



wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 11:23 pm BST

PDB ID : 3PIP
Title : Crystal structure of the synergistic antibiotic pair lankamycin and lankacidin in complex with the large ribosomal subunit
Authors : Belousoff, M.J.; Shapira, T.; Bashan, A.; Zimmerman, E.; Kinashi, H.; Rozenberg, H.; Yonath, A.
Deposited on : 2010-11-07
Resolution : 3.45 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

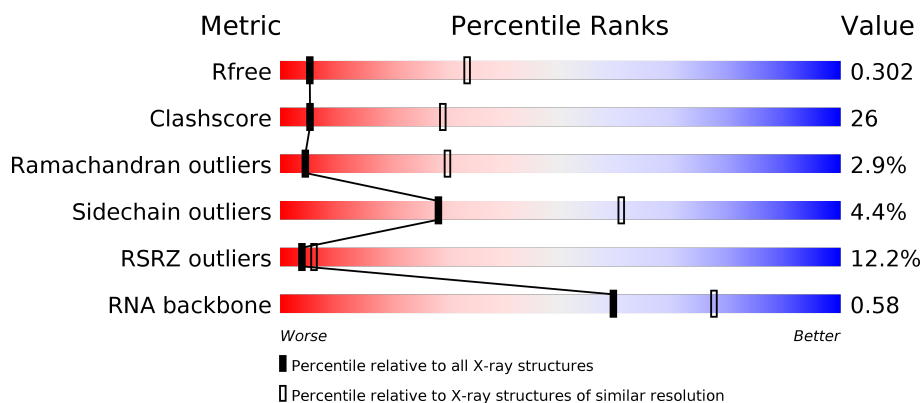
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 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	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)
RNA backbone	3102	1036 (3.96-2.96)

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	X	2880	
2	Y	123	
3	A	274	
4	B	211	

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Mol	Chain	Length	Quality of chain
5	C	205	
6	D	180	
7	E	185	
8	F	144	
9	G	174	
10	H	134	
11	I	156	
12	J	141	
13	K	116	
14	L	114	
15	M	166	
16	N	118	
17	O	100	
18	P	134	
19	Q	95	
20	R	115	
21	S	237	
22	T	91	
23	U	81	
24	V	67	
25	W	55	
26	Z	60	
27	1	55	
28	2	47	
29	3	66	

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Mol	Chain	Length	Quality of chain
30	4	37	<div> <div>89%</div> <div> <div></div> <div>62%</div> <div>35%</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
32	LMA	X	2882	-	-	X	-
33	MG	I	157	-	-	-	X
33	MG	X	2886	-	-	-	X
33	MG	X	2911	-	-	-	X
33	MG	X	2926	-	-	-	X
35	NA	X	2962	-	-	-	X

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 83963 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 RNA chain called RIBOSOMAL 23S RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	2644	Total	C	N	O	P	0	0	0
			56750	25314	10473	18320	2643			

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	120	Total	C	N	O	P	0	0	0
			2561	1143	471	827	120			

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	253	Total	C	N	O	S	0	0	0
			1920	1196	382	340	2			

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	205	Total	C	N	O	S	0	0	0
			1539	965	295	271	8			

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	194	Total	C	N	O	S	0	0	0
			1481	920	284	275	2			

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	177	Total	C	N	O	S	0	0	0
			1394	889	244	254	7			

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	171	Total	C	N	O	S	0	0	0
			1286	812	237	236	1			

- Molecule 8 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	63	Total	C	N	O	S	0	0	0
			451	280	82	86	3			

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	G	142	Total	C	N	O	S	0	0	0
			1114	704	209	198	3			

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	H	134	Total	C	N	O	S	0	0	0
			997	614	198	180	5			

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	I	134	Total	C	N	O	S	0	0	0
			1005	616	203	186				

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	J	136	Total	C	N	O	S	0	0	0
			1090	696	202	185	7			

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	113	Total	C	N	O	S	0	0	0
			878	541	178	157	2			

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	L	104	Total	C	N	O	0	0	0
			779	476	161	142			

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	M	108	Total	C	N	O	0	0	0
			871	543	172	156			

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	N	117	Total	C	N	O	S	0	0	0
			978	608	210	159	1			

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	O	94	Total	C	N	O	0	0	0
			741	465	139	137			

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	P	126	Total	C	N	O	S	0	0	0
			1004	633	197	172	2			

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Q	93	Total	C	N	O	S	0	0	0
			714	452	130	130	2			

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	110	Total	C	N	O	S	0	0	0
			825	513	160	151	1			

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	S	175	Total	C	N	O	S	0	0	0
			1345	849	236	254	6			

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	T	74	Total	C	N	O	S	0	0	0
			556	351	107	97	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	U	72	Total	C	N	O	S	0	0	0
			537	334	110	93				

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	V	65	Total	C	N	O	S	0	0	0
			525	322	106	95	2			

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	W	55	Total	C	N	O	S	0	0	0
			424	264	82	76	2			

- Molecule 26 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	57	Total	C	N	O	S	0	0	0
			452	278	93	76	5			

- Molecule 27 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1	53	Total	C	N	O	S	0	0	0
			431	274	80	76	1			

- Molecule 28 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	2	46	Total	C	N	O	S	0	0	0
			383	230	91	60	2			

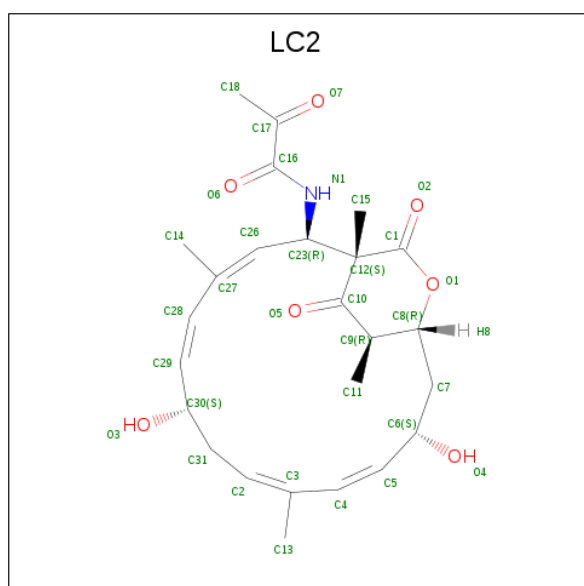
- Molecule 29 is a protein called 50S ribosomal protein L35.

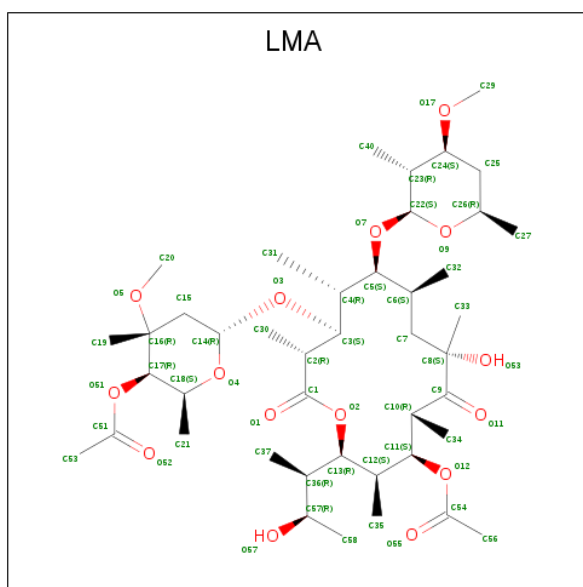
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	59	Total	C	N	O	S	0	0	0
			462	290	95	73	4			

- Molecule 30 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	4	37	Total	C	N	O	S	0	0	0
			297	179	66	47	5			

- Molecule 31 is N-[(1S,2R,3E,5E,7S,9E,11E,13S,15R,19R)-7,13-dihydroxy-1,4,10,19-tetramethyl-17,18-dioxo-16-oxabicyclo[13.2.2]nonadeca-3,5,9,11-tetraen-2-yl]-2-oxopropanamide (three-letter code: LC2) (formula: C₂₅H₃₃NO₇).





Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	X	1	Total	C O	0	0
			58	43 15		

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	X	71	Total	Mg	0	0
			71	71		
33	I	1	Total	Mg	0	0
			1	1		
33	U	1	Total	Mg	0	0
			1	1		

- Molecule 34 is POTASSIUM ION (three-letter code: K) (formula: K).

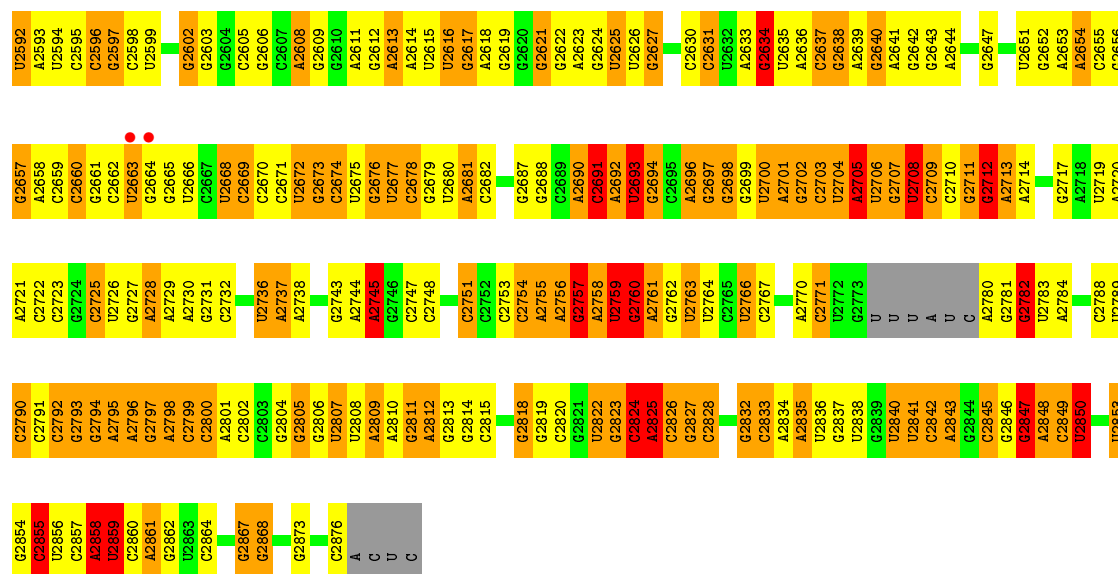
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	X	4	Total	K	0	0
			4	4		

- Molecule 35 is SODIUM ION (three-letter code: NA) (formula: Na).

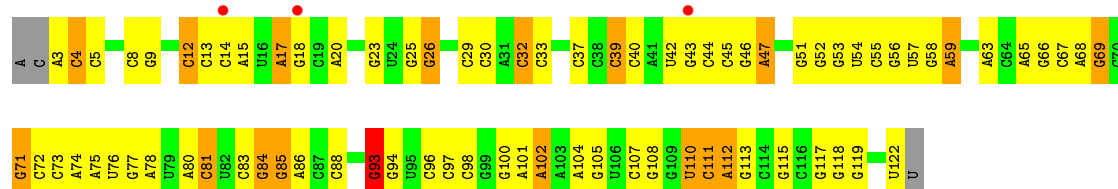
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	X	5	Total	Na	0	0
			5	5		

U1608	A1534	C1456	A1386	G	U1124	A1059	A992	G928	A862	A796	G734	A668
C1609	C1535	A1467	G1387	C	G1125	C1060	C993	G931	C863	A797	G735	G669
A1610	G1536	A1458	C1388	A	A1126	A1061	A994	G932	C864	G798	G736	U670
G1613	U1539	U1459	G	G1127	G1062	A995	A996	C993	C865	C799	C737	A671
C1614	C1540	C1460	A1391	G1128	C1063	C996	C997	G933	C869	U800	G738	C672
C1615	G1541	C1462	U1392	A1129	C1064	C997	C998	G934	C870	A801	G739	G673
C1616	G1542	A1463	G1394	U1130	A1065	C998	A999	C935	C871	A802	A740	U674
G1617	G1543	G1465	U1395	G1131	G1066	A999	A1001	C936	U871	G741	G741	C679
U1618	A1544	C1466	U1396	C1135	G1067	A1001	U1005	A937	C804	C803	G742	C679
A1619	G1545	U1467	G1397	U1136	A1068	A1001	C1006	G937	C804	C804	G742	U680
G1620	G1546	C1468	C1398	A1137	G1069	U1005	U1006	C938	C805	C805	G743	A681
C1621	U1548	U1469	C1399	A1138	U1070	C1007	A1007	C939	C806	C806	G744	A681
G1622	C1549	U1470	U1400	U1141	U1071	A1008	A1008	C940	C807	C807	G745	A682
C1623	C1550	G1471	G1330	G1142	U1072	C1009	C1009	U941	C808	C808	G746	A683
A1624	U1551	C1472	A1203	U1073	G1073	C1009	C1009	U942	C809	C809	G747	C684
A1625	C1552	U1473	G1204	G1143	C1075	C1009	C1009	U943	U810	U810	G748	U685
G1626	G1553	U1474	G1205	U1144	U1076	A1010	A1010	A944	G811	G811	G749	C686
C1627	G1554	A1474	G1206	U1145	U1077	U1011	U1011	A944	G812	G812	G750	G687
G1628	G1559	U1475	G1209	C1145	U1077	A1011	A1011	C947	A883	A883	G751	A688
C1629	C1560	G1476	C1210	G1146	A1078	A1012	A1012	C948	C884	C884	G752	A689
A1630	A1560	C1477	G1211	U1147	U1079	U1015	U1015	G949	A885	A885	U753	A690
C1631	A1561	U1478	U1212	G1148	A	C1016	C1016	C950	A886	A886	G754	C691
G1632	G1562	G1479	U1213	G1149	A1081	C1017	C1017	G951	C887	C887	G755	C692
C1633	U1563	C1480	C1214	C1150	G1082	C1018	C1018	A952	C888	C888	G756	A693
A1634	U1564	U1481	A1215	U1151	G1083	C1019	C1019	G953	C889	C889	G757	G694
G1635	G1565	U1482	G1216	C1152	G1085	A1020	A1020	U954	U890	U890	G758	G695
C1636	C1566	G1483	U1217	A1153	C1086	A1021	A1021	G955	A	A	G759	U696
U1637	G1567	U1484	C1218	A1154	C1087	A1022	A1022	A956	G	G	U760	G697
G1638	A1568	U1485	C1219	G1155	U1088	U1023	U1023	G957	C	C	G761	A698
C1639	U1569	U1490	C1220	G1156	C1089	G1089	G1089	G958	G	G	G762	G699
G1640	G1570	A1493	C1221	U1158	C1090	G1028	G1028	C959	C	C	G763	C700
C1641	U1571	U1494	G1222	A1159	C1091	C1029	C1029	U960	C	C	G764	U701
G1642	C1572	G1495	G1223	C1160	U1092	C1030	C1030	G961	C828	C828	G765	A702
A1643	G1573	G1496	A1224	U1093	U1093	C1031	C1031	C962	C829	C829	G766	A703
U1644	A1574	C1497	G1225	C1163	C1094	A964	A964	G963	C830	C830	G767	C704
G1645	C1575	C1498	A1226	G1164	A1095	C1032	C1032	G965	C831	C831	G768	C705
U1647	G1576	A1499	A1227	C1165	U1096	U1034	U1034	G966	A832	A832	G769	A706
C1648	U1577	U1500	G1228	A1166	A1097	G1035	G1035	G967	C833	C833	U770	U707
A1649	G1578	C1501	C1229	A1167	G1098	G1036	G1036	C968	C834	C834	G771	G708
G1650	C1579	U1502	C1230	U1168	A1099	U1037	U1037	U969	U835	U835	G772	A709
U1651	U1580	U1503	A1231	C1169	U1100	U1038	U1038	A970	C836	C836	G773	
C1652	C1581	U1504	U1232	U1170	U1101	G1041	G1041	G971	U837	U837	G774	A712
G1653	A1582	U1505	A1233	A1171	C1102	G1042	G1042	C972	A838	A838	G775	G713
A1654	U1583	C1506	C1234	U1172	G1103	A1043	A1043	G973	C	C	G776	G714
C1655	G1584	A1507	G1235	G1173	G1104	U1044	U1044	U974	U840	U840	G777	U715
U1656	A1585	G1439	C1236	U1174	A1107	G1045	G1045	C975	A842	A842	G778	U716
A1657	A1586	U1509	G1237	U1175	U1108	U1046	U1046	G976	G843	G843	G779	U717
G1658	U1587	U1510	A1238	U1176	U1109	U1047	U1047	G977	G844	G844	G780	A718
C1659	U1588	U1511	G1240	U1177	G1111	U1048	U1048	U978	U845	U845	G781	A719
G1660	C1589	U1521	G1241	C1178	A1114	C1049	C1049	U979	U846	U846	G782	A720
C1661	U1590	C	G1242	A1179	A1115	G1050	G1050	G980	G849	G849	U786	C724
G1662	A1591	A	G1243	C1180	C1115	U1051	U1051	C981	C850	C850	A787	C725
U1601	G1601	C	U1447	U1182	U1182	C1052	C1052	G982	C851	C851	U	U
G1602	A1602	A	G1246	C1183	U1119	G1053	G1053	G983	U852	U852	G789	G
A1603	C1449	U1526	G1382	G	U1119	C1054	C1054	A984	A923	A923	A790	A
U1604	G1450	G1527	C1383	C	C1120	A	A	G985	U857	U857	G791	C
A1605	C1451	U1528	A1384	G	A1121	U	U	C986	G858	G858	U792	A
C1606	U1452	G1533	C1385	A	A1122	A	A	G987	U859	U859	G793	C
A1669					G1123	G1058	G1058	A991	U860	U860	A794	A
									G861	G861	A795	

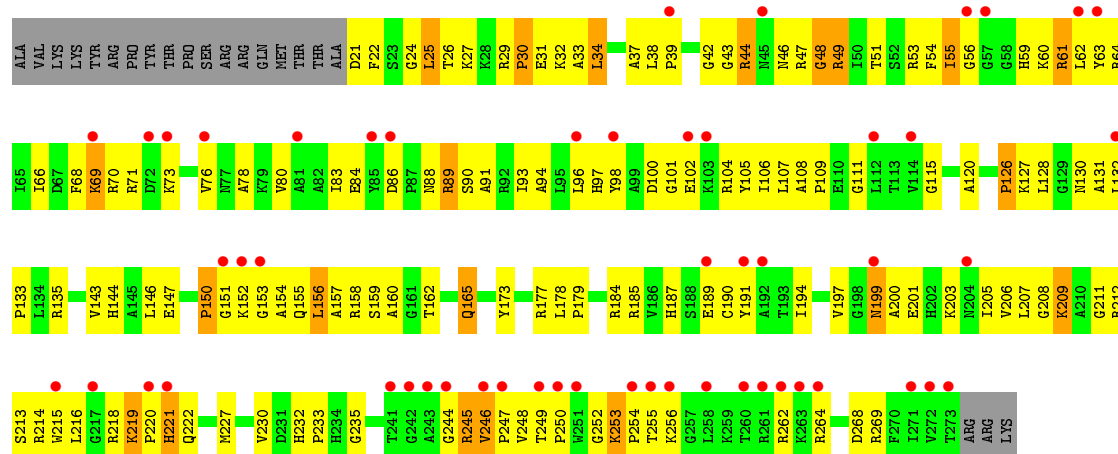
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U2533	C2338	G2473	A2409	G2261	C2194	U	A2063	U1999	U1939	G1874	G1798	G1735	A1672
U2534	G2474	U2410	A2339	C2262	C2195	U	G2064	U2000	C1940	G1879	A1800	C1736	C1673
C2535	G2475	A2411	G2340	C2263	U2196	G	A2065	G2001	C1941	G1882	C1801	C1737	C1674
G2536	G2476	A2412	G2341	C2264	U2197	G	G2066	G2002	C1942	G1883	A1802	U1738	C1675
C2537	G2477	U2413	U2342	A2265	U2198	G	G2067	A2003	C1943	G1884	G1803	G1739	U1676
C2538	G2478	A2414	C2343	A2266	C2199	G	U2068	U2004	C1944	G1885	A1804	C1740	C1677
C2539	G2479	G2415	G2344	G2267	G2200	U	G2069	U2005	C1945	G1886	G1805	G1741	G1678
A2540	C2480	G2481	A2345	U2270	G2201	C	G2070	G2006	U1946	C1887	G1806	C1742	U1679
A2543	A2482	C2483	C2346	U2271	G2202	G	G2071	G2007	C1947	C1888	A1807	C1743	U1680
A2544	U2483	G2484	G2347	C2271	G2203	G	C2072	C2008	C1948	G	C1808	G1744	A1681
A2545	G2485	C2485	A2348	C2272	A2204	U	A2073	U2009	C1949	G	C1809	G1745	A1682
G2546	C2486	G2486	G2349	C2273	C2205	G	U2074	G2010	C1950	U	G	A1746	G1683
C2547	C2487	G2487	G2350	C2274	C2206	G	U2075	A2011	C1951	C	U	G1747	G1684
G2548	C2488	U2275	G2351	U2276	G2207	A	C2082	A2012	A1952	C	U	C1748	A1685
G2549	C2489	A2277	G2352	C2276	U2208	G	G2083	A2013	A1953	C	A1812	G1749	A1686
C2550	C2489	A2278	G2353	A2277	G2209	G	G2084	A2014	A1954	C	A1813	C1750	C1687
C2551	U2490	A2278	G2354	A2278	C2210	C	G2085	G2015	G1955	U	A1814	A1751	U1688
C2552	C2491	G2282	A2355	G2282	U2211	A	U2086	A2016	G1956	A	G1815	U1752	U1689
G2553	G2492	G2283	A2356	G2283	G2216	A	U	U2017	C1957	C	G1816	C1753	U1690
C2554	U2493	U2284	A2357	U2284	G2217	C	U	G2018	U1958	U	G1817	G1754	C1692
G2555	C2494	U2285	G2362	U2285	U2218	G	C	C2019	C1959	A	U	G1755	C1693
C2556	A2495	G2286	G2363	G2286	U2219	U	U	G2020	A1960	A	U1819	C1756	A1693
G2557	C2496	G2287	C2364	G2287	A2220	G	C	G2021	A1961	U	G1820	C1757	A1694
C2558	A2497	A2288	U2365	A2288	G2221	C	U	C2022	C1962	A	A1821	C1758	U1695
U2559	U2498	A2289	G2366	U2289	G2222	A	U	C2023	G1963	C	G1822	C1759	C1696
C2560	C2499	A2290	U2367	G2290	U2223	A	G	U2024	A1964	C	G1823	U1760	U1697
G2561	G2500	U2291	G2371	U2291	U2224	C	C	A2025	U1965	G	C1824	C1761	C1698
C2562	U2501	G2292	A2372	G2292	U2225	U	U	G2026	C1966	G	C1825	C1762	A1699
U2563	G2502	G2293	C2373	G2293	G2226	C	A	U2030	U1967	U	C	G1763	C1700
U2564	U2503	U2294	C2374	U2294	A2227	C	G	A2031	G1968	C	C1828	A1764	C1701
C2565	G2504	C2295	G2375	C2295	G2228	C	G	C2032	C1969	U	C1829	C1765	C1702
G2566	U2505	C2296	U2376	C2296	U2229	A	A	C2033	G1970	G	G1830	U1766	C1703
C2567	C2506	U2298	U2377	U2298	G2230	C	U	A2034	C1971	A	G1831	G1767	G1704
C2568	U2507	A2299	G2378	A2299	U2231	C	A	G2035	G1972	A1911	C	U1768	U1705
A2569	G2508	G2300	G2379	G2300	G2232	U	G	G2036	C1973	U1912	C	U1769	A1706
C2570	U2510	A2301	U2380	A2301	G2233	G	G	A2037	U1974	G1913	C	U1770	A1707
G2571	G2511	C2302	C2381	C2302	G2234	A	U	C2038	G1975	U1914	G	U1771	C1708
C2572	U2512	C2303	C2382	C2303	C2237	G	C	U1915	U1976	A1915	C	C1772	U1709
G2573	A2513	U2311	G2383	U2311	C2238	A	U	G2039	C1977	G1916	C	C1773	C1710
C2574	G2514	A2312	U2386	A2312	C2239	A	G	A2040	U1978	C1917	A	A1774	A1839
U2575	U2515	C2313	C2386	C2313	U2240	C	C	A2041	C1979	G1918	C	A1775	G1712
C2576	G2516	A2314	G2392	A2314	C2241	A	G	A2042	A1980	U1919	G	A1776	G1713
G2577	U2517	A2315	G2393	A2315	C2242	C	C	A2043	C1981	A1920	C	A1777	A1714
C2578	C2518	G2316	G2394	G2316	C2243	C	U	G2044	C1982	U1921	C	U1778	A1715
U2579	U2519	U2323	U2395	U2323	C2244	C	C	A2045	G1983	U1922	C	C1779	G1716
C2580	A2520	G2324	C2396	G2324	A2245	C	G	C2047	C1984	C1924	C	G1847	A1717
A2581	U2521	A2325	A2397	A2325	A2246	C	C	C2048	G1985	G	A1851	C1781	A1718
G2582	G2522	C2326	U2398	C2326	A2247	A	G	C2049	G1986	U1927	G	G1782	G1719
U2583	C2523	U2327	C2399	U2327	U2251	A	A	G2050	C1987	G1928	C	G1783	G1720
C2584	G2524	G2400	G2401	U2328	A2252	C	A	U2051	A1988	C	U1852	G1784	G1721
G2585	U2525	C2328	A2402	G2328	A2253	C	C	G2052	C1989	U1929	C	U1787	G1722
C2586	U2526	U2329	U2402	G2329	G2256	U	G	C2053	U1990	C1930	C	U1788	U1723
G2587	G2527	A2331	C2403	G2330	A2257	C	C	G2054	C1991	G1931	C	G1864	C1724
U2588	U2528	G2335	A2404	G2335	G2258	G	G	G2055	C1992	U1932	C	G1865	C1725
C2589	G2529	A2331	A2405	A2331	G2259	C	C	C2056	G1993	G1933	C	C1791	C1726
U2590	C2530	G2335	C2406	U2335	G2259	C	C	U2057	U1994	U1934	C	A1792	G
C2591								U2058	A1996	A1936	C	A1793	G



- Molecule 2: 5S ribosomal RNA

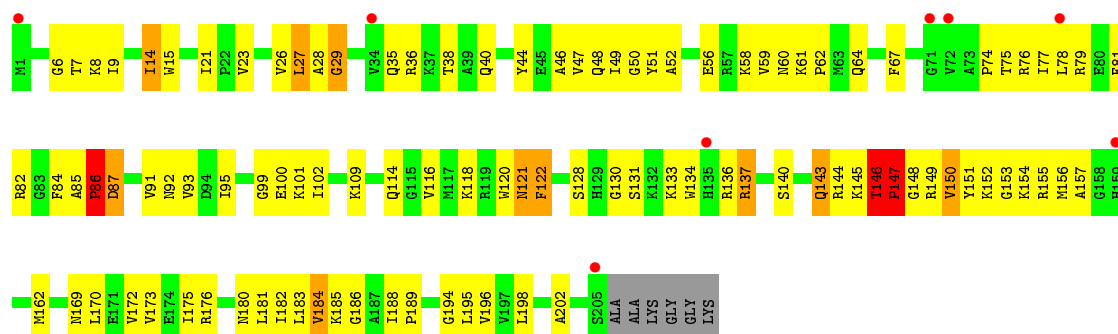


- Molecule 3: 50S ribosomal protein L2

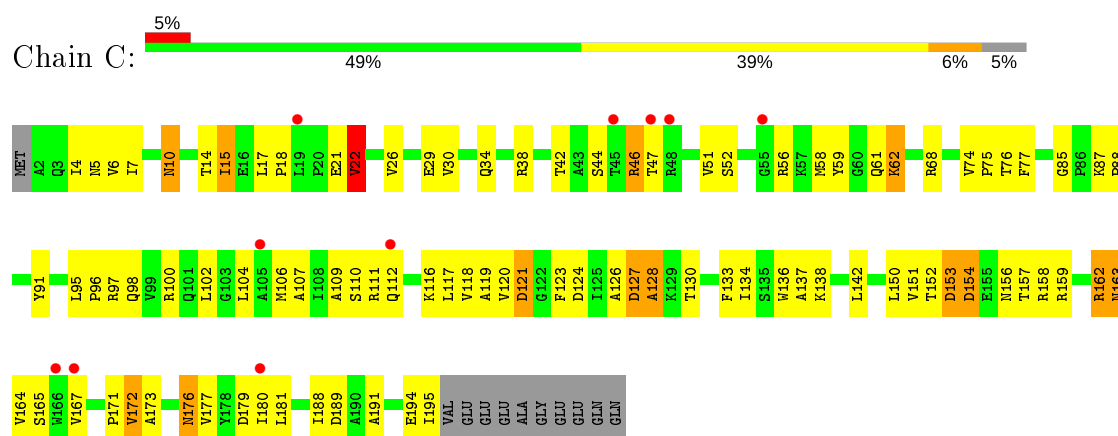


- Molecule 4: 50S ribosomal protein L3

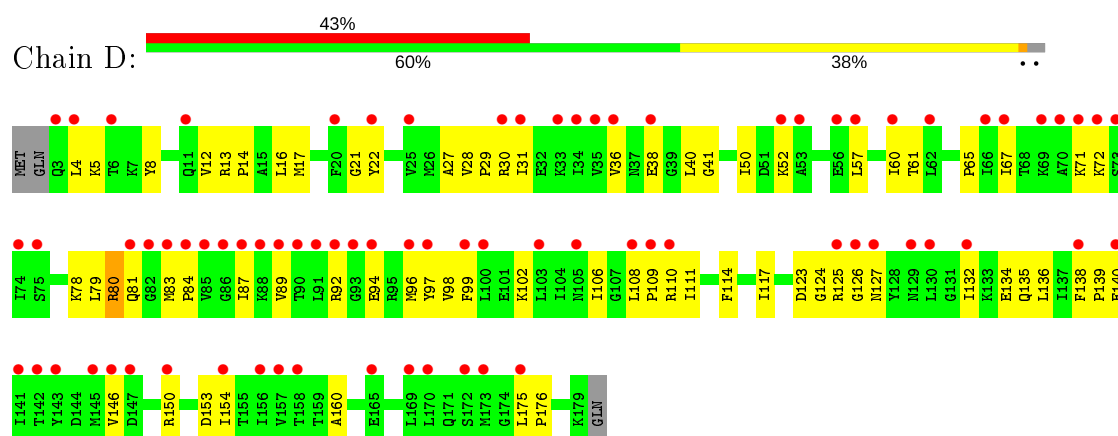




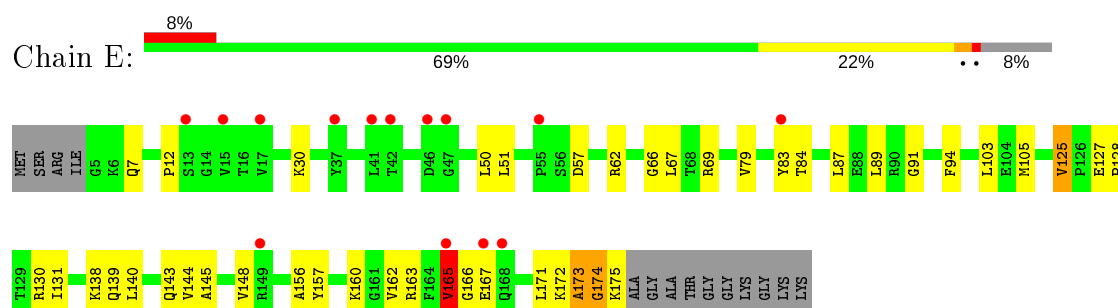
• Molecule 5: 50S ribosomal protein L4



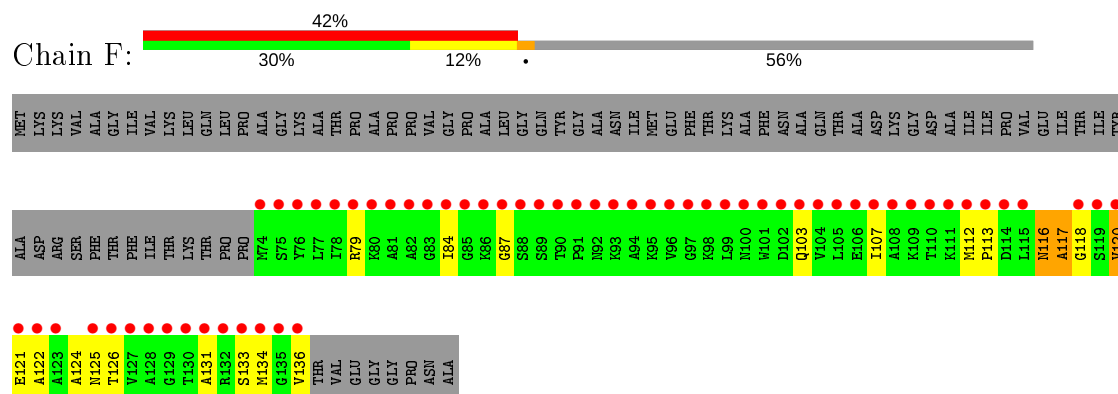
• Molecule 6: 50S ribosomal protein L5



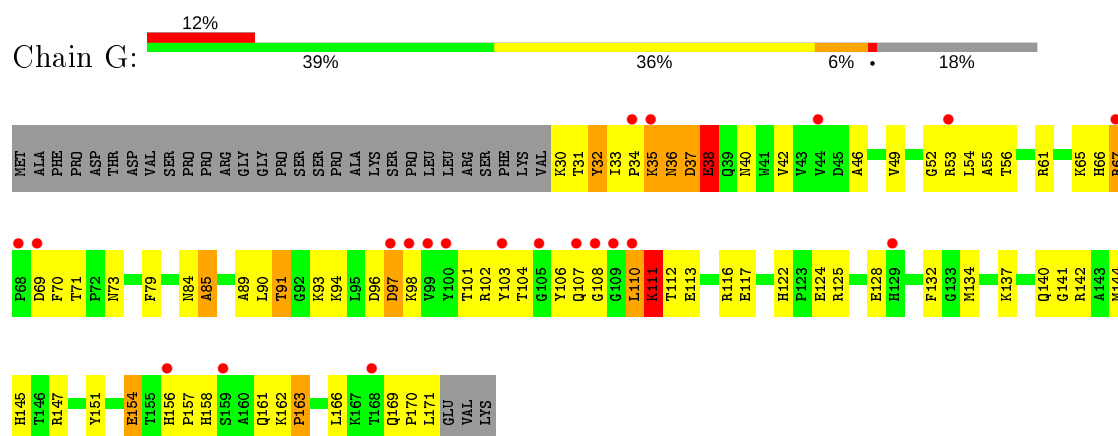
• Molecule 7: 50S ribosomal protein L6



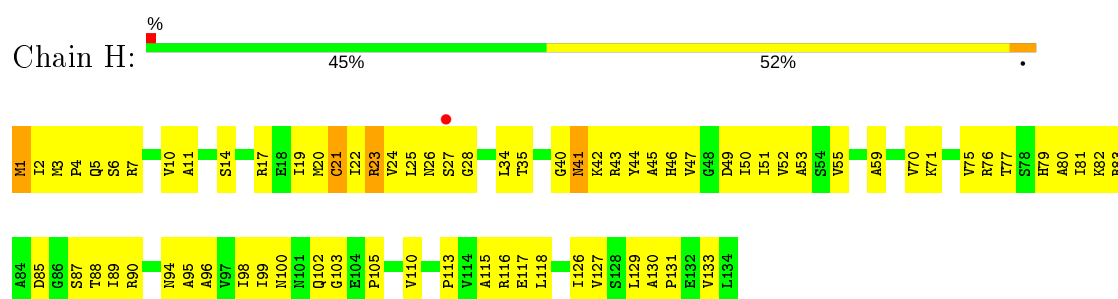
- Molecule 8: 50S ribosomal protein L11



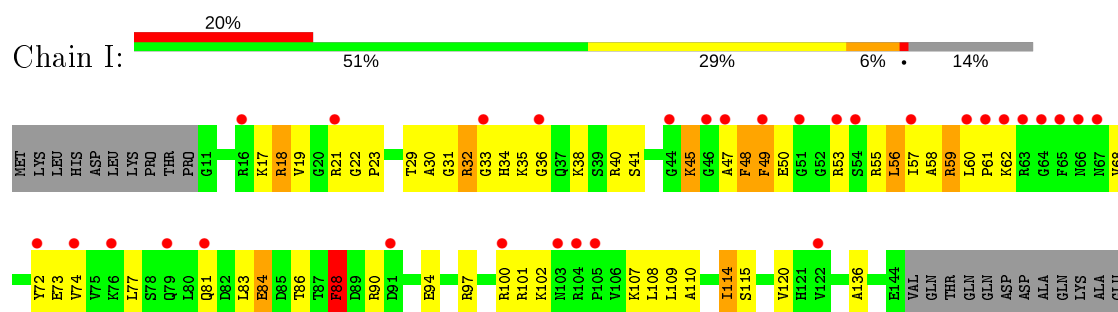
- Molecule 9: 50S ribosomal protein L13



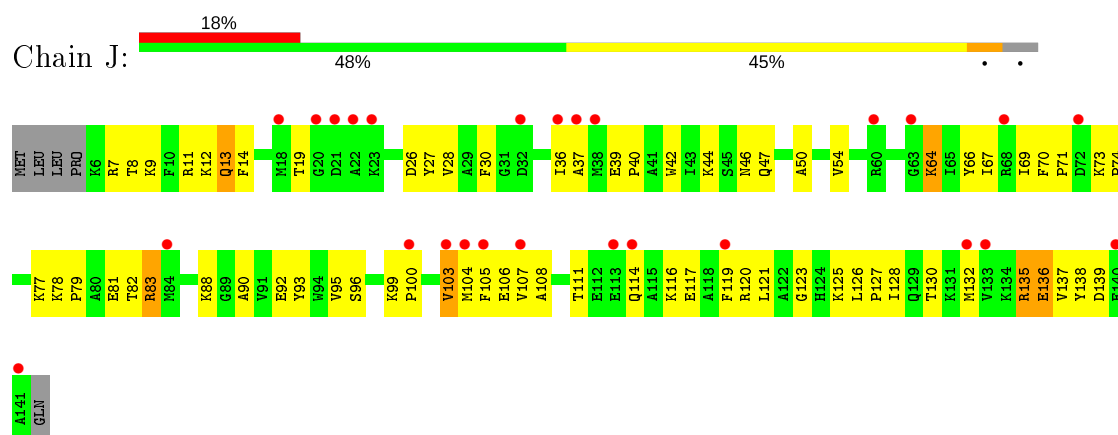
- Molecule 10: 50S ribosomal protein L14



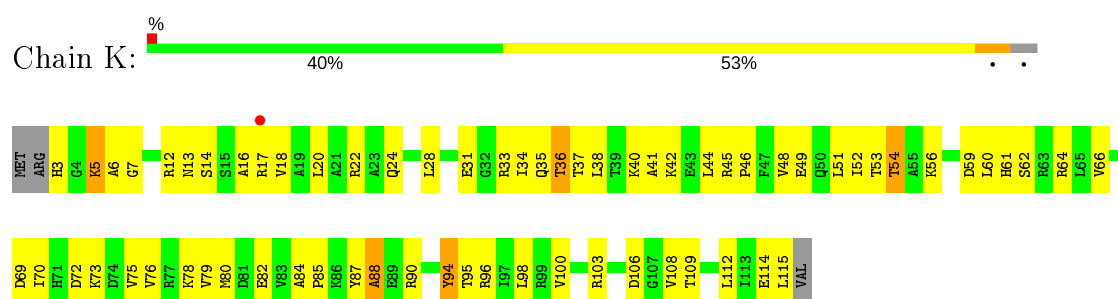
- Molecule 11: 50S ribosomal protein L15



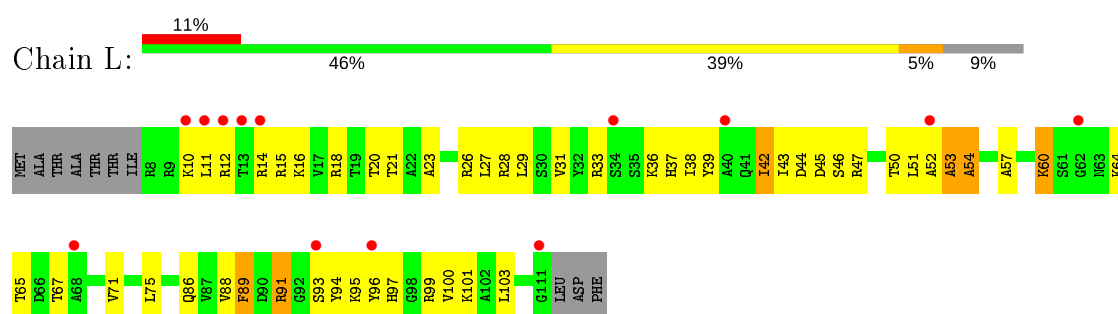
- Molecule 12: 50S ribosomal protein L16



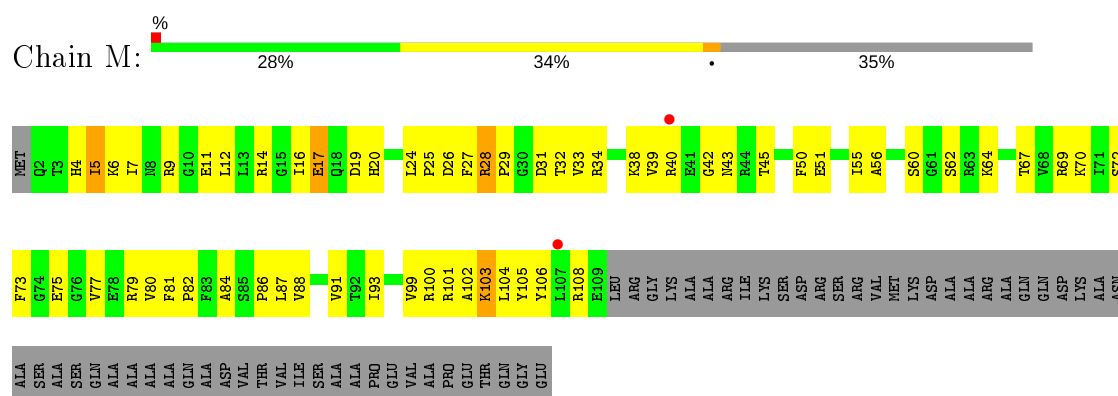
- Molecule 13: 50S ribosomal protein L17



- Molecule 14: 50S ribosomal protein L18



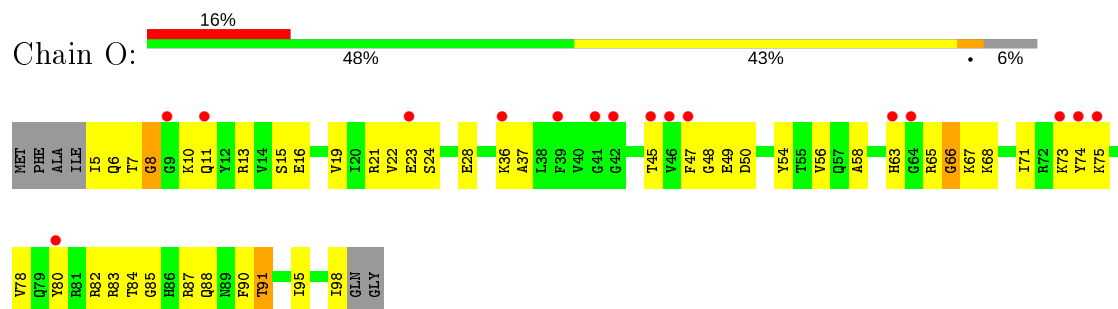
- Molecule 15: 50S ribosomal protein L19



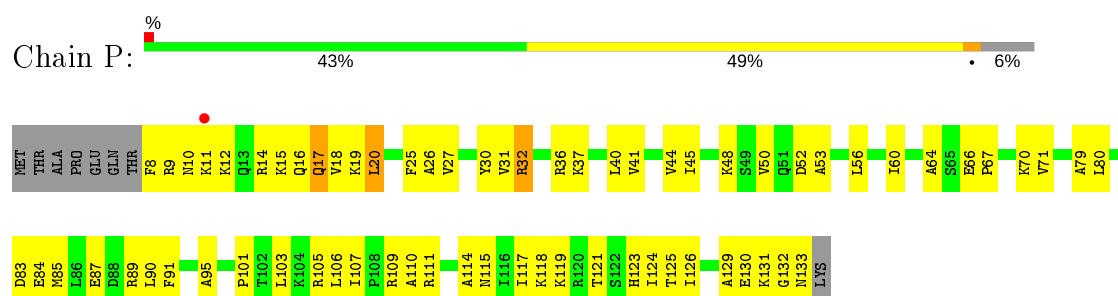
- Molecule 16: 50S ribosomal protein L20



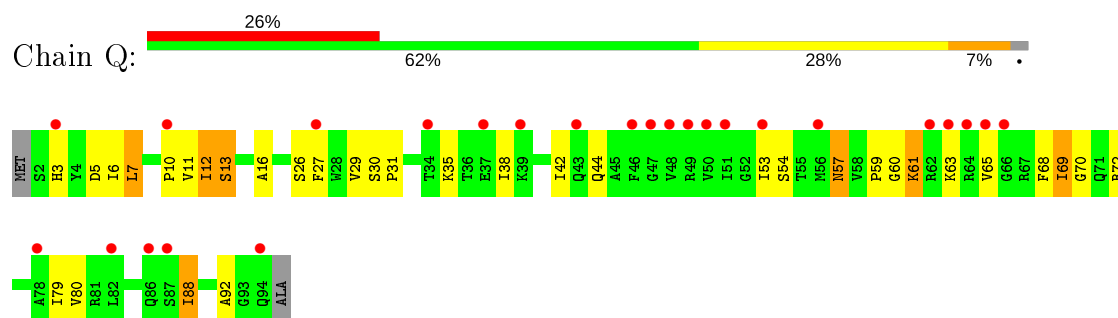
- Molecule 17: 50S ribosomal protein L21



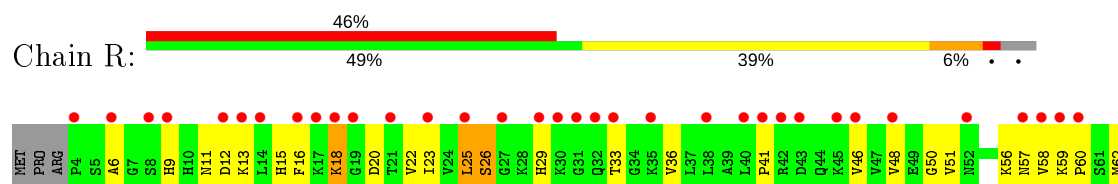
- Molecule 18: 50S ribosomal protein L22

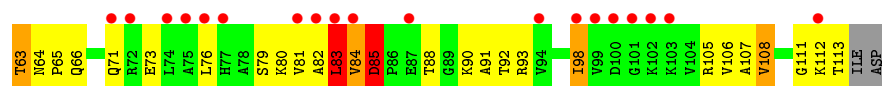


- Molecule 19: 50S ribosomal protein L23

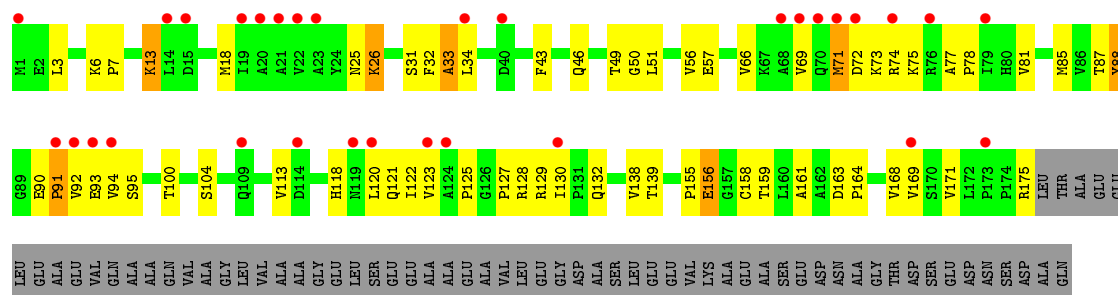


- Molecule 20: 50S ribosomal protein L24

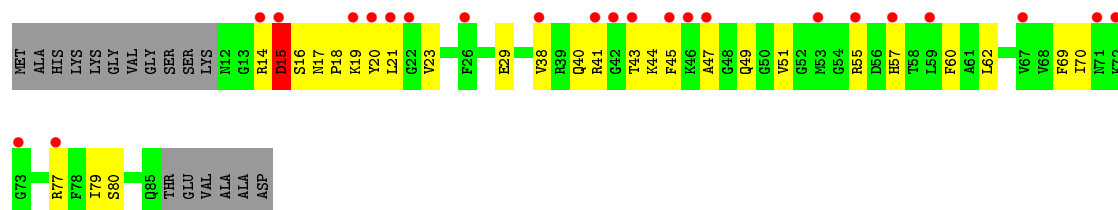




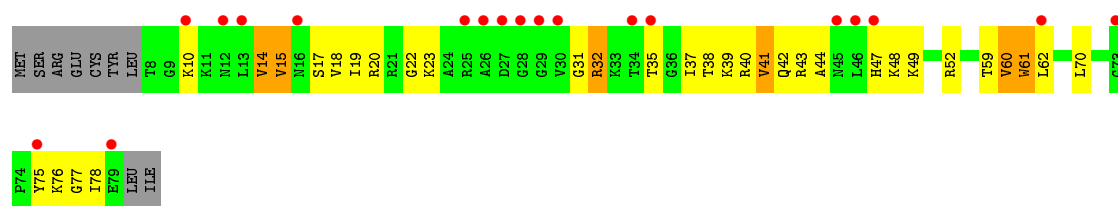
• Molecule 21: 50S ribosomal protein L25



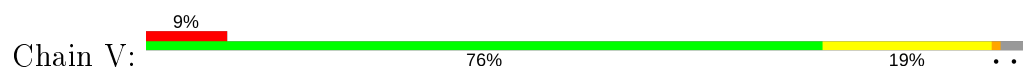
• Molecule 22: 50S ribosomal protein L27



• Molecule 23: 50S ribosomal protein L28



• Molecule 24: 50S ribosomal protein L29



• Molecule 25: 50S ribosomal protein L30





- Molecule 26: 50S ribosomal protein L32



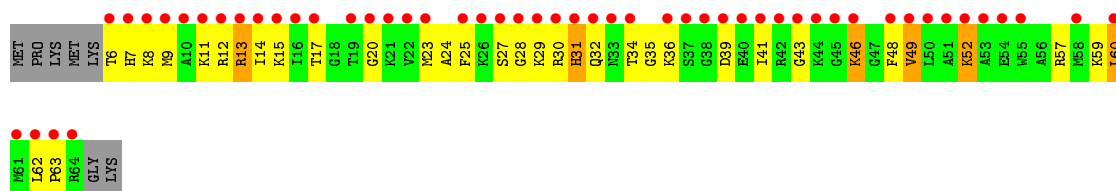
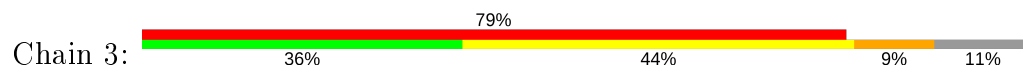
- Molecule 27: 50S ribosomal protein L33



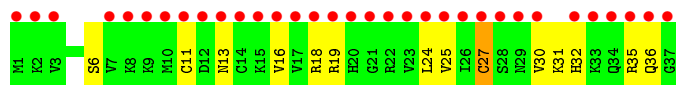
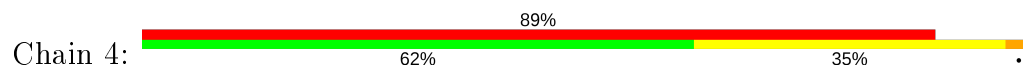
- Molecule 28: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L36



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	169.72Å 408.56Å 693.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.45 93.01 – 3.44	Depositor EDS
% Data completeness (in resolution range)	83.3 (20.00-3.45) 82.4 (93.01-3.44)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 3.41Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.257 , 0.301 0.262 , 0.302	Depositor DCC
R_{free} test set	2649 reflections (1.01%)	wwPDB-VP
Wilson B-factor (Å ²)	86.0	Xtriage
Anisotropy	0.732	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 76.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	83963	wwPDB-VP
Average B, all atoms (Å ²)	138.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% of the height of the origin peak. No significant pseudotranslation is detected.*

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: NA, K, LC2, MG, LMA

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	X	1.17	260/63542 (0.4%)	1.58	1813/99100 (1.8%)
2	Y	0.80	1/2863 (0.0%)	1.13	21/4461 (0.5%)
3	A	0.65	0/1958	0.83	2/2638 (0.1%)
4	B	0.85	0/1567	0.93	2/2105 (0.1%)
5	C	0.84	0/1504	0.84	1/2036 (0.0%)
6	D	0.46	0/1413	0.56	0/1896
7	E	0.57	0/1308	0.60	0/1771
8	F	0.37	0/455	0.45	0/611
9	G	0.75	0/1138	0.82	0/1539
10	H	0.94	0/1007	0.99	0/1352
11	I	0.62	0/1016	0.71	0/1359
12	J	0.80	0/1113	0.80	0/1486
13	K	0.93	1/886 (0.1%)	1.01	0/1188
14	L	0.72	0/785	0.93	1/1048 (0.1%)
15	M	0.99	0/884	1.07	1/1186 (0.1%)
16	N	0.93	0/994	0.85	0/1323
17	O	0.77	0/750	0.81	0/1000
18	P	1.01	2/1017 (0.2%)	0.97	1/1362 (0.1%)
19	Q	0.66	0/725	0.69	0/974
20	R	0.66	0/835	0.72	1/1121 (0.1%)
21	S	0.51	0/1370	0.60	1/1862 (0.1%)
22	T	0.74	0/563	0.77	0/747
23	U	0.57	0/541	0.70	1/723 (0.1%)
24	V	0.67	0/529	0.63	0/704
25	W	0.60	0/426	0.71	0/568
26	Z	0.89	0/464	0.94	1/622 (0.2%)
27	1	0.32	0/438	0.60	0/583
28	2	0.57	0/387	0.54	0/509
29	3	0.22	0/468	0.38	0/614
30	4	0.69	1/298 (0.3%)	0.58	0/390
All	All	1.06	265/91244 (0.3%)	1.42	1846/136878 (1.3%)

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
7	E	0	4
8	F	0	3
9	G	0	8
10	H	0	2
11	I	0	1
12	J	0	1
All	All	0	19

The worst 5 of 265 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	616	U	C3'-C2'	-13.53	1.37	1.52
1	X	1775	A	O3'-P	-11.52	1.47	1.61
1	X	1299	A	N9-C4	-11.34	1.31	1.37
1	X	1260	A	N9-C4	-11.21	1.31	1.37
1	X	2669	C	N1-C6	-10.57	1.30	1.37

The worst 5 of 1846 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	29	ARG	C-N-CD	-19.10	78.58	120.60
1	X	1678	G	N1-C6-O6	-18.90	108.56	119.90
1	X	2486	C	C5-C6-N1	17.23	129.62	121.00
1	X	2815	C	C6-N1-C2	17.04	127.12	120.30
14	L	54	ALA	CB-CA-C	16.51	134.87	110.10

There are no chirality outliers.

5 of 19 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	E	125	VAL	Peptide
7	E	130	ARG	Sidechain
7	E	165	VAL	Peptide
7	E	174	GLY	Peptide
8	F	116	ASN	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	X	56750	0	28598	2022	3
2	Y	2561	0	1306	67	0
3	A	1920	0	1974	255	0
4	B	1539	0	1600	168	0
5	C	1481	0	1504	122	0
6	D	1394	0	1470	73	0
7	E	1286	0	1336	30	0
8	F	451	0	474	21	0
9	G	1114	0	1144	113	0
10	H	997	0	1046	97	0
11	I	1005	0	1036	117	0
12	J	1090	0	1125	97	0
13	K	878	0	930	93	0
14	L	779	0	820	77	0
15	M	871	0	894	85	3
16	N	978	0	1020	107	0
17	O	741	0	756	66	0
18	P	1004	0	1083	70	0
19	Q	714	0	731	35	0
20	R	825	0	881	78	0
21	S	1345	0	1372	56	0
22	T	556	0	579	30	0
23	U	537	0	580	40	0
24	V	525	0	546	20	0
25	W	424	0	470	24	0
26	Z	452	0	457	39	0
27	1	431	0	456	91	0
28	2	383	0	414	51	0
29	3	462	0	506	78	0
30	4	297	0	330	18	0
31	X	33	0	33	18	0
32	X	58	0	69	43	0
33	I	1	0	0	0	0
33	U	1	0	0	0	0
33	X	71	0	0	0	0
34	X	4	0	0	0	0
35	X	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	83963	0	55540	3669	3

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 26.

The worst 5 of 3669 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:X:699:G:N2	28:2:5:TYR:CE1	1.89	1.36
27:1:28:ARG:HB2	27:1:30:ASN:OD1	1.24	1.34
1:X:699:G:N2	28:2:5:TYR:HE1	1.25	1.28
1:X:775:U:H5'	1:X:776:G:N2	1.49	1.26
1:X:699:G:N7	28:2:11:LYS:HG3	1.51	1.26

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1552:C:O2	15:M:43:ASN:ND2[8_455]	0.99	1.21
1:X:1552:C:O2	15:M:43:ASN:CG[8_455]	1.93	0.27
1:X:1552:C:C2	15:M:43:ASN:ND2[8_455]	2.03	0.17

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	
3	A	251/274 (92%)	207 (82%)	36 (14%)	8 (3%)	4	28
4	B	203/211 (96%)	174 (86%)	22 (11%)	7 (3%)	3	27
5	C	192/205 (94%)	153 (80%)	30 (16%)	9 (5%)	2	19
6	D	175/180 (97%)	146 (83%)	27 (15%)	2 (1%)	14	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	E	169/185 (91%)	147 (87%)	18 (11%)	4 (2%)	6	34
8	F	61/144 (42%)	51 (84%)	9 (15%)	1 (2%)	9	42
9	G	140/174 (80%)	118 (84%)	18 (13%)	4 (3%)	4	30
10	H	132/134 (98%)	115 (87%)	17 (13%)	0	100	100
11	I	132/156 (85%)	96 (73%)	29 (22%)	7 (5%)	2	16
12	J	134/141 (95%)	107 (80%)	25 (19%)	2 (2%)	10	43
13	K	111/116 (96%)	101 (91%)	9 (8%)	1 (1%)	17	54
14	L	102/114 (90%)	81 (79%)	20 (20%)	1 (1%)	15	52
15	M	106/166 (64%)	94 (89%)	9 (8%)	3 (3%)	5	31
16	N	115/118 (98%)	106 (92%)	7 (6%)	2 (2%)	9	40
17	O	92/100 (92%)	77 (84%)	12 (13%)	3 (3%)	4	27
18	P	124/134 (92%)	109 (88%)	13 (10%)	2 (2%)	9	42
19	Q	91/95 (96%)	66 (72%)	20 (22%)	5 (6%)	2	16
20	R	108/115 (94%)	82 (76%)	20 (18%)	6 (6%)	2	15
21	S	173/237 (73%)	140 (81%)	28 (16%)	5 (3%)	4	30
22	T	72/91 (79%)	57 (79%)	12 (17%)	3 (4%)	3	22
23	U	70/81 (86%)	44 (63%)	21 (30%)	5 (7%)	1	11
24	V	63/67 (94%)	58 (92%)	4 (6%)	1 (2%)	9	42
25	W	53/55 (96%)	49 (92%)	4 (8%)	0	100	100
26	Z	55/60 (92%)	42 (76%)	12 (22%)	1 (2%)	8	39
27	1	51/55 (93%)	31 (61%)	15 (29%)	5 (10%)	0	6
28	2	44/47 (94%)	37 (84%)	7 (16%)	0	100	100
29	3	57/66 (86%)	37 (65%)	18 (32%)	2 (4%)	3	26
30	4	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
All	All	3111/3558 (87%)	2556 (82%)	466 (15%)	89 (3%)	4	30

5 of 89 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	221	HIS
4	B	86	PRO
4	B	122	PHE
4	B	137	ARG
4	B	147	PRO

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	
3	A	194/215 (90%)	180 (93%)	14 (7%)	14	45
4	B	155/157 (99%)	147 (95%)	8 (5%)	23	55
5	C	154/163 (94%)	146 (95%)	8 (5%)	23	55
6	D	152/156 (97%)	151 (99%)	1 (1%)	84	93
7	E	136/144 (94%)	135 (99%)	1 (1%)	84	93
8	F	46/107 (43%)	46 (100%)	0	100	100
9	G	118/146 (81%)	111 (94%)	7 (6%)	19	52
10	H	103/103 (100%)	100 (97%)	3 (3%)	42	71
11	I	100/121 (83%)	93 (93%)	7 (7%)	15	46
12	J	110/115 (96%)	106 (96%)	4 (4%)	35	66
13	K	90/93 (97%)	85 (94%)	5 (6%)	21	53
14	L	74/82 (90%)	70 (95%)	4 (5%)	22	54
15	M	94/134 (70%)	90 (96%)	4 (4%)	29	61
16	N	96/97 (99%)	94 (98%)	2 (2%)	53	78
17	O	75/79 (95%)	73 (97%)	2 (3%)	44	73
18	P	108/115 (94%)	107 (99%)	1 (1%)	78	91
19	Q	73/76 (96%)	69 (94%)	4 (6%)	21	53
20	R	91/96 (95%)	83 (91%)	8 (9%)	10	36
21	S	149/192 (78%)	146 (98%)	3 (2%)	55	79
22	T	55/67 (82%)	54 (98%)	1 (2%)	59	81
23	U	54/66 (82%)	51 (94%)	3 (6%)	21	53
24	V	53/55 (96%)	53 (100%)	0	100	100
25	W	48/48 (100%)	48 (100%)	0	100	100
26	Z	51/53 (96%)	50 (98%)	1 (2%)	55	79
27	1	46/48 (96%)	36 (78%)	10 (22%)	1	4
28	2	39/40 (98%)	34 (87%)	5 (13%)	4	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	3	46/52 (88%)	41 (89%)	5 (11%)	6	27
30	4	35/35 (100%)	35 (100%)	0	100	100
All	All	2545/2855 (89%)	2434 (96%)	111 (4%)	28	61

5 of 111 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	J	103	VAL
15	M	5	ILE
28	2	9	ASN
12	J	135	ARG
13	K	54	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
9	G	169	GLN
10	H	46	HIS
21	S	118	HIS
7	E	111	HIS
9	G	73	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2630/2880 (91%)	470 (17%)	73 (2%)
2	Y	119/123 (96%)	22 (18%)	0
All	All	2749/3003 (91%)	492 (17%)	73 (2%)

5 of 492 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	4	C
1	X	14	A
1	X	34	U
1	X	35	G
1	X	39	C

5 of 73 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	1324	G
1	X	1496	G
1	X	2736	U
1	X	1441	A
1	X	1607	A

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 84 ligands modelled in this entry, 82 are monoatomic - leaving 2 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
32	LMA	X	2882	-	58,60,60	4.94	27 (46%)	75,90,90	1.30	6 (8%)
31	LC2	X	2881	-	29,34,34	1.82	6 (20%)	26,49,49	1.18	2 (7%)

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
32	LMA	X	2882	-	-	23/80/115/115	0/3/3/3
31	LC2	X	2881	-	-	5/33/61/61	0/0/2/2

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	X	2882	LMA	C30-C2	-19.81	1.10	1.53
32	X	2882	LMA	C2-C1	-16.96	1.13	1.51
32	X	2882	LMA	O53-C8	-10.28	1.25	1.43
32	X	2882	LMA	O2-C13	8.48	1.57	1.44
32	X	2882	LMA	C35-C12	-8.25	1.36	1.53

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	X	2882	LMA	O12-C54-C56	4.58	119.51	111.09
32	X	2882	LMA	O51-C51-C53	4.53	119.42	111.09
32	X	2882	LMA	O7-C5-C4	3.89	112.91	108.22
32	X	2882	LMA	C3-C2-C1	-2.75	104.39	110.01
32	X	2882	LMA	C25-C24-C23	-2.46	106.52	113.08

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	X	2882	LMA	C3-C4-C5-C6
32	X	2882	LMA	C3-C4-C5-O7
32	X	2882	LMA	C31-C4-C5-C6
32	X	2882	LMA	C12-C11-O12-C54
32	X	2882	LMA	O55-C54-O12-C11

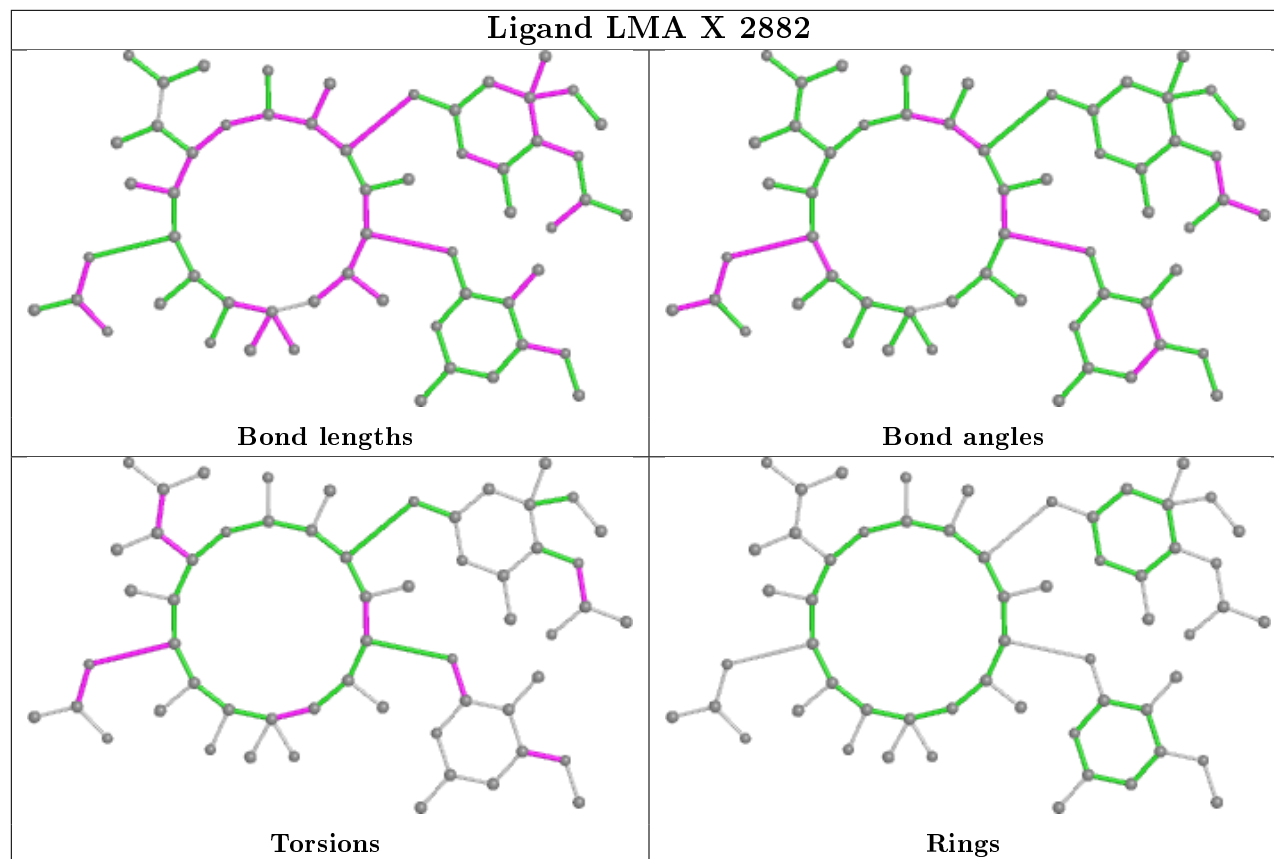
There are no ring outliers.

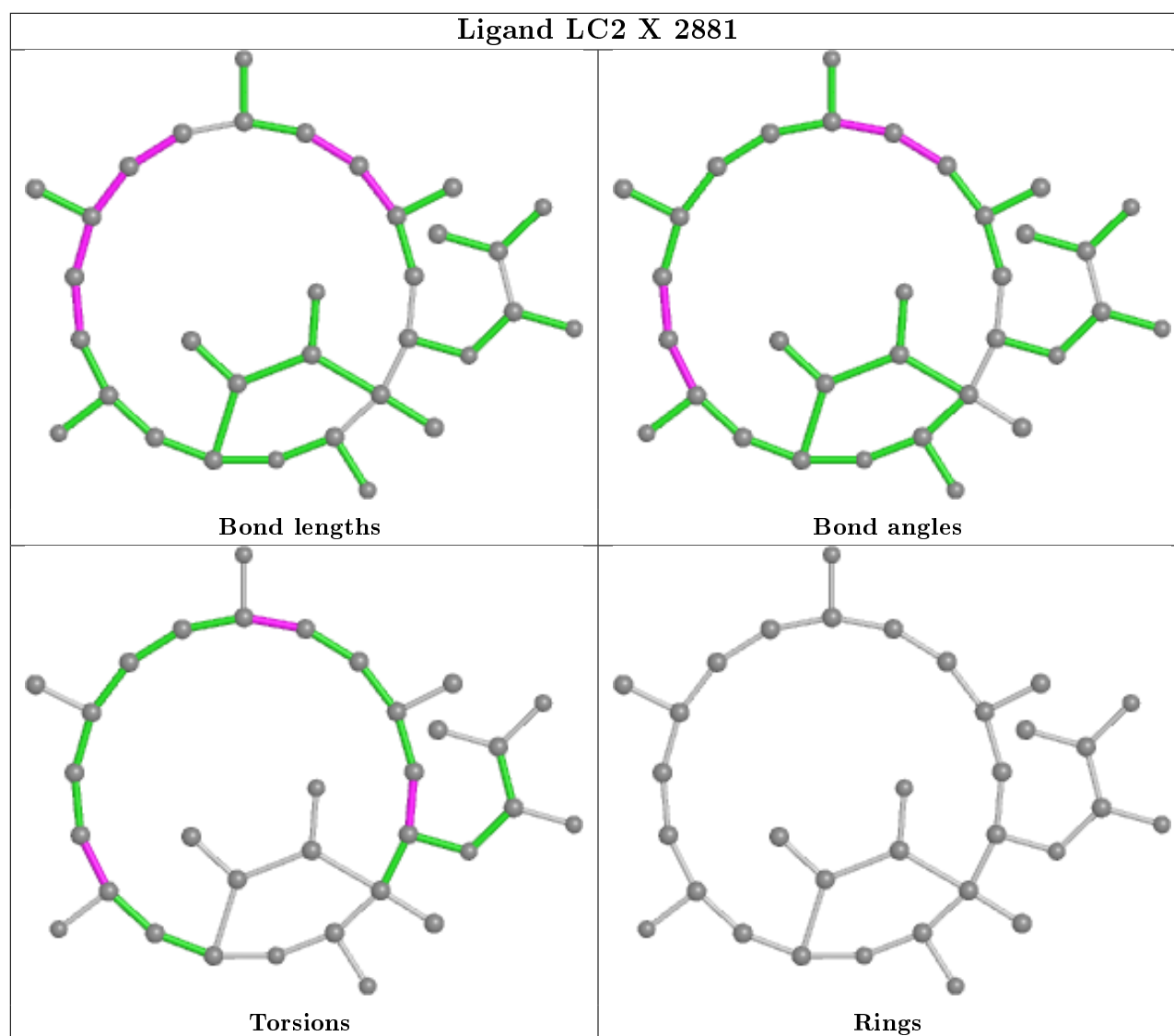
2 monomers are involved in 61 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	X	2882	LMA	43	0
31	X	2881	LC2	18	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	X	2644/2880 (91%)	0.10	83 (3%) 49 47	44, 115, 240, 575	0
2	Y	120/123 (97%)	-0.13	3 (2%) 57 54	108, 183, 252, 342	0
3	A	253/274 (92%)	1.01	53 (20%) 1 1	66, 158, 225, 423	0
4	B	205/211 (97%)	0.25	8 (3%) 39 38	35, 85, 159, 249	0
5	C	194/205 (94%)	0.03	10 (5%) 27 27	61, 142, 250, 381	0
6	D	177/180 (98%)	1.98	77 (43%) 0 0	174, 255, 358, 427	0
7	E	171/185 (92%)	0.32	14 (8%) 11 14	87, 183, 269, 354	0
8	F	63/144 (43%)	5.03	60 (95%) 0 0	208, 334, 476, 516	0
9	G	142/174 (81%)	0.65	21 (14%) 2 3	73, 126, 257, 421	0
10	H	134/134 (100%)	-0.20	1 (0%) 87 85	39, 71, 135, 248	0
11	I	134/156 (85%)	0.89	31 (23%) 0 0	75, 168, 261, 375	0
12	J	136/141 (96%)	0.93	26 (19%) 1 1	76, 135, 223, 388	0
13	K	113/116 (97%)	0.01	1 (0%) 84 81	32, 61, 101, 128	0
14	L	104/114 (91%)	0.36	13 (12%) 3 6	134, 193, 300, 325	0
15	M	108/166 (65%)	-0.06	2 (1%) 66 64	32, 73, 138, 298	0
16	N	117/118 (99%)	0.47	12 (10%) 6 9	57, 116, 177, 328	0
17	O	94/100 (94%)	0.72	16 (17%) 1 2	82, 145, 271, 322	0
18	P	126/134 (94%)	-0.19	1 (0%) 86 82	33, 84, 149, 226	0
19	Q	93/95 (97%)	1.34	25 (26%) 0 0	86, 134, 245, 329	0
20	R	110/115 (95%)	2.29	53 (48%) 0 0	93, 166, 332, 423	0
21	S	175/237 (73%)	0.79	31 (17%) 1 2	130, 202, 285, 326	0
22	T	74/91 (81%)	1.54	23 (31%) 0 0	112, 141, 201, 284	0
23	U	72/81 (88%)	1.55	19 (26%) 0 0	119, 188, 304, 349	0
24	V	65/67 (97%)	0.39	6 (9%) 9 11	116, 175, 235, 292	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	55/55 (100%)	0.93	12 (21%) 0 1	97, 126, 181, 194	0
26	Z	57/60 (95%)	-0.23	1 (1%) 68 65	44, 79, 182, 234	0
27	1	53/55 (96%)	2.99	34 (64%) 0 0	126, 192, 295, 403	0
28	2	46/47 (97%)	0.68	5 (10%) 5 8	72, 123, 258, 308	0
29	3	59/66 (89%)	4.22	52 (88%) 0 0	139, 213, 356, 435	0
30	4	37/37 (100%)	7.32	33 (89%) 0 0	152, 219, 307, 382	0
All	All	5931/6561 (90%)	0.55	726 (12%) 4 6	32, 131, 276, 575	0

The worst 5 of 726 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
23	U	28	GLY	23.8
8	F	113	PRO	15.2
30	4	28	SER	14.4
30	4	1	MET	13.8
30	4	24	LEU	13.8

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
33	MG	X	2911	1/1	0.28	0.63	124,124,124,124	0
33	MG	X	2912	1/1	0.66	0.20	62,62,62,62	0
33	MG	U	82	1/1	0.67	0.38	72,72,72,72	0
33	MG	I	157	1/1	0.74	0.47	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	MG	X	2917	1/1	0.75	0.32	104,104,104,104	0
33	MG	X	2886	1/1	0.76	1.10	54,54,54,54	0
35	NA	X	2962	1/1	0.79	1.12	98,98,98,98	0
33	MG	X	2926	1/1	0.79	0.45	67,67,67,67	0
32	LMA	X	2882	58/58	0.80	0.38	120,120,120,120	0
33	MG	X	2909	1/1	0.80	0.17	58,58,58,58	0
33	MG	X	2902	1/1	0.81	0.17	89,89,89,89	0
33	MG	X	2942	1/1	0.81	0.63	77,77,77,77	0
33	MG	X	2940	1/1	0.82	0.31	71,71,71,71	0
33	MG	X	2894	1/1	0.82	0.47	65,65,65,65	0
33	MG	X	2948	1/1	0.82	0.85	110,110,110,110	0
34	K	X	2956	1/1	0.83	0.39	146,146,146,146	0
31	LC2	X	2881	33/33	0.83	0.33	49,106,118,122	0
33	MG	X	2893	1/1	0.84	0.42	66,66,66,66	0
33	MG	X	2931	1/1	0.84	0.68	72,72,72,72	0
33	MG	X	2920	1/1	0.85	0.37	100,100,100,100	0
35	NA	X	2960	1/1	0.85	0.47	86,86,86,86	0
33	MG	X	2944	1/1	0.85	0.29	77,77,77,77	0
33	MG	X	2915	1/1	0.86	0.57	67,67,67,67	0
33	MG	X	2885	1/1	0.87	0.47	68,68,68,68	0
33	MG	X	2928	1/1	0.87	0.34	29,29,29,29	0
33	MG	X	2914	1/1	0.87	0.52	74,74,74,74	0
33	MG	X	2950	1/1	0.88	0.31	36,36,36,36	0
33	MG	X	2925	1/1	0.88	0.57	80,80,80,80	0
33	MG	X	2904	1/1	0.88	0.43	64,64,64,64	0
33	MG	X	2891	1/1	0.89	0.33	50,50,50,50	0
33	MG	X	2951	1/1	0.89	0.47	142,142,142,142	0
34	K	X	2957	1/1	0.89	0.57	82,82,82,82	0
33	MG	X	2941	1/1	0.89	0.23	71,71,71,71	0
33	MG	X	2910	1/1	0.90	0.37	44,44,44,44	0
33	MG	X	2903	1/1	0.90	0.54	65,65,65,65	0
33	MG	X	2916	1/1	0.90	0.20	44,44,44,44	0
33	MG	X	2895	1/1	0.90	0.29	26,26,26,26	0
33	MG	X	2938	1/1	0.91	0.62	62,62,62,62	0
35	NA	X	2958	1/1	0.91	0.47	48,48,48,48	0
35	NA	X	2959	1/1	0.91	0.25	60,60,60,60	0
33	MG	X	2905	1/1	0.91	0.67	50,50,50,50	0
33	MG	X	2921	1/1	0.91	0.17	61,61,61,61	0
35	NA	X	2961	1/1	0.92	0.43	75,75,75,75	0
33	MG	X	2908	1/1	0.92	0.67	80,80,80,80	0
33	MG	X	2883	1/1	0.92	0.54	23,23,23,23	0
33	MG	X	2922	1/1	0.92	0.36	53,53,53,53	0

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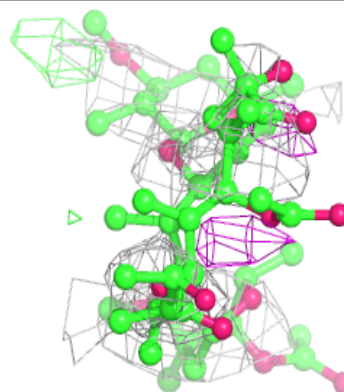
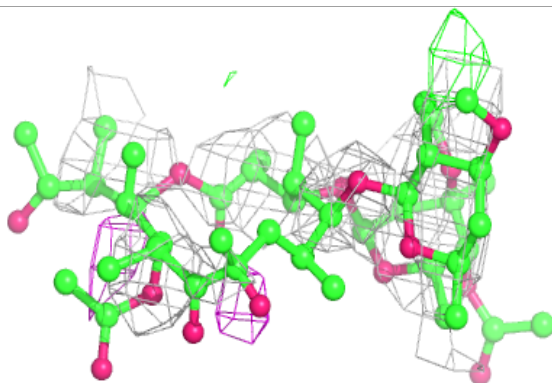
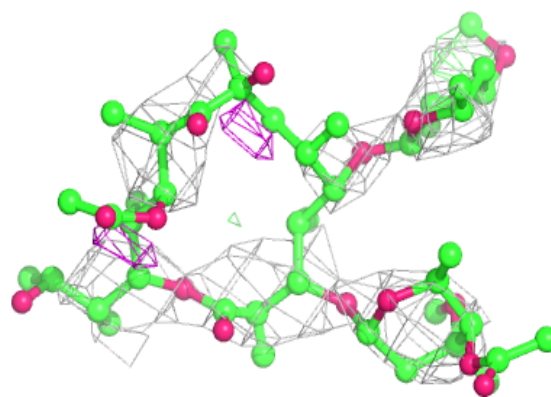
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	MG	X	2901	1/1	0.92	0.39	19,19,19,19	0
33	MG	X	2924	1/1	0.92	0.13	51,51,51,51	0
33	MG	X	2918	1/1	0.93	0.53	84,84,84,84	0
33	MG	X	2949	1/1	0.93	0.55	83,83,83,83	0
34	K	X	2955	1/1	0.93	0.15	113,113,113,113	0
33	MG	X	2884	1/1	0.93	1.00	72,72,72,72	0
33	MG	X	2929	1/1	0.93	0.83	61,61,61,61	0
33	MG	X	2923	1/1	0.93	0.15	97,97,97,97	0
33	MG	X	2900	1/1	0.94	0.64	42,42,42,42	0
33	MG	X	2932	1/1	0.94	0.35	62,62,62,62	0
33	MG	X	2919	1/1	0.94	0.33	65,65,65,65	0
33	MG	X	2907	1/1	0.94	0.36	46,46,46,46	0
33	MG	X	2935	1/1	0.94	0.23	36,36,36,36	0
33	MG	X	2936	1/1	0.94	0.25	55,55,55,55	0
33	MG	X	2937	1/1	0.94	0.38	109,109,109,109	0
33	MG	X	2946	1/1	0.94	0.16	123,123,123,123	0
33	MG	X	2934	1/1	0.94	0.41	56,56,56,56	0
33	MG	X	2952	1/1	0.95	0.35	59,59,59,59	0
33	MG	X	2933	1/1	0.95	0.37	83,83,83,83	0
33	MG	X	2896	1/1	0.95	0.26	24,24,24,24	0
33	MG	X	2887	1/1	0.95	0.41	35,35,35,35	0
33	MG	X	2945	1/1	0.95	0.17	67,67,67,67	0
33	MG	X	2927	1/1	0.95	0.74	65,65,65,65	0
33	MG	X	2892	1/1	0.95	0.30	71,71,71,71	0
33	MG	X	2943	1/1	0.95	0.20	43,43,43,43	0
33	MG	X	2906	1/1	0.96	0.38	52,52,52,52	0
33	MG	X	2890	1/1	0.96	0.40	59,59,59,59	0
33	MG	X	2888	1/1	0.96	0.49	51,51,51,51	0
33	MG	X	2897	1/1	0.96	0.14	79,79,79,79	0
34	K	X	2954	1/1	0.96	0.24	70,70,70,70	0
33	MG	X	2899	1/1	0.97	0.54	41,41,41,41	0
33	MG	X	2953	1/1	0.97	0.39	53,53,53,53	0
33	MG	X	2939	1/1	0.97	0.49	54,54,54,54	0
33	MG	X	2930	1/1	0.97	0.21	77,77,77,77	0
33	MG	X	2913	1/1	0.97	0.40	63,63,63,63	0
33	MG	X	2889	1/1	0.98	0.24	61,61,61,61	0
33	MG	X	2898	1/1	0.98	0.39	19,19,19,19	0
33	MG	X	2947	1/1	0.98	0.13	56,56,56,56	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.

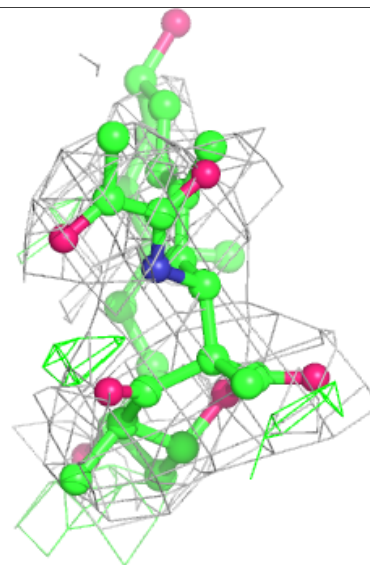
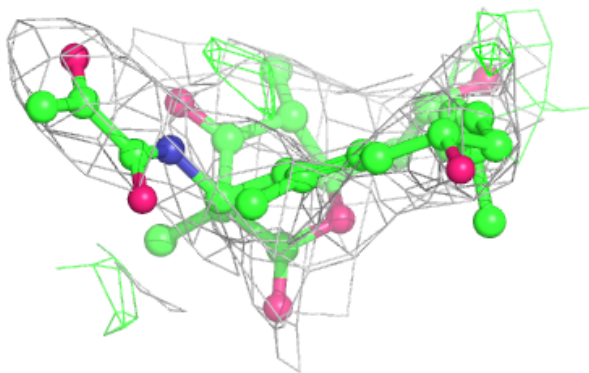
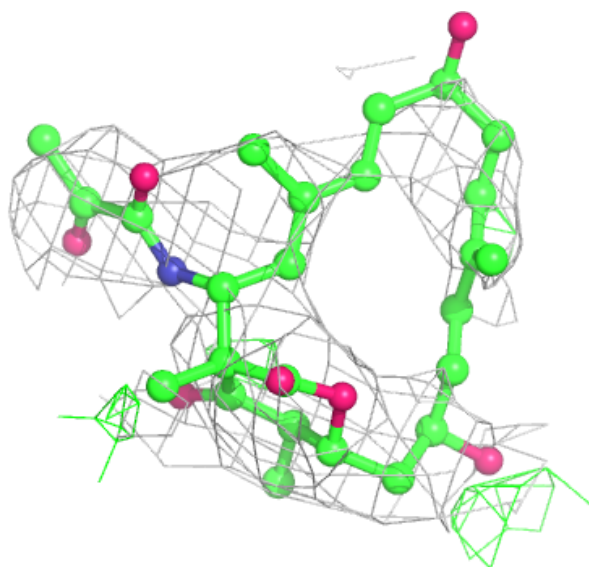
Electron density around LMA X 2882:

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



Electron density around LC2 X 2881:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.