



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 3, 2016 – 12:58 PM EDT

PDB ID : 5JVH
Title : The crystal structure large ribosomal subunit (50S) of *Deinococcus radiodurans* in complex with evernimicin
Authors : Yonath, A.
Deposited on : 2016-05-11
Resolution : 3.58 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	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028320
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)	:	rb-20028320

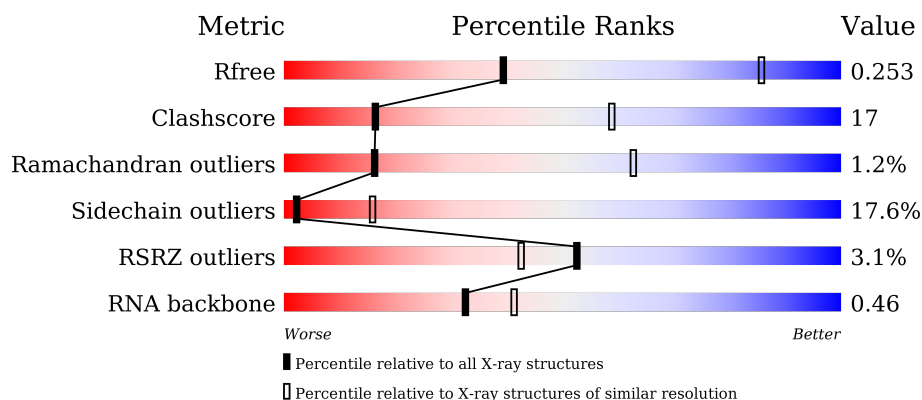
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

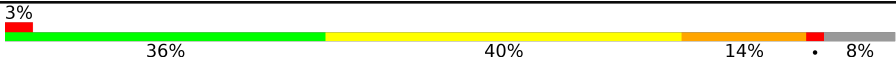

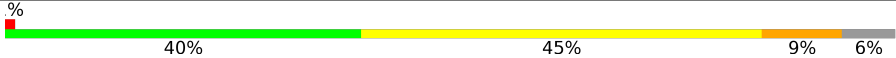

The reported resolution of this entry is 3.58 Å.

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.






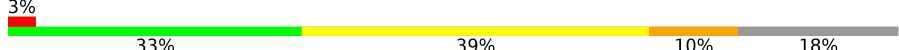

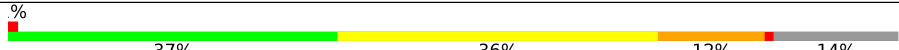
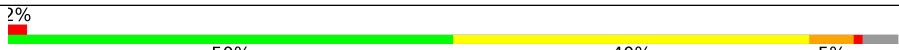
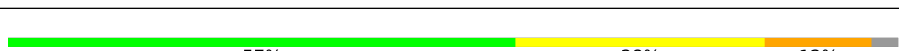
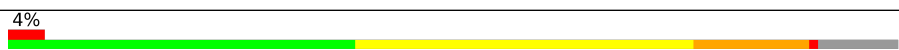
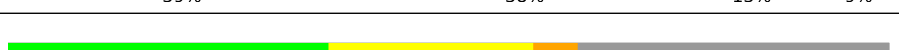
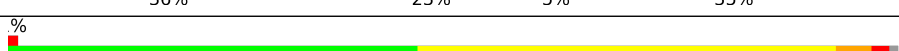

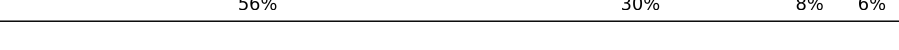
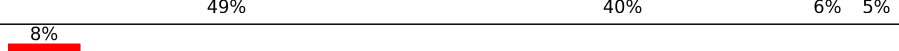
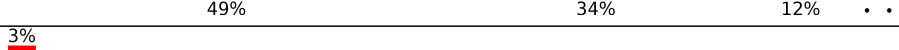
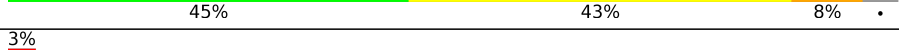


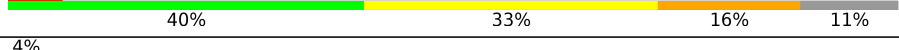

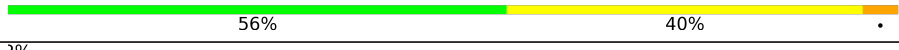
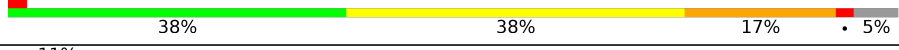
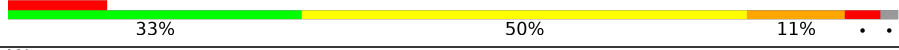
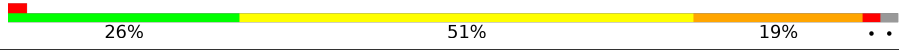
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1261 (3.76-3.40)
Clashscore	102246	1026 (3.72-3.44)
Ramachandran outliers	100387	1028 (3.74-3.42)
Sidechain outliers	100360	1028 (3.74-3.42)
RSRZ outliers	91569	1268 (3.76-3.40)
RNA backbone	2183	1057 (4.30-2.80)

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 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	 3% 36% 40% 14% 8%
2	Y	123	 2% 46% 41% 11% 2%
3	A	275	 0% 40% 45% 9% 6%
4	B	211	 0% 53% 38% 6% 3%

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Mol	Chain	Length	Quality of chain
5	C	205	
6	D	180	
7	E	185	
8	G	174	
9	H	134	
10	I	156	
11	J	141	
12	K	116	
13	L	114	
14	M	166	
15	N	118	
16	O	100	
17	P	134	
18	Q	95	
19	R	115	
20	S	237	
21	T	91	
22	U	81	
23	V	67	
24	W	55	
25	Z	60	
26	1	54	
27	2	47	
28	3	66	

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
29	6O1	X	2901	-	-	-	X
30	MG	K	201	-	-	-	X
30	MG	X	2903	-	-	-	X
30	MG	X	2906	-	-	-	X
30	MG	X	2907	-	-	-	X
30	MG	X	2910	-	-	-	X
30	MG	X	2911	-	-	-	X
30	MG	X	2912	-	-	-	X
30	MG	X	2915	-	-	-	X
30	MG	X	2916	-	-	-	X
30	MG	X	2918	-	-	-	X
30	MG	X	2921	-	-	-	X
30	MG	X	2924	-	-	-	X
30	MG	X	2925	-	-	-	X
30	MG	X	2926	-	-	-	X
30	MG	X	2931	-	-	-	X
30	MG	X	2935	-	-	-	X
30	MG	X	2936	-	-	-	X
30	MG	X	2939	-	-	-	X
30	MG	X	2941	-	-	-	X
30	MG	X	2946	-	-	-	X
30	MG	X	2947	-	-	-	X
30	MG	X	2952	-	-	-	X
30	MG	X	2953	-	-	-	X
30	MG	X	2954	-	-	-	X
30	MG	X	2957	-	-	-	X
30	MG	X	2959	-	-	-	X
30	MG	X	2963	-	-	-	X
30	MG	X	2964	-	-	-	X
30	MG	X	2969	-	-	-	X
30	MG	X	2970	-	-	-	X
30	MG	X	2975	-	-	-	X
30	MG	X	2977	-	-	-	X
30	MG	X	2978	-	-	-	X
30	MG	X	2980	-	-	-	X
30	MG	X	2981	-	-	-	X
30	MG	X	2983	-	-	-	X
30	MG	X	2990	-	-	-	X
30	MG	X	2992	-	-	-	X
30	MG	X	2993	-	-	-	X
30	MG	X	3008	-	-	-	X
30	MG	X	3011	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	MG	X	3014	-	-	-	X
30	MG	X	3017	-	-	-	X
30	MG	X	3020	-	-	-	X

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 83681 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	X	2658	Total	C	N	O	P	0	0	0
			57052	25450	10532	18413	2657			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	1526	U	C	conflict	GB 1026245073

- 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	259	Total	C	N	O	S	0	0	0
			1973	1226	395	349	3			

- 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 L13.

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

- Molecule 9 is a protein called 50S ribosomal protein L14.

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

- Molecule 10 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	134	Total	C	N	O	S	0	0	0
			1011	619	206	186				

- Molecule 11 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	136	Total	C	N	O	S	0	0	0
			1078	690	196	185	7			

- Molecule 12 is a protein called 50S ribosomal protein L17.

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

- Molecule 13 is a protein called 50S ribosomal protein L18.

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

- Molecule 14 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	M	108	Total	C	N	O	0	0	0
			859	537	166	156			

- Molecule 15 is a protein called 50S ribosomal protein L20.

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

- Molecule 16 is a protein called 50S ribosomal protein L21.

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

- Molecule 17 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	P	127	Total	C	N	O	S	0	0	0
			1014	639	199	174	2			

- Molecule 18 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Q	93	Total	C	N	O	S	0	0	0
			726	458	136	130	2			

- Molecule 19 is a protein called 50S ribosomal protein L24.

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

- Molecule 20 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	S	179	Total	C	N	O	S	0	0	0
			1374	867	240	261	6			

- Molecule 21 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	T	74	Total	C	N	O	S	0	0	0
			556	351	107	97	1			

- Molecule 22 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	U	72	Total	C	N	O	S	0	0	0
			552	341	116	95				

- Molecule 23 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	V	65	Total	C	N	O	S	0	0	0
			525	322	106	95	2			

- Molecule 24 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	W	55	Total	C	N	O	S	0	0	0
			424	264	82	76	2			

- Molecule 25 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Z	57	Total	C	N	O	S	0	0	0
			452	278	93	76	5			

- Molecule 26 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	1	53	Total	C	N	O	S	0	0	0
			427	271	79	76	1			

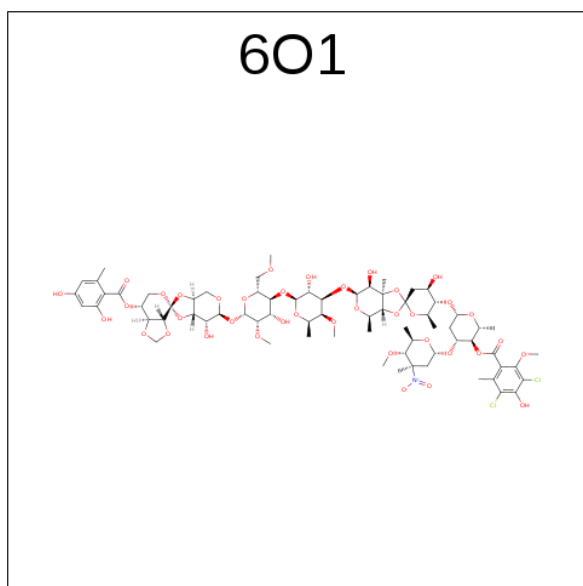
- Molecule 27 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	2	46	Total	C	N	O	S	0	0	0
			383	230	91	60	2			

- Molecule 28 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	3	59	Total	C	N	O	S	0	0	0
			462	290	95	73	4			

- Molecule 29 is Evernimicin (three-letter code: 6O1) (formula: $C_{70}H_{97}Cl_2NO_{38}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	X	1	Total	C	Cl	N	O	0	0
			111	70	2	1	38		

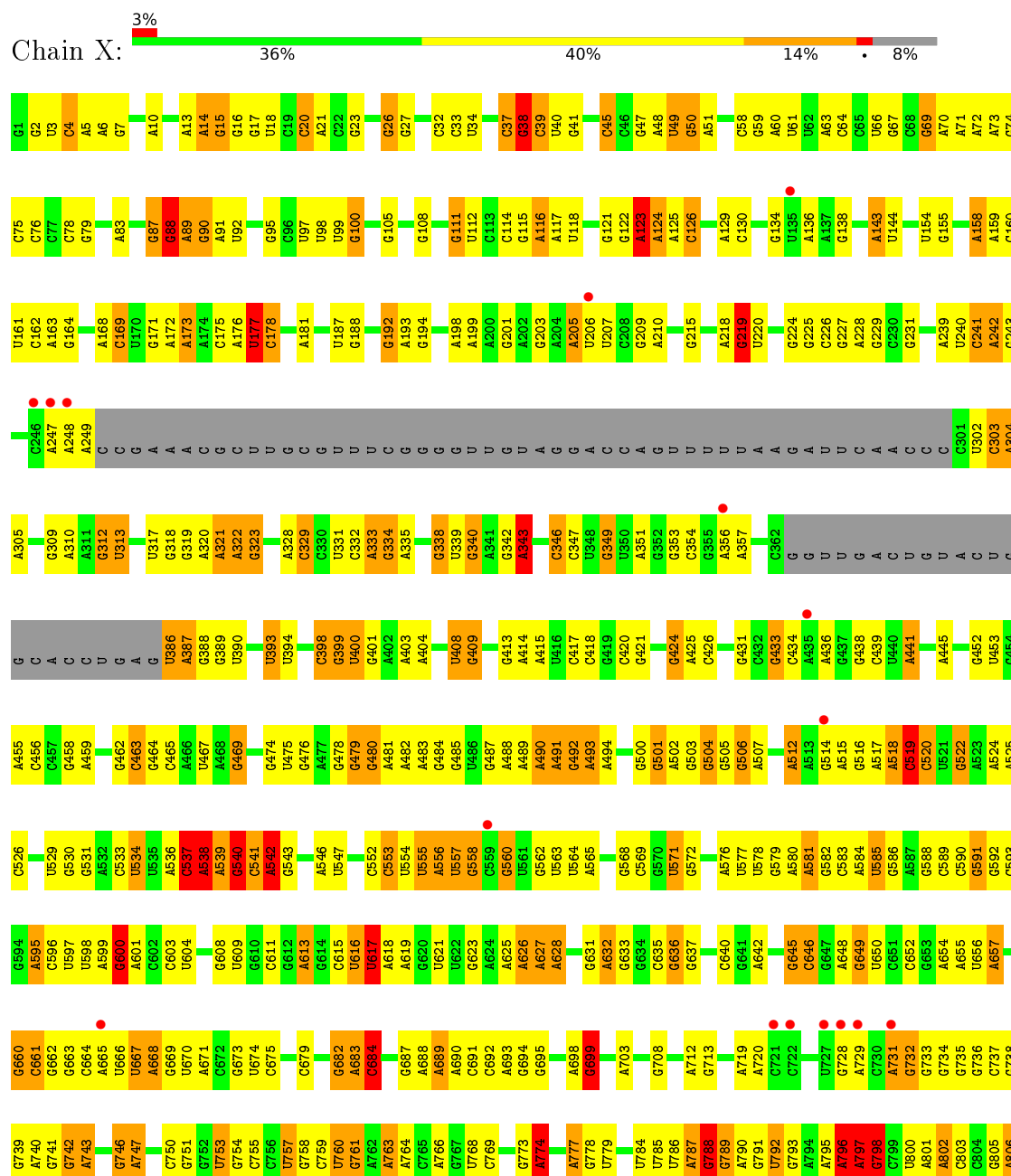
- Molecule 30 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	X	119	Total	Mg	0	0
			119	119		
30	Y	1	Total	Mg	0	0
			1	1		
30	K	2	Total	Mg	0	0
			2	2		
30	M	1	Total	Mg	0	0
			1	1		

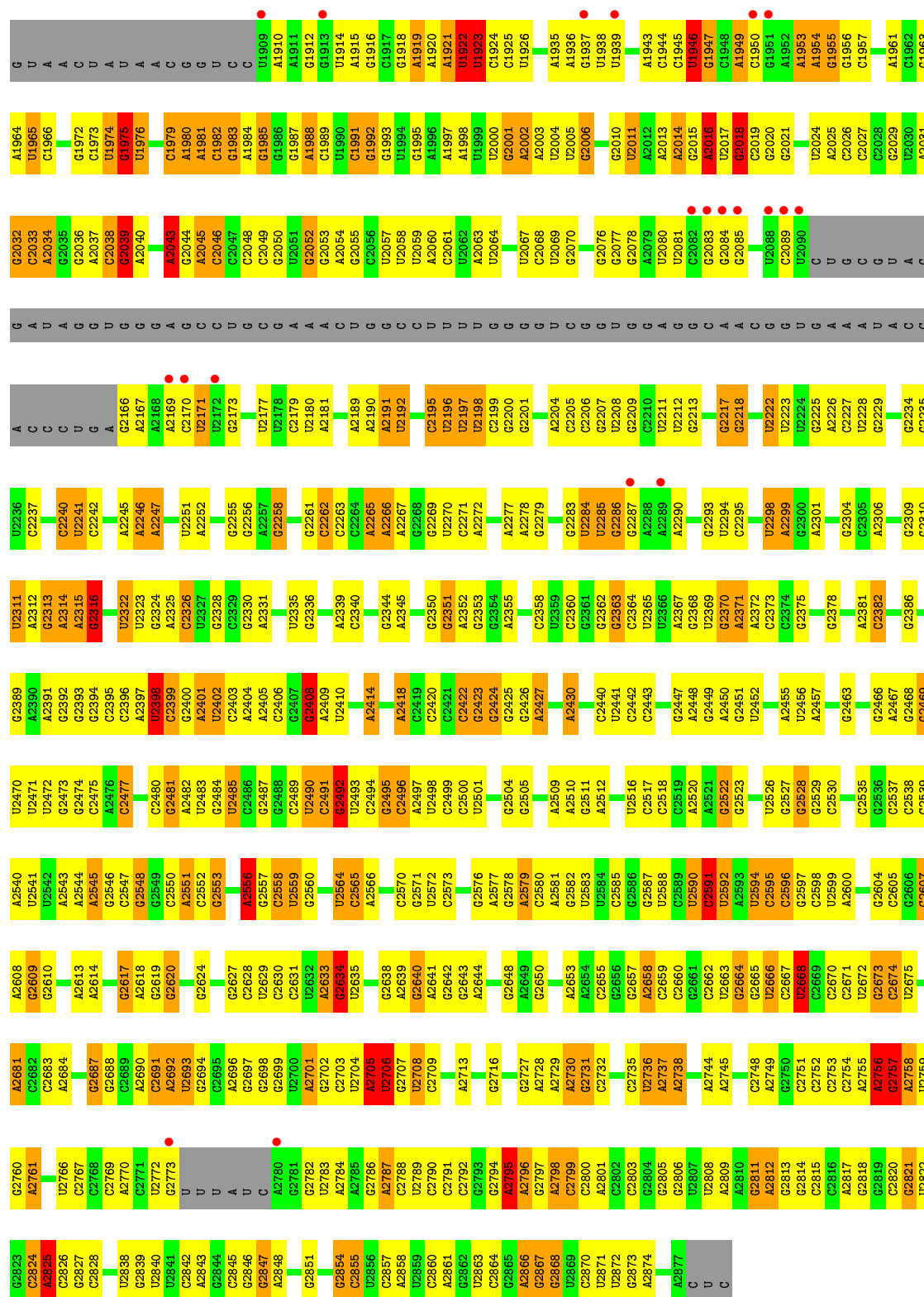
3 Residue-property plots

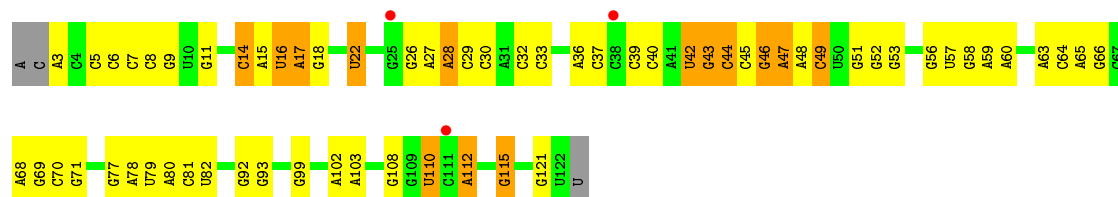
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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: 23S ribosomal RNA

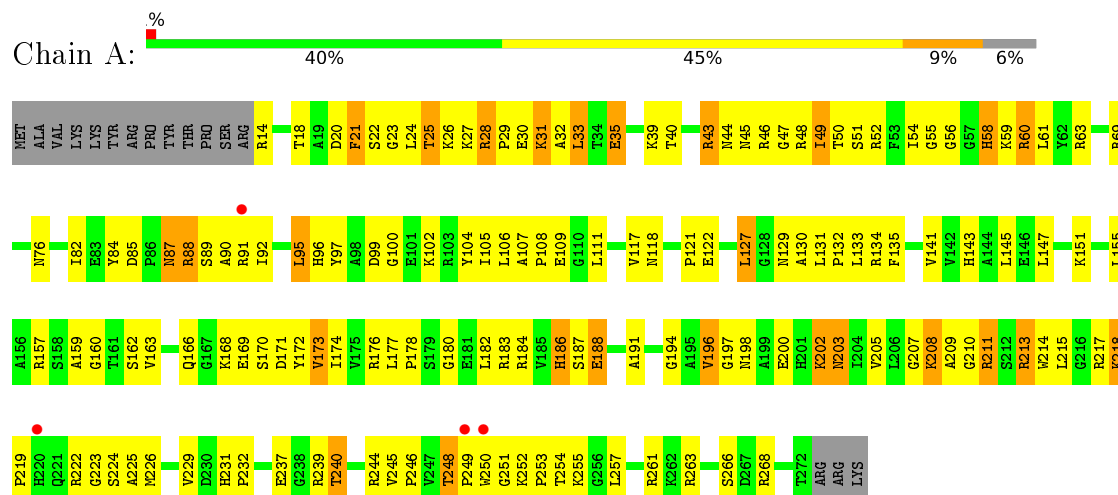


A1821	A1753	G1674	U1594	C1517	A1437	G1359	G1222	C1152	C	A1021	G945	G875	A807
A1822	G1754	C1675	A1595	G1517	G1438	G1360	G1223	A1153	A	A1022	U946	A876	C808
A1823	G1755	U1676	G1599	G1520	G1439	G1361	A1224	A1154	C	U1023	C947	C877	C809
A1824	G1756	C1677	G1599	U1521	G1440	C1362	A1225	G1155	C	G1024	C948	C878	U810
A1825	C1757	G1678	U1600	C1522	G1441	C1363	A1226	U1161	C	C1029	G951	C880	G811
A1826	C1758	U1679	U1601	A1523	G1442	G1364	A1227	A1162	U	U1030	A952	C881	G812
A1827	G1759	A1682	G1602	G1524	G1443	U1370	G1228	C1163	C	G1031	G953	U881	A813
A1830	G1760	A1683	A1603	C1524	A1444	A1372	C1230	C1164	U	U1032	U954	U882	G814
A1831	G1761	G1683	A1604	A1525	A1448	G1373	C1231	G1165	A	A1033	G955	A	A817
A1832	G1762	G1684	G1605	U1526	A1448	G1374	A1231	A1166	A	G1034	A956	G	G818
A1833	G1763	A1685	C1606	G1527	U1454	U1303	G1235	A1167	A	G1035	G957	G	C819
A1834	A1764	A1686	A1607	C1528	C1455	U1304	G1236	G1173	G	G1036	G958	G	U820
A1835	G1765	C1687	A1608	G1528	U1455	A1378	G1237	G1174	U101	U1037	C959	G	A821
A1836	U1766	U1688	G1609	C1531	U1459	G1381	G1237	G1175	U102	U1038	A964	G	U822
A1837	G1767	A1689	A1610	A1532	G1460	G1382	G1240	U1176	G103	A1040	G967	G	U823
A1838	U1768	C1691	G1611	G1533	C1461	G1383	A1241	A1177	C1104	G1041	G968	C	U824
A1839	U1769	A1692	C1614	A1534	C1462	G1385	G1242	C1178	U105	U1044	U969	A	C825
A1840	U1770	A1693	C1615	G1542	A1463	A1386	G1245	C1179	U106	G1045	A970	C	C829
A1841	A1771	G1694	G1616	A1544	A1464	G1390	G1246	A1180	A1107	U1046	A971	C	C830
A1842	U1772	U1697	C1623	A1544	G1465	A1391	U1247	C1181	U1108	G1047	C972	A	A832
A1843	C1776	C1698	A1624	U1547	C1466	U1392	U1248	G1182	U1109	U1048	G977	C	A833
A1844	A1777	A1699	A1625	U1548	U1467	G1393	G1249	C1183	G1110	C1049	U978	C	U835
A1845	C1778	C1700	A1625	U1549	A1468	G1393	G1251	C1184	U1112	G1050	U979	U	G836
A1846	U1779	G1701	A1630	C1550	U1469	A1397	G1252	C1185	U1113	U1051	A984	C	U837
A1847	A1780	C1702	C1631	U1551	G1470	G1398	C1253	G1186	C1113	C1052	G985	C	U840
A1848	C1781	U1705	A1632	C1552	U1475	G1398	G1254	A1187	C1114	G1053	A985	C	A841
A1849	A1782	U1705	C1633	G1553	C1476	U1403	C1255	A1188	C1115	G1054	G986	A911	A842
A1850	U1783	C1711	C1634	G1554	C1477	C1404	C1256	A1189	C1116	C1055	G987	A912	A842
A1851	A1784	G1712	G1635	A1555	U1478	G1404	C1257	C1190	C1117	U1056	G988	A913	A842
A1852	U1785	C1713	A1643	A1556	G1479	G1407	A1260	G1191	G1118	U1057	G989	C914	U845
A1853	C1786	G1713	G1646	C1557	U1480	A1408	G1261	A1192	U1119	A1058	G990	C915	A846
A1854	U1787	A1714	U1647	G1558	U1481	U1409	U1262	G1193	G1120	G1059	G991	U919	A847
A1855	C1788	C1715	C1648	G1559	U1482	G1433	G1263	U1194	G1121	A1059	G992	G920	C848
A1856	U1789	A1715	A1649	A1561	G1483	C1411	C1264	U1195	G1122	G993	A994	G921	C849
A1857	C1790	C1716	A1649	G1562	A1486	C1412	G1265	U1196	G1123	G994	A995	A922	C850
A1858	U1791	U1647	A1649	U1563	C1487	G1412	G1266	U1197	A1126	G995	C996	A923	C851
A1859	C1792	A1717	G1652	G1564	U1490	A1416	G1267	C1198	G1127	C996	C997	C924	C852
A1860	U1793	C1718	C1653	G1565	C1491	C1417	U1268	G1201	G1128	C997	C998	C924	C853
A1861	C1794	A1718	A1654	C1570	A1492	G1419	G1271	A1202	G1129	A999	C999	C925	C854
A1862	U1795	G1721	G1655	G1571	A1493	U1420	G1272	A1203	U1130	C1003	C1003	C926	C855
A1863	C1796	G1722	C1656	G1572	U1494	U1421	G1273	G1204	U1136	A1004	A1004	C927	U857
A1864	U1797	U1723	A1654	A1574	G1495	C1422	C1274	G1205	G1137	U1005	G998	G928	G858
A1865	G1866	C1724	U1655	C1575	G1496	A1423	A1275	G1206	A1137	C1006	A929	A929	U859
A1866	C1867	C1727	C1656	G1576	G1497	U1424	U1276	A1208	G1074	A1007	A930	A930	U860
A1867	U1799	A1728	U1657	G1577	C1498	U1425	G1277	A1209	C1075	A1008	G931	G931	G861
A1868	C1801	C1729	A1658	U1578	A1499	U1426	A1278	G1209	U1076	C1009	G932	G932	A862
A1869	G1803	G1734	G1659	G1579	U1500	G1427	G1279	U1212	U1077	C1010	G933	G933	C863
A1870	C1803	C1735	C1660	A1582	C1501	A1428	G1283	U1213	A1078	A1012	G934	G934	C864
A1871	U1807	G1735	G1661	A1583	U1505	U1429	C1284	G1214	G1079	G1013	G935	G935	U866
A1872	C1808	G1742	U1662	A1584	U1506	G1430	A1285	A1215	A1080	G1014	G936	G936	U867
A1873	U1809	C1743	C1663	G1585	A1507	A1353	U1286	G1216	A1081	U1015	G937	G937	C870
A1874	G1814	G1744	G1664	A1586	A1508	G1431	A1287	U1217	G1146	G1016	G938	G938	U868
A1875	C1815	A1746	A1665	A1587	G1506	U1433	A1288	C1218	G1147	C1017	G939	G939	G871
A1876	U1817	G1747	A1666	A1588	A1509	U1434	A1289	C1219	G1148	G1018	G940	G940	U872
A1877	G1818	A1750	A1667	A1589	U1509	G1435	A1290	G1220	U1150	U1019	U941	U941	U873
A1878	U1819	C1751	A1668	A1590	A1510	G1436	A1291	U1221	C	A1020	U942	U942	C874
A1879	C1820	U1752	C1673	A1591	A1511	G1436	A1292	C1221	U1511		A944	A944	A874

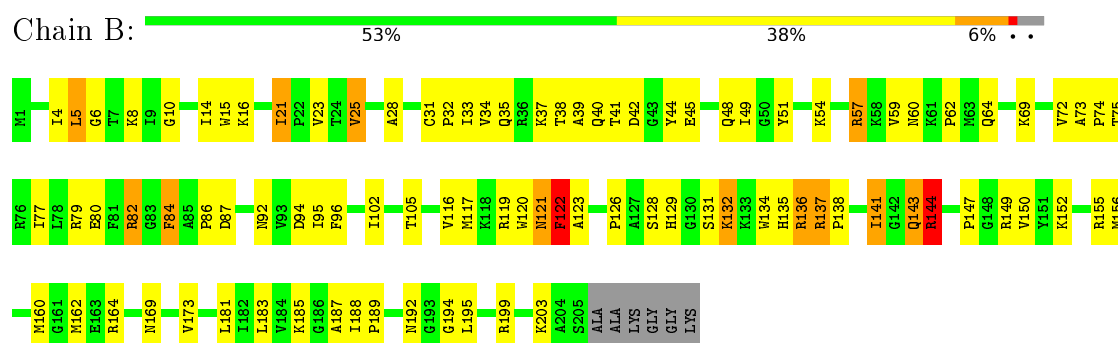




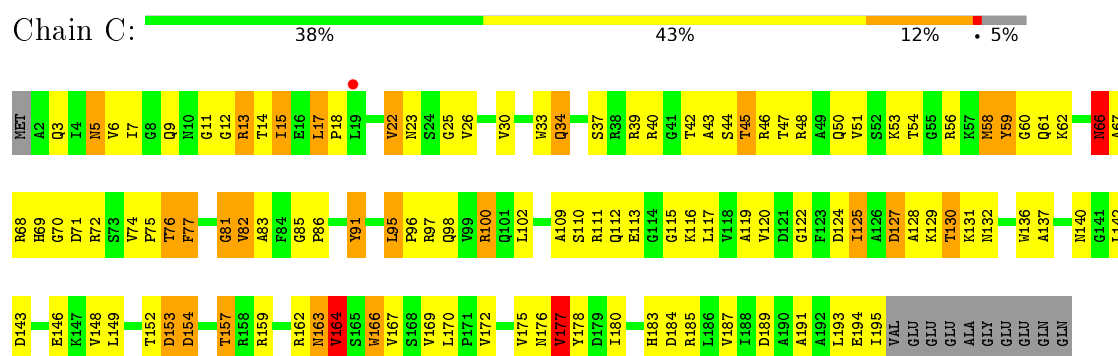
• Molecule 3: 50S ribosomal protein L2



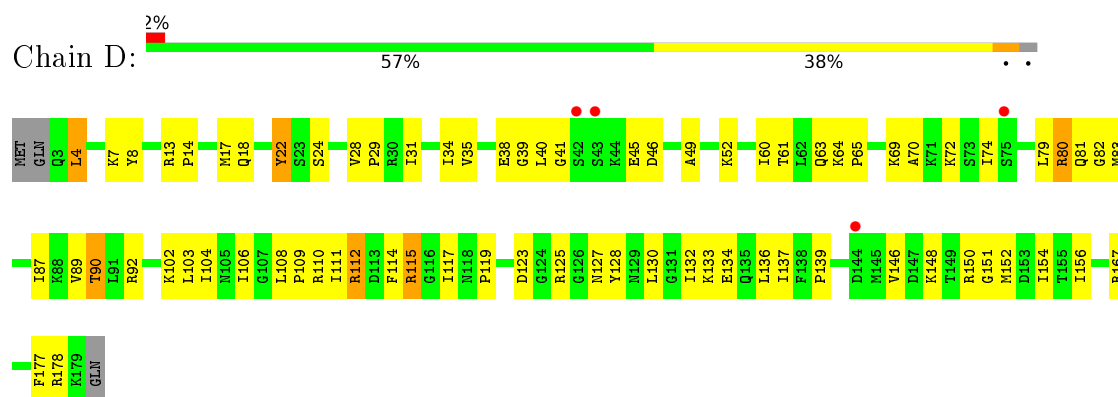
• Molecule 4: 50S ribosomal protein L3



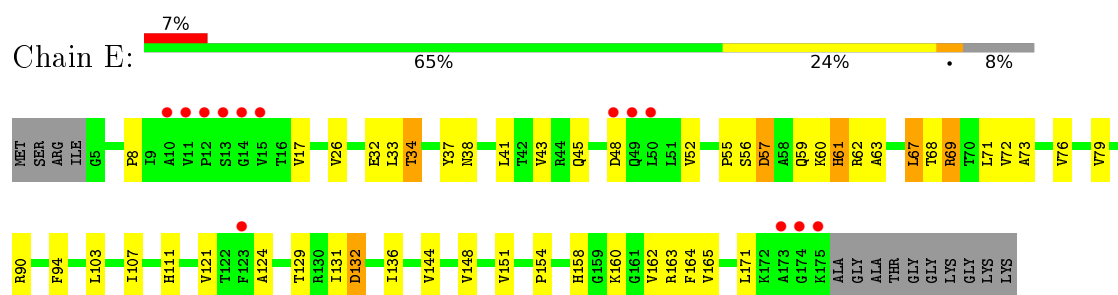
• Molecule 5: 50S ribosomal protein L4



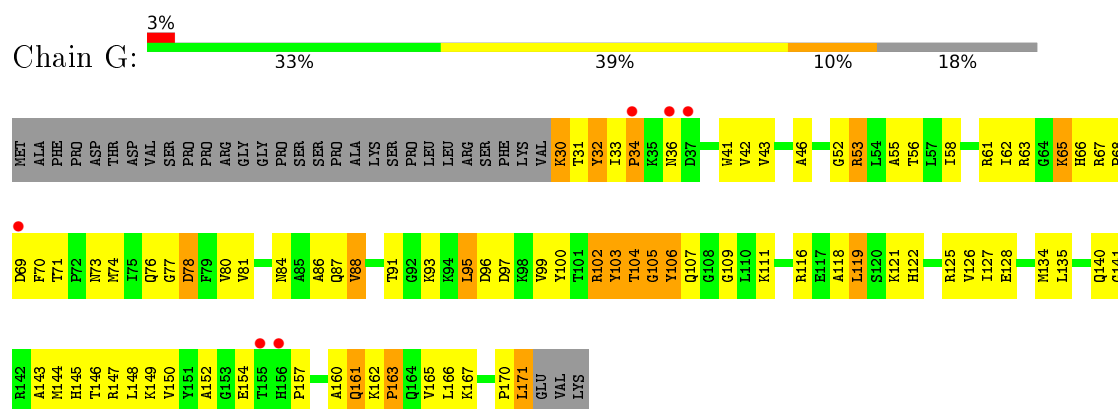
• Molecule 6: 50S ribosomal protein L5



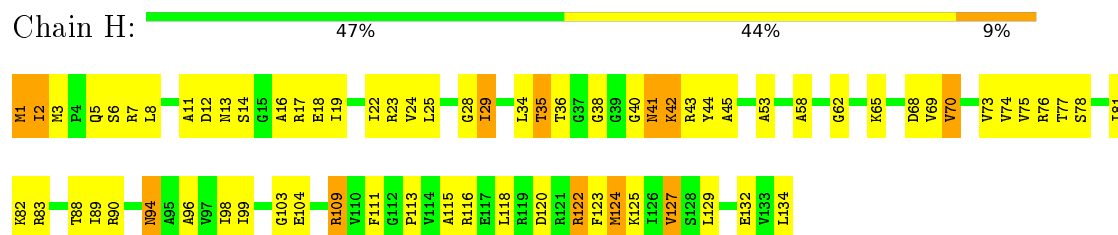
• Molecule 7: 50S ribosomal protein L6



• Molecule 8: 50S ribosomal protein L13

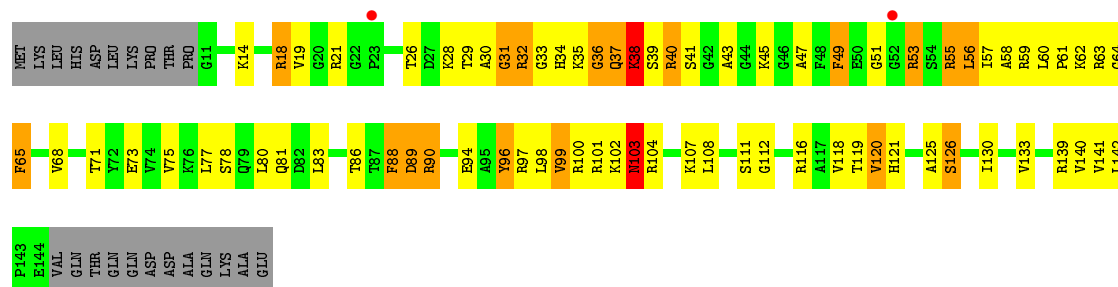


• Molecule 9: 50S ribosomal protein L14

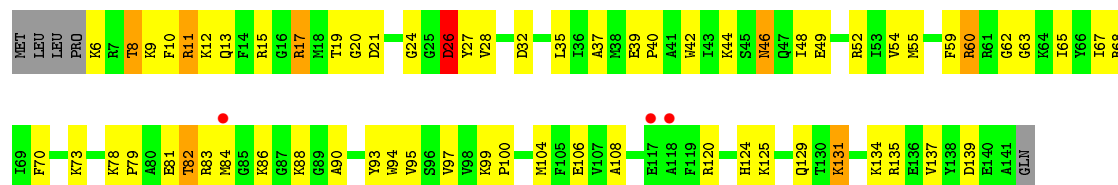


• Molecule 10: 50S ribosomal protein L15

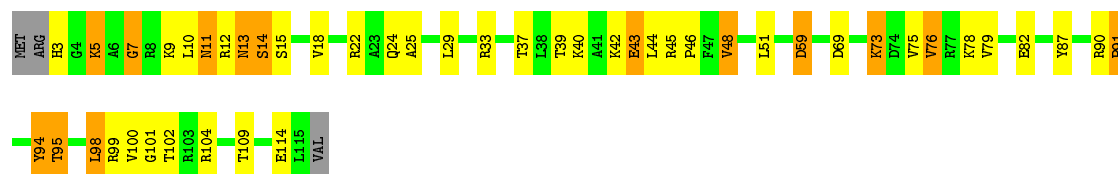




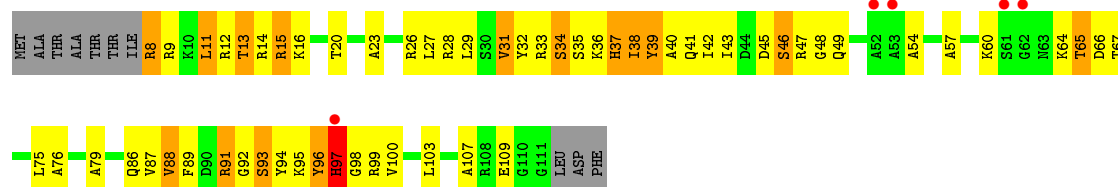
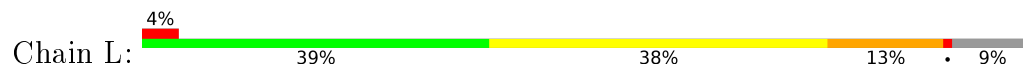
- Molecule 11: 50S ribosomal protein L16



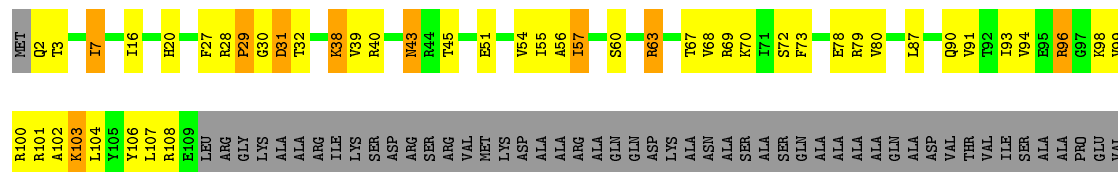
- Molecule 12: 50S ribosomal protein L17



- Molecule 13: 50S ribosomal protein L18

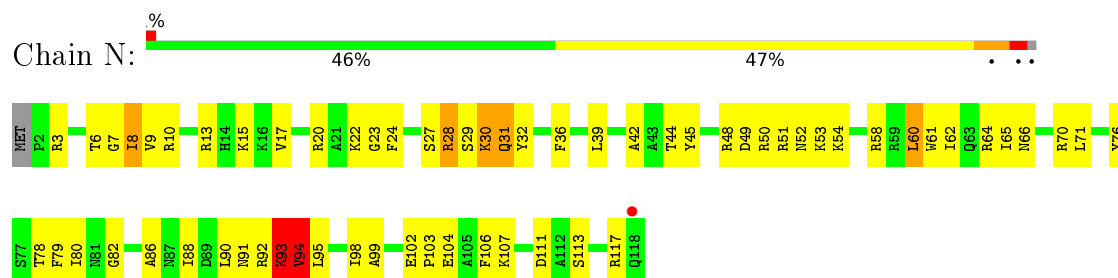


- Molecule 14: 50S ribosomal protein L19

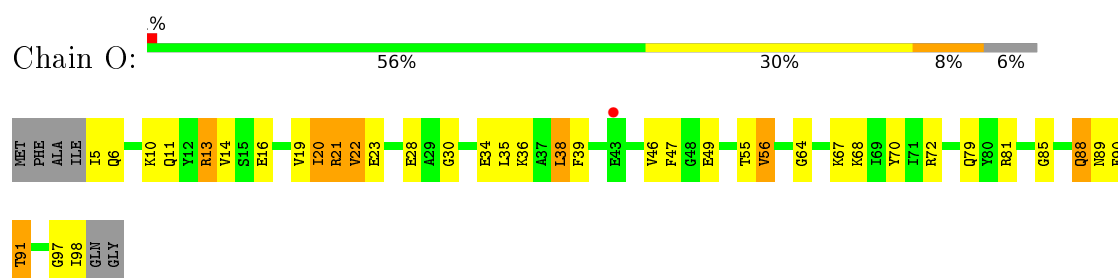


ALA
PRO
GLU
THR
GLN
GLY
GLU

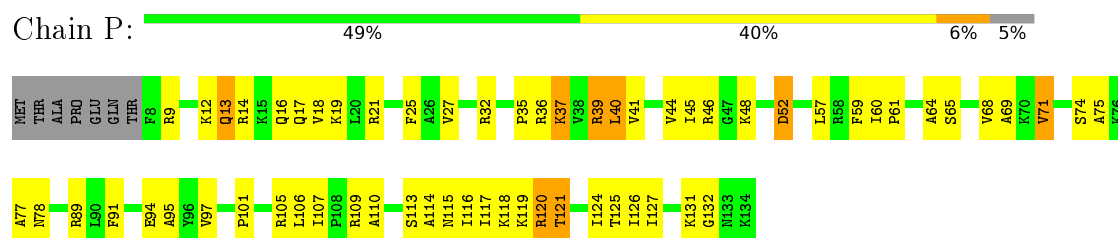
• Molecule 15: 50S ribosomal protein L20



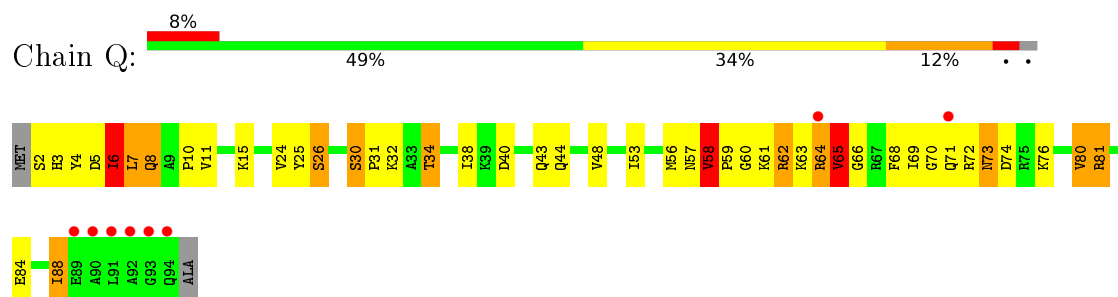
• Molecule 16: 50S ribosomal protein L21



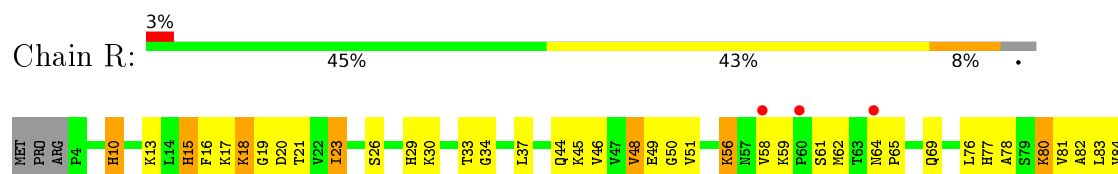
• Molecule 17: 50S ribosomal protein L22



• Molecule 18: 50S ribosomal protein L23

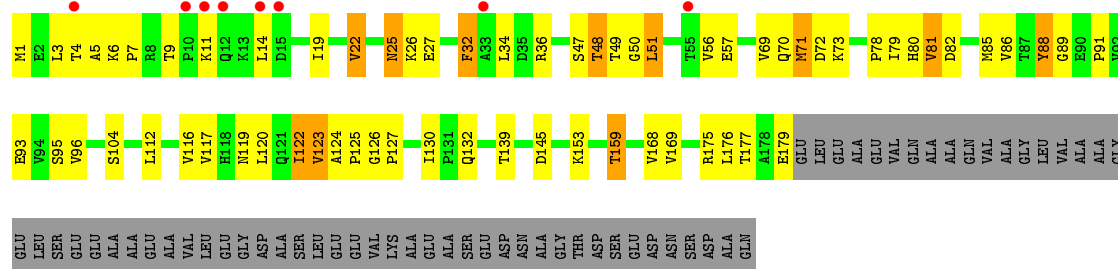


• Molecule 19: 50S ribosomal protein L24

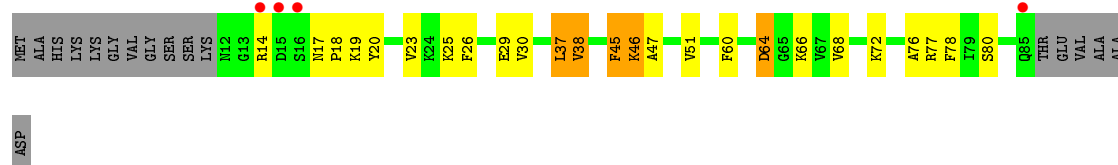




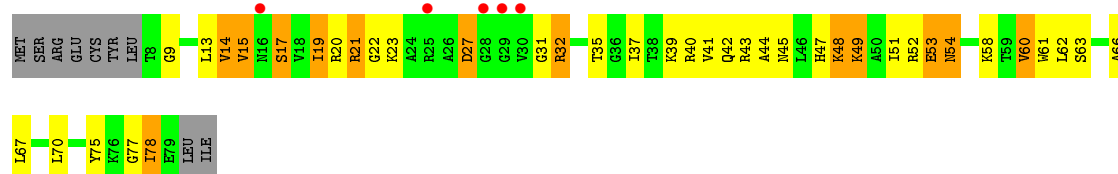
• Molecule 20: 50S ribosomal protein L25



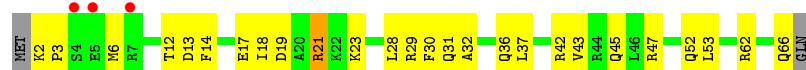
• Molecule 21: 50S ribosomal protein L27



• Molecule 22: 50S ribosomal protein L28



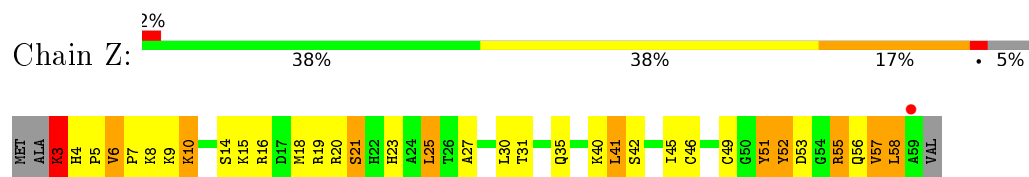
• Molecule 23: 50S ribosomal protein L29



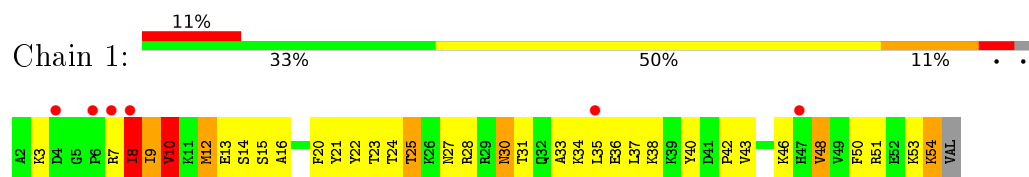
• Molecule 24: 50S ribosomal protein L30



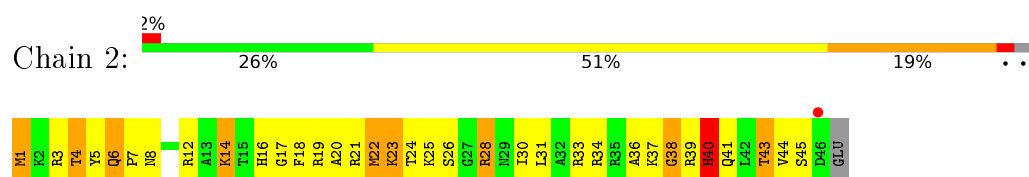
- Molecule 25: 50S ribosomal protein L32



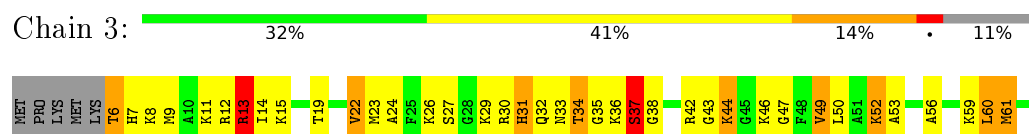
- Molecule 26: 50S ribosomal protein L33



- Molecule 27: 50S ribosomal protein L34



- Molecule 28: 50S ribosomal protein L35



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	169.47Å 407.38Å 692.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.84 – 3.58 29.84 – 3.57	Depositor EDS
% Data completeness (in resolution range)	94.3 (29.84-3.58) 94.2 (29.84-3.57)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 3.56Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.204 , 0.247 0.208 , 0.253	Depositor DCC
R_{free} test set	13342 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	112.0	Xtriage
Anisotropy	0.654	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 36.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	83681	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 6O1

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	20/63887 (0.0%)	1.25	500/99650 (0.5%)
2	Y	0.41	0/2863	0.93	0/4461
3	A	0.49	0/2011	0.79	4/2708 (0.1%)
4	B	0.58	0/1567	0.85	0/2105
5	C	0.49	0/1504	0.77	1/2036 (0.0%)
6	D	0.30	0/1419	0.51	0/1903
7	E	0.30	0/1308	0.54	0/1771
8	G	0.51	0/1138	0.81	1/1539 (0.1%)
9	H	0.56	0/1007	0.74	0/1352
10	I	0.61	0/1022	0.93	3/1366 (0.2%)
11	J	0.48	0/1101	0.71	0/1472
12	K	0.67	0/886	0.89	2/1188 (0.2%)
13	L	0.39	0/785	0.69	0/1048
14	M	0.67	1/872 (0.1%)	0.91	2/1172 (0.2%)
15	N	0.52	0/994	0.77	0/1323
16	O	0.46	0/750	0.81	2/1000 (0.2%)
17	P	0.58	0/1027	0.71	0/1373
18	Q	0.49	0/737	0.82	2/988 (0.2%)
19	R	0.45	0/835	0.75	0/1121
20	S	0.31	0/1399	0.57	0/1902
21	T	0.45	0/563	0.75	0/747
22	U	0.46	0/556	0.73	0/741
23	V	0.34	0/529	0.52	0/704
24	W	0.43	0/426	0.67	0/568
25	Z	0.56	0/464	0.77	0/622
26	1	0.55	0/434	0.83	0/579
27	2	0.58	0/387	1.04	2/509 (0.4%)
28	3	0.59	0/468	0.98	2/614 (0.3%)
All	All	0.63	21/90939 (0.0%)	1.14	521/136562 (0.4%)

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
3	A	0	1
4	B	0	1
5	C	0	2
8	G	0	4
10	I	0	5
11	J	0	1
13	L	0	1
15	N	0	2
19	R	0	1
25	Z	0	1
27	2	0	3
28	3	0	2
All	All	0	24

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	774	A	C5-C4	7.18	1.43	1.38
1	X	542	A	N9-C4	-7.12	1.33	1.37
14	M	29	PRO	CA-C	6.60	1.66	1.52
1	X	540	G	C2-N3	6.49	1.38	1.32
1	X	2548	G	C6-O6	6.47	1.29	1.24

The worst 5 of 521 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	774	A	N7-C8-N9	14.67	121.13	113.80
1	X	774	A	C8-N9-C4	-14.58	99.97	105.80
1	X	542	A	C2-N3-C4	-13.70	103.75	110.60
1	X	1333	G	N3-C4-N9	-12.51	118.49	126.00
1	X	2018	G	C4-C5-N7	11.72	115.49	110.80

There are no chirality outliers.

5 of 24 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	58	HIS	Peptide
4	B	122	PHE	Peptide
5	C	176	ASN	Peptide

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Mol	Chain	Res	Type	Group
5	C	66	ASN	Peptide
8	G	34	PRO	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	57052	0	28750	1265	0
2	Y	2561	0	1306	59	0
3	A	1973	0	2034	131	0
4	B	1539	0	1600	81	0
5	C	1481	0	1504	97	0
6	D	1400	0	1481	60	0
7	E	1286	0	1336	31	0
8	G	1114	0	1144	83	0
9	H	997	0	1046	55	0
10	I	1011	0	1047	76	0
11	J	1078	0	1103	47	0
12	K	878	0	930	34	0
13	L	779	0	820	49	0
14	M	859	0	872	35	0
15	N	978	0	1020	66	0
16	O	741	0	756	34	0
17	P	1014	0	1096	49	0
18	Q	726	0	753	29	0
19	R	825	0	881	57	0
20	S	1374	0	1401	44	0
21	T	556	0	579	24	0
22	U	552	0	604	42	0
23	V	525	0	546	14	0
24	W	424	0	470	16	0
25	Z	452	0	457	34	0
26	1	427	0	445	35	0
27	2	383	0	414	37	0
28	3	462	0	506	36	0
29	X	111	0	0	2	0
30	K	2	0	0	0	0
30	M	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	X	119	0	0	0	0
30	Y	1	0	0	0	0
All	All	83681	0	54901	2278	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 17.

The worst 5 of 2278 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:356:A:HO2'	1:X:357:A:H8	1.10	0.99
8:G:100:TYR:HB2	8:G:116:ARG:HE	1.25	0.96
10:I:56:LEU:H	10:I:59:ARG:HD3	1.30	0.94
1:X:1277:G:OP1	25:Z:19:ARG:NH2	2.01	0.93
1:X:1264:C:H5''	15:N:13:ARG:HH12	1.34	0.93

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	257/275 (94%)	219 (85%)	37 (14%)	1 (0%)	39	80
4	B	203/211 (96%)	183 (90%)	15 (7%)	5 (2%)	7	48
5	C	192/205 (94%)	161 (84%)	25 (13%)	6 (3%)	5	43
6	D	175/180 (97%)	151 (86%)	24 (14%)	0	100	100
7	E	169/185 (91%)	155 (92%)	13 (8%)	1 (1%)	30	74
8	G	140/174 (80%)	124 (89%)	15 (11%)	1 (1%)	26	72
9	H	132/134 (98%)	123 (93%)	8 (6%)	1 (1%)	24	69
10	I	132/156 (85%)	98 (74%)	30 (23%)	4 (3%)	5	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	J	134/141 (95%)	117 (87%)	16 (12%)	1 (1%)	26	72
12	K	111/116 (96%)	101 (91%)	9 (8%)	1 (1%)	21	67
13	L	102/114 (90%)	80 (78%)	22 (22%)	0	100	100
14	M	106/166 (64%)	100 (94%)	6 (6%)	0	100	100
15	N	115/118 (98%)	100 (87%)	13 (11%)	2 (2%)	11	55
16	O	92/100 (92%)	83 (90%)	9 (10%)	0	100	100
17	P	125/134 (93%)	121 (97%)	4 (3%)	0	100	100
18	Q	91/95 (96%)	69 (76%)	19 (21%)	3 (3%)	5	41
19	R	108/115 (94%)	80 (74%)	28 (26%)	0	100	100
20	S	177/237 (75%)	150 (85%)	25 (14%)	2 (1%)	17	64
21	T	72/91 (79%)	63 (88%)	9 (12%)	0	100	100
22	U	70/81 (86%)	51 (73%)	17 (24%)	2 (3%)	6	44
23	V	63/67 (94%)	58 (92%)	5 (8%)	0	100	100
24	W	53/55 (96%)	49 (92%)	4 (8%)	0	100	100
25	Z	55/60 (92%)	45 (82%)	10 (18%)	0	100	100
26	1	51/54 (94%)	36 (71%)	12 (24%)	3 (6%)	2	25
27	2	44/47 (94%)	37 (84%)	5 (11%)	2 (4%)	3	32
28	3	57/66 (86%)	44 (77%)	11 (19%)	2 (4%)	4	40
All	All	3026/3377 (90%)	2598 (86%)	391 (13%)	37 (1%)	16	63

5 of 37 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	N	94	VAL
18	Q	6	ILE
5	C	177	VAL
20	S	122	ILE
26	1	9	ILE

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	200/216 (93%)	160 (80%)	40 (20%)	1	11
4	B	155/157 (99%)	132 (85%)	23 (15%)	4	25
5	C	154/163 (94%)	117 (76%)	37 (24%)	1	6
6	D	153/156 (98%)	144 (94%)	9 (6%)	24	66
7	E	136/144 (94%)	124 (91%)	12 (9%)	12	50
8	G	118/146 (81%)	100 (85%)	18 (15%)	3	23
9	H	103/103 (100%)	83 (81%)	20 (19%)	2	12
10	I	101/121 (84%)	77 (76%)	24 (24%)	1	6
11	J	108/115 (94%)	89 (82%)	19 (18%)	2	16
12	K	90/93 (97%)	74 (82%)	16 (18%)	2	15
13	L	74/82 (90%)	50 (68%)	24 (32%)	0	2
14	M	92/134 (69%)	76 (83%)	16 (17%)	2	16
15	N	96/97 (99%)	87 (91%)	9 (9%)	11	47
16	O	75/79 (95%)	64 (85%)	11 (15%)	4	25
17	P	109/115 (95%)	90 (83%)	19 (17%)	2	16
18	Q	75/76 (99%)	53 (71%)	22 (29%)	0	4
19	R	91/96 (95%)	77 (85%)	14 (15%)	3	23
20	S	152/192 (79%)	130 (86%)	22 (14%)	4	26
21	T	55/67 (82%)	47 (86%)	8 (14%)	4	26
22	U	57/66 (86%)	43 (75%)	14 (25%)	1	6
23	V	53/55 (96%)	49 (92%)	4 (8%)	17	57
24	W	48/48 (100%)	42 (88%)	6 (12%)	6	31
25	Z	51/53 (96%)	36 (71%)	15 (29%)	0	4
26	1	45/47 (96%)	33 (73%)	12 (27%)	0	5
27	2	39/40 (98%)	29 (74%)	10 (26%)	0	5
28	3	46/52 (88%)	34 (74%)	12 (26%)	0	5
All	All	2476/2713 (91%)	2040 (82%)	436 (18%)	2	16

5 of 436 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	J	106	GLU

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Mol	Chain	Res	Type
14	M	31	ASP
26	1	8	ILE
12	K	11	ASN
13	L	15	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
10	I	103	ASN
12	K	35	GLN
25	Z	44	HIS
11	J	58	HIS
13	L	41	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2650/2880 (92%)	580 (21%)	49 (1%)
2	Y	119/123 (96%)	23 (19%)	1 (0%)
All	All	2769/3003 (92%)	603 (21%)	50 (1%)

5 of 603 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	2	G
1	X	4	C
1	X	7	G
1	X	10	A
1	X	14	A

5 of 50 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	1182	U
1	X	1475	U
1	X	2736	U
1	X	1223	G
1	X	1391	A

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 124 ligands modelled in this entry, 123 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	$\# Z > 2$
29	6O1	X	2901	-	114,123,123	1.39	12 (10%)	150,191,191	1.57	28 (18%)

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
29	6O1	X	2901	-	-	0/50/234/234	0/13/13/13

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	X	2901	6O1	C08-C05	-5.94	1.39	1.51
29	X	2901	6O1	C62-C61	-5.32	1.40	1.51
29	X	2901	6O1	C04-C09	-4.17	1.40	1.50
29	X	2901	6O1	C56-C55	-3.67	1.41	1.50
29	X	2901	6O1	C51-C50	-2.82	1.48	1.53

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	2901	6O1	C44-O44-C36	-5.82	105.27	114.40
29	X	2901	6O1	C36-C37-C38	-4.78	102.16	110.50
29	X	2901	6O1	C29-O33-C33	-3.51	107.33	113.76
29	X	2901	6O1	C45-C46-C47	-3.08	106.00	113.56
29	X	2901	6O1	C29-C30-C31	-3.04	104.61	110.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	X	2901	6O1	2	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	2658/2880 (92%)	-0.12	96 (3%) 46 37	30, 77, 204, 337	0
2	Y	120/123 (97%)	-0.07	3 (2%) 61 50	80, 150, 187, 207	0
3	A	259/275 (94%)	-0.19	4 (1%) 76 68	50, 105, 160, 212	0
4	B	205/211 (97%)	-0.49	0 100 100	30, 51, 113, 199	0
5	C	194/205 (94%)	-0.38	1 (0%) 91 88	35, 103, 180, 254	0
6	D	177/180 (98%)	-0.14	4 (2%) 64 53	128, 183, 249, 280	0
7	E	171/185 (92%)	-0.08	13 (7%) 17 13	70, 142, 203, 254	0
8	G	142/174 (81%)	-0.12	6 (4%) 40 31	38, 78, 188, 245	0
9	H	134/134 (100%)	-0.43	0 100 100	40, 55, 108, 175	0
10	I	134/156 (85%)	-0.10	2 (1%) 76 68	50, 120, 191, 236	0
11	J	136/141 (96%)	-0.04	3 (2%) 65 55	65, 106, 170, 225	0
12	K	113/116 (97%)	-0.53	0 100 100	30, 37, 91, 200	0
13	L	104/114 (91%)	0.01	5 (4%) 34 27	120, 154, 189, 241	0
14	M	108/166 (65%)	-0.66	0 100 100	37, 50, 117, 169	0
15	N	117/118 (99%)	-0.47	1 (0%) 85 79	42, 82, 136, 279	0
16	O	94/100 (94%)	-0.37	1 (1%) 82 74	48, 101, 170, 216	0
17	P	127/134 (94%)	-0.53	0 100 100	34, 53, 105, 192	0
18	Q	93/95 (97%)	-0.28	8 (8%) 13 11	49, 88, 174, 215	0
19	R	110/115 (95%)	-0.28	4 (3%) 46 37	62, 117, 213, 259	0
20	S	179/237 (75%)	-0.10	8 (4%) 37 29	97, 158, 213, 289	0
21	T	74/91 (81%)	-0.09	4 (5%) 29 23	67, 104, 157, 206	0
22	U	72/81 (88%)	0.10	5 (6%) 20 15	70, 125, 187, 215	0
23	V	65/67 (97%)	-0.23	3 (4%) 36 28	83, 125, 197, 216	0
24	W	55/55 (100%)	-0.61	0 100 100	68, 90, 135, 182	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Z	57/60 (95%)	-0.28	1 (1%) 71 62	32, 43, 104, 182	0
26	1	53/54 (98%)	0.36	6 (11%) 7 6	101, 129, 224, 259	0
27	2	46/47 (97%)	-0.29	1 (2%) 65 55	44, 59, 103, 162	0
28	3	59/66 (89%)	0.04	0 100 100	72, 100, 161, 239	0
All	All	5856/6380 (91%)	-0.19	179 (3%) 52 42	30, 91, 201, 337	0

The worst 5 of 179 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	1523	A	15.4
6	D	43	SER	8.2
22	U	29	GLY	6.4
1	X	1522	C	6.3
1	X	1073	G	6.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
30	MG	X	2977	1/1	0.96	1.03	85.12	78,78,78,78	0
30	MG	X	2935	1/1	0.88	2.21	66.25	41,41,41,41	0
30	MG	X	2952	1/1	0.97	1.28	43.51	54,54,54,54	0
30	MG	X	2992	1/1	0.90	1.05	42.15	34,34,34,34	0
30	MG	X	2970	1/1	0.94	1.03	33.37	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
30	MG	X	2947	1/1	0.94	1.18	32.51	52,52,52,52	0
30	MG	X	2921	1/1	0.96	0.98	30.70	37,37,37,37	0
30	MG	X	2975	1/1	0.89	1.38	30.37	49,49,49,49	0
30	MG	X	3020	1/1	0.54	1.57	29.07	64,64,64,64	0
30	MG	X	2910	1/1	0.94	0.62	27.03	34,34,34,34	0
30	MG	X	3008	1/1	0.94	0.62	23.65	39,39,39,39	0
30	MG	X	2911	1/1	0.97	0.66	19.97	46,46,46,46	0
30	MG	X	2906	1/1	0.91	0.87	19.73	42,42,42,42	0
30	MG	X	2916	1/1	0.82	1.05	18.56	51,51,51,51	0
30	MG	X	2912	1/1	0.95	0.46	16.76	34,34,34,34	0
30	MG	X	2939	1/1	0.96	0.61	15.65	30,30,30,30	0
30	MG	X	2907	1/1	0.90	1.25	14.61	49,49,49,49	0
30	MG	K	201	1/1	0.83	0.69	14.53	31,31,31,31	0
30	MG	X	2963	1/1	0.98	0.67	14.51	71,71,71,71	0
30	MG	X	2925	1/1	0.92	0.53	11.43	43,43,43,43	0
30	MG	X	2918	1/1	0.98	0.47	10.87	45,45,45,45	0
30	MG	X	2969	1/1	0.99	0.64	10.71	43,43,43,43	0
30	MG	X	2964	1/1	0.92	0.53	10.70	60,60,60,60	0
30	MG	X	2946	1/1	0.98	0.43	10.65	34,34,34,34	0
30	MG	X	2993	1/1	0.98	0.42	10.22	44,44,44,44	0
30	MG	X	2959	1/1	0.96	0.69	9.95	54,54,54,54	0
30	MG	X	2990	1/1	0.96	0.63	9.85	39,39,39,39	0
30	MG	X	2924	1/1	0.99	0.39	9.74	30,30,30,30	0
30	MG	X	2931	1/1	0.96	0.58	9.73	32,32,32,32	0
30	MG	X	2941	1/1	0.97	0.43	9.41	55,55,55,55	0
30	MG	X	2915	1/1	0.98	0.36	9.06	36,36,36,36	0
30	MG	X	2978	1/1	0.92	0.42	9.04	49,49,49,49	0
30	MG	X	2903	1/1	0.95	0.61	8.38	37,37,37,37	0
30	MG	X	2936	1/1	0.98	0.48	7.90	53,53,53,53	0
30	MG	X	2954	1/1	0.99	0.56	7.77	41,41,41,41	0
30	MG	X	2980	1/1	0.97	0.44	5.86	49,49,49,49	0
30	MG	X	3017	1/1	0.88	0.76	5.60	52,52,52,52	0
30	MG	X	2981	1/1	0.92	0.61	5.30	99,99,99,99	0
30	MG	X	2983	1/1	0.98	0.30	4.80	63,63,63,63	0
30	MG	X	2926	1/1	0.97	0.32	4.77	32,32,32,32	0
30	MG	X	2957	1/1	0.96	0.33	4.75	42,42,42,42	0
30	MG	X	3014	1/1	0.97	0.29	3.61	43,43,43,43	0
29	6O1	X	2901	111/111	0.91	0.39	3.50	106,116,136,139	0
30	MG	X	3011	1/1	0.94	0.34	3.27	58,58,58,58	0
30	MG	X	2953	1/1	0.97	0.29	2.01	38,38,38,38	0
30	MG	X	2943	1/1	0.95	0.29	1.75	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
30	MG	X	2942	1/1	0.91	0.25	1.23	31,31,31,31	0
30	MG	X	3018	1/1	0.96	0.28	0.90	32,32,32,32	0
30	MG	X	2917	1/1	0.94	0.21	0.73	33,33,33,33	0
30	MG	X	2951	1/1	0.97	0.22	0.71	35,35,35,35	0
30	MG	X	2998	1/1	0.94	0.22	0.47	35,35,35,35	0
30	MG	X	2996	1/1	0.98	0.19	0.03	43,43,43,43	0
30	MG	K	202	1/1	0.95	0.19	-0.39	31,31,31,31	0
30	MG	X	2932	1/1	0.95	0.32	-	53,53,53,53	0
30	MG	X	2902	1/1	0.94	1.16	-	32,32,32,32	0
30	MG	X	2967	1/1	0.90	0.37	-	55,55,55,55	0
30	MG	X	3013	1/1	0.98	0.49	-	47,47,47,47	0
30	MG	X	2973	1/1	0.94	0.35	-	52,52,52,52	0
30	MG	X	3005	1/1	0.96	0.92	-	66,66,66,66	0
30	MG	X	3002	1/1	0.95	0.31	-	44,44,44,44	0
30	MG	X	2965	1/1	0.97	0.48	-	40,40,40,40	0
30	MG	X	2997	1/1	0.99	0.36	-	38,38,38,38	0
30	MG	X	2999	1/1	0.80	0.77	-	74,74,74,74	0
30	MG	X	2955	1/1	0.96	0.39	-	31,31,31,31	0
30	MG	Y	201	1/1	0.96	0.90	-	77,77,77,77	0
30	MG	X	2909	1/1	0.94	0.72	-	36,36,36,36	0
30	MG	X	3001	1/1	0.79	1.63	-	86,86,86,86	0
30	MG	X	2950	1/1	0.97	0.51	-	36,36,36,36	0
30	MG	X	2961	1/1	0.96	0.68	-	68,68,68,68	0
30	MG	X	3006	1/1	0.74	0.50	-	34,34,34,34	0
30	MG	X	2940	1/1	0.92	0.41	-	34,34,34,34	0
30	MG	X	2982	1/1	0.89	0.86	-	31,31,31,31	0
30	MG	X	2937	1/1	0.93	0.73	-	32,32,32,32	0
30	MG	X	2986	1/1	0.96	0.48	-	46,46,46,46	0
30	MG	X	2987	1/1	0.93	0.46	-	43,43,43,43	0
30	MG	X	2908	1/1	0.95	0.67	-	34,34,34,34	0
30	MG	X	2974	1/1	0.87	0.85	-	30,30,30,30	0
30	MG	X	2920	1/1	0.95	0.74	-	34,34,34,34	0
30	MG	X	3016	1/1	0.71	1.26	-	74,74,74,74	0
30	MG	X	2938	1/1	0.94	0.33	-	36,36,36,36	0
30	MG	X	2968	1/1	0.94	0.26	-	35,35,35,35	0
30	MG	X	3009	1/1	0.99	0.33	-	41,41,41,41	0
30	MG	X	2923	1/1	0.98	0.38	-	30,30,30,30	0
30	MG	X	3019	1/1	0.83	1.06	-	46,46,46,46	0
30	MG	X	2928	1/1	0.91	0.17	-	41,41,41,41	0
30	MG	X	2995	1/1	0.93	0.82	-	83,83,83,83	0
30	MG	X	2966	1/1	0.98	0.34	-	37,37,37,37	0
30	MG	X	2930	1/1	0.97	0.64	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
30	MG	X	2913	1/1	0.91	0.63	-	36,36,36,36	0
30	MG	X	2976	1/1	0.94	0.49	-	53,53,53,53	0
30	MG	X	3015	1/1	0.89	0.55	-	98,98,98,98	0
30	MG	X	2945	1/1	0.93	1.19	-	55,55,55,55	0
30	MG	X	3012	1/1	0.74	0.39	-	52,52,52,52	0
30	MG	X	2985	1/1	0.98	0.27	-	55,55,55,55	0
30	MG	X	2905	1/1	0.97	0.82	-	30,30,30,30	0
30	MG	X	2933	1/1	0.88	1.35	-	38,38,38,38	0
30	MG	X	3004	1/1	0.96	0.30	-	54,54,54,54	0
30	MG	X	3007	1/1	0.88	0.50	-	40,40,40,40	0
30	MG	X	2948	1/1	0.97	0.26	-	30,30,30,30	0
30	MG	X	2927	1/1	0.79	0.54	-	57,57,57,57	0
30	MG	X	2971	1/1	0.92	0.62	-	33,33,33,33	0
30	MG	X	3010	1/1	0.97	0.27	-	41,41,41,41	0
30	MG	X	2972	1/1	0.92	0.63	-	36,36,36,36	0
30	MG	X	3000	1/1	0.98	0.28	-	39,39,39,39	0
30	MG	X	2962	1/1	0.98	0.20	-	41,41,41,41	0
30	MG	X	2922	1/1	0.95	0.45	-	35,35,35,35	0
30	MG	X	3003	1/1	0.95	0.87	-	63,63,63,63	0
30	MG	X	2984	1/1	0.97	0.56	-	49,49,49,49	0
30	MG	X	2956	1/1	0.95	0.58	-	32,32,32,32	0
30	MG	X	2904	1/1	0.91	1.01	-	32,32,32,32	0
30	MG	X	2989	1/1	0.96	0.67	-	56,56,56,56	0
30	MG	X	2979	1/1	0.90	0.29	-	46,46,46,46	0
30	MG	X	2994	1/1	0.94	0.37	-	77,77,77,77	0
30	MG	X	2949	1/1	0.96	0.35	-	32,32,32,32	0
30	MG	X	2914	1/1	0.96	0.46	-	43,43,43,43	0
30	MG	X	2944	1/1	0.93	0.88	-	37,37,37,37	0
30	MG	X	2991	1/1	0.96	0.69	-	72,72,72,72	0
30	MG	M	201	1/1	0.92	1.59	-	35,35,35,35	0
30	MG	X	2934	1/1	0.98	0.81	-	39,39,39,39	0
30	MG	X	2958	1/1	0.96	0.86	-	38,38,38,38	0
30	MG	X	2988	1/1	0.94	0.64	-	55,55,55,55	0
30	MG	X	2929	1/1	0.98	0.73	-	39,39,39,39	0
30	MG	X	2960	1/1	0.80	0.88	-	34,34,34,34	0
30	MG	X	2919	1/1	0.98	0.31	-	33,33,33,33	0

6.5 Other polymers

There are no such residues in this entry.