



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 05:36 PM UTC

PDB ID : 1N8R / pdb_00001n8r
Title : Structure of large ribosomal subunit in complex with virginiamycin M
Authors : Hansen, J.L.; Moore, P.B.; Steitz, T.A.
Deposited on : 2002-11-21
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

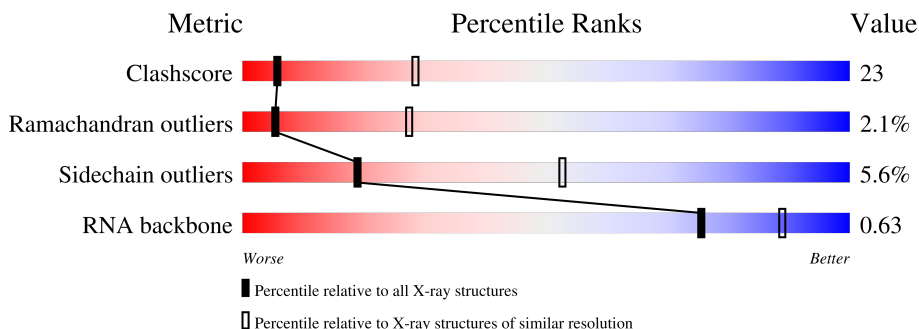
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RNA backbone	3983	1109 (3.20-2.80)

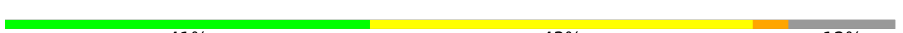
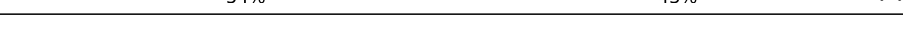
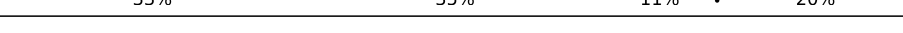
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	2922	
2	B	122	
3	C	239	
4	D	337	
5	E	246	
6	F	176	

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Mol	Chain	Length	Quality of chain
7	G	177	
8	H	119	
9	I	348	
10	J	167	
11	K	145	
12	L	132	
13	M	164	
14	N	194	
15	O	186	
16	P	115	
17	Q	148	
18	R	95	
19	S	154	
20	T	84	
21	U	119	
22	V	66	
23	W	70	
24	X	154	
25	Y	91	
26	Z	240	
27	1	73	
28	2	56	
29	3	48	
30	4	92	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	CL	M	8510	-	-	X	-
35	CL	N	8518	-	-	X	-

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 98569 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 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2754	Total	C	N	O	P	0	0	0
			59017	26346	10878	19048	2745			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	122	Total	C	N	O	P	0	0	0
			2600	1160	472	847	121			

- Molecule 3 is a protein called 50S ribosomal protein L2P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	237	Total	C	N	O	S	0	0	0
			1754	1072	352	325	5			

- Molecule 4 is a protein called 50S ribosomal protein L3P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	337	Total	C	N	O	S	0	0	0
			2624	1616	493	510	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	PRO	deletion	UNP P20279
D	310	ARG	PHE	conflict	UNP P20279

- Molecule 5 is a protein called 50S ribosomal protein L4E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	246	Total	C	N	O	S	0	0	0
			1858	1131	344	382	1			

- Molecule 6 is a protein called 50S ribosomal protein L5P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	140	Total	C	N	O	S	0	0	0
			1094	685	195	210	4			

- Molecule 7 is a protein called 50S ribosomal protein L6P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	172	Total	C	N	O	S	0	0	0
			1357	840	224	289	4			

- Molecule 8 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	119	Total	C	N	O	S	0	0	0
			885	552	141	191	1			

- Molecule 9 is a protein called Acidic ribosomal protein P0 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	29	Total	C	N	O	S	0	0	0
			240	149	39	51	1			

- Molecule 10 is a protein called 50S ribosomal protein L10e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	156	Total	C	N	O	S	0	0	0
			1215	766	233	212	4			

- Molecule 11 is a protein called 50S ribosomal protein L13P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	142	Total	C	N	O	S	0	0	0
			1119	696	199	221	3			

- Molecule 12 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	132	Total	C	N	O	S	0	0	0
			993	609	189	191	4			

- Molecule 13 is a protein called 50S ribosomal protein L15P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	145	Total	C	N	O	0	0	0
			1114	668	222	224			

- Molecule 14 is a protein called 50S ribosomal protein L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	194	Total	C	N	O	S	0	0	0
			1605	988	346	266	5			

- Molecule 15 is a protein called 50S ribosomal protein L18P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	186	Total	C	N	O	S	0	0	0
			1444	895	262	285	2			

- Molecule 16 is a protein called 50S ribosomal protein L18E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	P	115	Total	C	N	O	0	0	0
			864	529	161	174			

- Molecule 17 is a protein called 50S ribosomal protein L19E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	Q	143	Total	C	N	O	0	0	0
			1133	680	230	223			

- Molecule 18 is a protein called 50S ribosomal protein L21e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	95	Total	C	N	O	0	0	0
			734	450	141	143			

- Molecule 19 is a protein called 50S ribosomal protein L22P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	150	Total	C	N	O	S	0	0	0
			1149	713	209	223	4			

- Molecule 20 is a protein called 50S ribosomal protein L23P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	81	Total	C	N	O	S	0	0	0
			641	389	111	138	3			

- Molecule 21 is a protein called 50S ribosomal protein L24P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	U	119	Total	C	N	O		0	0	0
			949	568	180	201				

- Molecule 22 is a protein called 50S ribosomal protein L24E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	53	Total	C	N	O	S	0	0	0
			410	244	75	86	5			

- Molecule 23 is a protein called 50S ribosomal protein L29P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	65	Total	C	N	O	S	0	0	0
			499	304	94	100	1			

- Molecule 24 is a protein called 50S ribosomal protein L30P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	X	154	Total	C	N	O	S	0	0	0
			1195	737	209	243	6			

- Molecule 25 is a protein called 50S ribosomal protein L31E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Y	82	Total	C	N	O	S	0	0	0
			654	402	129	122	1			

- Molecule 26 is a protein called 50S ribosomal protein L32E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	142	Total	C	N	O		0	0	0
			1130	686	228	216				

- Molecule 27 is a protein called 50S ribosomal protein L37AE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1	73	Total	C	N	O	S	0	0	0
			563	359	111	86	7			

- Molecule 28 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	2	56	Total	C	N	O	S	0	0	0
			430	258	86	82	4			

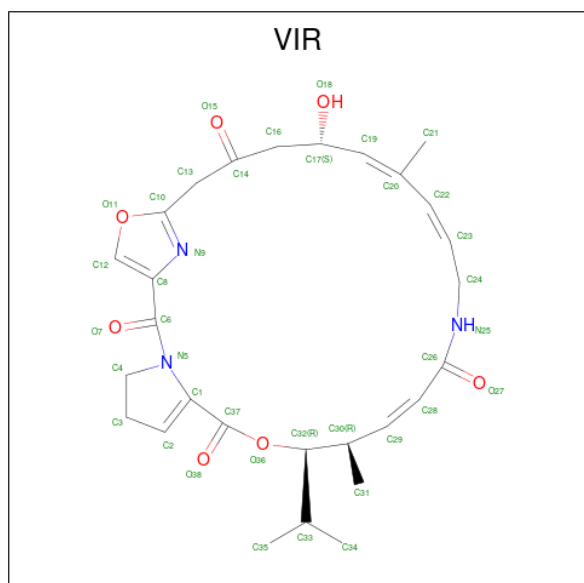
- Molecule 29 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	46	Total	C	N	O	S	0	0	0
			393	238	86	68	1			

- Molecule 30 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	4	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 31 is VIRGINIAMYCIN M1 (CCD ID: VIR) (formula: $C_{28}H_{35}N_3O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	N	O	0	0
			38	28	3	7		

- Molecule 32 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	A	109	Total 109	Mg 109	0	0
32	B	1	Total 1	Mg 1	0	0
32	C	2	Total 2	Mg 2	0	0
32	D	1	Total 1	Mg 1	0	0
32	L	1	Total 1	Mg 1	0	0
32	U	1	Total 1	Mg 1	0	0
32	Z	1	Total 1	Mg 1	0	0
32	4	1	Total 1	Mg 1	0	0

- Molecule 33 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	A	1	Total 1	K 1	0	0

- Molecule 34 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	A	71	Total 71	Na 71	0	0
34	B	2	Total 2	Na 2	0	0
34	C	1	Total 1	Na 1	0	0
34	E	1	Total 1	Na 1	0	0
34	J	2	Total 2	Na 2	0	0
34	K	1	Total 1	Na 1	0	0
34	M	1	Total 1	Na 1	0	0
34	N	1	Total 1	Na 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	R	1	Total 1	Na 1	0	0
34	S	2	Total 2	Na 2	0	0
34	T	1	Total 1	Na 1	0	0
34	U	1	Total 1	Na 1	0	0
34	4	1	Total 1	Na 1	0	0

- Molecule 35 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	A	8	Total 8	Cl 8	0	0
35	C	1	Total 1	Cl 1	0	0
35	D	1	Total 1	Cl 1	0	0
35	K	3	Total 3	Cl 3	0	0
35	L	1	Total 1	Cl 1	0	0
35	M	1	Total 1	Cl 1	0	0
35	N	1	Total 1	Cl 1	0	0
35	O	1	Total 1	Cl 1	0	0
35	P	1	Total 1	Cl 1	0	0
35	S	1	Total 1	Cl 1	0	0
35	Z	2	Total 2	Cl 2	0	0
35	4	1	Total 1	Cl 1	0	0

- Molecule 36 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	P	1	Total Cd 1 1	0	0
36	V	1	Total Cd 1 1	0	0
36	1	1	Total Cd 1 1	0	0
36	2	1	Total Cd 1 1	0	0
36	4	1	Total Cd 1 1	0	0

- Molecule 37 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	A	5881	Total O 5881 5881	0	0
37	B	146	Total O 146 146	0	0
37	C	135	Total O 135 135	0	0
37	D	141	Total O 141 141	0	0
37	E	178	Total O 178 178	0	0
37	F	49	Total O 49 49	0	0
37	G	43	Total O 43 43	0	0
37	H	30	Total O 30 30	0	0
37	I	21	Total O 21 21	0	0
37	J	76	Total O 76 76	0	0
37	K	55	Total O 55 55	0	0
37	L	64	Total O 64 64	0	0
37	M	85	Total O 85 85	0	0
37	N	141	Total O 141 141	0	0
37	O	67	Total O 67 67	0	0

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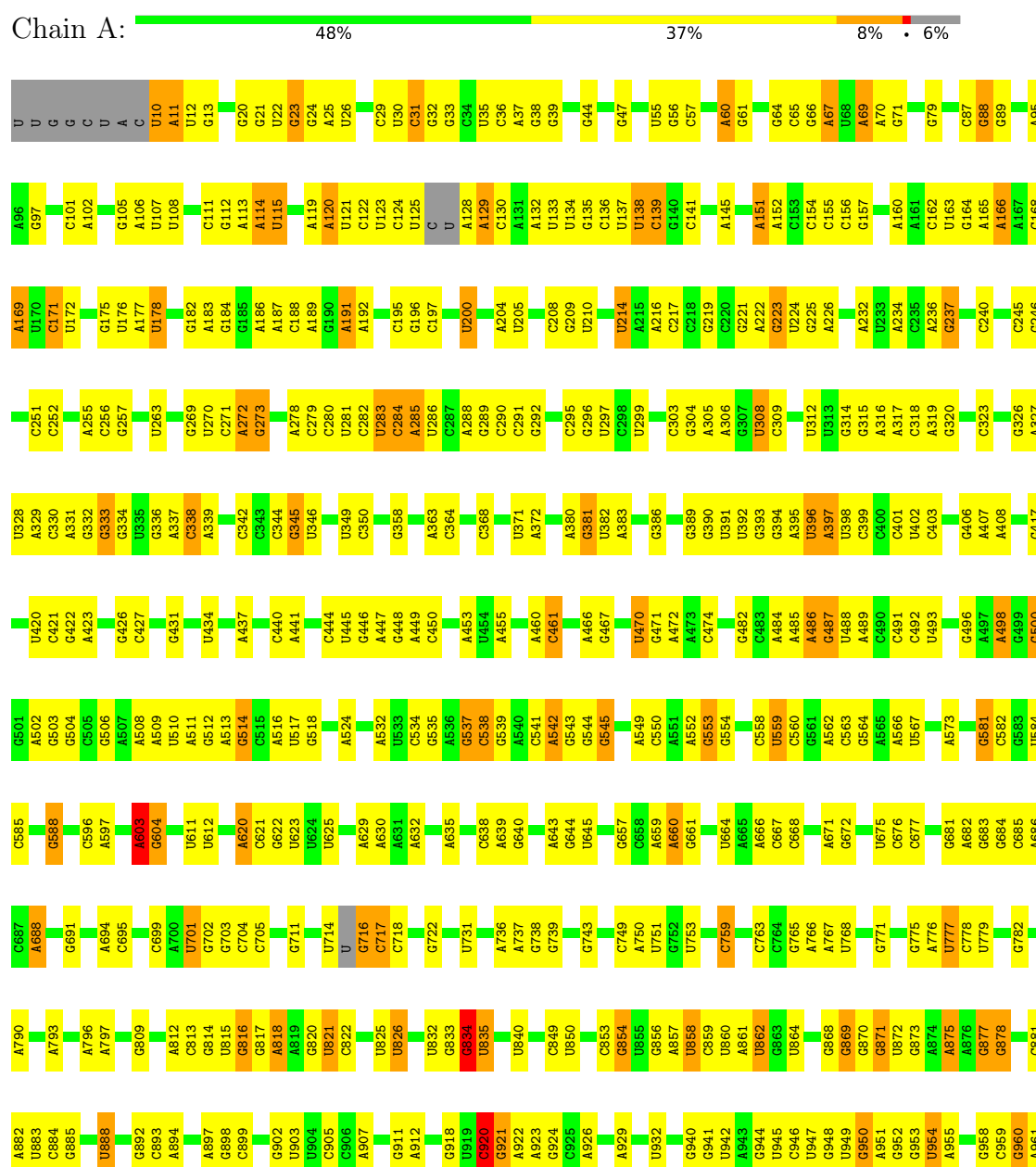
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	P	45	Total 45	O 45	0	0
37	Q	72	Total 72	O 72	0	0
37	R	57	Total 57	O 57	0	0
37	S	87	Total 87	O 87	0	0
37	T	34	Total 34	O 34	0	0
37	U	33	Total 33	O 33	0	0
37	V	27	Total 27	O 27	0	0
37	W	16	Total 16	O 16	0	0
37	X	68	Total 68	O 68	0	0
37	Y	27	Total 27	O 27	0	0
37	Z	100	Total 100	O 100	0	0
37	1	35	Total 35	O 35	0	0
37	2	57	Total 57	O 57	0	0
37	3	40	Total 40	O 40	0	0
37	4	72	Total 72	O 72	0	0

3 Residue-property plots

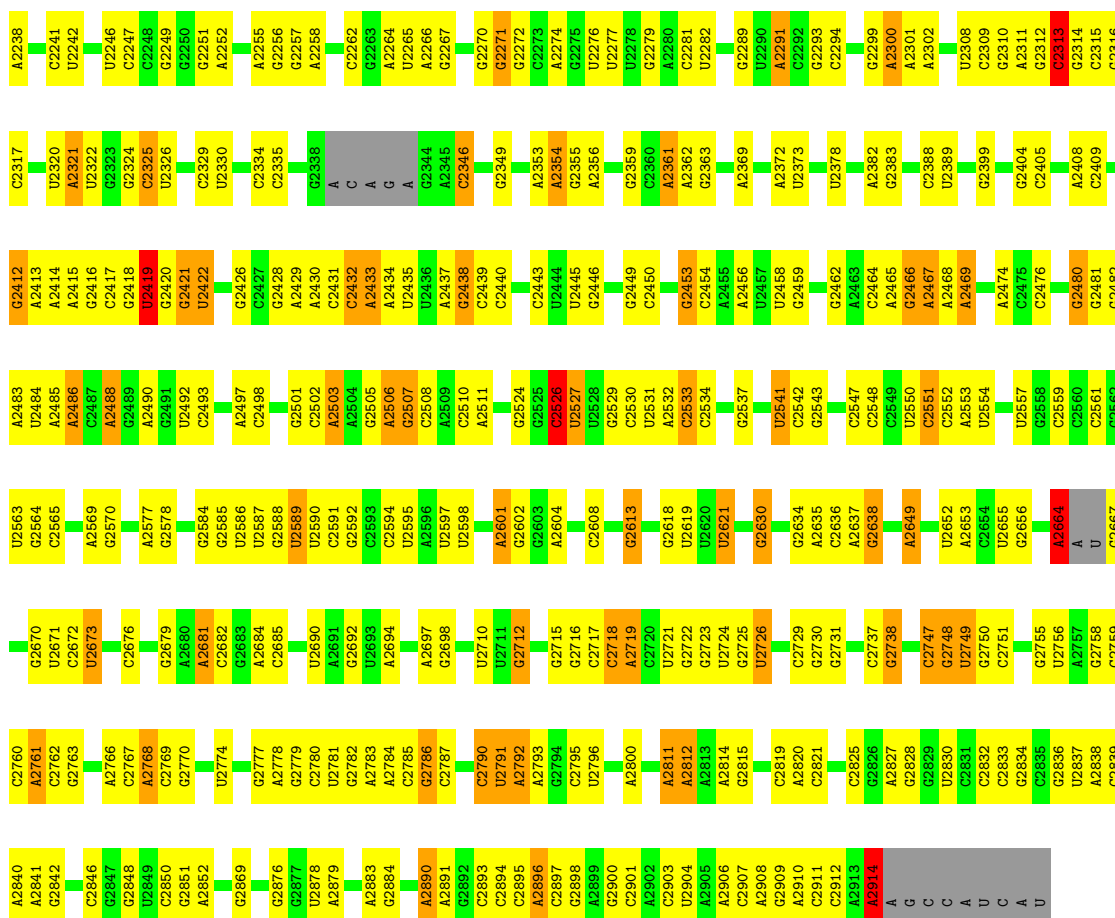
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

• Molecule 1: 23S ribosomal RNA

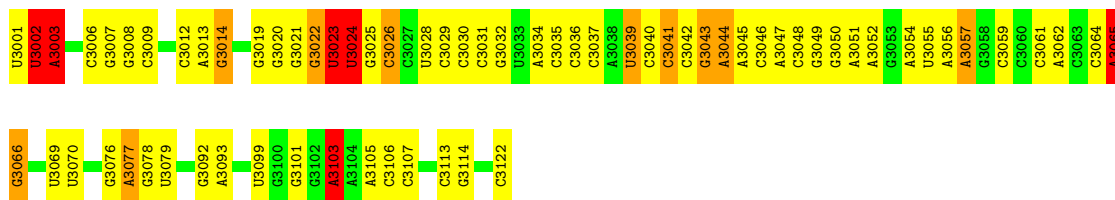


A	G	C2114	U2016	A1930	G1855	C1763	G1681	A1598	G1512	U1412	A1313	G1216	G1134	G1045	C962
G	C	U2115	A2019	C1936	C1856	U1766	A1682	G1601	C1512	U1413	U1314	G1226	G1135	G1061	C963
U	U	U2116	A2017	C1936	A1857	A1767	G1683	C1602	C1514	A1414	G1316	G1227	G1136	G1052	U970
C	A	A2118	G2023	U1939	A1858	C1768	A1685	A1603	A1515	G1417	G1319	C1228	G1143	G1053	G
A	C	C2119	C1940	A1859	A1858	C1769	A1686	G1604	A1516	U1418	G1324	U1234	G1151	G1055	U
C	C	U2120	U2028	U1941	U1860	U1770	C1687	G1605	U1517	U1419	G1325	G1235	G1152	G1056	G
C	C	G2121	C2029	A1942	C1861	C1772	G1688	A1606	G1523	U1420	G1326	U1236	G1153	U1067	U
C	C	C2122	C1943	C1862	C1863	C1773	C1692	A1607	U1524	U1421	G1327	G1237	G1154	A1057	C
C	C	A2123	U2032	G1863	C1864	G1773	C1692	G1608	U1525	U1422	A1328	U1237	G1155	A1058	C
G	G	G2126	U2034	G1865	C1866	G1777	C1699	G1609	U1526	U1423	A1329	U1238	G1156	G1059	G
U	U	U2127	C2035	G1866	C1867	A1778	C1700	G1610	A1527	U1424	A1330	G1239	G1161	C1060	C
A	A	G2128	A2038	G1867	C1868	A1779	A1701	C1613	U1528	A1435	A1331	G1240	G1162	C1061	U
G	G	U2133	A2039	A1868	C1869	C1787	U1702	G1614	U1529	U1436	C1332	A1242	G1163	U1062	C
G	G	G2134	G2040	A1869	C1870	U1788	G1706	A1615	U1530	A1437	C1333	C1243	G1164	C1063	C
G	G	A2135	G2041	A1870	C1871	U1789	G1707	U1616	U1531	A1438	C1334	C1244	G1165	A1067	C
C	C	G2136	A2042	C1872	C1873	U1790	A1710	C1617	G1535	G1441	G1340	A1246	G1166	G1068	A
C	C	A	G2043	U1874	U1875	C1792	A1711	U1625	C1536	G1442	A1341	A1247	G1167	G1069	G
C	C	C	A2054	G1878	A1879	G1795	A1712	A1626	U1543	G1443	A1342	A1248	G1168	A	
A	A	C	A2055	U1879	C1880	A1796	G1713	G1627	U1544	G1444	C1343	U1249	U1169	G	
C	C	C	U2063	C1881	C1882	C1798	A1717	G1633	G1545	G1445	G1349	C1250	U1170	A	
C	C	C	U2064	C1883	C1884	C1798	G1718	U1634	G1546	C1450	U1350	C1251	A1172	G	
A	A	C	C	U1887	C1888	C1804	G1722	U1635	A1547	C1451	G1351	C1252	A1173	U	
C	C	C	C	U1889	C1889	G1805	G1723	G1636	U1557	C1452	G1352	G1260	G1175	G	
G	G	C	C	U1890	C1890	G1806	U1724	A1637	C1558	G1453	C1353	A1261	G1176	A	
C	C	C	C	U1891	C1891	C1810	C1725	A1559	U	U1454	U1359	C1262	A1177	C	
A	A	C	C	U1892	C1892	C1811	G1728	A1642	U1561	U1461	C1360	G1265	U1180	A	
C	C	C	C	U1893	C1893	U1813	A1729	C1643	C1562	C1462	C1361	G1266	A1181	C	
C	C	C	C	U1894	C1894	C1818	G1730	U1644	C1563	A1463	C1362	C1268	A1182	A1088	
A	A	C	C	U1895	C1895	C1819	A1733	U1645	C1564	A1471	U1367	U1270	U1185	U1095	U1003
A	A	C	C	U1896	C1896	G1820	G1734	G1646	C1565	C1472	U1368	U1279	U1186	A1005	C1004
C	C	C	C	U1897	C1897	A1821	C1734	G1647	C1566	U1473	U1369	U1279	U1187	A1006	A1007
C	C	C	C	U1898	C1898	C1822	C1735	C1651	A1567	C1474	A1372	U1279	A1188	A1008	A1009
C	C	C	C	U1899	C1899	U1825	A1736	C1652	C1570	C1475	A1189	A1287	U1189	U1109	U1009
C	C	C	C	U1900	C1900	C1826	C1737	U1654	G1571	A1476	G1190	U1288	G1190	G1110	C1010
C	C	C	C	U1901	C1901	G1827	C1738	U1655	A1572	A1477	A1191	C1289	G1191	C1011	C1012
C	C	C	C	U1902	C1902	G1828	C1739	U1656	C1573	U1478	A1192	G1290	A1192	A1117	A1118
C	C	C	C	U1903	C1903	A1829	U1741	A1657	C1574	C1483	G1378	A1291	A1193	G1119	G1120
C	C	C	C	U1904	C1904	C1834	A1742	A1658	U1580	G1484	U1380	A1292	G1197	U1120	C1015
C	C	C	C	U1905	C1905	C1834	G1743	A1659	U1581	A1485	U1381	A1294	G1197	G1121	U1016
C	C	C	C	U1906	C1906	U1835	G1744	G1660	U1582	A1494	G1385	U1298	C1201	U1122	G1021
C	C	C	C	U1907	C1907	U1835	U1745	A1661	U1583	C1495	G1386	U1299	U1205	A1123	A1022
C	C	C	C	U1908	C1908	C1839	C1750	C1666	G1586	G1496	G1391	G1300	U1206	A1124	C1023
C	C	C	C	U1909	C1909	A1840	G1751	A1667	U1587	G1497	A1392	U1304	U1207	U1125	C1024
C	C	C	C	U1910	C1910	C1844	G1752	U1668	G1588	G1498	A1393	C1305	C1208	C1126	G1025
C	C	C	C	U1911	C1911	A1845	A1754	G1670	G1589	U1499	C1394	U1306	C1209	C1127	C1026
C	C	C	C	U1912	C1912	U1846	A1755	G1671	G1590	U1500	G1398	U1307	G1210	G1027	G1028
C	C	C	C	U1913	C1913	A1847	A1756	C1675	G1591	U1501	A1399	A1308	G1211	U1130	U1029
C	C	C	C	U1914	C1914	G1848	G1759	G1676	C1594	U1503	A1406	A1309	C1212	U1030	C1044
C	C	C	C	U1915	C1915	U1849	G1760	G1679	G1595	A1504	U1505	G1311	C1213	A1132	
C	C	C	C	U1916	C1916	U1850	G1761	C1680	U1597	U1506	A1407	G1312	A1215	A1133	
C	C	C	C	U1917	C1917	G1851	C1762								



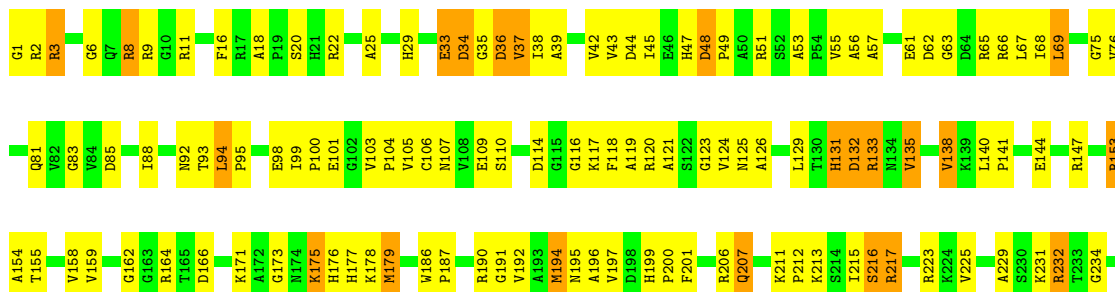
• Molecule 2: 5S ribosomal RNA

Chain B: 44% 43% 8% 5%



• Molecule 3: 50S ribosomal protein L2P

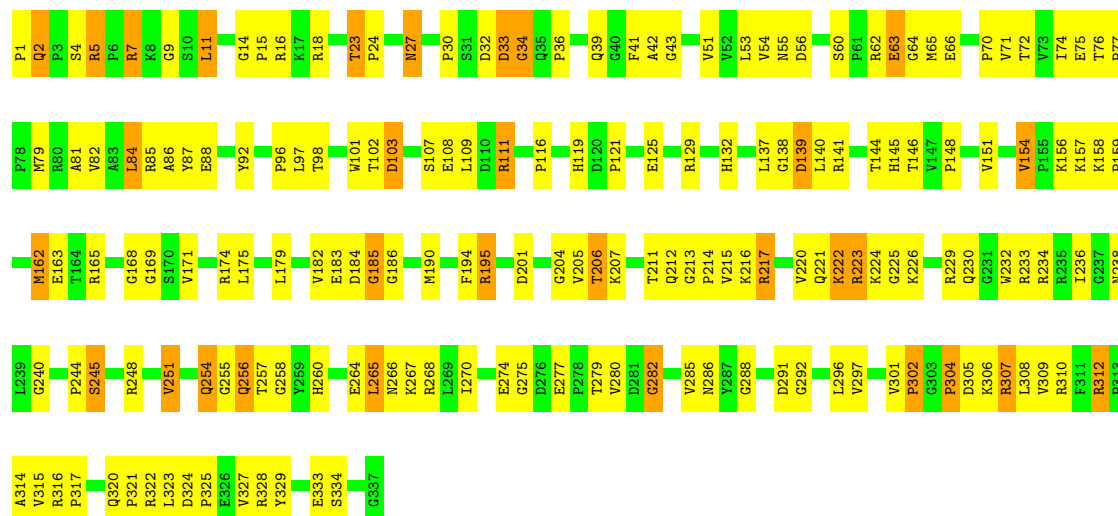
Chain C: 48% 42% 9%





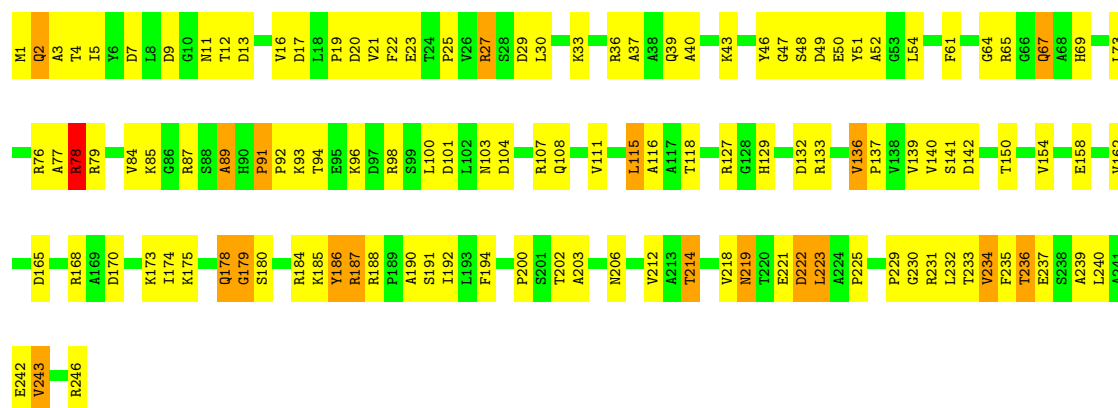
• Molecule 4: 50S ribosomal protein L3P

Chain D: 47% 44% 9%



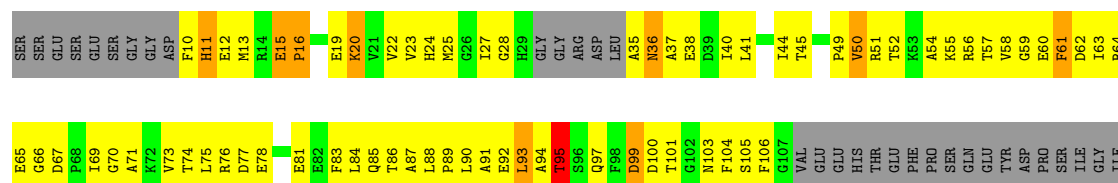
• Molecule 5: 50S ribosomal protein L4E

Chain E: 50% 42% 7%



• Molecule 6: 50S ribosomal protein L5P

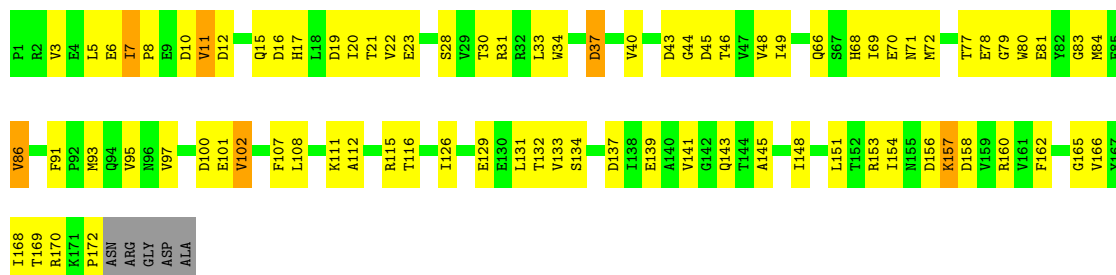
Chain F: 25% 45% 7% 20%





• Molecule 7: 50S ribosomal protein L6P

Chain G: 51% 43%



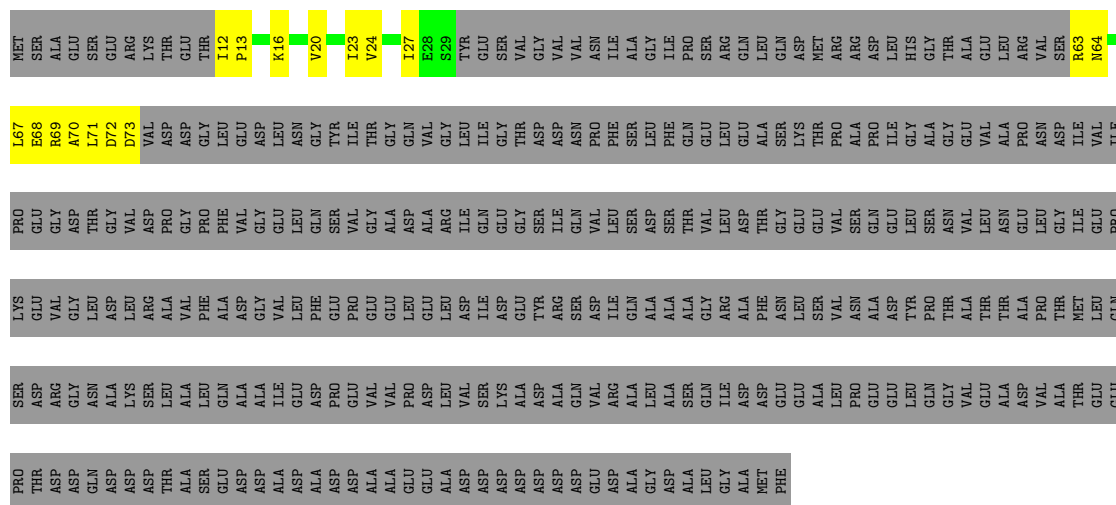
• Molecule 8: 50S ribosomal protein L7Ae

Chain H: 50% 45%



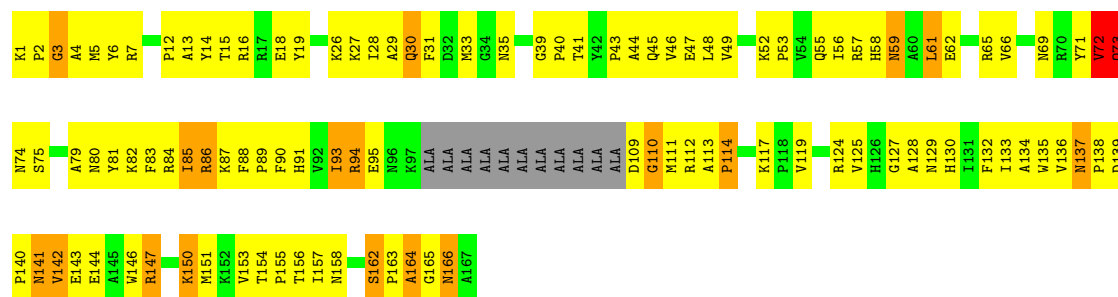
• Molecule 9: Acidic ribosomal protein P0 homolog

Chain I: 5% 92%



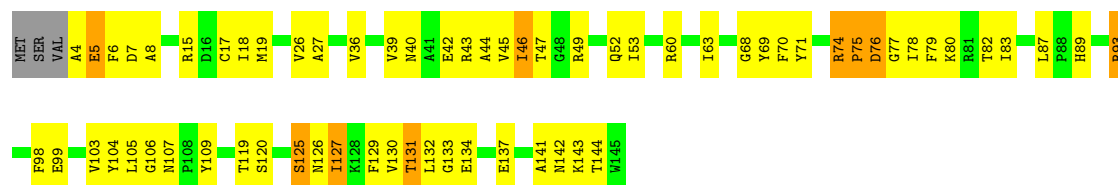
• Molecule 10: 50S ribosomal protein L10e

Chain J: 29% 52% 11% 7%



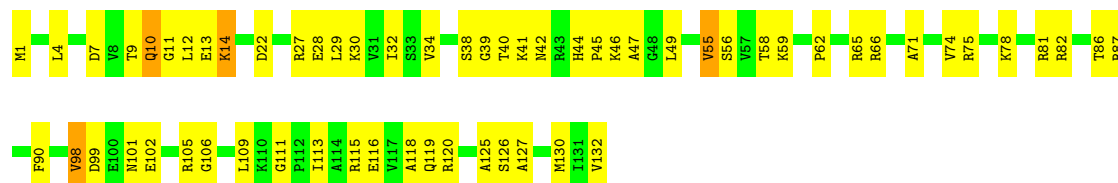
• Molecule 11: 50S ribosomal protein L13P

Chain K: 53% 39% 6%



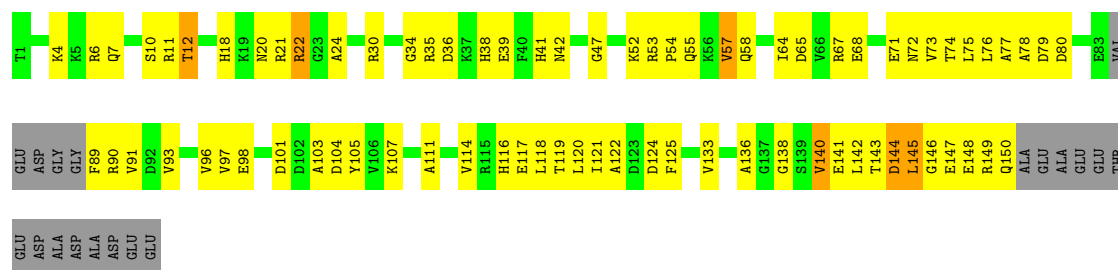
• Molecule 12: 50S ribosomal protein L14P

Chain L: 54% 43%



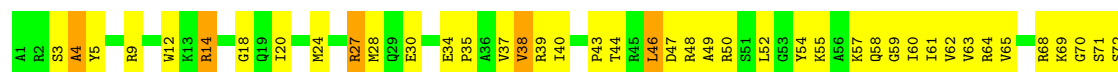
• Molecule 13: 50S ribosomal protein L15P

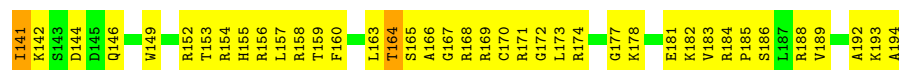
Chain M: 41% 43% 12%



• Molecule 14: 50S ribosomal protein L15E

Chain N: 32% 57% 10%





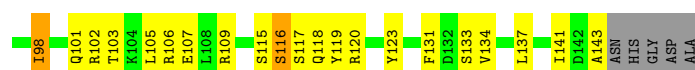
• Molecule 15: 50S ribosomal protein L18P



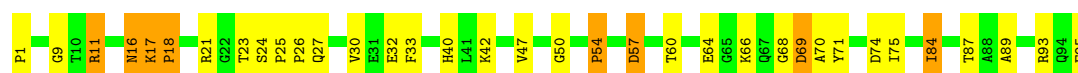
• Molecule 16: 50S ribosomal protein L18E



• Molecule 17: 50S ribosomal protein L19E



• Molecule 18: 50S ribosomal protein L21e



• Molecule 19: 50S ribosomal protein L22P

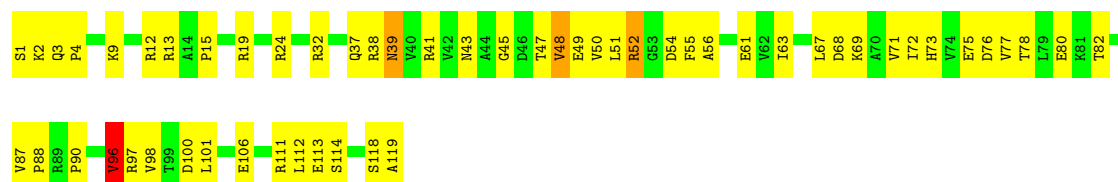




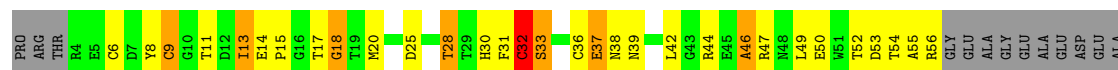
- Molecule 20: 50S ribosomal protein L23P



- Molecule 21: 50S ribosomal protein L24P



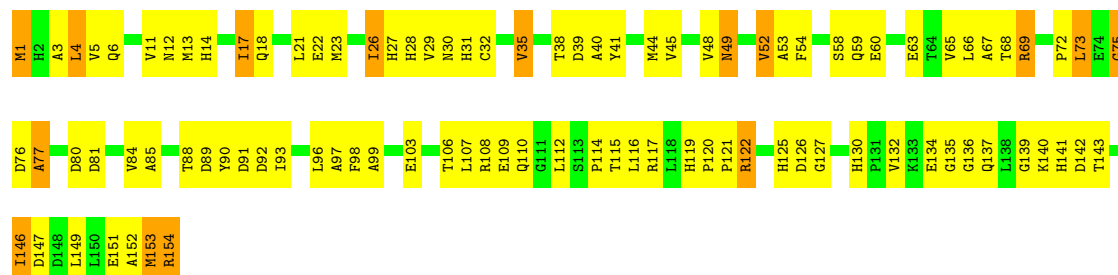
- Molecule 22: 50S ribosomal protein L24E



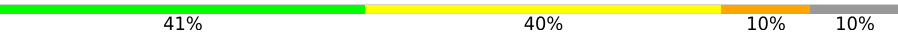
- Molecule 23: 50S ribosomal protein L29P

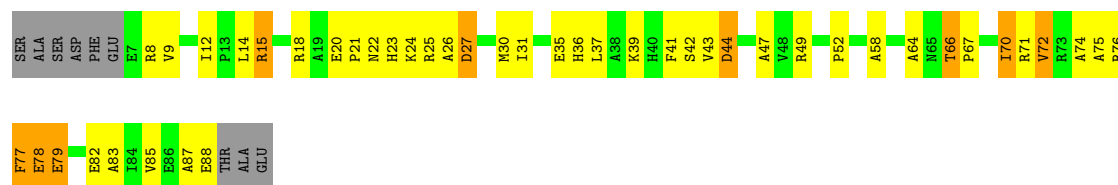


- Molecule 24: 50S ribosomal protein L30P

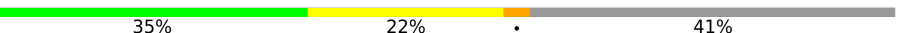


- Molecule 25: 50S ribosomal protein L31E

Chain Y:  41% 40% 10% 10%



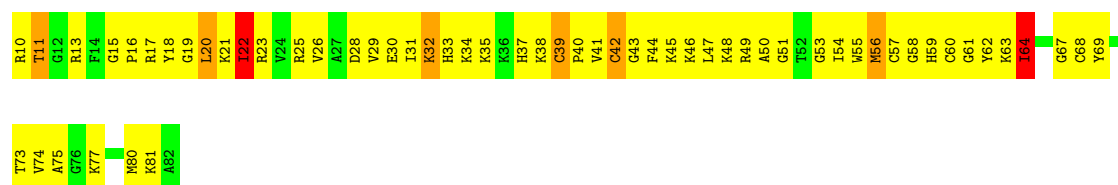
- Molecule 26: 50S ribosomal protein L32E

Chain Z:  35% 22% 41%



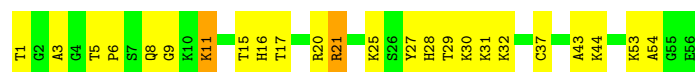
- Molecule 27: 50S ribosomal protein L37AE

Chain 1:  21% 68% 8% .



- Molecule 28: 50S ribosomal protein L37e

Chain 2:  57% 39% .

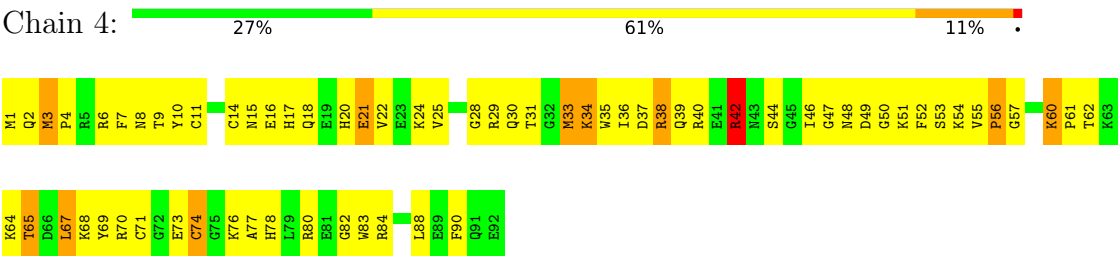


- Molecule 29: 50S ribosomal protein L39e

Chain 3:  54% 40% . .



● Molecule 30: 50S ribosomal protein L44E



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	212.90 Å 300.47 Å 575.18 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00	Depositor
% Data completeness (in resolution range)	94.6 (20.00-3.00)	Depositor
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.201 , 0.242	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	98569	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.49	5/66076 (0.0%)	0.73	44/103052 (0.0%)
2	B	0.72	8/2905 (0.3%)	0.89	14/4528 (0.3%)
3	C	0.58	1/1787 (0.1%)	1.12	11/2409 (0.5%)
4	D	0.54	0/2689	1.11	19/3652 (0.5%)
5	E	0.61	0/1883	1.12	11/2551 (0.4%)
6	F	0.47	0/1111	0.98	7/1498 (0.5%)
7	G	0.54	0/1382	0.98	7/1880 (0.4%)
8	H	0.49	0/896	0.97	3/1219 (0.2%)
9	I	0.47	0/241	0.82	0/324
10	J	0.62	0/1246	1.33	15/1686 (0.9%)
11	K	0.58	0/1135	1.04	5/1530 (0.3%)
12	L	0.55	0/1003	1.13	8/1351 (0.6%)
13	M	0.50	0/1126	1.13	11/1504 (0.7%)
14	N	0.80	3/1633 (0.2%)	1.29	19/2180 (0.9%)
15	O	0.52	0/1473	1.17	14/1999 (0.7%)
16	P	0.55	0/873	1.06	7/1181 (0.6%)
17	Q	0.55	0/1143	0.99	2/1521 (0.1%)
18	R	0.57	0/748	1.18	7/1005 (0.7%)
19	S	0.60	0/1172	1.11	10/1578 (0.6%)
20	T	0.50	0/648	1.01	4/875 (0.5%)
21	U	0.49	0/957	1.08	5/1289 (0.4%)
22	V	0.95	1/417 (0.2%)	1.23	5/562 (0.9%)
23	W	0.50	0/502	1.05	2/675 (0.3%)
24	X	0.72	2/1218 (0.2%)	1.07	5/1655 (0.3%)
25	Y	0.60	0/664	1.08	2/895 (0.2%)
26	Z	0.58	0/1146	1.06	4/1536 (0.3%)
27	1	0.94	1/575 (0.2%)	1.28	7/763 (0.9%)
28	2	0.66	0/437	1.14	4/578 (0.7%)
29	3	0.56	0/398	0.87	0/527
30	4	1.19	2/771 (0.3%)	1.16	5/1024 (0.5%)
All	All	0.54	23/98255 (0.0%)	0.85	257/147027 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	157
2	B	0	4
All	All	1	161

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3003	A	O5'-C5'	9.09	1.56	1.42
1	A	2488	A	O5'-C5'	-9.02	1.28	1.42
2	B	3024	U	O5'-C5'	8.96	1.55	1.42
30	4	33	MET	SD-CE	7.74	1.98	1.79
2	B	3019	G	O5'-C5'	7.51	1.53	1.42

The worst 5 of 257 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1164	U	OP2-P-O3'	-14.62	64.14	108.00
1	A	1164	U	OP1-P-O3'	-14.27	65.19	108.00
1	A	1979	G	C2'-C3'-O3'	14.26	130.90	109.50
1	A	1563	G	C2'-C3'-O3'	14.05	130.58	109.50
14	N	141	ILE	N-CA-C	-13.73	100.78	111.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1563	G	C3'

5 of 161 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	22	U	Sidechain
1	A	23	G	Sidechain
1	A	26	U	Sidechain
1	A	32	G	Sidechain
1	A	33	G	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	59017	0	29801	1311	0
2	B	2600	0	1326	85	0
3	C	1754	0	1763	149	0
4	D	2624	0	2533	205	0
5	E	1858	0	1816	150	0
6	F	1094	0	1085	139	0
7	G	1357	0	1266	88	0
8	H	885	0	854	77	0
9	I	240	0	231	24	0
10	J	1215	0	1215	172	0
11	K	1119	0	1098	70	0
12	L	993	0	1027	65	0
13	M	1114	0	1072	82	0
14	N	1605	0	1676	221	0
15	O	1444	0	1401	152	0
16	P	864	0	873	30	0
17	Q	1133	0	1127	70	0
18	R	734	0	729	29	0
19	S	1149	0	1122	69	0
20	T	641	0	605	27	0
21	U	949	0	923	53	0
22	V	410	0	368	48	0
23	W	499	0	511	34	0
24	X	1195	0	1137	125	0
25	Y	654	0	653	47	0
26	Z	1130	0	1133	63	0
27	1	563	0	601	85	0
28	2	430	0	426	31	0
29	3	393	0	406	22	0
30	4	755	0	732	91	0
31	A	38	0	34	3	0
32	4	1	0	0	0	0
32	A	109	0	0	0	0
32	B	1	0	0	0	0
32	C	2	0	0	0	0
32	D	1	0	0	0	0
32	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	U	1	0	0	0	0
32	Z	1	0	0	0	0
33	A	1	0	0	0	0
34	4	1	0	0	0	0
34	A	71	0	0	0	0
34	B	2	0	0	0	0
34	C	1	0	0	0	0
34	E	1	0	0	0	0
34	J	2	0	0	0	0
34	K	1	0	0	0	0
34	M	1	0	0	0	0
34	N	1	0	0	0	0
34	R	1	0	0	0	0
34	S	2	0	0	0	0
34	T	1	0	0	0	0
34	U	1	0	0	0	0
35	4	1	0	0	1	0
35	A	8	0	0	0	0
35	C	1	0	0	0	0
35	D	1	0	0	0	0
35	K	3	0	0	1	0
35	L	1	0	0	0	0
35	M	1	0	0	2	0
35	N	1	0	0	2	0
35	O	1	0	0	1	0
35	P	1	0	0	0	0
35	S	1	0	0	0	0
35	Z	2	0	0	0	0
36	1	1	0	0	0	0
36	2	1	0	0	0	0
36	4	1	0	0	0	0
36	P	1	0	0	0	0
36	V	1	0	0	0	0
37	1	35	0	0	15	0
37	2	57	0	0	2	0
37	3	40	0	0	6	0
37	4	72	0	0	11	0
37	A	5881	0	0	303	0
37	B	146	0	0	21	0
37	C	135	0	0	16	0
37	D	141	0	0	34	0
37	E	178	0	0	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	F	49	0	0	18	0
37	G	43	0	0	11	0
37	H	30	0	0	11	0
37	I	21	0	0	7	0
37	J	76	0	0	23	0
37	K	55	0	0	6	0
37	L	64	0	0	19	0
37	M	85	0	0	24	0
37	N	141	0	0	36	0
37	O	67	0	0	20	0
37	P	45	0	0	10	0
37	Q	72	0	0	10	0
37	R	57	0	0	3	0
37	S	87	0	0	9	0
37	T	34	0	0	5	0
37	U	33	0	0	6	0
37	V	27	0	0	6	0
37	W	16	0	0	2	0
37	X	68	0	0	11	0
37	Y	27	0	0	5	0
37	Z	100	0	0	14	0
All	All	98569	0	59544	3489	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 23.

The worst 5 of 3489 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)
10:J:86:ARG:NH1	10:J:133:ILE:HG13	1.52	1.20
10:J:165:GLY:HA3	37:J:8397:HOH:O	1.39	1.18
27:1:39:CYS:SG	27:1:47:LEU:HD21	1.84	1.17
14:N:87:MET:HG2	30:4:46:ILE:HG21	1.25	1.15
6:F:25:MET:HE2	6:F:41:LEU:HG	1.23	1.15

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	C	235/239 (98%)	200 (85%)	29 (12%)	6 (3%)	4	23
4	D	335/337 (99%)	302 (90%)	22 (7%)	11 (3%)	3	17
5	E	244/246 (99%)	222 (91%)	22 (9%)	0	100	100
6	F	134/176 (76%)	95 (71%)	27 (20%)	12 (9%)	0	3
7	G	170/177 (96%)	157 (92%)	12 (7%)	1 (1%)	21	56
8	H	117/119 (98%)	104 (89%)	10 (8%)	3 (3%)	4	23
9	I	25/348 (7%)	23 (92%)	1 (4%)	1 (4%)	2	14
10	J	152/167 (91%)	130 (86%)	17 (11%)	5 (3%)	3	17
11	K	140/145 (97%)	127 (91%)	8 (6%)	5 (4%)	2	16
12	L	130/132 (98%)	120 (92%)	8 (6%)	2 (2%)	8	35
13	M	141/164 (86%)	120 (85%)	20 (14%)	1 (1%)	18	53
14	N	192/194 (99%)	165 (86%)	24 (12%)	3 (2%)	7	34
15	O	184/186 (99%)	164 (89%)	12 (6%)	8 (4%)	2	12
16	P	113/115 (98%)	109 (96%)	4 (4%)	0	100	100
17	Q	141/148 (95%)	135 (96%)	5 (4%)	1 (1%)	18	53
18	R	93/95 (98%)	86 (92%)	3 (3%)	4 (4%)	2	12
19	S	148/154 (96%)	134 (90%)	13 (9%)	1 (1%)	18	53
20	T	79/84 (94%)	73 (92%)	6 (8%)	0	100	100
21	U	117/119 (98%)	110 (94%)	7 (6%)	0	100	100
22	V	51/66 (77%)	48 (94%)	3 (6%)	0	100	100
23	W	63/70 (90%)	58 (92%)	3 (5%)	2 (3%)	3	18
24	X	152/154 (99%)	142 (93%)	8 (5%)	2 (1%)	9	38
25	Y	80/91 (88%)	71 (89%)	5 (6%)	4 (5%)	1	10
26	Z	140/240 (58%)	133 (95%)	7 (5%)	0	100	100
27	1	71/73 (97%)	61 (86%)	7 (10%)	3 (4%)	2	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	2	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
29	3	42/48 (88%)	41 (98%)	1 (2%)	0	100	100
30	4	90/92 (98%)	83 (92%)	5 (6%)	2 (2%)	5	26
All	All	3633/4235 (86%)	3265 (90%)	291 (8%)	77 (2%)	5	27

5 of 77 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	139	ASP
6	F	93	LEU
6	F	95	THR
6	F	173	GLU
8	H	101	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	179/181 (99%)	166 (93%)	13 (7%)	13	42
4	D	282/282 (100%)	264 (94%)	18 (6%)	16	48
5	E	193/193 (100%)	176 (91%)	17 (9%)	9	35
6	F	117/147 (80%)	109 (93%)	8 (7%)	14	45
7	G	152/155 (98%)	149 (98%)	3 (2%)	48	76
8	H	92/92 (100%)	90 (98%)	2 (2%)	45	74
9	I	27/283 (10%)	27 (100%)	0	100	100
10	J	122/122 (100%)	107 (88%)	15 (12%)	4	21
11	K	118/121 (98%)	110 (93%)	8 (7%)	14	45
12	L	106/106 (100%)	102 (96%)	4 (4%)	29	63
13	M	112/126 (89%)	109 (97%)	3 (3%)	39	71
14	N	166/166 (100%)	159 (96%)	7 (4%)	26	61
15	O	149/149 (100%)	141 (95%)	8 (5%)	20	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	P	93/93 (100%)	89 (96%)	4 (4%)	26	60
17	Q	113/116 (97%)	110 (97%)	3 (3%)	39	71
18	R	79/79 (100%)	74 (94%)	5 (6%)	16	48
19	S	117/121 (97%)	113 (97%)	4 (3%)	32	66
20	T	71/73 (97%)	70 (99%)	1 (1%)	59	80
21	U	105/105 (100%)	102 (97%)	3 (3%)	37	70
22	V	44/52 (85%)	41 (93%)	3 (7%)	14	45
23	W	51/56 (91%)	50 (98%)	1 (2%)	48	76
24	X	130/130 (100%)	121 (93%)	9 (7%)	14	45
25	Y	66/73 (90%)	60 (91%)	6 (9%)	9	33
26	Z	120/195 (62%)	110 (92%)	10 (8%)	10	37
27	1	56/56 (100%)	49 (88%)	7 (12%)	4	20
28	2	46/46 (100%)	46 (100%)	0	100	100
29	3	42/44 (96%)	41 (98%)	1 (2%)	43	73
30	4	79/79 (100%)	71 (90%)	8 (10%)	7	29
All	All	3027/3441 (88%)	2856 (94%)	171 (6%)	19	52

5 of 171 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	R	54	PRO
25	Y	66	THR
19	S	39	THR
24	X	4	LEU
26	Z	189	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 107 such sidechains are listed below:

Mol	Chain	Res	Type
15	O	153	GLN
20	T	9	HIS
28	2	28	HIS
17	Q	66	GLN
19	S	61	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2747/2922 (94%)	256 (9%)	38 (1%)
2	B	121/122 (99%)	14 (11%)	4 (3%)
All	All	2868/3044 (94%)	270 (9%)	42 (1%)

5 of 270 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	11	A
1	A	31	C
1	A	60	A
1	A	67	A
1	A	69	A

5 of 42 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	2005	G
1	A	2718	C
1	A	2011	A
1	A	2467	A
1	A	2791	U

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 232 ligands modelled in this entry, 231 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	VIR	A	9403	-	38,40,40	2.51	17 (44%)	42,55,55	1.96	13 (30%)

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	VIR	A	9403	-	-	11/48/58/58	0/2/3/3

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	9403	VIR	C28-C29	-7.80	1.15	1.32
31	A	9403	VIR	C13-C10	-4.87	1.44	1.50
31	A	9403	VIR	C4-N5	4.41	1.53	1.47
31	A	9403	VIR	C17-C19	-3.50	1.46	1.50
31	A	9403	VIR	C28-C26	3.49	1.55	1.48

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	9403	VIR	O27-C26-C28	5.57	135.79	122.95
31	A	9403	VIR	C28-C26-N25	-5.30	103.44	115.07
31	A	9403	VIR	O7-C6-C8	3.39	123.92	118.65
31	A	9403	VIR	C12-C8-C6	-2.91	122.14	127.60
31	A	9403	VIR	C4-N5-C6	2.80	126.88	120.74

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

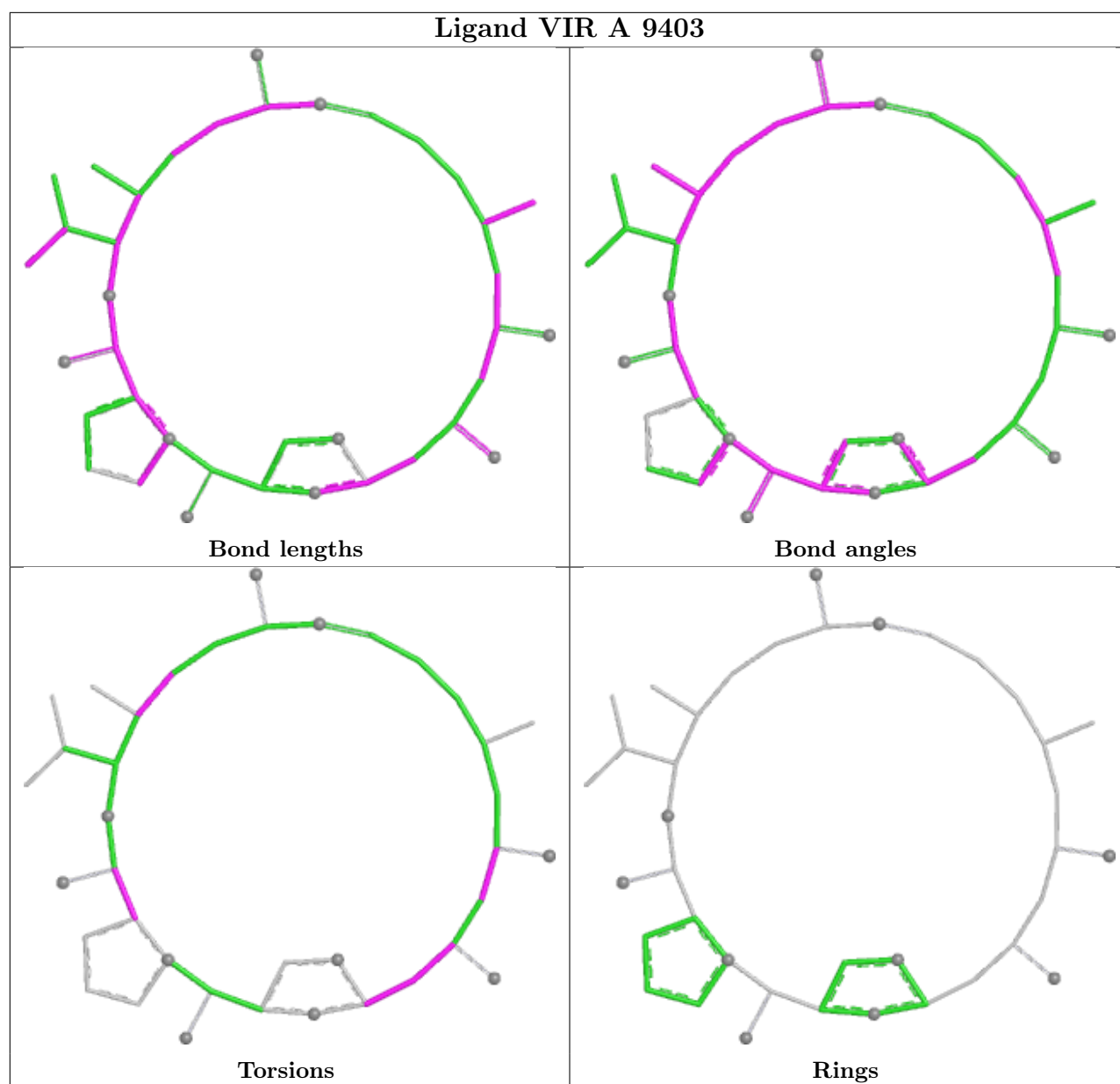
Mol	Chain	Res	Type	Atoms
31	A	9403	VIR	N9-C10-C13-C14
31	A	9403	VIR	O11-C10-C13-C14
31	A	9403	VIR	C14-C16-C17-O18
31	A	9403	VIR	N5-C1-C37-O38
31	A	9403	VIR	N5-C1-C37-O36

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	A	9403	VIR	3	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.