



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2020 – 11:19 am BST

PDB ID : 5DM6  
Title : Crystal structure of the 50S ribosomal subunit from *Deinococcus radiodurans*  
Authors : Kaminishi, T.; Schedlbauer, A.; Ochoa-Lizarralde, B.; Connell, S.R.; Fucini, P.  
Deposited on : 2015-09-08  
Resolution : 2.90 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

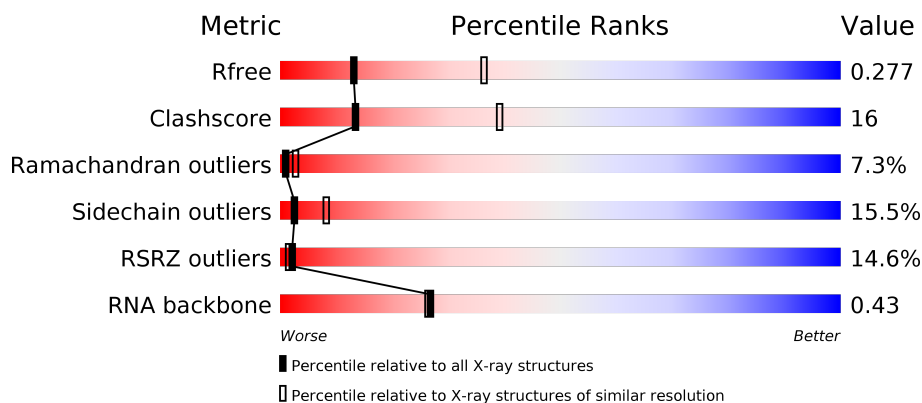
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
$R_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)
RNA backbone	3102	1007 (3.16-2.64)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	0	224	<div> <div>89%</div> <div> <div>54%</div> <div>38%</div> <div>8%</div> </div> </div>
2	A	274	<div> <div>11%</div> <div>58%</div> <div>37%</div> <div>5%</div> </div>
3	B	205	<div> <div>3%</div> <div>53%</div> <div>40%</div> <div>7%</div> </div>
4	C	197	<div> <div>8%</div> <div>44%</div> <div>46%</div> <div>10%</div> </div>

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Mol	Chain	Length	Quality of chain
5	D	177	
6	E	171	
7	F	144	
8	G	142	
9	H	134	
10	I	141	
11	J	136	
12	K	113	
13	L	104	
14	M	109	
15	N	117	
16	O	94	
17	P	127	
18	Q	93	
19	R	110	
20	S	175	
21	T	84	
22	U	72	
23	V	66	
24	W	55	
25	Z	57	
26	1	54	
27	2	47	
28	3	65	
29	X	2881	

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Mol	Chain	Length	Quality of chain
30	Y	122	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	MG	X	6014	-	-	-	X
31	MG	X	6038	-	-	-	X
31	MG	X	6046	-	-	-	X
31	MG	X	6048	-	-	-	X
31	MG	X	6058	-	-	-	X
31	MG	X	6093	-	-	-	X
31	MG	X	6098	-	-	-	X
31	MG	X	6099	-	-	-	X
31	MG	X	6107	-	-	-	X
31	MG	X	6108	-	-	-	X
31	MG	X	6111	-	-	-	X
31	MG	X	6113	-	-	-	X
31	MG	X	6119	-	-	-	X
31	MG	X	6121	-	-	-	X
31	MG	X	6133	-	-	-	X
31	MG	X	6138	-	-	-	X
31	MG	X	6141	-	-	-	X
31	MG	X	6146	-	-	-	X
31	MG	X	6156	-	-	-	X
31	MG	X	6159	-	-	-	X
31	MG	X	6162	-	-	-	X
31	MG	X	6167	-	-	-	X
31	MG	X	6170	-	-	-	X
31	MG	X	6175	-	-	-	X
31	MG	X	6177	-	-	-	X
31	MG	X	6179	-	-	-	X
31	MG	X	6180	-	-	-	X
31	MG	X	6183	-	-	-	X
31	MG	X	6186	-	-	-	X
31	MG	X	6187	-	-	-	X
31	MG	X	6191	-	-	-	X
31	MG	X	6192	-	-	-	X

## 2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 89337 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 protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	224	Total	C	N	O	S	0	0	0
			1651	1031	302	313	5			

- Molecule 2 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	274	Total	C	N	O	S	0	0	0
			2107	1313	423	368	3			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	LYS	ARG	conflict	UNP Q9RXJ9
A	25	ALA	THR	conflict	UNP Q9RXJ9
A	270	LEU	ILE	conflict	UNP Q9RXJ9

- Molecule 3 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	205	Total	C	N	O	S	0	0	0
			1540	965	295	272	8			

- Molecule 4 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	197	Total	C	N	O	S	0	0	0
			1507	935	287	283	2			

- Molecule 5 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	177	Total	C	N	O	S	0	0	0
			1401	892	247	255	7			

- Molecule 6 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	E	171	Total	C	N	O	S	0	0	0
			1287	812	237	237	1			

- Molecule 7 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	F	144	Total	C	N	O	S	0	0	0
			1048	663	183	197	5			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	1	MET	-	expression tag	UNP Q9RSS7
F	2	ARG	-	expression tag	UNP Q9RSS7
F	3	ARG	-	expression tag	UNP Q9RSS7

- 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
			1115	704	209	199	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	141	Total	C	N	O		0	0	0
			1068	655	216	197				

- 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
			1091	696	202	186	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
			879	541	178	158	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
			778	476	159	143			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	26	LYS	ARG	conflict	UNP Q9RSL2

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	M	109	Total	C	N	O	0	0	0
			867	540	171	156			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	107	GLY	-	expression tag	UNP Q9RWB4
M	108	LYS	-	expression tag	UNP Q9RWB4
M	109	ALA	-	expression tag	UNP Q9RWB4
M	110	ALA	-	expression tag	UNP Q9RWB4

- 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
			742	465	139	138			

- 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
			727	458	136	131	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
			826	513	160	152	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	S	175	Total	C	N	O	S	0	0	0
			1346	849	236	255	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	T	84	Total	C	N	O	S	0	0	0
			626	393	122	110	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	0	0	0
			553	341	116	96			

There is a discrepancy between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
U	67	ILE	LEU	conflict	UNP Q9RRG8

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	V	66	Total	C	N	O	S	0	0	0
			534	327	107	97	3			

- 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
			453	278	93	77	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	1	54	Total	C	N	O	S	0	0	0
			404	256	73	74	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	2	47	Total	C	N	O	S	0	0	0
			393	235	92	64	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	3	65	Total	C	N	O	S	0	0	0
			509	320	104	80	5			

- Molecule 29 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	X	2780	Total	C	N	O	P	0	0	0
			59673	26617	11011	19265	2780			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	1510	U	UNK	conflict	GB 11612676

- Molecule 30 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	Y	122	Total	C	N	O	P	0	0	0
			2601	1161	476	842	122			

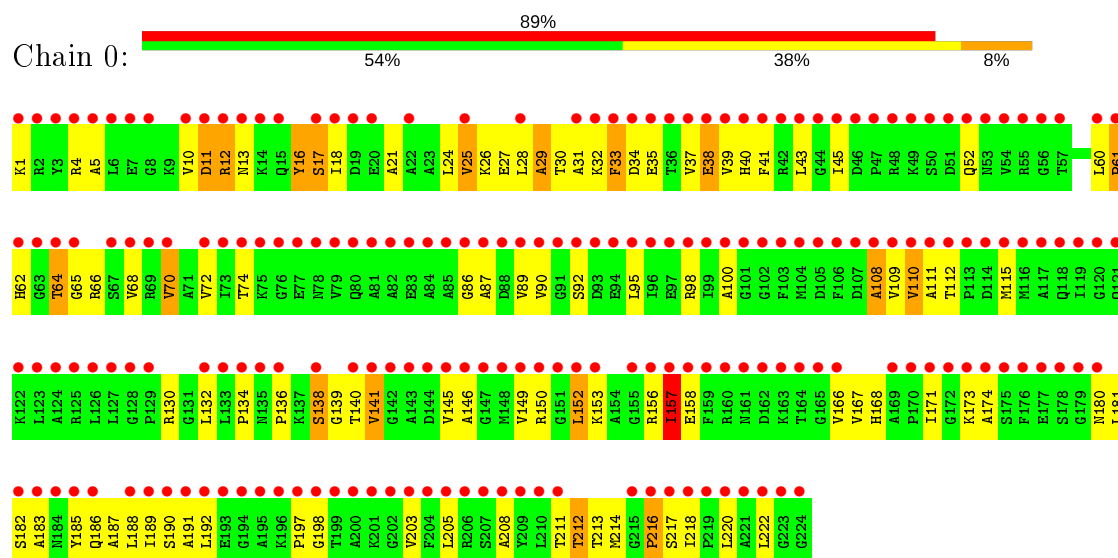
- Molecule 31 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
31	X	192	Total	Mg	0	0
			192	192		
31	Y	5	Total	Mg	0	0
			5	5		
31	M	1	Total	Mg	0	0
			1	1		

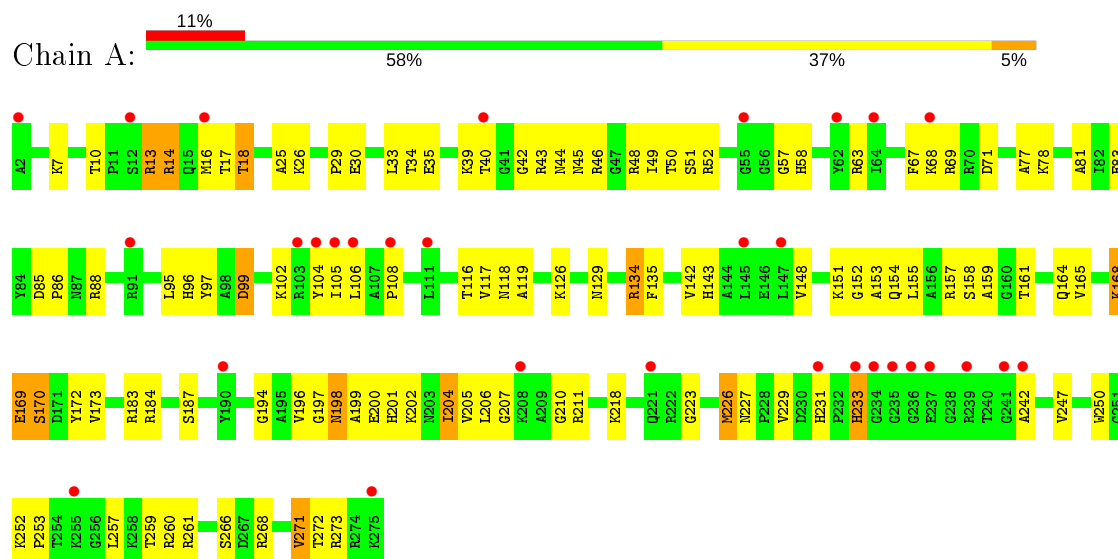
### 3 Residue-property plots [i](#)

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

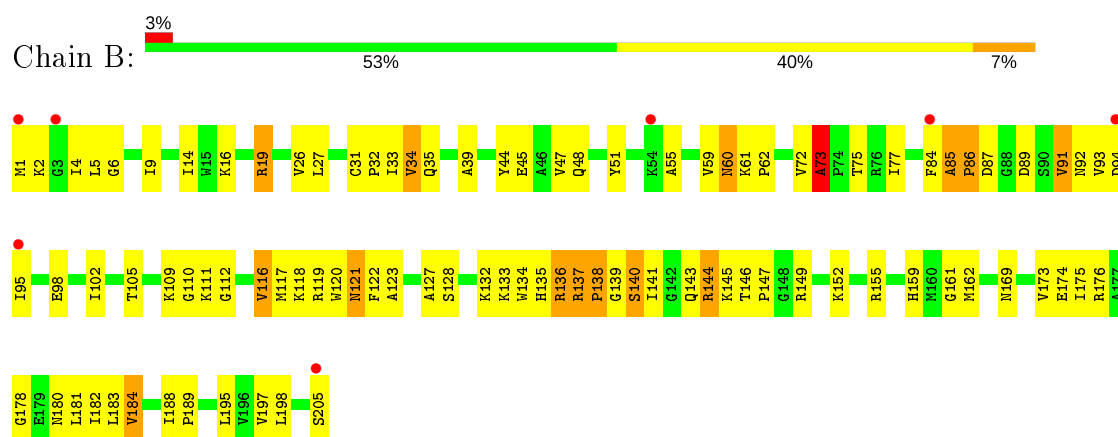
#### • Molecule 1: 50S ribosomal protein L1



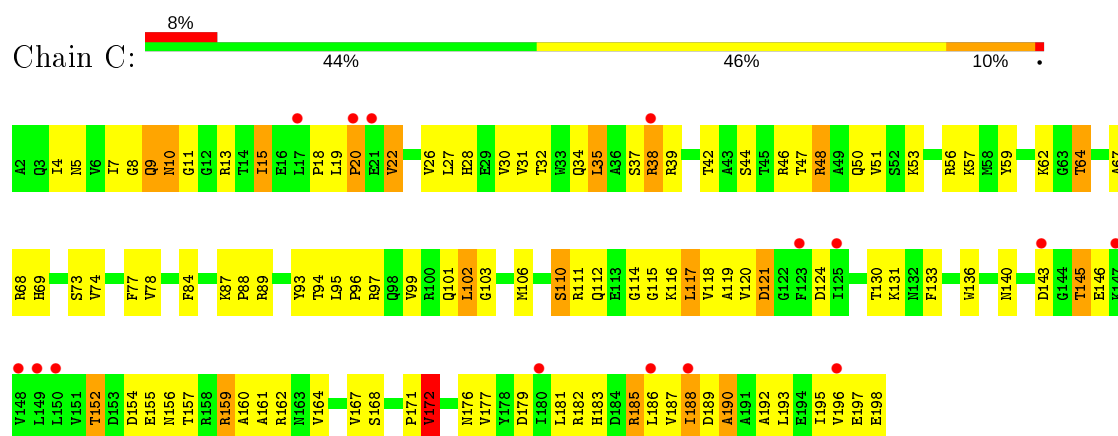
#### • Molecule 2: 50S ribosomal protein L2



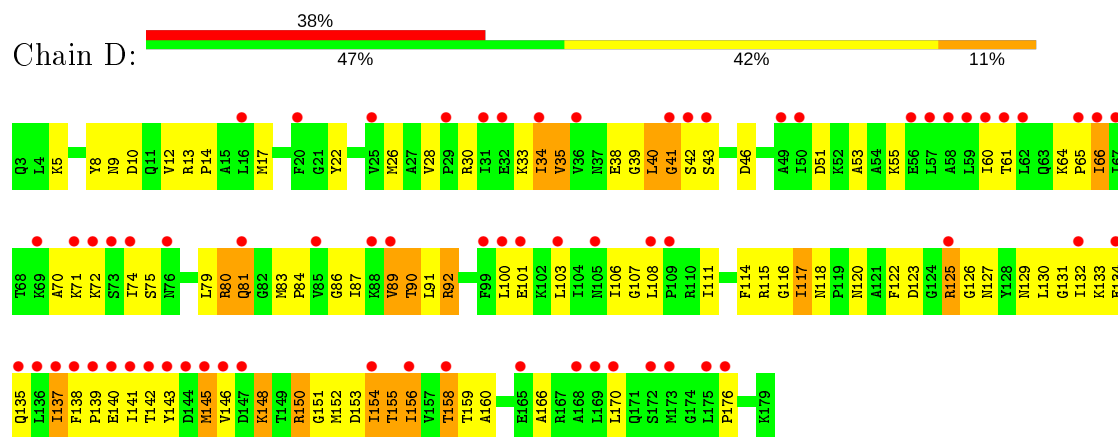
#### • Molecule 3: 50S ribosomal protein L3



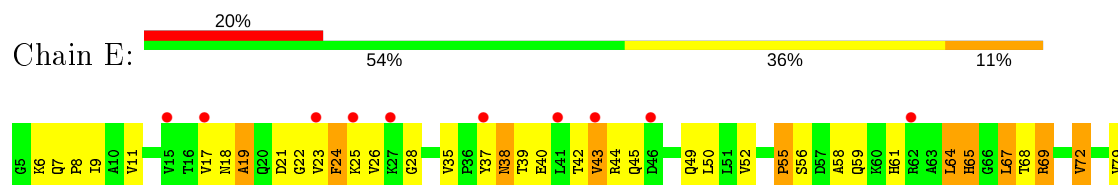
- Molecule 4: 50S ribosomal protein L4

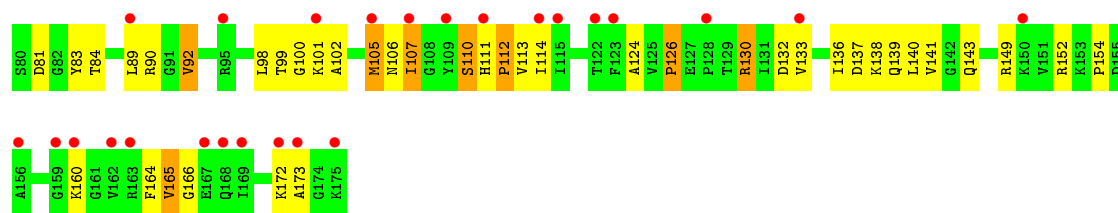


- Molecule 5: 50S ribosomal protein L5

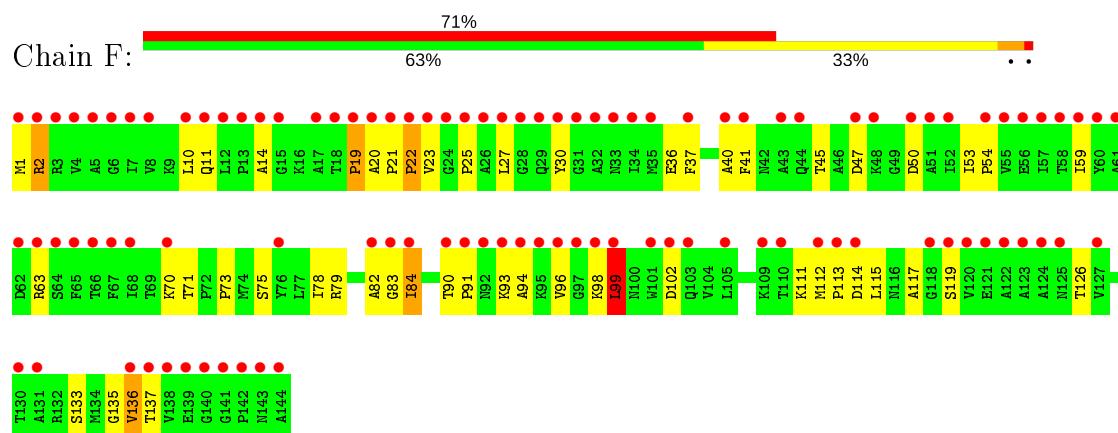


- Molecule 6: 50S ribosomal protein L6

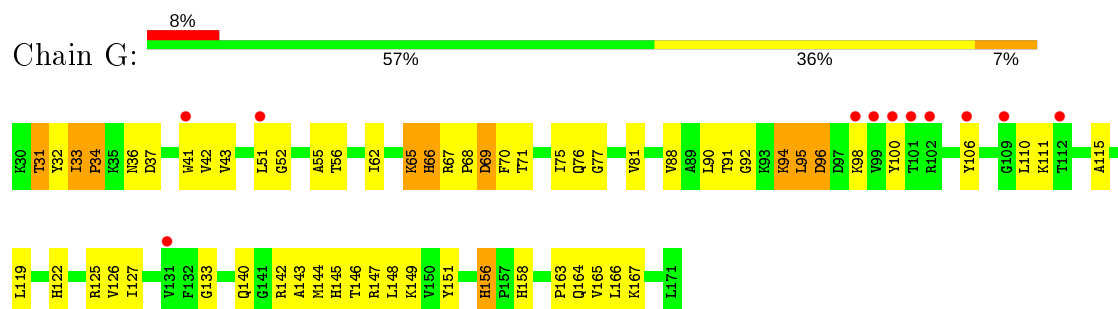




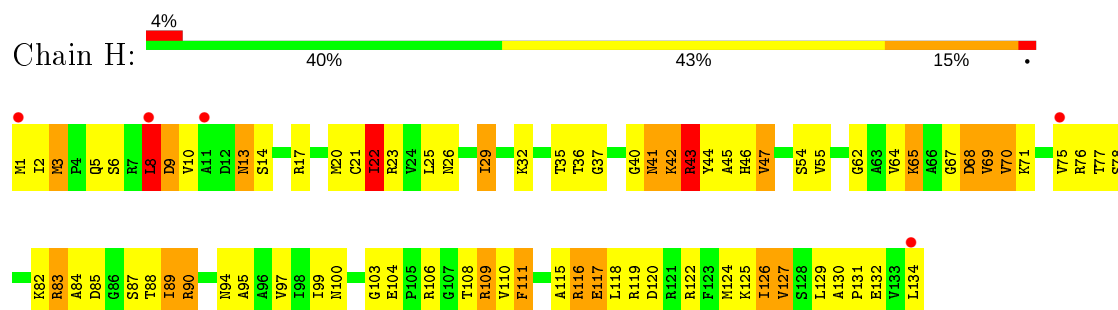
• Molecule 7: 50S ribosomal protein L11



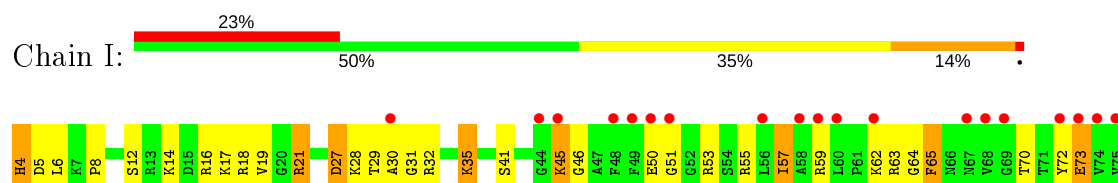
• Molecule 8: 50S ribosomal protein L13

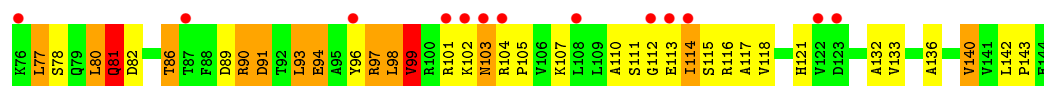


• Molecule 9: 50S ribosomal protein L14

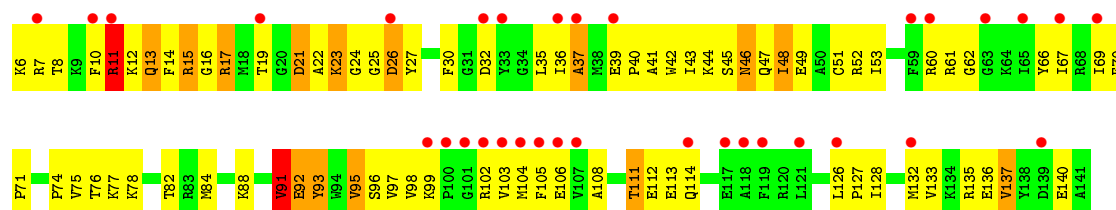


• Molecule 10: 50S ribosomal protein L15

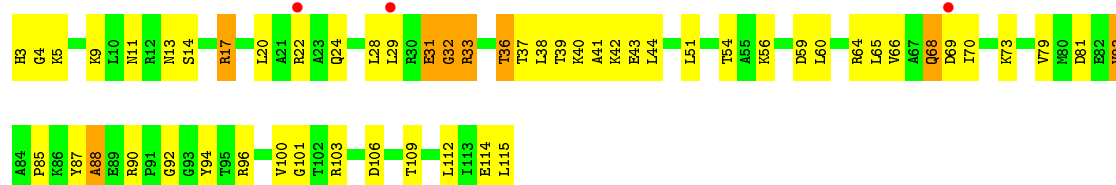




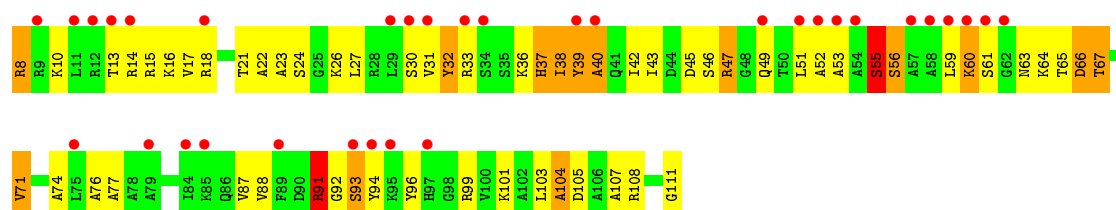
- Molecule 11: 50S ribosomal protein L16



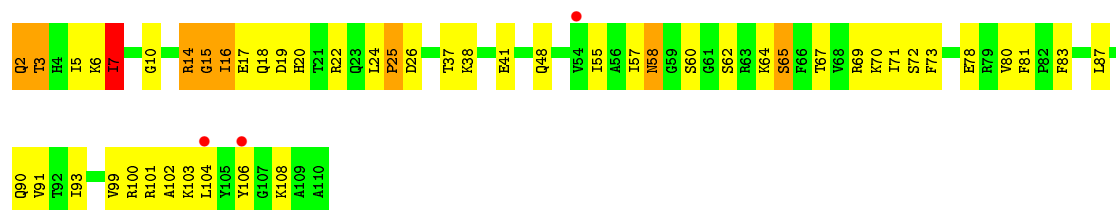
- Molecule 12: 50S ribosomal protein L17



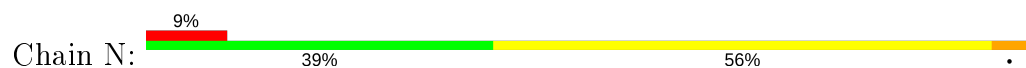
- Molecule 13: 50S ribosomal protein L18

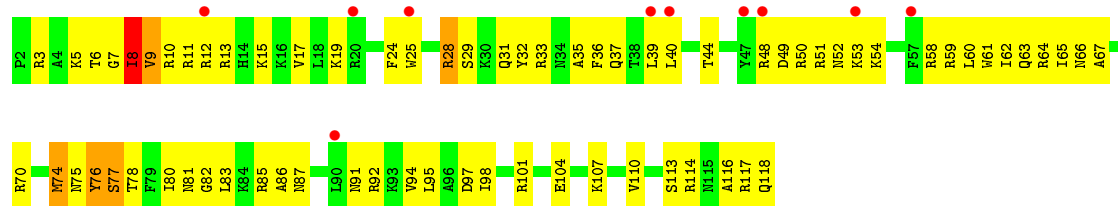


- Molecule 14: 50S ribosomal protein L19

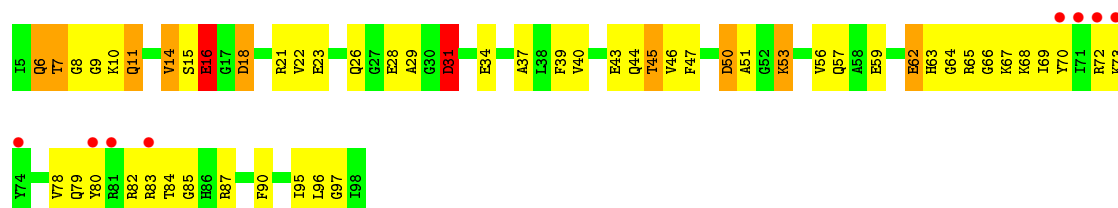


- Molecule 15: 50S ribosomal protein L20

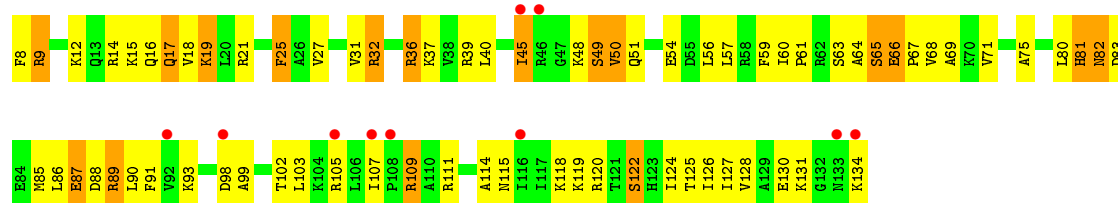
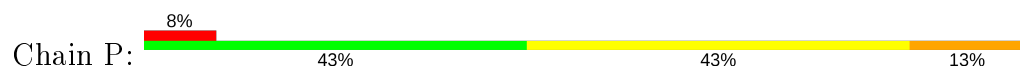




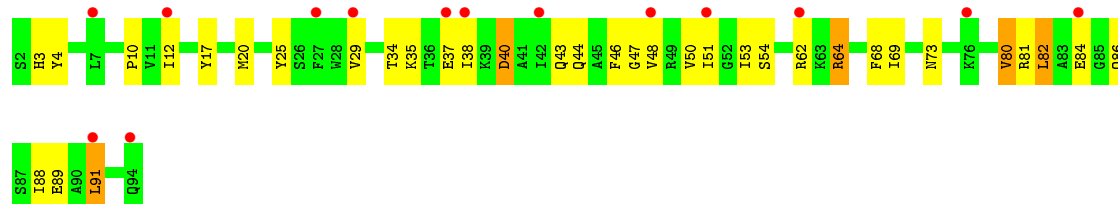
• Molecule 16: 50S ribosomal protein L21



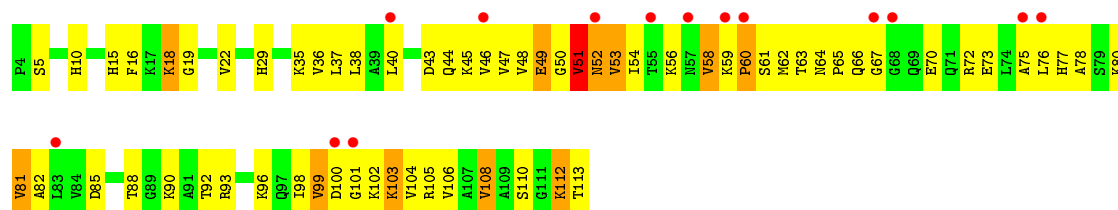
• Molecule 17: 50S ribosomal protein L22



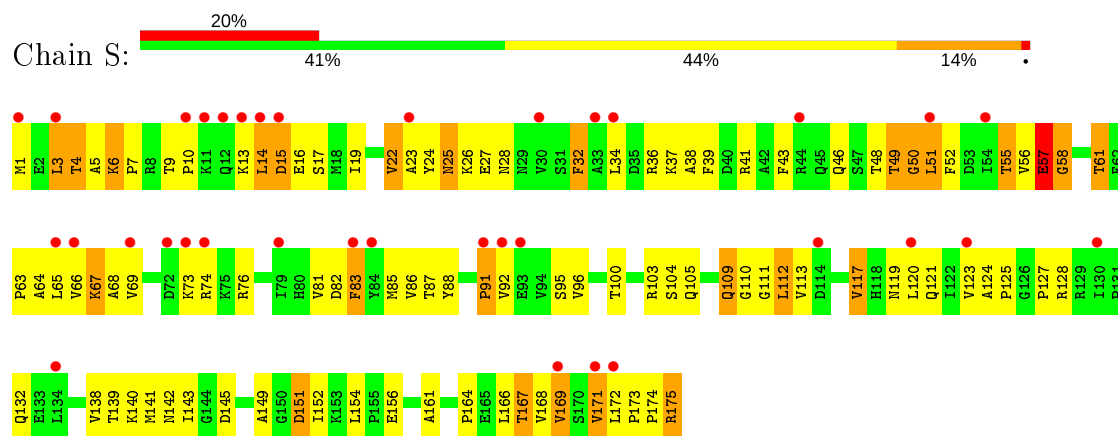
• Molecule 18: 50S ribosomal protein L23



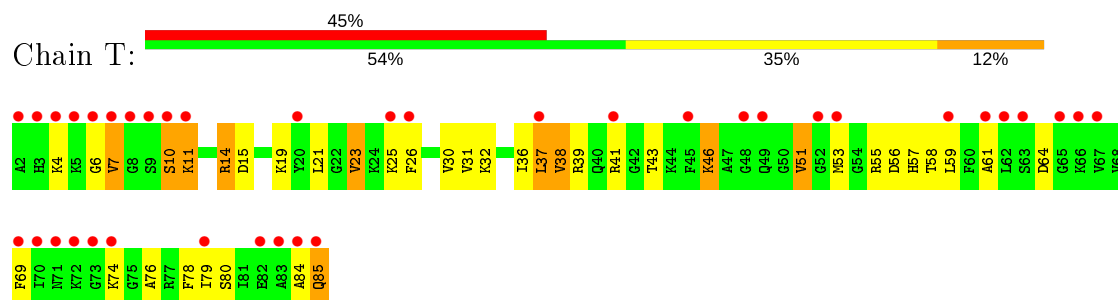
• Molecule 19: 50S ribosomal protein L24



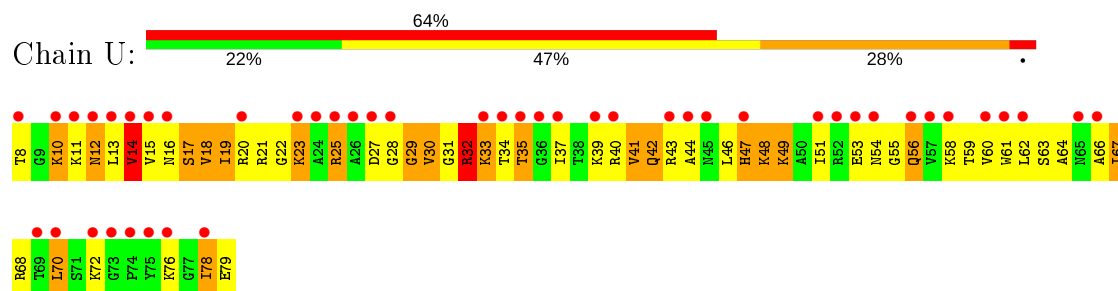
- Molecule 20: 50S ribosomal protein L25



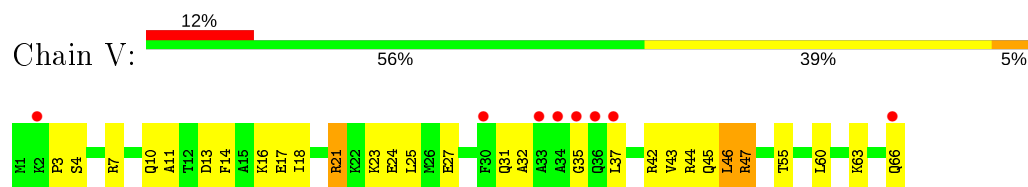
- Molecule 21: 50S ribosomal protein L27



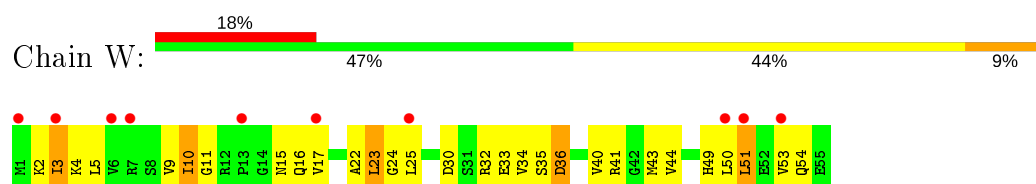
- Molecule 22: 50S ribosomal protein L28



- Molecule 23: 50S ribosomal protein L29



- Molecule 24: 50S ribosomal protein L30

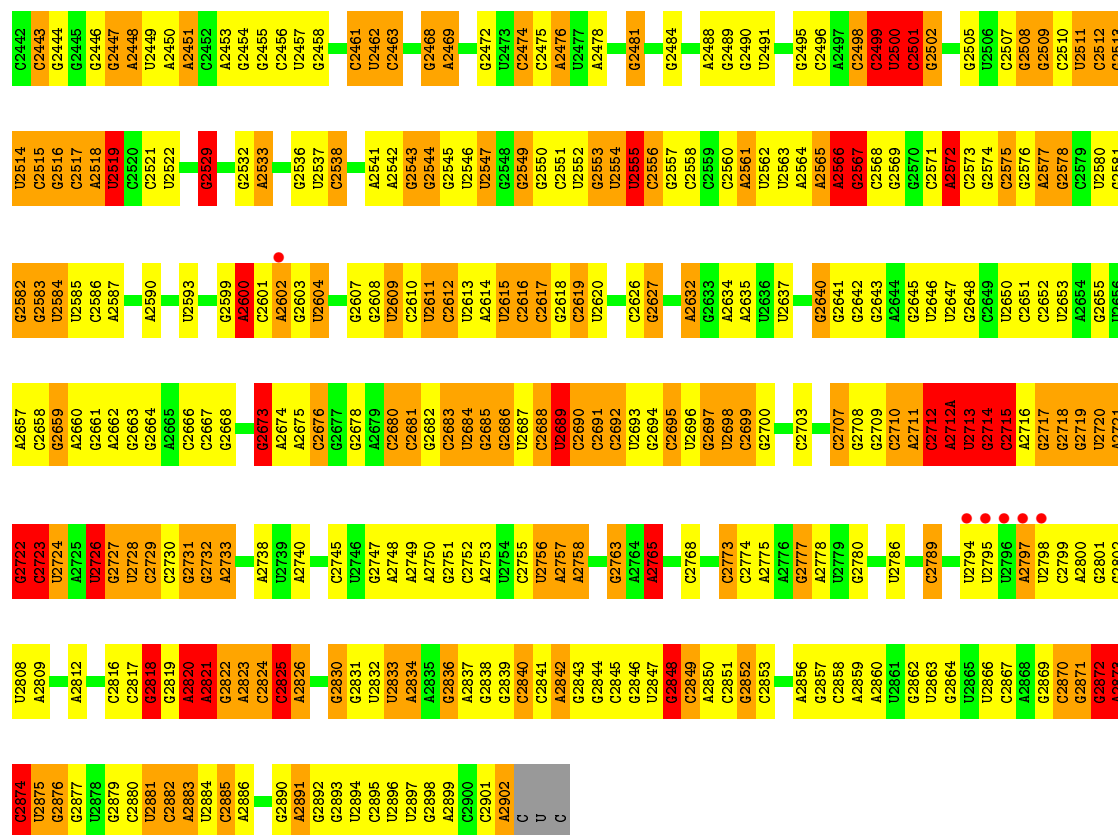




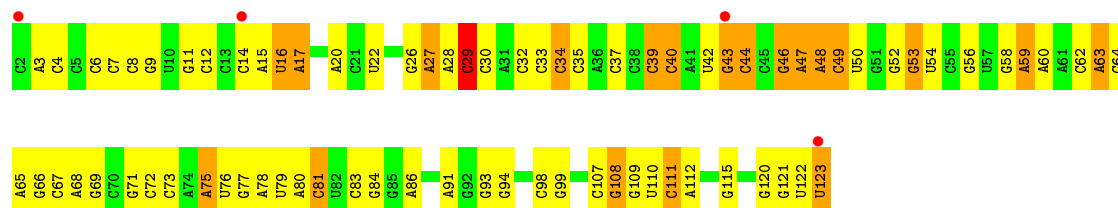


WORLDWIDE  
**PDB**  
PROTEIN DATA BANK

A2378	U2312	G2168	G2027	C1957	G1881	C1800	G1730	C1638	G1557	U1466	C1372
C2379	C2313	A2169	U2028	C1958	C1882	C1801	A1731	U1639	G1558	U1467	A1373
U2380	G2314	A2170	A2029	U1963	G1883	A1801	C1734	A1640	A1558	G1468	A1378
G2381	U2315	A2171	A2030	U1966	A1884	A1805	U1735	G1642	C1559	G1474	U1379
G2382	C2316	U2172	G2031	A1966	A1886	A1808	U1736	G1643	G1565	U1474	G1380
G2383	G2317	G2173	G2032	C1967	U1887	A1810	C1737	C1644	A1566	A1377	A1384
G2384	G2318	C2174	G2033	U1968	G1892	G1810	U1738	C1645	A1567	G1478	A1390
C2385	U2319	C2175	G2034	A1969	G1892	G1811	C1739	C1646	U1568	G1479	U1391
U2386	A2320	C2176	C2035	G1969	G1892	G1812	U1740	C1647	A1569	G1480	G1392
U2387	G2321	C2177	C2036	A1970	A1900	G1813	U1741	C1648	A1570	C1481	C1391
U2388	A2322	C2178	G2038	A1971	A1901	G1814	G1745	G1649	A1571	G1482	A1392
G2389	G2323	U2179	A2042	G1972	A1902	A1815	C1746	A1650	A1578	A1483	A1393
U2390	C2324	U2180	G2043	G1973	G1903	C1816	G1747	G1651	U1578	U1484	G1394
G2391	G2325	G2181	C2044	C1974	G1903	A1817	C1748	A1652	G1485	C1486	A1395
A2392	C2326	A2182	C2045	A1977	G1904	U1818	U1749	A1653	G1583	G1487	C1405
A2393	U2327	C2183	C2046	U1978	C1905	U1819	A1750	A1654	U1584	G1488	G1406
C2394	G2328	U2184	G2047	A1979	G1906	A1820	U1751	A1655	U1585	U1489	
A2395	A2329	A2185	U2048	G1980	G1907	A1821	G1752	C1656	A1586	C1490	U1412
G2396	G2330	C2187	G2049	U1981	C1908	G1822	U1753	C1657	U1587	U1491	G1413
	G2331	U2188	G2050	G1985	G1909	G1823	C1759	C1658	A1588	A1492	G1414
G2400	U2332	U2189	C2051	U1986	U1910	G1824	U1760	U1659	A1589	A1493	A1415
U2401	A2333	G2190	A2052	U1986	U1911	U1825	C1761	C1660	A1591	U1494	
A2402	G2334	G2191	G2053	G1990	A1912	G1826	U1762	C1661	U1592	U1495	G1416
C2403	C2335	A2192	G2054	U1981	A1913	U1827	U1763	U1662	U1593	U1496	U1417
C2404	A2336	U2194	A2055	G1982	G1914	G1828	G1764	U1663	A1594		G1418
G2405		U2195	C2056	U1983	U1915	A1829	C1765	A1664	C1598	U1497	
U2406	U2339	C2196	G2057	U1983	U1916	C1832	U1766	A1665	C1599	A1500	G1422
U2407	G2340	U2197	A2058	U1986	A1918	C1833	U1767	C1666	U1599	A1499	A1423
G2408	G2341	A2198	U2059	U1986	A1919	U1834	U1768	C1667	U1602	C1501	G1424
U2409	C2342	U2203	A2060	G1987	G1920	U1835	U1769	A1668	C1502	C1502	A1427
G2410	U2343	G2192	G2061	U1988	G1921	G1835	C1770	A1669	G1606	C1428	C1429
U2411	U2344	A2204	A2062	A1998	G1922	G1838	U1771	C1673	C1607	U1504	C1430
A2412	G2345	A2205	C2063	G2000	U1926	G1839	C1772	U1674	A1608	U1505	
G2413	A2346	A2210	G2064	A2001	A1927	G1840	U1773	C1675	A1609	G1506	G1435
G2414	C2347	A2211	C2065	G2002	A1928	U1841	U1774	A1676	A1610	A1507	G1436
G2415	U2348	A2212	G2066	G2003	G1929	G1842	U1775	A1677	C1611	C1508	
C2416	G2349	U2213	G2067	G2004	U1930	C1843	U1776	U1678	C1612	A1509	C1437
G2417	C2350	U2214	G2068	A2005	U1931	G1844	U1777	C1679	G1613	U1510	
A2418	G2351	U2217	G2069	C2006	U1931	A1848	U1779	C1684	A1614	C1512	U1440
U2419	A2352	U2218	C2141	U2007	A1936	G1849	A1780	C1685	A1615	G1525	U1444
G2420		U2219	C2142	C2008	A1937	G1850	C1781	C1686	A1616	G1526	G1445
G2421	C2355	C2220	U2143	G2009	A1938	U1851	C1782	U1687	U1621	G1529	
A2422	U2356	G2221	U2144	C2010	U1939	C1852	U1783	U1688	G1622	U1532	G1450
U2423	G2357	G2222	U2145	G2011	U1940	A1853	A1784	C1689	G1625A	C1533	U1452
C2424	A2358	G2223	U2146	U2012	C1941	A1854	C1785	A1697	A1626	U1534	A1453
A2425	C2359	G2224	G2147	A2013	U1942	A1854	A1786	C1694	G1627	U1535	U1454
A2426	A2360	A2225	G2148	A2014	U1943	G1858	C1787	C1695	U1628	C1536	G1455
C2427	G2361	U2229	G2149	A2015	U1944	G1858	U1788	G1696	U1629	U1537	U1458
G2428	U2362	G2230	U2151	U2016	U1945	G1862	C1789	A1698	A1700	A1538	A1459
G2429	C2363	C2152	C2153	U2017	G1945	G1863	A1791	A1699	A1701	U1630	U1460
A2430	G2364	G2154	G2154	A2018	G1949	U1864	C1790	A1699	U1704	U1634	G1461
A2431	C2365	G2155	G2155	A2019	U1949	U1864	C1791	A1699	A1704	U1634	
A2432	U2366	G2156	G2156	A2020	G1950	U1864	C1791	A1699	A1704	U1634	
A2433	G2367	G2157	G2157	A2021	U1951	C1875	A1791	A1699	A1704	U1634	
A2434	U2368	G2158	G2158	U2022	U1952	C1875	A1791	A1699	A1704	U1634	
		G2159	G2159	U2023	A1953	C1875	A1791	A1699	A1704	U1634	
U2438	G2369	G2238	G2159	U2024	U1954	C1875	A1791	A1699	A1704	U1634	
A2439	A2370	G2239	G2159	U2025	U1955	C1875	A1791	A1699	A1704	U1634	
C2440	U2371	G2240	G2159	U2026	U1956	C1875	A1791	A1699	A1704	U1634	
C2441	A2372	G2241	G2159	U2027	U1956	C1875	A1791	A1699	A1704	U1634	



● Molecule 30: 5S ribosomal RNA



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	169.90Å 410.76Å 696.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.96 – 2.90 58.96 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (58.96-2.90) 81.6 (58.96-2.90)	Depositor EDS
$R_{merge}$	0.24	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.61 (at 2.91Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.235 , 0.270 0.243 , 0.277	Depositor DCC
$R_{free}$ test set	24732 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	76.9	Xtriage
Anisotropy	0.500	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.22 , 65.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	89337	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.28% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

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	0.30	0/1674	0.49	0/2257
2	A	0.39	0/2149	0.59	0/2890
3	B	0.69	1/1568 (0.1%)	0.86	1/2105 (0.0%)
4	C	0.51	0/1530	0.73	1/2070 (0.0%)
5	D	0.36	0/1420	0.56	0/1903
6	E	0.39	0/1309	0.55	0/1771
7	F	0.33	0/1067	0.52	1/1446 (0.1%)
8	G	0.47	0/1139	0.67	0/1539
9	H	0.76	0/1007	0.91	2/1352 (0.1%)
10	I	0.52	0/1082	0.76	1/1448 (0.1%)
11	J	0.65	0/1114	0.78	0/1486
12	K	0.83	0/887	1.04	0/1188
13	L	0.52	0/784	0.73	0/1045
14	M	0.77	0/880	0.83	0/1179
15	N	0.64	0/994	0.80	1/1323 (0.1%)
16	O	0.53	0/751	0.73	0/1000
17	P	0.69	0/1027	0.83	0/1373
18	Q	0.45	0/738	0.59	0/988
19	R	0.54	0/836	0.72	0/1121
20	S	0.41	0/1371	0.67	0/1862
21	T	0.54	0/634	0.69	0/838
22	U	0.61	0/557	0.88	1/741 (0.1%)
23	V	0.41	0/538	0.57	0/714
24	W	0.51	0/426	0.68	0/568
25	Z	0.71	0/465	0.90	0/622
26	1	0.49	0/411	0.73	0/554
27	2	0.48	0/397	0.65	0/521
28	3	0.54	0/516	0.70	0/673
29	X	0.78	37/66826 (0.1%)	1.44	971/104247 (0.9%)
30	Y	0.64	0/2907	1.20	8/4529 (0.2%)
All	All	0.72	38/97004 (0.0%)	1.29	987/145353 (0.7%)

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	B	0	3
4	C	0	1
8	G	0	1
25	Z	0	2
All	All	0	7

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	X	761	A	C6-N1	8.06	1.41	1.35
29	X	1999	C	N3-C4	-7.01	1.29	1.33
29	X	1638	C	N1-C6	-6.80	1.33	1.37
29	X	1661	G	C6-N1	-6.69	1.34	1.39
29	X	1661	G	C5-C4	-6.50	1.33	1.38

The worst 5 of 987 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	761	A	N1-C6-N6	22.08	131.85	118.60
29	X	761	A	C5-N7-C8	-17.56	95.12	103.90
29	X	2713	U	O5'-P-OP2	-17.29	89.95	110.70
29	X	761	A	C4-C5-N7	16.33	118.87	110.70
29	X	761	A	C5-C6-N6	-14.62	112.00	123.70

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	178	GLY	Peptide
3	B	73	ALA	Peptide
3	B	85	ALA	Peptide
4	C	187	VAL	Peptide
8	G	37	ASP	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	0	1651	0	1693	59	0
2	A	2107	0	2190	82	0
3	B	1540	0	1600	75	0
4	C	1507	0	1525	80	0
5	D	1401	0	1481	64	0
6	E	1287	0	1336	49	0
7	F	1048	0	1088	23	0
8	G	1115	0	1144	47	0
9	H	997	0	1046	67	0
10	I	1068	0	1103	60	0
11	J	1091	0	1125	64	0
12	K	879	0	930	43	0
13	L	778	0	820	38	0
14	M	867	0	890	43	0
15	N	978	0	1020	72	0
16	O	742	0	756	37	0
17	P	1014	0	1096	60	0
18	Q	727	0	753	25	0
19	R	826	0	881	54	0
20	S	1346	0	1372	65	0
21	T	626	0	655	33	0
22	U	553	0	604	59	0
23	V	534	0	558	16	0
24	W	424	0	470	20	0
25	Z	453	0	455	38	0
26	1	404	0	416	21	0
27	2	393	0	420	19	0
28	3	509	0	565	40	0
29	X	59673	0	30060	1282	0
30	Y	2601	0	1327	57	0
31	M	1	0	0	0	0
31	X	192	0	0	0	0
31	Y	5	0	0	0	0
All	All	89337	0	59379	2369	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 16.



The worst 5 of 2369 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)
12:K:103:ARG:HD2	29:X:1287:A:H5'	1.33	1.04
9:H:41:ASN:ND2	29:X:2674:A:O2'	1.91	1.04
15:N:48:ARG:HD2	29:X:1156:A:H61	1.20	1.03
8:G:31:THR:HG21	15:N:61:TRP:HE1	1.26	1.00
29:X:500:G:H22	29:X:503:A:H5''	1.26	0.97

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	
1	0	222/224 (99%)	135 (61%)	65 (29%)	22 (10%)	0	1
2	A	272/274 (99%)	238 (88%)	25 (9%)	9 (3%)	4	15
3	B	203/205 (99%)	168 (83%)	24 (12%)	11 (5%)	2	6
4	C	195/197 (99%)	151 (77%)	30 (15%)	14 (7%)	1	3
5	D	175/177 (99%)	124 (71%)	39 (22%)	12 (7%)	1	3
6	E	169/171 (99%)	130 (77%)	22 (13%)	17 (10%)	0	1
7	F	142/144 (99%)	99 (70%)	34 (24%)	9 (6%)	1	4
8	G	140/142 (99%)	121 (86%)	13 (9%)	6 (4%)	2	10
9	H	132/134 (98%)	103 (78%)	19 (14%)	10 (8%)	1	2
10	I	139/141 (99%)	104 (75%)	23 (16%)	12 (9%)	1	2
11	J	134/136 (98%)	102 (76%)	20 (15%)	12 (9%)	1	1
12	K	111/113 (98%)	95 (86%)	11 (10%)	5 (4%)	2	9
13	L	102/104 (98%)	65 (64%)	21 (21%)	16 (16%)	0	0
14	M	107/109 (98%)	93 (87%)	7 (6%)	7 (6%)	1	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	N	115/117 (98%)	104 (90%)	8 (7%)	3 (3%)	5	20
16	O	92/94 (98%)	75 (82%)	11 (12%)	6 (6%)	1	3
17	P	125/127 (98%)	99 (79%)	16 (13%)	10 (8%)	1	2
18	Q	91/93 (98%)	87 (96%)	4 (4%)	0	100	100
19	R	108/110 (98%)	84 (78%)	14 (13%)	10 (9%)	0	1
20	S	173/175 (99%)	123 (71%)	32 (18%)	18 (10%)	0	1
21	T	82/84 (98%)	68 (83%)	11 (13%)	3 (4%)	3	13
22	U	70/72 (97%)	38 (54%)	16 (23%)	16 (23%)	0	0
23	V	64/66 (97%)	55 (86%)	5 (8%)	4 (6%)	1	4
24	W	53/55 (96%)	48 (91%)	3 (6%)	2 (4%)	3	13
25	Z	55/57 (96%)	41 (74%)	11 (20%)	3 (6%)	2	5
26	1	52/54 (96%)	33 (64%)	13 (25%)	6 (12%)	0	1
27	2	45/47 (96%)	40 (89%)	3 (7%)	2 (4%)	2	10
28	3	63/65 (97%)	47 (75%)	12 (19%)	4 (6%)	1	4
All	All	3431/3487 (98%)	2670 (78%)	512 (15%)	249 (7%)	1	3

5 of 249 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	28	LEU
1	0	30	THR
1	0	45	ILE
1	0	157	ILE
1	0	216	PRO

### 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	
1	0	167/167 (100%)	150 (90%)	17 (10%)	7	22
2	A	214/214 (100%)	190 (89%)	24 (11%)	6	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	B	155/155 (100%)	139 (90%)	16 (10%)	7	22
4	C	157/157 (100%)	137 (87%)	20 (13%)	4	13
5	D	153/153 (100%)	131 (86%)	22 (14%)	3	9
6	E	136/136 (100%)	114 (84%)	22 (16%)	2	7
7	F	107/107 (100%)	97 (91%)	10 (9%)	9	27
8	G	118/118 (100%)	108 (92%)	10 (8%)	10	31
9	H	103/103 (100%)	76 (74%)	27 (26%)	0	1
10	I	108/108 (100%)	85 (79%)	23 (21%)	1	3
11	J	110/110 (100%)	89 (81%)	21 (19%)	1	4
12	K	90/90 (100%)	78 (87%)	12 (13%)	4	11
13	L	74/74 (100%)	52 (70%)	22 (30%)	0	1
14	M	92/92 (100%)	79 (86%)	13 (14%)	3	10
15	N	96/96 (100%)	86 (90%)	10 (10%)	7	21
16	O	75/75 (100%)	57 (76%)	18 (24%)	0	2
17	P	109/109 (100%)	92 (84%)	17 (16%)	2	8
18	Q	75/75 (100%)	69 (92%)	6 (8%)	12	33
19	R	91/91 (100%)	76 (84%)	15 (16%)	2	7
20	S	149/149 (100%)	117 (78%)	32 (22%)	1	3
21	T	62/62 (100%)	48 (77%)	14 (23%)	1	2
22	U	57/57 (100%)	42 (74%)	15 (26%)	0	1
23	V	54/54 (100%)	48 (89%)	6 (11%)	6	19
24	W	48/48 (100%)	43 (90%)	5 (10%)	7	21
25	Z	51/51 (100%)	43 (84%)	8 (16%)	2	8
26	1	38/38 (100%)	30 (79%)	8 (21%)	1	3
27	2	40/40 (100%)	33 (82%)	7 (18%)	2	6
28	3	51/51 (100%)	40 (78%)	11 (22%)	1	3
All	All	2780/2780 (100%)	2349 (84%)	431 (16%)	2	8

5 of 431 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	J	26	ASP
13	L	71	VAL

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Mol	Chain	Res	Type
25	Z	9	LYS
11	J	92	GLU
12	K	60	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
5	D	127	ASN
8	G	161	GLN
18	Q	86	GLN
5	D	120	ASN
15	N	91	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
29	X	2776/2881 (96%)	655 (23%)	41 (1%)
30	Y	121/122 (99%)	35 (28%)	1 (0%)
All	All	2897/3003 (96%)	690 (23%)	42 (1%)

5 of 690 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
29	X	13	A
29	X	14	A
29	X	22	C
29	X	28	A
29	X	46	C

5 of 42 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
29	X	1413	G
29	X	1586	G
29	X	2756	U
29	X	1414	G
29	X	1510	U

## 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 198 ligands modelled in this entry, 198 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.

No monomer is involved in short contacts.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	0	224/224 (100%)	5.93	199 (88%) 0 0	238, 259, 280, 290	0
2	A	274/274 (100%)	0.53	31 (11%) 5 4	93, 135, 154, 161	0
3	B	205/205 (100%)	0.24	7 (3%) 45 40	60, 89, 107, 124	0
4	C	197/197 (100%)	0.37	15 (7%) 13 10	77, 125, 145, 159	0
5	D	177/177 (100%)	1.65	67 (37%) 0 0	155, 174, 190, 197	0
6	E	171/171 (100%)	0.85	35 (20%) 1 0	110, 148, 175, 177	0
7	F	144/144 (100%)	3.56	102 (70%) 0 0	213, 230, 235, 237	0
8	G	142/142 (100%)	0.27	11 (7%) 13 10	79, 112, 127, 144	0
9	H	134/134 (100%)	0.03	5 (3%) 41 37	62, 79, 94, 111	0
10	I	141/141 (100%)	0.98	32 (22%) 0 0	86, 138, 155, 161	0
11	J	136/136 (100%)	1.04	33 (24%) 0 0	94, 113, 135, 141	0
12	K	113/113 (100%)	0.14	3 (2%) 54 50	61, 72, 83, 88	0
13	L	104/104 (100%)	1.48	33 (31%) 0 0	121, 136, 153, 162	0
14	M	109/109 (100%)	-0.19	3 (2%) 53 49	65, 80, 98, 127	0
15	N	117/117 (100%)	0.40	10 (8%) 10 8	80, 107, 127, 133	0
16	O	94/94 (100%)	0.07	8 (8%) 10 8	89, 122, 141, 152	0
17	P	127/127 (100%)	0.40	10 (7%) 12 10	71, 85, 109, 156	0
18	Q	93/93 (100%)	0.94	14 (15%) 2 1	98, 124, 140, 144	0
19	R	110/110 (100%)	0.58	14 (12%) 3 2	110, 121, 146, 157	0
20	S	175/175 (100%)	0.72	35 (20%) 1 0	124, 151, 164, 168	0
21	T	84/84 (100%)	2.25	38 (45%) 0 0	102, 117, 133, 146	0
22	U	72/72 (100%)	2.89	46 (63%) 0 0	117, 148, 161, 164	0
23	V	66/66 (100%)	0.35	8 (12%) 4 3	129, 141, 159, 163	0
24	W	55/55 (100%)	0.70	10 (18%) 1 1	95, 110, 126, 139	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	Z	57/57 (100%)	-0.12	1 (1%) 68 67	74, 82, 104, 112	0
26	1	54/54 (100%)	1.45	20 (37%) 0 0	125, 136, 152, 168	0
27	2	47/47 (100%)	0.21	1 (2%) 63 61	91, 108, 116, 117	0
28	3	65/65 (100%)	2.07	32 (49%) 0 0	107, 118, 127, 129	0
29	X	2780/2881 (96%)	-0.13	108 (3%) 39 35	51, 111, 221, 347	0
30	Y	122/122 (100%)	-0.53	4 (3%) 46 41	96, 136, 161, 172	0
All	All	6389/6490 (98%)	0.57	935 (14%) 2 1	51, 119, 242, 347	0

The worst 5 of 935 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
29	X	2137	C	31.2
29	X	1916	A	26.7
1	0	54	VAL	23.5
29	X	2112	G	20.1
1	0	86	GLY	19.7

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	B-factors(Å <sup>2</sup> )	Q<0.9
31	MG	X	6108	1/1	0.36	0.64	120,120,120,120	0
31	MG	X	6119	1/1	0.46	0.53	128,128,128,128	0
31	MG	X	6177	1/1	0.48	0.59	113,113,113,113	0
31	MG	X	6159	1/1	0.49	0.44	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
31	MG	X	6093	1/1	0.52	0.69	106,106,106,106	0
31	MG	X	6046	1/1	0.56	0.40	91,91,91,91	0
31	MG	X	6167	1/1	0.56	0.57	103,103,103,103	0
31	MG	X	6183	1/1	0.58	0.71	105,105,105,105	0
31	MG	X	6179	1/1	0.61	0.54	117,117,117,117	0
31	MG	X	6175	1/1	0.64	0.41	121,121,121,121	0
31	MG	X	6098	1/1	0.65	1.04	97,97,97,97	0
31	MG	X	6144	1/1	0.65	0.37	87,87,87,87	0
31	MG	X	6162	1/1	0.67	0.81	111,111,111,111	0
31	MG	X	6041	1/1	0.69	0.35	83,83,83,83	0
31	MG	X	6038	1/1	0.71	0.67	85,85,85,85	0
31	MG	X	6099	1/1	0.72	0.68	89,89,89,89	0
31	MG	X	6186	1/1	0.72	1.02	134,134,134,134	0
31	MG	X	6133	1/1	0.73	1.20	111,111,111,111	0
31	MG	X	6170	1/1	0.73	1.97	127,127,127,127	0
31	MG	X	6191	1/1	0.74	1.56	101,101,101,101	0
31	MG	X	6141	1/1	0.74	0.60	122,122,122,122	0
31	MG	X	6138	1/1	0.75	0.78	94,94,94,94	0
31	MG	X	6058	1/1	0.76	0.52	97,97,97,97	0
31	MG	X	6085	1/1	0.76	0.36	101,101,101,101	0
31	MG	X	6187	1/1	0.77	0.57	92,92,92,92	0
31	MG	X	6111	1/1	0.77	0.70	98,98,98,98	0
31	MG	X	6113	1/1	0.77	0.53	115,115,115,115	0
31	MG	X	6192	1/1	0.77	0.69	138,138,138,138	0
31	MG	X	6014	1/1	0.78	0.42	91,91,91,91	0
31	MG	X	6048	1/1	0.78	0.80	102,102,102,102	0
31	MG	X	6117	1/1	0.78	0.36	90,90,90,90	0
31	MG	X	6020	1/1	0.78	0.34	79,79,79,79	0
31	MG	X	6180	1/1	0.78	1.59	101,101,101,101	0
31	MG	X	6156	1/1	0.79	0.63	105,105,105,105	0
31	MG	X	6107	1/1	0.79	0.75	113,113,113,113	0
31	MG	X	6121	1/1	0.79	0.80	99,99,99,99	0
31	MG	X	6146	1/1	0.80	1.51	129,129,129,129	0
31	MG	X	6022	1/1	0.80	0.40	77,77,77,77	0
31	MG	X	6006	1/1	0.81	0.48	69,69,69,69	0
31	MG	X	6164	1/1	0.81	0.99	124,124,124,124	0
31	MG	X	6122	1/1	0.81	0.46	100,100,100,100	0
31	MG	X	6171	1/1	0.82	0.80	111,111,111,111	0
31	MG	X	6110	1/1	0.82	0.38	130,130,130,130	0
31	MG	X	6157	1/1	0.82	0.31	111,111,111,111	0
31	MG	X	6100	1/1	0.83	0.59	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
31	MG	X	6090	1/1	0.83	0.45	117,117,117,117	0
31	MG	X	6155	1/1	0.83	0.33	115,115,115,115	0
31	MG	X	6013	1/1	0.83	0.57	76,76,76,76	0
31	MG	X	6136	1/1	0.83	0.81	122,122,122,122	0
31	MG	X	6018	1/1	0.83	0.46	74,74,74,74	0
31	MG	X	6080	1/1	0.83	0.71	108,108,108,108	0
31	MG	X	6154	1/1	0.83	1.09	113,113,113,113	0
31	MG	Y	205	1/1	0.83	0.90	129,129,129,129	0
31	MG	X	6016	1/1	0.84	0.35	77,77,77,77	0
31	MG	X	6109	1/1	0.84	0.31	101,101,101,101	0
31	MG	X	6190	1/1	0.84	1.33	129,129,129,129	0
31	MG	X	6028	1/1	0.84	0.33	88,88,88,88	0
31	MG	X	6172	1/1	0.84	0.66	124,124,124,124	0
31	MG	X	6011	1/1	0.85	0.45	89,89,89,89	0
31	MG	X	6174	1/1	0.85	0.72	87,87,87,87	0
31	MG	X	6030	1/1	0.85	1.19	83,83,83,83	0
31	MG	X	6052	1/1	0.85	0.52	97,97,97,97	0
31	MG	X	6003	1/1	0.85	0.49	70,70,70,70	0
31	MG	X	6137	1/1	0.85	0.57	135,135,135,135	0
31	MG	X	6173	1/1	0.85	1.91	102,102,102,102	0
31	MG	X	6142	1/1	0.86	0.77	89,89,89,89	0
31	MG	X	6012	1/1	0.86	0.50	82,82,82,82	0
31	MG	X	6127	1/1	0.86	0.59	122,122,122,122	0
31	MG	X	6143	1/1	0.86	1.04	100,100,100,100	0
31	MG	X	6074	1/1	0.86	0.74	80,80,80,80	0
31	MG	X	6158	1/1	0.86	2.46	114,114,114,114	0
31	MG	X	6105	1/1	0.86	1.40	118,118,118,118	0
31	MG	X	6066	1/1	0.86	1.08	84,84,84,84	0
31	MG	X	6151	1/1	0.86	0.34	98,98,98,98	0
31	MG	X	6072	1/1	0.86	0.56	102,102,102,102	0
31	MG	X	6135	1/1	0.86	0.76	91,91,91,91	0
31	MG	X	6124	1/1	0.87	1.14	107,107,107,107	0
31	MG	X	6160	1/1	0.87	0.68	104,104,104,104	0
31	MG	Y	204	1/1	0.87	0.96	109,109,109,109	0
31	MG	X	6189	1/1	0.87	0.75	120,120,120,120	0
31	MG	X	6147	1/1	0.87	1.00	82,82,82,82	0
31	MG	X	6023	1/1	0.87	0.52	97,97,97,97	0
31	MG	Y	201	1/1	0.87	0.85	112,112,112,112	0
31	MG	X	6034	1/1	0.88	0.81	90,90,90,90	0
31	MG	X	6176	1/1	0.88	0.50	107,107,107,107	0
31	MG	X	6008	1/1	0.88	0.42	81,81,81,81	0
31	MG	X	6114	1/1	0.88	0.55	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
31	MG	X	6083	1/1	0.88	0.80	91,91,91,91	0
31	MG	X	6182	1/1	0.88	0.97	120,120,120,120	0
31	MG	X	6149	1/1	0.88	0.59	94,94,94,94	0
31	MG	X	6123	1/1	0.88	0.48	130,130,130,130	0
31	MG	X	6057	1/1	0.88	0.99	93,93,93,93	0
31	MG	X	6165	1/1	0.88	0.99	99,99,99,99	0
31	MG	X	6027	1/1	0.89	1.04	86,86,86,86	0
31	MG	X	6039	1/1	0.89	1.17	104,104,104,104	0
31	MG	X	6037	1/1	0.89	0.41	86,86,86,86	0
31	MG	X	6132	1/1	0.89	0.54	94,94,94,94	0
31	MG	X	6035	1/1	0.89	0.43	86,86,86,86	0
31	MG	X	6115	1/1	0.89	0.74	103,103,103,103	0
31	MG	X	6047	1/1	0.89	0.54	74,74,74,74	0
31	MG	X	6021	1/1	0.90	0.70	75,75,75,75	0
31	MG	X	6168	1/1	0.90	0.84	107,107,107,107	0
31	MG	X	6055	1/1	0.90	0.64	90,90,90,90	0
31	MG	X	6067	1/1	0.90	0.49	79,79,79,79	0
31	MG	X	6059	1/1	0.90	0.46	87,87,87,87	0
31	MG	X	6017	1/1	0.91	0.48	83,83,83,83	0
31	MG	X	6104	1/1	0.91	0.59	86,86,86,86	0
31	MG	X	6064	1/1	0.91	0.63	96,96,96,96	0
31	MG	X	6075	1/1	0.91	0.85	103,103,103,103	0
31	MG	X	6140	1/1	0.91	1.02	97,97,97,97	0
31	MG	X	6019	1/1	0.91	0.81	77,77,77,77	0
31	MG	X	6082	1/1	0.91	0.76	83,83,83,83	0
31	MG	X	6015	1/1	0.91	0.55	77,77,77,77	0
31	MG	X	6071	1/1	0.91	0.40	81,81,81,81	0
31	MG	X	6188	1/1	0.91	0.44	98,98,98,98	0
31	MG	X	6051	1/1	0.91	0.39	69,69,69,69	0
31	MG	X	6001	1/1	0.92	0.56	69,69,69,69	0
31	MG	X	6084	1/1	0.92	0.30	93,93,93,93	0
31	MG	X	6010	1/1	0.92	0.83	69,69,69,69	0
31	MG	X	6045	1/1	0.92	1.03	89,89,89,89	0
31	MG	X	6076	1/1	0.92	0.73	102,102,102,102	0
31	MG	X	6004	1/1	0.92	0.36	76,76,76,76	0
31	MG	Y	202	1/1	0.92	0.43	125,125,125,125	0
31	MG	X	6095	1/1	0.92	0.85	79,79,79,79	0
31	MG	X	6056	1/1	0.92	0.88	85,85,85,85	0
31	MG	X	6101	1/1	0.93	0.87	89,89,89,89	0
31	MG	X	6097	1/1	0.93	1.26	93,93,93,93	0
31	MG	X	6161	1/1	0.93	0.68	95,95,95,95	0
31	MG	X	6120	1/1	0.93	1.04	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
31	MG	X	6092	1/1	0.93	0.26	93,93,93,93	0
31	MG	X	6163	1/1	0.93	0.37	156,156,156,156	0
31	MG	X	6033	1/1	0.93	0.53	98,98,98,98	0
31	MG	X	6002	1/1	0.93	0.33	78,78,78,78	0
31	MG	X	6178	1/1	0.93	0.58	103,103,103,103	0
31	MG	X	6118	1/1	0.93	0.72	90,90,90,90	0
31	MG	X	6024	1/1	0.93	0.61	87,87,87,87	0
31	MG	X	6081	1/1	0.93	0.42	78,78,78,78	0
31	MG	X	6129	1/1	0.93	0.89	104,104,104,104	0
31	MG	X	6094	1/1	0.93	0.45	92,92,92,92	0
31	MG	X	6128	1/1	0.93	0.81	97,97,97,97	0
31	MG	X	6007	1/1	0.93	0.46	70,70,70,70	0
31	MG	X	6150	1/1	0.94	0.69	111,111,111,111	0
31	MG	X	6044	1/1	0.94	0.29	73,73,73,73	0
31	MG	X	6130	1/1	0.94	0.67	108,108,108,108	0
31	MG	X	6078	1/1	0.94	0.57	93,93,93,93	0
31	MG	X	6145	1/1	0.94	0.20	104,104,104,104	0
31	MG	X	6112	1/1	0.94	0.68	84,84,84,84	0
31	MG	X	6029	1/1	0.94	0.43	69,69,69,69	0
31	MG	X	6036	1/1	0.94	0.84	82,82,82,82	0
31	MG	X	6062	1/1	0.94	0.41	85,85,85,85	0
31	MG	X	6169	1/1	0.94	0.57	101,101,101,101	0
31	MG	X	6088	1/1	0.94	0.87	99,99,99,99	0
31	MG	X	6077	1/1	0.94	0.65	98,98,98,98	0
31	MG	X	6026	1/1	0.94	0.41	91,91,91,91	0
31	MG	X	6126	1/1	0.94	1.19	94,94,94,94	0
31	MG	X	6040	1/1	0.94	0.78	80,80,80,80	0
31	MG	X	6106	1/1	0.94	0.54	80,80,80,80	0
31	MG	X	6032	1/1	0.94	0.34	78,78,78,78	0
31	MG	X	6103	1/1	0.94	0.32	117,117,117,117	0
31	MG	X	6091	1/1	0.94	1.11	88,88,88,88	0
31	MG	X	6102	1/1	0.94	0.25	89,89,89,89	0
31	MG	X	6131	1/1	0.94	0.86	101,101,101,101	0
31	MG	X	6068	1/1	0.94	0.66	90,90,90,90	0
31	MG	X	6139	1/1	0.95	0.54	126,126,126,126	0
31	MG	X	6089	1/1	0.95	0.51	90,90,90,90	0
31	MG	X	6031	1/1	0.95	0.53	69,69,69,69	0
31	MG	X	6079	1/1	0.95	0.35	102,102,102,102	0
31	MG	X	6073	1/1	0.95	0.79	85,85,85,85	0
31	MG	X	6152	1/1	0.95	0.93	112,112,112,112	0
31	MG	X	6185	1/1	0.95	0.59	109,109,109,109	0
31	MG	M	201	1/1	0.95	0.94	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
31	MG	X	6061	1/1	0.95	0.71	83,83,83,83	0
31	MG	X	6054	1/1	0.95	0.54	92,92,92,92	0
31	MG	X	6065	1/1	0.96	0.61	81,81,81,81	0
31	MG	X	6184	1/1	0.96	0.76	102,102,102,102	0
31	MG	X	6153	1/1	0.96	0.62	113,113,113,113	0
31	MG	X	6049	1/1	0.96	0.67	88,88,88,88	0
31	MG	X	6005	1/1	0.96	0.89	69,69,69,69	0
31	MG	X	6063	1/1	0.96	1.29	87,87,87,87	0
31	MG	X	6070	1/1	0.96	0.58	107,107,107,107	0
31	MG	X	6166	1/1	0.96	0.73	106,106,106,106	0
31	MG	X	6069	1/1	0.96	0.51	91,91,91,91	0
31	MG	X	6181	1/1	0.97	0.31	121,121,121,121	0
31	MG	X	6043	1/1	0.97	0.85	69,69,69,69	0
31	MG	X	6060	1/1	0.97	0.68	80,80,80,80	0
31	MG	X	6116	1/1	0.97	0.59	106,106,106,106	0
31	MG	X	6096	1/1	0.97	1.19	89,89,89,89	0
31	MG	X	6025	1/1	0.97	0.45	83,83,83,83	0
31	MG	X	6050	1/1	0.97	0.50	84,84,84,84	0
31	MG	X	6125	1/1	0.97	0.46	123,123,123,123	0
31	MG	Y	203	1/1	0.97	0.97	102,102,102,102	0
31	MG	X	6009	1/1	0.97	0.67	69,69,69,69	0
31	MG	X	6086	1/1	0.98	0.93	87,87,87,87	0
31	MG	X	6087	1/1	0.98	0.54	98,98,98,98	0
31	MG	X	6042	1/1	0.98	0.59	83,83,83,83	0
31	MG	X	6053	1/1	0.99	0.85	91,91,91,91	0
31	MG	X	6148	1/1	0.99	0.57	130,130,130,130	0
31	MG	X	6134	1/1	0.99	0.67	112,112,112,112	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.