



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 11:43 AM GMT

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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

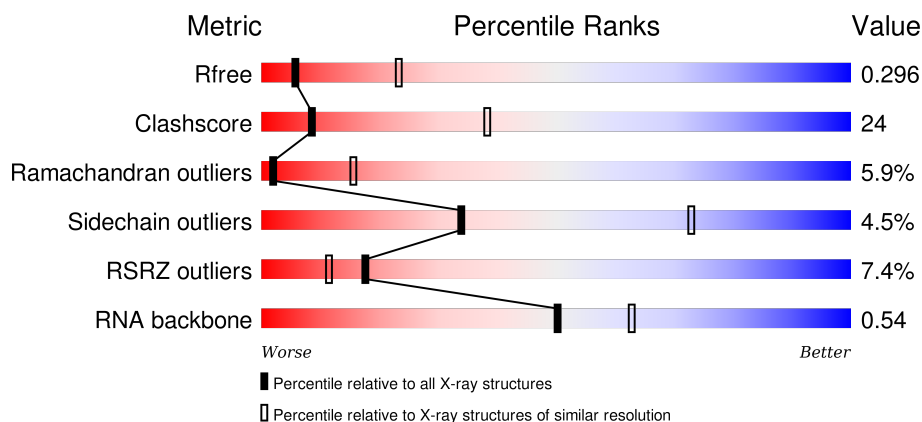
1 Overall quality at a glance

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}	91344	1092 (3.28-3.20)
Clashscore	102246	1227 (3.28-3.20)
Ramachandran outliers	100387	1204 (3.28-3.20)
Sidechain outliers	100360	1203 (3.28-3.20)
RSRZ outliers	91569	1097 (3.28-3.20)
RNA backbone	2183	1001 (3.74-2.74)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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>6%</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></div> <div>95%</div> <div>62%</div> <div>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
32	MG	X	2885	-	-	-	X
32	MG	X	2886	-	-	-	X
32	MG	X	2888	-	-	-	X
32	MG	X	2890	-	-	-	X
32	MG	X	2894	-	-	-	X
32	MG	X	2896	-	-	-	X
32	MG	X	2897	-	-	-	X
32	MG	X	2898	-	-	-	X
32	MG	X	2901	-	-	-	X
32	MG	X	2904	-	-	-	X
32	MG	X	2911	-	-	-	X
32	MG	X	2914	-	-	-	X
32	MG	X	2915	-	-	-	X
32	MG	X	2920	-	-	-	X
32	MG	X	2933	-	-	-	X
32	MG	X	2941	-	-	-	X
32	MG	X	2943	-	-	-	X
32	MG	X	2944	-	-	-	X
32	MG	X	2957	-	-	-	X
32	MG	X	2960	-	-	-	X
32	MG	X	2961	-	-	-	X
32	MG	X	2964	-	-	-	X
32	MG	X	2965	-	-	-	X
32	MG	X	2967	-	-	-	X
32	MG	X	2973	-	-	-	X
32	MG	X	2974	-	-	-	X
32	MG	X	2978	-	-	-	X
32	MG	X	2979	-	-	-	X
32	MG	X	2982	-	-	-	X
32	MG	X	2995	-	-	-	X
32	MG	X	3002	-	-	-	X
32	MG	X	3004	-	-	-	X
32	MG	X	3011	-	-	-	X
32	MG	X	3016	-	-	-	X
32	MG	X	3020	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	MG	X	3024	-	-	-	X
33	NA	X	3033	-	-	-	X
33	NA	X	3042	-	-	-	X
33	NA	X	3045	-	-	-	X
33	NA	X	3058	-	-	-	X
33	NA	Y	126	-	-	-	X
34	K	M	167	-	-	-	X
34	K	X	3070	-	-	-	X
34	K	X	3077	-	-	-	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			

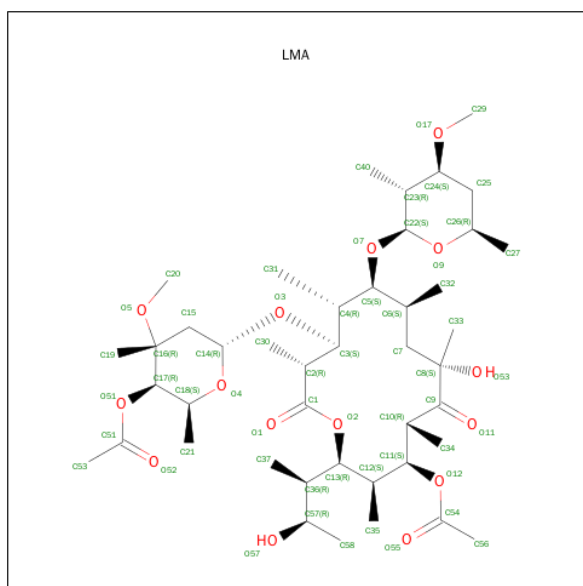
- Molecule 29 is a protein called 50S ribosomal protein L35.

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	C	1	Total 1	Mg 1	0	0
32	Y	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

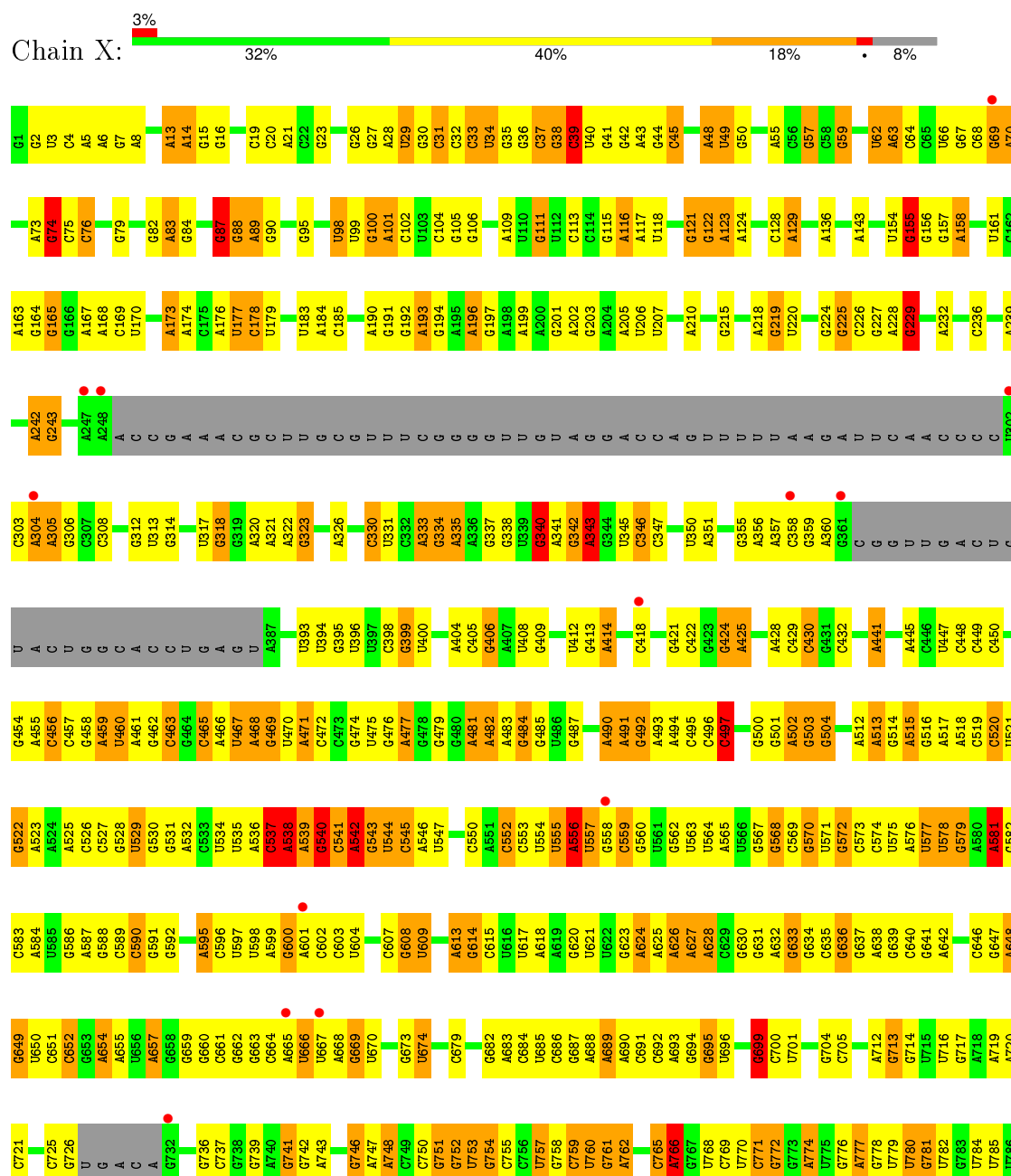
- Molecule 34 is POTASSIUM ION (three-letter code: K) (formula: K).

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

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

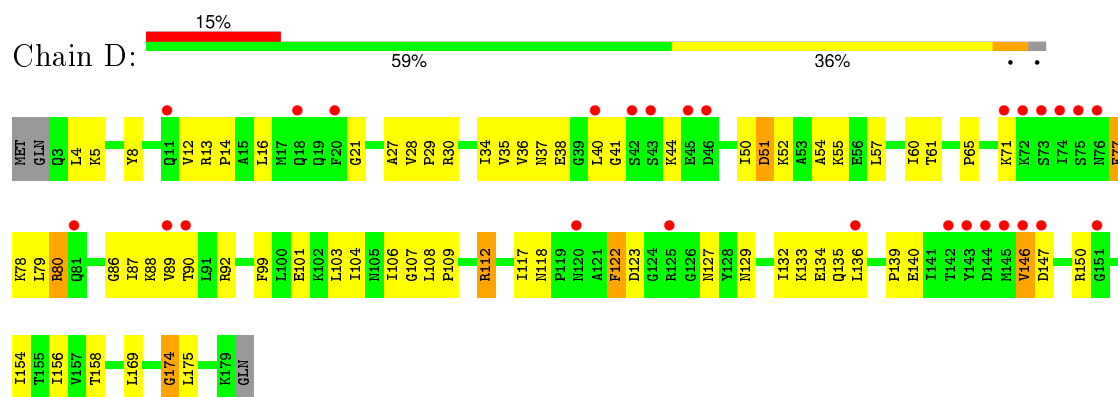
• Molecule 1: RIBOSOMAL 23S RNA



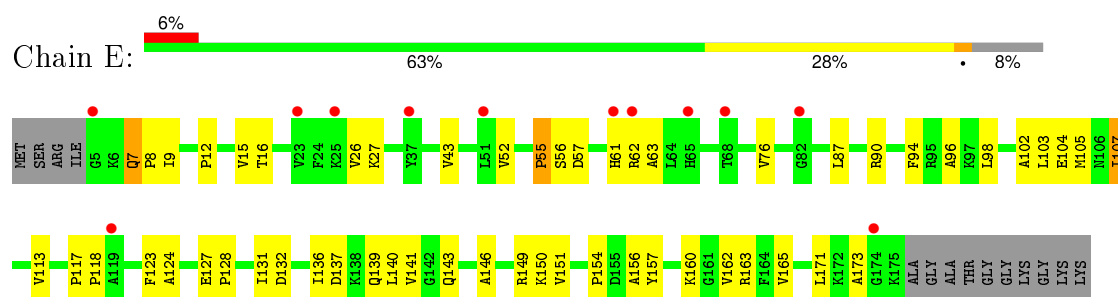
A1793	G1721	U1656	G1573	A1493	C1422	C1346	C1283	G1211	G1062	G989	A923	C853	A787
A1796	G1722	A1657	A1574	G1494	A1423	C1347	G1284	U1212	G1067	A994	C924	C854	G783
A1799	C1723	G1660	G1575	G1495	G1428	C1348	A1285	U1213	U1067	U925	C925	C855	G789
A1800	C1725	G1661	G1576	G1496	G1429	G1351	U1286	C1214	G1069	A999	C926	U859	G791
C1801	G1730	G1662	U1577	C1497	G1430	G1352	A1287	A1215	G1070	G1000	C927	U860	U792
A1802		C1663	U1578	A1498	U1431	A1353	A1288	U1216	U1071	A1001	C928	C861	G793
U1803	U1733	G1664	G1579	U1500	A1432	A1354	A1289	U1217	U1072	C1002	G931	U867	A794
U1804	C1734	C1665	G1584	U1505	A1433	A1355	U1291	C1218	G1073	C1003	G932	C867	A795
U1805	G1737	A1666	A1585	C1506	U1434	G1356	A1292	G1220	G1074	A1004	G933	U868	A796
A1806		G1667	U1592	U1507	G1435	U1357	A1293	G1223	U1075	U1005	G934	C869	A797
A1807	G1741	G1668	U1593	G1508	A1436	G1358	U1294	G1224	U1076	C1006	C935	C870	G798
C1808	G1742	U1594	U1595	A1509	A1437	G1359	U1295	A1225	A1077	A936	C937	U871	C799
G1809	G1743	G1671		G1510	G1438	G1360	G1296	G1226	A1078	G1008	C937	C872	U800
A1810	C1744	A1672	U1601	A1511	G1439	G1361	U1297	A1226	G1079	C1009	G938	U873	A801
A1811	G1745	C1673	U1602	A1512	G1440	A1362	A1298	G1227	G1080	C939	G939	U874	A802
A1812	A1746	C1674	A1603	U1513	A1441	C1363	A1299	C1229	A1081	A1011	G940	C875	C803
A1813	G1747	C1675	A1603	C1514	G1443	C1364	A1300	C1230	G1082	A876	U941	C876	C804
G1814	G1748	C1676		C1522	C1444	U1370	U1301	G1245	C1083	U1015	U942	C877	G805
G1815	U1749	C1677	A1607	A	U1447	G1371	U1302	C1246	A1084	C1016	U943	C878	A806
U1816	G1750	U1678	U1608	G1527	A1454	A1372	U1303	C1235	G1085	C1017	U944	C879	A807
U1817	A1751	U1679	G1609	C1528	C1455	G1373	U1304	G1236	C1086	C1018	G945	U882	C808
A1821	U1752	U1680	A1610	A	G1456	G1374	C1305	A1242	C1087	U1019	U946	C882	C809
C1822	U1753	U1681	U1611	U1526	A1457	U1374	U1306	G1245	C1088	A1020	C947	A883	U810
G1825	A1754	A1682	U1612	G1527	A1458	U1375	G1307	G1246	C1089	A1021	C948	U888	G811
G1826	G1755	G1683	G1613	C1528	U1459	A1376	U1308	G1249	U1093	U1023	G949	C889	A812
G1827	C1756	A1684	C1614	C1528	C1455	A1377	C1310	G1250	U1094	G1024	G950	C890	A813
U1827	G1757	A1685	C1615	C1531	C1456	G1381	G1312	A1251	C1095	A1025	A952	A	A815
C1830	C1758	A1686	C1615	C1531	A1457	G1382	G1313	G1252	A1096	U1170	G953	G	U816
G1831		C1687	A1619	U1537	U1458	G1383	A1314	C1253	A1097	U1171	U954	G	A817
G1834	G1761	U1688	G1622	U1538	U1459	A1386	A1315	C1254	G1098	C1031	G955	G	G818
C1835	C1762	U1689	C1623	U1539	C1460	G1387	G1316	A1255	G1099	A1032	A956	G	C819
G1836	A1763	G1691	A1624	G1541	C1461	A1391	G1317	C1256	A1099	G1033	C957	G	U820
G1837	G1765	C1692	A1625	G1542	A1462	U1392	U1321	U1257	A1175	U1034	C959	C	A821
G1838	U1766	A1694	C1626	G1543	A1463	G1393	G1322	G1258	A1176	G1035	U860	U	U822
A1839	G1767	U1695	C1627	A1544	G1464	G1397	G1323	A1259	U1177	G1036	G961	A	U824
A1840	U1768	C1696	C1628	C1550	U1465	A1397	U1324	C1264	G1104	U1037	C962	C	C825
G1841	U1769	U1697	G1629	U1551	U1466	G1398	U1325	G1265	A1105	G1042	G965	C	U826
G1842	U1770	C1698	C1630	C1552	A1468	C1399	U1326	A1267	A1106	A1043	A966	A	C827
	A1771	A1699	A1632	G1553	G1470	A1400	C1327	C1268	U1108	G1044	C967	G	C830
G1849	C1772	C1700	C1633	G1554	C1471	C1404	U1328	G1269	A1109	U1045	C968	U	G831
G1850	C1773	C1701	A1634	A1555	C1472	A1405	U1329	A1267	A1114	G1046	U969	U	A832
G1851	A1774	C1702	G1635	A1556	U1473	A1406	G1331	G1268	C1115	U1047	A970	A	G836
G1852	A1775	C1703			U1474	G1407	U1332	G1269	C1116	G1048	A971	C	U837
G1853	A1776	G1704			U1475	A1408	G1333	C1270	G1117	C1049	C972	C	A838
G1854	U1779	U1710	G1641	A1560	G1476	U1409	A1334	C1271	U1119	G1050	U973	A911	U839
G1855	A1780	C1711	G1642	A1561	C1477	U1410	A1335	G1272	C1120	U1051	U974	A912	U840
G1856	C1781	G1712	A1643	G1562	U1478	C1411	G1336	G1273	G1121	C1052	G977	A913	G841
G1857	A1782	U1713	G1644	U1563	U1479	A1412	U1337	C1274	G1122	G1053		C915	A842
G1864		G1714	U1481	G1565	G1480	U1413	G1338	A1275	U1124	A1055	C982	C915	G843
A1867	U1787	A1715	C1648	G1566	U1481	G1414	U1339	G1276	A1056	U1056	G983	U917	G844
A1868	C1788	G1716	U1651	A1567	U1482	C1415	G1340	G1277	A1126	A1057	A984	A918	
	U1789	A1717	G1652	A1568	G1483	C1418	U1202	A1278	C1127	G1058	G985	U919	G849
	G1790	A1718	G1653	A1569	U1490	G1419	U1203	G1279	G1128	A1059	A986	G920	C850
	C1791	G1719	A1654	C1570	U1491	A1420	C1344	A1280	A1129	C1060	G987	A1921	C851
	C1792		C1655	C1572	A1492	U1421	G1345	A1282	U1130	A1061	G988	A922	U852

U2850	A2784	A2658	U2584	U2516	G2433	A2371	A2390	U2211	U	A2073	C2007	A1943	C1878
G2851	A2787	C2659	U2587	C2517	U2436	A2372	U2291	G2217	G	U2074	C2008	C1944	G1879
G2852	A2788	C2660	U2588	C2518	U2437	C2373	C2292	G2218	A	U2075	C2009	C1945	G1880
G2853	A2789	C2661	U2589	C2519	U2438	C2374	G2293	G2219	G	C2082	U2010	U1946	U1881
G2854	A2790	C2662	U2590	A2520	U2441	G2375	U2298	G2220	G	C2083	A2011	G1947	A1884
G2855	A2791	C2663	U2591	A2521	C2442	G2376	A2299	G2221	C	G2084	A2012	C1948	A1885
G2856	A2792	C2664	U2592	G2522	C2443	U2377	A2300	G2222	C	G2085	A2013	A1949	C1885
G2857	A2793	C2665	U2593	G2523	C2444	G2378	G2300	U2223	A	G2086	A2014	C1950	G1886
A2858	G2794	U2666	U2594	G2524	C2445	U2379	A2301	U2224	C	U2087	A2015	G1951	G1887
U2859	A2795	C2667	U2595	G2525	C2446	U2380	G2302	U2225	G	U	A2016	A1952	A1888
G2860	A2796	U2668	U2596	G2526	C2447	A2381	A2306	C2227	C	C	U2017	A1953	G
A2861	G2797	C2669	U2597	G2527	U2448	G2382	A2307	U2228	G	U	G2018	A1954	C
G2862	A2798	C2670	U2598	C2530	U2449	G2383	G2308	G2229	U	C	G2019	G1955	C
U2863	G2799	C2671	U2599	U2531	U2450	G2384	G2310	G2230	G	U	C2023	G1956	C
A2866	G2800	U2672	U2600	G2532	C2452	U2385	U2311	C2233	A	U	U2024	A1960	G
G2867	A2801	C2673	U2601	U2533	C2453	G2386	A2312	G2234	A	G	A2025	U	U
G2868	G2802	C2674	U2602	U2534	C2454	U2387	G2313	G2235	U	C	G2026	G1963	A
G2873	G2803	U2675	G2604	A2545	C2455	G2388	A2314	G2236	A	U	C2027	A1964	C
G2876	G2804	C2676	C2605	U2546	U2457	G2389	A2315	U2237	C	A	G2028	U1965	U
G2877	G2805	U2677	U2606	U2547	U2458	A2390	G2321	C2238	C	G	C2029	U1966	A
G2878	G2806	C2678	A2608	U2548	U2459	A2391	U2322	G2239	C	G	G2030	U1967	U
G2879	G2807	U2679	G2609	A2549	A2467	G2392	U2323	C2240	A	A	U2031	G1968	U
U2880	U2808	C2680	G2610	A2544	G2468	G2393	U2324	G2241	C	U	A2032	G1969	A
G2881	G2809	A2681	A2611	A2545	G2469	G2394	G2325	C2242	C	A	G2033	G1970	C
A2810	A2810	C2682	G2612	G2546	U2470	C2395	C2326	U2243	U	G	A2034	C1971	G
G2811	G2811	C2683	A2613	C2547	U2471	C2396	U2327	A2245	G	U	G2035	G1972	G
A2812	G2812	A2684	A2614	G2548	U2472	A2397	G2328	A2246	A	U	G2036	G1973	U
G2813	G2813	C2685	U2615	G2549	C2473	U2398	G2329	A2247	A	G	A2037	U1974	C
G2814	G2814	C2686	G2616	A2550	C2474	A2401	G2330	U2251	A	G	G2038	G1975	C
G2815	G2815	U2617	U2617	A2551	C2475	U2402	A2331	A2252	A	A	G2039	U1976	U1909
G2816	G2816	A2618	A2618	C2552	C2476	C2403	A2332	A2253	G	G	A2040	C1977	A1910
G2817	G2817	C2688	U2619	G2553	C2477	A2404	G2333	A2254	C	A	A2041	U1978	A1911
A2818	G2818	A2689	G2622	C2554	C2478	C2405	G2334	G2255	C	U	A2042	G1979	G1912
G2819	G2819	C2690	A2623	G2555	C2479	A2406	U2337	C2256	U	U	A2043	A1980	G1913
G2820	G2820	A2691	G2624	A2556	C2480	C2407	G2338	G2257	C	U	G2044	A1981	U1914
G2821	G2821	A2692	U2625	G2557	A2481	G2408	A2339	G2258	U	G	A2045	C1982	C
G2822	G2822	U2693	U2626	C2558	U2482	G2409	C2340	G2259	C	C	C2046	G1983	G
G2823	G2823	C2694	U2627	U2559	G2483	A2409	G2341	G2260	G	U	G2047	A1984	G
G2824	G2824	C2695	U2628	G2560	C2484	U2410	U2342	G2261	A	A	C2048	U1987	G
A2825	A2825	A2696	C2630	U2561	C2485	A2413	A2348	C2262	A	A	G2049	A1988	A1921
G2826	G2826	G2697	U2631	G2562	U2486	A2414	G2349	G2263	C	C	G2050	C1989	U1922
G2827	G2827	C2698	G2632	U2563	C2491	G2415	G2350	C2264	U	U	U2051	U1990	U1923
G2828	G2828	U2700	A2635	U2564	C2492	U2416	A2190	A2191	G	G	G2052	C1991	C1924
G2832	G2832	A2701	A2636	C2565	U2493	U2417	A2192	A2265	C	U	G2053	G1992	C1925
U2836	U2836	C2702	G2637	A2566	U2494	A2418	G2354	A2266	C	U	A2054	G1993	U1926
G2837	G2837	C2703	A2638	G2567	G2495	C2419	A2355	A2267	C	U	G2055	U1994	U1927
U2838	G2838	U2704	G2639	A2568	C2496	C2420	A2356	A2268	U	U	C2056	G1995	G1928
G2839	G2839	A2705	A2641	A2569	C2497	C2421	A2357	A2269	C	U	U2057	U1996	U1929
U2840	U2840	G2706	G2642	C2570	U2498	C2422	G2360	A2272	U	U	U2058	A1997	G1930
G2841	G2841	U2708	U2643	U2572	C2499	G2423	G2361	C2273	U	U	A2059	A1998	G1931
C2842	C2842	C2709	G2650	C2573	U2500	G2424	G2362	C2274	U	U	A2060	A1999	G1932
A2843	A2843	G2710	U2651	U2574	U2501	G2425	G2363	G2282	G	G	G2061	U1999	U1933
G2844	G2844	G2711	G2652	G2575	U2502	G2426	C2364	G2283	U	U	U2062	U2000	U1934
G2845	G2845	G2712	G2653	G2576	C2505	A2427	U2365	U2284	G	G	A2063	G2001	A2002
G2846	G2846	A2713	A2654	G2578	C2506	U2428	U2366	U2285	U	U	U2064	A2003	G1839
G2847	G2847	G2716	C2655	U2507	U2507	A2429	A2367	G2286	C	C	A2065	A2004	U1940
G2848	G2848	G2717	G2656	G2508	U2508	A2430	G2368	G2287	U	U	G2066	U2005	G1941
G2849	G2849	A2718	U2582	A2509	A2509	C2431	U2369	A2288	G	G	U2067	G2006	G1942
			G2657	U2583		A2432	G2370	A2289	G	G			

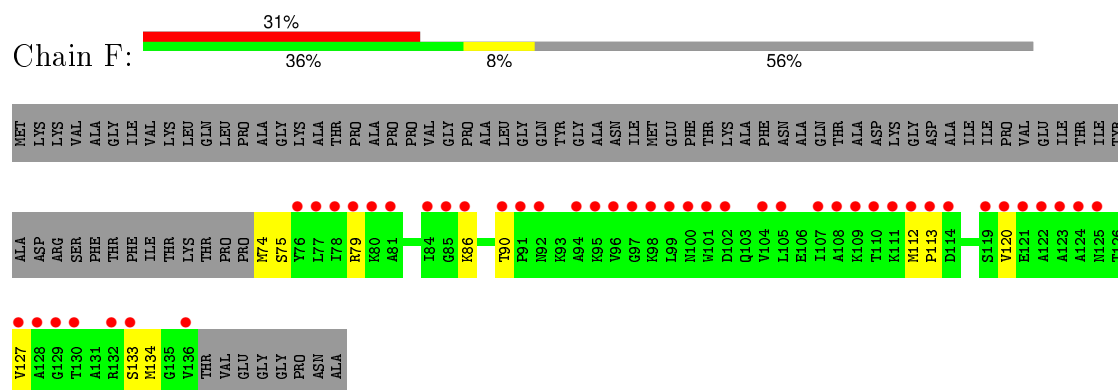
- Molecule 6: 50S ribosomal protein L5



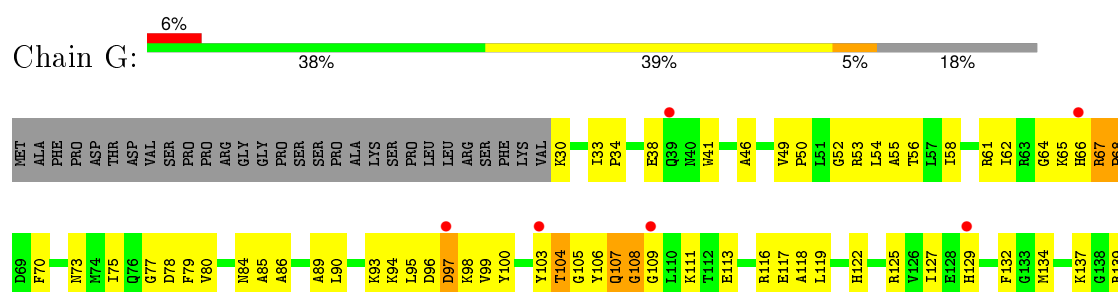
- Molecule 7: 50S ribosomal protein L6



- Molecule 8: 50S ribosomal protein L11

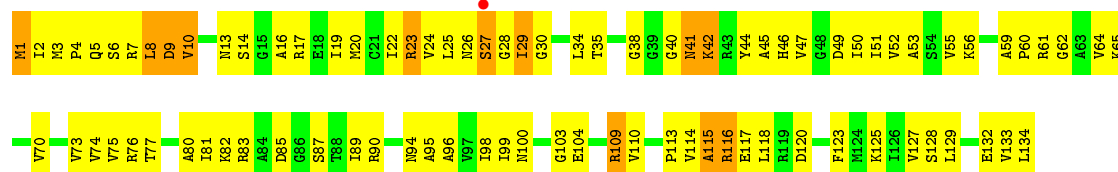


- Molecule 9: 50S ribosomal protein L13

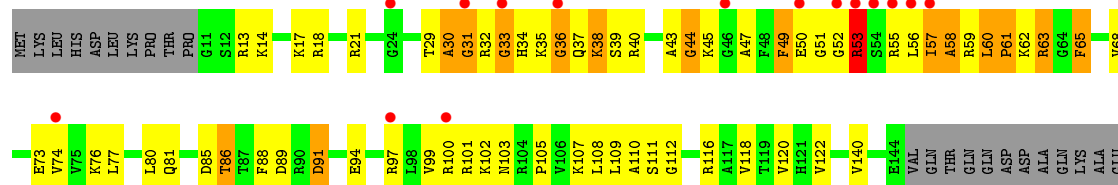




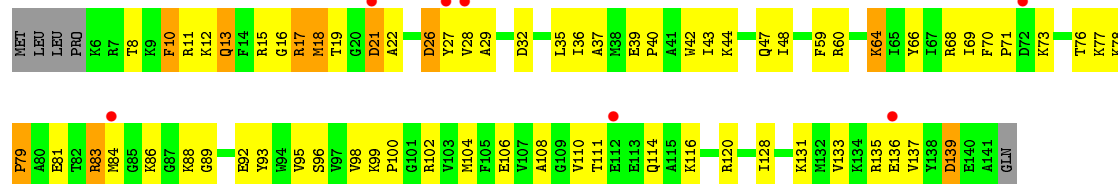
- Molecule 10: 50S ribosomal protein L14



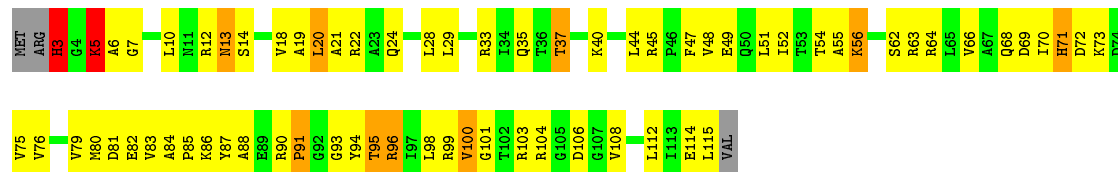
- Molecule 11: 50S ribosomal protein L15



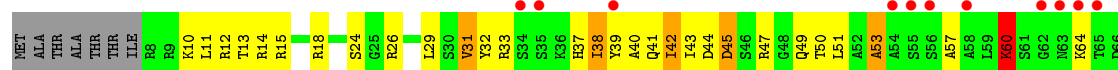
- Molecule 12: 50S ribosomal protein L16



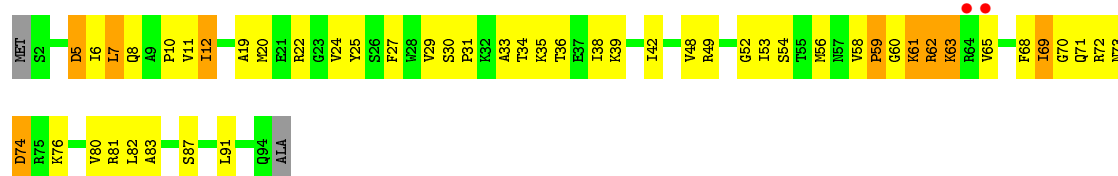
- Molecule 13: 50S ribosomal protein L17



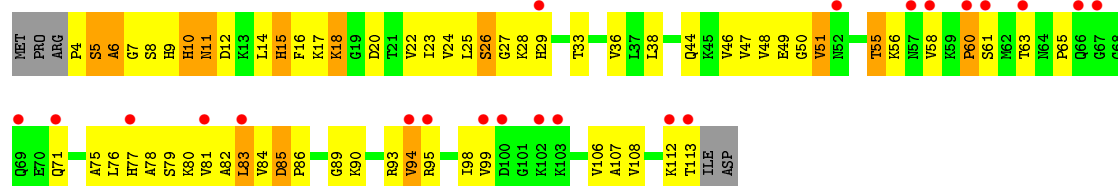
- Molecule 14: 50S ribosomal protein L18



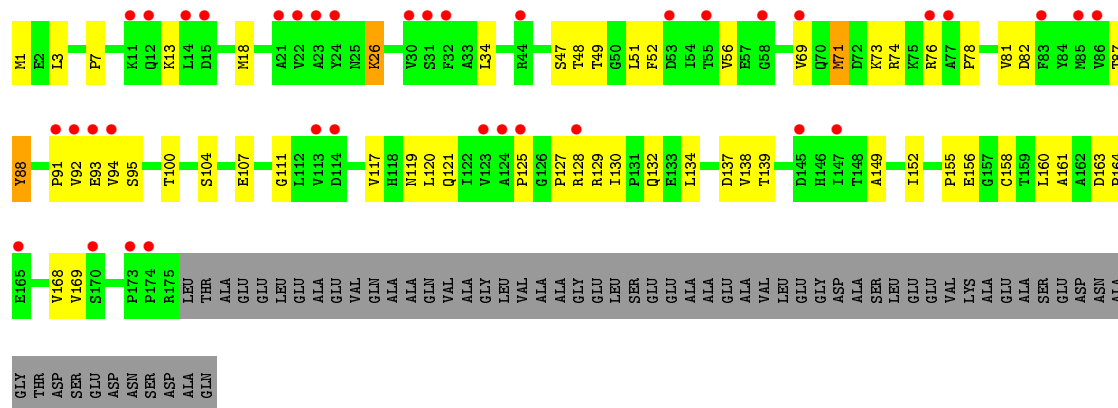




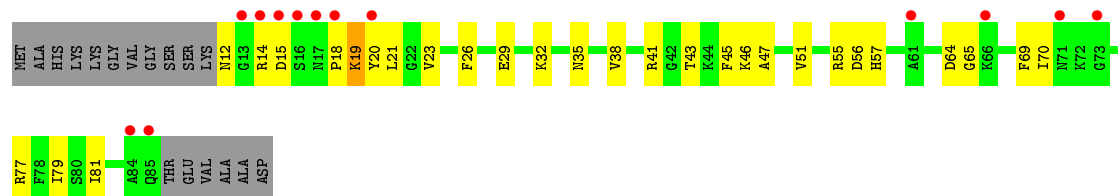
• Molecule 20: 50S ribosomal protein L24



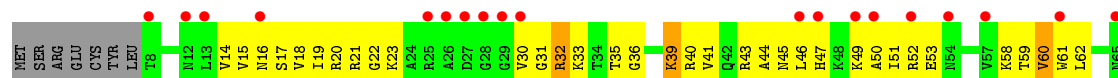
• Molecule 21: 50S ribosomal protein L25

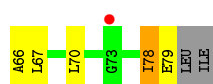


• Molecule 22: 50S ribosomal protein L27



• Molecule 23: 50S ribosomal protein L28





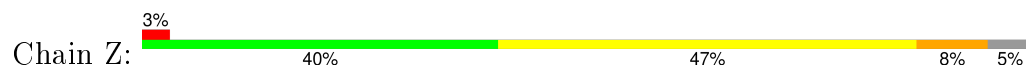
- Molecule 24: 50S ribosomal protein L29



- Molecule 25: 50S ribosomal protein L30



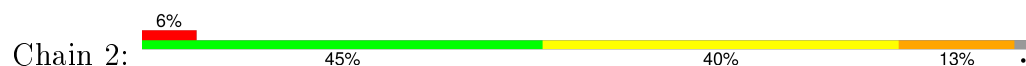
- Molecule 26: 50S ribosomal protein L32



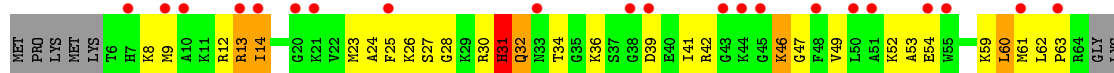
- Molecule 27: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L36



M1	R2	V3	R4	S5	S6	V7	R8	R9	M10	C11	D12	M13	C14	K15	V16	V17	R18	R19	R20	G21	R22	V23	L24	V25	I26	C27	S28	N29	V30	K31	H32	R33	Q34	R35	Q36	G37
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4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 3.25Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.6.4_486)	Depositor
R, R_{free}	0.252 , 0.294 0.257 , 0.296	Depositor DCC
R_{free} test set	3584 reflections (1.02%)	DCC
Wilson B-factor (Å ²)	73.8	Xtriage
Anisotropy	0.636	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 65.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 355752 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	84383	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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

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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%)	3	21
4	B	203/211 (96%)	160 (79%)	29 (14%)	14 (7%)	1	10
5	C	192/205 (94%)	143 (74%)	37 (19%)	12 (6%)	2	13
6	D	175/180 (97%)	137 (78%)	32 (18%)	6 (3%)	5	30
7	E	169/185 (91%)	142 (84%)	20 (12%)	7 (4%)	3	25
8	F	61/144 (42%)	48 (79%)	12 (20%)	1 (2%)	12	52
9	G	140/174 (80%)	104 (74%)	27 (19%)	9 (6%)	2	12
10	H	132/134 (98%)	111 (84%)	17 (13%)	4 (3%)	5	33
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	7
13	K	111/116 (96%)	89 (80%)	14 (13%)	8 (7%)	1	9
14	L	102/114 (90%)	73 (72%)	26 (26%)	3 (3%)	6	34
15	M	106/166 (64%)	82 (77%)	18 (17%)	6 (6%)	2	17
16	N	115/118 (98%)	95 (83%)	16 (14%)	4 (4%)	4	29
17	O	92/100 (92%)	68 (74%)	17 (18%)	7 (8%)	1	8
18	P	124/134 (92%)	101 (82%)	18 (14%)	5 (4%)	4	25
19	Q	91/95 (96%)	63 (69%)	19 (21%)	9 (10%)	1	4
20	R	108/115 (94%)	70 (65%)	26 (24%)	12 (11%)	0	3
21	S	173/237 (73%)	135 (78%)	32 (18%)	6 (4%)	4	29
22	T	72/91 (79%)	53 (74%)	18 (25%)	1 (1%)	14	55
23	U	70/81 (86%)	50 (71%)	13 (19%)	7 (10%)	1	4
24	V	63/67 (94%)	55 (87%)	5 (8%)	3 (5%)	3	21

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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	9
27	1	51/55 (93%)	30 (59%)	15 (29%)	6 (12%)	0	2
28	2	44/47 (94%)	37 (84%)	5 (11%)	2 (4%)	3	22
29	3	57/66 (86%)	34 (60%)	18 (32%)	5 (9%)	1	5
30	4	35/37 (95%)	29 (83%)	6 (17%)	0	100	100
All	All	3111/3558 (87%)	2371 (76%)	557 (18%)	183 (6%)	2	15

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%)	29	68
4	B	155/157 (99%)	149 (96%)	6 (4%)	39	76
5	C	154/163 (94%)	147 (96%)	7 (4%)	34	73
6	D	153/156 (98%)	150 (98%)	3 (2%)	63	87
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%)	55	84
10	H	103/103 (100%)	94 (91%)	9 (9%)	13	45
11	I	101/121 (84%)	97 (96%)	4 (4%)	38	76
12	J	110/115 (96%)	108 (98%)	2 (2%)	66	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	K	90/93 (97%)	82 (91%)	8 (9%)	12	43
14	L	74/82 (90%)	68 (92%)	6 (8%)	15	50
15	M	94/134 (70%)	87 (93%)	7 (7%)	17	55
16	N	96/97 (99%)	93 (97%)	3 (3%)	47	80
17	O	75/79 (95%)	72 (96%)	3 (4%)	38	76
18	P	108/115 (94%)	101 (94%)	7 (6%)	21	60
19	Q	75/76 (99%)	70 (93%)	5 (7%)	20	59
20	R	91/96 (95%)	84 (92%)	7 (8%)	16	52
21	S	149/192 (78%)	146 (98%)	3 (2%)	63	87
22	T	55/67 (82%)	53 (96%)	2 (4%)	42	77
23	U	57/66 (86%)	55 (96%)	2 (4%)	43	78
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%)	16	52
27	1	46/48 (96%)	41 (89%)	5 (11%)	8	33
28	2	39/40 (98%)	33 (85%)	6 (15%)	3	16
29	3	46/52 (88%)	43 (94%)	3 (6%)	21	60
30	4	35/35 (100%)	35 (100%)	0	100	100
All	All	2552/2855 (89%)	2437 (96%)	115 (4%)	34	73

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	-	59,60,60	4.60	24 (40%)	76,90,90	1.29	6 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMA	X	2881	-	-	0/80/115/115	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	X	2881	LMA	C30-C2	-18.34	1.10	1.53
31	X	2881	LMA	C2-C1	-16.09	1.13	1.51
31	X	2881	LMA	O53-C8	-9.82	1.25	1.43
31	X	2881	LMA	C33-C8	-7.75	1.41	1.52
31	X	2881	LMA	C35-C12	-7.57	1.36	1.53

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	X	2881	LMA	C3-C2-C1	-2.80	104.38	109.86
31	X	2881	LMA	C25-C24-C23	-2.46	106.55	113.55
31	X	2881	LMA	C13-C12-C11	-2.01	108.54	113.05
31	X	2881	LMA	O7-C5-C4	3.74	112.90	108.19
31	X	2881	LMA	O51-C51-C53	4.44	119.48	111.10

There are no chirality outliers.

There are no torsion outliers.

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	X	2657/2880 (92%)	-0.11	79 (2%) 54 42	32, 91, 207, 392	0
2	Y	120/123 (97%)	0.11	3 (2%) 61 49	85, 155, 211, 300	0
3	A	253/274 (92%)	0.46	16 (6%) 23 15	54, 119, 183, 297	0
4	B	205/211 (97%)	-0.32	3 (1%) 76 65	22, 64, 130, 298	0
5	C	194/205 (94%)	0.22	14 (7%) 18 12	44, 117, 220, 268	0
6	D	177/180 (98%)	0.92	27 (15%) 3 2	146, 209, 280, 370	0
7	E	171/185 (92%)	0.27	12 (7%) 19 12	86, 149, 209, 245	0
8	F	63/144 (43%)	3.18	45 (71%) 0 0	180, 261, 394, 440	0
9	G	142/174 (81%)	0.30	10 (7%) 19 12	55, 101, 188, 266	0
10	H	134/134 (100%)	-0.47	1 (0%) 89 83	35, 61, 108, 204	0
11	I	134/156 (85%)	0.69	15 (11%) 7 5	64, 145, 237, 367	0
12	J	136/141 (96%)	0.20	7 (5%) 32 21	76, 108, 190, 272	0
13	K	113/116 (97%)	-0.64	0 100 100	27, 46, 79, 105	0
14	L	104/114 (91%)	0.58	13 (12%) 5 4	117, 160, 248, 306	0
15	M	108/166 (65%)	-0.31	3 (2%) 56 44	36, 60, 135, 241	0
16	N	117/118 (99%)	-0.11	5 (4%) 39 27	44, 88, 156, 279	0
17	O	94/100 (94%)	0.18	6 (6%) 23 14	58, 119, 195, 238	0
18	P	126/134 (94%)	-0.39	0 100 100	29, 59, 118, 200	0
19	Q	93/95 (97%)	0.06	2 (2%) 65 54	59, 107, 182, 273	0
20	R	110/115 (95%)	0.70	22 (20%) 1 1	68, 127, 234, 359	0
21	S	175/237 (73%)	0.98	37 (21%) 1 1	112, 169, 237, 314	0
22	T	74/91 (81%)	0.66	13 (17%) 2 1	82, 123, 199, 271	0
23	U	72/81 (88%)	1.85	20 (27%) 1 1	89, 155, 302, 332	0
24	V	65/67 (97%)	0.31	4 (6%) 24 15	94, 126, 205, 256	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	55/55 (100%)	0.10	3 (5%) 29 18	73, 102, 166, 177	0
26	Z	57/60 (95%)	-0.13	2 (3%) 48 35	31, 63, 108, 191	0
27	1	53/55 (96%)	1.61	18 (33%) 0 1	106, 171, 261, 319	0
28	2	46/47 (97%)	0.25	3 (6%) 22 14	56, 85, 154, 195	0
29	3	59/66 (89%)	1.64	21 (35%) 0 1	97, 150, 276, 316	0
30	4	37/37 (100%)	6.56	35 (94%) 0 0	133, 223, 289, 323	0
All	All	5944/6561 (90%)	0.19	439 (7%) 17 11	22, 105, 230, 440	0

The worst 5 of 439 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
23	U	28	GLY	26.2
30	4	17	VAL	14.6
30	4	25	VAL	14.5
8	F	113	PRO	14.1
30	4	24	LEU	13.2

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
32	MG	X	2901	1/1	0.87	0.49	49.95	30,30,30,30	0
32	MG	X	2982	1/1	0.96	0.48	25.83	51,51,51,51	0
32	MG	X	2979	1/1	0.92	0.60	24.57	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	X	2886	1/1	0.98	0.37	20.14	16,16,16,16	0
32	MG	X	2943	1/1	0.94	0.52	17.34	29,29,29,29	0
32	MG	X	2914	1/1	0.93	0.61	15.29	60,60,60,60	0
32	MG	X	2896	1/1	0.98	0.41	14.14	28,28,28,28	0
32	MG	X	2961	1/1	0.92	0.36	12.89	61,61,61,61	0
32	MG	X	2933	1/1	0.96	0.50	11.53	59,59,59,59	0
33	NA	X	3033	1/1	0.97	0.44	11.52	38,38,38,38	0
32	MG	X	2904	1/1	0.98	0.49	11.22	39,39,39,39	0
32	MG	X	2915	1/1	0.97	0.55	10.46	47,47,47,47	0
32	MG	X	3004	1/1	0.90	0.39	10.42	71,71,71,71	0
32	MG	X	2957	1/1	0.94	0.40	9.73	35,35,35,35	0
32	MG	X	3016	1/1	0.97	0.35	8.97	39,39,39,39	0
34	K	M	167	1/1	0.97	0.38	8.83	44,44,44,44	0
32	MG	X	2898	1/1	0.99	0.38	8.46	8,8,8,8	0
33	NA	X	3045	1/1	0.98	0.45	8.17	31,31,31,31	0
32	MG	X	2941	1/1	0.95	0.42	8.06	46,46,46,46	0
32	MG	X	2885	1/1	0.95	0.49	7.86	21,21,21,21	0
32	MG	X	2964	1/1	0.96	0.44	7.54	50,50,50,50	0
32	MG	X	2965	1/1	0.97	0.31	7.42	42,42,42,42	0
33	NA	Y	126	1/1	0.80	0.40	7.27	85,85,85,85	0
32	MG	X	3011	1/1	0.97	0.54	7.11	45,45,45,45	0
32	MG	X	2995	1/1	0.94	0.63	7.11	42,42,42,42	0
33	NA	X	3042	1/1	0.95	0.49	6.20	45,45,45,45	0
34	K	X	3077	1/1	0.93	0.45	6.09	80,80,80,80	0
32	MG	X	2960	1/1	0.95	0.36	6.07	33,33,33,33	0
32	MG	X	2911	1/1	0.93	0.47	6.01	83,83,83,83	0
32	MG	X	2897	1/1	0.96	0.36	5.96	37,37,37,37	0
32	MG	X	2978	1/1	0.89	0.42	5.80	48,48,48,48	0
32	MG	X	2973	1/1	0.98	0.22	5.34	30,30,30,30	0
32	MG	X	2890	1/1	0.99	0.24	4.64	38,38,38,38	0
32	MG	X	3020	1/1	0.97	0.35	4.35	42,42,42,42	0
32	MG	X	2888	1/1	0.98	0.46	4.21	36,36,36,36	0
32	MG	X	2944	1/1	0.96	0.36	3.93	59,59,59,59	0
32	MG	X	3024	1/1	0.95	0.28	3.83	68,68,68,68	0
34	K	X	3070	1/1	0.91	0.52	3.76	72,72,72,72	0
32	MG	X	2974	1/1	0.96	0.18	3.02	37,37,37,37	0
32	MG	X	2967	1/1	0.98	0.31	2.87	50,50,50,50	0
32	MG	X	2920	1/1	0.96	0.37	2.75	31,31,31,31	0
32	MG	X	2894	1/1	0.91	0.24	2.73	33,33,33,33	0
32	MG	X	3002	1/1	0.95	0.22	2.71	34,34,34,34	0
33	NA	X	3058	1/1	0.89	0.36	2.64	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	X	2953	1/1	0.94	0.21	1.58	59,59,59,59	0
31	LMA	X	2881	58/58	0.90	0.27	1.56	22,83,114,128	0
32	MG	X	3007	1/1	0.93	0.20	1.53	37,37,37,37	0
32	MG	X	2926	1/1	0.97	0.17	1.51	35,35,35,35	0
32	MG	X	3025	1/1	0.98	0.19	0.92	62,62,62,62	0
32	MG	X	2991	1/1	0.98	0.38	0.67	51,51,51,51	0
32	MG	X	2917	1/1	0.99	0.27	0.60	52,52,52,52	0
32	MG	X	2976	1/1	0.96	0.24	0.48	32,32,32,32	0
32	MG	X	3009	1/1	0.97	0.25	0.37	53,53,53,53	0
32	MG	C	206	1/1	0.98	0.20	0.14	37,37,37,37	0
32	MG	X	2922	1/1	0.95	0.18	-0.39	19,19,19,19	0
33	NA	K	117	1/1	0.90	0.16	-0.39	28,28,28,28	0
32	MG	X	3028	1/1	0.93	0.19	-0.82	65,65,65,65	0
32	MG	X	2996	1/1	0.98	0.08	-3.49	42,42,42,42	0
32	MG	X	2994	1/1	0.96	0.10	-3.56	41,41,41,41	0
32	MG	X	2932	1/1	0.99	0.36	-	31,31,31,31	0
32	MG	X	2945	1/1	0.93	0.47	-	32,32,32,32	0
33	NA	X	3052	1/1	0.92	0.25	-	43,43,43,43	0
32	MG	X	2987	1/1	0.94	0.46	-	38,38,38,38	0
32	MG	X	2948	1/1	0.97	0.43	-	40,40,40,40	0
32	MG	X	2906	1/1	0.97	0.39	-	43,43,43,43	0
33	NA	X	3035	1/1	0.94	0.29	-	50,50,50,50	0
32	MG	X	2910	1/1	0.92	0.30	-	47,47,47,47	0
33	NA	X	3067	1/1	0.91	0.29	-	47,47,47,47	0
32	MG	X	2999	1/1	0.94	0.18	-	49,49,49,49	0
32	MG	X	2899	1/1	0.97	0.30	-	57,57,57,57	0
33	NA	X	3062	1/1	0.93	0.14	-	47,47,47,47	0
32	MG	X	3012	1/1	0.96	0.57	-	45,45,45,45	0
33	NA	X	3068	1/1	0.98	0.30	-	64,64,64,64	0
34	K	X	3081	1/1	0.97	0.36	-	91,91,91,91	0
32	MG	X	2975	1/1	0.86	0.23	-	73,73,73,73	0
32	MG	X	2986	1/1	0.98	0.26	-	54,54,54,54	0
32	MG	X	2988	1/1	0.91	0.29	-	63,63,63,63	0
32	MG	X	2950	1/1	0.93	0.25	-	49,49,49,49	0
34	K	X	3073	1/1	0.97	0.40	-	57,57,57,57	0
32	MG	X	2908	1/1	0.94	0.31	-	55,55,55,55	0
33	NA	X	3046	1/1	0.89	0.59	-	80,80,80,80	0
33	NA	X	3039	1/1	0.93	0.28	-	51,51,51,51	0
32	MG	X	2972	1/1	0.94	0.21	-	65,65,65,65	0
32	MG	X	2977	1/1	0.96	0.32	-	51,51,51,51	0
32	MG	X	2936	1/1	0.95	0.27	-	26,26,26,26	0
33	NA	X	3041	1/1	0.96	0.31	-	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	X	2952	1/1	0.86	0.44	-	57,57,57,57	0
33	NA	X	3060	1/1	0.98	0.70	-	73,73,73,73	0
32	MG	X	2882	1/1	0.98	0.33	-	5,5,5,5	0
32	MG	X	3022	1/1	0.92	0.14	-	43,43,43,43	0
32	MG	X	2900	1/1	0.95	0.41	-	37,37,37,37	0
34	K	X	3076	1/1	0.76	0.37	-	100,100,100,100	0
33	NA	X	3044	1/1	0.94	0.09	-	48,48,48,48	0
33	NA	X	3053	1/1	0.83	0.53	-	62,62,62,62	0
34	K	X	3075	1/1	0.95	0.22	-	68,68,68,68	0
33	NA	X	3049	1/1	0.93	0.49	-	68,68,68,68	0
34	K	X	3082	1/1	0.94	0.29	-	98,98,98,98	0
32	MG	X	2971	1/1	0.96	0.24	-	44,44,44,44	0
33	NA	X	3055	1/1	0.95	0.28	-	70,70,70,70	0
32	MG	X	2937	1/1	0.88	0.24	-	46,46,46,46	0
32	MG	X	2940	1/1	0.92	0.25	-	34,34,34,34	0
32	MG	X	2951	1/1	0.99	0.37	-	28,28,28,28	0
32	MG	X	2918	1/1	0.90	0.22	-	60,60,60,60	0
34	K	X	3083	1/1	0.96	0.28	-	103,103,103,103	0
32	MG	X	2992	1/1	0.84	0.23	-	44,44,44,44	0
32	MG	X	3023	1/1	0.85	0.32	-	73,73,73,73	0
32	MG	X	2998	1/1	0.96	0.38	-	29,29,29,29	0
32	MG	X	3021	1/1	0.96	0.54	-	70,70,70,70	0
32	MG	X	2925	1/1	0.93	0.35	-	72,72,72,72	0
32	MG	X	3003	1/1	0.95	0.48	-	55,55,55,55	0
33	NA	X	3066	1/1	0.92	0.41	-	48,48,48,48	0
32	MG	X	2887	1/1	0.90	0.31	-	37,37,37,37	0
32	MG	X	2963	1/1	0.94	0.27	-	69,69,69,69	0
32	MG	X	3018	1/1	0.92	0.41	-	59,59,59,59	0
34	K	X	3074	1/1	0.75	0.67	-	171,171,171,171	0
33	NA	X	3043	1/1	0.97	0.31	-	48,48,48,48	0
33	NA	X	3064	1/1	0.72	0.27	-	58,58,58,58	0
33	NA	X	3040	1/1	0.98	0.41	-	70,70,70,70	0
32	MG	X	2980	1/1	0.99	0.12	-	42,42,42,42	0
32	MG	X	2927	1/1	0.97	0.21	-	55,55,55,55	0
32	MG	X	2984	1/1	0.95	0.29	-	62,62,62,62	0
32	MG	X	2895	1/1	0.94	0.35	-	19,19,19,19	0
34	K	X	3072	1/1	0.95	0.21	-	104,104,104,104	0
34	K	X	3078	1/1	0.95	0.32	-	91,91,91,91	0
32	MG	X	2970	1/1	0.88	0.21	-	51,51,51,51	0
33	NA	X	3057	1/1	0.91	0.90	-	75,75,75,75	0
33	NA	X	3063	1/1	0.92	0.38	-	50,50,50,50	0
32	MG	X	2939	1/1	0.83	0.56	-	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	NA	X	3061	1/1	0.81	0.55	-	62,62,62,62	0
32	MG	X	3014	1/1	0.91	0.36	-	54,54,54,54	0
34	K	X	3071	1/1	0.96	0.23	-	86,86,86,86	0
32	MG	X	2968	1/1	0.93	0.26	-	56,56,56,56	0
32	MG	X	2883	1/1	0.92	0.33	-	34,34,34,34	0
32	MG	X	2969	1/1	0.94	0.24	-	31,31,31,31	0
32	MG	X	3013	1/1	0.97	0.11	-	60,60,60,60	0
32	MG	X	2989	1/1	0.95	0.39	-	83,83,83,83	0
32	MG	X	2924	1/1	0.98	0.31	-	26,26,26,26	0
32	MG	X	2966	1/1	0.87	0.29	-	60,60,60,60	0
34	K	X	3080	1/1	0.96	0.49	-	94,94,94,94	0
32	MG	X	2903	1/1	0.86	0.45	-	51,51,51,51	0
32	MG	X	2938	1/1	0.98	0.40	-	34,34,34,34	0
32	MG	X	2997	1/1	0.88	0.20	-	50,50,50,50	0
32	MG	X	3027	1/1	0.93	0.17	-	51,51,51,51	0
32	MG	X	3026	1/1	0.95	0.33	-	37,37,37,37	0
32	MG	X	2923	1/1	0.92	0.53	-	66,66,66,66	0
32	MG	X	2993	1/1	0.96	0.36	-	51,51,51,51	0
32	MG	X	2930	1/1	0.93	0.53	-	51,51,51,51	0
32	MG	X	2892	1/1	0.96	0.23	-	30,30,30,30	0
32	MG	X	2958	1/1	0.97	0.10	-	29,29,29,29	0
32	MG	X	2913	1/1	0.95	0.43	-	56,56,56,56	0
32	MG	X	3017	1/1	0.97	0.51	-	70,70,70,70	0
32	MG	X	2947	1/1	0.96	0.39	-	47,47,47,47	0
32	MG	X	3019	1/1	0.91	0.41	-	74,74,74,74	0
33	NA	X	3034	1/1	0.96	0.30	-	50,50,50,50	0
32	MG	X	3010	1/1	0.92	0.42	-	73,73,73,73	0
32	MG	X	2907	1/1	0.92	0.48	-	66,66,66,66	0
32	MG	X	2931	1/1	0.83	0.59	-	48,48,48,48	0
32	MG	X	3008	1/1	0.94	0.25	-	45,45,45,45	0
32	MG	X	3006	1/1	0.98	0.07	-	59,59,59,59	0
32	MG	X	2949	1/1	0.93	0.40	-	48,48,48,48	0
33	NA	X	3036	1/1	0.88	0.26	-	79,79,79,79	0
33	NA	Y	125	1/1	0.97	0.44	-	62,62,62,62	0
32	MG	X	3005	1/1	0.95	0.15	-	58,58,58,58	0
33	NA	X	3050	1/1	0.91	0.30	-	40,40,40,40	0
33	NA	A	277	1/1	0.83	0.43	-	72,72,72,72	0
32	MG	X	2928	1/1	0.89	0.40	-	41,41,41,41	0
32	MG	X	2905	1/1	0.97	0.37	-	57,57,57,57	0
33	NA	X	3069	1/1	0.84	0.94	-	74,74,74,74	0
32	MG	X	2934	1/1	0.91	0.20	-	62,62,62,62	0
32	MG	X	2889	1/1	0.97	0.26	-	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	NA	X	3037	1/1	0.83	0.26	-	53,53,53,53	0
32	MG	X	2891	1/1	0.78	0.20	-	56,56,56,56	0
33	NA	X	3048	1/1	0.95	0.26	-	71,71,71,71	0
32	MG	X	3000	1/1	0.90	0.25	-	65,65,65,65	0
32	MG	X	2919	1/1	0.96	0.35	-	61,61,61,61	0
33	NA	X	3065	1/1	0.96	0.38	-	58,58,58,58	0
32	MG	X	3001	1/1	0.97	0.46	-	84,84,84,84	0
32	MG	X	2912	1/1	0.95	0.34	-	24,24,24,24	0
32	MG	X	2954	1/1	0.97	0.31	-	31,31,31,31	0
33	NA	X	3051	1/1	0.96	0.24	-	43,43,43,43	0
32	MG	X	2981	1/1	0.97	0.47	-	65,65,65,65	0
32	MG	X	3031	1/1	0.98	0.15	-	48,48,48,48	0
32	MG	X	2893	1/1	0.95	0.48	-	25,25,25,25	0
32	MG	Y	124	1/1	0.96	0.11	-	40,40,40,40	0
33	NA	X	3056	1/1	0.93	0.70	-	76,76,76,76	0
32	MG	X	2956	1/1	0.95	0.66	-	71,71,71,71	0
33	NA	X	3047	1/1	0.94	0.59	-	75,75,75,75	0
32	MG	X	2884	1/1	0.97	0.54	-	38,38,38,38	0
34	K	X	3079	1/1	0.93	0.47	-	97,97,97,97	0
32	MG	X	2955	1/1	0.97	0.37	-	54,54,54,54	0
32	MG	X	2916	1/1	0.92	0.30	-	51,51,51,51	0
33	NA	X	3054	1/1	0.97	0.37	-	49,49,49,49	0
32	MG	X	2909	1/1	0.94	0.43	-	44,44,44,44	0
32	MG	X	2959	1/1	0.98	0.40	-	33,33,33,33	0
32	MG	X	2929	1/1	0.99	0.32	-	10,10,10,10	0
32	MG	X	2946	1/1	0.98	0.45	-	38,38,38,38	0
32	MG	X	2990	1/1	0.96	0.38	-	31,31,31,31	0
32	MG	X	3015	1/1	0.88	0.45	-	77,77,77,77	0
32	MG	X	3030	1/1	0.95	0.10	-	66,66,66,66	0
32	MG	X	2983	1/1	0.95	0.26	-	23,23,23,23	0
33	NA	X	3038	1/1	0.90	0.39	-	59,59,59,59	0
33	NA	Z	61	1/1	0.94	0.30	-	48,48,48,48	0
32	MG	X	2902	1/1	0.97	0.35	-	39,39,39,39	0
32	MG	X	2942	1/1	0.93	0.20	-	74,74,74,74	0
33	NA	X	3059	1/1	0.95	0.14	-	66,66,66,66	0
32	MG	I	157	1/1	0.88	0.35	-	50,50,50,50	0
32	MG	X	2935	1/1	0.94	0.31	-	55,55,55,55	0
32	MG	X	2985	1/1	0.92	0.17	-	50,50,50,50	0
32	MG	X	3032	1/1	0.93	0.38	-	74,74,74,74	0
32	MG	X	3029	1/1	0.94	0.41	-	63,63,63,63	0
32	MG	X	2962	1/1	0.96	0.13	-	70,70,70,70	0
32	MG	X	2921	1/1	0.94	0.23	-	52,52,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.