



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 12:59 AM GMT

PDB ID : 2AWB
Title : Crystal structure of the bacterial ribosome from Escherichia coli at 3.5 Å resolution. This file contains the 50S subunit of the second 70S ribosome. The entire crystal structure contains two 70S ribosomes and is described in remark 400.
Authors : Schuwirth, B.S.; Borovinskaya, M.A.; Hau, C.W.; Zhang, W.; Vila-Sanjurjo, A.; Holton, J.M.; Cate, J.H.D.
Deposited on : 2005-08-31
Resolution : 3.46 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>

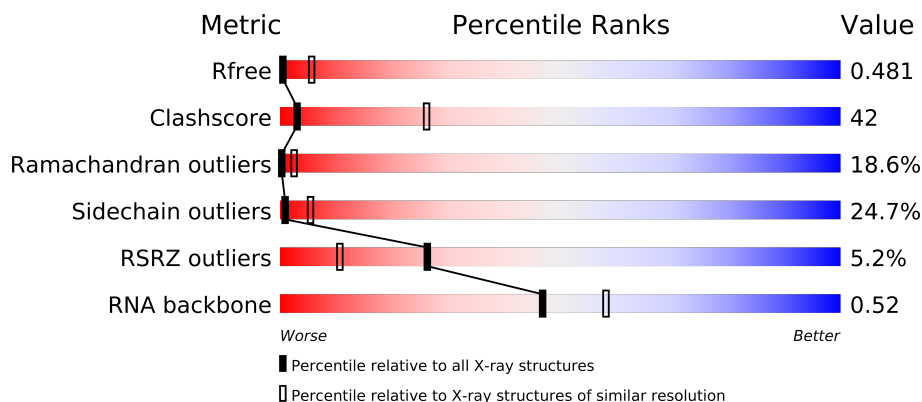
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
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 3.46 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}	66092	1149 (3.62-3.30)
Clashscore	79885	1012 (3.60-3.32)
Ramachandran outliers	78287	1401 (3.62-3.30)
Sidechain outliers	78261	1401 (3.62-3.30)
RSRZ outliers	66119	1149 (3.62-3.30)
RNA backbone	1838	1004 (4.10-2.76)

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 ≥ 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.

Mol	Chain	Length	Quality of chain
1	A	120	
2	B	2904	
3	V	94	
4	C	273	
5	D	209	
6	E	201	
7	F	178	
8	G	176	
9	H	149	
10	J	142	
11	K	123	
12	L	144	

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Mol	Chain	Length	Quality of chain
13	M	136	
14	N	127	
15	O	117	
16	P	114	
17	Q	117	
18	R	103	
19	S	110	
20	T	100	
21	U	103	
22	W	84	
23	X	63	
24	Y	58	
25	Z	70	
26	0	56	
27	1	54	
28	2	46	
29	3	64	
30	4	38	
31	I	141	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
32	MG	B	2938	-	X
32	MG	B	2952	-	X
32	MG	B	2956	-	X
32	MG	B	2969	-	X
32	MG	B	2973	-	X
32	MG	B	2980	-	X
32	MG	B	2990	-	X
32	MG	B	2998	-	X

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 90313 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 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	117	Total	C	N	O	P	0	0	0
			2507	1116	459	815	117			

- Molecule 2 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			

- Molecule 3 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	V	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			

- Molecule 4 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	267	Total	C	N	O	S	0	0	0
			2053	1271	416	359	7			

- Molecule 5 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			

- Molecule 6 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	E	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			

- Molecule 7 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	F	178	Total	C	N	O	S	0	0	0
			1420	905	251	258	6			

- Molecule 8 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	G	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			

- Molecule 9 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	149	Total	C	N	O	S	0	0	0
			1111	699	197	214	1			

- Molecule 10 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	140	Total	C	N	O	S	0	0	0
			1112	704	210	194	4			

- Molecule 11 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	121	Total	C	N	O	S	0	0	0
			930	582	179	164	5			

- Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	144	Total	C	N	O	S	0	0	0
			1053	654	207	190	2			

- Molecule 13 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			

- Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	127	Total	C	N	O	S	0	0	0
			1008	621	204	178	5			

- Molecule 15 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	117	Total	C	N	O	S	0	0	0
			900	557	179	163	1			

- Molecule 16 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			

- Molecule 17 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	117	Total	C	N	O	S	0	0	0
			947	604	192	151				

- Molecule 18 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	R	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			

- Molecule 19 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	99	Total	C	N	O	S	0	0	0
			777	491	145	139	2			

- Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	102	Total	C	N	O			
			779	492	146	141	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	W	84	Total	C	N	O	S		
			634	391	129	113	1	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	X	63	Total	C	N	O	S		
			509	313	99	95	2	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	Y	58	Total	C	N	O	S		
			449	281	87	79	2	0	0

- Molecule 25 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	Z	70	Total	C	N	O	S		
			549	339	104	100	6	0	0

- Molecule 26 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	0	56	Total	C	N	O	S		
			444	269	94	80	1	0	0

- Molecule 27 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
27	1	54	Total	C	N	O			
			441	284	81	76	0	0	0

- Molecule 28 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

- Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			

- Molecule 30 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

- Molecule 31 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	I	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	B	110	Total	Mg	0	0
			110	110		
32	N	1	Total	Mg	0	0
			1	1		

- Molecule 33 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	2	2	Total	O	0	0
			2	2		
33	B	499	Total	O	0	0
			499	499		
33	C	1	Total	O	0	0
			1	1		
33	D	1	Total	O	0	0
			1	1		
33	E	2	Total	O	0	0
			2	2		

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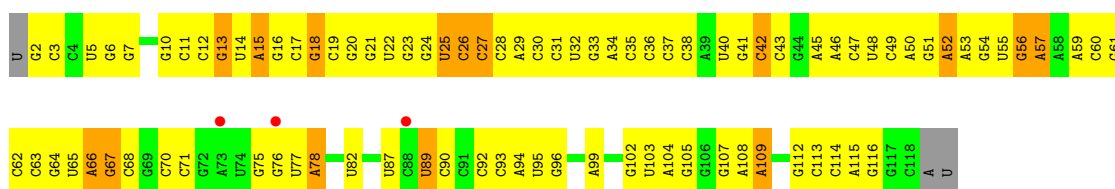
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	J	2	Total	O	0	0
			2	2		
33	L	1	Total	O	0	0
			1	1		
33	N	3	Total	O	0	0
			3	3		
33	Q	1	Total	O	0	0
			1	1		

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.

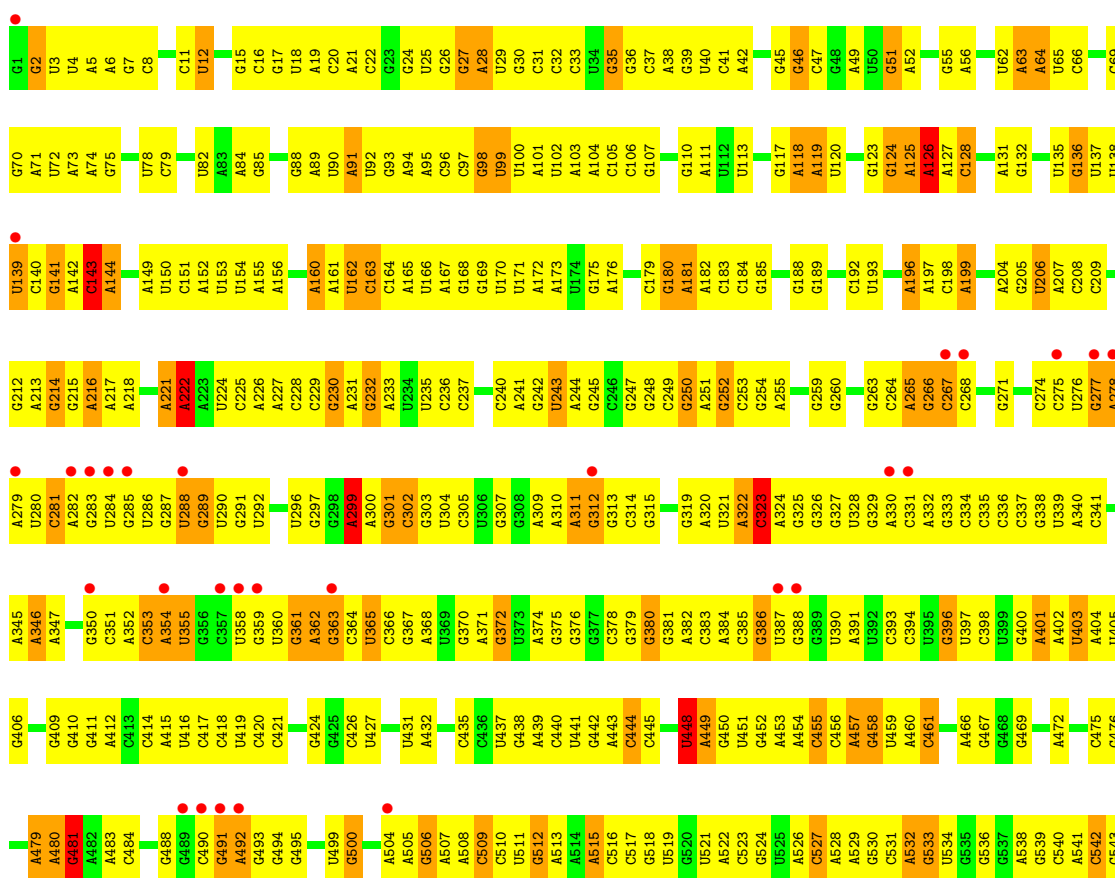
• Molecule 1: 5S ribosomal RNA

Chain A:



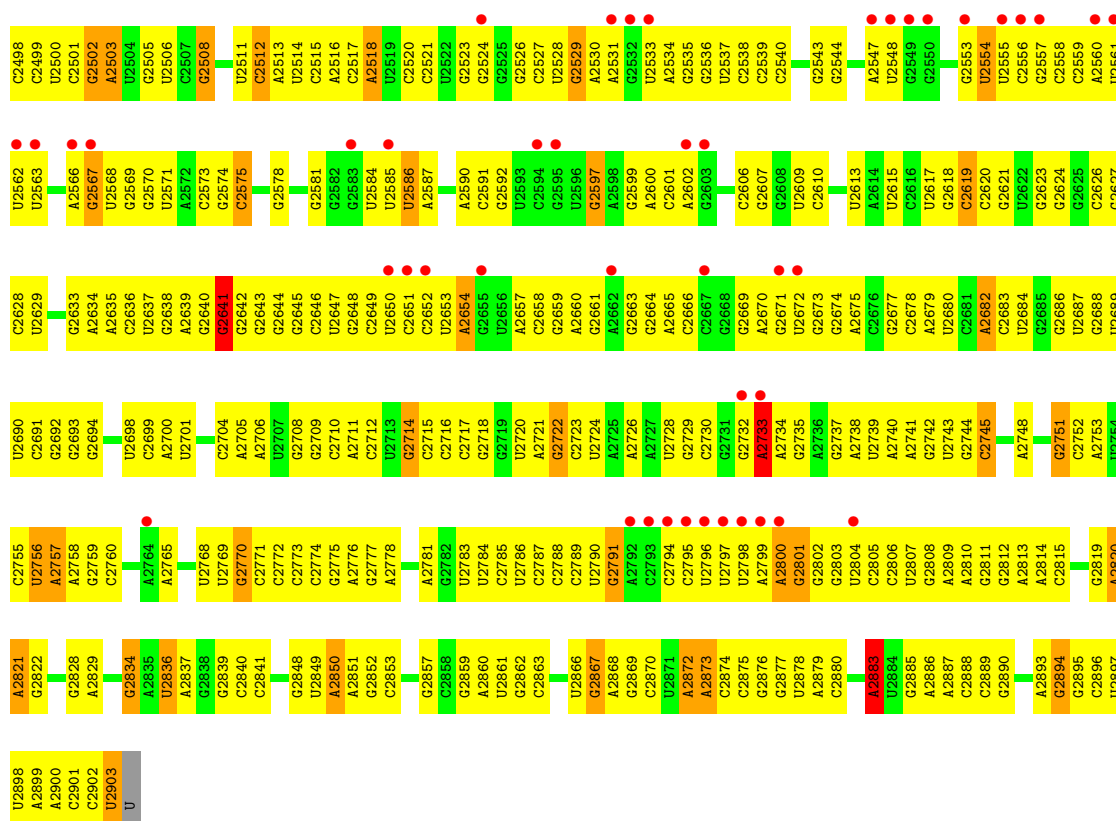
• Molecule 2: 23S ribosomal RNA

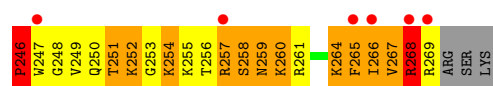
Chain B:





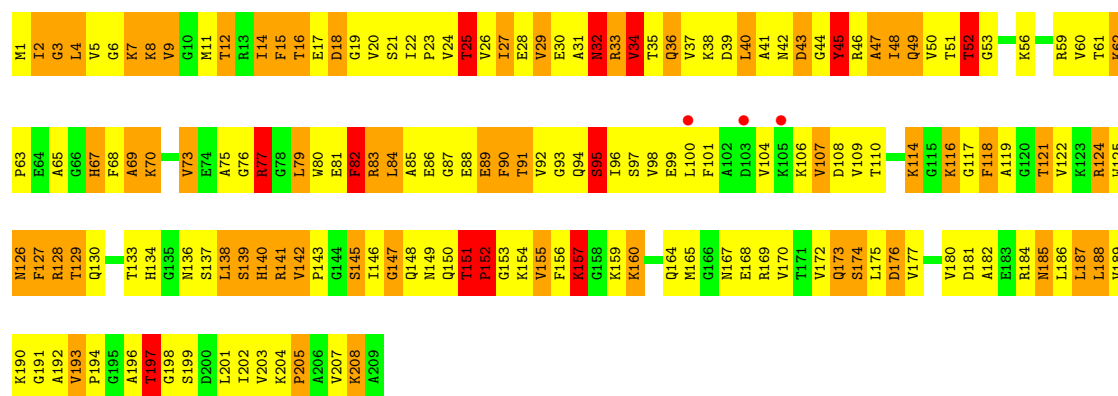
G2429	A2430	A2433	A2434	U2438	A2439	G2440	U2441	G2442	G2443	G2444	G2445	G2446	G2447	A2448	U2449	A2450	G2454	G2455	G2456	U2457	G2458	A2459	U2460	A2461	G2462	G2463	G2464	G2465	G2466	A2467	A2468	A2469	G2470	A2471	G2472	G2475	A2476	U2477	A2478	U2479	G2480	G2481	G2482	G2483	G2484	G2485	G2488	U2489	G2490	U2491	U2492	U2493	G2496	A2497									
G2363	G2364	G2365		A2369	G2370	G2371	U2372	G2373	G2374	G2375	A2376	A2377	A2378	G2379	G2380	A2381	G2382	G2383	G2384	G2385	A2386	U2387	A2388	G2389	U2390	G2391	A2392	U2393	G2394	G2395	G2396	G2397	U2398	G2399	G2400	U2401	U2402	G2405	A2406	G2410	A2411	A2412	G2413	G2414	G2415	G2416	G2417	A2418	U2419	G2423	G2424	A2425	A2426	U2427	A2428	G2429	G2432						
U2233	G2234	G2235	U2236	G2237	G2238	G2239	U2240	A2241	G2242	U2243	U2244	U2245	G2246	A2247	G2248	G2249	G2250	G2251	G2252	G2253	G2254	G2255	G2256	U2257	G2258	U2259	C2260	G2261	G2262	G2263	G2264	G2265	G2266	G2267	G2268	G2269	G2270	G2271	U2272	A2273	A2274	C2275	A2276	G2277	A2278	G2279	G2280	A2281	G2282	G2283	A2284	G2285	G2286	A2287	G2288	G2289	G2290	U2291	G2292	G2293	G2294	U2295	U2296
A	A	U	A	C	C	A	C	C	C2179	U2180	U2181	U2182	A2183	U2184	G2185	U2186	U2187	U2188	U2189	U2190	A2191	U2192	G2193	U2194	U2195	C2196	U2197	A2198	U2199	C2200	U2203	G2204	C2207	G2208	G2209	U2210	A2211	A2212	U2213	G2214	G2215	G2216	G2217	U2220	G2221	C2222	G2223	A2224	A2225	G2226	A2227	G2228	U2229	U2230	U2231	G2232							
U	G	U	U	A	G	A	U	A	A	G	G	U	A	U	G	G	A	G	C	U	U	U	G2133	A2134	A2135	G2136	U2137	G2138	U2139	G2140	G2141	A2142	G2143	G2144	U2085	U2086	G2087	A2088	C2089	A2090	G2091	U2092	G2093	A2094	A2095	G2096	G2097	U2098	U2099	G2100	A2101	G2102	C2103	G2104	U2105	U2106	A2107	A2108	U2109				
G1974	U1979	G1980	A1981	U1982	U1983	C1986	A1987	G1988	G1989	G1990	U1991	U1992	U1993	U1994	U1995	C1996	C1997	A1998	C1999	C2000	C2001	A2005	C2006	U2007	C2008	A2009	G2012	U2016	U2017	G2018	A2019	A2020	C2021	U2022	G2023	G2024	C2025	U2026	G2027	U2028	G2029	A2030	A2031	G2032	A2033	U2034	G2035	C2036	A2037	U2038	U2039	G2040	U2041	A2042									
U1911	A1912	C1913	A1914	U1915	U1916	U1917	A1918	A1919	G1920	G1921	G1922	U1923	C1924	A1927	A1928	G1929	U1930	U1931	A1932	G1933	C1934	G1935	A1936	A1937	A1938	U1939	U1940	C1941	U1942	U1943	U1944	U1945	U1946	C1947	G1948	U1949	G1950	U1951	A1952	A1953	G1954	U1955	U1956	C1957	C1958	G1959	U1963	G1964	C1965	A1966	C1967	G1968	A1969	U1970	U1971	U1972	G1973						
C1844	G1845	A1846	A1847	G1848	G1849	G1850	U1851	U1852	A1853	A1854	U1855	U1856	G1857	U1858	U1859	G1862	U1863	U1864	U1865	A1866	G1867	C1868	G1869	C1870	A1871	U1872	G1873	C1874	G1875	A1876	A1877	G1878	C1879	U1880	A1881	U1882	U1883	U1884	A1885	A1888	A1889	A1890	G1891	C1892	G1895	U1896	C1902	G1903	G1904	C1905	G1906	C1909	G1910										
G1776	U1779	U1781	A1784	A1785	U1786	U1787	C1788	A1789	C1790	A1791	G1792	A1793	A1794	U1795	U1796	U1797	U1798	C1800	G1801	A1802	A1803	C1804	G1805	G1806	A1807	U1810	G1811	U1812	G1813	A1814	G1815	C1816	G1817	U1818	A1819	U1820	U1821	C1822	G1823	U1824	U1825	U1826	U1827	G1828	A1829	C1832	G1833	U1834	G1835	C1836	U1837	U1838	U1841	G1842	C1843								
A1641	G1642	G1645	A1646	U1647	U1648	A1649	A1650	G1651	A1654	U1655	C1656	U1657	C1658	A1659	U1660	G1661	G1662	G1666	G1667	A1668	G1669	G1670	U1671	A1672	G1673	G1674	G1675	A1676	A1677	G1681	G1682	U1683	U1684	U1685	G1686	G1687	U1688	A1689	A1690	C1691	U1692	U1693	G1694	G1695	A1700	A1701	G1702	C1703	C1704	A1705	C1706	G1707	C1708	U1709	G1710								
C1565	A1566	G1567	G1568	A1569	A1570	A1571	A1572	G1573	C1574	U1578	A1579	A1580	A1583	U1584	C1585	U1586	G1587	G1588	U1589	A1590	A1591	C1592	A1593	U1594	C1595	U1599	G1600	A1601	U1602	A1603	C1606	C1607	A1608	A1609	A1610	C1611	C1612	G1613	A1616	C1617	A1618	G1622	G1623	G1624	G1633	A1634	A1635	U1636	A1637	C1638	C1639	A1640											
A1711	U1712	U1713	U1714	U1715	U1716	A1717	G1718	G1719	G1720	G1721	G1722	G1723	G1724	U1725	C1726	C1727	G1728	U1729	G1730	G1731	G1732	G1733	G1734	G1735	U1736	G1737	G1738	A1739	G1740	G1741	U1742	G1743	A1744	A1745	U1746	U1747	C1748	A1749	G1750	U1751	C1752	A1753	A1754	U1755	G1756	A1757	U1758	A1759	A1762	G1763	C1764	U1765	C1771	A1772	C1773	U1775							





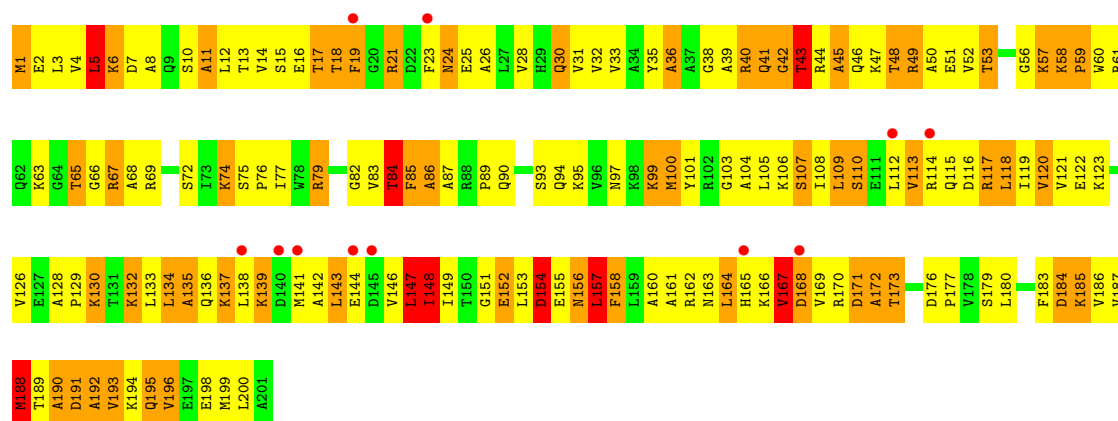
• Molecule 5: 50S ribosomal protein L3

Chain D:



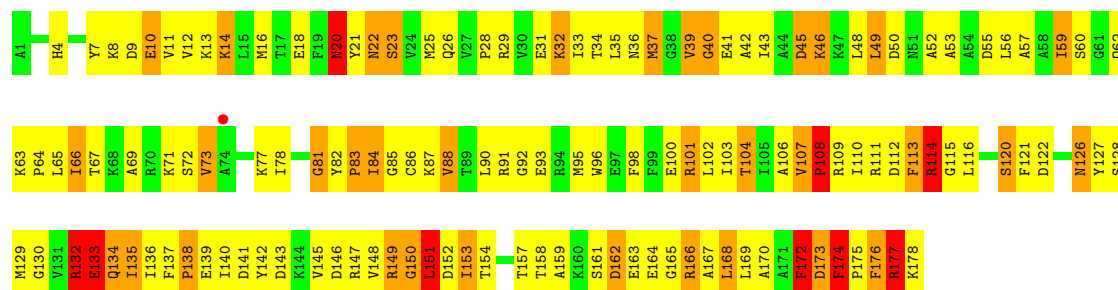
• Molecule 6: 50S ribosomal protein L4

Chain E:



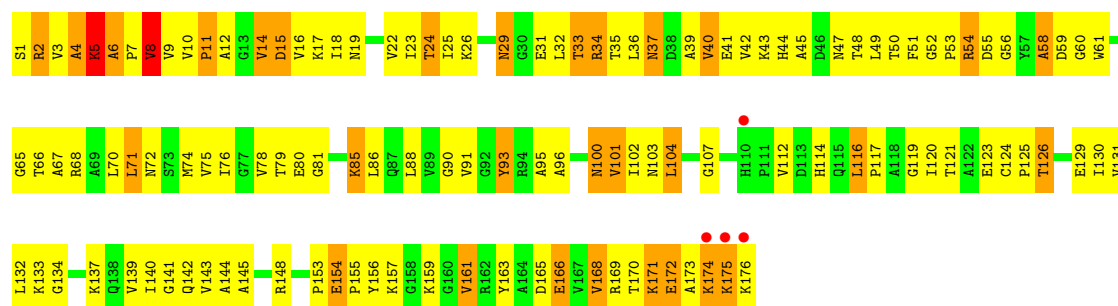
• Molecule 7: 50S ribosomal protein L5

Chain F:



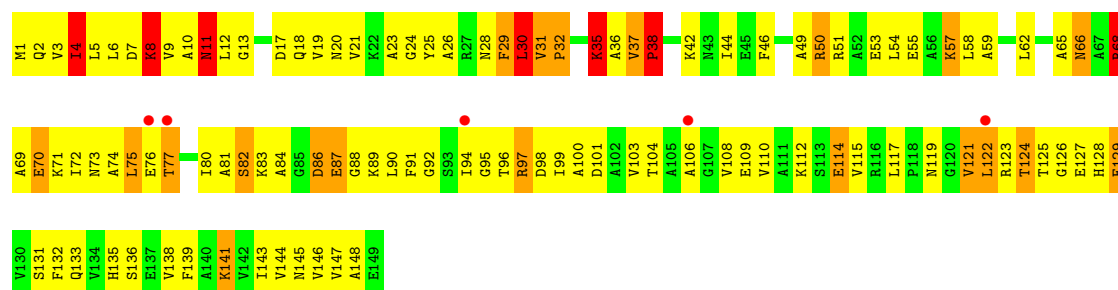
• Molecule 8: 50S ribosomal protein L6

Chain G:



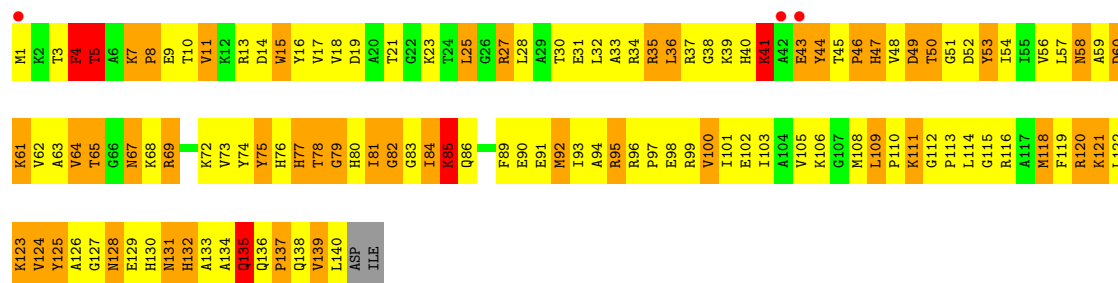
• Molecule 9: 50S ribosomal protein L9

Chain H:



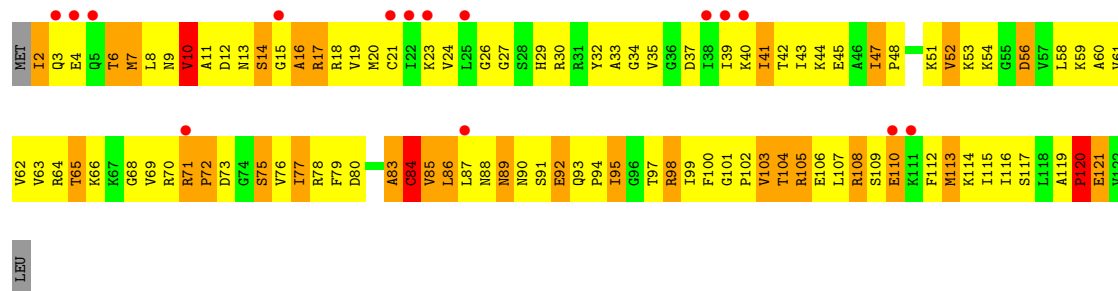
• Molecule 10: 50S ribosomal protein L13

Chain J:



• Molecule 11: 50S ribosomal protein L14

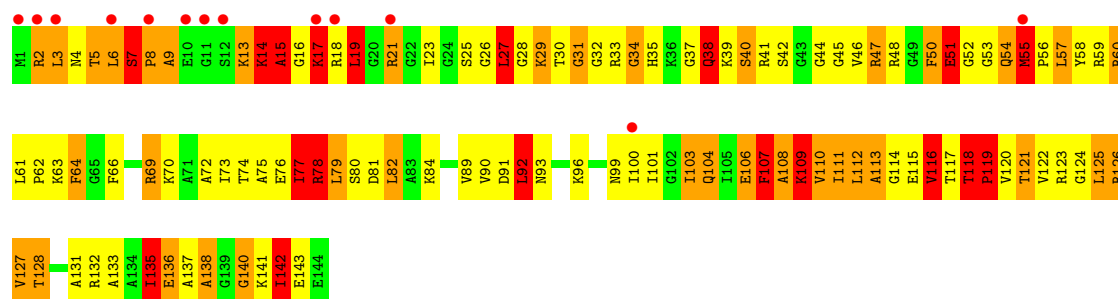
Chain K:



• Molecule 12: 50S ribosomal protein L15

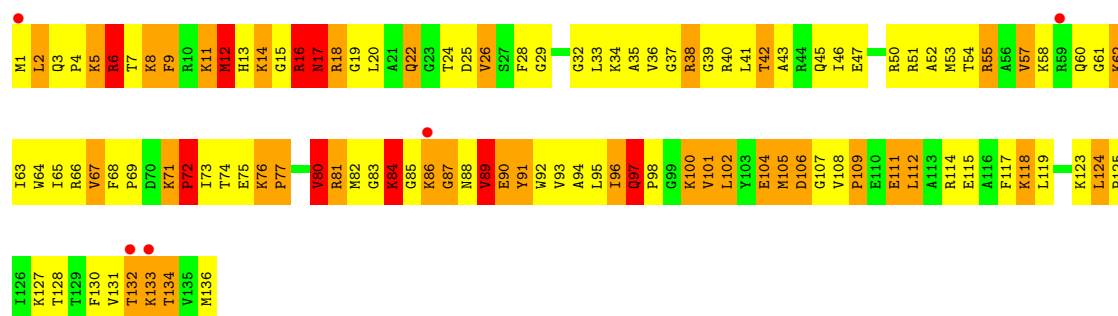
Chain L:





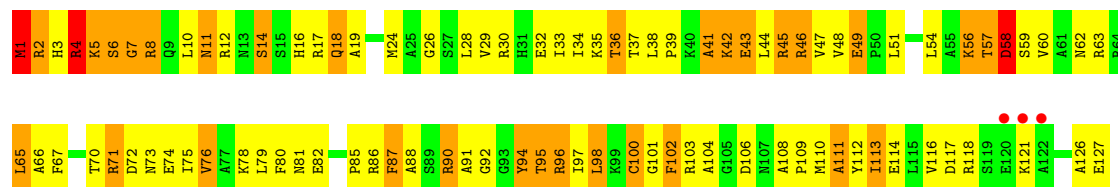
• Molecule 13: 50S ribosomal protein L16

Chain M:



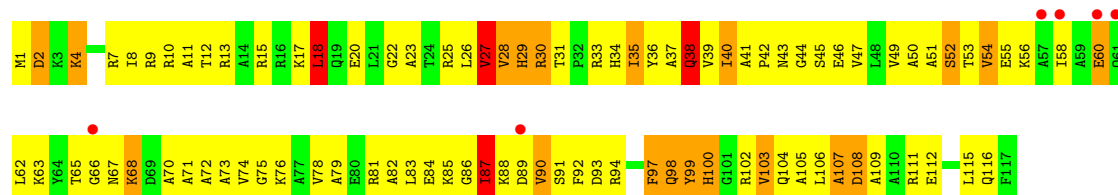
• Molecule 14: 50S ribosomal protein L17

Chain N:



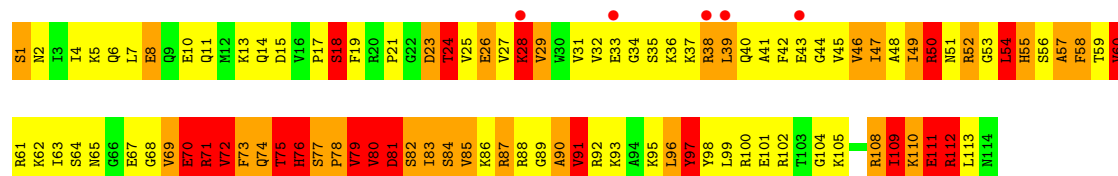
• Molecule 15: 50S ribosomal protein L18

Chain O:



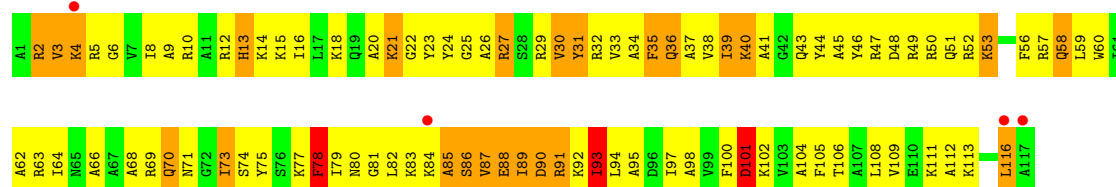
• Molecule 16: 50S ribosomal protein L19

Chain P:



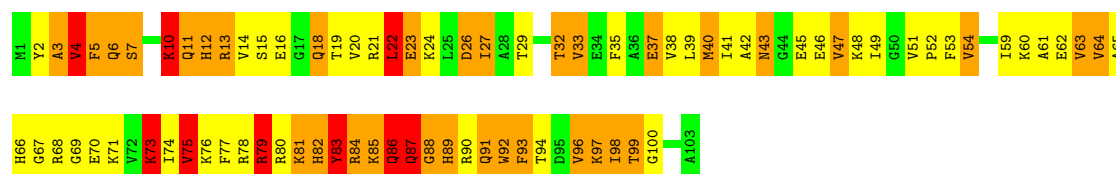
- Molecule 17: 50S ribosomal protein L20

Chain Q:



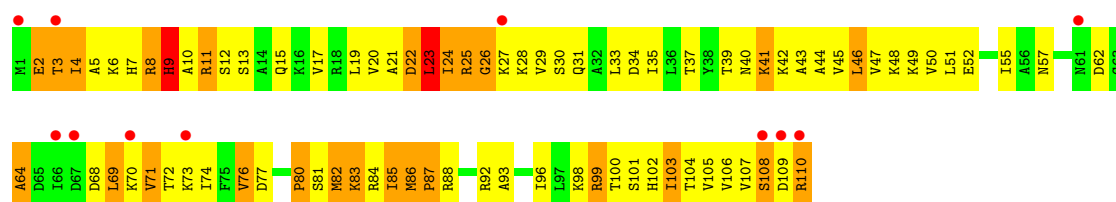
- Molecule 18: 50S ribosomal protein L21

Chain R:



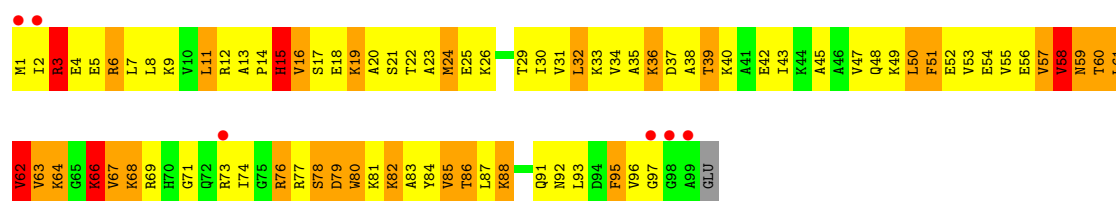
- Molecule 19: 50S ribosomal protein L22

Chain S:



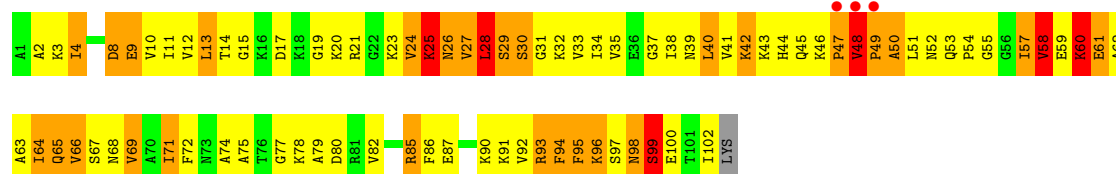
- Molecule 20: 50S ribosomal protein L23

Chain T:



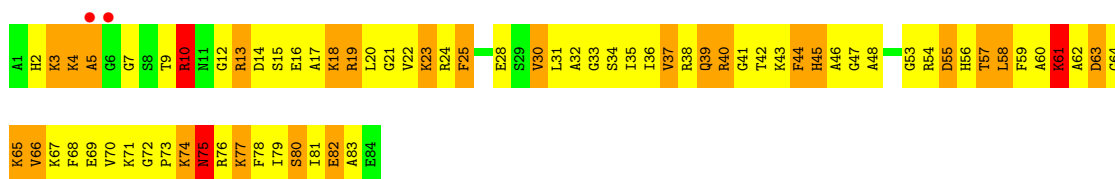
- Molecule 21: 50S ribosomal protein L24

Chain U:



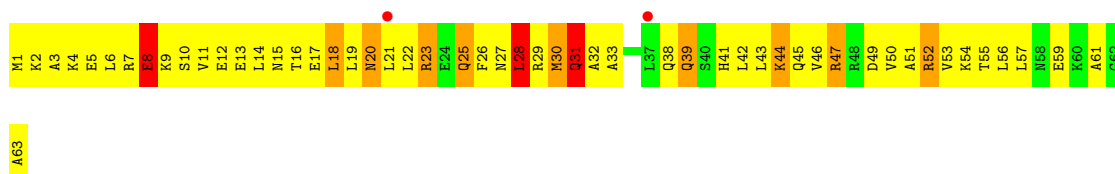
- Molecule 22: 50S ribosomal protein L27

Chain W:



- Molecule 23: 50S ribosomal protein L29

Chain X:



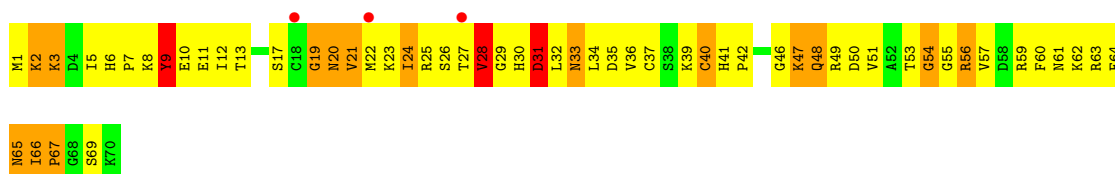
- Molecule 24: 50S ribosomal protein L30

Chain Y:



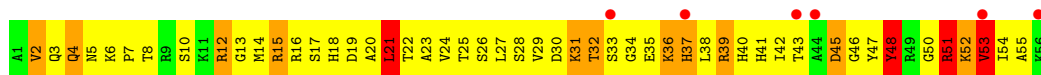
- Molecule 25: 50S ribosomal protein L31

Chain Z:



- Molecule 26: 50S ribosomal protein L32

Chain 0:



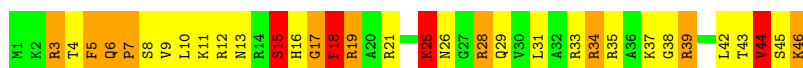
- Molecule 27: 50S ribosomal protein L33

Chain 1:



- Molecule 28: 50S ribosomal protein L34

Chain 2:



- Molecule 29: 50S ribosomal protein L35

P1	P2	P3	P4	P5	P6	P7	P8	P9	P10	P11	P12	P13	P14	P15	P16	P17	P18	P19	P20	P21	P22	P23	P24	P25	P26	P27	P28	P29	P30	P31	P32	P33	P34	P35	P36	P37	P38	P39	P40	P41	P42	P43	P44	P45	P46	P47	P48	P49	P50	P51	P52	P53	P54	P55	P56	P57	P58	P59	P60	P61	P62	P63	P64	P65	P66	P67	P68	P69	P70	P71	P72	P73	P74	P75	P76	P77	P78	P79	P80	P81	P82	P83	P84	P85	P86	P87	P88	P89	P90	P91	P92	P93	P94	P95	P96	P97	P98	P99	P100
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- Chain 4:

M1	K2	V3	R4	A5	S6	V7	K8	K9	L10	C11	R12	N13	C14	K15	I16	V17	K18	R19	D20	G21	V22	I23	R24	V25	I26	C27	S28	A29	E30	P31	K32	H33	K34	Q35	R36	Q37	G38
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- Chain I:

S134	M135	G136	L137	V138	V139	E140	D141	V69	T70	K71	T72	P73	P74	A75	A76	L78	L79	K80	K81	A82	A83	G84	I85	K86	S87	G88	S89	G90	K91	P92	N93	K94	D95	K96	V97	G98	K99	I100	R102	A103	Q104	L105	I108	A109	K112	D115	G118	I121	E122	T125	R126	S127	I128	E129	G130	T131	A132	V133	V134	V135	V136	V137	V138	V139	V140	V141	V142	V143	V144	V145	V146	V147	V148	V149	V150	V151	V152	V153	V154	V155	V156	V157	V158	T159	V160	D63	R64	S65	V66
A1	K2	K3	V4	Q5	A6	Y7	V8	K9	L10	L11	Q12	V13	V14	V15	V16	V17	V18	V19	V20	V21	V22	V23	G24	P25	A26	L27	G28	Q29	Q30	G31	V32	N33	I34	F37	C38	F41	N42	T45	I48	E49	L52	P53	S54	P55	V56	V57	I58	T59	V60	D63	R64	S65	V66																																				

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.85Å 379.20Å 739.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.00 – 3.46 163.96 – 3.46	Depositor EDS
% Data completeness (in resolution range)	91.6 (70.00-3.46) 91.6 (163.96-3.46)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 3.49Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.279 , 0.331 0.470 , 0.481	Depositor DCC
R_{free} test set	34223 reflections (4.94%)	DCC
Wilson B-factor (Å ²)	77.0	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 34.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 720727 reflections	Xtriage
F_o, F_c correlation	0.54	EDS
Total number of atoms	90313	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	A	0.28	0/2803	0.77	0/4371
2	B	0.34	18/68314 (0.0%)	0.79	75/106569 (0.1%)
3	V	0.25	0/766	0.46	0/1025
4	C	0.40	0/2092	0.90	8/2813 (0.3%)
5	D	0.37	0/1586	0.82	4/2134 (0.2%)
6	E	0.70	4/1571 (0.3%)	0.83	5/2113 (0.2%)
7	F	0.41	1/1444 (0.1%)	1.00	10/1937 (0.5%)
8	G	0.30	0/1343	0.67	1/1816 (0.1%)
9	H	0.34	0/1122	0.71	1/1515 (0.1%)
10	J	0.32	0/1135	0.76	3/1529 (0.2%)
11	K	0.35	0/939	0.99	4/1258 (0.3%)
12	L	0.74	1/1062 (0.1%)	1.58	25/1413 (1.8%)
13	M	0.39	0/1093	0.85	5/1460 (0.3%)
14	N	0.37	0/1021	0.80	3/1364 (0.2%)
15	O	0.31	0/910	0.64	0/1219
16	P	0.58	0/929	1.40	16/1242 (1.3%)
17	Q	0.36	0/960	0.75	0/1278
18	R	0.38	0/829	0.82	3/1107 (0.3%)
19	S	0.26	0/864	0.60	0/1156
20	T	0.45	1/784 (0.1%)	0.80	1/1048 (0.1%)
21	U	0.37	0/787	0.94	7/1051 (0.7%)
22	W	0.39	0/642	0.80	2/848 (0.2%)
23	X	0.29	0/510	0.66	0/677
24	Y	0.31	0/453	0.69	1/605 (0.2%)
25	Z	0.52	0/559	0.91	1/745 (0.1%)
26	0	0.41	0/450	0.97	3/599 (0.5%)
27	1	0.32	0/448	0.69	0/594
28	2	0.30	0/380	0.60	0/498
29	3	0.39	0/513	0.80	1/676 (0.1%)
30	4	0.32	0/303	0.77	0/397
31	I	0.60	4/1046 (0.4%)	0.76	4/1410 (0.3%)
All	All	0.36	29/97658 (0.0%)	0.81	183/146467 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	1	65
4	C	0	2
16	P	0	1
18	R	0	1
25	Z	0	1
26	0	0	1
All	All	1	72

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	79	ARG	CD-NE	18.29	1.77	1.46
2	B	1086	A	C5-C6	-17.70	1.25	1.41
2	B	448	U	O4'-C1'	12.68	1.58	1.41
6	E	79	ARG	CG-CD	10.76	1.78	1.51
2	B	1088	A	C6-N1	-10.45	1.28	1.35

The worst 5 of 183 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2791	G	O5'-P-OP2	-27.77	77.38	110.70
2	B	2791	G	O5'-P-OP1	18.50	132.90	110.70
2	B	448	U	N1-C1'-C2'	17.52	136.78	114.00
2	B	2790	U	OP2-P-O3'	14.81	137.79	105.20
12	L	77	ILE	CB-CA-C	-12.70	86.19	111.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	2076	U	C3'

5 of 72 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	78	A	Sidechain
2	B	136	G	Sidechain
2	B	214	G	Sidechain

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Mol	Chain	Res	Type	Group
2	B	221	A	Sidechain
2	B	28	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	A	2507	0	1270	97	0
2	B	60995	0	30677	2356	0
3	V	753	0	780	69	0
4	C	2053	0	2122	429	0
5	D	1565	0	1616	316	0
6	E	1552	0	1619	266	0
7	F	1420	0	1460	177	0
8	G	1323	0	1374	162	0
9	H	1111	0	1148	145	0
10	J	1112	0	1147	231	0
11	K	930	0	1000	125	0
12	L	1053	0	1129	227	0
13	M	1074	0	1157	189	0
14	N	1008	0	1045	133	0
15	O	900	0	935	128	0
16	P	917	0	965	206	0
17	Q	947	0	1022	161	0
18	R	816	0	839	180	0
19	S	857	0	922	111	0
20	T	777	0	840	129	0
21	U	779	0	834	134	0
22	W	634	0	656	156	0
23	X	509	0	543	90	0
24	Y	449	0	491	64	0
25	Z	549	0	552	101	0
26	0	444	0	461	80	0
27	1	441	0	485	69	0
28	2	377	0	418	66	0
29	3	504	0	574	113	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	4	302	0	343	80	0
31	I	1032	0	1088	214	0
32	B	110	0	0	0	0
32	N	1	0	0	0	0
33	2	2	0	0	0	0
33	B	499	0	0	7	0
33	C	1	0	0	0	0
33	D	1	0	0	0	0
33	E	2	0	0	0	0
33	J	2	0	0	1	0
33	L	1	0	0	0	0
33	N	3	0	0	0	0
33	Q	1	0	0	0	0
All	All	90313	0	59512	6243	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 42.

The worst 5 of 6243 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
31:I:3:LYS:CE	31:I:3:LYS:CD	1.74	1.64
6:E:79:ARG:CG	6:E:79:ARG:CD	1.78	1.57
31:I:3:LYS:CG	31:I:3:LYS:CD	1.81	1.56
6:E:79:ARG:NE	6:E:79:ARG:CD	1.77	1.47
2:B:1098:A:H3'	31:I:3:LYS:CA	1.73	1.17

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	V	92/94 (98%)	59 (64%)	27 (29%)	6 (6%)	2 27
4	C	265/273 (97%)	97 (37%)	93 (35%)	75 (28%)	0 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	D	207/209 (99%)	96 (46%)	67 (32%)	44 (21%)	0	2
6	E	199/201 (99%)	87 (44%)	63 (32%)	49 (25%)	0	1
7	F	176/178 (99%)	91 (52%)	53 (30%)	32 (18%)	0	3
8	G	174/176 (99%)	117 (67%)	39 (22%)	18 (10%)	1	12
9	H	147/149 (99%)	84 (57%)	44 (30%)	19 (13%)	0	8
10	J	138/142 (97%)	70 (51%)	36 (26%)	32 (23%)	0	1
11	K	119/123 (97%)	72 (60%)	25 (21%)	22 (18%)	0	2
12	L	142/144 (99%)	66 (46%)	37 (26%)	39 (28%)	0	0
13	M	134/136 (98%)	79 (59%)	31 (23%)	24 (18%)	0	3
14	N	125/127 (98%)	82 (66%)	32 (26%)	11 (9%)	1	17
15	O	115/117 (98%)	63 (55%)	33 (29%)	19 (16%)	0	4
16	P	112/114 (98%)	42 (38%)	38 (34%)	32 (29%)	0	0
17	Q	115/117 (98%)	79 (69%)	22 (19%)	14 (12%)	1	9
18	R	101/103 (98%)	42 (42%)	31 (31%)	28 (28%)	0	0
19	S	108/110 (98%)	67 (62%)	20 (18%)	21 (19%)	0	2
20	T	97/100 (97%)	42 (43%)	32 (33%)	23 (24%)	0	1
21	U	100/103 (97%)	46 (46%)	41 (41%)	13 (13%)	0	8
22	W	82/84 (98%)	31 (38%)	30 (37%)	21 (26%)	0	1
23	X	61/63 (97%)	38 (62%)	15 (25%)	8 (13%)	0	8
24	Y	56/58 (97%)	35 (62%)	17 (30%)	4 (7%)	2	24
25	Z	68/70 (97%)	37 (54%)	22 (32%)	9 (13%)	0	7
26	0	54/56 (96%)	30 (56%)	15 (28%)	9 (17%)	0	4
27	1	52/54 (96%)	21 (40%)	22 (42%)	9 (17%)	0	3
28	2	44/46 (96%)	24 (54%)	12 (27%)	8 (18%)	0	3
29	3	62/64 (97%)	35 (56%)	17 (27%)	10 (16%)	0	4
30	4	36/38 (95%)	13 (36%)	11 (31%)	12 (33%)	0	0
31	I	139/141 (99%)	123 (88%)	11 (8%)	5 (4%)	5	48
All	All	3320/3390 (98%)	1768 (53%)	936 (28%)	616 (19%)	0	2

5 of 616 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	C	21	PRO

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Mol	Chain	Res	Type
4	C	22	GLU
4	C	28	PRO
4	C	29	PHE
4	C	31	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	
3	V	78/78 (100%)	69 (88%)	9 (12%)	8	38
4	C	213/218 (98%)	150 (70%)	63 (30%)	0	3
5	D	164/164 (100%)	113 (69%)	51 (31%)	0	3
6	E	165/165 (100%)	127 (77%)	38 (23%)	1	7
7	F	149/149 (100%)	122 (82%)	27 (18%)	2	14
8	G	137/137 (100%)	111 (81%)	26 (19%)	2	12
9	H	114/114 (100%)	90 (79%)	24 (21%)	1	9
10	J	114/116 (98%)	85 (75%)	29 (25%)	1	5
11	K	102/104 (98%)	81 (79%)	21 (21%)	2	9
12	L	103/103 (100%)	68 (66%)	35 (34%)	0	2
13	M	109/109 (100%)	75 (69%)	34 (31%)	0	3
14	N	103/103 (100%)	76 (74%)	27 (26%)	1	4
15	O	87/87 (100%)	69 (79%)	18 (21%)	2	9
16	P	99/99 (100%)	67 (68%)	32 (32%)	0	2
17	Q	89/89 (100%)	71 (80%)	18 (20%)	2	10
18	R	84/84 (100%)	58 (69%)	26 (31%)	0	3
19	S	93/93 (100%)	77 (83%)	16 (17%)	3	17
20	T	83/84 (99%)	60 (72%)	23 (28%)	0	4
21	U	83/84 (99%)	60 (72%)	23 (28%)	0	4
22	W	62/62 (100%)	45 (73%)	17 (27%)	0	4
23	X	55/55 (100%)	43 (78%)	12 (22%)	1	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	Y	48/48 (100%)	33 (69%)	15 (31%)	0	3
25	Z	62/62 (100%)	46 (74%)	16 (26%)	1	4
26	0	47/47 (100%)	33 (70%)	14 (30%)	0	3
27	1	48/48 (100%)	33 (69%)	15 (31%)	0	3
28	2	38/38 (100%)	27 (71%)	11 (29%)	0	3
29	3	51/51 (100%)	40 (78%)	11 (22%)	1	8
30	4	34/34 (100%)	17 (50%)	17 (50%)	0	0
31	I	109/109 (100%)	104 (95%)	5 (5%)	37	81
All	All	2723/2734 (100%)	2050 (75%)	673 (25%)	1	5

5 of 673 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	L	64	PHE
14	N	87	PHE
27	1	26	LYS
12	L	107	PHE
13	M	76	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 83 such sidechains are listed below:

Mol	Chain	Res	Type
13	M	60	GLN
15	O	67	ASN
25	Z	65	ASN
13	M	97	GLN
14	N	73	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	116/120 (96%)	20 (17%)	1 (0%)
2	B	2837/2904 (97%)	482 (16%)	22 (0%)
All	All	2953/3024 (97%)	502 (16%)	23 (0%)

5 of 502 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	13	G
1	A	15	A
1	A	16	G
1	A	18	G
1	A	25	U

5 of 23 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	1133	A
2	B	1210	G
2	B	2425	A
2	B	1205	A
2	B	1211	C

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 111 ligands modelled in this entry, 111 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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	117/120 (97%)	0.13	3 (2%) 53 23	27, 62, 113, 180	0
2	B	2841/2904 (97%)	0.18	164 (5%) 22 9	5, 39, 133, 180	0
3	V	94/94 (100%)	1.28	24 (25%) 1 2	17, 71, 119, 130	0
4	C	267/273 (97%)	0.37	18 (6%) 17 8	5, 46, 139, 180	0
5	D	209/209 (100%)	0.10	3 (1%) 72 37	5, 60, 139, 180	0
6	E	201/201 (100%)	0.21	11 (5%) 24 10	5, 76, 164, 180	0
7	F	178/178 (100%)	-0.25	1 (0%) 86 58	29, 89, 138, 180	0
8	G	176/176 (100%)	-0.01	4 (2%) 57 26	20, 86, 154, 172	0
9	H	149/149 (100%)	0.12	5 (3%) 43 18	31, 100, 153, 180	0
10	J	140/142 (98%)	0.05	3 (2%) 60 28	14, 61, 136, 162	0
11	K	121/123 (98%)	0.95	15 (12%) 5 3	5, 37, 84, 143	0
12	L	144/144 (100%)	0.45	13 (9%) 10 6	7, 74, 150, 179	0
13	M	136/136 (100%)	0.26	5 (3%) 39 16	10, 66, 152, 180	0
14	N	127/127 (100%)	-0.04	3 (2%) 56 25	5, 45, 143, 180	0
15	O	117/117 (100%)	0.16	6 (5%) 27 11	20, 77, 150, 169	0
16	P	114/114 (100%)	0.06	5 (4%) 33 13	8, 69, 148, 180	0
17	Q	117/117 (100%)	0.12	4 (3%) 43 18	11, 57, 127, 180	0
18	R	103/103 (100%)	0.06	0 100 100	26, 92, 154, 180	0
19	S	110/110 (100%)	0.64	11 (10%) 8 5	5, 45, 137, 175	0
20	T	99/100 (99%)	0.33	6 (6%) 21 9	16, 84, 160, 180	0
21	U	102/103 (99%)	0.11	3 (2%) 49 22	11, 103, 161, 180	0
22	W	84/84 (100%)	0.25	2 (2%) 56 25	20, 81, 149, 180	0
23	X	63/63 (100%)	0.21	2 (3%) 45 19	47, 96, 162, 171	0
24	Y	58/58 (100%)	0.26	5 (8%) 11 6	5, 60, 129, 177	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Z	70/70 (100%)	0.21	3 (4%) 34 14	16, 59, 132, 180	0
26	0	56/56 (100%)	0.55	6 (10%) 6 4	12, 61, 148, 180	0
27	1	54/54 (100%)	0.68	7 (12%) 4 3	22, 77, 153, 173	0
28	2	46/46 (100%)	0.06	0 100 100	13, 48, 112, 129	0
29	3	64/64 (100%)	0.24	2 (3%) 47 21	8, 55, 125, 169	0
30	4	38/38 (100%)	0.00	0 100 100	20, 80, 168, 180	0
31	I	141/141 (100%)	-0.14	2 (1%) 72 37	84, 157, 180, 180	0
All	All	6336/6414 (98%)	0.20	336 (5%) 26 10	5, 55, 151, 180	0

The worst 5 of 336 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1533	C	14.4
2	B	1459	G	10.1
2	B	1532	A	9.1
2	B	1535	A	8.5
2	B	1536	C	7.9

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
32	MG	B	2969	1/1	0.27	19.15	47,47,47,47	1

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	B	2998	1/1	0.33	14.72	5,5,5,5	1
32	MG	B	2938	1/1	0.23	4.32	66,66,66,66	0
32	MG	B	2956	1/1	0.30	3.62	60,60,60,60	0
32	MG	B	2980	1/1	0.52	3.62	17,17,17,17	0
32	MG	B	2990	1/1	0.23	3.35	69,69,69,69	0
32	MG	B	2952	1/1	0.46	2.99	20,20,20,20	0
32	MG	B	2973	1/1	0.27	2.23	44,44,44,44	0
32	MG	B	2993	1/1	0.32	1.89	65,65,65,65	0
32	MG	B	2963	1/1	0.20	1.31	127,127,127,127	0
32	MG	B	2976	1/1	0.20	1.11	30,30,30,30	0
32	MG	B	2939	1/1	0.23	0.46	30,30,30,30	0
32	MG	B	3007	1/1	0.22	-0.06	50,50,50,50	0
32	MG	B	2916	1/1	0.16	-0.21	6,6,6,6	0
32	MG	B	2974	1/1	0.16	-0.35	46,46,46,46	0
32	MG	B	3013	1/1	0.16	-0.42	24,24,24,24	0
32	MG	B	2949	1/1	0.15	-0.57	61,61,61,61	0
32	MG	B	2950	1/1	0.15	-0.65	33,33,33,33	0
32	MG	B	2933	1/1	0.15	-0.70	41,41,41,41	0
32	MG	B	2940	1/1	0.21	-0.76	16,16,16,16	0
32	MG	B	2972	1/1	0.16	-0.80	14,14,14,14	0
32	MG	B	2999	1/1	0.23	-0.83	55,55,55,55	0
32	MG	B	2928	1/1	0.13	-0.95	36,36,36,36	0
32	MG	B	2964	1/1	0.15	-0.97	77,77,77,77	0
32	MG	B	2959	1/1	0.15	-1.05	19,19,19,19	0
32	MG	B	2924	1/1	0.14	-1.13	20,20,20,20	0
32	MG	B	2941	1/1	0.14	-1.14	13,13,13,13	0
32	MG	B	2914	1/1	0.11	-1.24	12,12,12,12	0
32	MG	B	2915	1/1	0.17	-1.24	8,8,8,8	0
32	MG	B	3005	1/1	0.12	-1.27	27,27,27,27	0
32	MG	B	2913	1/1	0.18	-1.32	7,7,7,7	0
32	MG	B	2918	1/1	0.14	-1.42	5,5,5,5	0
32	MG	B	2907	1/1	0.09	-1.54	14,14,14,14	0
32	MG	B	2986	1/1	0.14	-1.55	73,73,73,73	0
32	MG	B	2970	1/1	0.14	-1.56	5,5,5,5	0
32	MG	B	2997	1/1	0.15	-1.57	10,10,10,10	0
32	MG	B	2948	1/1	0.12	-1.61	7,7,7,7	0
32	MG	B	2987	1/1	0.11	-1.76	27,27,27,27	0
32	MG	B	2995	1/1	0.12	-1.79	96,96,96,96	0
32	MG	B	2961	1/1	0.04	-1.82	28,28,28,28	0
32	MG	B	2981	1/1	0.15	-1.83	57,57,57,57	0
32	MG	B	2954	1/1	0.12	-1.84	74,74,74,74	0
32	MG	B	2968	1/1	0.14	-1.88	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	B	3001	1/1	0.14	-1.92	15,15,15,15	0
32	MG	B	2905	1/1	0.12	-1.96	7,7,7,7	0
32	MG	B	2992	1/1	0.12	-2.00	35,35,35,35	0
32	MG	B	2967	1/1	0.05	-2.22	13,13,13,13	0
32	MG	B	2935	1/1	0.13	-2.29	18,18,18,18	0
32	MG	B	2955	1/1	0.08	-2.40	53,53,53,53	0
32	MG	B	2908	1/1	0.12	-2.47	19,19,19,19	0
32	MG	B	2906	1/1	0.10	-2.50	37,37,37,37	0
32	MG	B	2922	1/1	0.09	-2.55	29,29,29,29	0
32	MG	B	2983	1/1	0.10	-2.67	5,5,5,5	0
32	MG	B	3014	1/1	0.10	-2.68	54,54,54,54	0
32	MG	N	128	1/1	0.09	-2.69	49,49,49,49	0
32	MG	B	2978	1/1	0.12	-2.69	25,25,25,25	0
32	MG	B	2910	1/1	0.20	-2.74	5,5,5,5	0
32	MG	B	2944	1/1	0.12	-2.77	5,5,5,5	0
32	MG	B	2960	1/1	0.11	-2.78	11,11,11,11	0
32	MG	B	3006	1/1	0.12	-2.88	26,26,26,26	0
32	MG	B	2977	1/1	0.10	-3.05	16,16,16,16	0
32	MG	B	2979	1/1	0.06	-3.05	5,5,5,5	0
32	MG	B	2947	1/1	0.10	-3.16	9,9,9,9	0
32	MG	B	2923	1/1	0.08	-3.23	5,5,5,5	0
32	MG	B	2994	1/1	0.13	-3.40	28,28,28,28	0
32	MG	B	2982	1/1	0.08	-3.45	18,18,18,18	0
32	MG	B	2946	1/1	0.09	-3.45	27,27,27,27	0
32	MG	B	3011	1/1	0.08	-3.47	19,19,19,19	0
32	MG	B	3000	1/1	0.09	-3.48	20,20,20,20	0
32	MG	B	2996	1/1	0.08	-3.53	23,23,23,23	0
32	MG	B	2966	1/1	0.09	-3.57	43,43,43,43	0
32	MG	B	2975	1/1	0.10	-3.58	39,39,39,39	0
32	MG	B	3010	1/1	0.10	-3.60	21,21,21,21	0
32	MG	B	2919	1/1	0.10	-3.64	49,49,49,49	0
32	MG	B	3009	1/1	0.16	-3.68	23,23,23,23	0
32	MG	B	2931	1/1	0.06	-3.77	10,10,10,10	0
32	MG	B	2971	1/1	0.08	-3.81	17,17,17,17	0
32	MG	B	2929	1/1	0.05	-3.82	21,21,21,21	0
32	MG	B	2989	1/1	0.07	-3.92	17,17,17,17	0
32	MG	B	2934	1/1	0.10	-3.99	23,23,23,23	0
32	MG	B	3002	1/1	0.07	-4.01	18,18,18,18	0
32	MG	B	2942	1/1	0.05	-4.07	16,16,16,16	0
32	MG	B	2985	1/1	0.07	-4.17	25,25,25,25	0
32	MG	B	2984	1/1	0.14	-4.22	12,12,12,12	0
32	MG	B	2909	1/1	0.04	-4.38	9,9,9,9	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	B	2957	1/1	0.12	-4.41	27,27,27,27	0
32	MG	B	2937	1/1	0.19	-4.45	11,11,11,11	0
32	MG	B	2988	1/1	0.07	-4.60	8,8,8,8	0
32	MG	B	3003	1/1	0.05	-4.79	9,9,9,9	0
32	MG	B	3012	1/1	0.07	-4.86	5,5,5,5	0
32	MG	B	2925	1/1	0.11	-4.87	16,16,16,16	0
32	MG	B	2965	1/1	0.12	-4.87	78,78,78,78	0
32	MG	B	2932	1/1	0.10	-5.30	28,28,28,28	0
32	MG	B	2951	1/1	0.10	-5.35	17,17,17,17	0
32	MG	B	2920	1/1	0.10	-5.48	23,23,23,23	0
32	MG	B	2917	1/1	0.12	-5.49	34,34,34,34	0
32	MG	B	2921	1/1	0.08	-5.61	5,5,5,5	0
32	MG	B	2991	1/1	0.05	-5.92	6,6,6,6	0
32	MG	B	3008	1/1	0.05	-6.21	50,50,50,50	0
32	MG	B	2911	1/1	0.06	-6.50	12,12,12,12	0
32	MG	B	2945	1/1	0.09	-6.77	18,18,18,18	0
32	MG	B	2936	1/1	0.10	-6.80	46,46,46,46	0
32	MG	B	2930	1/1	0.10	-7.49	18,18,18,18	0
32	MG	B	2926	1/1	0.05	-7.98	15,15,15,15	0
32	MG	B	2912	1/1	0.09	-8.01	24,24,24,24	0
32	MG	B	2953	1/1	0.04	-8.72	5,5,5,5	0
32	MG	B	2943	1/1	0.06	-9.09	19,19,19,19	0
32	MG	B	2958	1/1	0.07	-9.61	15,15,15,15	0
32	MG	B	2962	1/1	0.10	-10.52	30,30,30,30	1
32	MG	B	3004	1/1	0.07	-10.60	11,11,11,11	0
32	MG	B	2927	1/1	0.07	-13.41	34,34,34,34	0

6.5 Other polymers ⓘ

There are no such residues in this entry.