



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 02:54 AM GMT

PDB ID : 1W2B  
Title : TRIGGER FACTOR RIBOSOME BINDING DOMAIN IN COMPLEX WITH 50S  
Authors : Ferbitz, L.; Maier, T.; Patzelt, H.; Bukau, B.; Deuerling, E.; Ban, N.  
Deposited on : 2004-07-01  
Resolution : 3.50 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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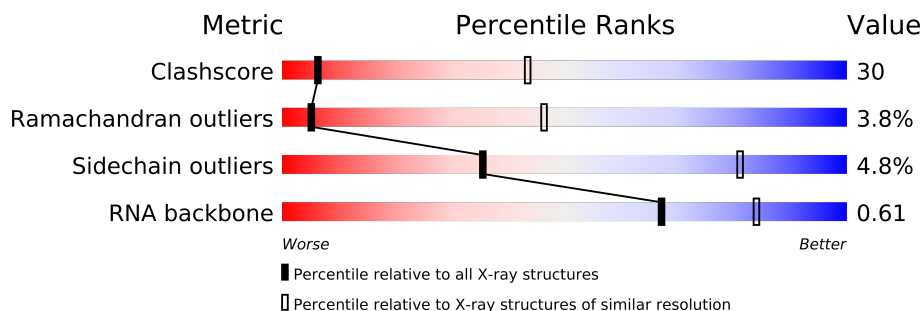
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.50 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	79885	1039 (3.66-3.34)
Ramachandran outliers	78287	1000 (3.66-3.34)
Sidechain outliers	78261	1000 (3.66-3.34)
RNA backbone	1838	1007 (4.22-2.76)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	0	2922	
2	1	48	
3	2	92	
4	5	144	
5	9	122	
6	A	239	
7	B	337	
8	C	246	
9	D	176	
10	E	177	
11	F	119	
12	G	348	
13	H	167	
14	I	145	
15	J	132	

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Mol	Chain	Length	Quality of chain
16	K	164	
17	L	194	
18	M	186	
19	N	115	
20	O	148	
21	P	95	
22	Q	154	
23	R	84	
24	S	119	
25	T	66	
26	U	70	
27	V	154	
28	W	91	
29	X	240	
30	Y	73	
31	Z	56	

## 2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 98859 atoms, of which 0 are hydrogen and 0 are deuterium.

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 RRNA.

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

- Molecule 2 is a protein called 50S RIBOSOMAL PROTEIN L39E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1	46	Total	C	N	O	S	0	0	0
			394	238	86	69	1			

- Molecule 3 is a protein called 50S RIBOSOMAL PROTEIN L44E LA, HLA, RIBOSOMAL PROTEIN L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	2	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 4 is a protein called TRIGGER FACTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	5	35	Total	C	N	O	S	0	0	0
			273	173	52	47	1			

- Molecule 5 is a RNA chain called 5S RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	9	122	Total	C	N	O	P	0	0	0
			2600	1160	472	847	121			

- Molecule 6 is a protein called 50S RIBOSOMAL PROTEIN L2P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	A	238	Total	C	N	O	S	0	0	1
			1755	1072	353	325	5			

- Molecule 7 is a protein called 50S RIBOSOMAL PROTEIN L3P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	B	337	Total	C	N	O	S	0	0	0
			2625	1616	493	511	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	310	ARG	PHE	CONFLICT	UNP P20279

- Molecule 8 is a protein called 50S RIBOSOMAL PROTEIN L4P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	C	246	Total	C	N	O	S	0	0	0
			1859	1131	344	383	1			

- Molecule 9 is a protein called 50S RIBOSOMAL PROTEIN L5P HMA15, HL13, RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	D	141	Total	C	N	O	S	0	0	1
			1095	685	196	210	4			

- Molecule 10 is a protein called 50S RIBOSOMAL PROTEIN L6P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	E	173	Total	C	N	O	S	0	0	1
			1358	840	225	289	4			

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L7AE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	F	119	Total	C	N	O	S	0	0	0
			886	552	141	192	1			

- Molecule 12 is a protein called 50S RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	G	30	Total	C	N	O	S	0	0	1
			241	149	40	51	1			

- Molecule 13 is a protein called 50S RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	H	156	Total	C	N	O	S	0	0	0
			1216	766	233	213	4			

- Molecule 14 is a protein called 50S RIBOSOMAL PROTEIN L13P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	I	142	Total	C	N	O	S	0	0	0
			1120	696	199	222	3			

- Molecule 15 is a protein called 50S RIBOSOMAL PROTEIN L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	J	132	Total	C	N	O	S	0	0	0
			994	609	189	192	4			

- Molecule 16 is a protein called 50S RIBOSOMAL PROTEIN L15P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	K	146	Total	C	N	O	S	0	0	1
			1115	668	223	224				

- Molecule 17 is a protein called 50S RIBOSOMAL PROTEIN L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	L	194	Total	C	N	O	S	0	0	0
			1606	988	346	267	5			

- Molecule 18 is a protein called 50S RIBOSOMAL PROTEIN L18P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	M	186	Total	C	N	O	S	0	0	0
			1445	895	262	286	2			

- Molecule 19 is a protein called 50S RIBOSOMAL PROTEIN L18E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	N	115	Total	C	N	O	0	0	0
			865	529	161	175			

- Molecule 20 is a protein called 50S RIBOSOMAL PROTEIN L19E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	O	144	Total	C	N	O	0	0	1
			1134	680	231	223			

- Molecule 21 is a protein called 50S RIBOSOMAL PROTEIN L21E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	P	95	Total	C	N	O	0	0	0
			735	450	141	144			

- Molecule 22 is a protein called 50S RIBOSOMAL PROTEIN L22P HMAL22, HL23, RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	Q	151	Total	C	N	O	S	0	0	1
			1150	713	210	223	4			

- Molecule 23 is a protein called 50S RIBOSOMAL PROTEIN L23P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	R	84	Total	C	N	O	S	0	0	0
			664	405	114	142	3			

- Molecule 24 is a protein called RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	S	119	Total	C	N	O	0	0	0
			950	568	180	202			

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L24P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	T	54	Total	C	N	O	S	0	0	1
			411	244	76	86	5			

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L24E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	U	66	Total	C	N	O	S	0	0	1
			500	304	95	100	1			

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L30P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	V	154	Total	C	N	O	S	0	0	0
			1196	737	209	244	6			

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L31E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	W	83	Total	C	N	O	S	0	0	1
			655	402	130	122	1			

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L32E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	X	143	Total	C	N	O	S	0	0	1
			1131	686	229	216				

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L37AE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	Y	73	Total	C	N	O	S	0	0	0
			564	359	111	87	7			

- Molecule 31 is a protein called RIBOSOMAL PROTEIN L37E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	Z	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	0	62	Total	Mg	0	0
			62	62		
32	J	1	Total	Mg	0	0
			1	1		
32	B	3	Total	Mg	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	A	1	Total 1	Mg 1	0	0
32	9	1	Total 1	Mg 1	0	0
32	3	49	Total 49	Mg 49	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	2	Total 2	K 2	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	56	Total 56	Na 56	0	0
34	P	1	Total 1	Na 1	0	0
34	Q	2	Total 2	Na 2	0	0
34	H	2	Total 2	Na 2	0	0
34	B	1	Total 1	Na 1	0	0
34	I	1	Total 1	Na 1	0	0
34	C	1	Total 1	Na 1	0	0
34	S	1	Total 1	Na 1	0	0
34	A	1	Total 1	Na 1	0	0
34	R	1	Total 1	Na 1	0	0
34	9	1	Total 1	Na 1	0	0
34	L	1	Total 1	Na 1	0	0
34	3	17	Total 17	Na 17	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	7	Total 7	Cl 7	0	0
35	P	1	Total 1	Cl 1	0	0
35	J	1	Total 1	Cl 1	0	0
35	Q	1	Total 1	Cl 1	0	0
35	K	1	Total 1	Cl 1	0	0
35	B	1	Total 1	Cl 1	0	0
35	I	3	Total 3	Cl 3	0	0
35	N	1	Total 1	Cl 1	0	0
35	X	1	Total 1	Cl 1	0	0
35	2	1	Total 1	Cl 1	0	0
35	L	1	Total 1	Cl 1	0	0
35	3	2	Total 2	Cl 2	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	2	1	Total 1	Cd 1	0	0
36	Y	1	Total 1	Cd 1	0	0
36	T	1	Total 1	Cd 1	0	0
36	Z	1	Total 1	Cd 1	0	0
36	N	1	Total 1	Cd 1	0	0

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	0	5944	Total 5944	O 5944	0	0
37	1	49	Total 49	O 49	0	0
37	2	66	Total 66	O 66	0	0
37	9	153	Total 153	O 153	0	0
37	A	132	Total 132	O 132	0	0
37	B	145	Total 145	O 145	0	0
37	C	160	Total 160	O 160	0	0
37	D	52	Total 52	O 52	0	0
37	E	41	Total 41	O 41	0	0
37	F	29	Total 29	O 29	0	0
37	G	20	Total 20	O 20	0	0
37	H	80	Total 80	O 80	0	0
37	I	52	Total 52	O 52	0	0
37	J	61	Total 61	O 61	0	0
37	K	91	Total 91	O 91	0	0
37	L	148	Total 148	O 148	0	0
37	M	59	Total 59	O 59	0	0
37	N	35	Total 35	O 35	0	0
37	O	64	Total 64	O 64	0	0
37	P	52	Total 52	O 52	0	0
37	Q	80	Total 80	O 80	0	0
37	R	29	Total 29	O 29	0	0

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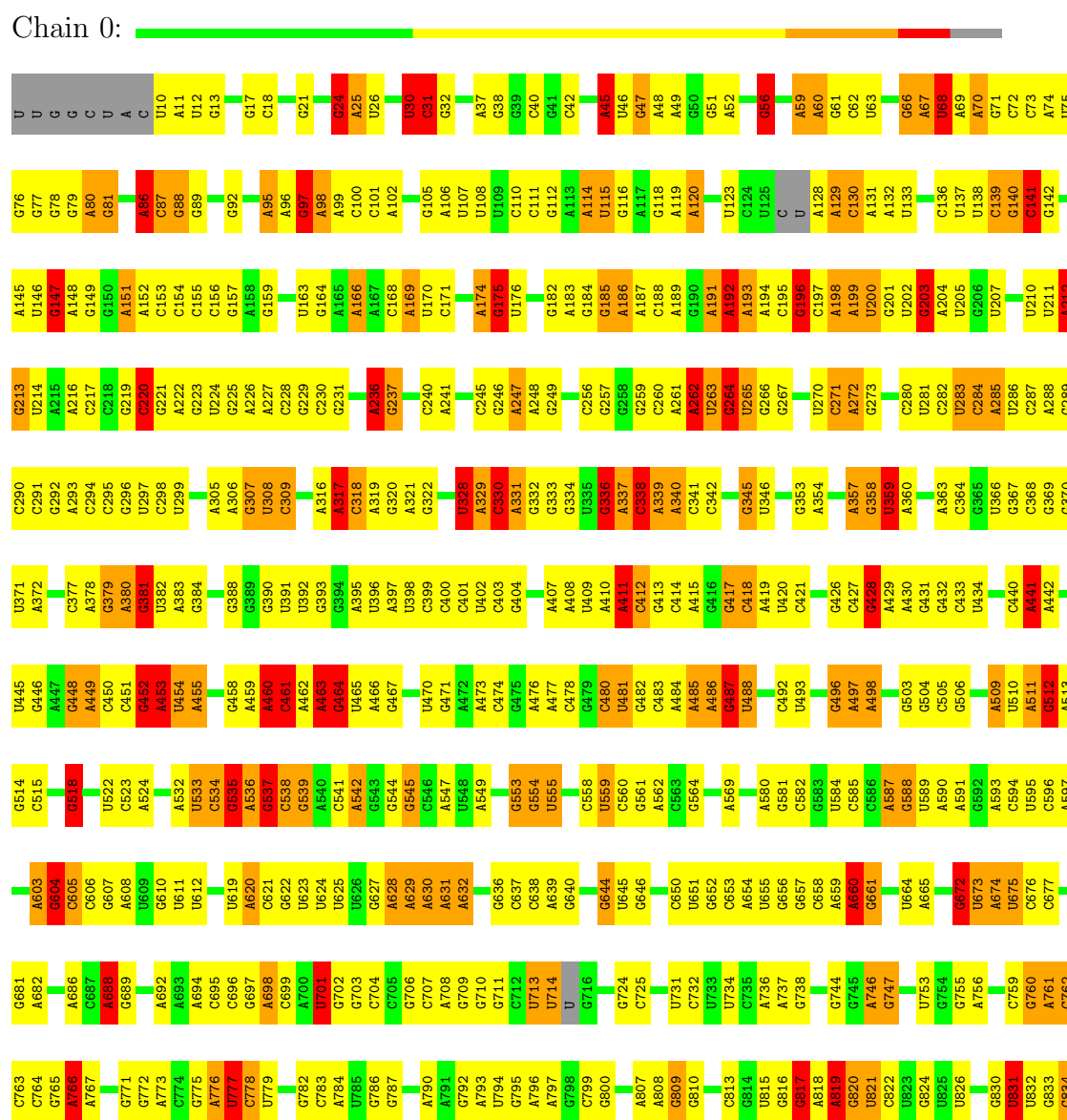
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	S	31	Total 31	O 31	0	0
37	T	25	Total 25	O 25	0	0
37	U	11	Total 11	O 11	0	0
37	V	69	Total 69	O 69	0	0
37	W	26	Total 26	O 26	0	0
37	X	101	Total 101	O 101	0	0
37	Y	35	Total 35	O 35	0	0
37	Z	47	Total 47	O 47	0	0

### 3 Residue-property plots

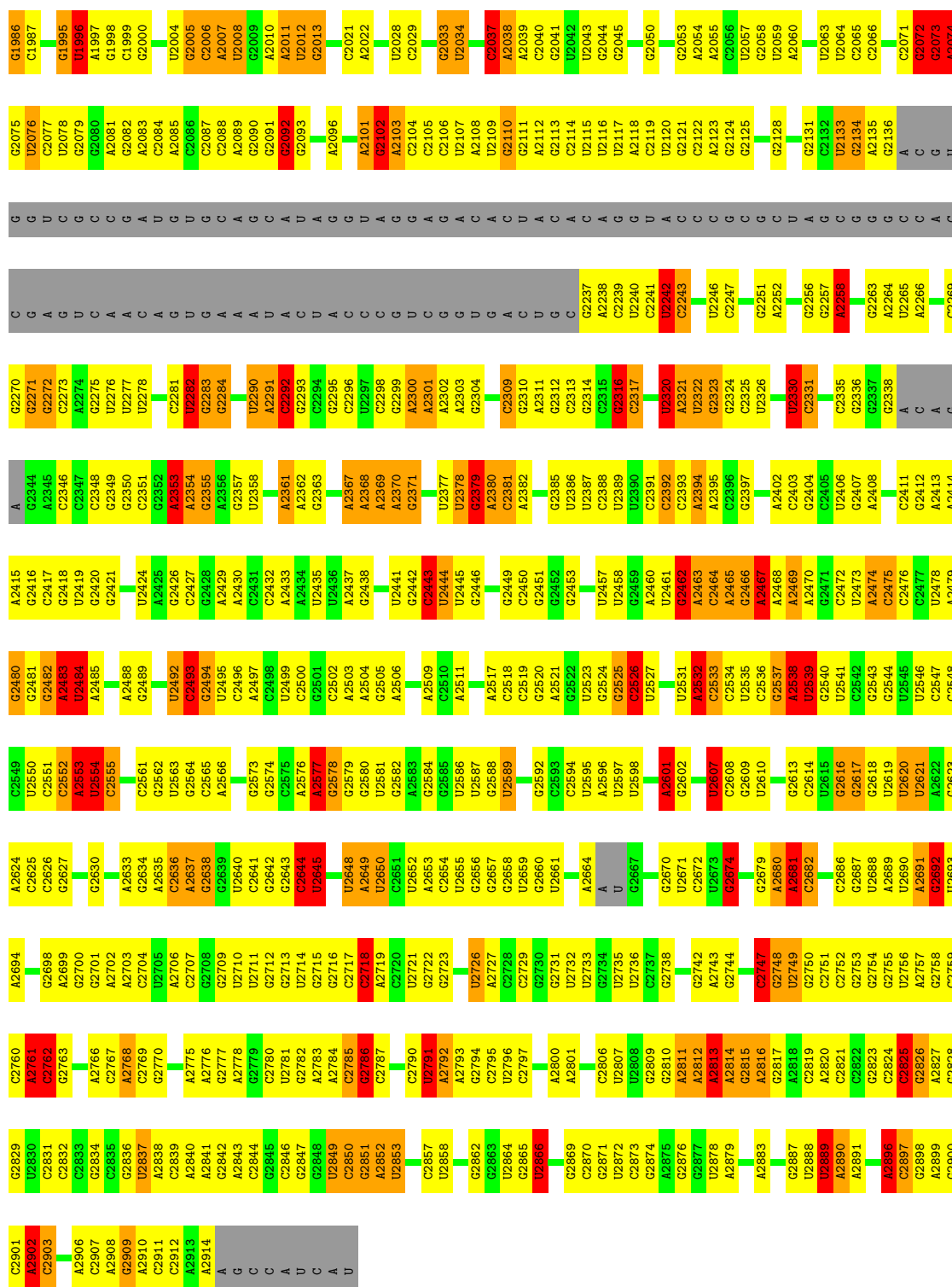
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

#### • Molecule 1: 23S rRNA

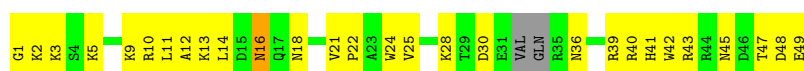


A1910	A1845	U1770	U1696	A1630	A1559	A1471	G1401	C1332	C1262	C1186	A1114	G1038	U903	U835
A1919	A1846	U1771	G1697	A1630	U	C1472	C1404	U1333	G1265	U1187	U1115	G1039	U904	G836
C1920	A1847	G1772	C1700	C1633	U1561	U1473	U1405	C1334	U1266	A1188	A1116	U1040	C905	U837
A1921	G1848	G1773	U1702	U1635	G1563	G1475	A1406	C1335	C1267	A1189	A1117	U1041	C906	U840
A1922	G1849	A1775	G1703	U1636	C1564	A1476	A1407	U1336	C1268	A1190	G1119	C1042	A907	A841
G1923	U1850	A1776	G1703	A1637	C1565	C1477	U1408	U1338	G1269	A1191	G1118	C1043	A908	A841
A1924	G1851	A1777	G1703	A1637	C1566	U1478	G1409	U1339	U1270	A1192	U1120	C1044	U909	C842
G1925	A1852	A1778	C1708	A1641	U1566	U1478	U1409	G1339	U1271	A1193	U1121	G1045	C910	A843
G1929	C1853	A1779	G1709	A1642	U1567	A1482	U1412	G1340	A1271	A1194	U1122	G1046	A844	A844
A1930	G1854	A1780	U1710	C1643	U1568	C1483	A1413	C1341	C1272	U1195	A1123	C1061	U919	U845
A1931	A1855	A1781	A1712	C1643	C1570	G1484	A1414	C1342	C1273	U1196	A1124	G1052	C920	A846
G1932	A1857	G1785	G1713	G1646	G1571	A1485	G1415	C1343	G1197	U1197	U1125	G1053	C921	C847
C1936	A1858	C1786	G1713	G1647	G1572	A1486	G1416	U1346	C1201	C1201	C1127	G1054	A922	C848
U1937	A1859	C1787	U1718	G1648	A1573	U1487	G1417	U1347	A1202	A1202	U1128	G1055	A923	C849
G1938	U1860	U1788	G1718	G1649	C1574	A1488	U1418	A1348	U1205	U1205	U1129	U1056	C924	U850
U1939	C1861	G1789	G1719	C1650	C1575	A1489	U1419	U1351	U1206	U1206	U1130	A1057	C925	C853
G1940	C1862	C1790	G1720	C1651	U1576	G1490	U1422	G1352	A1207	A1207	G1131	G1058	C926	C854
A1941	G1863	U1791	G1721	C1652	C1579	U1491	A1423	A1353	C1208	C1208	A1132	G1059	C931	U855
C1942	A1866	G1795	U1722	C1653	U1580	A1492	C1424	C1354	C1289	C1289	A1133	C1060	C932	G856
A1943	G1867	U1796	G1723	U1654	A1581	A1493	A1425	G1355	C1290	C1290	G1134	C1061	U932	A857
C1943	U1868	A1797	U1724	G1655	U1583	C1495	G1426	A1356	G1291	G1291	G1135	C1062	C933	U858
C1946	A1869	G1797	G1725	A1657	C1584	G1496	A1427	A1357	G1292	C1212	U1136	C1063	C934	C859
G1950	U1870	C1798	G1727	A1658	U1589	G1497	U1430	U1358	U1293	C1213	G1137	U1066	G935	U860
G1951	U1871	G1730	C1731	A1661	A1590	U1500	C1431	U1359	A1294	G1214	C1138	C1068	U1001	A861
U1964	C1872	A1804	C1805	C1662	A1591	A1501	U1432	C1360	G1295	A1215	C1148	C1069	U1002	A867
A1967	U1873	G1805	G1809	C1663	U1592	A1502	A1433	C1361	U1296	U1216	U1149	A1070	G1003	C868
A1968	A1881	G1810	G1812	C1664	U1593	A1503	U1434	C1362	U1297	U1297	A1150	A1071	C1004	G940
A1969	C1882	U1811	U1813	C1665	U1594	A1504	U1435	C1363	U1298	C1229	G1151	A1072	A1005	G941
A1970	U1883	G1814	G1815	C1666	U1595	A1505	U1436	C1364	U1299	A1230	A1152	A1073	A1006	U942
G1971	U1884	C1816	C1817	C1667	U1596	U1506	G1438	A1367	G1299	A1231	C1153	G1076	A1007	A943
A1972	A1885	U1817	U1818	C1668	U1597	U1507	U1439	A1368	G1302	A1232	C1154	G1077	U1008	U872
A1973	U1886	G1819	G1820	C1669	U1598	U1508	U1440	C1369	U1303	U1233	G1155	C1080	U1009	A875
G1974	U1887	U1820	G1821	C1670	U1599	U1509	U1441	C1370	C1304	U1234	C1156	A1081	U946	A876
U1977	U1888	C1821	C1822	C1671	U1600	G1601	U1442	A1371	U1305	G1235	G1157	A1082	U947	G877
A1978	C1889	G1823	G1824	C1672	G1602	C1603	U1443	A1372	U1306	G1236	C1158	A1083	G948	G878
G1979	U1890	U1824	U1825	C1673	U1603	C1604	U1444	A1373	U1307	U1237	G1159	C1084	C881	C881
U1980	A1891	C1826	C1827	C1674	U1604	U1605	U1445	A1374	U1308	C1238	G1160	C1085	G953	A882
A1981	C1892	U1827	U1828	C1675	U1606	U1607	U1446	A1375	U1309	G1239	A1161	A1086	A955	U883
C1982	U1900	G1829	G1830	C1676	U1608	U1609	U1447	A1376	U1310	G1240	G1162	G1087	C956	C884
U1983	G1901	C1831	C1832	C1677	U1610	U1611	U1448	A1377	U1311	G1241	G1163	A1088	A957	G885
U1984	U1902	U1833	U1834	C1678	U1612	U1613	U1449	A1378	U1312	A1242	G1164	G1089	G958	A886
U1985	C1903	G1835	G1836	C1679	U1614	U1615	U1450	U1380	U1313	C1243	G1165	G1090	G959	G887
A1986	U1904	U1837	U1838	C1680	U1616	U1617	U1451	A1381	U1314	U1244	A1166	U1096	C960	U888
A1987	C1905	C1839	C1840	C1681	U1618	U1619	U1452	A1382	G1315	C1245	G1167	A1097	A961	G889
A1988	U1906	U1841	U1842	C1682	U1620	U1621	U1453	A1383	G1316	A1246	C1168	C1098	C962	C890
A1989	C1907	G1843	G1844	C1683	U1622	U1623	U1454	U1384	A1317	A1247	U1169	A1099	C963	G891
A1990	U1908	C1845	C1846	C1684	U1624	U1625	U1455	U1385	G1318	A1248	G1172	G1100	G964	G892
A1991	C1909	U1847	U1848	C1685	U1626	U1627	U1456	U1386	U1320	C1250	A1173	C1104	U1028	C893
A1992	U1910	G1849	G1850	C1686	U1628	U1629	U1457	U1387	U1321	C1251	A1174	C1105	U1029	A894
A1993	C1910	U1851	U1852	C1687	U1630	U1631	U1458	U1388	G1325	A1252	G1175	A1106	C1030	A895
A1994	U1911	C1853	C1854	C1688	U1632	U1633	U1459	U1389	U1326	C1253	U1180	A1107	G1031	C896
A1995	C1911	G1855	G1856	C1689	U1634	U1635	U1460	U1390	G1327	C1254	U1181	G1108	C1032	A897
A1996	U1912	U1857	U1858	C1690	U1636	U1637	U1461	U1391	U1328	G1257	C1182	U1109	C1033	C898
A1997	C1912	C1859	C1860	C1691	U1638	U1639	U1462	U1392	A1328	C1260	C1183	G1110	G1034	C899
A1998	U1913	U1861	U1862	C1692	U1640	U1641	U1463	A1393	A1329	G1261	U1184	U1111	C1035	G901
A1999	C1913	G1863	G1864	C1693	U1642	U1643	U1464	U1394	U1330	A1330	C1184	C1036	U	C
A2000	U1914	C1865	C1866	C1694	U1644	U1645	U1465	U1395	A1331	A1331	U1185			G902



• Molecule 2: 50S RIBOSOMAL PROTEIN L39E

Chain 1:



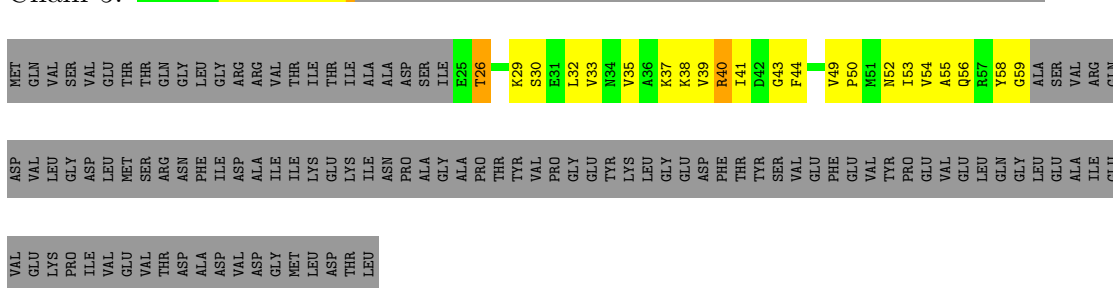
• Molecule 3: 50S RIBOSOMAL PROTEIN L44E LA, HLA, RIBOSOMAL PROTEIN L44E

Chain 2:



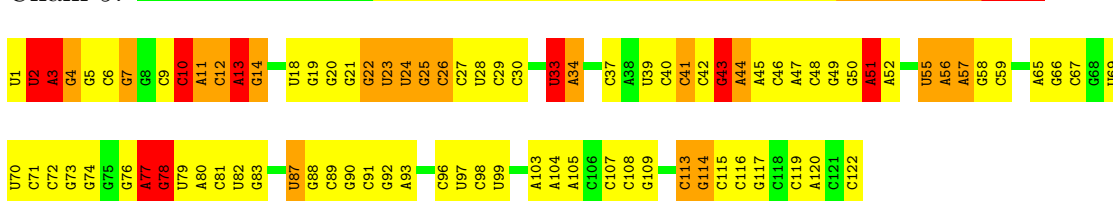
- Molecule 4: TRIGGER FACTOR

Chain 5:



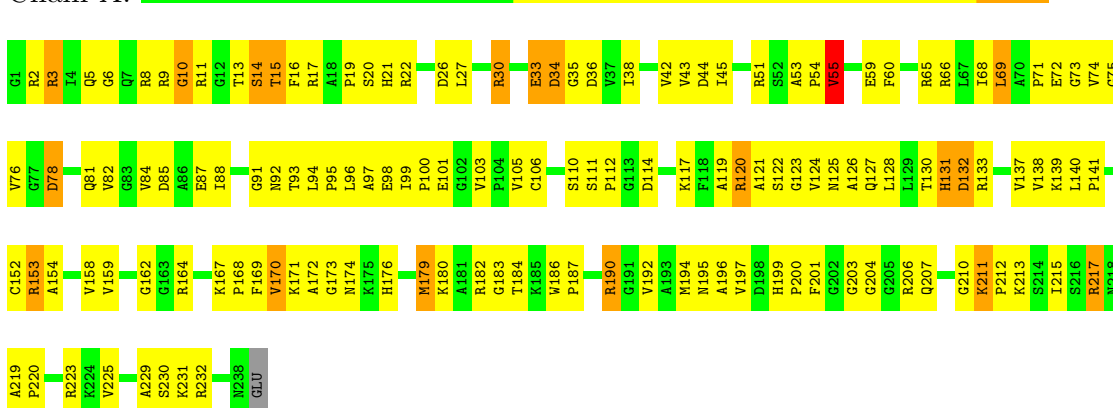
- Molecule 5: 5S rRNA

Chain 9:



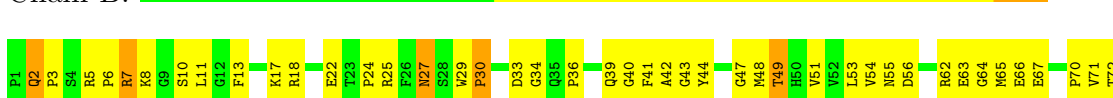
- Molecule 6: 50S RIBOSOMAL PROTEIN L2P

Chain A:

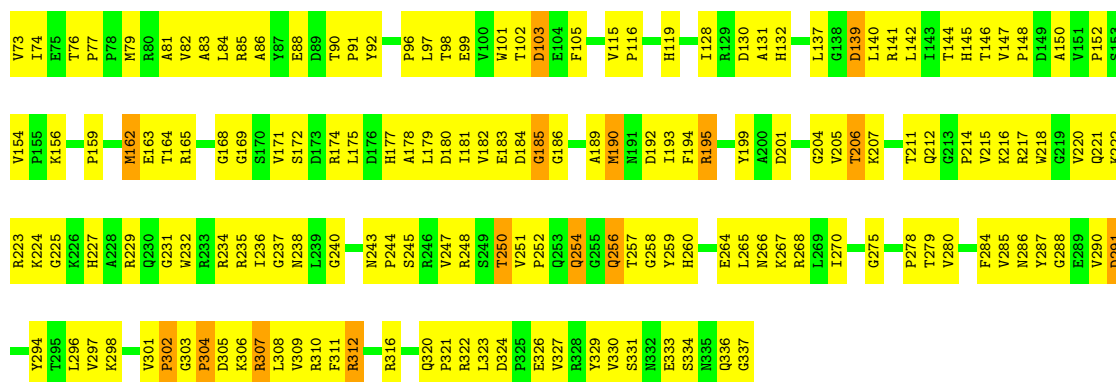


● Molecule 7: 50S RIBOSOMAL PROTEIN L3P

Chain B:

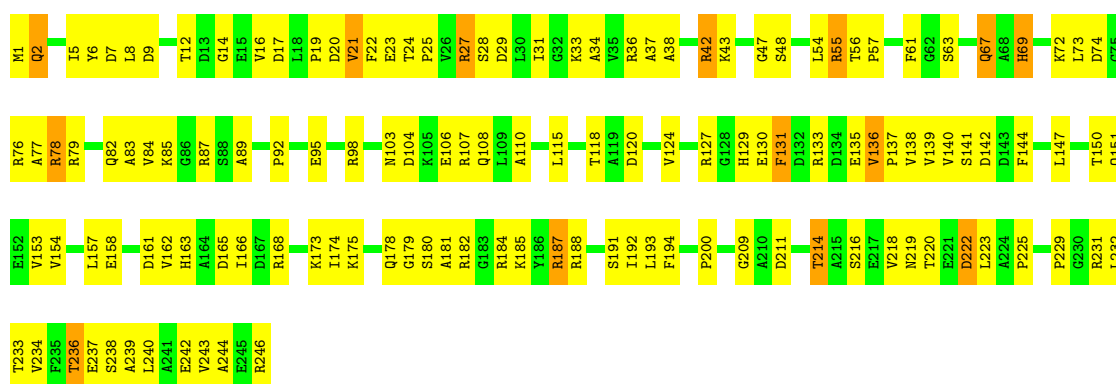






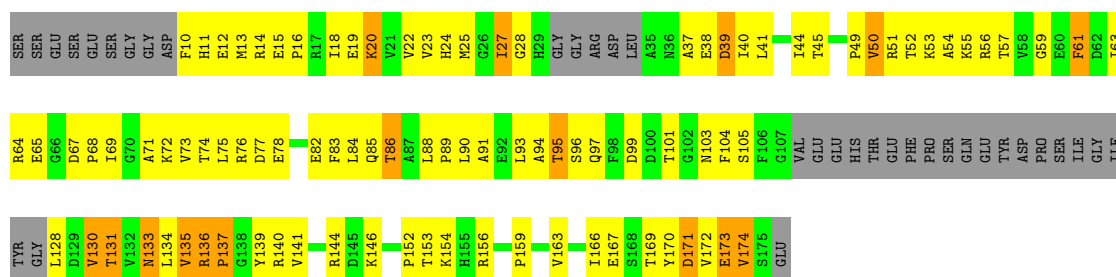
### • Molecule 8: 50S RIBOSOMAL PROTEIN L4P

Chain C:



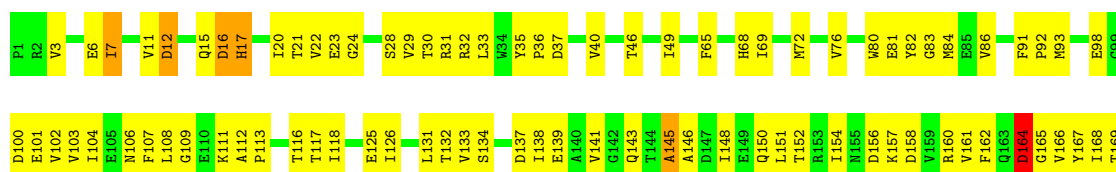
### • Molecule 9: 50S RIBOSOMAL PROTEIN L5P HMA15, HL13, RIBOSOMAL PROTEIN L5

Chain D:



### • Molecule 10: 50S RIBOSOMAL PROTEIN L6P

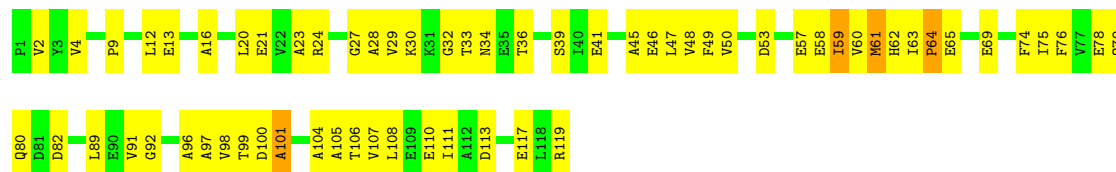
Chain E:





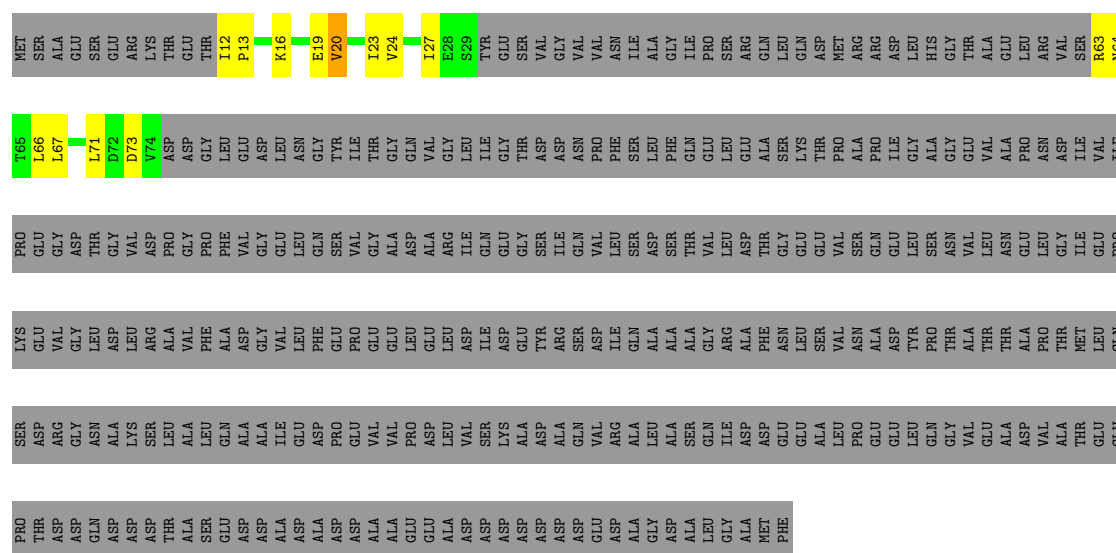
• Molecule 11: 50S RIBOSOMAL PROTEIN L7AE

Chain F:



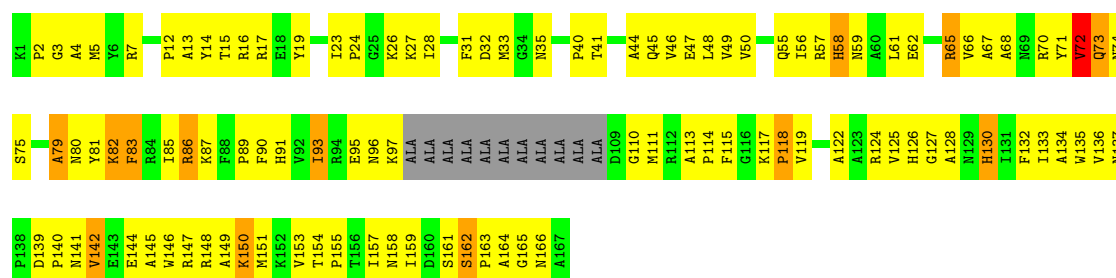
• Molecule 12: 50S RIBOSOMAL PROTEIN L10E

Chain G:



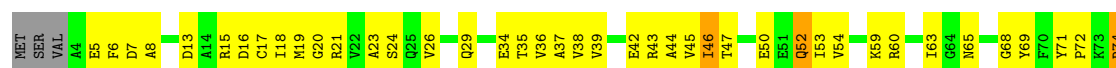
• Molecule 13: 50S RIBOSOMAL PROTEIN L10E

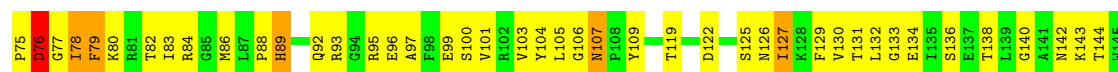
Chain H:



• Molecule 14: 50S RIBOSOMAL PROTEIN L13P

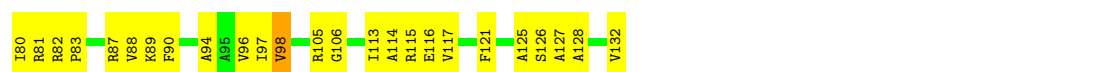
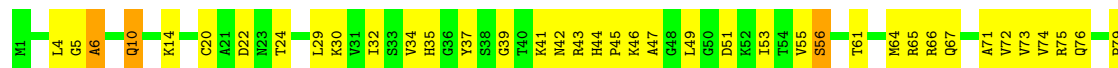
Chain I:





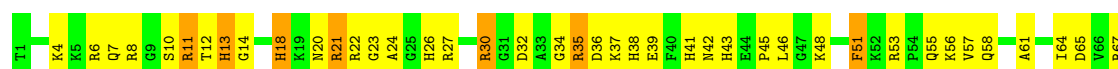
• Molecule 15: 50S RIBOSOMAL PROTEIN L14P

Chain J:



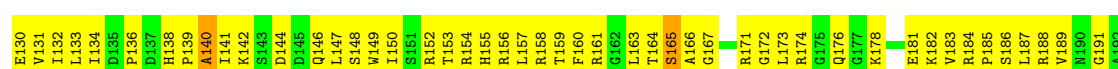
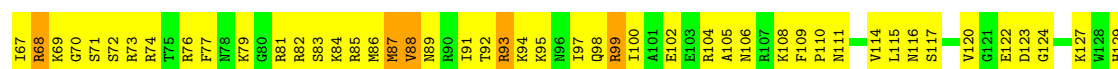
• Molecule 16: 50S RIBOSOMAL PROTEIN L15P

Chain K:



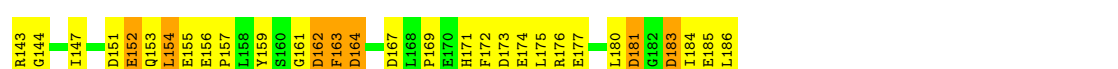
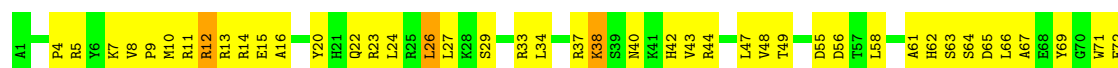
• Molecule 17: 50S RIBOSOMAL PROTEIN L15E

Chain L:

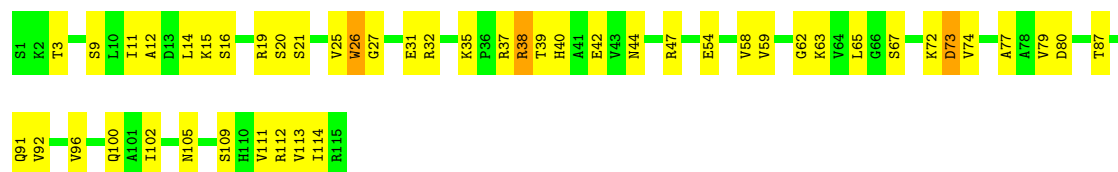


• Molecule 18: 50S RIBOSOMAL PROTEIN L18P

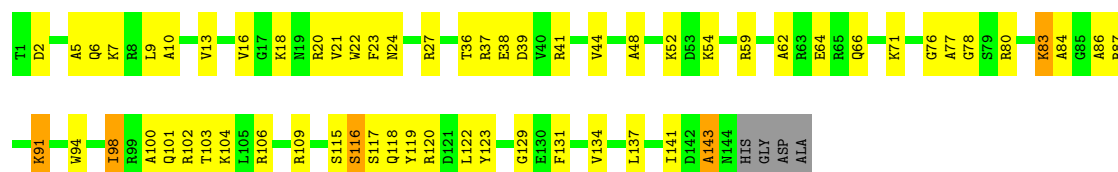
Chain M:



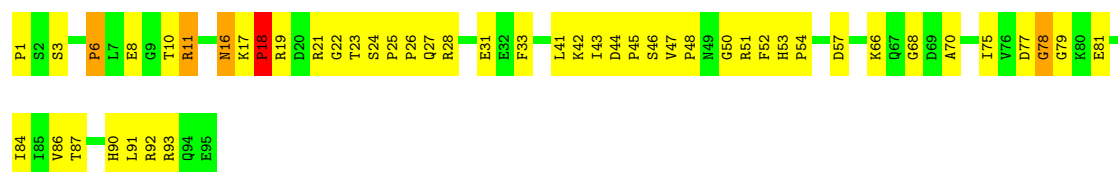
- Molecule 19: 50S RIBOSOMAL PROTEIN L18E

Chain N: 

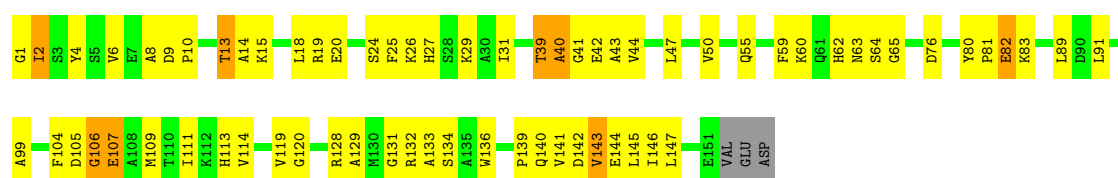
- Molecule 20: 50S RIBOSOMAL PROTEIN L19E

Chain O: 

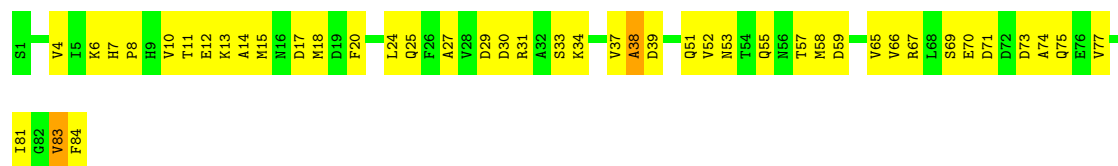
- Molecule 21: 50S RIBOSOMAL PROTEIN L21E

Chain P: 

- Molecule 22: 50S RIBOSOMAL PROTEIN L22P HMAL22, HL23, RIBOSOMAL PROTEIN L22

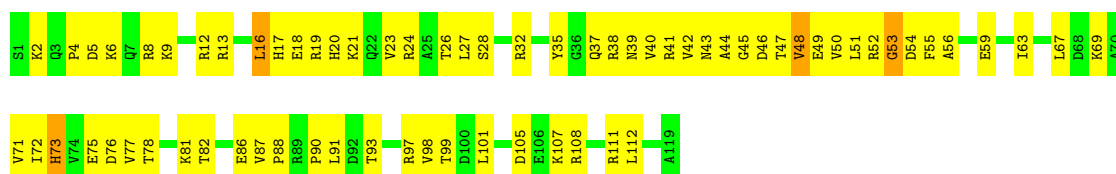
Chain Q: 

- Molecule 23: 50S RIBOSOMAL PROTEIN L23P

Chain R: 

- Molecule 24: RIBOSOMAL PROTEIN L24

Chain S: 



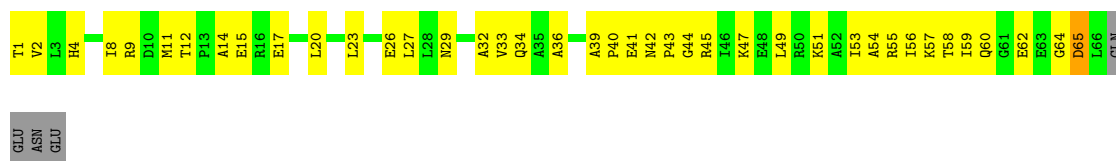
• Molecule 25: 50S RIBOSOMAL PROTEIN L24P

Chain T:



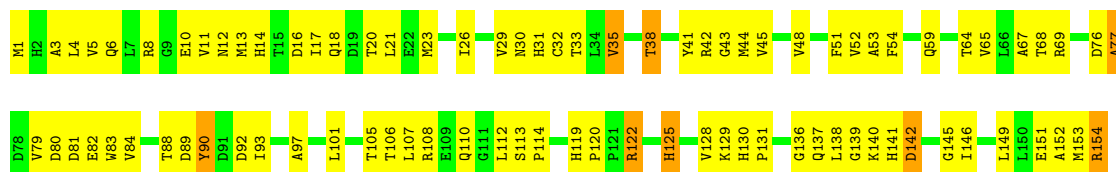
• Molecule 26: 50S RIBOSOMAL PROTEIN L24E

Chain U:



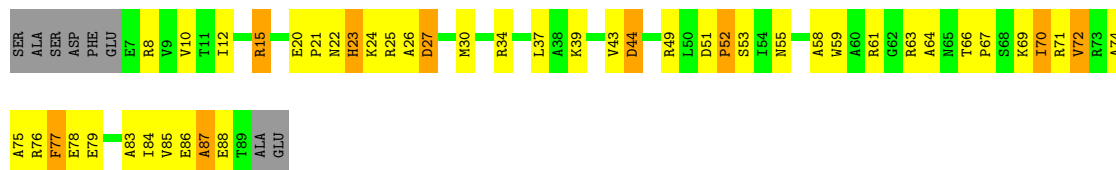
• Molecule 27: 50S RIBOSOMAL PROTEIN L30P

Chain V:



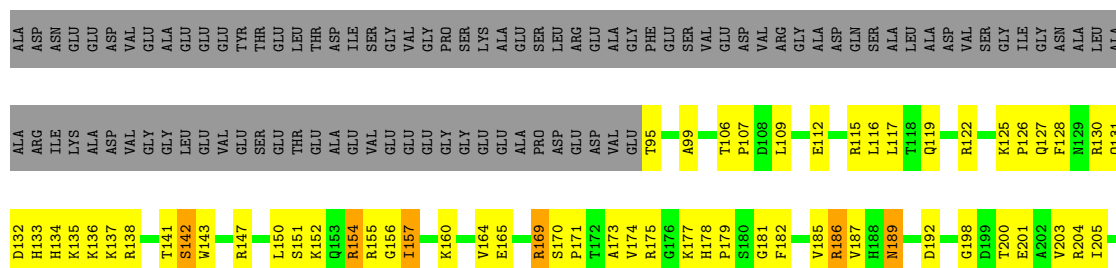
• Molecule 28: 50S RIBOSOMAL PROTEIN L31E

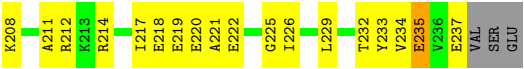
Chain W:



• Molecule 29: 50S RIBOSOMAL PROTEIN L32E

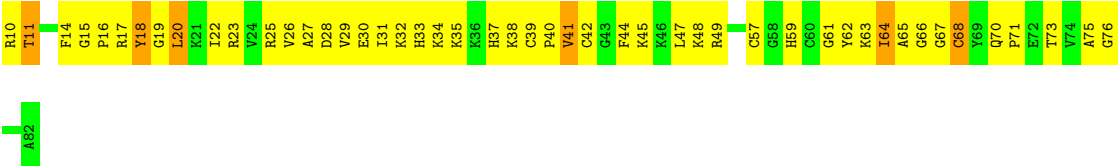
Chain X:





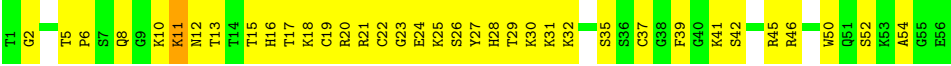
● Molecule 30: 50S RIBOSOMAL PROTEIN L37AE

Chain Y:



● Molecule 31: RIBOSOMAL PROTEIN L37E

Chain Z:



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.75Å 298.87Å 574.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.50	Depositor
% Data completeness (in resolution range)	80.3 (30.00-3.50)	Depositor
$R_{merge}$	0.26	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.192 , 0.268	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	98859	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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

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	0	0.49	0/66076	0.85	218/103052 (0.2%)
2	1	0.34	0/399	0.56	0/527
3	2	0.34	0/771	0.55	0/1024
4	5	0.38	0/275	0.77	0/366
5	9	0.44	0/2905	0.84	11/4528 (0.2%)
6	A	0.36	0/1788	0.65	0/2411
7	B	0.36	0/2690	0.65	0/3652
8	C	0.37	0/1884	0.62	0/2551
9	D	0.35	0/1112	0.59	0/1500
10	E	0.38	0/1383	0.63	0/1882
11	F	0.35	0/897	0.59	0/1219
12	G	0.41	0/242	0.53	0/326
13	H	0.38	0/1247	0.68	0/1686
14	I	0.37	0/1136	0.63	0/1530
15	J	0.39	0/1004	0.68	0/1351
16	K	0.34	0/1127	0.64	0/1506
17	L	0.40	0/1634	0.66	0/2180
18	M	0.32	0/1474	0.66	0/1999
19	N	0.35	0/874	0.65	0/1181
20	O	0.37	0/1144	0.55	0/1523
21	P	0.37	0/749	0.67	0/1005
22	Q	0.41	0/1173	0.63	0/1580
23	R	0.53	0/672	0.69	0/906
24	S	0.34	0/958	0.65	0/1289
25	T	0.40	0/418	0.57	0/564
26	U	0.36	0/503	0.59	0/677
27	V	0.37	0/1219	0.64	0/1655
28	W	0.37	0/665	0.61	0/897
29	X	0.38	0/1147	0.65	0/1538
30	Y	0.34	0/576	0.58	0/763
31	Z	0.40	0/438	0.63	0/578
All	All	0.45	0/98580	0.80	229/147446 (0.2%)



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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	65
5	9	0	4
27	V	0	1
All	All	0	70

There are no bond length outliers.

The worst 5 of 229 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	535	G	N9-C1'-C2'	10.05	127.07	114.00
1	0	537	G	N9-C1'-C2'	9.91	126.88	114.00
1	0	1235	G	O4'-C1'-N9	8.50	115.00	108.20
1	0	1702	U	N1-C1'-C2'	8.48	125.03	114.00
1	0	337	A	N9-C1'-C2'	8.44	124.97	114.00

There are no chirality outliers.

5 of 70 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	203	G	Sidechain
1	0	224	U	Sidechain
1	0	30	U	Sidechain
1	0	68	U	Sidechain
1	0	86	A	Sidechain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59017	0	29808	2081	0
2	1	394	0	406	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	2	755	0	732	81	0
4	5	273	0	296	23	0
5	9	2600	0	1326	119	0
6	A	1755	0	1763	185	0
7	B	2625	0	2533	240	0
8	C	1859	0	1816	166	0
9	D	1095	0	1085	125	0
10	E	1358	0	1266	95	0
11	F	886	0	854	75	0
12	G	241	0	231	20	0
13	H	1216	0	1215	169	0
14	I	1120	0	1098	92	0
15	J	994	0	1027	82	0
16	K	1115	0	1072	91	0
17	L	1606	0	1676	241	0
18	M	1445	0	1401	149	0
19	N	865	0	873	52	0
20	O	1134	0	1127	65	0
21	P	735	0	729	49	0
22	Q	1150	0	1122	76	0
23	R	664	0	626	50	0
24	S	950	0	924	80	0
25	T	411	0	368	35	0
26	U	500	0	511	45	0
27	V	1196	0	1137	120	0
28	W	655	0	653	55	0
29	X	1131	0	1133	100	0
30	Y	564	0	601	85	0
31	Z	431	0	426	45	0
32	0	62	0	0	0	0
32	3	49	0	0	0	0
32	9	1	0	0	0	0
32	A	1	0	0	0	0
32	B	3	0	0	0	0
32	J	1	0	0	0	0
33	0	2	0	0	0	0
34	0	56	0	0	0	0
34	3	17	0	0	0	0
34	9	1	0	0	0	0
34	A	1	0	0	0	0
34	B	1	0	0	0	0
34	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	H	2	0	0	0	0
34	I	1	0	0	0	0
34	L	1	0	0	0	0
34	P	1	0	0	0	0
34	Q	2	0	0	0	0
34	R	1	0	0	0	0
34	S	1	0	0	0	0
35	0	7	0	0	2	0
35	2	1	0	0	0	0
35	3	2	0	0	0	0
35	B	1	0	0	0	0
35	I	3	0	0	3	0
35	J	1	0	0	0	0
35	K	1	0	0	0	0
35	L	1	0	0	2	0
35	M	1	0	0	1	0
35	N	1	0	0	0	0
35	P	1	0	0	2	0
35	Q	1	0	0	0	0
35	X	1	0	0	2	0
36	2	1	0	0	0	0
36	N	1	0	0	0	0
36	T	1	0	0	0	0
36	Y	1	0	0	0	0
36	Z	1	0	0	0	0
37	0	5944	0	0	351	0
37	1	49	0	0	8	0
37	2	66	0	0	8	0
37	9	153	0	0	16	0
37	A	132	0	0	28	0
37	B	145	0	0	30	0
37	C	160	0	0	42	0
37	D	52	0	0	15	0
37	E	41	0	0	8	0
37	F	29	0	0	6	0
37	G	20	0	0	3	0
37	H	80	0	0	19	0
37	I	52	0	0	4	0
37	J	61	0	0	18	0
37	K	91	0	0	23	0
37	L	148	0	0	33	0
37	M	59	0	0	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	N	35	0	0	5	0
37	O	64	0	0	6	0
37	P	52	0	0	6	0
37	Q	80	0	0	6	0
37	R	29	0	0	6	0
37	S	31	0	0	4	0
37	T	25	0	0	6	0
37	U	11	0	0	2	0
37	V	69	0	0	10	0
37	W	26	0	0	6	0
37	X	101	0	0	13	0
37	Y	35	0	0	10	0
37	Z	47	0	0	2	0
All	All	98859	0	59835	4534	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 30.

The worst 5 of 4534 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:156:C:H5"	17:L:171:ARG:HD3	1.28	1.14
3:2:46:ILE:HG21	17:L:87:MET:HG2	1.24	1.14
26:U:12:THR:HG22	26:U:15:GLU:HG3	1.28	1.14
11:F:91:VAL:HG12	11:F:92:GLY:H	1.09	1.13
5:9:6:C:H5"	18:M:37:ARG:HH12	1.08	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	
2	1	42/48 (88%)	37 (88%)	5 (12%)	0	100	100
3	2	90/92 (98%)	82 (91%)	5 (6%)	3 (3%)	6	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	5	33/144 (23%)	24 (73%)	9 (27%)	0	100	100
6	A	236/239 (99%)	197 (84%)	27 (11%)	12 (5%)	3	36
7	B	335/337 (99%)	281 (84%)	40 (12%)	14 (4%)	4	43
8	C	244/246 (99%)	201 (82%)	37 (15%)	6 (2%)	9	57
9	D	135/176 (77%)	90 (67%)	31 (23%)	14 (10%)	1	14
10	E	171/177 (97%)	147 (86%)	21 (12%)	3 (2%)	13	65
11	F	117/119 (98%)	97 (83%)	16 (14%)	4 (3%)	6	50
12	G	26/348 (8%)	23 (88%)	2 (8%)	1 (4%)	5	46
13	H	152/167 (91%)	123 (81%)	21 (14%)	8 (5%)	3	35
14	I	140/145 (97%)	117 (84%)	17 (12%)	6 (4%)	4	42
15	J	130/132 (98%)	115 (88%)	13 (10%)	2 (2%)	15	69
16	K	142/164 (87%)	116 (82%)	20 (14%)	6 (4%)	4	43
17	L	192/194 (99%)	144 (75%)	40 (21%)	8 (4%)	4	43
18	M	184/186 (99%)	153 (83%)	24 (13%)	7 (4%)	5	46
19	N	113/115 (98%)	92 (81%)	17 (15%)	4 (4%)	6	50
20	O	142/148 (96%)	126 (89%)	12 (8%)	4 (3%)	8	55
21	P	93/95 (98%)	72 (77%)	16 (17%)	5 (5%)	3	35
22	Q	149/154 (97%)	127 (85%)	18 (12%)	4 (3%)	8	56
23	R	82/84 (98%)	68 (83%)	9 (11%)	5 (6%)	2	30
24	S	117/119 (98%)	101 (86%)	13 (11%)	3 (3%)	8	57
25	T	52/66 (79%)	49 (94%)	3 (6%)	0	100	100
26	U	64/70 (91%)	49 (77%)	13 (20%)	2 (3%)	7	53
27	V	152/154 (99%)	132 (87%)	19 (12%)	1 (1%)	30	83
28	W	81/91 (89%)	65 (80%)	11 (14%)	5 (6%)	2	30
29	X	141/240 (59%)	126 (89%)	12 (8%)	3 (2%)	11	62
30	Y	71/73 (97%)	59 (83%)	7 (10%)	5 (7%)	2	26
31	Z	54/56 (96%)	43 (80%)	7 (13%)	4 (7%)	2	24
All	All	3680/4379 (84%)	3056 (83%)	485 (13%)	139 (4%)	5	46

5 of 139 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	D	20	LYS

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Mol	Chain	Res	Type
9	D	93	LEU
9	D	95	THR
9	D	144	ARG
9	D	173	GLU

### 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	
2	1	42/44 (96%)	40 (95%)	2 (5%)	35	81
3	2	79/79 (100%)	75 (95%)	4 (5%)	33	79
4	5	29/122 (24%)	26 (90%)	3 (10%)	10	47
6	A	179/181 (99%)	167 (93%)	12 (7%)	23	70
7	B	282/282 (100%)	268 (95%)	14 (5%)	34	79
8	C	193/193 (100%)	181 (94%)	12 (6%)	26	73
9	D	117/147 (80%)	109 (93%)	8 (7%)	22	70
10	E	152/155 (98%)	147 (97%)	5 (3%)	50	88
11	F	92/92 (100%)	91 (99%)	1 (1%)	84	96
12	G	27/283 (10%)	27 (100%)	0	100	100
13	H	122/122 (100%)	111 (91%)	11 (9%)	14	55
14	I	118/121 (98%)	111 (94%)	7 (6%)	28	75
15	J	106/106 (100%)	102 (96%)	4 (4%)	44	85
16	K	112/126 (89%)	106 (95%)	6 (5%)	31	77
17	L	166/166 (100%)	160 (96%)	6 (4%)	47	87
18	M	149/149 (100%)	142 (95%)	7 (5%)	36	82
19	N	93/93 (100%)	90 (97%)	3 (3%)	51	89
20	O	113/116 (97%)	109 (96%)	4 (4%)	48	88
21	P	79/79 (100%)	74 (94%)	5 (6%)	25	73
22	Q	117/121 (97%)	113 (97%)	4 (3%)	49	88
23	R	73/73 (100%)	72 (99%)	1 (1%)	78	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	S	105/105 (100%)	101 (96%)	4 (4%)	44	85
25	T	44/52 (85%)	41 (93%)	3 (7%)	22	70
26	U	51/56 (91%)	51 (100%)	0	100	100
27	V	130/130 (100%)	124 (95%)	6 (5%)	37	82
28	W	66/73 (90%)	61 (92%)	5 (8%)	19	65
29	X	120/195 (62%)	115 (96%)	5 (4%)	40	84
30	Y	56/56 (100%)	51 (91%)	5 (9%)	14	56
31	Z	46/46 (100%)	46 (100%)	0	100	100
All	All	3058/3563 (86%)	2911 (95%)	147 (5%)	35	81

5 of 147 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	H	86	ARG
15	J	98	VAL
28	W	51	ASP
13	H	126	HIS
14	I	74	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 87 such sidechains are listed below:

Mol	Chain	Res	Type
14	I	107	ASN
17	L	58	GLN
29	X	119	GLN
15	J	10	GLN
16	K	42	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	542 (19%)	360 (13%)
5	9	121/122 (99%)	27 (22%)	14 (11%)
All	All	2866/3044 (94%)	569 (19%)	374 (13%)

5 of 569 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	24	G
1	0	25	A
1	0	31	C
1	0	32	G
1	0	46	U

5 of 374 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1354	G
1	0	1563	G
1	0	2791	U
1	0	1370	G
1	0	1430	G

## 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, 232 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.



## 5.8 Polymer linkage issues

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.