



# wwPDB X-ray Structure Validation Summary Report i

Feb 28, 2014 – 05:56 PM GMT

PDB ID : 2QBE  
Title : Crystal structure of the bacterial ribosome from Escherichia coli in complex with ribosome recycling factor (RRF). This file contains the 50S subunit of the first 70S ribosome, with RRF bound. The entire crystal structure contains two 70S ribosomes and is described in remark 400.  
Authors : Borovinskaya, M.A.; Pai, R.D.; Zhang, W.; Schuwirth, B.-S.; Holton, J.M.; Hirokawa, G.; Kaji, H.; Kaji, A.; Cate, J.H.D.  
Deposited on : 2007-06-16  
Resolution : 3.30 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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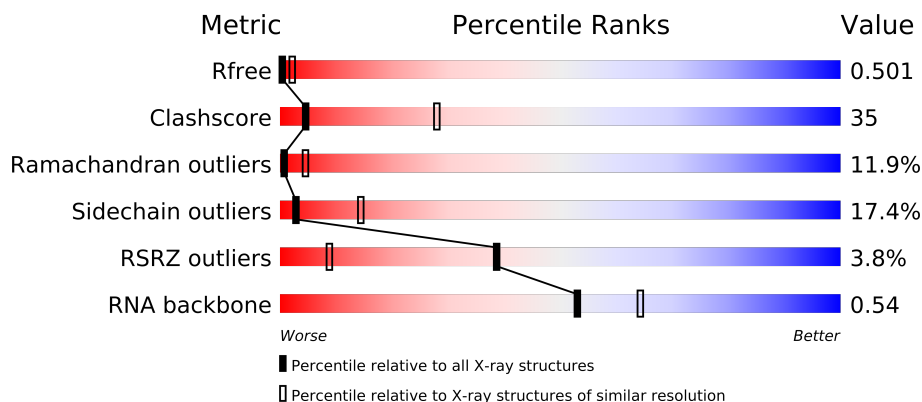
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	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 3.30 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	1341 (3.40-3.20)
Clashscore	79885	1696 (3.40-3.20)
Ramachandran outliers	78287	1664 (3.40-3.20)
Sidechain outliers	78261	1662 (3.40-3.20)
RSRZ outliers	66119	1342 (3.40-3.20)
RNA backbone	1838	1042 (3.90-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	120	
2	B	2904	
3	I	141	
4	C	272	
5	D	209	
6	K	123	
7	P	114	
8	E	201	
9	Y	58	
10	0	56	
11	4	38	
12	1	54	

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Mol	Chain	Length	Quality of chain
13	3	64	
14	V	94	
15	2	46	
16	L	144	
17	M	136	
18	X	63	
19	H	149	
20	J	142	
21	N	127	
22	O	117	
23	Q	117	
24	S	110	
25	U	103	
26	F	178	
27	G	176	
28	R	103	
29	T	100	
30	Z	78	
31	W	84	
32	6	185	

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

Mol	Type	Chain	Res	Geometry	Electron density
33	MG	B	3032	-	X
33	MG	B	3044	-	X
33	MG	B	3141	-	X
33	MG	B	3194	-	X
33	MG	B	3344	-	X
33	MG	B	3400	-	X
33	MG	B	3521	-	X
33	MG	B	3561	-	X

## 2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 91734 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 rRNA.

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 rRNA.

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 L11.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	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 L14.

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

- Molecule 7 is a protein called 50S ribosomal protein L19.

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

- Molecule 8 is a protein called 50S ribosomal protein L4.

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

- Molecule 9 is a protein called 50S ribosomal protein L30.

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

- Molecule 10 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			

- Molecule 11 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

- Molecule 12 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	1	50	Total	C	N	O	0	0	0
			409	263	75	71			

- Molecule 13 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			

- Molecule 14 is a protein called 50S ribosomal protein L25.

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

- Molecule 15 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

- Molecule 16 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	L	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			

- Molecule 17 is a protein called 50S ribosomal protein L16.

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

- Molecule 18 is a protein called 50S ribosomal protein L29.

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

- Molecule 19 is a protein called 50S ribosomal protein L9.

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

- Molecule 20 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	J	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			

- Molecule 21 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	N	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			

- Molecule 22 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	O	116	Total	C	N	O		0	0	0
			892	552	178	162				

- Molecule 23 is a protein called 50S ribosomal protein L20.

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

- Molecule 24 is a protein called 50S ribosomal protein L22.

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

- Molecule 25 is a protein called 50S ribosomal protein L24.

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

- Molecule 26 is a protein called 50S ribosomal protein L5.

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

- Molecule 27 is a protein called 50S ribosomal protein L6.

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

- Molecule 28 is a protein called 50S ribosomal protein L21.

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

- Molecule 29 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	T	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			

- Molecule 30 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	Z	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			

- Molecule 31 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	W	79	Total	C	N	O	S	0	0	0
			596	367	120	108	1			

- Molecule 32 is a protein called ribosome recycling factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	6	185	Total	C	N	O	S	0	0	0
			1478	924	270	282	2			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	B	110	Total	Mg	0	0
			110	110		

- Molecule 34 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	4	1	Total	Zn	0	0
			1	1		

- Molecule 35 is water.



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	B	495	Total 495	O 495	0	0
35	C	4	Total 4	O 4	0	0
35	D	1	Total 1	O 1	0	0
35	E	4	Total 4	O 4	0	0
35	L	1	Total 1	O 1	0	0
35	T	1	Total 1	O 1	0	0

### 3 Residue-property plots

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

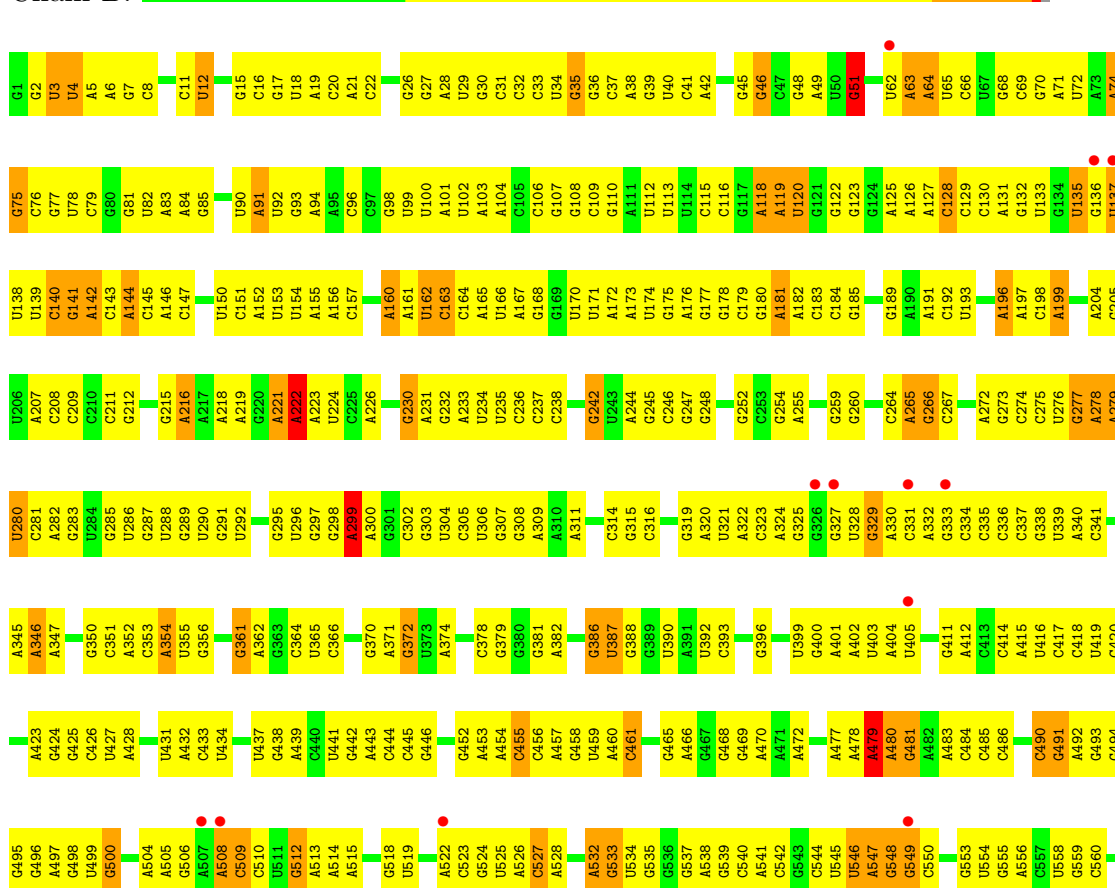
#### • Molecule 1: 5S rRNA

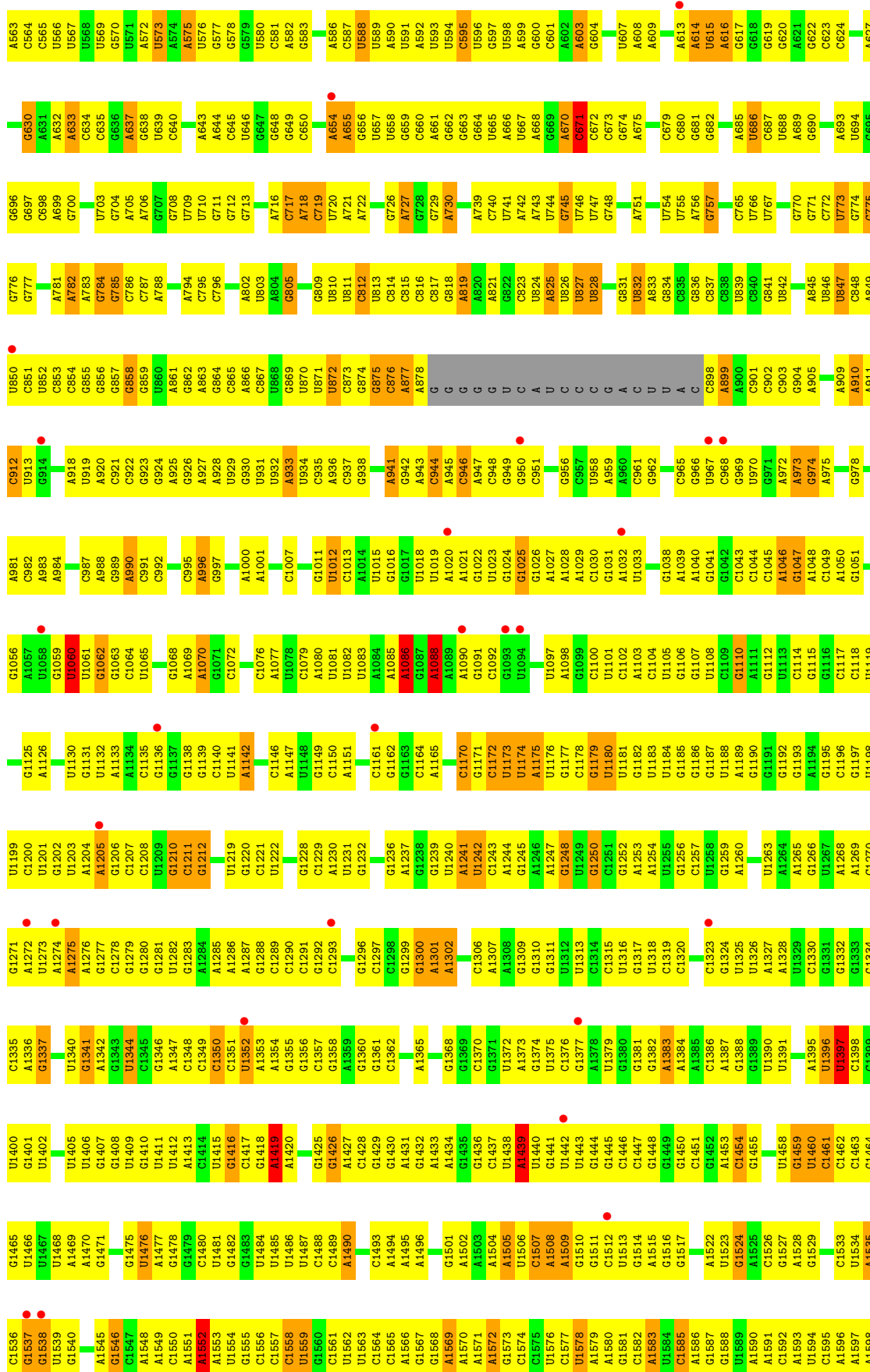
Chain A:



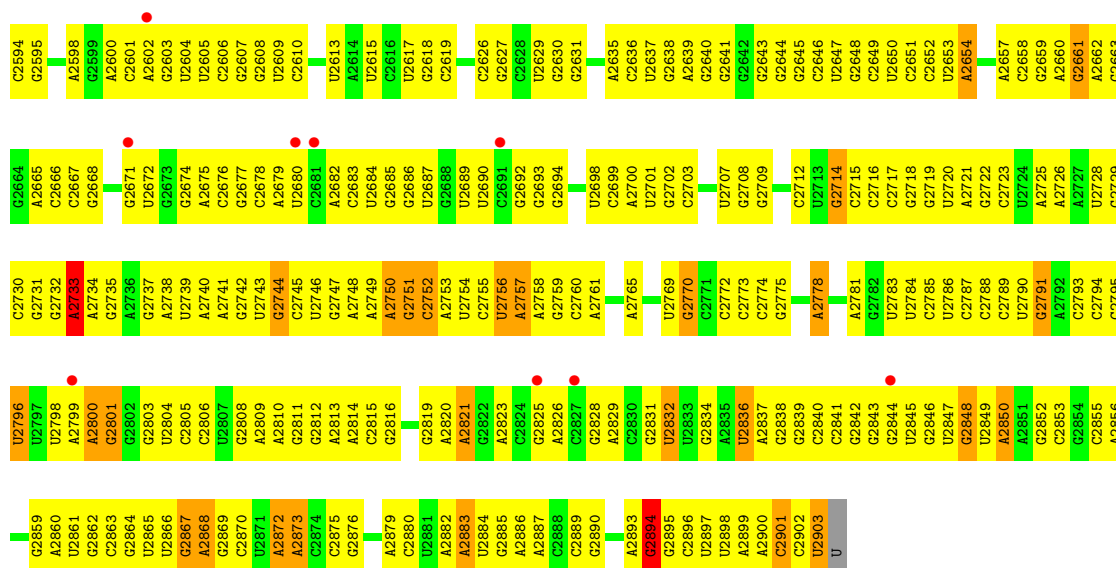
#### • Molecule 2: 23S rRNA

Chain B:



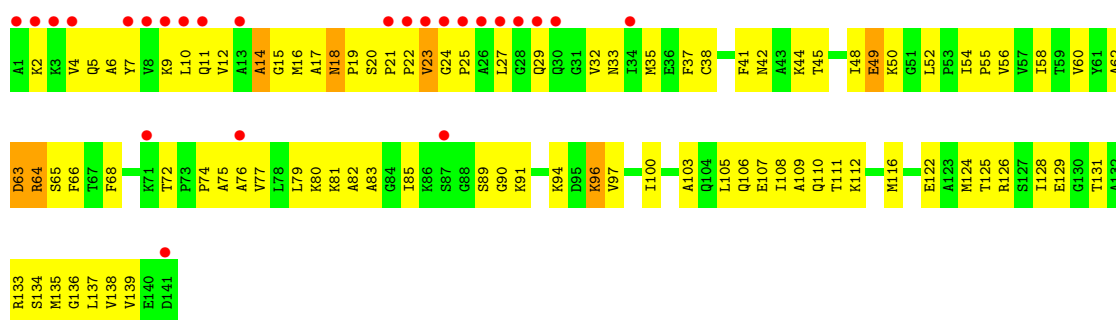


C2512	U2438	G2303	U2233	A	U	G2049	A1966	A1821	A1745	G1681	U1599
A2513	A2439	G2304	G2234	U	G	C2050	C1967	C1822	A1746	G1682	C1600
U2514	C2440	U2305	G2235	A	U	A2051	A1969	G1823	U1747	U1683	
C2515	U2441	C2306	U2236	C	A	G2052	A1970	G1824	C1748	G1684	A1603
A2516	C2442	G2307	G2237	C	G	G2053	U1971	U1825		G1685	
C2517	C2443	C2308	G2238	A	G	A2054	A1972	G1826	A1755	C1686	C1607
U2518	G2444	A2309	G2239	C	A	C2055	G1972	U1827	G1756	A1687	A1608
U2519	A2445	C2310	U2240	C	U	C2056	U1979	A1828	A1757	U1688	A1609
C2520	G2446	A2311	A2241	U	A	G2057	G1980	A1829	U1758	A1689	A1610
U2521	C2447	U2312	G2242	G	G			C1830	A1759	A1690	C1611
C2522	A2448	C2313	U2243	U	G			C1831	C1760	C1691	C1612
G2523	U2449	A2314	U2244	U	U			C1832	C1761	U1692	G1613
U2524	A2450	G2315	U2245	G	G				A1762	U1693	
G2525			G2246	A2183	U	A2060	G1984	C1838	G1763	A1616	
C2526	G2455	G2319	A2247	A2184	G	A2062	C1985		C1764	C1617	
U2527	C2456	U2320	C2248	U2185	A	C2063	A1987	G1842	A1700	G1622	
U2528	U2457	U2321	U2249	C2064	G	C2065	G1988	C1843	G1701	G1623	
G2529	G2458	A2322	G2250	U2187	G	C2066	U1991	C1844	G1702	U1624	
A2530	U2459		G2251	U2188	G	U2067	G1992	G1845	C1703		
C2531	U2460	G2325	C2254	U2189	C	U2068	U1993	G1846	A1705	A1632	
G2532	A2461	C2326		A2191	U	G2069		A1847	A1706	G1633	
U2533	C2462	A2327		U2192	U	A2070	C1996	A1848	G1707	G1634	
G2535	G2463	A2328	C2260		G	A2071	C1997		C1708	U1635	
U2537	U2464	U2329	U2261	U2195	A	C2072	A1998	A1854	U1709	A1636	
C2538		G2330	U2262	C2196	G	C2073	A1999	U1855	G1710	A1637	
C2539	C2467	C2331	C2263	U2197	G	U2074	C2000	G1856	A1711	C1638	
U2540	A2468	A2332	C2264	A2198	U	U2075	C2001	G1857	U1712	C1639	
		G2333	U2265	A2199	G	U2076	C2002	U1927	A1713	A1640	
C2543		U2334	A2266	C2200	G	A2077	C2008	A1928	U1714	A1641	
G2544	A2471	A2335	A2267	C2201	G	C2078	A2009	U1929	G1715	G1642	
U2545	C2472	C2336	A2268	U2202	G	U2079	G2010	U1931	A1789	G1643	
C2547	U2477	G2337	C2269	U2203	A	U2080		U1932	U1716		
U2548	A2478	C2338	A2270	G2204	G	U2081	A2013	G1933	A1717	U1647	
	C2480	A2340	U2271	C2206	G	U2085	A2014	C1934	G1718	U1648	
U2553	U2481	C2341	G2272	C2207	G	U2086	A2015	G1868	G1719	G1649	
U2554		U2342	C2275	C2208	U	G2087	U2016	G1869	U1720		
C2555					G	A2088		C1870	G1721		
U2556		U2343	A2281	A2211	G	C2089	A2020	A1871	A1722	A1652	
G2557	C2482	G2345	G2282	A2212	C	A2090	C2021	G1872	G1723	G1653	
C2558	G2484	A2346	C2283	U2213	G	C2091	U2022	A1873	G1724	A1654	
	U2485	C2347	A2284	C2214	A	U2092	C2023	G1874	U1725	A1655	
U2564	C2486	A2352	C2285	C2215	C	G2093	G2024	G1875	C1726	C1656	
C2565		G2353	G2286	G2216	U	A2094	C2025	A1801	C1727	U1657	
U2566		C2354	A2287	G2217	U	C2095	U2026	A1802	G1728	C1658	
G2567	G2490	G2355	G2288	U2218	G	A2096	U2027	A1803	U1729	G1659	
U2568	U2491	U2356	G2289	U2219	G	A2097	G1947	C1804	C1730	G1660	
G2569		G2357	G2290	G2220	A	U2098	G2029	U1882	G1731	G1661	
	C2496	A2358	U2291	G2221	G	A2099	A2030	U1883	C1732	U1662	
U2578	U2497	C2359	U2292	C2222	C	G2100	A2031	G1884	G1733		
C2579	C2498	G2360	G2293	G2223	C	A2101	G2032	A1809	A1734	A1665	
	U2500	A2425	G2294	G2224	G	G2102	A2033	A1810	A1735	G1666	
U2585	C2501	C2362	U2295	A2225	A			G1811	U1736	G1667	
U2586	G2502	G2363	U2296	C2226	C	C2104	A2037	U1812	G1737	A1668	
	U2584	G2428	A2297	A2227	U	U2105	G1957	G1813	G1738	A1669	
U2590	G2505	C2364	U2298	G2228	U	U2106	C1958	A1889	A1739		
C2591	U2506	G2365	U2299	U2229	G	G2107	G2040	G1816	G1740	G1674	
G2592		A2366	C2300	G2230	A	A2108	U2041	G1817	C1741	A1678	
U2593		C2368	U2302	C2232	A	U2109	A2042	U1818	U1742	A1679	
						G2110	C2043	G1819	G1743	U1680	



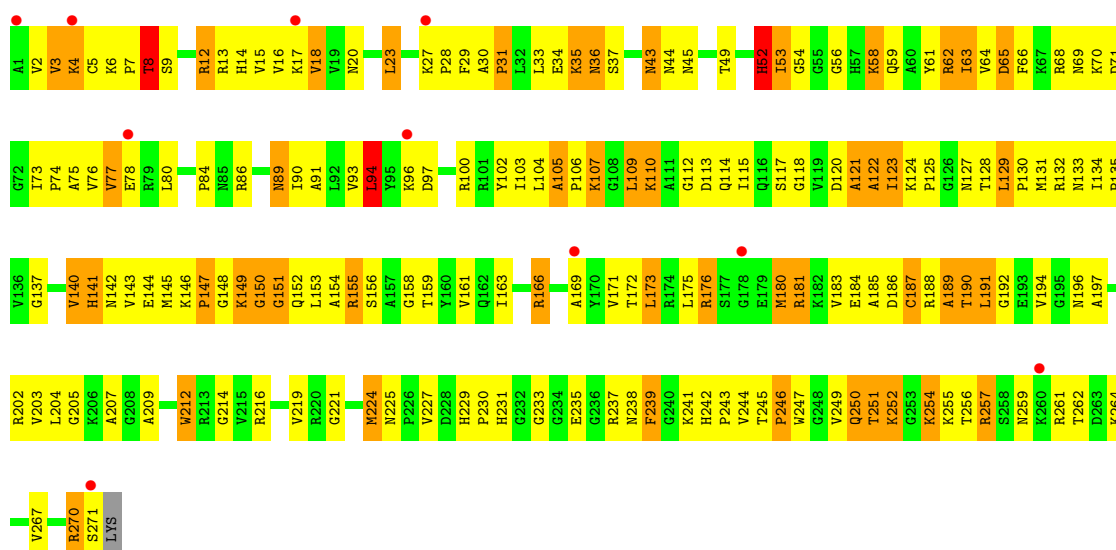
• Molecule 3: 50S ribosomal protein L11

Chain I:

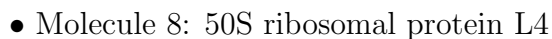


• Molecule 4: 50S ribosomal protein L2

Chain C:



• Molecule 5: 50S ribosomal protein L3



- Molecule 9: 50S ribosomal protein L30

Chain Y: 

- Molecule 10: 50S ribosomal protein L32

Chain 0: 

- Molecule 11: 50S ribosomal protein L36

Chain 4: 

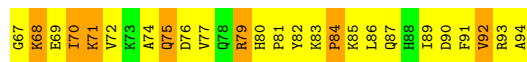
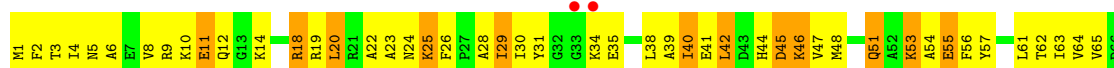
- Molecule 12: 50S ribosomal protein L33

Chain 1: 

- Molecule 13: 50S ribosomal protein L35

Chain 3: 

- Molecule 14: 50S ribosomal protein L25

Chain V: 

- Molecule 15: 50S ribosomal protein L34

Chain 2: 

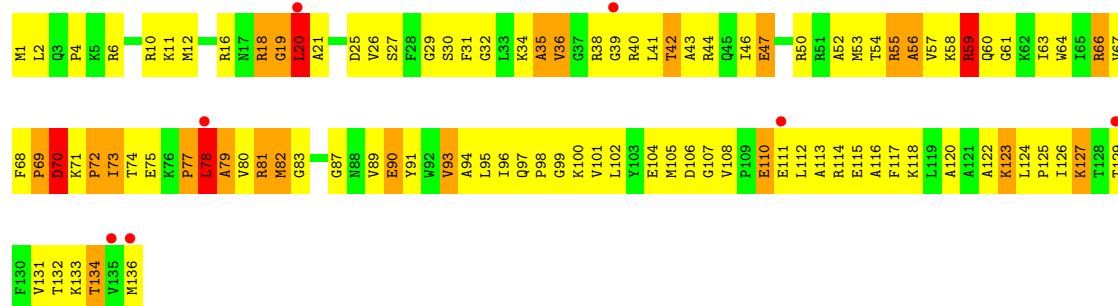
- Molecule 16: 50S ribosomal protein L15

Chain L: 



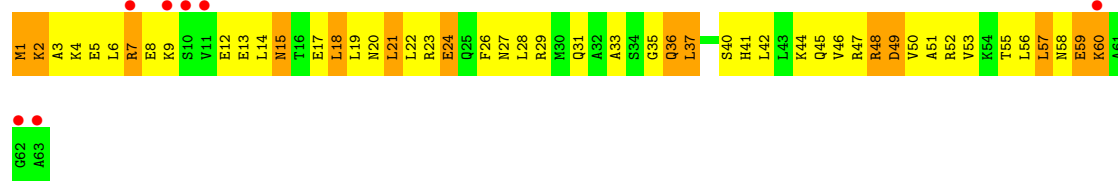
• Molecule 17: 50S ribosomal protein L16

Chain M:



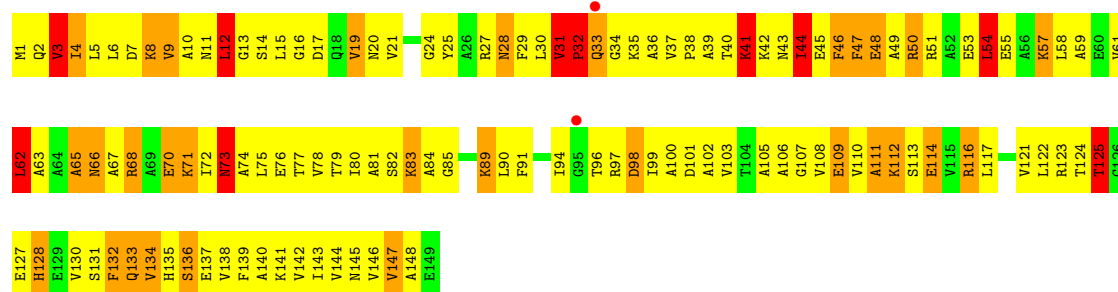
• Molecule 18: 50S ribosomal protein L29

Chain X:



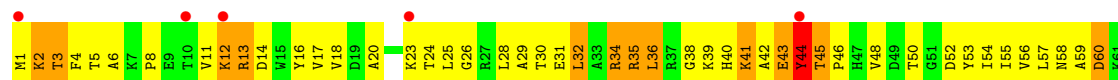
• Molecule 19: 50S ribosomal protein L9

Chain H:

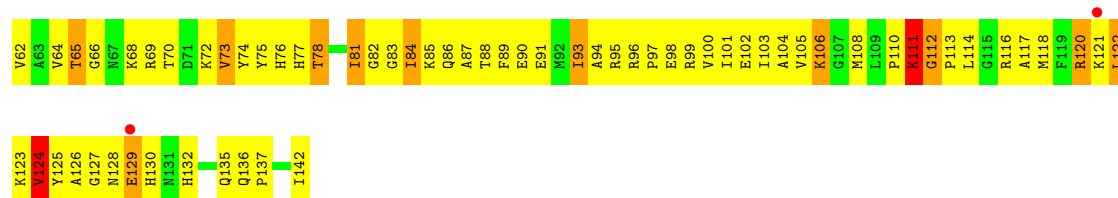


• Molecule 20: 50S ribosomal protein L13

Chain J:

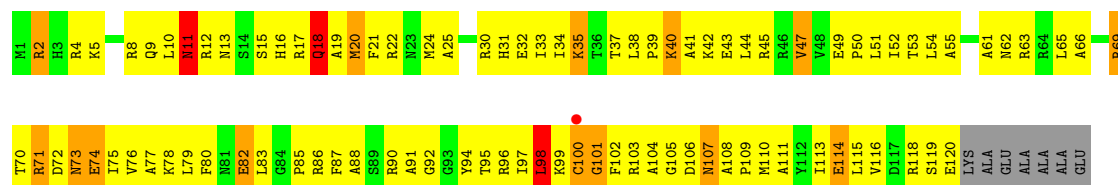






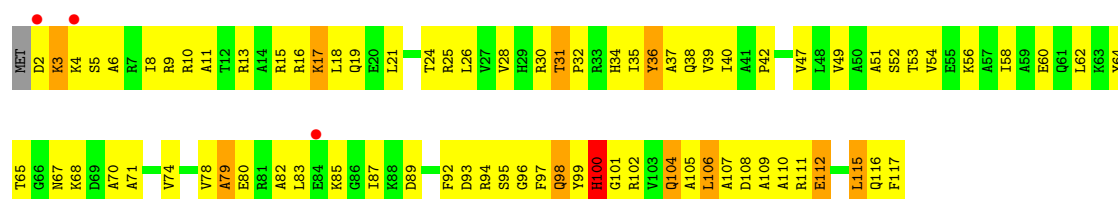
• Molecule 21: 50S ribosomal protein L17

Chain N:



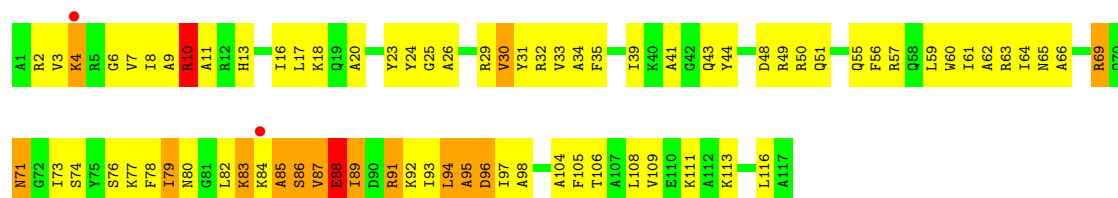
• Molecule 22: 50S ribosomal protein L18

Chain O:



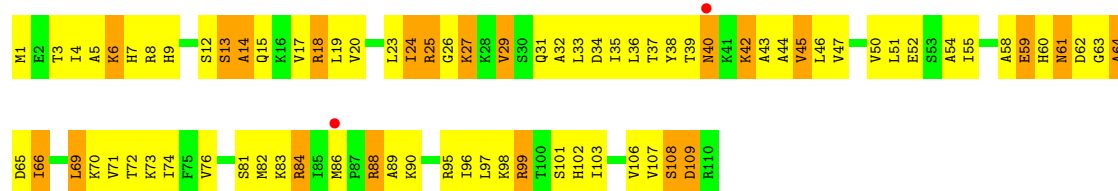
• Molecule 23: 50S ribosomal protein L20

Chain Q:



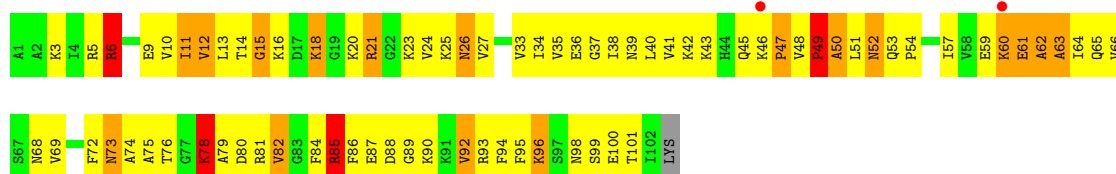
• Molecule 24: 50S ribosomal protein L22

Chain S:



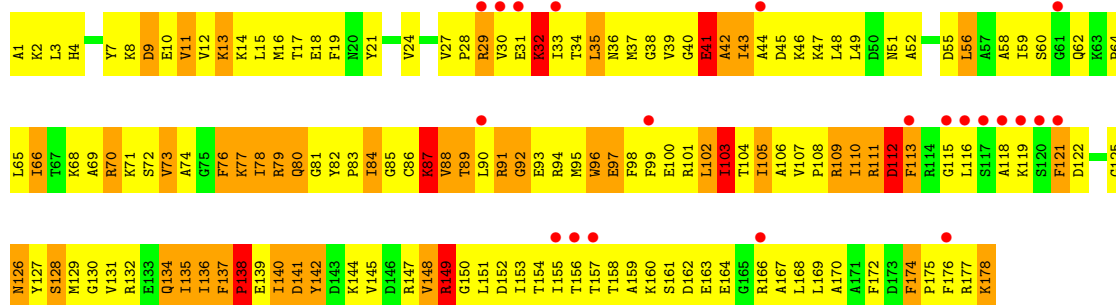
• Molecule 25: 50S ribosomal protein L24

Chain U:



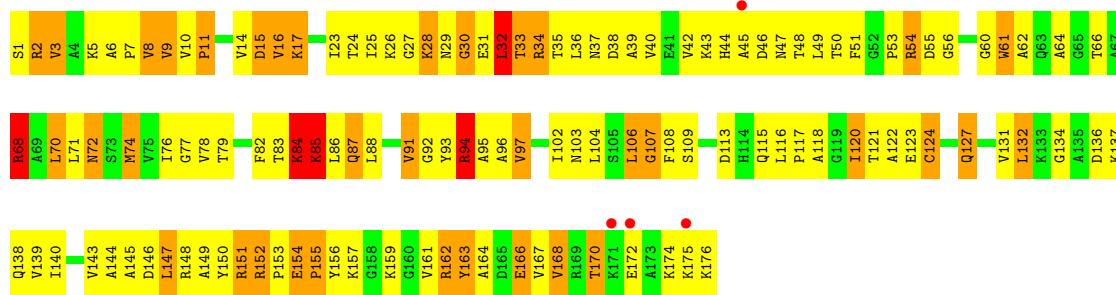
• Molecule 26: 50S ribosomal protein L5

Chain F:



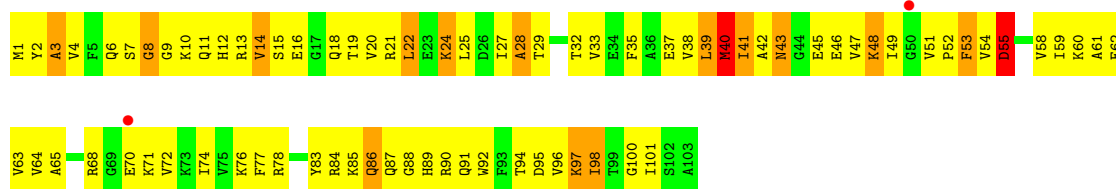
• Molecule 27: 50S ribosomal protein L6

Chain G:



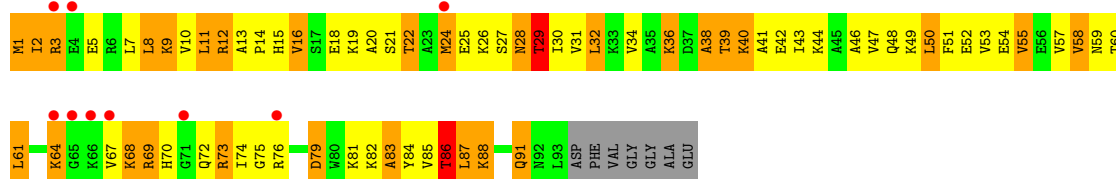
• Molecule 28: 50S ribosomal protein L21

Chain R:

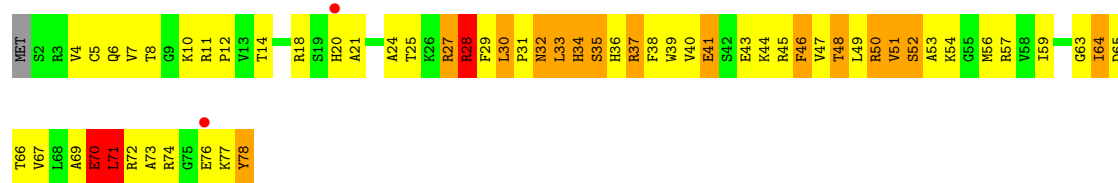


• Molecule 29: 50S ribosomal protein L23

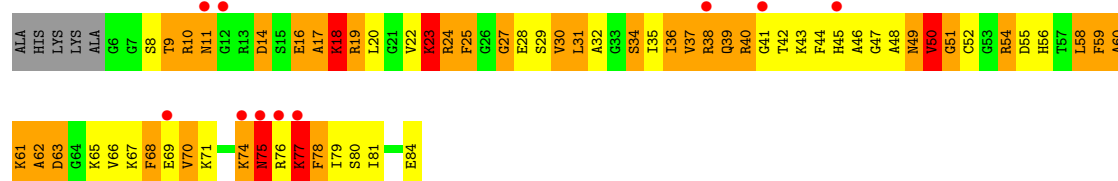
Chain T:



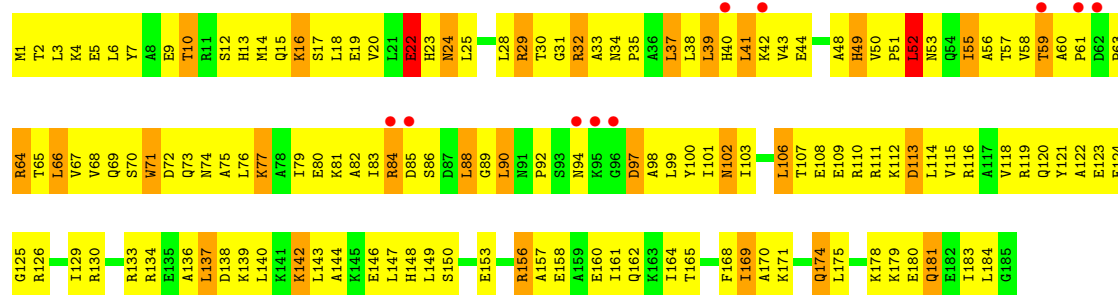
- Molecule 30: 50S ribosomal protein L28

Chain Z: 

- Molecule 31: 50S ribosomal protein L27

Chain W: 

- Molecule 32: ribosome recycling factor

Chain 6: 

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	207.90Å 378.20Å 736.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.30 82.86 – 3.32	Depositor EDS
% Data completeness (in resolution range)	85.8 (40.00-3.30) 87.1 (82.86-3.32)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.17 (at 3.33Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.275 , 0.304 0.496 , 0.501	Depositor DCC
$R_{free}$ test set	26469 reflections (3.58%)	DCC
Wilson B-factor (Å <sup>2</sup> )	83.9	Xtriage
Anisotropy	0.393	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 36.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 738833 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.56	EDS
Total number of atoms	91734	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.37% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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: ZN, 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	0.25	0/2803	0.74	1/4371 (0.0%)
2	B	0.28	6/68314 (0.0%)	0.77	55/106569 (0.1%)
3	I	0.24	0/1046	0.47	0/1410
4	C	0.22	0/2121	0.48	0/2852
5	D	0.24	0/1586	0.49	0/2134
6	K	0.24	0/939	0.55	0/1258
7	P	0.25	0/929	0.50	0/1242
8	E	0.24	0/1571	0.51	0/2113
9	Y	0.23	0/453	0.50	0/605
10	O	0.22	0/450	0.56	0/599
11	4	0.23	0/303	0.47	0/397
12	1	0.27	0/416	0.49	0/554
13	3	0.24	0/513	0.47	0/676
14	V	0.25	0/766	0.43	0/1025
15	2	0.26	0/380	0.48	0/498
16	L	0.23	0/1054	0.49	0/1403
17	M	0.25	0/1093	0.49	0/1460
18	X	0.24	0/510	0.52	0/677
19	H	0.25	0/1122	0.48	0/1515
20	J	0.23	0/1152	0.48	0/1551
21	N	0.24	0/973	0.51	0/1301
22	O	0.23	0/902	0.49	0/1209
23	Q	0.25	0/960	0.49	0/1278
24	S	0.22	0/864	0.52	0/1156
25	U	0.25	0/787	0.47	0/1051
26	F	0.26	0/1444	0.52	0/1937
27	G	0.23	0/1343	0.48	0/1816
28	R	0.25	0/829	0.49	0/1107
29	T	0.23	0/744	0.55	0/994
30	Z	0.25	0/635	0.52	0/848
31	W	0.28	0/603	0.52	0/797
32	6	0.24	0/1497	0.48	0/2017

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.27	6/99102 (0.0%)	0.71	56/148420 (0.0%)

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
2	B	0	29

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1086	A	C5-C6	-16.41	1.26	1.41
2	B	1088	A	C6-N1	-10.54	1.28	1.35
2	B	1060	U	C2-N3	7.86	1.43	1.37
2	B	2181	U	C4'-C3'	-7.35	1.45	1.53
2	B	1086	A	N3-C4	-6.62	1.30	1.34

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2204	G	O5'-P-OP2	-27.99	77.11	110.70
2	B	2791	G	O5'-P-OP1	-27.68	77.49	110.70
2	B	2204	G	O5'-P-OP1	17.95	132.24	110.70
2	B	2791	G	O5'-P-OP2	17.88	132.16	110.70
2	B	2790	U	OP1-P-O3'	14.44	136.96	105.20

There are no chirality outliers.

5 of 29 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	221	A	Sidechain
2	B	222	A	Sidechain
2	B	299	A	Sidechain
2	B	3	U	Sidechain
2	B	51	G	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	89	0
2	B	60995	0	30679	2161	0
3	I	1032	0	1088	112	0
4	C	2082	0	2157	231	0
5	D	1565	0	1616	186	0
6	K	930	0	1000	109	0
7	P	917	0	965	134	0
8	E	1552	0	1619	188	0
9	Y	449	0	491	52	0
10	O	444	0	461	39	0
11	4	302	0	340	50	0
12	1	409	0	440	51	0
13	3	504	0	574	54	0
14	V	753	0	780	86	0
15	2	377	0	418	34	0
16	L	1045	0	1117	138	0
17	M	1074	0	1157	120	0
18	X	509	0	543	56	0
19	H	1111	0	1148	220	0
20	J	1129	0	1162	156	0
21	N	960	0	1000	111	0
22	O	892	0	923	76	0
23	Q	947	0	1022	125	0
24	S	857	0	922	94	0
25	U	779	0	834	111	0
26	F	1420	0	1460	242	0
27	G	1323	0	1374	158	0
28	R	816	0	839	85	0
29	T	738	0	807	120	0
30	Z	625	0	652	63	0
31	W	596	0	610	138	0
32	6	1478	0	1526	204	0
33	B	110	0	0	0	0
34	4	1	0	0	0	0
35	B	495	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	C	4	0	0	0	0
35	D	1	0	0	0	0
35	E	4	0	0	0	0
35	L	1	0	0	0	0
35	T	1	0	0	0	0
All	All	91734	0	60994	5338	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 35.

The worst 5 of 5338 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:855:G:H21	31:W:23:LYS:HG2	1.08	1.11
16:L:143:GLU:HG2	16:L:144:GLU:H	1.13	1.11
8:E:21:ARG:HD2	8:E:107:SER:HB3	1.29	1.11
19:H:83:LYS:HA	19:H:148:ALA:HA	1.33	1.08
5:D:148:GLN:HG3	5:D:152:PRO:HG2	1.33	1.08

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	I	139/141 (99%)	119 (86%)	15 (11%)	5 (4%)	5	40
4	C	269/272 (99%)	176 (65%)	61 (23%)	32 (12%)	1	4
5	D	207/209 (99%)	123 (59%)	56 (27%)	28 (14%)	0	3
6	K	119/123 (97%)	80 (67%)	25 (21%)	14 (12%)	1	4
7	P	112/114 (98%)	68 (61%)	29 (26%)	15 (13%)	0	3
8	E	199/201 (99%)	126 (63%)	54 (27%)	19 (10%)	1	9
9	Y	56/58 (97%)	39 (70%)	11 (20%)	6 (11%)	1	6
10	0	54/56 (96%)	40 (74%)	5 (9%)	9 (17%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	4	36/38 (95%)	22 (61%)	5 (14%)	9 (25%)	0	0
12	1	48/54 (89%)	37 (77%)	6 (12%)	5 (10%)	1	7
13	3	62/64 (97%)	42 (68%)	14 (23%)	6 (10%)	1	8
14	V	92/94 (98%)	71 (77%)	18 (20%)	3 (3%)	6	43
15	2	44/46 (96%)	36 (82%)	7 (16%)	1 (2%)	10	54
16	L	141/144 (98%)	92 (65%)	31 (22%)	18 (13%)	0	3
17	M	134/136 (98%)	90 (67%)	24 (18%)	20 (15%)	0	2
18	X	61/63 (97%)	40 (66%)	17 (28%)	4 (7%)	2	19
19	H	147/149 (99%)	74 (50%)	50 (34%)	23 (16%)	0	1
20	J	140/142 (99%)	96 (69%)	31 (22%)	13 (9%)	1	9
21	N	118/127 (93%)	84 (71%)	25 (21%)	9 (8%)	2	15
22	O	114/117 (97%)	87 (76%)	21 (18%)	6 (5%)	3	26
23	Q	115/117 (98%)	81 (70%)	21 (18%)	13 (11%)	1	5
24	S	108/110 (98%)	72 (67%)	21 (19%)	15 (14%)	0	2
25	U	100/103 (97%)	58 (58%)	27 (27%)	15 (15%)	0	2
26	F	176/178 (99%)	106 (60%)	36 (20%)	34 (19%)	0	1
27	G	174/176 (99%)	108 (62%)	41 (24%)	25 (14%)	0	2
28	R	101/103 (98%)	74 (73%)	16 (16%)	11 (11%)	1	6
29	T	91/100 (91%)	52 (57%)	23 (25%)	16 (18%)	0	1
30	Z	75/78 (96%)	50 (67%)	16 (21%)	9 (12%)	1	4
31	W	77/84 (92%)	32 (42%)	20 (26%)	25 (32%)	0	0
32	6	183/185 (99%)	140 (76%)	36 (20%)	7 (4%)	5	37
All	All	3492/3582 (98%)	2315 (66%)	762 (22%)	415 (12%)	1	4

5 of 415 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	I	18	ASN
4	C	4	LYS
4	C	107	LYS
4	C	141	HIS
4	C	149	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	I	109/109 (100%)	107 (98%)	2 (2%)	71	93
4	C	216/217 (100%)	186 (86%)	30 (14%)	5	25
5	D	164/164 (100%)	146 (89%)	18 (11%)	9	38
6	K	102/104 (98%)	84 (82%)	18 (18%)	3	13
7	P	99/99 (100%)	78 (79%)	21 (21%)	1	7
8	E	165/165 (100%)	136 (82%)	29 (18%)	3	13
9	Y	48/48 (100%)	41 (85%)	7 (15%)	5	23
10	0	47/47 (100%)	37 (79%)	10 (21%)	1	7
11	4	34/34 (100%)	26 (76%)	8 (24%)	1	4
12	1	45/48 (94%)	39 (87%)	6 (13%)	6	27
13	3	51/51 (100%)	47 (92%)	4 (8%)	18	60
14	V	78/78 (100%)	59 (76%)	19 (24%)	1	3
15	2	38/38 (100%)	32 (84%)	6 (16%)	4	18
16	L	102/103 (99%)	92 (90%)	10 (10%)	12	45
17	M	109/109 (100%)	90 (83%)	19 (17%)	3	14
18	X	55/55 (100%)	43 (78%)	12 (22%)	1	7
19	H	114/114 (100%)	79 (69%)	35 (31%)	0	1
20	J	116/116 (100%)	96 (83%)	20 (17%)	3	15
21	N	100/103 (97%)	84 (84%)	16 (16%)	3	18
22	O	86/87 (99%)	74 (86%)	12 (14%)	5	25
23	Q	89/89 (100%)	78 (88%)	11 (12%)	7	31
24	S	93/93 (100%)	82 (88%)	11 (12%)	8	34
25	U	83/84 (99%)	71 (86%)	12 (14%)	5	23
26	F	149/149 (100%)	114 (76%)	35 (24%)	1	4
27	G	137/137 (100%)	106 (77%)	31 (23%)	1	5
28	R	84/84 (100%)	71 (84%)	13 (16%)	4	19
29	T	80/84 (95%)	59 (74%)	21 (26%)	1	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	Z	67/68 (98%)	52 (78%)	15 (22%)	1	6
31	W	59/62 (95%)	42 (71%)	17 (29%)	0	2
32	6	157/157 (100%)	126 (80%)	31 (20%)	2	9
All	All	2876/2896 (99%)	2377 (83%)	499 (17%)	3	14

5 of 499 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	H	31	VAL
21	N	35	LYS
31	W	49	ASN
19	H	50	ARG
19	H	141	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 117 such sidechains are listed below:

Mol	Chain	Res	Type
17	M	22	GLN
19	H	133	GLN
31	W	39	GLN
17	M	88	ASN
18	X	41	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	116/120 (96%)	18 (15%)	0
2	B	2837/2904 (97%)	448 (15%)	20 (0%)
All	All	2953/3024 (97%)	466 (15%)	20 (0%)

5 of 466 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	12	C
1	A	13	G
1	A	16	G
1	A	25	U
1	A	26	C

5 of 20 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	1301	A
2	B	1419	A
2	B	2425	A
2	B	1205	A
2	B	1210	G

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 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, 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	A	117/120 (97%)	-0.01	2 (1%) 67 21	46, 80, 115, 168	0
2	B	2841/2904 (97%)	0.08	74 (2%) 53 13	16, 56, 145, 180	0
3	I	141/141 (100%)	0.88	25 (17%) 2 1	62, 152, 180, 180	0
4	C	271/272 (99%)	0.24	10 (3%) 39 9	9, 45, 87, 170	0
5	D	209/209 (100%)	0.21	7 (3%) 44 10	22, 66, 124, 167	0
6	K	121/123 (98%)	0.16	5 (4%) 35 8	16, 67, 120, 154	0
7	P	114/114 (100%)	0.35	8 (7%) 16 4	27, 77, 122, 160	0
8	E	201/201 (100%)	0.15	9 (4%) 32 7	16, 67, 132, 148	0
9	Y	58/58 (100%)	0.35	1 (1%) 67 21	42, 73, 129, 143	0
10	0	56/56 (100%)	0.55	2 (3%) 41 9	33, 71, 126, 141	0
11	4	38/38 (100%)	0.47	2 (5%) 25 6	23, 75, 134, 149	0
12	1	50/54 (92%)	0.01	0 100 100	43, 79, 117, 132	0
13	3	64/64 (100%)	0.73	6 (9%) 9 3	31, 51, 91, 115	0
14	V	94/94 (100%)	0.10	2 (2%) 60 17	32, 90, 135, 169	0
15	2	46/46 (100%)	0.34	1 (2%) 59 16	13, 40, 87, 121	0
16	L	143/144 (99%)	0.12	4 (2%) 50 12	13, 64, 117, 161	0
17	M	136/136 (100%)	0.23	7 (5%) 27 6	24, 68, 124, 174	0
18	X	63/63 (100%)	0.23	7 (11%) 6 2	20, 86, 141, 171	0
19	H	149/149 (100%)	0.10	2 (1%) 74 27	37, 121, 160, 180	0
20	J	142/142 (100%)	0.31	7 (4%) 28 6	25, 73, 126, 137	0
21	N	120/127 (94%)	0.20	1 (0%) 83 39	20, 65, 117, 173	0
22	O	116/117 (99%)	0.03	3 (2%) 53 13	27, 82, 128, 179	0
23	Q	117/117 (100%)	0.06	2 (1%) 67 21	5, 64, 111, 163	0
24	S	110/110 (100%)	0.12	2 (1%) 65 20	15, 58, 112, 161	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	U	102/103 (99%)	0.13	2 (1%) 62 19	26, 75, 130, 171	0
26	F	178/178 (100%)	0.56	21 (11%) 5 2	42, 113, 160, 180	0
27	G	176/176 (100%)	0.10	4 (2%) 57 15	51, 103, 141, 162	0
28	R	103/103 (100%)	0.15	2 (1%) 64 20	27, 86, 128, 157	0
29	T	93/100 (93%)	0.34	9 (9%) 8 2	31, 70, 134, 164	0
30	Z	77/78 (98%)	0.18	2 (2%) 53 13	22, 50, 93, 129	0
31	W	79/84 (94%)	0.63	10 (12%) 4 2	29, 81, 126, 153	0
32	6	185/185 (100%)	0.30	10 (5%) 25 6	33, 116, 167, 180	0
All	All	6510/6606 (98%)	0.18	249 (3%) 38 9	5, 66, 147, 180	0

The worst 5 of 249 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	27	LEU	11.7
3	I	26	ALA	8.0
26	F	31	GLU	6.9
18	X	63	ALA	6.7
32	6	95	LYS	6.6

## 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, 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	B	3521	1/1	0.65	16.17	38,38,38,38	1
33	MG	B	3194	1/1	0.41	9.32	94,94,94,94	0
33	MG	B	3561	1/1	0.88	8.19	75,75,75,75	1
33	MG	B	3400	1/1	0.38	4.19	17,17,17,17	0
33	MG	B	3344	1/1	0.30	4.17	32,32,32,32	0
33	MG	B	3044	1/1	0.45	4.08	93,93,93,93	0
33	MG	B	3141	1/1	0.26	2.15	47,47,47,47	0
33	MG	B	3032	1/1	0.32	2.01	28,28,28,28	0
33	MG	B	3181	1/1	0.24	1.98	46,46,46,46	0
33	MG	B	3021	1/1	0.32	1.89	52,52,52,52	0
33	MG	B	3550	1/1	0.20	1.89	30,30,30,30	0
33	MG	B	3600	1/1	0.26	1.73	37,37,37,37	0
33	MG	B	3464	1/1	0.22	1.54	57,57,57,57	0
33	MG	B	3496	1/1	0.21	1.17	100,100,100,100	0
33	MG	B	3227	1/1	0.19	0.79	43,43,43,43	0
33	MG	B	3270	1/1	0.21	0.25	70,70,70,70	0
33	MG	B	3590	1/1	0.20	-0.03	36,36,36,36	0
33	MG	B	3169	1/1	0.16	-0.08	28,28,28,28	0
33	MG	B	3509	1/1	0.21	-0.14	78,78,78,78	0
33	MG	B	3206	1/1	0.18	-0.25	41,41,41,41	0
33	MG	B	3471	1/1	0.19	-0.28	35,35,35,35	0
33	MG	B	3130	1/1	0.19	-0.33	44,44,44,44	0
33	MG	B	3265	1/1	0.23	-0.39	69,69,69,69	0
33	MG	B	3555	1/1	0.20	-0.39	51,51,51,51	0
33	MG	B	3418	1/1	0.19	-0.41	44,44,44,44	0
33	MG	B	3369	1/1	0.32	-0.45	31,31,31,31	0
33	MG	B	3516	1/1	0.21	-0.46	51,51,51,51	0
33	MG	B	3096	1/1	0.18	-0.52	59,59,59,59	0
33	MG	B	3359	1/1	0.17	-0.58	41,41,41,41	0
33	MG	B	3157	1/1	0.12	-0.72	34,34,34,34	0
33	MG	B	3232	1/1	0.17	-0.75	60,60,60,60	0
33	MG	B	3240	1/1	0.14	-0.85	123,123,123,123	0
33	MG	B	3085	1/1	0.17	-0.97	40,40,40,40	0
34	ZN	4	617	1/1	0.07	-1.07	55,55,55,55	0
33	MG	B	3014	1/1	0.14	-1.18	47,47,47,47	0
33	MG	B	3028	1/1	0.13	-1.26	24,24,24,24	0
33	MG	B	3289	1/1	0.16	-1.44	28,28,28,28	0
33	MG	B	3476	1/1	0.15	-1.49	38,38,38,38	0
33	MG	B	3212	1/1	0.08	-1.60	39,39,39,39	0
33	MG	B	3038	1/1	0.12	-1.61	74,74,74,74	0
33	MG	B	3201	1/1	0.12	-1.63	35,35,35,35	0
33	MG	B	3607	1/1	0.09	-1.66	42,42,42,42	0
33	MG	B	3326	1/1	0.17	-1.67	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	B	3145	1/1	0.14	-1.67	49,49,49,49	0
33	MG	B	3612	1/1	0.07	-1.68	56,56,56,56	0
33	MG	B	3499	1/1	0.13	-1.71	75,75,75,75	0
33	MG	B	3217	1/1	0.05	-1.78	23,23,23,23	0
33	MG	B	3353	1/1	0.07	-1.79	38,38,38,38	0
33	MG	B	3001	1/1	0.11	-1.80	35,35,35,35	0
33	MG	B	3457	1/1	0.14	-1.80	63,63,63,63	0
33	MG	B	3596	1/1	0.08	-1.81	31,31,31,31	0
33	MG	B	3056	1/1	0.11	-1.84	70,70,70,70	0
33	MG	B	3331	1/1	0.12	-1.84	37,37,37,37	0
33	MG	B	3066	1/1	0.08	-1.85	32,32,32,32	0
33	MG	B	3221	1/1	0.06	-1.86	98,98,98,98	0
33	MG	B	3577	1/1	0.14	-1.89	20,20,20,20	0
33	MG	B	3428	1/1	0.13	-1.92	21,21,21,21	0
33	MG	B	3078	1/1	0.09	-1.98	58,58,58,58	0
33	MG	B	3061	1/1	0.09	-2.01	30,30,30,30	0
33	MG	B	3531	1/1	0.15	-2.03	25,25,25,25	0
33	MG	B	3276	1/1	0.12	-2.09	30,30,30,30	0
33	MG	B	3382	1/1	0.09	-2.16	21,21,21,21	0
33	MG	B	3164	1/1	0.11	-2.17	46,46,46,46	0
33	MG	B	3050	1/1	0.12	-2.19	87,87,87,87	0
33	MG	B	3282	1/1	0.12	-2.20	26,26,26,26	0
33	MG	B	3188	1/1	0.09	-2.21	34,34,34,34	0
33	MG	B	3135	1/1	0.08	-2.25	23,23,23,23	0
33	MG	B	3349	1/1	0.13	-2.25	47,47,47,47	0
33	MG	B	3364	1/1	0.14	-2.26	52,52,52,52	0
33	MG	B	3110	1/1	0.08	-2.43	37,37,37,37	0
33	MG	B	3090	1/1	0.12	-2.51	34,34,34,34	0
33	MG	B	3450	1/1	0.14	-2.52	47,47,47,47	0
33	MG	B	3394	1/1	0.13	-2.54	43,43,43,43	0
33	MG	B	3586	1/1	0.09	-2.57	65,65,65,65	0
33	MG	B	3488	1/1	0.07	-2.70	56,56,56,56	0
33	MG	B	3412	1/1	0.15	-2.73	25,25,25,25	0
33	MG	B	3480	1/1	0.11	-2.77	30,30,30,30	0
33	MG	B	3321	1/1	0.08	-2.88	41,41,41,41	0
33	MG	B	3376	1/1	0.08	-2.89	40,40,40,40	0
33	MG	B	3528	1/1	0.09	-2.91	21,21,21,21	0
33	MG	B	3423	1/1	0.06	-2.95	70,70,70,70	0
33	MG	B	3124	1/1	0.06	-2.95	43,43,43,43	0
33	MG	B	3505	1/1	0.12	-2.97	38,38,38,38	0
33	MG	B	3175	1/1	0.14	-3.00	40,40,40,40	0
33	MG	B	3389	1/1	0.07	-3.08	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	B	3007	1/1	0.08	-3.26	12,12,12,12	0
33	MG	B	3537	1/1	0.08	-3.35	37,37,37,37	0
33	MG	B	3568	1/1	0.11	-3.43	22,22,22,22	0
33	MG	B	3573	1/1	0.10	-3.47	38,38,38,38	0
33	MG	B	3103	1/1	0.15	-3.55	45,45,45,45	0
33	MG	B	3433	1/1	0.10	-3.66	37,37,37,37	0
33	MG	B	3582	1/1	0.06	-3.68	20,20,20,20	0
33	MG	B	3253	1/1	0.08	-3.71	70,70,70,70	0
33	MG	B	3246	1/1	0.12	-3.72	53,53,53,53	0
33	MG	B	3492	1/1	0.13	-3.84	45,45,45,45	0
33	MG	B	3259	1/1	0.10	-3.94	41,41,41,41	0
33	MG	B	3439	1/1	0.10	-4.19	43,43,43,43	0
33	MG	B	3406	1/1	0.10	-4.32	35,35,35,35	0
33	MG	B	3484	1/1	0.07	-4.45	38,38,38,38	0
33	MG	B	3072	1/1	0.06	-4.65	36,36,36,36	0
33	MG	B	3235	1/1	0.10	-4.78	22,22,22,22	0
33	MG	B	3316	1/1	0.06	-5.16	57,57,57,57	0
33	MG	B	3302	1/1	0.03	-5.29	25,25,25,25	0
33	MG	B	3444	1/1	0.07	-5.32	36,36,36,36	0
33	MG	B	3151	1/1	0.09	-5.55	28,28,28,28	0
33	MG	B	3295	1/1	0.07	-5.94	35,35,35,35	0
33	MG	B	3543	1/1	0.10	-6.00	101,101,101,101	0
33	MG	B	3512	1/1	0.09	-6.96	31,31,31,31	0
33	MG	B	3117	1/1	0.05	-7.18	20,20,20,20	0
33	MG	B	3309	1/1	0.11	-7.26	61,61,61,61	0
33	MG	B	3338	1/1	0.13	-10.63	33,33,33,33	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.