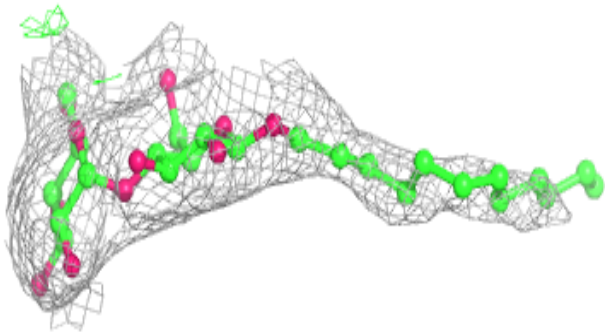


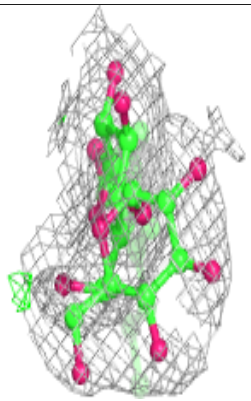


Electron density around LMT E 2032:

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

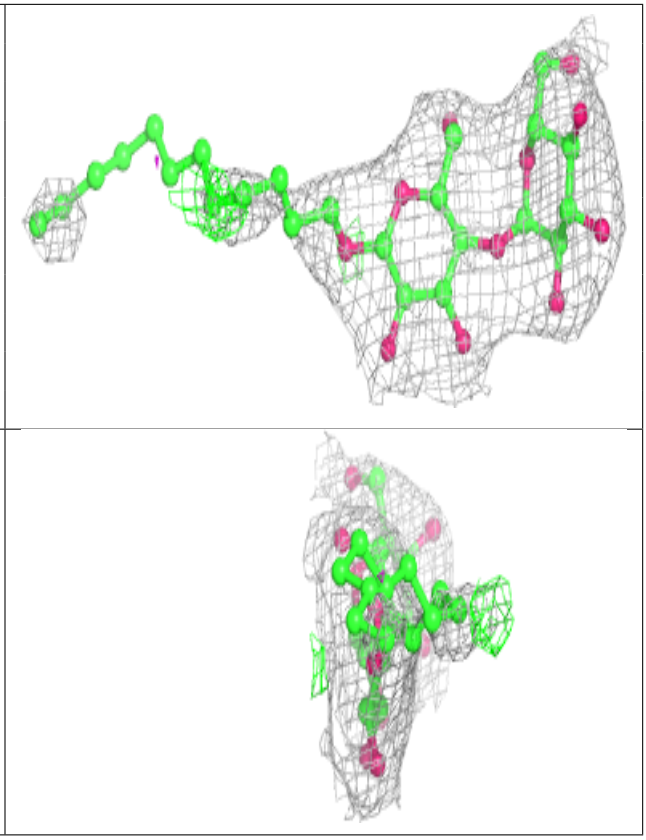






Electron density around LMT B 2032:

$2mF_o$-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.