



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2020 – 11:39 pm BST

PDB ID : 3PIO  
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.; Arakawa, K.; Kinashi, H.; Rozenberg, H.; Yonath, A.  
Deposited on : 2010-11-07  
Resolution : 3.25 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](mailto: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.

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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

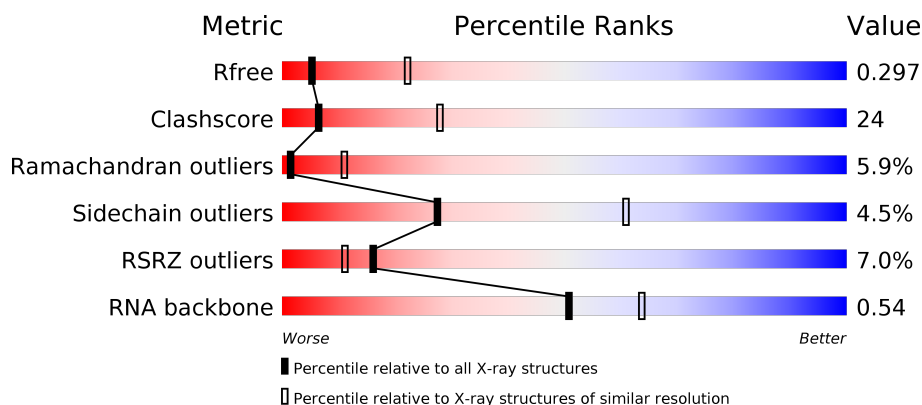
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.25 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	1619 (3.28-3.20)
Clashscore	141614	1755 (3.28-3.20)
Ramachandran outliers	138981	1728 (3.28-3.20)
Sidechain outliers	138945	1727 (3.28-3.20)
RSRZ outliers	127900	1567 (3.28-3.20)
RNA backbone	3102	1034 (3.58-2.90)

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  $\geq 3$ , 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	<div> <div>3%</div> <div>32% 40% 18% 8%</div> </div>
2	Y	123	<div> <div>2%</div> <div>48% 41% 8%</div> </div>
3	A	274	<div> <div>5%</div> <div>42% 45% 5% 8%</div> </div>
4	B	211	<div> <div>%</div> <div>48% 43% 6%</div> </div>

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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>95%</div> <div>62%38%</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
34	K	X	3074	-	-	-	X

## 2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 84383 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	2657	Total	C	N	O	P	0	0	0
			57035	25441	10530	18408	2656			

- 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
			1400	892	247	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
			1011	619	206	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
			726	458	136	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
			552	341	116	95				

- 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			

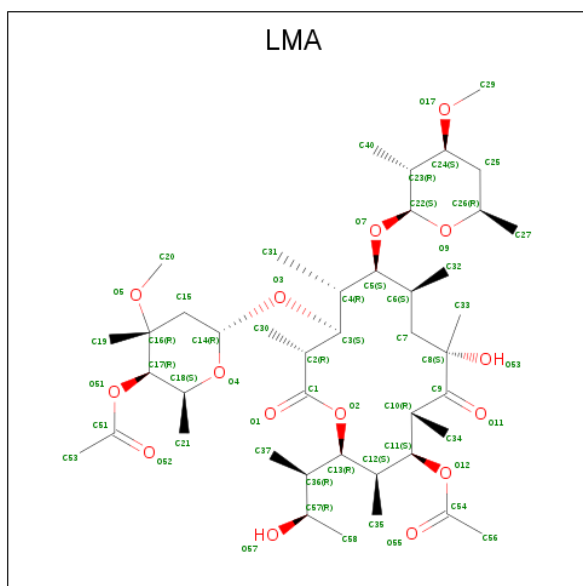
- Molecule 29 is a protein called 50S ribosomal protein L35.

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 Lankamycin (three-letter code: LMA) (formula:  $C_{43}H_{74}O_{15}$ ).



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

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	X	151	Total	Mg	0	0
			151	151		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	I	1	Total 1	Mg 1	0	0
32	Y	1	Total 1	Mg 1	0	0
32	C	1	Total 1	Mg 1	0	0

- Molecule 33 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	X	37	Total 37	Na 37	0	0
33	A	1	Total 1	Na 1	0	0
33	Z	1	Total 1	Na 1	0	0
33	Y	2	Total 2	Na 2	0	0
33	K	1	Total 1	Na 1	0	0

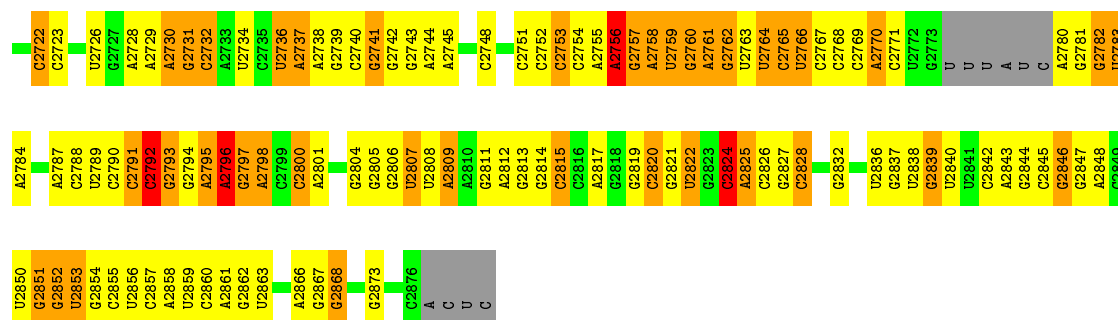
- Molecule 34 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	X	14	Total 14	K 14	0	0
34	M	1	Total 1	K 1	0	0

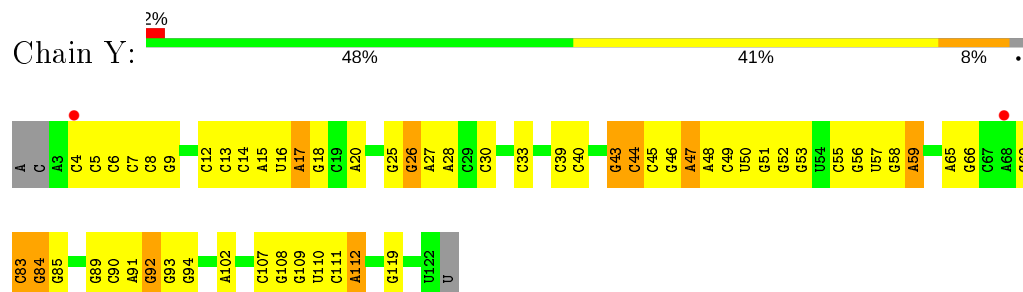


U1656	A1574	G1573	A1493	G1422	G1346	C1283	G1211	G1131	G1062	0989	A923	C853	A787	C721
A1657	G1575	A1574	G1494	A1423	C1347	G1284	U1212	G1132	G1067	A994	C924	G854	G788	C725
G1660	G1576	G1575	G1496	G1428	C1348	U1286	C1214	G1133	A1068	A999	U925	G855	G789	G726
G1662	G1577	G1576	G1497	A1429	G1351	A1287	A1215	G1135	G1069	A999	C926	U859	A790	U
G1663	G1578	G1577	G1498	G1430	G1352	A1288	G1216	G1136	G1070	G1000	C928	U860	G791	G
G1664	G1579	G1578	A1499	U1431	A1353	A1289	U1217	U1141	U1071	A1001	G928	G861	A792	A
C1665	G1584	G1584	U1500	A1432	A1354	A1290	C1218	G1142	U1072	C1002	G931	G867	C	C
A1666	A1585	A1585	U1505	A1433	A1355	G1291	C1219	G1143	G1073	C1003	G932	G867	A795	A
A1667	U1592	U1592	C1506	G1435	G1356	A1292	G1220	C1145	C1075	U1005	G933	U868	A796	G732
G1668	U1593	U1593	A1507	G1436	G1358	G1294	G1223	G1146	U1076	C1006	G934	U869	A797	G736
A1669	U1594	U1594	A1508	A1437	G1359	U1295	A1224	G1147	U1077	G1007	C935	U871	G798	C737
G1670	A1595	A1595	A1509	G1438	G1360	G1296	G1225	G1148	A1078	G1008	G936	G872	C799	G738
A1671	G1602	G1602	A1510	G1439	G1361	A1297	A1226	G1149	G1079	C1009	G937	U873	G799	G739
A1672	U1601	U1601	A1511	G1440	A1362	G1298	C1229	C1150	U1080	U1010	C938	A874	A801	G759
C1673	A1602	A1602	A1512	A1441	G1363	A1299	C1230	U1151	A1081	U1019	C939	A875	A802	G741
C1674	A1603	A1603	G1513	C1442	C1364	A1300	C1230	C1152	G1082	A1011	C940	G876	C803	G742
C1675			C1514	G1443	U1370	U1301	C1234	A1153	C1083	U1015	U942	G877	G805	A743
U1676			C1522	C1444	G1371	C1302	C1235	C1160	C1084	C1016	U943	C878	A806	G746
C1677			A	U1447	A1372	U1303	C1236	G1167	G1085	C1017	U944	A879	A807	A747
U1678			C	U1447	G1373	C1304	A1242	C1164	C1086	U1018	U945	G880	C808	A748
U1680			A	G1450	G1374	C1305	G1245	G1165	C1087	U1019	U946	C882	C809	U749
A1681			U1526			U1306	G1246	A1166	A1088	A1020	C947	A883	U810	G750
A1682			G1527			G1309	G1246	A1167	C1089	A1021	C948	G888	G811	G751
G1683			C1528			C1310	G1249	G1168	U1093	U1023	G949	C889	G812	G752
G1684			C1529			C1311	C1250	C1169	C1094	G1024	G951	U890	A813	G753
A1685			C1531			G1312	A1250	U1170	C1095	A1025	A952	A	A815	G754
A1686						C1313	G1251	A1171	A1095	U1026	G953	G	U816	G755
C1687						A1314	C1252	U1172	A1096	U1027	U954	G	A817	C756
C1687			U1537			A1315	C1253	G1173	A1097		G955	G	G818	U757
U1688			U1538			G1316	G1254	G1174	G1098	C1031	A956	G	G819	G758
U1689			U1539			G1317	G1255	A1175	A1099	A1033	G957	G	U820	G759
C1690			C1540			G1317	C1256	U1176	G1100	U1034	C959	C	A821	U760
G1691			G1541			A1321	U1257	U1177	G1104	U1035	U960	U	G822	G761
C1692			G1542			G1322	G1258	A1179	U1105	G1036	G961	A	U823	A762
A1693			G1543			G1323	A1259	U1182	U1106	U1037	C962	C	U824	
A1694			A1544			G1324	A1260	C1183	U1107			C	C825	C765
U1695						G1325	G1261	G1184	U1108	G1042	G965	A	U826	A766
C1696			C1546			U1326	C1264	C	A1109	A1043	A966	G	C827	G767
G1697			U1468			U1327	G1265	G	A1114	U1044	G967	C	U768	U768
C1698			U1469			G1328	G1266	A	C1115	U1045	C968	U	C830	C769
A1699			G1470			U1329	A1267	A	U1046	U1046	U969	C	U770	U770
C1700			G1471			G1330	U1268	G	G1116	G1047	A970	A	C771	C771
C1701			A1545			G1331	G1269	C	U1117	U1048	A971	C	G772	G772
C1702			G1554			G1332	G1270	G1191	G1118	C1049	C972	C	G773	G773
G1704			A1556			A1333	C1271	G1192	U1119	G1050	U973	A911	U774	U774
						A1334	G1272	G1193	C1120	U1051	U974	A912	G776	G776
						A1335	G1273	G1196	G1121	C1052		A913	A777	A777
						G1336	C1274	G1196	A1122	G1053	G977	C914	U778	U778
						G1337	A1275	G	G1123	C1054		C915	U779	U779
						U1338	U1276	G1200	A1055	U1046	C982	U916	U780	U780
						G1339	G1277	G1201	G1125	U1056	G983	U917	G843	G843
						C1414	G1278	U1202	A1126	A1057	A984	U918	G781	G781
						C1415	A1278	A1203	C1127	G1058	G985	U919	U782	U782
						G1418	G1279	A1203	G1128	U1059	A986	G920	G783	G783
						A1419	U1280	G1204	G1129	A1061	G987	U921	U784	U784
						C1344	A1281	G1205	U1130			G988	C851	U785
						U1421	A1282						U852	U786

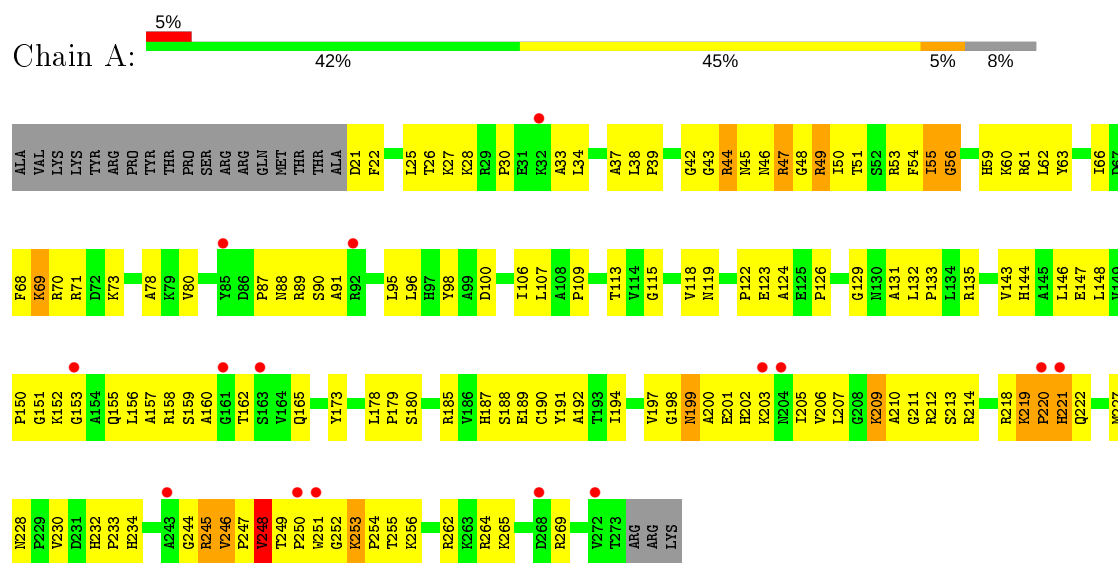
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C2660	G2661	G2588	C2517	U2436	A2372	U2291	G2217	G	U2074	C2008	C1944	G1879	A1796	G1722
G2662	G2663	U2590	C2519	G2437	C2373	C2292	G2218	A	U2075	U2009	C1945	U1881	G	U1723
U2664	U2665	G2591	A2520	U2441	G2375	G2293	U2219	G	C2082	G2010	A1946	U1881	G	C1724
U2666	U2667	U2592	G2521	U2442	G2376	U2298	G2220	G	G2083	A2011	G1947	A1884	A1800	C1725
C2668	C2669	U2593	G2522	C2443	U2377	A2299	G2221	C	G2084	A2012	C1948	C1885	C1801	G1730
U2669	U2670	G2594	G2523	C2444	G2378	G2300	U2222	A	G2085	A2013	A1949	C1886	A1802	U1733
C2671	C2672	U2595	G2524	C2445	G2379	A2301	U2223	A	U2087	A2014	G1951	G1887	U1804	C1734
G2673	G2674	G2596	G2525	C2446	U2380	G2302	U2224	C	U	A2015	A1952	C1888	G1805	U1737
U2675	U2676	U2597	G2526	G2447	C2382	A2306	G2227	G	C	U2016	A1953	G	G1806	G
C2677	C2678	U2598	U2527	U2448	G2383	G2310	U2228	U	C	C2018	A1954	C	A1807	G
G2679	G2680	A2600	G2532	U2452	U2385	U2311	G2229	G	C	C2019	G1955	C	C1808	G1741
U2681	U2682	G2604	U2534	C2453	U2386	A2312	C2233	A	U	C2023	A1960	G	G1809	G1742
C2683	C2684	C2605	U2540	C2454	U2387	G2313	C2234	A	C	U2024	U1810	U	A1811	C1743
U2685	U2686	G2606	U2541	C2455	U2388	A2314	G2235	U	C	A2025	G1963	A	U1812	G1744
C2687	C2688	U2607	U2542	U2456	U2389	A2315	U2236	A	U	C2026	A1964	C	A1813	G1745
U2689	U2690	A2608	U2543	U2457	A2390	C2321	C2237	C	U	C2027	U1965	U	A1746	A1747
G2691	G2692	G2609	A2544	U2458	U2391	U2322	C2238	C	G	G2028	C1966	A	G1748	U1747
U2693	U2694	U2611	A2545	G2468	U2392	U2323	C2239	A	G	U2029	U1967	U	G1749	U1750
C2695	C2696	G2612	A2546	G2469	G2393	G2324	U2241	C	A	A2030	G1968	A	U1816	A1751
U2697	U2698	A2613	G2547	U2470	G2394	A2325	C2242	C	U	U2031	C1969	A	U1817	U1752
C2699	C2700	U2614	U2548	U2471	U2395	C2326	C2243	U	G	G2032	G1970	C	A1821	A1753
U2701	U2702	G2615	G2549	C2475	A2396	U2327	A2245	G	U	C2033	C1971	G	G1822	G
G2703	G2704	U2616	C2550	U2476	U2397	G2328	A2246	A	G	U2034	G1972	G	C1825	G1754
U2705	U2706	G2617	U2551	C2477	U2398	C2329	A2247	G	C	A2037	C1973	C	U1826	G1755
C2707	C2708	U2618	C2552	U2478	A2401	G2330	U2251	A	G	G2038	U1976	U	C1827	C1757
U2709	U2710	G2619	G2553	C2479	U2402	A2331	A2252	G	A	G2039	C1977	A	G1830	C1758
G2711	G2712	U2620	U2554	U2480	G2413	A2336	A2253	G	U	A2040	C1978	U	G1831	G1761
A2713	A2714	U2621	C2555	C2481	U2414	U2337	C2254	C	G	A2041	U1979	U	C1832	C1762
G2715	G2716	G2622	G2556	G2482	G2415	G2338	G2255	C	C	A2042	C1979	U	G1833	G1763
U2717	U2718	A2623	C2557	U2483	U2416	U2339	G2256	C	U	A2043	A1981	U	C1834	A1764
C2719	C2720	G2624	A2558	G2484	U2417	C2340	A2257	G	U	A2044	C1982	U	C1835	G1765
U2721	U2722	U2625	U2559	G2485	U2418	G2341	G2258	C	C	C2046	G1983	U	C1836	U1766
G2723	G2724	U2626	G2560	U2486	U2419	U2342	G2259	G	G	C2047	A1984	U	G1837	G1767
U2725	U2726	U2627	U2561	U2487	G2420	A2343	C2260	A	A	C2048	A1985	U	G1838	U1768
C2727	C2728	U2628	U2562	C2491	U2421	A2344	G2261	A	U	A2049	C1987	U	A1840	U1769
U2729	U2730	G2629	U2563	U2492	G2414	G2345	C2262	G	C	G2050	A1988	U	G1841	A1770
G2731	G2732	U2630	C2564	U2493	U2415	G2350	C2263	U	U	U2051	C1989	U	G1842	A1771
U2733	U2734	A2631	G2565	U2494	U2416	G2351	C2264	C	C	G2052	U1990	U	C1843	C1772
C2735	C2736	G2632	A2566	C2495	U2417	G2352	A2265	G	G	G2053	C1991	U	C1844	C1773
U2737	U2738	U2633	U2567	G2496	A2418	A2353	A2266	C	C	A2054	G1992	U	G1845	A1774
G2739	G2740	G2634	A2568	C2497	C2419	A2354	A2267	U	U	G2055	G1993	U	A1851	A1775
U2741	U2742	U2635	U2569	U2498	C2420	A2355	C2268	C	C	C2056	U1994	U	G1852	A1776
C2743	C2744	G2636	C2570	U2499	C2421	A2356	A2272	U	U	U2057	G1995	U	G1853	G
U2745	U2746	U2637	U2571	C2499	C2422	C2360	C2273	U	U	G2058	A1996	U	G1854	G1779
G2747	G2748	U2638	U2572	U2500	G2423	G2361	C2274	U	U	U2059	A1997	U	G1855	A1780
U2749	U2750	U2639	C2573	U2501	G2424	G2362	G2275	G	G	A2060	C1998	U	C1781	A1782
C2751	C2752	G2640	U2574	G2502	G2425	G2363	G2282	C	C	G2061	U1999	U	G1856	G
U2753	U2754	U2641	G2575	C2503	G2426	G2364	G2283	G	G	U2062	U2000	U	G1857	U1787
G2755	G2756	U2642	U2576	G2504	A2427	U2365	U2284	C	U	A2063	G2001	U	A1867	C1788
U2757	U2758	U2643	U2577	C2505	U2428	U2366	U2285	C	C	U2064	A2002	U	A1868	U1789
C2759	C2760	U2644	G2578	G2506	U2429	A2367	G2286	U	U	A2065	A2003	U	G1869	G1790
U2761	U2762	U2645	A2581	U2507	A2430	G2368	G2287	C	C	G2066	U2004	U	C1791	C1792
G2763	G2764	G2646	G2582	U2508	A2431	U2369	A2288	G	G	U2067	G2005	U	G1871	G
U2765	U2766	U2647	U2583	A2509	A2432	G2370	A2289	G	G					



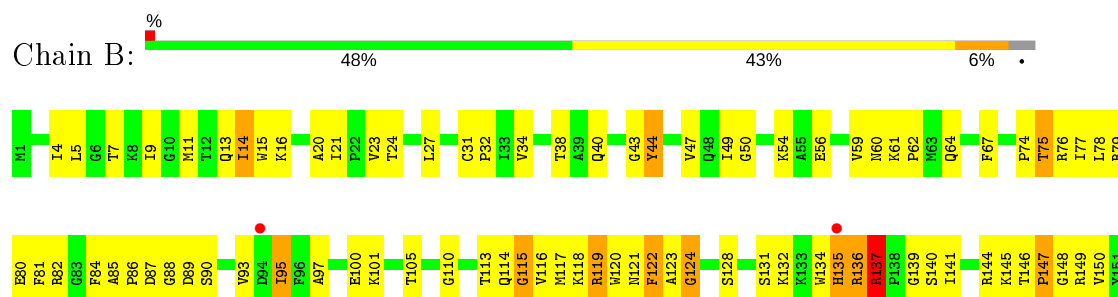
### • Molecule 2: 5S ribosomal RNA



### • Molecule 3: 50S ribosomal protein L2

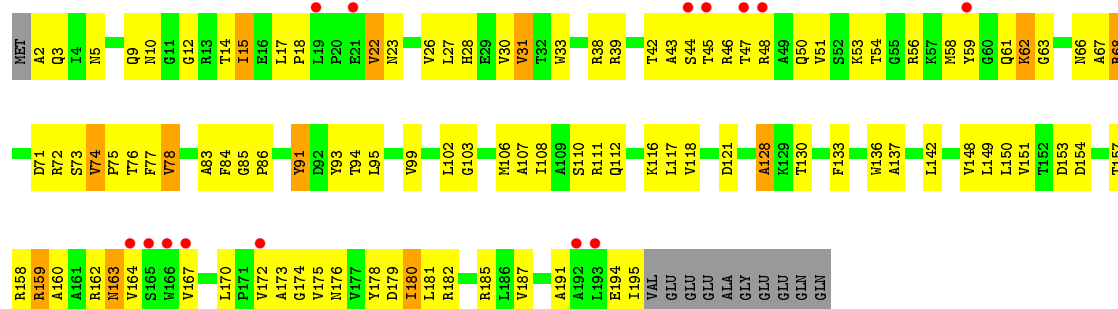
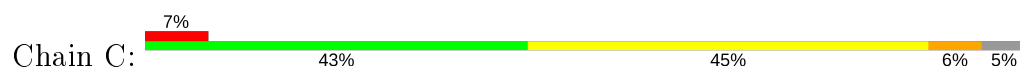


### • Molecule 4: 50S ribosomal protein L3

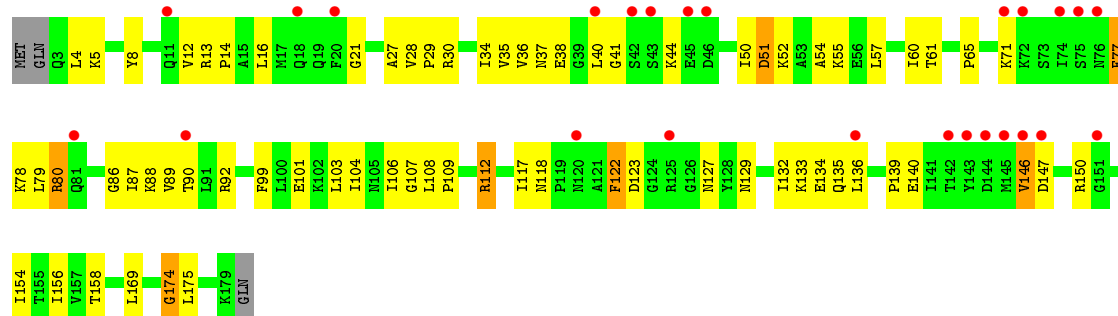




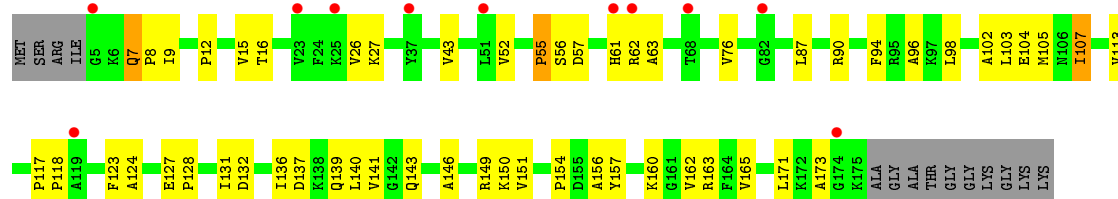
- Molecule 5: 50S ribosomal protein L4



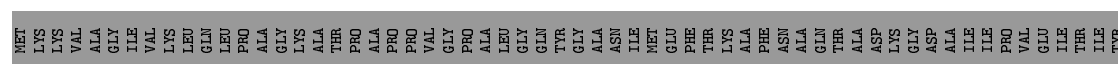
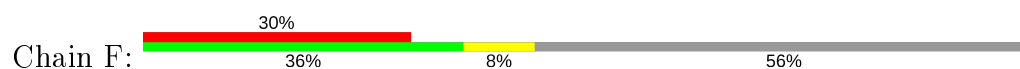
- Molecule 6: 50S ribosomal protein L5

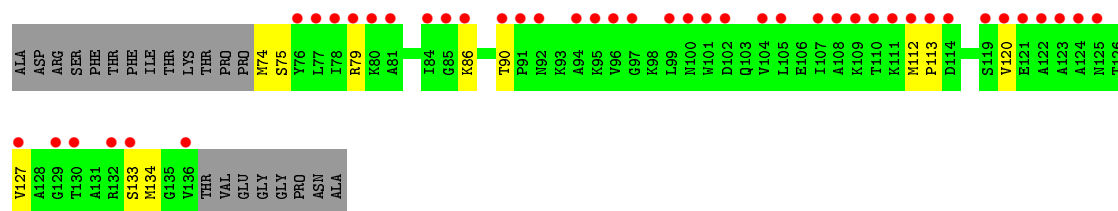


- Molecule 7: 50S ribosomal protein L6

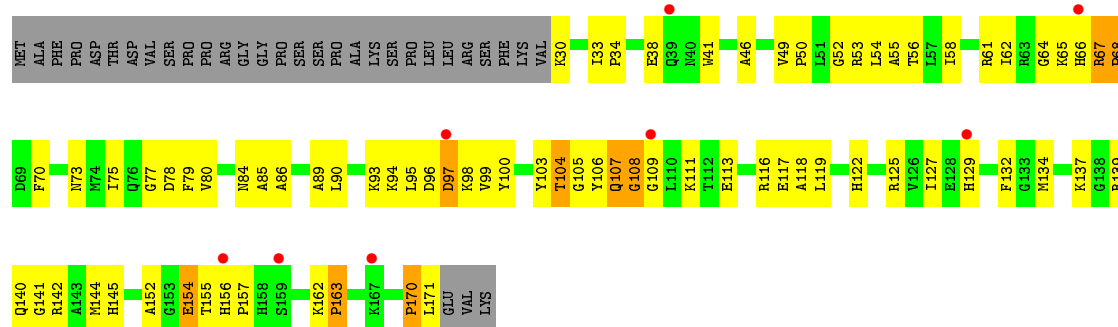


- Molecule 8: 50S ribosomal protein L11

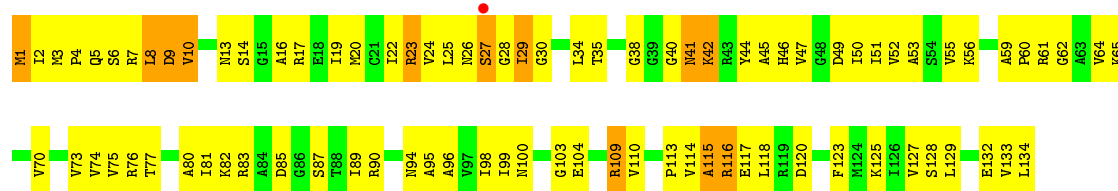




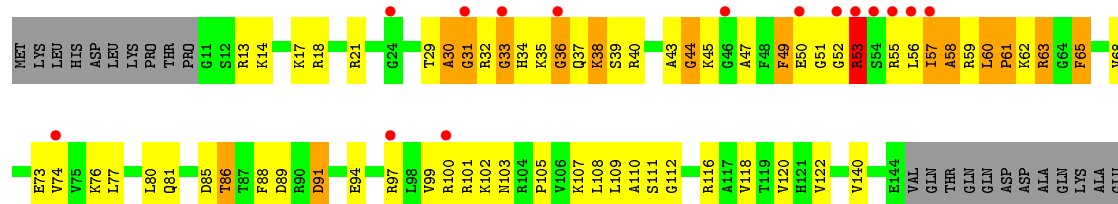
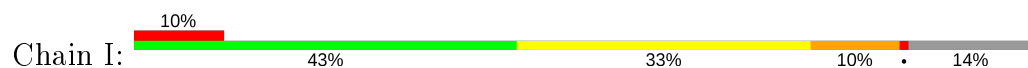
• Molecule 9: 50S ribosomal protein L13



• Molecule 10: 50S ribosomal protein L14



• Molecule 11: 50S ribosomal protein L15



• Molecule 12: 50S ribosomal protein L16

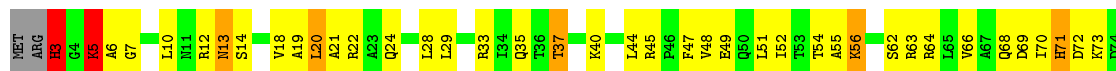






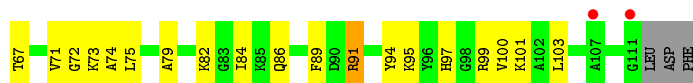
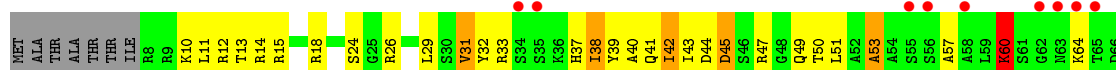
- Molecule 13: 50S ribosomal protein L17

Chain K: 38% 50% 8% . .



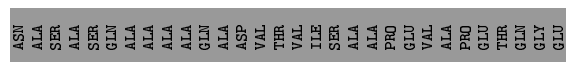
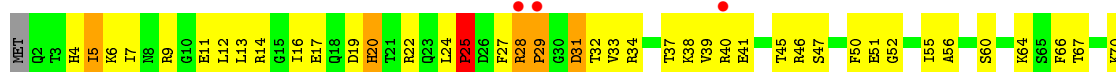
- Molecule 14: 50S ribosomal protein L18

Chain L: 10% 48% 37% 5% . 9%



- Molecule 15: 50S ribosomal protein L19

Chain M: 2% 26% 34% 5% . 35%

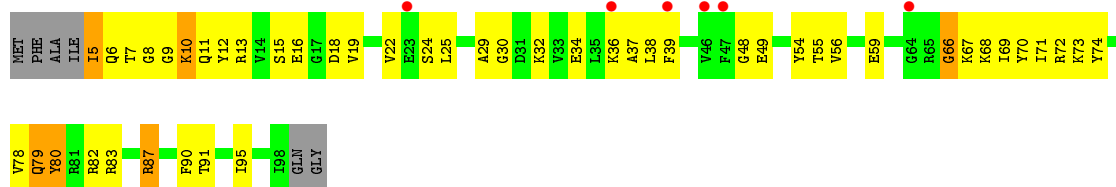


- Molecule 16: 50S ribosomal protein L20

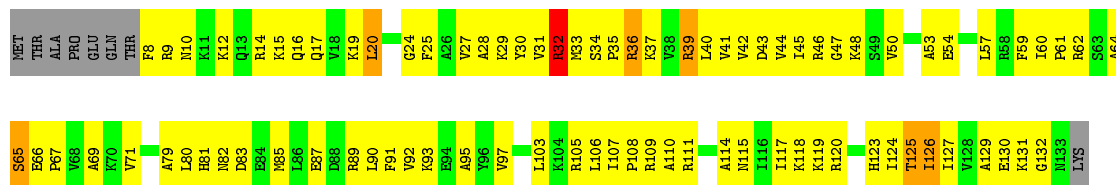
Chain N: 3% 42% 53% . .



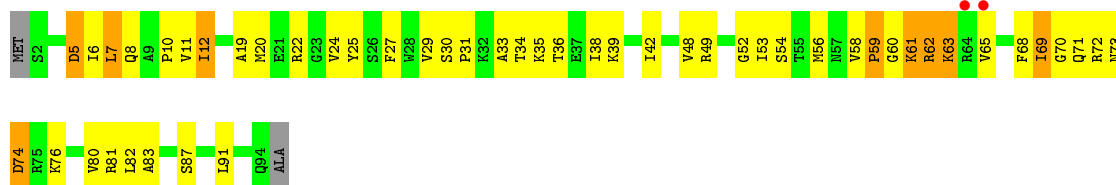
- Molecule 17: 50S ribosomal protein L21



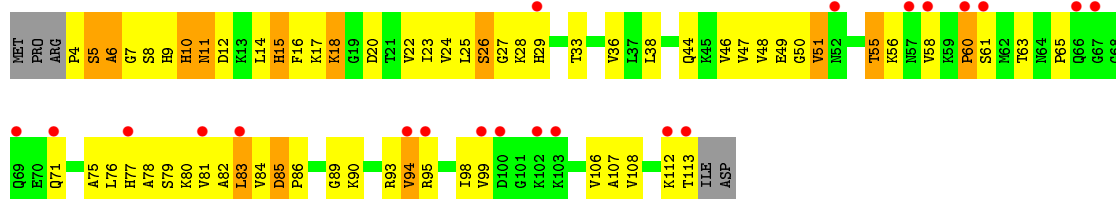
- Molecule 18: 50S ribosomal protein L22



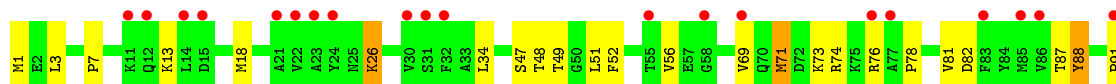
- Molecule 19: 50S ribosomal protein L23

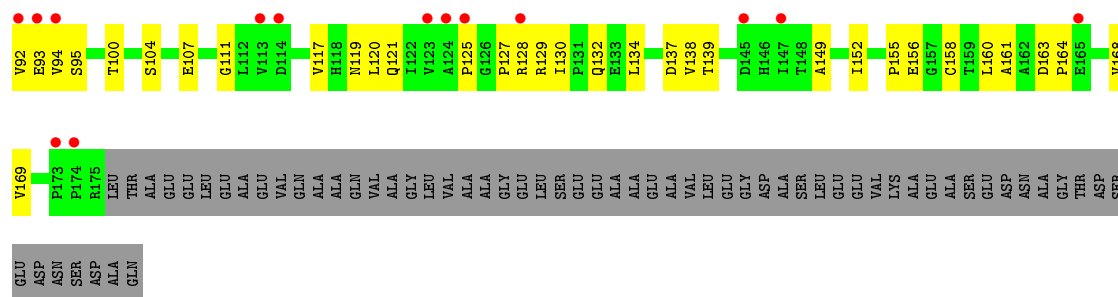


- Molecule 20: 50S ribosomal protein L24

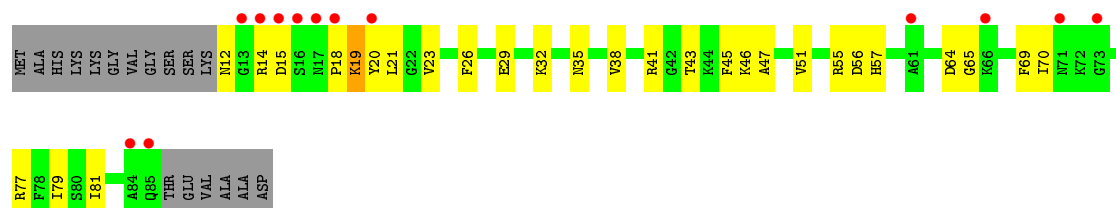


- Molecule 21: 50S ribosomal protein L25

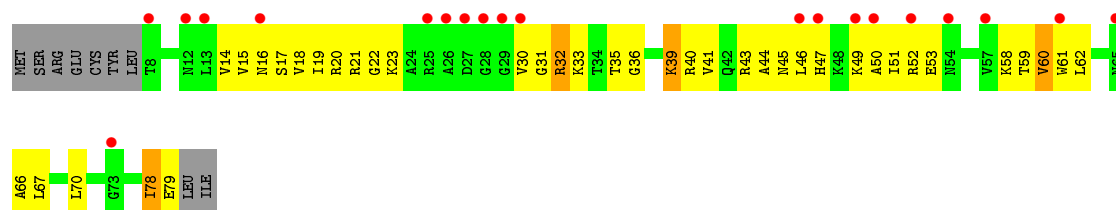
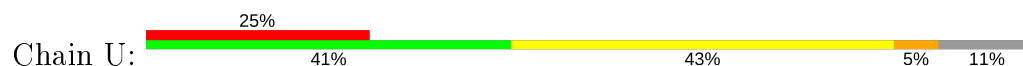




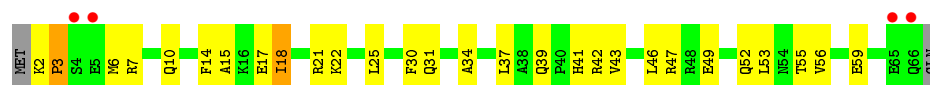
- Molecule 22: 50S ribosomal protein L27



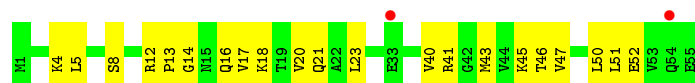
- Molecule 23: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L29

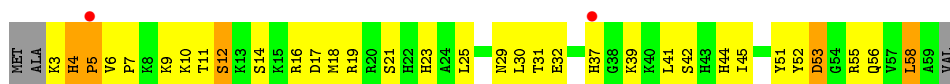


- Molecule 25: 50S ribosomal protein L30

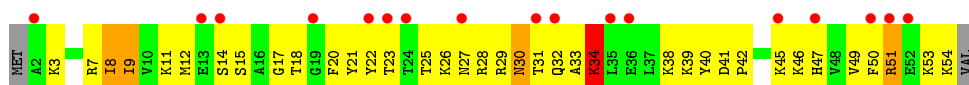


- Molecule 26: 50S ribosomal protein L32

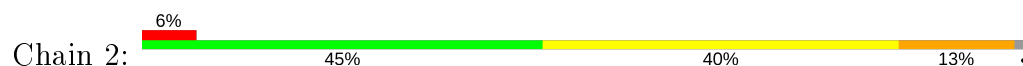




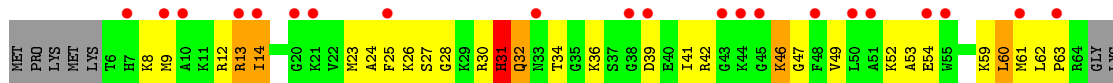
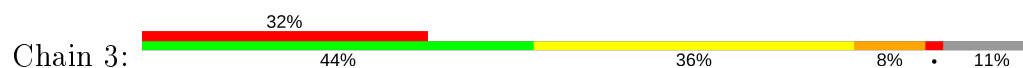
- Molecule 27: 50S ribosomal protein L33



- 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, $\alpha$ , $\beta$ , $\gamma$	170.59Å 410.20Å 695.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.25 34.75 – 3.25	Depositor EDS
% Data completeness (in resolution range)	93.3 (20.00-3.25) 93.3 (34.75-3.25)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.09 (at 3.25Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, $R_{free}$	0.252 , 0.294 0.258 , 0.297	Depositor DCC
$R_{free}$ test set	3585 reflections (1.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	73.8	Xtriage
Anisotropy	0.636	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.20 , 65.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	84383	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, 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	0.69	12/63867 (0.0%)	1.28	804/99618 (0.8%)
2	Y	0.46	0/2863	0.86	5/4461 (0.1%)
3	A	0.49	1/1958 (0.1%)	0.65	2/2638 (0.1%)
4	B	0.55	0/1567	0.79	0/2105
5	C	0.52	0/1504	0.67	0/2036
6	D	0.31	0/1419	0.45	0/1903
7	E	0.33	0/1308	0.48	0/1771
8	F	0.22	0/455	0.37	0/611
9	G	0.57	0/1138	0.70	0/1539
10	H	0.63	0/1007	0.84	0/1352
11	I	0.54	0/1022	0.64	0/1366
12	J	0.48	0/1113	0.63	0/1486
13	K	0.81	1/886 (0.1%)	1.06	6/1188 (0.5%)
14	L	0.40	0/785	0.56	0/1048
15	M	0.67	0/884	0.88	1/1186 (0.1%)
16	N	0.55	0/994	0.71	0/1323
17	O	0.44	0/750	0.62	0/1000
18	P	0.58	0/1017	0.79	1/1362 (0.1%)
19	Q	0.47	0/737	0.63	0/988
20	R	0.45	0/835	0.59	0/1121
21	S	0.33	0/1370	0.48	0/1862
22	T	0.43	0/563	0.56	0/747
23	U	0.40	0/556	0.58	0/741
24	V	0.31	0/529	0.47	0/704
25	W	0.39	0/426	0.65	0/568
26	Z	0.56	0/464	0.79	0/622
27	1	0.48	0/438	0.56	0/583
28	2	0.56	0/387	0.71	0/509
29	3	0.59	0/468	0.65	0/614
30	4	0.22	0/298	0.37	0/390
All	All	0.63	14/91608 (0.0%)	1.15	819/137442 (0.6%)

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	1977	C	P-O5'	-7.09	1.52	1.59
1	X	774	A	N7-C5	7.06	1.43	1.39
1	X	1333	G	O3'-P	-6.43	1.53	1.61
1	X	1202	U	O3'-P	-6.42	1.53	1.61
1	X	774	A	N9-C8	6.38	1.42	1.37

The worst 5 of 819 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1975	G	N1-C6-O6	-19.89	107.97	119.90
1	X	774	A	C5-N7-C8	-17.57	95.12	103.90
1	X	774	A	C4-C5-C6	-17.47	108.26	117.00
1	X	1670	G	C8-N9-C4	15.74	112.69	106.40
1	X	774	A	C4-C5-N7	14.89	118.15	110.70

There are no chirality outliers.

There are no planarity outliers.

## 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	57035	0	28741	1817	0
2	Y	2561	0	1306	48	0
3	A	1920	0	1974	176	0
4	B	1539	0	1600	147	0
5	C	1481	0	1504	120	0
6	D	1400	0	1481	61	0
7	E	1286	0	1336	44	0
8	F	451	0	474	7	0
9	G	1114	0	1144	100	0
10	H	997	0	1046	98	0
11	I	1011	0	1047	98	0
12	J	1090	0	1125	78	0
13	K	878	0	930	80	0
14	L	779	0	820	72	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	M	871	0	894	99	0
16	N	978	0	1020	82	0
17	O	741	0	756	45	0
18	P	1004	0	1083	88	0
19	Q	726	0	753	50	0
20	R	825	0	881	69	0
21	S	1345	0	1372	43	0
22	T	556	0	579	38	0
23	U	552	0	604	48	0
24	V	525	0	546	29	0
25	W	424	0	470	17	0
26	Z	452	0	457	53	0
27	1	431	0	456	58	0
28	2	383	0	414	52	0
29	3	462	0	506	63	0
30	4	297	0	330	23	0
31	X	58	0	69	13	0
32	C	1	0	0	0	0
32	I	1	0	0	0	0
32	X	151	0	0	0	0
32	Y	1	0	0	0	0
33	A	1	0	0	0	0
33	K	1	0	0	0	0
33	X	37	0	0	0	0
33	Y	2	0	0	0	0
33	Z	1	0	0	0	0
34	M	1	0	0	0	0
34	X	14	0	0	0	0
All	All	84383	0	55718	3336	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 24.

The worst 5 of 3336 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:2044:G:OP1	5:C:62:LYS:HG3	1.36	1.18
15:M:28:ARG:HB2	15:M:29:PRO:HD3	1.29	1.14
9:G:103:TYR:HB3	9:G:107:GLN:HE21	1.14	1.12
4:B:9:ILE:HD11	4:B:27:LEU:HB2	1.32	1.10
4:B:116:VAL:HG22	4:B:136:ARG:NE	1.69	1.05



There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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%)	195 (78%)	44 (18%)	12 (5%)	2	15
4	B	203/211 (96%)	160 (79%)	29 (14%)	14 (7%)	1	7
5	C	192/205 (94%)	143 (74%)	37 (19%)	12 (6%)	1	9
6	D	175/180 (97%)	137 (78%)	32 (18%)	6 (3%)	3	22
7	E	169/185 (91%)	142 (84%)	20 (12%)	7 (4%)	3	18
8	F	61/144 (42%)	48 (79%)	12 (20%)	1 (2%)	9	40
9	G	140/174 (80%)	104 (74%)	27 (19%)	9 (6%)	1	9
10	H	132/134 (98%)	111 (84%)	17 (13%)	4 (3%)	4	25
11	I	132/156 (85%)	82 (62%)	31 (24%)	19 (14%)	0	1
12	J	134/141 (95%)	96 (72%)	27 (20%)	11 (8%)	1	5
13	K	111/116 (96%)	89 (80%)	14 (13%)	8 (7%)	1	6
14	L	102/114 (90%)	73 (72%)	26 (26%)	3 (3%)	4	25
15	M	106/166 (64%)	82 (77%)	18 (17%)	6 (6%)	1	12
16	N	115/118 (98%)	95 (83%)	16 (14%)	4 (4%)	3	21
17	O	92/100 (92%)	68 (74%)	17 (18%)	7 (8%)	1	6
18	P	124/134 (92%)	101 (82%)	18 (14%)	5 (4%)	3	18
19	Q	91/95 (96%)	63 (69%)	19 (21%)	9 (10%)	0	3
20	R	108/115 (94%)	70 (65%)	26 (24%)	12 (11%)	0	2
21	S	173/237 (73%)	135 (78%)	32 (18%)	6 (4%)	3	21
22	T	72/91 (79%)	53 (74%)	18 (25%)	1 (1%)	11	43
23	U	70/81 (86%)	50 (71%)	13 (19%)	7 (10%)	0	3
24	V	63/67 (94%)	55 (87%)	5 (8%)	3 (5%)	2	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	W	53/55 (96%)	47 (89%)	6 (11%)	0	100	100
26	Z	55/60 (92%)	42 (76%)	9 (16%)	4 (7%)	1	6
27	1	51/55 (93%)	30 (59%)	15 (29%)	6 (12%)	0	2
28	2	44/47 (94%)	37 (84%)	5 (11%)	2 (4%)	2	16
29	3	57/66 (86%)	34 (60%)	18 (32%)	5 (9%)	1	4
30	4	35/37 (95%)	29 (83%)	6 (17%)	0	100	100
All	All	3111/3558 (87%)	2371 (76%)	557 (18%)	183 (6%)	1	11

5 of 183 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	220	PRO
3	A	221	HIS
3	A	248	VAL
4	B	135	HIS
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%)	184 (95%)	10 (5%)	23	56
4	B	155/157 (99%)	149 (96%)	6 (4%)	32	65
5	C	154/163 (94%)	147 (96%)	7 (4%)	27	61
6	D	153/156 (98%)	150 (98%)	3 (2%)	55	78
7	E	136/144 (94%)	136 (100%)	0	100	100
8	F	46/107 (43%)	46 (100%)	0	100	100
9	G	118/146 (81%)	115 (98%)	3 (2%)	47	74
10	H	103/103 (100%)	94 (91%)	9 (9%)	10	35
11	I	101/121 (84%)	97 (96%)	4 (4%)	31	64
12	J	110/115 (96%)	108 (98%)	2 (2%)	59	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	K	90/93 (97%)	82 (91%)	8 (9%)	9	34
14	L	74/82 (90%)	68 (92%)	6 (8%)	11	39
15	M	94/134 (70%)	87 (93%)	7 (7%)	13	43
16	N	96/97 (99%)	93 (97%)	3 (3%)	40	70
17	O	75/79 (95%)	72 (96%)	3 (4%)	31	64
18	P	108/115 (94%)	101 (94%)	7 (6%)	17	49
19	Q	75/76 (99%)	70 (93%)	5 (7%)	16	47
20	R	91/96 (95%)	84 (92%)	7 (8%)	13	41
21	S	149/192 (78%)	146 (98%)	3 (2%)	55	78
22	T	55/67 (82%)	53 (96%)	2 (4%)	35	66
23	U	57/66 (86%)	55 (96%)	2 (4%)	36	67
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%)	47 (92%)	4 (8%)	12	41
27	1	46/48 (96%)	41 (89%)	5 (11%)	6	25
28	2	39/40 (98%)	33 (85%)	6 (15%)	2	12
29	3	46/52 (88%)	43 (94%)	3 (6%)	17	49
30	4	35/35 (100%)	35 (100%)	0	100	100
All	All	2552/2855 (89%)	2437 (96%)	115 (4%)	27	61

5 of 115 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	L	31	VAL
15	M	98	LYS
28	2	5	TYR
14	L	38	ILE
15	M	5	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
12	J	47	GLN
16	N	14	HIS
22	T	35	ASN

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Mol	Chain	Res	Type
13	K	24	GLN
14	L	41	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2647/2880 (91%)	473 (17%)	54 (2%)
2	Y	119/123 (96%)	18 (15%)	0
All	All	2766/3003 (92%)	491 (17%)	54 (1%)

5 of 491 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	4	C
1	X	13	A
1	X	14	A
1	X	34	U
1	X	35	G

5 of 54 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	1313	U
1	X	1601	U
1	X	2692	A
1	X	1357	U
1	X	1441	A

## 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 212 ligands modelled in this entry, 211 are monoatomic - leaving 1 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
31	LMA	X	2881	-	58,60,60	4.94	26 (44%)	75,90,90	1.30	5 (6%)

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
31	LMA	X	2881	-	-	20/80/115/115	0/3/3/3

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	X	2881	LMA	C30-C2	-19.79	1.10	1.53
31	X	2881	LMA	C2-C1	-17.00	1.13	1.51
31	X	2881	LMA	O53-C8	-10.30	1.25	1.43
31	X	2881	LMA	O2-C13	8.52	1.57	1.44
31	X	2881	LMA	C35-C12	-8.22	1.36	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	X	2881	LMA	O12-C54-C56	4.58	119.52	111.09
31	X	2881	LMA	O51-C51-C53	4.56	119.48	111.09
31	X	2881	LMA	O7-C5-C4	3.88	112.90	108.22
31	X	2881	LMA	C3-C2-C1	-2.76	104.38	110.01
31	X	2881	LMA	C25-C24-C23	-2.45	106.55	113.08

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
31	X	2881	LMA	C3-C4-C5-C6

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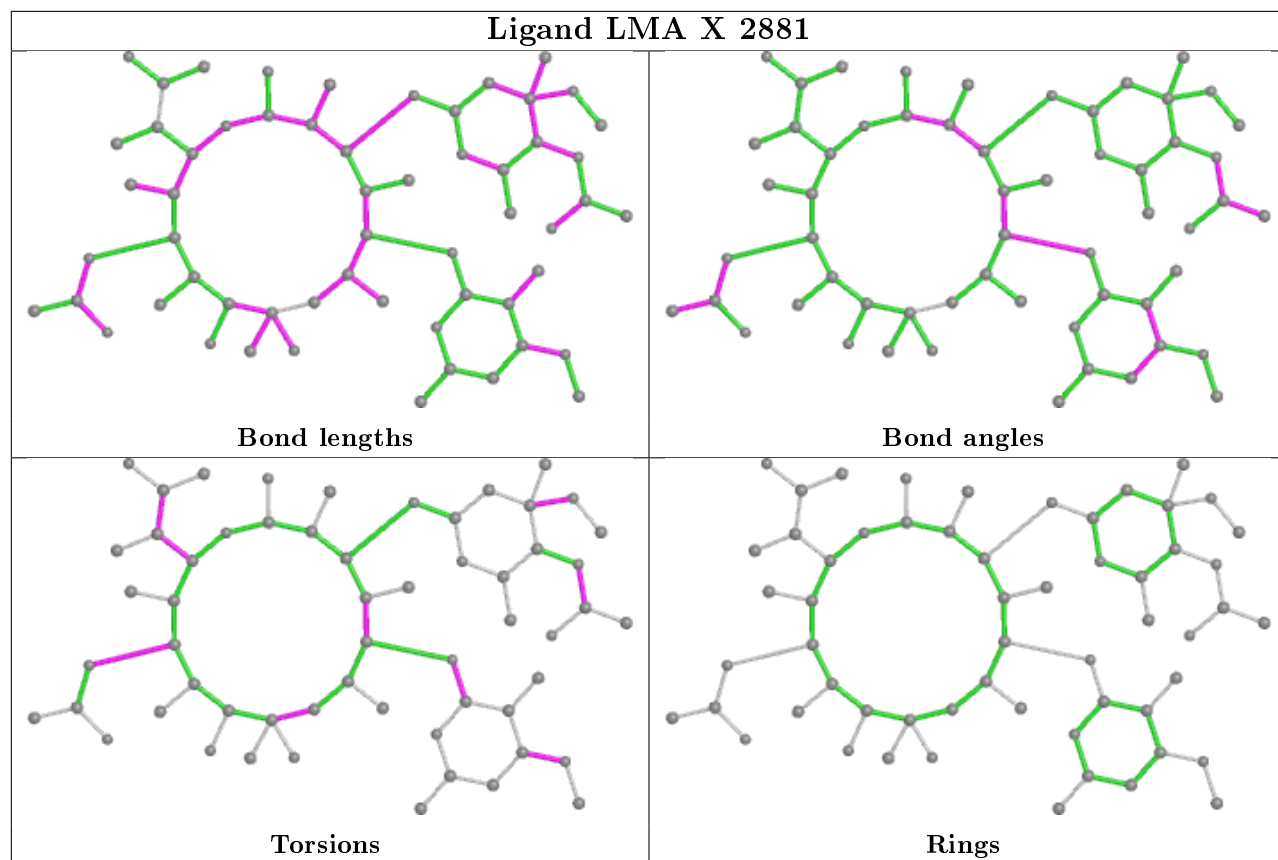
Mol	Chain	Res	Type	Atoms
31	X	2881	LMA	C3-C4-C5-O7
31	X	2881	LMA	C31-C4-C5-C6
31	X	2881	LMA	C12-C11-O12-C54
31	X	2881	LMA	C13-C36-C57-O57

There are no ring outliers.

1 monomer is involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	X	2881	LMA	13	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	X	2657/2880 (92%)	-0.13	75 (2%) 53 41	32, 91, 207, 392	0
2	Y	120/123 (97%)	0.08	2 (1%) 70 60	85, 155, 211, 300	0
3	A	253/274 (92%)	0.42	15 (5%) 22 15	54, 119, 183, 297	0
4	B	205/211 (97%)	-0.34	3 (1%) 73 64	22, 64, 130, 298	0
5	C	194/205 (94%)	0.19	14 (7%) 15 10	44, 117, 220, 268	0
6	D	177/180 (98%)	0.88	25 (14%) 2 2	146, 209, 280, 370	0
7	E	171/185 (92%)	0.24	11 (6%) 19 13	86, 149, 209, 245	0
8	F	63/144 (43%)	3.09	43 (68%) 0 0	180, 261, 394, 440	0
9	G	142/174 (81%)	0.27	8 (5%) 24 15	55, 101, 188, 266	0
10	H	134/134 (100%)	-0.48	1 (0%) 87 83	35, 61, 108, 204	0
11	I	134/156 (85%)	0.65	15 (11%) 5 4	64, 145, 237, 367	0
12	J	136/141 (96%)	0.17	7 (5%) 28 18	76, 108, 190, 272	0
13	K	113/116 (97%)	-0.65	0 100 100	27, 46, 79, 105	0
14	L	104/114 (91%)	0.54	11 (10%) 6 5	117, 160, 248, 306	0
15	M	108/166 (65%)	-0.33	3 (2%) 53 41	36, 60, 135, 241	0
16	N	117/118 (99%)	-0.12	4 (3%) 45 33	44, 88, 156, 279	0
17	O	94/100 (94%)	0.15	6 (6%) 19 13	58, 119, 195, 238	0
18	P	126/134 (94%)	-0.40	0 100 100	29, 59, 118, 200	0
19	Q	93/95 (97%)	0.04	2 (2%) 62 52	59, 107, 182, 273	0
20	R	110/115 (95%)	0.66	21 (19%) 1 1	68, 127, 234, 359	0
21	S	175/237 (73%)	0.93	34 (19%) 1 1	112, 169, 237, 314	0
22	T	74/91 (81%)	0.63	13 (17%) 1 1	82, 123, 199, 271	0
23	U	72/81 (88%)	1.79	20 (27%) 0 0	89, 155, 302, 332	0
24	V	65/67 (97%)	0.29	4 (6%) 20 13	94, 126, 205, 256	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	W	55/55 (100%)	0.08	2 (3%) 42 31	73, 102, 166, 177	0
26	Z	57/60 (95%)	-0.15	2 (3%) 44 32	31, 63, 108, 191	0
27	1	53/55 (96%)	1.55	17 (32%) 0 0	106, 171, 261, 319	0
28	2	46/47 (97%)	0.22	3 (6%) 18 12	56, 85, 154, 195	0
29	3	59/66 (89%)	1.58	21 (35%) 0 0	97, 150, 276, 316	0
30	4	37/37 (100%)	6.38	35 (94%) 0 0	133, 223, 289, 323	0
All	All	5944/6561 (90%)	0.16	417 (7%) 16 11	22, 105, 230, 440	0

The worst 5 of 417 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
23	U	28	GLY	25.4
30	4	25	VAL	14.2
8	F	113	PRO	14.0
30	4	17	VAL	13.9
30	4	24	LEU	12.9

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
33	NA	X	3064	1/1	0.72	0.27	58,58,58,58	0
34	K	X	3074	1/1	0.75	0.67	171,171,171,171	0
34	K	X	3076	1/1	0.76	0.36	100,100,100,100	0
32	MG	X	2891	1/1	0.78	0.20	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
33	NA	Y	126	1/1	0.80	0.40	85,85,85,85	0
33	NA	X	3061	1/1	0.81	0.55	62,62,62,62	0
32	MG	X	2939	1/1	0.83	0.56	79,79,79,79	0
32	MG	X	2931	1/1	0.83	0.59	48,48,48,48	0
33	NA	A	277	1/1	0.83	0.43	72,72,72,72	0
33	NA	X	3037	1/1	0.83	0.26	53,53,53,53	0
33	NA	X	3053	1/1	0.83	0.53	62,62,62,62	0
32	MG	X	2992	1/1	0.84	0.23	44,44,44,44	0
33	NA	X	3069	1/1	0.84	0.94	74,74,74,74	0
32	MG	X	3023	1/1	0.85	0.32	73,73,73,73	0
32	MG	X	2903	1/1	0.86	0.45	51,51,51,51	0
32	MG	X	2975	1/1	0.86	0.23	73,73,73,73	0
32	MG	X	2952	1/1	0.86	0.44	57,57,57,57	0
32	MG	X	2901	1/1	0.87	0.49	30,30,30,30	0
32	MG	X	2966	1/1	0.87	0.29	60,60,60,60	0
32	MG	X	2997	1/1	0.88	0.20	50,50,50,50	0
32	MG	X	2970	1/1	0.88	0.21	51,51,51,51	0
32	MG	X	2937	1/1	0.88	0.24	46,46,46,46	0
32	MG	X	3015	1/1	0.88	0.45	77,77,77,77	0
32	MG	I	157	1/1	0.88	0.35	50,50,50,50	0
33	NA	X	3036	1/1	0.88	0.26	79,79,79,79	0
32	MG	X	2978	1/1	0.89	0.42	48,48,48,48	0
33	NA	X	3046	1/1	0.89	0.59	80,80,80,80	0
32	MG	X	2928	1/1	0.89	0.40	41,41,41,41	0
33	NA	X	3058	1/1	0.89	0.35	69,69,69,69	0
32	MG	X	2934	1/1	0.90	0.20	62,62,62,62	0
32	MG	X	2918	1/1	0.90	0.21	60,60,60,60	0
33	NA	K	117	1/1	0.90	0.16	28,28,28,28	0
32	MG	X	3000	1/1	0.90	0.25	65,65,65,65	0
33	NA	X	3038	1/1	0.90	0.39	59,59,59,59	0
32	MG	X	2887	1/1	0.90	0.31	37,37,37,37	0
32	MG	X	3004	1/1	0.90	0.39	71,71,71,71	0
31	LMA	X	2881	58/58	0.90	0.27	22,83,114,128	0
33	NA	X	3067	1/1	0.91	0.29	47,47,47,47	0
33	NA	X	3063	1/1	0.91	0.38	50,50,50,50	0
32	MG	X	3019	1/1	0.91	0.41	74,74,74,74	0
32	MG	X	2894	1/1	0.91	0.24	33,33,33,33	0
33	NA	X	3057	1/1	0.91	0.89	75,75,75,75	0
32	MG	X	2988	1/1	0.91	0.29	63,63,63,63	0
33	NA	X	3050	1/1	0.91	0.30	40,40,40,40	0
32	MG	X	3014	1/1	0.91	0.36	54,54,54,54	0
34	K	X	3070	1/1	0.91	0.53	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	X	2979	1/1	0.92	0.60	50,50,50,50	0
33	NA	X	3052	1/1	0.92	0.25	43,43,43,43	0
32	MG	X	2940	1/1	0.92	0.25	34,34,34,34	0
32	MG	X	3022	1/1	0.92	0.14	43,43,43,43	0
32	MG	X	2883	1/1	0.92	0.33	34,34,34,34	0
32	MG	X	2910	1/1	0.92	0.29	47,47,47,47	0
32	MG	X	2961	1/1	0.92	0.36	61,61,61,61	0
32	MG	X	2916	1/1	0.92	0.30	51,51,51,51	0
33	NA	X	3066	1/1	0.92	0.42	48,48,48,48	0
32	MG	X	3018	1/1	0.92	0.40	59,59,59,59	0
32	MG	X	3010	1/1	0.92	0.43	73,73,73,73	0
32	MG	X	2923	1/1	0.92	0.52	66,66,66,66	0
32	MG	X	2985	1/1	0.92	0.17	50,50,50,50	0
32	MG	X	2907	1/1	0.93	0.48	66,66,66,66	0
33	NA	X	3062	1/1	0.93	0.14	47,47,47,47	0
32	MG	X	2949	1/1	0.93	0.41	48,48,48,48	0
32	MG	X	2925	1/1	0.93	0.35	72,72,72,72	0
32	MG	X	2930	1/1	0.93	0.53	51,51,51,51	0
32	MG	X	2950	1/1	0.93	0.25	49,49,49,49	0
33	NA	X	3039	1/1	0.93	0.28	51,51,51,51	0
32	MG	X	2914	1/1	0.93	0.61	60,60,60,60	0
32	MG	X	3032	1/1	0.93	0.37	74,74,74,74	0
32	MG	X	3028	1/1	0.93	0.18	65,65,65,65	0
33	NA	X	3056	1/1	0.93	0.70	76,76,76,76	0
33	NA	X	3049	1/1	0.93	0.49	68,68,68,68	0
34	K	X	3077	1/1	0.93	0.45	80,80,80,80	0
32	MG	X	2945	1/1	0.93	0.46	32,32,32,32	0
32	MG	X	3007	1/1	0.93	0.20	37,37,37,37	0
32	MG	X	3027	1/1	0.93	0.17	51,51,51,51	0
32	MG	X	2968	1/1	0.93	0.26	56,56,56,56	0
32	MG	X	2942	1/1	0.93	0.20	74,74,74,74	0
34	K	X	3079	1/1	0.93	0.47	97,97,97,97	0
32	MG	X	2963	1/1	0.94	0.27	69,69,69,69	0
32	MG	X	2921	1/1	0.94	0.23	52,52,52,52	0
33	NA	X	3044	1/1	0.94	0.09	48,48,48,48	0
32	MG	X	2953	1/1	0.94	0.21	59,59,59,59	0
32	MG	X	2984	1/1	0.94	0.29	62,62,62,62	0
32	MG	X	2895	1/1	0.94	0.35	19,19,19,19	0
32	MG	X	2957	1/1	0.94	0.40	35,35,35,35	0
33	NA	X	3035	1/1	0.94	0.30	50,50,50,50	0
34	K	X	3082	1/1	0.94	0.29	98,98,98,98	0
32	MG	X	2999	1/1	0.94	0.18	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
33	NA	X	3047	1/1	0.94	0.59	75,75,75,75	0
32	MG	X	2969	1/1	0.94	0.24	31,31,31,31	0
32	MG	X	2943	1/1	0.94	0.52	29,29,29,29	0
32	MG	X	2995	1/1	0.94	0.63	42,42,42,42	0
32	MG	X	2909	1/1	0.94	0.43	44,44,44,44	0
32	MG	X	2972	1/1	0.94	0.21	65,65,65,65	0
32	MG	X	2911	1/1	0.94	0.47	83,83,83,83	0
33	NA	Z	61	1/1	0.94	0.30	48,48,48,48	0
32	MG	X	2987	1/1	0.94	0.46	38,38,38,38	0
32	MG	X	3029	1/1	0.94	0.41	63,63,63,63	0
32	MG	X	2908	1/1	0.94	0.32	55,55,55,55	0
32	MG	X	3005	1/1	0.95	0.15	58,58,58,58	0
32	MG	X	2935	1/1	0.95	0.32	55,55,55,55	0
32	MG	X	3024	1/1	0.95	0.28	68,68,68,68	0
32	MG	X	2993	1/1	0.95	0.36	51,51,51,51	0
33	NA	X	3055	1/1	0.95	0.28	70,70,70,70	0
32	MG	X	2989	1/1	0.95	0.40	83,83,83,83	0
32	MG	X	2885	1/1	0.95	0.50	21,21,21,21	0
33	NA	X	3048	1/1	0.95	0.26	71,71,71,71	0
32	MG	X	3002	1/1	0.95	0.22	34,34,34,34	0
32	MG	X	2960	1/1	0.95	0.36	33,33,33,33	0
32	MG	X	2912	1/1	0.95	0.34	24,24,24,24	0
32	MG	X	2893	1/1	0.95	0.48	25,25,25,25	0
33	NA	X	3042	1/1	0.95	0.48	45,45,45,45	0
32	MG	X	2956	1/1	0.95	0.66	71,71,71,71	0
32	MG	X	2936	1/1	0.95	0.27	26,26,26,26	0
32	MG	X	2941	1/1	0.95	0.43	46,46,46,46	0
32	MG	X	3030	1/1	0.95	0.10	66,66,66,66	0
32	MG	X	3026	1/1	0.95	0.33	37,37,37,37	0
32	MG	X	2900	1/1	0.95	0.41	37,37,37,37	0
32	MG	X	2913	1/1	0.95	0.43	56,56,56,56	0
34	K	X	3072	1/1	0.95	0.21	104,104,104,104	0
32	MG	X	2983	1/1	0.95	0.26	23,23,23,23	0
34	K	X	3078	1/1	0.95	0.32	91,91,91,91	0
34	K	X	3075	1/1	0.95	0.22	68,68,68,68	0
33	NA	X	3059	1/1	0.95	0.13	66,66,66,66	0
32	MG	X	3008	1/1	0.95	0.25	45,45,45,45	0
32	MG	X	3003	1/1	0.95	0.48	55,55,55,55	0
32	MG	X	2922	1/1	0.95	0.18	19,19,19,19	0
32	MG	X	2998	1/1	0.96	0.38	29,29,29,29	0
32	MG	X	2964	1/1	0.96	0.44	50,50,50,50	0
32	MG	X	2994	1/1	0.96	0.10	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	X	2920	1/1	0.96	0.36	31,31,31,31	0
32	MG	X	2944	1/1	0.96	0.35	59,59,59,59	0
33	NA	X	3051	1/1	0.96	0.24	43,43,43,43	0
32	MG	X	2947	1/1	0.96	0.39	47,47,47,47	0
32	MG	Y	124	1/1	0.96	0.11	40,40,40,40	0
32	MG	X	3021	1/1	0.96	0.54	70,70,70,70	0
33	NA	X	3034	1/1	0.96	0.31	50,50,50,50	0
32	MG	X	2976	1/1	0.96	0.24	32,32,32,32	0
32	MG	X	2892	1/1	0.96	0.22	30,30,30,30	0
32	MG	X	2990	1/1	0.96	0.39	31,31,31,31	0
32	MG	X	2919	1/1	0.96	0.35	61,61,61,61	0
34	K	X	3071	1/1	0.96	0.23	86,86,86,86	0
32	MG	X	2971	1/1	0.96	0.24	44,44,44,44	0
33	NA	X	3065	1/1	0.96	0.38	58,58,58,58	0
32	MG	X	2977	1/1	0.96	0.32	51,51,51,51	0
33	NA	X	3041	1/1	0.96	0.30	37,37,37,37	0
32	MG	X	2933	1/1	0.96	0.49	59,59,59,59	0
32	MG	X	3012	1/1	0.96	0.57	45,45,45,45	0
34	K	X	3083	1/1	0.96	0.28	103,103,103,103	0
32	MG	X	2974	1/1	0.96	0.18	37,37,37,37	0
32	MG	X	2982	1/1	0.96	0.48	51,51,51,51	0
32	MG	X	2962	1/1	0.96	0.13	70,70,70,70	0
32	MG	X	2897	1/1	0.96	0.36	37,37,37,37	0
34	K	X	3081	1/1	0.97	0.36	91,91,91,91	0
32	MG	X	3001	1/1	0.97	0.46	84,84,84,84	0
32	MG	X	3020	1/1	0.97	0.35	42,42,42,42	0
33	NA	X	3043	1/1	0.97	0.31	48,48,48,48	0
32	MG	X	2981	1/1	0.97	0.47	65,65,65,65	0
32	MG	X	2926	1/1	0.97	0.17	35,35,35,35	0
32	MG	X	2927	1/1	0.97	0.21	55,55,55,55	0
32	MG	X	3013	1/1	0.97	0.11	60,60,60,60	0
32	MG	X	2884	1/1	0.97	0.54	38,38,38,38	0
32	MG	X	2965	1/1	0.97	0.31	42,42,42,42	0
34	K	X	3080	1/1	0.97	0.49	94,94,94,94	0
33	NA	Y	125	1/1	0.97	0.44	62,62,62,62	0
32	MG	X	3011	1/1	0.97	0.55	45,45,45,45	0
32	MG	X	2955	1/1	0.97	0.37	54,54,54,54	0
33	NA	X	3054	1/1	0.97	0.38	49,49,49,49	0
32	MG	X	2882	1/1	0.97	0.33	5,5,5,5	0
34	K	X	3073	1/1	0.97	0.39	57,57,57,57	0
33	NA	X	3033	1/1	0.97	0.44	38,38,38,38	0
32	MG	X	2905	1/1	0.97	0.37	57,57,57,57	0

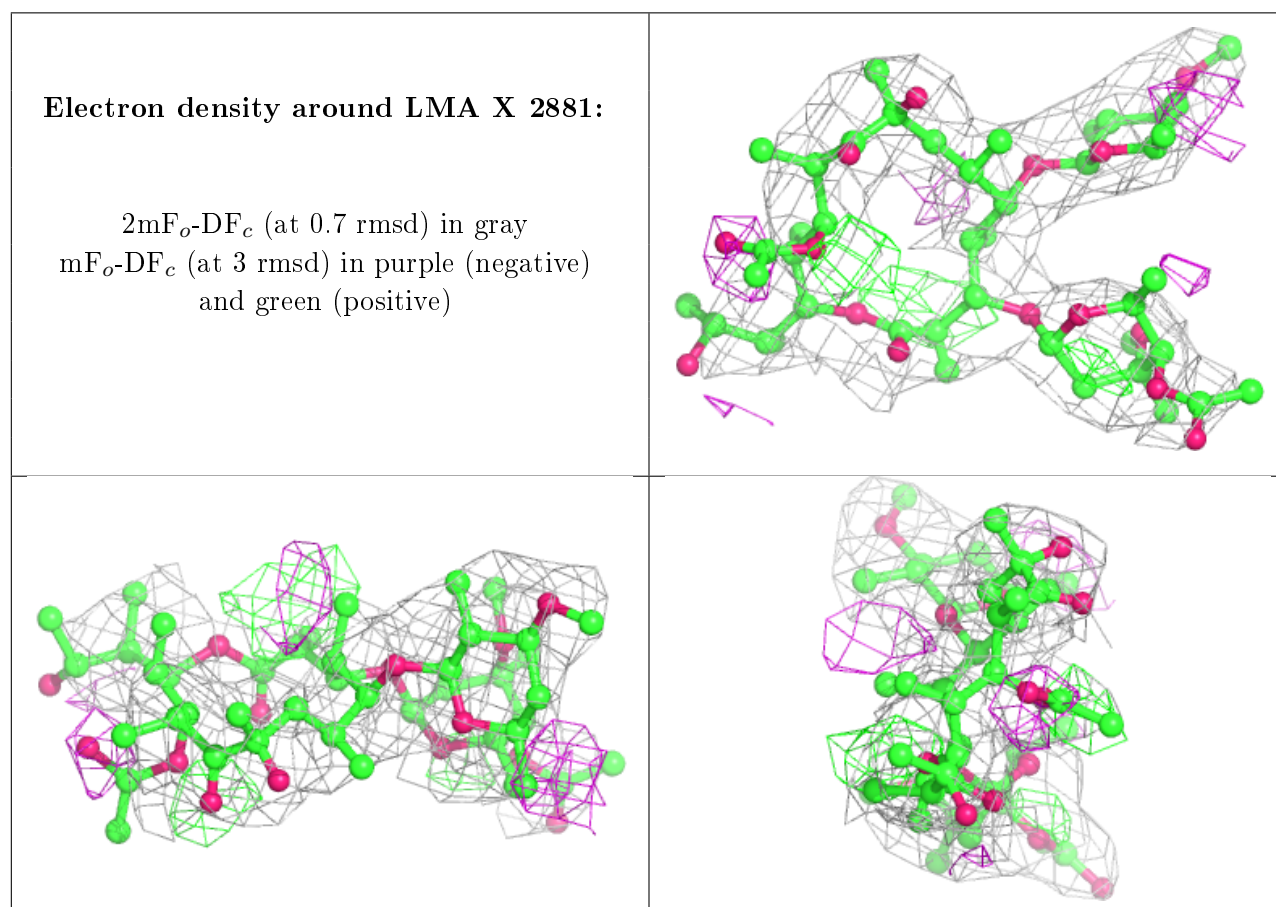
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	X	2899	1/1	0.97	0.30	57,57,57,57	0
32	MG	X	2948	1/1	0.97	0.43	40,40,40,40	0
32	MG	X	2902	1/1	0.97	0.35	39,39,39,39	0
32	MG	X	3016	1/1	0.97	0.35	39,39,39,39	0
32	MG	X	2889	1/1	0.97	0.26	26,26,26,26	0
32	MG	X	2915	1/1	0.97	0.55	47,47,47,47	0
34	K	M	167	1/1	0.97	0.38	44,44,44,44	0
32	MG	X	2958	1/1	0.97	0.10	29,29,29,29	0
32	MG	X	3009	1/1	0.97	0.24	53,53,53,53	0
32	MG	X	2906	1/1	0.97	0.39	43,43,43,43	0
32	MG	X	3017	1/1	0.97	0.51	70,70,70,70	0
32	MG	X	2924	1/1	0.98	0.31	26,26,26,26	0
32	MG	X	3025	1/1	0.98	0.19	62,62,62,62	0
32	MG	X	2904	1/1	0.98	0.49	39,39,39,39	0
33	NA	X	3068	1/1	0.98	0.31	64,64,64,64	0
32	MG	X	2896	1/1	0.98	0.41	28,28,28,28	0
32	MG	X	2959	1/1	0.98	0.40	33,33,33,33	0
32	MG	X	2946	1/1	0.98	0.45	38,38,38,38	0
32	MG	X	2886	1/1	0.98	0.36	16,16,16,16	0
33	NA	X	3060	1/1	0.98	0.70	73,73,73,73	0
32	MG	X	3006	1/1	0.98	0.07	59,59,59,59	0
32	MG	X	2938	1/1	0.98	0.40	34,34,34,34	0
33	NA	X	3045	1/1	0.98	0.45	31,31,31,31	0
32	MG	X	2954	1/1	0.98	0.30	31,31,31,31	0
32	MG	X	2991	1/1	0.98	0.38	51,51,51,51	0
32	MG	X	2967	1/1	0.98	0.31	50,50,50,50	0
32	MG	X	3031	1/1	0.98	0.15	48,48,48,48	0
32	MG	X	2986	1/1	0.98	0.26	54,54,54,54	0
32	MG	C	206	1/1	0.98	0.20	37,37,37,37	0
33	NA	X	3040	1/1	0.98	0.41	70,70,70,70	0
32	MG	X	2973	1/1	0.98	0.22	30,30,30,30	0
32	MG	X	2888	1/1	0.98	0.46	36,36,36,36	0
32	MG	X	2996	1/1	0.98	0.08	42,42,42,42	0
32	MG	X	2980	1/1	0.99	0.12	42,42,42,42	0
32	MG	X	2929	1/1	0.99	0.32	10,10,10,10	0
32	MG	X	2890	1/1	0.99	0.24	38,38,38,38	0
32	MG	X	2898	1/1	0.99	0.39	8,8,8,8	0
32	MG	X	2932	1/1	0.99	0.36	31,31,31,31	0
32	MG	X	2917	1/1	0.99	0.27	52,52,52,52	0
32	MG	X	2951	1/1	0.99	0.36	28,28,28,28	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.



## 6.5 Other polymers ⓘ

There are no such residues in this entry.