



wwPDB X-ray Structure Validation Summary Report i

Feb 28, 2014 – 09:20 AM GMT

PDB ID : 3CF5
Title : Thiopeptide antibiotic Thiostrepton bound to the large ribosomal subunit of *Deinococcus radiodurans*
Authors : Harms, J.M.; Wilson, D.N.; Schlutzen, F.; Connell, S.R.; Stachelhaus, T.; Zaborowska, Z.; Spahn, C.M.T.; Fucini, P.
Deposited on : 2008-03-02
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
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

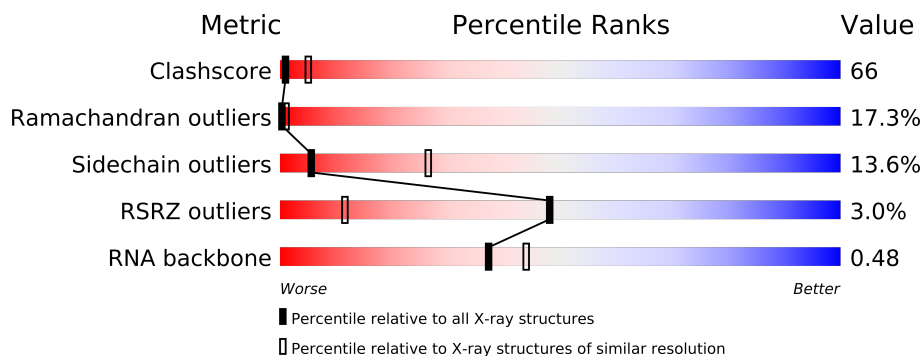
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.30 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))
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 ≥ 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	1	55	
2	2	47	
3	3	66	
4	4	37	
5	5	19	
6	A	274	
7	B	211	
8	C	205	
9	D	180	
10	E	185	
11	F	144	
12	G	174	
13	H	134	
14	I	156	

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Mol	Chain	Length	Quality of chain
15	J	142	
16	K	116	
17	L	114	
18	M	166	
19	N	118	
20	O	100	
21	P	134	
22	Q	95	
23	R	115	
24	S	237	
25	T	91	
26	U	81	
27	V	67	
28	W	55	
29	X	2880	
30	Y	60	
31	Z	123	

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	M	167	-	X
32	MG	X	2881	-	X
32	MG	X	2882	-	X
32	MG	X	2884	-	X
32	MG	X	2885	-	X
32	MG	X	2886	-	X
32	MG	X	2887	-	X
32	MG	X	2888	-	X
32	MG	X	2889	-	X
32	MG	X	2890	-	X
32	MG	X	2891	-	X
32	MG	X	2893	-	X
32	MG	X	2894	-	X
32	MG	X	2896	-	X
32	MG	X	2897	-	X
32	MG	X	2898	-	X
32	MG	X	2899	-	X
32	MG	X	2900	-	X
32	MG	X	2902	-	X
32	MG	X	2903	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
32	MG	X	2904	-	X
32	MG	X	2905	-	X
32	MG	X	2907	-	X
32	MG	X	2909	-	X
32	MG	X	2910	-	X
32	MG	Z	124	-	X
32	MG	Z	125	-	X
32	MG	Z	126	-	X
32	MG	Z	127	-	X

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 84475 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 protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	1	53	Total C 53 53	0	0	53

- Molecule 2 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	2	46	Total C 46 46	0	0	46

- Molecule 3 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	3	63	Total C 63 63	0	0	63

- Molecule 4 is a protein called 50S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	4	37	Total C N O S 297 179 66 47 5	0	0	0

- Molecule 5 is a protein called THIOSTREPTON.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	5	19	Total C N O S 114 72 19 18 5	0	0	1

- Molecule 6 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	A	240	Total C N O S 1826 1137 366 321 2	0	0	0

- Molecule 7 is a protein called 50S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	B	205	Total	C	N	O	S	0	0	0
			1539	965	295	271	8			

- Molecule 8 is a protein called 50S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	C	197	Total	C	N	O	S	0	0	0
			1506	935	287	282	2			

- Molecule 9 is a protein called 50S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	D	177	Total	C	N	O	S	0	0	0
			1400	892	247	254	7			

- Molecule 10 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	E	171	Total	C	N	O	S	0	0	0
			1286	812	237	236	1			

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	F	144	Total	C	N	O	S	0	0	0
			1044	663	179	197	5			

- Molecule 12 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	G	142	Total	C	N	O	S	0	0	0
			1114	704	209	198	3			

- Molecule 13 is a protein called 50S RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	H	134	Total	C	N	O	S	0	0	0
			997	614	198	180	5			

- Molecule 14 is a protein called 50S RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	I	141	Total	C	N	O	0	0	0
			1067	655	216	196			

- Molecule 15 is a protein called 50S RIBOSOMAL PROTEIN L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	J	136	Total	C	N	O	S	0	0	0
			1090	696	202	185	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	1	MET	-	INITIATING METHIONINE	UNP Q9RXJ5

- Molecule 16 is a protein called 50S RIBOSOMAL PROTEIN L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	K	113	Total	C	N	O	S	0	0	0
			878	541	178	157	2			

- Molecule 17 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	L	104	Total	C	N	O	0	0	0
			779	476	161	142			

- Molecule 18 is a protein called 50S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	M	108	Total	C	N	O	0	0	0
			871	543	172	156			

- Molecule 19 is a protein called 50S RIBOSOMAL PROTEIN L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	N	117	Total	C	N	O	S	0	0	0
			978	608	210	159	1			

- Molecule 20 is a protein called 50S RIBOSOMAL PROTEIN L21.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	O	94	Total	C	N	O	0	0	0
			741	465	139	137			

- Molecule 21 is a protein called 50S RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	P	127	Total	C	N	O	S	0	0	0
			1014	639	199	174	2			

- Molecule 22 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	Q	93	Total	C	N	O	S	0	0	0
			726	458	136	130	2			

- Molecule 23 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	R	110	Total	C	N	O	S	0	0	0
			825	513	160	151	1			

- Molecule 24 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	S	175	Total	C	N	O	S	0	0	0
			1345	849	236	254	6			

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	T	84	Total	C	N	O	S	0	0	0
			625	393	122	109	1			

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	U	72	Total	C	N	O	0	0	0
			552	341	116	95			

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	V	66	Total	C	N	O	S	0	0	0
			533	327	107	96	3			

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	W	55	Total	C	N	O	S	0	0	0
			424	264	82	76	2			

- Molecule 29 is a RNA chain called RRNA-23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	X	2686	Total	C	N	O	P	0	0	0
			57651	25718	10642	18606	2685			

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	Y	58	Total	C	N	O	S	0	0	0
			457	281	94	77	5			

- Molecule 31 is a RNA chain called RRNA-5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	Z	122	Total	C	N	O	P	0	0	0
			2598	1161	476	840	121			

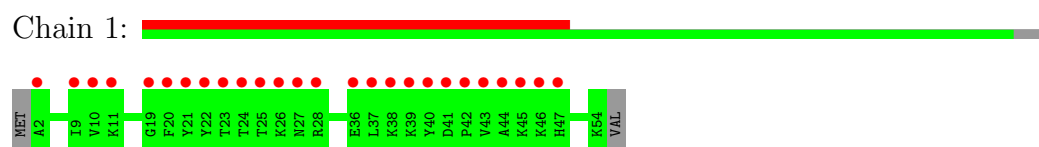
- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	X	30	Total	Mg	0	0
			30	30		
32	Z	5	Total	Mg	0	0
			5	5		
32	M	1	Total	Mg	0	0
			1	1		

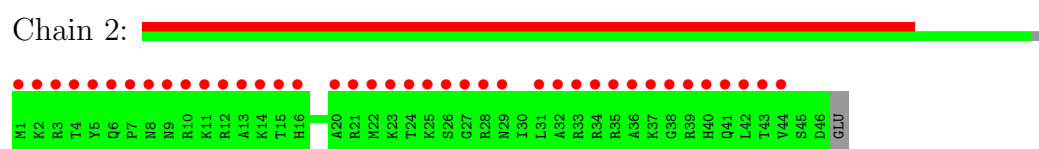
3 Residue-property plots

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

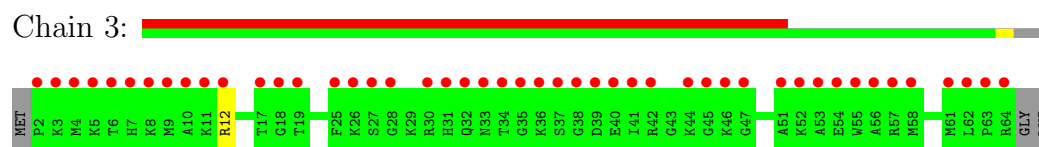
- Molecule 1: 50S RIBOSOMAL PROTEIN L33



- Molecule 2: 50S RIBOSOMAL PROTEIN L34



- Molecule 3: 50S RIBOSOMAL PROTEIN L35



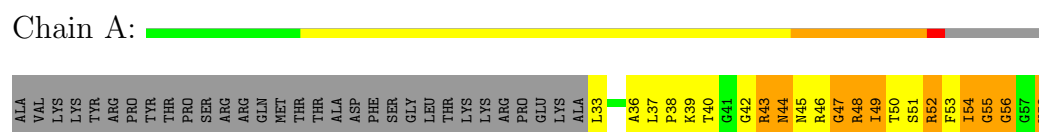
- Molecule 4: 50S RIBOSOMAL PROTEIN L36

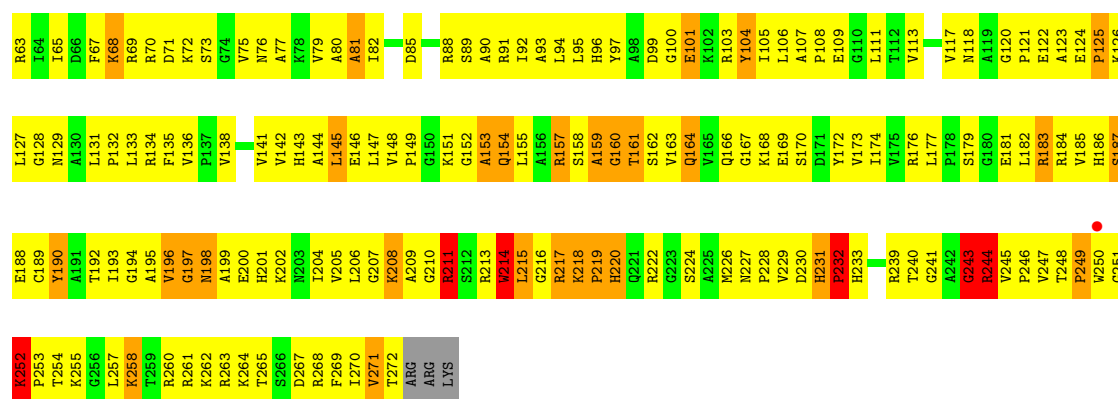


- Molecule 5: THIOSTREPTON



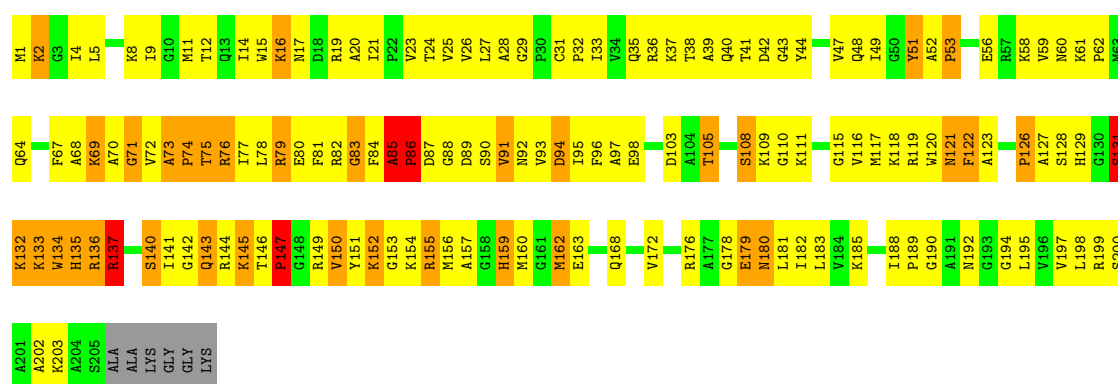
- Molecule 6: 50S RIBOSOMAL PROTEIN L2





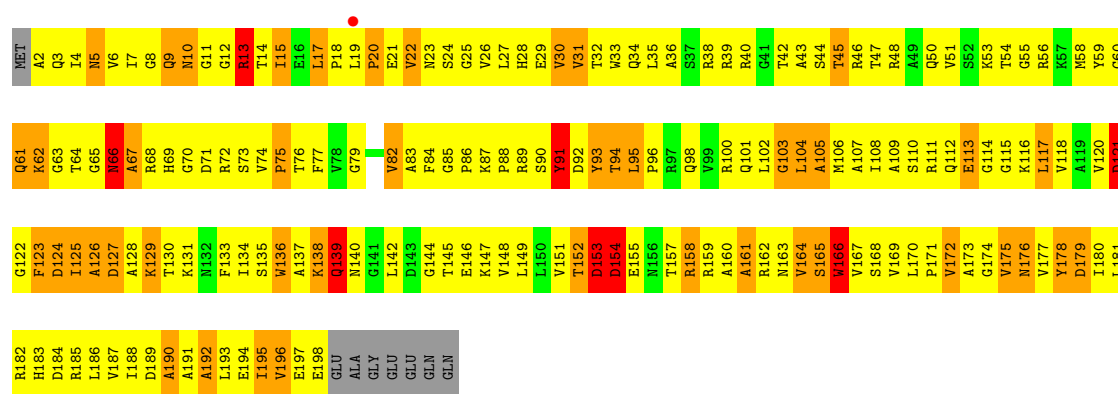
• Molecule 7: 50S RIBOSOMAL PROTEIN L3

Chain B:



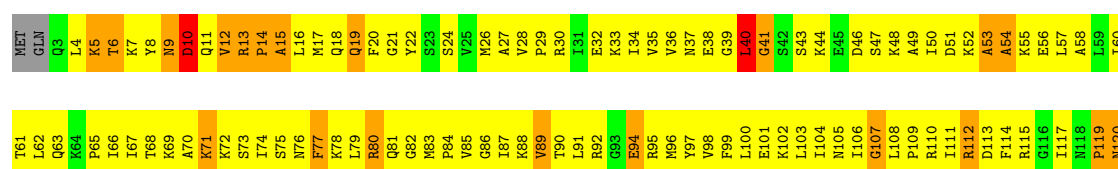
• Molecule 8: 50S RIBOSOMAL PROTEIN L4

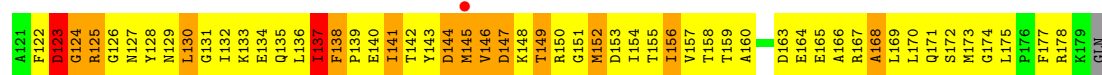
Chain C:



• Molecule 9: 50S RIBOSOMAL PROTEIN L5

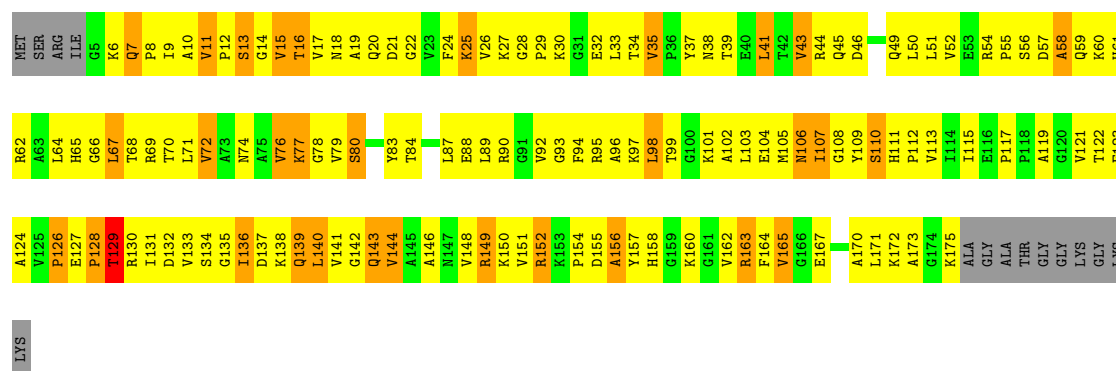
Chain D:





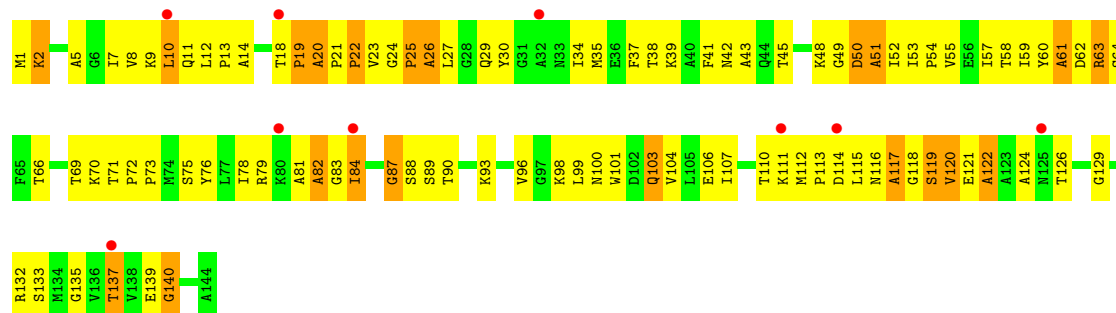
• Molecule 10: 50S RIBOSOMAL PROTEIN L6

Chain E:



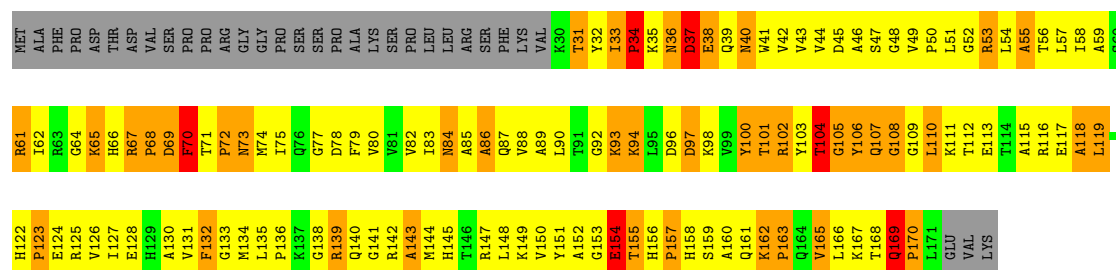
• Molecule 11: 50S RIBOSOMAL PROTEIN L11

Chain F:



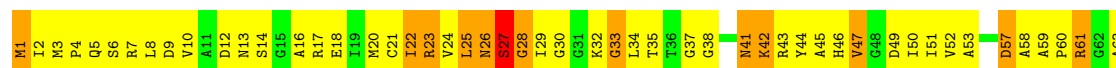
• Molecule 12: 50S RIBOSOMAL PROTEIN L13

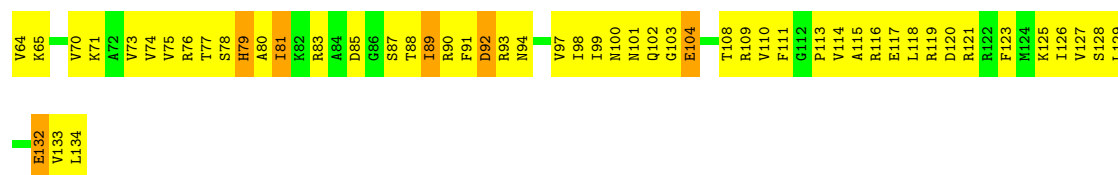
Chain G:



• Molecule 13: 50S RIBOSOMAL PROTEIN L14

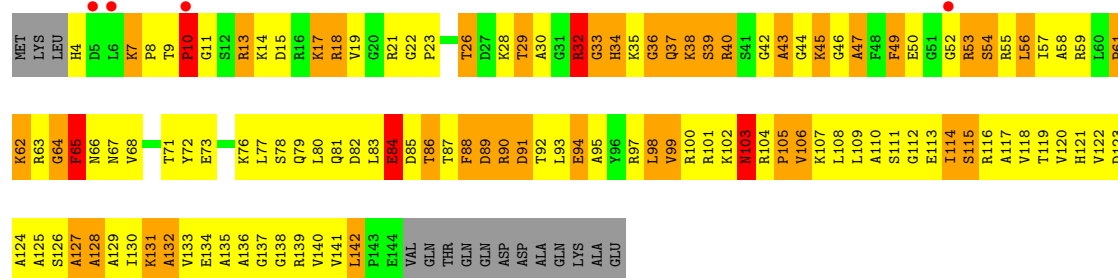
Chain H:





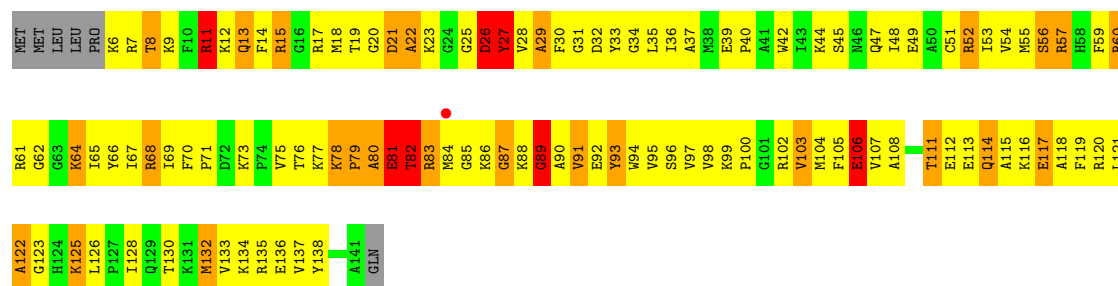
• Molecule 14: 50S RIBOSOMAL PROTEIN L15

Chain I:



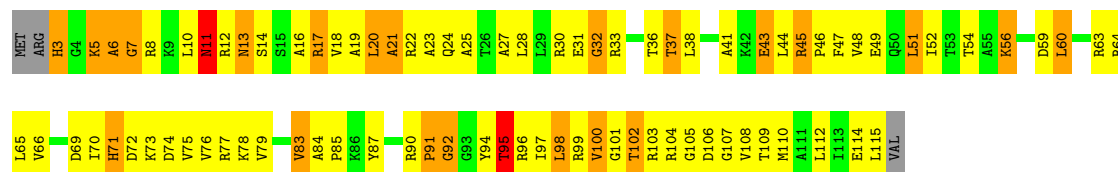
• Molecule 15: 50S RIBOSOMAL PROTEIN L16

Chain J:



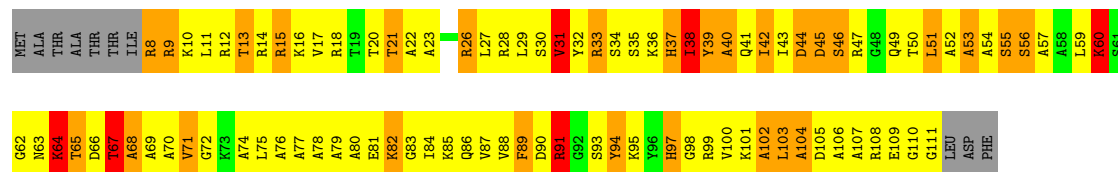
• Molecule 16: 50S RIBOSOMAL PROTEIN L17

Chain K:



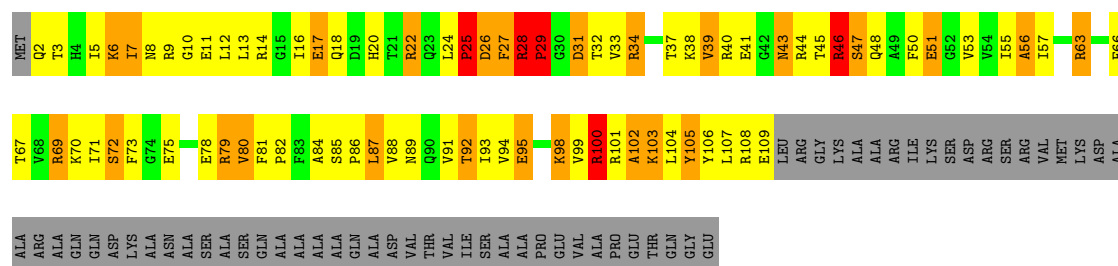
• Molecule 17: 50S RIBOSOMAL PROTEIN L18

Chain L:



• Molecule 18: 50S RIBOSOMAL PROTEIN L19

Chain M:



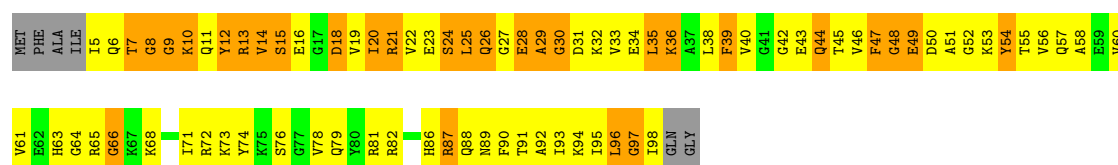
• Molecule 19: 50S RIBOSOMAL PROTEIN L20

Chain N:



• Molecule 20: 50S RIBOSOMAL PROTEIN L21

Chain O:



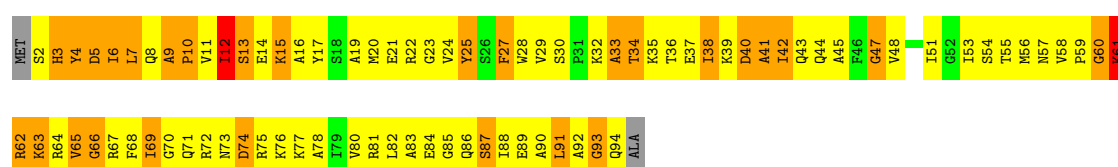
• Molecule 21: 50S RIBOSOMAL PROTEIN L22

Chain P:



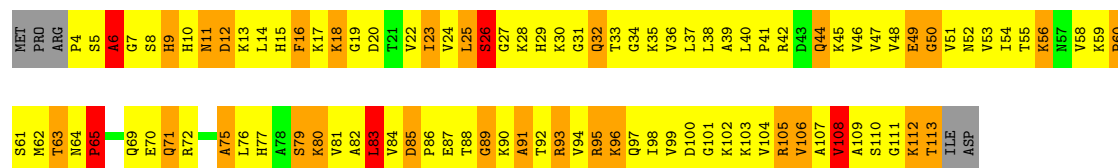
• Molecule 22: 50S RIBOSOMAL PROTEIN L23

Chain Q:



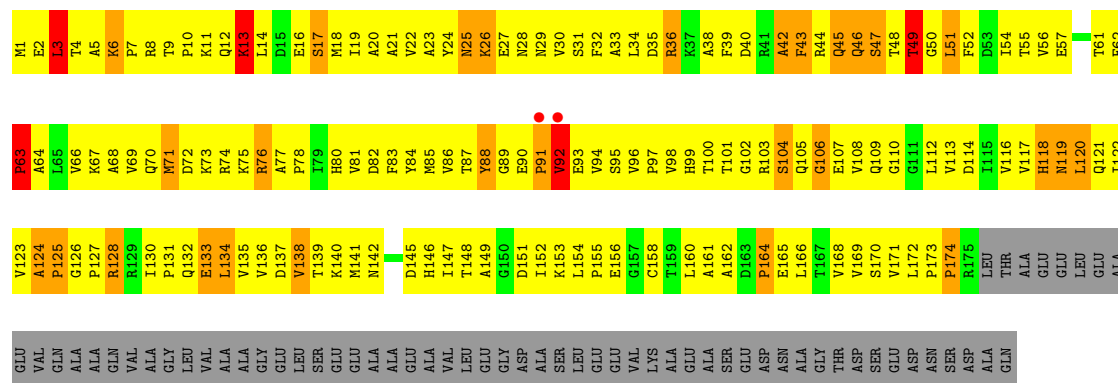
• Molecule 23: 50S RIBOSOMAL PROTEIN L24

Chain R:



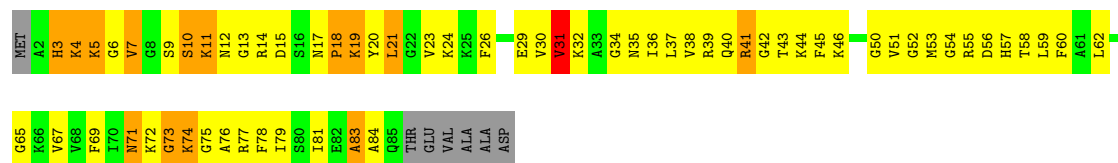
• Molecule 24: 50S RIBOSOMAL PROTEIN L25

Chain S:



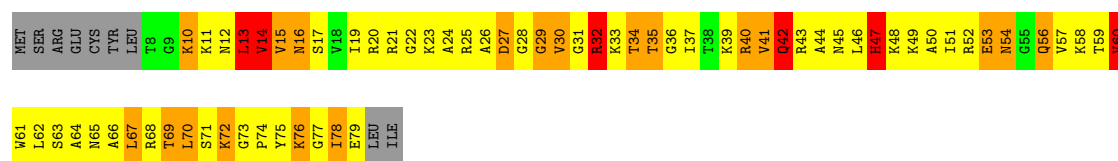
• Molecule 25: 50S RIBOSOMAL PROTEIN L27

Chain T:



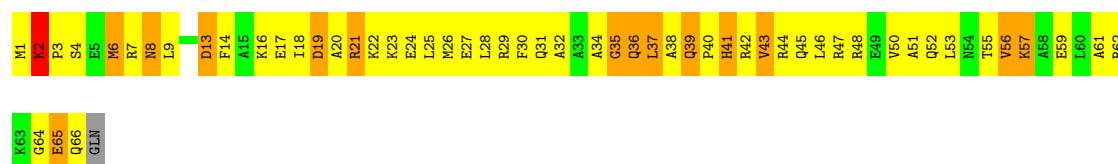
• Molecule 26: 50S RIBOSOMAL PROTEIN L28

Chain U:



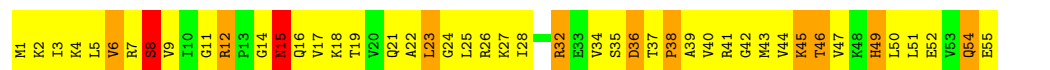
• Molecule 27: 50S RIBOSOMAL PROTEIN L29

Chain V:



• Molecule 28: 50S RIBOSOMAL PROTEIN L30

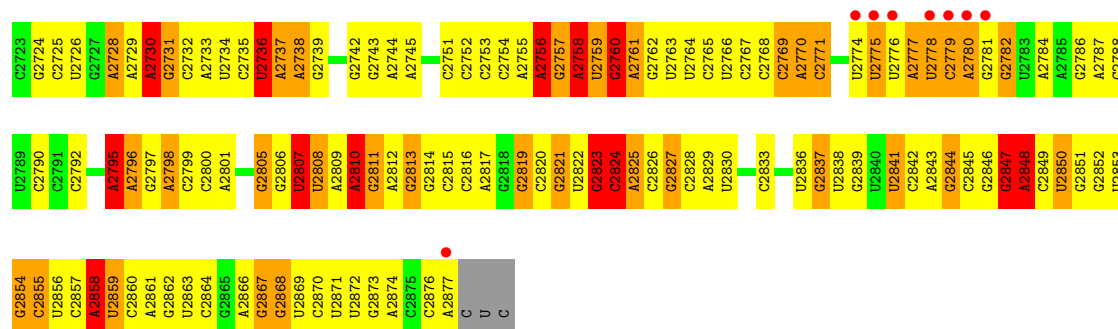
Chain W:





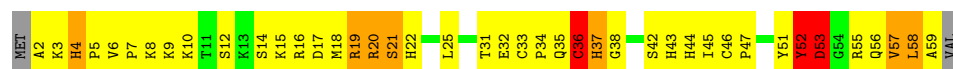
WORLDWIDE
PDB
PROTEIN DATA BANK

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C2662	A2600	C2535	C2475	A2413	G2363	G2287	C2227	A2167	G	A2045	G1986	U1922	G1861	A1800
U2663	C2601	C2539	A2476	A2414	G2354	A2288	U2228	A2168	A	C2046	G1987	U1923	G1862	A1801
G2664	G2602	G2540	C2477	G2415	A2355	A2289	G2229	A2169	G	C2047	G1988	U1924	U1863	A1802
G2665	G2603	A2541	U2478	U2416	A2356	A2290	G2230	G2230	C	C2048	A1988	C1925	U1864	U1804
U2666	G2604	U2542	U2479	U2417	A2357	U2291	G2231	U2171	C	C2049	C1989	U1926	C1865	U1805
C2667	C2605	U2543	C2480	A2418	G2358	C2292	G2232	U2172	C	G2050	U1990	U1927	G1866	G1806
U2668	G2606	A2544	G2481	C2419	U2359	G2293	G2233	G2173	U	U2051	C1991	U1928	A1867	A1807
C2669	C2607	A2544	A2482	C2420	U2360	G2294	G2234	G2174	G	G2052	C1992	U1929	A1868	G1808
C2670	A2608	U2545	U2483	C2421	G2361	U2298	U2235	G2175	C	A2054	G1993	U1930	A1869	C1809
G2671	G2609	G2546	G2484	G2422	G2362	A2299	U2236	U2176	A	G2055	G1994	G1933	G1871	U1810
U2672	U2610	C2547	U2485	G2423	G2363	A2299	G2237	U2177	A	G2056	G1995	U1934	A1872	A1811
G2673	G2611	G2548	C2486	G2424	C2364	G2300	G2238	U2178	A	U2057	A1996	U1934	U1872	U1812
C2674	C2612	G2549	G2487	G2425	U2365	A2301	G2239	C2179	A	U2058	A1997	A1935	A1873	A1813
U2675	A2613	C2550	G2488	G2426	U2366	G2302	C2240	U2180	C	U2059	A1998	U1936	G1876	G1830
G2676	U2614	A2551	C2489	A2427	U2367	G2303	U2241	A2181	G	U2060	G1999	G1937	C1877	G1831
U2677	U2615	C2552	U2490	U2428	G2368	G2304	G2242	A2182	G	C2061	U2000	U1938	G1878	G1832
G2678	G2616	G2553	U2491	A2429	U2369	C2305	A2243	G2183	C	U2062	G2001	U1939	G1879	U1833
	U2617	G2554	G2492	A2430	G2370	A2306	C2244	C2184	C	A2002	G2002	A1940	A1884	G1834
	A2618	G2555	U2493	A2431	A2371	A2307	A2245	U2185	C	A2063	A2003	C1941	G1885	C1836
	G2619	A2556	C2494	A2432	A2372	A2308	A2246	U2186	C	U2064	U2004	C1942	G1886	G1837
G2620	C2620	C2557	G2495	G2433	C2373	G2309	A2247	A2187	U	A2065	U2005	G1941	G1887	G1838
		C2558	C2496	G2434	C2374	A2310	A2248	A2188	U	G2066	G2006	C1943	A1882	A1839
	U2621	G2559	C2497	U2435	G2375	U2311	U2249	A2189	U	U2067	G2007	U1946	A1883	A1840
G2622	G2625	G2560	U2498	U2436	G2376	A2312	G2250	A2190	U	C2068	C2008	G1947	A1884	G1841
U2626	U2626	G2561	C2499	G2437	U2377	G2313	U2251	A2191	G	U2069	U2009	C1948	A1885	G1842
G2627	C2627	U2562	G2500	A2438	G2378	A2314	A2252	U2192	G	G2070	G2010	A1949	G1886	G1843
U2628	U2628	G2563	U2501	U2439	G2379	A2315	A2253	U2193	G	G2071	U2011	U1950	G1887	C1835
G2629	A2690	U2564	G2502	C2440	U2380	C2315	G2254	A2194	U	C2072	A2012	G1951	A1888	G1836
C2630	C2630	G2565	U2503	U2441	A2381	A2316	G2255	C2195	C	A2073	A2013	A1952	G	G1837
G2631	G2631	A2566	G2504	C2442	C2382	U2318	G2256	U2196	G	U2074	A2014	A1953	C	G1838
	U2632	G2567	G2505	C2443	C2383	G2320	A2257	U2197	G	U2075	G2015	A1954	C	G1839
U2633	A2633	A2568	C2506	C2445	G2384	C2321	G2258	U2198	U	G2076	A2016	G1956	G	G1840
G2634	U2634	A2569	G2507	C2446	U2385	U2322	G2259	C2199	G	U2080	U2017	C1957	C	U1833
U2635	G2635	G2570	C2447	G2448	G2386	U2323	G2260	G2200	A	U2081	G2018	G1958	A	A1834
G2636	A2636	G2571	A2448	G2449	U2387	G2324	G2261	G2201	A	U2082	C2019	U1959	C	C1835
G2637	G2637	U2572	G2450	A2450	G2388	A2325	C2262	G2202	C	G2083	G2020	U1960	C	C1836
G2638	G2638		G2451	G2451	G2389	C2326	C2263	G2203	G	G2084	G2021	A1961	U	G1837
A2639	A2639	G2576	A2512	U2452	A2390	U2327	A2264	A2204	C	G2085	C2022	C1962	A	G1838
A2701	G2640	A2577	A2513	U2453	A2391	G2328	A2265	C2205	A	U2086	C2023	G1963	U	A1839
G2702	G2641	G2578	G2514	C2453	G2392	G2329	A2266	C2206	A	U2087	U2024	A1964	A	A1840
C2703	G2642	A2579	U2515	G2454	G2393	G2330	A2267	G2207	C	U2088	A2025	U1965	A	G1841
U2704	G2643	A2580	U2516	A2455	G2394	A2331	G2268	U2208	G	C2089	C2026	U1966	C	G1842
G2705	A2644	A2581	C2517	U2456	G2395	G2332	G2269	G2209	G	U2090	C2027	C1967	G	U1843
U2706	C2645	G2582	C2518	A2457	C2396	A2333	U2270	C2210	U	G2091	C2028	U1968	G	G1844
G2707	G2646		C2519	U2458	A2397	U2334	G2271	U2211	G	C	G2029	G1969	U	A1845
U2708	G2647	G2585	A2520	C2459	U2398	U2335	A2272	U2212	A	U	U2030	C1970	C	A1846
C2709	G2648	G2586	A2521	G2460	C2399	G2336	G2273	G2213	A	G	A2031	G1971	C	G1847
G2710	A2649	G2587	G2522	G2461	G2400	A2337	G2274	G2214	A	C	G2032	C1971	U1909	U1848
G2711	G2650	U2588	G2523	G2463	A2401	U2342	U2275	C2215	U	G	C2033	G1972	A1910	G1849
A2712	U2651	G2589	G2524	G2464	U2402	C2343	G2276	G2216	C	A	A2034	C1973	A1911	G1850
G2713	G2652	U2590	C2403	G2465	C2403	U2344	A2277	G2217	C	A	G2035	U1974	A1912	A1851
A2714	A2653	G2591	A2404	G2466	A2404	A2345	A2278	G2218	C	G	G2036	G1975	G1913	G1852
C2715	C2715	U2592	G2527	A2467	A2405	G2346	G2279	U2219	A	G	A2037	U1976	G1914	C1853
		U2593	G2528	G2468	G2406	A2280	A2280	G2220	C	A	C2038	C1977	A1915	G1854
G2716	G2655	U2594	G2529	G2469	C2407	G2347	G2281	G2221	C	U	G2039	U1978	G1916	G1855
U2718	G2657	C2595	G2530	U2470	G2408	A2348	G2282	U2222	C	A	A2040	C1979	C1917	U1856
U2719	A2658	U2596	U2531	U2471	A2409	G2349	G2283	U2223	C	A	A2041	A1980	G1918	U1857
C2720	C2659	G2597	U2472	U2472	U2410	G2350	U2284	U2224	U	G	A2042	A1981	A1919	C1858
G2722	C2660	C2598	U2533	G2473	A2411	G2351	U2285	G2225	A2165	U	A2043	C1982	A1920	A1859



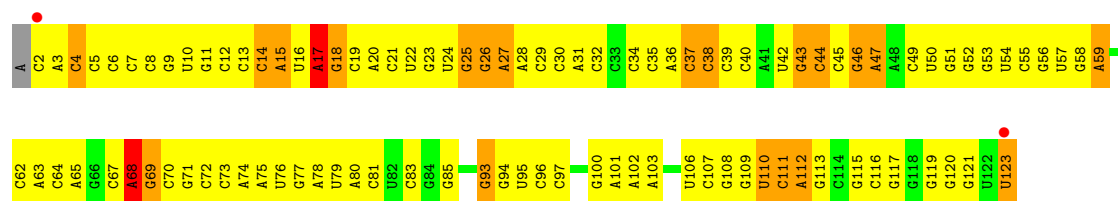
• Molecule 30: 50S RIBOSOMAL PROTEIN L32

Chain Y:



• Molecule 31: RRNA-5S RIBOSOMAL RNA

Chain Z:



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	169.90Å 408.90Å 694.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.30 29.76 – 3.31	Depositor EDS
% Data completeness (in resolution range)	94.1 (30.00-3.30) 93.3 (29.76-3.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 3.31Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.276 , 0.318 0.242 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	67.5	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.17 , 19.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	1 of 332876 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	84475	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% 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, DCY, DHA, QUA, BB9, NH2, MH6, DBU, TS9

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$
4	4	0.46	0/298	0.67	0/390
5	5	1.46	0/31	1.18	0/38
6	A	0.55	0/1862	0.85	2/2510 (0.1%)
7	B	0.77	0/1567	1.04	4/2105 (0.2%)
8	C	0.63	0/1529	0.91	0/2070
9	D	0.48	0/1419	0.71	0/1903
10	E	0.48	0/1308	0.80	1/1771 (0.1%)
11	F	0.50	0/1063	0.71	0/1440
12	G	0.69	0/1138	1.00	3/1539 (0.2%)
13	H	0.79	0/1007	0.96	1/1352 (0.1%)
14	I	0.65	0/1081	0.94	3/1448 (0.2%)
15	J	0.67	0/1113	0.91	2/1486 (0.1%)
16	K	0.87	0/886	1.06	2/1188 (0.2%)
17	L	0.52	0/785	0.86	0/1048
18	M	0.73	0/884	1.20	6/1186 (0.5%)
19	N	0.63	0/994	0.89	0/1323
20	O	0.61	0/750	0.90	0/1000
21	P	0.77	0/1027	0.93	1/1373 (0.1%)
22	Q	0.67	0/737	0.98	4/988 (0.4%)
23	R	0.55	0/835	0.95	2/1121 (0.2%)
24	S	0.50	0/1370	0.75	0/1862
25	T	0.56	0/633	0.83	1/838 (0.1%)
26	U	0.58	0/556	0.95	1/741 (0.1%)
27	V	0.44	0/537	0.67	0/714
28	W	0.56	0/426	0.84	0/568
29	X	0.88	59/64561 (0.1%)	1.05	497/100708 (0.5%)
30	Y	0.70	0/469	1.11	2/629 (0.3%)
31	Z	0.55	0/2904	0.76	0/4525
All	All	0.81	59/91770 (0.1%)	1.01	532/137864 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	A	0	1
19	N	0	2
22	Q	0	1
29	X	2	257
30	Y	0	1
31	Z	0	4
All	All	2	266

The worst 5 of 59 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	X	1856	U	C4'-C3'	-9.30	1.43	1.53
29	X	1856	U	O3'-P	-8.64	1.50	1.61
29	X	1056	U	P-O5'	8.52	1.68	1.59
29	X	1855	G	O3'-P	-8.11	1.51	1.61
29	X	551	A	O3'-P	-8.05	1.51	1.61

The worst 5 of 532 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	1055	A	N9-C1'-C2'	-29.46	75.70	114.00
29	X	2324	G	N9-C1'-C2'	22.22	142.88	114.00
29	X	557	U	N1-C1'-C2'	19.61	139.50	114.00
29	X	417	C	N1-C1'-C2'	18.73	138.35	114.00
18	M	28	ARG	C-N-CD	-18.52	79.85	120.60

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
29	X	1278	A	C1'
29	X	2592	U	C1'

5 of 266 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	A	104	TYR	Sidechain
19	N	32	TYR	Sidechain
19	N	76	TYR	Sidechain
22	Q	25	TYR	Sidechain

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Mol	Chain	Res	Type	Group
29	X	12	U	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	1	53	0	0	0	0
2	2	46	0	0	0	0
3	3	63	0	0	1	0
4	4	297	0	330	62	0
5	5	114	0	79	5	0
6	A	1826	0	1885	451	0
7	B	1539	0	1600	303	0
8	C	1506	0	1525	371	0
9	D	1400	0	1481	373	0
10	E	1286	0	1336	264	0
11	F	1044	0	1088	176	0
12	G	1114	0	1144	310	0
13	H	997	0	1046	194	0
14	I	1067	0	1103	301	0
15	J	1090	0	1125	273	0
16	K	878	0	930	135	0
17	L	779	0	820	231	0
18	M	871	0	894	208	0
19	N	978	0	1020	239	0
20	O	741	0	756	186	0
21	P	1014	0	1096	181	0
22	Q	726	0	753	150	0
23	R	825	0	881	266	0
24	S	1345	0	1372	303	0
25	T	625	0	655	111	0
26	U	552	0	604	207	0
27	V	533	0	558	109	0
28	W	424	0	470	83	0
29	X	57651	0	29049	4301	0
30	Y	457	0	462	86	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	Z	2598	0	1328	185	0
32	M	1	0	0	0	0
32	X	30	0	0	0	0
32	Z	5	0	0	0	0
All	All	84475	0	55390	9214	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 66.

The worst 5 of 9214 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:B:116:VAL:N	7:B:136:ARG:HE	1.23	1.30
29:X:1053:G:H2'	29:X:1054:C:C6	1.70	1.26
29:X:2196:U:H2'	29:X:2197:U:O4'	1.31	1.23
29:X:2736:U:O2'	29:X:2737:A:H5''	1.36	1.21
29:X:2496:C:O2'	29:X:2497:A:H3'	1.40	1.19

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	
4	4	35/37 (95%)	20 (57%)	10 (29%)	5 (14%)	0	2
5	5	5/19 (26%)	4 (80%)	1 (20%)	0	100	100
6	A	238/274 (87%)	154 (65%)	50 (21%)	34 (14%)	0	2
7	B	203/211 (96%)	148 (73%)	32 (16%)	23 (11%)	1	5
8	C	195/205 (95%)	97 (50%)	54 (28%)	44 (23%)	0	0
9	D	175/180 (97%)	95 (54%)	48 (27%)	32 (18%)	0	1
10	E	169/185 (91%)	100 (59%)	38 (22%)	31 (18%)	0	1
11	F	142/144 (99%)	94 (66%)	29 (20%)	19 (13%)	0	3
12	G	140/174 (80%)	76 (54%)	34 (24%)	30 (21%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	H	132/134 (98%)	105 (80%)	18 (14%)	9 (7%)	2	18
14	I	139/156 (89%)	59 (42%)	45 (32%)	35 (25%)	0	0
15	J	134/142 (94%)	82 (61%)	31 (23%)	21 (16%)	0	1
16	K	111/116 (96%)	74 (67%)	25 (22%)	12 (11%)	1	6
17	L	102/114 (90%)	59 (58%)	19 (19%)	24 (24%)	0	0
18	M	106/166 (64%)	70 (66%)	23 (22%)	13 (12%)	1	4
19	N	115/118 (98%)	57 (50%)	40 (35%)	18 (16%)	0	1
20	O	92/100 (92%)	57 (62%)	10 (11%)	25 (27%)	0	0
21	P	125/134 (93%)	89 (71%)	21 (17%)	15 (12%)	1	4
22	Q	91/95 (96%)	39 (43%)	28 (31%)	24 (26%)	0	0
23	R	108/115 (94%)	62 (57%)	27 (25%)	19 (18%)	0	1
24	S	173/237 (73%)	93 (54%)	46 (27%)	34 (20%)	0	1
25	T	82/91 (90%)	47 (57%)	19 (23%)	16 (20%)	0	1
26	U	70/81 (86%)	35 (50%)	16 (23%)	19 (27%)	0	0
27	V	64/67 (96%)	35 (55%)	16 (25%)	13 (20%)	0	1
28	W	53/55 (96%)	38 (72%)	9 (17%)	6 (11%)	1	5
30	Y	56/60 (93%)	40 (71%)	9 (16%)	7 (12%)	1	4
All	All	3055/3410 (90%)	1829 (60%)	698 (23%)	528 (17%)	0	1

5 of 528 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	A	59	LYS
6	A	145	LEU
6	A	168	LYS
6	A	217	ARG
6	A	220	HIS

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	
4	4	35/35 (100%)	32 (91%)	3 (9%)	15	54
5	5	3/4 (75%)	3 (100%)	0	100	100
6	A	185/215 (86%)	161 (87%)	24 (13%)	6	29
7	B	155/157 (99%)	132 (85%)	23 (15%)	4	21
8	C	157/163 (96%)	131 (83%)	26 (17%)	3	16
9	D	153/156 (98%)	138 (90%)	15 (10%)	12	45
10	E	136/144 (94%)	128 (94%)	8 (6%)	28	73
11	F	107/107 (100%)	100 (94%)	7 (6%)	24	69
12	G	118/146 (81%)	96 (81%)	22 (19%)	2	11
13	H	103/103 (100%)	88 (85%)	15 (15%)	5	23
14	I	108/121 (89%)	91 (84%)	17 (16%)	4	19
15	J	110/116 (95%)	89 (81%)	21 (19%)	2	10
16	K	90/93 (97%)	76 (84%)	14 (16%)	4	19
17	L	74/82 (90%)	54 (73%)	20 (27%)	1	2
18	M	94/134 (70%)	72 (77%)	22 (23%)	1	4
19	N	96/97 (99%)	83 (86%)	13 (14%)	6	27
20	O	75/79 (95%)	70 (93%)	5 (7%)	23	67
21	P	109/115 (95%)	100 (92%)	9 (8%)	16	56
22	Q	75/76 (99%)	67 (89%)	8 (11%)	10	39
23	R	91/96 (95%)	72 (79%)	19 (21%)	1	8
24	S	149/192 (78%)	137 (92%)	12 (8%)	17	58
25	T	62/67 (92%)	57 (92%)	5 (8%)	17	58
26	U	57/66 (86%)	44 (77%)	13 (23%)	1	5
27	V	54/55 (98%)	48 (89%)	6 (11%)	9	37
28	W	48/48 (100%)	38 (79%)	10 (21%)	2	8
30	Y	51/53 (96%)	48 (94%)	3 (6%)	28	73
All	All	2495/2720 (92%)	2155 (86%)	340 (14%)	5	26

5 of 340 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	I	65	PHE
16	K	83	VAL
26	U	47	HIS

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Mol	Chain	Res	Type
14	I	103	ASN
15	J	82	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 78 such sidechains are listed below:

Mol	Chain	Res	Type
13	H	41	ASN
16	K	13	ASN
27	V	45	GLN
13	H	79	HIS
14	I	66	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
29	X	2680/2880 (93%)	688 (25%)	313 (11%)
31	Z	121/123 (98%)	24 (19%)	1 (0%)
All	All	2801/3003 (93%)	712 (25%)	314 (11%)

5 of 712 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
29	X	2	G
29	X	4	C
29	X	13	A
29	X	14	A
29	X	27	G

5 of 314 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
29	X	1261	G
29	X	1552	C
29	X	2660	C
29	X	1278	A
29	X	1345	G

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

11 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	TS9	5	10	5	8,8,10	0.79	0	10,12,15	0.96	0
5	BB9	5	11	5	3,5,6	3.15	2 (66%)	1,5,7	2.99	1 (100%)
5	BB9	5	13	5	2,4,6	2.32	2 (100%)	1,4,7	3.58	1 (100%)
5	MH6	5	14	5	2,3,6	0.43	0	0,3,7	0.00	-
5	BB9	5	15	5	3,5,6	6.58	2 (66%)	1,5,7	4.81	1 (100%)
5	DHA	5	16	5	3,4,5	5.84	2 (66%)	1,4,6	0.56	0
5	DHA	5	17	5	3,4,5	2.44	1 (33%)	1,4,6	2.35	1 (100%)
5	DHA	5	3	5	3,4,5	2.70	2 (66%)	1,4,6	0.27	0
5	BB9	5	6	5	3,5,6	3.77	2 (66%)	1,5,7	4.88	1 (100%)
5	DBU	5	8	5	3,4,6	3.54	1 (33%)	2,4,7	0.81	0
5	DCY	5	9	5	5,5,6	6.01	1 (20%)	3,5,7	2.02	1 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	TS9	5	10	5	-	0/7/12/16	0/0/0/0
5	BB9	5	11	5	-	0/0/4/6	0/0/0/0
5	BB9	5	13	5	-	0/0/2/6	0/0/0/0
5	MH6	5	14	5	-	0/0/0/6	0/0/0/0
5	BB9	5	15	5	-	0/0/4/6	0/0/0/0
5	DHA	5	16	5	-	0/0/2/4	0/0/0/0
5	DHA	5	17	5	-	0/0/2/4	0/0/0/0
5	DHA	5	3	5	-	0/0/2/4	0/0/0/0
5	BB9	5	6	5	-	0/0/4/6	0/0/0/0
5	DBU	5	8	5	-	0/0/2/6	0/0/0/0
5	DCY	5	9	5	-	0/2/4/6	0/0/0/0

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	5	9	DCY	O-C	13.29	1.20	1.11
5	5	15	BB9	CB-CA	10.74	1.51	1.34
5	5	16	DHA	CA-N	9.86	1.55	1.35
5	5	8	DBU	CA-N	6.04	1.47	1.34
5	5	6	BB9	CB-CA	5.39	1.43	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	5	6	BB9	CB-CA-N	-4.88	112.61	123.34
5	5	15	BB9	CB-CA-N	-4.81	112.77	123.34
5	5	13	BB9	CB-CA-N	-3.58	113.96	122.77
5	5	9	DCY	CA-CB-SG	-3.45	104.20	115.14
5	5	11	BB9	CB-CA-N	-2.99	116.77	123.34

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 36 ligands modelled in this entry, 36 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	1	53/55 (96%)	1.98	26 (49%) 1 0	48, 56, 77, 82	0
2	2	46/47 (97%)	3.27	40 (86%) 0 0	9, 29, 38, 40	0
3	3	63/66 (95%)	2.97	47 (74%) 0 0	23, 41, 51, 57	0
4	4	37/37 (100%)	0.70	3 (8%) 12 3	60, 69, 77, 81	0
5	5	19/19 (100%)	0.66	1 (5%) 25 6	77, 85, 88, 89	2 (10%)
6	A	240/274 (87%)	-0.11	1 (0%) 90 57	25, 63, 77, 84	0
7	B	205/211 (97%)	-0.47	0 100 100	3, 22, 49, 63	0
8	C	197/205 (96%)	-0.22	1 (0%) 88 51	8, 51, 73, 83	0
9	D	177/180 (98%)	-0.04	1 (0%) 86 46	60, 75, 85, 91	0
10	E	171/185 (92%)	-0.26	0 100 100	44, 66, 79, 88	0
11	F	144/144 (100%)	0.75	9 (6%) 19 5	74, 89, 98, 102	0
12	G	142/174 (81%)	-0.22	0 100 100	22, 43, 67, 72	0
13	H	134/134 (100%)	-0.50	0 100 100	3, 16, 37, 45	0
14	I	141/156 (90%)	0.11	4 (2%) 50 12	22, 62, 77, 85	0
15	J	136/142 (95%)	-0.25	1 (0%) 84 42	27, 51, 73, 80	0
16	K	113/116 (97%)	-0.56	0 100 100	3, 9, 24, 34	0
17	L	104/114 (91%)	-0.08	0 100 100	43, 62, 72, 75	0
18	M	108/166 (65%)	-0.49	0 100 100	4, 19, 43, 64	0
19	N	117/118 (99%)	-0.38	0 100 100	4, 40, 62, 73	0
20	O	94/100 (94%)	-0.30	0 100 100	18, 53, 71, 81	0
21	P	127/134 (94%)	-0.48	0 100 100	4, 18, 53, 76	0
22	Q	93/95 (97%)	-0.26	0 100 100	32, 50, 69, 80	0
23	R	110/115 (95%)	-0.14	0 100 100	36, 54, 80, 87	0
24	S	175/237 (73%)	0.06	2 (1%) 77 30	61, 71, 82, 87	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
25	T	84/91 (92%)	-0.06	0	100	100	35, 51, 80, 90	0
26	U	72/81 (88%)	0.02	0	100	100	45, 61, 72, 78	0
27	V	66/67 (98%)	-0.36	0	100	100	49, 61, 81, 88	0
28	W	55/55 (100%)	-0.33	0	100	100	23, 41, 61, 78	0
29	X	2686/2880 (93%)	-0.45	48 (1%)	65	20	4, 41, 116, 151	0
30	Y	58/60 (96%)	-0.38	0	100	100	4, 17, 44, 52	0
31	Z	122/123 (99%)	-0.19	2 (1%)	68	22	30, 75, 102, 129	0
All	All	6089/6581 (92%)	-0.22	186 (3%)	48	11	3, 49, 95, 151	2 (0%)

The worst 5 of 186 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
31	Z	123	U	6.7
29	X	731	A	6.4
3	3	39	ASP	6.2
2	2	1	MET	6.1
2	2	37	LYS	6.0

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

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
5	BB9	5	15	6/7	0.43	7.61	88,88,88,88	0
5	DHA	5	16	5/6	0.45	2.08	83,83,85,86	0
5	DHA	5	3	5/6	0.51	1.92	82,83,84,85	0
5	MH6	5	14	4/7	0.30	1.18	86,86,87,87	0
5	TS9	5	10	9/11	0.35	0.37	87,88,89,89	0
5	DHA	5	17	5/6	0.33	-0.47	76,77,78,80	2
5	BB9	5	11	6/7	0.22	-0.72	85,87,87,88	0
5	BB9	5	13	5/7	0.21	-0.85	85,86,86,87	0
5	BB9	5	6	6/7	0.19	-1.60	82,84,85,86	0
5	DCY	5	9	6/7	0.18	-3.75	87,87,87,87	0
5	DBU	5	8	5/7	0.15	-4.02	85,86,87,87	0

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	X	2885	1/1	0.40	73.23	56,56,56,56	0
32	MG	X	2907	1/1	0.69	50.99	17,17,17,17	0
32	MG	X	2897	1/1	0.46	46.65	3,3,3,3	0
32	MG	X	2902	1/1	0.31	41.60	24,24,24,24	0
32	MG	Z	126	1/1	0.39	40.27	25,25,25,25	0
32	MG	X	2890	1/1	0.34	35.05	49,49,49,49	0
32	MG	X	2899	1/1	0.52	30.97	3,3,3,3	0
32	MG	X	2894	1/1	0.38	27.99	15,15,15,15	0
32	MG	X	2889	1/1	0.73	22.91	3,3,3,3	0
32	MG	X	2898	1/1	0.54	22.38	19,19,19,19	0
32	MG	X	2891	1/1	0.39	20.48	12,12,12,12	0
32	MG	X	2900	1/1	0.24	19.95	3,3,3,3	0
32	MG	Z	125	1/1	0.28	19.25	9,9,9,9	0
32	MG	X	2882	1/1	0.35	19.05	12,12,12,12	0
32	MG	X	2886	1/1	0.29	17.11	41,41,41,41	0
32	MG	X	2884	1/1	0.78	14.36	55,55,55,55	0
32	MG	M	167	1/1	0.53	14.15	3,3,3,3	0
32	MG	X	2910	1/1	0.35	11.54	19,19,19,19	0
32	MG	X	2896	1/1	0.26	10.85	3,3,3,3	0
32	MG	X	2888	1/1	0.30	9.75	3,3,3,3	0
32	MG	X	2905	1/1	0.48	9.64	13,13,13,13	0
32	MG	X	2909	1/1	0.24	7.55	3,3,3,3	0
32	MG	Z	124	1/1	0.31	7.54	26,26,26,26	0
32	MG	X	2904	1/1	0.31	6.92	6,6,6,6	0
32	MG	X	2903	1/1	0.33	5.98	3,3,3,3	0
32	MG	X	2887	1/1	0.18	5.67	3,3,3,3	0
32	MG	X	2893	1/1	0.14	4.33	13,13,13,13	0
32	MG	X	2881	1/1	0.23	2.83	59,59,59,59	0
32	MG	Z	127	1/1	0.19	2.65	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	X	2895	1/1	0.24	1.16	3,3,3,3	0
32	MG	X	2906	1/1	0.15	0.91	58,58,58,58	0
32	MG	X	2883	1/1	0.12	-0.52	49,49,49,49	0
32	MG	Z	128	1/1	0.09	-1.56	41,41,41,41	0
32	MG	X	2908	1/1	0.11	-2.82	3,3,3,3	0
32	MG	X	2901	1/1	0.09	-3.48	60,60,60,60	0
32	MG	X	2892	1/1	0.15	-	22,22,22,22	0

6.5 Other polymers

There are no such residues in this entry.