



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 27, 2026 – 03:25 AM UTC

PDB ID : 7O3M / pdb_00007o3m
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 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

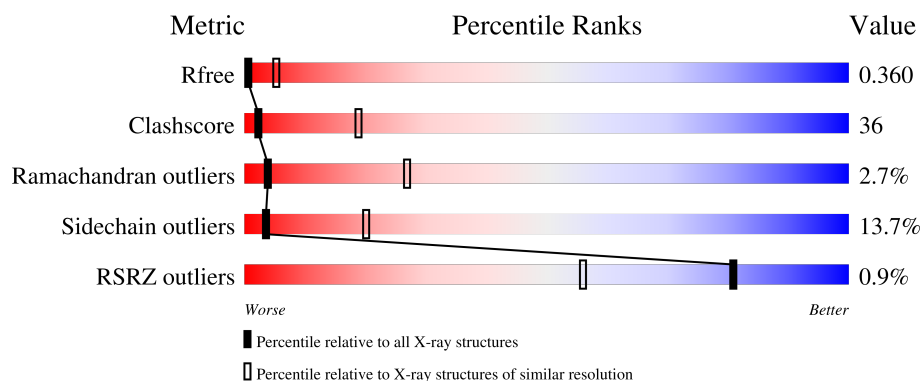
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.55 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}	180053	1410 (3.62-3.50)
Clashscore	190562	1480 (3.62-3.50)
Ramachandran outliers	187476	1440 (3.62-3.50)
Sidechain outliers	187428	1441 (3.62-3.50)
RSRZ outliers	180081	1409 (3.62-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	 38% 49% 10% ..
1	B	1069	 39% 47% 11% .
1	C	1069	 37% 49% 11% ..
1	D	1069	 37% 48% 12% ..
1	E	1069	 35% 50% 11% ..

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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

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
1	A	1044	Total	C	N	O	S	0	0	0
			7936	5102	1312	1479	43			
1	B	1042	Total	C	N	O	S	0	0	0
			7919	5092	1308	1476	43			
1	C	1044	Total	C	N	O	S	0	0	0
			7936	5102	1312	1479	43			
1	D	1044	Total	C	N	O	S	0	0	0
			7936	5102	1312	1479	43			
1	E	1042	Total	C	N	O	S	0	0	0
			7919	5092	1308	1476	43			
1	F	1044	Total	C	N	O	S	0	0	0
			7936	5102	1312	1479	43			

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
B	-3	ARG	-	expression tag	UNP E2QH56
B	-2	GLY	-	expression tag	UNP E2QH56
B	-1	SER	-	expression tag	UNP E2QH56
B	0	HIS	-	expression tag	UNP E2QH56
B	620	ALA	ARG	engineered mutation	UNP E2QH56
C	-19	MET	-	initiating methionine	UNP E2QH56
C	-18	GLY	-	expression tag	UNP E2QH56
C	-17	SER	-	expression tag	UNP E2QH56
C	-16	SER	-	expression tag	UNP E2QH56
C	-15	HIS	-	expression tag	UNP E2QH56
C	-14	HIS	-	expression tag	UNP E2QH56
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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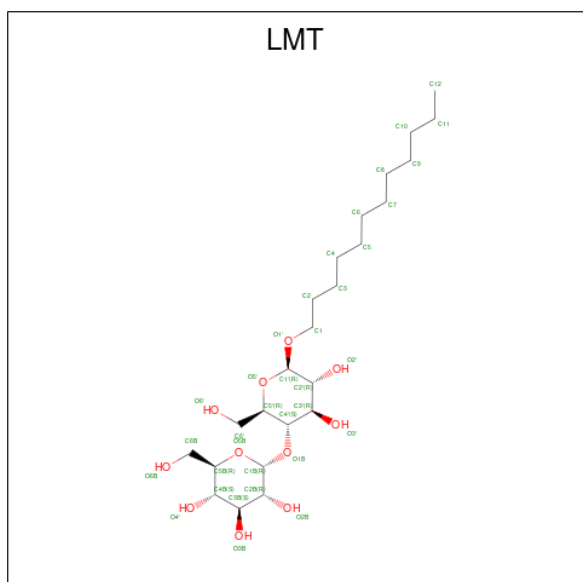
Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP E2QH56
C	-1	SER	-	expression tag	UNP E2QH56
C	0	HIS	-	expression tag	UNP E2QH56
C	620	ALA	ARG	engineered mutation	UNP E2QH56
D	-19	MET	-	initiating methionine	UNP E2QH56
D	-18	GLY	-	expression tag	UNP E2QH56
D	-17	SER	-	expression 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-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).

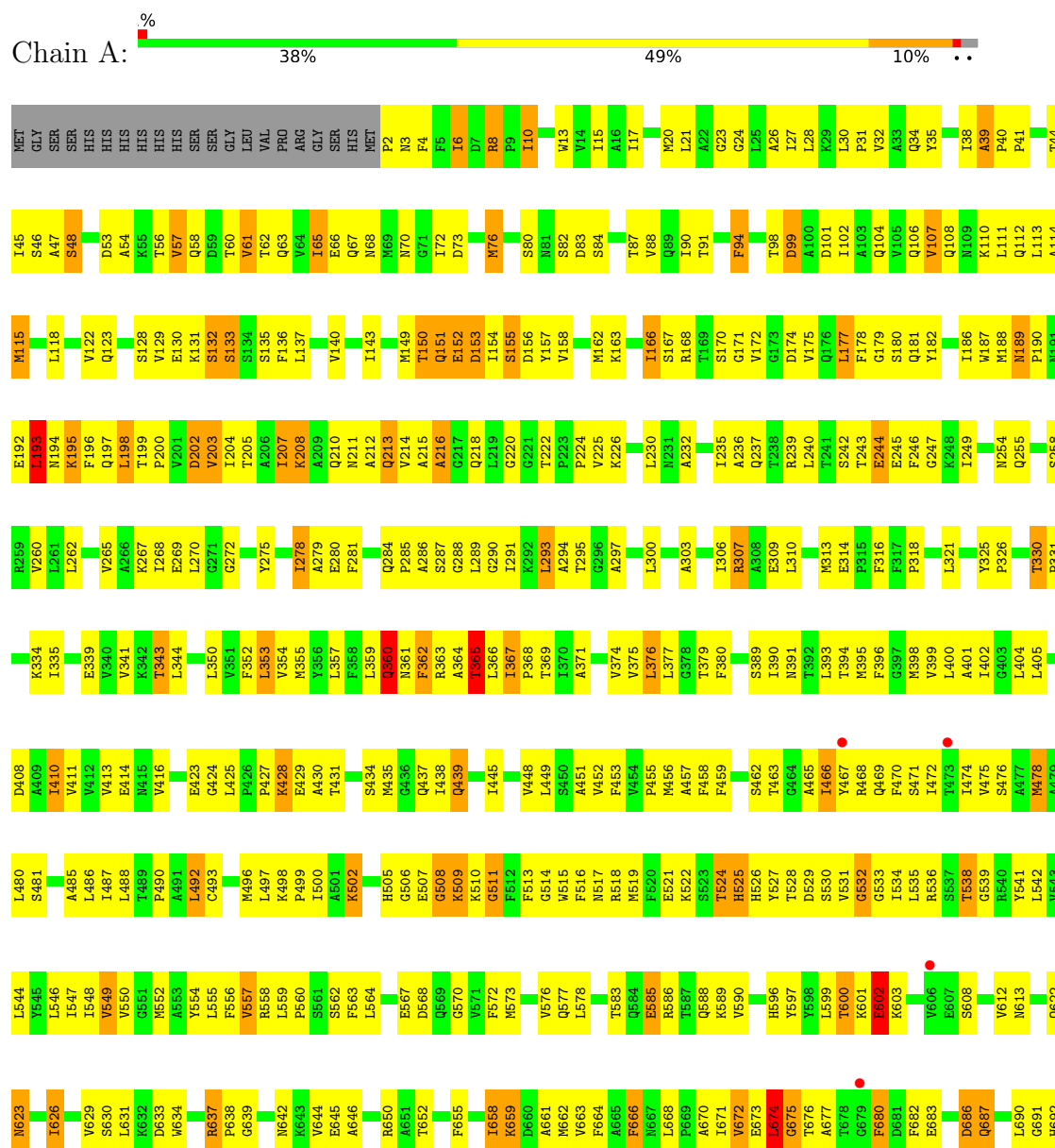


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			35	24	11		
2	B	1	Total	C	O	0	0
			35	24	11		
2	C	1	Total	C	O	0	0
			35	24	11		
2	D	1	Total	C	O	0	0
			35	24	11		
2	E	1	Total	C	O	0	0
			35	24	11		
2	F	1	Total	C	O	0	0
			35	24	11		

3 Residue-property plots

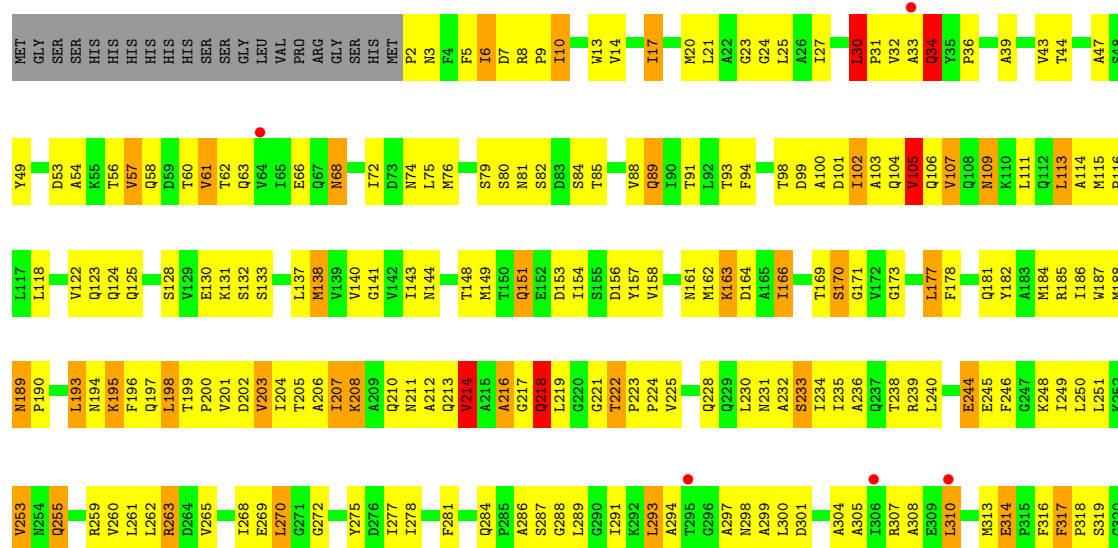
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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









M188	M189	P190	N191	E192	L193	N194	K195	F196	Q197	P200	V201	D202	V203	I204	T205	A206	I207	K208	N211	A215	A216	G217	Q218	L219	T222	P223	P224	V225	Q228	Q229	L230	N231	A232	I235	A236	Q237	T238	R239	L240	T243	E244	E245	F246	G247	K248	I249	L250	L251	K252	N254																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
Q255	R259	V260	L261	L262	V265	T268	E269	L270	L271	G272	E273	D274	D275	D276	I277	I278	A279	E280	A286	S287	Q288	L289	G290	L291	K292	L293	A294	A297	T302	A303	I306	R307	A308	E309	L310	A311	K312	E313	P315	F316	F317	P318	S319	G320	L321	K322	L323	V324	Y327																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
D328	T329	P331	V332	V333	S336	I337	H338	V340	V341	K342	T343	L344	V345	L350	V351	F352	L353	V354	M355	Y356	L357	F358	L359	Q360	N361	K362	R363	A364	T365	L366	I367	P368	T369	I370	A371	V372	P373	V374	V375	L376	L377	G378	T379	F380	A381	V382	L383	S389	I390	N391	T392	L393	T394	M395																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
F396	G397	V399	L400	A401	L402	L405	V406	D407	E408	L409	L410	V411	V412	V413	E414	N415	R418	V419	N420	A421	E422	E423	G424	P426	P427	K428	E429	R432	K433	S434	M435	G436	Q437	Q438	Q439	O440	A441	L442	V443	G444	L445	A446	N447	V448	L449	S450	A451	V452	F453	V454	P455	N456	T457	F458																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
F459	S462	L466	Y467	Q468	Q469	F470	S471	L472	L473	L474	V475	S476	A477	N478	S481	L482	L483	V484	A485	L488	T489	P490	L491	L492	C493	A494	T495	R496	L497	K498	P499	L500	A501	R502	H505	G506	E507	G508	V509	F516	N517	R518	M519	S523	T524	H525	H526	Y527	S530	V531																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
G532	G533	L534	L535	S536	T538	G539	S541	L542	Y545	L546	L547	P548	V549	V550	G551	H552	L555	F556	V557	R558	L559	P560	S561	S562	F563	L564	Q569	G570	V571	F572	N573	T574	H575	V576	Q577	L578	P579	T583	G584	T587	O588	V589	V594	T595	H596	Y597	V598	L599	T600	K601																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
E602	V606	V609	N613	G614	Q622	L626	A627	F628	G629	S630	L631	V632	D633	W634	R637	P638	G639	E640	E641	N642	S643	S644	L645	F646	L647	V648	T649	T650	T651	T652	T653	T654	T655	T656	T657	T658	T659	D660	A661	M662	V663	F664	A665	F666	R667	L668	I671	V672	S673	L674	G675	G679																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
F680	D681	E682	E683	I685	D686	G691	H692	K694	L695	T696	Q697	A698	R699	N700	L701	L702	L703	A704	E705	A706	H709	P710	D711	M712	L713	T714	S715	V716	T717	R718	L721	E722	D723	T724	P725	Q726	L727	K728	F729	M730	D731	A736	Q737	A738	L739	G740	V741	S742	L743	N744	D745	P746	N747																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
T748	T749	L750	A753	A754	Y755	Y758	V759	N760	D761	F762	L763	D764	R765	G766	V767	V768	K769	W770	V771	V772	V773	V774	S775	E776	A777	G778	D779	S780	T781	L782	D785	I786	S787	Y788	Q789	R790	V791	R792	A793	L794	D795	G796	Q797	M798	V799	P800	F801	S802	F803	S805	V806	W807	S808	V809	V810	V811	V812	V813	V814	V815	V816	V817	V818	V819	V820	V821	V822	V823	V824	V825	V826	V827	V828	V829	V830	V831	V832	V833	V834	V835	V836	V837	V838	V839	V840	V841	V842	V843	V844	V845	V846	V847	V848	V849	V850	V851	V852	V853	V854	V855	V856	V857	V858	V859	V860	V861	V862	V863	V864	V865	V866	V867	V868	V869	V870	V871	V872	V873	V874	V875	V876	V877	V878	V879	V880	V881	V882	V883	V884	V885	V886	V887	V888	V889	V890	V891	V892	V893	V894	V895	V896	V897	V898	V899	V900	V901	V902	V903	V904	V905	V906	V907	V908	V909	V910	V911	V912	V913	V914	V915	V916	V917	V918	V919	V920	V921	V922	V923	V924	V925	V926	V927	V928	V929	V930	V931	V932	V933	V934	V935	V936	V937	V938	V939	V940	V941	V942	V943	V944	V945	V946	V947	V948	V949	V950	V951	V952	V953	V954	V955	V956	V957	V958	V959	V960	V961	V962	V963	V964	V965	V966	V967	V968	V969	V970	V971	V972	V973	V974	V975	V976	V977	V978	V979	V980	V981	V982	V983	V984	V985	V986	V987	V988	V989	V990	V991	V992	V993	V994	V995	V996	V997	V998	V999	V1000	V1001	V1002	V1003	V1004	V1005	V1006	V1007	V1008	V1009	V1010	V1011	V1012	V1013	V1014	V1015	V1016	V1017	V1018	V1019	V1020	V1021	V1022	V1023	V1024	V1025	V1026	V1027	V1028	V1029	V1030	V1031	V1032	V1033	V1034	V1035	V1036	V1037	V1038	V1039	V1040	V1041	V1042	V1043	V1044	V1045	V1046	V1047	V1048	V1049	V1050	V1051	V1052	V1053	V1054	V1055	V1056	V1057	V1058	V1059	V1060	V1061	V1062	V1063	V1064	V1065	V1066	V1067	V1068	V1069	V1070	V1071	V1072	V1073	V1074	V1075	V1076	V1077	V1078	V1079	V1080	V1081	V1082	V1083	V1084	V1085	V1086	V1087	V1088	V1089	V1090	V1091	V1092	V1093	V1094	V1095	V1096	V1097	V1098	V1099	V1100	V1101	V1102	V1103	V1104	V1105	V1106	V1107	V1108	V1109	V1110	V1111	V1112	V1113	V1114	V1115	V1116	V1117	V1118	V1119	V1120	V1121	V1122	V1123	V1124	V1125	V1126	V1127	V1128	V1129	V1130	V1131	V1132	V1133	V1134	V1135	V1136	V1137	V1138	V1139	V1140	V1141	V1142	V1143	V1144	V1145	V1146	V1147	V1148	V1149	V1150	V1151	V1152	V1153	V1154	V1155	V1156	V1157	V1158	V1159	V1160	V1161	V1162	V1163	V1164	V1165	V1166	V1167	V1168	V1169	V1170	V1171	V1172	V1173	V1174	V1175	V1176	V1177	V1178	V1179	V1180	V1181	V1182	V1183	V1184	V1185	V1186	V1187	V1188	V1189	V1190	V1191	V1192	V1193	V1194	V1195	V1196	V1197	V1198	V1199	V1200	V1201	V1202	V1203	V1204	V1205	V1206	V1207	V1208	V1209	V1210	V1211	V1212	V1213	V1214	V1215	V1216	V1217	V1218	V1219	V1220	V1221	V1222	V1223	V1224	V1225	V1226	V1227	V1228	V1229	V1230	V1231	V1232	V1233	V1234	V1235	V1236	V1237	V1238	V1239	V1240	V1241	V1242	V1243	V1244	V1245	V1246	V1247	V1248	V1249	V1250	V1251	V1252	V1253	V1254	V1255	V1256	V1257	V1258	V1259	V1260	V1261	V1262	V1263	V1264	V1265	V1266	V1267	V1268	V1269	V1270	V1271	V1272	V1273	V1274	V1275	V1276	V1277	V1278	V1279	V1280	V1281	V1282	V1283	V1284	V1285	V1286	V1287	V1288	V1289	V1290	V1291	V1292	V1293	V1294	V1295	V1296	V1297	V1298	V1299	V1300	V1301	V1302	V1303	V1304	V1305	V1306	V1307	V1308	V1309	V1310	V1311	V1312	V1313	V1314	V1315	V1316	V1317	V1318	V1319	V1320	V1321	V1322	V1323	V1324	V1325	V1326	V1327	V1328	V1329	V1330	V1331	V1332	V1333	V1334	V1335	V1336	V1337	V1338	V1339	V1340	V1341	V1342	V1343	V1344	V1345	V1346	V1347	V1348	V1349	V1350	V1351	V1352	V1353	V1354	V1355	V1356	V1357	V1358	V1359	V1360	V1361	V1362	V1363	V1364	V1365	V1366	V1367	V1368	V1369	V1370	V1371	V1372	V1373	V1374	V1375	V1376	V1377	V1378	V1379	V1380	V1381	V1382	V1383	V1384	V1385	V1386	V1387	V1388	V1389	V1390	V1391	V1392	V1393	V1394	V1395	V1396	V1397	V1398	V1399	V1400	V1401	V1402	V1403	V1404	V1405	V1406	V1407	V1408	V1409	V1410	V1411	V1412	V1413	V1414	V1415	V1416	V1417	V1418	V1419	V1420	V1421	V1422	V1423	V1424	V1425	V1426	V1427	V1428	V1429	V1430	V1431	V1432	V1433	V1434	V1435	V1436	V1437	V1438	V1439	V1440	V1441	V1442	V1443	V1444	V1445	V1446	V1447	V1448	V1449	V1450	V1451	V1452	V1453	V1454	V1455	V1456	V1457	V1458	V1459	V1460	V1461	V1462	V1463	V1464	V1465	V1466	V1467	V1468	V1469	V1470	V1471	V1472	V1473	V1474	V1475	V1476	V1477	V1478	V1479	V1480	V1481	V1482	V1483	V1484	V1485	V1486	V1487	V1488	V1489	V1490	V1491	V1492	V1493	V1494	V1495	V1496	V1497	V1498	V1499	V1500	V1501	V1502	V1503	V1504	V1505	V1506	V1507	V1508	V1509	V1510	V1511	V1512	V1513	V1514	V1515	V1516	V1517	V1518	V1519	V1520	V1521	V1522	V1523	V1524	V1525	V1526	V1527	V1528	V1529	V1530	V1531	V1532	V1533	V1534	V1535	V1536	V1537	V1538	V1539	V1540	V1541	V1542	V1543	V1544	V1545	V1546	V1547	V1548	V1549	V1550	V1551	V1552	V1553	V1554	V1555	V1556	V1557	V1558	V1559	V1560	V1561	V1562	V1563	V1564	V1565	V1566	V1567	V1568	V1569	V1570	V1571	V1572	V1573	V1574	V1575	V1576	V1577	V1578	V1579	V1580	V1581	V1582	V1583	V1584	V1585	V1586	V1587	V1588	V1589	V1590	V1591	V1592	V1593	V1594	V1595	V1596	V1597	V1598	V1599	V1600	V1601	V1602	V1603	V1604	V1605	V1606	V1607	V1608	V1609	V1610	V1611	V1612	V1613	V1614	V1615	V1616	V1617	V1618	V1619	V1620	V1621	V1622	V1623	V1624	V1625	V1626	V1627	V1628	V1629	V1630	V1631	V1632	V1633	V1634	V1635	V1636	V1637	V1638	V1639	V1640	V1641	V1642	V1643	V1644	V1645	V1646	V1647	V1648	V1649	V1650	V1651	V1652	V1653	V1654	V1655	V1656	V1657	V1658	V1659	V1660	V1661	V1662	V1663	V1664	V1665	V1666	V1667	V1668	V1669	V1670	V1671	V1672	V1673	V1674	V1675	V1676	V1677	V1678	V1679	V1680	V1681	V1682	V1683	V1684	V1685	V1686	V1687	V1688	V1689	V1690	V1691	V1692	V1693	V1694	V1695	V1696	V1697	V1698	V1699	V1700	V1701	V1702	V1703	V1704	V1705	V1706	V1707	V1708	V1709	V1710	V1711	V1712	V1713	V1714	V1715	V1716	V1717	V1718	V1719	V1720	V1721	V1722	V1723	V1724	V1725	V1726	V1727	V1728	V1729	V1730	V1731	V1732	V1733	V1734	V1735	V1736	V1737	V1738	V1739	V1740	V1741	V1742	V1743	V1744	V1745	V1746	V1747	V1748	V1749	V1750	V1751	V1752	V1753	V1754	V1755	V1756	V1757	V1758	V1759	V1760	V1761

A1014	K940	R867	F801	L739	A685	T587	A457	I390	F317	F246	G179	A114	S48
T1015	H941	G870	F804	G740	F686	Q588	S523	N391	P318	F247	S180	M115	Y49
V1016	A942	G871		V741	I687	K589	T524	T392	S319	K248	Q181	L116	D53
L1017	I943	N870		S742	L688	V590	H525	L393	G320	L463	Y182	L117	A54
A1018		K872	R808	I743	F689	L591	H526	T394	L321	L249	M184	L118	K55
L1019	V946	A873	R809	N744	A670	N592	Y527	M395		L250	M183	P119	A54
F1020	F947			D745	A671	E593	T528	T395	P326	L251	R185	T56	V57
F1021	F948	S880	S813	I746	V672	V594	D529	G397	Y327	K252	I186	E121	Q58
V1022	A949		P814	N747	E673	T595	S520	M398	T330	V253	W187	V122	D59
P1023	K950	V883	R815	T748	G675	H596	S530	V399		G257	M188	Q123	T60
F1024	D951	L816	L816	T749	G675		F470	L400	F331	R258	P190	Q125	D59
F1025	L952	F885	E817	L750	T676	L599	G533	A401	F332	R259	P191	G126	V61
F1026	K953	L886	R818	G751	A677	T600	I534	I402	V333	R259	N191	G126	T62
V1027	F954	C887	Y819	A752	T678	K601	L555	G403	K334	V260	E192	V127	Q63
V1028	K955	L888	N820	A753	G679	K602	R536	L404	I337	L262	L193		V64
V1029		A889	G821	W754	F680	K603	S537	L405		L262	N194	S132	T65
R1030	G959	A890	L822		D681	S608	T538	V406	H338	V265	K195		N68
R1031	L960	L891	P823	Y758	F682	V609	G539	D407	E339		F196	S135	M69
R1032	R961	Y892	S824	V759	E683	R540	R540	D408	V340	F136		F136	M70
F1033	E962	E893	M825	N760	L684	F610	Y541	A479	V341	L137		L137	
S1034	A963	S894	E826	D761	T685	A611	L542	L480	K342	M138		M138	G71
R1035		S895	I827	F762	D686	V612	V543	S481	L343	L270		V139	T72
K1036	V968	S896	L828	I763		N613	L544	V482	L344	D202		V140	D73
N1037		I897	I827		G691		Y545	E414		G272		G141	N74
	K970	P898	Q830	D764	H692	F617	L546	L483	L350	E273		V140	L75
	R971	P898	Q830	R765	E693	A618	L547	L483	V351	N274		G141	M76
	L972	S900	A832	R767	E694	G619	L548	R418	F352	Y275		I143	M77
H1041	R973	V901	P833	V768	K694		V549	L487	L353	Y275		N144	M78
S1043	P974	M902	G834	K769	T696	Q622	L549	M420	V354	L278		G147	S79
H1044		L903	K835	K770	G697	M623	M552	A421	M355				S80
T1045	K977	V904	S836	V771	A698	L631	L559	E422	Y356	F281		M149	M81
VAL	T978	V905	T837	V772	R699	L626	Y554	E423	L357				S82
ASP	S979	P906	G838	V773	N700	A627	L555	E424	F358	Q284		M149	
HIS	L980	L907	E839	M774	Q701	F628	F556	L425	T285	T150		Q151	D83
	A981	G908	A840	S775	L702	V629	V557	P427	A216	A216			T87
	F982	V909	E776	E776	L703	S630	F557	P499	G217	G217		D153	
	I983	I910	E842	A777		L631	R558	T495	N361	G218		I154	I90
	L984	G911	L843	K778	W712	K632	L559	M496	F362	G218		S155	T91
	G985	A912	M844	Y779	L713	D633	S561	L497	R363	L219		D156	T92
	V986	L913	E945	R780	W716	W634	S562	K498	A364	G220		V157	L92
	N987	L914	Q846	M781	R717	P638	F563	I500	T365	G221		V158	T93
	P988		L847	L782	F718		L564	A501	L366	T222		A159	F94
			A848	A778	W719	K644	P565	K502	I367	P223		G161	E95
	V990	T922	S849	D783	G720	E645	D568	G503	P368	P224		A160	S96
	I991	N923	K850	D785	L721	E645			T369	G97		N162	G97
		D924	L851	I786	E722	M649	V571	G506	I370	V225		M162	T98
		V925		G787	D723	R650	F572	G508	A299	Q228		K163	D99
		Y926	G854	D788			F572	G508	L300	Q229		D164	A100
		F927	G855	W789	Q726	R653	M573	K509	P372	L230		D301	D101
		Q928	G856	Y790	A654	T574	T574	K510	P373	N231		I166	D101
		V929	T857	V791	K659	A654	M575	G511	T302	A232		S167	I102
		G930	D858	R792	K728	A654	V576	M447	L376	A232		R168	A103
		L931	W859	A793	L731	F655	F576	L448	R307	S233		S170	Q104
		L932	T860	A794	S656	S656	F512	L449	T377	T234		G173	V105
		T933	G861	D795	A654	A654	F513	S450	G378	T235		S170	Q106
		K934	G862	G796	D732	K659	L578	A451	A236	A236		G173	V107
		I835	M862	G796	Q733	D660	W515	A451	Q237	A236		G173	Q108
		G936	S863	Q797	Q733	A651	F516	A451	A236	A236		G173	N109
		V1007	Y864	M798	A736	M652	M517	F453	N313	L310		V175	K110
		M1008	Q865	V799	Q737	V663	M518	V454	E314	A311		Q176	L111
		G1009	L937		A738	F664	E585	M519	P315	K312		Q176	L112
		G1010					T583		S389	F316		F178	L113
		M1011					Q584						
		V1012					E585						
		T1013					R586						

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) 99.0 (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 0.278 , 0.360	Depositor DCC
R_{free} test set	6185 reflections (4.98%)	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)	0.26 , 33.6	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	0.90	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

5.1 Standard geometry

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	0.88	5/8088 (0.1%)	1.29	60/10983 (0.5%)
1	B	0.93	5/8070 (0.1%)	1.32	68/10958 (0.6%)
1	C	0.92	5/8088 (0.1%)	1.33	83/10983 (0.8%)
1	D	0.84	2/8088 (0.0%)	1.26	55/10983 (0.5%)
1	E	0.87	4/8070 (0.0%)	1.29	62/10958 (0.6%)
1	F	0.87	3/8088 (0.0%)	1.33	93/10983 (0.8%)
All	All	0.89	24/48492 (0.0%)	1.30	421/65848 (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	1
1	F	0	1
All	All	0	2

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1022	VAL	CA-CB	8.15	1.58	1.54
1	A	905	VAL	CA-CB	7.38	1.57	1.54
1	F	897	ILE	CA-CB	6.93	1.58	1.54
1	C	676	THR	CA-CB	6.12	1.62	1.53
1	F	150	THR	CA-CB	6.11	1.62	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	8	ARG	CA-C-N	13.77	133.55	119.64
1	F	8	ARG	C-N-CA	13.77	133.55	119.64
1	A	35	TYR	CA-C-N	-11.16	108.98	120.03
1	A	35	TYR	C-N-CA	-11.16	108.98	120.03
1	E	325	TYR	CA-C-N	10.95	130.69	119.64

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

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	552	0
1	B	7919	0	8058	537	0
1	C	7936	0	8072	569	0
1	D	7936	0	8072	582	0
1	E	7919	0	8058	637	0
1	F	7936	0	8072	710	0
2	A	35	0	46	1	0
2	B	35	0	46	12	0
2	C	35	0	46	5	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	3466	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 36.

The worst 5 of 3466 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
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
1:C:559:LEU:HD22	1:C:560:PRO:HD2	1.47	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	1042/1069 (98%)	880 (84%)	133 (13%)	29 (3%)	4	26
1	B	1040/1069 (97%)	894 (86%)	116 (11%)	30 (3%)	3	26
1	C	1042/1069 (98%)	901 (86%)	114 (11%)	27 (3%)	4	27
1	D	1042/1069 (98%)	888 (85%)	126 (12%)	28 (3%)	4	27
1	E	1040/1069 (97%)	895 (86%)	119 (11%)	26 (2%)	4	28
1	F	1042/1069 (98%)	884 (85%)	132 (13%)	26 (2%)	4	28
All	All	6248/6414 (97%)	5342 (86%)	740 (12%)	166 (3%)	4	27

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 ⓘ

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%)	739 (87%)	110 (13%)	4	21
1	B	847/871 (97%)	746 (88%)	101 (12%)	5	24
1	C	849/871 (98%)	734 (86%)	115 (14%)	4	21
1	D	849/871 (98%)	728 (86%)	121 (14%)	3	18
1	E	847/871 (97%)	717 (85%)	130 (15%)	3	16
1	F	849/871 (98%)	727 (86%)	122 (14%)	3	18
All	All	5090/5226 (97%)	4391 (86%)	699 (14%)	3	20

5 of 699 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	118	LEU
1	E	1024	VAL
1	E	218	GLN
1	E	111	LEU
1	E	563	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 69 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	667	ASN
1	E	846	GLN
1	F	592	ASN
1	C	211	ASN
1	C	112	GLN

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](#)

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	1.85	9 (25%)	47,47,47	1.40	8 (17%)
2	LMT	F	2000	-	36,36,36	1.90	10 (27%)	47,47,47	1.53	9 (19%)
2	LMT	B	2000	-	36,36,36	1.94	10 (27%)	47,47,47	1.29	7 (14%)
2	LMT	C	2000	-	36,36,36	1.80	9 (25%)	47,47,47	1.76	10 (21%)
2	LMT	A	2000	-	36,36,36	2.01	10 (27%)	47,47,47	1.57	11 (23%)
2	LMT	D	2000	-	36,36,36	2.01	9 (25%)	47,47,47	1.35	6 (12%)

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	F	2000	-	3/3/10/10	12/21/61/61	0/2/2/2
2	LMT	B	2000	-	1/1/10/10	13/21/61/61	0/2/2/2
2	LMT	C	2000	-	3/3/10/10	6/21/61/61	0/2/2/2
2	LMT	A	2000	-	2/2/10/10	14/21/61/61	0/2/2/2
2	LMT	D	2000	-	2/2/10/10	11/21/61/61	0/2/2/2

The worst 5 of 57 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2000	LMT	O5'-C5'	4.95	1.56	1.44
2	D	2000	LMT	O1'-C1'	4.76	1.48	1.40
2	B	2000	LMT	O1'-C1'	4.70	1.48	1.40
2	A	2000	LMT	O1'-C1'	4.53	1.47	1.40
2	E	2000	LMT	O5'-C5'	4.43	1.55	1.44

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'	5.24	121.58	109.68
2	F	2000	LMT	O1'-C1'-C2'	4.92	115.75	108.27
2	C	2000	LMT	O1'-C1'-C2'	4.17	114.61	108.27
2	D	2000	LMT	C1'-O5'-C5'	3.87	121.28	113.72
2	E	2000	LMT	C1B-O1B-C4'	-3.78	109.02	117.98

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	C1B
2	C	2000	LMT	C2B

5 of 66 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	B	2000	LMT	O5B-C1B-O1B-C4'

There are no ring outliers.

6 monomers are involved in 29 short contacts:

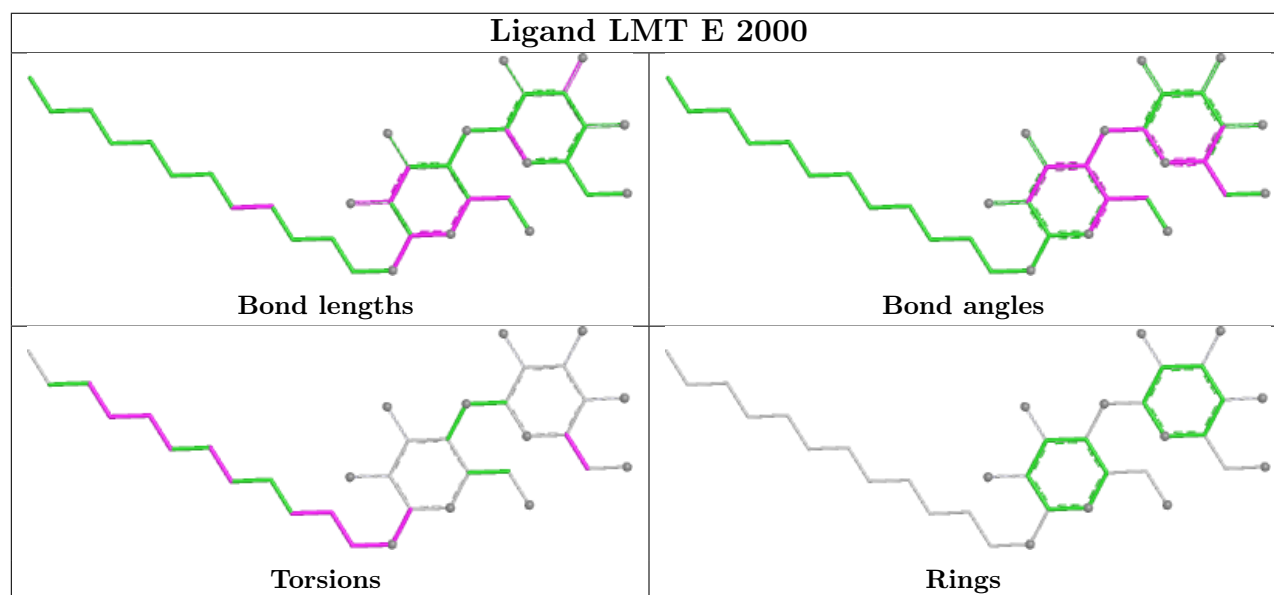
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2000	LMT	6	0
2	F	2000	LMT	2	0
2	B	2000	LMT	12	0
2	C	2000	LMT	5	0

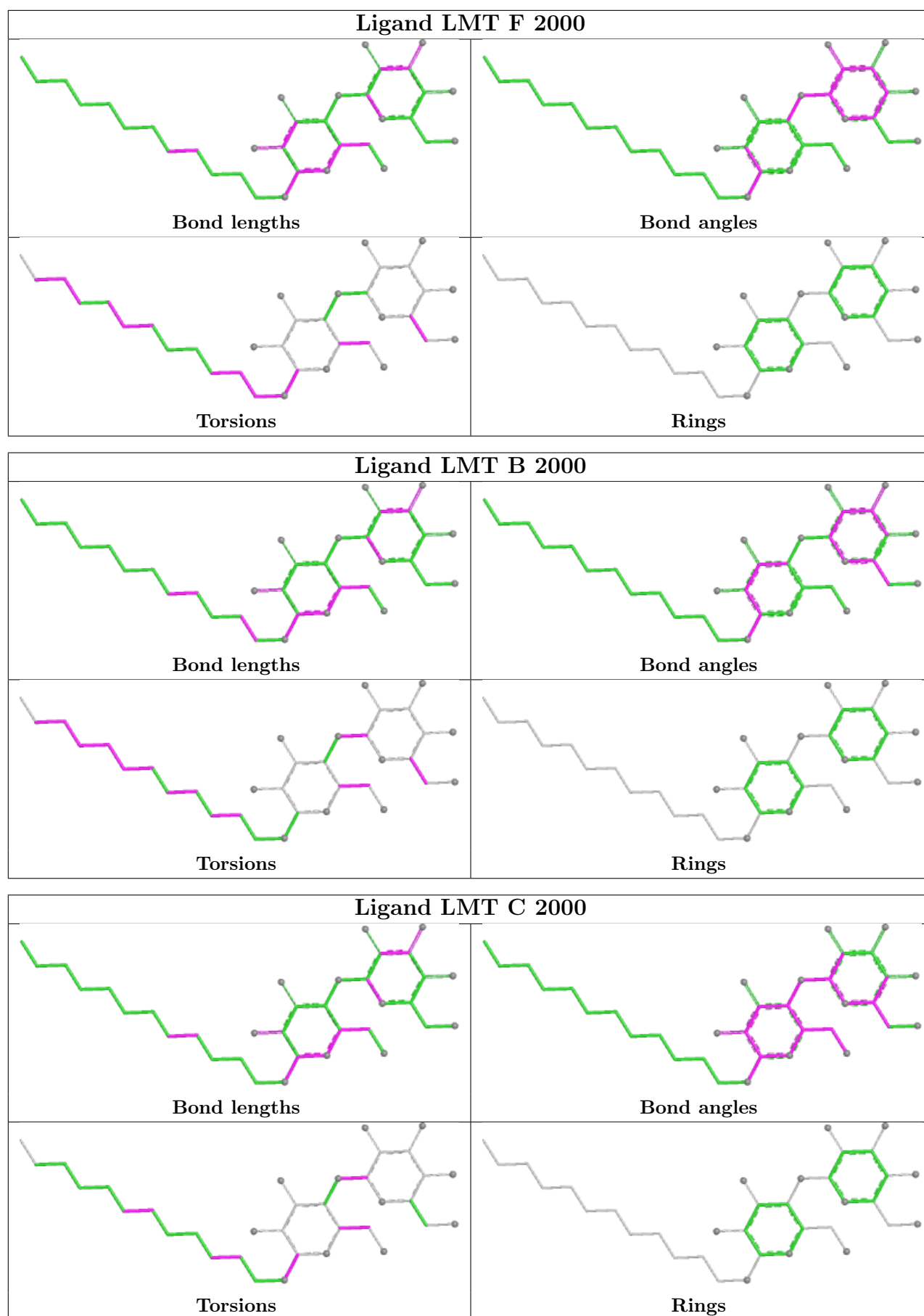
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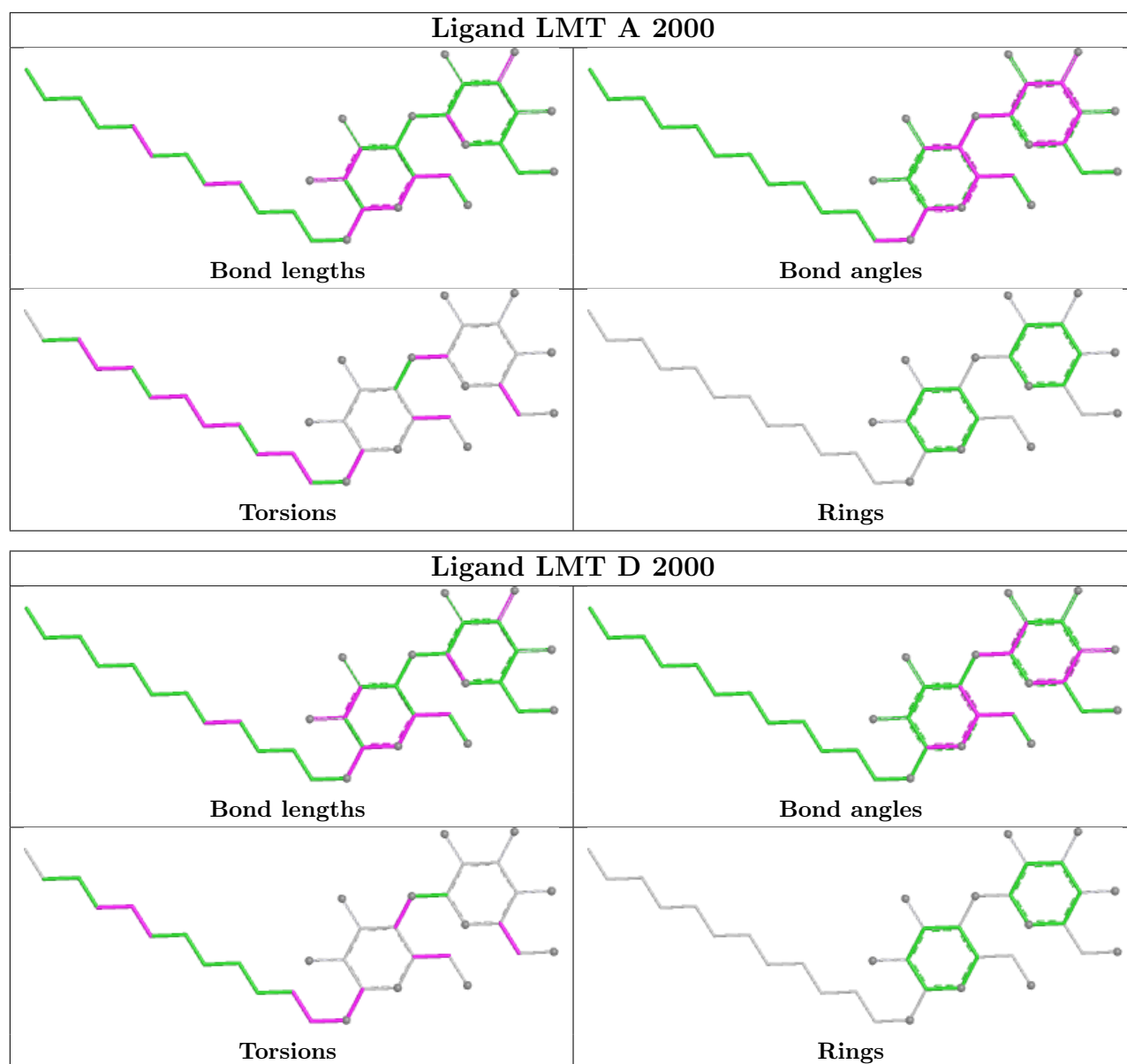
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2000	LMT	1	0
2	D	2000	LMT	3	0

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	1044/1069 (97%)	-0.28	6 (0%) 85 63	5, 35, 83, 118	0
1	B	1042/1069 (97%)	-0.48	1 (0%) 92 85	3, 27, 62, 108	0
1	C	1044/1069 (97%)	-0.40	1 (0%) 92 85	4, 29, 60, 88	0
1	D	1044/1069 (97%)	-0.18	8 (0%) 82 58	10, 49, 88, 114	0
1	E	1042/1069 (97%)	-0.15	12 (1%) 76 49	5, 46, 100, 129	0
1	F	1044/1069 (97%)	-0.04	29 (2%) 55 30	5, 54, 104, 142	0
All	All	6260/6414 (97%)	-0.26	57 (0%) 81 56	3, 39, 90, 142	0

The worst 5 of 57 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	706	ALA	5.8
1	D	295	THR	4.3
1	F	116	PRO	4.3
1	F	856	GLY	3.8
1	F	848	ALA	3.7

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 [i](#)

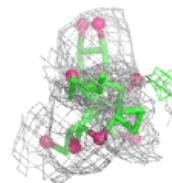
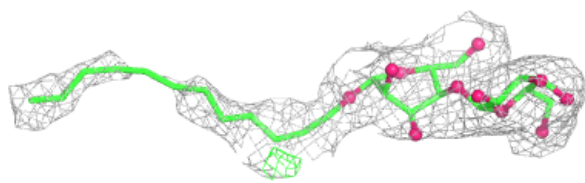
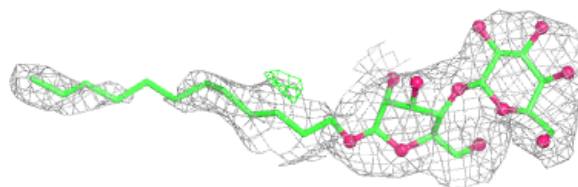
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	LMT	A	2000	35/35	0.75	0.11	2,31,49,54	0
2	LMT	B	2000	35/35	0.77	0.10	6,32,47,61	0
2	LMT	E	2000	35/35	0.78	0.11	3,34,48,49	0
2	LMT	D	2000	35/35	0.84	0.09	1,25,38,40	0
2	LMT	C	2000	35/35	0.88	0.08	5,22,46,50	0
2	LMT	F	2000	35/35	0.89	0.08	13,38,54,58	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.

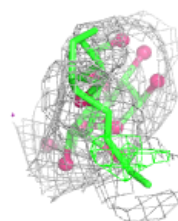
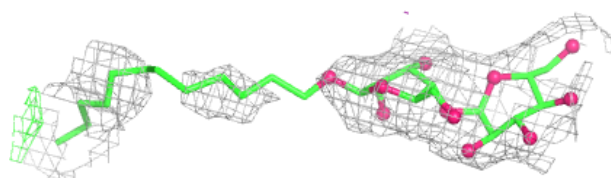
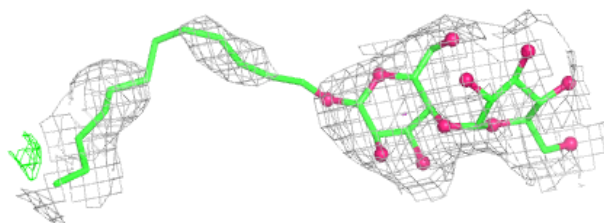
Electron density around LMT A 2000:

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

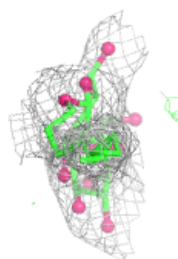
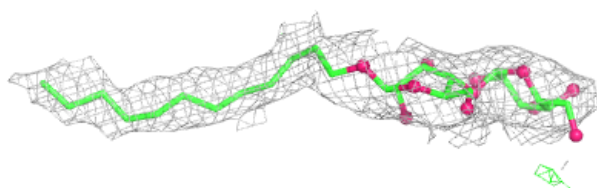
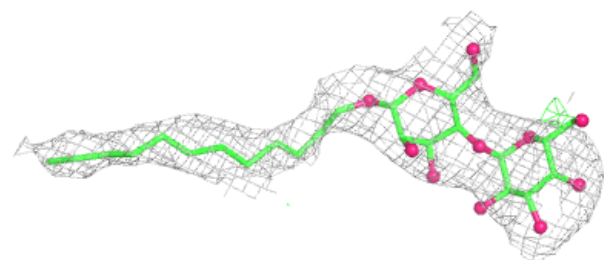


Electron density around LMT B 2000:

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

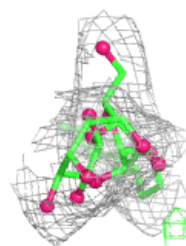
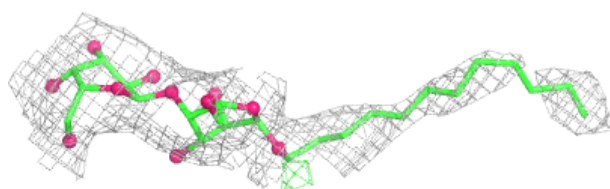
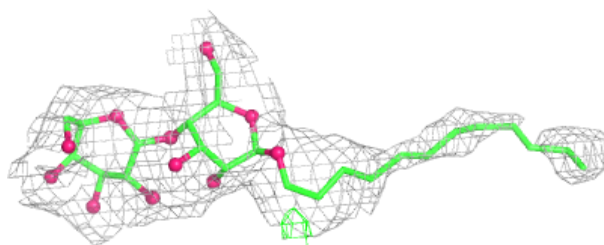
**Electron density around LMT E 2000:**

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and green (positive)

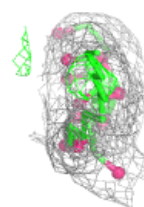
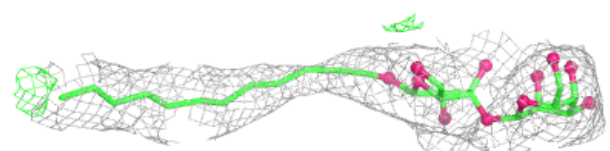
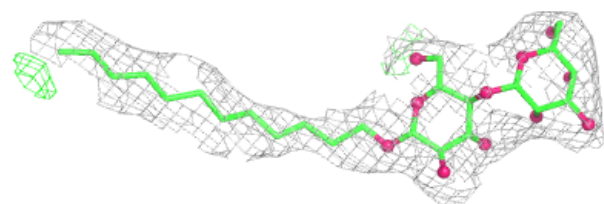


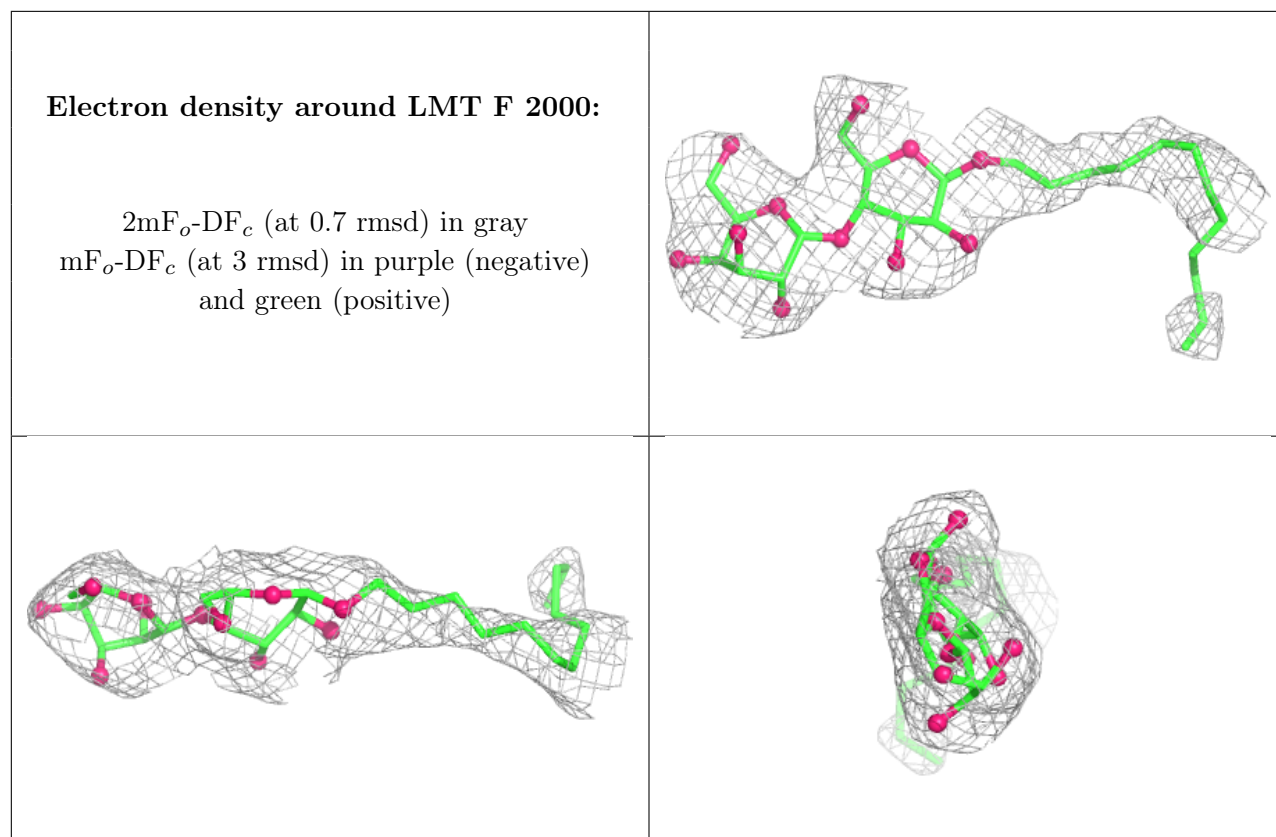
Electron density around LMT D 2000:

$2mF_o-DF_c$ (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)





6.5 Other polymers [i](#)

There are no such residues in this entry.