



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 5, 2022 – 01:18 pm BST

PDB ID : 7O3M
Title : Crystal Structure of AcrB Single Mutant - 1
Authors : Ababou, A.
Deposited on : 2021-04-02
Resolution : 3.55 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.27
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.27

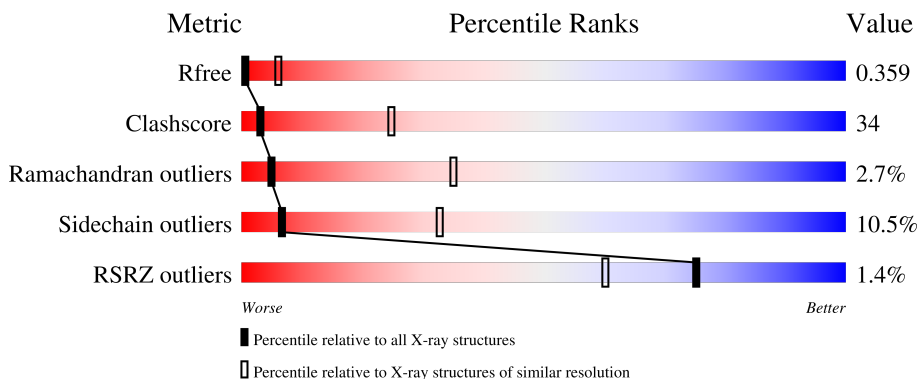
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.55 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	1020 (3.62-3.50)
Clashscore	141614	1100 (3.62-3.50)
Ramachandran outliers	138981	1065 (3.62-3.50)
Sidechain outliers	138945	1066 (3.62-3.50)
RSRZ outliers	127900	1009 (3.64-3.48)

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	1069	 41% 51% 6%
1	B	1069	 44% 45% 7%
1	C	1069	 41% 49% 7%
1	D	1069	 42% 48% 8%
1	E	1069	 38% 52% 7%

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Mol	Chain	Length	Quality of chain
1	F	1069	

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	A	2000	X	-	-	-
2	LMT	B	2000	X	-	-	-
2	LMT	C	2000	X	-	-	-
2	LMT	D	2000	X	-	-	-
2	LMT	E	2000	X	-	-	-
2	LMT	F	2000	X	-	-	-

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 47792 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 Efflux pump membrane transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1044	7936	5102	1312	1479	43	0	0	0
1	B	1042	7919	5092	1308	1476	43	0	0	0
1	C	1044	7936	5102	1312	1479	43	0	0	0
1	D	1044	7936	5102	1312	1479	43	0	0	0
1	E	1042	7919	5092	1308	1476	43	0	0	0
1	F	1044	7936	5102	1312	1479	43	0	0	0

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP E2QH56
A	-18	GLY	-	expression tag	UNP E2QH56
A	-17	SER	-	expression tag	UNP E2QH56
A	-16	SER	-	expression tag	UNP E2QH56
A	-15	HIS	-	expression tag	UNP E2QH56
A	-14	HIS	-	expression tag	UNP E2QH56
A	-13	HIS	-	expression tag	UNP E2QH56
A	-12	HIS	-	expression tag	UNP E2QH56
A	-11	HIS	-	expression tag	UNP E2QH56
A	-10	HIS	-	expression tag	UNP E2QH56
A	-9	SER	-	expression tag	UNP E2QH56
A	-8	SER	-	expression tag	UNP E2QH56
A	-7	GLY	-	expression tag	UNP E2QH56
A	-6	LEU	-	expression tag	UNP E2QH56
A	-5	VAL	-	expression tag	UNP E2QH56
A	-4	PRO	-	expression tag	UNP E2QH56
A	-3	ARG	-	expression tag	UNP E2QH56

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP E2QH56
A	-1	SER	-	expression tag	UNP E2QH56
A	0	HIS	-	expression tag	UNP E2QH56
A	620	ALA	ARG	engineered mutation	UNP E2QH56
B	-19	MET	-	initiating methionine	UNP E2QH56
B	-18	GLY	-	expression tag	UNP E2QH56
B	-17	SER	-	expression tag	UNP E2QH56
B	-16	SER	-	expression tag	UNP E2QH56
B	-15	HIS	-	expression tag	UNP E2QH56
B	-14	HIS	-	expression tag	UNP E2QH56
B	-13	HIS	-	expression tag	UNP E2QH56
B	-12	HIS	-	expression tag	UNP E2QH56
B	-11	HIS	-	expression tag	UNP E2QH56
B	-10	HIS	-	expression tag	UNP E2QH56
B	-9	SER	-	expression tag	UNP E2QH56
B	-8	SER	-	expression tag	UNP E2QH56
B	-7	GLY	-	expression tag	UNP E2QH56
B	-6	LEU	-	expression tag	UNP E2QH56
B	-5	VAL	-	expression tag	UNP E2QH56
B	-4	PRO	-	expression tag	UNP E2QH56
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C	-13	HIS	-	expression tag	UNP E2QH56
C	-12	HIS	-	expression tag	UNP E2QH56
C	-11	HIS	-	expression tag	UNP E2QH56
C	-10	HIS	-	expression tag	UNP E2QH56
C	-9	SER	-	expression tag	UNP E2QH56
C	-8	SER	-	expression tag	UNP E2QH56
C	-7	GLY	-	expression tag	UNP E2QH56
C	-6	LEU	-	expression tag	UNP E2QH56
C	-5	VAL	-	expression tag	UNP E2QH56
C	-4	PRO	-	expression tag	UNP E2QH56
C	-3	ARG	-	expression tag	UNP E2QH56

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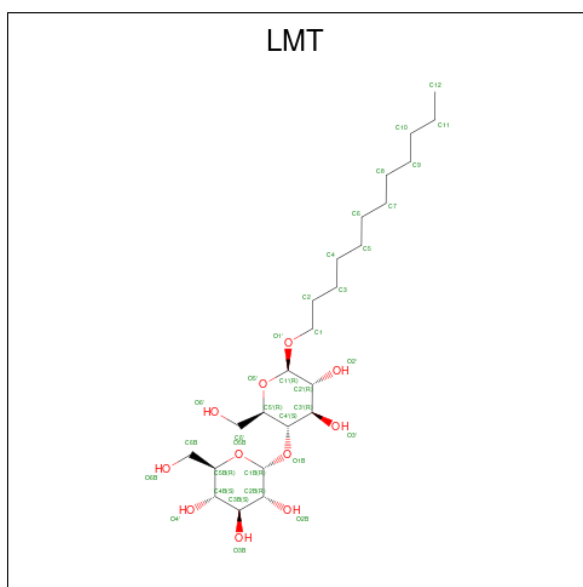
Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP E2QH56
C	-1	SER	-	expression tag	UNP E2QH56
C	0	HIS	-	expression tag	UNP E2QH56
C	620	ALA	ARG	engineered mutation	UNP E2QH56
D	-19	MET	-	initiating methionine	UNP E2QH56
D	-18	GLY	-	expression tag	UNP E2QH56
D	-17	SER	-	expression tag	UNP E2QH56
D	-16	SER	-	expression tag	UNP E2QH56
D	-15	HIS	-	expression tag	UNP E2QH56
D	-14	HIS	-	expression tag	UNP E2QH56
D	-13	HIS	-	expression tag	UNP E2QH56
D	-12	HIS	-	expression tag	UNP E2QH56
D	-11	HIS	-	expression tag	UNP E2QH56
D	-10	HIS	-	expression tag	UNP E2QH56
D	-9	SER	-	expression tag	UNP E2QH56
D	-8	SER	-	expression tag	UNP E2QH56
D	-7	GLY	-	expression tag	UNP E2QH56
D	-6	LEU	-	expression tag	UNP E2QH56
D	-5	VAL	-	expression tag	UNP E2QH56
D	-4	PRO	-	expression tag	UNP E2QH56
D	-3	ARG	-	expression tag	UNP E2QH56
D	-2	GLY	-	expression tag	UNP E2QH56
D	-1	SER	-	expression tag	UNP E2QH56
D	0	HIS	-	expression tag	UNP E2QH56
D	620	ALA	ARG	engineered mutation	UNP E2QH56
E	-19	MET	-	initiating methionine	UNP E2QH56
E	-18	GLY	-	expression tag	UNP E2QH56
E	-17	SER	-	expression tag	UNP E2QH56
E	-16	SER	-	expression tag	UNP E2QH56
E	-15	HIS	-	expression tag	UNP E2QH56
E	-14	HIS	-	expression tag	UNP E2QH56
E	-13	HIS	-	expression tag	UNP E2QH56
E	-12	HIS	-	expression tag	UNP E2QH56
E	-11	HIS	-	expression tag	UNP E2QH56
E	-10	HIS	-	expression tag	UNP E2QH56
E	-9	SER	-	expression tag	UNP E2QH56
E	-8	SER	-	expression tag	UNP E2QH56
E	-7	GLY	-	expression tag	UNP E2QH56
E	-6	LEU	-	expression tag	UNP E2QH56
E	-5	VAL	-	expression tag	UNP E2QH56
E	-4	PRO	-	expression tag	UNP E2QH56
E	-3	ARG	-	expression tag	UNP E2QH56

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP E2QH56
E	-1	SER	-	expression tag	UNP E2QH56
E	0	HIS	-	expression tag	UNP E2QH56
E	620	ALA	ARG	engineered mutation	UNP E2QH56
F	-19	MET	-	initiating methionine	UNP E2QH56
F	-18	GLY	-	expression tag	UNP E2QH56
F	-17	SER	-	expression tag	UNP E2QH56
F	-16	SER	-	expression tag	UNP E2QH56
F	-15	HIS	-	expression tag	UNP E2QH56
F	-14	HIS	-	expression tag	UNP E2QH56
F	-13	HIS	-	expression tag	UNP E2QH56
F	-12	HIS	-	expression tag	UNP E2QH56
F	-11	HIS	-	expression tag	UNP E2QH56
F	-10	HIS	-	expression tag	UNP E2QH56
F	-9	SER	-	expression tag	UNP E2QH56
F	-8	SER	-	expression tag	UNP E2QH56
F	-7	GLY	-	expression tag	UNP E2QH56
F	-6	LEU	-	expression tag	UNP E2QH56
F	-5	VAL	-	expression tag	UNP E2QH56
F	-4	PRO	-	expression tag	UNP E2QH56
F	-3	ARG	-	expression tag	UNP E2QH56
F	-2	GLY	-	expression tag	UNP E2QH56
F	-1	SER	-	expression tag	UNP E2QH56
F	0	HIS	-	expression tag	UNP E2QH56
F	620	ALA	ARG	engineered mutation	UNP E2QH56

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

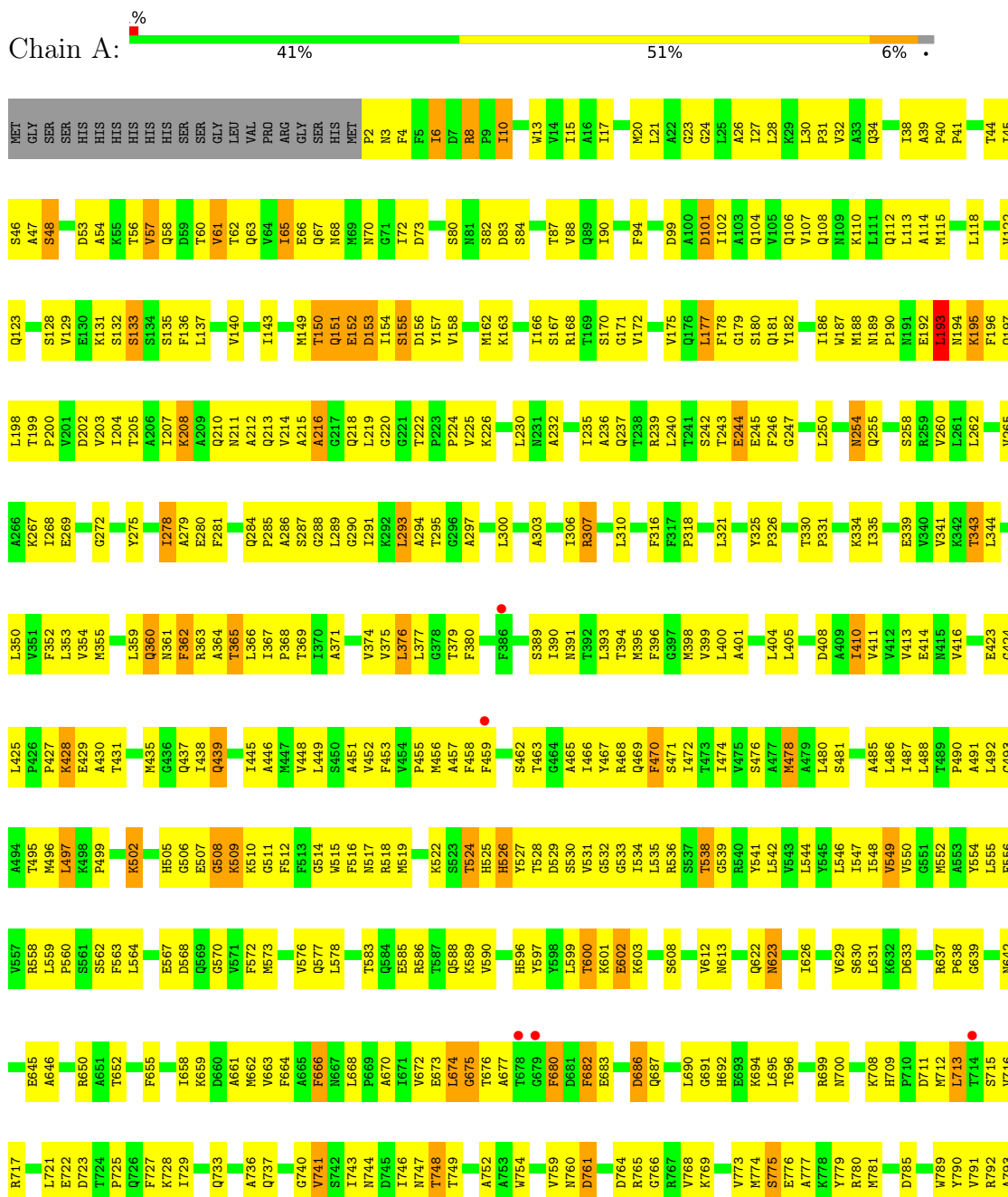


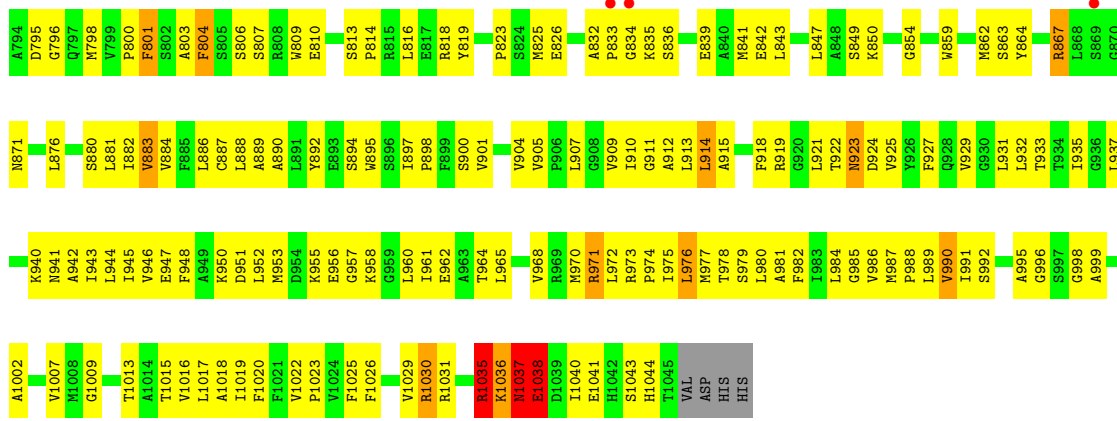
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			35	24	11		
2	B	1	Total	C	O	0	0
			35	24	11		
2	C	1	Total	C	O	0	0
			35	24	11		
2	D	1	Total	C	O	0	0
			35	24	11		
2	E	1	Total	C	O	0	0
			35	24	11		
2	F	1	Total	C	O	0	0
			35	24	11		

3 Residue-property plots

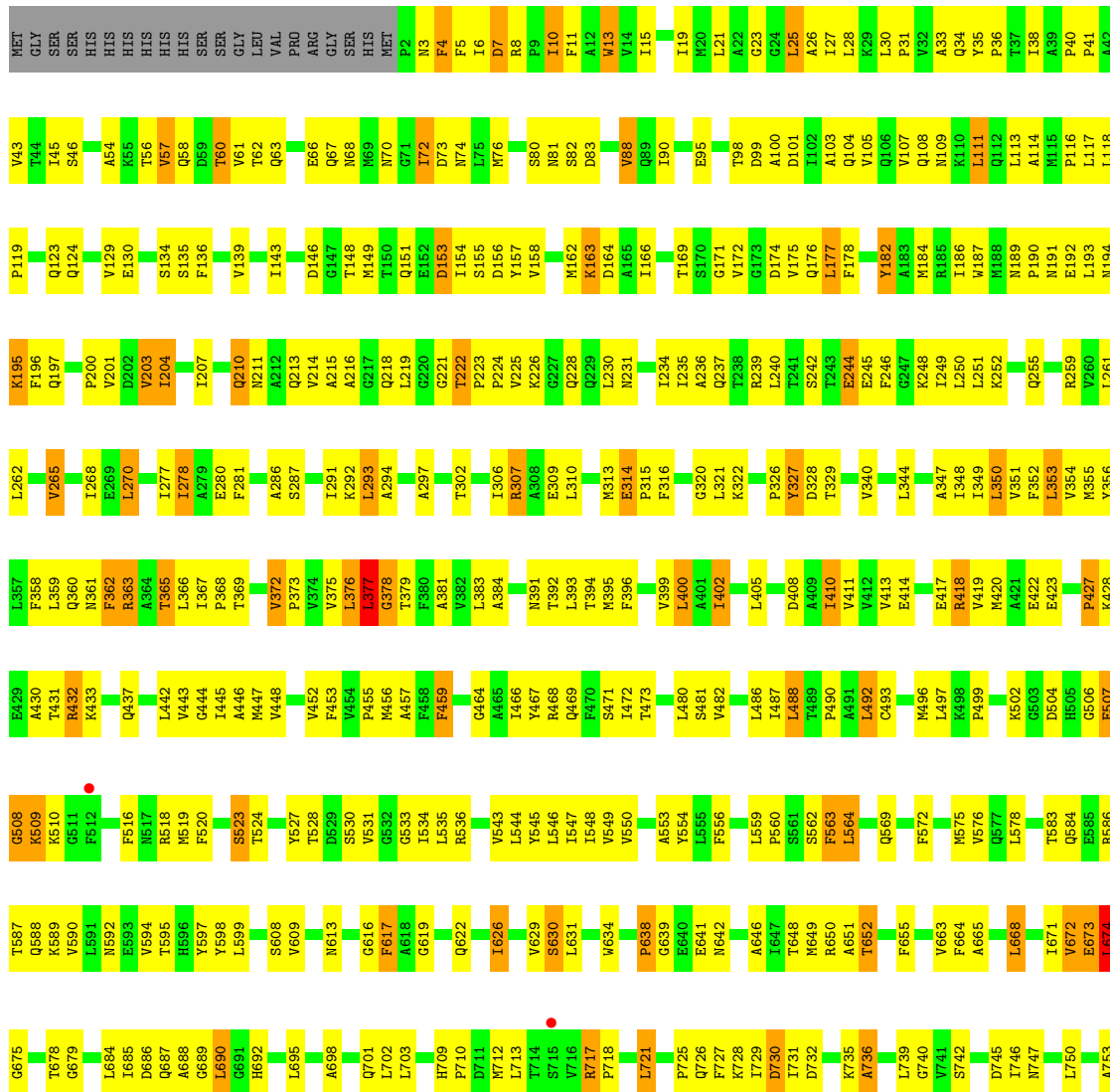
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

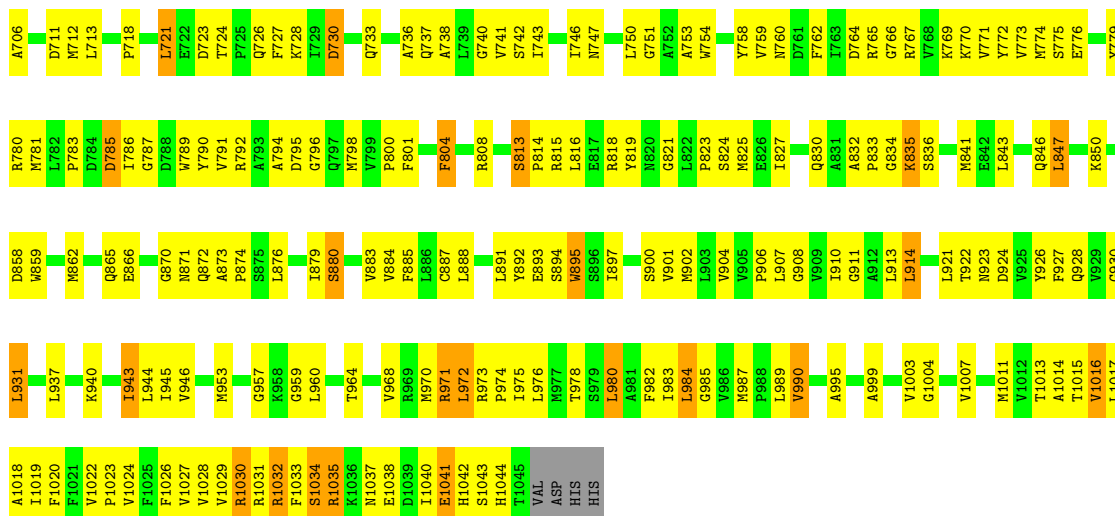
- Molecule 1: Efflux pump membrane transporter



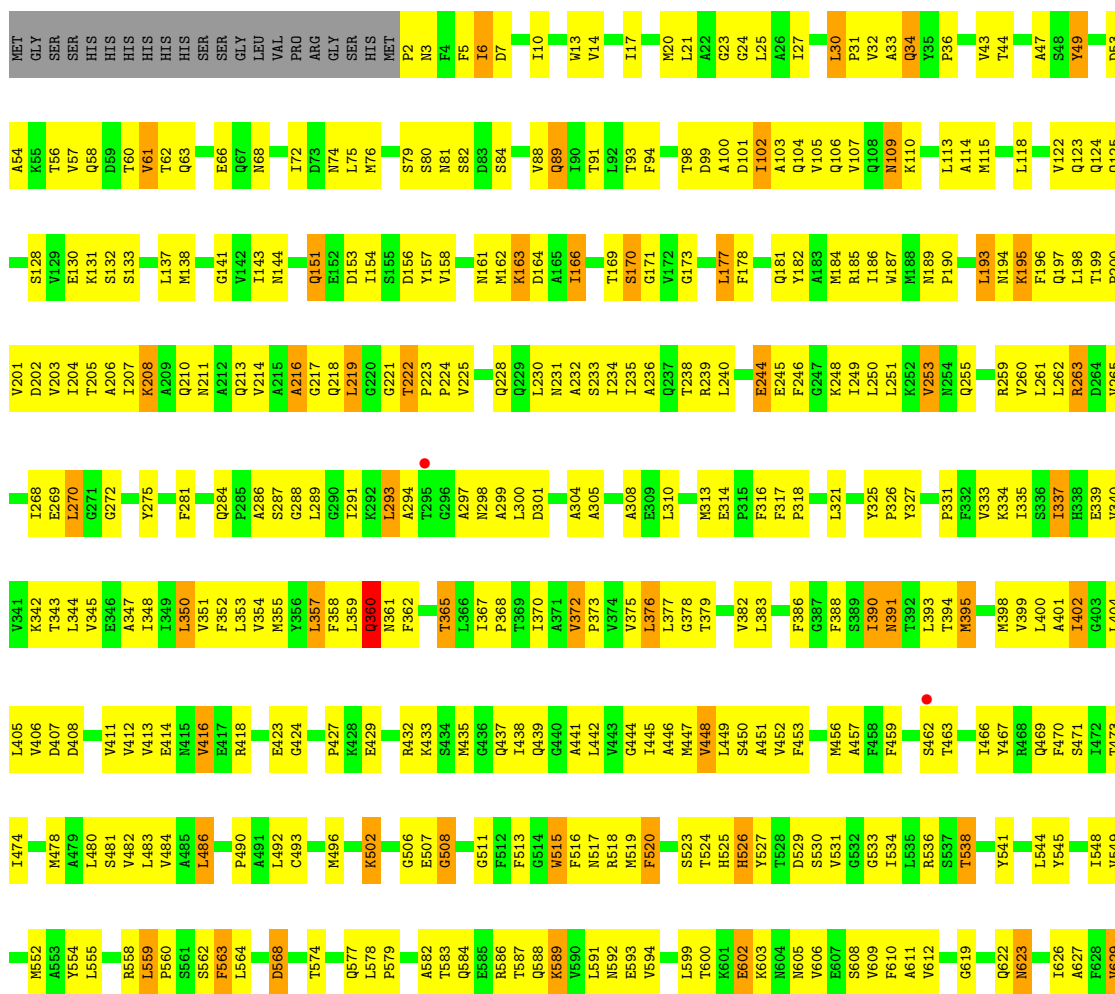


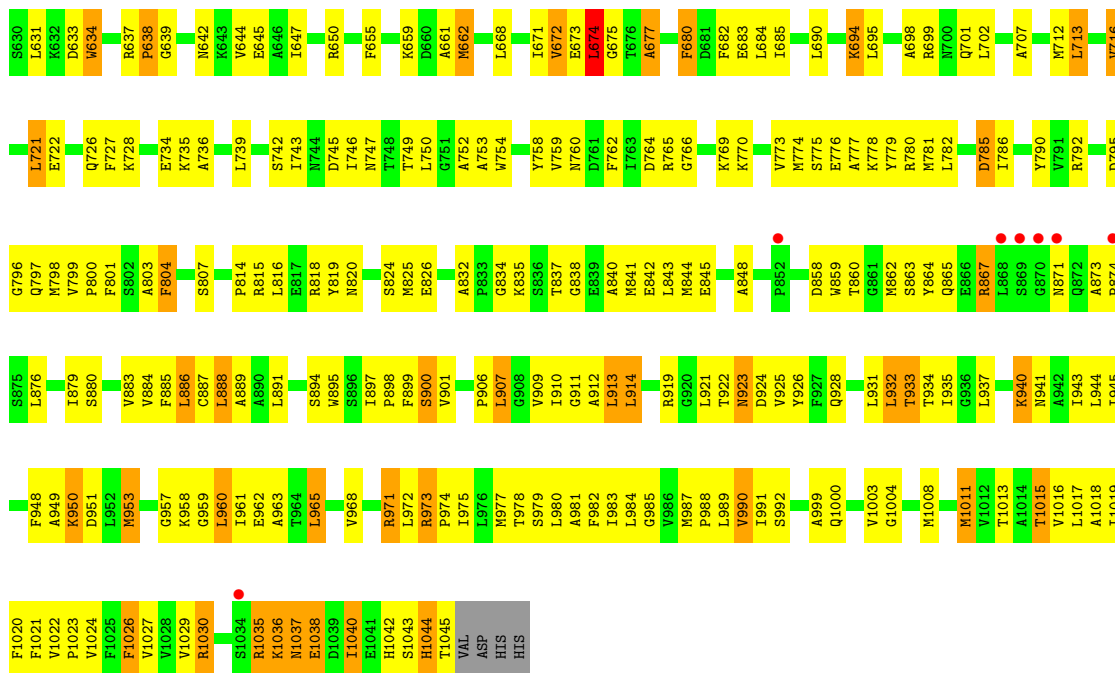
• Molecule 1: Efflux pump membrane transporter



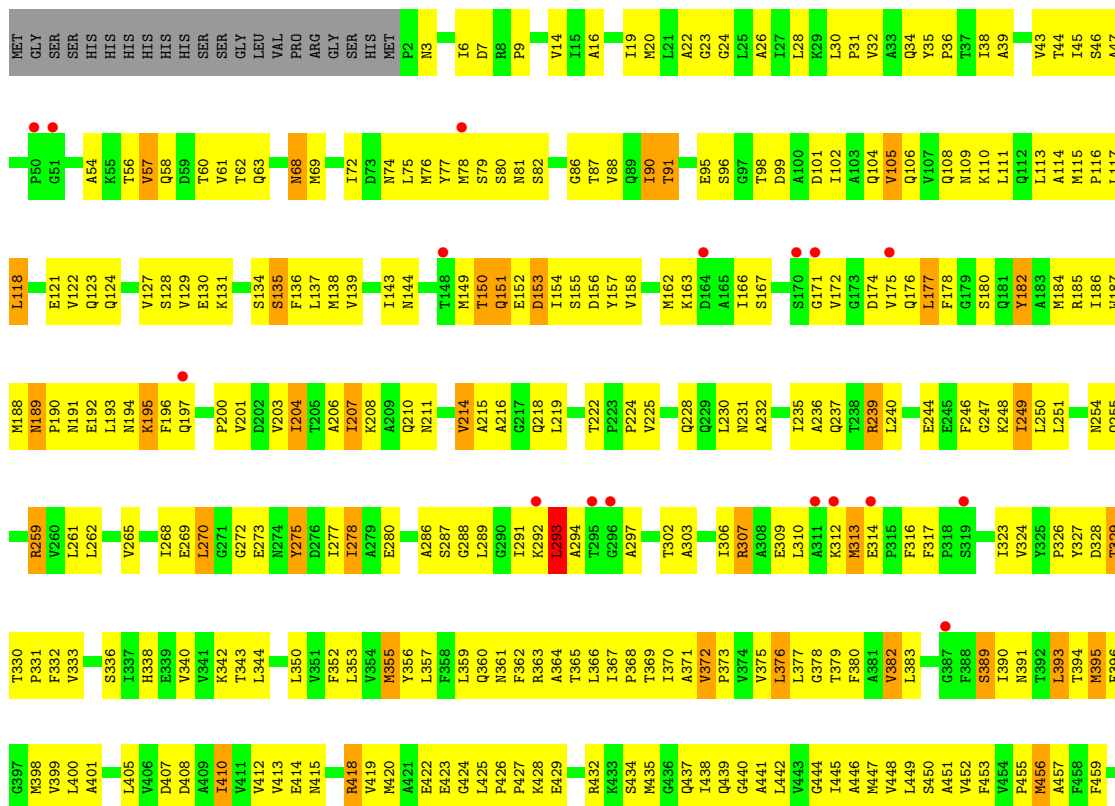


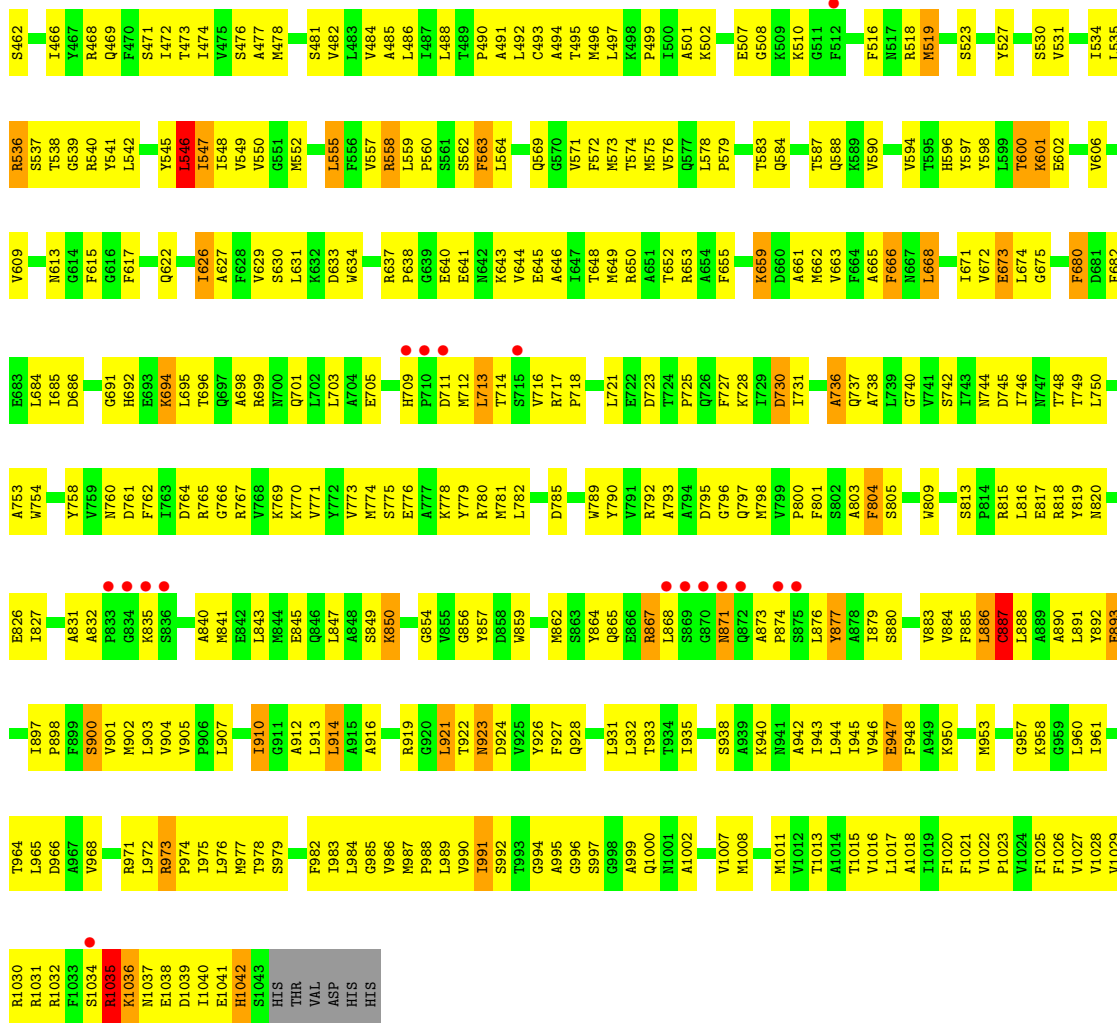
● Molecule 1: Efflux pump membrane transporter



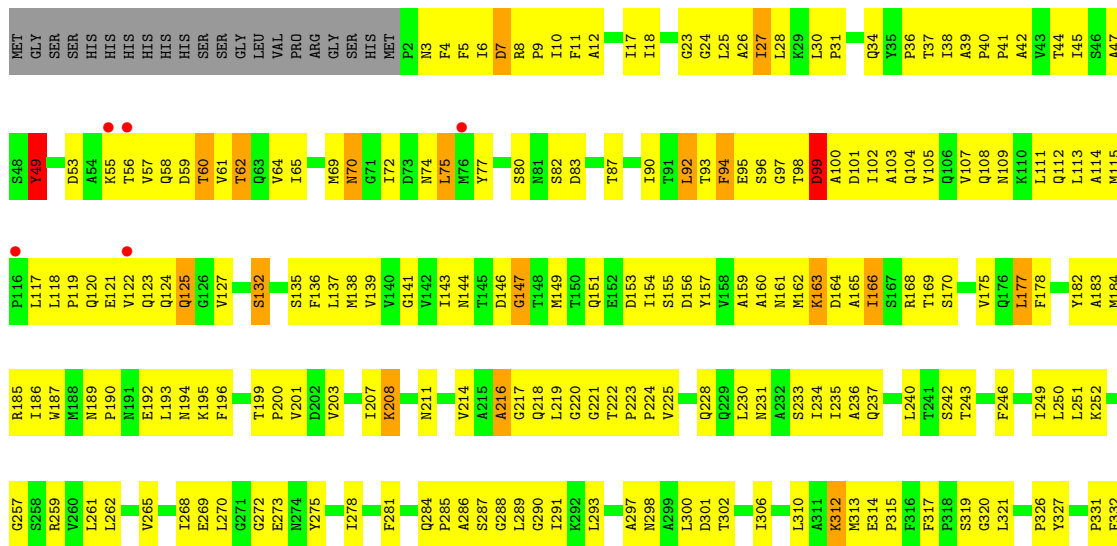


• Molecule 1: Efflux pump membrane transporter





● Molecule 1: Efflux pump membrane transporter



F1033	V333	L472	I534	T600	T676	G751	R818	Y892	E962	F1033
S1034	K334	T473	L535	R601	A677	A752	T619	E893	A963	S1034
R1035	L404	T474	R536	E602	T678	A753	T620	S894	T964	R1035
K1036	V406	V475	R537	K603	G679	W754	G821	W895	L965	K1036
M1037	D407	S476	T538	E607	F680	Y758	L822	S896	R966	M1037
E1038	D408	A477	G539	S608	D681	Y759	R823	T897	V968	E1038
D1039	A409	M478	R540	V609	F682	W759	S824	P898	R969	D1039
I1040	V412	L479	Y641	F610	E683	N760	H825	F899	M970	I1040
H1042	V413	L480	L542	L694	E684	D761	E826	S900	R971	H1042
S1043	E411	L489	V543	A611	I685	I762	R827	Y901	L972	S1043
H1044	V482	V480	L544	B612	D686	I763	L828	N902	R973	H1044
T1045	M415	V483	V545	M613	M613	D764	G829	L903	P974	T1045
VAL	R418	V484	L546	I947	L690	R765	G830	Y904	M977	VAL
ASP	V419	A485	I948	A618	G691	G766	H831	V905	T978	ASP
HIS	M420	L486	V549	G619	H692	R767	R832	P906	T979	HIS
	M421	L487	V549	G619	E693	R768	R833	L907	S979	
	A421	L488	M552	Q622	K694	K769	G834	G908	L980	
	E422	T489	A453	M623	A698	K770	R835	Y909	A981	
	E423	P490	A554	R699	R699	V772	T837	G911	F982	
	E424	A491	L555	I626	M700	M773	G838	A912	L983	
	P426	C493	F556	F627	Q701	M774	G839	L913	L984	
	P427	A494	V557	F628	L702	S775	M841	L914	G985	
	K428	T495	R558	V629	L703	E776	E842	L921	M987	
	E429	M496	L559	S630	A704	A777	L843	L922	P988	
	A430	L497	P560	L631	M712	K776	Q846	T923	L989	
	T431	K498	S561	R632	L713	Y779	L847	N923	V990	
		P499	D633	W634	L714	R780	R848	D924	I991	
		S434	F563	M634	V716	M781	R849	Y925	G994	
	M435	L500	L564	P638	L782	L782	R850	Y926	A995	
		A501	L564	V644	R717	P783	L851	F927	G996	
		K502	P565	E644	P718	D784	D785	Q928	S997	
		G503	D568	E645	M719	D786	I786	Y929	G998	
			V571	E645	Q720	G787	L787	L931	A999	
			F572	M649	E722	D788	D858	L932	M1008	
			T574	R650	E723	Y789	R859	T933	G1009	
			M575	R653	F727	Y791	G860	F934	G1009	
			F512	A654	K728	R792	G861	L935	G1010	
			F513	F655	E729	A793	M862	G936	M1011	
			G514	Q577	I731	A794	S863	L937	V1012	
			M515	L578	D732	D795	Y864	L937	T1013	
			F516	P579	Q733	G796	Q865	K940	A1014	
			M517	T587	F733	Q797	E866	I941	T1015	
			R518	Q588	A736	M798	G870	A942	V1016	
			M519	K588	Q737	Y799	N871	L943	L1017	
			F520	R586	A738	P800	Q872	Y946	I1018	
				Q588	L739	F801	S880	F947	I1019	
				K589	G740	F804	Y883	F948	F1020	
				V590	V741	F804	Y884	A949	V1021	
				L591	S742	R808	Y885	K950	P1022	
				M592	I743	W809	F884	D951	P1023	
				E593	N744	R809	F885	L952	F1026	
				V594	A670	E970	F886	L952	V1027	
				T595	I671	D745	C887	K955	M1028	
				H596	M672	M747	L888	Y959	V1029	
				E596	E673	T748	R815	G959	R1030	
				L599	L674	L749	R815	L960	R1031	
					L675	L750	E817	L891	R1032	

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	152.37Å 156.80Å 218.65Å 90.00° 92.48° 90.00°	Depositor
Resolution (Å)	19.95 – 3.55 19.95 – 3.55	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.95-3.55) 99.6 (19.95-3.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 3.52Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.277 , 0.359 0.277 , 0.359	Depositor DCC
R_{free} test set	6134 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	101.9	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.074 for -k,-h,-l 0.095 for k,h,-l 0.089 for h,-k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	47792	wwPDB-VP
Average B, all atoms (Å ²)	42.0	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 48.61 % 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 8.4003e-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 [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	0.66	0/8088	0.88	6/10983 (0.1%)
1	B	0.69	0/8070	0.90	11/10958 (0.1%)
1	C	0.67	0/8088	0.90	12/10983 (0.1%)
1	D	0.61	1/8088 (0.0%)	0.85	7/10983 (0.1%)
1	E	0.64	0/8070	0.87	6/10958 (0.1%)
1	F	0.63	0/8088	0.88	8/10983 (0.1%)
All	All	0.65	1/48492 (0.0%)	0.88	50/65848 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	F	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	515	TRP	CB-CG	5.94	1.60	1.50

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	971	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	C	400	LEU	CA-CB-CG	8.33	134.46	115.30
1	F	486	LEU	CA-CB-CG	7.42	132.38	115.30
1	E	357	LEU	CA-CB-CG	7.28	132.05	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	30	LEU	CA-CB-CG	7.08	131.58	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1038	GLU	Peptide
1	F	7	ASP	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7936	0	8072	516	0
1	B	7919	0	8058	500	0
1	C	7936	0	8072	533	0
1	D	7936	0	8072	541	0
1	E	7919	0	8058	610	0
1	F	7936	0	8072	669	0
2	A	35	0	46	1	0
2	B	35	0	46	12	0
2	C	35	0	46	6	0
2	D	35	0	46	3	0
2	E	35	0	46	6	0
2	F	35	0	46	2	0
All	All	47792	0	48680	3253	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 34.

The worst 5 of 3253 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:235:ILE:HD11	1:B:726:GLN:HB2	1.41	1.03
1:F:559:LEU:HD22	1:F:560:PRO:HD2	1.40	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:PHE:HD1	1:A:369:THR:HG1	1.09	0.99
1:F:74:ASN:HB3	1:F:95:GLU:HB2	1.41	0.99
1:D:971:ARG:HG2	1:D:974:PRO:HG2	1.47	0.96

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	1042/1069 (98%)	880 (84%)	133 (13%)	29 (3%)	5	34
1	B	1040/1069 (97%)	894 (86%)	116 (11%)	30 (3%)	4	34
1	C	1042/1069 (98%)	901 (86%)	114 (11%)	27 (3%)	5	35
1	D	1042/1069 (98%)	888 (85%)	126 (12%)	28 (3%)	5	35
1	E	1040/1069 (97%)	895 (86%)	119 (11%)	26 (2%)	5	36
1	F	1042/1069 (98%)	884 (85%)	132 (13%)	26 (2%)	5	36
All	All	6248/6414 (97%)	5342 (86%)	740 (12%)	166 (3%)	5	35

5 of 166 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	360	GLN
1	A	508	GLY
1	A	638	PRO
1	A	833	PRO
1	A	871	ASN

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	849/871 (98%)	766 (90%)	83 (10%)	8	35
1	B	847/871 (97%)	758 (90%)	89 (10%)	7	33
1	C	849/871 (98%)	757 (89%)	92 (11%)	6	32
1	D	849/871 (98%)	757 (89%)	92 (11%)	6	32
1	E	847/871 (97%)	755 (89%)	92 (11%)	6	31
1	F	849/871 (98%)	761 (90%)	88 (10%)	7	33
All	All	5090/5226 (97%)	4554 (90%)	536 (10%)	7	33

5 of 536 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	177	LEU
1	F	419	VAL
1	F	166	ILE
1	F	910	ILE
1	C	269	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	106	GLN
1	F	588	GLN
1	E	108	GLN
1	F	70	ASN
1	C	588	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](#)

6 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	2000	-	36,36,36	1.86	8 (22%)	47,47,47	1.38	8 (17%)
2	LMT	C	2000	-	36,36,36	1.80	8 (22%)	47,47,47	1.74	10 (21%)
2	LMT	F	2000	-	36,36,36	1.90	9 (25%)	47,47,47	1.50	9 (19%)
2	LMT	A	2000	-	36,36,36	2.01	9 (25%)	47,47,47	1.54	12 (25%)
2	LMT	D	2000	-	36,36,36	2.01	9 (25%)	47,47,47	1.33	5 (10%)
2	LMT	B	2000	-	36,36,36	1.93	9 (25%)	47,47,47	1.27	7 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LMT	E	2000	-	2/2/10/10	10/21/61/61	0/2/2/2
2	LMT	C	2000	-	3/3/10/10	6/21/61/61	0/2/2/2
2	LMT	F	2000	-	3/3/10/10	12/21/61/61	0/2/2/2
2	LMT	A	2000	-	2/2/10/10	14/21/61/61	0/2/2/2
2	LMT	D	2000	-	2/2/10/10	10/21/61/61	0/2/2/2
2	LMT	B	2000	-	1/1/10/10	13/21/61/61	0/2/2/2

The worst 5 of 52 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2000	LMT	O5'-C5'	5.00	1.56	1.44
2	D	2000	LMT	O1'-C1'	4.64	1.48	1.40
2	B	2000	LMT	O1'-C1'	4.59	1.48	1.40
2	E	2000	LMT	O5'-C5'	4.48	1.55	1.44
2	A	2000	LMT	O1'-C1'	4.42	1.47	1.40

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2000	LMT	C2'-C3'-C4'	5.21	121.58	109.68
2	F	2000	LMT	O1'-C1'-C2'	4.77	115.75	108.30
2	C	2000	LMT	O1'-C1'-C2'	4.04	114.61	108.30
2	D	2000	LMT	C1'-O5'-C5'	3.87	121.28	113.69
2	E	2000	LMT	C1B-O1B-C4'	-3.61	109.02	117.96

5 of 13 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	2000	LMT	C3'
2	A	2000	LMT	C4B
2	B	2000	LMT	C3'
2	C	2000	LMT	C2B
2	C	2000	LMT	C1B

5 of 65 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2000	LMT	C2'-C1'-O1'-C1
2	A	2000	LMT	O5'-C1'-O1'-C1
2	D	2000	LMT	O5'-C1'-O1'-C1
2	E	2000	LMT	O5'-C1'-O1'-C1
2	E	2000	LMT	C2-C1-O1'-C1'

There are no ring outliers.

6 monomers are involved in 30 short contacts:

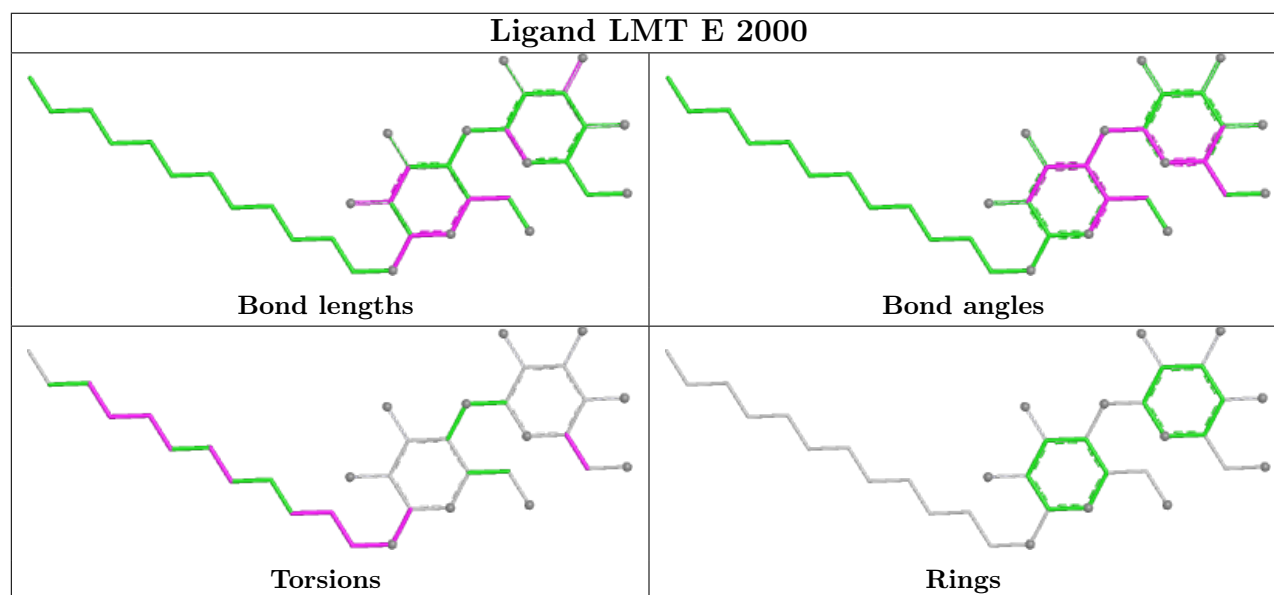
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2000	LMT	6	0
2	C	2000	LMT	6	0
2	F	2000	LMT	2	0
2	A	2000	LMT	1	0

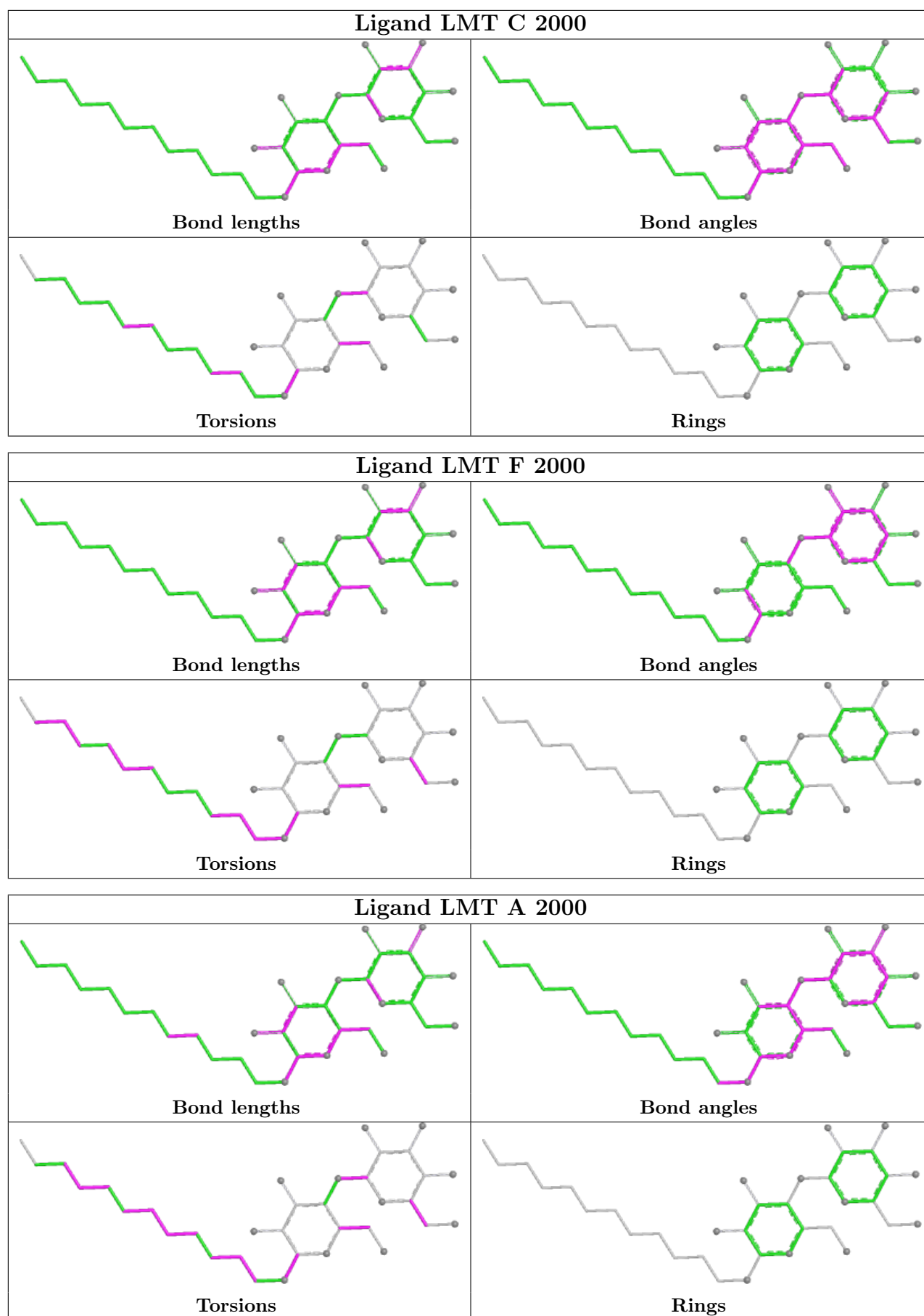
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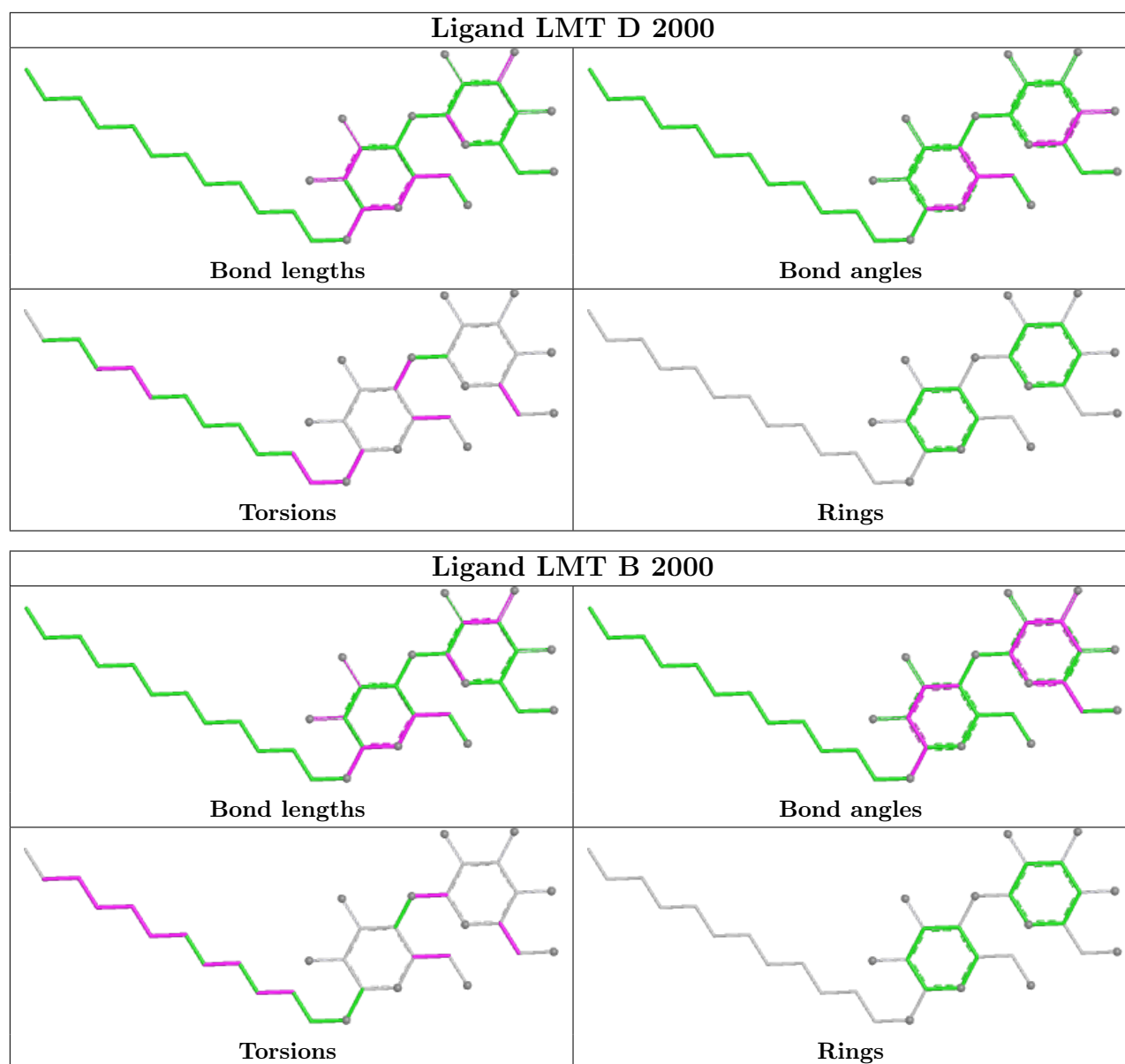
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2000	LMT	3	0
2	B	2000	LMT	12	0

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	1044/1069 (97%)	-0.45	8 (0%) 86 74	5, 35, 83, 118	0
1	B	1042/1069 (97%)	-0.55	7 (0%) 87 78	3, 27, 62, 108	0
1	C	1044/1069 (97%)	-0.55	5 (0%) 91 83	4, 29, 60, 88	0
1	D	1044/1069 (97%)	-0.36	9 (0%) 84 72	10, 49, 88, 114	0
1	E	1042/1069 (97%)	-0.26	34 (3%) 46 32	5, 46, 100, 129	0
1	F	1044/1069 (97%)	-0.24	23 (2%) 62 45	5, 54, 104, 142	0
All	All	6260/6414 (97%)	-0.40	86 (1%) 75 60	3, 39, 90, 142	0

The worst 5 of 86 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	715	SER	6.5
1	F	849	SER	6.4
1	E	295	THR	5.2
1	E	834	GLY	4.5
1	E	170	SER	4.5

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](#)

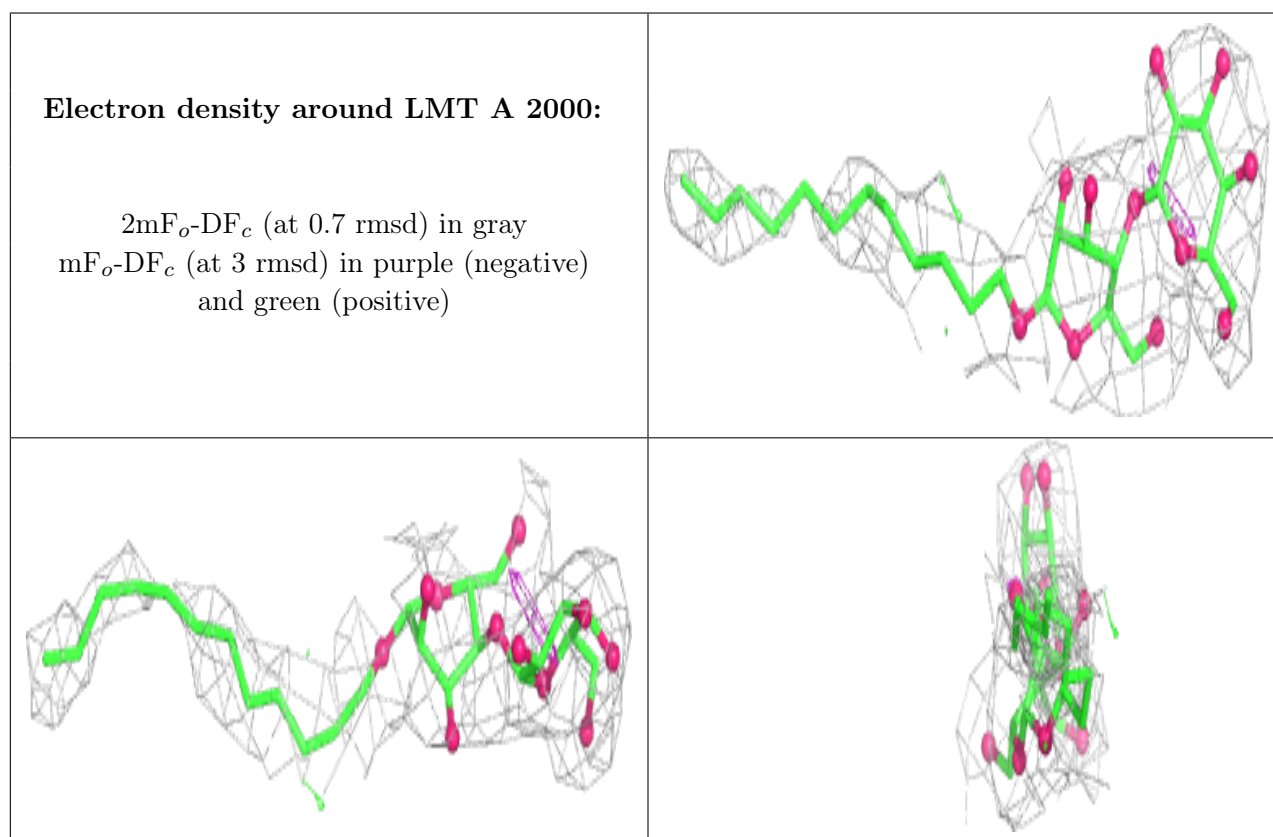
There are no monosaccharides in this entry.

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.

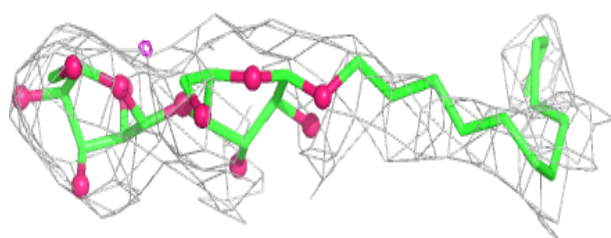
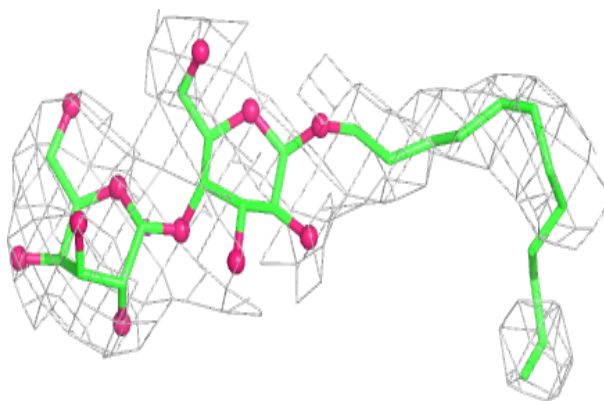
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	LMT	A	2000	35/35	0.86	0.37	2,31,49,54	0
2	LMT	F	2000	35/35	0.86	0.34	13,38,54,58	0
2	LMT	D	2000	35/35	0.87	0.26	1,25,38,40	0
2	LMT	C	2000	35/35	0.88	0.25	5,22,46,50	0
2	LMT	B	2000	35/35	0.89	0.29	6,32,47,61	0
2	LMT	E	2000	35/35	0.90	0.34	3,34,48,49	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.

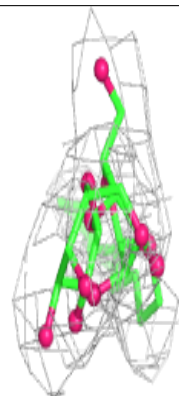
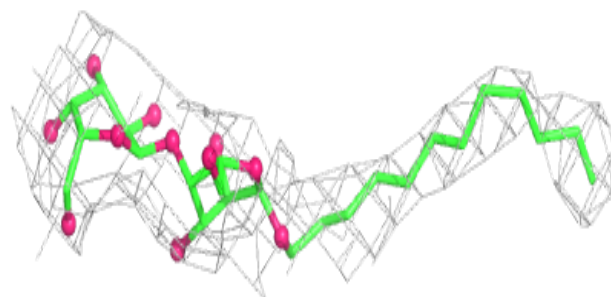
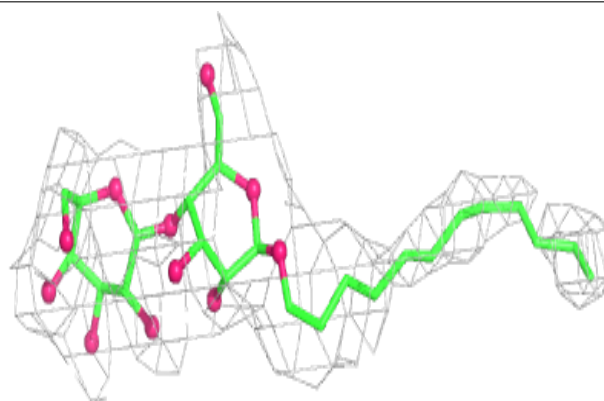


Electron density around LMT F 2000:

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

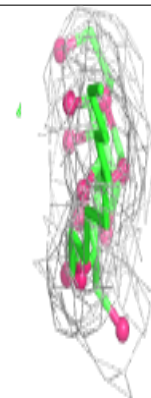
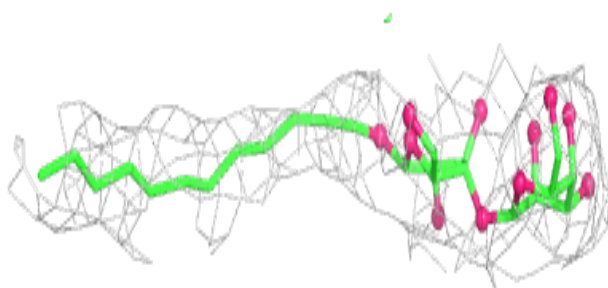
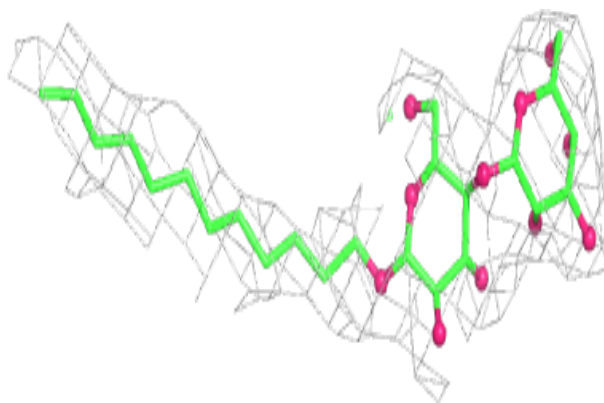
**Electron density around LMT D 2000:**

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

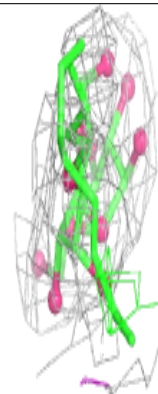
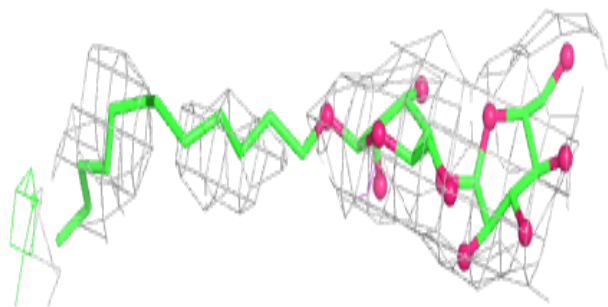
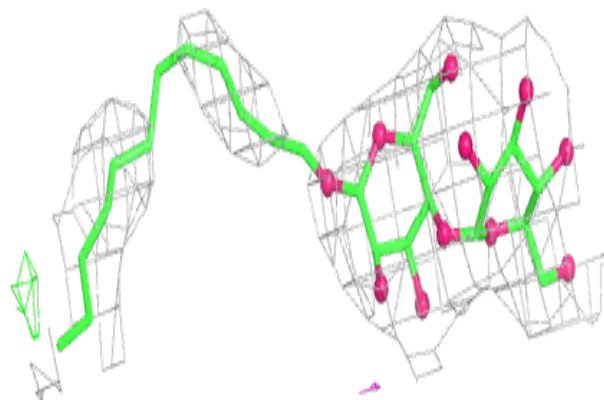


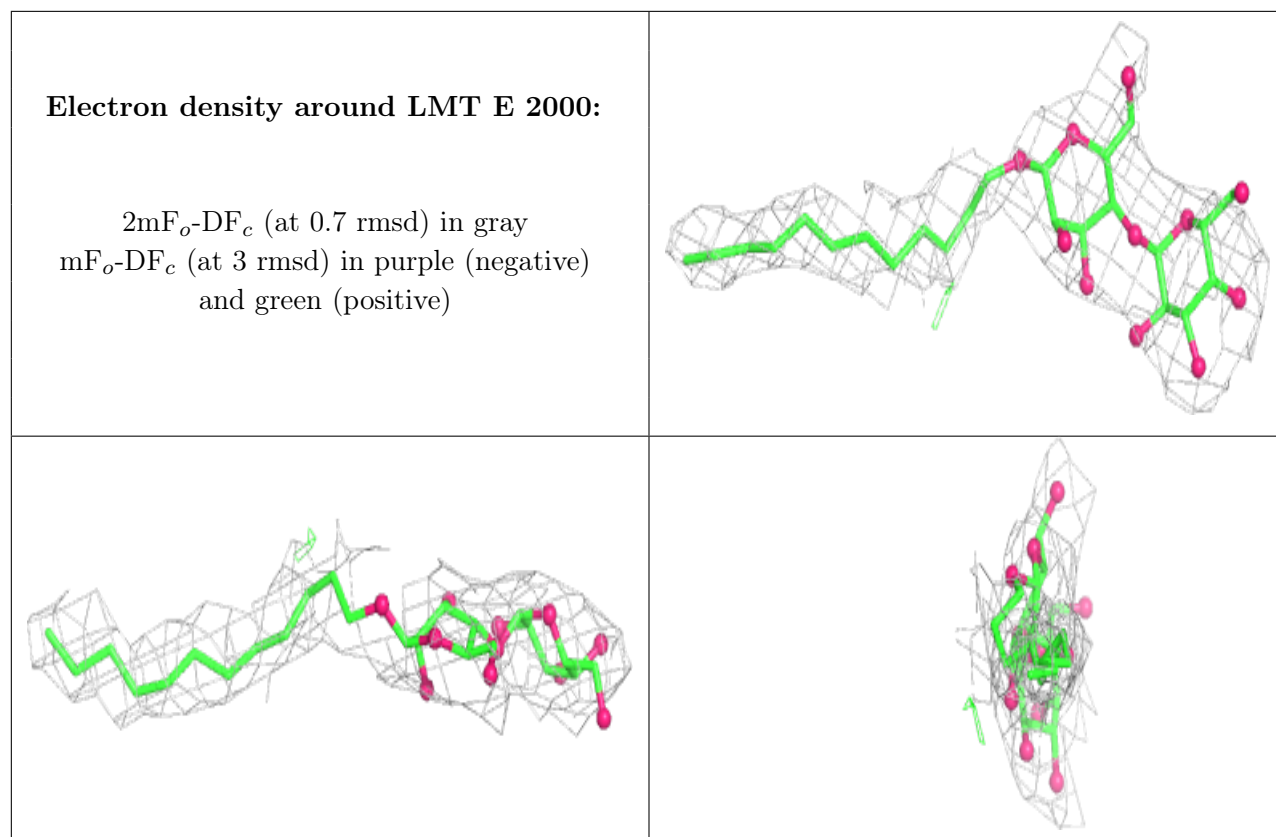
Electron density around LMT C 2000:

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

**Electron density around LMT 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.