



# wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 01:46 AM GMT

PDB ID : 3V23  
Title : Crystal structure of RMF bound to the 70S ribosome. This PDB entry contains coordinates for the 50S subunit of the 1st ribosome in the ASU  
Authors : Polikanov, Y.S.; Blaha, G.M.; Steitz, T.A.  
Deposited on : 2011-12-11  
Resolution : 3.00 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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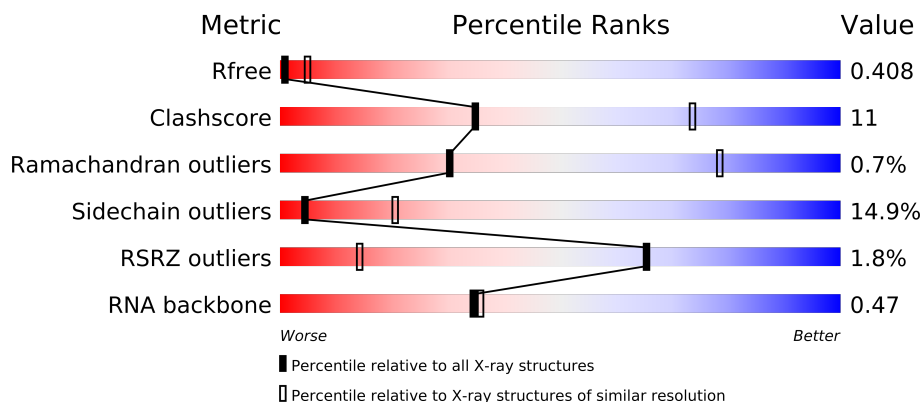
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.00 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	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)
RNA backbone	1838	1070 (3.50-2.50)

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	2915	
2	B	122	
3	D	276	
4	E	206	
5	F	210	
6	G	182	
7	H	180	
8	I	148	
9	N	140	
10	O	122	
11	P	150	
12	Q	141	

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Mol	Chain	Length	Quality of chain
13	R	118	
14	S	112	
15	T	146	
16	U	118	
17	V	101	
18	W	113	
19	X	96	
20	Y	110	
21	Z	206	
22	0	85	
23	1	98	
24	2	72	
25	3	60	
26	4	71	
27	5	60	
28	6	54	
29	7	49	
30	8	65	
31	9	37	

## 2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 91974 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 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2809	Total	C	N	O	P	0	0	0
			60512	26930	11328	19446	2808			

- Molecule 2 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

- Molecule 3 is a protein called 50S Ribosomal Protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			

- Molecule 4 is a protein called 50S Ribosomal Protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	204	Total	C	N	O	S	0	0	0
			1555	982	297	270	6			

- Molecule 5 is a protein called 50S Ribosomal Protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	203	Total	C	N	O	S	0	0	1
			1580	1007	298	273	2			

- Molecule 6 is a protein called 50S Ribosomal Protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	181	Total	C	N	O	S	0	0	0
			1368	879	242	244	3			

- Molecule 7 is a protein called 50S Ribosomal Protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	174	Total	C	N	O	S	0	0	0
			1317	837	243	236	1			

- Molecule 8 is a protein called 50S Ribosomal Protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	146	Total	C	N	O	S	0	0	0
			1040	669	180	190	1			

- Molecule 9 is a protein called 50S Ribosomal Protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	N	140	Total	C	N	O	S	0	0	0
			1112	717	207	184	4			

- Molecule 10 is a protein called 50S Ribosomal Protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	O	122	Total	C	N	O	S	0	0	0
			923	583	168	168	4			

- Molecule 11 is a protein called 50S Ribosomal Protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	P	149	Total	C	N	O	S	0	0	0
			1131	703	229	196	3			

- Molecule 12 is a protein called 50S Ribosomal Protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	Q	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 13 is a protein called 50S Ribosomal Protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	R	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 14 is a protein called 50S Ribosomal Protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	S	110	Total	C	N	O			
			865	544	172	149	0	0	0

- Molecule 15 is a protein called 50S Ribosomal Protein L19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	T	131	Total	C	N	O	S		
			1063	666	213	183	1	0	0

- Molecule 16 is a protein called 50S Ribosomal Protein L20.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	U	116	Total	C	N	O	S		
			959	608	201	149	1	0	0

- Molecule 17 is a protein called 50S Ribosomal Protein L21.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	V	100	Total	C	N	O	S		
			760	490	136	133	1	0	0

- Molecule 18 is a protein called 50S Ribosomal Protein L22.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	W	112	Total	C	N	O	S		
			881	554	172	153	2	0	0

- Molecule 19 is a protein called 50S Ribosomal Protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	X	95	Total	C	N	O	S		
			742	483	134	124	1	0	0

- Molecule 20 is a protein called 50S Ribosomal Protein L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	Y	107	Total	C	N	O	S		
			785	503	145	131	6	0	0

- Molecule 21 is a protein called 50S Ribosomal Protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	Z	198	Total	C	N	O	S	0	0	0
			1522	972	269	279	2			

- Molecule 22 is a protein called 50S Ribosomal Protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	0	76	Total	C	N	O	S	0	0	0
			594	368	125	100	1			

- Molecule 23 is a protein called 50S Ribosomal Protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	1	97	Total	C	N	O	S	0	0	0
			745	469	144	131	1			

- Molecule 24 is a protein called 50S Ribosomal Protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

- Molecule 25 is a protein called 50S Ribosomal Protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	3	59	Total	C	N	O	0	0	0
			458	293	87	78			

- Molecule 26 is a protein called 50S Ribosomal Protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	4	46	Total	C	N	O	S	0	0	0
			349	223	57	64	5			

- Molecule 27 is a protein called 50S Ribosomal Protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	5	59	Total	C	N	O	S	0	0	0
			455	286	90	74	5			

- Molecule 28 is a protein called 50S Ribosomal Protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	6	53	Total	C	N	O	S	0	0	0
			449	278	90	77	4			

- Molecule 29 is a protein called 50S Ribosomal Protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 30 is a protein called 50S Ribosomal Protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	8	64	Total	C	N	O	S	0	0	0
			509	326	99	82	2			

- Molecule 31 is a protein called 50S Ribosomal Protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	9	36	Total	C	N	O	S	0	0	0
			297	182	66	46	3			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	P	1	Total	Mg	0	0
			1	1		
32	0	2	Total	Mg	0	0
			2	2		
32	Q	3	Total	Mg	0	0
			3	3		
32	D	3	Total	Mg	0	0
			3	3		
32	E	6	Total	Mg	0	0
			6	6		
32	B	17	Total	Mg	0	0
			17	17		
32	8	2	Total	Mg	0	0
			2	2		
32	V	1	Total	Mg	0	0
			1	1		
32	1	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	W	1	Total 1	Mg 1	0	0
32	A	621	Total 621	Mg 621	0	0
32	U	2	Total 2	Mg 2	0	0
32	3	1	Total 1	Mg 1	0	0
32	R	2	Total 2	Mg 2	0	0
32	9	1	Total 1	Mg 1	0	0
32	2	1	Total 1	Mg 1	0	0
32	F	2	Total 2	Mg 2	0	0

- Molecule 33 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	9	1	Total 1	Zn 1	0	0
33	Y	1	Total 1	Zn 1	0	0
33	4	1	Total 1	Zn 1	0	0
33	6	1	Total 1	Zn 1	0	0
33	5	1	Total 1	Zn 1	0	0

- Molecule 34 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	A	1418	Total 1418	O 1418	0	0
34	B	31	Total 31	O 31	0	0
34	D	10	Total 10	O 10	0	0
34	E	7	Total 7	O 7	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	F	10	Total 10	O 10	0	0
34	H	1	Total 1	O 1	0	0
34	N	2	Total 2	O 2	0	0
34	O	1	Total 1	O 1	0	0
34	P	5	Total 5	O 5	0	0
34	Q	2	Total 2	O 2	0	0
34	R	5	Total 5	O 5	0	0
34	U	2	Total 2	O 2	0	0
34	V	2	Total 2	O 2	0	0
34	W	4	Total 4	O 4	0	0
34	X	1	Total 1	O 1	0	0
34	0	6	Total 6	O 6	0	0
34	3	1	Total 1	O 1	0	0
34	4	1	Total 1	O 1	0	0
34	5	5	Total 5	O 5	0	0
34	7	2	Total 2	O 2	0	0
34	8	8	Total 8	O 8	0	0
34	9	2	Total 2	O 2	0	0



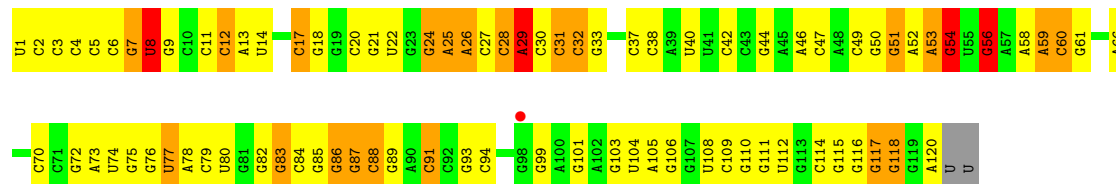


G2833	A2764	U2698	A2614	G2550	G2479	G2413	G2341	G2280	C2200	U2130	G2069	G2009	U1931	A1829
G2834	A2765	C2699	G2615	C2551	C2480	G2414	C2342	C2281	C2200	G2131	G2070	G2010	G1830	G1831
A2835	C2766	C2700	C2616	U2552	U2553	G2415	U2343	G2282	U2203	U2132	A2071	U2011	G1832	G1833
A2836	C2767	G2701	C2617	G2553	G2483	C2416	U2344	C2283	G2205	G2133	G2072	G2012	G1834	G1835
G2837	C2768	U2702	G2618	U2554	G2484	U2419	G2345	C2284	G2206	A2134	C2073	A2013	U1833	U1834
G2838	C2769	C2703	C2619	G2555	G2485	G2420	A2346	C2285	G2207	A2135	U2074	A2014	U1837	U1838
G2839	C2770	G2704	C2620	G2557	G2486	C2421	C2347	A2286	G2208	G2140	U2075	A2015	A1838	G1835
G2840	C2772	A2705	A2621	C2558	G2487	G2422	U2348	A2287	U2218	G2141	A2076	U2016	U1839	C1836
U2841	C2773	G2706	G2622	C2559	A2488	U2423	C2350	G2289	G2220	C2142	G2078	U2017	G1839	G1840
G2842	C2774	G2707	G2623	U2560	G2489	U2424	G2351	G2290	G2221	C2143	U2079	A2018	G1841	G1842
G2843	C2775	G2708	G2624	U2561	G2490	U2425	A2352	U2291	G2222	U2144	G2080	A2020	C1844	C1845
G2844	C2776	G2709	G2625	U2562	U2491	A2426	G2353	C2292	G2223	C2145	C2081	C2021	U1847	U1848
G2845	C2777	A2710	G2626	A2563	U2492	C2427	G2354	C2293	A2225	G2146	A2082	U2022	A1849	A1850
G2846	C2778	G2711	G2627	A2564	U2493	U2428	U2357	C2294	C2226	G2147	G2083	G2023	A1851	A1852
G2847	C2779	G2712	G2628	A2565	U2494	G2429	U2358	C2295	A2227	G2148	C2084	G2024	G1855	G1856
G2848	C2780	G2713	G2629	A2566	G2495	A2430	C2358	G2296	G2228	G2149	U1954	G2025	G1857	G1858
G2849	C2781	A2714	G2630	G2567	G2496	U2431	C2359	C2297	C2229	U2150	U2088	G2026	G1859	G1860
G2850	C2782	G2715	G2631	A2568	A2497	A2432	A2360	A2298	C2230	G2161	G2094	A2033	C1861	C1862
G2851	C2783	C2716	A2632	A2569	C2499	A2433	A2361	G2299	U2232	G2162	C2095	U2036	G1863	G1864
G2852	C2784	U2717	U2637	C2570	U2500	A2434	G2362	G2300	U2233	G2163	U2096	G2035	G1865	G1866
G2853	C2785	G2718	G2638	C2571	G2499	U2435	C2363	C2301	G2234	A2158	U2091	A2030	G1867	G1868
G2854	C2786	G2719	G2639	C2572	C2499	A2436	C2364	C2302	G2235	G2159	U2092	A2031	C1869	C1870
G2855	C2787	U2720	G2640	C2573	C2499	U2437	G2365	G2303	C2236	G2160	G2093	G2032	C1871	C1872
G2856	C2788	G2721	G2641	C2574	U2501	A2438	G2366	C2304	C2237	G2161	C2094	A2033	A1876	A1877
G2857	C2789	G2722	G2642	C2575	G2502	U2439	G2367	C2305	G2238	G2162	C2095	U2036	G1878	G1879
G2858	C2790	C2723	G2643	C2576	U2503	U2440	G2368	C2306	C2240	G2163	U2096	G2036	G1880	G1881
G2859	C2791	G2724	G2644	C2577	G2504	A2441	G2369	C2307	C2241	G2164	C2097	G2037	C1882	C1883
G2860	C2792	C2725	G2645	C2578	U2505	C2442	G2370	C2308	U2243	U2167	U2100	G2038	A1884	A1885
G2861	C2793	A2726	U2646	C2579	G2506	U2443	G2371	A2309	U2244	U2168	G2101	G2039	C1886	C1887
G2862	C2794	U2727	G2647	U2580	G2507	C2444	G2372	A2310	U2245	G2169	U2102	U2041	A1889	A1890
G2863	C2795	G2728	G2648	G2581	G2508	C2445	G2373	C2311	U2246	A2170	C2103	A2042	A1891	G1891
G2864	C2796	U2729	G2649	G2582	C2510	U2446	G2374	C2312	U2247	A2171	G2104	C2043	G1892	G1893
G2865	C2797	G2730	G2650	C2583	G2511	G2447	G2375	C2313	U2248	A2172	C2105	C2044	G1894	G1895
G2866	C2798	U2731	U2651	U2584	G2512	C2448	G2376	C2314	U2249	A2173	C2106	C2045	G1896	G1897
G2867	C2799	G2732	G2652	U2585	G2513	U2449	G2377	C2315	G2250	C2174	C2107	U2047	G1898	G1899
G2868	C2800	A2733	G2653	U2586	G2514	A2450	G2378	C2316	G2251	C2175	U2109	G2048	A1891	A1892
G2869	C2801	G2734	G2654	G2587	G2515	C2451	G2379	C2317	G2252	A2176	C2111	C2050	G1900	G1901
G2870	C2802	U2735	G2655	A2588	G2516	C2452	G2380	G2318	G2253	U2180	C2112	A2051	G1902	G1903
G2871	C2803	G2736	G2656	U2589	G2517	A2453	G2381	A2319	G2254	G2181	U2113	G2052	G1904	G1905
G2872	C2804	U2737	G2657	C2590	G2518	G2454	G2382	A2320	G2255	G2182	G2114	G2053	G1906	G1907
G2873	C2805	G2738	G2658	U2591	G2519	C2455	G2383	A2321	G2256	G2183	A2119	A2054	G1908	G1909
G2874	C2806	A2740	G2659	C2592	G2520	U2456	G2384	G2322	C2257	G2184	G2120	A2055	G1910	G1911
G2875	C2807	G2739	G2660	U2593	G2521	G2457	G2385	A2323	G2258	G2185	G2121	G2056	G1912	G1913
G2876	C2808	U2741	G2661	G2594	G2522	U2458	G2386	A2324	C2259	G2186	U2122	G2057	G1914	G1915
G2877	C2809	A2742	G2662	U2595	G2523	C2459	G2387	A2325	G2260	G2187	A2117	A2058	U1917	U1918
G2878	C2810	G2743	G2663	G2596	G2524	U2460	G2388	A2326	C2261	G2188	G2123	A2059	G1919	G1920
G2879	C2811	U2744	G2664	U2597	G2525	U2461	G2389	A2327	C2262	G2189	G2124	A2060	G1921	G1922
G2880	C2812	G2745	G2665	G2598	G2526	C2462	G2390	A2328	C2263	U2190	G2125	C2061	G1923	G1924
G2881	C2813	A2746	G2666	U2599	G2527	U2463	G2391	A2329	G2264	G2191	A2126	C2062	C1925	C1926
G2882	C2814	G2747	G2667	G2600	G2528	U2464	G2392	A2330	C2265	G2192	G2127	C2063	U1927	U1928
G2883	C2815	U2748	G2668	A2601	G2529	C2465	G2393	A2331	C2266	G2193	C2128	C2064	A1929	A1930
G2884	C2816	A2749	G2669	U2602	G2530	U2466	G2394	A2332	C2267	G2194	G2129	C2065	G1931	G1932
G2885	C2817	G2750	G2670	A2603	G2531	C2467	G2395	A2333	G2270	G2195	A2127	C2066	G1933	G1934
G2886	C2818	U2751	G2671	G2604	G2532	U2468	G2396	A2334	G2271	G2196	G2128	C2067	G1935	G1936
G2887	C2819	G2752	G2672	U2605	G2533	U2469	G2397	A2335	U2272	C2197	C2129	C2068	G1937	G1938
G2888	C2820	A2753	G2673	A2606	G2534	C2470	G2398	A2336	A2273	A2198	G2130	C2069	G1939	G1940
G2889	C2821	G2754	G2674	U2607	G2535	U2471	G2399	A2337	C2274	G2199	G2131	C2070	G1941	G1942
G2890	C2822	U2755	G2675	A2608	G2536	C2472	G2400	A2338	A2275	G2200	G2132	C2071	G1943	G1944
G2891	C2823	G2756	G2676	G2609	G2537	U2473	C2401	A2339	G2276	G2201	G2133	C2072	G1945	G1946
G2892	C2824	A2756	G2677	U2610	G2538	U2474	G2402	A2340	G2277	G2202	G2134	C2073	G1947	G1948
G2893	C2825	G2757	G2678	A2611	G2539	C2475	C2403	A2341	U2278	A2205	G2135	C2074	G1949	G1950
G2894	C2826	U2758	G2679	U2612	G2540	U2476	G2404	A2342	A2279	G2206	G2136	C2075	G1951	G1952
G2895	C2827	A2759	G2680	G2613	G2541	C2477	G2405	A2343	G2280	G2207	G2137	C2076	G1953	G1954
G2896	C2828	G2760	G2681	C2614	G2542	U2478	G2406	A2344	U2281	G2208	G2138	C2077	G1955	G1956
G2897	C2829	U2761	G2682	U2615	G2543	U2479	G2407	A2345	A2282	G2209	G2139	C2078	G1957	G1958
G2898	C2830	G2762	G2683	G2616	G2544	C2480	G2408	A2346	C2283	G2210	G2140	C2079	G1959	G1960
G2899	C2831	U2763	G2684	U2617	G2545	U2481	G2409	A2347	C2284	G2211	G2141	C2080	G1961	G1962
G2900	C2832	G2764	G2685	G2618	G2546	U2482	G2410	A2348	C2285	G2212	G2142	C2081	G1963	G1964
G2901	C2833	U2765	G2686	U2619	G2547	U2483	G2411	A2349	A2286	G2213	G2143	C2082	G1965	G1966
G2902	C2834	A2766	G2687	A2620	G2548	U2484	G2412	A2350	A2287	G2214	G2144	C2083	G1967	G1968
G2903	C2835	G2767	G2688	U2621	G2549	U2485	G2413	A2351	A2288	G2215	G2145	C2084	G1969	G1970
G2904	C2836	U2768	G2689	G2622	G2550	U2486	G2414	A2352	A2289	G2216	G2146	C2085	G1971	G1972
G2905	C2837	A2769	G2690	U2623	G2551	U2487	G2415	A2353	A2290	G2217	G2147	C2086	G1973	G1974
G2906	C2838	G2769	G2691	A2623	G2552	U2488	G2416	A2354	C2291	G2218	G2148	C2087	G1975	G1976
G2907	C2839	U2770	G2692	U2624	G2553	U2489	G2417	A2355	C2292	G2219	G2149	C2088	G1977	G1978
G2908	C2840	A2771	G2693	G2625	G2554	U2490	G2418	A2356	A2293	G2220	G2150	C2089	G1979	G1980
G2909	C2841	G2772	G2694	U2626	G2555	U2491	G2419	A2357	C2294	G2221	G2151	C2090	G1981	G1982
G2910	C2842	U2773	G2695	A2626	G2556	U2492	G2420	A2358	A2295	G2222	G2152	C2091	G1983	G1984
G2911	C2843	A2774	G2696	U2627	G2557	U2493	G2421	A2359	C2296	G2223	G2153	C2092	G1985	G1986
G2912	C2844	G2775	G2697	A2628	G2558	U2494	G2422	A2360	A2297	G2224	G2154	C2093	G1987	G1988
G2913	C2845	U2776	G2698	G2629	G2559	U2495	G2423	A2361	C2298	G2225	G2155	C2094	G1989	G1990
G2914	C2846	A2777	G2699	U2630	G2560	U2496	G2424	A2362	A2299	G2226	G2156	C2095	G1991	G1992
G2915	C2847	G2778	G2700	G2631	G2561	U2497	G2425	A2363	G2300	G2227	G2157	C2096	G1993	G1994
G2916	C2848	U2779	C2701	G2632	G2562	U2498	G2426	A2364	C2301	G2228	G2158	C2097	G1995	G1996
G2917	C2849	G2780	G2702	G2633	G2563	U2499	G2427	A2365	C2302	G2229	G2159	C2098	G1997	G1998
G2918	C2850	A2781	U2703	G2634	G2564	U2500	G2428	G2366	C2303	C2230	G2160	C2099	G1999	G2000
G2919	C2851	G2782	C2704	G2635	G2565	U2501	G2429	G2367	C2304	C2231	G2161	C2100	G200	

C

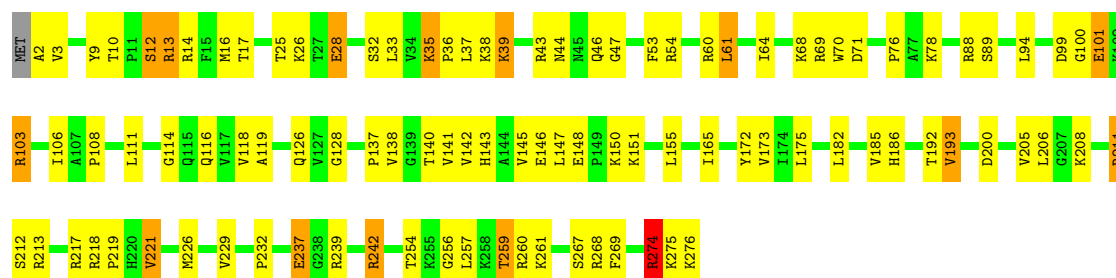
- Molecule 2: 5S Ribosomal RNA

Chain B:



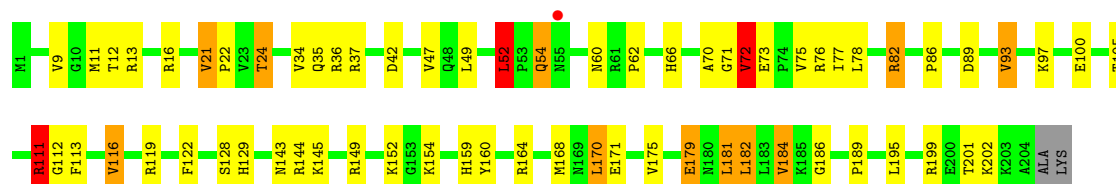
- Molecule 3: 50S Ribosomal Protein L2

Chain D:



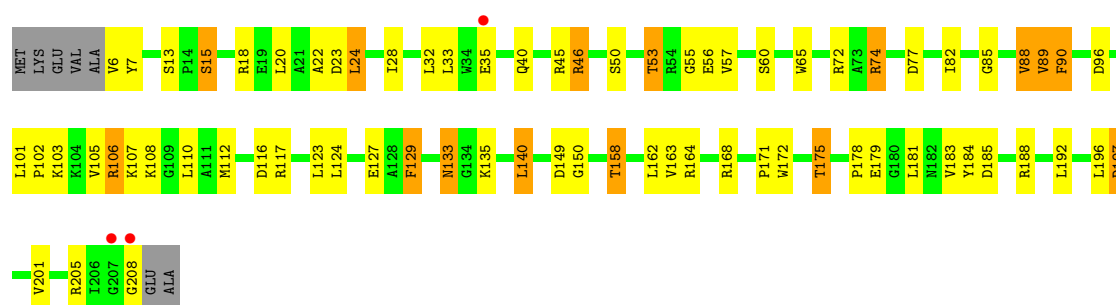
- Molecule 4: 50S Ribosomal Protein L3

Chain E:



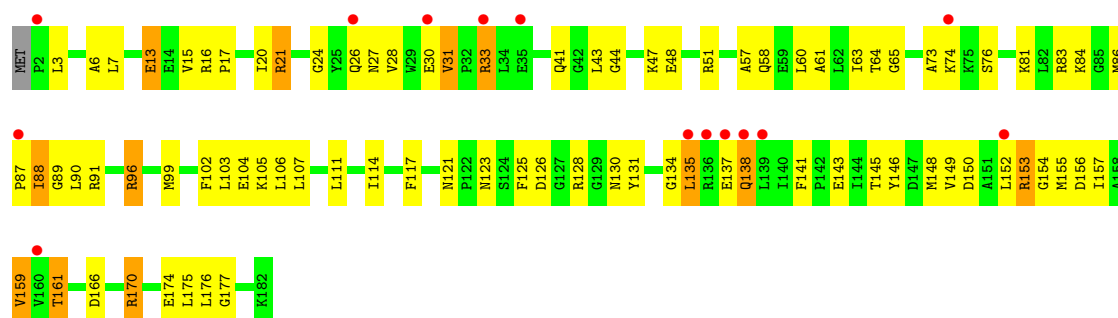
- Molecule 5: 50S Ribosomal Protein L4

Chain F:



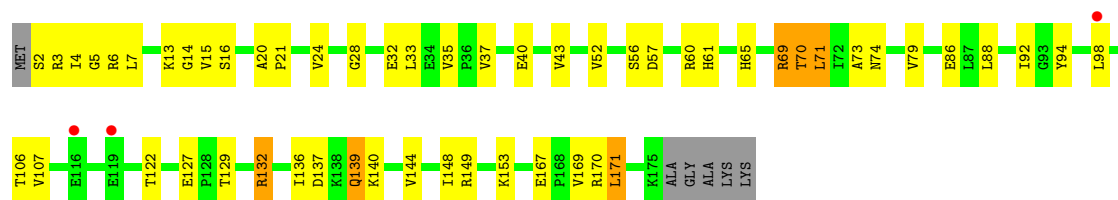
- Molecule 6: 50S Ribosomal Protein L5

Chain G:



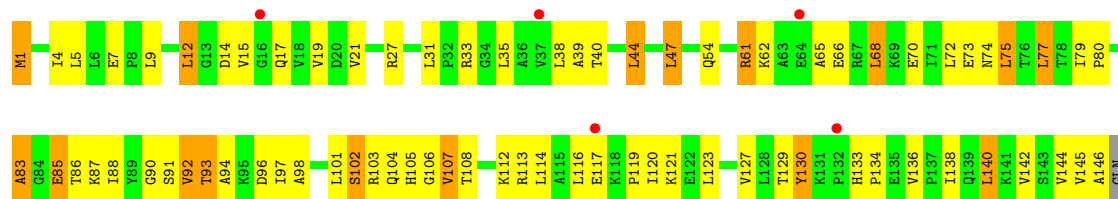
• Molecule 7: 50S Ribosomal Protein L6

Chain H:



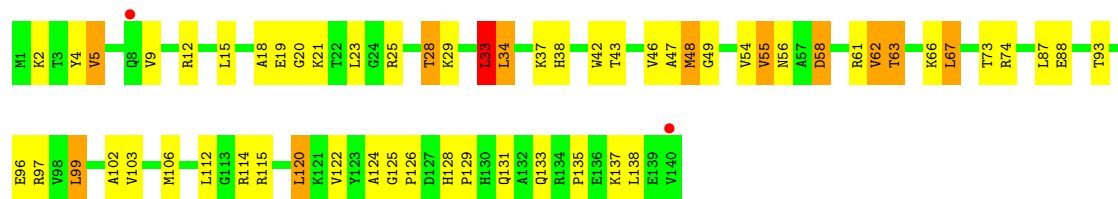
• Molecule 8: 50S Ribosomal Protein L9

Chain I:



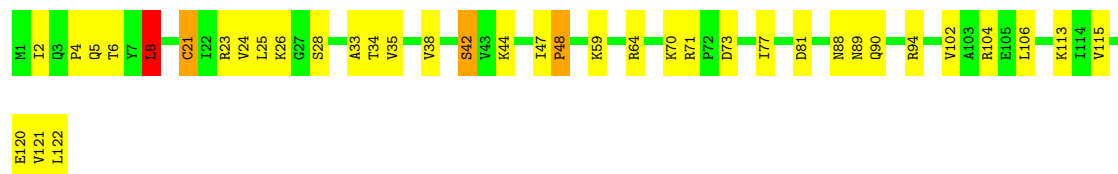
• Molecule 9: 50S Ribosomal Protein L13

Chain N:



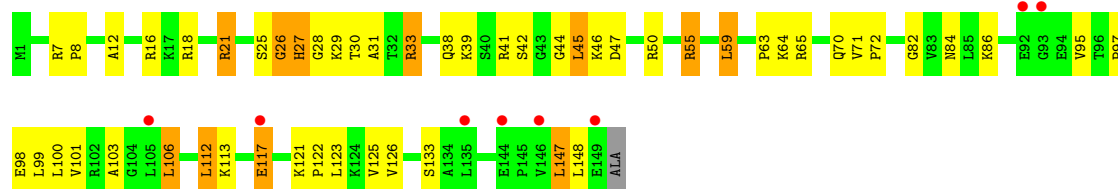
• Molecule 10: 50S Ribosomal Protein L14

Chain O:



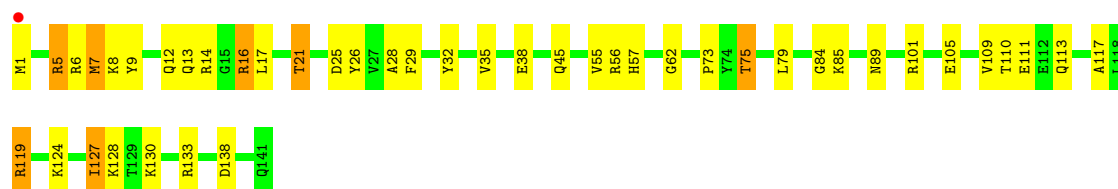
- Molecule 11: 50S Ribosomal Protein L15

Chain P:



- Molecule 12: 50S Ribosomal Protein L16

Chain Q:



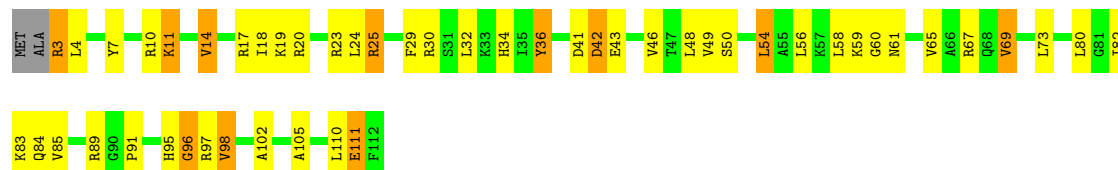
- Molecule 13: 50S Ribosomal Protein L17

Chain R:



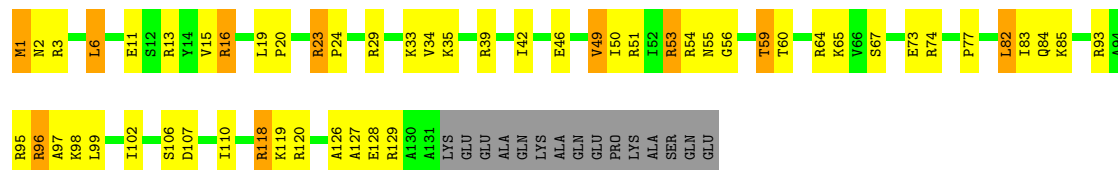
- Molecule 14: 50S Ribosomal Protein L18

Chain S:



- Molecule 15: 50S Ribosomal Protein L19

Chain T:



- Molecule 16: 50S Ribosomal Protein L20

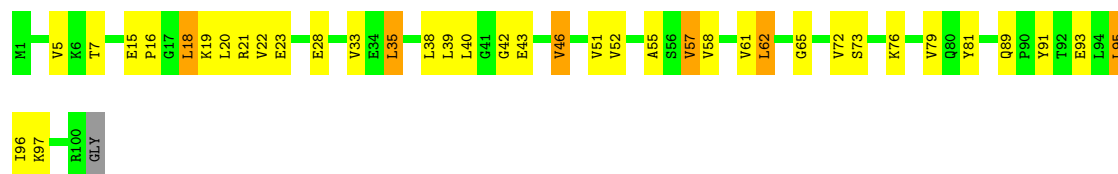
Chain U:





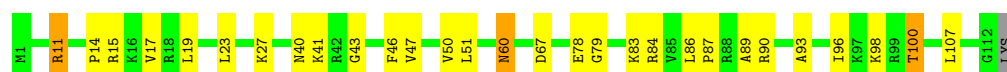
- Molecule 17: 50S Ribosomal Protein L21

Chain V:



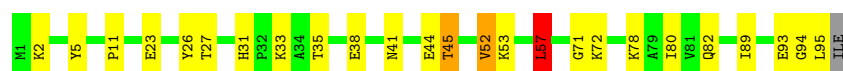
- Molecule 18: 50S Ribosomal Protein L22

Chain W:



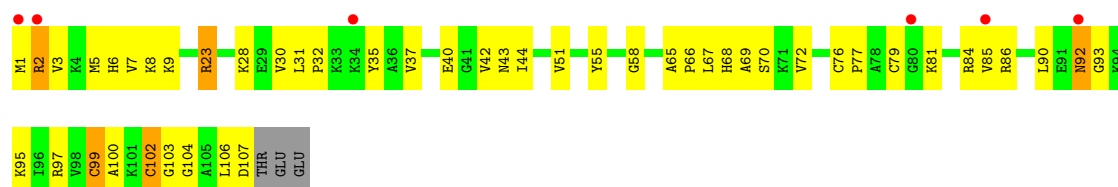
- Molecule 19: 50S Ribosomal Protein L23

Chain X:



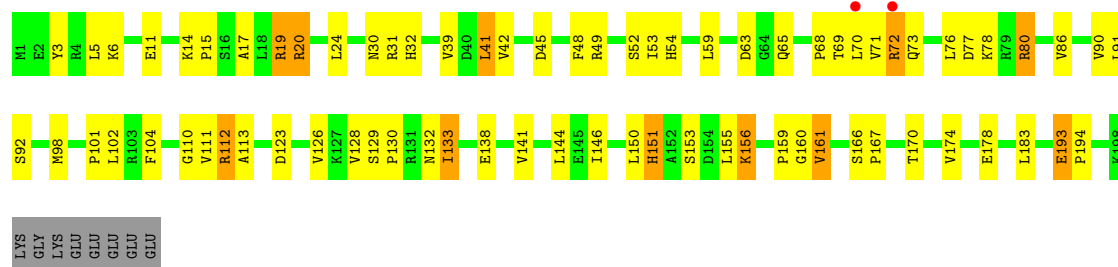
- Molecule 20: 50S Ribosomal Protein L24

Chain Y:



- Molecule 21: 50S Ribosomal Protein L25

Chain Z:



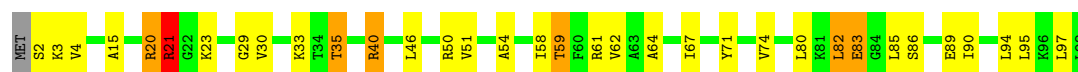
- Molecule 22: 50S Ribosomal Protein L27

Chain 0:



- Molecule 23: 50S Ribosomal Protein L28

Chain 1: 



- Molecule 24: 50S Ribosomal Protein L29

Chain 2: 



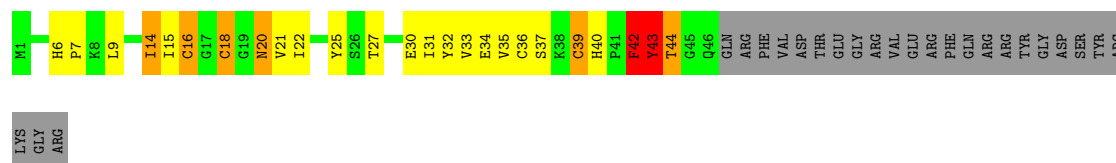
- Molecule 25: 50S Ribosomal Protein L30

Chain 3: 



- Molecule 26: 50S Ribosomal Protein L31

Chain 4: 



- Molecule 27: 50S Ribosomal Protein L32

Chain 5: 



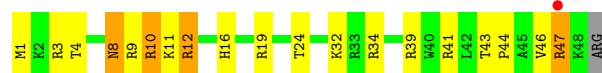
- Molecule 28: 50S Ribosomal Protein L33

Chain 6: 



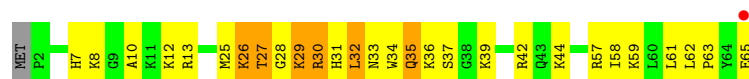
- Molecule 29: 50S Ribosomal Protein L34

Chain 7: 



- Molecule 30: 50S Ribosomal Protein L35

Chain 8: 



- Molecule 31: 50S Ribosomal Protein L36

Chain 9: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.24Å 451.44Å 621.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.75 – 3.00 49.75 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.9 (49.75-3.00) 98.0 (49.75-3.00)	Depositor EDS
$R_{merge}$	0.27	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.34 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, $R_{free}$	0.218 , 0.254 0.403 , 0.408	Depositor DCC
$R_{free}$ test set	57194 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	68.3	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 25.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 1142037 reflections	Xtriage
$F_o, F_c$ correlation	0.68	EDS
Total number of atoms	91974	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% 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	1.60	727/67771 (1.1%)	1.72	2179/105789 (2.1%)
2	B	1.11	3/2878 (0.1%)	1.57	62/4490 (1.4%)
3	D	0.88	3/2186 (0.1%)	0.96	0/2944
4	E	0.89	0/1588	0.96	3/2145 (0.1%)
5	F	0.88	1/1615 (0.1%)	0.86	0/2188
6	G	0.53	0/1393	0.71	0/1892
7	H	0.68	0/1343	0.80	3/1820 (0.2%)
8	I	0.64	0/1055	0.83	0/1445
9	N	0.86	0/1139	0.87	2/1538 (0.1%)
10	O	0.79	1/933 (0.1%)	0.86	1/1257 (0.1%)
11	P	0.80	0/1148	0.93	1/1529 (0.1%)
12	Q	0.79	0/1143	0.89	0/1527
13	R	0.82	0/982	0.94	2/1312 (0.2%)
14	S	0.65	0/875	0.88	0/1168
15	T	0.74	0/1077	0.87	0/1444
16	U	1.02	0/977	0.89	0/1301
17	V	0.89	0/771	0.84	0/1037
18	W	1.04	0/891	0.99	2/1197 (0.2%)
19	X	0.87	0/756	0.88	1/1016 (0.1%)
20	Y	0.81	0/798	0.88	0/1073
21	Z	0.62	0/1555	0.82	1/2118 (0.0%)
22	0	0.83	0/602	0.86	0/804
23	1	0.80	0/752	1.00	3/1003 (0.3%)
24	2	0.81	0/590	0.82	0/781
25	3	0.79	0/463	0.86	1/623 (0.2%)
26	4	0.64	0/358	0.82	1/487 (0.2%)
27	5	1.01	0/469	0.99	1/634 (0.2%)
28	6	0.84	1/456 (0.2%)	0.86	0/609
29	7	1.07	0/426	1.16	2/561 (0.4%)
30	8	0.88	0/516	1.00	2/679 (0.3%)
31	9	0.85	0/300	0.91	0/395
All	All	1.41	736/97806 (0.8%)	1.55	2267/146806 (1.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	D	0	1
4	E	0	2
5	F	0	2
6	G	0	1
8	I	0	1
9	N	0	1
10	O	0	1
11	P	0	4
14	S	0	2
15	T	0	1
19	X	0	1
20	Y	0	1
21	Z	0	1
23	1	0	1
26	4	0	3
All	All	0	23

The worst 5 of 736 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	530	G	C2-N3	-14.25	1.21	1.32
1	A	1142(A)	A	N9-C4	-13.60	1.29	1.37
1	A	2335	A	C6-N6	-12.80	1.23	1.33
1	A	2296	U	C4-C5	11.32	1.53	1.43
1	A	528	A	N9-C4	-11.10	1.31	1.37

The worst 5 of 2267 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1779	U	C5-C6-N1	-24.54	110.43	122.70
1	A	2296	U	C5-C6-N1	-19.55	112.93	122.70
1	A	2296	U	C2-N3-C4	-18.06	116.16	127.00
1	A	2296	U	N1-C2-N3	17.62	125.47	114.90
1	A	530	G	N3-C2-N2	-17.53	107.63	119.90

There are no chirality outliers.

5 of 23 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	274	ARG	Peptide
4	E	70	ALA	Peptide
4	E	72	VAL	Peptide
5	F	129	PHE	Peptide
5	F	85	GLY	Peptide

## 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	60512	0	30492	876	0
2	B	2573	0	1304	45	0
3	D	2136	0	2218	67	0
4	E	1555	0	1607	39	0
5	F	1580	0	1621	51	0
6	G	1368	0	1324	51	0
7	H	1317	0	1376	30	0
8	I	1040	0	1045	55	0
9	N	1112	0	1180	37	0
10	O	923	0	981	23	0
11	P	1131	0	1201	38	0
12	Q	1122	0	1179	33	0
13	R	968	0	1033	22	0
14	S	865	0	905	46	0
15	T	1063	0	1103	37	0
16	U	959	0	1019	24	0
17	V	760	0	816	20	0
18	W	881	0	935	17	0
19	X	742	0	799	17	0
20	Y	785	0	828	31	0
21	Z	1522	0	1511	49	0
22	0	594	0	604	23	0
23	1	745	0	804	31	0
24	2	588	0	643	19	0
25	3	458	0	503	9	0
26	4	349	0	336	20	0
27	5	455	0	472	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	6	449	0	462	19	0
29	7	418	0	467	11	0
30	8	509	0	565	23	0
31	9	297	0	316	8	0
32	0	2	0	0	0	0
32	1	1	0	0	0	0
32	2	1	0	0	0	0
32	3	1	0	0	0	0
32	8	2	0	0	0	0
32	9	1	0	0	0	0
32	A	621	0	0	0	0
32	B	17	0	0	0	0
32	D	3	0	0	0	0
32	E	6	0	0	0	0
32	F	2	0	0	0	0
32	P	1	0	0	0	0
32	Q	3	0	0	0	0
32	R	2	0	0	0	0
32	U	2	0	0	0	0
32	V	1	0	0	0	0
32	W	1	0	0	0	0
33	4	1	0	0	0	0
33	5	1	0	0	0	0
33	6	1	0	0	0	0
33	9	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	6	0	0	0	0
34	3	1	0	0	0	0
34	4	1	0	0	0	0
34	5	5	0	0	1	0
34	7	2	0	0	0	0
34	8	8	0	0	0	0
34	9	2	0	0	1	0
34	A	1418	0	0	86	0
34	B	31	0	0	1	0
34	D	10	0	0	4	0
34	E	7	0	0	0	0
34	F	10	0	0	0	0
34	H	1	0	0	0	0
34	N	2	0	0	0	0
34	O	1	0	0	0	0
34	P	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	Q	2	0	0	0	0
34	R	5	0	0	0	0
34	U	2	0	0	0	0
34	V	2	0	0	0	0
34	W	4	0	0	0	0
34	X	1	0	0	0	0
All	All	91974	0	59649	1569	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 11.

The worst 5 of 1569 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2296:U:O4	1:A:2335:A:N6	1.76	1.15
1:A:2057:A:OP2	34:A:4248:HOH:O	1.72	1.05
1:A:1310:G:OP2	29:7:9:ARG:NH1	1.94	1.00
1:A:2304:G:H1	1:A:2312:U:H3	1.11	0.97
1:A:139(A):G:N2	19:X:44:GLU:OE1	1.97	0.97

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	D	273/276 (99%)	258 (94%)	14 (5%)	1 (0%)	43 87
4	E	202/206 (98%)	188 (93%)	12 (6%)	2 (1%)	22 70
5	F	201/210 (96%)	187 (93%)	13 (6%)	1 (0%)	38 84
6	G	179/182 (98%)	151 (84%)	28 (16%)	0	100 100
7	H	172/180 (96%)	156 (91%)	14 (8%)	2 (1%)	19 64
8	I	144/148 (97%)	114 (79%)	27 (19%)	3 (2%)	11 47
9	N	138/140 (99%)	128 (93%)	6 (4%)	4 (3%)	7 35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	O	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
11	P	147/150 (98%)	134 (91%)	12 (8%)	1 (1%)	30	78
12	Q	139/141 (99%)	127 (91%)	12 (9%)	0	100	100
13	R	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
14	S	108/112 (96%)	96 (89%)	11 (10%)	1 (1%)	25	73
15	T	129/146 (88%)	125 (97%)	4 (3%)	0	100	100
16	U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
17	V	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
18	W	110/113 (97%)	106 (96%)	4 (4%)	0	100	100
19	X	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
20	Y	105/110 (96%)	94 (90%)	9 (9%)	2 (2%)	12	51
21	Z	196/206 (95%)	178 (91%)	15 (8%)	3 (2%)	15	58
22	0	74/85 (87%)	71 (96%)	3 (4%)	0	100	100
23	1	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
24	2	68/72 (94%)	65 (96%)	3 (4%)	0	100	100
25	3	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
26	4	44/71 (62%)	37 (84%)	7 (16%)	0	100	100
27	5	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
28	6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
29	7	46/49 (94%)	44 (96%)	1 (2%)	1 (2%)	10	45
30	8	62/65 (95%)	59 (95%)	2 (3%)	1 (2%)	14	56
31	9	34/37 (92%)	34 (100%)	0	0	100	100
All	All	3372/3526 (96%)	3116 (92%)	234 (7%)	22 (1%)	30	78

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	P	27	HIS
5	F	90	PHE
8	I	113	ARG
9	N	23	LEU
20	Y	103	GLY

### 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	D	215/218 (99%)	181 (84%)	34 (16%)	4	18
4	E	163/166 (98%)	138 (85%)	25 (15%)	4	19
5	F	159/166 (96%)	133 (84%)	26 (16%)	3	16
6	G	128/156 (82%)	106 (83%)	22 (17%)	3	14
7	H	141/148 (95%)	127 (90%)	14 (10%)	11	40
8	I	99/124 (80%)	75 (76%)	24 (24%)	1	5
9	N	117/119 (98%)	92 (79%)	25 (21%)	1	8
10	O	98/100 (98%)	90 (92%)	8 (8%)	17	52
11	P	114/116 (98%)	98 (86%)	16 (14%)	5	23
12	Q	111/111 (100%)	95 (86%)	16 (14%)	5	22
13	R	101/101 (100%)	82 (81%)	19 (19%)	2	12
14	S	84/88 (96%)	69 (82%)	15 (18%)	2	13
15	T	110/127 (87%)	95 (86%)	15 (14%)	5	24
16	U	93/94 (99%)	84 (90%)	9 (10%)	12	42
17	V	79/82 (96%)	62 (78%)	17 (22%)	1	8
18	W	89/92 (97%)	78 (88%)	11 (12%)	7	28
19	X	75/78 (96%)	70 (93%)	5 (7%)	23	64
20	Y	80/91 (88%)	66 (82%)	14 (18%)	3	14
21	Z	159/179 (89%)	141 (89%)	18 (11%)	9	33
22	0	59/67 (88%)	54 (92%)	5 (8%)	15	51
23	1	78/83 (94%)	67 (86%)	11 (14%)	5	23
24	2	65/67 (97%)	59 (91%)	6 (9%)	13	46
25	3	49/52 (94%)	43 (88%)	6 (12%)	7	29
26	4	39/63 (62%)	29 (74%)	10 (26%)	1	4
27	5	50/52 (96%)	45 (90%)	5 (10%)	11	39
28	6	50/52 (96%)	39 (78%)	11 (22%)	1	7
29	7	41/42 (98%)	32 (78%)	9 (22%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	8	52/55 (94%)	43 (83%)	9 (17%)	3	14
31	9	32/34 (94%)	29 (91%)	3 (9%)	13	44
All	All	2730/2923 (93%)	2322 (85%)	408 (15%)	4	20

5 of 408 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	P	64	LYS
13	R	111	LEU
28	6	14	THR
11	P	112	LEU
12	Q	119	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
15	T	84	GLN
16	U	72	HIS
21	Z	151	HIS
10	O	89	ASN
19	X	31	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2802/2915 (96%)	556 (19%)	62 (2%)
2	B	119/122 (97%)	21 (17%)	0
All	All	2921/3037 (96%)	577 (19%)	62 (2%)

5 of 577 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	G
1	A	15	G
1	A	34	C
1	A	36	G
1	A	45	C

5 of 62 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1033	U
1	A	1210	A
1	A	2610	C
1	A	1049	C
1	A	1379	A

## 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 672 ligands modelled in this entry, 672 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	2809/2915 (96%)	-0.20	60 (2%) 60 12	31, 50, 134, 186	0
2	B	120/122 (98%)	-0.07	1 (0%) 83 26	46, 72, 94, 119	0
3	D	275/276 (99%)	-0.07	0 100 100	34, 52, 69, 117	0
4	E	204/206 (99%)	-0.06	1 (0%) 88 36	32, 55, 78, 95	0
5	F	203/210 (96%)	-0.02	3 (1%) 70 16	30, 60, 92, 136	0
6	G	181/182 (99%)	0.48	14 (7%) 13 3	80, 120, 143, 152	0
7	H	174/180 (96%)	-0.01	3 (1%) 67 15	58, 79, 97, 110	0
8	I	146/148 (98%)	0.18	5 (3%) 43 8	57, 90, 108, 120	0
9	N	140/140 (100%)	-0.13	2 (1%) 72 18	39, 55, 83, 98	0
10	O	122/122 (100%)	0.00	0 100 100	43, 58, 79, 85	0
11	P	149/150 (99%)	0.36	8 (5%) 25 5	34, 63, 98, 109	0
12	Q	141/141 (100%)	0.16	1 (0%) 84 28	43, 61, 77, 91	0
13	R	118/118 (100%)	-0.12	0 100 100	38, 50, 70, 78	0
14	S	110/112 (98%)	0.01	0 100 100	58, 75, 93, 101	0
15	T	131/146 (89%)	-0.04	0 100 100	51, 63, 98, 117	0
16	U	116/118 (98%)	-0.16	0 100 100	35, 48, 69, 81	0
17	V	100/101 (99%)	0.05	0 100 100	34, 62, 81, 91	0
18	W	112/113 (99%)	-0.28	0 100 100	36, 43, 64, 102	0
19	X	95/96 (98%)	-0.09	0 100 100	41, 51, 74, 98	0
20	Y	107/110 (97%)	0.18	6 (5%) 24 5	52, 64, 89, 107	0
21	Z	198/206 (96%)	0.15	2 (1%) 79 22	65, 85, 111, 126	0
22	0	76/85 (89%)	0.09	1 (1%) 74 19	48, 55, 71, 87	0
23	1	97/98 (98%)	0.08	0 100 100	37, 57, 89, 103	0
24	2	70/72 (97%)	0.37	3 (4%) 34 7	50, 66, 84, 103	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
25	3	59/60 (98%)	-0.00	0	100	100	43, 57, 85, 101	0
26	4	46/71 (64%)	-0.04	0	100	100	106, 141, 151, 154	0
27	5	59/60 (98%)	-0.24	0	100	100	33, 51, 68, 89	0
28	6	53/54 (98%)	0.31	0	100	100	53, 61, 75, 78	0
29	7	48/49 (97%)	0.39	1 (2%)	60	12	32, 37, 61, 78	0
30	8	64/65 (98%)	-0.07	1 (1%)	68	16	42, 49, 58, 70	0
31	9	36/37 (97%)	0.53	0	100	100	49, 59, 72, 83	0
All	All	6359/6563 (96%)	-0.06	112 (1%)	65	14	30, 57, 120, 186	0

The worst 5 of 112 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2107	C	7.8
1	A	2175	C	7.6
1	A	2108	C	7.0
1	A	2169	A	5.5
1	A	2109	U	5.1

## 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(Å <sup>2</sup> )	Q<0.9
32	MG	A	3504	1/1	0.10	-	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3305	1/1	0.21	-	36,36,36,36	0
32	MG	A	3316	1/1	0.16	-	71,71,71,71	0
32	MG	A	3447	1/1	0.13	-	61,61,61,61	0
32	MG	A	3262	1/1	0.35	-	50,50,50,50	0
32	MG	A	3041	1/1	0.20	-	56,56,56,56	0
32	MG	A	3011	1/1	0.24	-	103,103,103,103	0
32	MG	A	3184	1/1	0.15	-	69,69,69,69	0
32	MG	A	3110	1/1	0.34	-	56,56,56,56	0
32	MG	A	3071	1/1	0.58	-	53,53,53,53	0
32	MG	A	3096	1/1	0.28	-	41,41,41,41	0
32	MG	A	3142	1/1	0.34	-	59,59,59,59	0
32	MG	A	3133	1/1	0.30	-	44,44,44,44	0
32	MG	A	3372	1/1	0.37	-	74,74,74,74	0
32	MG	A	3558	1/1	0.77	-	49,49,49,49	0
32	MG	A	3109	1/1	0.15	-	49,49,49,49	0
32	MG	A	3154	1/1	0.23	-	73,73,73,73	0
32	MG	A	3450	1/1	0.26	-	37,37,37,37	0
32	MG	A	3054	1/1	0.24	-	52,52,52,52	0
32	MG	A	3298	1/1	0.08	-	48,48,48,48	0
32	MG	A	3600	1/1	0.06	-	26,26,26,26	0
32	MG	A	3192	1/1	0.80	-	46,46,46,46	0
32	MG	Q	203	1/1	0.18	-	44,44,44,44	0
32	MG	A	3126	1/1	0.22	-	68,68,68,68	0
32	MG	A	3158	1/1	0.11	-	57,57,57,57	0
32	MG	A	3452	1/1	0.16	-	49,49,49,49	0
32	MG	A	3419	1/1	0.09	-	46,46,46,46	0
32	MG	A	3025	1/1	0.77	-	68,68,68,68	0
32	MG	A	3463	1/1	0.15	-	58,58,58,58	0
32	MG	A	3009	1/1	0.58	-	50,50,50,50	0
32	MG	A	3399	1/1	0.30	-	23,23,23,23	0
32	MG	W	201	1/1	0.16	-	51,51,51,51	0
32	MG	A	3277	1/1	0.37	-	41,41,41,41	0
32	MG	A	3066	1/1	0.28	-	45,45,45,45	0
32	MG	A	3225	1/1	0.85	-	57,57,57,57	0
32	MG	A	3537	1/1	0.42	-	76,76,76,76	0
32	MG	O	102	1/1	0.27	-	56,56,56,56	0
32	MG	A	3597	1/1	0.10	-	70,70,70,70	0
32	MG	Q	202	1/1	0.48	-	53,53,53,53	0
32	MG	A	3541	1/1	0.18	-	70,70,70,70	0
32	MG	A	3002	1/1	0.24	-	41,41,41,41	0
32	MG	A	3249	1/1	0.31	-	53,53,53,53	0
32	MG	A	3295	1/1	0.09	-	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3328	1/1	0.29	-	30,30,30,30	0
32	MG	A	3005	1/1	0.25	-	36,36,36,36	0
33	ZN	4	101	1/1	0.04	-	200,200,200,200	0
32	MG	A	3296	1/1	0.16	-	37,37,37,37	0
32	MG	A	3405	1/1	0.06	-	47,47,47,47	0
32	MG	A	3088	1/1	0.36	-	57,57,57,57	0
32	MG	A	3460	1/1	0.09	-	91,91,91,91	0
32	MG	A	3195	1/1	0.26	-	50,50,50,50	0
32	MG	A	3013	1/1	0.72	-	75,75,75,75	0
32	MG	A	3488	1/1	0.23	-	60,60,60,60	0
32	MG	A	3402	1/1	0.10	-	41,41,41,41	0
32	MG	A	3612	1/1	0.10	-	51,51,51,51	0
32	MG	A	3037	1/1	0.13	-	36,36,36,36	0
32	MG	A	3398	1/1	0.05	-	32,32,32,32	0
32	MG	A	3442	1/1	0.29	-	53,53,53,53	0
32	MG	A	3318	1/1	0.18	-	34,34,34,34	0
32	MG	A	3217	1/1	0.10	-	61,61,61,61	0
32	MG	A	3264	1/1	0.27	-	32,32,32,32	0
32	MG	A	3619	1/1	0.24	-	82,82,82,82	0
32	MG	A	3492	1/1	0.14	-	38,38,38,38	0
32	MG	2	101	1/1	0.59	-	60,60,60,60	0
32	MG	A	3545	1/1	0.17	-	60,60,60,60	0
32	MG	A	3014	1/1	0.60	-	42,42,42,42	0
32	MG	A	3369	1/1	0.06	-	50,50,50,50	0
32	MG	A	3406	1/1	0.14	-	44,44,44,44	0
32	MG	A	3476	1/1	0.31	-	59,59,59,59	0
32	MG	A	3234	1/1	0.72	-	54,54,54,54	0
32	MG	A	3178	1/1	0.68	-	69,69,69,69	0
32	MG	A	3526	1/1	0.11	-	79,79,79,79	0
32	MG	A	3173	1/1	0.41	-	67,67,67,67	0
32	MG	A	3144	1/1	0.44	-	53,53,53,53	0
32	MG	9	102	1/1	0.60	-	45,45,45,45	0
32	MG	A	3365	1/1	0.07	-	73,73,73,73	0
32	MG	A	3434	1/1	0.20	-	34,34,34,34	0
32	MG	A	3338	1/1	0.17	-	55,55,55,55	0
32	MG	A	3329	1/1	0.11	-	34,34,34,34	0
32	MG	A	3252	1/1	0.40	-	47,47,47,47	0
32	MG	A	3038	1/1	0.67	-	64,64,64,64	0
32	MG	A	3143	1/1	0.31	-	65,65,65,65	0
32	MG	A	3269	1/1	0.64	-	53,53,53,53	0
32	MG	A	3020	1/1	0.15	-	33,33,33,33	0
32	MG	A	3048	1/1	0.29	-	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3248	1/1	0.75	-	49,49,49,49	0
32	MG	A	3524	1/1	0.10	-	41,41,41,41	0
32	MG	A	3480	1/1	0.11	-	45,45,45,45	0
32	MG	A	3049	1/1	0.41	-	54,54,54,54	0
32	MG	A	3516	1/1	0.28	-	66,66,66,66	0
32	MG	A	3309	1/1	0.10	-	29,29,29,29	0
32	MG	A	3429	1/1	0.24	-	28,28,28,28	0
32	MG	A	3175	1/1	0.82	-	65,65,65,65	0
32	MG	A	3461	1/1	0.14	-	45,45,45,45	0
32	MG	A	3276	1/1	0.18	-	81,81,81,81	0
32	MG	A	3242	1/1	0.36	-	64,64,64,64	0
32	MG	A	3427	1/1	0.17	-	32,32,32,32	0
32	MG	A	3519	1/1	0.15	-	39,39,39,39	0
32	MG	A	3015	1/1	0.50	-	57,57,57,57	0
32	MG	A	3400	1/1	0.11	-	31,31,31,31	0
32	MG	A	3292	1/1	0.31	-	47,47,47,47	0
32	MG	A	3104	1/1	0.31	-	59,59,59,59	0
32	MG	A	3061	1/1	0.54	-	64,64,64,64	0
32	MG	B	211	1/1	0.16	-	51,51,51,51	0
32	MG	A	3076	1/1	0.46	-	55,55,55,55	0
32	MG	A	3032	1/1	0.77	-	40,40,40,40	0
32	MG	A	3383	1/1	0.29	-	50,50,50,50	0
32	MG	A	3059	1/1	0.28	-	49,49,49,49	0
32	MG	A	3302	1/1	0.12	-	37,37,37,37	0
32	MG	A	3454	1/1	0.10	-	34,34,34,34	0
32	MG	A	3153	1/1	0.28	-	62,62,62,62	0
32	MG	A	3324	1/1	0.13	-	45,45,45,45	0
32	MG	A	3621	1/1	0.21	-	85,85,85,85	0
32	MG	A	3473	1/1	0.12	-	35,35,35,35	0
32	MG	A	3026	1/1	0.31	-	56,56,56,56	0
32	MG	A	3360	1/1	0.19	-	47,47,47,47	0
32	MG	A	3340	1/1	0.12	-	33,33,33,33	0
32	MG	A	3529	1/1	0.10	-	28,28,28,28	0
32	MG	A	3190	1/1	0.65	-	43,43,43,43	0
32	MG	A	3586	1/1	0.11	-	50,50,50,50	0
32	MG	A	3125	1/1	0.29	-	43,43,43,43	0
32	MG	A	3530	1/1	0.10	-	51,51,51,51	0
32	MG	A	3012	1/1	0.27	-	57,57,57,57	0
32	MG	A	3620	1/1	0.13	-	93,93,93,93	0
32	MG	A	3308	1/1	0.10	-	51,51,51,51	0
32	MG	A	3479	1/1	0.22	-	44,44,44,44	0
32	MG	A	3187	1/1	0.26	-	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3327	1/1	0.16	-	47,47,47,47	0
32	MG	A	3416	1/1	0.14	-	31,31,31,31	0
32	MG	E	301	1/1	0.32	-	43,43,43,43	0
32	MG	A	3618	1/1	0.10	-	91,91,91,91	0
32	MG	A	3422	1/1	0.11	-	35,35,35,35	0
32	MG	A	3165	1/1	0.53	-	42,42,42,42	0
32	MG	A	3431	1/1	0.14	-	35,35,35,35	0
32	MG	A	3176	1/1	1.15	-	71,71,71,71	0
32	MG	A	3227	1/1	0.35	-	61,61,61,61	0
32	MG	A	3553	1/1	0.16	-	37,37,37,37	0
32	MG	A	3306	1/1	0.08	-	27,27,27,27	0
32	MG	A	3084	1/1	0.41	-	71,71,71,71	0
32	MG	A	3374	1/1	0.10	-	67,67,67,67	0
32	MG	A	3129	1/1	0.34	-	51,51,51,51	0
32	MG	A	3300	1/1	0.17	-	53,53,53,53	0
32	MG	E	304	1/1	0.07	-	32,32,32,32	0
32	MG	A	3007	1/1	0.22	-	59,59,59,59	0
32	MG	A	3086	1/1	1.56	-	56,56,56,56	0
32	MG	A	3155	1/1	0.23	-	53,53,53,53	0
32	MG	A	3112	1/1	0.18	-	23,23,23,23	0
32	MG	A	3559	1/1	0.15	-	58,58,58,58	0
32	MG	A	3466	1/1	0.19	-	36,36,36,36	0
32	MG	A	3425	1/1	0.09	-	27,27,27,27	0
32	MG	A	3472	1/1	0.26	-	77,77,77,77	0
32	MG	A	3401	1/1	0.09	-	36,36,36,36	0
32	MG	A	3339	1/1	0.11	-	46,46,46,46	0
32	MG	D	302	1/1	0.17	-	38,38,38,38	0
32	MG	A	3535	1/1	0.11	-	35,35,35,35	0
32	MG	A	3232	1/1	0.35	-	50,50,50,50	0
32	MG	A	3301	1/1	0.29	-	38,38,38,38	0
32	MG	A	3366	1/1	0.26	-	74,74,74,74	0
32	MG	A	3532	1/1	0.29	-	86,86,86,86	0
32	MG	A	3490	1/1	0.29	-	94,94,94,94	0
32	MG	B	201	1/1	0.28	-	61,61,61,61	0
32	MG	A	3239	1/1	0.80	-	56,56,56,56	0
32	MG	A	3282	1/1	0.46	-	89,89,89,89	0
32	MG	A	3345	1/1	0.06	-	57,57,57,57	0
32	MG	A	3050	1/1	0.27	-	46,46,46,46	0
32	MG	A	3413	1/1	0.20	-	34,34,34,34	0
32	MG	A	3034	1/1	0.14	-	45,45,45,45	0
32	MG	A	3403	1/1	0.11	-	34,34,34,34	0
32	MG	A	3326	1/1	0.21	-	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	E	302	1/1	0.34	-	52,52,52,52	0
32	MG	A	3567	1/1	0.17	-	36,36,36,36	0
32	MG	A	3063	1/1	0.15	-	60,60,60,60	0
32	MG	A	3486	1/1	0.08	-	57,57,57,57	0
32	MG	A	3157	1/1	0.29	-	64,64,64,64	0
32	MG	A	3549	1/1	0.21	-	57,57,57,57	0
32	MG	A	3200	1/1	0.23	-	29,29,29,29	0
32	MG	A	3444	1/1	0.21	-	35,35,35,35	0
32	MG	A	3236	1/1	0.19	-	34,34,34,34	0
32	MG	A	3459	1/1	0.41	-	89,89,89,89	0
32	MG	A	3550	1/1	0.15	-	31,31,31,31	0
32	MG	A	3509	1/1	0.15	-	61,61,61,61	0
32	MG	A	3424	1/1	0.20	-	36,36,36,36	0
32	MG	A	3231	1/1	0.24	-	51,51,51,51	0
32	MG	A	3047	1/1	0.30	-	50,50,50,50	0
32	MG	A	3075	1/1	0.10	-	67,67,67,67	0
32	MG	A	3575	1/1	0.20	-	49,49,49,49	0
32	MG	B	214	1/1	0.17	-	67,67,67,67	0
32	MG	A	3407	1/1	0.06	-	46,46,46,46	0
32	MG	A	3599	1/1	0.10	-	46,46,46,46	0
32	MG	A	3548	1/1	0.16	-	79,79,79,79	0
32	MG	A	3443	1/1	0.14	-	63,63,63,63	0
32	MG	F	302	1/1	0.32	-	62,62,62,62	0
32	MG	A	3216	1/1	0.32	-	34,34,34,34	0
32	MG	1	101	1/1	0.68	-	50,50,50,50	0
32	MG	A	3080	1/1	0.39	-	38,38,38,38	0
32	MG	A	3093	1/1	0.46	-	47,47,47,47	0
32	MG	A	3343	1/1	0.52	-	65,65,65,65	0
32	MG	A	3508	1/1	0.17	-	76,76,76,76	0
32	MG	A	3191	1/1	0.56	-	46,46,46,46	0
32	MG	A	3214	1/1	0.22	-	47,47,47,47	0
32	MG	A	3287	1/1	0.40	-	59,59,59,59	0
32	MG	A	3095	1/1	0.96	-	81,81,81,81	0
32	MG	A	3380	1/1	0.34	-	69,69,69,69	0
32	MG	A	3464	1/1	0.26	-	38,38,38,38	0
32	MG	A	3177	1/1	0.27	-	70,70,70,70	0
32	MG	A	3347	1/1	0.41	-	52,52,52,52	0
32	MG	A	3580	1/1	0.38	-	58,58,58,58	0
32	MG	B	204	1/1	0.24	-	67,67,67,67	0
32	MG	A	3609	1/1	0.10	-	29,29,29,29	0
32	MG	A	3021	1/1	0.18	-	57,57,57,57	0
32	MG	A	3052	1/1	0.15	-	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
33	ZN	Y	201	1/1	0.04	-	74,74,74,74	0
32	MG	A	3201	1/1	0.34	-	31,31,31,31	0
32	MG	A	3030	1/1	0.84	-	41,41,41,41	0
32	MG	A	3502	1/1	0.21	-	107,107,107,107	0
32	MG	A	3456	1/1	0.47	-	74,74,74,74	0
32	MG	A	3591	1/1	0.48	-	86,86,86,86	0
32	MG	A	3008	1/1	0.33	-	48,48,48,48	0
32	MG	A	3208	1/1	0.39	-	68,68,68,68	0
32	MG	A	3152	1/1	0.69	-	61,61,61,61	0
32	MG	A	3250	1/1	0.16	-	50,50,50,50	0
32	MG	A	3414	1/1	0.16	-	43,43,43,43	0
32	MG	A	3017	1/1	0.23	-	72,72,72,72	0
32	MG	A	3610	1/1	0.07	-	38,38,38,38	0
32	MG	A	3162	1/1	0.25	-	46,46,46,46	0
32	MG	A	3169	1/1	1.57	-	68,68,68,68	0
32	MG	A	3583	1/1	0.18	-	61,61,61,61	0
32	MG	A	3560	1/1	0.36	-	42,42,42,42	0
33	ZN	9	101	1/1	0.05	-	69,69,69,69	0
32	MG	A	3386	1/1	0.28	-	71,71,71,71	0
32	MG	A	3311	1/1	0.12	-	38,38,38,38	0
32	MG	A	3511	1/1	0.15	-	40,40,40,40	0
32	MG	B	208	1/1	1.06	-	70,70,70,70	0
32	MG	A	3576	1/1	0.40	-	55,55,55,55	0
32	MG	A	3098	1/1	0.80	-	63,63,63,63	0
32	MG	A	3180	1/1	0.32	-	58,58,58,58	0
32	MG	A	3317	1/1	0.27	-	84,84,84,84	0
32	MG	A	3377	1/1	0.09	-	75,75,75,75	0
32	MG	A	3604	1/1	0.12	-	33,33,33,33	0
32	MG	A	3219	1/1	0.43	-	51,51,51,51	0
32	MG	A	3489	1/1	0.13	-	48,48,48,48	0
32	MG	A	3453	1/1	0.29	-	71,71,71,71	0
32	MG	A	3124	1/1	0.39	-	56,56,56,56	0
32	MG	A	3448	1/1	0.13	-	56,56,56,56	0
32	MG	B	202	1/1	0.97	-	46,46,46,46	0
32	MG	A	3147	1/1	1.04	-	78,78,78,78	0
32	MG	A	3546	1/1	0.17	-	59,59,59,59	0
32	MG	A	3307	1/1	0.15	-	37,37,37,37	0
32	MG	A	3185	1/1	1.76	-	76,76,76,76	0
32	MG	A	3613	1/1	0.07	-	56,56,56,56	0
32	MG	A	3565	1/1	0.26	-	43,43,43,43	0
32	MG	A	3381	1/1	0.13	-	38,38,38,38	0
32	MG	A	3221	1/1	0.44	-	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3068	1/1	0.14	-	43,43,43,43	0
32	MG	A	3467	1/1	0.15	-	41,41,41,41	0
32	MG	A	3036	1/1	0.17	-	52,52,52,52	0
32	MG	A	3470	1/1	0.15	-	73,73,73,73	0
32	MG	A	3294	1/1	0.21	-	44,44,44,44	0
32	MG	A	3114	1/1	0.28	-	47,47,47,47	0
32	MG	A	3193	1/1	0.28	-	45,45,45,45	0
32	MG	A	3385	1/1	0.11	-	58,58,58,58	0
32	MG	A	3336	1/1	0.12	-	43,43,43,43	0
32	MG	A	3430	1/1	0.14	-	32,32,32,32	0
32	MG	A	3579	1/1	0.21	-	41,41,41,41	0
32	MG	A	3031	1/1	0.48	-	67,67,67,67	0
32	MG	A	3206	1/1	0.91	-	47,47,47,47	0
32	MG	A	3085	1/1	0.48	-	56,56,56,56	0
32	MG	A	3555	1/1	0.16	-	38,38,38,38	0
32	MG	A	3212	1/1	1.06	-	57,57,57,57	0
32	MG	8	302	1/1	0.15	-	51,51,51,51	0
32	MG	A	3094	1/1	0.38	-	55,55,55,55	0
32	MG	A	3161	1/1	0.29	-	66,66,66,66	0
32	MG	A	3106	1/1	0.38	-	48,48,48,48	0
32	MG	A	3611	1/1	0.20	-	87,87,87,87	0
32	MG	A	3415	1/1	0.10	-	41,41,41,41	0
32	MG	A	3585	1/1	0.07	-	54,54,54,54	0
32	MG	A	3121	1/1	0.25	-	39,39,39,39	0
32	MG	A	3092	1/1	0.25	-	45,45,45,45	0
32	MG	A	3089	1/1	0.47	-	56,56,56,56	0
32	MG	A	3428	1/1	0.11	-	37,37,37,37	0
32	MG	A	3273	1/1	0.33	-	60,60,60,60	0
32	MG	A	3587	1/1	0.44	-	68,68,68,68	0
32	MG	A	3263	1/1	0.29	-	59,59,59,59	0
32	MG	A	3146	1/1	0.19	-	54,54,54,54	0
32	MG	A	3475	1/1	0.14	-	29,29,29,29	0
32	MG	A	3344	1/1	0.11	-	69,69,69,69	0
32	MG	A	3462	1/1	0.22	-	130,130,130,130	0
32	MG	A	3315	1/1	0.20	-	42,42,42,42	0
32	MG	A	3522	1/1	0.54	-	90,90,90,90	0
32	MG	A	3118	1/1	0.82	-	56,56,56,56	0
32	MG	A	3224	1/1	0.19	-	51,51,51,51	0
32	MG	A	3441	1/1	0.15	-	38,38,38,38	0
32	MG	A	3484	1/1	0.12	-	76,76,76,76	0
32	MG	A	3073	1/1	0.48	-	49,49,49,49	0
32	MG	A	3615	1/1	0.24	-	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3148	1/1	0.22	-	52,52,52,52	0
32	MG	A	3569	1/1	0.11	-	40,40,40,40	0
32	MG	A	3556	1/1	0.16	-	70,70,70,70	0
32	MG	A	3033	1/1	0.53	-	46,46,46,46	0
32	MG	A	3364	1/1	0.27	-	53,53,53,53	0
32	MG	A	3497	1/1	0.29	-	44,44,44,44	0
32	MG	A	3426	1/1	0.10	-	30,30,30,30	0
32	MG	A	3607	1/1	0.09	-	36,36,36,36	0
32	MG	A	3223	1/1	0.18	-	51,51,51,51	0
32	MG	A	3288	1/1	0.39	-	52,52,52,52	0
32	MG	A	3230	1/1	0.40	-	26,26,26,26	0
32	MG	A	3170	1/1	0.40	-	52,52,52,52	0
32	MG	A	3045	1/1	0.73	-	62,62,62,62	0
32	MG	A	3251	1/1	0.32	-	70,70,70,70	0
32	MG	A	3478	1/1	0.19	-	53,53,53,53	0
32	MG	A	3284	1/1	0.23	-	43,43,43,43	0
32	MG	V	201	1/1	0.47	-	74,74,74,74	0
32	MG	8	301	1/1	0.98	-	61,61,61,61	0
32	MG	A	3601	1/1	0.07	-	39,39,39,39	0
32	MG	A	3341	1/1	0.12	-	30,30,30,30	0
32	MG	A	3103	1/1	0.20	-	51,51,51,51	0
32	MG	A	3540	1/1	0.15	-	38,38,38,38	0
32	MG	A	3127	1/1	0.38	-	50,50,50,50	0
32	MG	B	205	1/1	0.69	-	57,57,57,57	0
32	MG	A	3362	1/1	0.07	-	49,49,49,49	0
32	MG	A	3064	1/1	0.19	-	69,69,69,69	0
32	MG	A	3465	1/1	0.07	-	25,25,25,25	0
32	MG	A	3608	1/1	0.07	-	30,30,30,30	0
32	MG	A	3542	1/1	0.05	-	61,61,61,61	0
32	MG	A	3378	1/1	0.31	-	46,46,46,46	0
32	MG	A	3016	1/1	0.26	-	47,47,47,47	0
32	MG	A	3375	1/1	0.13	-	50,50,50,50	0
32	MG	A	3150	1/1	0.39	-	54,54,54,54	0
32	MG	A	3183	1/1	0.27	-	48,48,48,48	0
32	MG	A	3503	1/1	0.14	-	33,33,33,33	0
32	MG	A	3222	1/1	0.33	-	79,79,79,79	0
32	MG	A	3087	1/1	1.11	-	63,63,63,63	0
32	MG	A	3527	1/1	0.23	-	77,77,77,77	0
32	MG	A	3349	1/1	0.13	-	45,45,45,45	0
32	MG	A	3358	1/1	0.32	-	54,54,54,54	0
32	MG	A	3274	1/1	0.32	-	65,65,65,65	0
32	MG	A	3440	1/1	0.17	-	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3506	1/1	0.15	-	68,68,68,68	0
32	MG	A	3209	1/1	0.43	-	59,59,59,59	0
32	MG	A	3237	1/1	0.15	-	45,45,45,45	0
32	MG	A	3266	1/1	0.39	-	38,38,38,38	0
32	MG	A	3268	1/1	0.86	-	48,48,48,48	0
32	MG	A	3551	1/1	0.26	-	41,41,41,41	0
32	MG	A	3001	1/1	0.34	-	29,29,29,29	0
32	MG	A	3235	1/1	0.15	-	59,59,59,59	0
32	MG	A	3105	1/1	0.35	-	67,67,67,67	0
32	MG	A	3254	1/1	0.21	-	44,44,44,44	0
32	MG	A	3046	1/1	0.28	-	49,49,49,49	0
32	MG	A	3577	1/1	0.08	-	41,41,41,41	0
32	MG	A	3395	1/1	0.07	-	55,55,55,55	0
32	MG	B	213	1/1	0.18	-	69,69,69,69	0
32	MG	A	3582	1/1	0.22	-	53,53,53,53	0
32	MG	A	3367	1/1	0.15	-	46,46,46,46	0
32	MG	A	3314	1/1	0.09	-	50,50,50,50	0
32	MG	E	303	1/1	0.61	-	54,54,54,54	0
32	MG	A	3141	1/1	0.37	-	53,53,53,53	0
32	MG	A	3534	1/1	0.22	-	49,49,49,49	0
32	MG	A	3117	1/1	0.31	-	43,43,43,43	0
32	MG	A	3357	1/1	0.08	-	49,49,49,49	0
32	MG	A	3070	1/1	0.17	-	70,70,70,70	0
32	MG	A	3065	1/1	0.81	-	84,84,84,84	0
32	MG	A	3101	1/1	0.30	-	52,52,52,52	0
32	MG	A	3439	1/1	0.23	-	38,38,38,38	0
32	MG	A	3167	1/1	0.47	-	56,56,56,56	0
32	MG	A	3379	1/1	0.30	-	55,55,55,55	0
32	MG	D	303	1/1	0.50	-	58,58,58,58	0
32	MG	A	3164	1/1	0.33	-	62,62,62,62	0
32	MG	A	3337	1/1	0.16	-	42,42,42,42	0
32	MG	D	301	1/1	0.39	-	41,41,41,41	0
32	MG	A	3496	1/1	0.11	-	52,52,52,52	0
32	MG	A	3396	1/1	0.13	-	38,38,38,38	0
32	MG	A	3501	1/1	0.10	-	69,69,69,69	0
32	MG	A	3210	1/1	0.22	-	54,54,54,54	0
32	MG	A	3330	1/1	0.06	-	27,27,27,27	0
32	MG	A	3539	1/1	0.06	-	82,82,82,82	0
32	MG	A	3240	1/1	0.26	-	32,32,32,32	0
32	MG	A	3616	1/1	0.14	-	109,109,109,109	0
32	MG	A	3370	1/1	0.09	-	33,33,33,33	0
32	MG	A	3156	1/1	0.14	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3617	1/1	0.40	-	94,94,94,94	0
32	MG	A	3593	1/1	0.19	-	82,82,82,82	0
32	MG	A	3091	1/1	0.22	-	46,46,46,46	0
32	MG	A	3469	1/1	0.11	-	67,67,67,67	0
32	MG	A	3457	1/1	0.13	-	34,34,34,34	0
32	MG	A	3334	1/1	0.36	-	60,60,60,60	0
32	MG	A	3384	1/1	0.09	-	49,49,49,49	0
32	MG	A	3408	1/1	0.16	-	38,38,38,38	0
32	MG	A	3495	1/1	0.15	-	78,78,78,78	0
32	MG	A	3179	1/1	0.40	-	45,45,45,45	0
32	MG	A	3285	1/1	0.57	-	56,56,56,56	0
32	MG	A	3272	1/1	0.26	-	74,74,74,74	0
32	MG	A	3455	1/1	0.10	-	62,62,62,62	0
32	MG	A	3512	1/1	0.14	-	85,85,85,85	0
32	MG	A	3346	1/1	0.21	-	91,91,91,91	0
32	MG	A	3120	1/1	0.50	-	57,57,57,57	0
32	MG	A	3566	1/1	0.34	-	67,67,67,67	0
32	MG	A	3275	1/1	0.31	-	66,66,66,66	0
32	MG	A	3188	1/1	0.36	-	64,64,64,64	0
32	MG	A	3138	1/1	0.35	-	73,73,73,73	0
32	MG	A	3388	1/1	0.17	-	73,73,73,73	0
32	MG	A	3572	1/1	0.34	-	68,68,68,68	0
32	MG	A	3417	1/1	0.18	-	26,26,26,26	0
32	MG	A	3299	1/1	0.07	-	35,35,35,35	0
32	MG	A	3072	1/1	0.54	-	61,61,61,61	0
32	MG	A	3563	1/1	0.10	-	29,29,29,29	0
32	MG	A	3485	1/1	0.12	-	58,58,58,58	0
32	MG	A	3003	1/1	0.58	-	42,42,42,42	0
32	MG	A	3361	1/1	0.18	-	64,64,64,64	0
32	MG	A	3215	1/1	0.40	-	64,64,64,64	0
32	MG	A	3202	1/1	0.94	-	51,51,51,51	0
32	MG	A	3510	1/1	0.26	-	53,53,53,53	0
32	MG	A	3149	1/1	0.29	-	57,57,57,57	0
32	MG	A	3283	1/1	0.22	-	56,56,56,56	0
32	MG	A	3397	1/1	0.07	-	29,29,29,29	0
32	MG	A	3140	1/1	0.32	-	54,54,54,54	0
32	MG	A	3590	1/1	0.08	-	66,66,66,66	0
32	MG	B	215	1/1	0.13	-	77,77,77,77	0
32	MG	A	3035	1/1	0.38	-	49,49,49,49	0
32	MG	A	3356	1/1	0.13	-	28,28,28,28	0
32	MG	3	101	1/1	0.50	-	54,54,54,54	0
32	MG	A	3420	1/1	0.13	-	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3303	1/1	0.13	-	62,62,62,62	0
32	MG	A	3468	1/1	0.11	-	38,38,38,38	0
32	MG	A	3332	1/1	0.18	-	36,36,36,36	0
32	MG	A	3160	1/1	0.56	-	51,51,51,51	0
32	MG	A	3130	1/1	0.41	-	53,53,53,53	0
32	MG	A	3533	1/1	0.27	-	84,84,84,84	0
32	MG	A	3289	1/1	0.22	-	65,65,65,65	0
32	MG	A	3389	1/1	0.19	-	77,77,77,77	0
32	MG	A	3245	1/1	0.46	-	117,117,117,117	0
32	MG	A	3471	1/1	0.14	-	38,38,38,38	0
32	MG	A	3057	1/1	1.10	-	46,46,46,46	0
32	MG	A	3321	1/1	0.20	-	68,68,68,68	0
32	MG	A	3261	1/1	0.24	-	51,51,51,51	0
33	ZN	5	101	1/1	0.04	-	58,58,58,58	0
32	MG	A	3313	1/1	0.24	-	60,60,60,60	0
32	MG	A	3196	1/1	0.53	-	79,79,79,79	0
32	MG	A	3412	1/1	0.10	-	26,26,26,26	0
32	MG	A	3097	1/1	0.30	-	45,45,45,45	0
32	MG	A	3028	1/1	0.09	-	83,83,83,83	0
32	MG	A	3186	1/1	0.42	-	66,66,66,66	0
32	MG	A	3561	1/1	0.12	-	61,61,61,61	0
32	MG	A	3517	1/1	0.21	-	97,97,97,97	0
32	MG	A	3055	1/1	0.34	-	58,58,58,58	0
32	MG	A	3493	1/1	0.18	-	53,53,53,53	0
32	MG	A	3432	1/1	0.12	-	29,29,29,29	0
32	MG	A	3592	1/1	0.09	-	70,70,70,70	0
32	MG	A	3257	1/1	0.70	-	65,65,65,65	0
32	MG	A	3062	1/1	0.24	-	51,51,51,51	0
32	MG	A	3547	1/1	0.21	-	91,91,91,91	0
32	MG	A	3500	1/1	0.14	-	55,55,55,55	0
32	MG	A	3557	1/1	0.25	-	58,58,58,58	0
32	MG	A	3022	1/1	0.24	-	52,52,52,52	0
32	MG	A	3483	1/1	0.09	-	70,70,70,70	0
32	MG	B	206	1/1	0.40	-	62,62,62,62	0
32	MG	A	3102	1/1	0.54	-	72,72,72,72	0
32	MG	A	3411	1/1	0.15	-	34,34,34,34	0
32	MG	A	3040	1/1	0.48	-	33,33,33,33	0
32	MG	A	3320	1/1	0.18	-	73,73,73,73	0
32	MG	A	3168	1/1	0.35	-	58,58,58,58	0
32	MG	A	3043	1/1	0.54	-	54,54,54,54	0
32	MG	A	3090	1/1	0.31	-	46,46,46,46	0
32	MG	A	3297	1/1	0.09	-	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3280	1/1	0.32	-	43,43,43,43	0
32	MG	A	3115	1/1	0.27	-	35,35,35,35	0
32	MG	A	3602	1/1	0.08	-	50,50,50,50	0
32	MG	A	3596	1/1	0.20	-	70,70,70,70	0
32	MG	A	3446	1/1	0.23	-	41,41,41,41	0
32	MG	A	3554	1/1	0.14	-	40,40,40,40	0
32	MG	A	3350	1/1	0.14	-	55,55,55,55	0
32	MG	R	201	1/1	0.58	-	58,58,58,58	0
32	MG	A	3267	1/1	0.15	-	30,30,30,30	0
32	MG	A	3220	1/1	0.51	-	54,54,54,54	0
32	MG	A	3390	1/1	0.18	-	33,33,33,33	0
32	MG	A	3348	1/1	0.09	-	45,45,45,45	0
32	MG	A	3029	1/1	0.60	-	37,37,37,37	0
32	MG	A	3189	1/1	0.24	-	30,30,30,30	0
32	MG	A	3333	1/1	0.19	-	51,51,51,51	0
32	MG	U	202	1/1	0.40	-	62,62,62,62	0
32	MG	A	3067	1/1	0.61	-	47,47,47,47	0
32	MG	A	3458	1/1	0.23	-	42,42,42,42	0
32	MG	A	3449	1/1	0.05	-	40,40,40,40	0
32	MG	A	3060	1/1	0.38	-	45,45,45,45	0
32	MG	A	3056	1/1	0.43	-	48,48,48,48	0
32	MG	P	201	1/1	0.21	-	43,43,43,43	0
32	MG	A	3107	1/1	0.27	-	40,40,40,40	0
32	MG	A	3174	1/1	0.62	-	71,71,71,71	0
32	MG	A	3437	1/1	0.20	-	36,36,36,36	0
32	MG	B	203	1/1	0.28	-	80,80,80,80	0
32	MG	A	3325	1/1	0.13	-	40,40,40,40	0
32	MG	A	3243	1/1	0.41	-	62,62,62,62	0
32	MG	A	3331	1/1	0.11	-	45,45,45,45	0
32	MG	A	3410	1/1	0.17	-	35,35,35,35	0
32	MG	A	3259	1/1	0.97	-	64,64,64,64	0
32	MG	A	3039	1/1	0.56	-	44,44,44,44	0
32	MG	A	3538	1/1	0.14	-	70,70,70,70	0
32	MG	A	3171	1/1	0.47	-	60,60,60,60	0
32	MG	A	3531	1/1	0.17	-	43,43,43,43	0
32	MG	A	3069	1/1	0.14	-	35,35,35,35	0
32	MG	A	3265	1/1	0.14	-	41,41,41,41	0
32	MG	A	3199	1/1	0.22	-	62,62,62,62	0
32	MG	A	3181	1/1	0.24	-	48,48,48,48	0
32	MG	A	3376	1/1	0.21	-	55,55,55,55	0
32	MG	A	3544	1/1	0.17	-	54,54,54,54	0
32	MG	A	3581	1/1	0.28	-	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3108	1/1	0.46	-	48,48,48,48	0
32	MG	A	3518	1/1	0.15	-	46,46,46,46	0
32	MG	A	3418	1/1	0.07	-	49,49,49,49	0
32	MG	A	3523	1/1	0.08	-	67,67,67,67	0
32	MG	A	3027	1/1	0.25	-	46,46,46,46	0
32	MG	A	3335	1/1	0.08	-	36,36,36,36	0
32	MG	A	3514	1/1	0.18	-	33,33,33,33	0
32	MG	A	3584	1/1	0.18	-	47,47,47,47	0
32	MG	A	3371	1/1	0.21	-	34,34,34,34	0
32	MG	A	3310	1/1	0.20	-	51,51,51,51	0
32	MG	A	3355	1/1	0.22	-	53,53,53,53	0
32	MG	B	212	1/1	0.12	-	68,68,68,68	0
32	MG	A	3521	1/1	0.12	-	59,59,59,59	0
32	MG	A	3083	1/1	0.36	-	66,66,66,66	0
32	MG	A	3588	1/1	0.39	-	54,54,54,54	0
32	MG	A	3392	1/1	0.12	-	33,33,33,33	0
32	MG	A	3312	1/1	0.13	-	44,44,44,44	0
32	MG	A	3079	1/1	0.32	-	43,43,43,43	0
32	MG	A	3528	1/1	0.15	-	112,112,112,112	0
32	MG	A	3006	1/1	0.12	-	32,32,32,32	0
32	MG	A	3078	1/1	0.23	-	70,70,70,70	0
32	MG	A	3197	1/1	0.29	-	84,84,84,84	0
32	MG	A	3363	1/1	0.24	-	53,53,53,53	0
32	MG	A	3019	1/1	0.20	-	34,34,34,34	0
32	MG	A	3281	1/1	0.43	-	54,54,54,54	0
32	MG	A	3423	1/1	0.31	-	41,41,41,41	0
32	MG	A	3589	1/1	0.37	-	58,58,58,58	0
32	MG	A	3435	1/1	0.13	-	31,31,31,31	0
32	MG	A	3233	1/1	0.30	-	45,45,45,45	0
32	MG	A	3614	1/1	0.06	-	70,70,70,70	0
32	MG	A	3573	1/1	0.14	-	36,36,36,36	0
32	MG	A	3228	1/1	0.39	-	62,62,62,62	0
32	MG	A	3131	1/1	0.30	-	49,49,49,49	0
32	MG	A	3247	1/1	0.24	-	36,36,36,36	0
32	MG	A	3042	1/1	0.24	-	47,47,47,47	0
32	MG	A	3207	1/1	0.28	-	61,61,61,61	0
32	MG	A	3010	1/1	0.21	-	34,34,34,34	0
32	MG	A	3368	1/1	0.09	-	84,84,84,84	0
32	MG	A	3136	1/1	0.19	-	44,44,44,44	0
32	MG	A	3595	1/1	0.09	-	51,51,51,51	0
32	MG	A	3291	1/1	0.39	-	50,50,50,50	0
32	MG	A	3260	1/1	0.21	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3451	1/1	0.20	-	33,33,33,33	0
32	MG	A	3122	1/1	0.36	-	42,42,42,42	0
32	MG	A	3594	1/1	0.07	-	56,56,56,56	0
32	MG	A	3322	1/1	0.22	-	57,57,57,57	0
32	MG	A	3058	1/1	0.37	-	56,56,56,56	0
32	MG	A	3505	1/1	0.08	-	41,41,41,41	0
32	MG	A	3198	1/1	0.40	-	80,80,80,80	0
32	MG	A	3507	1/1	0.28	-	28,28,28,28	0
32	MG	A	3571	1/1	0.17	-	60,60,60,60	0
32	MG	A	3211	1/1	0.61	-	67,67,67,67	0
32	MG	A	3132	1/1	0.27	-	32,32,32,32	0
32	MG	A	3290	1/1	0.34	-	33,33,33,33	0
32	MG	F	301	1/1	0.46	-	56,56,56,56	0
32	MG	U	201	1/1	0.34	-	51,51,51,51	0
32	MG	A	3481	1/1	0.21	-	92,92,92,92	0
32	MG	A	3213	1/1	0.13	-	53,53,53,53	0
32	MG	E	305	1/1	0.10	-	32,32,32,32	0
32	MG	A	3100	1/1	0.20	-	54,54,54,54	0
32	MG	A	3474	1/1	0.08	-	38,38,38,38	0
32	MG	A	3359	1/1	0.18	-	59,59,59,59	0
32	MG	A	3606	1/1	0.10	-	30,30,30,30	0
32	MG	A	3024	1/1	0.16	-	52,52,52,52	0
32	MG	A	3605	1/1	0.08	-	24,24,24,24	0
32	MG	A	3445	1/1	0.14	-	31,31,31,31	0
32	MG	B	207	1/1	1.01	-	69,69,69,69	0
32	MG	A	3082	1/1	0.32	-	42,42,42,42	0
32	MG	A	3256	1/1	0.66	-	67,67,67,67	0
32	MG	A	3271	1/1	0.24	-	54,54,54,54	0
32	MG	A	3482	1/1	0.14	-	35,35,35,35	0
32	MG	A	3520	1/1	0.20	-	51,51,51,51	0
32	MG	A	3304	1/1	0.21	-	45,45,45,45	0
32	MG	A	3351	1/1	0.12	-	37,37,37,37	0
32	MG	A	3113	1/1	0.29	-	57,57,57,57	0
32	MG	A	3182	1/1	0.53	-	51,51,51,51	0
32	MG	A	3391	1/1	0.20	-	54,54,54,54	0
32	MG	A	3051	1/1	0.80	-	52,52,52,52	0
32	MG	A	3241	1/1	0.37	-	38,38,38,38	0
32	MG	A	3382	1/1	0.07	-	56,56,56,56	0
32	MG	A	3487	1/1	0.17	-	40,40,40,40	0
32	MG	A	3166	1/1	0.35	-	39,39,39,39	0
32	MG	A	3226	1/1	0.65	-	61,61,61,61	0
32	MG	A	3570	1/1	0.14	-	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	Q	201	1/1	0.47	-	49,49,49,49	0
32	MG	A	3134	1/1	0.20	-	31,31,31,31	0
32	MG	A	3477	1/1	0.40	-	66,66,66,66	0
32	MG	A	3404	1/1	0.08	-	45,45,45,45	0
32	MG	A	3342	1/1	0.13	-	91,91,91,91	0
32	MG	A	3246	1/1	0.37	-	45,45,45,45	0
32	MG	A	3494	1/1	0.21	-	65,65,65,65	0
32	MG	A	3578	1/1	0.28	-	54,54,54,54	0
32	MG	R	202	1/1	0.14	-	49,49,49,49	0
32	MG	A	3128	1/1	0.36	-	57,57,57,57	0
32	MG	B	216	1/1	0.15	-	46,46,46,46	0
32	MG	A	3319	1/1	0.23	-	51,51,51,51	0
32	MG	A	3159	1/1	0.58	-	46,46,46,46	0
32	MG	A	3352	1/1	0.18	-	39,39,39,39	0
32	MG	B	209	1/1	0.35	-	79,79,79,79	0
32	MG	A	3218	1/1	0.17	-	52,52,52,52	0
32	MG	A	3258	1/1	0.57	-	69,69,69,69	0
32	MG	A	3293	1/1	0.66	-	59,59,59,59	0
32	MG	A	3238	1/1	0.16	-	50,50,50,50	0
32	MG	A	3229	1/1	0.17	-	42,42,42,42	0
32	MG	A	3323	1/1	0.08	-	65,65,65,65	0
32	MG	A	3409	1/1	0.14	-	40,40,40,40	0
32	MG	A	3081	1/1	0.19	-	68,68,68,68	0
32	MG	A	3253	1/1	0.29	-	63,63,63,63	0
32	MG	A	3053	1/1	0.29	-	53,53,53,53	0
32	MG	A	3145	1/1	0.17	-	45,45,45,45	0
32	MG	A	3151	1/1	0.24	-	49,49,49,49	0
32	MG	A	3099	1/1	0.25	-	58,58,58,58	0
32	MG	A	3270	1/1	0.65	-	44,44,44,44	0
32	MG	A	3387	1/1	0.10	-	62,62,62,62	0
32	MG	A	3436	1/1	0.17	-	35,35,35,35	0
32	MG	A	3394	1/1	0.17	-	38,38,38,38	0
32	MG	A	3205	1/1	0.37	-	69,69,69,69	0
32	MG	A	3564	1/1	0.14	-	49,49,49,49	0
32	MG	A	3074	1/1	0.24	-	59,59,59,59	0
32	MG	A	3543	1/1	0.12	-	61,61,61,61	0
32	MG	A	3116	1/1	0.27	-	43,43,43,43	0
32	MG	A	3373	1/1	0.07	-	66,66,66,66	0
32	MG	A	3562	1/1	0.14	-	39,39,39,39	0
32	MG	A	3421	1/1	0.10	-	54,54,54,54	0
32	MG	A	3525	1/1	0.13	-	68,68,68,68	0
32	MG	A	3498	1/1	0.13	-	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3044	1/1	0.31	-	49,49,49,49	0
32	MG	A	3244	1/1	0.45	-	66,66,66,66	0
32	MG	A	3354	1/1	0.15	-	57,57,57,57	0
32	MG	A	3278	1/1	0.83	-	56,56,56,56	0
32	MG	A	3163	1/1	0.13	-	54,54,54,54	0
32	MG	A	3513	1/1	0.10	-	33,33,33,33	0
32	MG	A	3499	1/1	0.29	-	79,79,79,79	0
32	MG	A	3574	1/1	0.13	-	76,76,76,76	0
32	MG	B	217	1/1	0.15	-	42,42,42,42	0
33	ZN	6	101	1/1	0.03	-	54,54,54,54	0
32	MG	A	3194	1/1	0.29	-	43,43,43,43	0
32	MG	A	3111	1/1	1.04	-	57,57,57,57	0
32	MG	A	3552	1/1	0.12	-	68,68,68,68	0
32	MG	A	3077	1/1	0.24	-	53,53,53,53	0
32	MG	A	3286	1/1	0.57	-	40,40,40,40	0
32	MG	A	3598	1/1	0.41	-	82,82,82,82	0
32	MG	A	3135	1/1	0.30	-	31,31,31,31	0
32	MG	A	3491	1/1	0.09	-	34,34,34,34	0
32	MG	A	3393	1/1	0.12	-	29,29,29,29	0
32	MG	A	3123	1/1	0.14	-	38,38,38,38	0
32	MG	A	3023	1/1	0.46	-	48,48,48,48	0
32	MG	A	3172	1/1	0.28	-	52,52,52,52	0
32	MG	B	210	1/1	0.22	-	67,67,67,67	0
32	MG	A	3438	1/1	0.22	-	36,36,36,36	0
32	MG	A	3279	1/1	0.44	-	66,66,66,66	0
32	MG	E	306	1/1	0.24	-	56,56,56,56	0
32	MG	A	3203	1/1	0.60	-	79,79,79,79	0
32	MG	A	3433	1/1	0.14	-	30,30,30,30	0
32	MG	A	3004	1/1	0.19	-	44,44,44,44	0
32	MG	A	3204	1/1	0.39	-	65,65,65,65	0
32	MG	A	3568	1/1	0.19	-	90,90,90,90	0
32	MG	O	101	1/1	0.59	-	75,75,75,75	0
32	MG	A	3137	1/1	0.54	-	54,54,54,54	0
32	MG	A	3255	1/1	0.99	-	38,38,38,38	0
32	MG	A	3603	1/1	0.15	-	31,31,31,31	0
32	MG	A	3515	1/1	0.31	-	45,45,45,45	0
32	MG	A	3536	1/1	0.06	-	48,48,48,48	0
32	MG	A	3018	1/1	0.48	-	39,39,39,39	0
32	MG	A	3139	1/1	0.36	-	38,38,38,38	0
32	MG	A	3119	1/1	0.27	-	31,31,31,31	0
32	MG	A	3353	1/1	0.17	-	60,60,60,60	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.