



wwPDB X-ray Structure Validation Summary Report ⓘ

May 17, 2020 – 04:09 am BST

PDB ID : 1N8R
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 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

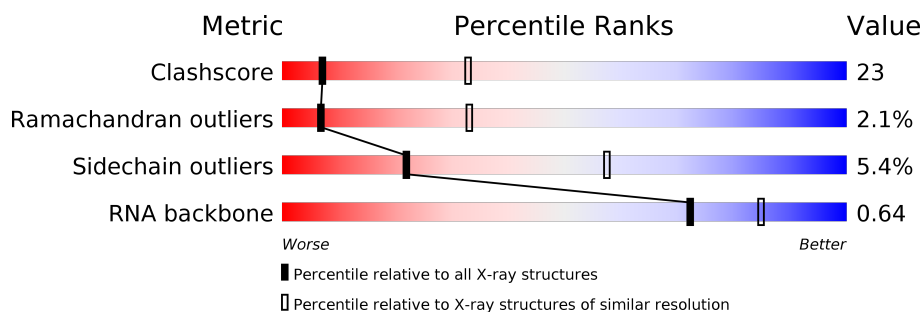
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)









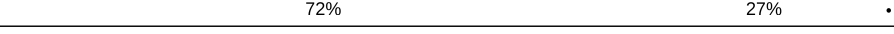







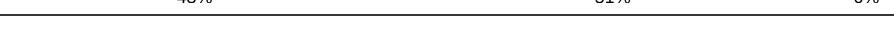
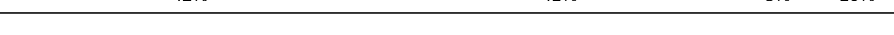

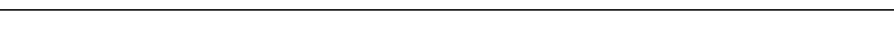
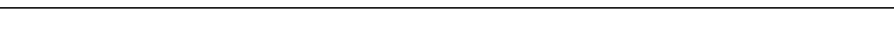
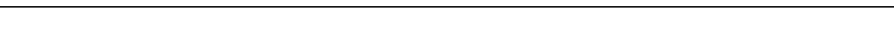
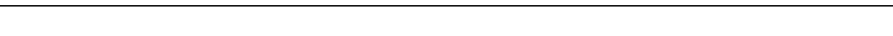
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	2922	48% 37% 8% 6%
2	B	122	43% 43% 10% .
3	C	239	50% 43% 6% .
4	D	337	49% 45% 7%
5	E	246	52% 43% .
6	F	176	26% 45% 7% . 20%
7	G	177	54% 42% . .

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Mol	Chain	Length	Quality of chain
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 criteria:

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			

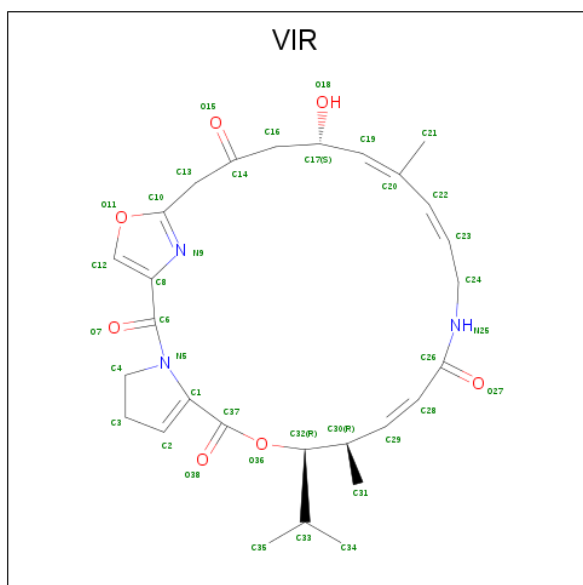
- Molecule 29 is a protein called 50S ribosomal protein L39e.

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 (three-letter code: 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 (three-letter code: MG) (formula: Mg).

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

- Molecule 33 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 34 is SODIUM ION (three-letter code: NA) (formula: Na).

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

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

- Molecule 35 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 36 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	P	1	Total Cd 1 1	0	0
36	2	1	Total Cd 1 1	0	0
36	1	1	Total Cd 1 1	0	0
36	4	1	Total Cd 1 1	0	0
36	V	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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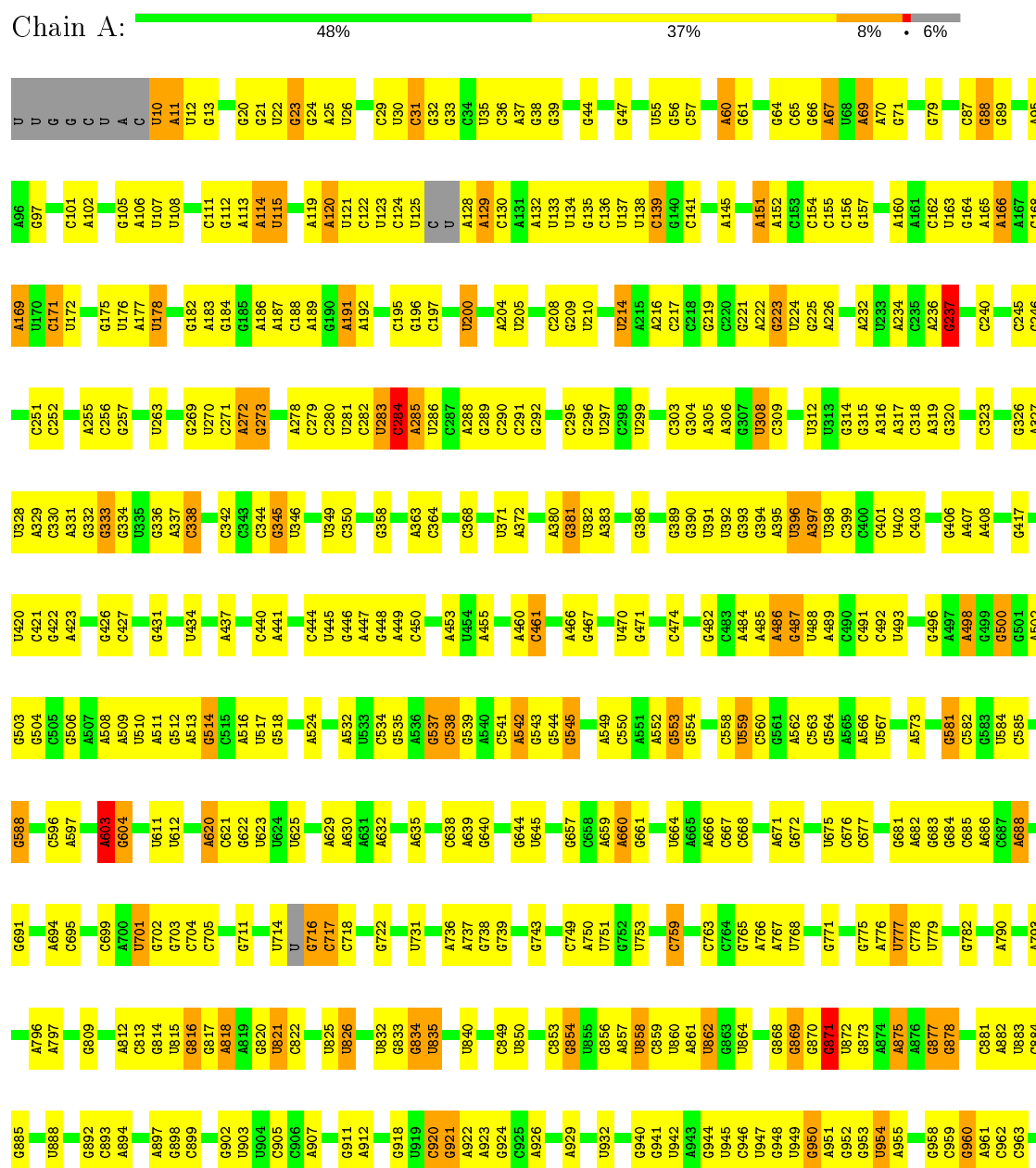
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	P	45	Total 45	O 45	0	0
37	Q	72	Total 72	O 72	0	0
37	R	57	Total 57	O 57	0	0
37	S	87	Total 87	O 87	0	0
37	T	34	Total 34	O 34	0	0
37	U	33	Total 33	O 33	0	0
37	V	27	Total 27	O 27	0	0
37	W	16	Total 16	O 16	0	0
37	X	68	Total 68	O 68	0	0
37	Y	27	Total 27	O 27	0	0
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

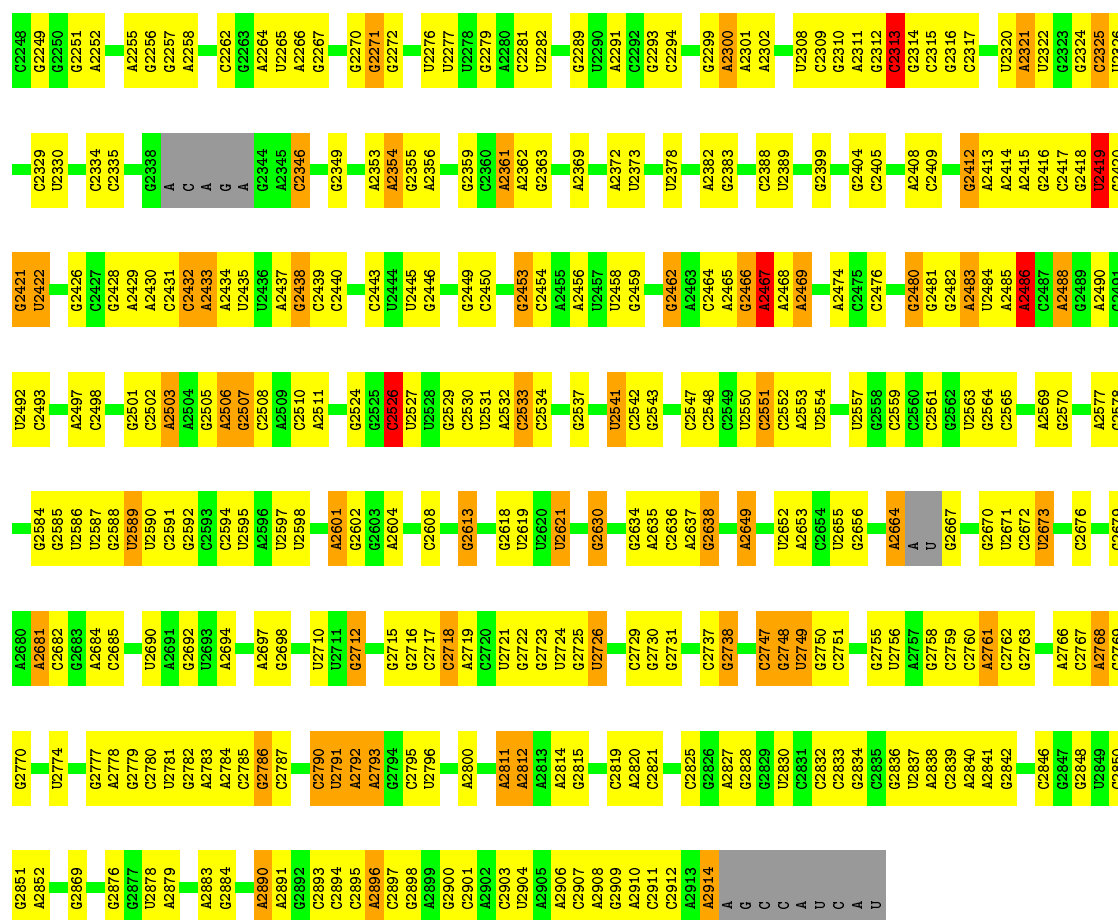
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

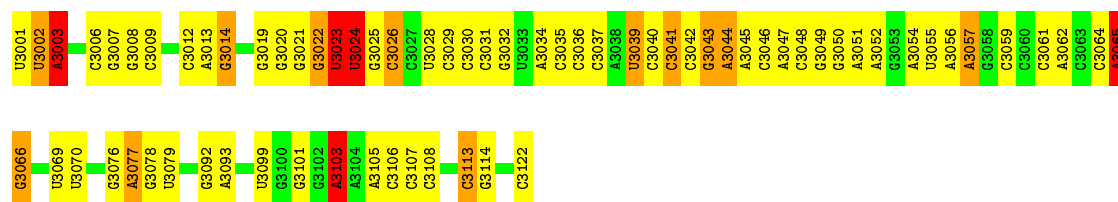
• Molecule 1: 23S ribosomal RNA



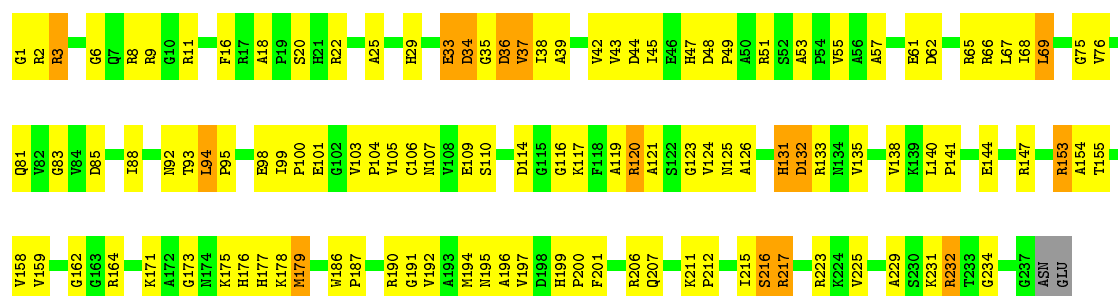
C	G	C2029	A1859	C1768	A1685	A1603	C1516	G1416	C1228	G1143	G1052	U970
C2121	C2122	C2032	U1860	C1769	C1686	G1604	U1517	G1417	C1229	G1143	G1053	G
A2123	A2123	U2032	C1861	U1770	C1687	G1605	U1517	U1418	U1234	G1151	G1054	U
C2126	C2126	G2033	C1862	U1771	G1688	A1606	G1523	U1419	U1234	G1151	G1055	U
U2127	U2127	U2034	G1863	C1772	C1689	A1607	G1524	C1420	G1235	G1158	A1057	C
G2128	G2128	C2035	C1864	G1773	C1692	A1608	G1525	C1421	G1236	G1159	A1058	C
A	A	A	A1865	G1777	C1693	C1609	A1526	C1422	U1237	G1160	G1059	C
C	C	C	A1866	G1778	C1699	G1610	A1527	C1423	G1238	A1161	C1060	C
C	C	C	G1867	A1779	C1700	C1613	G1529	A1434	G1239	G1162	U1062	C
C	C	C	A1868	U1778	C1701	G1614	U1530	C1435	A1242	G1163	U1063	C
C	C	C	A1869	U1779	C1702	A1615	U1531	U1436	U1244	G1164	C1064	C
C	C	C	C1870	U1780	G1706	A1616	U1532	C1437	C1245	G1165	C1065	C
C	C	C	G1871	U1781	A1710	C1617	C1536	A1437	A1246	A1067	C1066	C
C	C	C	U1872	C1791	A1711	U1625	C1536	G1441	A1247	C1068	C1069	C
C	C	C	G1873	C1792	A1712	U1626	C1537	A1442	U1248	G1072	C1070	C
C	C	C	U1874	C1793	G1713	G1627	U1543	A1443	U1249	A1073	G1071	C
C	C	C	U1875	U1795	A1714	C1628	G1544	C1343	U1170	G1074	G1072	C
C	C	C	U1876	U1796	G1715	C1629	U1545	C1344	C1250	G1075	G1073	C
C	C	C	C1877	A1797	U1717	C1633	G1546	G1444	C1251	A1171	G1076	C
C	C	C	A1878	C1798	G1718	G1634	A1547	U1445	A1252	A1172	G1077	C
C	C	C	U1879	U1799	G1719	U1635	G1557	C1450	C1253	A1173	G1078	C
C	C	C	U1880	A1804	U1722	G1636	C1558	C1451	G1260	G1175	A1081	C
C	C	C	A1881	G1805	G1723	A1637	U1559	G1452	A1261	C1176	A1082	C
C	C	C	U1882	G1806	U1724	C1638	U	U1454	C1262	A1177	C1083	C
C	C	C	A1883	C1810	C1725	A1641	U1561	U1461	G1265	U1180	A1084	C
C	C	C	U1884	U1813	G1728	C1642	U1562	C1361	U1181	A1085	A1085	C
C	C	C	A1885	U1814	A1729	C1643	C1563	C1362	C1182	A1086	A1086	C
C	C	C	U1886	U1815	G1730	U1644	G1564	C1363	C1183	A1087	A1087	C
C	C	C	A1887	C1816	C1731	G1645	C1565	G1364	C1184	A1088	A1088	C
C	C	C	U1888	U1817	A1732	G1646	C1566	U1471	U1270	U1095	U1095	C
C	C	C	C1889	G1819	A1733	G1647	C1567	C1472	C1279	A1098	A1098	C
C	C	C	U1890	U1820	C1734	C1651	C1570	C1473	U1279	A1099	A1099	C
C	C	C	A1891	A1822	C1735	C1652	G1571	U1474	A1287	A1109	A1109	C
C	C	C	U1892	U1823	A1736	U1654	A1572	U1475	C1288	G1110	G1110	C
C	C	C	G1902	C1825	C1738	C1655	C1573	C1476	C1289	U1116	U1116	C
C	C	C	U1903	G1826	C1739	C1656	C1574	U1477	G1290	A1117	A1117	C
C	C	C	A1904	G1827	U1741	A1657	C1575	C1478	A1291	A1118	A1118	C
C	C	C	U1905	G1828	A1742	A1658	C1579	U1484	U1293	A1119	A1119	C
C	C	C	A1906	A1829	G1743	A1659	A1580	A1485	U1294	U1120	U1120	C
C	C	C	U1907	C1834	U1748	G1660	U1583	A1494	A1294	G1121	G1121	C
C	C	C	G1916	U1835	U1749	A1661	U1584	C1495	U1298	U1122	U1122	C
C	C	C	U1917	A1840	C1750	C1666	G1586	G1496	G1299	A1123	A1123	C
C	C	C	U1918	U1841	G1751	A1667	U1587	G1497	G1300	U1205	U1205	C
C	C	C	C1919	C1842	G1752	U1668	G1588	G1498	A1206	A1206	A1206	C
C	C	C	A1920	A1843	C1753	A1669	G1589	U1499	C1208	C1208	C1208	C
C	C	C	U1921	U1844	A1754	G1670	G1590	U1500	U1304	C1209	C1209	C
C	C	C	G1922	A1845	A1755	C1671	G1591	U1501	U1305	G1210	U1128	C
C	C	C	A1923	U1846	A1756	C1672	G1592	U1502	A1307	G1211	G1211	C
C	C	C	U1924	A1847	A1757	C1673	G1593	A1504	A1308	C1212	U1130	C
C	C	C	G1925	G1848	A1758	G1676	C1594	U1505	U1309	C1213	G1027	C
C	C	C	A1926	U1849	G1760	G1677	U1595	U1506	U1310	C1214	U1131	C
C	C	C	U1927	U1850	U1761	C1678	U1596	A1407	G1311	A1215	A1133	C
C	C	C	C1928	G1851	C1762	C1679	A1597	U1407	G1312	G1216	G1134	C
C	C	C	U1929	G1852	C1763	C1680	A1598	U1412	A1313	G1226	G1135	C
C	C	C	A1930	G1853	C1764	G1681	A1599	A1413	A1314	U1227	U1136	C
C	C	C	U1931	G1854	C1765	G1682	A1601	U1414	G1315	C1227	C1051	C
C	C	C	C1932	G1855	C1766	G1683	C1602	A1515	G1316			C
C	C	C	U1933	G1856	U1766	G1684						C
C	C	C	A1934	A1857	U1767	A1684						C
C	C	C	U1935	G1858	U1768	A1685						C
C	C	C	C1936	G1859	U1769	A1686						C
C	C	C	U1937	G1860	U1770	A1687						C
C	C	C	A1938	G1861	U1771	A1688						C
C	C	C	U1939	G1862	U1772	A1689						C
C	C	C	C1940	G1863	U1773	A1690						C
C	C	C	U1941	G1864	U1774	A1691						C
C	C	C	A1942	G1865	U1775	A1692						C
C	C	C	U1943	G1866	U1776	A1693						C
C	C	C	C1944	G1867	U1777	A1694						C
C	C	C	G1945	G1868	U1778	A1695						C
C	C	C	U1946	G1869	U1779	A1696						C
C	C	C	G1947	G1870	U1780	A1697						C
C	C	C	U1948	G1871	U1781	A1698						C
C	C	C	G1949	G1872	U1782	A1699						C
C	C	C	U1950	G1873	U1783	A1700						C
C	C	C	A1951	G1874	U1784	A1701						C
C	C	C	U1952	G1875	U1785	A1702						C
C	C	C	G1953	G1876	U1786	A1703						C
C	C	C	A1954	G1877	U1787	A1704						C
C	C	C	U1955	G1878	U1788	A1705						C
C	C	C	G1956	G1879	U1789	A1706						C
C	C	C	U1957	G1880	U1790	A1707						C
C	C	C	A1958	G1881	U1791	A1708						C
C	C	C	U1959	G1882	U1792	A1709						C
C	C	C	G1960	G1883	U1793	A1710						C
C	C	C	U1961	G1884	U1794	A1711						C
C	C	C	A1962	G1885	U1795	A1712						C
C	C	C	U1963	G1886	U1796	A1713						C
C	C	C	G1964	G1887	U1797	A1714						C
C	C	C	U1965	G1888	U1798	A1715						C
C	C	C	A1966	G1889	U1799	A1716						C
C	C	C	U1967	G1890	U1800	A1717						C
C	C	C	G1968	G1891	U1801	A1718						C
C	C	C	U1969	G1892	U1802	A1719						C
C	C	C	A1970	G1893	U1803	A1720						C
C	C	C	U1971	G1894	U1804	A1721						C
C	C	C	G1972	G1895	U1805	A1722						C
C	C	C	U1973	G1896	U1806	A1723						C
C	C	C	A1974	G1897	U1807	A1724						C
C	C	C	U1975	G1898	U1808	A1725						C
C	C	C	G1976	G1899	U1809	A1726						C
C	C	C	U1977	G1900	U1810	A1727						C
C	C	C	A1978	G1901	U1811	A1728						C
C	C	C	U1979	G1902	U1812	A1729						C
C	C	C	G1980	G1903	U1813	A1730						C
C	C	C	U1981	U1904	U1814	A1731						C
C	C	C	A1982	G1905	U1815	A1732						C
C	C	C	U1983	G1906	U1816	A1733						C
C	C	C	G1984	G1907	U1817	A1734						C
C	C	C	U1985	G1908	U1818	A1735						C
C	C	C	A1986	G1909	U1819	A1736						C
C	C	C	U1987	G1910	U1820	A1737						C
C	C	C	G1988	G1911	U1821	A1738						C
C	C	C	U1989	G1912	U1822	A1739						C
C	C	C	A1990	G1913	U1823	A1740						C
C	C	C	U1991	G1914	U1824	A1741						C
C	C	C	G1992	G1915	U1825	A1742						C
C	C	C	U1993	G1916	U1826	A1743						C
C	C	C	A1994	G1917	U1827	A1744						C
C	C	C	U1995	G1918	U1828	A1745						C
C	C	C	G1996	G1919	U1829	A1746						C
C	C	C	U1997	G1920	U1830	A1747						C
C	C	C	A1998	G1921	U1831	A1748						C
C	C	C	U1999	G1922	U1832	A1749						C
C	C	C	G1999	G1923	U1833	A1750						C
C	C	C	U2000	G1924	U1834	A1751						C
C	C	C	A2001	G1925	U1835	A1752						C
C	C	C	U2002	G1926	U1836	A1753						C
C	C	C	G1927	G1927</								



• Molecule 2: 5S ribosomal RNA

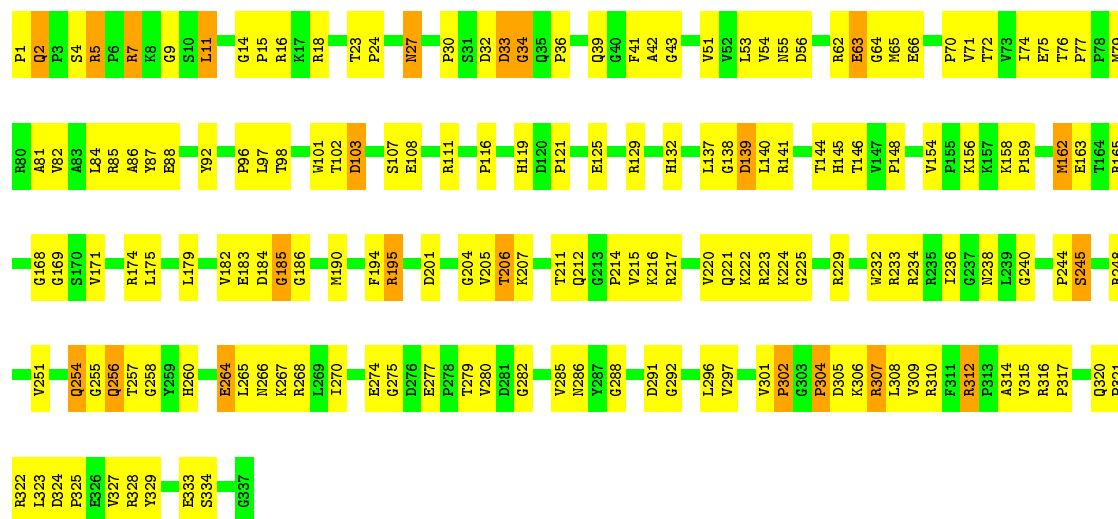


• Molecule 3: 50S ribosomal protein L2P



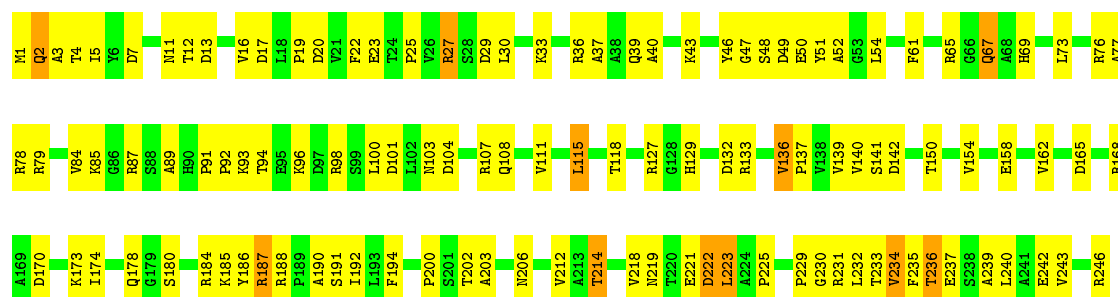
- Molecule 4: 50S ribosomal protein L3P

Chain D:  49% 45% 7%



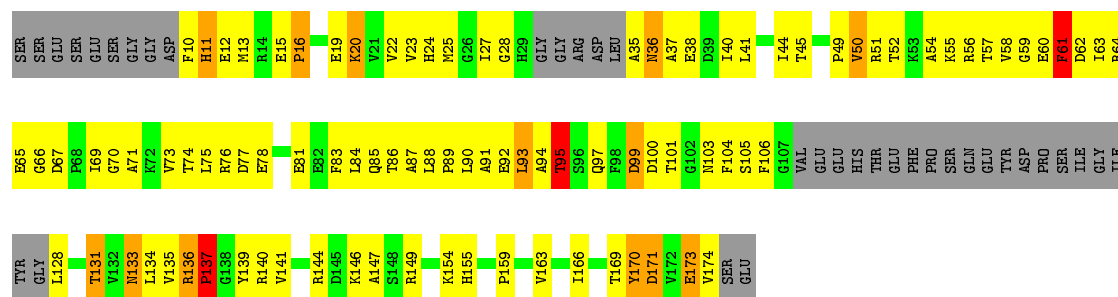
- Molecule 5: 50S ribosomal protein L4E

Chain E:  52% 43% .



- Molecule 6: 50S ribosomal protein L5P

Chain F:  26% 45% 7% 20%



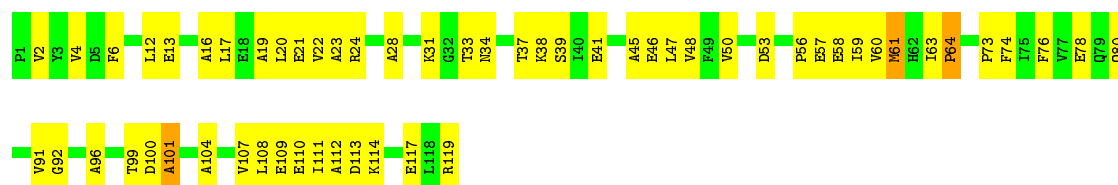
- Molecule 7: 50S ribosomal protein L6P

Chain G:  54% 42% ..



- Molecule 8: 50S ribosomal protein L7Ae

Chain H: 52% 45%



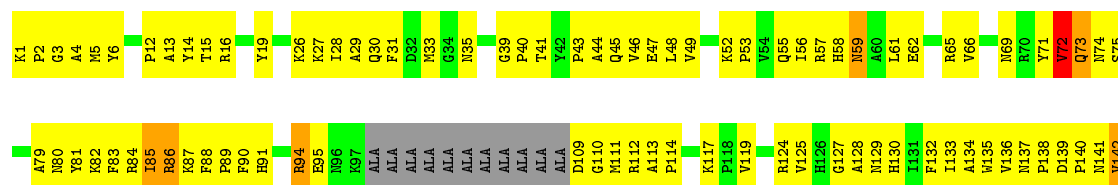
- Molecule 9: Acidic ribosomal protein P0 homolog

Chain I: 5% 92%



- Molecule 10: 50S ribosomal protein L10e

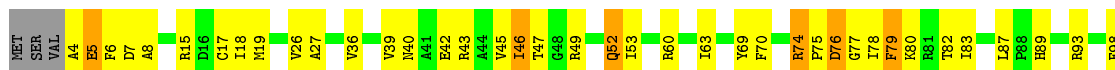
Chain J: 33% 54% 6% 7%





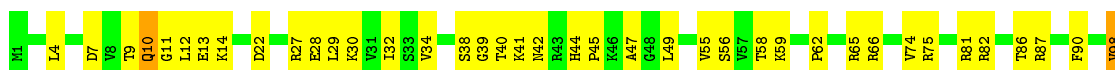
- Molecule 11: 50S ribosomal protein L13P

Chain K: 54% 37% 7%



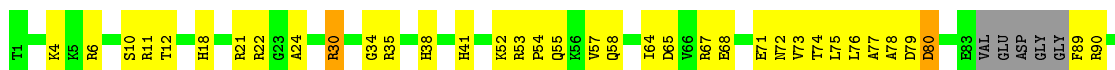
- Molecule 12: 50S ribosomal protein L14P

Chain L: 60% 39%



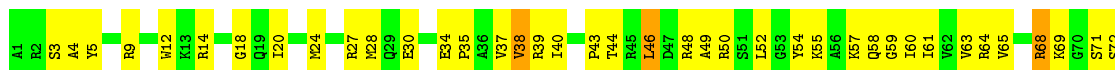
- Molecule 13: 50S ribosomal protein L15P

Chain M: 46% 41% 12%



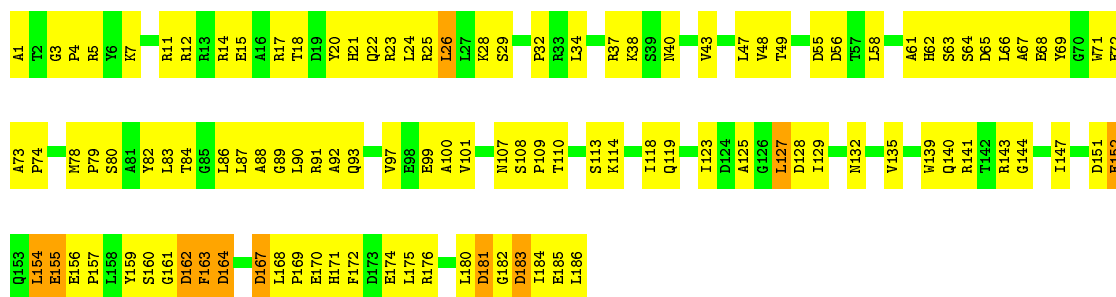
- Molecule 14: 50S ribosomal protein L15E

Chain N: 37% 59% 5%



- Molecule 15: 50S ribosomal protein L18P

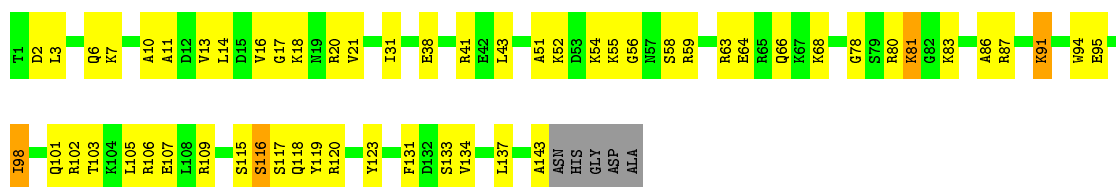
Chain O: 40% 54% 6%



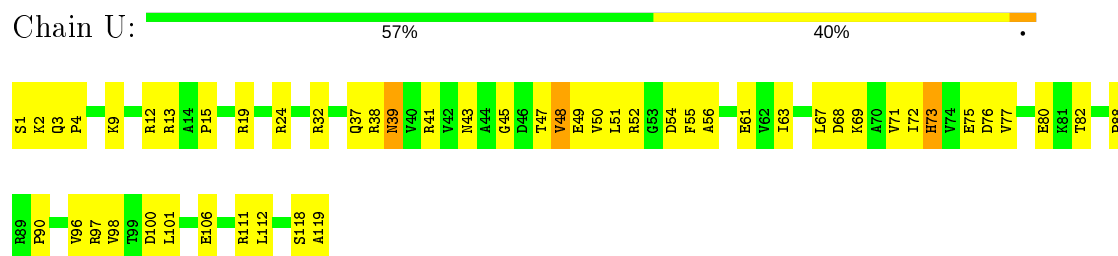
- Molecule 16: 50S ribosomal protein L18E



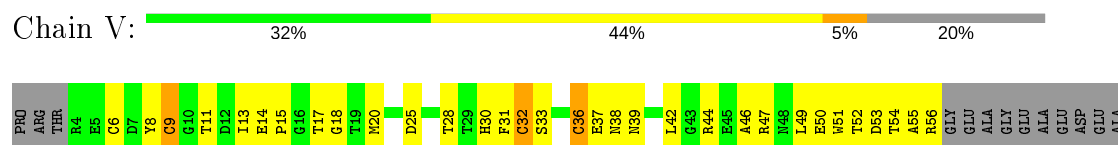
- Molecule 17: 50S ribosomal protein L19E



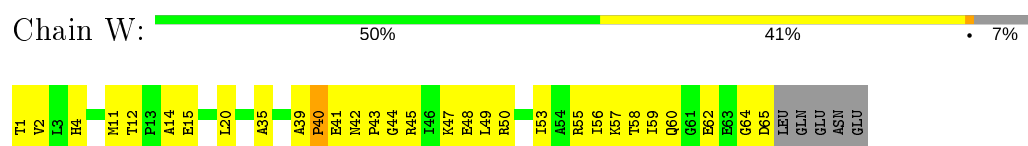
- Molecule 21: 50S ribosomal protein L24P



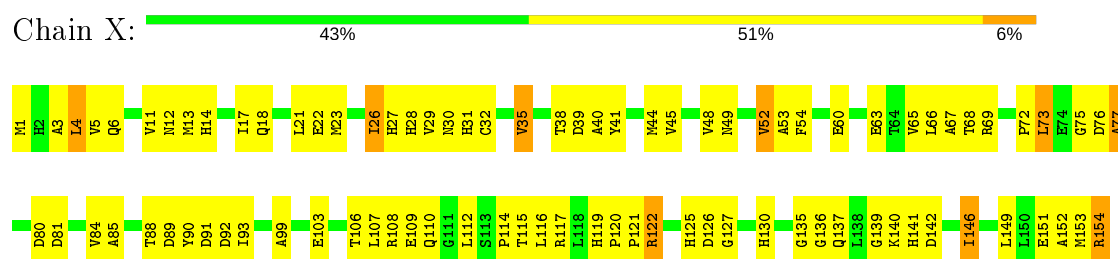
- Molecule 22: 50S ribosomal protein L24E



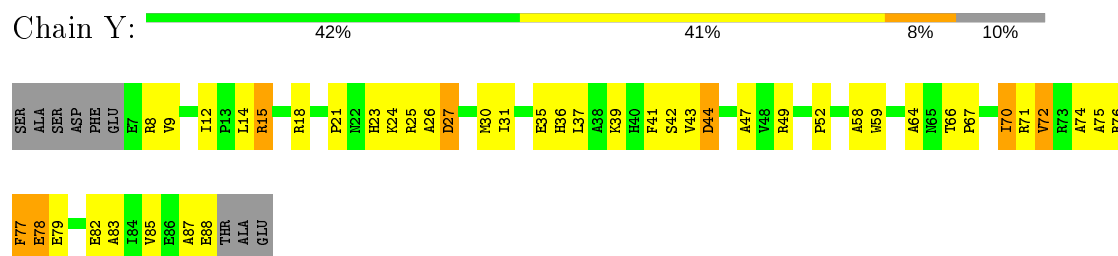
- Molecule 23: 50S ribosomal protein L29P



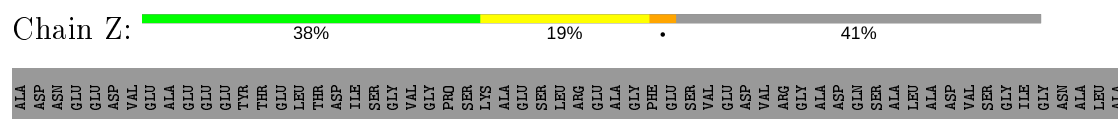
- Molecule 24: 50S ribosomal protein L30P



- Molecule 25: 50S ribosomal protein L31E



- Molecule 26: 50S ribosomal protein L32E





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: MG, CL, NA, K, CD, VIR

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	0.57	9/66076 (0.0%)	0.76	37/103052 (0.0%)
2	B	0.81	10/2905 (0.3%)	0.91	17/4528 (0.4%)
3	C	0.44	0/1787	0.75	0/2409
4	D	0.41	0/2689	0.71	0/3652
5	E	0.48	0/1883	0.74	0/2551
6	F	0.40	0/1111	0.64	0/1498
7	G	0.44	0/1382	0.66	0/1880
8	H	0.40	0/896	0.63	0/1219
9	I	0.33	0/241	0.53	0/324
10	J	0.46	0/1246	0.83	2/1686 (0.1%)
11	K	0.46	0/1135	0.70	0/1530
12	L	0.43	0/1003	0.75	0/1351
13	M	0.42	0/1126	0.75	0/1504
14	N	0.63	0/1633	0.86	1/2180 (0.0%)
15	O	0.42	0/1473	0.71	0/1999
16	P	0.45	0/873	0.71	0/1181
17	Q	0.44	0/1143	0.64	0/1521
18	R	0.45	0/748	0.79	0/1005
19	S	0.45	0/1172	0.76	0/1578
20	T	0.41	0/648	0.65	0/875
21	U	0.38	0/957	0.70	0/1289
22	V	0.82	0/417	0.81	1/562 (0.2%)
23	W	0.40	0/502	0.61	0/675
24	X	0.50	0/1218	0.73	0/1655
25	Y	0.44	0/664	0.70	0/895
26	Z	0.46	0/1146	0.72	0/1536
27	1	0.77	0/575	0.82	0/763
28	2	0.54	0/437	0.78	0/578
29	3	0.42	0/398	0.63	0/527
30	4	0.98	0/771	0.81	0/1024
All	All	0.56	19/98255 (0.0%)	0.76	58/147027 (0.0%)

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 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2488	A	O5'-C5'	-8.71	1.28	1.42
2	B	3025	G	C2'-O2'	-7.62	1.31	1.41
2	B	3003	A	O5'-C5'	7.52	1.56	1.44
2	B	3024	U	O5'-C5'	7.15	1.55	1.44
2	B	3023	U	C4'-O4'	7.08	1.54	1.45

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1164	U	OP2-P-O3'	-18.66	64.14	105.20
1	A	1164	U	OP1-P-O3'	-18.19	65.19	105.20
1	A	1979	G	C2'-C3'-O3'	9.72	130.90	109.50
1	A	1563	G	C2'-C3'-O3'	9.58	130.58	109.50
1	A	1165	G	O5'-P-OP1	-8.38	98.16	105.70

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	1306	0
2	B	2600	0	1326	85	0
3	C	1754	0	1763	144	0
4	D	2624	0	2533	195	0
5	E	1858	0	1816	146	0
6	F	1094	0	1085	135	0
7	G	1357	0	1266	79	0
8	H	885	0	854	73	0
9	I	240	0	231	23	0
10	J	1215	0	1215	168	0
11	K	1119	0	1098	70	0
12	L	993	0	1027	60	0
13	M	1114	0	1072	79	0
14	N	1605	0	1676	212	0
15	O	1444	0	1401	152	0
16	P	864	0	873	29	0
17	Q	1133	0	1127	68	0
18	R	734	0	729	27	0
19	S	1149	0	1122	68	0
20	T	641	0	605	26	0
21	U	949	0	923	52	0
22	V	410	0	368	48	0
23	W	499	0	511	30	0
24	X	1195	0	1137	115	0
25	Y	654	0	653	48	0
26	Z	1130	0	1133	62	0
27	1	563	0	601	83	0
28	2	430	0	426	30	0
29	3	393	0	406	22	0
30	4	755	0	732	89	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	1	0
37	3	40	0	0	6	0
37	4	72	0	0	11	0
37	A	5881	0	0	302	0
37	B	146	0	0	21	0
37	C	135	0	0	15	0
37	D	141	0	0	33	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	17	0
37	G	43	0	0	10	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	16	0
37	M	85	0	0	21	0
37	N	141	0	0	35	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	10	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	3401	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 3401 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
21:U:71:VAL:HG11	21:U:90:PRO:HB3	1.31	1.11

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%)	5	27
4	D	335/337 (99%)	302 (90%)	22 (7%)	11 (3%)	4	21
5	E	244/246 (99%)	222 (91%)	22 (9%)	0	100	100
6	F	134/176 (76%)	95 (71%)	27 (20%)	12 (9%)	1	3
7	G	170/177 (96%)	157 (92%)	12 (7%)	1 (1%)	25	64
8	H	117/119 (98%)	104 (89%)	10 (8%)	3 (3%)	5	27
9	I	25/348 (7%)	23 (92%)	1 (4%)	1 (4%)	3	17
10	J	152/167 (91%)	130 (86%)	17 (11%)	5 (3%)	4	21
11	K	140/145 (97%)	127 (91%)	8 (6%)	5 (4%)	3	19
12	L	130/132 (98%)	120 (92%)	8 (6%)	2 (2%)	10	42
13	M	141/164 (86%)	120 (85%)	20 (14%)	1 (1%)	22	60
14	N	192/194 (99%)	165 (86%)	24 (12%)	3 (2%)	9	40
15	O	184/186 (99%)	164 (89%)	12 (6%)	8 (4%)	2	15
16	P	113/115 (98%)	109 (96%)	4 (4%)	0	100	100
17	Q	141/148 (95%)	135 (96%)	5 (4%)	1 (1%)	22	60
18	R	93/95 (98%)	86 (92%)	3 (3%)	4 (4%)	2	15
19	S	148/154 (96%)	134 (90%)	13 (9%)	1 (1%)	22	60
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%)	4	22
24	X	152/154 (99%)	142 (93%)	8 (5%)	2 (1%)	12	45
25	Y	80/91 (88%)	71 (89%)	5 (6%)	4 (5%)	2	12
26	Z	140/240 (58%)	133 (95%)	7 (5%)	0	100	100
27	1	71/73 (97%)	61 (86%)	7 (10%)	3 (4%)	3	16

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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%)	6	31
All	All	3633/4235 (86%)	3265 (90%)	291 (8%)	77 (2%)	7	33

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%)	14	44
4	D	282/282 (100%)	264 (94%)	18 (6%)	17	51
5	E	193/193 (100%)	178 (92%)	15 (8%)	12	42
6	F	117/147 (80%)	106 (91%)	11 (9%)	8	32
7	G	152/155 (98%)	148 (97%)	4 (3%)	46	78
8	H	92/92 (100%)	91 (99%)	1 (1%)	73	90
9	I	27/283 (10%)	27 (100%)	0	100	100
10	J	122/122 (100%)	111 (91%)	11 (9%)	9	35
11	K	118/121 (98%)	107 (91%)	11 (9%)	9	33
12	L	106/106 (100%)	102 (96%)	4 (4%)	33	69
13	M	112/126 (89%)	108 (96%)	4 (4%)	35	70
14	N	166/166 (100%)	158 (95%)	8 (5%)	25	62
15	O	149/149 (100%)	144 (97%)	5 (3%)	37	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	P	93/93 (100%)	91 (98%)	2 (2%)	52	81
17	Q	113/116 (97%)	109 (96%)	4 (4%)	36	71
18	R	79/79 (100%)	75 (95%)	4 (5%)	24	60
19	S	117/121 (97%)	113 (97%)	4 (3%)	37	72
20	T	71/73 (97%)	69 (97%)	2 (3%)	43	77
21	U	105/105 (100%)	102 (97%)	3 (3%)	42	76
22	V	44/52 (85%)	42 (96%)	2 (4%)	27	64
23	W	51/56 (91%)	51 (100%)	0	100	100
24	X	130/130 (100%)	121 (93%)	9 (7%)	15	48
25	Y	66/73 (90%)	61 (92%)	5 (8%)	13	43
26	Z	120/195 (62%)	110 (92%)	10 (8%)	11	39
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%)	49	79
30	4	79/79 (100%)	73 (92%)	6 (8%)	13	43
All	All	3027/3441 (88%)	2863 (95%)	164 (5%)	22	57

5 of 164 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	K	52	GLN
13	M	117	GLU
27	1	32	LYS
11	K	76	ASP
11	K	131	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 95 such sidechains are listed below:

Mol	Chain	Res	Type
13	M	116	HIS
18	R	40	HIS
29	3	18	ASN
14	N	58	GLN
15	O	153	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2747/2922 (94%)	248 (9%)	38 (1%)
2	B	121/122 (99%)	14 (11%)	4 (3%)
All	All	2868/3044 (94%)	262 (9%)	42 (1%)

5 of 262 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	1352	A
1	A	1667	A
2	B	3023	U
1	A	1377	C
1	A	1474	C

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 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	-	34,40,40	2.51	16 (47%)	36,55,55	2.42	11 (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	-	-	11/42/58/58	0/2/3/3

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	9403	VIR	C28-C29	-7.33	1.15	1.32
31	A	9403	VIR	C4-N5	4.21	1.53	1.47
31	A	9403	VIR	C28-C26	3.53	1.55	1.48
31	A	9403	VIR	C17-C19	-3.49	1.46	1.50
31	A	9403	VIR	C13-C10	-3.33	1.44	1.50

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	9403	VIR	C28-C26-N25	-6.11	103.44	114.97
31	A	9403	VIR	C8-C6-N5	-6.09	110.64	118.48
31	A	9403	VIR	O27-C26-C28	5.60	135.79	123.03
31	A	9403	VIR	C4-N5-C6	5.39	126.88	118.83
31	A	9403	VIR	O36-C37-C1	3.31	114.56	110.53

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

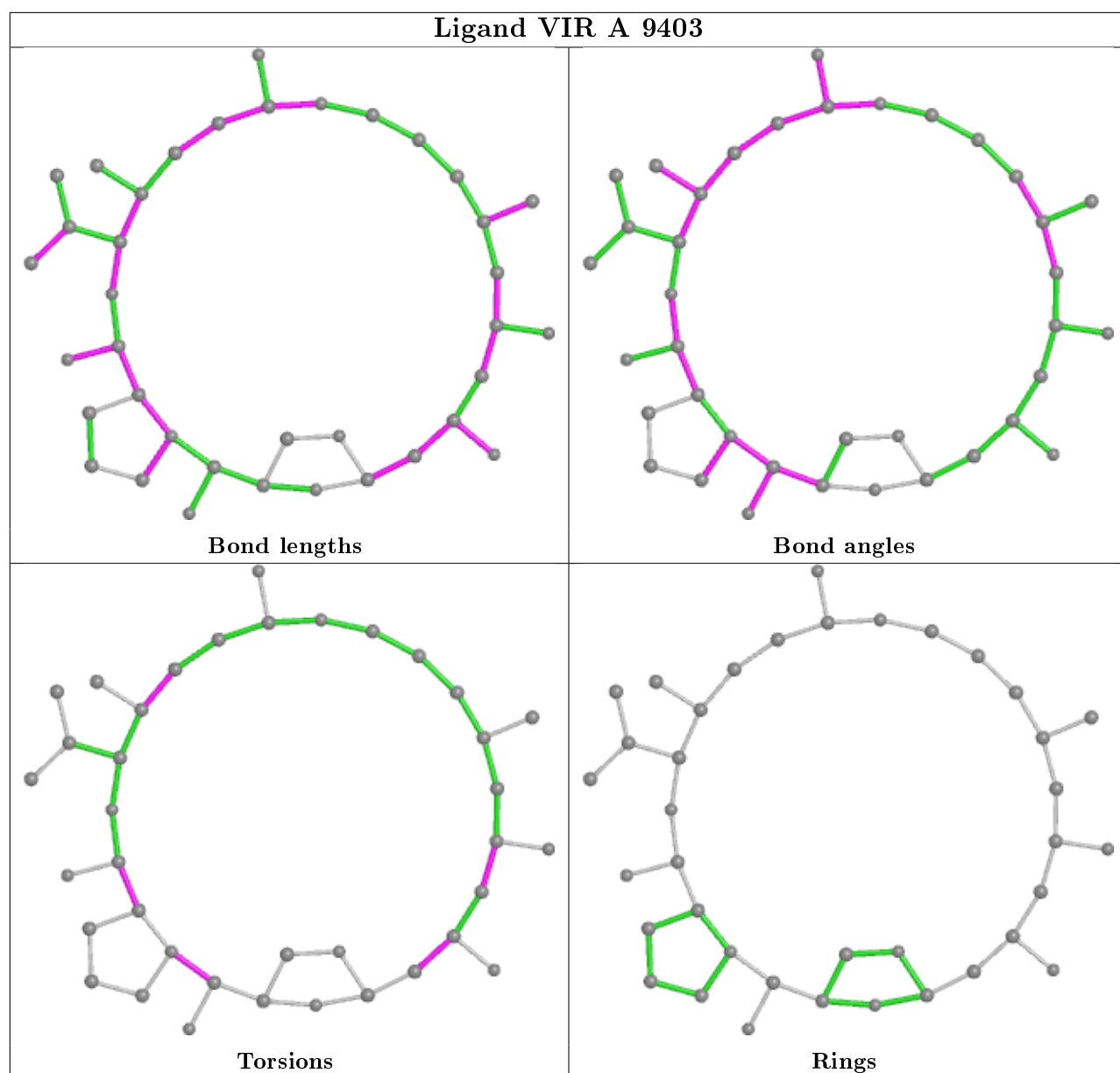
Mol	Chain	Res	Type	Atoms
31	A	9403	VIR	C14-C16-C17-O18
31	A	9403	VIR	N5-C1-C37-O38
31	A	9403	VIR	N5-C1-C37-O36
31	A	9403	VIR	C14-C16-C17-C19
31	A	9403	VIR	C10-C13-C14-O15

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.