wwPDB X-ray Structure Validation Summary Report (i)

Nov 7, 2023 – 07:07 PM EST

PDB ID	:	1SM1
Title	:	COMPLEX OF THE LARGE RIBOSOMAL SUBUNIT FROM DEINOCOCCUS RADIODURANS WITH QUINUPRISTIN AND DALFOPRISTIN
Authors	:	Harms, J.M.; Schluenzen, F.; Fucini, P.; Bartels, H.; Yonath, A.
Deposited on	:	2004-03-08
Resolution	:	3.42 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

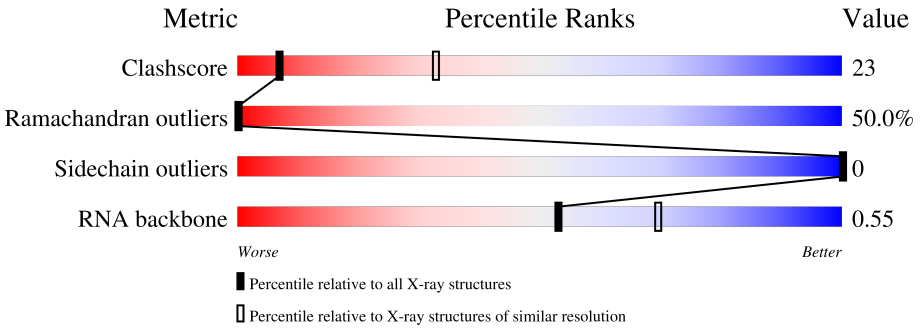
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.42 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	141614	1572 (3.50-3.34)
Ramachandran outliers	138981	1534 (3.50-3.34)
Sidechain outliers	138945	1535 (3.50-3.34)
RNA backbone	3102	1012 (3.88-2.96)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	0	2880	29% 53% 13%
2	1	82	65% 35%
3	2	47	98%
4	3	66	95% 5%
5	4	37	95% 5%
6	5	8	25% 50% 12% 12%

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Mol	Chain	Length	Quality of chain
7	9	124	36% 54% 5% 5%
8	A	275	98%
9	B	211	97%
10	C	205	96%
11	D	180	99%
12	E	212	83% 17%
13	F	146	36% 64%
14	G	144	99%
15	H	174	82% 18%
16	I	134	99%
17	J	156	90% 10%
18	K	142	87% 13%
19	L	116	97%
20	M	114	97%
21	N	166	75% 25%
22	O	118	97%
23	P	100	100%
24	Q	134	97%
25	R	95	98%
26	S	115	98%
27	T	253	88% 12%
28	U	91	95% 5%
29	W	67	97%
30	X	55	100%
31	Y	73	100%

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Mol	Chain	Length	Quality of chain
32	Z	60	95%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	DOL	0	2882	X	-	-	-
6	DBB	5	3	-	-	X	-

2 Entry composition (i)

There are 33 unique types of molecules in this entry. The entry contains 65418 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	0	2766	59359	26479	10949	19166	2765	0	0	0

- Molecule 2 is a protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
			Total	C			
2	1	53	53	53	0	0	53

- Molecule 3 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
			Total	C			
3	2	46	46	46	0	0	46

- Molecule 4 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
			Total	C			
4	3	63	63	63	0	0	63

- Molecule 5 is a protein called 50S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
			Total	C			
5	4	35	35	35	0	0	35

- Molecule 6 is a protein called QUINUPRISTIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	5	8	73	53	9	10	1	0	0	0

- Molecule 7 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	9	118	Total	C	N	O	P	0	0	0
			2516	1124	464	811	117			

- Molecule 8 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
8	A	270	Total	C	0	0	270
			270	270			

- Molecule 9 is a protein called 50S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
9	B	205	Total	C	0	0	205
			205	205			

- Molecule 10 is a protein called 50S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
10	C	197	Total	C	0	0	197
			197	197			

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
11	D	178	Total	C	0	0	178
			178	178			

- Molecule 12 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
12	E	177	Total	C	0	0	177
			177	177			

- Molecule 13 is a protein called 50S RIBOSOMAL PROTEIN L9.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
13	F	52	Total	C	0	0	52
			52	52			

- Molecule 14 is a protein called 50S RIBOSOMAL PROTEIN L11.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
14	G	143	Total C 143 143	0	0	143

- Molecule 15 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
15	H	143	Total C 143 143	0	0	143

- Molecule 16 is a protein called 50S RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
16	I	132	Total C 132 132	0	0	132

- Molecule 17 is a protein called 50S RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
17	J	141	Total C 141 141	0	0	141

- Molecule 18 is a protein called 50S RIBOSOMAL PROTEIN L16.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
18	K	124	Total C 124 124	0	0	124

- Molecule 19 is a protein called 50S RIBOSOMAL PROTEIN L17.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
19	L	114	Total C 114 114	0	0	114

- Molecule 20 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
20	M	111	Total C 111 111	8	0	111

- Molecule 21 is a protein called 50S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
21	N	125	Total C 125 125	0	0	125

- Molecule 22 is a protein called 50S RIBOSOMAL PROTEIN L20.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
22	O	117	Total C 117 117	16	0	117

- Molecule 23 is a protein called 50S RIBOSOMAL PROTEIN L21.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
23	P	100	Total C 100 100	0	0	100

- Molecule 24 is a protein called 50S RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
24	Q	130	Total C 130 130	0	0	130

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
25	R	93	Total C 93 93	0	0	93

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
26	S	113	Total C 113 113	0	0	113

- Molecule 27 is a protein called GENERAL STRESS PROTEIN CTC.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
27	T	223	Total C 223 223	43	0	223

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
28	U	86	Total C 86 86	0	0	86

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
29	W	65	Total C 65 65	0	0	65

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
30	X	55	Total C 55 55	4	0	55

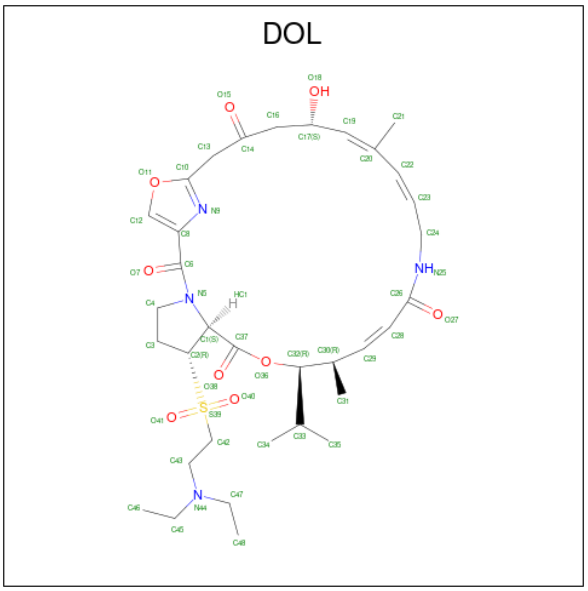
- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
31	Y	73	Total C 73 73	0	0	73

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
32	Z	58	Total C 58 58	0	0	58

- Molecule 33 is 5-(2-DIETHYLAMINO-ETHANESULFONYL)-21-HYDROXY-10-ISOPROPYL-11,19-DIMETHYL-9,26-DIOXA-3,15,28-TRIAZA-TRICYCLO[23.2.1.00,255]OCTACOSA-1(27),12,17,19,25(28)-PENTAENE-2,8,14,23-TETRAONE (three-letter code: DOL) (formula: $C_{34}H_{50}N_4O_9S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
33	0	1	Total	C	N	O	S	0	0
			48	34	4	9	1		

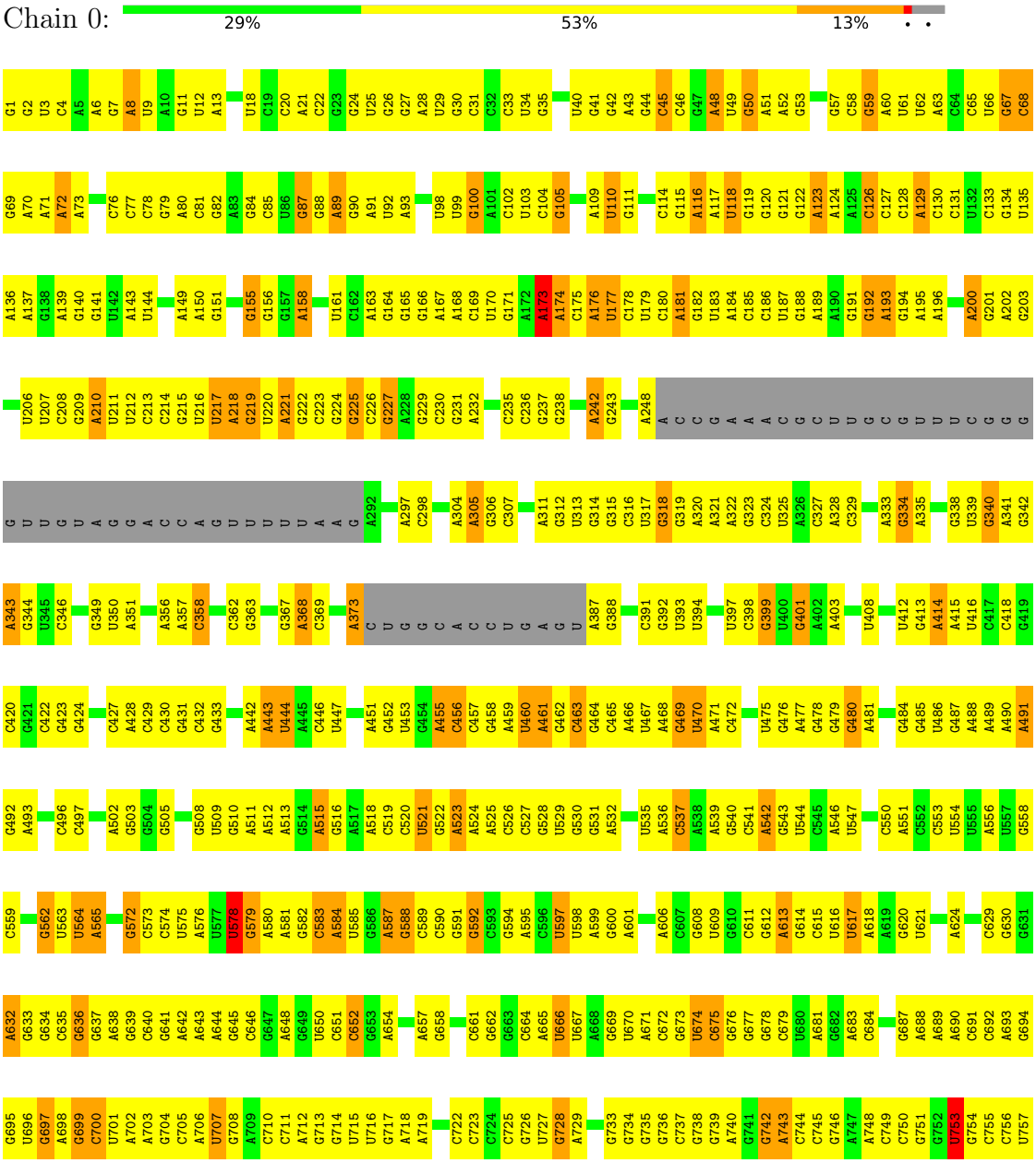
3 Residue-property plots (i)

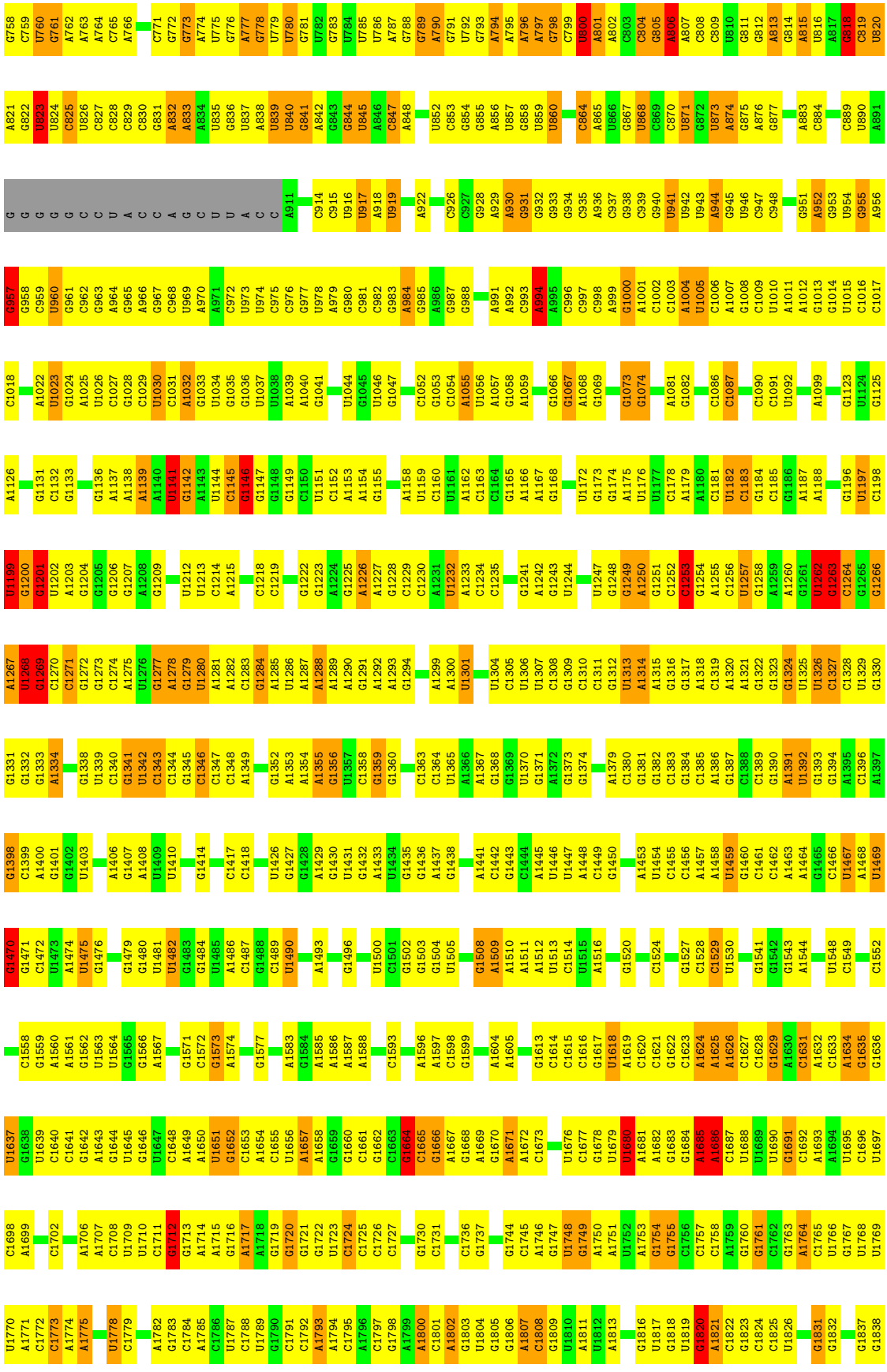
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

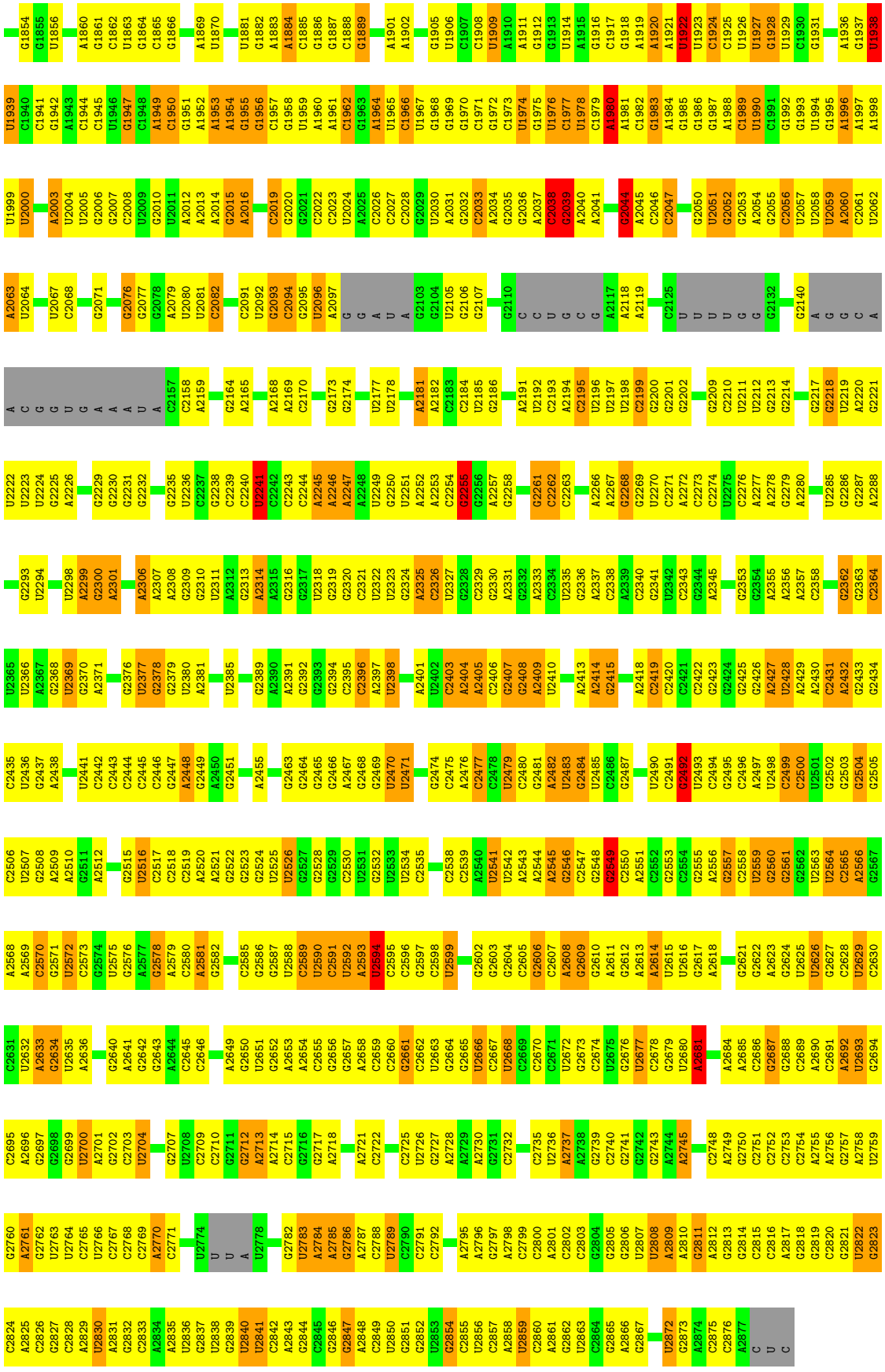
Note EDS was not executed.

- Molecule 1: 23S RIBOSOMAL RNA

Chain 0:






G1854 G1855 U1856 A1860 G1861 C1862 U1863 G1864 C1865 C1866 A1869 U1870 U1881 G1882 A1883 A1884 C1885 G1886 G1887 C1888 G1889 A1901 A1902 G1905 U1906 C1907 C1908 U1909 A1910 A1911 G1912 G1913 U1914 A1915 G1916 C1917 G1918 A1919 A1920 A1921 U1922 U1923 C1924 C1925 U1926 U1927 G1928 U1929 C1930 G1931 A1936 G1937 U1938
U1939 C1940 C1941 G1942 A1943 C1944 C1945 U1946 G1947 C1948 A1949 C1950 G1951 A1952 A1953 A1954 G1955 G1956 C1957 G1958 U1959 A1960 A1961 C1962 G1963 A1964 U1965 C1966 U1967 G1968 G1969 G1970 C1971 G1972 C1973 U1974 A1975 G1912 G1913 U1914 A1915 A1980 A1981 A1982 A1983 A1984 A1996 A1997 A1998
U1999 U2000 A2003 U2004 U2005 G2006 G2007 C2008 U2009 G2010 U2011 A2012 A2013 A2014 G2015 A2016 C2019 G2020 G2021 C2022 C2023 U2024 A2025 C2026 C2027 C2028 G2029 U2030 A2031 G2032 C2033 A2034 G2035 G2036 A2037 C2038 C2039 A2040 A2041 G2044 A2045 C2046 C2047 G2050 U2051 G2052 G2053 A2054 G2055 C2056 U2057 U2058 U2059 A2060 C2061 U2062
A2063 U2064 U2067 C2068 G2071 G2076 G2077 G2078 A2079 U2080 U2081 C2082 C2091 U2092 G2093 C2094 G2095 U2096 A2097 G G A U A G2103 G2104 U2105 G2106 G2107 G2110 C C U G C G A2117 A2118 A2119 C2125 U U U U G G G2132 G2140 A G G C A
A C G G U G A A A U A C2157 C2158 A2159 G2164 A2165 A2168 A2169 C2170 G2173 G2174 U2177 U2178 A2181 A2182 C2183 C2184 U2185 G2186 A2191 U2192 C2193 A2194 C2195 U2196 U2197 U2198 C2199 G2200 G2201 G2202 G2209 C2210 U2211 U2212 G2213 G2214 G2217 G2218 U2219 A2220 G2221
U2222 U2223 U2224 G2225 A2226 G2229 G2230 G2231 G2232 G2235 U2236 C2237 G2238 C2239 C2240 U2241 C2242 C2243 C2244 A2245 A2246 A2247 A2248 U2249 G2250 U2251 A2252 A2253 C2254 G2255 G2256 A2257 G2258 G2261 C2262 C2263 A2266 A2267 G2268 G2269 U2270 C2271 A2272 C2273 C2274 U2275 C2276 A2277 A2278 A2279 A2280 U2285 G2286 G2287 A2288
G2293 U2294 U2298 A2299 G2300 A2301 A2306 A2307 A2308 G2309 G2310 U2311 A2312 G2313 A2314 A2315 G2316 G2317 U2318 G2319 G2320 C2321 U2322 U2323 G2324 A2325 C2326 U2327 G2328 C2329 G2330 A2331 G2332 A2333 C2334 U2335 G2336 A2337 C2338 A2339 C2340 G2341 U2342 C2343 G2344 A2345 G2353 G2354 A2355 A2356 A2357 C2358 G2362 G2363 C2364
U2365 U2366 A2367 G2368 U2369 G2370 A2371 G2376 U2377 G2378 C2379 U2380 A2381 U2385 G2389 A2390 A2391 G2392 G2393 G2394 C2395 C2396 A2397 U2398 A2401 U2402 C2403 A2404 A2405 C2406 G2407 G2408 A2409 U2410 A2413 A2414 G2415 A2418 C2419 C2420 C2421 A2272 C2422 G2423 G2424 G2425 G2426 A2427 A2278 U2428 A2429 G2430 C2431 A2432 G2433 C2434
C2435 U2436 G2437 A2438 U2441 C2442 C2443 C2444 C2445 C2446 G2447 A2448 G2449 A2450 G2451 A2455 G2463 G2464 G2465 G2466 A2467 G2468 G2469 U2470 U2471 G2474 C2475 A2476 C2477 C2478 U2479 C2480 G2481 A2482 U2483 G2484 U2485 C2486 G2487 U2490 C2491 G2492 U2493 C2494 G2495 C2496 A2497 U2498 C2499 C2500 U2501 G2502 G2503 G2504 G2505
C2506 U2507 G2508 A2509 A2510 G2511 A2512 G2515 U2516 C2517 C2518 C2519 A2520 A2521 G2522 G2523 G2524 U2525 U2526 G2527 G2528 G2529 C2530 U2531 G2532 U2533 U2534 C2535 C2538 C2539 A2540 U2541 U2542 A2543 A2544 A2545 G2546 C2547 G2548 G2549 C2550 A2551 C2552 G2553 C2554 C2555 A2556 G2557 C2558 U2559 G2560 G2561 G2562 U2563 U2564 C2565 A2566 G2567
A2568 A2569 C2570 G2571 U2572 C2573 G2574 U2575 G2576 A2577 G2578 A2579 C2580 A2581 G2582 C2585 G2586 G2587 U2588 C2589 U2590 C2591 U2592 A2593 U2594 C2595 C2596 G2597 C2598 U2599 G2602 G2603 G2604 C2605 G2606 C2607 A2608 G2609 G2610 A2611 G2612 A2613 A2614 U2615 U2616 G2617 A2618 G2621 G2622 A2623 G2624 U2625 U2626 G2627 C2628 U2629 C2630
C2631 U2632 A2633 G2634 U2635 A2636 G2640 A2641 G2642 G2643 A2644 C2645 C2646 A2649 G2650 U2651 G2652 A2653 A2654 C2655 G2656 G2657 A2658 C2659 C2660 G2661 C2662 U2663 G2664 G2665 U2666 C2667 U2668 C2669 C2670 C2671 U2672 G2673 C2674 U2675 G2676 U2677 C2678 G2679 U2680 A2681 A2684 A2685 C2686 G2687 G2688 C2689 A2690 C2691 A2692 U2693 G2694
C2695 A2696 G2697 G2698 G2699 U2700 A2701 G2702 C2703 U2704 G2707 U2708 C2709 C2710 G2711 G2712 A2713 A2714 C2715 G2716 G2717 A2718 A2721 C2722 C2725 U2726 G2727 A2728 A2729 A2730 G2731 C2732 C2735 U2736 A2737 A2738 G2739 C2740 G2741 G2742 G2743 A2744 A2745 C2748 A2749 G2750 C2751 C2752 C2753 C2754 A2755 A2756 G2757 A2758 U2759
G2760 A2761 G2762 U2763 U2764 C2765 U2766 C2767 C2768 C2769 A2770 C2771 U2774 U U A U2778 G2782 U2783 A2784 A2785 G2786 A2787 C2788 U2789 C2790 C2791 C2792 A2795 A2796 G2797 A2798 C2799 C2800 A2801 C2802 C2803 G2804 G2805 G2806 U2807 U2808 A2809 A2810 G2811 A2812 G2813 G2814 C2815 C2816 A2817 G2818 G2819 C2820 G2821 U2822 G2823
C2824 A2825 C2826 G2827 C2828 A2829 U2830 A2831 G2832 C2833 A2834 A2835 U2836 G2837 U2838 G2839 U2840 U2841 C2842 A2843 G2844 C2845 G2846 G2847 A2848 C2849 U2850 G2851 G2852 U2853 G2854 C2855 U2856 C2857 A2858 U2859 C2860 A2861 G2862 U2863 C2864 G2865 A2866 G2867 U2872 G2873 A2874 C2875 C2876 A2877 C U C

• Molecule 2: 50S RIBOSOMAL PROTEIN L33

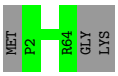
Chain 1:

• Molecule 3: 50S RIBOSOMAL PROTEIN L34

Chain 2:

• Molecule 4: 50S RIBOSOMAL PROTEIN L35

Chain 3:

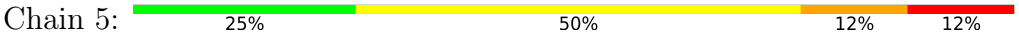


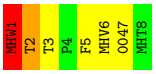
• Molecule 5: 50S RIBOSOMAL PROTEIN L36

Chain 4:

• Molecule 6: QUINUPRISTIN

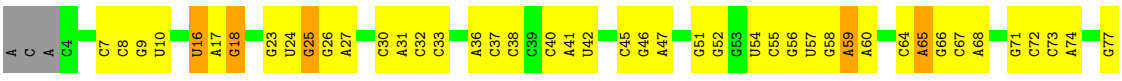
Chain 5:





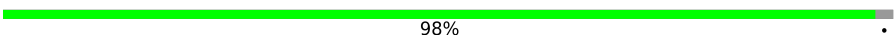
• Molecule 7: 5S RIBOSOMAL RNA

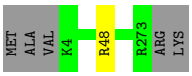
Chain 9:



• Molecule 8: 50S RIBOSOMAL PROTEIN L2

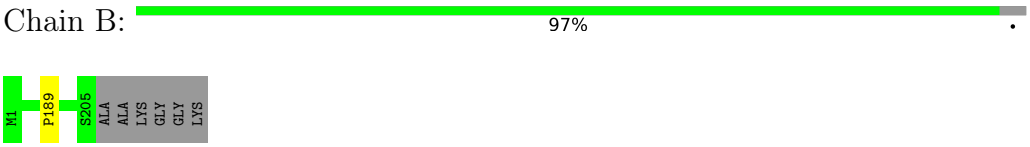
Chain A:





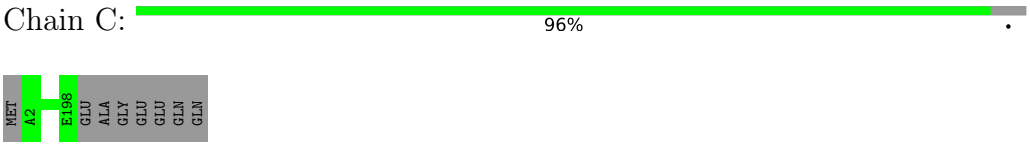
• Molecule 9: 50S RIBOSOMAL PROTEIN L3

Chain B:



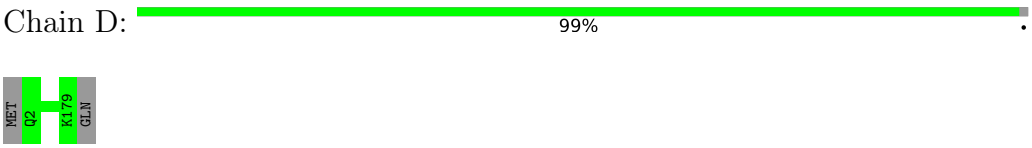
• Molecule 10: 50S RIBOSOMAL PROTEIN L4

Chain C:



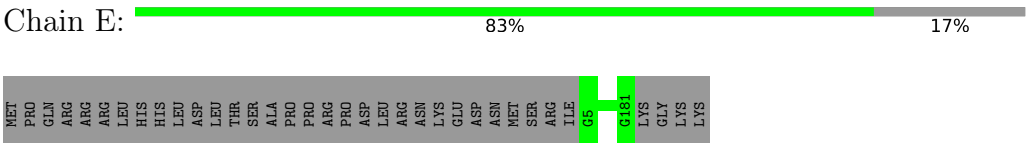
• Molecule 11: 50S RIBOSOMAL PROTEIN L5

Chain D:



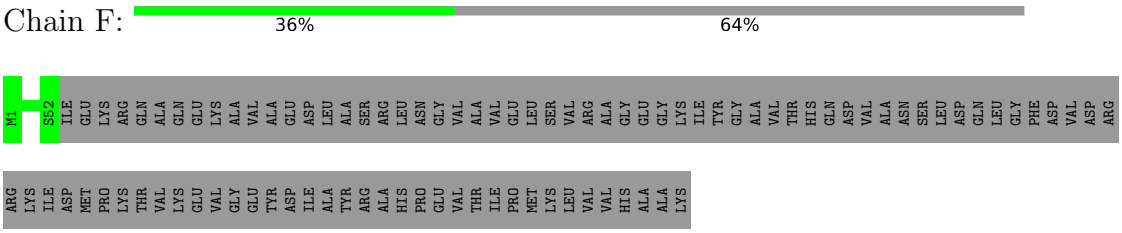
• Molecule 12: 50S RIBOSOMAL PROTEIN L6

Chain E:



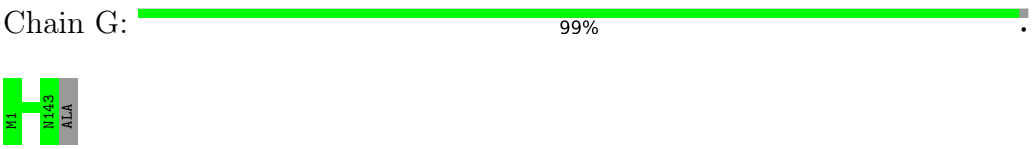
• Molecule 13: 50S RIBOSOMAL PROTEIN L9

Chain F:



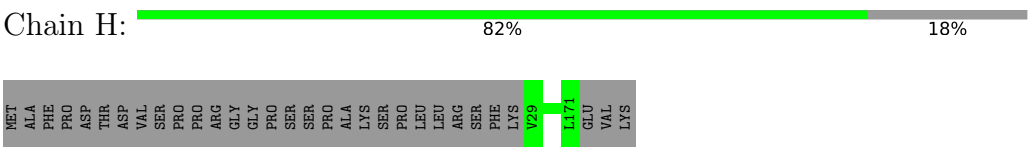
• Molecule 14: 50S RIBOSOMAL PROTEIN L11

Chain G:



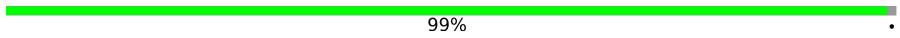
• Molecule 15: 50S RIBOSOMAL PROTEIN L13

Chain H:



• Molecule 16: 50S RIBOSOMAL PROTEIN L14

Chain I:

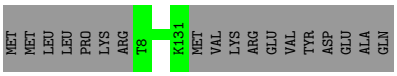


• Molecule 17: 50S RIBOSOMAL PROTEIN L15

Chain J:

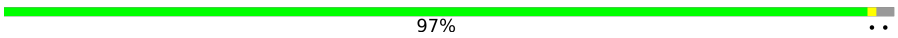
• Molecule 18: 50S RIBOSOMAL PROTEIN L16

Chain K:



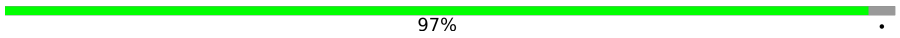
• Molecule 19: 50S RIBOSOMAL PROTEIN L17

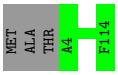
Chain L:



• Molecule 20: 50S RIBOSOMAL PROTEIN L18

Chain M:



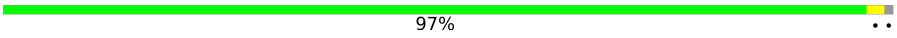


• Molecule 21: 50S RIBOSOMAL PROTEIN L19

Chain N:

• Molecule 22: 50S RIBOSOMAL PROTEIN L20

Chain O:



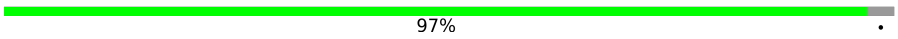
• Molecule 23: 50S RIBOSOMAL PROTEIN L21

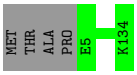
Chain P:

There are no outlier residues recorded for this chain.

• Molecule 24: 50S RIBOSOMAL PROTEIN L22

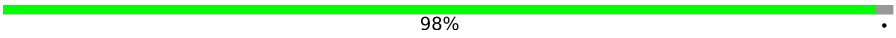
Chain Q:





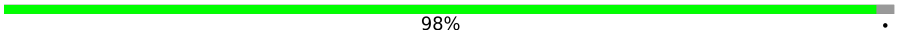
• Molecule 25: 50S RIBOSOMAL PROTEIN L23

Chain R:



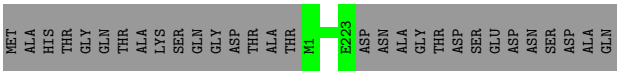
• Molecule 26: 50S RIBOSOMAL PROTEIN L24

Chain S:



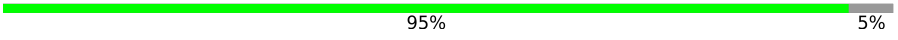
• Molecule 27: GENERAL STRESS PROTEIN CTC

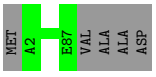
Chain T:



• Molecule 28: 50S RIBOSOMAL PROTEIN L27

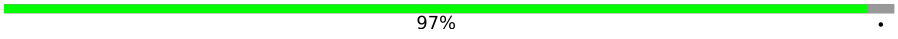
Chain U:





• Molecule 29: 50S RIBOSOMAL PROTEIN L29

Chain W:

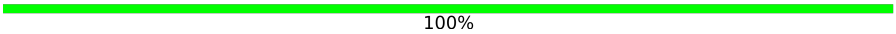


• Molecule 30: 50S RIBOSOMAL PROTEIN L30

Chain X:

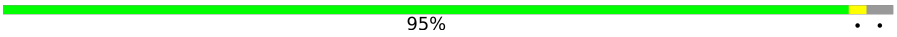
There are no outlier residues recorded for this chain.

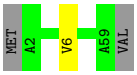
• Molecule 31: 50S RIBOSOMAL PROTEIN L31

Chain Y: 

There are no outlier residues recorded for this chain.

• Molecule 32: 50S RIBOSOMAL PROTEIN L32

Chain Z: 



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	168.50Å 406.00Å 693.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.42	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-3.42)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.278 , 0.348	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	65418	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 004, MHU, MHW, DOL, MHV, MHT, DBB

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	0	0.70	16/66467 (0.0%)	0.74	12/103673 (0.0%)
6	5	0.85	0/13	0.67	0/15
7	9	0.50	0/2813	0.65	0/4384
All	All	0.70	16/69293 (0.0%)	0.73	12/108072 (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
1	0	0	146
6	5	1	1
7	9	0	1
All	All	1	148

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	1962	C	N1-C2	-7.46	1.32	1.40
1	0	2255	G	C5-C6	-7.28	1.35	1.42
1	0	2789	U	N1-C2	6.94	1.44	1.38
1	0	868	U	N1-C2	6.93	1.44	1.38
1	0	806	A	C5-C6	6.88	1.47	1.41

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	0	994	A	N9-C1'-C2'	-6.36	105.00	112.00
1	0	800	U	OP2-P-O3'	6.27	119.00	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	0	2056	C	N1-C1'-C2'	-6.04	105.36	112.00
1	0	1686	A	C5'-C4'-O4'	5.86	116.13	109.10
1	0	1938	U	C2'-C3'-O3'	5.75	122.90	113.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	5	8	MHT	C3

5 of 148 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	126	C	Sidechain
1	0	174	A	Sidechain
1	0	211	U	Sidechain
1	0	33	C	Sidechain
1	0	8	A	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59359	0	29917	2138	0
2	1	53	0	0	0	0
3	2	46	0	0	0	0
4	3	63	0	0	0	0
5	4	35	0	0	0	0
6	5	73	0	64	6	0
7	9	2516	0	1286	66	0
8	A	270	0	0	1	0
9	B	205	0	0	1	0
10	C	197	0	0	0	0
11	D	178	0	0	0	0
12	E	177	0	0	0	0
13	F	52	0	0	0	0
14	G	143	0	0	0	0
15	H	143	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	I	132	0	0	0	0
17	J	141	0	0	0	0
18	K	124	0	0	0	0
19	L	114	0	0	1	0
20	M	111	0	0	0	0
21	N	125	0	0	0	0
22	O	117	0	0	2	0
23	P	100	0	0	0	0
24	Q	130	0	0	0	0
25	R	93	0	0	0	0
26	S	113	0	0	0	0
27	T	223	0	0	0	0
28	U	86	0	0	0	0
29	W	65	0	0	0	0
30	X	55	0	0	0	0
31	Y	73	0	0	0	0
32	Z	58	0	0	2	0
33	0	48	0	47	16	0
All	All	65418	0	31314	2213	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

The worst 5 of 2213 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1463:A:H1'	1:0:1543:G:H22	1.05	1.14
1:0:128:C:H2'	1:0:129:A:H5"	1.19	1.10
1:0:1656:U:H2'	1:0:1657:A:H5"	1.34	1.10
1:0:940:G:H3'	1:0:941:U:H5"	1.23	1.09
1:0:2607:C:H3'	1:0:2608:A:H5'	1.10	1.08

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
6	5	2/8 (25%)	1 (50%)	0	1 (50%)	0 0

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	5	2	THR

5.3.2 Protein sidechains (i)

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
6	5	2/2 (100%)	2 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2757/2880 (95%)	433 (15%)	19 (0%)
7	9	117/124 (94%)	12 (10%)	0
All	All	2874/3004 (95%)	445 (15%)	19 (0%)

5 of 445 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	45	C
1	0	48	A
1	0	49	U
1	0	50	G
1	0	59	G

5 of 19 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	2015	G
1	0	2377	U
1	0	2404	A
1	0	2261	G
1	0	1354	A

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

5 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	$\#\|Z\| > 2$
6	004	5	7	6	9,10,11	1.69	2 (22%)	9,12,14	1.27	1 (11%)
6	MHW	5	1	6	9,9,10	0.76	0	10,11,13	1.56	1 (10%)
6	MHV	5	6	6	7,9,10	0.67	0	7,11,13	1.68	2 (28%)
6	MHU	5	5	6	14,15,16	1.14	1 (7%)	18,19,21	1.11	1 (5%)
6	DBB	5	3	6	4,5,6	0.58	0	1,5,7	0.06	0

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
6	004	5	7	6	-	2/4/6/8	0/1/1/1
6	MHW	5	1	6	-	2/2/2/4	0/1/1/1
6	MHV	5	6	6	-	0/1/12/14	0/1/1/1
6	MHU	5	5	6	-	2/9/12/14	0/1/1/1
6	DBB	5	3	6	-	1/3/4/6	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	5	7	004	CB-CA	3.12	1.55	1.52
6	5	7	004	CG2-CB	-2.70	1.34	1.39
6	5	5	MHU	CZ1-NZ	-2.59	1.39	1.45

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	5	1	MHW	O-C-CA	-4.20	120.24	124.22
6	5	6	MHV	CE-CD2-CG	3.22	117.29	111.89
6	5	5	MHU	O-C-CA	-2.83	117.37	124.78
6	5	7	004	CG2-CB-CA	2.31	124.38	120.65
6	5	6	MHV	CB-CA-N	-2.02	108.33	112.50

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	5	1	MHW	O-C-CA-N
6	5	1	MHW	O-C-CA-CB
6	5	3	DBB	O-C-CA-CB
6	5	5	MHU	N-CA-CB-CG
6	5	5	MHU	C-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	5	1	MHW	1	0
6	5	3	DBB	5	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
33	DOL	0	2882	-	43,50,50	4.58	11 (25%)	51,70,70	3.94	18 (35%)

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
33	DOL	0	2882	-	2/2/14/20	20/58/77/77	0/2/3/3

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	0	2882	DOL	O40-S39	18.61	1.77	1.44
33	0	2882	DOL	O41-S39	18.41	1.76	1.44
33	0	2882	DOL	C28-C29	-8.71	1.11	1.32
33	0	2882	DOL	C1-C37	4.83	1.62	1.52
33	0	2882	DOL	C8-C6	-4.51	1.42	1.50

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	0	2882	DOL	C4-N5-C1	-14.71	94.37	112.45
33	0	2882	DOL	O18-C17-C16	13.82	145.78	109.73
33	0	2882	DOL	C28-C26-N25	-9.38	97.30	114.97
33	0	2882	DOL	O40-S39-O41	-7.23	109.95	118.19
33	0	2882	DOL	O27-C26-C28	6.58	138.02	123.03

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
33	0	2882	DOL	C17
33	0	2882	DOL	C2

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
33	0	2882	DOL	O7-C6-N5-C1
33	0	2882	DOL	C8-C6-N5-C1
33	0	2882	DOL	C1-C2-S39-O41
33	0	2882	DOL	C1-C2-S39-O40
33	0	2882	DOL	C1-C2-S39-C42

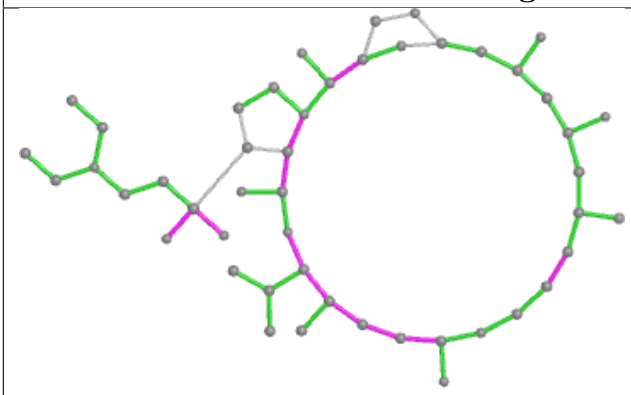
There are no ring outliers.

1 monomer is involved in 16 short contacts:

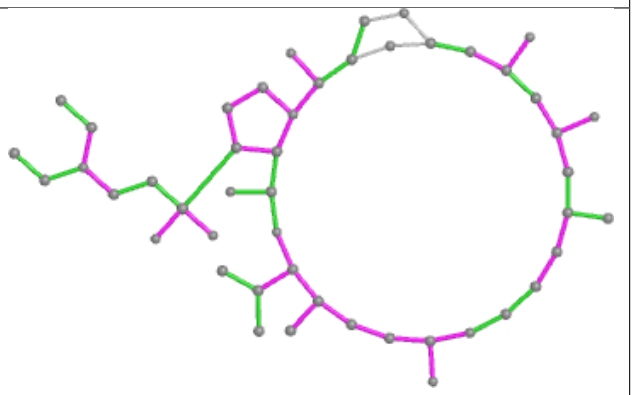
Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	0	2882	DOL	16	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

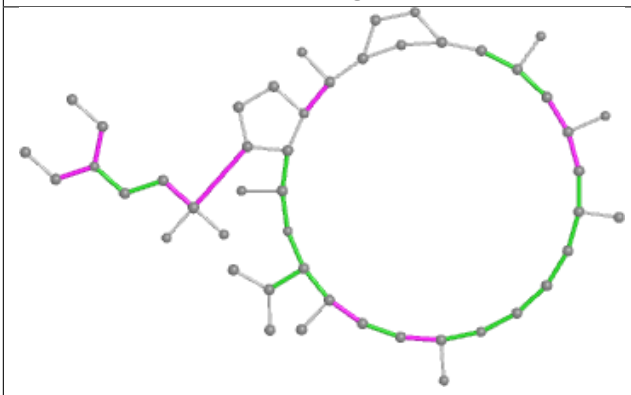
Ligand DOL 0 2882



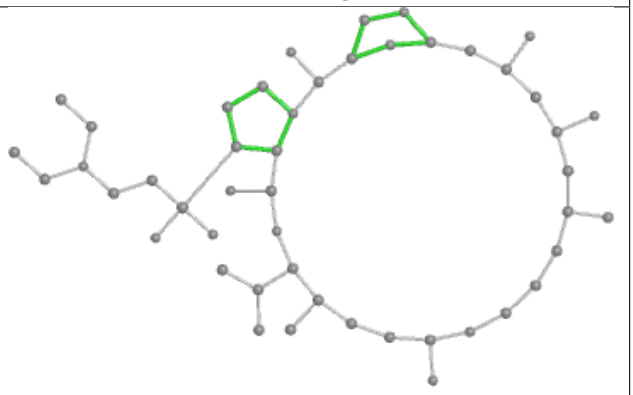
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.