



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2026 – 12:54 AM UTC

PDB ID : 4ZIW / pdb_00004ziw
Title : Crystal structure of AcrB deletion mutant in P21 space group
Authors : Ababou, A.; Koronakis, V.
Deposited on : 2015-04-28
Resolution : 3.40 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

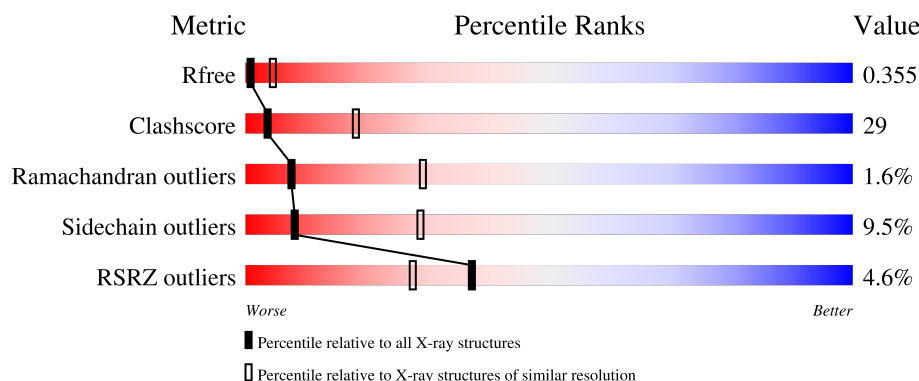
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1044	5% 43% 48% 8% .
1	B	1044	3% 47% 46% 6% .
1	C	1044	3% 42% 48% 9% ..
1	D	1044	4% 39% 51% 8% ..
1	E	1044	6% 45% 45% 9% ..

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Mol	Chain	Length	Quality of chain
1	F	1044	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LMT	D	2000	X	-	-	-
2	LMT	E	1101	X	-	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 47532 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 efflux pump subunit AcrB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1038	Total	C	N	O	S	0	0	0
			7893	5072	1306	1472	43			
1	B	1039	Total	C	N	O	S	0	0	0
			7900	5076	1307	1474	43			
1	C	1035	Total	C	N	O	S	0	0	0
			7867	5057	1299	1468	43			
1	D	1038	Total	C	N	O	S	0	0	0
			7893	5072	1306	1472	43			
1	E	1037	Total	C	N	O	S	0	0	0
			7883	5066	1303	1471	43			
1	F	1037	Total	C	N	O	S	0	0	0
			7883	5066	1303	1471	43			

There are 36 discrepancies between the modelled and reference sequences:

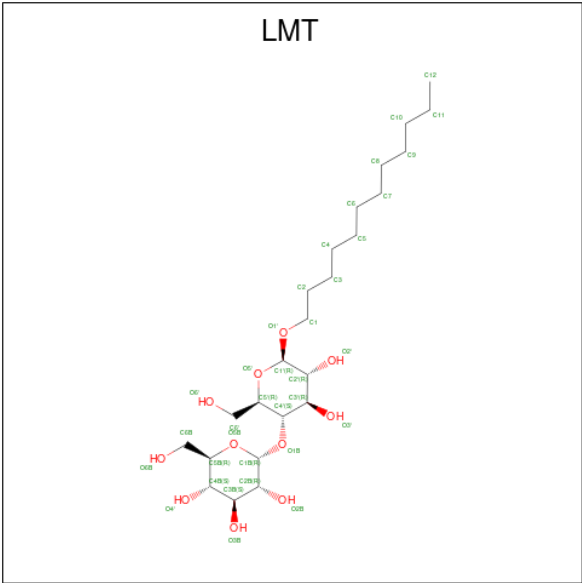
Chain	Residue	Modelled	Actual	Comment	Reference
A	615	GLY	PHE	engineered mutation	UNP P31224
A	?	-	GLY	deletion	UNP P31224
A	?	-	PHE	deletion	UNP P31224
A	?	-	ALA	deletion	UNP P31224
A	?	-	GLY	deletion	UNP P31224
A	?	-	ARG	deletion	UNP P31224
B	615	GLY	PHE	engineered mutation	UNP P31224
B	?	-	GLY	deletion	UNP P31224
B	?	-	PHE	deletion	UNP P31224
B	?	-	ALA	deletion	UNP P31224
B	?	-	GLY	deletion	UNP P31224
B	?	-	ARG	deletion	UNP P31224
C	615	GLY	PHE	engineered mutation	UNP P31224
C	?	-	GLY	deletion	UNP P31224
C	?	-	PHE	deletion	UNP P31224
C	?	-	ALA	deletion	UNP P31224
C	?	-	GLY	deletion	UNP P31224

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	ARG	deletion	UNP P31224
D	615	GLY	PHE	engineered mutation	UNP P31224
D	?	-	GLY	deletion	UNP P31224
D	?	-	PHE	deletion	UNP P31224
D	?	-	ALA	deletion	UNP P31224
D	?	-	GLY	deletion	UNP P31224
D	?	-	ARG	deletion	UNP P31224
E	615	GLY	PHE	engineered mutation	UNP P31224
E	?	-	GLY	deletion	UNP P31224
E	?	-	PHE	deletion	UNP P31224
E	?	-	ALA	deletion	UNP P31224
E	?	-	GLY	deletion	UNP P31224
E	?	-	ARG	deletion	UNP P31224
F	615	GLY	PHE	engineered mutation	UNP P31224
F	?	-	GLY	deletion	UNP P31224
F	?	-	PHE	deletion	UNP P31224
F	?	-	ALA	deletion	UNP P31224
F	?	-	GLY	deletion	UNP P31224
F	?	-	ARG	deletion	UNP P31224

- Molecule 2 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



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

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

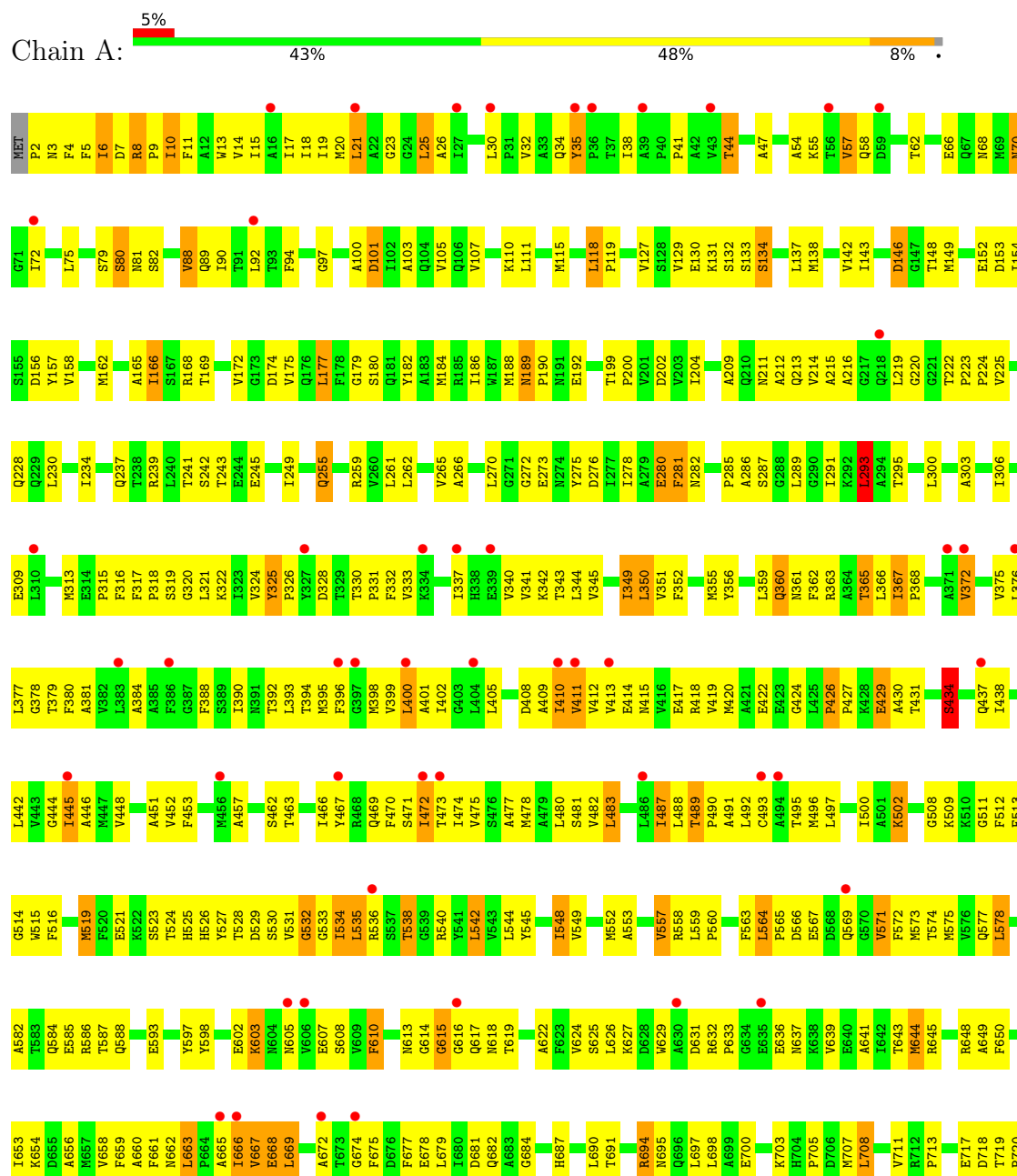
- Molecule 3 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

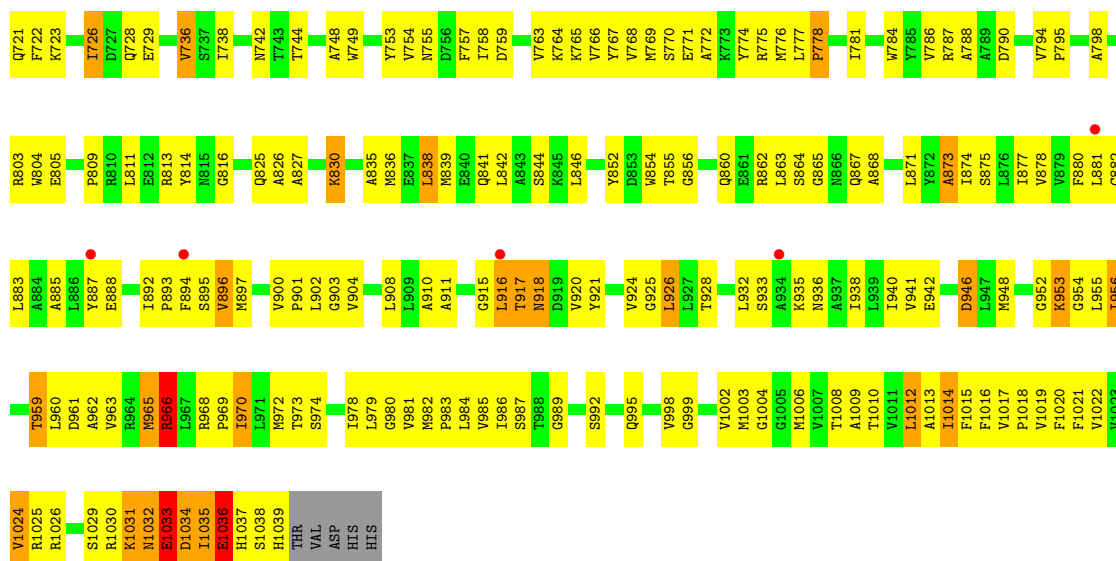
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ni	0	0
			1	1		
3	C	1	Total	Ni	0	0
			1	1		
3	E	1	Total	Ni	0	0
			1	1		

3 Residue-property plots

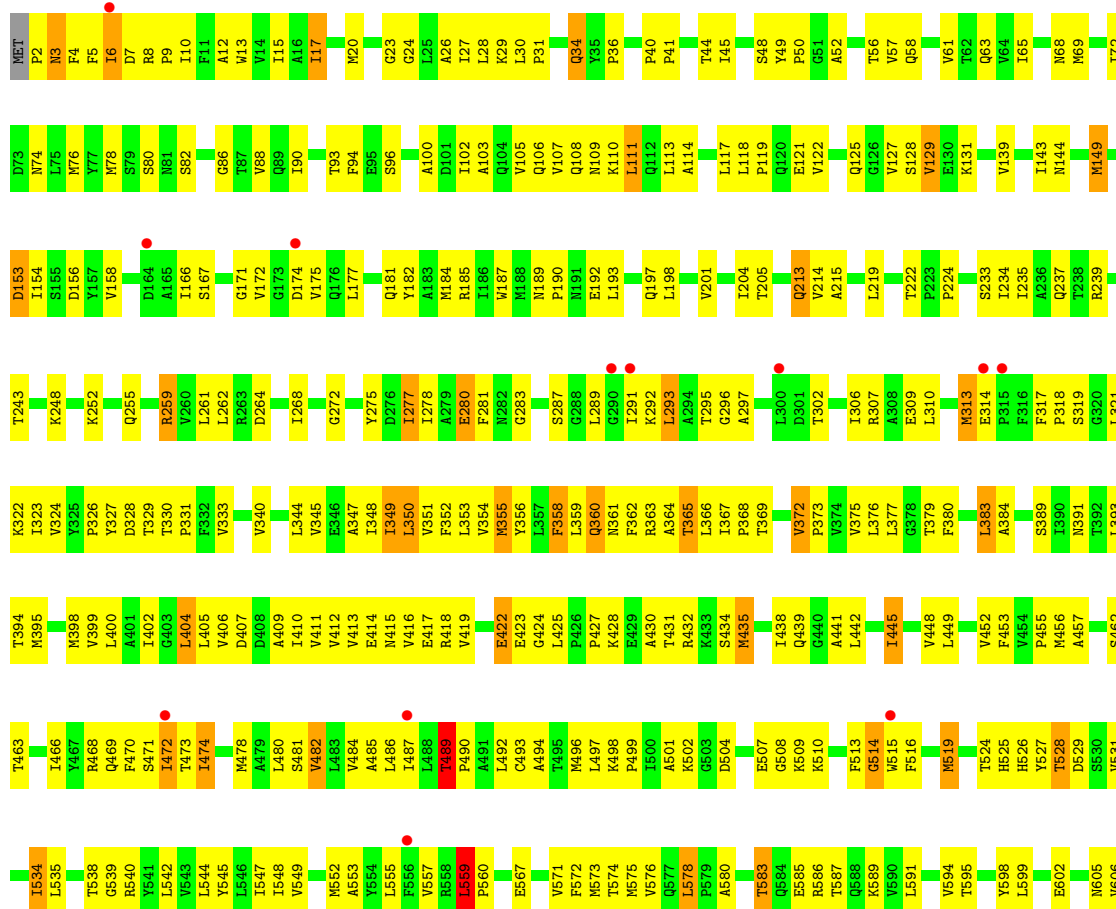
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

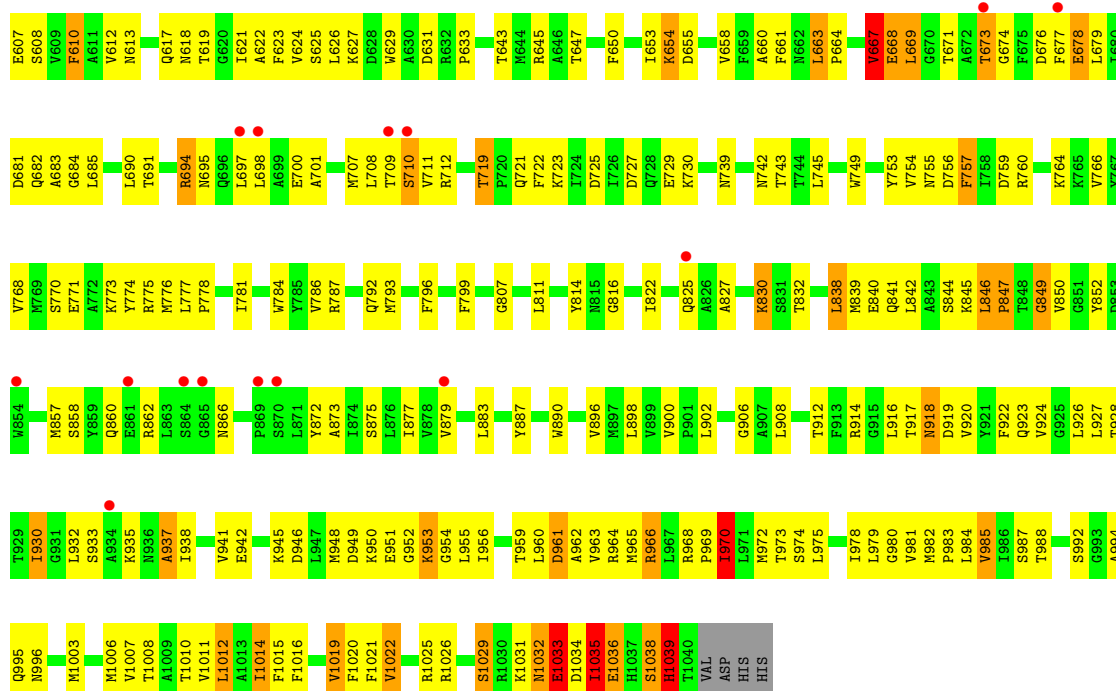
- Molecule 1: Multidrug efflux pump subunit AcrB

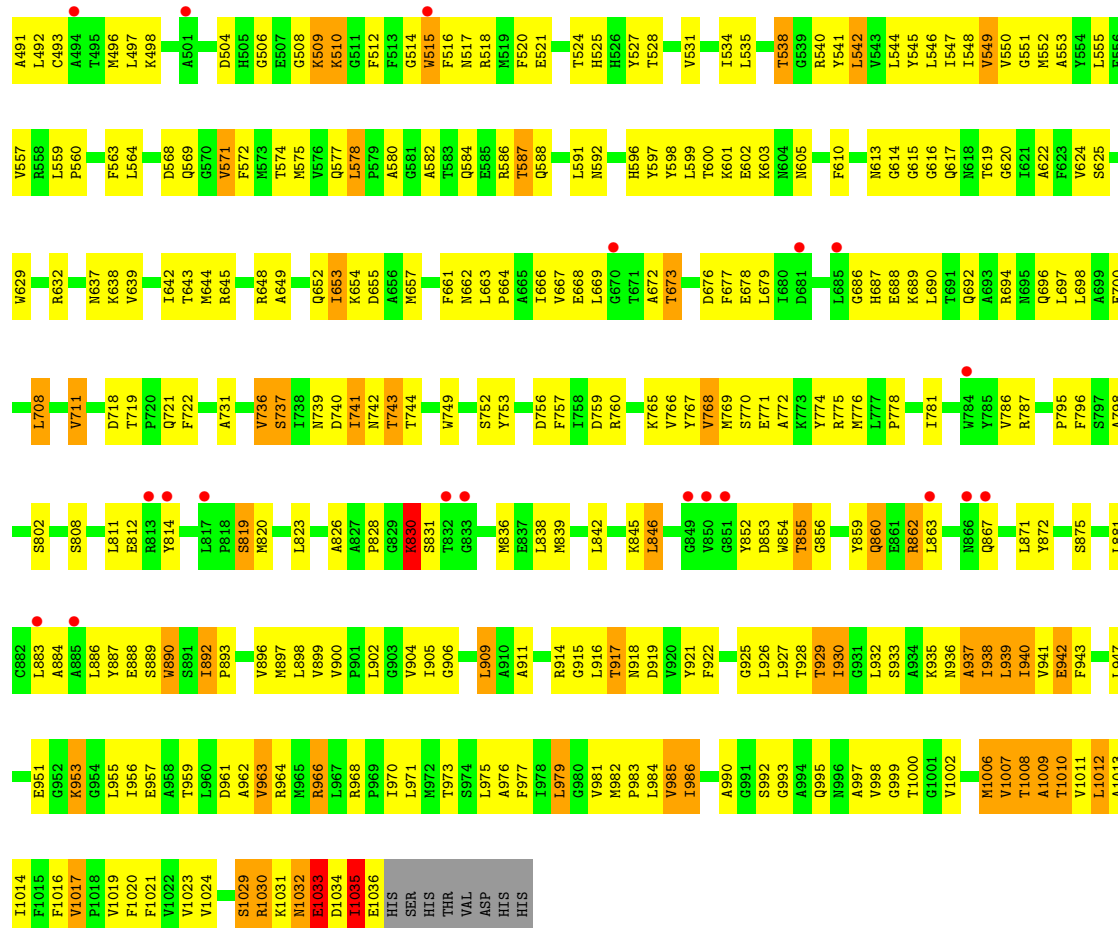




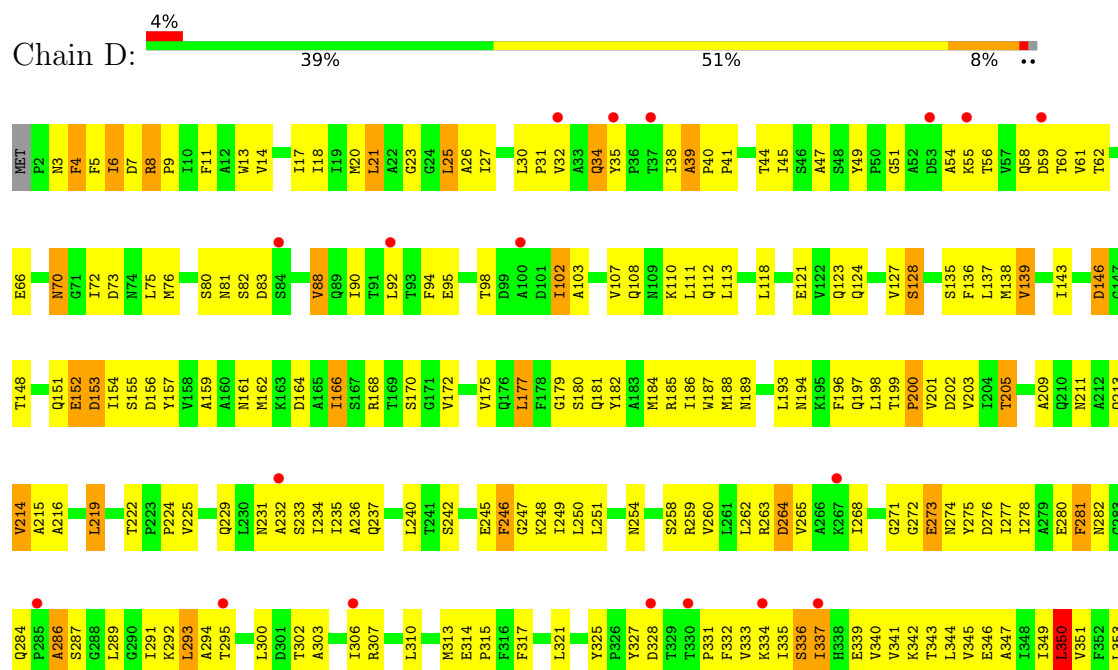
• Molecule 1: Multidrug efflux pump subunit AcrB

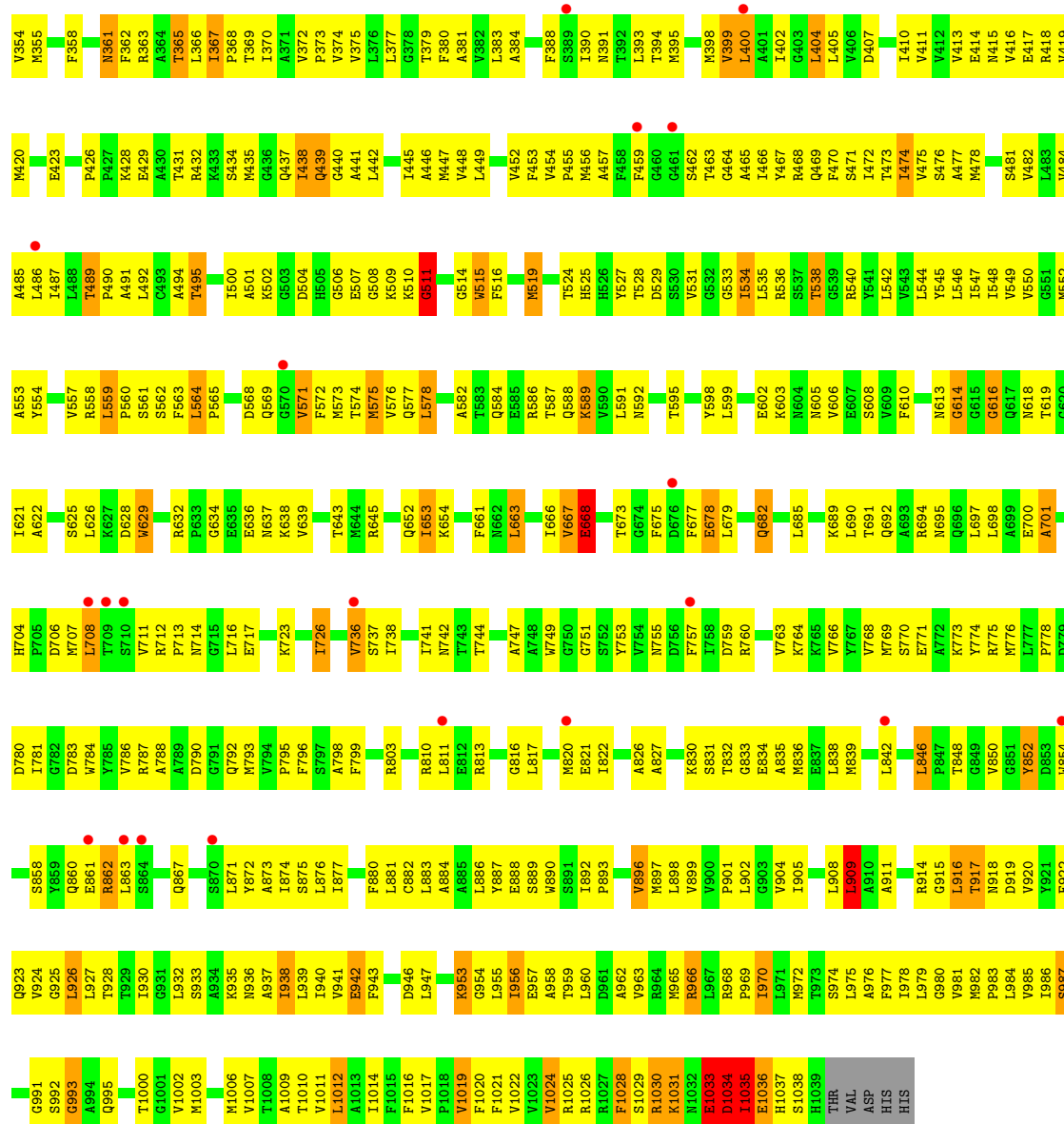






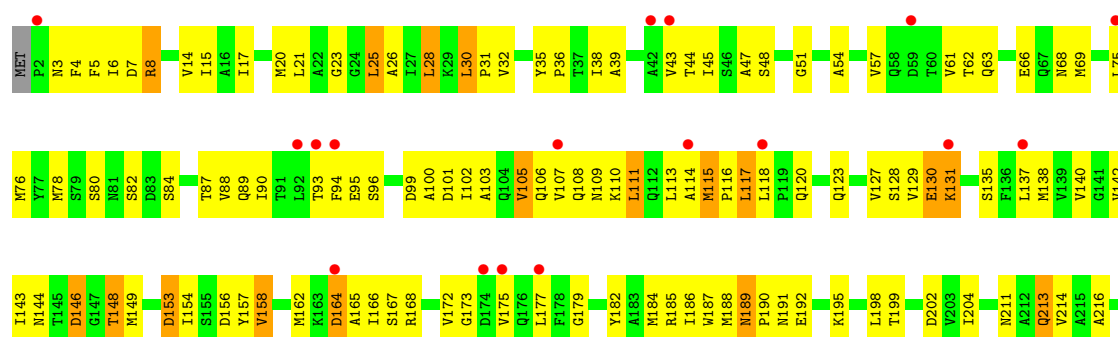
● Molecule 1: Multidrug efflux pump subunit AcrB

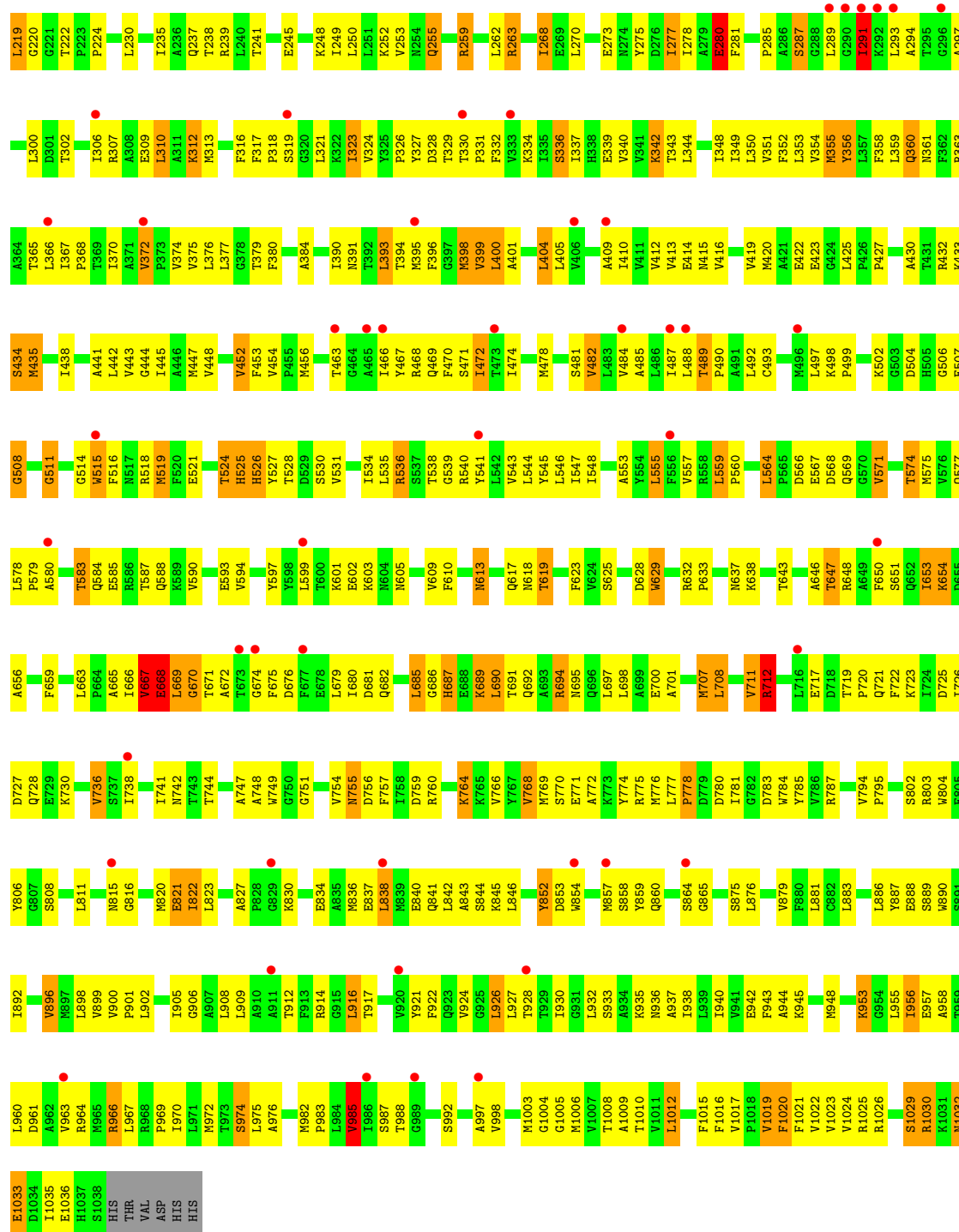




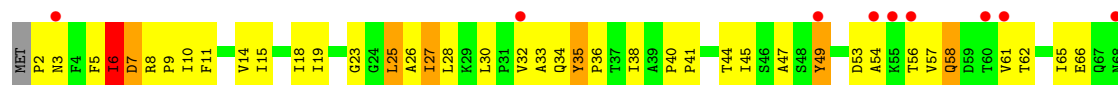
• Molecule 1: Multidrug efflux pump subunit AcrB

Chain E: 6% 45% 45% 9% ..





● Molecule 1: Multidrug efflux pump subunit AcrB



V1007	A934	R862	G791	M707	A641	F563	M496	R432	R363	N298	Q218	S133	M69
T1008	K935	L863	Q792	L708	T643	L564	L497	K433	A364		L219	S134	M70
A1009	N936	L863	M793	T709	T643	P565		S434	T365			S135	G71
T1010	A937	A868	V794	S710	M644	D566	I500	M435	L366	D301	T222	M138	I72
V1011	L938	V795	F795	V711	R645		A501	A501	T367	T302	P223	V139	M74
L1012	L939	L871	F796	R712	A646	V571	K502	Q439	P368	A393	P224	V140	M75
A1013	I940	Y872	S797	T713	T647		G503	A441	A371	A304	V225		M76
F1015	V941		A798	G715	R648	F650	H505	L442		L306	Q228	I143	M77
	K945	S875	R803		F650		G506	V443	V375	R307	Q229	N144	M78
P1017	D946	L876	W804	D718	I653		E507	G444	L376	A308	L230	T145	
L947	V878	V877	E805	T719	K654	L578	G508	I445	T379	E309	N231	D146	N81
V1019	M948	V879		P720	R654		K509	A446	F380	L310	G147	S82	
F1020	F880	F880	S808	Q721	A656	A582	K510	M447	F380	A311	I234	D83	
F1021	K953	L881	P809	F722	A656	T583	G511	V448	A381	K312	T234	T148	S84
V1022	G954	C882	R810	K723	M657	Q584	F512	V382	V382	M313	Q237	T150	T85
G1023	L955	L883	L811	I724	V658	E585	F513	L383	L383	E314	T238	Q151	G86
V1024	I956	A884	E812	D725	F659	R586	G514	V452	A384	P315	R239	E152	T87
			R813	I726	S787		W515	F453		F316	L240	E153	Q88
		Y887		Q728	Q727	Q588	F516	V454	I390	F317	L240	D154	Q89
F1028	T959		N815	Q728	L663	N592	M517	M456	T392	P318	T243	I58	I90
S1029	D961	S889	G816	I738	A665		M519		L393	S319			T91
R1030	A962	W890	L817		I666	T595	F520	F459	T394	G390	F246	V158	
K1031	V963	S891	P816		V667		E521	G460	M395	L321	Q247	D164	T93
E1033	R964	R892	S819	I741	R667	Y598	K522	G461		K321	K248	A165	F94
D1034	P965	P993	M820	N742	E668	L599	S523	S462		Y325	L249	E95	
I1035	R966	F894	E821	L745	L669	T600	T524	T463	M398	P326	L250	R168	S96
E1036	L967	S895	L822		G670		H525	G464	V399		L251	T169	G97
H1037	R968	V896	L823	W749	T671	E602	H526	A465	L400		K252	S170	
S1038	P969	M937			A672	R603	Y527	I466	A401	T329		G171	D101
HIS	I970		A827		T673			Y467	L402				I102
THR	L971	V900		N755	G674	N604		G403	G403		R259	S180	A103
VAL	M972	P901	K830	D756	F675	N605	V531	Q469	L404	V333	L261		Q104
ASP	T973	L902	S831	F757	D676	V606		R468	L405	K334	L262	M184	V105
HIS	S974	G903	T832	I768	F677		I534	F470	V406	S336	R263	R185	
HIS	L975	V904	G833	D759	E878	F610	L535	S471	D407	I337		I186	G106
	A976	I905	E834		L879	A611	R536	I472	D408	H338	A266	W187	V107
	F977		A835	R762	T680	V612	L536	T473	A409	E339	K267	M188	Q108
P1078	L978	L909	M836		D681	N613	T538	I474	L410	V340	L268	K110	M109
L979	A910	A910	E837	V766	Q682	G614	G539	V475	V411	K342	E269	L111	
G980	A911	A911	L838	V767	A683	G615	R540	S476	V412	V341	L270	Q112	
V981			M839	V768	G684	G616	Y541	A477	V413	T343	E192	L113	
	R914	R914		M769	L885	Q617	L542	M478	E414	L344	G271	L193	
P983	G915	G915	L842	S770	G686	N618	V543	A479	M415	V345	E272	N194	A114
L984	L916	L916	E771	H687	T619	G686	L544	L480	V416	V346	G273	M115	M115
V985	T917	T917	K845	A772	E688	G620	Y545	E417	A347	A346	N274	F196	P116
	N918	N918	L846	K773	K689	I621	L546	S481	A347	E347	Y275	Q197	L117
	D919	D919		Y774		A622	I547	V482	R418	I348	L278	L198	L118
	V920	V920	W850	R775	Q692	A622	F548	L483	M419	I349	I278	T199	F119
	Q923	Q923	G851	M776	A693	S625	V549	V484	A421	L350	A279	P200	Q120
	V924	V924	W852	L777	R694		V550	L486	E422	V351	E280	V201	V122
			D853	P778		W629		I487	E423	F352	F281		E123
			K854		Q696		A553	L488	G424	M355	Q284	T205	Q124
	L927	L927	T855	I781	L697	D631		T489	L425	Y356		W211	V127
	T928	T928	G856			R632	V557	P490	P426	L357	S287	A212	S128
G1001	T1000	T929	M857	W784	E700	P633	R558	A491	P427	F358	G288	Q213	
V1002	I930	I930	S858	V785			L559	L492	K428	L359	L289	W214	
M1003		G931	V786	K703		K638	P560	C493	E429	Q360	L289	A215	E130
			H859			V639	S561	A494	A430	N361	L293	A216	
		S922	D860	R787	D706	T640	S562	T405	T430	F362	A293	C217	S132

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	152.07Å 157.78Å 219.39Å 90.00° 93.14° 90.00°	Depositor
Resolution (Å)	20.00 – 3.40 20.00 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-3.40) 97.4 (20.00-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 3.41Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.275 , 0.349 0.288 , 0.355	Depositor DCC
R_{free} test set	7110 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	98.9	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 57.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	47532	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.48 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.8623e-05.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NI, 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	0.87	3/8043 (0.0%)	1.32	68/10922 (0.6%)
1	B	0.88	4/8050 (0.0%)	1.29	56/10932 (0.5%)
1	C	0.91	5/8015 (0.1%)	1.31	71/10884 (0.7%)
1	D	0.83	2/8043 (0.0%)	1.30	77/10922 (0.7%)
1	E	0.81	2/8032 (0.0%)	1.29	72/10907 (0.7%)
1	F	0.82	2/8032 (0.0%)	1.34	77/10907 (0.7%)
All	All	0.85	18/48215 (0.0%)	1.31	421/65474 (0.6%)

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	3
1	B	0	2
1	C	0	1
1	D	0	1
1	F	0	1
All	All	0	8

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	564	LEU	CA-C	-6.25	1.47	1.52
1	F	426	PRO	CA-C	5.90	1.55	1.51
1	A	513	PHE	CA-C	5.80	1.56	1.52
1	C	6	ILE	CA-C	5.76	1.60	1.52
1	B	534	ILE	CA-CB	5.75	1.61	1.54

The worst 5 of 421 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	559	LEU	CA-C-N	12.63	132.78	119.78
1	B	559	LEU	C-N-CA	12.63	132.78	119.78
1	F	7	ASP	CA-C-N	12.36	133.86	122.37
1	F	7	ASP	C-N-CA	12.36	133.86	122.37
1	A	674	GLY	N-CA-C	12.30	126.13	110.38

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1033	GLU	Peptide
1	A	1034	ASP	Peptide
1	A	1036	GLU	Peptide
1	B	1033	GLU	Peptide
1	B	1035	ILE	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7893	0	8034	484	0
1	B	7900	0	8041	407	0
1	C	7867	0	8015	480	0
1	D	7893	0	8034	546	0
1	E	7883	0	8027	484	0
1	F	7883	0	8027	503	0
2	A	35	0	46	4	0
2	B	35	0	46	3	0
2	C	35	0	46	2	0
2	D	35	0	46	3	0
2	E	35	0	46	8	0
2	F	35	0	46	1	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
All	All	47532	0	48454	2810	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 29.

The worst 5 of 2810 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:536:ARG:NE	2:E:1101:LMT:O3B	1.81	1.13
1:A:424:GLY:HA3	1:A:502:LYS:HG2	1.38	1.04
1:D:954:GLY:HA2	1:D:1034:ASP:H	1.23	1.03
1:C:686:GLY:HA3	1:C:689:LYS:HD3	1.42	1.01
1:D:533:GLY:HA2	1:D:536:ARG:HD3	1.48	0.95

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	1036/1044 (99%)	942 (91%)	79 (8%)	15 (1%)	9	31
1	B	1037/1044 (99%)	942 (91%)	85 (8%)	10 (1%)	12	40
1	C	1033/1044 (99%)	931 (90%)	84 (8%)	18 (2%)	7	28
1	D	1036/1044 (99%)	934 (90%)	83 (8%)	19 (2%)	6	26
1	E	1035/1044 (99%)	937 (90%)	87 (8%)	11 (1%)	11	38
1	F	1035/1044 (99%)	926 (90%)	84 (8%)	25 (2%)	4	22
All	All	6212/6264 (99%)	5612 (90%)	502 (8%)	98 (2%)	7	29

5 of 98 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	672	ALA
1	A	986	ILE
1	A	1029	SER
1	A	1033	GLU
1	B	617	GLN

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	846/852 (99%)	768 (91%)	78 (9%)	8	29
1	B	847/852 (99%)	766 (90%)	81 (10%)	8	28
1	C	843/852 (99%)	753 (89%)	90 (11%)	6	23
1	D	846/852 (99%)	771 (91%)	75 (9%)	9	31
1	E	845/852 (99%)	763 (90%)	82 (10%)	8	28
1	F	845/852 (99%)	767 (91%)	78 (9%)	8	29
All	All	5072/5112 (99%)	4588 (90%)	484 (10%)	8	29

5 of 484 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	892	ILE
1	F	519	MET
1	D	559	LEU
1	F	447	MET
1	F	961	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	867	GLN
1	E	605	ASN
1	F	613	ASN
1	D	918	ASN
1	E	231	ASN

5.3.3 RNA ⓘ

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](#)

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 for Mogul analysis.

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	1101	-	36,36,36	1.84	10 (27%)	47,47,47	1.95	9 (19%)
2	LMT	C	1101	-	36,36,36	1.85	10 (27%)	47,47,47	1.43	7 (14%)
2	LMT	A	1101	-	36,36,36	1.80	12 (33%)	47,47,47	1.38	6 (12%)
2	LMT	D	2000	-	36,36,36	1.87	11 (30%)	47,47,47	1.72	8 (17%)
2	LMT	F	2000	-	36,36,36	1.86	8 (22%)	47,47,47	1.15	4 (8%)
2	LMT	B	2000	-	36,36,36	1.81	9 (25%)	47,47,47	1.52	8 (17%)

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	1101	-	1/1/10/10	12/21/61/61	0/2/2/2
2	LMT	C	1101	-	-	12/21/61/61	0/2/2/2
2	LMT	A	1101	-	-	8/21/61/61	0/2/2/2
2	LMT	D	2000	-	1/1/10/10	12/21/61/61	0/2/2/2
2	LMT	F	2000	-	-	15/21/61/61	0/2/2/2
2	LMT	B	2000	-	-	13/21/61/61	0/2/2/2

The worst 5 of 60 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1101	LMT	O1'-C1'	4.30	1.47	1.40
2	C	1101	LMT	O5'-C5'	4.06	1.54	1.44
2	F	2000	LMT	O1'-C1'	4.05	1.46	1.40
2	D	2000	LMT	O1'-C1'	4.03	1.46	1.40
2	F	2000	LMT	O5'-C1'	4.03	1.52	1.41

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1101	LMT	O1B-C4'-C5'	-5.45	95.18	109.48
2	D	2000	LMT	O1'-C1'-C2'	5.27	116.28	108.27
2	C	1101	LMT	O1'-C1'-C2'	5.03	115.91	108.27
2	E	1101	LMT	C4B-C3B-C2B	4.79	119.23	110.83
2	D	2000	LMT	C1-O1'-C1'	4.66	121.63	113.68

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	2000	LMT	C3B
2	E	1101	LMT	C2B

5 of 72 torsion outliers are listed below:

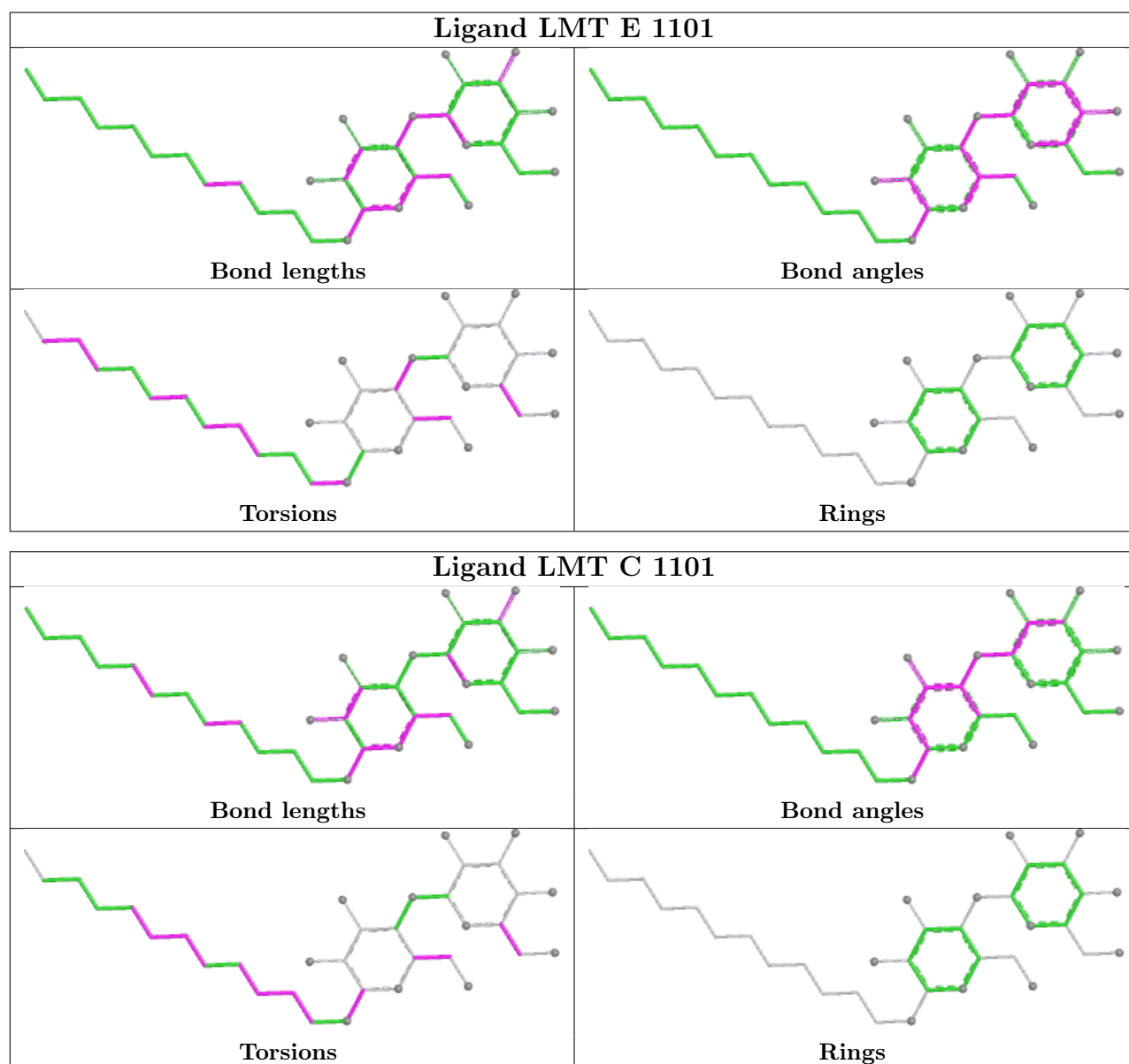
Mol	Chain	Res	Type	Atoms
2	F	2000	LMT	C2'-C1'-O1'-C1
2	E	1101	LMT	C4B-C5B-C6B-O6B
2	A	1101	LMT	O5'-C5'-C6'-O6'
2	F	2000	LMT	O5'-C5'-C6'-O6'
2	C	1101	LMT	O5B-C5B-C6B-O6B

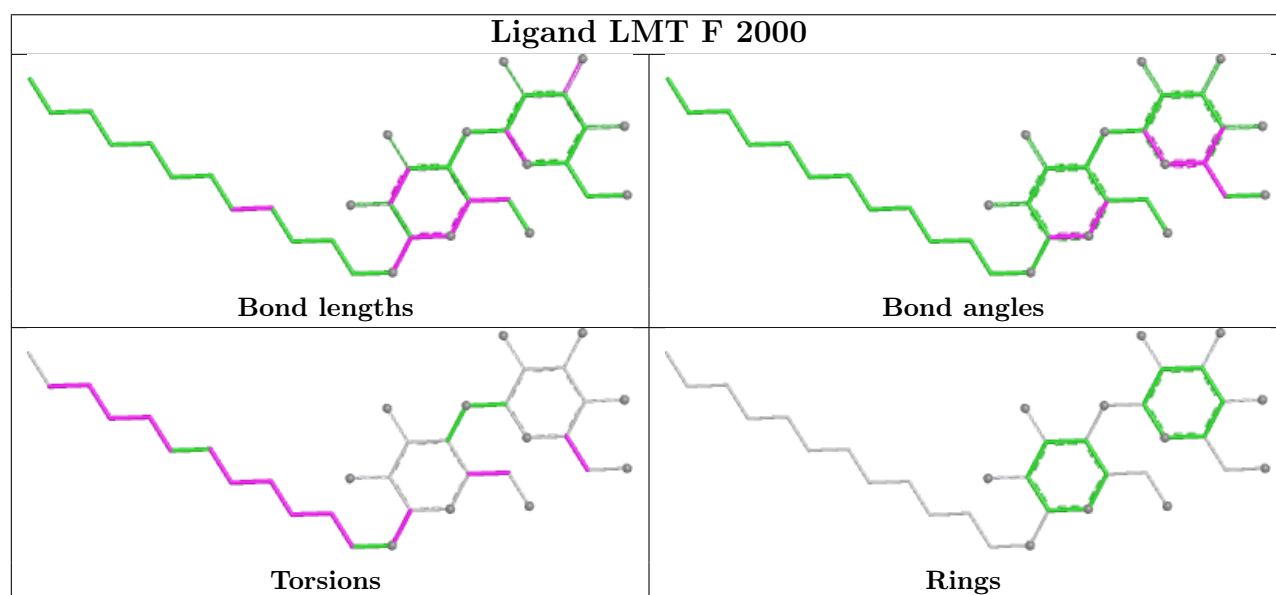
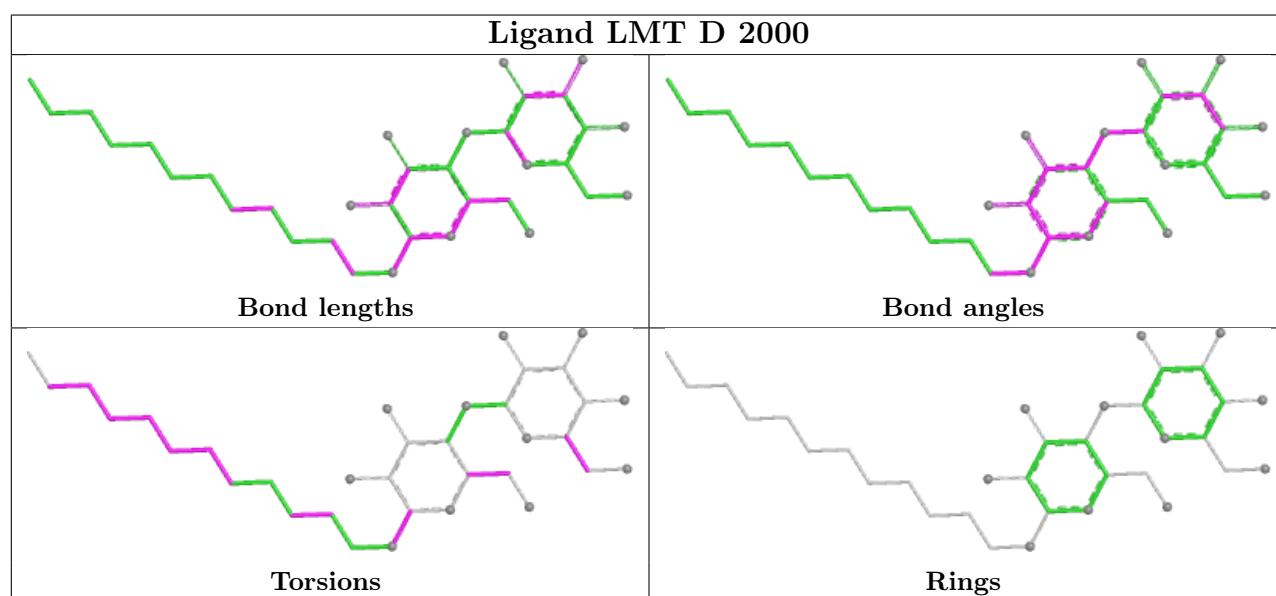
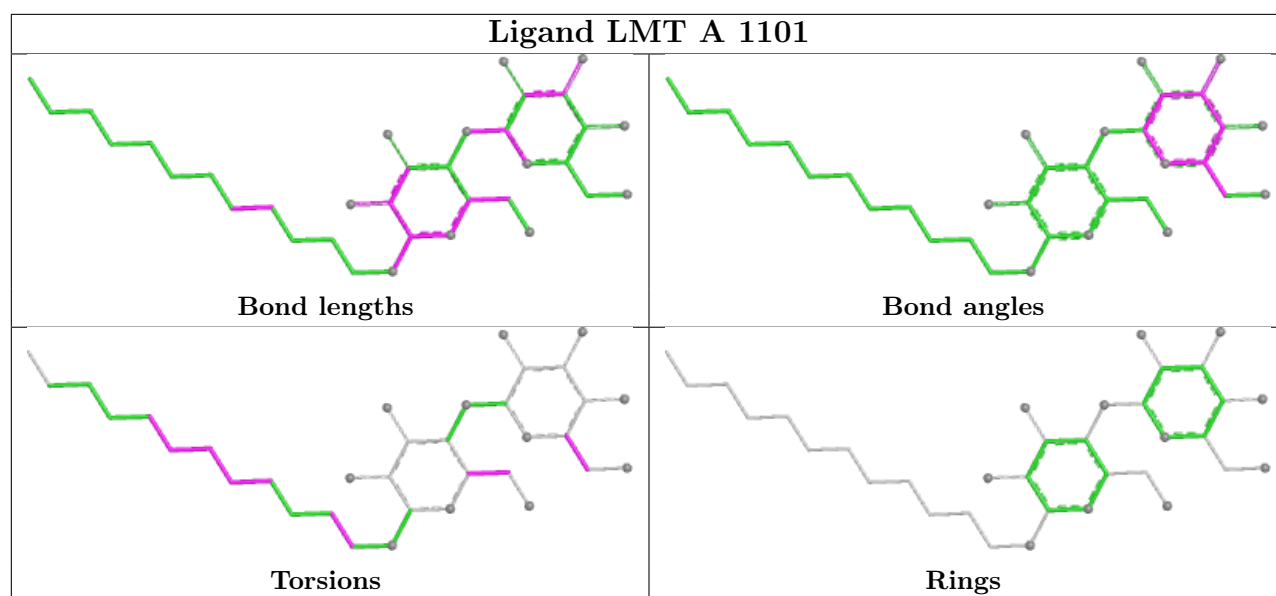
There are no ring outliers.

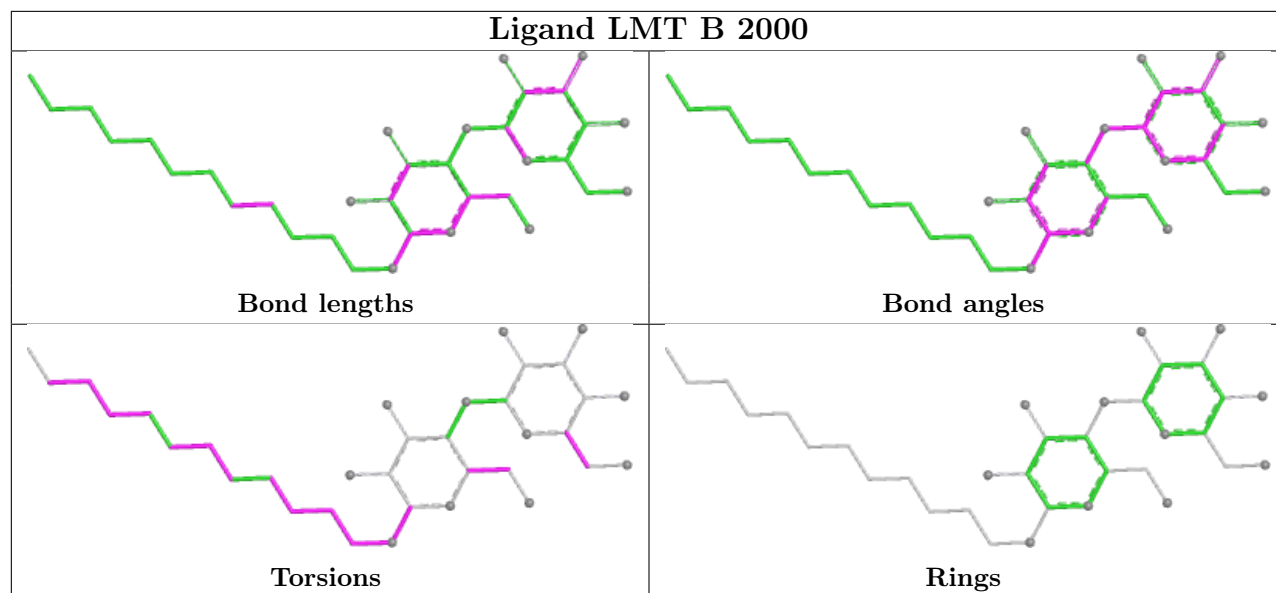
6 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1101	LMT	8	0
2	C	1101	LMT	2	0
2	A	1101	LMT	4	0
2	D	2000	LMT	3	0
2	F	2000	LMT	1	0
2	B	2000	LMT	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	1038/1044 (99%)	0.27	55 (5%)	32	24	27, 75, 109, 132	0
1	B	1039/1044 (99%)	0.04	27 (2%)	57	42	18, 68, 104, 130	0
1	C	1035/1044 (99%)	0.10	34 (3%)	49	36	17, 69, 104, 126	0
1	D	1038/1044 (99%)	0.29	38 (3%)	45	32	16, 90, 130, 173	0
1	E	1037/1044 (99%)	0.44	64 (6%)	26	21	40, 91, 115, 134	0
1	F	1037/1044 (99%)	0.42	67 (6%)	25	20	24, 84, 118, 142	0
All	All	6224/6264 (99%)	0.26	285 (4%)	37	27	16, 80, 115, 173	0

The worst 5 of 285 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	291	ILE	8.1
1	D	59	ASP	7.6
1	B	710	SER	6.6
1	A	383	LEU	6.3
1	E	864	SER	6.2

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](#)

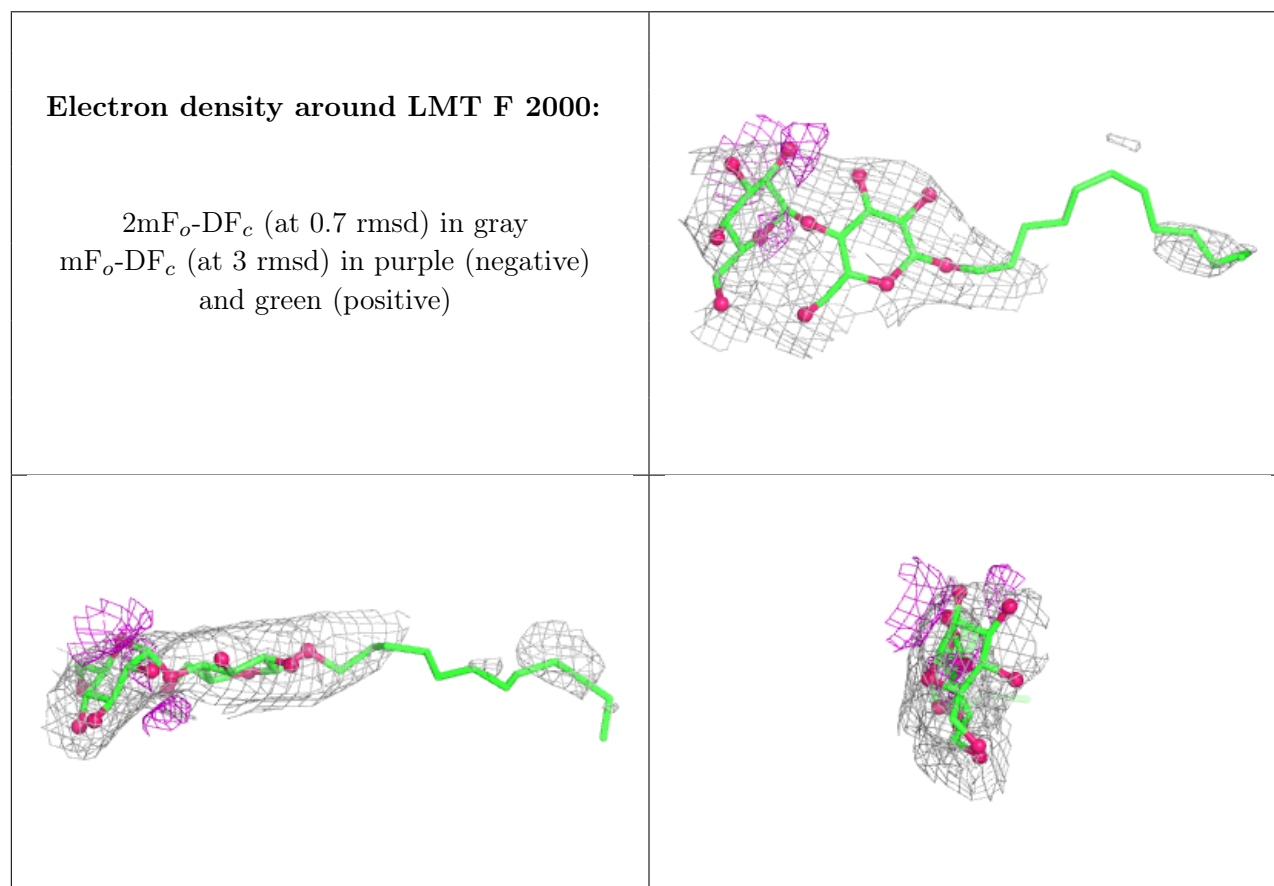
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

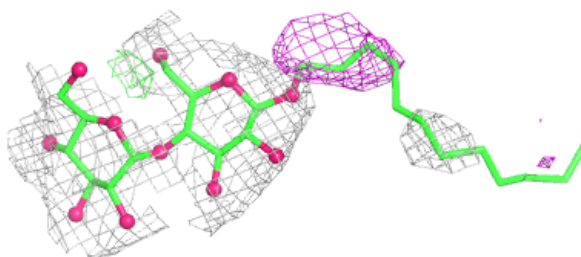
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	LMT	F	2000	35/35	0.79	0.13	40,64,89,94	0
2	LMT	B	2000	35/35	0.84	0.15	31,50,60,69	0
2	LMT	E	1101	35/35	0.85	0.11	41,74,104,107	0
2	LMT	D	2000	35/35	0.90	0.09	21,41,56,63	0
2	LMT	C	1101	35/35	0.91	0.07	12,41,56,72	0
2	LMT	A	1101	35/35	0.92	0.09	31,41,90,99	0
3	NI	E	1102	1/1	0.95	0.06	170,170,170,170	0
3	NI	A	1102	1/1	0.96	0.06	154,154,154,154	0
3	NI	C	1102	1/1	1.00	0.05	41,41,41,41	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.

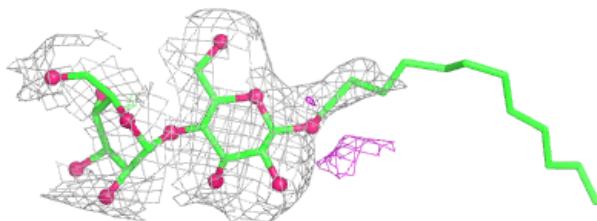


Electron density around LMT B 2000:

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

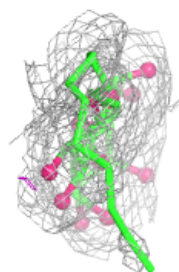
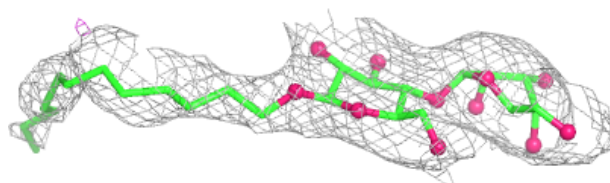
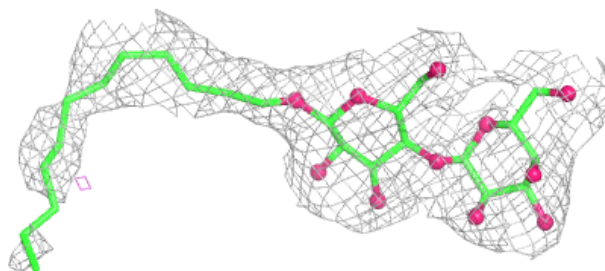
**Electron density around LMT E 1101:**

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

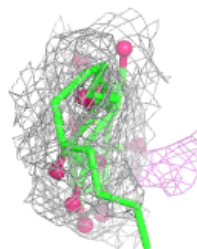
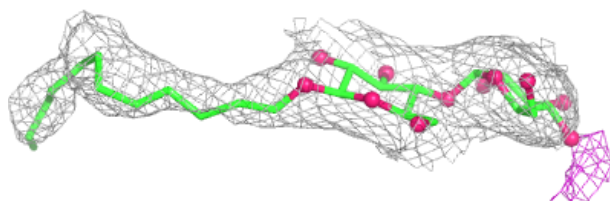
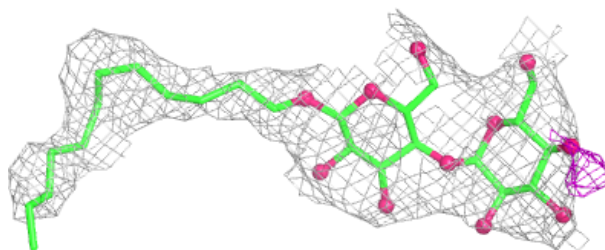


Electron density around LMT D 2000:

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

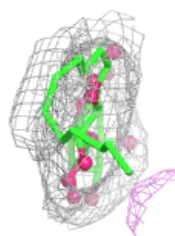
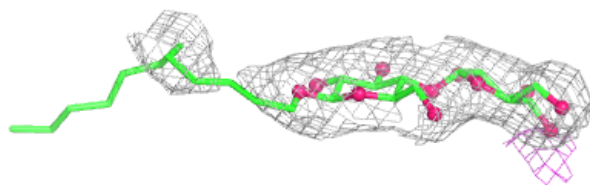
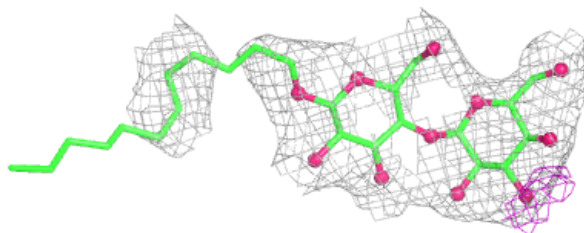
**Electron density around LMT C 1101:**

$2mF_o-DF_c$ (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)



6.5 Other polymers ⓘ

There are no such residues in this entry.