



wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 05:14 pm BST

PDB ID : 4ZJQ
Title : Crystal structure of AcrB deletion mutant in complex with antibiotic in P21 space group
Authors : Ababou, A.; Koronakis, V.
Deposited on : 2015-04-29
Resolution : 3.59 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

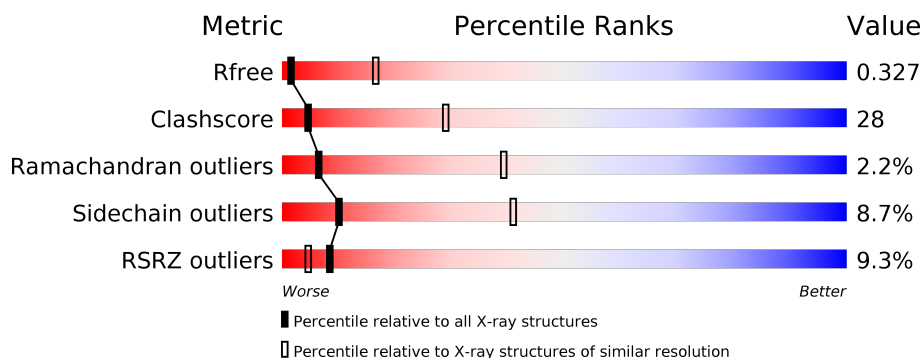
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.59 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	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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 on 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	<div> <div>7%</div> <div>48%</div> <div>47%</div> <div>• •</div> </div>
1	B	1044	<div> <div>7%</div> <div>48%</div> <div>46%</div> <div>6%</div> <div>•</div> </div>
1	C	1044	<div> <div>9%</div> <div>45%</div> <div>48%</div> <div>6%</div> <div>•</div> </div>
1	D	1044	<div> <div>7%</div> <div>48%</div> <div>45%</div> <div>6%</div> <div>•</div> </div>
1	E	1044	<div> <div>11%</div> <div>47%</div> <div>46%</div> <div>6%</div> <div>•</div> </div>
1	F	1044	<div> <div>13%</div> <div>43%</div> <div>49%</div> <div>6%</div> <div>• •</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ERY	A	1101	-	-	-	X
2	ERY	D	1101	-	-	-	X
3	LMT	A	1102	-	-	-	X
3	LMT	B	2100	-	-	-	X
3	LMT	C	1101	-	-	-	X
3	LMT	D	1102	-	-	-	X
3	LMT	D	1103	-	-	-	X
3	LMT	F	2100	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 47697 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	1037	Total	C	N	O	S	0	0	0
			7883	5066	1303	1471	43			
1	C	1036	Total	C	N	O	S	0	0	0
			7877	5063	1302	1469	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:

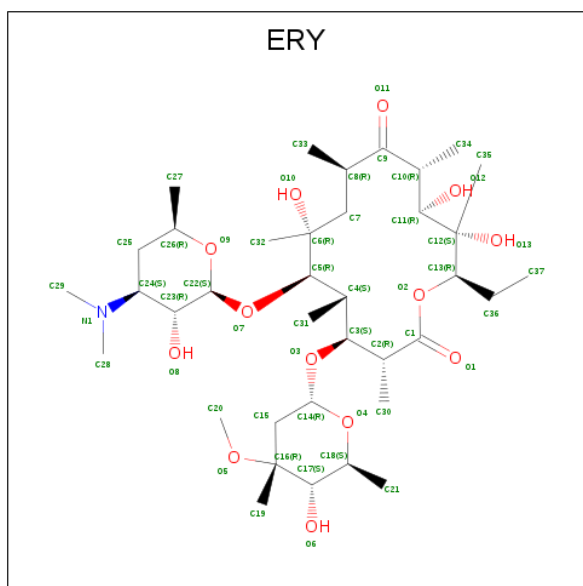
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	GLY	PHE	engineered mutation	UNP P31224
A	?	-	GLY	deletion	UNP P31224
A	?	-	PHE	deletion	UNP P31224
A	?	-	ALA	deletion	UNP P31224
A	?	-	GLY	deletion	UNP P31224
A	?	-	ARG	deletion	UNP P31224
B	?	GLY	PHE	engineered mutation	UNP P31224
B	?	-	GLY	deletion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

Continued on next page...

Continued from previous page...

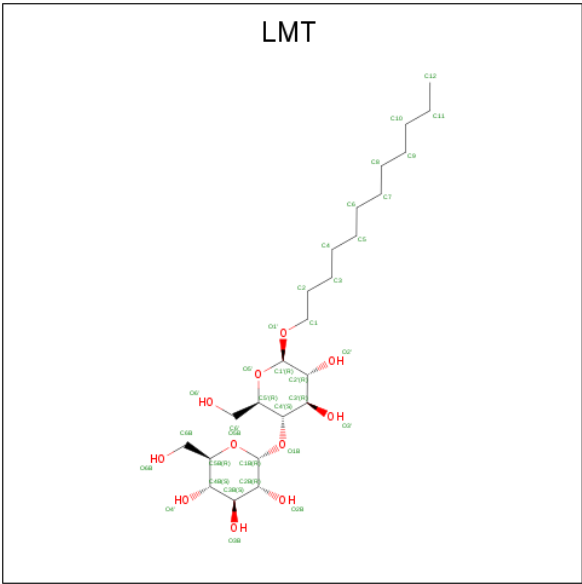
Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	ARG	deletion	UNP P31224
D	?	GLY	PHE	engineered mutation	UNP P31224
D	?	-	GLY	deletion	UNP P31224
D	?	-	PHE	deletion	UNP P31224
D	?	-	ALA	deletion	UNP P31224
D	?	-	GLY	deletion	UNP P31224
D	?	-	ARG	deletion	UNP P31224
E	?	GLY	PHE	engineered mutation	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	?	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 ERYTHROMYCIN A (three-letter code: ERY) (formula: $C_{37}H_{67}NO_{13}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			51	37	1	13		
2	D	1	Total	C	N	O	0	0
			51	37	1	13		

- Molecule 3 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



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

- Molecule 4 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

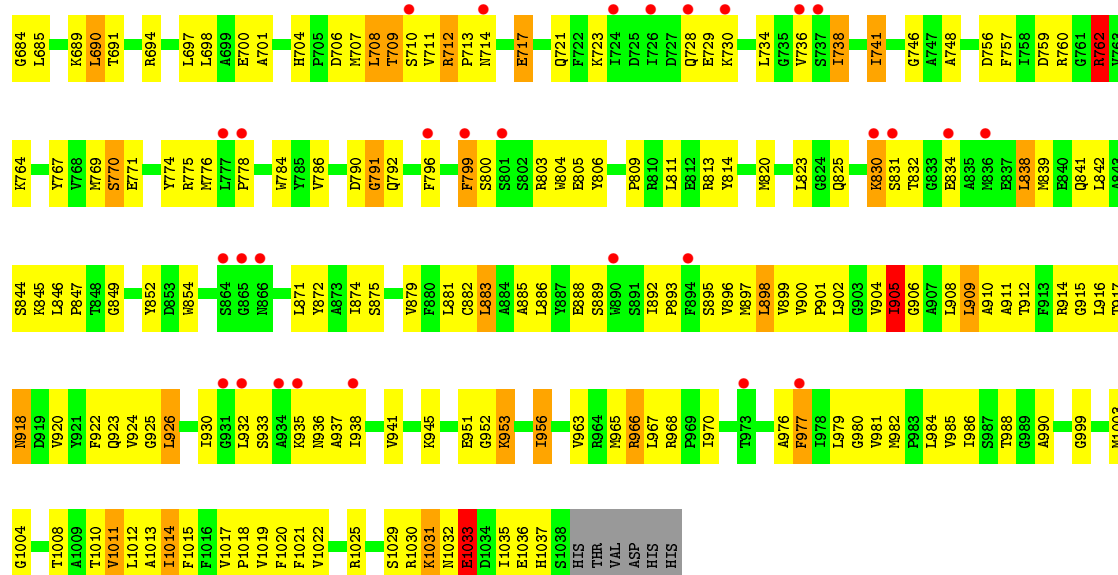
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ni	0	0
			1	1		
4	C	1	Total	Ni	0	0
			1	1		

Continued on next page...

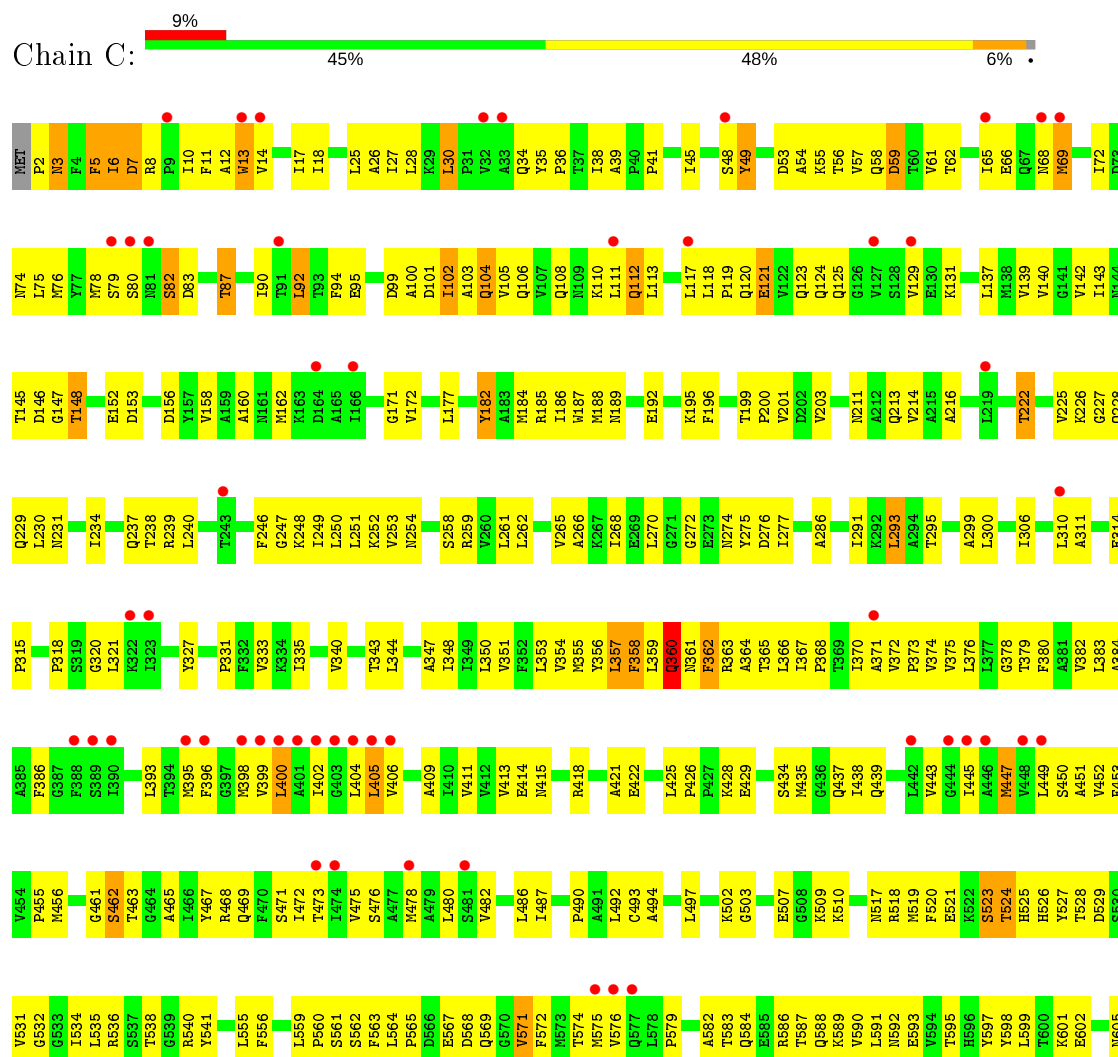
Continued from previous page...

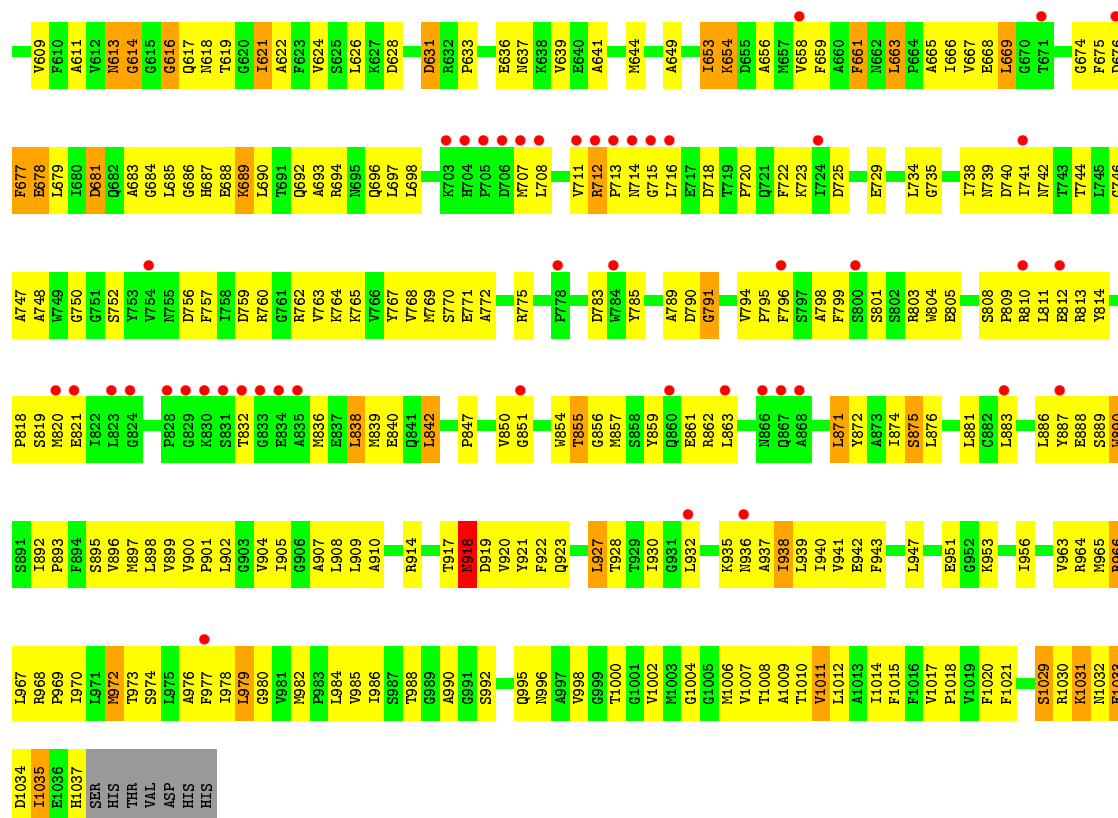
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	1	Total	Ni	0	0
			1	1		



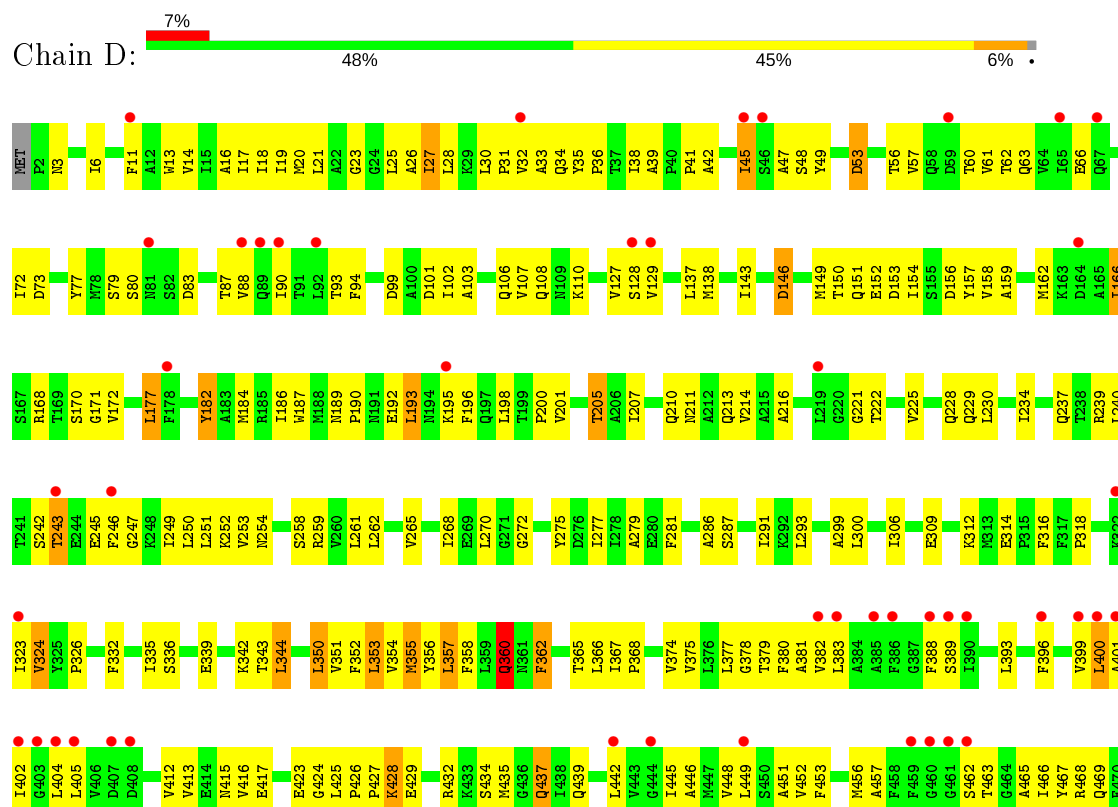


• Molecule 1: Multidrug efflux pump subunit AcrB





- Molecule 1: Multidrug efflux pump subunit AcrB



G1004	G1005	M1006	V1007	T1008	A1009	T1010	V1011	L1012	A1013	I1014	L1015	F1016	V1017	P1018	V1019	F1020	F1021	V1022	V1023	V1024	F1028	S1029	R1030	K1031	E1032	E1033	D1034	I1035	E1036	H1037	S1038	HIS	THR	VAL	ASP	HIS	HIS																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
V920	V921	F922	L926	L927	T928	T929	T930	G931	L932	S933	A934	K935	N936	A937	L938	T939	T940	V941	E942	F943	N948	E951	G952	K953	G954	L955	L956	E957	A958	V963	R964	N965	R966	L967	R968	F969	I970	L971	N972	T973	S974	F977	T978	L979	G980	L984	V985	L986	S987	T988	T1000																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
L946	M954	T955	G956	M957	S958	T959	Q960	E961	R962	L963	S964	G965	Q967	L971	L974	T976	S977	L978	L979	L980	L981	L982	L983	L984	L985	L986	L987	L988	L989	L990	L991	L992	L993	L994	L995	L996	L997	L998	L999	L1000	L1001	L1002	L1003	L1004	L1005	L1006	L1007	L1008	L1009	L1010	L1011	L1012	L1013	L1014	L1015	L1016	L1017	L1018	L1019	L1020	L1021	L1022	L1023	L1024	L1025	L1026	L1027	L1028	L1029	L1030	L1031	L1032	L1033	L1034	L1035	L1036	L1037	L1038	L1039	L1040	L1041	L1042	L1043	L1044	L1045	L1046	L1047	L1048	L1049	L1050	L1051	L1052	L1053	L1054	L1055	L1056	L1057	L1058	L1059	L1060	L1061	L1062	L1063	L1064	L1065	L1066	L1067	L1068	L1069	L1070	L1071	L1072	L1073	L1074	L1075	L1076	L1077	L1078	L1079	L1080	L1081	L1082	L1083	L1084	L1085	L1086	L1087	L1088	L1089	L1090	L1091	L1092	L1093	L1094	L1095	L1096	L1097	L1098	L1099	L1100	L1101	L1102	L1103	L1104	L1105	L1106	L1107	L1108	L1109	L1110	L1111	L1112	L1113	L1114	L1115	L1116	L1117	L1118	L1119	L1120	L1121	L1122	L1123	L1124	L1125	L1126	L1127	L1128	L1129	L1130	L1131	L1132	L1133	L1134	L1135	L1136	L1137	L1138	L1139	L1140	L1141	L1142	L1143	L1144	L1145	L1146	L1147	L1148	L1149	L1150	L1151	L1152	L1153	L1154	L1155	L1156	L1157	L1158	L1159	L1160	L1161	L1162	L1163	L1164	L1165	L1166	L1167	L1168	L1169	L1170	L1171	L1172	L1173	L1174	L1175	L1176	L1177	L1178	L1179	L1180	L1181	L1182	L1183	L1184	L1185	L1186	L1187	L1188	L1189	L1190	L1191	L1192	L1193	L1194	L1195	L1196	L1197	L1198	L1199	L1200	L1201	L1202	L1203	L1204	L1205	L1206	L1207	L1208	L1209	L1210	L1211	L1212	L1213	L1214	L1215	L1216	L1217	L1218	L1219	L1220	L1221	L1222	L1223	L1224	L1225	L1226	L1227	L1228	L1229	L1230	L1231	L1232	L1233	L1234	L1235	L1236	L1237	L1238	L1239	L1240	L1241	L1242	L1243	L1244	L1245	L1246	L1247	L1248	L1249	L1250	L1251	L1252	L1253	L1254	L1255	L1256	L1257	L1258	L1259	L1260	L1261	L1262	L1263	L1264	L1265	L1266	L1267	L1268	L1269	L1270	L1271	L1272	L1273	L1274	L1275	L1276	L1277	L1278	L1279	L1280	L1281	L1282	L1283	L1284	L1285	L1286	L1287	L1288	L1289	L1290	L1291	L1292	L1293	L1294	L1295	L1296	L1297	L1298	L1299	L1300	L1301	L1302	L1303	L1304	L1305	L1306	L1307	L1308	L1309	L1310	L1311	L1312	L1313	L1314	L1315	L1316	L1317	L1318	L1319	L1320	L1321	L1322	L1323	L1324	L1325	L1326	L1327	L1328	L1329	L1330	L1331	L1332	L1333	L1334	L1335	L1336	L1337	L1338	L1339	L1340	L1341	L1342	L1343	L1344	L1345	L1346	L1347	L1348	L1349	L1350	L1351	L1352	L1353	L1354	L1355	L1356	L1357	L1358	L1359	L1360	L1361	L1362	L1363	L1364	L1365	L1366	L1367	L1368	L1369	L1370	L1371	L1372	L1373	L1374	L1375	L1376	L1377	L1378	L1379	L1380	L1381	L1382	L1383	L1384	L1385	L1386	L1387	L1388	L1389	L1390	L1391	L1392	L1393	L1394	L1395	L1396	L1397	L1398	L1399	L1400	L1401	L1402	L1403	L1404	L1405	L1406	L1407	L1408	L1409	L1410	L1411	L1412	L1413	L1414	L1415	L1416	L1417	L1418	L1419	L1420	L1421	L1422	L1423	L1424	L1425	L1426	L1427	L1428	L1429	L1430	L1431	L1432	L1433	L1434	L1435	L1436	L1437	L1438	L1439	L1440	L1441	L1442	L1443	L1444	L1445	L1446	L1447	L1448	L1449	L1450	L1451	L1452	L1453	L1454	L1455	L1456	L1457	L1458	L1459	L1460	L1461	L1462	L1463	L1464	L1465	L1466	L1467	L1468	L1469	L1470	L1471	L1472	L1473	L1474	L1475	L1476	L1477	L1478	L1479	L1480	L1481	L1482	L1483	L1484	L1485	L1486	L1487	L1488	L1489	L1490	L1491	L1492	L1493	L1494	L1495	L1496	L1497	L1498	L1499	L1500	L1501	L1502	L1503	L1504	L1505	L1506	L1507	L1508	L1509	L1510	L1511	L1512	L1513	L1514	L1515	L1516	L1517	L1518	L1519	L1520	L1521	L1522	L1523	L1524	L1525	L1526	L1527	L1528	L1529	L1530	L1531	L1532	L1533	L1534	L1535	L1536	L1537	L1538	L1539	L1540	L1541	L1542	L1543	L1544	L1545	L1546	L1547	L1548	L1549	L1550	L1551	L1552	L1553	L1554	L1555	L1556	L1557	L1558	L1559	L1560	L1561	L1562	L1563	L1564	L1565	L1566	L1567	L1568	L1569	L1570	L1571	L1572	L1573	L1574	L1575	L1576	L1577	L1578	L1579	L1580	L1581	L1582	L1583	L1584	L1585	L1586	L1587	L1588	L1589	L1590	L1591	L1592	L1593	L1594	L1595	L1596	L1597	L1598	L1599	L1600	L1601	L1602	L1603	L1604	L1605	L1606	L1607	L1608	L1609	L1610	L1611	L1612	L1613	L1614	L1615	L1616	L1617	L1618	L1619	L1620	L1621	L1622	L1623	L1624	L1625	L1626	L1627	L1628	L1629	L1630	L1631	L1632	L1633	L1634	L1635	L1636	L1637	L1638	L1639	L1640	L1641	L1642	L1643	L1644	L1645	L1646	L1647	L1648	L1649	L1650	L1651	L1652	L1653	L1654	L1655	L1656	L1657	L1658	L1659	L1660	L1661	L1662	L1663	L1664	L1665	L1666	L1667	L1668	L1669	L1670	L1671	L1672	L1673	L1674	L1675	L1676	L1677	L1678	L1679	L1680	L1681	L1682	L1683	L1684	L1685	L1686	L1687	L1688	L1689	L1690	L1691	L1692	L1693	L1694	L1695	L1696	L1697	L1698	L1699	L1700	L1701	L1702	L1703	L1704	L1705	L1706	L1707	L1708	L1709	L1710	L1711	L1712	L1713	L1714	L1715	L1716	L1717	L1718	L1719	L1720	L1721	L1722	L1723	L1724	L1725	L1726	L1727	L1728	L1729	L1730	L1731	L1732	L1733	L1734	L1735	L1736	L1737	L1738	L1739	L1740	L1741	L1742	L1743	L1744	L1745	L1746	L1747	L1748	L1749	L1750	L1751	L1752	L1753	L1754	L1755	L1756	L1757	L1758	L1759	L1760	L1761	L1762	L1763	L1764	L1765	L1766	L1767	L1768	L1769	L1770	L1771	L1772	L1773	L1774	L1775	L1776	L1777	L1778	L1779	L1780	L1781	L1782	L1783	L1784	L1785	L1786	L1787	L1788	L1789	L1790	L1791	L1792	L1793	L1794	L1795	L1796	L1797	L1798	L1799	L1800	L1801	L1802	L1803	L1804	L1805	L1806	L1807	L1808	L1809	L1810	L1811	L1812	L1813	L1814	L1815	L1816	L1817	L1818	L1819	L1820	L1821	L1822	L1823	L1824	L1825	L1826	L1827	L1828	L1829	L1830	L1831	L1832	L1833	L1834	L1835	L1836	L1837	L1838	L1839	L1840	L1841	L1842	L1843	L1844	L1845	L1846	L1847	L1848	L1849	L1850	L1851	L1852	L1853	L1854	L1855	L1856	L1857	L1858	L1859	L1860	L1861	L1862	L1863	L1864	L1865	L1866	L1867	L1868	L1869	L1870	L1871	L1872	L1873	L1874	L1875	L1876	L1877	L1878	L1879	L1880	L1881	L1882	L1883	L1884	L1885	L1886	L1887	L1888	L1889	L1890	L1891	L1892	L1893	L1894	L1895	L1896	L1897	L1898	L1899	L1900	L1901	L1902	L1903	L1904	L1905	L1906	L1907	L1908	L1909	L1910	L1911	L1912	L1913	L1914	L1915	L1916	L1917	L1918	L1919	L1920	L1921	L1922	L1923	L1924	L1925	L1926	L1927	L1928	L1929	L1930	L1931	L1932	L1933	L1934	L1935	L1936	L1937	L1938	L1939	L1940	L1941	L1942	L1943	L1944	L1945	L1946	L1947	L1948	L1949	L1950	L1951	L1952	L1953	L1954	L1955	L1956	L1957	L1958	L1959	L1960	L1961	L1962	L1963	L1964	L1965	L1966	L1967	L1968	L1969	L1970	L1971	L1972	L1973	L1974	L1975	L1976	L1977	L1978	L1979	L1980	L1981	L1982	L1983	L1984	L1985	L1986	L1987	L1988	L1989	L1990	L1991	L1992	L1993	L1994	L1995	L1996	L1997	L1998	L1999	L2000	L2001	L2002	L2003	L2004	L2005	L2006	L2007	L2008	L2009	L2010	L2011	L2012	L2013	L2014	L2015	L2016	L2017	L2018	L2019	L2020	L2021	L2022	L2023	L2024	L2025	L2026	L2027	L2028	L2029	L2030	L2031	L2032	L2033	L2034	L2035	L2036	L2037	L2038	L2039	L2040	L2041	L2042	L2043	L2044	L2045	L2046	L2047	L2048	L2049	L2050	L2051	L2052	L2053	L2054	L2055	L2056	L2057	L2058	L2059	L2060	L2061	L2062	L2063	L2064	L2065	L2066	L2067	L2068	L2069	L2070	L2071	L2072	L2073	L2074	L2075	L2076	L2077	L2078	L2079	L2080	L2081	L2082	L2083	L2084	L2085	L2086	L2087	L2088	L2089	L2090	L2091	L2092	L2093	L2094	L2095	L2096	L2097	L2098	L2099	L2100	L2101	L2102	L2103	L2104	L2105	L2106	L2107	L2108	L2109	L2110	L2111	L2112	L2113	L2114	L2115	L2116	L2117	L2118	L2119	L2120	L2121	L2122	L2123	L2124	L2125	L2126	L2127	L2128	L2129	L2130	L2131	L2132	L2133	L2134	L2135	L2136	L2137	L2138	L2139	L2140	L2141	L2142	L2143	L2144	L2145	L2146	L2147	L2148	L2149	L2150	L2151	L2152	L2153	L2154	L2155	L2156	L2157	L2158	L2159	L2160	L2161	L2162	L2163	L2164	L2165	L2166	L2167	L2168	L2169	L2170	L2171	L2172	L2173	L2174	L2175	L2176	L2177	L2178	L2179	L2180	L2181	L2182	L2183	L2184	L2185	L2186	L2187	L2188	L2189	L2190	L2191	L2192	L2193	L2194	L2195	L2196	L2197	L2198	L2199	L2200	L2201	L2202	L2203	L2204	L2205	L2206	L2207	L2208	L2209	L2210	L2211	L2212	L2213	L2214	L2215	L2216	L2217	L2218	L2219	L2220	L2221	L2222	L2223	L2224	L2225	L2226	L2227	L2228	L2229	L2230	L2231	L2232	L2233	L2234	L2235	L2236	L2237	L2238	L2239	L2240	L2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	150.06Å 154.57Å 215.74Å 90.00° 92.42° 90.00°	Depositor
Resolution (Å)	19.96 – 3.59 125.61 – 3.59	Depositor EDS
% Data completeness (in resolution range)	99.2 (19.96-3.59) 96.5 (125.61-3.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 3.58Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.246 , 0.319 0.258 , 0.327	Depositor DCC
R_{free} test set	5715 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	110.6	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 61.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.055 for -k,-h,-l 0.070 for k,h,-l 0.068 for h,-k,-l	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	47697	wwPDB-VP
Average B, all atoms (Å ²)	81.0	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 51.06 % 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 5.9200e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: NI, LMT, ERY

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	0.59	0/8043	0.85	10/10922 (0.1%)
1	B	0.59	0/8032	0.83	11/10907 (0.1%)
1	C	0.59	0/8026	0.87	7/10899 (0.1%)
1	D	0.56	1/8043 (0.0%)	0.81	9/10922 (0.1%)
1	E	0.57	1/8032 (0.0%)	0.82	10/10907 (0.1%)
1	F	0.56	0/8032	0.83	5/10907 (0.0%)
All	All	0.57	2/48208 (0.0%)	0.84	52/65464 (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	B	0	1
1	D	0	1
1	F	0	2
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	515	TRP	CB-CG	7.12	1.63	1.50
1	D	515	TRP	CB-CG	6.58	1.62	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	529	ASP	CB-CG-OD1	10.28	127.55	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	529	ASP	CB-CG-OD1	9.49	126.84	118.30
1	F	113	LEU	CA-CB-CG	9.17	136.39	115.30
1	A	529	ASP	CB-CG-OD1	8.95	126.36	118.30
1	E	529	ASP	CB-CG-OD1	7.96	125.46	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1034	ASP	Peptide
1	B	1033	GLU	Peptide
1	D	1032	ASN	Peptide
1	F	1033	GLU	Peptide
1	F	1034	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	7893	0	8034	443	0
1	B	7883	0	8027	442	0
1	C	7877	0	8022	481	0
1	D	7893	0	8034	470	0
1	E	7883	0	8027	467	0
1	F	7883	0	8027	497	0
2	A	51	0	67	5	0
2	D	51	0	67	4	0
3	A	70	0	92	7	0
3	B	35	0	46	7	0
3	C	35	0	46	1	0
3	D	70	0	92	13	0
3	E	35	0	46	10	0
3	F	35	0	46	2	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
All	All	47697	0	48673	2723	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 28.

The worst 5 of 2723 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:F:34:GLN:HB2	1:F:333:VAL:HG22	1.45	0.98
1:A:225:VAL:H	1:B:776:MET:HE1	1.25	0.97
1:D:344:LEU:HD22	1:D:402:ILE:HD11	1.45	0.97
1:A:776:MET:HE1	1:C:225:VAL:H	1.29	0.96
1:B:213:GLN:HG2	1:B:239:ARG:HG3	1.44	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	1036/1044 (99%)	902 (87%)	117 (11%)	17 (2%)	9	46
1	B	1035/1044 (99%)	896 (87%)	117 (11%)	22 (2%)	7	40
1	C	1034/1044 (99%)	896 (87%)	119 (12%)	19 (2%)	8	43
1	D	1036/1044 (99%)	894 (86%)	116 (11%)	26 (2%)	5	36
1	E	1035/1044 (99%)	894 (86%)	116 (11%)	25 (2%)	6	37
1	F	1035/1044 (99%)	891 (86%)	118 (11%)	26 (2%)	5	36
All	All	6211/6264 (99%)	5373 (86%)	703 (11%)	135 (2%)	6	39

5 of 135 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	987	SER
1	A	1033	GLU
1	B	357	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	508	GLY
1	B	672	ALA

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%)	782 (92%)	64 (8%)	13	45
1	B	845/852 (99%)	772 (91%)	73 (9%)	10	41
1	C	844/852 (99%)	766 (91%)	78 (9%)	9	39
1	D	846/852 (99%)	779 (92%)	67 (8%)	12	44
1	E	845/852 (99%)	775 (92%)	70 (8%)	11	42
1	F	845/852 (99%)	758 (90%)	87 (10%)	7	34
All	All	5071/5112 (99%)	4632 (91%)	439 (9%)	10	41

5 of 439 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	838	LEU
1	D	571	VAL
1	F	681	ASP
1	C	890	TRP
1	D	152	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	918	ASN
1	D	112	GLN
1	F	70	ASN
1	C	996	ASN
1	D	58	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 3 are monoatomic - leaving 10 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$
3	LMT	D	1103	-	36,36,36	1.92	8 (22%)	47,47,47	1.31	7 (14%)
2	ERY	D	1101	-	53,53,53	1.28	2 (3%)	82,82,82	2.03	27 (32%)
3	LMT	A	1103	-	36,36,36	1.89	10 (27%)	47,47,47	1.58	9 (19%)
3	LMT	F	2100	-	36,36,36	1.74	8 (22%)	47,47,47	1.11	4 (8%)
3	LMT	A	1102	-	36,36,36	1.76	9 (25%)	47,47,47	1.14	4 (8%)
3	LMT	B	2100	-	36,36,36	1.73	9 (25%)	47,47,47	1.93	14 (29%)
3	LMT	D	1102	-	36,36,36	1.81	9 (25%)	47,47,47	1.41	7 (14%)
3	LMT	E	1101	-	36,36,36	1.89	11 (30%)	47,47,47	1.63	8 (17%)
3	LMT	C	1101	-	36,36,36	1.79	8 (22%)	47,47,47	1.43	6 (12%)
2	ERY	A	1101	-	53,53,53	1.14	2 (3%)	82,82,82	1.86	18 (21%)

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
3	LMT	D	1103	-	-	14/21/61/61	0/2/2/2
2	ERY	D	1101	-	-	48/72/107/107	0/3/3/3
3	LMT	A	1103	-	-	14/21/61/61	0/2/2/2
3	LMT	F	2100	-	-	12/21/61/61	0/2/2/2
3	LMT	A	1102	-	-	13/21/61/61	0/2/2/2
3	LMT	B	2100	-	-	11/21/61/61	0/2/2/2
3	LMT	D	1102	-	-	11/21/61/61	0/2/2/2
3	LMT	E	1101	-	-	11/21/61/61	0/2/2/2
3	LMT	C	1101	-	-	12/21/61/61	0/2/2/2
2	ERY	A	1101	-	-	33/72/107/107	0/3/3/3

The worst 5 of 76 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1101	ERY	O2-C1	5.43	1.47	1.34
2	A	1101	ERY	O2-C1	5.17	1.46	1.34
3	A	1103	LMT	O5'-C5'	4.58	1.55	1.44
3	D	1103	LMT	O5'-C5'	4.51	1.55	1.44
3	D	1102	LMT	O3B-C3B	4.36	1.53	1.43

The worst 5 of 104 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1103	LMT	O5B-C5B-C4B	5.53	119.73	109.69
3	E	1101	LMT	C1B-C2B-C3B	-5.51	98.53	110.00
2	D	1101	ERY	C20-O5-C16	5.24	128.48	117.55
3	C	1101	LMT	C4B-C3B-C2B	5.07	119.67	110.82
2	A	1101	ERY	C20-O5-C16	4.72	127.40	117.55

There are no chirality outliers.

5 of 179 torsion outliers are listed below:

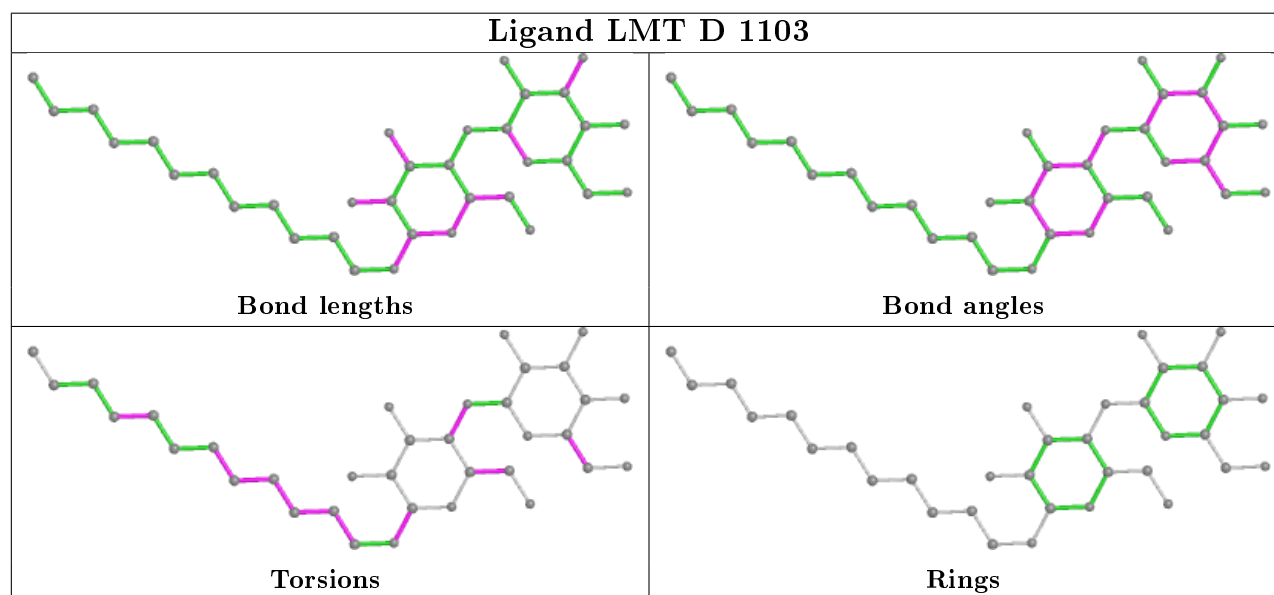
Mol	Chain	Res	Type	Atoms
3	D	1103	LMT	C2'-C1'-O1'-C1
3	D	1103	LMT	O5'-C1'-O1'-C1
2	D	1101	ERY	C9-C10-C11-C12
2	D	1101	ERY	C10-C11-C12-C13
2	D	1101	ERY	C10-C11-C12-C35

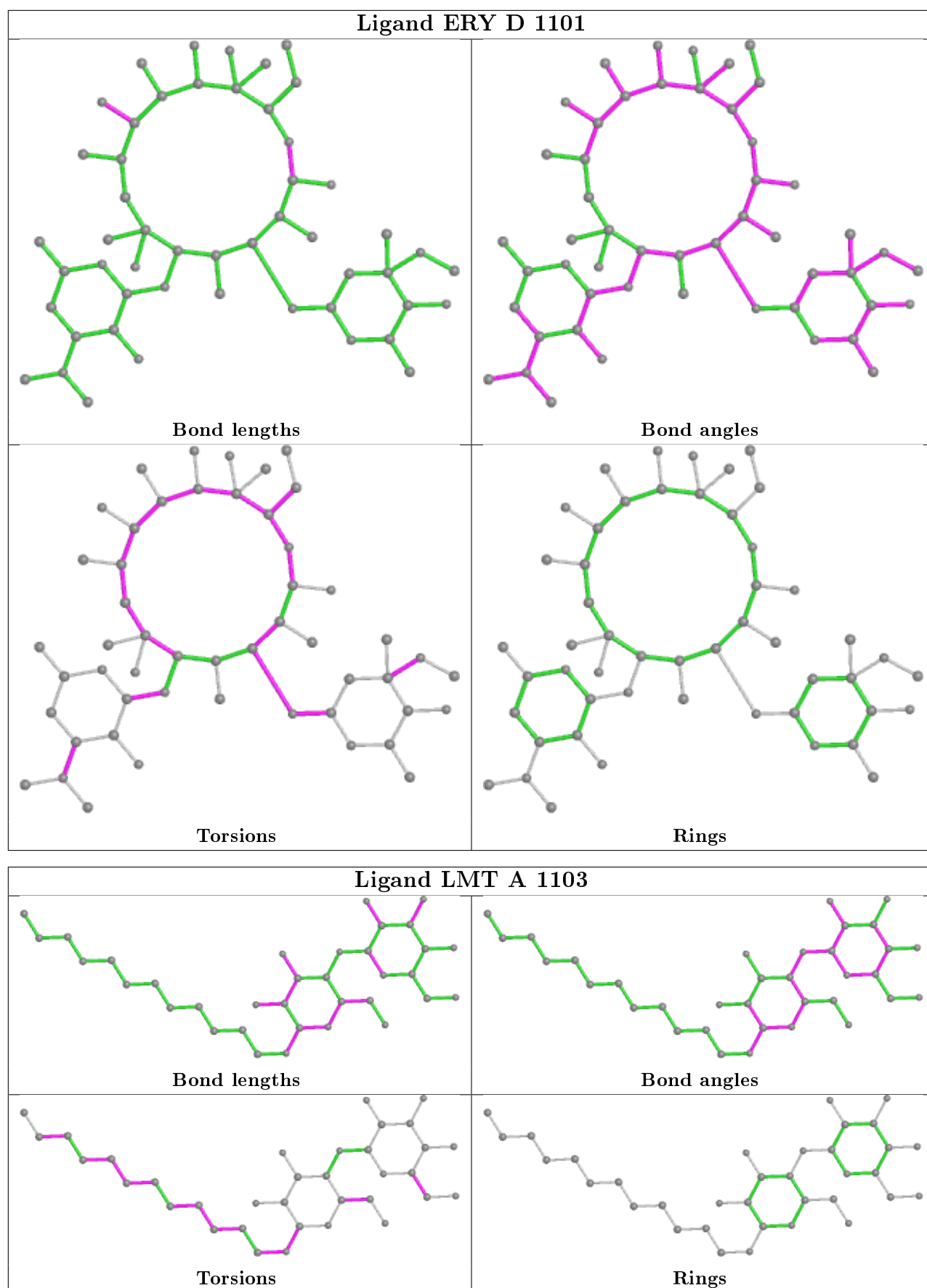
There are no ring outliers.

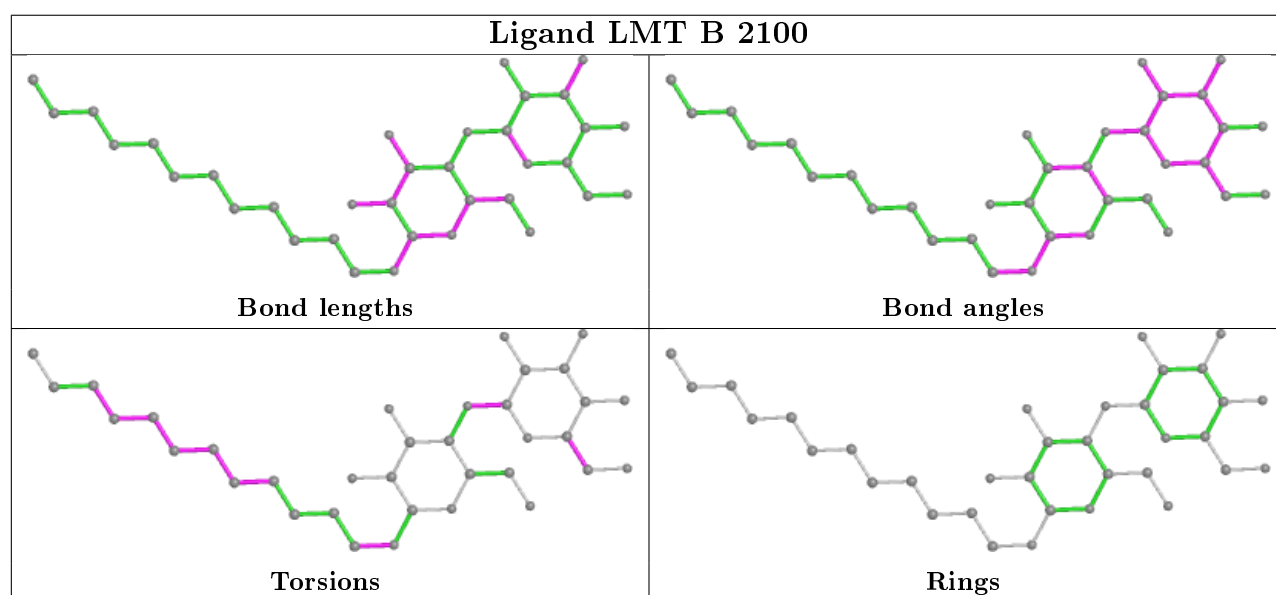
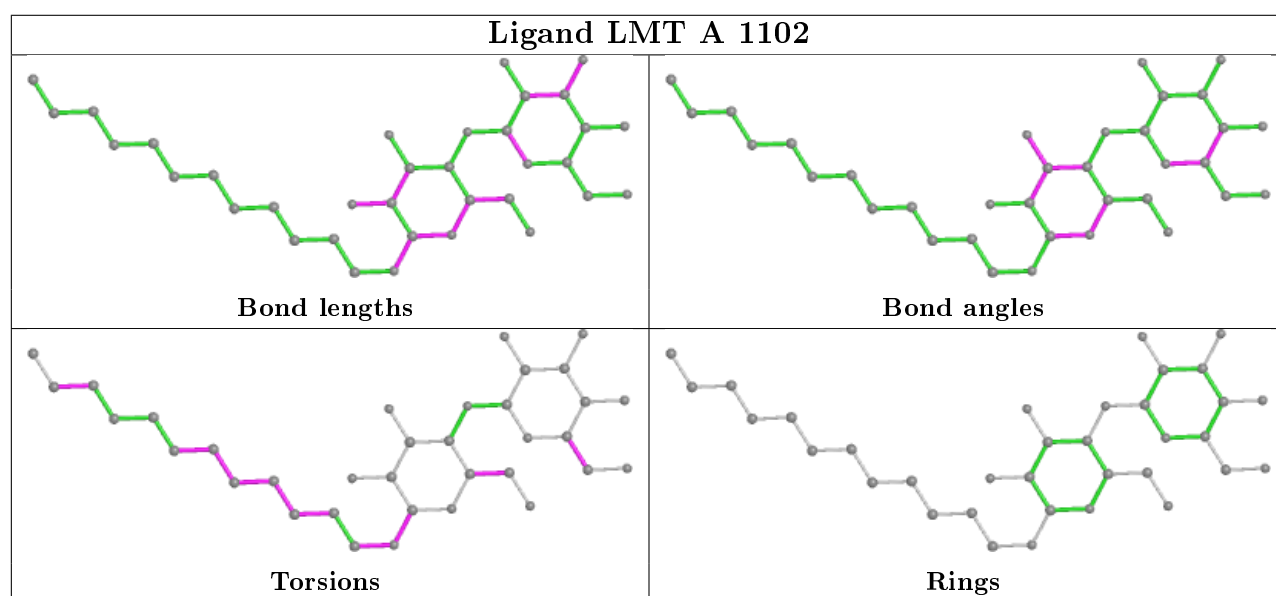
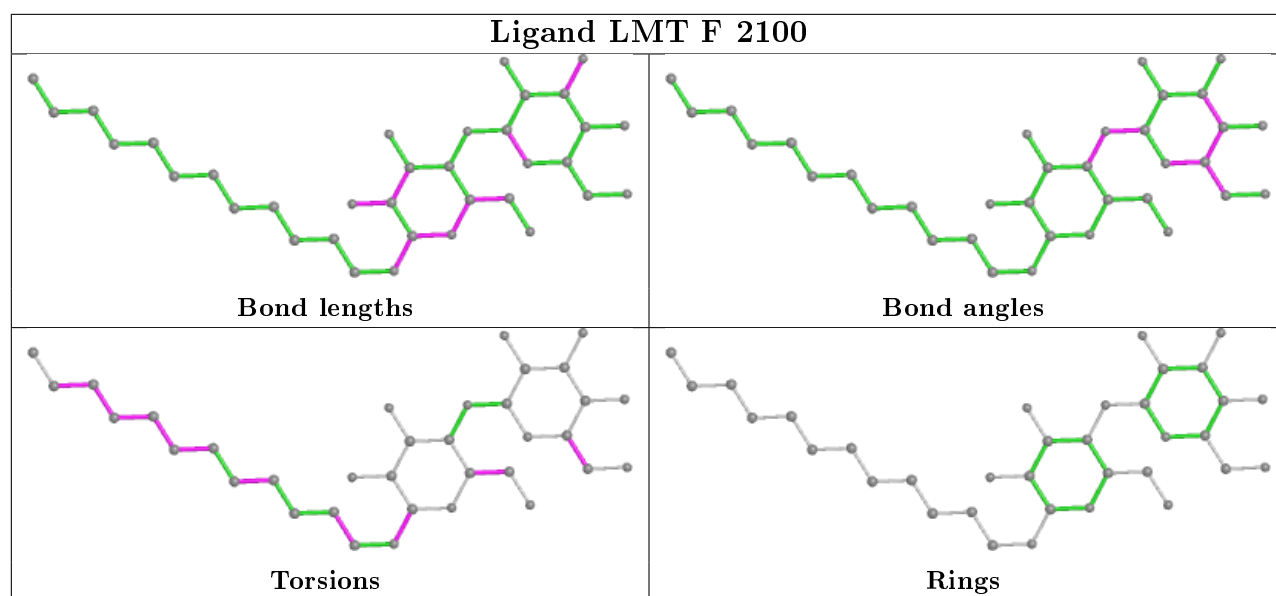
10 monomers are involved in 49 short contacts:

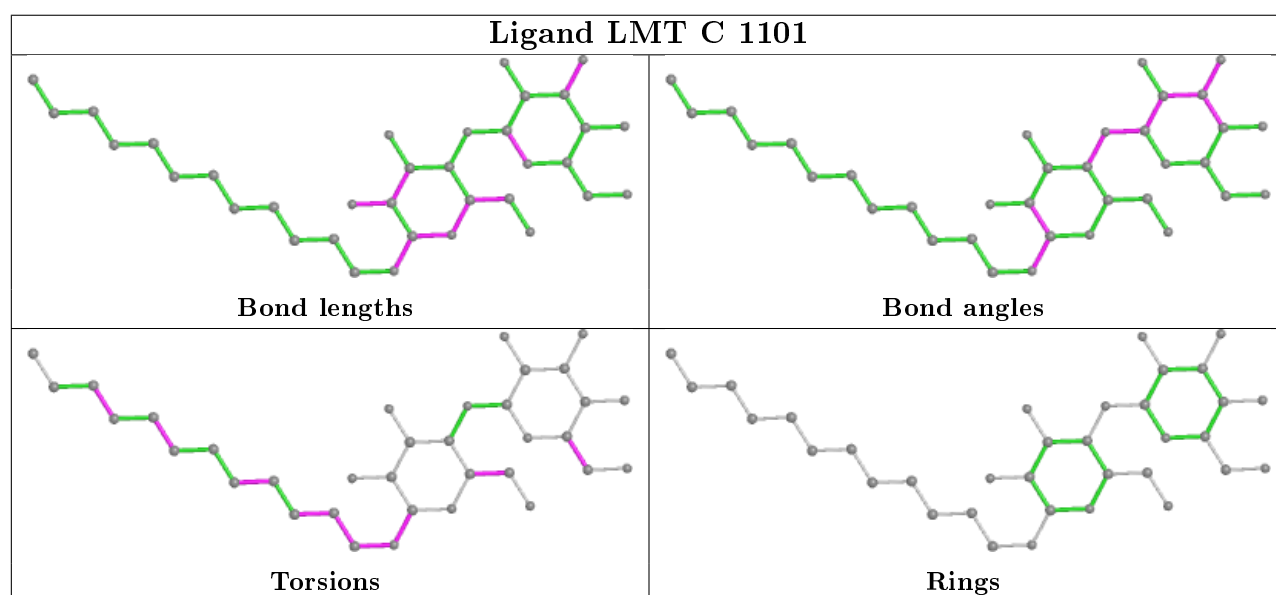
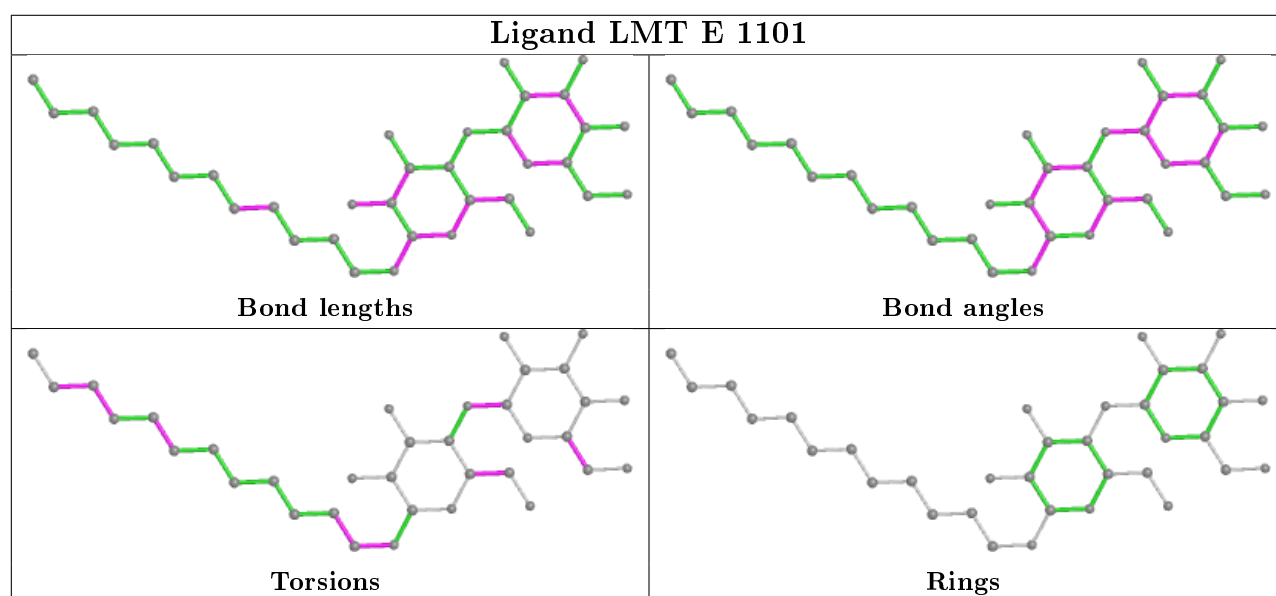
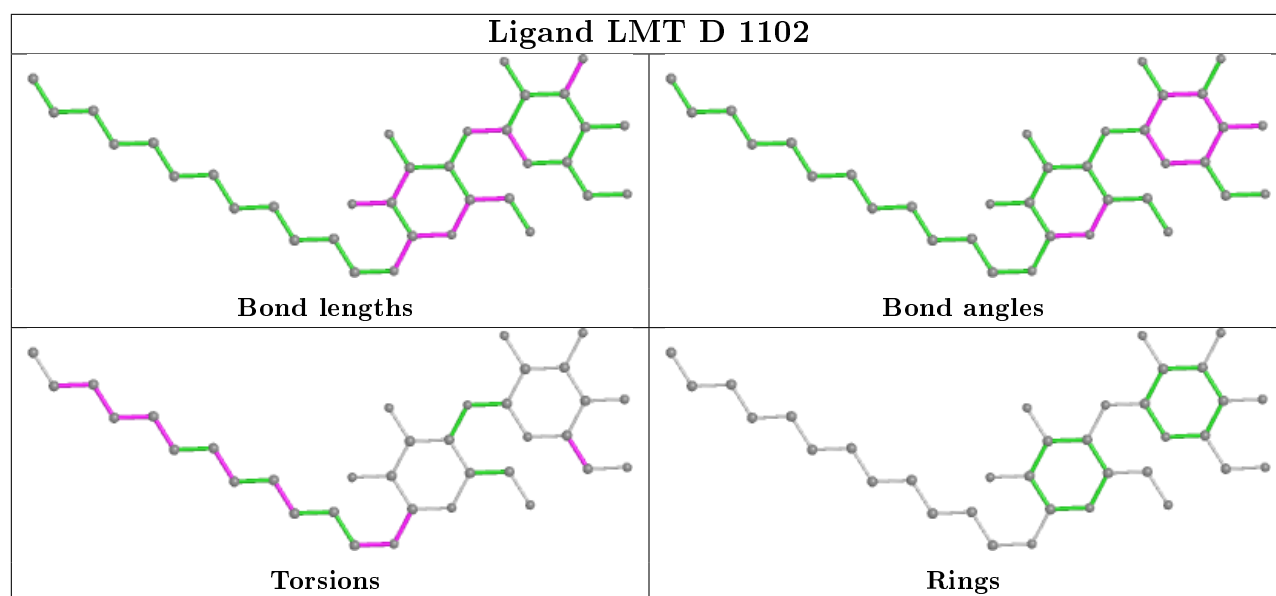
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1103	LMT	6	0
2	D	1101	ERY	4	0
3	A	1103	LMT	2	0
3	F	2100	LMT	2	0
3	A	1102	LMT	5	0
3	B	2100	LMT	7	0
3	D	1102	LMT	7	0
3	E	1101	LMT	10	0
3	C	1101	LMT	1	0
2	A	1101	ERY	5	0

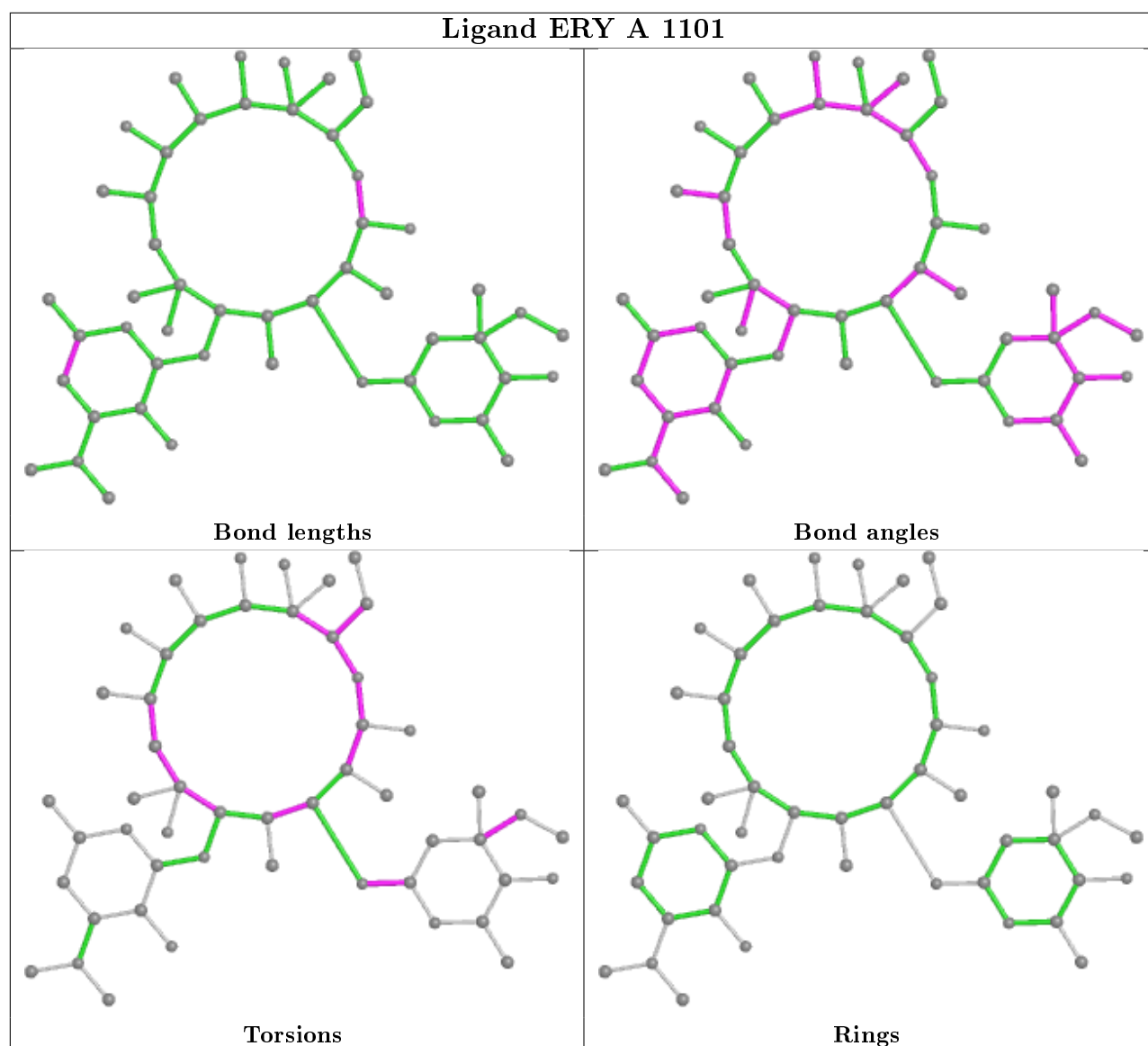
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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%)	0.17	76 (7%) 15 9	36, 75, 109, 154	0
1	B	1037/1044 (99%)	0.13	75 (7%) 15 9	31, 73, 111, 151	0
1	C	1036/1044 (99%)	0.33	99 (9%) 8 4	35, 76, 112, 139	0
1	D	1038/1044 (99%)	0.15	74 (7%) 16 9	34, 84, 123, 154	0
1	E	1037/1044 (99%)	0.32	119 (11%) 4 3	46, 87, 118, 148	0
1	F	1037/1044 (99%)	0.47	136 (13%) 3 2	41, 85, 119, 143	0
All	All	6223/6264 (99%)	0.26	579 (9%) 8 4	31, 81, 116, 154	0

The worst 5 of 579 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	714	ASN	10.9
1	C	714	ASN	10.3
1	C	715	GLY	9.4
1	E	314	GLU	9.1
1	A	404	LEU	9.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

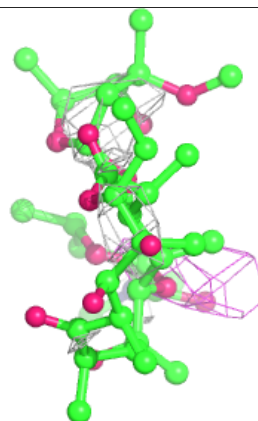
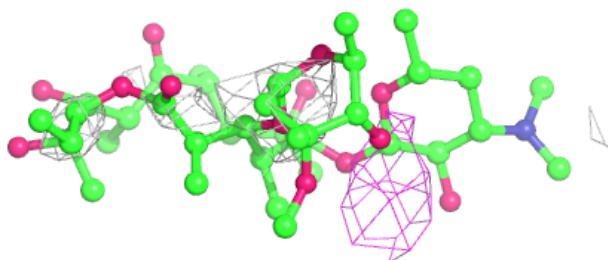
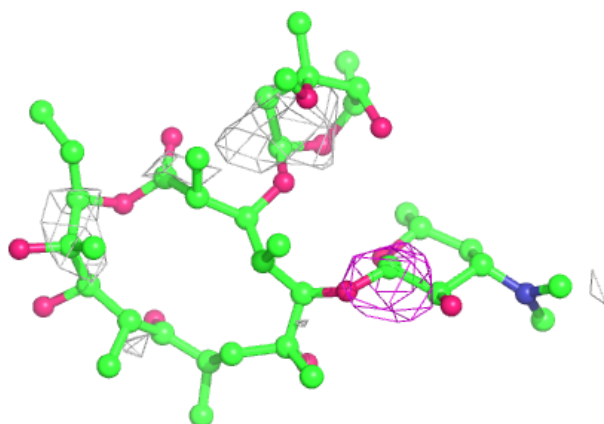
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	ERY	D	1101	51/51	0.68	1.24	62,93,101,108	51
3	LMT	D	1103	35/35	0.73	0.41	77,92,105,106	0
3	LMT	D	1102	35/35	0.76	0.43	38,74,82,84	0
3	LMT	F	2100	35/35	0.77	0.51	49,75,87,96	0
2	ERY	A	1101	51/51	0.77	1.26	81,93,101,104	51
3	LMT	A	1102	35/35	0.79	0.41	49,70,79,82	0
3	LMT	C	1101	35/35	0.79	0.41	62,75,83,87	0
3	LMT	B	2100	35/35	0.79	0.48	34,66,78,87	0
3	LMT	E	1101	35/35	0.80	0.45	63,72,86,108	0
3	LMT	A	1103	35/35	0.85	0.80	65,90,106,109	0
4	NI	C	1102	1/1	0.99	0.21	77,77,77,77	0
4	NI	A	1104	1/1	0.99	0.21	67,67,67,67	0
4	NI	E	1102	1/1	0.99	0.21	73,73,73,73	0

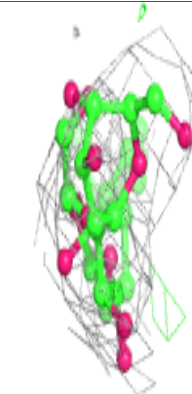
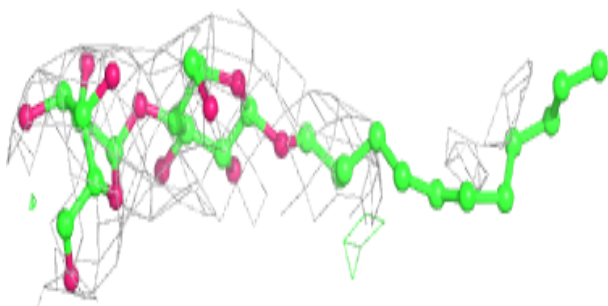
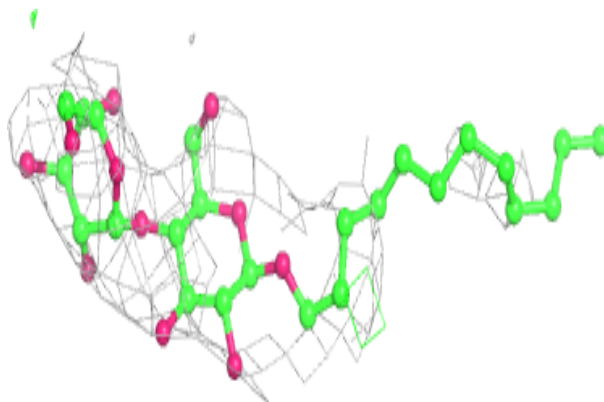
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ERY D 1101:

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

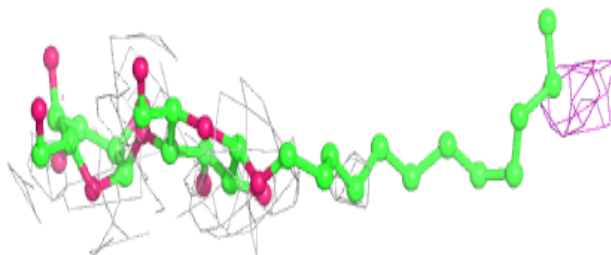
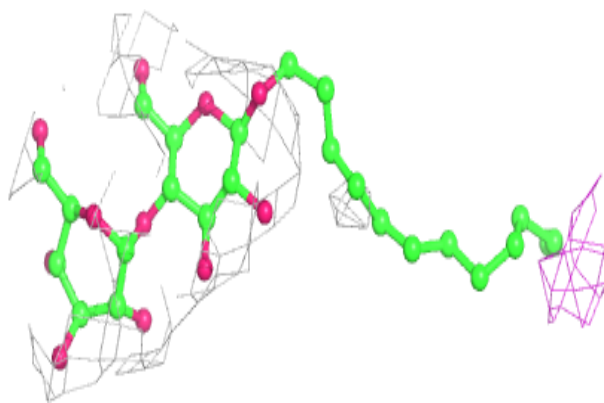
**Electron density around LMT D 1103:**

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

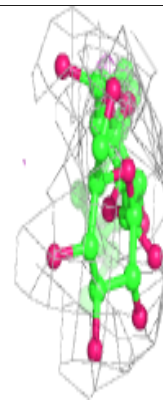
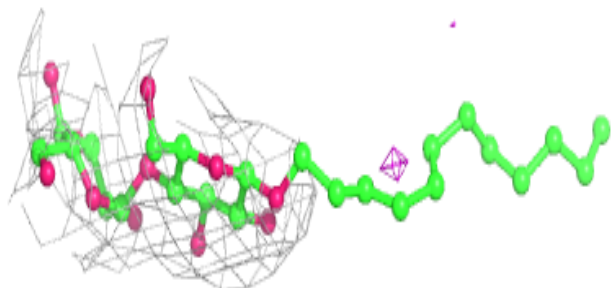
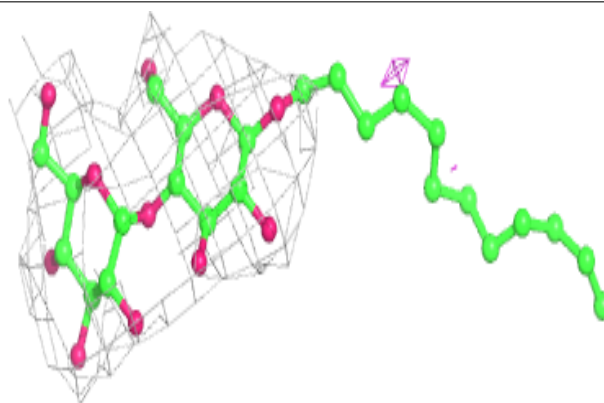


Electron density around LMT D 1102:

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

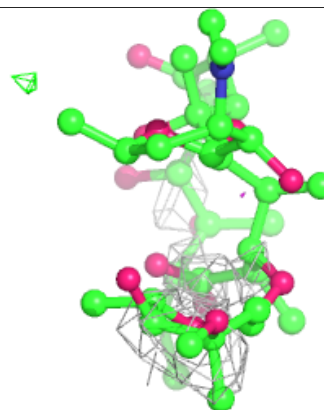
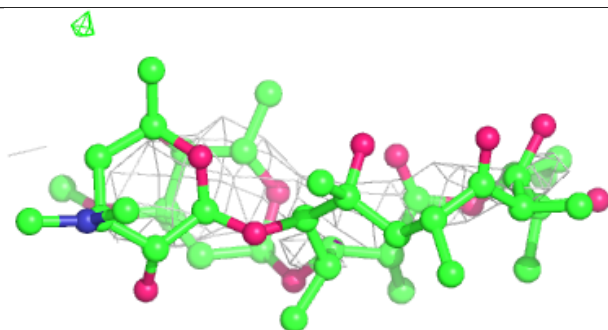
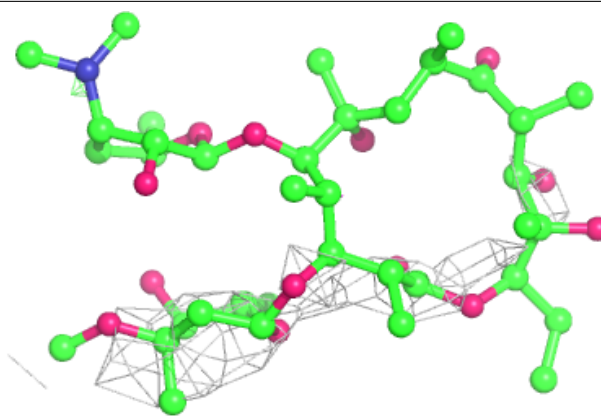
**Electron density around LMT F 2100:**

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

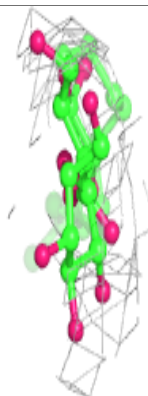
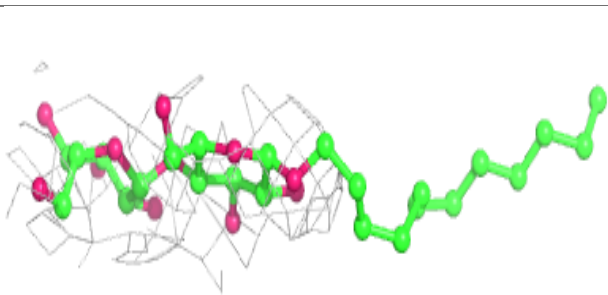
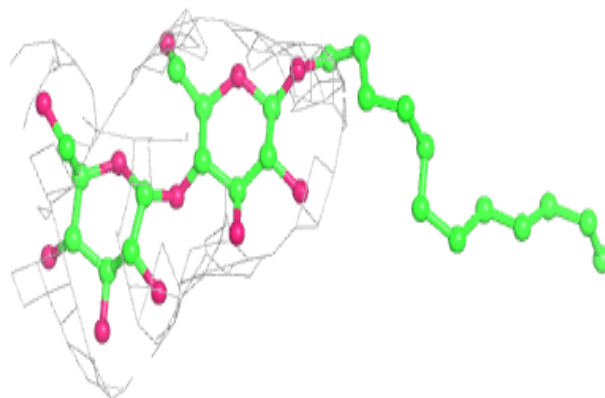


Electron density around ERY A 1101:

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

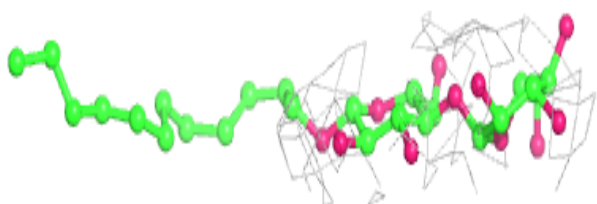
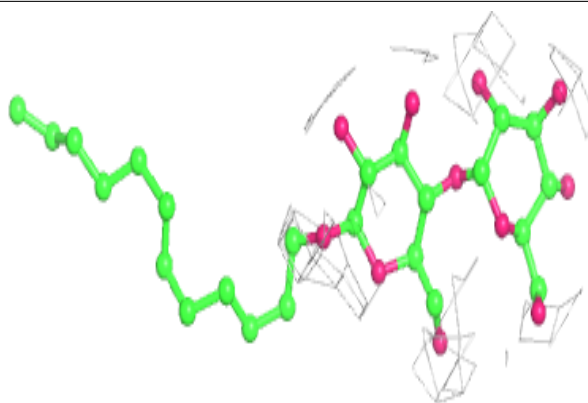
**Electron density around LMT A 1102:**

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

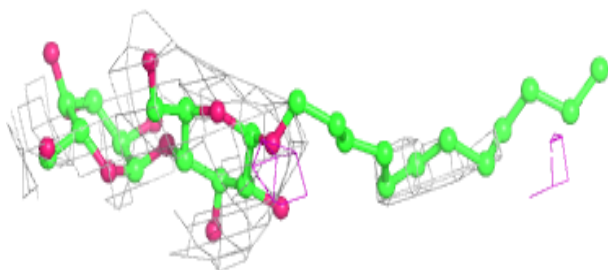
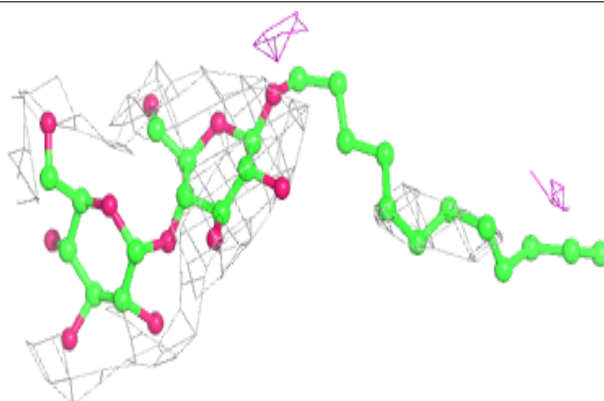


Electron density around LMT C 1101:

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

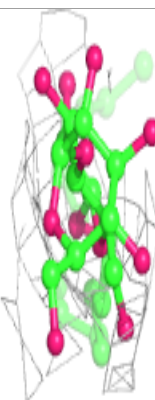
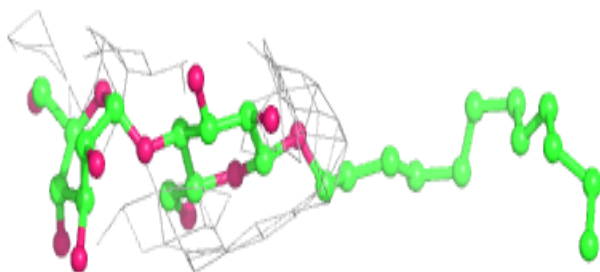
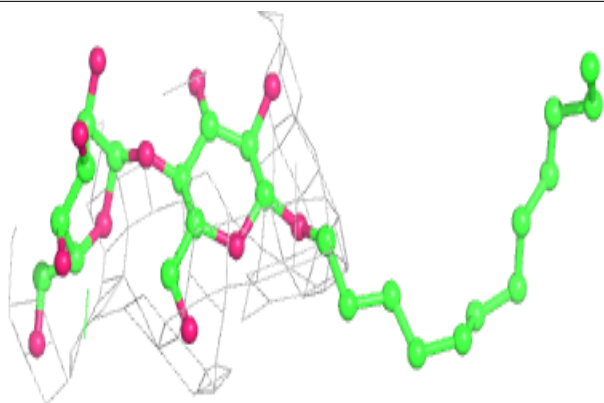
**Electron density around LMT B 2100:**

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

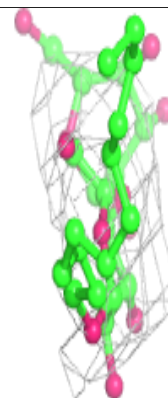
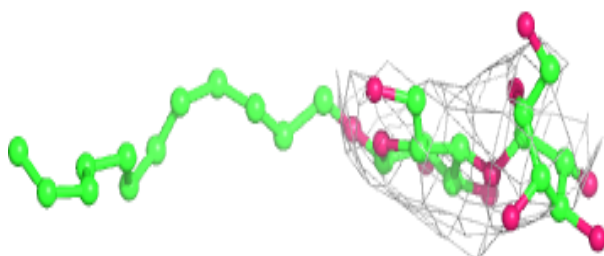
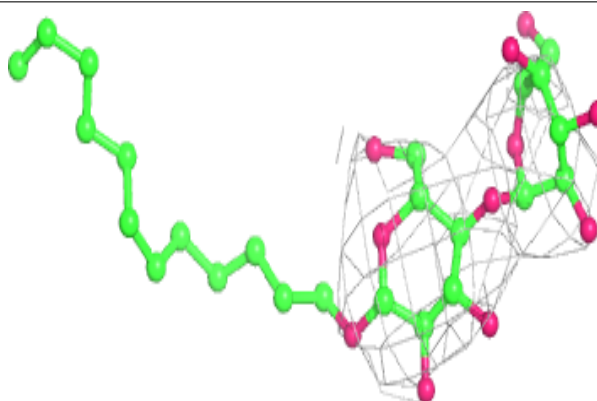


Electron density around LMT E 1101:

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

**Electron density around LMT A 1103:**

$2mF_o-DF_c$ (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.