



wwPDB X-ray Structure Validation Summary Report

Sep 15, 2014 – 12:01 PM EDT

PDB ID : 1VXJ
Title : Crystal Structure of tRNA Proline (CGG) Bound to Codon CCC-U on the Ribosome
Authors : Maehigashi, T.; Dunkle, J.A.; Dunham, C.M.
Deposited on : 2013-07-12
Resolution : 2.94 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

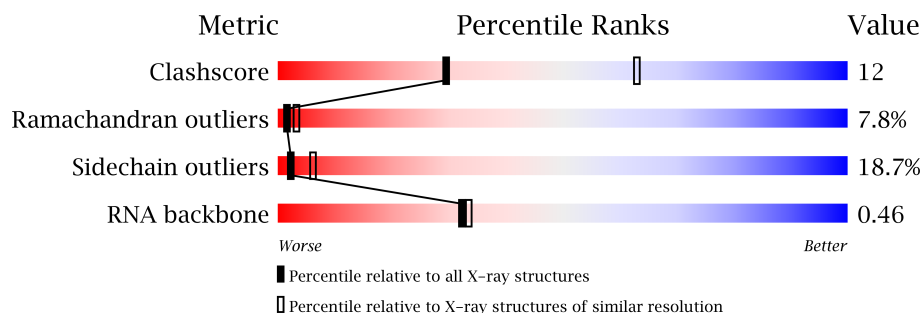
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 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) : stable23489

1 Overall quality at a glance

The reported resolution of this entry is 2.94 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	1761 (2.98-2.90)
Ramachandran outliers	78287	1708 (2.98-2.90)
Sidechain outliers	78261	1710 (2.98-2.90)
RNA backbone	1838	1002 (3.44-2.44)

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. 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	A	2916	
2	B	122	
3	D	276	
4	E	206	
5	F	210	
6	G	182	
7	H	180	
8	I	148	
9	N	140	
10	O	122	
11	P	150	
12	Q	141	
13	R	118	
14	S	112	

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Mol	Chain	Length	Quality of chain
15	T	146	
16	U	118	
17	V	101	
18	W	113	
19	X	96	
20	Y	110	
21	Z	206	
22	0	85	
23	1	98	
24	2	72	
25	3	60	
26	4	71	
27	5	60	
28	6	54	
29	7	49	
30	8	65	
31	9	37	
32	a	3	

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 92288 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	A	2883	Total	C	N	O	P	0	0	0
			62091	27636	11613	19960	2882			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	N	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	O	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	P	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	Q	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	R	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	S	111	Total	C	N	O			
			882	556	176	150	0	0	0

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	T	137	Total	C	N	O	S		
			1141	710	234	196	1	0	0

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	U	117	Total	C	N	O	S		
			964	610	202	151	1	0	0

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	V	101	Total	C	N	O	S		
			779	501	142	135	1	0	0

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	W	113	Total	C	N	O	S		
			900	566	177	155	2	0	0

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	X	92	Total	C	N	O			
			725	471	131	123		0	0

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	Y	102	Total	C	N	O	S		
			785	505	150	125	5	0	0

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	Z	183	Total	C	N	O	S	0	0	0
			1461	933	260	265	3			

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	0	82	Total	C	N	O	S	0	0	0
			648	401	138	108	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	1	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	2	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	3	59	Total	C	N	O	0	0	0
			469	298	90	81			

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	4	71	Total	C	N	O	S	0	0	0
			581	364	108	104	5			

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	6	49	Total	C	N	O	S	0	0	0
			424	264	87	69	4			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 32 is a RNA chain called tRNA acceptor end mimic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	a	3	Total	C	N	O	P	0	0	0
			74	40	13	19	2			

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	P	2	Total	Mg	0	0
			2	2		
33	Q	1	Total	Mg	0	0
			1	1		
33	E	1	Total	Mg	0	0
			1	1		
33	B	3	Total	Mg	0	0
			3	3		
33	A	268	Total	Mg	0	0
			268	268		
33	5	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	X	1	Total	Mg	0	0
			1	1		

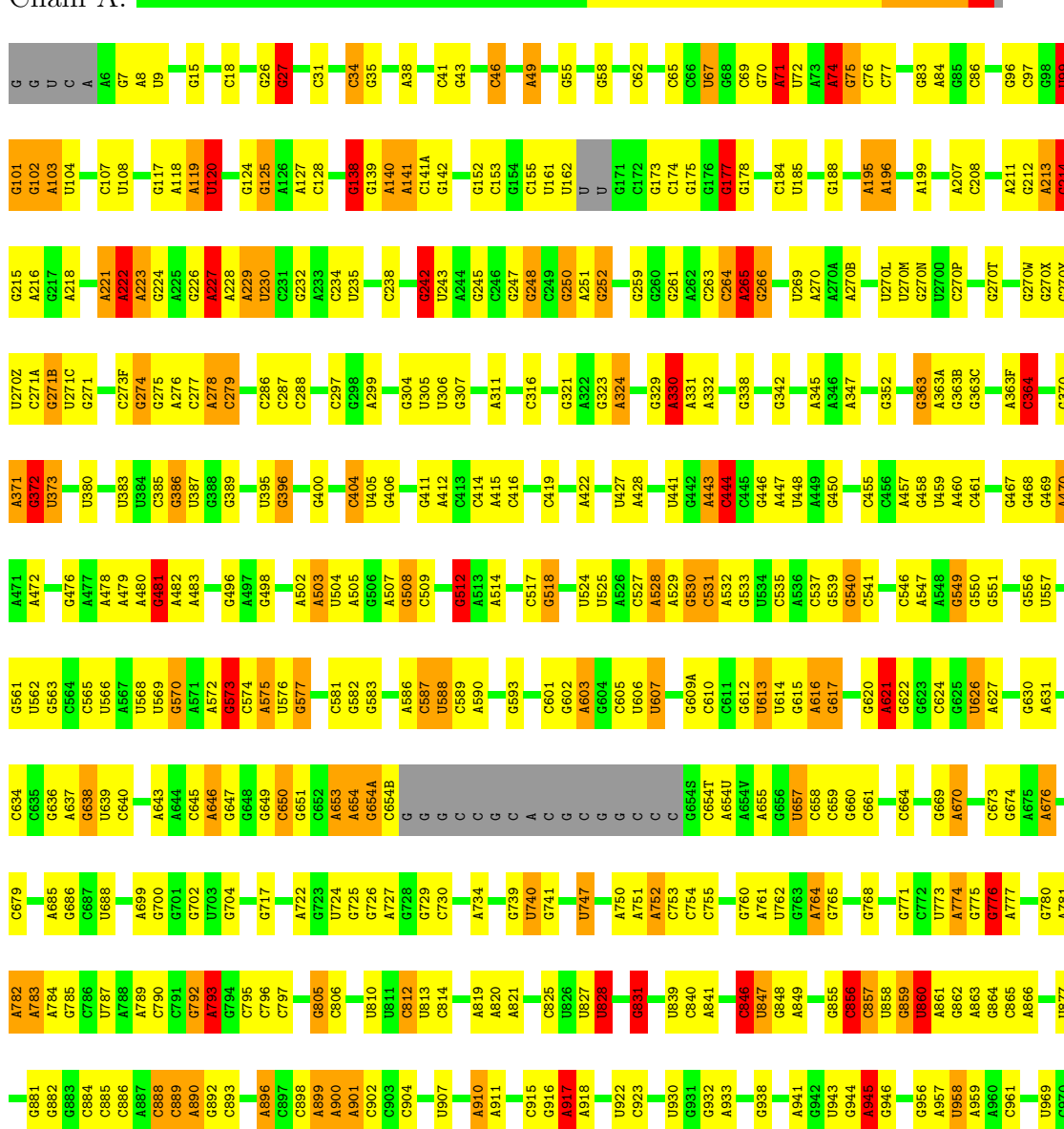
3 Residue-property plots

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 ($RSRZ > 2$). 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.

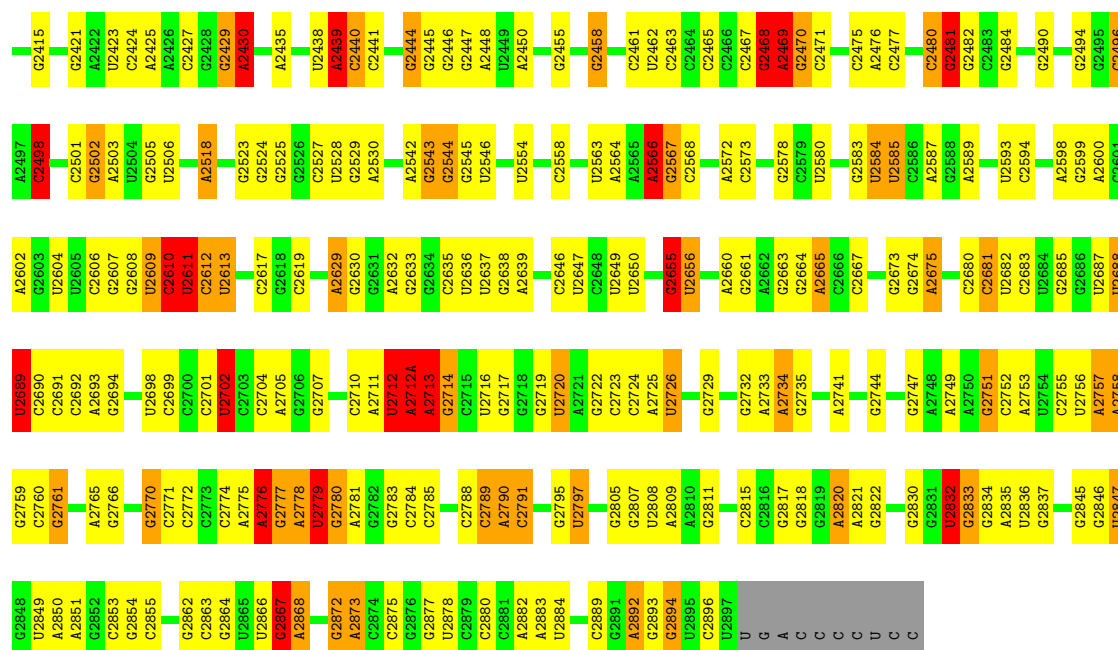
Note EDS was not executed.

• Molecule 1: 23S rRNA

Chain A:

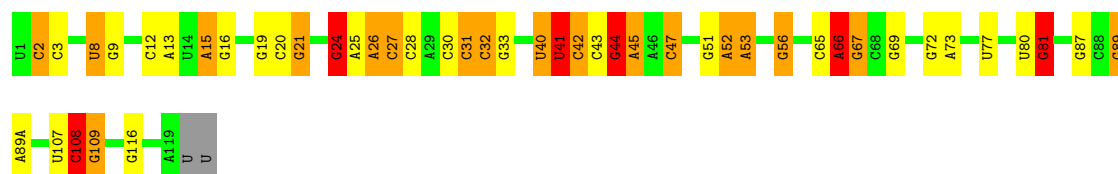


A2328	G2329	G2330	G2331	G2334	G2345	G2346	G2347	G2350	G2351	G2352	G2355	G2356	G2357	A2360	A2361	G2364	G2365	G2366	A2369	G2370	A2377	A2378	G2379	G2382	G2383	G2384	G2385	G2386	G2387	A2388	G2389	G2390	G2391	A2392	A2393	G2394	G2395	U2401	G2402	G2403	G2404	G2405	U2406	G2410	A2411										
U2245	G2246	G2250	G2254	G2257	G2258	U2262	U2265	A2268	G2271	U2272	A2273	A2274	G2276	G2277	G2281	G2282	G2283	G2284	G2285	A2286	A2287	A2288	U2291	G2292	G2293	G2294	A2298	G2299	G2302	G2306	G2307	G2308	G2391	A2392	A2393	G2394	G2395	U2401	G2402	G2403	G2404	G2405	U2406	G2410	A2411										
G2133	A2134	G2135	G2136	G2146	G2147	G2148	G2149	U2150	G2151	G2152	G2157	A2158	G2163	G2164	G2165	G2166	U2167	G2168	A2169	G2170	A2171	U2172	G2173	G2174	G2175	G2176	G2177	G2178	G2190	G2191	G2192	G2193	G2194	U2197	A2198	A2199	G2210	G2211	G2212	A2213	G2215	G2216	A2225	G2233	G2234	G2235	G2236	G2237	U2132						
C2043	C2044	C2045	C2050	A2051	C2055	C2056	A2057	A2058	A2059	A2060	G2061	A2062	C2063	C2064	C2065	C2066	G2067	U2068	G2069	G2070	A2071	U2074	U2075	U2089	U2093	C2097	U2098	U2099	C2100	C2108	U2109	G2110	C2111	C2112	U2113	A2114	G2115	G2116	A2117	U2118	A2119	G2120	G2123	G2124	G2125	A2126	G2127	C2128	G2131	U2132					
G1941	G1947	G1950	U1951	A1952	U1955	A1947	A1948	G1958	A1959	U1963	G1964	G1965	A1966	C1967	C1968	A1969	A1970	A1971	A1972	C1979	G1980	C1982	G1987	G1988	G1989	U1991	G1992	U1993	G1996	U2011	A2014	A2015	A2020	C2021	U2022	U2023	G2024	C2025	G2026	U2028	A2031	G2032	A2033	U2034	A2042										
G1835	G1836	G1839	A1847	A1848	G1858	A1859	G1862	G1863	U1864	G1869	A1871	A1872	G1878	C1879	G1882	G1883	A1884	A1889	G1896	G1898	G1899	C1902	C1905	G1906	C1914	U1915	A1916	U1917	A1918	A1919	C1920	C1924	C1925	G1929	G1930	U1931	A1932	G1933	A1936	A1937	U1938	U1939	U1940												
G1750	G1753	G1754	G1755	G1756	A1759	A1762	G1763	A1764	G1771	G1772	A1773	C1774	G1775	G1776	U1777	U1778	A1779	A1780	C1781	A1784	A1785	A1786	C1790	A1791	G1792	U1794	C1795	G1796	C1797	U1798	G1799	C1800	A1801	A1802	A1803	U1805	G1811	G1816	A1819	U1820	A1821	G1822	G1823	G1824	A1825	G1826	A1829								
C1638	U1639	C1640	G1647	C1648	G1649	A1652	G1653	A1654	A1655	C1656	G1657	A1665	G1666	G1667	A1668	G1674	G1678	G1679	G1684	G1688	A1689	U1693	G1694	G1695	G1696	G1697	A1698	A1699	A1700	A1701	U1709	C1710	G1725	G1728	U1729	A1730	G1731	A1732	G1733	C1734	C1742	G1743	A1744	A1745											
A1545A	C1546	C1547	C1548	C1549	C1550	C1551	A1554	C1557	A1558	G1559	C1565	A1567	G1568	A1569	A1570	A1571	C1577	U1578	A1580	G1581	C1585	A1586	A1587	C1588	U1590	A1591	G1592	G1593	G1594	G1595	C1598	A1603	C1607	A1608	A1609	A1610	A1614	G1615	C1617	A1618	G1622	A1634	A1637												
G1461	C1467	C1468	G1469	G1470	A1471	G1479	A1480	G1482	G1483	G1484	G1485	A1486	G1487	A1490	C1493	A1494	A1495	A1496	A1497	C1498	C1499	G1500	C1505	A1507	A1508	U1510	A1511	G1512	C1513	U1514	G1519	A1528	A1529	G1530	C1531	C1532	C1533	G1534	U1536	A1537	G1538	G1542	A1543	C1544	A1545										
C1386	C1387	G1388	G1389	U1390	U1391	A1392	A1393	U1394	A1395	U1396	U1397	C1398	C1399	G1400	C1403	C1404	U1405	U1406	C1407	C1408	C1411	A1412	G1413	G1416	C1417	G1418	A1419	G1421	G1424	G1425	G1426	A1427	C1428	G1429	C1430	U1431	A1434	A1444A	C1445	G1448	A1449	G1449A	G1455	C1458	G1459	A1460									
U1300	A1301	G1309	G1310	U1313	C1314	C1315	G1316	A1317	C1318	A1319	A1321	A1322	G1328	U1329	C1330	A1331	G1332	U1333	U1334	U1335	G1338	G1339	U1340	A1342	C1345	G1348	A1349	U1352	A1353	A1354	A1359	A1360	G1364	A1365	G1368	G1371	U1372	A1373	G1374	C1375	A1379	A1381	G1382	C1383	G1385										
G1205	G1206	C1207	C1208	U1210	U1211	G1212	A1213	G1216	A1220	C1221	C1222	G1228	G1238	G1239	U1240	A1241	G1242	G1243	G1244	G1245	G1250	A1253	G1256	C1257	U1263	G1264	A1265	G1266	U1267	A1268	A1269	C1270	G1271	A1272	U1273	A1278	G1283	A1284	G1285	A1286	U1287	U1288	C1289	G1290	C1291	U1292	C1293								
A1126	A1127	A1128	U1130	G1131	C1135	G1136	G1137	G1138	G1139	G1140	U1141	U1142	A1148	G1149	C1150	C1153	G1154	A1155	A1156	G1164	U1165	C1166	G1169	G1170	G1171	A1174	U1175	G1176	A1177	C1178	C1179	C1180	G1184	G1187	U1188	A1189	G1190	G1191	G1192	G1193	A1194	G1195	U1198	U1199	G1200	C1201	A1204								
G1055	G1056	A1057	G1058	U1059	U1060	U1061	G1062	G1063	U1066	A1067	G1068	A1069	A1070	G1071	G1076	A1077	U1078	U1079	G1080	U1081	U1082	U1083	A1084	A1085	A1086	G1087	A1088	U1089	U1090	G1093	U1094	A1095	A1096	U1097	A1098	G1099	C1100	U1101	G1102	C1103	A1103	C1104	G1105	G1106	G1107	U1108	G1109	G1110	A1111	G1112	G1113	G1114	G1122	C1123	G1125
C971	C972	A973	G974	C974A	G975	A980	A981	C982	A983	G987	A990	C991	C992	G993	C994	C995	A996	G997	A1000	G1003	C1004	A1005	C1006	C1007	G1011	U1012	C1013	U1019	A1020	A1021	G1022	U1023	G1024	G1025	U1026	A1027	A1028	A1029	A1032	U1033	G1036	A1045	A1046	G1047	A1048	C1049	A1050	A1054							



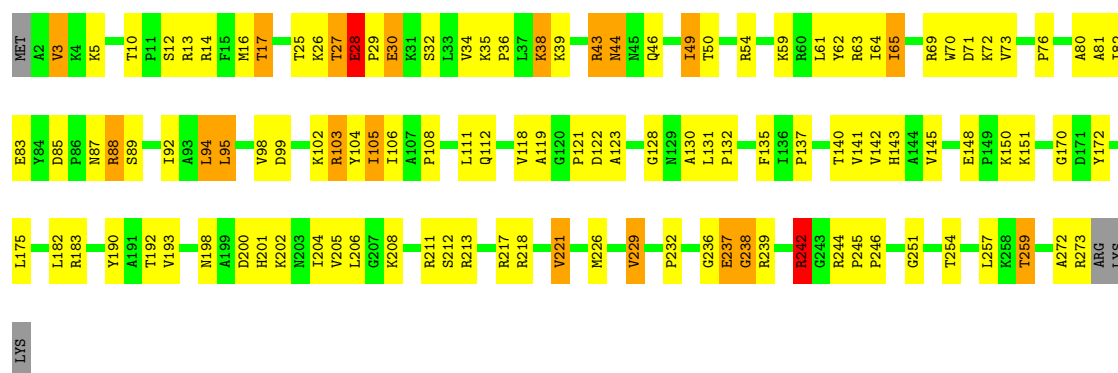
• Molecule 2: 5S rRNA

Chain B:



• Molecule 3: 50S ribosomal protein L2

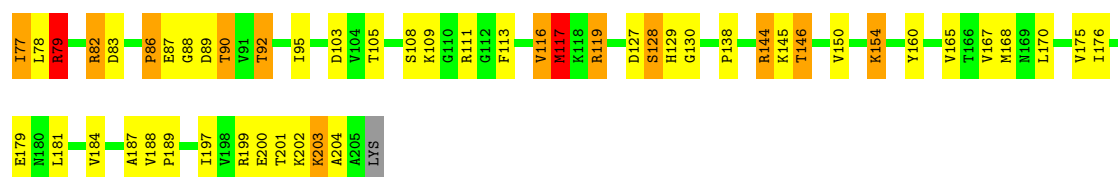
Chain D:



• Molecule 4: 50S ribosomal protein L3

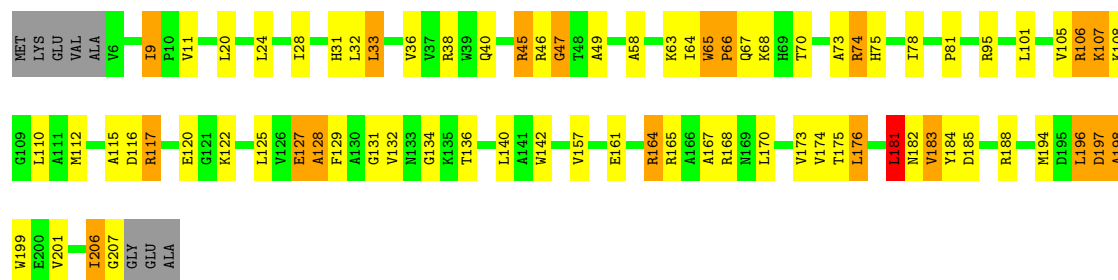
Chain E:





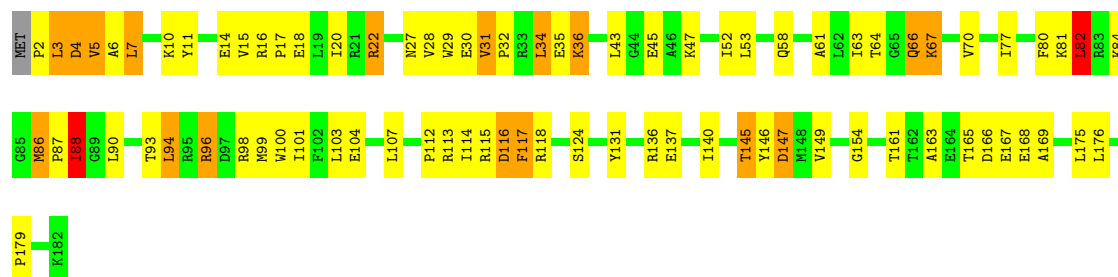
• Molecule 5: 50S ribosomal protein L4

Chain F:



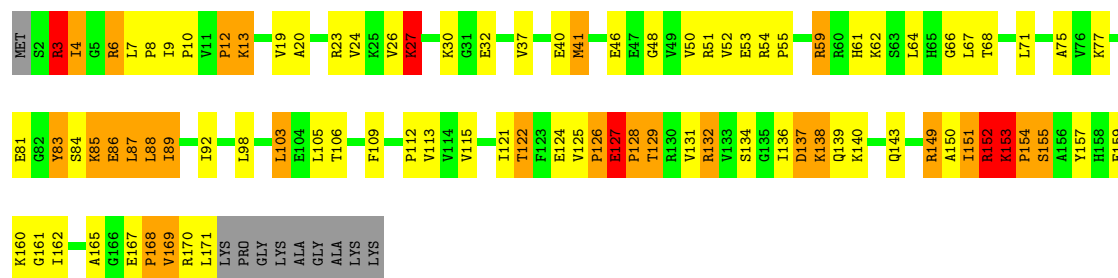
• Molecule 6: 50S ribosomal protein L5

Chain G:



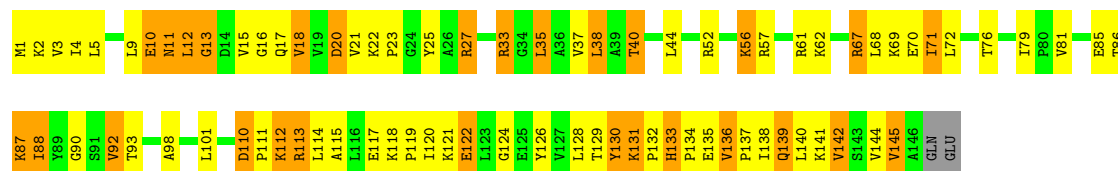
• Molecule 7: 50S ribosomal protein L6

Chain H:



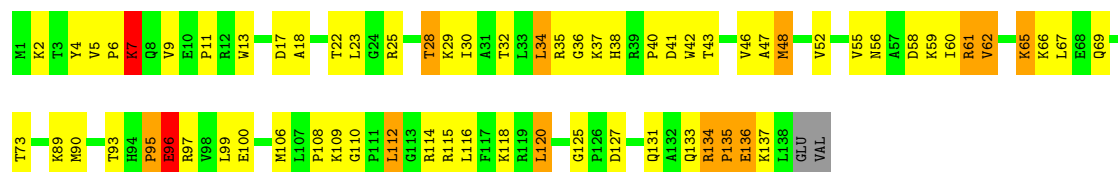
• Molecule 8: 50S ribosomal protein L9

Chain I:



- Molecule 9: 50S ribosomal protein L13

Chain N:



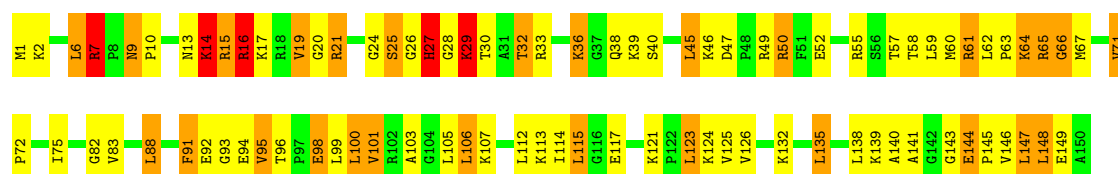
- Molecule 10: 50S ribosomal protein L14

Chain O:



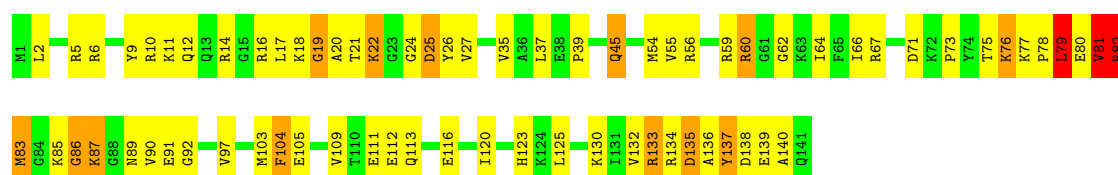
- Molecule 11: 50S ribosomal protein L15

Chain P:



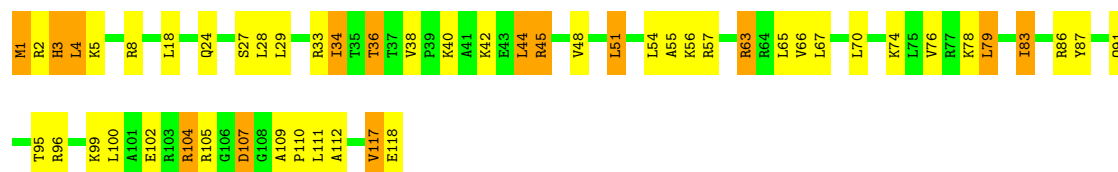
- Molecule 12: 50S ribosomal protein L16

Chain Q:



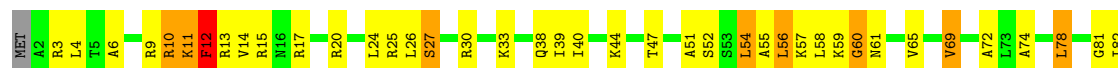
- Molecule 13: 50S ribosomal protein L17

Chain R:



- Molecule 14: 50S ribosomal protein L18

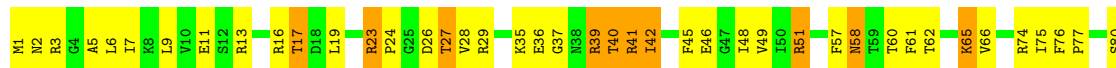
Chain S:





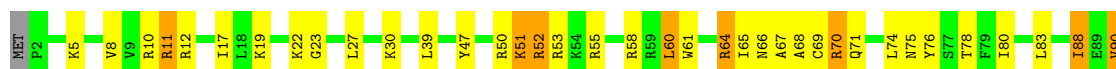
- Molecule 15: 50S ribosomal protein L19

Chain T:



- Molecule 16: 50S ribosomal protein L20

Chain U:



- Molecule 17: 50S ribosomal protein L21

Chain V:



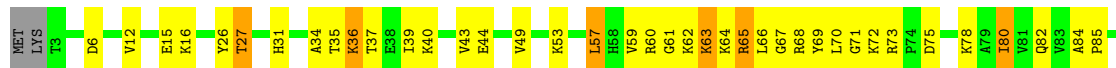
- Molecule 18: 50S ribosomal protein L22

Chain W:



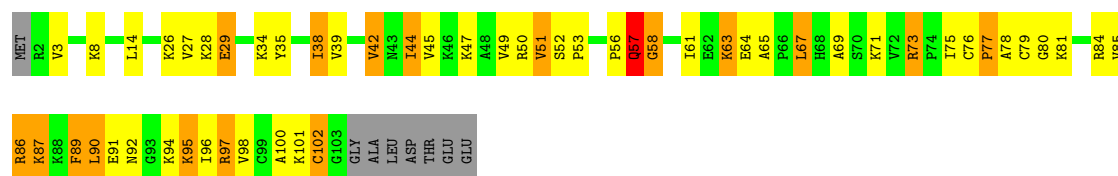
- Molecule 19: 50S ribosomal protein L23

Chain X:



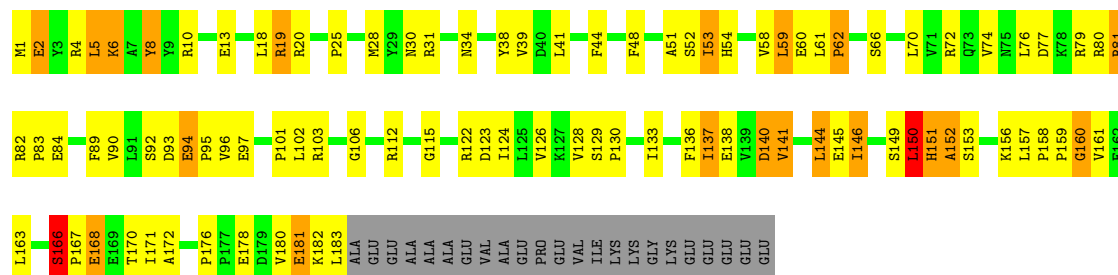
- Molecule 20: 50S ribosomal protein L24

Chain Y: 



- Molecule 21: 50S ribosomal protein L25

Chain Z: 



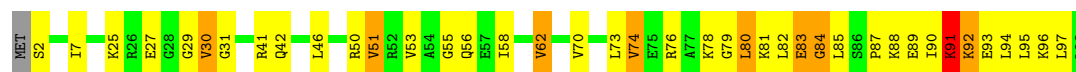
- Molecule 22: 50S ribosomal protein L27

Chain 0: 



- Molecule 23: 50S ribosomal protein L28

Chain 1: 



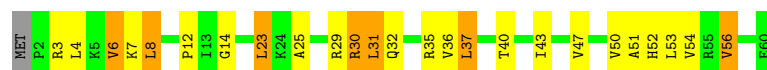
- Molecule 24: 50S ribosomal protein L29

Chain 2: 



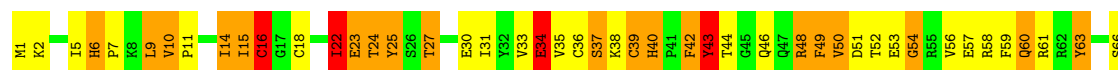
- Molecule 25: 50S ribosomal protein L30

Chain 3: 



- Molecule 26: 50S ribosomal protein L31

Chain 4: 





- Molecule 27: 50S ribosomal protein L32

Chain 5:



- Molecule 28: 50S ribosomal protein L33

Chain 6:



- Molecule 29: 50S ribosomal protein L34

Chain 7:



- Molecule 30: 50S ribosomal protein L35

Chain 8:



- Molecule 31: 50S ribosomal protein L36

Chain 9:



- Molecule 32: tRNA acceptor end mimic

Chain a:



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.81Å 449.41Å 620.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	155.22 – 2.94	Depositor
% Data completeness (in resolution range)	98.6 (155.22-2.94)	Depositor
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PHENIX	Depositor
R, R_{free}	0.219 , 0.265	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	92288	wwPDB-VP
Average B, all atoms (Å ²)	39.0	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, PPU

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	0.72	19/69543 (0.0%)	1.26	504/108563 (0.5%)
2	B	0.56	0/2878	1.15	18/4490 (0.4%)
3	D	0.58	0/2165	0.78	1/2919 (0.0%)
4	E	0.46	0/1601	0.75	2/2160 (0.1%)
5	F	0.48	0/1620	0.71	1/2194 (0.0%)
6	G	0.39	0/1499	0.60	0/2016
7	H	0.45	0/1332	0.73	0/1802
8	I	0.35	0/1151	0.66	0/1558
9	N	0.43	0/1131	0.64	0/1525
10	O	0.49	0/943	0.65	0/1269
11	P	0.49	0/1162	0.90	2/1544 (0.1%)
12	Q	0.57	0/1143	0.80	1/1527 (0.1%)
13	R	0.44	0/982	0.73	0/1312
14	S	0.40	0/892	0.75	1/1187 (0.1%)
15	T	0.44	0/1155	0.67	0/1542
16	U	0.50	0/982	0.68	0/1306
17	V	0.45	0/790	0.73	1/1057 (0.1%)
18	W	0.45	0/911	0.68	0/1220
19	X	0.50	0/739	0.66	0/993
20	Y	0.46	0/798	0.69	0/1064
21	Z	0.37	0/1493	0.64	2/2026 (0.1%)
22	0	0.48	0/657	0.69	0/874
23	1	0.46	0/770	0.69	0/1022
24	2	0.52	0/583	0.73	0/771
25	3	0.41	0/474	0.59	0/635
26	4	0.37	0/594	0.68	0/795
27	5	0.43	0/473	0.77	1/639 (0.2%)
28	6	0.37	0/431	0.67	0/575
29	7	0.57	0/438	0.71	0/575
30	8	0.58	0/525	0.82	0/691
31	9	0.32	0/310	0.48	0/407
32	a	0.78	0/40	1.81	1/60 (1.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.65	19/100205 (0.0%)	1.14	535/150318 (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
4	E	0	1
5	F	0	1
7	H	0	2
14	S	0	1
21	Z	0	1
24	2	0	1
30	8	0	2
All	All	0	9

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	528	A	N9-C4	-9.10	1.32	1.37
1	A	783	A	N9-C4	-7.66	1.33	1.37
1	A	783	A	N3-C4	-7.55	1.30	1.34
1	A	676	A	N9-C4	-7.13	1.33	1.37
1	A	1786	A	N3-C4	-6.80	1.30	1.34

The worst 5 of 535 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1786	A	N7-C8-N9	13.21	120.41	113.80
1	A	528	A	C2-N3-C4	-13.10	104.05	110.60
1	A	783	A	C2-N3-C4	-12.39	104.41	110.60
1	A	1786	A	C5-N7-C8	-12.26	97.77	103.90
1	A	1786	A	C2-N3-C4	-11.73	104.73	110.60

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	E	21	VAL	Peptide
5	F	47	GLY	Peptide

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Mol	Chain	Res	Type	Group
7	H	127	GLU	Peptide
7	H	153	LYS	Peptide
14	S	109	GLY	Peptide

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	A	62091	0	31295	865	0
2	B	2573	0	1306	32	0
3	D	2115	0	2195	97	0
4	E	1568	0	1634	64	0
5	F	1585	0	1632	64	0
6	G	1474	0	1535	57	0
7	H	1307	0	1382	66	0
8	I	1136	0	1223	46	0
9	N	1104	0	1180	50	0
10	O	933	0	996	23	0
11	P	1145	0	1227	94	0
12	Q	1122	0	1178	48	0
13	R	968	0	1033	36	0
14	S	882	0	943	40	0
15	T	1141	0	1202	47	0
16	U	964	0	1022	58	0
17	V	779	0	852	42	0
18	W	900	0	964	28	0
19	X	725	0	778	25	0
20	Y	785	0	878	39	0
21	Z	1461	0	1493	56	0
22	0	648	0	672	27	0
23	1	763	0	848	28	0
24	2	581	0	629	26	0
25	3	469	0	518	17	0
26	4	581	0	574	41	0
27	5	459	0	480	33	0
28	6	424	0	450	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	7	430	0	480	17	0
30	8	517	0	582	40	0
31	9	307	0	338	7	0
32	a	74	0	51	0	0
33	5	1	0	0	0	0
33	A	268	0	0	0	0
33	B	3	0	0	0	0
33	E	1	0	0	0	0
33	P	2	0	0	0	0
33	Q	1	0	0	0	0
33	X	1	0	0	0	0
All	All	92288	0	61570	1851	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 12.

The worst 5 of 1851 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2701:C:H3'	1:A:2702:U:H5''	1.32	1.07
3:D:43:ARG:NH1	3:D:44:ASN:OD1	1.86	1.06
1:A:1359:A:N6	1:A:1372:U:O4	1.92	1.02
1:A:1771:C:HO2'	1:A:1786:A:H8	1.01	0.98
1:A:1496:A:H8	1:A:1577:C:HO2'	1.10	0.97

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	D	270/276 (98%)	227 (84%)	34 (13%)	9 (3%)	6	23
4	E	203/206 (98%)	142 (70%)	41 (20%)	20 (10%)	1	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	F	200/210 (95%)	167 (84%)	25 (12%)	8 (4%)	5	16
6	G	179/182 (98%)	142 (79%)	25 (14%)	12 (7%)	2	4
7	H	168/180 (93%)	121 (72%)	23 (14%)	24 (14%)	0	1
8	I	144/148 (97%)	104 (72%)	23 (16%)	17 (12%)	1	1
9	N	136/140 (97%)	106 (78%)	16 (12%)	14 (10%)	1	2
10	O	120/122 (98%)	108 (90%)	10 (8%)	2 (2%)	14	45
11	P	148/150 (99%)	108 (73%)	23 (16%)	17 (12%)	1	1
12	Q	139/141 (99%)	98 (70%)	22 (16%)	19 (14%)	0	1
13	R	116/118 (98%)	99 (85%)	11 (10%)	6 (5%)	3	9
14	S	109/112 (97%)	78 (72%)	18 (16%)	13 (12%)	1	1
15	T	135/146 (92%)	108 (80%)	17 (13%)	10 (7%)	2	4
16	U	115/118 (98%)	101 (88%)	10 (9%)	4 (4%)	6	21
17	V	99/101 (98%)	79 (80%)	12 (12%)	8 (8%)	1	3
18	W	111/113 (98%)	100 (90%)	9 (8%)	2 (2%)	13	43
19	X	90/96 (94%)	82 (91%)	6 (7%)	2 (2%)	10	37
20	Y	100/110 (91%)	70 (70%)	18 (18%)	12 (12%)	1	1
21	Z	181/206 (88%)	124 (68%)	40 (22%)	17 (9%)	1	2
22	0	80/85 (94%)	73 (91%)	7 (9%)	0	100	100
23	1	95/98 (97%)	72 (76%)	17 (18%)	6 (6%)	2	5
24	2	67/72 (93%)	55 (82%)	6 (9%)	6 (9%)	1	2
25	3	57/60 (95%)	52 (91%)	4 (7%)	1 (2%)	13	43
26	4	69/71 (97%)	35 (51%)	15 (22%)	19 (28%)	0	0
27	5	57/60 (95%)	46 (81%)	9 (16%)	2 (4%)	6	21
28	6	47/54 (87%)	22 (47%)	17 (36%)	8 (17%)	0	0
29	7	47/49 (96%)	43 (92%)	3 (6%)	1 (2%)	11	39
30	8	62/65 (95%)	48 (77%)	10 (16%)	4 (6%)	2	5
31	9	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
All	All	3379/3526 (96%)	2641 (78%)	475 (14%)	263 (8%)	1	3

5 of 263 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	26	LYS

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Mol	Chain	Res	Type
3	D	28	GLU
3	D	122	ASP
3	D	123	ALA
4	E	2	LYS

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	D	214/218 (98%)	181 (85%)	33 (15%)	4	11
4	E	165/166 (99%)	137 (83%)	28 (17%)	3	8
5	F	161/166 (97%)	137 (85%)	24 (15%)	4	12
6	G	155/156 (99%)	133 (86%)	22 (14%)	5	13
7	H	142/148 (96%)	115 (81%)	27 (19%)	2	6
8	I	122/124 (98%)	92 (75%)	30 (25%)	1	2
9	N	117/119 (98%)	96 (82%)	21 (18%)	2	7
10	O	100/100 (100%)	89 (89%)	11 (11%)	9	26
11	P	116/116 (100%)	82 (71%)	34 (29%)	0	1
12	Q	111/111 (100%)	92 (83%)	19 (17%)	3	8
13	R	101/101 (100%)	80 (79%)	21 (21%)	2	4
14	S	87/88 (99%)	68 (78%)	19 (22%)	1	4
15	T	120/127 (94%)	98 (82%)	22 (18%)	2	6
16	U	93/94 (99%)	77 (83%)	16 (17%)	3	8
17	V	82/82 (100%)	67 (82%)	15 (18%)	2	6
18	W	92/92 (100%)	76 (83%)	16 (17%)	3	8
19	X	74/78 (95%)	60 (81%)	14 (19%)	2	6
20	Y	85/91 (93%)	64 (75%)	21 (25%)	1	2
21	Z	162/179 (90%)	130 (80%)	32 (20%)	2	5
22	0	65/67 (97%)	59 (91%)	6 (9%)	13	37
23	1	82/83 (99%)	70 (85%)	12 (15%)	5	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	2	64/67 (96%)	47 (73%)	17 (27%)	1	2
25	3	51/52 (98%)	43 (84%)	8 (16%)	4	10
26	4	63/63 (100%)	43 (68%)	20 (32%)	0	1
27	5	51/52 (98%)	37 (72%)	14 (28%)	0	1
28	6	48/52 (92%)	38 (79%)	10 (21%)	2	4
29	7	42/42 (100%)	35 (83%)	7 (17%)	3	8
30	8	54/55 (98%)	41 (76%)	13 (24%)	1	2
31	9	34/34 (100%)	32 (94%)	2 (6%)	28	63
All	All	2853/2923 (98%)	2319 (81%)	534 (19%)	2	6

5 of 534 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	Q	82	ARG
15	T	65	LYS
27	5	36	CYS
12	Q	139	GLU
14	S	12	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
15	T	58	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2880/2916 (98%)	623 (21%)	75 (2%)
2	B	119/122 (97%)	29 (24%)	3 (2%)
32	a	1/3 (33%)	0	0
All	All	3000/3041 (98%)	652 (21%)	78 (2%)

5 of 652 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	U
1	A	15	G

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Mol	Chain	Res	Type
1	A	27	G
1	A	34	C
1	A	35	G

5 of 78 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1109	C
1	A	1558	A
1	A	2776	A
1	A	1130	U
1	A	1204	A

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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
32	PPU	a	76	1,32	38,40,41	2.42	9 (23%)	54,57,60	2.61	14 (25%)

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
32	PPU	a	76	1,32	-	0/26/43/44	0/4/4/4

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	a	76	PPU	O-C	9.19	1.41	1.23
32	a	76	PPU	C9-N6	-5.44	1.32	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	a	76	PPU	C-N3'	5.37	1.46	1.34
32	a	76	PPU	C10-N6	-5.11	1.32	1.45
32	a	76	PPU	C4-N9	-3.15	1.33	1.37

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	a	76	PPU	N3-C2-N1	-8.55	121.37	128.89
32	a	76	PPU	C3'-N3'-C	-8.15	110.22	123.19
32	a	76	PPU	C5-C4-N3	-6.29	119.85	125.98
32	a	76	PPU	C2'-C1'-N9	-5.46	98.49	113.35
32	a	76	PPU	C2'-C3'-N3'	5.17	125.08	113.08

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 277 ligands modelled in this entry, 277 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.