



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 01:39 pm BST

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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

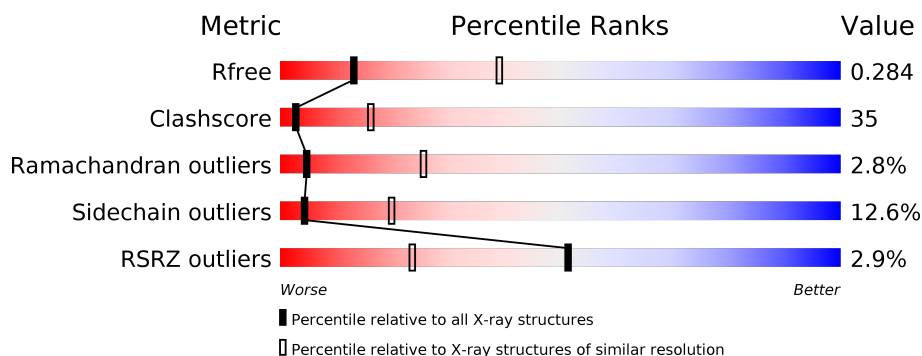
# 1 Overall quality at a glance

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>0%</div> <div> <div>37%</div> <div>46%</div> <div>12%</div> <div>• •</div> </div> </div>
1	B	1052	<div> <div>2%</div> <div> <div>46%</div> <div>44%</div> <div>8%</div> <div>•</div> </div> </div>
1	C	1052	<div> <div>4%</div> <div> <div>46%</div> <div>45%</div> <div>7%</div> <div>•</div> </div> </div>
1	D	1052	<div> <div>2%</div> <div> <div>38%</div> <div>46%</div> <div>11%</div> <div>• 5%</div> </div> </div>
1	E	1052	<div> <div>4%</div> <div> <div>44%</div> <div>44%</div> <div>8%</div> <div>•</div> </div> </div>
1	F	1052	<div> <div>4%</div> <div> <div>46%</div> <div>45%</div> <div>7%</div> <div>•</div> </div> </div>

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

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
1	A	1005	Total	C	N	O	S	6	0	0
			7634	4920	1265	1410	39			
1	B	1030	Total	C	N	O	S	0	0	0
			7812	5027	1298	1447	40			
1	C	1030	Total	C	N	O	S	12	0	0
			7812	5027	1298	1447	40			
1	D	998	Total	C	N	O	S	0	0	0
			7582	4888	1255	1399	40			
1	E	1012	Total	C	N	O	S	0	0	0
			7696	4956	1279	1421	40			
1	F	1030	Total	C	N	O	S	0	0	0
			7812	5027	1298	1447	40			

There are 36 discrepancies between the modelled and reference sequences:

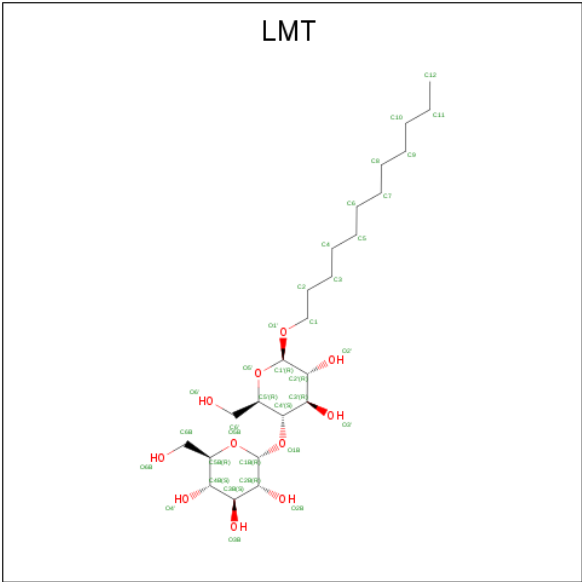
Chain	Residue	Modelled	Actual	Comment	Reference
A	1047	HIS	-	expression tag	UNP P52002
A	1048	HIS	-	expression tag	UNP P52002
A	1049	HIS	-	expression tag	UNP P52002
A	1050	HIS	-	expression tag	UNP P52002
A	1051	HIS	-	expression tag	UNP P52002
A	1052	HIS	-	expression tag	UNP P52002
B	1047	HIS	-	expression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

*Continued on next page...*

Continued from previous page...

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<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



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

Continued on next page...

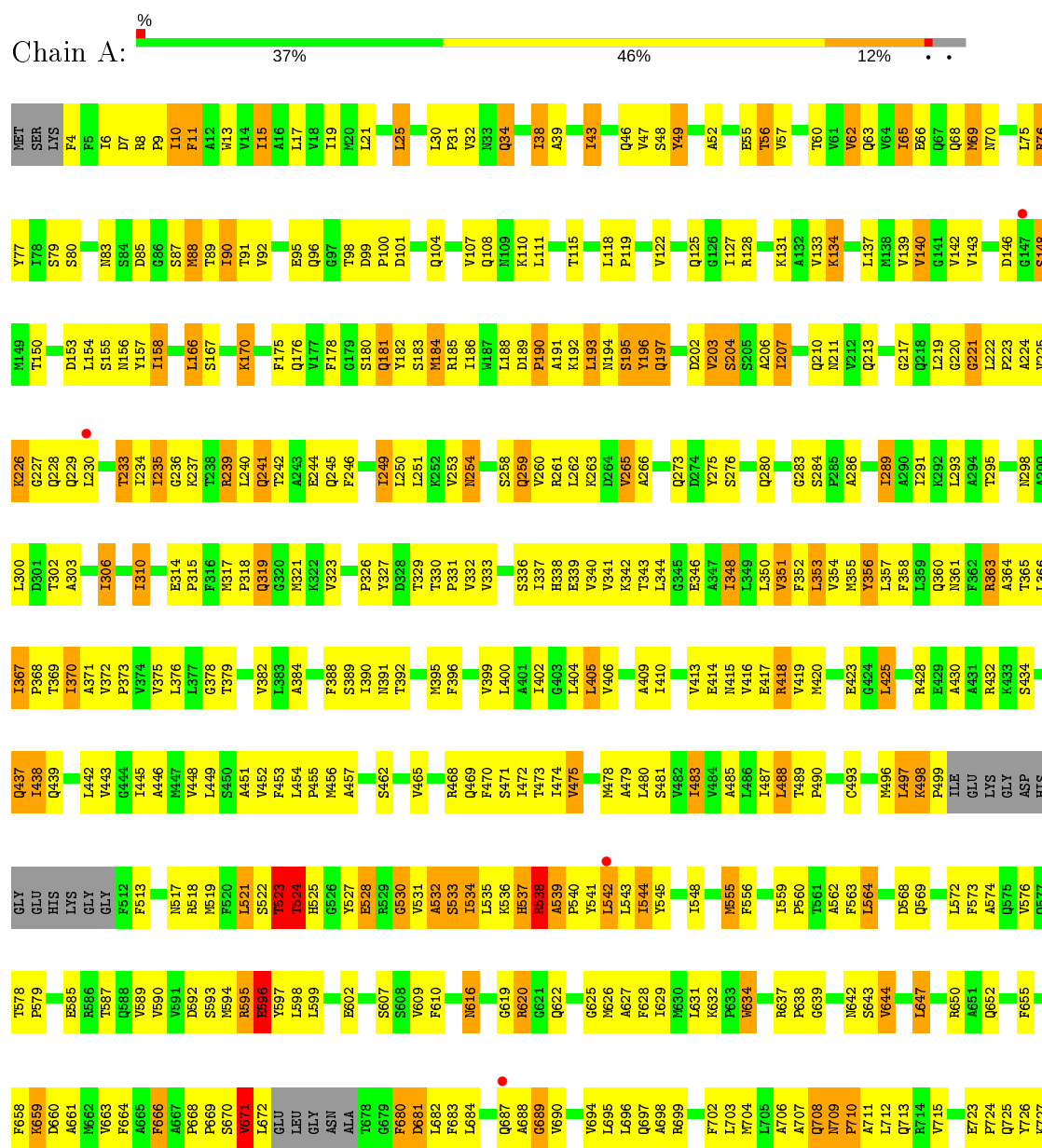
*Continued from previous page...*

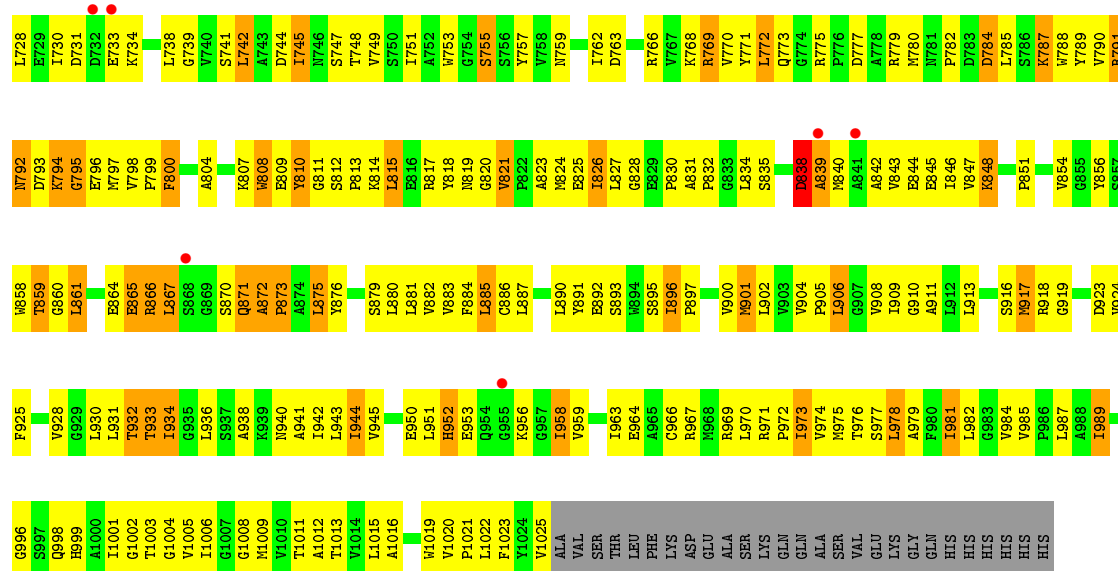
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			35	24	11		
2	B	1	Total	C	O	0	0
			35	24	11		
2	B	1	Total	C	O	0	0
			35	24	11		
2	D	1	Total	C	O	0	0
			35	24	11		
2	E	1	Total	C	O	0	0
			35	24	11		
2	E	1	Total	C	O	0	0
			35	24	11		
2	E	1	Total	C	O	0	0
			35	24	11		

### 3 Residue-property plots

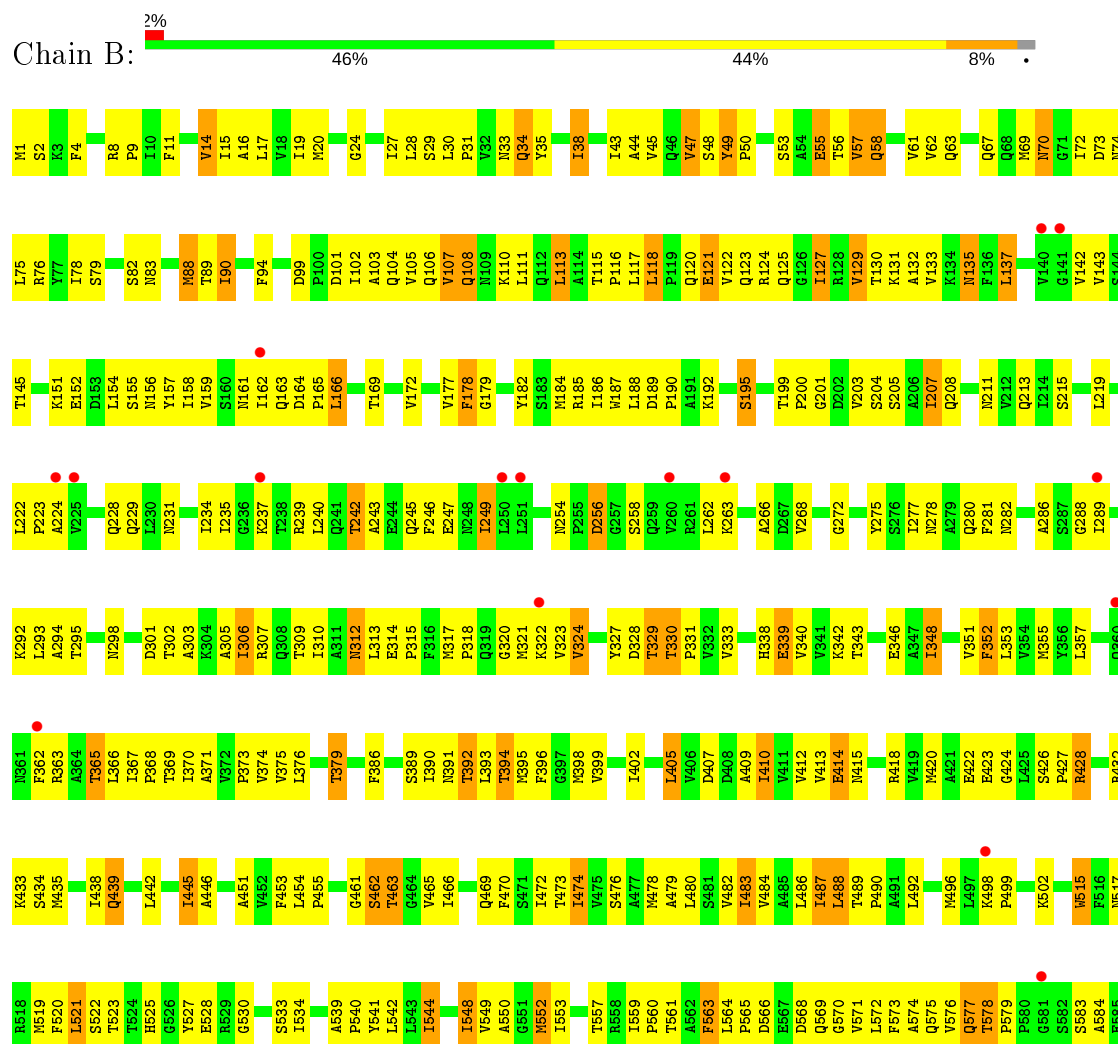
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

#### • Molecule 1: MULTIDRUG RESISTANCE PROTEIN MEXB

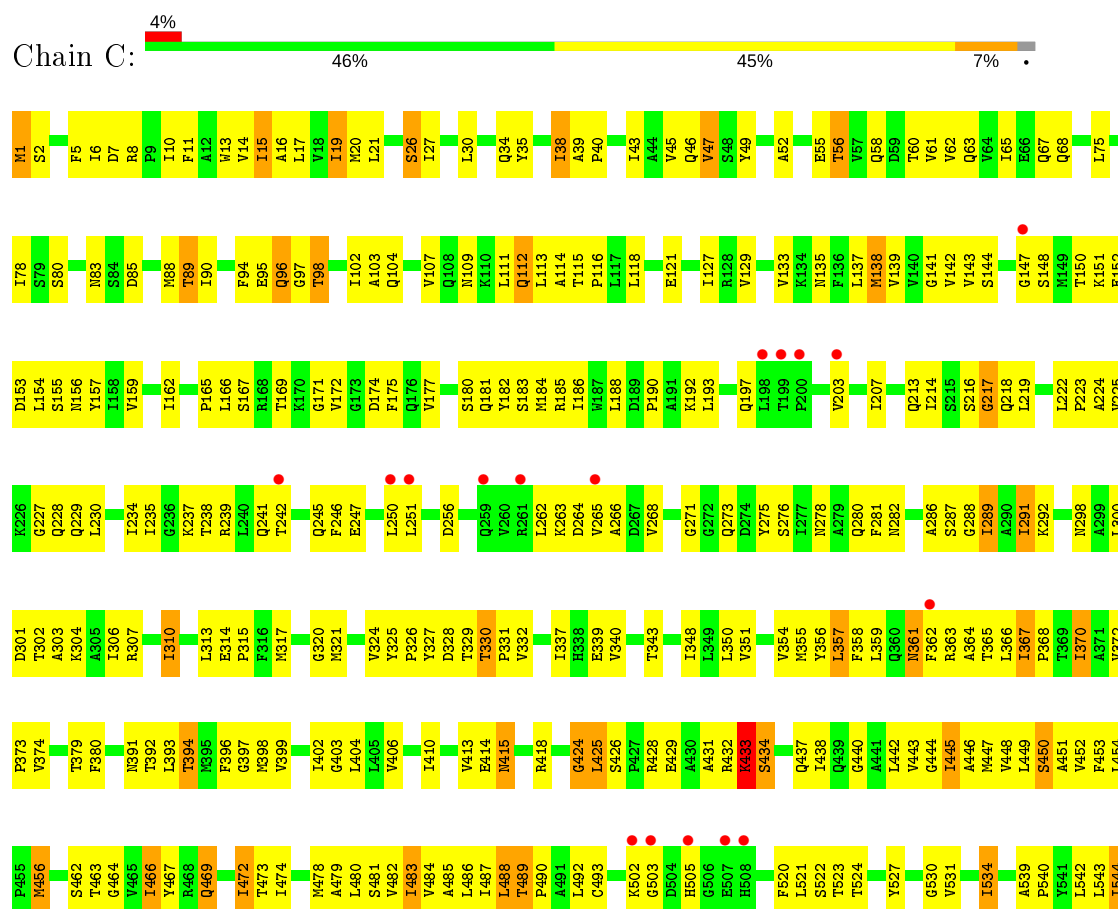


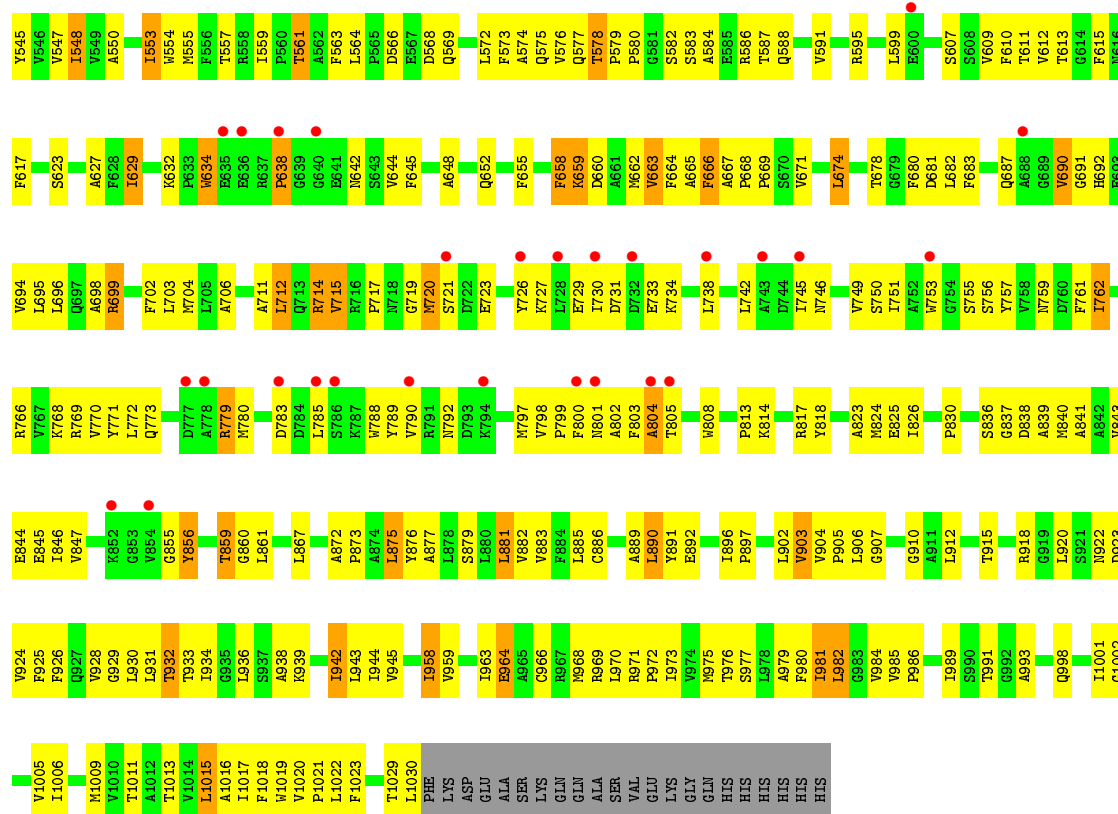


### • Molecule 1: MULTIDRUG RESISTANCE PROTEIN MEXB

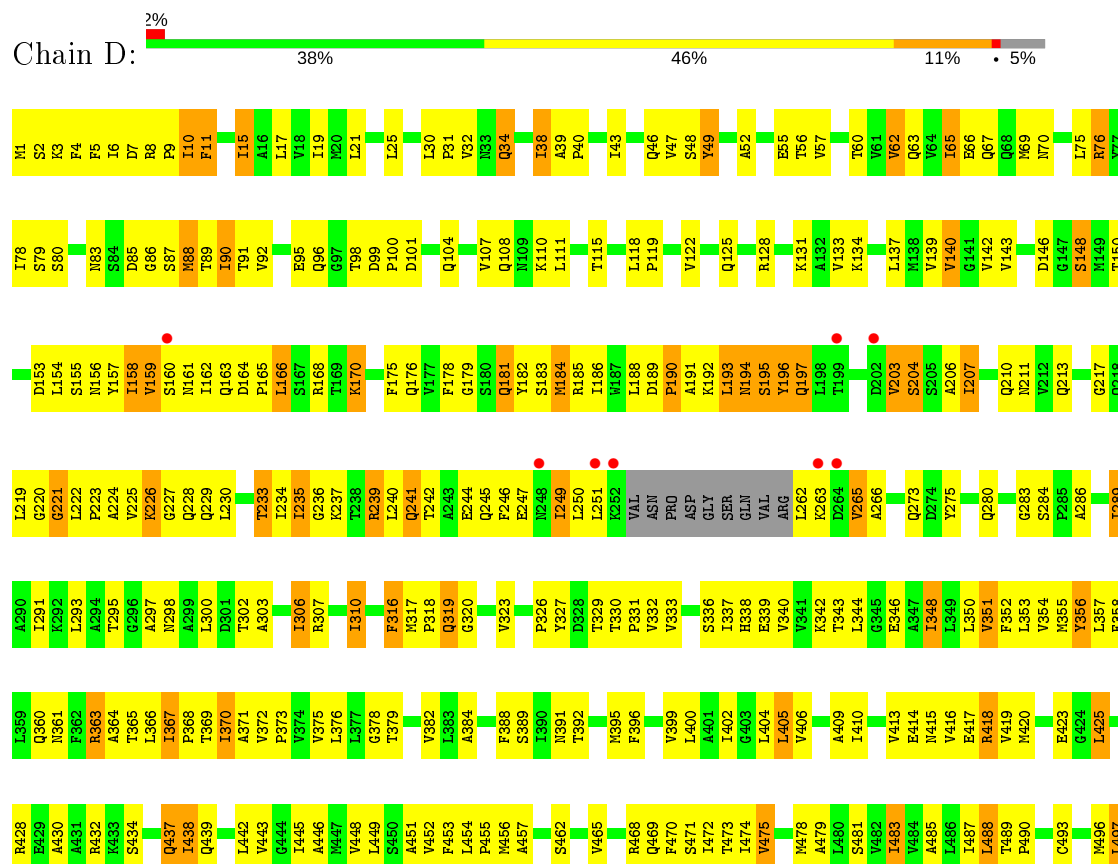




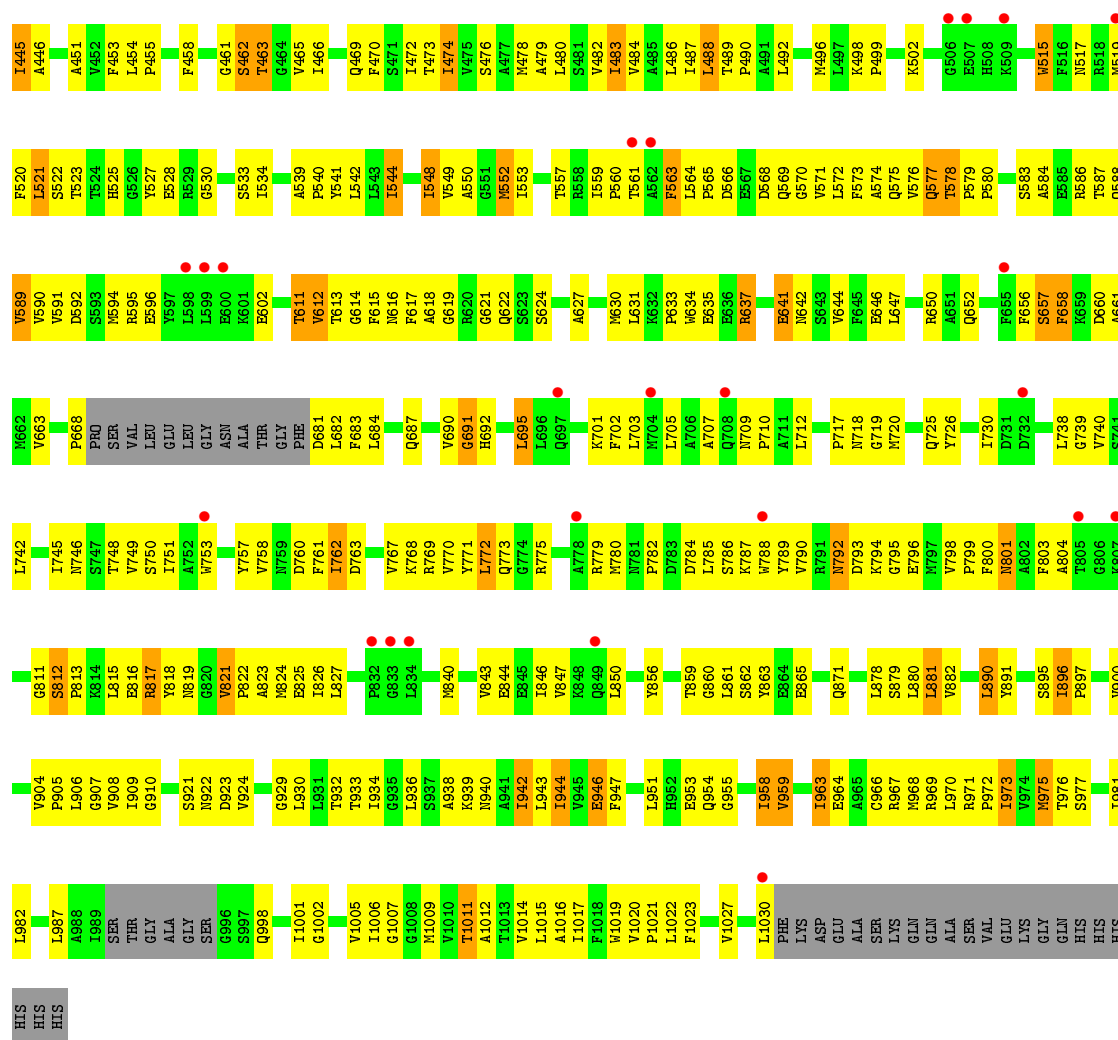




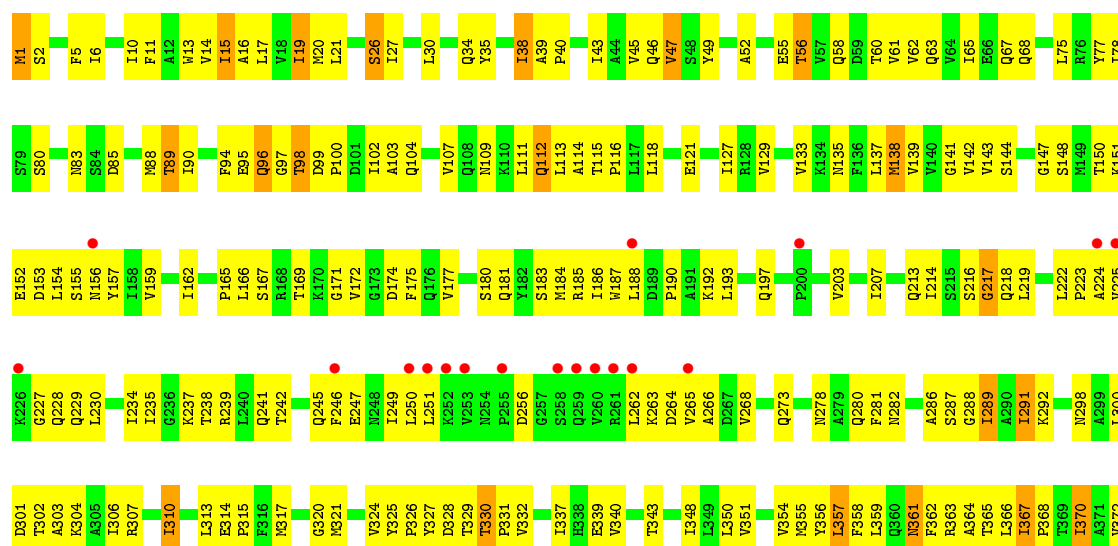
• Molecule 1: MULTIDRUG RESISTANCE PROTEIN MEXB







• Molecule 1: MULTIDRUG RESISTANCE PROTEIN MEXB



A1012	T1013	T932	I846	R766	L696	F617	Y545	P455	P373
V1014	I934	I933	V847	V767	Q897	S623	I548	M456	V374
A1016	I935	I934	G855	K768	R699	M626	V549	S462	T379
I1017	I936	I935	Y856	R769	F702	F628	A550	T463	F380
F1018	S937	I936	T859	V770	L703	I629	I553	G464	I831
I1019	A938	I937	G860	L772	M704	L705	M554	I466	T392
V1020	I939	I938	L867	Q773	A706	K632	F556	Y467	L393
P1021	I942	I941	A872	R779	M709	P633	T557	R468	T394
L1022	I944	I943	P873	M780	P710	M634	R558	M395	I839
F1023	I945	I944	A874	D783	A711	P638	I559	F396	G397
T1029	I946	I945	L875	D784	L712	G639	P560	G397	M398
PHE	I958	I957	L876	L785	Q713	E640	T561	Q469	V399
LYS	V959	I958	A877	L786	R714	E641	I562	I472	I402
ASP	I963	I962	L878	W788	R715	N642	F563	I473	G403
GLU	I964	I963	S879	Y789	R716	S643	I564	I480	I404
ALA	E965	I964	L880	V790	P717	F644	P566	S481	I405
SER	A966	I965	L881	R791	M718	F645	D567	V482	V406
LYS	C966	I966	V882	N792	G719	A648	D568	I483	D407
GLN	R967	I967	V883	D793	M720	Q652	I569	V484	D408
GLN	N968	I968	F884	K794	S721	Q652	I572	A485	A409
ALA	R969	I969	L885	G795	D722	F655	F573	I486	I410
SER	L970	I970	C886	E796	E723	F655	A574	I487	I411
VAL	R971	I971	A889	M797	P724	F655	Q575	L488	V413
GLU	P972	I972	L890	N798	Q725	F655	Q575	T489	E414
LYS	I973	I973	Y891	P799	Y726	F658	V576	P490	N415
GLY	V974	I974	L891	F800	Y726	K659	D577	A491	R418
GLN	N975	I975	E892	N801	E729	D660	T578	L492	G424
HIS	T976	I976	I896	A802	I730	A661	P579	C493	L426
HIS	S977	I977	P897	F803	D731	M662	P580	K502	S426
HIS	A979	I978	L897	A804	D732	V663	S582	G503	P427
HIS	F980	I979	I902	T805	E733	F664	S583	D604	R428
HIS	I981	I980	V903	W808	K734	A665	A584	H505	E429
HIS	L982	I981	V904	L808	L738	F666	E585	G506	R433
G983	G983	I982	P905	S812	L742	A667	R586	E507	S434
V984	V984	I983	P813	P813	A743	P668	T587	F520	Q437
V985	V985	I984	K814	K814	D744	P669	Q588	L521	I438
P986	P986	I985	G910	R817	I745	V671	V591	S522	Q439
I989	I989	I989	G911	Y818	I746	L674	R595	T523	G440
S990	S990	I990	L912	Y818	S747	T678	I599	H525	A441
T991	T991	I991	T915	A823	V748	G679	L599	G526	L442
G992	G992	I992	T915	M824	V749	F680	R601	Y527	V443
A993	A993	I993	E825	E825	S750	D681	I601	G530	G444
I998	I998	I998	I826	I826	I751	L682	S607	I445	I445
Q998	Q998	I999	S921	P830	A752	F683	S608	A446	A446
I1001	I1001	I1001	N922	G837	G753	Q687	V609	I534	M447
G1002	G1002	I1002	D923	D838	S755	Q687	F610	A539	V448
V1005	V1005	I1005	F925	A839	S756	V690	T611	P540	L449
I1006	I1006	I1006	F926	A839	Y757	G691	V612	A451	S450
I1006	I1006	I1006	Q927	W840	V758	H692	T613	I541	A451
V928	V928	I1007	V928	A841	N759	E693	G614	L542	V452
G929	G929	I1008	G929	A842	D760	V694	F614	L543	F453
L930	L930	I1009	L930	V843	F761	I695	I616	I544	L454
T1011	T1011	I1011	I931	I843	I762				

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	88.4	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 66.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.30	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

*Continued on next page...*

*Continued from previous page...*

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:HH11	1:A:76:ARG:HG2	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:HH11	1:C:699:ARG:HG3	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 ⓘ

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	C	578	THR
1	D	249	ILE
1	F	450	SER
1	C	704	MET
1	D	15	ILE

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

Mol	Chain	Res	Type
1	C	437	GLN
1	D	213	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	282	ASN
1	C	469	GLN
1	D	68	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	E	2032	-	36,36,36	0.62	1 (2%)	47,47,47	1.40	5 (10%)
2	LMT	D	2026	-	36,36,36	0.71	1 (2%)	47,47,47	1.76	8 (17%)
2	LMT	E	2033	-	36,36,36	1.11	4 (11%)	47,47,47	3.55	18 (38%)
2	LMT	B	2033	-	36,36,36	1.19	3 (8%)	47,47,47	3.63	19 (40%)
2	LMT	A	2026	-	36,36,36	0.57	0	47,47,47	1.44	6 (12%)
2	LMT	B	2032	-	36,36,36	0.76	1 (2%)	47,47,47	2.01	9 (19%)
2	LMT	B	2031	-	36,36,36	0.97	1 (2%)	47,47,47	1.42	9 (19%)
2	LMT	E	2031	-	36,36,36	0.89	1 (2%)	47,47,47	1.81	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	E	2032	-	-	5/21/61/61	0/2/2/2
2	LMT	D	2026	-	-	4/21/61/61	0/2/2/2
2	LMT	E	2033	-	-	7/21/61/61	0/2/2/2
2	LMT	B	2033	-	-	7/21/61/61	0/2/2/2
2	LMT	A	2026	-	-	6/21/61/61	0/2/2/2
2	LMT	B	2032	-	-	0/21/61/61	0/2/2/2
2	LMT	B	2031	-	-	1/21/61/61	0/2/2/2
2	LMT	E	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(°)	Ideal(°)
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:

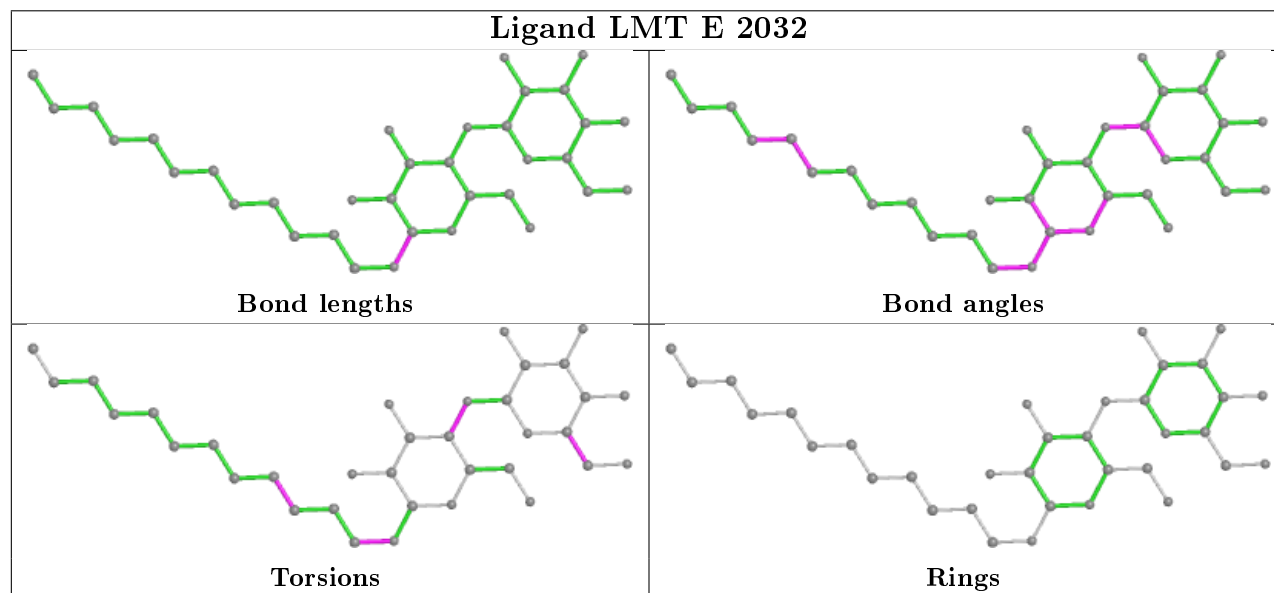
Mol	Chain	Res	Type	Atoms
2	D	2026	LMT	C2'-C1'-O1'-C1
2	D	2026	LMT	O5'-C1'-O1'-C1
2	E	2033	LMT	O5'-C1'-O1'-C1
2	E	2033	LMT	C2-C1-O1'-C1'
2	B	2033	LMT	O5'-C1'-O1'-C1

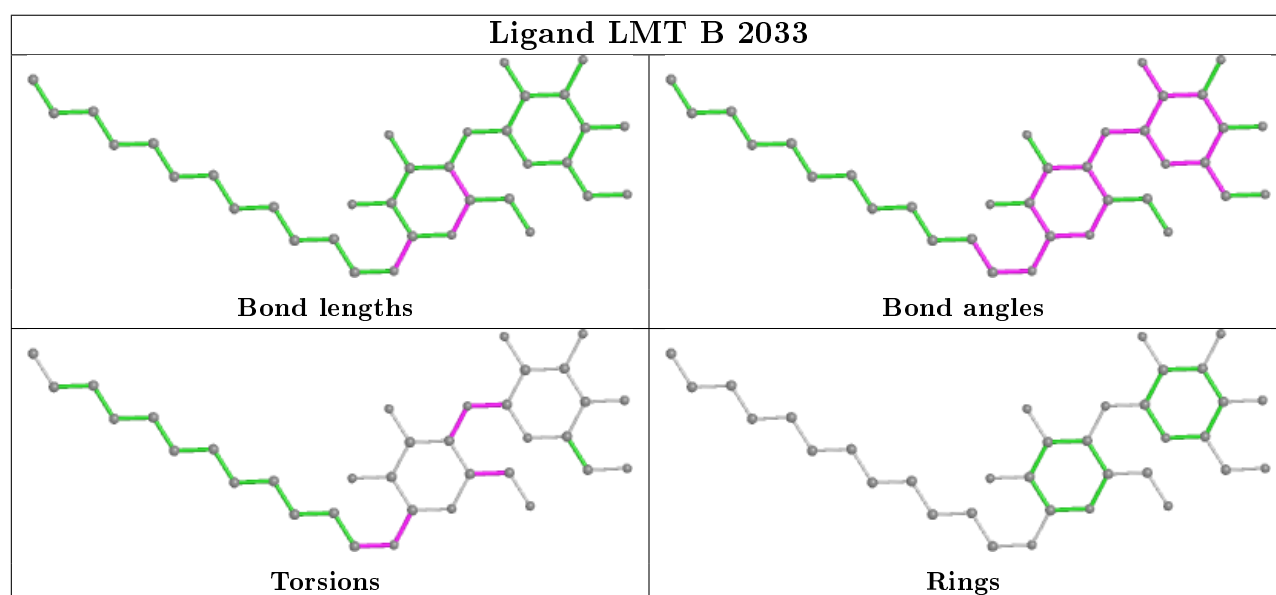
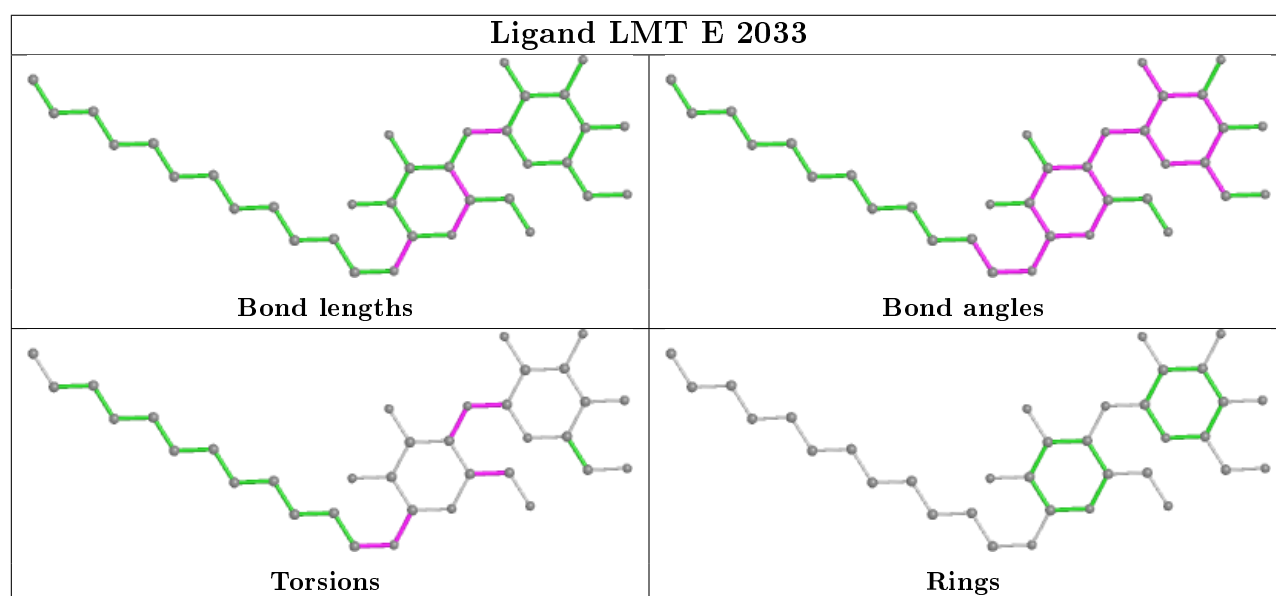
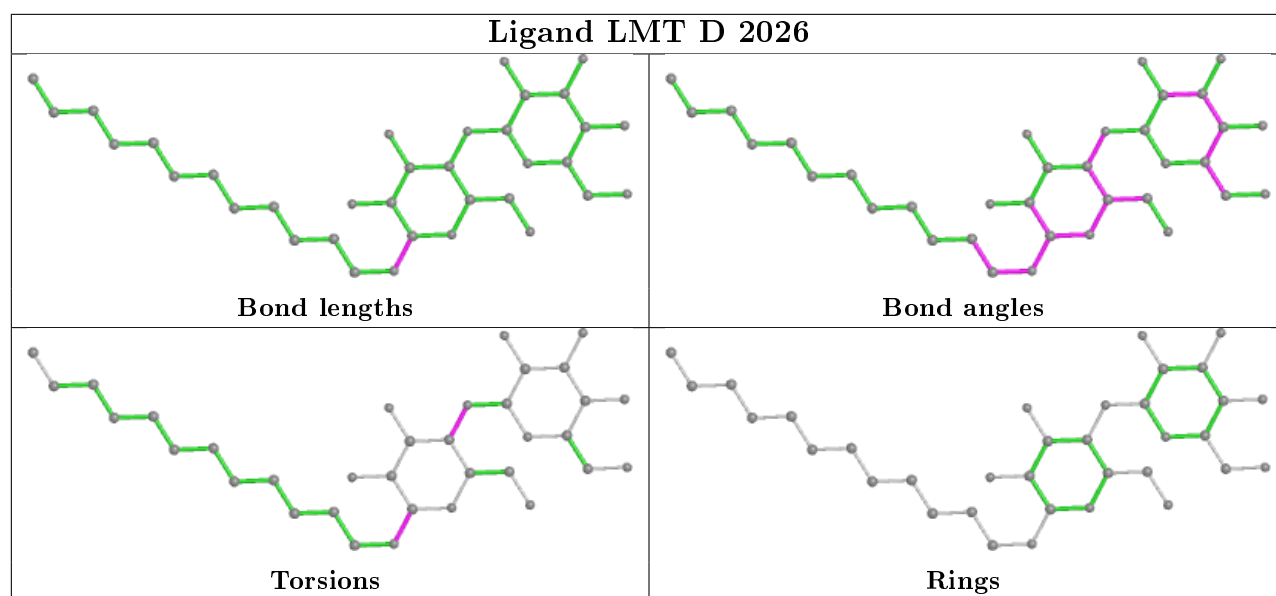
There are no ring outliers.

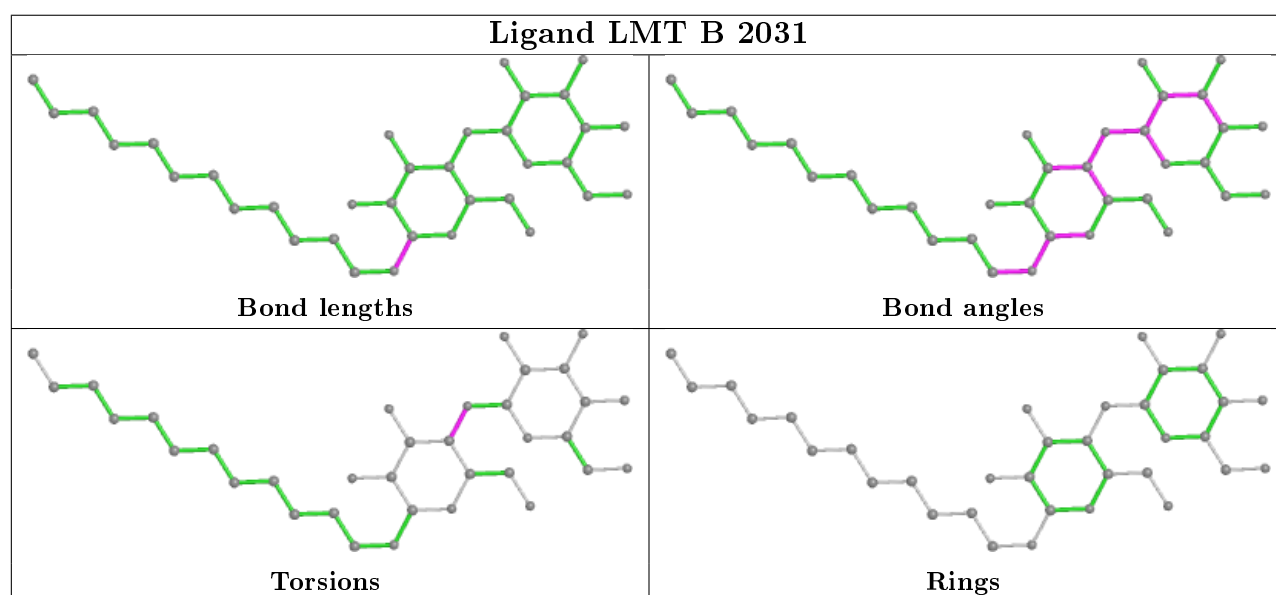
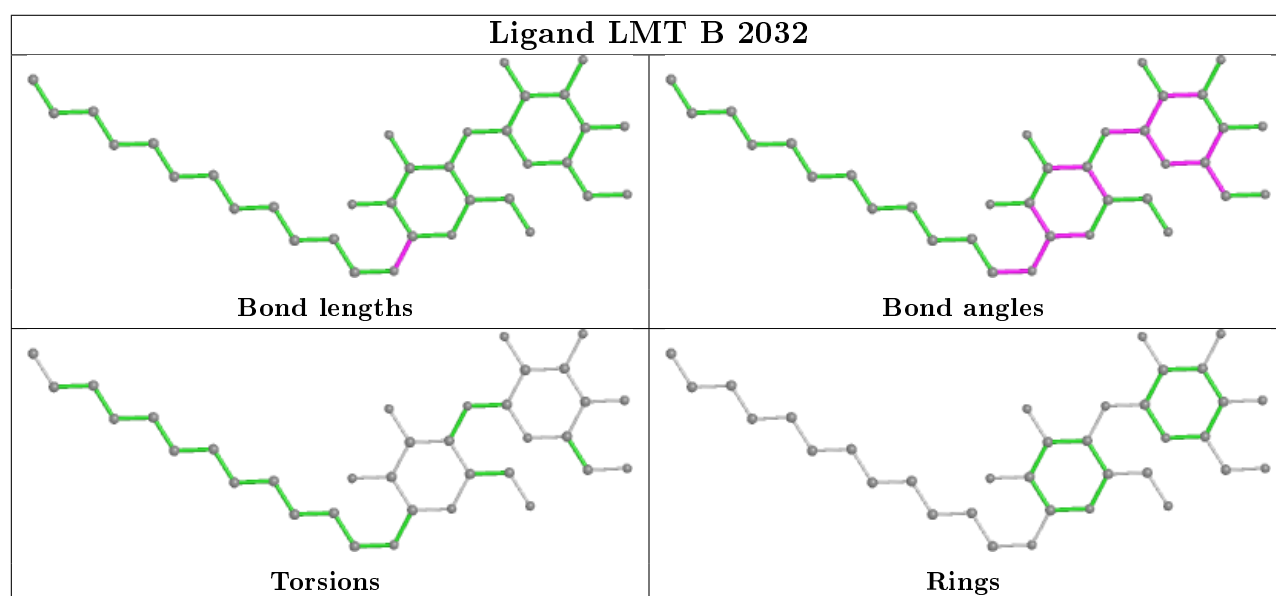
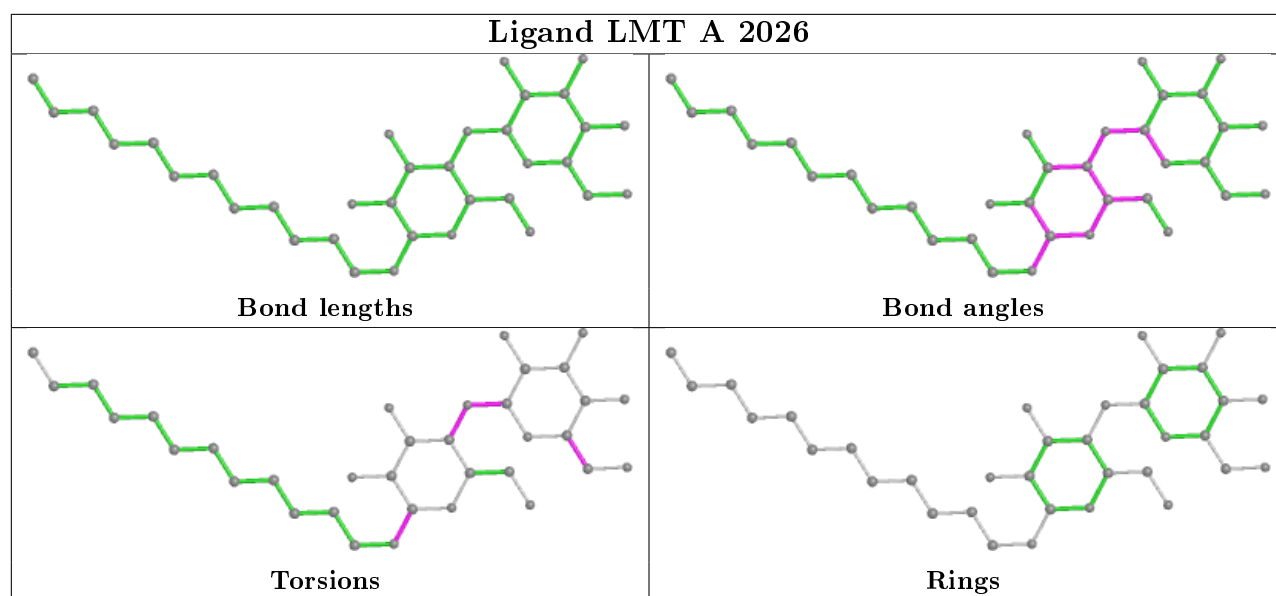
8 monomers are involved in 54 short contacts:

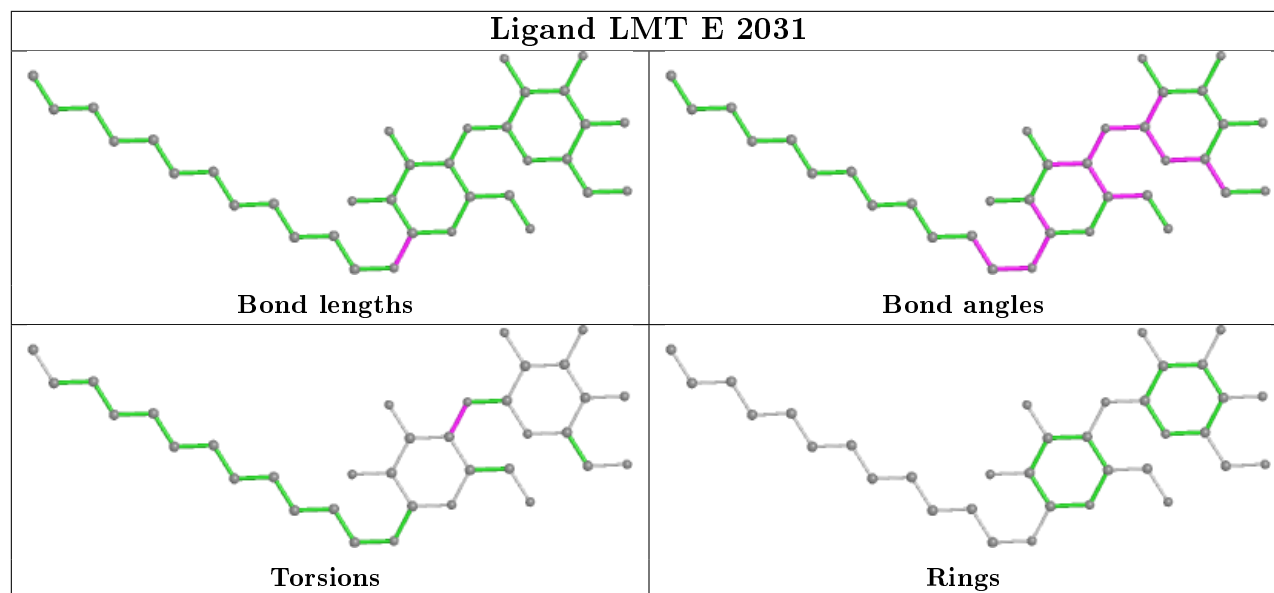
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2032	LMT	8	0
2	D	2026	LMT	5	0
2	E	2033	LMT	10	0
2	B	2033	LMT	8	0
2	A	2026	LMT	10	0
2	B	2032	LMT	4	0
2	B	2031	LMT	5	0
2	E	2031	LMT	4	0

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, 95<sup>th</sup> 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 <sup>2</sup> )	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 carbohydrates in this entry.

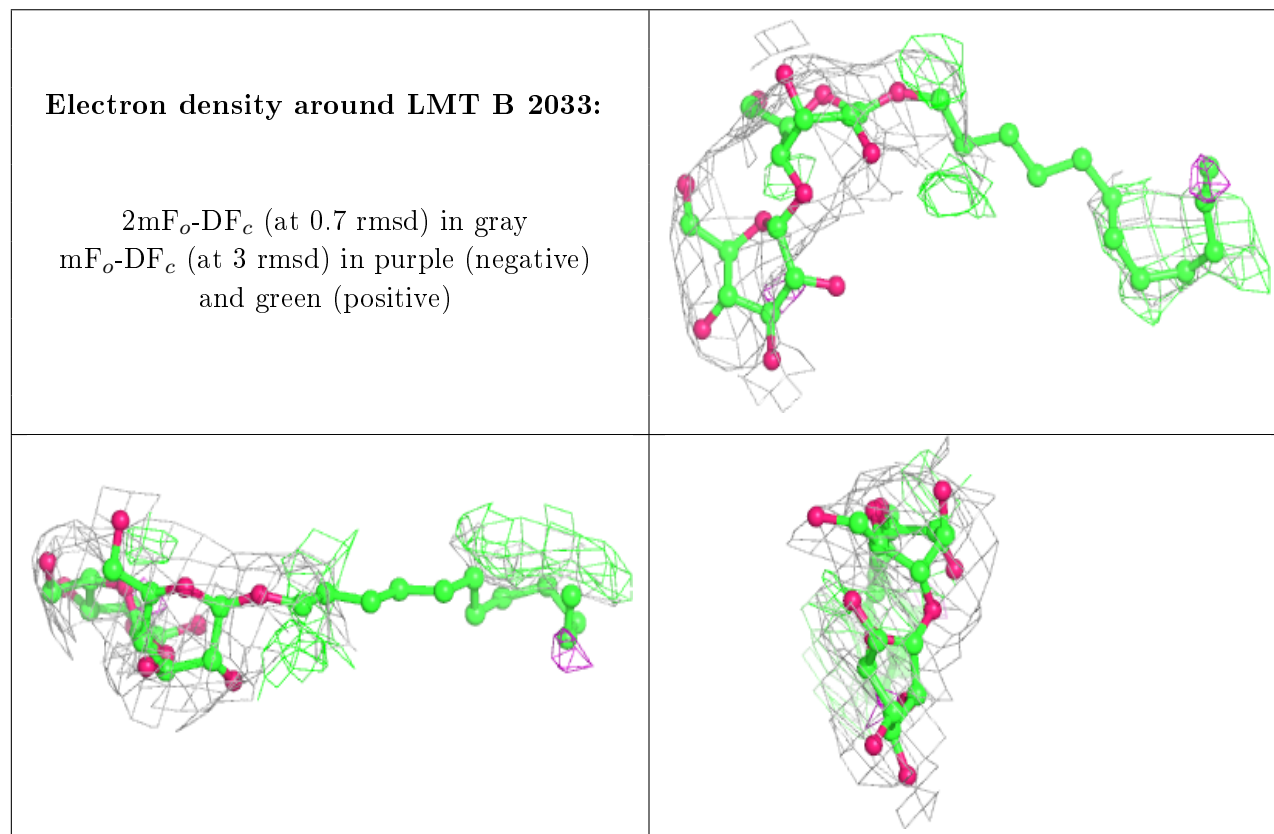


## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

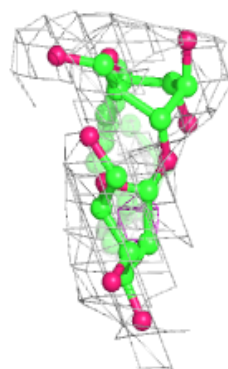
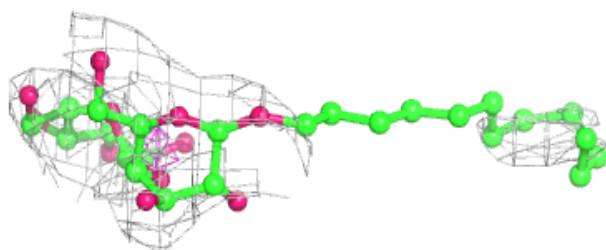
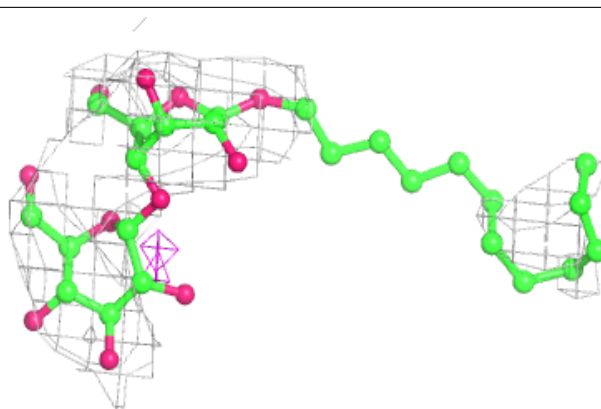
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	LMT	B	2033	35/35	0.72	0.42	100,155,176,183	0
2	LMT	E	2033	35/35	0.76	0.33	111,146,174,179	0
2	LMT	E	2031	35/35	0.85	0.23	72,95,121,130	0
2	LMT	B	2031	35/35	0.90	0.20	59,82,109,114	0
2	LMT	A	2026	35/35	0.90	0.21	80,110,145,173	0
2	LMT	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.

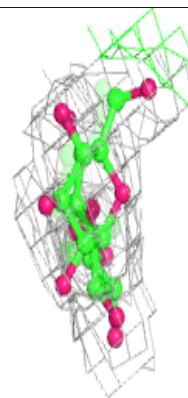
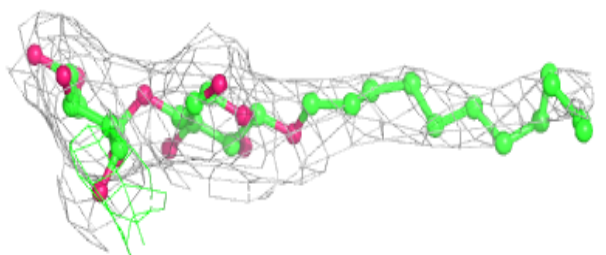
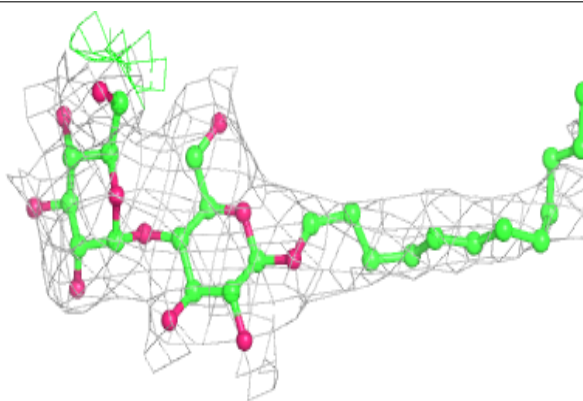


**Electron density around LMT E 2033:**

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

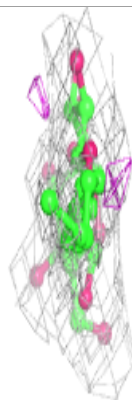
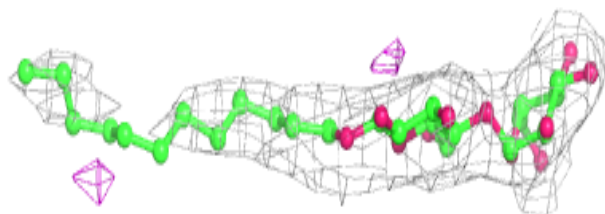
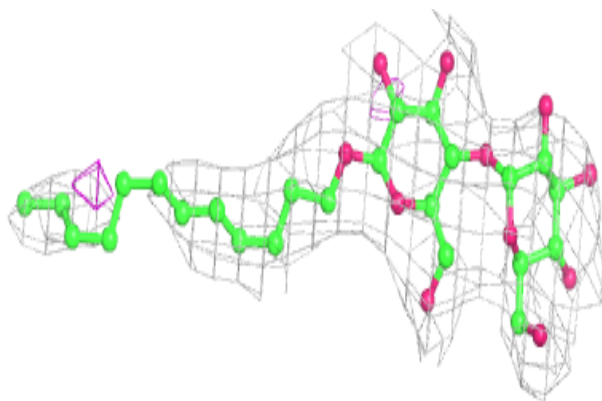
**Electron density around LMT E 2031:**

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

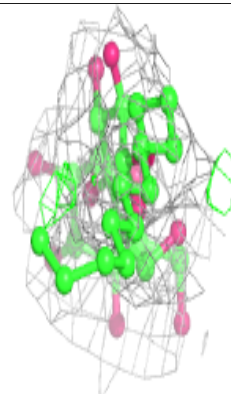
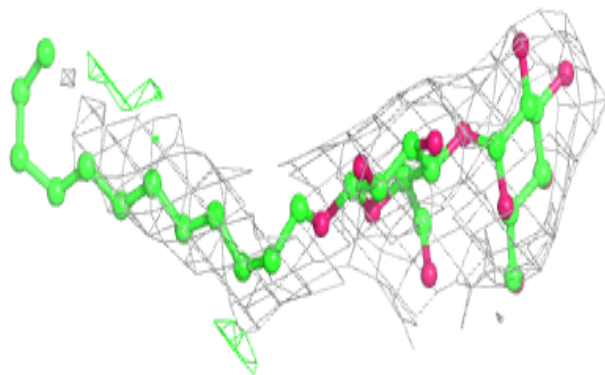
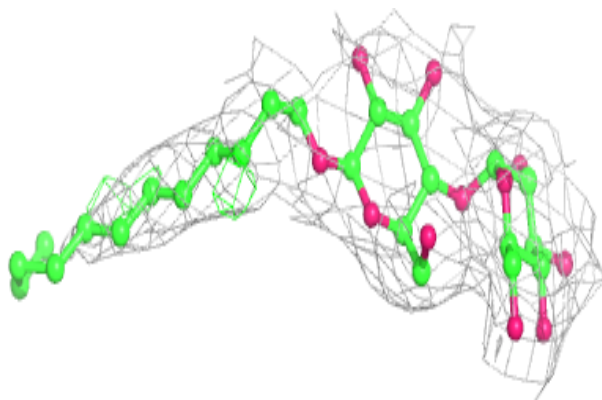


**Electron density around LMT B 2031:**

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

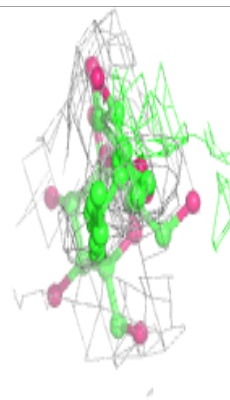
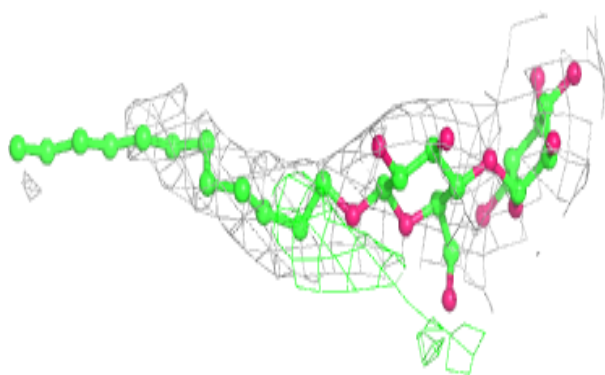
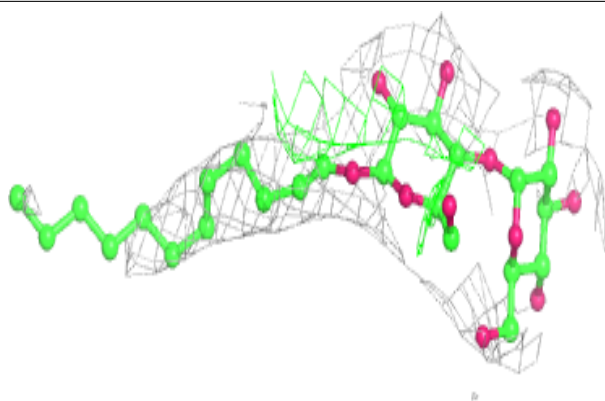
**Electron density around LMT A 2026:**

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

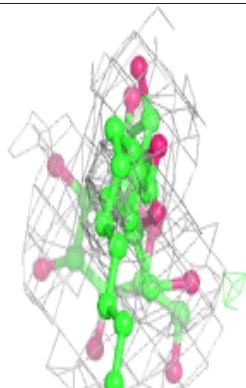
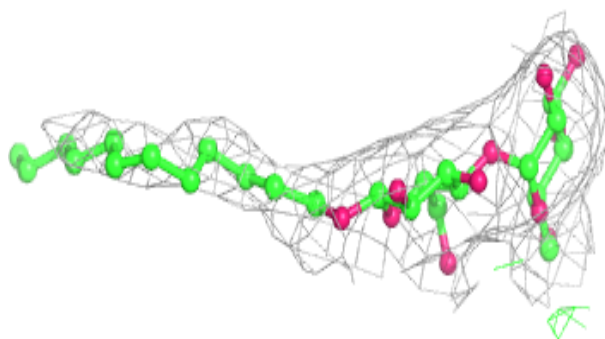
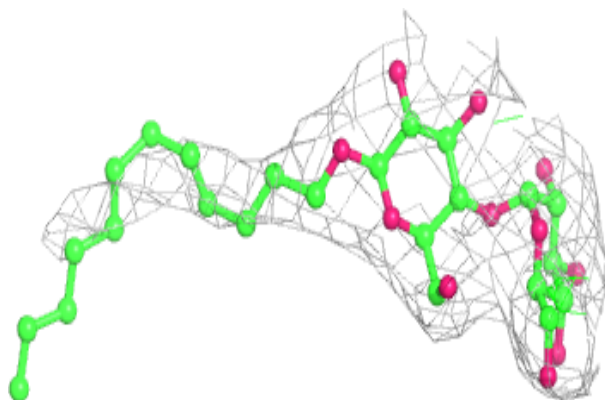


**Electron density around LMT D 2026:**

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

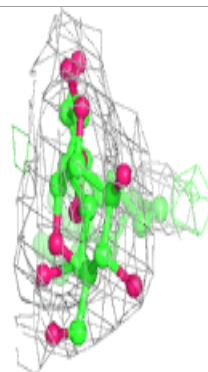
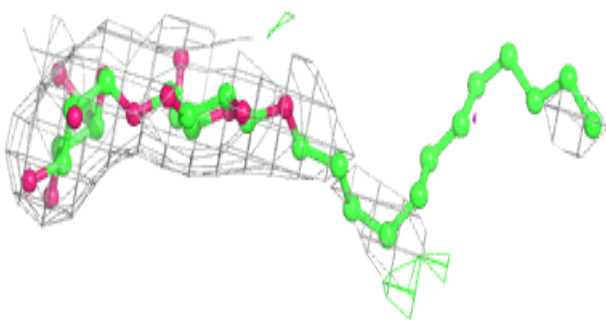
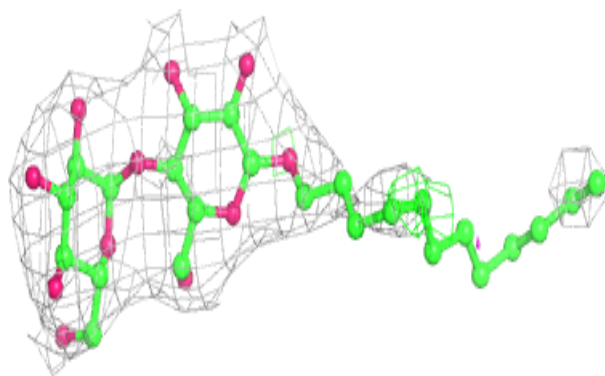
**Electron density around LMT E 2032:**

$2mF_o-DF_c$  (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.