



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 28, 2023 – 11:49 PM EDT

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](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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.35  
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) : 2.35

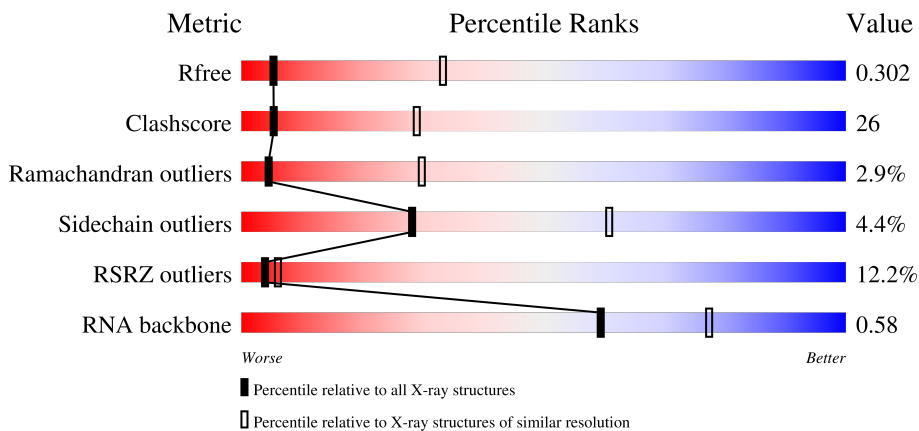
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

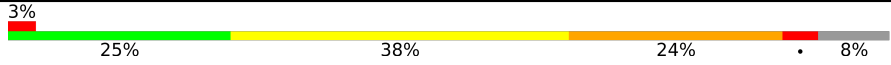


The reported resolution of this entry is 3.45 Å.

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 of 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	
2	Y	123	
3	A	274	



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Mol	Chain	Length	Quality of chain
4	B	211	4% 48% 43% 5% ..
5	C	205	5% 49% 39% 6% 5%
6	D	180	43% 60% 38% ..
7	E	185	8% 69% 22% .. 8%
8	F	144	42% 30% 12% . 56%
9	G	174	12% 39% 36% 6% . 18%
10	H	134	% 45% 52% .
11	I	156	20% 51% 29% 6% . 14%
12	J	141	18% 48% 45% . .
13	K	116	% 40% 53% . .
14	L	114	11% 46% 39% 5% 9%
15	M	166	% 28% 34% . 35%
16	N	118	10% 49% 47% ..
17	O	100	16% 48% 43% . 6%
18	P	134	% 43% 49% . 6%
19	Q	95	26% 62% 28% 7% .
20	R	115	46% 49% 39% 6% ..
21	S	237	13% 47% 24% . 26%
22	T	91	25% 51% 30% . 19%
23	U	81	23% 48% 33% 7% 11%
24	V	67	9% 76% 19% ..
25	W	55	22% 51% 49%
26	Z	60	2% 48% 42% 5% 5%
27	1	55	62% 18% 60% 16% ..
28	2	47	11% 47% 40% 11% .

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Mol	Chain	Length	Quality of chain
29	3	66	 <p>79%</p> <p>36% 44% 9% 11%</p>
30	4	37	 <p>89%</p> <p>62% 35%</p>

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 [i](#)

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
			Total	C	N	O	P			
1	X	2644	56750	25314	10473	18320	2643	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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	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
			Total	C	N	O	S			
28	2	46	Total 383	C 230	N 91	O 60	S 2	0	0	0

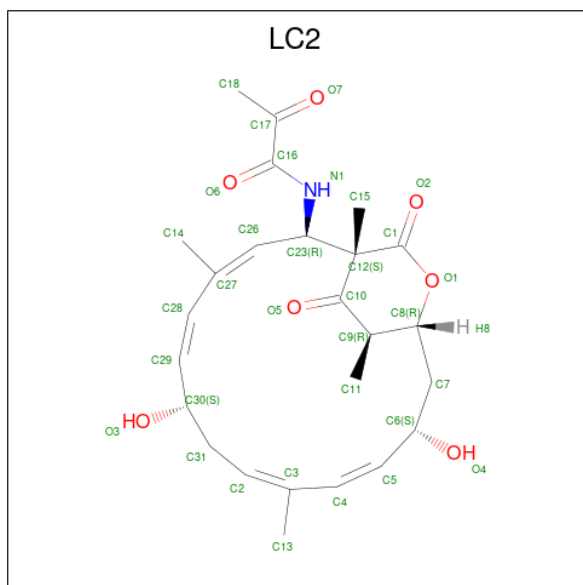
- Molecule 29 is a protein called 50S ribosomal protein L35.

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

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

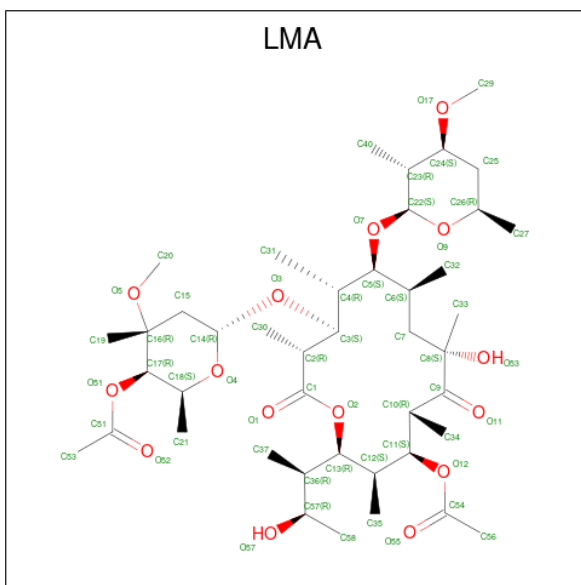
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
30	4	37	Total 297	C 179	N 66	O 47	S 5	0	0	0

- 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: C<sub>25</sub>H<sub>33</sub>NO<sub>7</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
31	X	1	Total 33	C 25	N 1	O 7	0	0

- Molecule 32 is Lankamycin (three-letter code: LMA) (formula: C<sub>43</sub>H<sub>74</sub>O<sub>15</sub>).



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).

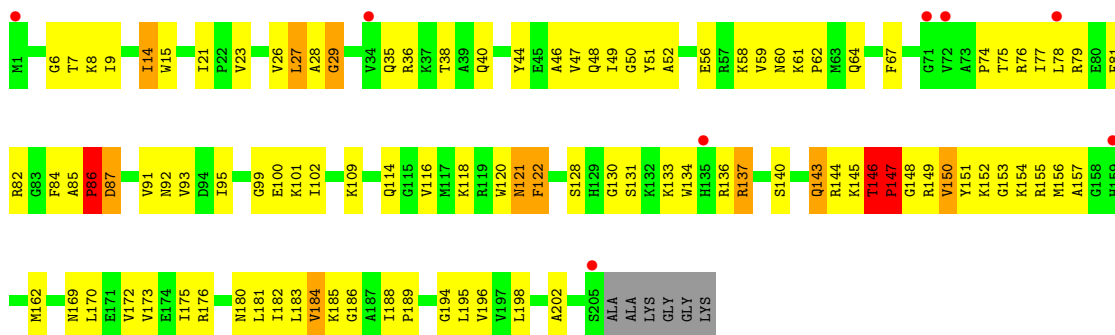
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	X	5	Total	Na	0	0
			5	5		



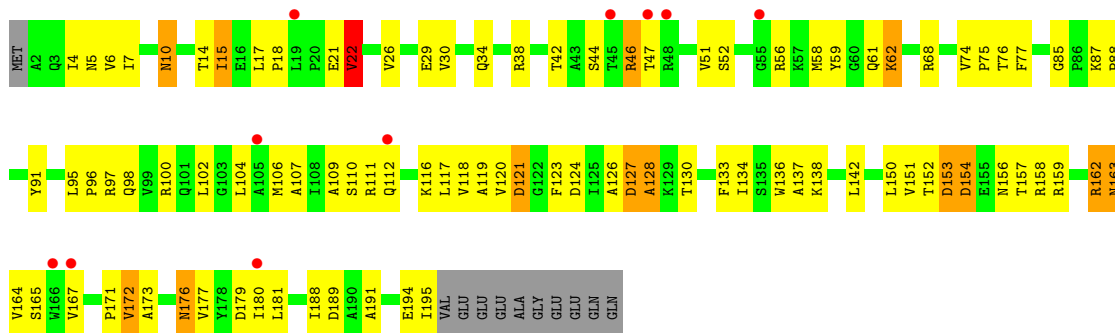
U1608	A1534	C1466	A1314	G1253	U1124	A1059	A922	G928	A862	A796	G734	A668
G1609	C1535	A1457	A1315	G1254	G1125	C1060	C993	G931	C863	A797	G735	G669
A1610	G1536	A1458	G1316	A1255	A1126	G1062	A994	C932	C864	C799	G736	U670
G1613	U1539	U1459	G1317	C1256	C1127	A1063	A995	C933	A865	C799	G737	A671
C1614	A1540	G1460	A1318	U1257	A1128	C1064	C996	C934	C869	A801	G738	C672
C1615	G1541	G1461	G1322	G1258	G1129	C1065	C997	G935	C870	A802	G739	C673
C1616	A1542	A1462	G1323	A1259	U1130	A1065	C998	C936	U871	A803	G740	U674
C1617	G1543	A1463	G1324	A1260	G1131	G1066	A999	A937	C803	C803	G741	
U1618	A1544	U1261	G1325	G1261	C1135	A1068	G1000	C937	C804	C804	G742	C679
A1619	G1545	U1262	U1326	U1263	G1136	A1069	A1001	A938	U872	C805	G743	U680
C1620	U1548	U1263	G1327	G1264	A1137	U1070	U1005	C939	U873	A806	G744	A681
G1621	C1549	G1467	C1328	G1265	U1071	U1071	C1006	U941	A874	A807	G745	G682
G1622	A1550	U1468	U1329	G1266	U1072	U1072	A1007	U942	A875	C808	G746	A683
C1623	U1551	A1469	G1330	A1267	G1073	G1073	G1008	U943	C877	C809	A747	C684
A1624	C1552	G1470	A1331	U1268	G1141	G1074	G1008	A944	C878	U810	A748	U685
A1625	U1553	G1471	G1332	G1269	G1142	G1075	C1009	A945	A879	G811	A749	C686
C1626	G1554	U1472	A1333	C1270	A1143	U1075	U1010	U946	A883	G812	C750	G687
G1628	G1559	U1473	A1334	C1271	U1144	U1076	U1011	C947	C884	A815	G752	A688
C1629	A1560	U1474	G1335	G1272	C1145	U1077	A1012	C948	C885	U816	G753	A690
A1630	A1561	G1476	A1336	A1273	G1146	A1078	U1015	C949	A886	A817	G754	C691
C1631	U1562	U1477	G1337	C1274	G1147	A	C1016	G950	A887	G818	C755	C692
A1632	G1563	U1478	A1338	A1275	G1148	A1081	C1017	C951	C888	C819	C756	A693
C1633	U1564	G1479	A1339	U1276	C1150	G1082	C1018	C952	C889	U820	G757	G694
A1634	G1565	U1480	G1341	C1277	U1151	C1083	U1019	U954	U890	A821	G758	G695
G1635	G1566	U1481	U1342	A1278	C1152	G1085	A1020	C955	A	C822	C759	U686
C1636	U1567	U1482	C1343	U1279	C1153	C1086	A1021	C956	G	U823	G760	G697
U1637	A1568	G1483	C1344	U1280	A1154	C1087	A1022	C957	G	U824	G761	A698
G1638	U1569	U1484	A1345	A1281	G1149	A1088	G1083	C958	C	U825	G762	G699
C1641	A1570	G1485	G1346	A1282	C1150	C1089	U1023	C959	G	U826	A763	C700
G1642	C1571	U1486	U1347	C1283	U1151	C1090	G1028	U960	C	C827	G764	U701
A1643	U1572	U1425	C1348	G1284	A1158	C1091	C1029	C961	C	C828	C765	A702
G1644	A1573	U1426	G1351	A1285	U1159	C1092	C1030	C962	C	C829	A766	A703
U1645	U1574	G	A1354	U1286	C1160	U1093	C1031	C963	U	C830	G767	G704
C1646	A1575	A1428	A1355	A1287	C1163	C1094	A1032	A964	A	C831	G768	C705
U1647	G1576	U1429	G1356	A1288	C1164	A1095	G1033	C965	C	A832	C769	A706
C1648	U1577	U1430	U1357	A1289	G1165	A1096	U1034	C966	C	A833	U770	U707
A1649	A1578	G1431	A1358	A1290	A1166	A1097	G1035	C967	A	A834	C771	G708
C1650	U1579	U1432	C1359	G1291	A1167	C1098	G1036	C968	G	U835	G772	A709
U1651	C1580	U1433	G1364	A1292	C1168	A1099	U1037	C969	C	G836	G773	
A1581	A1581	G1435	U1365	A1293	C1169	U1100	U1038	U970	U	U837	A774	A712
A1582	U1582	U1436	U1366	G1294	U1170	G1101	G1041	C971	U	U838	U775	G713
A1583	A1583	A1437	U1367	A1295	A1171	G1102	G1042	C972	U	U839	G776	G714
G1584	U1584	G1438	U1368	G1296	U1172	C1103	U1043	C973	C	U840	A777	U715
A1585	A1585	U1439	A1369	A1297	G1173	G1104	A1044	C974	C	U841	G778	U716
A1586	U1586	G1440	U1370	A1298	U1174	A1107	U1044	C975	A911	A842	G779	G717
A1587	A1587	U1441	G1371	A1299	U1175	U1108	G1045	C976	C	G843	U780	A718
U1589	U1589	A1442	U1374	A1300	U1177	U1109	U1046	C977	C	G844	G781	A719
C1589	C1589	G1443	G1377	U1301	C1178	G1111	U1047	C978	C	U845	U782	A720
C1590	C1590	C1444	A1378	U1304	A1179	G1112	U1048	C979	C	U846		
C1591	C1591	A1445	A1379	C1305	A1180	A1114	C1049	C980	C	U849	U786	C724
C1661	C1661	U1446	A1378	C1306	C1181	C1115	G1050	C981	C	C850	A787	C725
C1662	C1662	U1447	A1379	U1307	U1182	C1118	C1051	C982	U	C851	G788	G
G1601	G1601	A1448	A1380	U1308	C1183	C1119	C1052	C983	G	U852	G789	U
A1602	A1602	C1449	G1381	C1309	C	U1118	G1053	C984	A	A923	A790	G
A1603	A1603	U1449	U1382	G1310	C	U1119	C1064	C985	A	U857	G791	G
A1604	A1604	G1450	G1383	C1311	C	C1120	C1064	C986	C	C858	U792	C
A1605	A1605	U1451	C1384	C1312	G	U1121	A	C987	C	U859	G793	A
C1606	C1606	U1452	C1385	U1313	A	A1122	U	C987	C	U860	A794	G732
A1669	A1669	G1533	C1385	U1313	A	C1252	G1058	A991	C	U861	A795	G733

G1670	A1796	U1937	A1987	U2059	U1912	G2360	G2336	G2407	U2471	G2581
A1671	C1797	U1938	A1988	A2060	C2193	G2260	A2337	G2408	U2472	G2582
C1672	G1798	U1939	A1989	A2061	A2194	G2261	C2338	G2409	G2473	G2583
C1673	A1799	C1940	U2000	U2062	C2195	C2262	A2339	A2409	G2474	U2584
C1674	G1736	C1941	G2001	U2063	U2196	C2263	G2340	A2410	G2475	C2585
C1675	U1737	C1942	A2002	A2064	U2197	A2264	G2341	A2411	A2476	G2586
U1676	C1801	A1943	A2003	A2065	U2198	A2265	U2342	A2412	C2477	G2587
C1677	A1802	C1944	U2004	G2066	C2199	A2266	G2343	A2413	C2478	C2588
C1678	G1803	C1945	U2005	C2067	G2200	G2267	G2344	A2414	U2479	G2589
C1679	A1804	U1946	G2006	U2068	G2201	G2268	A2345	G2415	C2480	A2590
U1680	G1805	C1947	G2007	G2071	G2202	G2269	G2346	G2416	G2481	G2591
A1681	C1806	U1948	C2008	A2072	G2203	U2270	A2347	A2417	U2482	U2592
G1682	A1807	C1949	U2009	A2073	G2204	A2271	A2348	A2418	U2483	C2593
G1683	C1808	C1950	G2010	U2074	C2205	G2272	G2349	A2419	G2484	G2594
G1684	G	U1951	U2011	U2075	C2206	C2273	G2350	G2420	G2485	G2595
A1685	A1810	A1952	A2012	G2082	G2207	C2274	G2351	G2421	U2486	G2596
A1686	U1748	A1953	A2013	G2083	G2208	U2275	A2352	G2422	U2487	C2597
C1687	U1749	C1954	A2014	G2084	U2209	C2276	A2353	G2423	G2488	G2598
U1688	A1813	A1955	A2015	G2085	G2210	A2277	G2354	G2424	U2489	C2599
U1689	A1814	G1956	G2016	G2086	U2211	A2278	A2355	A2425	U2490	G2600
U1690	G1815	C1957	A2017	U2086	G2216	G2282	A2356	A2426	C2491	G2601
C1691	A1816	U1958	U2018	U	G2217	U2283	A2357	A2427	U2492	G2602
C1692	U1817	C1959	C2019	U	G2218	U2284	G2362	A2428	U2493	G2603
A1693	G1818	U1960	A2020	C	G2219	U2285	G2363	A2429	U2494	G2604
U1694	U1819	A1961	G2021	U	U2220	G2286	C2364	A2430	U2495	G2605
U1695	C1756	C1962	C2022	C	U2221	G2287	U2365	A2431	U2496	G2606
U1696	C1757	C1963	C2023	U	U2222	A2288	U2366	A2432	U2497	G2607
U1697	C1758	A1964	U2024	U	U2223	A2289	U2367	A2433	U2498	G2608
U1698	C1759	C1965	A2025	G	U2224	A2290	U2368	A2434	U2499	G2609
U1699	C1760	U1967	C2026	C	U2225	U2291	A2372	A2435	U2500	G2610
C1700	C1828	U1968	U2030	A	G2226	G2292	C2373	A2436	U2501	G2611
C1701	C1829	C1969	A2031	U	C2227	U2294	C2374	A2437	U2502	G2612
C1702	C1830	G1970	G2032	G	U2228	C2295	G2375	U2441	G2603	G2613
C1703	G1831	C1971	C2033	A	U2229	C2296	G2376	U2442	G2604	G2614
G1704	G1831	G1972	A2034	C	U2230	U2298	U2377	U2443	G2605	G2615
U1705	U1768	C1973	G2035	C	U2231	U2299	U2378	U2444	G2606	G2616
A1706	U1769	C1974	G2036	C	U2232	U2300	U2379	U2445	G2607	G2617
U1707	U1770	U1974	G2037	G	G2233	G2301	U2380	U2446	G2608	G2618
C1708	A1771	U1975	A2037	U	G2234	A2302	U2381	G2447	G2609	G2619
U1709	C1772	U1976	C2038	U	G2235	C2303	C2382	G2448	A2510	G2620
U1710	C1773	C1977	G2039	G	C2237	C2304	C2383	G2449	G2511	G2621
C1711	A1774	U1978	A2040	C	G2238	C2305	C2384	G2450	A2512	G2622
G1712	A1775	U1979	A2041	C	C2239	U2298	U2385	G2451	G2513	G2623
G1713	G1841	C1979	A2042	A	C2240	U2299	U2386	G2452	G2514	G2624
A1714	G1842	A1980	A2043	G	U2241	U2300	U2387	G2453	G2515	G2625
G1716	C1844	C1982	A2044	C	C2242	A2314	G2392	C2454	U2516	G2626
G1717	C1844	G1983	A2045	C	C2243	A2315	G2393	C2455	C2517	G2627
A1717	G1847	A1984	C2046	U	C2244	G2316	G2394	U2456	C2518	G2628
G1718	G1847	C1985	C2047	C	A2245	U2317	C2395	A2457	C2519	G2629
G1719	C1851	G1986	C2048	C	A2246	U2318	G2396	U2458	A2520	G2630
G1720	C1852	C1987	C2049	C	A2247	G2324	A2397	U2459	A2521	G2631
U1721	C1853	A1988	G2050	A	U2251	A2325	U2398	G2459	G2522	G2632
U1722	U1787	C1989	U2051	A	U2252	C2326	C2399	C2460	G2523	G2633
U1723	C1788	U1990	G2052	A	A2253	U2327	G2400	G2461	G2524	G2634
C1724	U1789	C1991	G2053	C	U2254	G2328	A2401	G2462	G2525	G2635
C1725	U1790	G1992	A2054	U	A2255	G2329	U2402	G2463	U2526	G2636
C1726	C1866	C1993	G2055	G	G2256	G2330	C2403	G2464	G2527	G2637
G1730	A1867	U1994	C2056	G	A2257	A2331	A2404	G2465	U2528	G2638
A1869	A1935	G1995	U2057	C	A2190	G2335	A2405	G2466	G2529	G2639
	A1869	A1996	U2058	C	A2191	G2259			C2530	

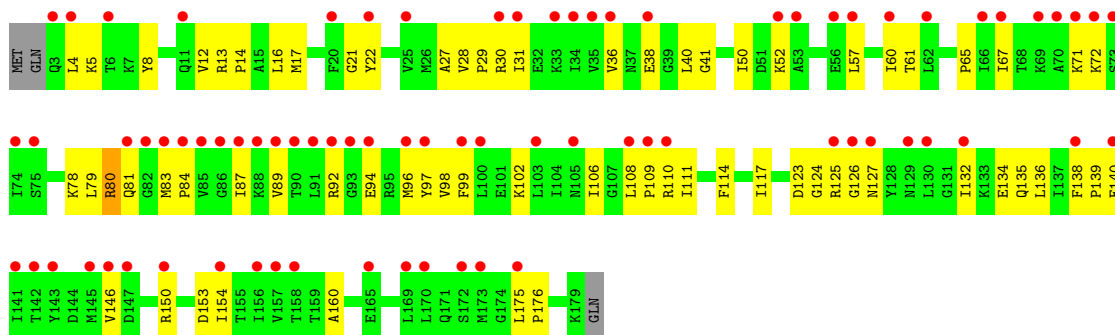
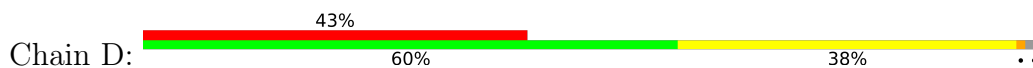




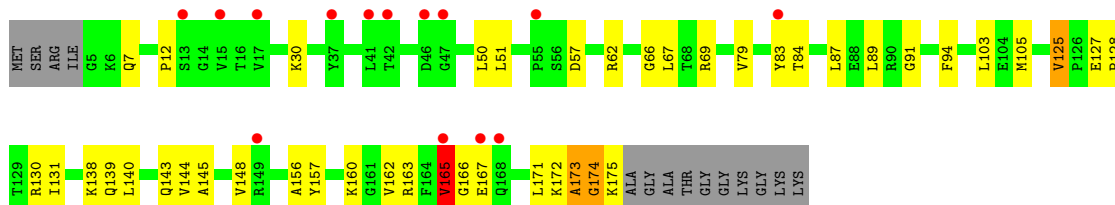
- Molecule 5: 50S ribosomal protein L4



- Molecule 6: 50S ribosomal protein L5

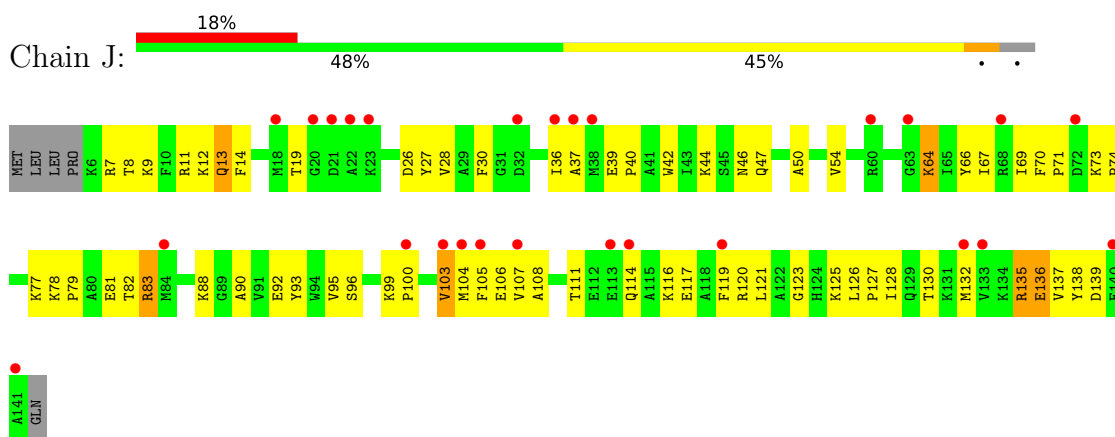


- Molecule 7: 50S ribosomal protein L6

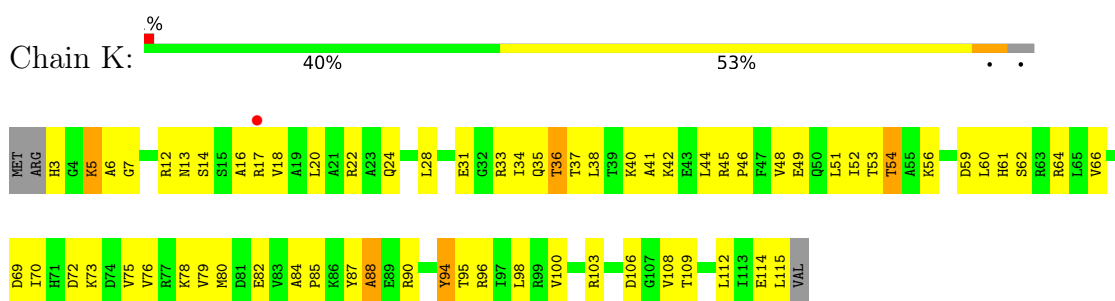




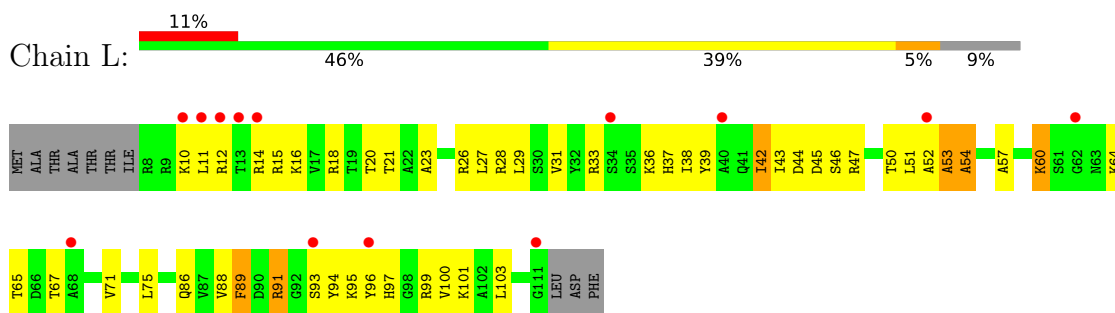




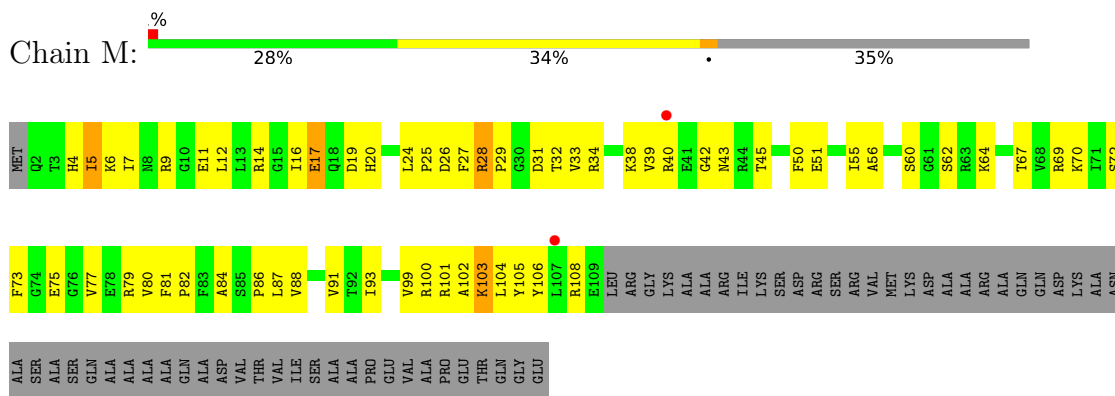
- Molecule 13: 50S ribosomal protein L17



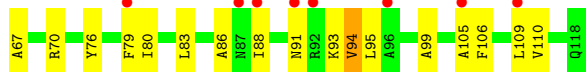
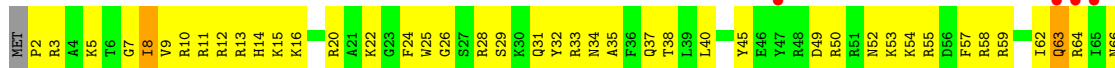
- Molecule 14: 50S ribosomal protein L18



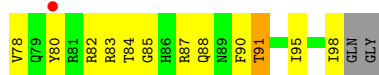
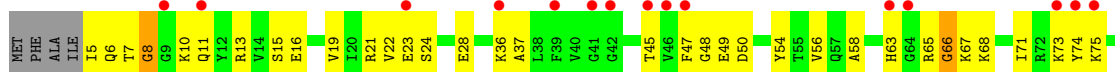
- Molecule 15: 50S ribosomal protein L19



- Molecule 16: 50S ribosomal protein L20



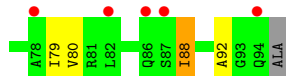
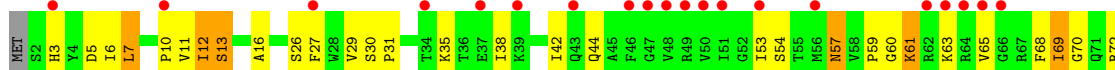
- Molecule 17: 50S ribosomal protein L21



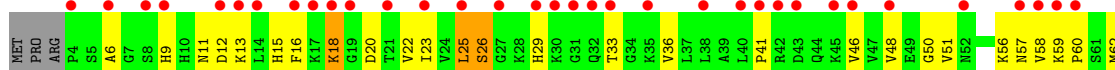
- Molecule 18: 50S ribosomal protein L22

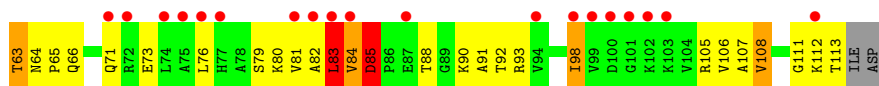


- Molecule 19: 50S ribosomal protein L23

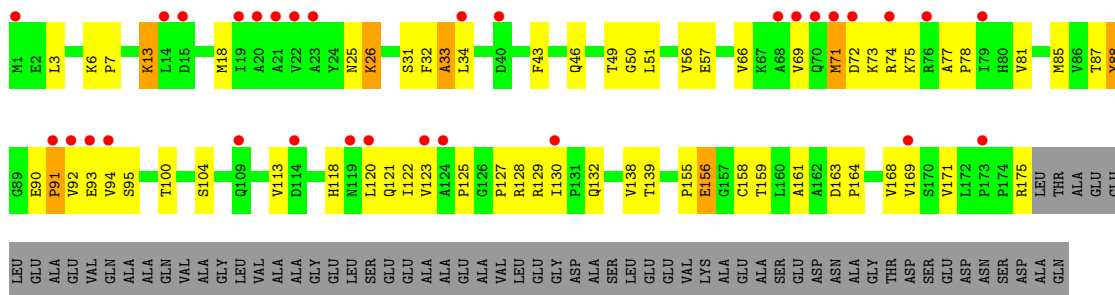


- Molecule 20: 50S ribosomal protein L24

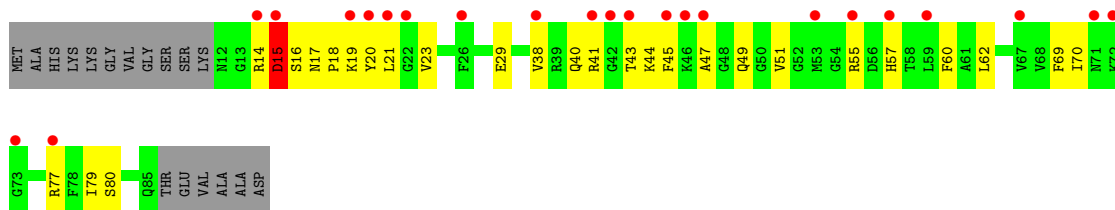




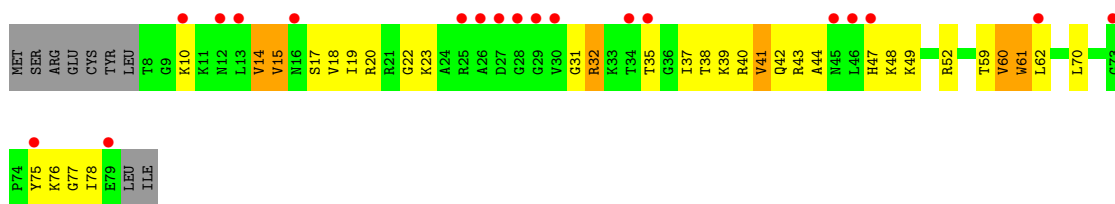
- Molecule 21: 50S ribosomal protein L25



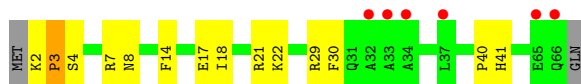
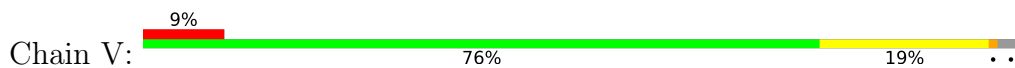
- Molecule 22: 50S ribosomal protein L27



- Molecule 23: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L29



- Molecule 25: 50S ribosomal protein L30





- Molecule 26: 50S ribosomal protein L32



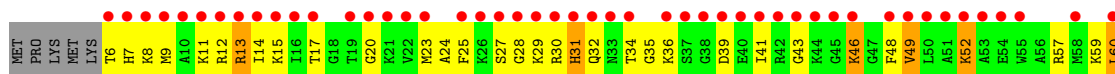
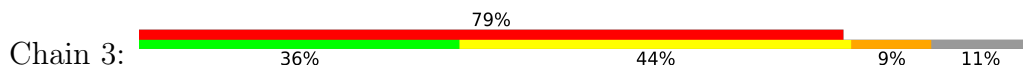
- Molecule 27: 50S ribosomal protein L33



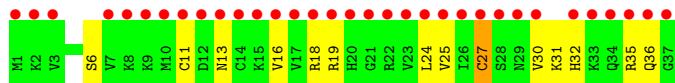
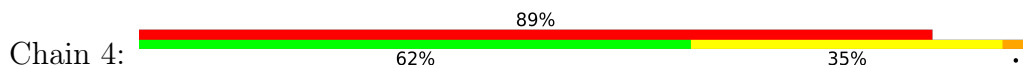
- Molecule 28: 50S ribosomal protein L34



- 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 3.41Å)	Xtrriage
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 <sup>2</sup> )	86.0	Xtrriage
Anisotropy	0.732	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.20 , 76.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	83963	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	138.0	wwPDB-VP

Xtrriage'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.*

<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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: K, NA, LC2, LMA, MG

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 [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
13	K	94	TYR
29	3	52	LYS
19	Q	7	LEU
29	3	49	VAL
27	1	51	ARG

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

Mol	Chain	Res	Type
18	P	82	ASN
21	S	121	GLN
24	V	54	ASN
23	U	47	HIS
6	D	127	ASN

### 5.3.3 RNA [i](#)

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	2245	A
1	X	2842	C
1	X	2404	A
1	X	2705	A
1	X	1031	C

#### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

#### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

#### 5.6 Ligand geometry [i](#)

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
31	LC2	X	2881	-	29,34,34	1.82	6 (20%)	26,49,49	1.18	2 (7%)
32	LMA	X	2882	-	58,60,60	4.94	27 (46%)	75,90,90	1.30	6 (8%)

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

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
31	X	2881	LC2	C12-C23-C26-C27
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

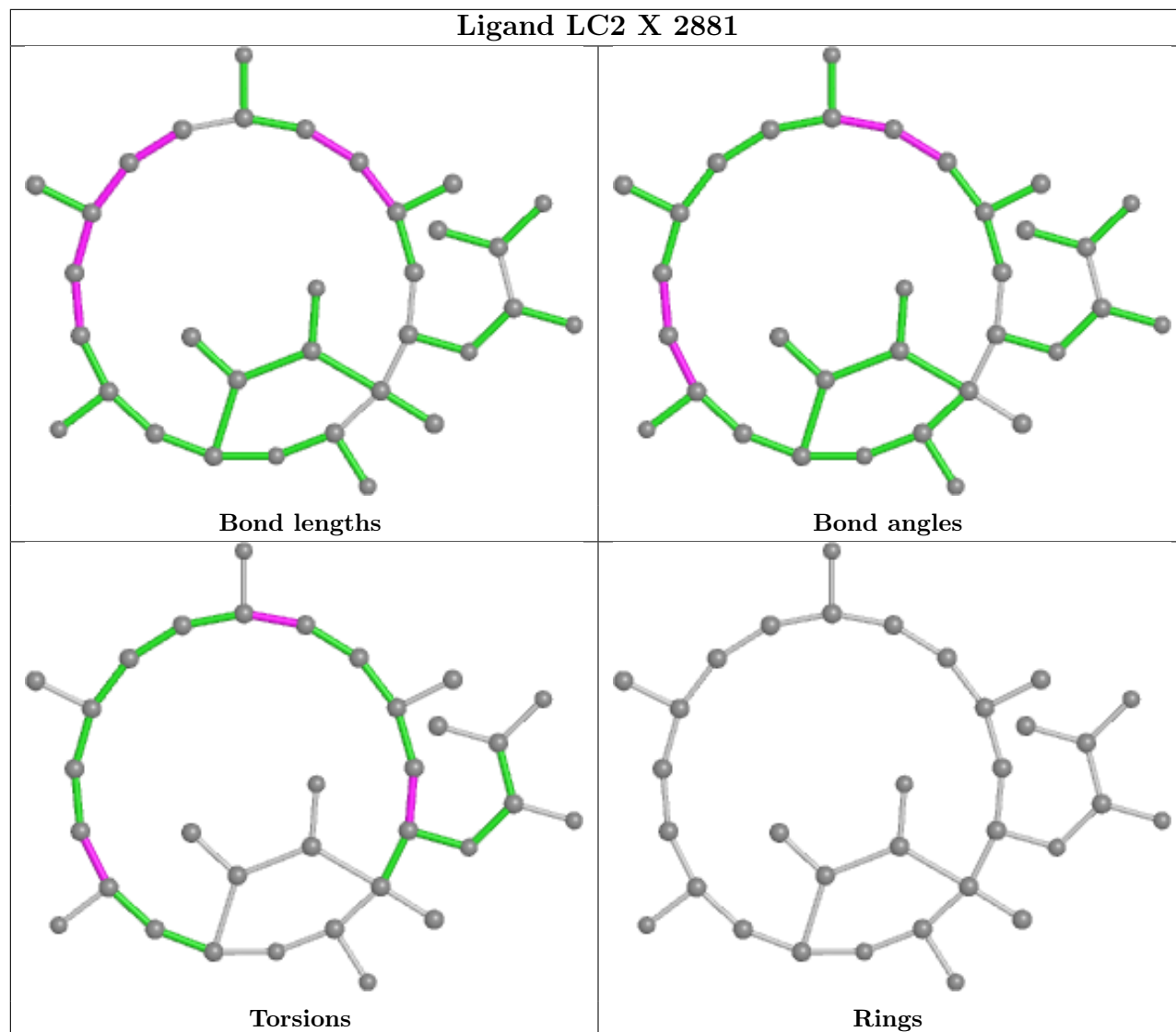
There are no ring outliers.

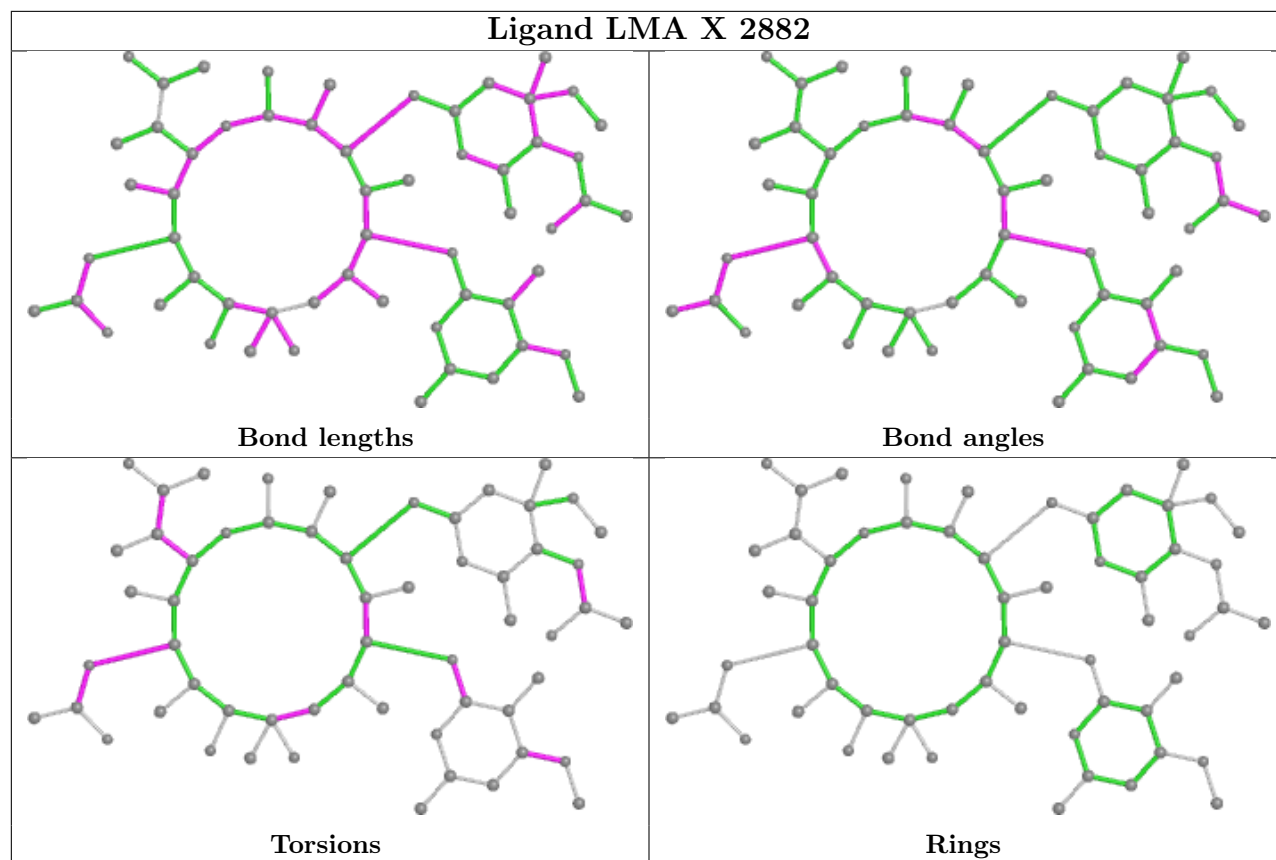
2 monomers are involved in 61 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	X	2881	LC2	18	0
32	X	2882	LMA	43	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.



## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	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 <sup>2</sup> )	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 [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	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(Å <sup>2</sup> )	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
33	MG	X	2926	1/1	0.79	0.45	67,67,67,67	0
35	NA	X	2962	1/1	0.79	1.12	98,98,98,98	0
33	MG	X	2909	1/1	0.80	0.17	58,58,58,58	0
32	LMA	X	2882	58/58	0.80	0.38	120,120,120,120	0
33	MG	X	2942	1/1	0.81	0.63	77,77,77,77	0
33	MG	X	2902	1/1	0.81	0.17	89,89,89,89	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	2931	1/1	0.84	0.68	72,72,72,72	0
33	MG	X	2893	1/1	0.84	0.42	66,66,66,66	0
33	MG	X	2944	1/1	0.85	0.29	77,77,77,77	0
35	NA	X	2960	1/1	0.85	0.47	86,86,86,86	0
33	MG	X	2920	1/1	0.85	0.37	100,100,100,100	0
33	MG	X	2915	1/1	0.86	0.57	67,67,67,67	0
33	MG	X	2914	1/1	0.87	0.52	74,74,74,74	0
33	MG	X	2928	1/1	0.87	0.34	29,29,29,29	0
33	MG	X	2885	1/1	0.87	0.47	68,68,68,68	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	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	2891	1/1	0.89	0.33	50,50,50,50	0
33	MG	X	2941	1/1	0.89	0.23	71,71,71,71	0
33	MG	X	2916	1/1	0.90	0.20	44,44,44,44	0
33	MG	X	2903	1/1	0.90	0.54	65,65,65,65	0
33	MG	X	2910	1/1	0.90	0.37	44,44,44,44	0
33	MG	X	2895	1/1	0.90	0.29	26,26,26,26	0
33	MG	X	2921	1/1	0.91	0.17	61,61,61,61	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	2938	1/1	0.91	0.62	62,62,62,62	0
33	MG	X	2905	1/1	0.91	0.67	50,50,50,50	0
33	MG	X	2901	1/1	0.92	0.39	19,19,19,19	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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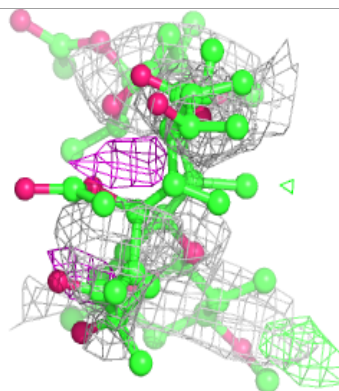
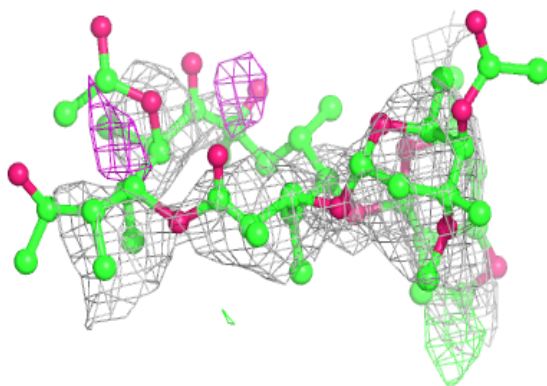
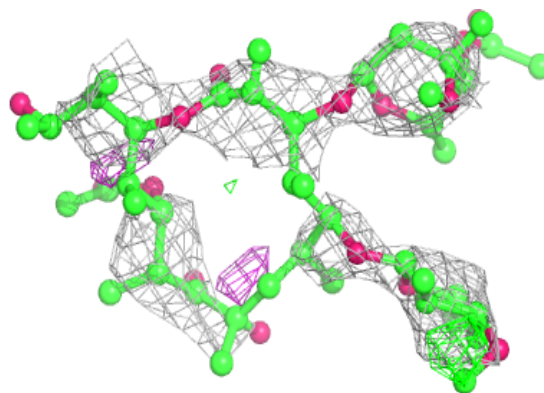
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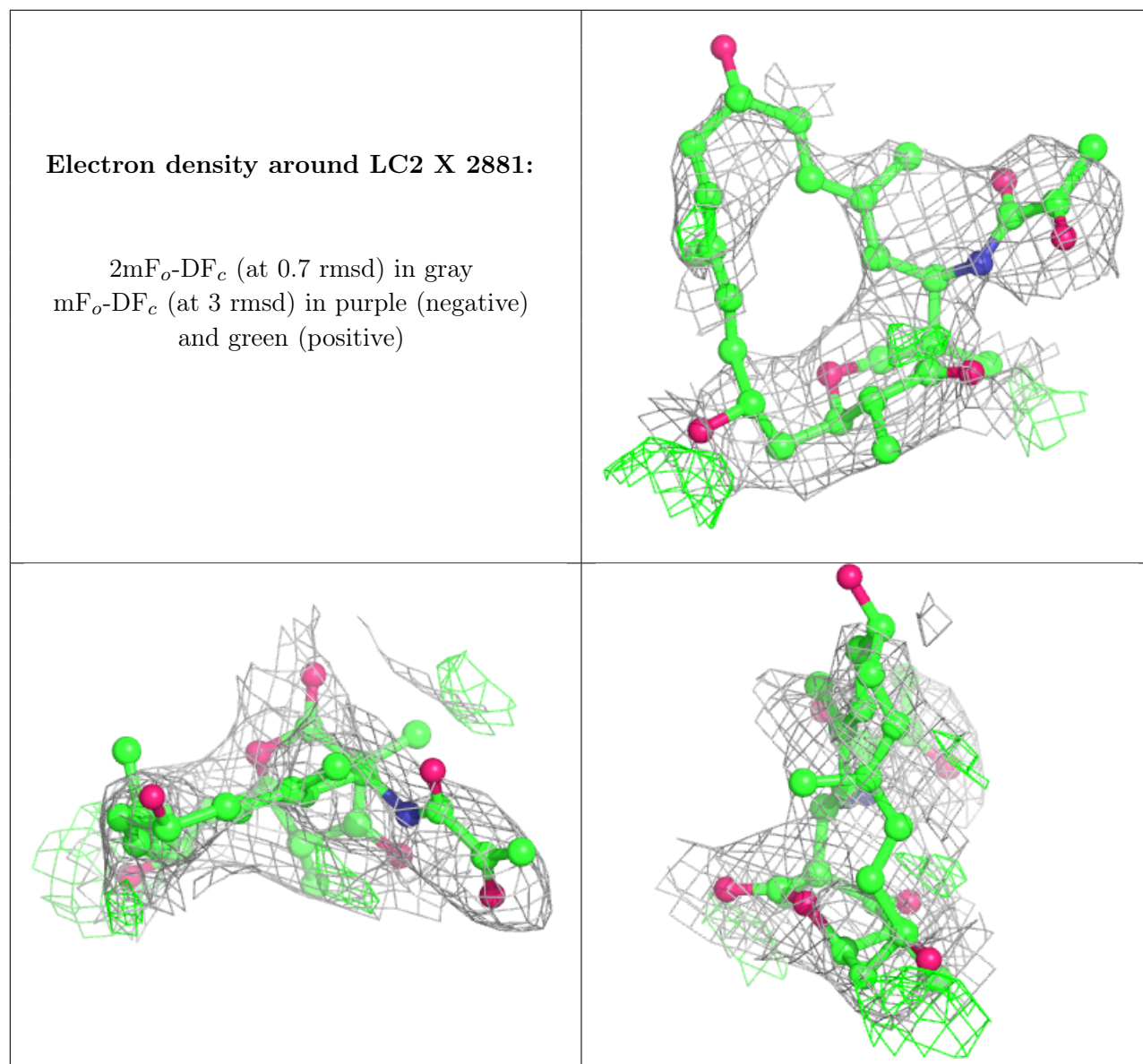
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	X	2961	1/1	0.92	0.43	75,75,75,75	0
33	MG	X	2924	1/1	0.92	0.13	51,51,51,51	0
33	MG	X	2929	1/1	0.93	0.83	61,61,61,61	0
33	MG	X	2884	1/1	0.93	1.00	72,72,72,72	0
33	MG	X	2923	1/1	0.93	0.15	97,97,97,97	0
33	MG	X	2918	1/1	0.93	0.53	84,84,84,84	0
34	K	X	2955	1/1	0.93	0.15	113,113,113,113	0
33	MG	X	2949	1/1	0.93	0.55	83,83,83,83	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	2934	1/1	0.94	0.41	56,56,56,56	0
33	MG	X	2946	1/1	0.94	0.16	123,123,123,123	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	2907	1/1	0.94	0.36	46,46,46,46	0
33	MG	X	2919	1/1	0.94	0.33	65,65,65,65	0
33	MG	X	2933	1/1	0.95	0.37	83,83,83,83	0
33	MG	X	2887	1/1	0.95	0.41	35,35,35,35	0
33	MG	X	2896	1/1	0.95	0.26	24,24,24,24	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	2952	1/1	0.95	0.35	59,59,59,59	0
33	MG	X	2927	1/1	0.95	0.74	65,65,65,65	0
33	MG	X	2945	1/1	0.95	0.17	67,67,67,67	0
33	MG	X	2906	1/1	0.96	0.38	52,52,52,52	0
34	K	X	2954	1/1	0.96	0.24	70,70,70,70	0
33	MG	X	2888	1/1	0.96	0.49	51,51,51,51	0
33	MG	X	2890	1/1	0.96	0.40	59,59,59,59	0
33	MG	X	2897	1/1	0.96	0.14	79,79,79,79	0
33	MG	X	2899	1/1	0.97	0.54	41,41,41,41	0
33	MG	X	2913	1/1	0.97	0.40	63,63,63,63	0
33	MG	X	2939	1/1	0.97	0.49	54,54,54,54	0
33	MG	X	2953	1/1	0.97	0.39	53,53,53,53	0
33	MG	X	2930	1/1	0.97	0.21	77,77,77,77	0
33	MG	X	2947	1/1	0.98	0.13	56,56,56,56	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

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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.