



Full wwPDB X-ray Structure Validation 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 full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

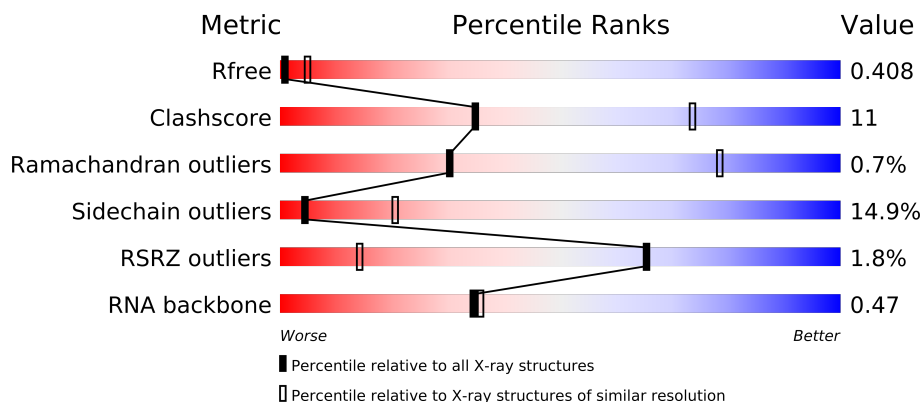
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.00 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.









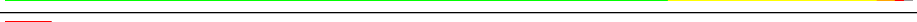


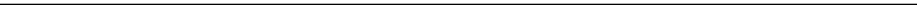




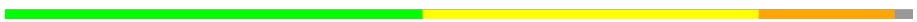




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)
RNA backbone	1838	1070 (3.50-2.50)

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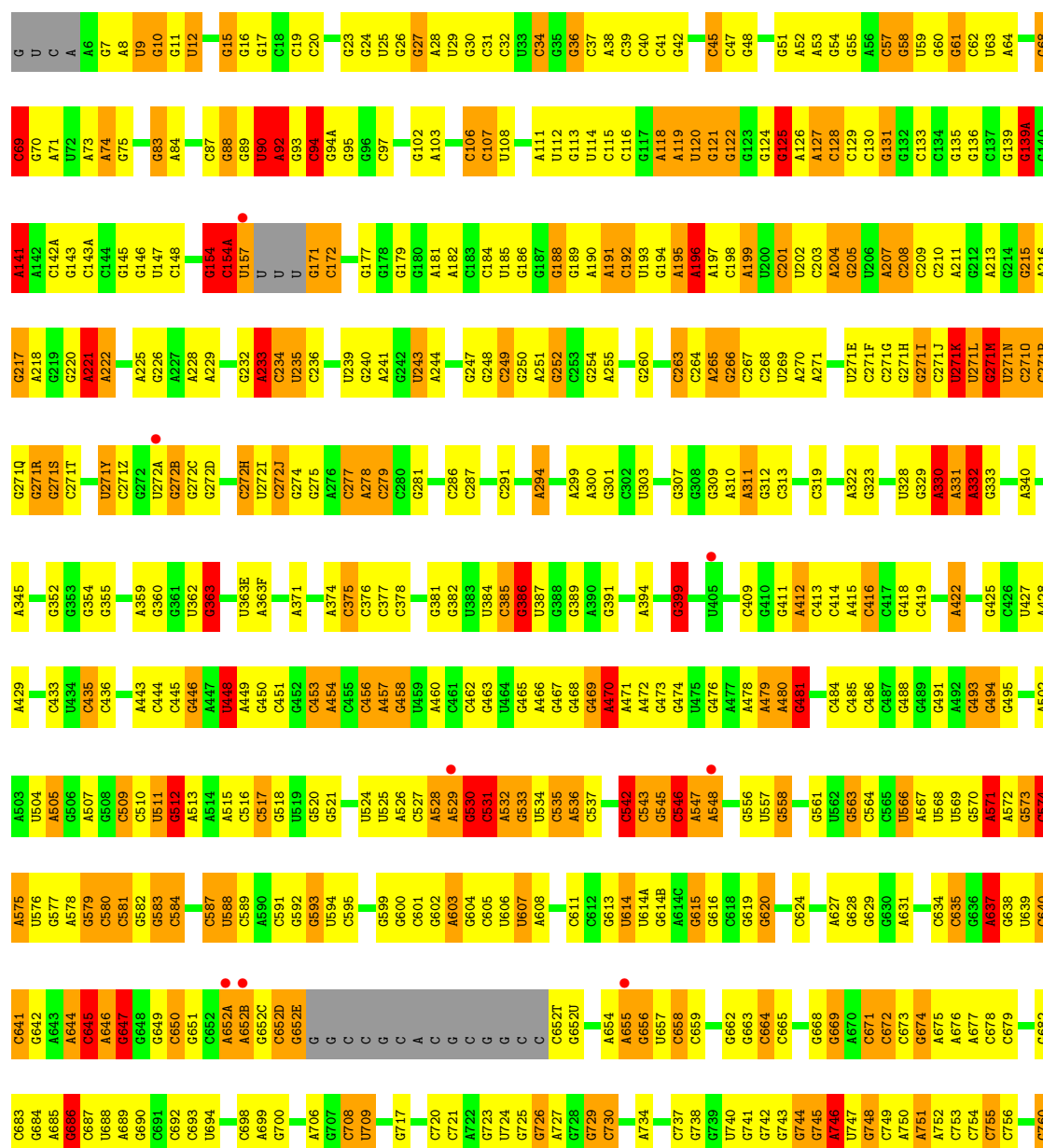
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	F	10	Total 10	O 10	0	0
34	H	1	Total 1	O 1	0	0
34	N	2	Total 2	O 2	0	0
34	O	1	Total 1	O 1	0	0
34	P	5	Total 5	O 5	0	0
34	Q	2	Total 2	O 2	0	0
34	R	5	Total 5	O 5	0	0
34	U	2	Total 2	O 2	0	0
34	V	2	Total 2	O 2	0	0
34	W	4	Total 4	O 4	0	0
34	X	1	Total 1	O 1	0	0
34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

3 Residue-property plots

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

• Molecule 1: 23S Ribosomal RNA

Chain A: 



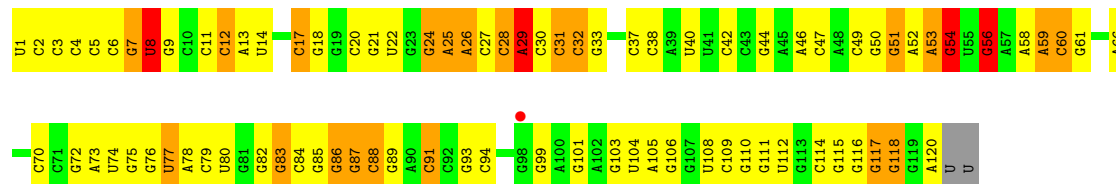


G2833	A2764	U2698	A2614	G2550	G2479	G2413	G2341	G2280	C2200	U2130	G2069	G2009	U1931	A1829
G2834	A2765	G2699	G2615	G2551	G2480	G2414	C2342	C2281	C2200	G2131	G2070	G2010	G1830	G1831
A2835	G2766	G2700	G2616	G2552	G2481	G2415	U2343	G2282	U2203	U2132	A2071	G2011	G1832	G1833
A2836	G2767	G2701	G2617	G2553	G2482	G2416	U2344	C2283	G2205	G2133	G2072	G2012	G1834	G1835
G2837	G2768	U2702	G2618	G2554	G2483	G2417	G2345	C2284	G2206	A2134	C2073	A2013	U1833	U1834
G2838	G2769	G2703	G2619	G2555	G2484	U2419	A2346	C2285	G2207	A2135	U2074	A2014	U1837	U1838
G2839	G2770	G2704	G2620	G2556	G2485	G2420	C2347	A2286	G2208	G2140	U2075	A2015	G1835	G1836
G2840	G2771	A2705	A2621	G2557	G2486	G2421	U2348	A2287	U2218	G2141	A2076	U2016	U1839	U1840
G2841	G2772	G2706	G2622	G2558	G2487	G2422	U2349	A2288	G2219	G2142	A2077	U2017	G1843	G1844
G2842	G2773	G2707	G2623	G2559	A2488	A2422	C2350	G2289	G2220	C2143	U2078	A2018	G1845	G1846
G2843	G2774	G2708	G2624	G2560	G2489	U2423	G2351	G2290	G2221	U2144	U2079	A2019	U1945	U1946
G2844	G2775	G2709	G2625	U2563	U2491	A2424	A2352	U2291	G2222	U2145	G2080	A2020	C1947	C1948
G2845	G2776	A2710	G2626	U2492	U2492	A2425	G2353	C2292	G2223	G2146	A2082	G2021	U1951	U1952
G2846	G2777	G2711	G2627	U2493	U2493	C2427	G2354	C2293	A2225	G2147	U2083	U2022	A1947	A1948
G2847	G2778	G2712	G2628	A2566	G2494	G2428	U2357	C2294	C2226	G2148	G2083	G2023	A1953	A1954
G2848	G2779	G2713	G2629	G2567	G2495	G2429	C2358	C2295	A2227	U2149	G2084	G2024	G1855	G1856
G2849	G2780	A2713	G2630	G2568	G2496	A2430	G2359	C2296	G2228	U2150	U2085	G2025	U1955	U1956
G2850	G2781	G2714	G2631	G2569	A2497	U2431	C2360	A2298	C2229	G2151	U2088	G2026	U1957	U1958
G2851	G2782	G2715	A2632	G2570	C2498	A2432	A2361	G2299	U2232	G2157	U2089	G2027	G1858	G1859
G2852	G2783	G2716	U2637	C2571	C2499	A2433	G2362	G2300	U2233	A2158	U2091	U2028	G1861	G1862
G2853	G2784	G2717	G2641	G2572	U2500	A2434	C2363	C2301	G2234	G2159	U2092	A2031	C1866	C1867
G2854	G2785	G2718	G2642	G2573	G2501	A2435	C2364	C2302	G2235	G2160	G2093	G2032	A1876	A1877
G2855	G2786	G2719	G2643	G2574	G2502	G2436	G2365	G2303	C2236	G2161	G2094	A2033	A1878	A1879
G2856	G2787	G2720	G2644	G2575	U2503	U2437	G2366	A2305	G2238	G2162	U2096	U2035	G1870	G1871
G2857	G2788	G2721	G2645	G2576	U2504	U2438	G2367	A2306	G2239	C2163	U2097	G2036	C1872	C1873
G2858	G2789	G2722	G2646	G2577	G2505	A2439	G2368	C2307	C2240	G2164	U2098	G2037	A1884	A1885
G2859	G2790	G2723	G2647	G2578	U2506	C2440	G2369	G2308	G2241	U2167	U2099	G2038	A1886	A1887
G2860	G2791	G2724	G2648	G2579	G2507	C2441	G2370	A2309	U2243	U2168	G2101	G2039	A1889	A1890
G2861	G2792	G2725	G2649	G2580	G2508	C2442	G2371	G2310	U2244	G2169	U2102	U2041	A1891	A1892
G2862	G2793	G2726	G2650	G2581	G2509	G2443	G2372	C2311	U2245	A2170	G2103	A2042	G1893	G1894
G2863	G2794	U2727	G2651	G2582	C2510	G2444	G2373	C2312	G2246	A2171	G2104	C2043	G1895	G1896
G2864	G2795	G2728	G2652	G2583	G2511	G2445	G2374	C2313	U2247	U2172	G2105	C2044	G1897	G1898
G2865	G2796	G2729	G2653	G2584	G2512	G2446	G2375	C2314	G2248	A2173	G2106	C2045	G1899	G1900
G2866	G2797	G2730	G2654	G2585	G2513	G2447	G2376	C2315	U2249	C2174	G2107	C2046	A1901	A1902
G2867	G2798	G2731	G2655	G2586	U2514	A2448	G2377	C2316	G2250	C2175	U2108	U2047	G1903	G1904
G2868	G2799	G2732	G2656	G2587	G2515	U2449	G2378	C2317	G2251	G2176	G2110	G2048	C1982	C1983
G2869	G2800	G2733	G2657	G2588	G2516	A2450	G2379	G2318	G2252	A2177	G2111	G2049	G1984	G1985
G2870	G2801	G2734	G2658	G2589	G2517	C2451	G2380	G2319	G2253	G2188	G2112	A2051	G1987	G1988
G2871	G2802	G2735	G2659	G2590	U2518	C2452	G2381	A2320	G2254	G2189	U2113	G2052	U1911	U1912
G2872	G2803	G2736	G2660	G2591	G2519	A2453	G2382	G2321	G2255	G2182	G2114	A2053	A1912	A1913
G2873	G2804	G2737	G2661	G2592	G2520	G2454	G2383	G2322	G2256	G2183	G2115	G2054	G1914	G1915
G2874	G2805	G2738	G2662	G2593	G2521	G2455	G2384	A2323	G2257	U2189	G2116	A2055	U1917	U1918
G2875	G2806	G2739	G2663	G2594	G2522	G2456	G2385	G2324	G2258	G2190	G2117	G2056	G1919	G1920
G2876	G2807	A2740	G2664	G2595	G2523	U2457	G2386	G2325	G2259	G2191	G2118	A2057	G1921	G1922
G2877	G2808	G2741	G2665	G2596	G2524	A2459	G2387	G2326	C2260	G2192	G2119	G2058	C1923	C1924
G2878	G2809	G2742	G2666	G2597	G2525	U2460	G2388	G2327	G2261	G2193	G2120	A2059	C1925	C1926
G2879	G2810	G2743	G2667	G2598	G2526	G2461	G2389	G2328	G2262	G2194	G2121	A2060	U1927	U1928
G2880	G2811	G2744	G2668	G2599	G2527	U2462	A2393	G2329	C2263	G2195	G2122	A2061	C1929	C1930
G2881	G2812	G2745	G2669	G2600	G2528	G2463	G2394	G2330	A2267	G2196	G2123	A2062	G1931	G1932
G2882	G2813	G2746	G2670	G2601	A2533	G2464	G2395	G2331	A2268	G2197	G2124	A2063	U1933	U1934
G2883	G2814	G2747	G2671	G2602	G2534	G2465	G2396	G2332	G2269	G2198	G2125	A2064	G1935	G1936
G2884	G2815	G2748	G2672	G2603	G2535	C2466	G2397	G2333	A2270	G2199	G2126	A2065	U1937	U1938
G2885	G2816	G2749	G2673	G2604	G2536	G2467	G2398	G2334	A2271	G2200	G2127	A2066	C1939	C1940
G2886	G2817	G2750	G2674	G2605	G2537	U2468	G2399	G2335	A2272	G2201	G2128	A2067	G1941	G1942
G2887	G2818	G2751	G2675	G2606	G2538	G2469	A2403	G2336	A2273	G2202	G2129	A2068	U1943	U1944
G2888	G2819	G2752	G2676	G2607	G2539	G2470	G2404	G2337	A2274	G2203	G2130	A2069	G1945	G1946
G2889	G2820	G2753	G2677	G2608	G2540	A2471	G2405	G2338	A2275	G2204	G2131	A2070	U1947	U1948
G2890	G2821	G2754	G2678	G2609	G2541	U2472	G2406	G2339	A2276	G2205	G2132	A2071	G1949	G1950
G2891	G2822	G2755	G2679	G2610	G2542	G2473	G2407	G2340	G2277	G2206	G2133	A2072	U1951	U1952
G2892	G2823	G2756	G2680	G2611	G2543	U2474	G2408	G2341	G2278	G2207	G2134	A2073	C1953	C1954
G2893	G2824	G2757	G2681	G2612	G2544	G2475	G2409	G2342	A2279	G2208	G2135	A2074	U1955	U1956
G2894	G2825	G2758	G2682	G2613	G2545	G2476	G2410	G2343	A2280	G2209	G2136	A2075	A1957	A1958
G2895	G2826	G2759	G2683	G2614	G2546	U2477	G2411	G2344	A2281	G2210	G2137	A2076	C1959	C1960
G2896	G2827	G2760	G2684	G2615	G2547	G2478	G2412	G2345	A2282	G2211	G2138	A2077	U1961	U1962
G2897	G2828	G2761	G2685	G2616	G2548	G2479	G2413	G2346	A2283	G2212	G2139	A2078	G1963	G1964
G2898	G2829	G2762	G2686	G2617	G2549	G2480	G2414	G2347	A2284	G2213	G2140	A2079	C1965	C1966
G2899	G2830	G2763	G2687	G2618	G2550	G2481	G2415	G2348	A2285	G2214	G2141	A2080	U1967	U1968
G2900	G2831	G2764	G2688	G2619	G2551	G2482	G2416	G2349	A2286	G2215	G2142	A2081	G1969	G1970
G2901	G2832	G2765	G2689	G2620	G2552	G2483	G2417	G2350	A2287	G2216	G2143	A2082	C1971	C1972
G2902	G2833	G2766	G2690	G2621	G2553	G2484	G2418	G2351	A2288	G2217	G2144	A2083	G1973	G1974
G2903	G2834	G2767	G2691	G2622	G2554	G2485	G2419	G2352	A2289	G2218	G2145	A2084	A1975	A1976
G2904	G2835	G2768	G2692	G2623	G2555	G2486	G2420	G2353	A2290	G2219	G2146	A2085	G1977	G1978
G2905	G2836	G2769	G2693	G2624	G2556	G2487	G2421	G2354	A2291	G2220	G2147	A2086	C1979	C1980
G2906	G2837	G2770	G2694	G2625	G2557	G2488	G2422	G2355	A2292	G2221	G2148	A2087	G1981	G1982
G2907	G2838	G2771	G2695	G2626	G2558	G2489	G2423	G2356	A2293	G2222	G2149	A2088	C1983	C1984
G2908	G2839	G2772	G2696	G2627	G2559	G2490	G2424	G2357	A2294	G2223	G2150	A2089	G1985	G1986
G2909	G2840	G2773	G2697	G2628	G2560	G2491	G2425	G2358	A2295	G2224	G2151	A2090	C1987	C1988
G2910	G2841	G2774	G2698	G2629	G2561	G2492	G2426	G2359	A2296	G2225	G2152	A2091	G1989	G1990
G2911	G2842	G2775	G2699	G2630	G2562	G2493	G2427	G2360	A2297	G2226	G2153	A2092	C1991	C1992
G2912	G2843	G2776	G2700	G2631	G2563	G2494	G2428	G2361	A2298	G2227	G2154	A2093	G1993	G1994
G2913	G2844	G2777	G2701	G2632	G2564	G2495	G2429	G2362	A2299	G2228	G2155	A2094	C1995	C1996
G2914	G2845	G2778	G2702	G2633	G2565	G2496	G2430	G2363	A2300	G2229	G2156	A2095	G1997	G1998
G2915	G2846	G2779	G2703	G2634	G2566	G2497	G2431	G2364	A2301	G2230	G2157	A2096	C1999	C2000
G2916	G2847	G2780	G2704	G2635	G2567	G2498	G2432	G2365	A2302	G2231	G2158	A2097	G2001	G2002
G2917	G2848	G2781	G2705	G2636	G2568	G2499	G2433	G2366	A2303	G2232	G2159	A2098	C2003	C2004
G2918	G2849	G2782	G2706	G2637	G2569	G2500	G2434	G2367	A2304	G2233	G2160	A2099	U1999	U2000
G29														

C

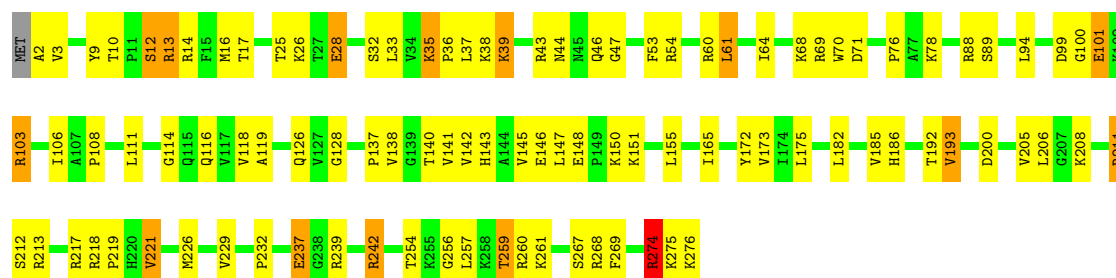
- Molecule 2: 5S Ribosomal RNA

Chain B:



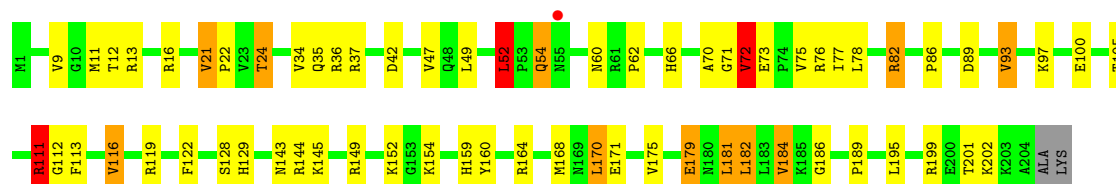
- Molecule 3: 50S Ribosomal Protein L2

Chain D:



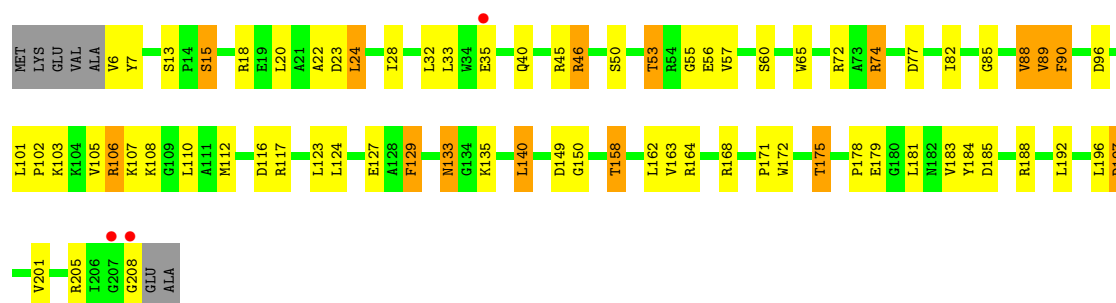
- Molecule 4: 50S Ribosomal Protein L3

Chain E:



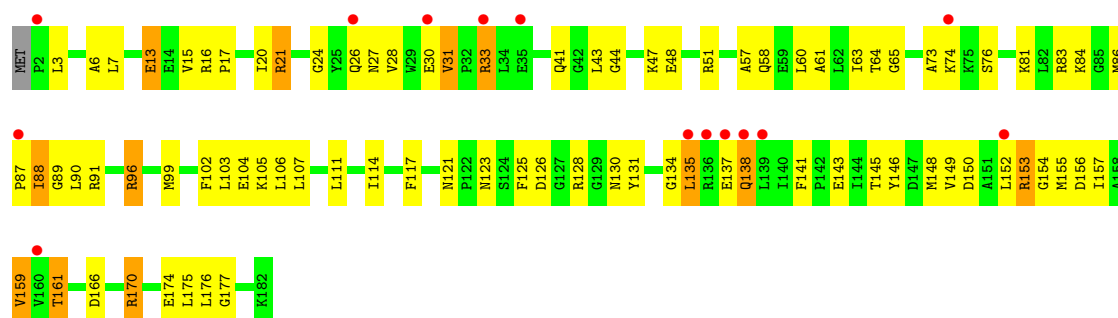
- Molecule 5: 50S Ribosomal Protein L4

Chain F:



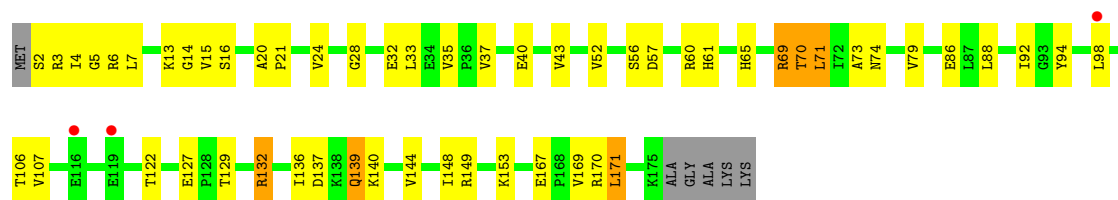
- Molecule 6: 50S Ribosomal Protein L5

Chain G:



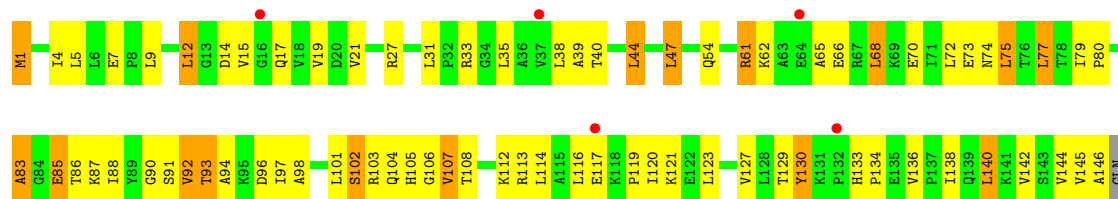
• Molecule 7: 50S Ribosomal Protein L6

Chain H:



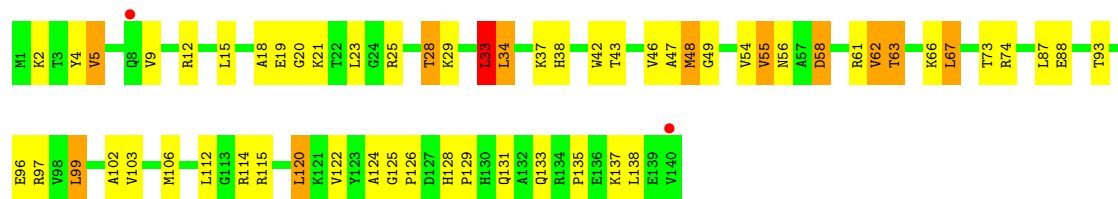
• Molecule 8: 50S Ribosomal Protein L9

Chain I:



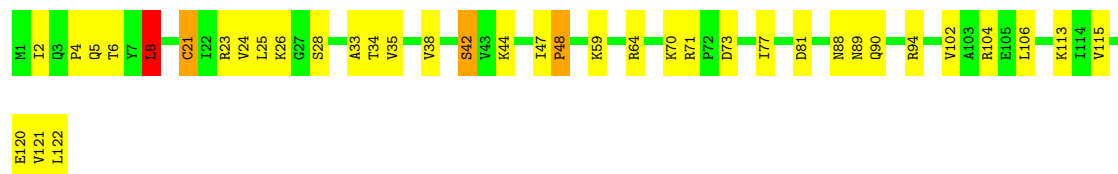
• Molecule 9: 50S Ribosomal Protein L13

Chain N:

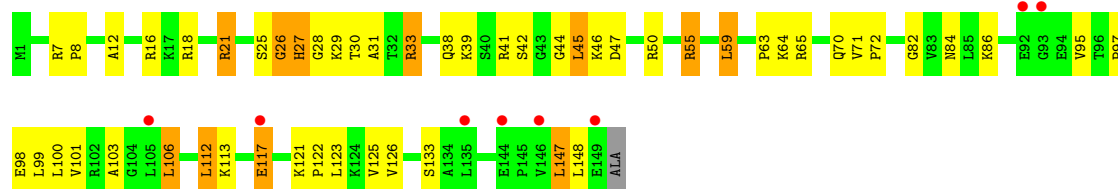


• Molecule 10: 50S Ribosomal Protein L14

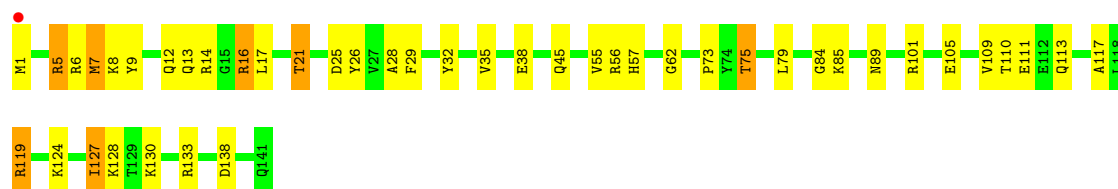
Chain O:



- Molecule 11: 50S Ribosomal Protein L15

Chain P: 

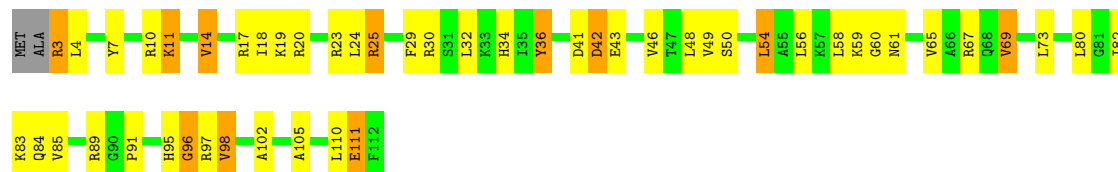
- Molecule 12: 50S Ribosomal Protein L16

Chain Q: 

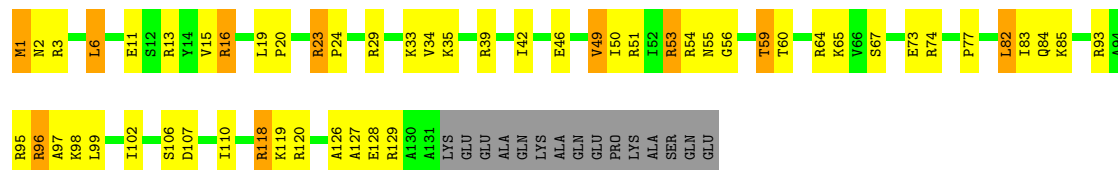
- Molecule 13: 50S Ribosomal Protein L17

Chain R: 

- Molecule 14: 50S Ribosomal Protein L18

Chain S: 

- Molecule 15: 50S Ribosomal Protein L19

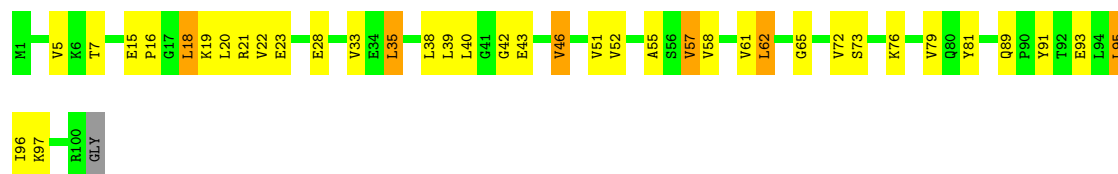
Chain T: 

- Molecule 16: 50S Ribosomal Protein L20

Chain U: 

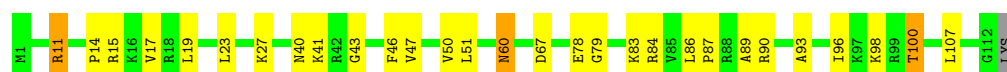
- Molecule 17: 50S Ribosomal Protein L21

Chain V:



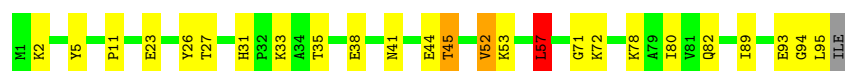
- Molecule 18: 50S Ribosomal Protein L22

Chain W:



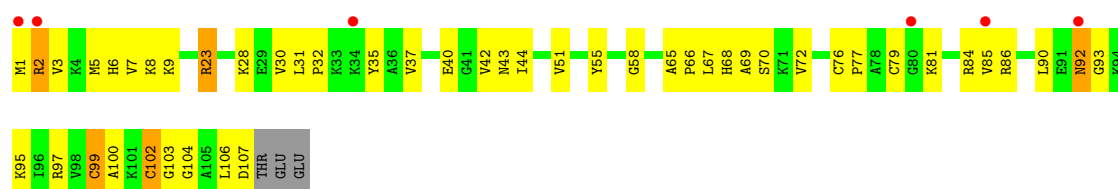
- Molecule 19: 50S Ribosomal Protein L23

Chain X:



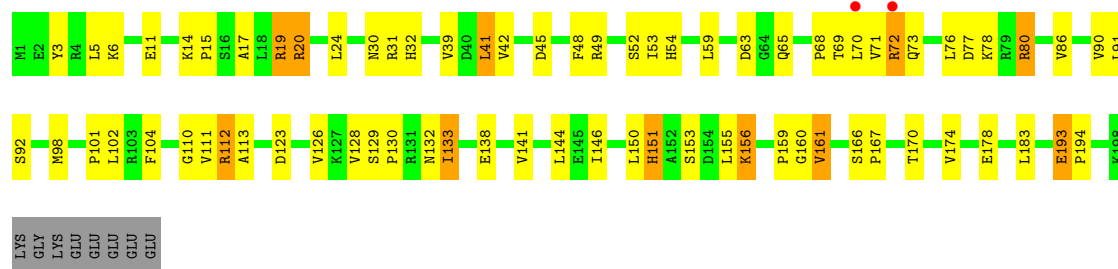
- Molecule 20: 50S Ribosomal Protein L24

Chain Y:



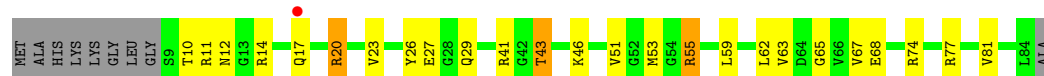
- Molecule 21: 50S Ribosomal Protein L25

Chain Z:



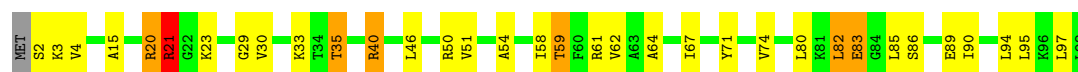
- Molecule 22: 50S Ribosomal Protein L27

Chain 0:



- Molecule 23: 50S Ribosomal Protein L28

Chain 1: 



- Molecule 24: 50S Ribosomal Protein L29

Chain 2: 



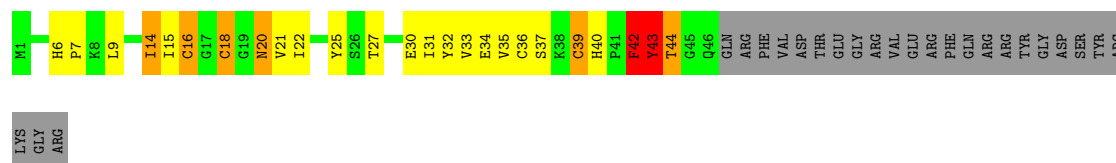
- Molecule 25: 50S Ribosomal Protein L30

Chain 3: 



- Molecule 26: 50S Ribosomal Protein L31

Chain 4: 



- Molecule 27: 50S Ribosomal Protein L32

Chain 5: 



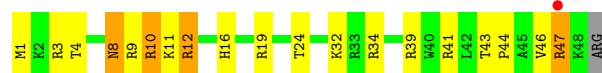
- Molecule 28: 50S Ribosomal Protein L33

Chain 6: 



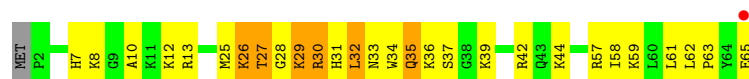
- Molecule 29: 50S Ribosomal Protein L34

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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	68.3	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	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 ²)	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.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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

All (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
2	B	120	A	C6-N6	-10.88	1.25	1.33
1	A	478	A	N3-C4	-10.54	1.28	1.34
1	A	1142(A)	A	N3-C4	-10.26	1.28	1.34
1	A	1762	A	N9-C4	9.95	1.43	1.37
1	A	1325	G	P-O5'	-9.34	1.50	1.59
1	A	467	G	P-OP1	-9.32	1.33	1.49
1	A	2296	U	N1-C2	9.29	1.47	1.38
1	A	2296	U	C4-O4	9.21	1.31	1.23
1	A	2825	C	N1-C6	-9.20	1.31	1.37
1	A	330	A	N9-C4	-9.13	1.32	1.37
1	A	467	G	P-O5'	-9.09	1.50	1.59
1	A	1210	A	N7-C5	-9.07	1.33	1.39
1	A	1204	A	N7-C5	-8.98	1.33	1.39
1	A	198	C	N1-C6	-8.97	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1254	A	P-OP1	-8.91	1.33	1.49
1	A	530	G	N9-C8	8.80	1.44	1.37
1	A	2058	A	N3-C4	-8.78	1.29	1.34
1	A	1210	A	N9-C4	-8.74	1.32	1.37
1	A	2070	G	N7-C5	-8.74	1.34	1.39
1	A	965	C	N3-C4	-8.54	1.27	1.33
1	A	26	G	N7-C5	-8.52	1.34	1.39
1	A	2252	G	C5-C4	-8.48	1.32	1.38
1	A	1614	A	N9-C4	-8.47	1.32	1.37
1	A	2570	G	N9-C4	-8.37	1.31	1.38
1	A	2499	C	N1-C6	-8.31	1.32	1.37
1	A	1393	A	N3-C4	-8.21	1.29	1.34
1	A	2452	C	N1-C6	-8.20	1.32	1.37
1	A	2060	A	C6-N1	-8.05	1.29	1.35
1	A	2620	C	N1-C6	-8.05	1.32	1.37
1	A	2055	C	P-OP2	-8.00	1.35	1.49
1	A	2515	C	C4-C5	-7.89	1.36	1.43
1	A	528	A	N9-C8	7.89	1.44	1.37
1	A	2055	C	P-OP1	-7.86	1.35	1.49
1	A	2497	A	N7-C5	-7.84	1.34	1.39
1	A	2017	U	C2-N3	-7.83	1.32	1.37
1	A	469	G	N9-C8	-7.81	1.32	1.37
1	A	2497	A	N9-C8	-7.79	1.31	1.37
1	A	1137	G	C5-C4	-7.77	1.32	1.38
1	A	2515	C	N3-C4	-7.73	1.28	1.33
1	A	2032	G	C6-N1	-7.70	1.34	1.39
1	A	2244	U	N3-C4	-7.70	1.31	1.38
1	A	1638	C	N1-C6	-7.70	1.32	1.37
1	A	530	G	C8-N7	7.67	1.35	1.30
1	A	567	A	N7-C5	-7.64	1.34	1.39
1	A	1204	A	C5-C6	-7.60	1.34	1.41
1	A	2287	A	N9-C4	-7.60	1.33	1.37
1	A	272(A)	U	C1'-N1	7.59	1.60	1.48
1	A	2600	A	N7-C5	-7.51	1.34	1.39
1	A	467	G	C5-C4	-7.46	1.33	1.38
1	A	2617	C	N1-C6	-7.46	1.32	1.37
1	A	2361	A	N9-C4	-7.43	1.33	1.37
1	A	1210	A	C5-C6	-7.34	1.34	1.41
1	A	2445	G	N9-C8	-7.34	1.32	1.37
1	A	2456	C	N1-C6	-7.32	1.32	1.37
1	A	2032	G	N7-C5	-7.30	1.34	1.39
1	A	980	A	N9-C4	-7.29	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2063	C	N1-C6	-7.29	1.32	1.37
1	A	964	C	N3-C4	-7.28	1.28	1.33
1	A	2441	C	P-O5'	-7.28	1.52	1.59
1	A	1791	A	N9-C4	-7.26	1.33	1.37
1	A	2730	C	N3-C4	-7.26	1.28	1.33
1	A	2502	G	N9-C8	-7.24	1.32	1.37
1	A	189	G	N7-C5	-7.22	1.34	1.39
1	A	2542	A	C5-C4	-7.22	1.33	1.38
1	A	2335	A	C5-C6	-7.17	1.34	1.41
1	A	2028	U	C2-N3	-7.15	1.32	1.37
1	A	1322	A	N7-C5	-7.15	1.34	1.39
1	A	582	G	N9-C8	-7.14	1.32	1.37
1	A	1131	G	C6-N1	-7.13	1.34	1.39
1	A	2499	C	N3-C4	-7.13	1.28	1.33
1	A	1779	U	N3-C4	-7.12	1.32	1.38
1	A	1022	G	N3-C4	-7.10	1.30	1.35
1	A	37	C	N1-C6	-7.07	1.32	1.37
1	A	1254	A	P-O5'	-7.05	1.52	1.59
1	A	579	G	N9-C8	-7.05	1.32	1.37
1	A	2104	G	N1-C2	-7.05	1.32	1.37
1	A	2822	G	N9-C8	-7.04	1.32	1.37
1	A	195	A	N9-C4	-7.02	1.33	1.37
2	B	120	A	C6-N1	7.02	1.40	1.35
1	A	1325	G	P-OP1	-7.01	1.37	1.49
1	A	801	G	N9-C8	-7.00	1.32	1.37
1	A	467	G	P-OP2	-6.97	1.37	1.49
1	A	1572	A	N3-C4	-6.97	1.30	1.34
1	A	2044	C	N1-C6	-6.96	1.32	1.37
1	A	2026	C	N1-C6	-6.95	1.32	1.37
1	A	1379	A	N9-C4	-6.95	1.33	1.37
1	A	2018	G	N3-C4	-6.94	1.30	1.35
1	A	1614	A	N3-C4	-6.91	1.30	1.34
1	A	1427	A	C6-N1	-6.90	1.30	1.35
1	A	27	G	N3-C4	-6.89	1.30	1.35
1	A	2730	C	C2-N3	-6.87	1.30	1.35
1	A	1332	G	C6-O6	-6.86	1.18	1.24
1	A	2030	A	C5-C4	-6.85	1.33	1.38
1	A	975	C	N3-C4	-6.84	1.29	1.33
1	A	2045	C	N1-C6	-6.83	1.33	1.37
1	A	2500	U	C4-O4	-6.82	1.18	1.23
1	A	1325	G	P-OP2	-6.82	1.37	1.49
1	A	2104	G	C6-N1	-6.82	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	794	G	N1-C2	-6.81	1.32	1.37
1	A	195	A	N3-C4	-6.80	1.30	1.34
1	A	1660	C	C2-O2	-6.77	1.18	1.24
1	A	1403	C	N1-C6	-6.77	1.33	1.37
1	A	794	G	C6-N1	-6.76	1.34	1.39
1	A	1633	G	N7-C5	-6.74	1.35	1.39
1	A	1571	A	N9-C4	-6.72	1.33	1.37
1	A	2515	C	N1-C6	-6.71	1.33	1.37
1	A	1608	A	N7-C5	-6.70	1.35	1.39
1	A	126	A	N7-C5	-6.68	1.35	1.39
1	A	2504	U	P-O5'	-6.67	1.53	1.59
1	A	756	C	N1-C6	-6.67	1.33	1.37
1	A	2872	G	N7-C5	-6.67	1.35	1.39
1	A	2286	A	N7-C5	-6.66	1.35	1.39
1	A	2015	A	N7-C5	-6.66	1.35	1.39
1	A	2727	G	N7-C5	-6.65	1.35	1.39
1	A	31	C	N1-C6	-6.64	1.33	1.37
1	A	27	G	P-OP2	-6.64	1.37	1.49
1	A	2690	C	N1-C6	-6.62	1.33	1.37
1	A	2055	C	P-O5'	-6.62	1.53	1.59
1	A	1137	G	N7-C5	-6.62	1.35	1.39
1	A	1195	G	N7-C5	-6.61	1.35	1.39
1	A	2055	C	O3'-P	-6.61	1.53	1.61
1	A	2430	A	N9-C4	-6.60	1.33	1.37
1	A	532	A	N7-C5	-6.59	1.35	1.39
1	A	529	A	N3-C4	-6.59	1.30	1.34
1	A	678	C	N1-C6	-6.58	1.33	1.37
1	A	578	A	N7-C5	-6.58	1.35	1.39
1	A	2041	U	N1-C2	-6.58	1.32	1.38
1	A	780	G	N7-C5	-6.57	1.35	1.39
1	A	2503	A	C5-C6	-6.57	1.35	1.41
1	A	1605	C	N3-C4	-6.57	1.29	1.33
1	A	1322	A	N9-C4	-6.56	1.33	1.37
1	A	1251	C	P-O5'	-6.55	1.53	1.59
1	A	448	U	N3-C4	-6.54	1.32	1.38
1	A	16	G	N3-C4	-6.54	1.30	1.35
1	A	515	A	N7-C5	-6.54	1.35	1.39
1	A	2587	A	N7-C5	-6.54	1.35	1.39
1	A	466	A	P-OP2	-6.53	1.37	1.49
1	A	1132	A	N3-C4	-6.52	1.30	1.34
1	A	818	G	C6-N1	-6.50	1.34	1.39
1	A	819	A	N3-C4	-6.50	1.30	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	73	A	N3-C4	-6.49	1.30	1.34
1	A	1755	A	C6-N1	-6.48	1.31	1.35
1	A	818	G	N3-C4	-6.48	1.30	1.35
1	A	1393	A	C5-C4	-6.48	1.34	1.38
1	A	566	U	C2-N3	-6.47	1.33	1.37
1	A	2578	G	N1-C2	-6.47	1.32	1.37
1	A	983	A	C6-N1	-6.45	1.31	1.35
1	A	788	A	N7-C5	-6.45	1.35	1.39
1	A	682	G	C5-C4	-6.44	1.33	1.38
1	A	2834	G	N7-C5	-6.44	1.35	1.39
1	A	2424	C	N1-C6	-6.43	1.33	1.37
1	A	1250	G	N7-C5	-6.43	1.35	1.39
1	A	2059	A	C5-C4	-6.42	1.34	1.38
1	A	582	G	N7-C5	-6.42	1.35	1.39
1	A	675	A	C6-N1	-6.42	1.31	1.35
1	A	1791	A	N7-C5	-6.42	1.35	1.39
1	A	24	G	N1-C2	-6.42	1.32	1.37
1	A	1254	A	P-OP2	-6.42	1.38	1.49
1	A	2689	U	N3-C4	-6.41	1.32	1.38
1	A	516	C	N1-C6	-6.40	1.33	1.37
1	A	2011	U	C4-O4	-6.39	1.18	1.23
1	A	2335	A	N9-C4	-6.39	1.34	1.37
1	A	793	A	N3-C4	-6.38	1.31	1.34
1	A	2056	G	P-OP2	-6.38	1.38	1.49
1	A	981	A	C5-C4	-6.38	1.34	1.38
1	A	1248	G	C2-N3	-6.37	1.27	1.32
1	A	780	G	N9-C8	-6.37	1.33	1.37
1	A	2741	A	N9-C4	-6.36	1.34	1.37
1	A	528	A	N3-C4	-6.36	1.31	1.34
1	A	2524	G	N9-C8	-6.36	1.33	1.37
1	A	1226	A	N7-C5	-6.35	1.35	1.39
1	A	1204	A	N3-C4	-6.34	1.31	1.34
1	A	676	A	P-O5'	-6.33	1.53	1.59
1	A	973	A	P-O5'	-6.33	1.53	1.59
1	A	2070	G	C2-N2	-6.32	1.28	1.34
1	A	2030	A	N3-C4	-6.32	1.31	1.34
1	A	575	A	P-OP1	-6.32	1.38	1.49
1	A	1315	C	N3-C4	-6.32	1.29	1.33
1	A	47	C	N3-C4	-6.30	1.29	1.33
1	A	235	U	C2-N3	-6.30	1.33	1.37
1	A	760	G	N9-C8	-6.28	1.33	1.37
1	A	2346	A	N3-C4	-6.28	1.31	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2621	A	P-O5'	-6.28	1.53	1.59
1	A	2327	A	N9-C4	-6.27	1.34	1.37
1	A	2490	G	N3-C4	-6.27	1.31	1.35
1	A	70	G	C6-N1	-6.27	1.35	1.39
1	A	564	C	N3-C4	-6.27	1.29	1.33
1	A	233	A	N3-C4	-6.26	1.31	1.34
1	A	457	A	C6-N1	-6.25	1.31	1.35
1	A	575	A	N7-C5	-6.25	1.35	1.39
1	A	2577	A	N7-C5	-6.25	1.35	1.39
1	A	2581	G	N1-C2	-6.24	1.32	1.37
1	A	469	G	N7-C5	-6.24	1.35	1.39
1	A	1335	U	N1-C6	-6.24	1.32	1.38
1	A	2064	C	N1-C6	-6.24	1.33	1.37
1	A	781	A	C5-C4	-6.23	1.34	1.38
1	A	933	A	N9-C4	-6.22	1.34	1.37
1	A	1131	G	N1-C2	-6.22	1.32	1.37
1	A	769	G	C2-N3	-6.22	1.27	1.32
1	A	2050	C	N1-C6	-6.21	1.33	1.37
1	A	2557	G	C2-N3	-6.21	1.27	1.32
1	A	2625	G	C2-N3	-6.21	1.27	1.32
1	A	570	G	C6-N1	-6.20	1.35	1.39
1	A	2614	A	P-O5'	-6.20	1.53	1.59
1	A	570	G	C5-C4	-6.20	1.34	1.38
1	A	533	G	C6-N1	-6.19	1.35	1.39
1	A	190	A	C6-N1	-6.19	1.31	1.35
1	A	1600	C	N1-C6	-6.19	1.33	1.37
1	A	467	G	N9-C8	-6.18	1.33	1.37
1	A	467	G	C8-N7	-6.17	1.27	1.30
1	A	2002	G	N7-C5	-6.17	1.35	1.39
1	A	939	G	C5-C4	-6.16	1.34	1.38
1	A	2765	A	N7-C5	-6.15	1.35	1.39
1	A	2239	G	N1-C2	-6.15	1.32	1.37
1	A	575	A	P-OP2	-6.14	1.38	1.49
1	A	2610	C	N1-C6	-6.13	1.33	1.37
1	A	2030	A	N9-C4	-6.13	1.34	1.37
1	A	571	A	N9-C4	-6.13	1.34	1.37
1	A	1247	A	N7-C5	-6.13	1.35	1.39
1	A	1432	C	N1-C6	-6.12	1.33	1.37
1	A	964	C	C4-C5	-6.11	1.38	1.43
1	A	389	G	N3-C4	-6.10	1.31	1.35
1	A	453	C	P-OP1	-6.09	1.38	1.49
1	A	2578	G	P-OP2	-6.09	1.38	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	738	G	N7-C5	-6.09	1.35	1.39
1	A	2346	A	N7-C5	-6.09	1.35	1.39
1	A	1992	G	P-O5'	-6.08	1.53	1.59
3	D	237	GLU	CD-OE1	6.08	1.32	1.25
1	A	1190	G	N7-C5	-6.08	1.35	1.39
1	A	2007	C	P-OP2	-6.08	1.38	1.49
1	A	265	A	C5-C6	-6.07	1.35	1.41
1	A	2765	A	N9-C4	-6.07	1.34	1.37
1	A	466	A	P-OP1	-6.07	1.38	1.49
1	A	955	C	N3-C4	-6.07	1.29	1.33
1	A	57	C	N1-C6	-6.05	1.33	1.37
1	A	48	G	N1-C2	-6.05	1.32	1.37
1	A	2286	A	C5-C6	-6.05	1.35	1.41
1	A	2516	G	C6-N1	-6.05	1.35	1.39
1	A	2014	A	C5-C4	-6.04	1.34	1.38
1	A	1570	A	N9-C4	-6.04	1.34	1.37
1	A	130	C	N1-C6	-6.04	1.33	1.37
1	A	1786	A	N3-C4	-6.03	1.31	1.34
1	A	330	A	N3-C4	-6.02	1.31	1.34
1	A	2383	G	N7-C5	-6.02	1.35	1.39
1	A	2043	C	N3-C4	-6.02	1.29	1.33
1	A	2515	C	C5-C6	-6.02	1.29	1.34
1	A	1605	C	N1-C6	-6.01	1.33	1.37
1	A	27	G	C2-N3	-6.01	1.27	1.32
1	A	2466	C	N1-C6	-6.01	1.33	1.37
1	A	19	C	N1-C6	-6.00	1.33	1.37
1	A	1137	G	N1-C2	-6.00	1.32	1.37
1	A	567	A	C5-C6	-6.00	1.35	1.41
1	A	2069	G	C5-C4	-6.00	1.34	1.38
1	A	2020	A	C6-N6	-5.99	1.29	1.33
1	A	73	A	C6-N1	-5.98	1.31	1.35
1	A	265	A	N9-C4	-5.98	1.34	1.37
1	A	465	G	C6-N1	-5.98	1.35	1.39
1	A	527	C	N3-C4	-5.97	1.29	1.33
1	A	819	A	P-OP1	-5.96	1.38	1.49
1	A	23	G	N3-C4	-5.95	1.31	1.35
1	A	1204	A	N9-C4	-5.95	1.34	1.37
1	A	2790	A	N9-C4	5.95	1.41	1.37
1	A	528	A	C5-C6	-5.94	1.35	1.41
1	A	197	A	N9-C4	-5.94	1.34	1.37
1	A	37	C	N3-C4	-5.93	1.29	1.33
1	A	777	A	C6-N1	-5.93	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2577	A	N9-C8	-5.93	1.33	1.37
1	A	2718	G	N3-C4	-5.93	1.31	1.35
1	A	516	C	P-O5'	-5.92	1.53	1.59
1	A	2712	U	P-O5'	-5.92	1.53	1.59
1	A	1783	A	N7-C5	-5.92	1.35	1.39
1	A	970	C	N3-C4	-5.92	1.29	1.33
1	A	2622	C	N3-C4	-5.91	1.29	1.33
1	A	528	A	C2-N3	-5.91	1.28	1.33
1	A	1266	G	C5-C4	-5.91	1.34	1.38
1	A	1338	G	C8-N7	-5.91	1.27	1.30
1	A	60	G	C5-C4	-5.90	1.34	1.38
1	A	2826	A	C5-C4	-5.90	1.34	1.38
1	A	1131	G	C5-C4	-5.89	1.34	1.38
1	A	2045	C	N3-C4	-5.88	1.29	1.33
1	A	800	A	N3-C4	-5.88	1.31	1.34
1	A	1271	G	N9-C8	-5.88	1.33	1.37
1	A	2079	U	P-O5'	-5.88	1.53	1.59
1	A	678	C	C2-N3	-5.88	1.31	1.35
1	A	1202	C	N1-C6	-5.87	1.33	1.37
1	A	119	A	P-O5'	-5.87	1.53	1.59
1	A	1020	A	N7-C5	-5.87	1.35	1.39
1	A	1158	C	N3-C4	-5.87	1.29	1.33
1	A	2430	A	N3-C4	-5.86	1.31	1.34
1	A	209	C	N3-C4	-5.86	1.29	1.33
1	A	119	A	N9-C8	-5.85	1.33	1.37
1	A	58	G	C6-N1	-5.85	1.35	1.39
1	A	2641	G	P-O5'	-5.84	1.53	1.59
1	A	23	G	N1-C2	-5.84	1.33	1.37
1	A	818	G	C5-C4	-5.84	1.34	1.38
1	A	1261	C	N3-C4	-5.83	1.29	1.33
1	A	2070	G	N9-C8	-5.83	1.33	1.37
1	A	2497	A	P-O5'	-5.83	1.53	1.59
1	A	1328	G	C8-N7	-5.83	1.27	1.30
1	A	493	G	C2-N3	-5.82	1.28	1.32
1	A	2580	U	P-O5'	-5.82	1.53	1.59
1	A	2044	C	N3-C4	-5.82	1.29	1.33
1	A	2499	C	C4-N4	-5.82	1.28	1.33
1	A	2873	A	C6-N1	-5.82	1.31	1.35
1	A	2017	U	N1-C6	-5.81	1.32	1.38
1	A	984	A	C6-N1	-5.81	1.31	1.35
1	A	1030	G	C6-N1	-5.81	1.35	1.39
1	A	192	C	N3-C4	-5.80	1.29	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	820	A	N9-C4	-5.80	1.34	1.37
1	A	2608	G	N3-C4	-5.80	1.31	1.35
1	A	488	G	N9-C8	-5.80	1.33	1.37
1	A	2623	G	N1-C2	-5.80	1.33	1.37
1	A	2823	A	C5-C6	-5.79	1.35	1.41
1	A	202	U	N1-C6	-5.79	1.32	1.38
1	A	1773	A	C5-C4	-5.78	1.34	1.38
1	A	2015	A	C5-C6	-5.77	1.35	1.41
1	A	1783	A	C6-N1	-5.77	1.31	1.35
1	A	141	A	C5-C6	-5.77	1.35	1.41
1	A	463	G	C6-N1	-5.77	1.35	1.39
1	A	939	G	N9-C8	-5.77	1.33	1.37
1	A	1378	A	N3-C4	-5.77	1.31	1.34
1	A	1647	G	C5-C4	-5.77	1.34	1.38
1	A	1324	G	O3'-P	-5.77	1.54	1.61
1	A	2000	G	C6-N1	-5.77	1.35	1.39
1	A	2730	C	N1-C6	-5.76	1.33	1.37
1	A	1608	A	N9-C8	-5.76	1.33	1.37
1	A	806	C	C4-C5	-5.76	1.38	1.43
1	A	2574	G	C5-C4	-5.75	1.34	1.38
1	A	2620	C	N3-C4	-5.75	1.29	1.33
1	A	1572	A	C6-N1	-5.74	1.31	1.35
1	A	945	A	N9-C4	-5.74	1.34	1.37
1	A	512	G	P-O5'	-5.74	1.54	1.59
1	A	2587	A	N9-C8	-5.74	1.33	1.37
1	A	2781	A	C6-N1	-5.73	1.31	1.35
1	A	783	A	N7-C5	-5.72	1.35	1.39
1	A	38	A	N3-C4	-5.72	1.31	1.34
1	A	1424	G	N3-C4	-5.72	1.31	1.35
1	A	2061	G	N7-C5	-5.72	1.35	1.39
1	A	2502	G	N7-C5	-5.72	1.35	1.39
1	A	2489	G	N9-C8	-5.72	1.33	1.37
1	A	28	A	N7-C5	-5.71	1.35	1.39
1	A	1786	A	C5-C4	-5.71	1.34	1.38
1	A	1360	A	N9-C4	-5.71	1.34	1.37
1	A	2063	C	C4-C5	-5.71	1.38	1.43
1	A	70	G	N1-C2	-5.70	1.33	1.37
1	A	2013	A	O3'-P	-5.70	1.54	1.61
1	A	746	A	N9-C4	-5.70	1.34	1.37
1	A	2020	A	P-O5'	-5.70	1.54	1.59
1	A	2053	G	N9-C8	-5.70	1.33	1.37
1	A	2333	A	N7-C5	-5.69	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2084	C	N1-C6	-5.69	1.33	1.37
1	A	2725	A	N9-C4	-5.69	1.34	1.37
1	A	2611	U	P-OP2	-5.69	1.39	1.49
1	A	1601	G	N1-C2	-5.68	1.33	1.37
1	A	2024	G	C8-N7	-5.68	1.27	1.30
1	A	530	G	N3-C4	-5.68	1.31	1.35
1	A	774	A	N7-C5	-5.68	1.35	1.39
1	A	2037	G	C8-N7	-5.68	1.27	1.30
1	A	1359	A	C6-N6	-5.67	1.29	1.33
1	A	2053	G	C5-C4	-5.67	1.34	1.38
1	A	1269	A	N3-C4	-5.66	1.31	1.34
1	A	1611	C	C2-N3	-5.66	1.31	1.35
1	A	20	C	N1-C6	-5.66	1.33	1.37
1	A	848	G	N9-C8	-5.66	1.33	1.37
1	A	454	A	N7-C5	-5.66	1.35	1.39
1	A	1771	C	N3-C4	-5.66	1.29	1.33
1	A	2200	C	N1-C6	-5.66	1.33	1.37
1	A	2574	G	C6-N1	-5.66	1.35	1.39
1	A	2719	G	N1-C2	-5.66	1.33	1.37
1	A	2497	A	C5-C4	-5.65	1.34	1.38
1	A	1008	C	N1-C6	-5.65	1.33	1.37
1	A	1661	G	N9-C8	-5.64	1.33	1.37
1	A	90	U	C2-N3	5.64	1.41	1.37
1	A	1784	A	C8-N7	-5.64	1.27	1.31
1	A	194	G	N9-C8	-5.64	1.33	1.37
1	A	2442	C	N3-C4	-5.64	1.30	1.33
1	A	234	C	N3-C4	-5.63	1.30	1.33
1	A	566	U	C5-C6	-5.63	1.29	1.34
1	A	2611	U	C2-O2	-5.63	1.17	1.22
1	A	2872	G	N9-C8	-5.62	1.33	1.37
2	B	76	G	C5-C4	-5.62	1.34	1.38
1	A	800	A	N7-C5	-5.62	1.35	1.39
1	A	16	G	C6-N1	-5.62	1.35	1.39
1	A	1698	A	N9-C4	-5.62	1.34	1.37
1	A	2393	A	C6-N1	-5.62	1.31	1.35
1	A	191	A	N7-C5	-5.62	1.35	1.39
1	A	266	G	N7-C5	-5.61	1.35	1.39
1	A	2382	G	N7-C5	-5.61	1.35	1.39
1	A	139(A)	G	N9-C8	5.61	1.41	1.37
1	A	2711	A	N9-C4	-5.61	1.34	1.37
1	A	2268	A	N7-C5	-5.61	1.35	1.39
1	A	593	G	N7-C5	-5.61	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	686	G	N7-C5	-5.60	1.35	1.39
1	A	119	A	C6-N1	-5.60	1.31	1.35
1	A	466	A	O3'-P	-5.60	1.54	1.61
1	A	2543	G	C5-C4	-5.60	1.34	1.38
1	A	2068	U	N1-C2	-5.60	1.33	1.38
1	A	2466	C	C4-C5	-5.60	1.38	1.43
1	A	793	A	C6-N1	-5.60	1.31	1.35
1	A	2052	G	C2-N3	-5.59	1.28	1.32
1	A	750	A	C6-N1	-5.59	1.31	1.35
1	A	1257	C	N1-C6	-5.58	1.33	1.37
1	A	684	G	N1-C2	-5.58	1.33	1.37
1	A	211	A	C5-C4	-5.58	1.34	1.38
1	A	815	C	N1-C6	-5.58	1.33	1.37
1	A	458	G	N3-C4	-5.57	1.31	1.35
1	A	574	C	N3-C4	-5.57	1.30	1.33
1	A	125	G	P-O5'	-5.56	1.54	1.59
1	A	265	A	N7-C5	-5.56	1.35	1.39
1	A	678	C	C5-C6	-5.56	1.29	1.34
1	A	2497	A	N3-C4	-5.56	1.31	1.34
1	A	2020	A	C5-C6	-5.55	1.36	1.41
1	A	2432	A	C5-C4	-5.55	1.34	1.38
1	A	1972	A	C5-C4	-5.55	1.34	1.38
1	A	1195	G	C6-N1	-5.55	1.35	1.39
1	A	2447	G	N7-C5	-5.55	1.35	1.39
1	A	1132	A	C6-N1	-5.55	1.31	1.35
1	A	2333	A	N9-C4	-5.54	1.34	1.37
1	A	2515	C	C4-N4	-5.54	1.28	1.33
1	A	989	G	N9-C8	-5.53	1.33	1.37
1	A	478	A	C6-N1	-5.53	1.31	1.35
1	A	1022	G	N1-C2	-5.53	1.33	1.37
1	A	2505	G	N1-C2	-5.53	1.33	1.37
1	A	1786	A	C6-N1	-5.53	1.31	1.35
1	A	1798	U	C2-N3	-5.52	1.33	1.37
1	A	55	G	C5-C4	-5.52	1.34	1.38
1	A	2344	U	N3-C4	-5.52	1.33	1.38
1	A	413	C	N1-C6	-5.52	1.33	1.37
1	A	451	C	N1-C6	-5.52	1.33	1.37
1	A	967	C	C2-N3	-5.52	1.31	1.35
1	A	771	G	N1-C2	-5.51	1.33	1.37
1	A	2060	A	N9-C8	-5.51	1.33	1.37
1	A	2267	A	N3-C4	-5.51	1.31	1.34
1	A	469	G	C5-C4	-5.51	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2578	G	P-OP1	-5.51	1.39	1.49
1	A	678	C	N3-C4	-5.50	1.30	1.33
1	A	1154	G	C5-C4	-5.50	1.34	1.38
1	A	579	G	C8-N7	-5.50	1.27	1.30
1	A	837	C	C4-C5	-5.50	1.38	1.43
1	A	1217	C	N1-C6	-5.50	1.33	1.37
1	A	128	C	C2-N3	-5.50	1.31	1.35
1	A	1127	A	N3-C4	-5.50	1.31	1.34
1	A	2335	A	C6-N1	-5.49	1.31	1.35
1	A	20	C	N3-C4	-5.49	1.30	1.33
1	A	192	C	N1-C6	-5.49	1.33	1.37
1	A	763	G	N3-C4	-5.48	1.31	1.35
1	A	1131	G	N3-C4	-5.48	1.31	1.35
1	A	567	A	N9-C4	-5.48	1.34	1.37
1	A	2716	U	C2-N3	-5.48	1.33	1.37
1	A	673	C	N1-C6	-5.48	1.33	1.37
1	A	2000	G	C5-C4	-5.47	1.34	1.38
1	A	195	A	N7-C5	-5.47	1.35	1.39
1	A	1129	A	C6-N1	-5.47	1.31	1.35
1	A	1779	U	C2-N3	-5.47	1.33	1.37
1	A	2490	G	C5-C4	-5.47	1.34	1.38
1	A	2778	A	P-O5'	-5.47	1.54	1.59
1	A	835	A	C5-C4	-5.47	1.34	1.38
1	A	2722	G	C6-N1	-5.47	1.35	1.39
1	A	2271	G	C6-N1	-5.46	1.35	1.39
1	A	818	G	P-O5'	-5.46	1.54	1.59
1	A	2066	C	N1-C6	-5.46	1.33	1.37
1	A	1027	A	N7-C5	-5.46	1.35	1.39
1	A	2000	G	N1-C2	-5.46	1.33	1.37
1	A	2697	G	N7-C5	-5.45	1.35	1.39
1	A	2057	A	N9-C8	-5.45	1.33	1.37
1	A	394	A	N9-C4	-5.44	1.34	1.37
1	A	1132	A	N7-C5	-5.44	1.35	1.39
1	A	1982	C	N3-C4	-5.44	1.30	1.33
1	A	2072	G	C2-N3	-5.44	1.28	1.32
1	A	2051	A	N7-C5	-5.44	1.35	1.39
1	A	2497	A	N9-C4	-5.43	1.34	1.37
1	A	2823	A	N7-C5	-5.43	1.35	1.39
1	A	777	A	N3-C4	-5.43	1.31	1.34
1	A	570	G	N1-C2	-5.42	1.33	1.37
1	A	1312	U	N3-C4	-5.42	1.33	1.38
1	A	2564	A	C5-C4	-5.42	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	561	G	N1-C2	-5.42	1.33	1.37
1	A	972	G	C2-N3	-5.42	1.28	1.32
1	A	2820	A	P-OP2	-5.42	1.39	1.49
1	A	793	A	P-OP2	-5.42	1.39	1.49
1	A	1126	A	N3-C4	-5.41	1.31	1.34
1	A	964	C	N1-C6	-5.41	1.33	1.37
1	A	472	A	N3-C4	-5.41	1.31	1.34
1	A	2451	A	C6-N1	-5.41	1.31	1.35
1	A	2621	A	N9-C4	-5.40	1.34	1.37
1	A	1275	A	C6-N1	-5.40	1.31	1.35
1	A	2822	G	O3'-P	-5.40	1.54	1.61
1	A	807	U	C2-N3	5.40	1.41	1.37
1	A	207	A	N7-C5	-5.39	1.36	1.39
1	A	1328	G	C6-O6	-5.39	1.19	1.24
1	A	1367	A	N3-C4	-5.39	1.31	1.34
1	A	1608	A	C5-C4	-5.39	1.34	1.38
10	O	21	CYS	CB-SG	-5.39	1.73	1.81
1	A	2032	G	N3-C4	-5.39	1.31	1.35
1	A	1213	A	N3-C4	-5.38	1.31	1.34
1	A	2692	C	N3-C4	-5.38	1.30	1.33
1	A	530	G	C6-O6	-5.38	1.19	1.24
1	A	799	G	C2-N3	-5.38	1.28	1.32
1	A	1568	G	C6-N1	-5.38	1.35	1.39
1	A	706	A	N3-C4	-5.37	1.31	1.34
1	A	836	G	C6-N1	-5.37	1.35	1.39
1	A	1303	G	C6-N1	-5.37	1.35	1.39
1	A	1754	C	N1-C6	-5.37	1.33	1.37
1	A	2249	U	C2-N3	-5.37	1.33	1.37
1	A	27	G	P-OP1	-5.37	1.39	1.49
1	A	454	A	N3-C4	-5.37	1.31	1.34
1	A	2764	A	N9-C4	-5.37	1.34	1.37
1	A	2589	A	N9-C4	-5.36	1.34	1.37
1	A	791	C	N1-C6	-5.36	1.33	1.37
1	A	2619	C	N1-C6	-5.36	1.33	1.37
1	A	980	A	C5-C4	-5.36	1.34	1.38
1	A	2041	U	C2-N3	-5.36	1.33	1.37
1	A	2233	U	C2-O2	-5.36	1.17	1.22
1	A	2830	G	N1-C2	-5.35	1.33	1.37
1	A	2454	G	N1-C2	-5.35	1.33	1.37
1	A	87	C	N3-C4	-5.34	1.30	1.33
1	A	20	C	C4-C5	-5.34	1.38	1.43
1	A	801	G	N9-C4	-5.33	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	800	A	P-OP1	-5.33	1.39	1.49
1	A	1384	A	N7-C5	-5.33	1.36	1.39
1	A	583	G	C5-C6	-5.33	1.37	1.42
1	A	1190	G	C5-C4	-5.33	1.34	1.38
1	A	776	G	P-O5'	-5.32	1.54	1.59
1	A	2548	G	C5-C4	-5.32	1.34	1.38
1	A	1154	G	N3-C4	-5.32	1.31	1.35
1	A	2024	G	N9-C8	-5.32	1.34	1.37
1	A	2504	U	P-OP2	-5.32	1.40	1.49
1	A	310	A	N9-C4	-5.32	1.34	1.37
1	A	502	A	C6-N1	-5.32	1.31	1.35
1	A	2678	C	N1-C6	-5.32	1.33	1.37
3	D	28	GLU	CG-CD	5.32	1.59	1.51
1	A	131	G	N3-C4	-5.31	1.31	1.35
1	A	1617	C	N1-C6	-5.31	1.33	1.37
1	A	202	U	C4-C5	-5.30	1.38	1.43
1	A	1214	A	C6-N1	-5.30	1.31	1.35
1	A	2346	A	N9-C8	-5.30	1.33	1.37
1	A	570	G	C5-C6	-5.30	1.37	1.42
1	A	2029	G	N9-C8	-5.29	1.34	1.37
1	A	196	A	N9-C8	-5.29	1.33	1.37
1	A	2051	A	C5-C4	-5.29	1.35	1.38
1	A	2359	C	C2-O2	-5.29	1.19	1.24
1	A	118	A	C5-C4	-5.28	1.35	1.38
1	A	2044	C	P-OP1	-5.28	1.40	1.49
1	A	2822	G	N9-C4	-5.28	1.33	1.38
1	A	1367	A	N9-C8	-5.28	1.33	1.37
1	A	2577	A	N3-C4	-5.28	1.31	1.34
1	A	828	U	C2-N3	-5.27	1.34	1.37
1	A	520	G	N1-C2	-5.27	1.33	1.37
1	A	2542	A	N7-C5	-5.27	1.36	1.39
1	A	462	C	C4-C5	-5.27	1.38	1.43
1	A	748	G	C6-N1	-5.26	1.35	1.39
1	A	744	G	N3-C4	-5.26	1.31	1.35
1	A	769	G	N9-C8	-5.26	1.34	1.37
1	A	107	C	C4-C5	-5.26	1.38	1.43
1	A	2018	G	C6-N1	-5.26	1.35	1.39
28	6	16	CYS	CB-SG	-5.26	1.73	1.81
1	A	770	G	C6-N1	-5.26	1.35	1.39
1	A	2456	C	C4-C5	-5.26	1.38	1.43
1	A	1809	A	C6-N1	-5.25	1.31	1.35
1	A	2372	G	C6-N1	5.25	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	967	C	N1-C6	-5.25	1.33	1.37
1	A	1653	G	C3'-O3'	5.24	1.49	1.42
1	A	2568	C	N1-C6	-5.24	1.34	1.37
1	A	1344	G	C2-N3	-5.24	1.28	1.32
1	A	1367	A	C5-C4	-5.24	1.35	1.38
1	A	2014	A	N9-C8	-5.24	1.33	1.37
1	A	954	G	N1-C2	-5.24	1.33	1.37
1	A	1003	G	N3-C4	-5.24	1.31	1.35
1	A	1614	A	P-OP1	-5.24	1.40	1.49
1	A	2243	U	N1-C2	-5.24	1.33	1.38
1	A	2617	C	C4-C5	-5.23	1.38	1.43
1	A	2488	A	C5-C4	-5.23	1.35	1.38
1	A	574	C	C2-N3	-5.23	1.31	1.35
1	A	837	C	N3-C4	-5.23	1.30	1.33
1	A	1006	C	N3-C4	-5.23	1.30	1.33
1	A	51	G	C6-N1	-5.22	1.35	1.39
1	A	1674	G	N7-C5	-5.22	1.36	1.39
1	A	817	C	C4-N4	-5.22	1.29	1.33
1	A	1638	C	N3-C4	-5.22	1.30	1.33
1	A	211	A	N9-C4	-5.22	1.34	1.37
1	A	502	A	N3-C4	-5.21	1.31	1.34
1	A	2520	C	N1-C6	-5.21	1.34	1.37
1	A	807	U	P-O5'	-5.21	1.54	1.59
1	A	2541	A	N7-C5	-5.21	1.36	1.39
1	A	2296	U	C5-C6	5.21	1.38	1.34
1	A	2452	C	C4-C5	-5.21	1.38	1.43
1	A	2322	A	N9-C4	5.20	1.41	1.37
1	A	2488	A	N7-C5	-5.20	1.36	1.39
1	A	88	G	N7-C5	-5.20	1.36	1.39
1	A	1303	G	C5-C4	-5.20	1.34	1.38
1	A	2081	C	N1-C6	-5.20	1.34	1.37
1	A	1269	A	C6-N1	-5.20	1.31	1.35
1	A	1290	C	C2-O2	-5.20	1.19	1.24
1	A	836	G	N1-C2	-5.19	1.33	1.37
1	A	1154	G	C8-N7	-5.19	1.27	1.30
1	A	1210	A	N3-C4	-5.19	1.31	1.34
1	A	1642	G	C6-N1	-5.19	1.35	1.39
1	A	763	G	C6-N1	-5.19	1.35	1.39
1	A	2020	A	C6-N1	-5.19	1.31	1.35
1	A	1125	G	N9-C4	-5.18	1.33	1.38
1	A	1627	G	N1-C2	-5.18	1.33	1.37
1	A	2732	G	C6-N1	-5.18	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	191	A	N9-C8	-5.18	1.33	1.37
1	A	446	G	C2-N3	-5.18	1.28	1.32
1	A	469	G	P-O5'	-5.18	1.54	1.59
1	A	1672	C	N1-C6	-5.18	1.34	1.37
1	A	2056	G	P-O5'	-5.18	1.54	1.59
1	A	511	U	N3-C4	-5.17	1.33	1.38
1	A	957	A	N9-C4	-5.17	1.34	1.37
1	A	2073	C	N1-C6	-5.17	1.34	1.37
1	A	2600	A	C5-C6	-5.17	1.36	1.41
1	A	194	G	C6-N1	-5.17	1.35	1.39
1	A	198	C	P-OP1	-5.17	1.40	1.49
1	A	2548	G	N7-C5	-5.17	1.36	1.39
1	A	516	C	C2-O2	-5.16	1.19	1.24
1	A	1190	G	N9-C8	-5.16	1.34	1.37
1	A	535	C	N3-C4	-5.16	1.30	1.33
1	A	2051	A	N3-C4	-5.16	1.31	1.34
1	A	107	C	N1-C6	-5.16	1.34	1.37
1	A	976	C	N3-C4	-5.16	1.30	1.33
1	A	2046	G	N7-C5	-5.16	1.36	1.39
1	A	2490	G	N1-C2	-5.16	1.33	1.37
1	A	2508	G	N1-C2	-5.15	1.33	1.37
1	A	1782	C	N1-C6	-5.15	1.34	1.37
1	A	446	G	N9-C8	-5.15	1.34	1.37
1	A	480	A	N7-C5	-5.15	1.36	1.39
1	A	2229	C	N1-C6	-5.15	1.34	1.37
1	A	312	G	P-O5'	-5.14	1.54	1.59
1	A	2822	G	N7-C5	-5.14	1.36	1.39
1	A	983	A	N9-C4	-5.14	1.34	1.37
1	A	1778	U	N3-C4	-5.14	1.33	1.38
1	A	802	A	N7-C5	-5.13	1.36	1.39
1	A	2054	A	O3'-P	-5.13	1.54	1.61
1	A	2081	C	N3-C4	-5.13	1.30	1.33
1	A	2403	C	N1-C6	-5.13	1.34	1.37
1	A	2497	A	C6-N1	-5.13	1.31	1.35
1	A	495	G	N9-C8	-5.13	1.34	1.37
1	A	1132	A	C5-C6	-5.13	1.36	1.41
1	A	2730	C	C4-C5	-5.13	1.38	1.43
1	A	1671	U	C2-N3	-5.13	1.34	1.37
1	A	2570	G	N3-C4	-5.13	1.31	1.35
1	A	683	C	C4-C5	-5.12	1.38	1.43
1	A	2333	A	N9-C8	-5.12	1.33	1.37
1	A	805	G	N7-C5	-5.12	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	474	G	N7-C5	-5.12	1.36	1.39
1	A	580	C	N1-C6	-5.12	1.34	1.37
1	A	698	C	N1-C6	-5.12	1.34	1.37
1	A	2271	G	N7-C5	-5.12	1.36	1.39
1	A	748	G	C5-C4	-5.12	1.34	1.38
1	A	933	A	C5-C4	5.12	1.42	1.38
1	A	1269	A	C5-C4	-5.12	1.35	1.38
1	A	2621	A	C6-N6	-5.12	1.29	1.33
1	A	520	G	C6-N1	-5.11	1.35	1.39
1	A	1675	C	N3-C4	-5.11	1.30	1.33
1	A	1284	A	N3-C4	5.11	1.38	1.34
1	A	1365	A	C5-C6	-5.11	1.36	1.41
1	A	1122	G	N9-C8	-5.11	1.34	1.37
1	A	1128	A	C5-C6	-5.11	1.36	1.41
1	A	1826	G	C6-N1	-5.11	1.35	1.39
1	A	2252	G	C5-C6	-5.10	1.37	1.42
1	A	2360	A	N3-C4	-5.10	1.31	1.34
1	A	1556	C	N3-C4	-5.10	1.30	1.33
1	A	2244	U	C2-O2	-5.10	1.17	1.22
1	A	31	C	P-OP1	-5.10	1.40	1.49
1	A	1332	G	N7-C5	-5.10	1.36	1.39
1	A	2594	C	N1-C6	-5.10	1.34	1.37
1	A	822	U	P-O5'	-5.10	1.54	1.59
1	A	684	G	C6-N1	-5.09	1.35	1.39
1	A	1297	C	N3-C4	-5.09	1.30	1.33
1	A	567	A	N3-C4	-5.09	1.31	1.34
1	A	569	U	N1-C2	-5.09	1.33	1.38
1	A	1754	C	N3-C4	-5.09	1.30	1.33
1	A	2235	G	C8-N7	-5.09	1.27	1.30
1	A	2572	A	N9-C4	-5.09	1.34	1.37
1	A	1647	G	C2-N3	-5.09	1.28	1.32
1	A	1393	A	C6-N1	-5.08	1.31	1.35
1	A	2007	C	P-O5'	-5.08	1.54	1.59
1	A	952	G	N1-C2	-5.08	1.33	1.37
1	A	2570	G	N9-C8	-5.08	1.34	1.37
1	A	1620	G	C6-N1	-5.08	1.35	1.39
1	A	2691	C	N1-C6	-5.08	1.34	1.37
1	A	377	C	N1-C6	-5.07	1.34	1.37
1	A	573	G	N7-C5	-5.07	1.36	1.39
1	A	755	C	N1-C6	-5.07	1.34	1.37
1	A	189	G	C5-C4	-5.07	1.34	1.38
1	A	450	G	N9-C8	-5.07	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1778	U	O3'-P	-5.07	1.55	1.61
1	A	2030	A	N9-C8	-5.07	1.33	1.37
5	F	89	VAL	C-O	-5.07	1.13	1.23
1	A	2327	A	C5-C4	-5.07	1.35	1.38
1	A	751	A	P-OP1	-5.06	1.40	1.49
1	A	1324	G	N9-C8	-5.06	1.34	1.37
1	A	2013	A	N9-C4	-5.06	1.34	1.37
1	A	700	G	C5-C4	-5.06	1.34	1.38
1	A	2588	G	C6-N1	-5.05	1.36	1.39
1	A	1376	C	N1-C6	-5.05	1.34	1.37
1	A	1953	A	N7-C5	-5.05	1.36	1.39
1	A	2424	C	N3-C4	-5.05	1.30	1.33
1	A	2819	G	C6-N1	-5.05	1.36	1.39
1	A	1570	A	N3-C4	-5.05	1.31	1.34
1	A	32	C	N3-C4	-5.05	1.30	1.33
1	A	1659	U	N1-C2	-5.05	1.34	1.38
1	A	2621	A	C6-N1	-5.05	1.32	1.35
1	A	663	G	C5-C4	-5.04	1.34	1.38
1	A	532	A	N9-C4	-5.04	1.34	1.37
1	A	971	C	C2-O2	-5.04	1.20	1.24
1	A	1334	G	C6-N1	-5.04	1.36	1.39
1	A	1677	A	N9-C4	-5.04	1.34	1.37
1	A	1797	C	N1-C6	-5.04	1.34	1.37
1	A	2248	C	N1-C6	-5.04	1.34	1.37
3	D	28	GLU	CB-CG	5.04	1.61	1.52
1	A	215	G	N1-C2	-5.04	1.33	1.37
1	A	254	G	N7-C5	-5.04	1.36	1.39
1	A	943	U	C2-O2	-5.03	1.17	1.22
1	A	1029	A	C5-C6	-5.03	1.36	1.41
1	A	1904	G	N7-C5	-5.03	1.36	1.39
1	A	684	G	P-O5'	-5.03	1.54	1.59
1	A	1197	G	C6-N1	-5.03	1.36	1.39
1	A	2428	G	N1-C2	-5.03	1.33	1.37
1	A	2505	G	C6-N1	-5.03	1.36	1.39
1	A	131	G	C6-N1	-5.02	1.36	1.39
1	A	476	G	C2-N3	-5.02	1.28	1.32
1	A	2553	G	N7-C5	-5.02	1.36	1.39
1	A	465	G	O3'-P	-5.02	1.55	1.61
1	A	1274	A	N3-C4	-5.02	1.31	1.34
1	A	2692	C	N1-C6	-5.02	1.34	1.37
1	A	2335	A	C5-C4	-5.01	1.35	1.38
1	A	2360	A	N9-C4	-5.01	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2441	C	N1-C6	-5.01	1.34	1.37
1	A	2446	G	N9-C8	-5.01	1.34	1.37
1	A	517	C	P-O5'	-5.00	1.54	1.59

All (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
1	A	1142(A)	A	C2-N3-C4	-17.48	101.86	110.60
1	A	2104	G	N3-C2-N2	17.45	132.12	119.90
1	A	141	A	C5-N7-C8	-16.96	95.42	103.90
1	A	528	A	C2-N3-C4	-16.90	102.15	110.60
1	A	2296	U	N3-C4-O4	-16.80	107.64	119.40
1	A	528	A	N3-C4-C5	16.40	138.28	126.80
1	A	141	A	N7-C8-N9	16.09	121.84	113.80
1	A	2296	U	C2-N1-C1'	-15.91	98.60	117.70
1	A	528	A	N3-C4-N9	-15.85	114.72	127.40
1	A	2296	U	C5-C4-O4	15.77	135.36	125.90
1	A	2322	A	C6-N1-C2	-15.01	109.60	118.60
1	A	2335	A	C5-C6-N1	14.94	125.17	117.70
1	A	2185	C	N1-C2-O2	14.54	127.62	118.90
1	A	330	A	C2-N3-C4	-14.43	103.39	110.60
1	A	1779	U	C4-C5-C6	14.21	128.22	119.70
1	A	130	C	C6-N1-C2	14.18	125.97	120.30
1	A	530	G	N3-C4-N9	-13.88	117.67	126.00
1	A	1698	A	C2-N3-C4	-13.86	103.67	110.60
1	A	2296	U	N3-C2-O2	-13.71	112.61	122.20
1	A	933	A	C5-N7-C8	-13.63	97.08	103.90
1	A	2104	G	C5-C6-O6	13.54	136.73	128.60
1	A	2296	U	C6-N1-C1'	13.53	140.14	121.20
1	A	530	G	C8-N9-C4	-13.32	101.07	106.40
1	A	2104	G	N1-C2-N2	-13.30	104.23	116.20
2	B	120	A	C5-C6-N1	-13.28	111.06	117.70
1	A	2322	A	N1-C6-N6	-13.27	110.64	118.60
1	A	933	A	N7-C8-N9	13.12	120.36	113.80
1	A	1332	G	C5-C6-N1	13.11	118.06	111.50
1	A	221	A	C8-N9-C4	-13.05	100.58	105.80
1	A	2104	G	N1-C6-O6	-12.89	112.16	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2515	C	N3-C4-C5	12.68	126.97	121.90
1	A	530	G	N1-C2-N2	12.65	127.58	116.20
1	A	1107	G	C4-N9-C1'	12.62	142.90	126.50
1	A	1359	A	N1-C6-N6	-12.54	111.07	118.60
1	A	2296	U	C4-C5-C6	12.53	127.22	119.70
1	A	1779	U	N1-C2-N3	12.48	122.39	114.90
2	B	5	C	C6-N1-C2	12.44	125.28	120.30
1	A	141	A	N1-C6-N6	12.39	126.03	118.60
1	A	139(A)	G	C4-C5-N7	12.37	115.75	110.80
1	A	139(A)	G	C5-N7-C8	-12.36	98.12	104.30
1	A	2346	A	N9-C4-C5	12.33	110.73	105.80
1	A	1142(A)	A	C5-C6-N1	-12.31	111.54	117.70
1	A	1107	G	C6-C5-N7	-12.29	123.03	130.40
1	A	856	C	C6-N1-C2	-12.25	115.40	120.30
1	A	1210	A	C5-N7-C8	-12.24	97.78	103.90
1	A	141	A	C4-C5-N7	12.20	116.80	110.70
1	A	2322	A	C5-C6-N1	12.18	123.79	117.70
1	A	2286	A	N1-C6-N6	12.17	125.90	118.60
2	B	120	A	C6-N1-C2	12.11	125.86	118.60
1	A	1107	G	C8-N9-C1'	-12.04	111.34	127.00
1	A	2286	A	C6-C5-N7	-11.97	123.92	132.30
1	A	1107	G	N1-C6-O6	11.87	127.02	119.90
1	A	139(A)	G	N7-C8-N9	11.79	119.00	113.10
1	A	1204	A	C6-C5-N7	-11.63	124.16	132.30
1	A	1142(A)	A	N3-C4-N9	-11.58	118.14	127.40
1	A	1204	A	C2-N3-C4	-11.58	104.81	110.60
1	A	794	G	N1-C6-O6	-11.47	113.02	119.90
1	A	409	C	C6-N1-C2	11.34	124.84	120.30
1	A	473	G	N1-C6-O6	-11.33	113.10	119.90
1	A	141	A	C6-C5-N7	-11.27	124.41	132.30
1	A	959	A	C8-N9-C4	-11.26	101.30	105.80
1	A	1108	U	N3-C2-O2	-11.21	114.36	122.20
1	A	1107	G	C5-C6-O6	-11.16	121.91	128.60
1	A	528	A	C6-N1-C2	11.12	125.27	118.60
1	A	2322	A	N9-C4-C5	11.08	110.23	105.80
1	A	2823	A	N1-C6-N6	11.05	125.23	118.60
1	A	1328	G	C5-C6-N1	11.00	117.00	111.50
2	B	120	A	N1-C2-N3	-10.98	123.81	129.30
1	A	1204	A	C4-C5-N7	10.97	116.18	110.70
1	A	265	A	N1-C6-N6	10.86	125.12	118.60
1	A	1204	A	C5-N7-C8	-10.86	98.47	103.90
1	A	141	A	C8-N9-C4	-10.84	101.46	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1210	A	N7-C8-N9	10.84	119.22	113.80
1	A	1762	A	C8-N9-C4	-10.84	101.47	105.80
1	A	106	C	C6-N1-C2	-10.83	115.97	120.30
1	A	1107	G	C4-C5-N7	10.74	115.09	110.80
2	B	6	C	C6-N1-C2	10.71	124.58	120.30
1	A	1779	U	C2-N3-C4	-10.70	120.58	127.00
1	A	2689	U	C5-C4-O4	10.57	132.24	125.90
1	A	2035	G	C8-N9-C4	-10.54	102.19	106.40
1	A	208	C	C6-N1-C2	10.46	124.48	120.30
1	A	1142(A)	A	N3-C4-C5	10.40	134.08	126.80
1	A	234	C	C6-N1-C2	-10.39	116.14	120.30
1	A	2497	A	C6-N1-C2	-10.39	112.37	118.60
1	A	1210	A	N1-C6-N6	10.34	124.80	118.60
1	A	1210	A	C6-C5-N7	-10.33	125.07	132.30
1	A	2002	G	C8-N9-C4	-10.30	102.28	106.40
1	A	141	A	C2-N3-C4	-10.26	105.47	110.60
1	A	446	G	N1-C6-O6	10.25	126.05	119.90
1	A	933	A	C8-N9-C4	-10.19	101.72	105.80
1	A	1779	U	C2-N1-C1'	-10.15	105.52	117.70
1	A	265	A	C2-N3-C4	-10.10	105.55	110.60
1	A	2286	A	C5-N7-C8	-10.10	98.85	103.90
1	A	1192	G	N7-C8-N9	-10.08	108.06	113.10
1	A	2499	C	N1-C2-O2	-10.04	112.88	118.90
1	A	1129	A	C8-N9-C4	-10.01	101.80	105.80
1	A	1779	U	C5-C4-O4	10.00	131.90	125.90
1	A	690	G	C5-C6-N1	9.95	116.47	111.50
1	A	645	C	N1-C2-O2	9.94	124.86	118.90
1	A	839	U	C5-C4-O4	9.92	131.85	125.90
1	A	675	A	C8-N9-C4	9.91	109.76	105.80
1	A	2346	A	C8-N9-C4	-9.90	101.84	105.80
1	A	1192	G	C8-N9-C4	9.88	110.35	106.40
1	A	463	G	C5-C6-O6	9.86	134.52	128.60
1	A	2062	A	N1-C6-N6	9.86	124.52	118.60
1	A	530	G	N9-C4-C5	9.85	109.34	105.40
1	A	729	G	C8-N9-C4	-9.83	102.47	106.40
1	A	1142(A)	A	C5-N7-C8	-9.82	98.99	103.90
1	A	2185	C	C2-N3-C4	9.81	124.81	119.90
1	A	1107	G	N3-C4-N9	9.77	131.86	126.00
1	A	27	G	N3-C2-N2	-9.77	113.06	119.90
1	A	531	C	N1-C2-O2	-9.75	113.05	118.90
1	A	566	U	C4-C5-C6	-9.75	113.85	119.70
1	A	2286	A	N7-C8-N9	9.75	118.67	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	624	C	N3-C4-C5	9.60	125.74	121.90
1	A	205	G	N3-C2-N2	9.60	126.62	119.90
1	A	528	A	C5-C6-N1	-9.60	112.90	117.70
1	A	2103	C	C2-N3-C4	9.59	124.69	119.90
1	A	1620	G	N1-C6-O6	-9.58	114.15	119.90
1	A	130	C	N3-C4-C5	9.57	125.73	121.90
2	B	101	G	N9-C4-C5	-9.56	101.57	105.40
1	A	2689	U	N3-C4-O4	-9.55	112.72	119.40
1	A	1332	G	C6-N1-C2	-9.54	119.38	125.10
1	A	1204	A	N1-C6-N6	9.52	124.31	118.60
1	A	1022	G	N9-C4-C5	9.51	109.20	105.40
1	A	2082	A	C6-N1-C2	-9.49	112.91	118.60
1	A	1558	A	C2-N3-C4	-9.48	105.86	110.60
1	A	528	A	C4-C5-C6	-9.46	112.27	117.00
1	A	774	A	C8-N9-C4	-9.43	102.03	105.80
1	A	391	G	C5-C6-O6	-9.41	122.95	128.60
1	A	2363	C	C6-N1-C2	9.41	124.06	120.30
1	A	652(T)	C	C2-N3-C4	9.40	124.60	119.90
1	A	2361	A	C8-N9-C4	9.37	109.55	105.80
1	A	458	G	C8-N9-C4	-9.35	102.66	106.40
1	A	2322	A	C4-C5-N7	-9.33	106.03	110.70
1	A	2689	U	N1-C2-N3	9.32	120.49	114.90
1	A	1107	G	N9-C4-C5	-9.31	101.67	105.40
1	A	265	A	C6-C5-N7	-9.28	125.80	132.30
1	A	528	A	C5-N7-C8	-9.28	99.26	103.90
1	A	209	C	N3-C4-C5	9.27	125.61	121.90
1	A	2236	C	N3-C4-C5	-9.25	118.20	121.90
1	A	2499	C	C2-N3-C4	-9.23	115.28	119.90
1	A	2244	U	C5-C4-O4	9.23	131.44	125.90
1	A	27	G	N9-C4-C5	9.23	109.09	105.40
1	A	932	G	C5-C6-O6	-9.22	123.07	128.60
1	A	265	A	C5-N7-C8	-9.21	99.30	103.90
1	A	781	A	C8-N9-C4	9.20	109.48	105.80
1	A	1607	C	N3-C4-N4	9.20	124.44	118.00
1	A	2037	G	C5-N7-C8	9.17	108.89	104.30
1	A	1192	G	C5-N7-C8	9.16	108.88	104.30
1	A	473	G	C5-C6-O6	9.15	134.09	128.60
1	A	2335	A	C5-C6-N6	-9.14	116.39	123.70
1	A	2271	G	N3-C4-C5	-9.12	124.04	128.60
1	A	1792	G	N1-C6-O6	-9.07	114.46	119.90
1	A	265	A	C4-C5-N7	9.04	115.22	110.70
1	A	1204	A	N1-C2-N3	9.04	133.82	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2690	C	N3-C4-C5	-9.03	118.29	121.90
1	A	2244	U	N3-C4-O4	-9.03	113.08	119.40
2	B	101	G	C8-N9-C4	9.01	110.00	106.40
1	A	1779	U	N1-C2-O2	-9.00	116.50	122.80
1	A	1022	G	N3-C4-N9	-8.99	120.61	126.00
1	A	377	C	C6-N1-C2	8.98	123.89	120.30
1	A	940	G	C8-N9-C4	-8.98	102.81	106.40
1	A	1616	A	C5-N7-C8	-8.97	99.42	103.90
1	A	566	U	N3-C4-C5	8.95	119.97	114.60
1	A	2107	C	C5-C4-N4	8.93	126.45	120.20
1	A	2182	G	C5-C6-O6	8.93	133.96	128.60
1	A	2252	G	N7-C8-N9	-8.92	108.64	113.10
2	B	104	U	C5-C6-N1	-8.92	118.24	122.70
1	A	1142(A)	A	N1-C2-N3	8.91	133.75	129.30
1	A	584	C	N1-C2-O2	-8.91	113.56	118.90
1	A	130	C	N1-C2-O2	8.90	124.24	118.90
1	A	2286	A	C4-C5-N7	8.89	115.15	110.70
1	A	394	A	C8-N9-C4	8.88	109.35	105.80
1	A	1698	A	N1-C2-N3	8.85	133.72	129.30
1	A	139(A)	G	C8-N9-C4	-8.84	102.86	106.40
1	A	1827	C	N3-C2-O2	-8.84	115.71	121.90
1	A	2286	A	C2-N3-C4	-8.83	106.18	110.60
1	A	2286	A	C8-N9-C4	-8.83	102.27	105.80
1	A	794	G	C5-C6-O6	8.82	133.89	128.60
1	A	391	G	N1-C6-O6	8.82	125.19	119.90
1	A	2191	G	C5-C6-O6	-8.81	123.31	128.60
1	A	1755	A	N1-C6-N6	-8.80	113.32	118.60
1	A	1899	G	N3-C2-N2	-8.80	113.74	119.90
1	A	121	G	C5-C6-O6	-8.79	123.33	128.60
1	A	1972	A	C2-N3-C4	8.78	114.99	110.60
1	A	530	G	N3-C4-C5	8.78	132.99	128.60
1	A	1253	A	C5-N7-C8	8.77	108.28	103.90
1	A	478	A	N1-C2-N3	8.77	133.68	129.30
1	A	2007	C	C6-N1-C2	-8.76	116.80	120.30
1	A	375	C	C6-N1-C2	8.76	123.80	120.30
1	A	959	A	N7-C8-N9	8.75	118.17	113.80
1	A	2449	U	C5-C4-O4	-8.74	120.66	125.90
1	A	527	C	C5-C4-N4	8.74	126.32	120.20
1	A	836	G	N1-C6-O6	-8.74	114.66	119.90
1	A	1708	C	C6-N1-C2	8.73	123.79	120.30
1	A	2361	A	N9-C4-C5	-8.73	102.31	105.80
1	A	2694	G	C5-C6-O6	-8.72	123.37	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	777	A	N1-C6-N6	-8.71	113.37	118.60
1	A	1108	U	N1-C2-O2	8.70	128.89	122.80
1	A	458	G	N9-C4-C5	8.67	108.87	105.40
1	A	1049	C	C6-N1-C2	-8.66	116.83	120.30
1	A	73	A	N9-C4-C5	8.66	109.26	105.80
1	A	1049	C	C5-C6-N1	8.65	125.33	121.00
1	A	2568	C	C6-N1-C2	8.64	123.76	120.30
1	A	1799	G	N3-C4-C5	-8.64	124.28	128.60
1	A	1563	G	N9-C4-C5	-8.63	101.95	105.40
1	A	1334	G	C8-N9-C4	-8.62	102.95	106.40
1	A	1210	A	C4-C5-N7	8.62	115.01	110.70
1	A	2473	U	C2-N1-C1'	8.61	128.03	117.70
1	A	966	G	N1-C6-O6	-8.60	114.74	119.90
1	A	763	G	N9-C4-C5	8.59	108.84	105.40
1	A	272(C)	G	C8-N9-C4	8.58	109.83	106.40
1	A	530	G	C8-N9-C1'	8.58	138.15	127.00
1	A	1393	A	N9-C4-C5	8.58	109.23	105.80
1	A	675	A	N9-C4-C5	-8.56	102.38	105.80
1	A	1108	U	C2-N1-C1'	8.55	127.96	117.70
1	A	2312	U	N3-C2-O2	-8.55	116.22	122.20
1	A	1190	G	C5-N7-C8	8.49	108.55	104.30
1	A	1383	C	N1-C2-O2	-8.47	113.82	118.90
1	A	1600	C	C5-C6-N1	-8.47	116.77	121.00
1	A	1620	G	C5-C6-O6	8.45	133.67	128.60
1	A	52	A	N7-C8-N9	8.45	118.03	113.80
2	B	58	A	C8-N9-C4	8.44	109.18	105.80
1	A	847	U	C5-C6-N1	-8.44	118.48	122.70
1	A	1445(A)	C	C6-N1-C2	-8.43	116.93	120.30
1	A	330	A	N1-C2-N3	8.43	133.51	129.30
1	A	1253	A	N7-C8-N9	-8.42	109.59	113.80
1	A	463	G	N1-C6-O6	-8.42	114.85	119.90
1	A	1210	A	C2-N3-C4	-8.42	106.39	110.60
1	A	2625	G	N3-C2-N2	-8.42	114.00	119.90
1	A	1127	A	C8-N9-C4	-8.42	102.43	105.80
1	A	374	A	C2-N3-C4	-8.39	106.41	110.60
1	A	1616	A	N7-C8-N9	8.37	117.98	113.80
1	A	465	G	C8-N9-C4	-8.36	103.06	106.40
1	A	1792	G	C5-C6-O6	8.35	133.61	128.60
1	A	2346	A	C4-C5-N7	-8.32	106.54	110.70
1	A	2067	G	C8-N9-C4	-8.31	103.07	106.40
1	A	2540	C	C6-N1-C2	8.31	123.62	120.30
1	A	148	C	C6-N1-C2	8.31	123.62	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2287	A	C2-N3-C4	-8.30	106.45	110.60
1	A	1393	A	N1-C6-N6	-8.29	113.63	118.60
1	A	530	G	C4-C5-C6	-8.29	113.83	118.80
1	A	2035	G	N9-C4-C5	8.28	108.71	105.40
1	A	1204	A	N7-C8-N9	8.27	117.94	113.80
1	A	777	A	N1-C2-N3	8.26	133.43	129.30
1	A	729	G	N3-C2-N2	-8.26	114.12	119.90
1	A	2182	G	C6-N1-C2	8.25	130.05	125.10
1	A	12	U	N3-C2-O2	-8.25	116.42	122.20
1	A	933	A	C4-C5-N7	8.23	114.82	110.70
1	A	1256	G	C8-N9-C4	8.22	109.69	106.40
1	A	1784	A	C8-N9-C4	8.22	109.09	105.80
1	A	2438	U	N3-C2-O2	-8.22	116.44	122.20
1	A	2503	A	N1-C6-N6	8.22	123.53	118.60
1	A	221	A	N7-C8-N9	8.20	117.90	113.80
1	A	584	C	C2-N3-C4	-8.20	115.80	119.90
1	A	978	G	C8-N9-C4	8.20	109.68	106.40
1	A	614	U	C5-C4-O4	8.20	130.82	125.90
1	A	2823	A	C4-C5-N7	8.19	114.80	110.70
1	A	766	C	N1-C2-O2	-8.19	113.99	118.90
1	A	2007	C	C5-C6-N1	8.19	125.09	121.00
1	A	1128	A	N1-C6-N6	8.18	123.51	118.60
1	A	1043	C	C6-N1-C2	-8.17	117.03	120.30
1	A	2515	C	C2-N3-C4	-8.16	115.82	119.90
1	A	27	G	N3-C4-N9	-8.15	121.11	126.00
1	A	2185	C	N3-C2-O2	-8.14	116.20	121.90
1	A	784	A	C5-C6-N6	8.13	130.21	123.70
1	A	2497	A	N1-C2-N3	8.13	133.37	129.30
1	A	425	G	N3-C4-C5	-8.13	124.53	128.60
1	A	488	G	C4-C5-N7	-8.12	107.55	110.80
1	A	1698	A	C5-N7-C8	-8.13	99.84	103.90
1	A	133	C	C6-N1-C2	8.12	123.55	120.30
1	A	51	G	N1-C6-O6	-8.09	115.05	119.90
1	A	73	A	N1-C6-N6	-8.09	113.75	118.60
1	A	2236	C	C6-N1-C2	-8.08	117.07	120.30
1	A	1415	U	C5-C4-O4	8.05	130.73	125.90
1	A	781	A	N7-C8-N9	-8.04	109.78	113.80
1	A	2346	A	C6-N1-C2	-8.04	113.77	118.60
1	A	31	C	C6-N1-C2	8.04	123.52	120.30
1	A	26	G	C8-N9-C4	-8.02	103.19	106.40
1	A	2441	C	N3-C4-N4	-8.02	112.38	118.00
2	B	28	C	C6-N1-C2	-8.02	117.09	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1368	G	C5-C6-N1	8.02	115.51	111.50
1	A	1256	G	N1-C2-N3	8.01	128.71	123.90
1	A	1800	C	C4-C5-C6	8.01	121.40	117.40
1	A	286	C	N1-C2-O2	8.00	123.70	118.90
1	A	570	G	C5-C6-N1	8.00	115.50	111.50
1	A	940	G	C2-N3-C4	8.00	115.90	111.90
18	W	11	ARG	NE-CZ-NH1	8.00	124.30	120.30
1	A	52	A	C8-N9-C4	-7.99	102.60	105.80
1	A	1028	A	C8-N9-C4	7.98	108.99	105.80
1	A	2575	C	C6-N1-C2	7.97	123.49	120.30
1	A	583	G	C5-C6-O6	-7.96	123.82	128.60
1	A	2059	A	N7-C8-N9	-7.96	109.82	113.80
1	A	139(A)	G	C5-C6-N1	7.95	115.48	111.50
1	A	1142(A)	A	N7-C8-N9	7.94	117.77	113.80
1	A	2826	A	N7-C8-N9	-7.94	109.83	113.80
1	A	468	G	C5-C6-O6	7.93	133.36	128.60
1	A	2682	U	N3-C2-O2	-7.92	116.66	122.20
1	A	491	G	N1-C6-O6	-7.92	115.15	119.90
1	A	982	C	C5-C6-N1	7.92	124.96	121.00
1	A	2574	G	C5-C6-N1	7.91	115.46	111.50
1	A	139(A)	G	C5-C6-O6	-7.90	123.86	128.60
1	A	2828	C	N1-C2-O2	-7.90	114.16	118.90
1	A	330	A	N3-C4-C5	7.88	132.32	126.80
1	A	2463	C	C6-N1-C2	7.88	123.45	120.30
1	A	2346	A	N1-C6-N6	-7.88	113.87	118.60
1	A	2107	C	C2-N3-C4	7.88	123.84	119.90
1	A	2723	C	N3-C2-O2	-7.87	116.39	121.90
1	A	2286	A	C4-C5-C6	7.87	120.93	117.00
2	B	99	G	C8-N9-C4	7.87	109.55	106.40
1	A	2499	C	N1-C2-N3	7.86	124.70	119.20
1	A	1047	G	N3-C4-C5	-7.86	124.67	128.60
23	1	21	ARG	NE-CZ-NH2	-7.85	116.37	120.30
2	B	75	G	C5-C6-O6	-7.85	123.89	128.60
1	A	2540	C	N3-C4-C5	7.84	125.04	121.90
1	A	234	C	N3-C2-O2	-7.84	116.41	121.90
1	A	1802	A	C5-C6-N6	-7.83	117.44	123.70
1	A	530	G	C5-N7-C8	-7.82	100.39	104.30
1	A	847	U	C5-C4-O4	7.82	130.59	125.90
1	A	1328	G	C5-C6-O6	-7.82	123.91	128.60
1	A	784	A	N1-C6-N6	-7.82	113.91	118.60
1	A	2519	U	C2-N3-C4	-7.82	122.31	127.00
1	A	2075	U	C5-C6-N1	-7.81	118.80	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	864	G	N1-C6-O6	-7.79	115.22	119.90
19	X	57	LEU	CA-CB-CG	7.78	133.20	115.30
1	A	1376	C	C5-C4-N4	-7.77	114.76	120.20
1	A	1365	A	N1-C6-N6	7.76	123.26	118.60
1	A	1368	G	C8-N9-C4	-7.74	103.31	106.40
1	A	2726	U	N1-C2-O2	-7.73	117.39	122.80
1	A	127	A	N7-C8-N9	-7.73	109.93	113.80
1	A	129	C	C5-C4-N4	-7.73	114.79	120.20
1	A	2823	A	C5-C6-N6	-7.73	117.52	123.70
1	A	1109	C	C4-C5-C6	7.72	121.26	117.40
1	A	811	U	C5-C6-N1	-7.71	118.84	122.70
1	A	2077	A	C8-N9-C4	-7.71	102.72	105.80
1	A	729	G	N1-C2-N2	7.71	123.14	116.20
1	A	1047	G	N3-C4-N9	7.69	130.62	126.00
1	A	1254	A	C8-N9-C4	-7.69	102.72	105.80
1	A	664	C	N3-C4-C5	7.69	124.98	121.90
1	A	2427	C	N1-C2-O2	-7.68	114.29	118.90
1	A	1324	G	N3-C2-N2	-7.68	114.52	119.90
1	A	949	C	C2-N3-C4	-7.68	116.06	119.90
1	A	1328	G	N9-C4-C5	-7.67	102.33	105.40
1	A	2791	C	C2-N1-C1'	7.67	127.24	118.80
1	A	201	C	C2-N3-C4	-7.67	116.06	119.90
1	A	1025	G	C8-N9-C4	-7.67	103.33	106.40
1	A	2363	C	C5-C6-N1	-7.67	117.17	121.00
1	A	2037	G	C4-C5-N7	-7.65	107.74	110.80
1	A	2722	G	N1-C6-O6	-7.64	115.32	119.90
1	A	847	U	N1-C2-N3	7.61	119.46	114.90
1	A	1600	C	C2-N3-C4	-7.61	116.10	119.90
1	A	446	G	C5-C6-O6	-7.60	124.04	128.60
1	A	763	G	C8-N9-C4	-7.59	103.36	106.40
1	A	658	C	N3-C2-O2	-7.58	116.59	121.90
1	A	448	U	C5-C4-O4	7.57	130.44	125.90
1	A	674	G	N1-C6-O6	7.57	124.44	119.90
1	A	2020	A	C5-C6-N1	7.56	121.48	117.70
1	A	591	C	N1-C2-O2	-7.54	114.38	118.90
1	A	1045	A	N9-C4-C5	-7.54	102.79	105.80
1	A	1751	C	N1-C2-O2	-7.53	114.38	118.90
1	A	1957	C	N1-C2-O2	7.53	123.42	118.90
1	A	1563	G	C8-N9-C4	7.53	109.41	106.40
1	A	1029	A	N1-C6-N6	7.53	123.12	118.60
1	A	766	C	N3-C4-C5	-7.51	118.89	121.90
1	A	488	G	C6-N1-C2	-7.51	120.59	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	13	ARG	NE-CZ-NH1	-7.51	116.55	120.30
1	A	148	C	N3-C4-C5	7.50	124.90	121.90
1	A	47	C	N3-C4-N4	-7.50	112.75	118.00
1	A	2407	G	C6-C5-N7	-7.50	125.90	130.40
1	A	527	C	N3-C2-O2	-7.49	116.65	121.90
23	1	21	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	A	530	G	N7-C8-N9	7.49	116.84	113.10
1	A	777	A	N9-C4-C5	7.48	108.79	105.80
1	A	2322	A	C2-N3-C4	7.48	114.34	110.60
1	A	478	A	N9-C4-C5	7.47	108.79	105.80
1	A	60	G	C8-N9-C4	7.47	109.39	106.40
1	A	267	C	N3-C4-C5	7.46	124.88	121.90
1	A	572	A	N1-C6-N6	-7.46	114.12	118.60
1	A	791	C	N1-C2-O2	7.46	123.38	118.90
1	A	778	G	C5-C6-O6	7.45	133.07	128.60
1	A	2503	A	C5-C6-N6	-7.43	117.76	123.70
1	A	2719	G	C5-C6-N1	7.42	115.21	111.50
1	A	1814	G	C5-C6-N1	7.42	115.21	111.50
1	A	1128	A	C5-C6-N6	-7.41	117.77	123.70
1	A	2082	A	C5-C6-N1	7.41	121.40	117.70
1	A	2463	C	N3-C4-C5	7.39	124.86	121.90
1	A	1210	A	C8-N9-C4	-7.39	102.84	105.80
1	A	860	U	C6-N1-C2	-7.39	116.57	121.00
1	A	982	C	C6-N1-C2	-7.37	117.35	120.30
1	A	2252	G	C8-N9-C4	7.37	109.35	106.40
1	A	2500	U	N1-C2-O2	7.37	127.96	122.80
1	A	2430	A	N1-C2-N3	7.36	132.98	129.30
1	A	2513	G	C8-N9-C4	-7.36	103.46	106.40
1	A	527	C	N3-C4-N4	-7.35	112.85	118.00
1	A	2791	C	N1-C2-O2	7.35	123.31	118.90
1	A	1253	A	C4-C5-N7	-7.35	107.03	110.70
1	A	1493	C	C2-N1-C1'	7.35	126.88	118.80
1	A	844	C	C6-N1-C2	7.34	123.24	120.30
1	A	1164	G	C5-C6-N1	-7.33	107.83	111.50
1	A	635	C	C6-N1-C2	-7.32	117.37	120.30
1	A	330	A	C5-C6-N1	-7.31	114.05	117.70
1	A	2335	A	C6-N1-C2	-7.31	114.22	118.60
1	A	1972	A	C5-C6-N6	-7.30	117.86	123.70
1	A	829	A	C2-N3-C4	-7.29	106.95	110.60
1	A	1820	U	C6-N1-C2	7.29	125.37	121.00
1	A	32	C	N3-C4-N4	-7.29	112.90	118.00
1	A	1653	G	C8-N9-C4	-7.27	103.49	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2039	C	N3-C4-C5	7.27	124.81	121.90
1	A	1382	G	C5-C6-O6	-7.27	124.24	128.60
1	A	816	C	N3-C4-C5	7.27	124.81	121.90
1	A	495	G	C8-N9-C4	7.26	109.31	106.40
1	A	2694	G	N1-C6-O6	7.26	124.25	119.90
1	A	799	G	C5-C6-O6	7.26	132.95	128.60
1	A	1605	C	C4-C5-C6	7.26	121.03	117.40
1	A	2591	C	C2-N3-C4	-7.25	116.28	119.90
1	A	2716	U	C5-C6-N1	-7.25	119.08	122.70
1	A	147	U	C5-C6-N1	-7.24	119.08	122.70
1	A	2344	U	C5-C4-O4	7.24	130.25	125.90
1	A	655	A	N7-C8-N9	7.24	117.42	113.80
1	A	857	C	C6-N1-C2	-7.24	117.41	120.30
1	A	2104	G	C6-N1-C2	7.23	129.44	125.10
1	A	2638	G	C8-N9-C4	-7.23	103.51	106.40
1	A	659	C	C6-N1-C2	7.23	123.19	120.30
1	A	2008	C	C6-N1-C2	-7.23	117.41	120.30
1	A	2124	G	C5-C6-O6	7.23	132.94	128.60
1	A	983	A	N1-C6-N6	-7.22	114.27	118.60
1	A	2494	G	C8-N9-C4	-7.22	103.51	106.40
1	A	964	C	C6-N1-C2	-7.22	117.41	120.30
1	A	2247	A	N1-C2-N3	7.22	132.91	129.30
1	A	676	A	C8-N9-C4	7.21	108.69	105.80
1	A	2322	A	C5-N7-C8	7.21	107.51	103.90
1	A	2755	C	C2-N1-C1'	7.21	126.73	118.80
1	A	394	A	N7-C8-N9	-7.20	110.20	113.80
1	A	726	G	C5-C6-O6	7.20	132.92	128.60
1	A	1760	A	N1-C6-N6	-7.20	114.28	118.60
1	A	1814	G	N1-C6-O6	-7.19	115.58	119.90
1	A	775	G	N1-C2-N2	-7.19	109.73	116.20
1	A	755	C	C6-N1-C2	-7.19	117.42	120.30
1	A	2243	U	C6-N1-C2	-7.18	116.69	121.00
1	A	1900	A	N1-C2-N3	7.18	132.89	129.30
1	A	2312	U	N1-C2-O2	7.18	127.83	122.80
1	A	1671	U	C5-C6-N1	-7.18	119.11	122.70
1	A	205	G	N3-C4-N9	7.18	130.31	126.00
1	A	271(Y)	U	C2-N3-C4	-7.18	122.69	127.00
1	A	690	G	N1-C6-O6	-7.17	115.60	119.90
2	B	7	G	C5-C6-O6	-7.17	124.30	128.60
1	A	865	C	N3-C2-O2	7.17	126.92	121.90
1	A	2433	A	N1-C6-N6	7.17	122.90	118.60
1	A	2473	U	N1-C2-O2	7.16	127.81	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2037	G	N7-C8-N9	-7.16	109.52	113.10
1	A	2441	C	C2-N3-C4	-7.15	116.32	119.90
1	A	1698	A	C6-C5-N7	-7.15	127.29	132.30
1	A	1779	U	N3-C4-O4	-7.14	114.40	119.40
1	A	2500	U	N3-C4-C5	7.14	118.89	114.60
1	A	1368	G	C2-N3-C4	7.14	115.47	111.90
1	A	671	C	N3-C2-O2	-7.12	116.91	121.90
1	A	491	G	C5-C6-O6	7.12	132.87	128.60
1	A	1488	G	C8-N9-C4	-7.12	103.55	106.40
1	A	1780	A	C8-N9-C4	-7.12	102.95	105.80
1	A	1956	U	N1-C2-N3	7.12	119.17	114.90
1	A	1574	C	N3-C4-C5	7.12	124.75	121.90
1	A	1805	U	C6-N1-C2	-7.12	116.73	121.00
1	A	534	U	N3-C4-O4	7.12	124.38	119.40
1	A	614	U	N3-C2-O2	-7.12	117.22	122.20
1	A	965	C	N3-C4-N4	-7.12	113.02	118.00
1	A	2062	A	C5-N7-C8	-7.11	100.34	103.90
1	A	2834	G	C8-N9-C4	-7.11	103.56	106.40
1	A	528	A	C8-N9-C1'	7.11	140.50	127.70
1	A	478	A	C6-N1-C2	-7.10	114.34	118.60
1	A	1638	C	C4-C5-C6	7.10	120.95	117.40
1	A	12	U	C2-N1-C1'	7.10	126.22	117.70
1	A	641	C	N3-C4-C5	-7.09	119.06	121.90
1	A	119	A	N1-C2-N3	7.09	132.84	129.30
1	A	2335	A	C4-C5-N7	7.08	114.24	110.70
1	A	655	A	C8-N9-C4	-7.08	102.97	105.80
7	H	71	LEU	CA-CB-CG	7.07	131.56	115.30
1	A	2883	A	C8-N9-C4	-7.06	102.98	105.80
1	A	613	G	C8-N9-C4	-7.05	103.58	106.40
1	A	2826	A	C8-N9-C4	7.05	108.62	105.80
1	A	1214	A	N7-C8-N9	-7.05	110.28	113.80
1	A	640	C	C5-C6-N1	7.05	124.52	121.00
1	A	801	G	N9-C4-C5	7.05	108.22	105.40
1	A	1320	C	C6-N1-C2	7.04	123.12	120.30
1	A	978	G	N7-C8-N9	-7.04	109.58	113.10
1	A	774	A	N7-C8-N9	7.04	117.32	113.80
1	A	2361	A	N1-C6-N6	7.04	122.82	118.60
1	A	2607	G	C6-C5-N7	-7.03	126.18	130.40
1	A	864	G	C2-N3-C4	7.03	115.42	111.90
1	A	1795	C	C5-C4-N4	-7.03	115.28	120.20
1	A	1623	G	C5-C6-N1	7.03	115.02	111.50
2	B	6	C	C5-C6-N1	-7.03	117.49	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2006	C	C6-N1-C2	-7.02	117.49	120.30
1	A	2226	C	C6-N1-C2	7.02	123.11	120.30
1	A	527	C	N1-C2-N3	7.02	124.11	119.20
1	A	1427	A	N1-C6-N6	-7.01	114.39	118.60
1	A	1365	A	C5-C6-N6	-7.01	118.09	123.70
1	A	1616	A	N1-C6-N6	7.01	122.81	118.60
1	A	15	G	N3-C2-N2	-7.01	114.99	119.90
1	A	2070	G	C2-N3-C4	-7.01	108.39	111.90
1	A	2335	A	C4-C5-C6	-7.01	113.50	117.00
1	A	823	G	C8-N9-C4	-7.01	103.60	106.40
1	A	2423	U	C5-C6-N1	-7.00	119.20	122.70
1	A	2683	C	N3-C2-O2	-7.00	117.00	121.90
1	A	527	C	C6-N1-C2	-7.00	117.50	120.30
1	A	2059	A	C8-N9-C4	6.99	108.60	105.80
1	A	1223	G	N1-C6-O6	-6.99	115.70	119.90
1	A	2290	G	C2-N3-C4	-6.99	108.41	111.90
1	A	777	A	C5-C6-N6	6.99	129.29	123.70
1	A	2290	G	C8-N9-C4	6.99	109.19	106.40
1	A	201	C	N3-C4-C5	6.98	124.69	121.90
1	A	2346	A	C4-C5-C6	6.98	120.49	117.00
1	A	1824	G	C5-C6-O6	-6.98	124.41	128.60
1	A	1607	C	C5-C4-N4	-6.97	115.32	120.20
1	A	683	C	C4-C5-C6	-6.97	113.91	117.40
1	A	121	G	N1-C6-O6	6.97	124.08	119.90
1	A	1190	G	N7-C8-N9	-6.97	109.62	113.10
1	A	1256	G	C6-N1-C2	-6.97	120.92	125.10
1	A	1639	U	N3-C2-O2	-6.96	117.33	122.20
1	A	2710	C	C4-C5-C6	6.96	120.88	117.40
1	A	1025	G	N9-C4-C5	6.96	108.18	105.40
1	A	330	A	N3-C4-N9	-6.95	121.84	127.40
1	A	2461	C	C6-N1-C2	-6.95	117.52	120.30
1	A	2441	C	C5-C6-N1	-6.94	117.53	121.00
1	A	799	G	N9-C4-C5	6.93	108.17	105.40
1	A	1307	A	C8-N9-C4	6.93	108.57	105.80
1	A	2428	G	N3-C2-N2	6.93	124.75	119.90
1	A	52	A	C5-N7-C8	-6.93	100.44	103.90
1	A	529	A	C5-N7-C8	-6.92	100.44	103.90
1	A	647	G	C8-N9-C4	-6.92	103.63	106.40
1	A	652(T)	C	N1-C2-O2	6.92	123.05	118.90
1	A	1952	A	C8-N9-C4	-6.92	103.03	105.80
1	A	737	C	N1-C2-O2	-6.92	114.75	118.90
1	A	799	G	N1-C6-O6	-6.92	115.75	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1616	A	C4-C5-N7	6.91	114.16	110.70
1	A	2415	G	N3-C2-N2	-6.91	115.06	119.90
1	A	2345	G	N1-C2-N3	6.91	128.04	123.90
1	A	488	G	N3-C4-C5	-6.90	125.15	128.60
1	A	194	G	N1-C2-N3	6.90	128.04	123.90
1	A	62	C	C5-C6-N1	-6.90	117.55	121.00
1	A	1558	A	N1-C2-N3	6.90	132.75	129.30
1	A	2446	G	N3-C4-C5	-6.89	125.16	128.60
1	A	2286	A	C5-C6-N1	-6.89	114.26	117.70
1	A	2030	A	N1-C6-N6	6.88	122.73	118.60
1	A	240	G	C8-N9-C4	6.88	109.15	106.40
1	A	2181	G	C6-N1-C2	6.88	129.23	125.10
1	A	1130	U	N3-C2-O2	-6.88	117.38	122.20
1	A	1328	G	C8-N9-C4	6.88	109.15	106.40
1	A	381	G	N3-C4-C5	-6.87	125.16	128.60
1	A	729	G	N7-C8-N9	6.87	116.54	113.10
1	A	932	G	C5-C6-N1	6.87	114.94	111.50
1	A	1125	G	N1-C6-O6	6.87	124.02	119.90
1	A	1376	C	N3-C4-N4	6.87	122.81	118.00
1	A	1955	U	C2-N1-C1'	-6.87	109.45	117.70
1	A	254	G	C8-N9-C4	-6.87	103.65	106.40
1	A	2407	G	C4-N9-C1'	6.87	135.43	126.50
1	A	1984	G	N1-C6-O6	-6.87	115.78	119.90
1	A	512	G	O4'-C1'-N9	6.86	113.69	108.20
1	A	2475	C	C6-N1-C2	-6.86	117.56	120.30
1	A	2075	U	N3-C2-O2	-6.86	117.40	122.20
1	A	2191	G	N1-C6-O6	6.85	124.01	119.90
1	A	2346	A	N1-C2-N3	6.85	132.73	129.30
1	A	808	G	N3-C4-C5	-6.85	125.17	128.60
1	A	1524	G	N1-C6-O6	-6.85	115.79	119.90
1	A	2791	C	C6-N1-C2	-6.85	117.56	120.30
1	A	2024	G	C8-N9-C4	6.84	109.14	106.40
1	A	2548	G	N9-C4-C5	6.84	108.14	105.40
1	A	127	A	C8-N9-C4	6.84	108.53	105.80
1	A	599	G	C8-N9-C4	6.84	109.13	106.40
1	A	987	G	N9-C4-C5	6.83	108.13	105.40
1	A	737	C	C6-N1-C2	6.83	123.03	120.30
1	A	2446	G	N3-C2-N2	6.83	124.68	119.90
1	A	311	A	N1-C6-N6	6.83	122.69	118.60
1	A	345	A	C5-C6-N6	-6.82	118.24	123.70
1	A	965	C	C5-C4-N4	6.82	124.97	120.20
1	A	1026	U	N1-C2-O2	6.82	127.58	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1899	G	N1-C6-O6	6.82	123.99	119.90
1	A	2280	G	C5-C6-O6	6.82	132.69	128.60
1	A	1128	A	C8-N9-C4	6.81	108.53	105.80
1	A	2048	G	C8-N9-C4	-6.80	103.68	106.40
1	A	2508	G	C5-C6-N1	6.80	114.90	111.50
1	A	221	A	N9-C4-C5	6.80	108.52	105.80
1	A	1214	A	C8-N9-C4	6.80	108.52	105.80
1	A	42	G	N7-C8-N9	-6.80	109.70	113.10
1	A	2103	C	N3-C4-C5	-6.80	119.18	121.90
30	8	30	ARG	NE-CZ-NH1	-6.80	116.90	120.30
1	A	1039	G	C8-N9-C4	6.79	109.12	106.40
1	A	199	A	C2-N3-C4	6.79	113.99	110.60
1	A	386	G	C8-N9-C4	-6.79	103.68	106.40
1	A	1415	U	N3-C4-O4	-6.79	114.65	119.40
1	A	847	U	C2-N1-C1'	-6.78	109.56	117.70
1	A	1755	A	C8-N9-C4	-6.78	103.09	105.80
1	A	2306	C	N1-C2-O2	6.78	122.97	118.90
1	A	1992	G	C8-N9-C4	-6.78	103.69	106.40
1	A	2306	C	C2-N1-C1'	6.78	126.26	118.80
1	A	2508	G	C2-N3-C4	6.78	115.29	111.90
1	A	2781	A	N1-C6-N6	-6.78	114.53	118.60
1	A	1332	G	C5-C6-O6	-6.78	124.53	128.60
1	A	1937	A	N1-C2-N3	6.78	132.69	129.30
1	A	478	A	C8-N9-C4	-6.77	103.09	105.80
1	A	2122	U	C5-C4-O4	6.77	129.96	125.90
1	A	1762	A	N7-C8-N9	6.76	117.18	113.80
1	A	215	G	C8-N9-C4	6.76	109.11	106.40
1	A	37	C	N3-C2-O2	-6.76	117.17	121.90
1	A	816	C	C2-N3-C4	-6.76	116.52	119.90
1	A	2848	G	C4-C5-N7	-6.76	108.10	110.80
1	A	1602	U	N1-C2-N3	6.75	118.95	114.90
1	A	573	G	N3-C2-N2	-6.75	115.17	119.90
1	A	1899	G	C5-C6-O6	-6.75	124.55	128.60
1	A	2581	G	C5-C6-O6	6.75	132.65	128.60
1	A	2791	C	C5-C6-N1	6.75	124.38	121.00
27	5	15	ARG	NE-CZ-NH1	-6.75	116.93	120.30
1	A	59	U	N1-C2-O2	6.75	127.52	122.80
1	A	2501	C	C2-N3-C4	-6.74	116.53	119.90
1	A	2070	G	N1-C2-N2	-6.74	110.14	116.20
1	A	678	C	C6-N1-C2	6.73	122.99	120.30
1	A	1539	G	C6-C5-N7	-6.73	126.36	130.40
1	A	1669	A	N1-C6-N6	-6.73	114.56	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2093	G	C2-N3-C4	-6.73	108.54	111.90
1	A	1831	G	C8-N9-C4	-6.73	103.71	106.40
1	A	2725	A	C2-N3-C4	-6.73	107.24	110.60
1	A	1827	C	C6-N1-C2	-6.73	117.61	120.30
1	A	453	C	C2-N3-C4	-6.72	116.54	119.90
1	A	1572	A	C2-N3-C4	-6.72	107.24	110.60
1	A	1858	G	N3-C4-C5	-6.72	125.24	128.60
1	A	678	C	N3-C4-C5	6.72	124.59	121.90
1	A	1359	A	C5-C6-N6	6.72	129.08	123.70
1	A	2244	U	C5-C6-N1	-6.72	119.34	122.70
1	A	1605	C	C6-N1-C2	-6.71	117.61	120.30
1	A	744	G	C5-C6-O6	6.70	132.62	128.60
1	A	839	U	C2-N3-C4	6.70	131.02	127.00
1	A	2446	G	N1-C2-N2	-6.69	110.17	116.20
1	A	837	C	C6-N1-C2	-6.69	117.62	120.30
11	P	147	LEU	CA-CB-CG	6.69	130.69	115.30
1	A	130	C	C5-C6-N1	-6.69	117.66	121.00
1	A	1858	G	C8-N9-C4	-6.69	103.72	106.40
1	A	1128	A	N9-C4-C5	-6.69	103.13	105.80
1	A	931	G	N3-C4-C5	-6.68	125.26	128.60
1	A	679	C	C6-N1-C2	6.68	122.97	120.30
1	A	2498	C	C6-N1-C2	6.68	122.97	120.30
1	A	2508	G	C6-C5-N7	6.68	134.41	130.40
1	A	1164	G	C5-C6-O6	6.68	132.61	128.60
1	A	476	G	N3-C4-N9	-6.68	121.99	126.00
1	A	2692	C	N3-C2-O2	-6.68	117.23	121.90
1	A	385	C	C4-C5-C6	-6.67	114.06	117.40
1	A	2379	G	N3-C4-N9	6.67	130.00	126.00
1	A	678	C	N3-C4-N4	-6.67	113.33	118.00
1	A	195	A	N1-C2-N3	6.67	132.63	129.30
1	A	1793	C	N1-C2-O2	-6.67	114.90	118.90
1	A	2069	G	C5-C6-O6	-6.66	124.60	128.60
1	A	1333	C	C6-N1-C2	6.66	122.97	120.30
1	A	640	C	N3-C4-N4	6.66	122.66	118.00
1	A	741	G	N1-C6-O6	-6.66	115.90	119.90
1	A	1204	A	C3'-C2'-C1'	-6.66	96.17	101.50
1	A	931	G	C2-N3-C4	6.66	115.23	111.90
1	A	2440	C	N1-C2-O2	6.66	122.89	118.90
1	A	271(Y)	U	N3-C2-O2	-6.66	117.54	122.20
1	A	968	G	N1-C6-O6	-6.65	115.91	119.90
1	A	2440	C	N3-C4-N4	-6.65	113.34	118.00
1	A	1336	A	C5-N7-C8	6.65	107.22	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1698	A	C5-C6-N1	-6.64	114.38	117.70
1	A	2015	A	C2-N3-C4	-6.64	107.28	110.60
1	A	2346	A	N3-C4-C5	-6.64	122.15	126.80
1	A	1188	U	N3-C4-C5	6.64	118.58	114.60
1	A	425	G	N3-C4-N9	6.64	129.98	126.00
1	A	1783	A	N9-C4-C5	6.64	108.45	105.80
1	A	1123	C	C6-N1-C2	6.63	122.95	120.30
1	A	217	G	N1-C6-O6	6.62	123.87	119.90
1	A	263	C	N3-C2-O2	-6.62	117.26	121.90
1	A	856	C	C5-C6-N1	6.62	124.31	121.00
1	A	1185	C	C5-C4-N4	6.62	124.84	120.20
1	A	1333	C	N3-C4-C5	6.62	124.55	121.90
1	A	36	G	C5-C6-O6	6.62	132.57	128.60
1	A	193	U	C6-N1-C2	-6.62	117.03	121.00
1	A	516	C	C4-C5-C6	6.62	120.71	117.40
1	A	1191	G	C4-C5-N7	-6.62	108.15	110.80
1	A	1899	G	C8-N9-C4	-6.62	103.75	106.40
1	A	2407	G	C8-N9-C1'	-6.62	118.40	127.00
1	A	37	C	N1-C2-O2	6.61	122.87	118.90
1	A	2581	G	N1-C2-N2	-6.61	110.25	116.20
1	A	785	G	N3-C4-C5	6.61	131.91	128.60
1	A	2869	G	C8-N9-C4	-6.61	103.75	106.40
1	A	1351	C	N3-C4-C5	6.61	124.54	121.90
1	A	1382	G	N1-C6-O6	6.61	123.86	119.90
1	A	57	C	C6-N1-C2	6.61	122.94	120.30
1	A	971	C	C2-N3-C4	-6.61	116.60	119.90
1	A	73	A	C6-N1-C2	-6.60	114.64	118.60
2	B	80	U	C5-C4-O4	6.60	129.86	125.90
1	A	2407	G	N1-C6-O6	6.60	123.86	119.90
1	A	641	C	C6-N1-C2	-6.59	117.66	120.30
1	A	2319	G	C5-N7-C8	-6.59	101.00	104.30
1	A	975	C	N3-C4-N4	-6.59	113.39	118.00
1	A	154(A)	C	C6-N1-C1'	-6.58	112.90	120.80
1	A	2353	G	C2-N3-C4	-6.58	108.61	111.90
1	A	2296	U	C3'-C2'-C1'	-6.58	96.24	101.50
1	A	1308	A	N1-C6-N6	-6.58	114.66	118.60
1	A	2628	C	N3-C4-C5	6.57	124.53	121.90
1	A	2442	C	C2-N3-C4	-6.57	116.61	119.90
1	A	272(D)	G	C8-N9-C4	6.57	109.03	106.40
1	A	243	U	C5-C6-N1	6.57	125.98	122.70
1	A	2359	C	N3-C2-O2	-6.57	117.30	121.90
1	A	154(A)	C	C2-N1-C1'	6.56	126.02	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2730	C	N3-C4-C5	6.56	124.53	121.90
1	A	783	A	C2-N3-C4	6.56	113.88	110.60
1	A	1659	U	N1-C2-O2	-6.56	118.21	122.80
1	A	2110	G	N3-C4-N9	6.56	129.94	126.00
1	A	2322	A	N1-C2-N3	6.56	132.58	129.30
1	A	2296	U	O4'-C1'-N1	6.55	113.44	108.20
1	A	1633	G	N1-C6-O6	6.55	123.83	119.90
1	A	2866	U	C5-C4-O4	6.55	129.83	125.90
1	A	584	C	C5-C4-N4	-6.55	115.62	120.20
1	A	2107	C	N3-C4-N4	-6.55	113.42	118.00
1	A	2578	G	N3-C2-N2	6.55	124.48	119.90
1	A	940	G	N7-C8-N9	6.54	116.37	113.10
1	A	141	A	C5-C6-N6	-6.54	118.47	123.70
1	A	2674	G	C8-N9-C4	-6.54	103.78	106.40
1	A	2285	C	C6-N1-C2	6.53	122.91	120.30
1	A	768	G	N3-C4-C5	-6.53	125.34	128.60
2	B	104	U	C2-N3-C4	-6.53	123.08	127.00
1	A	572	A	N9-C4-C5	6.52	108.41	105.80
1	A	2499	C	C6-N1-C2	-6.52	117.69	120.30
1	A	448	U	N1-C2-N3	6.52	118.81	114.90
1	A	830	G	C5-C6-O6	6.52	132.51	128.60
1	A	1368	G	N9-C4-C5	6.52	108.01	105.40
1	A	1403	C	C5-C6-N1	-6.52	117.74	121.00
1	A	2322	A	C6-C5-N7	6.52	136.86	132.30
1	A	1204	A	C8-N9-C4	-6.51	103.19	105.80
1	A	1755	A	N9-C4-C5	6.51	108.41	105.80
2	B	83	G	N3-C2-N2	-6.51	115.34	119.90
1	A	12	U	C6-N1-C2	-6.51	117.09	121.00
1	A	520	G	N1-C6-O6	-6.51	115.99	119.90
1	A	2676	C	N3-C4-C5	6.51	124.50	121.90
2	B	75	G	N1-C6-O6	6.51	123.81	119.90
1	A	1334	G	N9-C4-C5	6.51	108.00	105.40
1	A	2449	U	N3-C4-O4	6.51	123.96	119.40
1	A	2233	U	N1-C2-N3	6.51	118.80	114.90
1	A	2243	U	C5-C6-N1	6.50	125.95	122.70
1	A	267	C	N3-C4-N4	-6.50	113.45	118.00
1	A	1972	A	C5-C6-N1	6.50	120.95	117.70
1	A	2283	C	N3-C4-N4	6.50	122.55	118.00
1	A	1108	U	C6-N1-C2	-6.50	117.10	121.00
7	H	127	GLU	C-N-CD	6.49	142.03	128.40
1	A	505	A	C8-N9-C4	-6.49	103.20	105.80
1	A	51	G	C5-C6-O6	6.49	132.50	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2244	U	N1-C2-N3	6.49	118.80	114.90
1	A	2447	G	N9-C4-C5	6.49	108.00	105.40
1	A	488	G	N9-C4-C5	6.49	108.00	105.40
1	A	528	A	C4-C5-N7	6.49	113.94	110.70
1	A	655	A	C5-N7-C8	-6.49	100.66	103.90
1	A	2195	C	C5-C6-N1	-6.48	117.76	121.00
1	A	2540	C	C5-C6-N1	-6.48	117.76	121.00
1	A	817	C	N3-C4-C5	6.48	124.49	121.90
1	A	2332	U	C5-C6-N1	-6.48	119.46	122.70
1	A	2393	A	N1-C6-N6	-6.48	114.72	118.60
1	A	2591	C	N1-C2-O2	-6.48	115.01	118.90
1	A	12	U	N1-C2-O2	6.47	127.33	122.80
1	A	957	A	C2-N3-C4	-6.47	107.36	110.60
1	A	2008	C	N3-C4-C5	-6.47	119.31	121.90
1	A	1792	G	C5-N7-C8	6.46	107.53	104.30
1	A	2709	G	N3-C4-C5	-6.46	125.37	128.60
1	A	2114	A	N7-C8-N9	6.46	117.03	113.80
1	A	1630	G	N1-C6-O6	-6.45	116.03	119.90
1	A	69	C	N3-C2-O2	-6.45	117.39	121.90
1	A	1204	A	C4-N9-C1'	6.45	137.91	126.30
1	A	1918	A	C8-N9-C4	6.45	108.38	105.80
1	A	2032	G	N1-C2-N3	6.44	127.77	123.90
1	A	2593	U	N1-C2-N3	6.44	118.76	114.90
1	A	1539	G	C4-N9-C1'	6.44	134.87	126.50
1	A	2344	U	N3-C4-C5	-6.44	110.74	114.60
1	A	2682	U	C2-N1-C1'	6.44	125.42	117.70
1	A	1784	A	N9-C4-C5	-6.43	103.23	105.80
1	A	698	C	C6-N1-C2	6.43	122.87	120.30
1	A	2114	A	C8-N9-C4	-6.43	103.23	105.80
1	A	777	A	C4-C5-N7	-6.42	107.49	110.70
1	A	1638	C	N3-C4-C5	-6.42	119.33	121.90
1	A	1681	G	C4-C5-N7	6.42	113.37	110.80
1	A	2062	A	N7-C8-N9	6.42	117.01	113.80
1	A	1393	A	C4-C5-N7	-6.42	107.49	110.70
1	A	2077	A	N7-C8-N9	6.42	117.01	113.80
1	A	2191	G	N3-C4-N9	6.41	129.85	126.00
1	A	2515	C	C5-C4-N4	-6.41	115.71	120.20
1	A	2823	A	N9-C4-C5	-6.41	103.24	105.80
1	A	1681	G	N1-C6-O6	6.40	123.74	119.90
1	A	2463	C	C5-C6-N1	-6.40	117.80	121.00
1	A	2488	A	C5-N7-C8	6.40	107.10	103.90
1	A	566	U	N3-C4-O4	-6.40	114.92	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	580	C	N1-C2-O2	-6.40	115.06	118.90
1	A	941	A	C8-N9-C4	-6.40	103.24	105.80
1	A	1334	G	N1-C6-O6	-6.40	116.06	119.90
1	A	124	G	C4-C5-N7	6.40	113.36	110.80
1	A	2348	U	N3-C4-O4	-6.40	114.92	119.40
1	A	2446	G	N3-C4-N9	6.40	129.84	126.00
1	A	663	G	C2-N3-C4	6.40	115.10	111.90
1	A	1200	C	N1-C2-O2	-6.40	115.06	118.90
1	A	936	C	C6-N1-C2	6.39	122.86	120.30
1	A	2422	A	C8-N9-C4	-6.39	103.24	105.80
1	A	2439	A	C8-N9-C4	-6.39	103.24	105.80
1	A	2487	G	C2-N3-C4	-6.39	108.71	111.90
1	A	188	G	N1-C6-O6	-6.39	116.07	119.90
1	A	2648	C	C6-N1-C2	6.38	122.85	120.30
1	A	429	A	N1-C6-N6	6.38	122.43	118.60
1	A	2271	G	C8-N9-C4	-6.38	103.85	106.40
1	A	1802	A	C5-C6-N1	6.38	120.89	117.70
1	A	2057	A	N1-C2-N3	6.38	132.49	129.30
1	A	2419	U	C5-C6-N1	6.38	125.89	122.70
1	A	1368	G	N1-C6-O6	-6.38	116.07	119.90
1	A	769	G	C5-C6-N1	-6.38	108.31	111.50
1	A	1249	U	C5-C6-N1	-6.37	119.51	122.70
1	A	2862	G	C8-N9-C4	6.37	108.95	106.40
1	A	1814	G	C6-N1-C2	-6.37	121.28	125.10
1	A	785	G	C6-N1-C2	6.37	128.92	125.10
1	A	433	C	C6-N1-C2	-6.37	117.75	120.30
1	A	1131	G	N1-C6-O6	-6.36	116.08	119.90
1	A	1558	A	C5-C6-N1	-6.36	114.52	117.70
1	A	684	G	N3-C4-C5	-6.36	125.42	128.60
1	A	1764	G	N1-C6-O6	-6.36	116.09	119.90
1	A	748	G	C5-C6-O6	6.35	132.41	128.60
1	A	726	G	N1-C6-O6	-6.35	116.09	119.90
1	A	1783	A	N1-C6-N6	-6.35	114.79	118.60
1	A	1653	G	P-O3'-C3'	6.35	127.32	119.70
1	A	2017	U	N3-C2-O2	-6.35	117.76	122.20
1	A	2312	U	C2-N1-C1'	6.34	125.31	117.70
1	A	25	U	N3-C2-O2	6.34	126.64	122.20
1	A	474	G	C8-N9-C4	-6.34	103.86	106.40
1	A	2487	G	N9-C4-C5	-6.34	102.86	105.40
1	A	1330	C	C5-C4-N4	-6.34	115.76	120.20
1	A	2029	G	C5-C6-O6	-6.34	124.80	128.60
1	A	1934	C	C6-N1-C2	6.33	122.83	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	51	G	N9-C4-C5	-6.33	102.87	105.40
1	A	419	C	C6-N1-C2	6.33	122.83	120.30
1	A	1792	G	C4-C5-N7	-6.33	108.27	110.80
1	A	967	C	N3-C2-O2	-6.32	117.47	121.90
1	A	1904	G	N1-C6-O6	-6.32	116.11	119.90
1	A	1142(A)	A	C8-N9-C4	-6.32	103.27	105.80
1	A	2092	U	C5-C6-N1	6.32	125.86	122.70
1	A	42	G	C5-N7-C8	6.31	107.46	104.30
1	A	456	C	N3-C2-O2	6.31	126.32	121.90
29	7	3	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	A	139	G	C8-N9-C4	-6.30	103.88	106.40
1	A	2542	A	C2-N3-C4	6.30	113.75	110.60
1	A	652(E)	G	N3-C2-N2	6.30	124.31	119.90
1	A	194	G	N3-C2-N2	-6.30	115.49	119.90
1	A	2389	G	C5-C6-N1	-6.30	108.35	111.50
1	A	760	G	N1-C6-O6	6.30	123.68	119.90
1	A	1602	U	C4-C5-C6	6.30	123.48	119.70
1	A	2540	C	C2-N3-C4	-6.30	116.75	119.90
2	B	77	U	C5-C4-O4	-6.30	122.12	125.90
1	A	1028	A	N9-C4-C5	-6.30	103.28	105.80
1	A	1992	G	N3-C4-C5	-6.29	125.45	128.60
1	A	2726	U	N3-C2-O2	6.29	126.61	122.20
1	A	1618	A	C2-N3-C4	6.29	113.75	110.60
1	A	2372	G	N1-C6-O6	6.29	123.67	119.90
1	A	142(A)	C	C6-N1-C2	6.29	122.82	120.30
1	A	580	C	N3-C4-N4	6.29	122.40	118.00
1	A	2071	A	C5-C6-N1	6.29	120.84	117.70
1	A	272(H)	C	C2-N1-C1'	6.29	125.71	118.80
1	A	1296	G	C5-C6-N1	6.29	114.64	111.50
1	A	1519	G	C8-N9-C4	-6.29	103.89	106.40
1	A	614	U	N1-C2-N3	6.28	118.67	114.90
1	A	975	C	C5-C4-N4	6.28	124.60	120.20
1	A	2031	A	C8-N9-C4	6.28	108.31	105.80
1	A	2509	G	N3-C4-N9	6.28	129.77	126.00
1	A	1029	A	N9-C4-C5	-6.28	103.29	105.80
1	A	847	U	N3-C4-O4	-6.27	115.01	119.40
1	A	1827	C	N1-C2-O2	6.27	122.66	118.90
1	A	2428	G	N1-C2-N2	-6.27	110.56	116.20
1	A	2221	G	C8-N9-C4	-6.27	103.89	106.40
1	A	2825	C	C4-C5-C6	6.27	120.53	117.40
1	A	2253	G	N1-C6-O6	6.27	123.66	119.90
1	A	92	A	N7-C8-N9	6.26	116.93	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2460	U	N3-C2-O2	-6.26	117.81	122.20
1	A	146	G	C5-N7-C8	6.26	107.43	104.30
1	A	2123	G	C8-N9-C1'	6.26	135.14	127.00
1	A	933	A	C6-C5-N7	-6.26	127.92	132.30
1	A	73	A	N1-C2-N3	6.26	132.43	129.30
1	A	2070	G	N1-C2-N3	6.26	127.65	123.90
1	A	2620	C	C6-N1-C2	6.26	122.80	120.30
1	A	2123	G	C4-N9-C1'	-6.25	118.37	126.50
1	A	784	A	N9-C4-C5	6.25	108.30	105.80
1	A	2816	C	C6-N1-C2	-6.25	117.80	120.30
1	A	473	G	N1-C2-N2	-6.25	110.58	116.20
1	A	58	G	N1-C6-O6	-6.24	116.15	119.90
1	A	763	G	N1-C6-O6	-6.24	116.15	119.90
1	A	2473	U	C6-N1-C1'	-6.24	112.46	121.20
1	A	122	G	N1-C6-O6	6.24	123.64	119.90
1	A	129	C	N3-C2-O2	6.24	126.27	121.90
1	A	1582	C	C5-C6-N1	-6.24	117.88	121.00
2	B	101	G	C4-C5-N7	6.23	113.29	110.80
1	A	1981	A	N1-C6-N6	-6.23	114.86	118.60
1	A	1939	U	N3-C4-C5	6.23	118.34	114.60
1	A	1253	A	N1-C6-N6	-6.23	114.86	118.60
1	A	961	C	C5-C6-N1	-6.22	117.89	121.00
1	A	1710	C	C6-N1-C2	6.22	122.79	120.30
1	A	1137	G	N3-C2-N2	6.22	124.25	119.90
1	A	1777	U	N3-C4-O4	6.22	123.75	119.40
1	A	2062	A	C6-C5-N7	-6.22	127.95	132.30
1	A	2494	G	N7-C8-N9	6.21	116.21	113.10
1	A	1620	G	C6-C5-N7	6.21	134.13	130.40
1	A	2344	U	C2-N3-C4	6.21	130.73	127.00
1	A	470	A	N7-C8-N9	6.20	116.90	113.80
1	A	1955	U	C2-N3-C4	-6.20	123.28	127.00
1	A	2103	C	C5-C4-N4	6.20	124.54	120.20
1	A	2245	U	C5-C6-N1	-6.20	119.60	122.70
1	A	616	G	C8-N9-C4	6.20	108.88	106.40
1	A	1403	C	C4-C5-C6	6.20	120.50	117.40
1	A	2287	A	N3-C4-C5	6.20	131.14	126.80
1	A	1698	A	C4-C5-N7	6.19	113.80	110.70
1	A	1805	U	N3-C2-O2	-6.19	117.86	122.20
1	A	1956	U	N1-C2-O2	-6.19	118.47	122.80
1	A	1196	C	C2-N3-C4	-6.19	116.81	119.90
1	A	53	A	C8-N9-C4	-6.19	103.32	105.80
1	A	1042	G	C5-C6-O6	-6.19	124.89	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1310	G	N1-C6-O6	6.19	123.61	119.90
1	A	1368	G	N3-C4-C5	-6.19	125.51	128.60
1	A	1488	G	N7-C8-N9	6.19	116.19	113.10
1	A	2273	A	C5-C6-N1	6.19	120.79	117.70
1	A	2322	A	N3-C4-C5	-6.19	122.47	126.80
1	A	422	A	N1-C2-N3	6.18	132.39	129.30
1	A	2432	A	C8-N9-C4	6.18	108.27	105.80
1	A	802	A	C8-N9-C4	-6.18	103.33	105.80
1	A	1107	G	N7-C8-N9	6.18	116.19	113.10
1	A	1954	G	C5-C6-N1	-6.18	108.41	111.50
1	A	2415	G	C5-C6-O6	-6.18	124.89	128.60
1	A	2873	A	C8-N9-C4	-6.18	103.33	105.80
1	A	839	U	N3-C4-C5	-6.17	110.90	114.60
1	A	2107	C	C6-N1-C1'	6.17	128.21	120.80
1	A	567	A	C5-N7-C8	-6.17	100.81	103.90
1	A	468	G	C2-N3-C4	-6.17	108.82	111.90
1	A	2343	C	N1-C2-O2	-6.17	115.20	118.90
1	A	645	C	N3-C2-O2	-6.16	117.59	121.90
1	A	106	C	C5-C6-N1	6.16	124.08	121.00
1	A	2359	C	C6-N1-C2	-6.16	117.84	120.30
1	A	528	A	C4-N9-C1'	-6.16	115.22	126.30
1	A	1351	C	C5-C4-N4	-6.16	115.89	120.20
1	A	1771	C	N3-C4-N4	-6.16	113.69	118.00
1	A	673	C	C5-C4-N4	-6.16	115.89	120.20
1	A	2739	U	C4-C5-C6	6.16	123.39	119.70
1	A	2825	C	N3-C4-C5	-6.16	119.44	121.90
2	B	104	U	C6-N1-C2	6.15	124.69	121.00
1	A	2239	G	N1-C2-N2	-6.15	110.67	116.20
1	A	1129	A	N9-C4-C5	6.15	108.26	105.80
4	E	111	ARG	NE-CZ-NH2	-6.15	117.23	120.30
1	A	2186	G	C6-N1-C2	6.15	128.79	125.10
1	A	2383	G	N3-C4-N9	6.15	129.69	126.00
1	A	1222	C	N1-C2-O2	-6.14	115.21	118.90
1	A	445	C	C5-C6-N1	6.14	124.07	121.00
1	A	445	C	C2-N3-C4	6.14	122.97	119.90
1	A	1024	G	N1-C6-O6	-6.14	116.22	119.90
1	A	386	G	N7-C8-N9	6.14	116.17	113.10
1	A	760	G	N3-C2-N2	-6.14	115.61	119.90
1	A	1779	U	C6-N1-C1'	6.14	129.79	121.20
1	A	2430	A	C6-N1-C2	-6.13	114.92	118.60
1	A	121	G	C4-C5-N7	6.13	113.25	110.80
1	A	1338	G	N1-C6-O6	-6.13	116.22	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	114	U	C2-N1-C1'	6.13	125.05	117.70
1	A	2075	U	C2-N3-C4	-6.13	123.32	127.00
1	A	2107	C	C2-N1-C1'	-6.13	112.06	118.80
1	A	668	G	C2-N3-C4	-6.13	108.84	111.90
1	A	1358	G	N1-C2-N2	-6.13	110.69	116.20
1	A	1829	A	N1-C6-N6	-6.13	114.92	118.60
1	A	2519	U	C5-C4-O4	-6.13	122.22	125.90
1	A	399	G	C8-N9-C4	6.12	108.85	106.40
1	A	1689	A	C8-N9-C4	-6.12	103.35	105.80
1	A	1779	U	C6-N1-C2	6.12	124.67	121.00
1	A	2548	G	C4-C5-N7	-6.12	108.35	110.80
1	A	2581	G	N1-C6-O6	-6.12	116.23	119.90
1	A	240	G	N7-C8-N9	-6.12	110.04	113.10
1	A	1797	C	N1-C2-O2	-6.12	115.23	118.90
1	A	2025	C	N3-C4-N4	-6.12	113.72	118.00
1	A	115	C	N3-C4-N4	6.12	122.28	118.00
1	A	445	C	C6-N1-C2	-6.12	117.85	120.30
1	A	563	G	C4-C5-N7	6.12	113.25	110.80
1	A	817	C	C5-C6-N1	6.12	124.06	121.00
1	A	2239	G	C5-C6-O6	6.12	132.27	128.60
1	A	1007	C	C2-N3-C4	-6.12	116.84	119.90
1	A	146	G	N7-C8-N9	-6.11	110.04	113.10
1	A	864	G	C8-N9-C4	-6.11	103.95	106.40
1	A	1698	A	N7-C8-N9	6.11	116.86	113.80
1	A	2063	C	N3-C4-N4	6.11	122.28	118.00
1	A	2319	G	N7-C8-N9	6.11	116.16	113.10
1	A	2728	U	N1-C2-O2	-6.11	118.52	122.80
1	A	1186	G	C2-N3-C4	-6.11	108.84	111.90
1	A	791	C	N3-C2-O2	-6.11	117.62	121.90
1	A	2006	C	C5-C6-N1	6.11	124.06	121.00
1	A	2848	G	C5-C6-O6	6.11	132.26	128.60
1	A	1279	G	C8-N9-C4	-6.11	103.96	106.40
1	A	1305	C	C2-N3-C4	-6.11	116.85	119.90
1	A	1698	A	N1-C6-N6	6.11	122.27	118.60
1	A	2316	C	C5-C6-N1	6.11	124.05	121.00
1	A	2371	G	N9-C4-C5	-6.11	102.96	105.40
1	A	776	G	N1-C2-N3	6.11	127.56	123.90
1	A	1773	A	C6-N1-C2	-6.11	114.94	118.60
1	A	1937	A	C8-N9-C4	6.11	108.24	105.80
1	A	577	G	C5-C6-O6	-6.10	124.94	128.60
2	B	86	G	C8-N9-C4	6.10	108.84	106.40
13	R	1	MET	CG-SD-CE	-6.10	90.44	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	494	G	C8-N9-C4	-6.10	103.96	106.40
1	A	2067	G	N7-C8-N9	6.10	116.15	113.10
1	A	573	G	C6-N1-C2	-6.10	121.44	125.10
1	A	756	C	N3-C4-C5	-6.10	119.46	121.90
1	A	36	G	N1-C6-O6	-6.09	116.24	119.90
1	A	658	C	N1-C2-O2	6.09	122.56	118.90
1	A	2091	U	N3-C2-O2	-6.09	117.94	122.20
1	A	2719	G	C4-C5-N7	6.09	113.24	110.80
1	A	2318	G	N3-C4-C5	-6.09	125.56	128.60
1	A	2620	C	C5-C6-N1	-6.09	117.96	121.00
1	A	2723	C	C5-C6-N1	-6.09	117.96	121.00
1	A	2296	U	C1'-O4'-C4'	-6.09	105.03	109.90
1	A	1180	C	C6-N1-C2	6.08	122.73	120.30
1	A	806	C	N3-C4-C5	6.08	124.33	121.90
1	A	531	C	N3-C2-O2	6.07	126.15	121.90
1	A	1004	C	N1-C2-O2	-6.07	115.26	118.90
1	A	121	G	C6-C5-N7	-6.07	126.76	130.40
1	A	186	G	C8-N9-C4	6.07	108.83	106.40
1	A	391	G	C6-C5-N7	-6.07	126.76	130.40
1	A	2306	C	C6-N1-C1'	-6.07	113.51	120.80
1	A	2123	G	C6-C5-N7	6.07	134.04	130.40
1	A	154(A)	C	N1-C2-O2	6.07	122.54	118.90
1	A	2239	G	N3-C2-N2	6.07	124.15	119.90
1	A	2447	G	C6-N1-C2	-6.07	121.46	125.10
1	A	186	G	C5-C6-O6	-6.07	124.96	128.60
1	A	1633	G	C6-C5-N7	-6.07	126.76	130.40
1	A	2730	C	N1-C2-O2	6.07	122.54	118.90
1	A	27	G	N1-C2-N2	6.06	121.66	116.20
1	A	1245	G	N1-C6-O6	-6.06	116.26	119.90
1	A	2372	G	N3-C2-N2	-6.06	115.66	119.90
1	A	1827	C	C5-C4-N4	6.06	124.44	120.20
1	A	2504	U	N3-C4-O4	-6.06	115.16	119.40
1	A	2699	C	C5-C4-N4	-6.06	115.96	120.20
1	A	645	C	C2-N1-C1'	6.06	125.46	118.80
1	A	1558	A	N1-C6-N6	6.05	122.23	118.60
1	A	2062	A	C4-C5-N7	6.05	113.73	110.70
1	A	2375	G	C5-C6-N1	6.05	114.53	111.50
1	A	1377	G	N3-C4-C5	-6.05	125.57	128.60
1	A	145	G	N7-C8-N9	-6.05	110.07	113.10
1	A	2826	A	C5-N7-C8	6.05	106.93	103.90
1	A	272(B)	G	C8-N9-C4	6.05	108.82	106.40
1	A	2592	G	N3-C4-C5	-6.05	125.58	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	613	G	N3-C2-N2	-6.05	115.67	119.90
1	A	145	G	C8-N9-C4	6.04	108.82	106.40
1	A	1373	A	C5-N7-C8	6.04	106.92	103.90
2	B	6	C	N3-C4-C5	6.04	124.32	121.90
1	A	446	G	N3-C2-N2	-6.04	115.67	119.90
1	A	1602	U	N3-C2-O2	-6.04	117.97	122.20
1	A	799	G	C8-N9-C4	-6.04	103.98	106.40
1	A	807	U	C4-C5-C6	6.04	123.32	119.70
1	A	1327	C	N1-C2-O2	-6.04	115.28	118.90
1	A	1977	A	C8-N9-C4	6.04	108.22	105.80
1	A	1955	U	N3-C4-O4	-6.04	115.17	119.40
1	A	2094	G	C8-N9-C4	-6.04	103.98	106.40
1	A	2335	A	N9-C4-C5	-6.04	103.38	105.80
1	A	591	C	C5-C6-N1	-6.04	117.98	121.00
2	B	18	G	C5-C6-O6	-6.04	124.98	128.60
1	A	518	G	C5-C6-N1	-6.04	108.48	111.50
1	A	558	G	C5-C6-O6	6.04	132.22	128.60
1	A	217	G	C5-C6-O6	-6.03	124.98	128.60
1	A	1417	C	C6-N1-C2	6.03	122.71	120.30
1	A	2342	C	C5-C4-N4	-6.03	115.98	120.20
1	A	1652	A	C8-N9-C4	-6.03	103.39	105.80
1	A	652(E)	G	C6-N1-C2	6.03	128.72	125.10
1	A	775	G	N3-C2-N2	6.03	124.12	119.90
1	A	1762	A	C2-N3-C4	6.03	113.61	110.60
1	A	2371	G	C8-N9-C4	6.03	108.81	106.40
1	A	1804	C	C5-C6-N1	6.03	124.01	121.00
1	A	694	U	N3-C2-O2	-6.02	117.98	122.20
1	A	1253	A	C6-C5-N7	6.02	136.52	132.30
1	A	2271	G	N1-C6-O6	-6.02	116.29	119.90
1	A	1403	C	C2-N3-C4	-6.02	116.89	119.90
1	A	1934	C	N1-C2-O2	6.02	122.51	118.90
1	A	476	G	C5-C6-N1	-6.02	108.49	111.50
1	A	17	G	N9-C4-C5	-6.01	103.00	105.40
1	A	26	G	N7-C8-N9	6.01	116.11	113.10
1	A	975	C	N3-C2-O2	-6.01	117.69	121.90
1	A	1567	A	C8-N9-C4	-6.01	103.39	105.80
1	A	2067	G	N9-C4-C5	6.01	107.80	105.40
1	A	2440	C	C2-N1-C1'	-6.01	112.19	118.80
1	A	32	C	N3-C2-O2	-6.01	117.69	121.90
2	B	118	G	C8-N9-C4	6.01	108.80	106.40
1	A	472	A	C8-N9-C4	-6.01	103.40	105.80
1	A	1192	G	C4-C5-N7	-6.00	108.40	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1008	C	N3-C4-C5	-6.00	119.50	121.90
2	B	30	C	C6-N1-C2	-6.00	117.90	120.30
21	Z	151	HIS	N-CA-C	6.00	127.20	111.00
1	A	563	G	C5-N7-C8	-6.00	101.30	104.30
1	A	2182	G	N3-C4-N9	-6.00	122.40	126.00
1	A	2258	C	N3-C4-N4	6.00	122.20	118.00
1	A	1381	G	C8-N9-C4	-5.99	104.00	106.40
1	A	2060	A	N1-C6-N6	-5.99	115.00	118.60
1	A	1383	C	N3-C4-N4	5.99	122.19	118.00
1	A	2018	G	N7-C8-N9	5.99	116.09	113.10
1	A	766	C	C4-C5-C6	5.99	120.39	117.40
1	A	1328	G	C6-N1-C2	-5.99	121.51	125.10
1	A	377	C	C5-C6-N1	-5.99	118.01	121.00
1	A	1344	G	N3-C2-N2	-5.99	115.71	119.90
1	A	1692	U	N1-C2-N3	5.99	118.49	114.90
1	A	1937	A	N7-C8-N9	-5.99	110.81	113.80
1	A	1107	G	C5-N7-C8	-5.98	101.31	104.30
1	A	1151	G	N3-C2-N2	-5.98	115.71	119.90
1	A	512	G	N3-C2-N2	5.98	124.08	119.90
1	A	2016	U	C4-C5-C6	5.98	123.29	119.70
1	A	729	G	N1-C6-O6	5.97	123.48	119.90
1	A	1256	G	N1-C2-N2	-5.97	110.82	116.20
1	A	817	C	C6-N1-C2	-5.97	117.91	120.30
1	A	1291	C	C5-C4-N4	5.97	124.38	120.20
1	A	940	G	N3-C4-C5	-5.97	125.61	128.60
1	A	386	G	N3-C4-C5	-5.97	125.62	128.60
1	A	620	G	C6-N1-C2	-5.97	121.52	125.10
1	A	1255	U	C5-C4-O4	-5.97	122.32	125.90
1	A	2105	C	C6-N1-C2	-5.97	117.91	120.30
1	A	2012	G	C4-C5-N7	5.96	113.19	110.80
1	A	2533	A	C8-N9-C4	5.96	108.19	105.80
1	A	966	G	C5-C6-O6	5.96	132.18	128.60
1	A	1659	U	N1-C2-N3	5.96	118.48	114.90
1	A	1811	G	C4-C5-N7	-5.95	108.42	110.80
1	A	692	C	N1-C2-O2	-5.95	115.33	118.90
1	A	613	G	N7-C8-N9	5.95	116.07	113.10
1	A	614	U	C6-N1-C2	-5.95	117.43	121.00
1	A	1203	G	C5-C6-O6	5.95	132.17	128.60
1	A	2002	G	N7-C8-N9	5.95	116.07	113.10
1	A	2683	C	C6-N1-C2	-5.95	117.92	120.30
1	A	1780	A	N7-C8-N9	5.95	116.77	113.80
1	A	1954	G	N1-C6-O6	5.95	123.47	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	C	N3-C4-C5	5.94	124.28	121.90
1	A	671	C	C6-N1-C2	-5.94	117.92	120.30
1	A	985	C	N3-C4-C5	5.94	124.28	121.90
1	A	2498	C	C5-C6-N1	-5.94	118.03	121.00
1	A	154	G	C5-C6-O6	-5.94	125.04	128.60
1	A	836	G	C5-C6-O6	5.94	132.16	128.60
1	A	2886	G	C8-N9-C4	-5.94	104.03	106.40
1	A	286	C	N3-C2-O2	-5.94	117.75	121.90
1	A	567	A	C6-C5-N7	-5.94	128.14	132.30
1	A	265	A	N7-C8-N9	5.93	116.77	113.80
1	A	294	A	C8-N9-C4	5.93	108.17	105.80
1	A	572	A	C8-N9-C4	-5.93	103.43	105.80
1	A	978	G	N9-C4-C5	-5.93	103.03	105.40
1	A	60	G	N9-C4-C5	-5.93	103.03	105.40
1	A	2306	C	C2-N3-C4	5.93	122.87	119.90
1	A	817	C	C4-C5-C6	-5.93	114.43	117.40
1	A	1780	A	N9-C4-C5	5.93	108.17	105.80
1	A	2024	G	N1-C6-O6	5.93	123.46	119.90
1	A	1022	G	C8-N9-C1'	5.93	134.71	127.00
1	A	2110	G	C4-N9-C1'	5.93	134.21	126.50
1	A	1320	C	C5-C6-N1	-5.92	118.04	121.00
1	A	1324	G	C5-C6-O6	-5.92	125.05	128.60
1	A	748	G	N1-C6-O6	-5.92	116.35	119.90
1	A	2699	C	C6-N1-C2	5.92	122.67	120.30
1	A	1606	G	N3-C2-N2	-5.92	115.76	119.90
1	A	2586	C	N1-C2-O2	-5.91	115.35	118.90
1	A	2638	G	N7-C8-N9	5.91	116.06	113.10
1	A	470	A	C5-N7-C8	-5.91	100.94	103.90
1	A	1204	A	O4'-C1'-N9	5.91	112.93	108.20
1	A	1349	A	N1-C6-N6	5.91	122.15	118.60
1	A	583	G	N1-C6-O6	5.91	123.44	119.90
1	A	941	A	N7-C8-N9	5.91	116.75	113.80
1	A	1495	A	C8-N9-C4	-5.91	103.44	105.80
1	A	1784	A	N7-C8-N9	-5.90	110.85	113.80
1	A	2043	C	C6-N1-C2	-5.90	117.94	120.30
1	A	319	C	C5-C6-N1	-5.90	118.05	121.00
1	A	674	G	N7-C8-N9	5.90	116.05	113.10
1	A	2447	G	C4-C5-C6	5.90	122.34	118.80
1	A	801	G	C4-C5-N7	-5.90	108.44	110.80
1	A	2816	C	C5-C6-N1	5.90	123.95	121.00
1	A	805	G	C8-N9-C4	-5.89	104.04	106.40
1	A	1008	C	C4-C5-C6	5.89	120.35	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2248	C	N1-C2-O2	-5.89	115.36	118.90
1	A	2428	G	N1-C6-O6	-5.89	116.36	119.90
1	A	1307	A	N7-C8-N9	-5.89	110.85	113.80
1	A	2592	G	C8-N9-C4	-5.89	104.04	106.40
1	A	693	C	N3-C2-O2	-5.89	117.78	121.90
1	A	1359	A	N9-C4-C5	5.89	108.16	105.80
1	A	1367	A	C8-N9-C4	5.89	108.16	105.80
1	A	2501	C	C6-N1-C2	5.89	122.66	120.30
1	A	1131	G	C5-C6-O6	5.89	132.13	128.60
1	A	1937	A	C5-N7-C8	5.89	106.84	103.90
1	A	476	G	N3-C4-C5	5.88	131.54	128.60
1	A	2823	A	C6-C5-N7	-5.88	128.18	132.30
1	A	574	C	C5-C4-N4	5.88	124.32	120.20
1	A	2661	G	N3-C4-N9	5.88	129.53	126.00
1	A	652(T)	C	C5-C4-N4	5.88	124.32	120.20
1	A	532	A	C8-N9-C4	-5.88	103.45	105.80
1	A	1207	C	N1-C2-O2	-5.88	115.37	118.90
1	A	2715	C	C5-C6-N1	-5.88	118.06	121.00
1	A	688	U	N3-C4-O4	5.88	123.51	119.40
1	A	1751	C	N3-C2-O2	5.88	126.01	121.90
1	A	1296	G	C8-N9-C4	-5.88	104.05	106.40
1	A	1336	A	N7-C8-N9	-5.88	110.86	113.80
1	A	271(Y)	U	N1-C2-N3	5.87	118.42	114.90
1	A	763	G	N3-C4-C5	-5.87	125.66	128.60
1	A	2193	G	C5-C6-N1	-5.87	108.56	111.50
1	A	2570	G	N3-C4-C5	5.87	131.54	128.60
1	A	2038	G	C6-C5-N7	-5.87	126.88	130.40
1	A	45	C	C6-N1-C2	-5.87	117.95	120.30
1	A	205	G	N1-C2-N2	-5.87	110.92	116.20
1	A	1488	G	C4-N9-C1'	5.87	134.13	126.50
1	A	446	G	C6-C5-N7	-5.87	126.88	130.40
1	A	1333	C	C4-C5-C6	-5.87	114.47	117.40
1	A	1811	G	N3-C2-N2	-5.87	115.79	119.90
1	A	2383	G	C4-N9-C1'	5.86	134.12	126.50
1	A	2079	U	C5-C6-N1	-5.86	119.77	122.70
1	A	2280	G	C8-N9-C4	-5.86	104.06	106.40
1	A	2283	C	N1-C2-O2	-5.86	115.38	118.90
1	A	2380	C	C2-N3-C4	-5.86	116.97	119.90
1	A	2104	G	N9-C4-C5	-5.86	103.06	105.40
1	A	650	C	C6-N1-C2	-5.86	117.96	120.30
1	A	2459	A	C8-N9-C4	-5.86	103.46	105.80
1	A	236	C	C5-C6-N1	-5.85	118.07	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	571	A	N1-C6-N6	5.85	122.11	118.60
1	A	778	G	N3-C2-N2	5.85	124.00	119.90
1	A	1121	C	C2-N3-C4	-5.85	116.97	119.90
1	A	1939	U	C5-C4-O4	-5.85	122.39	125.90
1	A	270	A	C8-N9-C4	5.85	108.14	105.80
1	A	1804	C	C4-C5-C6	-5.85	114.48	117.40
1	A	1784	A	C2-N3-C4	-5.85	107.68	110.60
1	A	2032	G	C5-N7-C8	5.84	107.22	104.30
1	A	509	C	N3-C2-O2	-5.84	117.81	121.90
1	A	1372	U	C5-C4-O4	5.84	129.41	125.90
1	A	1616	A	C5-C6-N6	-5.84	119.03	123.70
1	A	2467	C	N3-C2-O2	-5.84	117.81	121.90
1	A	527	C	C4-C5-C6	5.84	120.32	117.40
1	A	647	G	N7-C8-N9	5.84	116.02	113.10
1	A	1210	A	C4-C5-C6	5.84	119.92	117.00
1	A	516	C	N1-C2-N3	5.84	123.29	119.20
1	A	1028	A	N1-C2-N3	-5.84	126.38	129.30
1	A	2176	A	C6-N1-C2	5.84	122.10	118.60
1	A	1298	C	N3-C4-C5	5.84	124.23	121.90
1	A	2253	G	C2-N3-C4	-5.84	108.98	111.90
1	A	2383	G	N3-C2-N2	5.84	123.98	119.90
1	A	1981	A	N9-C4-C5	5.83	108.13	105.80
1	A	2018	G	C5-N7-C8	-5.83	101.38	104.30
1	A	2247	A	C2-N3-C4	-5.83	107.68	110.60
1	A	481	G	C8-N9-C4	-5.83	104.07	106.40
1	A	1324	G	C6-N1-C2	-5.83	121.60	125.10
1	A	310	A	C8-N9-C4	5.83	108.13	105.80
1	A	2084	C	C4-C5-C6	5.83	120.31	117.40
1	A	2545	G	N1-C6-O6	5.83	123.40	119.90
1	A	2683	C	N1-C2-O2	5.83	122.40	118.90
1	A	777	A	C8-N9-C4	-5.83	103.47	105.80
1	A	570	G	N3-C4-N9	5.82	129.49	126.00
1	A	2261	C	C6-N1-C2	-5.82	117.97	120.30
1	A	53	A	C4-C5-C6	5.82	119.91	117.00
1	A	208	C	C5-C6-N1	-5.82	118.09	121.00
1	A	751	A	C6-N1-C2	-5.82	115.11	118.60
1	A	194	G	C2-N3-C4	-5.82	108.99	111.90
1	A	381	G	C6-N1-C2	-5.82	121.61	125.10
1	A	70	G	N3-C2-N2	5.82	123.97	119.90
1	A	2026	C	C4-C5-C6	5.82	120.31	117.40
1	A	2497	A	C5-C6-N1	5.82	120.61	117.70
1	A	194	G	C5-N7-C8	5.81	107.21	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	333	G	C4-N9-C1'	5.81	134.06	126.50
1	A	1397	U	N3-C4-C5	5.81	118.09	114.60
1	A	2035	G	N3-C4-N9	-5.81	122.51	126.00
1	A	2185	C	C5-C4-N4	5.81	124.27	120.20
1	A	2297	C	N1-C2-O2	-5.81	115.41	118.90
1	A	2628	C	C6-N1-C2	5.81	122.62	120.30
1	A	122	G	C2-N3-C4	-5.81	109.00	111.90
1	A	2200	C	C4-C5-C6	5.81	120.31	117.40
1	A	1155	A	C8-N9-C4	-5.81	103.48	105.80
1	A	1806	C	N3-C4-C5	-5.81	119.58	121.90
1	A	1998	G	C5-C6-N1	-5.81	108.60	111.50
1	A	53	A	N3-C4-C5	-5.81	122.74	126.80
1	A	1129	A	N7-C8-N9	5.81	116.70	113.80
1	A	34	C	C6-N1-C2	-5.80	117.98	120.30
1	A	2057	A	C2-N3-C4	-5.80	107.70	110.60
1	A	2501	C	C2-N1-C1'	-5.80	112.42	118.80
1	A	2715	C	C2-N3-C4	-5.80	117.00	119.90
1	A	28	A	N1-C2-N3	-5.80	126.40	129.30
1	A	2045	C	N3-C2-O2	-5.80	117.84	121.90
1	A	2383	G	C8-N9-C1'	-5.80	119.46	127.00
1	A	2441	C	N3-C2-O2	-5.80	117.84	121.90
1	A	62	C	C6-N1-C2	5.80	122.62	120.30
1	A	2719	G	C4-C5-C6	-5.80	115.32	118.80
2	B	6	C	C2-N1-C1'	-5.80	112.42	118.80
1	A	94	C	C6-N1-C2	-5.79	117.98	120.30
1	A	2258	C	C5-C4-N4	-5.79	116.14	120.20
1	A	1524	G	C5-C6-O6	5.79	132.07	128.60
1	A	118	A	C2-N3-C4	5.79	113.49	110.60
1	A	1977	A	C2-N3-C4	-5.79	107.70	110.60
1	A	2273	A	C5-C6-N6	-5.79	119.07	123.70
1	A	480	A	C8-N9-C4	-5.79	103.48	105.80
1	A	1489	U	C5-C4-O4	5.78	129.37	125.90
1	A	62	C	C2-N3-C4	-5.78	117.01	119.90
1	A	129	C	C6-N1-C2	5.78	122.61	120.30
1	A	1186	G	C8-N9-C4	5.78	108.71	106.40
1	A	2394	C	N1-C2-O2	-5.78	115.44	118.90
1	A	1656	C	C6-N1-C2	-5.77	117.99	120.30
1	A	2111	C	C6-N1-C2	-5.77	117.99	120.30
2	B	120	A	C5-C6-N6	5.77	128.32	123.70
1	A	195	A	C6-N1-C2	-5.77	115.14	118.60
1	A	694	U	N1-C2-O2	5.77	126.84	122.80
1	A	2069	G	C6-N1-C2	-5.77	121.64	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1977	A	C5-C6-N1	-5.76	114.82	117.70
1	A	1809	A	N1-C6-N6	-5.76	115.14	118.60
1	A	333	G	C8-N9-C4	-5.76	104.10	106.40
1	A	2873	A	N1-C6-N6	-5.76	115.14	118.60
1	A	495	G	N7-C8-N9	-5.76	110.22	113.10
1	A	533	G	C8-N9-C4	-5.76	104.10	106.40
1	A	19	C	N3-C4-C5	-5.75	119.60	121.90
1	A	1925	C	N1-C2-O2	-5.75	115.45	118.90
1	A	2123	G	N3-C4-N9	-5.75	122.55	126.00
1	A	1024	G	N3-C2-N2	5.75	123.93	119.90
1	A	1817	G	N9-C4-C5	-5.75	103.10	105.40
1	A	2075	U	N1-C2-N3	5.75	118.35	114.90
1	A	2236	C	N1-C2-O2	-5.75	115.45	118.90
1	A	2616	C	C6-N1-C2	-5.75	118.00	120.30
1	A	488	G	N1-C2-N3	5.75	127.35	123.90
1	A	2318	G	C8-N9-C4	-5.75	104.10	106.40
2	B	31	C	C2-N1-C1'	-5.75	112.47	118.80
1	A	1194	A	C2-N3-C4	-5.75	107.72	110.60
1	A	2069	G	N3-C4-C5	-5.75	125.73	128.60
1	A	1154	G	N3-C4-C5	-5.75	125.73	128.60
1	A	1938	A	C4-C5-C6	5.75	119.87	117.00
1	A	671	C	N1-C2-O2	5.74	122.35	118.90
1	A	2832	U	N3-C2-O2	5.74	126.22	122.20
1	A	205	G	N3-C4-C5	-5.74	125.73	128.60
1	A	25	U	N1-C2-O2	-5.74	118.78	122.80
1	A	60	G	N1-C6-O6	5.74	123.34	119.90
1	A	1395	A	C8-N9-C4	5.74	108.10	105.80
1	A	1984	G	C8-N9-C4	-5.74	104.10	106.40
1	A	785	G	N3-C4-N9	-5.74	122.56	126.00
1	A	2271	G	N3-C4-N9	5.74	129.44	126.00
1	A	209	C	C2-N3-C4	-5.74	117.03	119.90
1	A	530	G	C6-C5-N7	5.74	133.84	130.40
1	A	928	G	C6-C5-N7	-5.73	126.96	130.40
1	A	2718	G	C8-N9-C4	-5.73	104.11	106.40
1	A	655	A	C2-N3-C4	-5.73	107.74	110.60
1	A	1600	C	N1-C2-N3	5.72	123.21	119.20
1	A	2306	C	C5-C6-N1	5.72	123.86	121.00
1	A	469	G	C8-N9-C4	-5.72	104.11	106.40
1	A	687	C	C6-N1-C2	5.72	122.59	120.30
1	A	1809	A	C8-N9-C4	-5.72	103.51	105.80
1	A	2301	C	C6-N1-C2	-5.72	118.01	120.30
1	A	2730	C	N3-C2-O2	-5.72	117.90	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	186	G	N1-C6-O6	5.71	123.33	119.90
1	A	1814	G	N3-C4-C5	-5.71	125.74	128.60
1	A	59	U	C2-N1-C1'	5.71	124.55	117.70
1	A	2728	U	C5-C4-O4	-5.71	122.47	125.90
1	A	563	G	C5-C6-N1	5.71	114.36	111.50
1	A	1806	C	N1-C2-O2	-5.71	115.47	118.90
1	A	97	C	N3-C2-O2	-5.71	117.90	121.90
1	A	205	G	C8-N9-C4	5.71	108.68	106.40
1	A	476	G	C2-N3-C4	-5.71	109.05	111.90
1	A	521	G	C8-N9-C4	-5.71	104.12	106.40
1	A	740	U	C5-C6-N1	-5.71	119.85	122.70
1	A	1805	U	N1-C2-N3	5.71	118.32	114.90
1	A	966	G	C4-C5-N7	-5.71	108.52	110.80
1	A	951	C	N3-C4-C5	5.70	124.18	121.90
1	A	1563	G	C4-C5-N7	5.70	113.08	110.80
1	A	2447	G	N3-C4-C5	-5.70	125.75	128.60
1	A	1253	A	C5-C6-N6	5.70	128.26	123.70
1	A	2841	C	C6-N1-C2	-5.70	118.02	120.30
1	A	73	A	C8-N9-C4	-5.70	103.52	105.80
1	A	1027	A	C5-C6-N6	-5.70	119.14	123.70
1	A	1332	G	N3-C4-C5	-5.70	125.75	128.60
1	A	1677	A	C2-N3-C4	-5.70	107.75	110.60
1	A	2705	A	N1-C6-N6	5.70	122.02	118.60
2	B	61	G	C8-N9-C4	-5.70	104.12	106.40
1	A	1606	G	N1-C6-O6	5.70	123.32	119.90
1	A	462	C	C6-N1-C2	-5.69	118.02	120.30
1	A	1505	C	C6-N1-C2	-5.69	118.02	120.30
1	A	1582	C	C6-N1-C2	5.69	122.58	120.30
1	A	2880	C	C6-N1-C2	-5.69	118.02	120.30
1	A	2885	C	N1-C2-O2	5.69	122.31	118.90
1	A	592	G	N3-C4-C5	-5.69	125.75	128.60
1	A	2307	G	N7-C8-N9	5.69	115.95	113.10
1	A	2358	G	C5-C6-O6	5.69	132.01	128.60
1	A	2359	C	N1-C2-N3	5.69	123.18	119.20
4	E	111	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	A	1623	G	C6-N1-C2	-5.69	121.69	125.10
1	A	2079	U	C4-C5-C6	5.69	123.11	119.70
1	A	2082	A	N1-C2-N3	5.69	132.14	129.30
1	A	2319	G	C2-N3-C4	-5.68	109.06	111.90
10	O	8	LEU	CA-CB-CG	5.68	128.38	115.30
1	A	575	A	C4-C5-C6	5.68	119.84	117.00
1	A	1488	G	N3-C4-C5	-5.68	125.76	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2341	G	N3-C2-N2	5.68	123.88	119.90
1	A	2723	C	N3-C4-N4	-5.68	114.02	118.00
1	A	129	C	N3-C4-C5	5.68	124.17	121.90
1	A	186	G	N7-C8-N9	-5.68	110.26	113.10
1	A	763	G	C5-C6-O6	5.68	132.01	128.60
1	A	1045	A	C8-N9-C4	5.68	108.07	105.80
1	A	1415	U	C5-C6-N1	-5.68	119.86	122.70
1	A	2104	G	N3-C4-N9	5.68	129.41	126.00
1	A	2503	A	N1-C2-N3	-5.68	126.46	129.30
1	A	2737	G	N3-C2-N2	-5.68	115.92	119.90
1	A	1204	A	C1'-O4'-C4'	-5.68	105.36	109.90
1	A	2001	A	C8-N9-C4	-5.67	103.53	105.80
1	A	2713	A	C5-C6-N6	-5.67	119.16	123.70
1	A	978	G	N1-C2-N2	-5.67	111.10	116.20
29	7	41	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	A	412	A	C2-N3-C4	-5.67	107.77	110.60
1	A	780	G	N1-C6-O6	5.67	123.30	119.90
1	A	2181	G	C5-C6-O6	5.67	132.00	128.60
1	A	983	A	C5-C6-N6	5.67	128.23	123.70
1	A	512	G	C5-C6-O6	5.66	132.00	128.60
1	A	674	G	C6-C5-N7	-5.66	127.00	130.40
1	A	1660	C	N3-C2-O2	-5.66	117.94	121.90
1	A	2287	A	C5-N7-C8	-5.66	101.07	103.90
1	A	2862	G	N7-C8-N9	-5.66	110.27	113.10
1	A	2883	A	N7-C8-N9	5.66	116.63	113.80
1	A	668	G	N3-C2-N2	5.66	123.86	119.90
1	A	425	G	N1-C2-N2	-5.66	111.11	116.20
1	A	1139	G	C5-C6-O6	-5.66	125.20	128.60
1	A	1971	A	C2-N3-C4	5.66	113.43	110.60
1	A	569	U	C5-C6-N1	-5.66	119.87	122.70
1	A	1796	U	C5-C6-N1	-5.66	119.87	122.70
1	A	1817	G	C2-N3-C4	-5.66	109.07	111.90
1	A	59	U	N3-C2-O2	-5.66	118.24	122.20
1	A	2181	G	N3-C2-N2	5.66	123.86	119.90
1	A	2377	A	C2-N3-C4	-5.66	107.77	110.60
1	A	2741	A	C8-N9-C4	5.66	108.06	105.80
1	A	375	C	C5-C6-N1	-5.65	118.17	121.00
1	A	1035	U	C2-N1-C1'	-5.65	110.92	117.70
1	A	1308	A	C8-N9-C4	-5.65	103.54	105.80
1	A	1619	G	C2-N3-C4	5.65	114.73	111.90
1	A	2371	G	C5-C6-O6	-5.65	125.21	128.60
1	A	2436	G	C8-N9-C4	5.65	108.66	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2626	C	C6-N1-C2	5.65	122.56	120.30
1	A	265	A	C5-C6-N6	-5.65	119.18	123.70
1	A	331	A	C2-N3-C4	5.65	113.42	110.60
1	A	446	G	N1-C2-N3	5.65	127.29	123.90
1	A	449	A	C4-C5-N7	5.65	113.53	110.70
1	A	1254	A	N7-C8-N9	5.65	116.62	113.80
1	A	2002	G	N3-C4-C5	-5.65	125.78	128.60
1	A	515	A	C5-C6-N6	-5.65	119.18	123.70
1	A	1127	A	N7-C8-N9	5.65	116.62	113.80
1	A	1800	C	C5-C6-N1	-5.65	118.18	121.00
1	A	2342	C	C5-C6-N1	5.65	123.82	121.00
2	B	78	A	C8-N9-C4	5.65	108.06	105.80
1	A	122	G	C5-C6-O6	-5.64	125.21	128.60
1	A	647	G	C4-N9-C1'	5.64	133.84	126.50
1	A	1119	C	C5-C6-N1	-5.64	118.18	121.00
1	A	1119	C	C6-N1-C2	5.64	122.56	120.30
1	A	53	A	N1-C2-N3	5.64	132.12	129.30
1	A	391	G	C4-C5-N7	5.64	113.06	110.80
1	A	1308	A	N9-C4-C5	5.64	108.06	105.80
1	A	1954	G	N3-C4-N9	-5.64	122.62	126.00
1	A	1930	G	C4-N9-C1'	-5.64	119.17	126.50
1	A	756	C	C6-N1-C2	-5.63	118.05	120.30
1	A	2325	G	C5-C6-O6	-5.63	125.22	128.60
1	A	580	C	N3-C4-C5	-5.63	119.65	121.90
1	A	2050	C	N3-C2-O2	-5.63	117.96	121.90
1	A	2072	G	N3-C2-N2	-5.63	115.96	119.90
1	A	1267	U	C5-C4-O4	5.63	129.28	125.90
1	A	213	A	C8-N9-C4	5.63	108.05	105.80
1	A	1372	U	C5-C6-N1	-5.63	119.89	122.70
1	A	936	C	C5-C6-N1	-5.62	118.19	121.00
1	A	1324	G	N3-C4-C5	-5.62	125.79	128.60
1	A	2191	G	C4-C5-N7	5.62	113.05	110.80
1	A	2195	C	C2-N3-C4	-5.62	117.09	119.90
1	A	806	C	C4-C5-C6	-5.61	114.59	117.40
1	A	2287	A	N1-C6-N6	5.61	121.97	118.60
1	A	309	G	N1-C6-O6	-5.61	116.53	119.90
1	A	371	A	C5-C6-N6	-5.61	119.21	123.70
1	A	1914	C	N1-C2-O2	5.61	122.27	118.90
2	B	58	A	N7-C8-N9	-5.61	110.99	113.80
1	A	835	A	C2-N3-C4	5.61	113.41	110.60
1	A	2062	A	C5-C6-N6	-5.61	119.21	123.70
1	A	1029	A	C4-C5-N7	5.61	113.50	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2010	G	C8-N9-C4	-5.61	104.16	106.40
1	A	19	C	C4-C5-C6	5.61	120.20	117.40
1	A	1539	G	C8-N9-C1'	-5.61	119.71	127.00
1	A	1834	U	C5-C6-N1	5.61	125.50	122.70
1	A	2287	A	C4-C5-N7	5.61	113.50	110.70
1	A	32	C	C5-C4-N4	5.60	124.12	120.20
1	A	520	G	N3-C2-N2	5.60	123.82	119.90
1	A	1599	C	N1-C2-O2	-5.60	115.54	118.90
1	A	1633	G	C5-C6-O6	-5.60	125.24	128.60
1	A	2545	G	C5-C6-O6	-5.60	125.24	128.60
1	A	127	A	C5-N7-C8	5.60	106.70	103.90
1	A	1158	C	N3-C4-N4	-5.60	114.08	118.00
1	A	1814	G	N1-C2-N2	-5.60	111.16	116.20
1	A	2002	G	N1-C6-O6	-5.60	116.54	119.90
1	A	2100	G	N3-C4-N9	5.60	129.36	126.00
1	A	328	U	C5-C4-O4	-5.59	122.54	125.90
1	A	2124	G	C6-N1-C2	5.59	128.46	125.10
1	A	2552	U	N1-C2-N3	5.59	118.26	114.90
1	A	737	C	N3-C2-O2	5.59	125.81	121.90
1	A	1028	A	N7-C8-N9	-5.59	111.01	113.80
1	A	1395	A	N7-C8-N9	-5.59	111.01	113.80
1	A	2071	A	C2-N3-C4	5.59	113.39	110.60
1	A	1225	G	C5-N7-C8	-5.58	101.51	104.30
1	A	2032	G	C2-N3-C4	-5.58	109.11	111.90
1	A	1632	A	C5-N7-C8	-5.58	101.11	103.90
1	A	2191	G	C6-C5-N7	-5.58	127.05	130.40
1	A	933	A	N1-C6-N6	5.58	121.95	118.60
1	A	1206	G	N1-C6-O6	-5.58	116.55	119.90
1	A	1497	U	N3-C4-O4	-5.58	115.50	119.40
1	A	1661	G	C5-N7-C8	5.58	107.09	104.30
1	A	2253	G	C5-C6-N1	-5.58	108.71	111.50
1	A	2307	G	C6-C5-N7	-5.58	127.05	130.40
1	A	2508	G	N1-C6-O6	-5.58	116.55	119.90
1	A	1791	A	N1-C6-N6	5.57	121.94	118.60
1	A	1438	U	C5-C6-N1	5.57	125.49	122.70
1	A	2047	U	C5-C6-N1	-5.57	119.91	122.70
1	A	1206	G	N9-C4-C5	5.57	107.63	105.40
1	A	1760	A	C5-C6-N6	5.57	128.16	123.70
1	A	512	G	N1-C6-O6	-5.57	116.56	119.90
1	A	1546	C	C2-N1-C1'	5.57	124.92	118.80
1	A	2578	G	N1-C2-N2	-5.57	111.19	116.20
1	A	971	C	N1-C2-N3	5.57	123.09	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2070	G	N9-C4-C5	-5.57	103.17	105.40
1	A	686	G	C6-C5-N7	-5.56	127.06	130.40
1	A	1980	G	N9-C4-C5	5.56	107.63	105.40
1	A	773	U	N3-C2-O2	-5.56	118.31	122.20
1	A	450	G	N3-C2-N2	-5.56	116.01	119.90
1	A	659	C	C5-C6-N1	-5.56	118.22	121.00
1	A	1367	A	N7-C8-N9	-5.56	111.02	113.80
1	A	2710	C	C5-C6-N1	-5.56	118.22	121.00
1	A	1315	C	N3-C4-N4	-5.56	114.11	118.00
1	A	313	C	C6-N1-C2	-5.56	118.08	120.30
1	A	2304	G	C2-N3-C4	5.56	114.68	111.90
2	B	1	U	C2-N1-C1'	5.56	124.37	117.70
1	A	533	G	C5-C6-O6	5.55	131.93	128.60
1	A	1954	G	N3-C2-N2	-5.55	116.01	119.90
1	A	2110	G	C8-N9-C1'	-5.55	119.78	127.00
1	A	1042	G	N1-C6-O6	5.55	123.23	119.90
1	A	1365	A	N9-C4-C5	-5.55	103.58	105.80
1	A	1563	G	N3-C2-N2	5.55	123.79	119.90
2	B	91	C	C6-N1-C2	5.55	122.52	120.30
1	A	1378	A	C8-N9-C4	-5.55	103.58	105.80
1	A	1791	A	C2-N3-C4	-5.55	107.83	110.60
1	A	2489	G	C6-C5-N7	-5.55	127.07	130.40
1	A	1574	C	C2-N3-C4	-5.55	117.13	119.90
1	A	2271	G	C4-N9-C1'	5.55	133.71	126.50
1	A	54	G	N1-C6-O6	5.54	123.23	119.90
1	A	1614	A	C2-N3-C4	-5.54	107.83	110.60
1	A	2519	U	N1-C2-O2	-5.54	118.92	122.80
1	A	429	A	C5-N7-C8	-5.54	101.13	103.90
1	A	1302	A	N7-C8-N9	-5.54	111.03	113.80
1	A	2325	G	C4-N9-C1'	5.54	133.70	126.50
1	A	2733	A	N1-C6-N6	5.54	121.92	118.60
1	A	1568	G	N1-C6-O6	-5.54	116.58	119.90
1	A	2056	G	N9-C4-C5	-5.54	103.19	105.40
1	A	2705	A	C5-C6-N6	-5.54	119.27	123.70
1	A	536	A	N1-C6-N6	-5.54	115.28	118.60
1	A	2623	G	N3-C4-C5	-5.54	125.83	128.60
1	A	1605	C	N3-C2-O2	-5.54	118.03	121.90
18	W	11	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	A	136	G	C8-N9-C4	5.53	108.61	106.40
1	A	269	U	C2-N1-C1'	5.53	124.34	117.70
1	A	2020	A	C5-C6-N6	-5.53	119.28	123.70
1	A	940	G	N9-C4-C5	5.53	107.61	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2503	A	C4-C5-N7	5.53	113.47	110.70
2	B	51	G	N3-C4-N9	5.53	129.32	126.00
1	A	1622	G	N3-C2-N2	-5.53	116.03	119.90
1	A	775	G	C8-N9-C4	5.53	108.61	106.40
1	A	801	G	N3-C4-N9	-5.53	122.69	126.00
1	A	847	U	C6-N1-C1'	5.53	128.94	121.20
1	A	2373	G	C8-N9-C4	5.53	108.61	106.40
1	A	2381	C	C2-N3-C4	-5.53	117.14	119.90
1	A	2562	U	C5-C6-N1	-5.53	119.94	122.70
1	A	468	G	C8-N9-C4	5.52	108.61	106.40
1	A	567	A	C2-N3-C4	-5.52	107.84	110.60
1	A	2088	G	N1-C6-O6	5.52	123.22	119.90
1	A	2437	U	C4-C5-C6	5.52	123.01	119.70
1	A	546	C	C5-C6-N1	5.52	123.76	121.00
1	A	1274	A	C5-N7-C8	-5.52	101.14	103.90
1	A	32	C	C5-C6-N1	-5.52	118.24	121.00
1	A	2732	G	N1-C6-O6	-5.52	116.59	119.90
1	A	516	C	C5-C6-N1	-5.52	118.24	121.00
1	A	576	U	N3-C4-O4	-5.52	115.54	119.40
1	A	1510	G	N3-C4-N9	5.52	129.31	126.00
1	A	210	C	N3-C4-C5	5.51	124.11	121.90
1	A	512	G	N9-C4-C5	5.51	107.61	105.40
1	A	1221(A)	C	C6-N1-C2	5.51	122.51	120.30
1	A	2495	G	C2-N3-C4	-5.51	109.14	111.90
1	A	512	G	C4-C5-N7	-5.51	108.59	110.80
1	A	2088	G	C5-C6-O6	-5.51	125.29	128.60
1	A	910	A	C5-N7-C8	5.51	106.66	103.90
1	A	2255	G	N1-C6-O6	-5.51	116.59	119.90
1	A	2473	U	N3-C2-O2	-5.51	118.35	122.20
1	A	194	G	C4-C5-C6	5.50	122.10	118.80
1	A	961	C	C4-C5-C6	5.50	120.15	117.40
1	A	2379	G	N3-C2-N2	5.50	123.75	119.90
1	A	2493	U	N3-C2-O2	-5.50	118.35	122.20
1	A	385	C	C5-C6-N1	5.50	123.75	121.00
1	A	1397	U	C2-N3-C4	-5.50	123.70	127.00
1	A	2387	U	C5-C6-N1	-5.50	119.95	122.70
1	A	518	G	C5-C6-O6	5.50	131.90	128.60
2	B	117	G	C8-N9-C4	5.50	108.60	106.40
1	A	291	C	N1-C2-O2	-5.50	115.60	118.90
1	A	1039	G	C6-C5-N7	5.50	133.70	130.40
1	A	1234	U	N3-C2-O2	-5.50	118.35	122.20
1	A	2450	A	C8-N9-C4	5.50	108.00	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2846	G	C8-N9-C4	-5.50	104.20	106.40
1	A	1209	G	C5-C6-N1	-5.49	108.75	111.50
1	A	1992	G	P-O3'-C3'	5.49	126.29	119.70
1	A	2325	G	N1-C6-O6	5.49	123.20	119.90
1	A	2440	C	C6-N1-C2	5.49	122.50	120.30
1	A	2689	U	N3-C2-O2	-5.49	118.36	122.20
1	A	1505	C	N3-C2-O2	-5.49	118.06	121.90
1	A	2544	G	C8-N9-C4	5.49	108.59	106.40
1	A	2581	G	N3-C2-N2	5.49	123.74	119.90
1	A	1319	G	C4-N9-C1'	5.49	133.63	126.50
1	A	2881	C	C6-N1-C2	-5.49	118.11	120.30
1	A	2505	G	N1-C2-N2	-5.48	111.27	116.20
1	A	2345	G	C8-N9-C4	-5.48	104.21	106.40
1	A	1641	A	C2-N3-C4	-5.48	107.86	110.60
1	A	2592	G	C2-N3-C4	5.48	114.64	111.90
1	A	2503	A	C2-N3-C4	5.48	113.34	110.60
1	A	674	G	C5-C6-N1	-5.48	108.76	111.50
1	A	987	G	N3-C4-N9	-5.48	122.71	126.00
1	A	516	C	C2-N3-C4	-5.48	117.16	119.90
1	A	1186	G	N9-C4-C5	-5.47	103.21	105.40
1	A	1765	C	N3-C4-C5	5.47	124.09	121.90
1	A	2098	U	C2-N3-C4	5.47	130.28	127.00
2	B	104	U	N3-C4-C5	5.47	117.88	114.60
1	A	435	C	C5-C4-N4	-5.47	116.37	120.20
1	A	2591	C	N3-C4-C5	5.47	124.09	121.90
1	A	1411	C	N3-C4-C5	5.47	124.09	121.90
1	A	2315	G	C8-N9-C4	5.47	108.59	106.40
1	A	1582	C	C2-N3-C4	-5.47	117.17	119.90
1	A	1606	G	C5-C6-O6	-5.47	125.32	128.60
1	A	53	A	N9-C4-C5	5.47	107.99	105.80
1	A	1135	C	C5-C6-N1	5.47	123.73	121.00
1	A	2574	G	N1-C6-O6	-5.47	116.62	119.90
1	A	47	C	C5-C4-N4	5.46	124.03	120.20
1	A	199	A	C5-C6-N1	5.46	120.43	117.70
1	A	333	G	N7-C8-N9	5.46	115.83	113.10
1	A	1290	C	C6-N1-C2	-5.46	118.11	120.30
1	A	1358	G	N3-C2-N2	5.46	123.72	119.90
1	A	148	C	C5-C4-N4	-5.46	116.38	120.20
1	A	1563	G	N1-C2-N2	-5.46	111.28	116.20
1	A	1164	G	C5-N7-C8	5.46	107.03	104.30
1	A	2069	G	N3-C4-N9	5.46	129.28	126.00
1	A	2312	U	C6-N1-C2	-5.46	117.72	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1028	A	N1-C6-N6	5.46	121.87	118.60
1	A	2566	A	N9-C4-C5	5.46	107.98	105.80
1	A	2226	C	N3-C4-C5	5.45	124.08	121.90
1	A	1352	U	C6-N1-C2	-5.45	117.73	121.00
1	A	1429	G	C8-N9-C1'	-5.45	119.91	127.00
1	A	272(C)	G	C2-N3-C4	-5.45	109.17	111.90
1	A	662	G	N1-C6-O6	-5.45	116.63	119.90
1	A	1130	U	N1-C2-O2	5.45	126.62	122.80
1	A	1816	G	C4-N9-C1'	5.45	133.59	126.50
1	A	2044	C	C4-C5-C6	5.45	120.12	117.40
1	A	2195	C	C2-N1-C1'	-5.45	112.81	118.80
1	A	1210	A	C5-C6-N1	-5.45	114.98	117.70
1	A	1328	G	N3-C4-N9	5.45	129.27	126.00
1	A	1368	G	C6-N1-C2	-5.45	121.83	125.10
1	A	2090	G	C4-C5-N7	-5.45	108.62	110.80
1	A	2501	C	C5-C6-N1	-5.45	118.28	121.00
1	A	309	G	N3-C2-N2	5.45	123.71	119.90
1	A	1049	C	C4-C5-C6	-5.45	114.68	117.40
1	A	2463	C	C2-N3-C4	-5.45	117.18	119.90
1	A	996	A	N1-C6-N6	-5.44	115.33	118.60
1	A	830	G	N1-C2-N2	-5.44	111.30	116.20
1	A	1437	C	N1-C2-O2	5.44	122.17	118.90
1	A	1839	G	N9-C4-C5	-5.44	103.22	105.40
1	A	2075	U	C4-C5-C6	5.44	122.97	119.70
1	A	1959	G	N1-C6-O6	-5.44	116.64	119.90
1	A	584	C	N3-C4-C5	5.44	124.08	121.90
1	A	570	G	N3-C2-N2	5.44	123.70	119.90
1	A	727	A	C2-N3-C4	-5.44	107.88	110.60
1	A	1775	U	C5-C4-O4	-5.44	122.64	125.90
1	A	1783	A	C8-N9-C4	-5.43	103.63	105.80
1	A	2699	C	N3-C4-N4	5.43	121.80	118.00
1	A	450	G	C4-C5-N7	-5.43	108.63	110.80
1	A	1572	A	N1-C2-N3	5.43	132.02	129.30
1	A	2319	G	C4-C5-N7	5.43	112.97	110.80
1	A	2571	C	C2-N1-C1'	5.43	124.78	118.80
1	A	2315	G	N9-C4-C5	-5.43	103.23	105.40
1	A	210	C	C6-N1-C2	5.43	122.47	120.30
1	A	1112	G	C4-N9-C1'	-5.43	119.44	126.50
1	A	1269	A	C5-C6-N1	5.43	120.41	117.70
1	A	1899	G	N1-C2-N2	5.43	121.09	116.20
1	A	2596	U	N1-C2-O2	-5.43	119.00	122.80
1	A	139(A)	G	C6-C5-N7	-5.42	127.14	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1615	C	C2-N3-C4	5.42	122.61	119.90
1	A	435	C	N3-C4-N4	5.42	121.80	118.00
2	B	114	C	C6-N1-C2	-5.42	118.13	120.30
1	A	949	C	C5-C6-N1	-5.42	118.29	121.00
1	A	2442	C	N3-C4-C5	5.42	124.07	121.90
1	A	1614	A	N3-C4-N9	-5.42	123.07	127.40
1	A	2015	A	C5-C6-N1	-5.42	114.99	117.70
1	A	2145	C	C6-N1-C2	-5.41	118.13	120.30
1	A	599	G	N9-C4-C5	-5.41	103.23	105.40
1	A	773	U	C6-N1-C2	-5.41	117.75	121.00
1	A	528	A	C5-C6-N6	5.41	128.03	123.70
1	A	774	A	N9-C4-C5	5.41	107.96	105.80
1	A	1509	C	N1-C2-O2	5.41	122.15	118.90
1	A	1939	U	N3-C2-O2	5.41	125.99	122.20
1	A	871	U	N3-C2-O2	5.41	125.99	122.20
1	A	2028	U	C5-C6-N1	-5.41	120.00	122.70
1	A	2030	A	C8-N9-C4	5.41	107.96	105.80
1	A	2466	C	N3-C4-N4	5.41	121.79	118.00
1	A	1930	G	C8-N9-C1'	5.41	134.03	127.00
1	A	38	A	C6-N1-C2	-5.41	115.36	118.60
1	A	116	C	N1-C2-O2	-5.41	115.66	118.90
1	A	1383	C	N3-C4-C5	-5.41	119.74	121.90
1	A	1791	A	C5-N7-C8	-5.40	101.20	103.90
1	A	69	C	C4-C5-C6	5.40	120.10	117.40
1	A	542	C	C3'-C2'-C1'	-5.40	97.18	101.50
1	A	640	C	N3-C2-O2	5.40	125.68	121.90
1	A	830	G	N1-C6-O6	-5.40	116.66	119.90
1	A	1119	C	C2-N1-C1'	-5.40	112.86	118.80
1	A	130	C	N1-C2-N3	-5.40	115.42	119.20
1	A	131	G	N1-C2-N2	-5.40	111.34	116.20
1	A	1188	U	N3-C2-O2	5.39	125.98	122.20
1	A	2063	C	N3-C4-C5	-5.39	119.74	121.90
1	A	2508	G	C4-C5-N7	-5.39	108.64	110.80
1	A	47	C	C5-C6-N1	-5.39	118.30	121.00
1	A	154	G	N1-C6-O6	5.39	123.14	119.90
1	A	69	C	N1-C2-N3	5.39	122.97	119.20
1	A	281	G	C8-N9-C4	5.39	108.56	106.40
1	A	750	A	C5-C6-N6	5.39	128.01	123.70
1	A	2420	C	N3-C2-O2	5.39	125.67	121.90
1	A	744	G	N1-C6-O6	-5.39	116.67	119.90
1	A	1698	A	N3-C4-C5	5.39	130.57	126.80
1	A	375	C	C2-N3-C4	-5.39	117.21	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	679	C	N3-C2-O2	5.39	125.67	121.90
1	A	917	A	N9-C4-C5	-5.39	103.65	105.80
1	A	2705	A	C6-N1-C2	-5.39	115.37	118.60
1	A	45	C	N1-C2-N3	5.38	122.97	119.20
1	A	1348	G	C5-C6-O6	-5.38	125.37	128.60
1	A	1772	G	C8-N9-C4	5.38	108.55	106.40
1	A	2191	G	N9-C4-C5	-5.38	103.25	105.40
1	A	2372	G	C5-C6-O6	-5.38	125.37	128.60
1	A	1928	A	C5-C6-N1	5.38	120.39	117.70
1	A	2618	G	C2-N3-C4	5.38	114.59	111.90
1	A	1214	A	C5-N7-C8	5.38	106.59	103.90
1	A	864	G	N3-C4-C5	-5.38	125.91	128.60
1	A	2024	G	N9-C4-C5	-5.38	103.25	105.40
1	A	2296	U	N1-C1'-C2'	5.38	120.99	114.00
1	A	780	G	C5-C6-O6	-5.38	125.38	128.60
1	A	2060	A	C5-C6-N6	5.38	128.00	123.70
1	A	2411	A	N9-C4-C5	-5.38	103.65	105.80
1	A	1708	C	N3-C2-O2	5.37	125.66	121.90
1	A	2239	G	N1-C6-O6	-5.37	116.68	119.90
1	A	2383	G	N1-C2-N2	-5.37	111.36	116.20
1	A	271(M)	G	N3-C4-N9	5.37	129.22	126.00
1	A	330	A	C5-N7-C8	-5.37	101.21	103.90
1	A	729	G	C5-C6-O6	-5.37	125.38	128.60
2	B	54	G	N9-C4-C5	-5.37	103.25	105.40
1	A	2570	G	N3-C4-N9	-5.37	122.78	126.00
1	A	1740	G	C8-N9-C4	-5.37	104.25	106.40
1	A	2221	G	N7-C8-N9	5.37	115.78	113.10
9	N	74	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	A	807	U	N3-C4-C5	-5.37	111.38	114.60
1	A	990	A	N1-C6-N6	5.37	121.82	118.60
1	A	2271	G	C5-C6-N1	5.37	114.18	111.50
1	A	469	G	N3-C4-C5	-5.36	125.92	128.60
1	A	2232	U	C5-C6-N1	-5.36	120.02	122.70
1	A	2606	C	C5-C6-N1	-5.36	118.32	121.00
1	A	2048	G	C4-N9-C1'	5.36	133.47	126.50
2	B	22	U	C6-N1-C2	-5.36	117.78	121.00
1	A	418	G	C6-C5-N7	-5.36	127.18	130.40
1	A	1914	C	N3-C2-O2	-5.36	118.15	121.90
1	A	2022	U	N1-C2-O2	-5.36	119.05	122.80
1	A	2071	A	C6-N1-C2	-5.36	115.38	118.60
1	A	783	A	C8-N9-C4	-5.36	103.66	105.80
1	A	1431	U	C5-C6-N1	5.36	125.38	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4	C	C6-N1-C2	5.36	122.44	120.30
1	A	546	C	C6-N1-C2	-5.36	118.16	120.30
1	A	556	G	C5-C6-N1	-5.36	108.82	111.50
1	A	2063	C	N3-C2-O2	5.36	125.65	121.90
1	A	2590	A	N1-C6-N6	-5.36	115.39	118.60
1	A	68	G	N1-C2-N3	5.36	127.11	123.90
1	A	1652	A	C2-N3-C4	5.35	113.28	110.60
1	A	1962	C	C5-C6-N1	5.35	123.67	121.00
1	A	2497	A	C4-C5-C6	5.35	119.68	117.00
1	A	1290	C	C5-C4-N4	5.35	123.94	120.20
1	A	1799	G	N1-C6-O6	-5.35	116.69	119.90
1	A	512	G	N1-C2-N2	-5.35	111.39	116.20
1	A	1222	C	C2-N1-C1'	-5.35	112.92	118.80
1	A	2432	A	N7-C8-N9	-5.35	111.13	113.80
1	A	2051	A	N9-C4-C5	5.35	107.94	105.80
1	A	1424	G	N1-C2-N3	5.34	127.11	123.90
1	A	2510	C	N3-C4-N4	-5.34	114.26	118.00
1	A	2491	U	C5-C4-O4	-5.34	122.69	125.90
1	A	2723	C	N1-C2-O2	5.34	122.11	118.90
2	B	42	C	C6-N1-C2	5.34	122.44	120.30
1	A	1544	A	N9-C4-C5	5.34	107.94	105.80
1	A	2248	C	N1-C2-N3	5.34	122.94	119.20
1	A	2503	A	C6-C5-N7	-5.34	128.56	132.30
1	A	2588	G	C8-N9-C4	-5.34	104.26	106.40
1	A	446	G	N9-C4-C5	-5.34	103.27	105.40
1	A	577	G	N3-C4-N9	5.34	129.20	126.00
1	A	2690	C	C6-N1-C2	-5.34	118.17	120.30
1	A	546	C	N3-C4-N4	5.33	121.73	118.00
1	A	1338	G	N3-C2-N2	5.33	123.64	119.90
2	B	116	G	C2-N3-C4	-5.33	109.23	111.90
1	A	690	G	C6-N1-C2	-5.33	121.90	125.10
1	A	806	C	C5-C4-N4	-5.33	116.47	120.20
1	A	978	G	N3-C2-N2	5.33	123.63	119.90
1	A	1039	G	C4-N9-C1'	-5.33	119.57	126.50
1	A	932	G	C6-N1-C2	-5.33	121.90	125.10
1	A	377	C	C5-C4-N4	-5.33	116.47	120.20
1	A	448	U	N1-C2-O2	-5.33	119.07	122.80
1	A	772	C	N3-C4-C5	-5.33	119.77	121.90
1	A	910	A	C4-C5-N7	-5.33	108.04	110.70
1	A	1335	U	C4-C5-C6	5.33	122.90	119.70
1	A	529	A	C8-N9-C4	-5.32	103.67	105.80
1	A	1226	A	N1-C2-N3	-5.32	126.64	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1459	G	N3-C4-C5	-5.32	125.94	128.60
1	A	1833	U	N1-C2-N3	5.32	118.09	114.90
1	A	2451	A	N1-C6-N6	-5.32	115.41	118.60
1	A	252	G	N1-C2-N3	5.32	127.09	123.90
1	A	2572	A	C5-N7-C8	-5.32	101.24	103.90
1	A	60	G	N3-C4-C5	5.32	131.26	128.60
1	A	2066	C	C2-N3-C4	-5.32	117.24	119.90
1	A	1238	G	C5-C6-O6	-5.32	125.41	128.60
1	A	1121	C	C5-C6-N1	-5.32	118.34	121.00
1	A	1434	A	N1-C6-N6	-5.32	115.41	118.60
1	A	1997	G	C2-N3-C4	5.32	114.56	111.90
1	A	2689	U	C6-N1-C2	-5.32	117.81	121.00
2	B	7	G	N1-C6-O6	5.32	123.09	119.90
1	A	70	G	C8-N9-C4	-5.32	104.27	106.40
1	A	271(K)	U	C2-N1-C1'	5.32	124.08	117.70
1	A	1204	A	C4-C5-C6	5.32	119.66	117.00
1	A	1696	G	N1-C6-O6	-5.32	116.71	119.90
9	N	33	LEU	CA-CB-CG	5.32	127.53	115.30
1	A	959	A	N9-C4-C5	5.31	107.93	105.80
1	A	1708	C	N3-C4-C5	5.31	124.03	121.90
1	A	2070	G	C5-N7-C8	5.31	106.96	104.30
1	A	2500	U	N3-C4-O4	-5.31	115.68	119.40
1	A	2409	G	C6-C5-N7	-5.31	127.21	130.40
1	A	2673	G	C5-N7-C8	-5.31	101.64	104.30
1	A	664	C	C6-N1-C2	5.31	122.42	120.30
1	A	2163	C	C6-N1-C2	-5.31	118.18	120.30
1	A	2476	A	C4-C5-C6	5.31	119.66	117.00
23	1	46	LEU	CA-CB-CG	5.31	127.51	115.30
1	A	59	U	C6-N1-C1'	-5.31	113.77	121.20
1	A	521	G	N9-C4-C5	5.31	107.52	105.40
1	A	726	G	C4-C5-N7	-5.31	108.68	110.80
1	A	1149	G	N1-C6-O6	5.30	123.08	119.90
1	A	1773	A	C5-C6-N1	5.30	120.35	117.70
1	A	2016	U	N3-C2-O2	-5.30	118.49	122.20
1	A	1974	C	N1-C2-O2	5.30	122.08	118.90
1	A	2163	C	C5-C6-N1	5.30	123.65	121.00
1	A	2755	C	C5-C6-N1	5.30	123.65	121.00
1	A	792	G	N3-C4-C5	-5.30	125.95	128.60
1	A	645	C	C5-C6-N1	5.30	123.65	121.00
1	A	1302	A	C8-N9-C4	5.30	107.92	105.80
1	A	1539	G	N1-C6-O6	5.30	123.08	119.90
2	B	60	C	C5-C6-N1	5.30	123.65	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	454	A	N9-C4-C5	5.29	107.92	105.80
1	A	608	A	C2-N3-C4	-5.29	107.95	110.60
1	A	1312	U	C5-C6-N1	-5.29	120.06	122.70
1	A	481	G	N9-C4-C5	5.29	107.52	105.40
1	A	981	A	N7-C8-N9	-5.29	111.16	113.80
1	A	2186	G	C5-C6-O6	5.29	131.77	128.60
1	A	1546	C	C5-C6-N1	5.29	123.64	121.00
1	A	2487	G	C4-C5-N7	5.29	112.91	110.80
1	A	332	A	N9-C4-C5	5.28	107.91	105.80
1	A	2379	G	C8-N9-C1'	-5.28	120.13	127.00
13	R	60	LEU	CA-CB-CG	5.28	127.45	115.30
1	A	690	G	C2-N3-C4	5.28	114.54	111.90
1	A	2387	U	C2-N3-C4	-5.28	123.83	127.00
2	B	29	A	C8-N9-C4	-5.28	103.69	105.80
1	A	202	U	C6-N1-C2	5.28	124.17	121.00
1	A	205	G	N7-C8-N9	-5.28	110.46	113.10
1	A	600	G	N1-C2-N2	-5.28	111.45	116.20
1	A	611	C	N3-C2-O2	-5.28	118.21	121.90
1	A	1219	G	N9-C4-C5	-5.28	103.29	105.40
1	A	1998	G	N1-C6-O6	5.28	123.06	119.90
1	A	40	C	N1-C2-O2	-5.27	115.74	118.90
1	A	113	G	N1-C6-O6	5.27	123.06	119.90
1	A	2363	C	C2-N3-C4	-5.27	117.26	119.90
1	A	1191	G	N9-C4-C5	5.27	107.51	105.40
1	A	146	G	C4-C5-N7	-5.27	108.69	110.80
1	A	2319	G	C8-N9-C4	-5.27	104.29	106.40
1	A	2562	U	C2-N3-C4	-5.27	123.84	127.00
1	A	1641	A	N1-C2-N3	5.27	131.93	129.30
1	A	2615	U	N3-C4-C5	5.27	117.76	114.60
1	A	594	U	C5-C4-O4	5.26	129.06	125.90
1	A	914	C	N1-C2-O2	5.26	122.06	118.90
1	A	1204	A	C5-C6-N6	-5.26	119.49	123.70
1	A	1661	G	C4-C5-N7	-5.26	108.69	110.80
1	A	2072	G	N1-C6-O6	5.26	123.06	119.90
1	A	2182	G	C5-C6-N1	-5.26	108.87	111.50
1	A	2700	C	C5-C4-N4	-5.26	116.52	120.20
1	A	2616	C	N1-C2-N3	5.26	122.88	119.20
1	A	2622	C	N3-C2-O2	-5.26	118.22	121.90
1	A	839	U	C6-N1-C2	-5.26	117.84	121.00
1	A	2237	G	N3-C2-N2	5.26	123.58	119.90
1	A	745	G	N7-C8-N9	5.26	115.73	113.10
1	A	2071	A	N3-C4-C5	-5.26	123.12	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2005	A	N1-C2-N3	-5.26	126.67	129.30
1	A	567	A	N1-C6-N6	5.26	121.75	118.60
1	A	734	A	N1-C6-N6	5.26	121.75	118.60
1	A	2142	C	C5-C6-N1	5.26	123.63	121.00
1	A	1831	G	C5-C6-O6	5.25	131.75	128.60
1	A	533	G	N7-C8-N9	5.25	115.73	113.10
1	A	568	U	N3-C4-O4	5.25	123.08	119.40
1	A	2509	G	C5-C6-N1	5.25	114.13	111.50
1	A	2692	C	N1-C2-N3	5.25	122.88	119.20
1	A	2098	U	C5-C6-N1	5.25	125.33	122.70
1	A	2268	A	N1-C6-N6	5.25	121.75	118.60
25	3	30	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	A	669	G	C4-C5-N7	5.25	112.90	110.80
1	A	1331	A	C2-N3-C4	-5.25	107.97	110.60
1	A	2387	U	N1-C2-N3	5.25	118.05	114.90
1	A	47	C	N3-C2-O2	-5.25	118.23	121.90
1	A	205	G	C5-N7-C8	5.25	106.92	104.30
1	A	556	G	C6-N1-C2	5.25	128.25	125.10
1	A	613	G	N1-C6-O6	5.25	123.05	119.90
26	4	42	PHE	C-N-CA	5.25	134.82	121.70
1	A	1788	C	C2-N1-C1'	5.25	124.57	118.80
1	A	2361	A	C4-C5-N7	5.25	113.32	110.70
1	A	2439	A	N7-C8-N9	5.25	116.42	113.80
1	A	2505	G	N3-C2-N2	5.25	123.57	119.90
1	A	2571	C	C6-N1-C1'	-5.25	114.51	120.80
2	B	1	U	C5-C6-N1	5.25	125.32	122.70
1	A	1630	G	C8-N9-C4	-5.24	104.30	106.40
1	A	2335	A	C8-N9-C4	5.24	107.90	105.80
1	A	2492	U	C6-N1-C2	-5.24	117.86	121.00
1	A	2345	G	N9-C4-C5	5.24	107.50	105.40
1	A	2709	G	N3-C4-N9	5.24	129.14	126.00
1	A	737	C	C5-C6-N1	-5.24	118.38	121.00
1	A	755	C	N3-C4-C5	-5.24	119.81	121.90
1	A	2621	A	C2-N3-C4	-5.24	107.98	110.60
1	A	291	C	N3-C2-O2	5.24	125.56	121.90
1	A	331	A	C6-N1-C2	-5.24	115.46	118.60
1	A	2013	A	C5-C6-N1	5.24	120.32	117.70
2	B	56	G	N1-C6-O6	-5.24	116.76	119.90
1	A	1861	G	C8-N9-C1'	5.23	133.80	127.00
1	A	2045	C	C5-C6-N1	-5.23	118.38	121.00
1	A	2294	C	N1-C2-O2	5.23	122.04	118.90
1	A	254	G	N3-C4-C5	-5.23	125.98	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1275	A	C2-N3-C4	-5.23	107.98	110.60
1	A	1573	G	C8-N9-C4	5.23	108.49	106.40
1	A	2430	A	C2-N3-C4	-5.23	107.99	110.60
30	8	57	ARG	NE-CZ-NH2	5.23	122.92	120.30
1	A	177	G	N3-C2-N2	5.23	123.56	119.90
1	A	1795	C	N3-C4-C5	5.23	123.99	121.90
1	A	2261	C	C4-C5-C6	5.23	120.01	117.40
1	A	2480	C	C6-N1-C2	-5.23	118.21	120.30
1	A	171	G	N3-C2-N2	5.22	123.56	119.90
1	A	531	C	C5-C4-N4	-5.22	116.54	120.20
1	A	1365	A	C8-N9-C4	5.22	107.89	105.80
1	A	2293	C	C6-N1-C2	5.22	122.39	120.30
1	A	2848	G	C5-N7-C8	5.22	106.91	104.30
1	A	613	G	C5-C6-O6	-5.22	125.47	128.60
1	A	1338	G	C5-C6-O6	5.22	131.73	128.60
1	A	1980	G	N3-C4-C5	-5.22	125.99	128.60
1	A	2245	U	C6-N1-C2	5.22	124.13	121.00
1	A	2489	G	C8-N9-C1'	-5.22	120.21	127.00
1	A	1398	C	C5-C6-N1	5.22	123.61	121.00
1	A	26	G	C6-C5-N7	-5.22	127.27	130.40
1	A	1493	C	C6-N1-C1'	-5.22	114.54	120.80
1	A	529	A	N7-C8-N9	5.21	116.41	113.80
1	A	1429	G	C4-N9-C1'	5.21	133.28	126.50
1	A	1931	U	C5-C6-N1	5.21	125.31	122.70
1	A	2008	C	C4-C5-C6	5.21	120.01	117.40
1	A	271(K)	U	N1-C2-O2	5.21	126.45	122.80
1	A	1319	G	N7-C8-N9	5.21	115.71	113.10
1	A	61	G	N1-C2-N3	5.21	127.03	123.90
1	A	119	A	N1-C6-N6	-5.21	115.47	118.60
1	A	2325	G	C8-N9-C1'	-5.21	120.22	127.00
1	A	1299	G	C5-C6-N1	-5.21	108.89	111.50
1	A	2248	C	C2-N3-C4	-5.21	117.30	119.90
1	A	189	G	C6-N1-C2	-5.21	121.97	125.10
1	A	2630	G	C5-C6-O6	-5.21	125.47	128.60
1	A	118	A	N7-C8-N9	-5.21	111.20	113.80
1	A	454	A	C8-N9-C4	-5.21	103.72	105.80
1	A	1252	G	C4-N9-C1'	-5.20	119.73	126.50
1	A	1802	A	C6-N1-C2	-5.20	115.48	118.60
1	A	2019	A	C6-N1-C2	-5.20	115.48	118.60
2	B	75	G	C6-N1-C2	-5.20	121.98	125.10
1	A	949	C	C4-C5-C6	5.20	120.00	117.40
1	A	2248	C	C4-C5-C6	5.20	120.00	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	74	A	C8-N9-C4	-5.20	103.72	105.80
1	A	1296	G	N7-C8-N9	5.20	115.70	113.10
1	A	2145	C	C5-C6-N1	5.20	123.60	121.00
1	A	2589	A	N1-C6-N6	5.20	121.72	118.60
1	A	1124	C	N1-C2-O2	-5.20	115.78	118.90
2	B	74	U	C4-C5-C6	5.20	122.82	119.70
1	A	1359	A	C6-C5-N7	5.20	135.94	132.30
1	A	2620	C	C6-N1-C1'	-5.20	114.56	120.80
1	A	27	G	C8-N9-C4	-5.20	104.32	106.40
1	A	956	G	C4-C5-C6	5.20	121.92	118.80
1	A	2104	G	C8-N9-C1'	-5.20	120.25	127.00
1	A	2411	A	N1-C6-N6	5.20	121.72	118.60
1	A	2486	G	C8-N9-C1'	-5.20	120.25	127.00
1	A	749	C	C2-N1-C1'	5.19	124.51	118.80
1	A	2295	C	C5-C4-N4	-5.19	116.56	120.20
1	A	534	U	N1-C2-O2	-5.19	119.17	122.80
1	A	788	A	C4-C5-C6	5.19	119.59	117.00
1	A	1611	C	N3-C2-O2	-5.19	118.27	121.90
1	A	1036	G	N9-C4-C5	-5.19	103.32	105.40
1	A	42	G	C8-N9-C4	5.19	108.47	106.40
1	A	141	A	N1-C2-N3	5.19	131.89	129.30
1	A	271	A	N1-C2-N3	5.19	131.89	129.30
1	A	778	G	N1-C6-O6	-5.19	116.79	119.90
1	A	1200	C	C5-C6-N1	-5.19	118.41	121.00
1	A	1755	A	C5-C6-N6	5.19	127.85	123.70
1	A	2248	C	C5-C6-N1	-5.19	118.41	121.00
1	A	679	C	N1-C2-O2	-5.18	115.79	118.90
7	H	171	LEU	CA-CB-CG	5.18	127.23	115.30
1	A	672	C	N1-C2-O2	-5.18	115.79	118.90
1	A	811	U	C4-C5-C6	5.18	122.81	119.70
1	A	1600	C	N3-C2-O2	-5.18	118.27	121.90
1	A	1602	U	C5-C6-N1	-5.18	120.11	122.70
1	A	2505	G	C8-N9-C4	5.18	108.47	106.40
1	A	2619	C	N3-C4-C5	5.18	123.97	121.90
1	A	970	C	N1-C2-O2	-5.18	115.79	118.90
1	A	2803	C	C6-N1-C2	-5.18	118.23	120.30
1	A	592	G	C2-N3-C4	5.18	114.49	111.90
1	A	949	C	C5-C4-N4	-5.18	116.58	120.20
1	A	124	G	C5-N7-C8	-5.18	101.71	104.30
1	A	190	A	N1-C6-N6	-5.18	115.49	118.60
2	B	37	C	C6-N1-C2	-5.18	118.23	120.30
2	B	99	G	N7-C8-N9	-5.18	110.51	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	194	G	C4-C5-N7	-5.17	108.73	110.80
1	A	659	C	N3-C4-C5	5.17	123.97	121.90
1	A	2251	G	C4-C5-N7	-5.17	108.73	110.80
1	A	1939	U	N1-C2-O2	-5.17	119.18	122.80
1	A	1703	G	C8-N9-C4	-5.17	104.33	106.40
1	A	1372	U	N3-C4-O4	-5.17	115.78	119.40
1	A	1753	G	N3-C4-C5	-5.17	126.02	128.60
1	A	2491	U	N3-C4-C5	5.17	117.70	114.60
1	A	2500	U	N3-C2-O2	-5.17	118.58	122.20
1	A	2606	C	C6-N1-C2	5.17	122.37	120.30
1	A	1765	C	C4-C5-C6	-5.17	114.82	117.40
1	A	2767	C	N3-C4-N4	5.16	121.61	118.00
1	A	2077	A	C5-N7-C8	-5.16	101.32	103.90
1	A	1253	A	C2-N3-C4	5.16	113.18	110.60
1	A	1601	G	N1-C6-O6	-5.16	116.80	119.90
1	A	271(S)	G	C5-C6-N1	-5.16	108.92	111.50
1	A	945	A	C8-N9-C4	5.16	107.86	105.80
1	A	1603	A	C8-N9-C4	-5.16	103.74	105.80
1	A	2820	A	N9-C4-C5	-5.16	103.74	105.80
1	A	509	C	C4-C5-C6	5.16	119.98	117.40
1	A	1219	G	C4-C5-N7	5.16	112.86	110.80
1	A	1939	U	C4-C5-C6	-5.16	116.61	119.70
1	A	2253	G	N3-C4-C5	5.16	131.18	128.60
1	A	193	U	N3-C4-C5	-5.15	111.51	114.60
1	A	1450(A)	C	N1-C2-O2	-5.15	115.81	118.90
1	A	119	A	C6-N1-C2	-5.15	115.51	118.60
1	A	239	U	C5-C6-N1	-5.15	120.12	122.70
1	A	1820	U	N3-C2-O2	5.15	125.81	122.20
1	A	2552	U	C4-C5-C6	5.15	122.79	119.70
2	B	59	A	N1-C2-N3	-5.15	126.73	129.30
1	A	1621	U	N3-C4-C5	-5.15	111.51	114.60
1	A	1844	C	N3-C2-O2	5.15	125.50	121.90
1	A	2051	A	C8-N9-C4	-5.15	103.74	105.80
1	A	2002	G	N9-C4-C5	5.15	107.46	105.40
1	A	2622	C	C5-C4-N4	5.15	123.80	120.20
1	A	1145	C	C6-N1-C2	-5.14	118.24	120.30
1	A	2672	G	C8-N9-C1'	-5.14	120.31	127.00
1	A	611	C	N1-C2-O2	5.14	121.98	118.90
1	A	1544	A	C8-N9-C4	-5.14	103.74	105.80
1	A	943	U	N3-C2-O2	-5.14	118.60	122.20
1	A	2419	U	C6-N1-C2	-5.14	117.92	121.00
1	A	564	C	N1-C2-O2	-5.14	115.82	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	581	C	N1-C2-N3	5.14	122.80	119.20
1	A	2565	A	C8-N9-C4	5.14	107.86	105.80
1	A	591	C	C2-N3-C4	-5.14	117.33	119.90
1	A	41	C	N3-C4-C5	5.14	123.95	121.90
1	A	949	C	N1-C2-O2	-5.14	115.82	118.90
1	A	1036	G	N1-C2-N2	-5.14	111.58	116.20
1	A	1119	C	C2-N3-C4	-5.14	117.33	119.90
1	A	1627	G	N3-C4-C5	-5.14	126.03	128.60
1	A	2053	G	N3-C2-N2	-5.14	116.30	119.90
1	A	2037	G	C5-C6-O6	5.13	131.68	128.60
1	A	2038	G	C5-C6-N1	-5.13	108.93	111.50
1	A	2234	G	N3-C4-N9	5.13	129.08	126.00
1	A	2894	G	C4-N9-C1'	5.13	133.18	126.50
1	A	202	U	C6-N1-C1'	-5.13	114.01	121.20
1	A	613	G	C5-N7-C8	-5.13	101.73	104.30
1	A	852	G	N1-C6-O6	-5.13	116.82	119.90
1	A	978	G	C5-N7-C8	5.13	106.86	104.30
1	A	2035	G	C8-N9-C1'	5.13	133.67	127.00
1	A	2433	A	N9-C4-C5	-5.13	103.75	105.80
2	B	5	C	C5-C6-N1	-5.13	118.44	121.00
1	A	1858	G	C4-N9-C1'	5.13	133.17	126.50
1	A	2307	G	C4-N9-C1'	5.13	133.17	126.50
1	A	473	G	C4-C5-N7	-5.13	108.75	110.80
1	A	505	A	N9-C4-C5	5.13	107.85	105.80
1	A	645	C	C2-N3-C4	5.13	122.46	119.90
1	A	1459	G	N1-C6-O6	-5.13	116.82	119.90
1	A	2091	U	N1-C2-O2	5.13	126.39	122.80
1	A	1107	G	C4-C5-C6	5.12	121.88	118.80
1	A	119	A	C4-C5-N7	-5.12	108.14	110.70
1	A	587	C	N1-C2-O2	5.12	121.97	118.90
1	A	683	C	C5-C6-N1	5.12	123.56	121.00
1	A	1039	G	N7-C8-N9	-5.12	110.54	113.10
1	A	2846	G	N9-C4-C5	5.12	107.45	105.40
1	A	1442	G	N1-C6-O6	5.12	122.97	119.90
1	A	1802	A	N1-C6-N6	5.12	121.67	118.60
1	A	2453	A	N1-C2-N3	-5.12	126.74	129.30
1	A	28	A	C2-N3-C4	5.12	113.16	110.60
1	A	1799	G	C2-N3-C4	5.12	114.46	111.90
1	A	126	A	N1-C2-N3	-5.12	126.74	129.30
1	A	570	G	N3-C4-C5	-5.12	126.04	128.60
1	A	2880	C	N3-C4-C5	-5.12	119.85	121.90
2	B	26	A	C2-N3-C4	-5.12	108.04	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	542	C	C6-N1-C2	-5.12	118.25	120.30
1	A	756	C	N3-C2-O2	-5.12	118.32	121.90
1	A	1786	A	N7-C8-N9	-5.12	111.24	113.80
1	A	470	A	C8-N9-C4	-5.12	103.75	105.80
1	A	805	G	N7-C8-N9	5.12	115.66	113.10
1	A	2030	A	C5-C6-N6	-5.12	119.61	123.70
2	B	22	U	C5-C6-N1	5.12	125.26	122.70
1	A	87	C	N3-C4-N4	-5.11	114.42	118.00
1	A	1578	U	N3-C2-O2	-5.11	118.62	122.20
1	A	2506	U	C2-N3-C4	-5.11	123.93	127.00
1	A	2737	G	N1-C2-N2	5.11	120.80	116.20
1	A	202	U	C5-C6-N1	-5.11	120.14	122.70
1	A	1285	G	C8-N9-C4	-5.11	104.36	106.40
1	A	61	G	C2-N3-C4	-5.11	109.34	111.90
1	A	651	G	N3-C4-C5	-5.11	126.05	128.60
1	A	1639	U	C5-C6-N1	-5.11	120.14	122.70
1	A	2000	G	C8-N9-C4	-5.11	104.36	106.40
1	A	2260	C	C5-C6-N1	-5.11	118.44	121.00
1	A	1983	C	C2-N3-C4	-5.11	117.35	119.90
1	A	2033	A	C2-N3-C4	5.11	113.16	110.60
1	A	2848	G	N3-C4-C5	-5.11	126.05	128.60
1	A	567	A	C8-N9-C4	-5.11	103.76	105.80
1	A	847	U	C2-N3-C4	-5.11	123.94	127.00
1	A	2533	A	N1-C6-N6	-5.11	115.53	118.60
1	A	2894	G	N1-C6-O6	-5.11	116.84	119.90
2	B	104	U	N3-C4-O4	-5.11	115.82	119.40
1	A	468	G	C5-C6-N1	-5.11	108.95	111.50
1	A	1980	G	C8-N9-C4	-5.11	104.36	106.40
1	A	2672	G	N1-C6-O6	5.11	122.96	119.90
1	A	507	A	C8-N9-C4	5.10	107.84	105.80
1	A	566	U	C5-C6-N1	5.10	125.25	122.70
1	A	1762	A	N3-C4-C5	-5.10	123.23	126.80
1	A	2037	G	C8-N9-C4	5.10	108.44	106.40
1	A	2607	G	C8-N9-C4	-5.10	104.36	106.40
1	A	954	G	C6-N1-C2	-5.10	122.04	125.10
1	A	272(C)	G	N7-C8-N9	-5.09	110.55	113.10
1	A	1626	G	N9-C4-C5	5.09	107.44	105.40
1	A	2261	C	N1-C2-N3	5.09	122.77	119.20
1	A	69	C	C6-N1-C2	-5.09	118.26	120.30
1	A	378	C	C5-C6-N1	5.09	123.55	121.00
1	A	730	C	C4-C5-C6	5.09	119.95	117.40
1	A	1359	A	C4-C5-C6	-5.09	114.45	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1236	G	N3-C4-C5	5.09	131.14	128.60
1	A	2069	G	N7-C8-N9	-5.09	110.56	113.10
1	A	2789	C	C6-N1-C2	5.09	122.34	120.30
1	A	1206	G	C5-C6-O6	5.09	131.65	128.60
1	A	1671	U	N3-C4-O4	-5.09	115.84	119.40
1	A	1799	G	C4-C5-N7	-5.09	108.77	110.80
1	A	1858	G	N7-C8-N9	5.09	115.64	113.10
1	A	2125	G	C8-N9-C4	-5.08	104.37	106.40
1	A	363	G	N3-C2-N2	-5.08	116.34	119.90
1	A	784	A	N3-C4-N9	-5.08	123.33	127.40
1	A	1022	G	C8-N9-C4	-5.08	104.37	106.40
1	A	780	G	N3-C2-N2	-5.08	116.34	119.90
1	A	1109	C	N3-C4-C5	-5.08	119.87	121.90
1	A	2682	U	N1-C2-O2	5.08	126.36	122.80
1	A	2078	C	N3-C4-N4	5.08	121.56	118.00
1	A	668	G	C5-C6-N1	-5.08	108.96	111.50
1	A	817	C	N3-C4-N4	-5.08	114.44	118.00
1	A	1562	A	N1-C6-N6	5.08	121.65	118.60
1	A	2130	U	C5-C6-N1	5.08	125.24	122.70
1	A	2501	C	N3-C4-C5	5.08	123.93	121.90
1	A	1196	C	C4-C5-C6	5.08	119.94	117.40
1	A	381	G	C8-N9-C4	-5.08	104.37	106.40
1	A	699	A	C2-N3-C4	-5.08	108.06	110.60
1	A	268	C	N3-C4-C5	5.07	123.93	121.90
1	A	2286	A	N1-C2-N3	5.07	131.84	129.30
1	A	2505	G	C6-C5-N7	-5.07	127.36	130.40
1	A	2819	G	C5-C6-O6	5.07	131.64	128.60
2	B	99	G	N9-C4-C5	-5.07	103.37	105.40
1	A	1799	G	P-O3'-C3'	5.07	125.79	119.70
2	B	8	U	C5-C6-N1	5.07	125.24	122.70
1	A	977	G	N1-C6-O6	-5.07	116.86	119.90
1	A	1211	U	N3-C2-O2	5.07	125.75	122.20
1	A	1599	C	C4-C5-C6	5.07	119.94	117.40
1	A	1445	A	C2-N3-C4	5.07	113.14	110.60
1	A	975	C	C6-N1-C2	-5.07	118.27	120.30
1	A	1436	G	C8-N9-C4	-5.07	104.37	106.40
1	A	2048	G	C5-C6-O6	5.07	131.64	128.60
1	A	2519	U	C5-C6-N1	-5.07	120.17	122.70
1	A	2441	C	C5-C4-N4	5.07	123.75	120.20
1	A	668	G	C6-N1-C2	5.06	128.14	125.10
1	A	1256	G	C8-N9-C1'	-5.06	120.42	127.00
1	A	2599	G	N1-C6-O6	-5.06	116.86	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2816	C	C2-N3-C4	5.06	122.43	119.90
1	A	1721	G	C4-C5-N7	5.06	112.82	110.80
1	A	2689	U	P-O3'-C3'	5.06	125.77	119.70
1	A	2812	G	C4-C5-N7	-5.06	108.78	110.80
1	A	1238	G	N1-C6-O6	5.06	122.94	119.90
1	A	2292	C	C5-C6-N1	-5.06	118.47	121.00
1	A	2488	A	N7-C8-N9	-5.06	111.27	113.80
1	A	2492	U	C5-C6-N1	5.06	125.23	122.70
2	B	17	C	N1-C2-O2	5.06	121.94	118.90
1	A	1013	C	C6-N1-C2	5.05	122.32	120.30
1	A	1904	G	C5-C6-N1	5.05	114.03	111.50
1	A	135	G	C5-C6-N1	5.05	114.03	111.50
1	A	945	A	N1-C6-N6	5.05	121.63	118.60
1	A	595	C	N3-C4-C5	5.05	123.92	121.90
1	A	1914	C	C6-N1-C2	-5.05	118.28	120.30
1	A	1951	U	N3-C4-O4	5.05	122.94	119.40
1	A	2455	G	N1-C2-N3	5.05	126.93	123.90
1	A	2648	C	C2-N3-C4	-5.05	117.38	119.90
1	A	2719	G	C2-N3-C4	5.05	114.43	111.90
1	A	509	C	N1-C2-N3	5.05	122.73	119.20
1	A	2018	G	C8-N9-C4	-5.05	104.38	106.40
1	A	333	G	N3-C4-C5	-5.05	126.08	128.60
1	A	1791	A	C6-C5-N7	-5.05	128.77	132.30
1	A	2125	G	N7-C8-N9	5.05	115.62	113.10
1	A	74	A	N7-C8-N9	5.05	116.32	113.80
1	A	260	G	C2-N3-C4	-5.05	109.38	111.90
1	A	269	U	C5-C6-N1	5.04	125.22	122.70
1	A	291	C	C5-C4-N4	-5.04	116.67	120.20
1	A	2001	A	C2-N3-C4	5.04	113.12	110.60
1	A	981	A	C5-C6-N1	5.04	120.22	117.70
1	A	2174	C	C2-N3-C4	5.04	122.42	119.90
1	A	2442	C	N3-C4-N4	-5.04	114.47	118.00
1	A	2456	C	C6-N1-C2	5.04	122.32	120.30
1	A	526	A	N9-C4-C5	5.04	107.82	105.80
1	A	781	A	C5-N7-C8	5.04	106.42	103.90
1	A	979	G	N3-C2-N2	-5.04	116.37	119.90
1	A	1296	G	N3-C4-C5	-5.04	126.08	128.60
1	A	2427	C	N3-C2-O2	5.04	125.43	121.90
1	A	179	G	N7-C8-N9	-5.04	110.58	113.10
1	A	60	G	N7-C8-N9	-5.04	110.58	113.10
1	A	637	A	C8-N9-C4	5.04	107.81	105.80
1	A	2322	A	C8-N9-C4	-5.04	103.79	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	310	A	C2-N3-C4	-5.03	108.08	110.60
1	A	546	C	C2-N1-C1'	5.03	124.34	118.80
1	A	798	G	C2-N3-C4	-5.03	109.38	111.90
1	A	954	G	N3-C4-C5	-5.03	126.08	128.60
1	A	2280	G	N9-C4-C5	5.03	107.41	105.40
1	A	70	G	N1-C6-O6	-5.03	116.88	119.90
1	A	491	G	N9-C4-C5	5.03	107.41	105.40
1	A	1955	U	N3-C4-C5	5.03	117.62	114.60
1	A	775	G	N3-C4-N9	5.03	129.02	126.00
1	A	1824	G	C5-C6-N1	5.03	114.02	111.50
1	A	2053	G	N3-C4-C5	-5.03	126.08	128.60
1	A	2487	G	C6-C5-N7	-5.03	127.38	130.40
1	A	2868	A	C8-N9-C4	-5.03	103.79	105.80
1	A	542	C	C6-N1-C1'	5.03	126.83	120.80
1	A	1266	G	C2-N3-C4	5.03	114.41	111.90
1	A	2641	G	C5-C6-O6	5.03	131.62	128.60
1	A	429	A	C4-C5-N7	5.03	113.21	110.70
1	A	655	A	C6-C5-N7	-5.03	128.78	132.30
1	A	1653	G	C5-C6-O6	5.03	131.62	128.60
1	A	2085	C	C6-N1-C2	5.03	122.31	120.30
1	A	2686	G	N9-C4-C5	-5.03	103.39	105.40
1	A	271(J)	C	C6-N1-C2	5.03	122.31	120.30
1	A	453	C	N3-C4-C5	5.03	123.91	121.90
1	A	345	A	N1-C6-N6	5.02	121.61	118.60
1	A	2559	C	C5-C4-N4	-5.02	116.68	120.20
1	A	1600	C	C4-C5-C6	5.02	119.91	117.40
1	A	1983	C	C5-C6-N1	-5.02	118.49	121.00
1	A	2236	C	C4-C5-C6	5.02	119.91	117.40
1	A	1997	G	N3-C4-C5	-5.02	126.09	128.60
1	A	2485	G	N1-C6-O6	5.02	122.91	119.90
1	A	954	G	C5-C6-N1	5.02	114.01	111.50
1	A	2206	G	N3-C2-N2	5.02	123.41	119.90
1	A	2250	G	C8-N9-C4	-5.02	104.39	106.40
1	A	811	U	C2-N3-C4	-5.02	123.99	127.00
2	B	101	G	C5-C6-O6	-5.02	125.59	128.60
1	A	486	C	C4-C5-C6	5.01	119.91	117.40
1	A	1653	G	N9-C4-C5	5.01	107.41	105.40
1	A	822	U	N1-C2-N3	5.01	117.91	114.90
1	A	2219	G	C8-N9-C4	5.01	108.40	106.40
1	A	641	C	N3-C4-N4	5.01	121.51	118.00
1	A	1769	G	N1-C6-O6	5.01	122.91	119.90
1	A	2316	C	C2-N1-C1'	5.01	124.31	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2454	G	N1-C6-O6	-5.01	116.89	119.90
1	A	1125	G	N3-C2-N2	-5.01	116.39	119.90
1	A	1185	C	N3-C4-N4	-5.01	114.50	118.00
1	A	1627	G	N3-C4-N9	5.00	129.00	126.00
1	A	2200	C	N3-C4-C5	-5.00	119.90	121.90
1	A	769	G	C6-N1-C2	5.00	128.10	125.10

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
23	1	83	GLU	Peptide
26	4	42	PHE	Peptide
26	4	43	TYR	Peptide
26	4	44	THR	Peptide
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
6	G	13	GLU	Peptide
8	I	83	ALA	Peptide
9	N	124	ALA	Peptide
10	O	48	PRO	Peptide
11	P	103	ALA	Peptide
11	P	25	SER	Peptide
11	P	26	GLY	Peptide
11	P	44	GLY	Peptide
14	S	82	ILE	Peptide
14	S	96	GLY	Peptide
15	T	126	ALA	Peptide
19	X	93	GLU	Peptide
20	Y	102	CYS	Peptide
21	Z	159	PRO	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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.

All (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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
1:A:1784:A:OP2	34:A:3893:HOH:O	1.84	0.95
1:A:2059:A:OP2	34:A:4439:HOH:O	1.85	0.95
1:A:2322:A:H61	1:A:2335:A:N6	1.65	0.95
1:A:2122:U:H3	1:A:2176:A:H61	1.12	0.93
1:A:2714:G:OP2	34:A:4484:HOH:O	1.86	0.92
1:A:1664:A:OP1	34:A:4521:HOH:O	1.87	0.92
6:G:61:ALA:HB1	26:4:7:PRO:HG3	1.51	0.92
1:A:1774:C:OP1	34:A:4509:HOH:O	1.88	0.92
20:Y:76:CYS:HB3	20:Y:79:CYS:HB2	1.52	0.91
23:1:21:ARG:HH11	23:1:21:ARG:HG2	1.35	0.91
1:A:27:G:N2	1:A:512:G:O2'	2.02	0.91
1:A:9:U:N3	1:A:2629:A:N1	2.17	0.91
30:8:7:HIS:HD2	30:8:10:ALA:H	1.20	0.89
1:A:2322:A:OP2	34:A:4625:HOH:O	1.88	0.89
1:A:1154:G:N7	34:A:4279:HOH:O	2.04	0.89
5:F:46:ARG:HG2	5:F:46:ARG:HH11	1.37	0.89
1:A:631:A:OP1	11:P:65:ARG:NH1	2.05	0.89
1:A:571:A:H5'	1:A:2030:A:H62	1.38	0.88
1:A:1779:U:H5	1:A:1784:A:N7	1.71	0.88
1:A:446:G:OP2	34:A:3953:HOH:O	1.90	0.87
1:A:2319:G:H22	14:S:3:ARG:HE	1.21	0.87
11:P:39:LYS:HB2	11:P:45:LEU:HG	1.54	0.87
4:E:54:GLN:HG3	4:E:76:ARG:HB3	1.56	0.87
1:A:422:A:OP2	34:A:3934:HOH:O	1.93	0.86
8:I:104:GLN:HB3	8:I:105:HIS:HD2	1.38	0.86
1:A:1359:A:N6	1:A:1372:U:O4	2.08	0.86
1:A:1855:G:N7	34:A:4949:HOH:O	2.08	0.86
1:A:2499:C:OP1	34:A:4023:HOH:O	1.94	0.86
8:I:92:VAL:HG13	8:I:120:ILE:HB	1.55	0.85
1:A:27:G:N2	1:A:512:G:HO2'	1.73	0.85
1:A:1204:A:H2	1:A:1241:A:H62	1.25	0.85
1:A:2115:G:N2	1:A:2119:A:OP2	2.10	0.85
1:A:1235:G:OP1	34:A:4110:HOH:O	1.96	0.84
1:A:90:U:HO2'	1:A:92:A:H8	0.88	0.83
1:A:1970:A:OP1	34:A:4425:HOH:O	1.96	0.83
1:A:1654:A:OP1	13:R:1:MET:N	2.09	0.83
1:A:2108:C:H2'	1:A:2109:U:O5'	1.79	0.82
1:A:1332:G:O6	34:A:4817:HOH:O	1.97	0.82

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1352:U:OP2	34:A:3903:HOH:O	1.98	0.82
1:A:243:U:OP2	30:8:8:LYS:NZ	2.11	0.82
1:A:2576:G:OP1	34:A:4391:HOH:O	1.97	0.82
1:A:2306:C:H5'	1:A:2307:G:H2'	1.61	0.82
28:6:23:THR:OG1	28:6:24:GLU:N	2.10	0.82
1:A:1689:A:H62	1:A:1698:A:H2	1.26	0.81
6:G:131:TYR:HB3	6:G:159:VAL:HG13	1.60	0.81
1:A:1109:C:H5	1:A:1110:G:C2	1.99	0.81
1:A:2602:A:H4'	1:A:2603:G:OP1	1.80	0.81
1:A:2448:A:N1	34:A:3924:HOH:O	2.14	0.81
1:A:1439:A:OP1	34:A:4047:HOH:O	1.97	0.80
1:A:2108:C:C2'	1:A:2109:U:O5'	2.30	0.80
1:A:271(I):G:H1	1:A:271(O):C:H42	1.27	0.80
1:A:27:G:H22	1:A:512:G:HO2'	1.25	0.80
15:T:64:ARG:HB2	15:T:73:GLU:HG2	1.62	0.80
1:A:2615:U:OP1	34:A:4793:HOH:O	2.01	0.79
1:A:882:G:H1	1:A:894:C:H42	1.27	0.79
1:A:548:A:H62	17:V:19:LYS:HB2	1.47	0.79
1:A:2777:G:H5''	1:A:2778:A:H5'	1.64	0.78
1:A:399:G:OP2	34:A:3932:HOH:O	2.02	0.78
1:A:2222:G:N7	34:A:4597:HOH:O	2.15	0.78
15:T:95:ARG:HG2	15:T:95:ARG:HH11	1.48	0.78
1:A:2322:A:N6	1:A:2335:A:N6	2.33	0.77
1:A:301:G:OP2	20:Y:84:ARG:NH2	2.17	0.77
1:A:1403:C:H5''	1:A:1471:A:H1'	1.66	0.77
1:A:2134:A:H61	1:A:2157:G:H1'	1.50	0.77
1:A:2588:G:OP1	34:A:4238:HOH:O	2.02	0.77
1:A:69:C:N4	34:A:3941:HOH:O	2.17	0.77
25:3:8:LEU:HD13	25:3:31:LEU:HD23	1.67	0.76
31:9:11:CYS:SG	31:9:32:HIS:HE1	2.08	0.76
1:A:120:U:OP1	34:A:3882:HOH:O	2.01	0.76
6:G:76:SER:HA	6:G:83:ARG:HA	1.67	0.76
1:A:2104:G:N7	1:A:2186:G:N2	2.33	0.76
1:A:2820:A:OP2	13:R:2:ARG:NH2	2.19	0.76
1:A:827:U:OP1	34:A:4305:HOH:O	2.02	0.76
1:A:2407:G:OP1	34:A:4294:HOH:O	2.03	0.76
1:A:2134:A:N6	1:A:2157:G:H1'	2.01	0.76
1:A:587:C:OP2	11:P:21:ARG:NH2	2.18	0.76
1:A:106:C:O4'	20:Y:1:MET:HB2	1.86	0.76
1:A:1980:G:O2'	1:A:1982:C:OP2	2.05	0.75
1:A:1494:A:H2'	1:A:1495:A:C8	2.21	0.75
7:H:70:THR:O	7:H:71:LEU:HB2	1.85	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:28:GLU:OE1	34:D:402:HOH:O	2.04	0.75
23:1:3:LYS:HB2	23:1:61:ARG:NH1	2.01	0.75
1:A:90:U:O2	34:A:4781:HOH:O	2.01	0.75
1:A:2140:C:N3	1:A:2151:G:O6	2.19	0.75
5:F:185:ASP:OD1	5:F:188:ARG:NH1	2.20	0.74
1:A:90:U:O2'	1:A:92:A:H8	1.65	0.74
13:R:33:ARG:NH2	27:5:57:VAL:O	2.14	0.74
1:A:2181:G:H2'	1:A:2182:G:C8	2.23	0.74
1:A:287:C:O2	1:A:354:G:N2	2.16	0.74
1:A:2562:U:H1'	10:O:23:ARG:HH11	1.51	0.74
1:A:530:G:N3	1:A:530:G:O4'	2.20	0.74
1:A:1026:U:O2'	1:A:1027:A:O5'	2.03	0.73
15:T:60:THR:HG22	15:T:77:PRO:HA	1.68	0.73
1:A:1366:A:OP1	23:1:3:LYS:NZ	2.21	0.73
1:A:1798:U:H5'	3:D:259:THR:HG22	1.70	0.73
1:A:1669:A:OP2	34:A:4861:HOH:O	2.05	0.73
26:4:9:LEU:HD23	26:4:27:THR:HG23	1.70	0.73
1:A:1322:A:N7	34:A:4618:HOH:O	2.21	0.73
1:A:2036:C:H6	1:A:2036:C:H5'	1.54	0.73
1:A:990:A:OP2	34:A:4322:HOH:O	2.06	0.72
1:A:531:C:OP2	34:A:4355:HOH:O	2.05	0.72
15:T:56:GLY:O	15:T:59:THR:HG23	1.88	0.72
1:A:226:G:H21	1:A:228:A:H62	1.37	0.72
20:Y:30:VAL:HG22	20:Y:37:VAL:HG12	1.71	0.72
14:S:102:ALA:HA	14:S:105:ALA:HB3	1.70	0.72
1:A:2405:G:H4'	1:A:2406:U:OP2	1.89	0.72
11:P:126:VAL:HG12	11:P:148:LEU:HD22	1.70	0.72
24:2:51:ARG:HA	24:2:54:LYS:HB2	1.72	0.72
1:A:2786:U:O2'	4:E:62:PRO:O	2.07	0.72
1:A:1038:C:H42	1:A:1117:G:H1	1.38	0.72
1:A:639:U:H2'	1:A:640:C:C6	2.25	0.72
11:P:95:VAL:HA	11:P:99:LEU:HD12	1.72	0.71
1:A:1210:A:H5'	1:A:1210:A:H8	1.53	0.71
26:4:18:CYS:HB2	26:4:39:CYS:SG	2.30	0.71
1:A:747:U:O2	1:A:2014:A:H1'	1.90	0.71
1:A:2357:U:OP1	22:0:20:ARG:NH1	2.23	0.71
23:1:20:ARG:HG2	23:1:20:ARG:HH11	1.55	0.71
8:I:102:SER:HA	8:I:106:GLY:HA3	1.73	0.71
15:T:16:ARG:NH2	15:T:83:ILE:O	2.23	0.71
1:A:1817:G:OP1	3:D:88:ARG:NH2	2.22	0.71
1:A:2158:A:H4'	1:A:2159:G:OP1	1.90	0.70
1:A:2122:U:H3	1:A:2176:A:N6	1.86	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1669:A:OP1	34:A:4892:HOH:O	2.10	0.70
12:Q:38:GLU:HB2	12:Q:127:ILE:HG22	1.72	0.70
1:A:2839:G:H5'	13:R:46:GLY:HA2	1.74	0.70
1:A:39:C:O2	5:F:46:ARG:NH2	2.25	0.70
1:A:1858:G:O2'	1:A:1884:A:N6	2.23	0.70
21:Z:45:ASP:OD2	21:Z:49:ARG:NH1	2.25	0.70
1:A:2445:G:OP1	5:F:74:ARG:NH2	2.24	0.70
1:A:221:A:H4'	1:A:222:A:O5'	1.92	0.69
1:A:1243:G:O2'	11:P:7:ARG:NH2	2.25	0.69
26:4:16:CYS:HA	26:4:33:VAL:HB	1.74	0.69
1:A:2308:G:O2'	1:A:2310:A:OP2	2.07	0.69
28:6:10:LEU:HD12	28:6:54:ILE:HA	1.73	0.69
23:1:54:ALA:HB1	23:1:83:GLU:HB2	1.73	0.69
5:F:7:TYR:H	5:F:22:ALA:HB3	1.56	0.69
1:A:2327:A:H2'	1:A:2328:A:C8	2.27	0.69
1:A:1359:A:N6	1:A:1372:U:C4	2.61	0.69
1:A:2124:G:N2	1:A:2174:C:C2	2.61	0.69
1:A:833:U:O2	11:P:55:ARG:NH2	2.26	0.69
8:I:93:THR:HG23	8:I:96:ASP:H	1.57	0.69
1:A:2296:U:C4	1:A:2335:A:N6	2.61	0.69
1:A:141:A:H8	1:A:1408:C:HO2'	1.41	0.69
1:A:141:A:H8	1:A:1408:C:O2'	1.76	0.69
1:A:2646:C:OP2	1:A:2732:G:O2'	2.09	0.69
11:P:47:ASP:OD2	11:P:50:ARG:NH2	2.26	0.68
7:H:28:GLY:HA3	7:H:79:VAL:HB	1.74	0.68
1:A:2760:C:H2'	1:A:2761:G:H5''	1.74	0.68
13:R:67:LEU:HD13	13:R:76:VAL:HG21	1.76	0.68
1:A:120:U:OP2	34:A:3881:HOH:O	2.11	0.68
24:2:35:LEU:HD12	24:2:53:LEU:HD12	1.75	0.68
8:I:104:GLN:HB3	8:I:105:HIS:CD2	2.25	0.68
8:I:72:LEU:HD21	8:I:107:VAL:HG11	1.74	0.68
1:A:677:A:OP1	34:A:4096:HOH:O	2.11	0.68
1:A:528:A:N1	1:A:2042:A:H2'	2.09	0.67
6:G:16:ARG:HE	6:G:31:VAL:HG11	1.60	0.67
14:S:34:HIS:CE1	14:S:54:LEU:HD12	2.30	0.67
1:A:2319:G:N2	14:S:3:ARG:HE	1.93	0.67
1:A:1010:A:OP2	34:A:4343:HOH:O	2.12	0.67
1:A:1036:G:H1	1:A:1119:C:H42	1.43	0.67
1:A:1653:G:H3'	13:R:2:ARG:HD3	1.77	0.67
1:A:141:A:C8	1:A:1408:C:O2'	2.47	0.67
2:B:38:C:O4'	14:S:95:HIS:NE2	2.27	0.67
23:1:85:LEU:HB3	23:1:89:GLU:HG3	1.77	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1022:G:H22	1:A:1142(A):A:H2	1.43	0.66
22:0:65:GLY:HA3	22:0:81:VAL:HG12	1.77	0.66
20:Y:23:ARG:HG2	20:Y:42:VAL:HG22	1.76	0.66
1:A:2285:C:OP2	28:6:6:ARG:NH1	2.28	0.66
1:A:1486:A:H2'	1:A:1487:G:H8	1.58	0.66
1:A:1019:U:H3	1:A:1142(A):A:H62	1.42	0.66
2:B:27:C:H5''	14:S:54:LEU:HD11	1.76	0.66
1:A:879:G:H22	1:A:899:A:H1'	1.61	0.66
1:A:271(E):U:H2'	1:A:271(F):C:C6	2.31	0.66
8:I:88:ILE:HD11	8:I:123:LEU:HB3	1.76	0.66
1:A:90:U:O2'	1:A:92:A:O5'	2.14	0.66
1:A:1250:G:N7	11:P:18:ARG:NH2	2.44	0.66
4:E:11:MET:HG2	4:E:24:THR:HB	1.77	0.66
1:A:1278:A:OP1	13:R:36:THR:HG23	1.94	0.66
1:A:1494:A:H2'	1:A:1495:A:H8	1.60	0.66
9:N:20:GLY:HA2	9:N:61:ARG:HG2	1.78	0.66
1:A:1361:G:N7	34:A:4712:HOH:O	2.28	0.65
20:Y:79:CYS:HB3	20:Y:81:LYS:H	1.61	0.65
9:N:120:LEU:HD22	9:N:122:VAL:HG23	1.78	0.65
2:B:31:C:O2'	2:B:53:A:N6	2.30	0.65
1:A:2140:C:O2	1:A:2151:G:N1	2.22	0.65
2:B:60:C:N4	34:B:326:HOH:O	2.18	0.65
1:A:2099:U:H3	1:A:2190:G:H1	1.43	0.65
1:A:1153:C:OP1	16:U:92:ARG:NH1	2.30	0.65
3:D:275:LYS:HG3	3:D:276:LYS:HG2	1.77	0.65
1:A:1673:U:OP1	34:A:4559:HOH:O	2.15	0.65
22:0:27:GLU:HG3	22:0:68:GLU:HA	1.78	0.64
1:A:88:G:OP1	34:A:4653:HOH:O	2.15	0.64
1:A:2134:A:O2'	1:A:2159:G:N2	2.28	0.64
1:A:220:G:O2'	1:A:233:A:N3	2.29	0.64
21:Z:69:THR:HG22	21:Z:90:VAL:HA	1.78	0.64
1:A:2107:C:C5	1:A:2108:C:N4	2.65	0.64
5:F:53:THR:HG23	5:F:55:GLY:H	1.61	0.64
8:I:88:ILE:HG22	8:I:90:GLY:H	1.62	0.64
1:A:784:A:H5'	1:A:785:G:OP1	1.97	0.64
1:A:686:G:H5''	29:7:11:LYS:HE2	1.78	0.64
26:4:42:PHE:HB3	26:4:43:TYR:HB2	1.80	0.64
7:H:149:ARG:NH1	7:H:167:GLU:OE1	2.31	0.64
2:B:50:G:H5''	14:S:61:ASN:HD21	1.63	0.64
30:8:34:TRP:CG	30:8:35:GLN:N	2.65	0.64
1:A:1186:G:OP1	34:A:4246:HOH:O	2.15	0.64
1:A:847:U:OP2	34:A:4697:HOH:O	2.14	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:O:34:THR:OG1	10:O:35:VAL:N	2.29	0.64
11:P:59:LEU:HD11	30:8:10:ALA:HB2	1.78	0.64
1:A:271(I):G:H1	1:A:271(O):C:N4	1.96	0.64
2:B:24:G:N7	2:B:56:G:H2'	2.13	0.64
2:B:49:C:OP1	14:S:97:ARG:HB2	1.97	0.63
1:A:1866:C:H2'	1:A:1876:A:O4'	1.97	0.63
5:F:13:SER:HB3	5:F:15:SER:HB2	1.78	0.63
1:A:2887:U:H2'	1:A:2888:C:C6	2.33	0.63
1:A:1045:A:N3	1:A:1045:A:H2'	2.12	0.63
1:A:249:C:O2	30:8:12:LYS:NZ	2.31	0.63
1:A:2497:A:H5''	34:A:3874:HOH:O	1.99	0.63
1:A:252:G:OP2	11:P:50:ARG:NH1	2.30	0.63
4:E:47:VAL:HG21	4:E:86:PRO:HD2	1.80	0.63
12:Q:32:TYR:OH	12:Q:111:GLU:OE1	2.15	0.63
1:A:1803:A:O2'	3:D:259:THR:HG21	1.98	0.63
4:E:72:VAL:HA	4:E:73:GLU:HB3	1.80	0.63
3:D:145:VAL:HG12	3:D:146:GLU:O	1.99	0.63
20:Y:92:ASN:N	20:Y:93:GLY:HA2	2.13	0.63
8:I:72:LEU:HA	8:I:75:LEU:HD22	1.80	0.62
1:A:2206:G:H5'	1:A:2207:G:C5	2.34	0.62
18:W:86:LEU:HD22	18:W:96:ILE:HD11	1.81	0.62
23:1:3:LYS:HB2	23:1:61:ARG:HH12	1.63	0.62
11:P:38:GLN:O	11:P:39:LYS:HB3	1.99	0.62
21:Z:111:VAL:C	21:Z:113:ALA:H	2.03	0.62
5:F:53:THR:CG2	5:F:55:GLY:H	2.12	0.62
16:U:36:ARG:HD2	16:U:40:PHE:CZ	2.34	0.62
8:I:65:ALA:HB1	8:I:136:VAL:HG11	1.80	0.62
11:P:121:LYS:HG2	11:P:123:LEU:HG	1.81	0.62
3:D:33:LEU:O	3:D:64:ILE:HG13	1.99	0.62
1:A:2602:A:H8	34:A:3856:HOH:O	1.83	0.62
1:A:277:C:H1'	1:A:278:A:OP2	1.99	0.62
1:A:2637:U:H5''	4:E:82:ARG:HH21	1.65	0.62
1:A:1358:G:H2'	1:A:1359:A:C2	2.35	0.62
1:A:2306:C:C5'	1:A:2307:G:H2'	2.30	0.62
1:A:1754:C:OP1	15:T:96:ARG:NH1	2.30	0.62
15:T:65:LYS:HE2	15:T:67:SER:HB2	1.82	0.62
1:A:1488:G:H5'	1:A:1489:U:OP2	1.99	0.62
24:2:50:ILE:O	24:2:51:ARG:HB3	1.97	0.62
3:D:69:ARG:NH2	3:D:128:GLY:O	2.30	0.62
17:V:76:LYS:HB2	17:V:81:TYR:HB3	1.82	0.62
13:R:20:LEU:HD21	13:R:40:LYS:HD3	1.81	0.62
5:F:28:ILE:HG12	5:F:116:ASP:HB2	1.81	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1358:G:H2'	1:A:1359:A:H2	1.64	0.61
7:H:3:ARG:HG3	7:H:4:ILE:N	2.15	0.61
1:A:1991:U:H2'	1:A:1992:G:H5''	1.81	0.61
1:A:546:C:H6	1:A:547:A:H5'	1.64	0.61
12:Q:16:ARG:HG2	12:Q:16:ARG:HH11	1.66	0.61
1:A:615:G:OP1	5:F:40:GLN:NE2	2.33	0.61
1:A:300:A:P	20:Y:86:ARG:HH22	2.23	0.61
1:A:2867:G:OP2	15:T:119:LYS:NZ	2.31	0.61
1:A:2602:A:H1'	1:A:2603:G:H5''	1.82	0.61
15:T:51:ARG:HG3	15:T:98:LYS:HE3	1.81	0.61
1:A:1798:U:C5'	3:D:259:THR:HG22	2.30	0.61
8:I:112:LYS:C	8:I:114:LEU:H	2.03	0.61
1:A:1430:C:H2'	1:A:1431:U:C6	2.36	0.61
1:A:2849:U:OP2	15:T:95:ARG:NH1	2.33	0.61
10:O:24:VAL:HB	10:O:33:ALA:HB2	1.83	0.61
8:I:94:ALA:HA	8:I:97:ILE:HD12	1.82	0.61
12:Q:62:GLY:O	21:Z:178:GLU:HG2	2.01	0.61
1:A:207:A:H2'	1:A:208:C:O4'	2.01	0.61
2:B:32:C:C2	2:B:51:G:N2	2.69	0.61
25:3:18:ASP:OD1	25:3:18:ASP:N	2.33	0.61
9:N:67:LEU:O	9:N:88:GLU:HG3	2.00	0.61
1:A:1434:A:H61	1:A:1558:A:N6	1.99	0.61
12:Q:21:THR:HG21	12:Q:101:ARG:HB2	1.82	0.61
6:G:15:VAL:HG13	6:G:175:LEU:HB3	1.81	0.61
1:A:203:C:H3'	1:A:204:A:H5''	1.82	0.61
1:A:1405:U:H2'	1:A:1406:U:C6	2.35	0.61
1:A:1778:U:H2'	1:A:1784:A:N6	2.15	0.60
1:A:873:G:N2	1:A:905:U:O2	2.33	0.60
3:D:108:PRO:HB3	3:D:143:HIS:HE1	1.66	0.60
3:D:148:GLU:HB2	3:D:151:LYS:HD2	1.83	0.60
1:A:805:G:OP1	34:A:4311:HOH:O	2.16	0.60
1:A:2123:G:H1	1:A:2175:C:H42	1.48	0.60
1:A:271(M):G:H4'	1:A:271(N):U:OP1	2.00	0.60
1:A:879:G:N2	1:A:899:A:H1'	2.16	0.60
24:2:9:GLN:HE22	24:2:56:GLN:HB3	1.66	0.60
1:A:2022:U:O2'	1:A:2617:C:H5'	2.00	0.60
1:A:1495:A:H2'	1:A:1496:A:C8	2.37	0.60
16:U:92:ARG:HA	16:U:95:LEU:HB2	1.82	0.60
19:X:41:ASN:O	19:X:45:THR:HG23	2.01	0.60
5:F:102:PRO:HB2	5:F:105:VAL:HG23	1.83	0.60
1:A:2723:C:OP1	13:R:3:HIS:ND1	2.27	0.60
1:A:1106:G:O2'	1:A:1107:G:OP1	2.18	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
16:U:74:LEU:H	16:U:74:LEU:HD12	1.67	0.60
1:A:1506:C:H2'	1:A:1507:A:H5'	1.84	0.60
1:A:535:C:O3'	16:U:53:ARG:NH1	2.35	0.60
21:Z:17:ALA:HA	21:Z:20:ARG:HD2	1.83	0.60
1:A:1530:C:O2'	1:A:1531:C:O4'	2.20	0.60
1:A:1026:U:H2'	1:A:1026:U:O2	1.99	0.60
21:Z:160:GLY:HA2	21:Z:161:VAL:HB	1.82	0.60
23:1:80:LEU:HD23	23:1:82:LEU:HD21	1.83	0.60
1:A:1603:A:OP1	34:A:4686:HOH:O	2.16	0.60
14:S:10:ARG:HH21	14:S:91:PRO:HB2	1.67	0.60
7:H:56:SER:HB3	7:H:61:HIS:ND1	2.16	0.59
5:F:46:ARG:CG	5:F:46:ARG:HH11	2.14	0.59
1:A:2104:G:N2	1:A:2105:C:C2	2.70	0.59
1:A:2364:C:H2'	1:A:2365:G:O4'	2.01	0.59
1:A:1153:C:H2'	1:A:1154:G:O4'	2.02	0.59
3:D:71:ASP:OD1	3:D:103:ARG:NH2	2.34	0.59
1:A:995:C:OP2	16:U:54:LYS:HE3	2.03	0.59
9:N:42:TRP:HD1	9:N:48:MET:HE1	1.68	0.59
18:W:60:ASN:N	18:W:60:ASN:HD22	1.99	0.59
26:4:14:ILE:HG13	26:4:22:ILE:HB	1.82	0.59
1:A:2331:G:O3'	22:0:43:THR:HG22	2.03	0.59
6:G:137:GLU:HG2	6:G:138:GLN:H	1.68	0.59
1:A:528:A:H4'	34:A:4289:HOH:O	2.02	0.59
1:A:11:G:H2'	1:A:12:U:H5'	1.83	0.59
1:A:1107:G:N7	1:A:1108:U:N3	2.50	0.59
7:H:3:ARG:HG2	7:H:6:ARG:HE	1.67	0.59
1:A:1593:G:H2'	1:A:1594:G:C8	2.38	0.59
1:A:548:A:N6	17:V:19:LYS:H	2.01	0.59
8:I:91:SER:HB2	8:I:119:PRO:HB2	1.84	0.59
1:A:1427:A:H4'	1:A:1428:C:O5'	2.01	0.59
1:A:2228:G:OP1	3:D:261:LYS:NZ	2.31	0.59
1:A:546:C:H2'	1:A:547:A:H5'	1.85	0.59
6:G:126:ASP:HB3	6:G:130:ASN:H	1.67	0.59
4:E:105:THR:OG1	4:E:199:ARG:NH2	2.36	0.59
1:A:271(R):G:H2'	1:A:271(S):G:H8	1.68	0.58
17:V:40:LEU:HB2	17:V:46:VAL:HG13	1.84	0.58
1:A:796:C:H2'	1:A:797:C:C6	2.38	0.58
3:D:206:LEU:HD22	3:D:211:ARG:HG2	1.84	0.58
1:A:2126:A:N1	1:A:2162:G:O2'	2.30	0.58
15:T:54:ARG:HA	15:T:59:THR:HB	1.85	0.58
3:D:267:SER:O	3:D:268:ARG:HB3	2.03	0.58
7:H:137:ASP:HB3	7:H:140:LYS:HB3	1.85	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
18:W:79:GLY:HA3	18:W:100:THR:HG22	1.84	0.58
5:F:181:LEU:HB3	5:F:205:ARG:HH22	1.69	0.58
1:A:2315:G:H2'	1:A:2316:C:C6	2.37	0.58
8:I:97:ILE:O	8:I:101:LEU:N	2.36	0.58
1:A:862:G:OP2	34:A:4187:HOH:O	2.16	0.58
1:A:307:G:H21	1:A:330:A:H62	1.52	0.58
12:Q:16:ARG:HG2	12:Q:16:ARG:NH1	2.18	0.58
21:Z:52:SER:OG	21:Z:53:ILE:N	2.36	0.58
1:A:184:C:H2'	1:A:185:U:C6	2.38	0.58
1:A:1108:U:O2'	1:A:1109:C:O5'	2.21	0.58
11:P:38:GLN:HA	11:P:41:ARG:HG2	1.86	0.58
1:A:1359:A:N6	1:A:1372:U:C5	2.71	0.58
1:A:548:A:N6	17:V:19:LYS:HB2	2.17	0.58
8:I:5:LEU:HD11	8:I:19:VAL:HG22	1.86	0.58
1:A:185:U:H4'	1:A:218:A:H4'	1.86	0.58
15:T:106:SER:O	15:T:110:ILE:HG13	2.04	0.58
1:A:2690:C:OP2	13:R:14:SER:HB3	2.04	0.58
1:A:2308:G:H4'	1:A:2309:A:OP2	2.02	0.58
17:V:35:LEU:HB2	17:V:57:VAL:HG13	1.84	0.58
1:A:993:G:OP1	16:U:50:ARG:NH2	2.37	0.58
1:A:517:C:OP1	27:5:16:ARG:NH2	2.36	0.57
24:2:13:ALA:HA	24:2:16:LEU:HD12	1.85	0.57
1:A:2309:A:N6	1:A:2310:A:N1	2.51	0.57
8:I:72:LEU:O	8:I:73:GLU:HB2	2.03	0.57
1:A:12:U:O2	1:A:12:U:H2'	2.04	0.57
28:6:8:LYS:HD3	30:8:34:TRP:CD2	2.39	0.57
23:1:50:ARG:HG2	23:1:59:THR:HB	1.86	0.57
30:8:39:LYS:HA	30:8:42:ARG:NH1	2.18	0.57
8:I:61:ARG:HB3	8:I:133:HIS:HD2	1.68	0.57
1:A:1722:A:C2	1:A:1740:G:C8	2.92	0.57
14:S:58:LEU:HD12	14:S:65:VAL:HG13	1.86	0.57
3:D:254:THR:O	3:D:254:THR:OG1	2.22	0.57
5:F:6:VAL:HA	5:F:23:ASP:H	1.67	0.57
1:A:708:C:H42	1:A:723:G:H1	1.51	0.57
23:1:21:ARG:NH1	23:1:21:ARG:HG2	2.07	0.57
1:A:8:A:H2'	1:A:9:U:C6	2.39	0.57
26:4:18:CYS:CB	26:4:39:CYS:SG	2.90	0.57
1:A:2611:U:C4	27:5:3:LYS:HG2	2.40	0.57
1:A:1040:C:H2'	1:A:1041:C:O4'	2.05	0.57
4:E:16:ARG:NH1	4:E:171:GLU:OE2	2.37	0.57
12:Q:84:GLY:O	12:Q:85:LYS:HB2	2.04	0.57
1:A:1568:G:N7	34:D:402:HOH:O	2.32	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:861:A:C2	1:A:917:A:C4	2.92	0.57
8:I:31:LEU:HD21	8:I:38:LEU:HG	1.87	0.57
1:A:2712:U:OP1	1:A:2714:G:H4'	2.05	0.57
26:4:15:ILE:HB	26:4:32:TYR:CD2	2.40	0.57
8:I:88:ILE:HG12	8:I:121:LYS:O	2.04	0.57
1:A:299:A:H5''	20:Y:86:ARG:HH21	1.70	0.57
3:D:108:PRO:HB3	3:D:143:HIS:CE1	2.40	0.57
1:A:443:A:N7	5:F:45:ARG:HG2	2.20	0.57
1:A:652(D):C:H2'	1:A:652(E):G:O4'	2.05	0.57
1:A:1292:U:H2'	1:A:1293:C:C6	2.40	0.57
17:V:15:GLU:O	17:V:18:LEU:HB2	2.05	0.57
8:I:102:SER:OG	8:I:103:ARG:N	2.36	0.57
1:A:2892:A:H2'	1:A:2893:G:H5''	1.85	0.57
1:A:1507:A:O2'	1:A:1508:A:O5'	2.22	0.57
8:I:70:GLU:O	8:I:74:ASN:HB2	2.05	0.57
19:X:31:HIS:CD2	19:X:33:LYS:H	2.23	0.57
1:A:2292:C:OP1	14:S:17:ARG:NH2	2.37	0.57
1:A:1639:U:C2'	1:A:1640:C:H5''	2.35	0.57
1:A:2683:C:OP1	15:T:53:ARG:NH2	2.38	0.57
12:Q:5:ARG:O	21:Z:194:PRO:HD2	2.04	0.57
1:A:2291:U:H2'	1:A:2292:C:C6	2.40	0.56
1:A:628:G:H2'	1:A:629:G:H8	1.70	0.56
29:7:8:ASN:OD1	29:7:8:ASN:C	2.43	0.56
1:A:602:G:O2'	1:A:655:A:N6	2.38	0.56
1:A:2131:G:N3	1:A:2133:G:N2	2.51	0.56
5:F:32:LEU:HD11	5:F:105:VAL:HG13	1.86	0.56
23:1:64:ALA:HA	23:1:67:ILE:HG13	1.87	0.56
1:A:761:A:N7	34:A:3897:HOH:O	2.33	0.56
1:A:1796:U:H2'	1:A:1797:C:C6	2.39	0.56
2:B:87:G:H5''	2:B:88:C:OP2	2.06	0.56
14:S:83:LYS:O	14:S:111:GLU:HG3	2.06	0.56
1:A:1557:C:OP2	1:A:1558:A:O2'	2.18	0.56
1:A:795:C:H2'	1:A:796:C:H6	1.70	0.56
17:V:42:GLY:O	17:V:43:GLU:HG2	2.06	0.56
1:A:271(L):U:H4'	1:A:271(M):G:OP1	2.04	0.56
1:A:2384:G:OP2	22:0:55:ARG:NH1	2.39	0.56
1:A:2118:U:OP1	1:A:2147:G:O2'	2.22	0.56
2:B:8:U:H6	2:B:8:U:H5''	1.70	0.56
14:S:25:ARG:NH1	14:S:42:ASP:OD2	2.39	0.56
1:A:1364:G:OP2	23:1:3:LYS:HG2	2.05	0.56
20:Y:51:VAL:HG22	20:Y:58:GLY:H	1.70	0.56
1:A:2131:G:H5''	1:A:2132:U:H5''	1.88	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1593:G:H2'	1:A:1594:G:H8	1.71	0.56
1:A:63:U:OP2	34:A:4694:HOH:O	2.18	0.56
1:A:2107:C:C5	1:A:2108:C:C4	2.93	0.56
1:A:528:A:O2'	1:A:529:A:H5'	2.06	0.56
14:S:59:LYS:HB3	14:S:60:GLY:CA	2.35	0.56
27:5:49:CYS:SG	27:5:51:TYR:HB2	2.46	0.56
1:A:579:G:H2'	1:A:580:C:C6	2.41	0.56
20:Y:2:ARG:HH11	20:Y:2:ARG:HA	1.70	0.56
1:A:2113:U:H2'	1:A:2114:A:C8	2.40	0.56
1:A:2036:C:C6	1:A:2036:C:H5'	2.40	0.56
1:A:107:C:H2'	1:A:108:U:H6	1.70	0.56
30:8:7:HIS:CD2	30:8:10:ALA:H	2.12	0.55
1:A:2305:A:H1'	6:G:135:LEU:O	2.06	0.55
1:A:2328:A:H2'	1:A:2329:G:C8	2.41	0.55
1:A:1141:U:OP2	9:N:63:THR:OG1	2.19	0.55
7:H:139:GLN:HG3	7:H:140:LYS:N	2.20	0.55
1:A:2424:C:O2	1:A:2429:G:O2'	2.20	0.55
1:A:1509(B):A:H2'	1:A:1510:G:C8	2.41	0.55
10:O:115:VAL:HG13	10:O:121:VAL:HG21	1.88	0.55
5:F:107:LYS:HE3	5:F:205:ARG:O	2.07	0.55
1:A:271(F):C:H2'	1:A:271(G):C:H6	1.72	0.55
1:A:1309:G:N7	34:A:4011:HOH:O	2.33	0.55
1:A:848:G:OP1	34:A:3712:HOH:O	2.18	0.55
1:A:2109:U:H3'	1:A:2109:U:H6	1.72	0.55
1:A:1109:C:C5	1:A:1110:G:C2	2.88	0.55
1:A:1762:A:H8	1:A:1762:A:O5'	1.89	0.55
24:2:53:LEU:O	24:2:57:ILE:HG13	2.07	0.55
20:Y:8:LYS:HG2	20:Y:9:LYS:O	2.07	0.55
8:I:112:LYS:O	8:I:114:LEU:N	2.36	0.55
15:T:127:ALA:HA	15:T:128:GLU:C	2.27	0.55
1:A:154(A):C:N4	1:A:172:C:N3	2.54	0.55
1:A:1007:C:OP1	9:N:37:LYS:NZ	2.38	0.55
20:Y:68:HIS:ND1	20:Y:70:SER:HB3	2.22	0.55
1:A:2306:C:H3'	1:A:2307:G:C8	2.41	0.55
14:S:46:VAL:HG12	14:S:48:LEU:HD12	1.89	0.55
16:U:76:TYR:CZ	16:U:80:ILE:HG13	2.42	0.55
1:A:2126:A:H4'	1:A:2127:G:O5'	2.07	0.55
11:P:148:LEU:H	11:P:148:LEU:HD23	1.71	0.55
23:1:82:LEU:HA	23:1:85:LEU:HD23	1.87	0.55
1:A:1140:C:O3'	9:N:25:ARG:NH1	2.39	0.55
1:A:2287:A:N6	1:A:2344:U:N3	2.54	0.55
25:3:6:VAL:HG12	25:3:54:VAL:HG11	1.89	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:956:G:OP2	12:Q:14:ARG:NH2	2.40	0.55
1:A:547:A:H1'	1:A:548:A:H4'	1.88	0.55
1:A:2134:A:C2	1:A:2159:G:H1'	2.42	0.55
1:A:330:A:HO2'	1:A:331:A:H8	1.51	0.55
1:A:2610:C:H4'	1:A:2611:U:OP2	2.05	0.55
14:S:84:GLN:HB3	14:S:111:GLU:HB2	1.89	0.55
5:F:129:PHE:CD2	5:F:163:VAL:HG21	2.42	0.55
1:A:2321:G:OP2	34:A:4626:HOH:O	2.18	0.55
1:A:2790:A:N3	1:A:2790:A:H2'	2.22	0.55
1:A:1364:G:OP1	23:1:2:SER:HA	2.07	0.54
1:A:443:A:H1'	1:A:1201:C:O4'	2.06	0.54
21:Z:101:PRO:O	21:Z:102:LEU:HD12	2.08	0.54
23:1:15:ALA:O	23:1:40:ARG:HG3	2.07	0.54
1:A:2115:G:O2'	1:A:2166:G:N2	2.39	0.54
1:A:638:G:H2'	1:A:639:U:C6	2.42	0.54
1:A:1141:U:OP1	9:N:25:ARG:NH1	2.40	0.54
1:A:1486:A:H2'	1:A:1487:G:C8	2.42	0.54
1:A:271(E):U:H2'	1:A:271(F):C:H6	1.73	0.54
1:A:907:U:O2'	12:Q:101:ARG:NH2	2.41	0.54
1:A:2144:U:H1'	1:A:2147:G:H1	1.72	0.54
19:X:2:LYS:HE2	19:X:38:GLU:OE2	2.07	0.54
1:A:1786:A:H1'	1:A:1938:A:N6	2.22	0.54
1:A:2822:G:C8	34:A:4408:HOH:O	2.61	0.54
1:A:192:C:O2'	1:A:802:A:N3	2.38	0.54
4:E:97:LYS:N	4:E:100:GLU:OE1	2.39	0.54
1:A:1570:A:H5'	3:D:36:PRO:HG3	1.89	0.54
34:A:4341:HOH:O	11:P:16:ARG:HG2	2.07	0.54
15:T:118:ARG:HG3	15:T:118:ARG:HH11	1.71	0.54
29:7:34:ARG:NH1	29:7:39:ARG:HG3	2.21	0.54
6:G:134:GLY:HA2	6:G:156:ASP:HA	1.89	0.54
1:A:1047:G:H2'	1:A:1110:G:N2	2.22	0.54
1:A:1364:G:C8	23:1:3:LYS:HD3	2.41	0.54
3:D:17:THR:O	3:D:211:ARG:NH2	2.37	0.54
1:A:1412:A:N6	34:A:4496:HOH:O	2.40	0.54
11:P:82:GLY:HA2	11:P:113:LYS:O	2.07	0.54
1:A:1657:C:H2'	1:A:1658:C:C6	2.43	0.54
1:A:2016:U:H1'	27:5:6:VAL:HG13	1.89	0.54
11:P:100:LEU:HD12	11:P:112:LEU:HD11	1.89	0.54
1:A:646:A:H2'	1:A:647:G:O4'	2.06	0.54
1:A:1434:A:H61	1:A:1558:A:H62	1.56	0.54
1:A:2477:C:O2	31:9:4:ARG:NH2	2.37	0.54
1:A:744:G:OP1	34:A:4394:HOH:O	2.18	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:674:G:H1'	5:F:74:ARG:HD3	1.90	0.54
14:S:59:LYS:HB3	14:S:60:GLY:HA2	1.89	0.54
1:A:2361:A:OP1	30:8:27:THR:HG23	2.08	0.54
1:A:2834:G:H8	1:A:2834:G:H5''	1.72	0.54
1:A:645:C:H2'	1:A:645:C:O2	2.07	0.54
1:A:330:A:H2	1:A:1210:A:H2'	1.72	0.54
1:A:2575:C:H5'	4:E:143:ASN:O	2.07	0.54
1:A:628:G:H2'	1:A:629:G:C8	2.43	0.54
1:A:857:C:OP2	22:0:77:ARG:NH2	2.40	0.54
34:A:3808:HOH:O	12:Q:119:ARG:HD2	2.07	0.54
31:9:14:CYS:HA	31:9:27:CYS:HB2	1.89	0.54
1:A:2025:C:P	34:A:4199:HOH:O	2.65	0.54
1:A:1043:C:H2'	1:A:1044:G:O4'	2.08	0.53
6:G:156:ASP:O	6:G:157:ILE:HG13	2.07	0.53
1:A:1026:U:HO2'	1:A:1027:A:P	2.27	0.53
8:I:14:ASP:O	8:I:17:GLN:HB3	2.08	0.53
14:S:102:ALA:HA	14:S:105:ALA:CB	2.38	0.53
1:A:607:U:OP1	5:F:102:PRO:HA	2.08	0.53
1:A:1790:C:H5''	1:A:1791:A:OP1	2.08	0.53
12:Q:110:THR:HG23	12:Q:113:GLN:OE1	2.07	0.53
1:A:2506:U:H2'	34:A:3796:HOH:O	2.07	0.53
5:F:53:THR:HG22	5:F:56:GLU:HG3	1.91	0.53
20:Y:28:LYS:CG	20:Y:40:GLU:HG2	2.38	0.53
6:G:106:LEU:HG	6:G:111:LEU:HG	1.89	0.53
1:A:2319:G:C2	14:S:3:ARG:HA	2.44	0.53
1:A:2166:G:N2	1:A:2172:U:O4	2.40	0.53
1:A:1721:G:H5'	1:A:1722:A:OP2	2.08	0.53
1:A:234:C:H2'	1:A:235:U:O4'	2.09	0.53
11:P:8:PRO:HB2	11:P:12:ALA:HB3	1.91	0.53
1:A:277:C:H4'	1:A:278:A:O5'	2.09	0.53
1:A:184:C:H2'	1:A:185:U:H6	1.74	0.53
8:I:61:ARG:HH11	8:I:61:ARG:HA	1.72	0.53
1:A:154:G:H5'	1:A:154(A):C:OP2	2.09	0.53
9:N:56:ASN:H	9:N:125:GLY:HA3	1.73	0.53
1:A:2784:C:H1'	4:E:37:ARG:HH12	1.72	0.53
3:D:2:ALA:N	3:D:200:ASP:OD2	2.42	0.53
14:S:3:ARG:HG3	14:S:4:LEU:N	2.22	0.53
1:A:1038:C:N4	1:A:1117:G:H1	2.03	0.53
1:A:1022:G:N7	9:N:66:LYS:HE2	2.23	0.53
1:A:1531:C:H42	1:A:1538:G:H1	1.57	0.53
21:Z:54:HIS:ND1	21:Z:101:PRO:HG3	2.24	0.53
1:A:2272:U:H5''	1:A:2273:A:OP1	2.09	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:G:48:GLU:O	6:G:51:ARG:N	2.42	0.53
21:Z:68:PRO:O	21:Z:91:LEU:HB2	2.08	0.53
1:A:2114:A:H2'	1:A:2115:G:O4'	2.08	0.53
1:A:2805:G:H2'	1:A:2807:G:H8	1.74	0.53
5:F:150:GLY:HA2	5:F:172:TRP:CD2	2.43	0.53
1:A:588:U:H2'	1:A:589:C:C6	2.43	0.53
3:D:44:ASN:OD1	3:D:46:GLN:HB2	2.09	0.53
1:A:1031:G:H21	31:9:36:GLN:HE22	1.56	0.53
12:Q:12:GLN:HG2	12:Q:73:PRO:HD2	1.91	0.53
1:A:1899:G:H2'	1:A:1899:G:N3	2.22	0.53
1:A:226:G:H21	1:A:228:A:N6	2.05	0.52
8:I:68:LEU:C	8:I:70:GLU:H	2.12	0.52
1:A:2144:U:O2'	1:A:2145:C:H2'	2.08	0.52
1:A:974:G:O6	34:A:4094:HOH:O	2.19	0.52
1:A:2557:G:H2'	1:A:2558:C:C6	2.44	0.52
1:A:2712:U:O2'	1:A:2713:A:H5'	2.09	0.52
4:E:111:ARG:HG3	4:E:160:TYR:CD1	2.44	0.52
3:D:232:PRO:HA	34:D:406:HOH:O	2.07	0.52
26:4:18:CYS:SG	26:4:39:CYS:HB2	2.49	0.52
14:S:14:VAL:O	14:S:18:ILE:HG12	2.09	0.52
18:W:43:GLY:O	18:W:47:VAL:HG23	2.10	0.52
1:A:2031:A:C6	1:A:2498:C:H1'	2.45	0.52
1:A:2751:G:C5	7:H:2:SER:N	2.78	0.52
1:A:1816:G:H1	3:D:35:LYS:HD3	1.73	0.52
1:A:1779:U:H6	1:A:1784:A:H62	1.57	0.52
1:A:2133:G:H2'	1:A:2157:G:H22	1.75	0.52
30:8:28:GLY:O	30:8:36:LYS:NZ	2.43	0.52
1:A:2014:A:OP1	34:A:4828:HOH:O	2.18	0.52
1:A:1815:A:OP2	3:D:54:ARG:NH2	2.40	0.52
1:A:2887:U:H2'	1:A:2888:C:H6	1.74	0.52
1:A:2815:C:H5'	27:5:29:THR:HG21	1.90	0.52
7:H:24:VAL:HG13	7:H:37:VAL:HG21	1.92	0.52
20:Y:23:ARG:HB2	20:Y:23:ARG:NH1	2.24	0.52
13:R:37:THR:OG1	13:R:40:LYS:HG3	2.09	0.52
4:E:170:LEU:HB3	4:E:184:VAL:HG22	1.90	0.52
21:Z:92:SER:O	21:Z:130:PRO:HG2	2.10	0.52
1:A:2567:G:H2'	1:A:2568:C:C6	2.44	0.52
1:A:975(A):G:H1'	1:A:990:A:C2	2.44	0.52
1:A:2854:G:H2'	1:A:2855:C:C6	2.45	0.52
1:A:1503:U:H2'	1:A:1504:C:C6	2.44	0.52
2:B:105:A:OP1	21:Z:72:ARG:NH1	2.43	0.52
1:A:2102:U:O2	1:A:2187:G:O6	2.27	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:725:G:C6	1:A:726:G:N1	2.78	0.52
1:A:2483:C:N3	12:Q:124:LYS:NZ	2.58	0.52
16:U:74:LEU:HD11	16:U:110:VAL:HG13	1.92	0.52
1:A:795:C:H2'	1:A:796:C:C6	2.45	0.52
6:G:111:LEU:HD22	6:G:114:ILE:HD11	1.91	0.52
17:V:16:PRO:HA	17:V:96:ILE:HG22	1.91	0.52
1:A:863:A:H2'	1:A:864:G:H8	1.75	0.52
7:H:40:GLU:OE2	7:H:60:ARG:NH1	2.42	0.52
1:A:1048:A:O2'	1:A:1049:C:OP2	2.25	0.52
1:A:217:G:OP2	34:A:3937:HOH:O	2.19	0.52
1:A:2250:G:O2'	1:A:2496:C:OP1	2.20	0.52
6:G:16:ARG:HH21	6:G:31:VAL:HB	1.74	0.51
5:F:103:LYS:HA	5:F:106:ARG:HG3	1.93	0.51
1:A:1005:C:O2'	9:N:28:THR:HG21	2.10	0.51
9:N:102:ALA:O	9:N:106:MET:HG3	2.09	0.51
9:N:47:ALA:HB2	9:N:112:LEU:HD11	1.91	0.51
1:A:587:C:O2	11:P:33:ARG:NH2	2.32	0.51
13:R:36:THR:HG22	13:R:37:THR:H	1.74	0.51
21:Z:102:LEU:HD13	21:Z:123:ASP:HA	1.92	0.51
1:A:2163:C:OP2	1:A:2164:C:N4	2.42	0.51
24:2:44:LEU:HG	24:2:45:SER:O	2.10	0.51
1:A:720:C:H2'	1:A:721:C:H6	1.75	0.51
1:A:566:U:H5''	11:P:29:LYS:HE3	1.92	0.51
20:Y:76:CYS:CB	20:Y:79:CYS:HB2	2.35	0.51
1:A:2305:A:H2'	1:A:2306:C:O4'	2.10	0.51
6:G:27:ASN:HB3	6:G:30:GLU:HG3	1.93	0.51
10:O:102:VAL:HB	10:O:106:LEU:HD12	1.91	0.51
3:D:142:VAL:HG23	3:D:193:VAL:HA	1.92	0.51
1:A:2727:G:O2'	10:O:70:LYS:HE2	2.10	0.51
12:Q:29:PHE:N	12:Q:105:GLU:OE2	2.40	0.51
1:A:2275:C:H5'	1:A:2275:C:H6	1.75	0.51
1:A:2162:G:H4'	1:A:2172:U:O2'	2.10	0.51
1:A:2131:G:H8	1:A:2131:G:OP2	1.94	0.51
1:A:2144:U:HO2'	1:A:2145:C:H6	1.56	0.51
6:G:41:GLN:NE2	6:G:154:GLY:O	2.39	0.51
25:3:43:ILE:O	25:3:47:VAL:HG23	2.11	0.51
1:A:2317:C:H2'	1:A:2318:G:H5'	1.93	0.51
20:Y:23:ARG:HH11	20:Y:23:ARG:HB2	1.76	0.51
1:A:1720:U:H2'	1:A:1721:G:O4'	2.11	0.51
1:A:958:U:H5''	12:Q:14:ARG:HD3	1.92	0.51
1:A:1891:G:N7	34:A:4690:HOH:O	2.32	0.51
1:A:829:A:N7	1:A:2248:C:H5'	2.25	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
18:W:14:PRO:HG2	18:W:78:GLU:HG2	1.93	0.51
1:A:271(Q):G:O2'	1:A:271(R):G:OP2	2.28	0.51
1:A:1364:G:P	23:1:3:LYS:HG2	2.51	0.51
1:A:2023:G:H5'	1:A:2617:C:H4'	1.92	0.51
1:A:263:C:H2'	1:A:264:C:O4'	2.11	0.51
3:D:9:TYR:CZ	3:D:13:ARG:HG2	2.46	0.51
1:A:1946:U:H2'	1:A:1947:C:C6	2.46	0.51
1:A:529:A:H62	1:A:2041:U:H3	1.57	0.51
14:S:7:TYR:CE1	14:S:91:PRO:HG3	2.46	0.51
15:T:42:ILE:HG12	15:T:84:GLN:OE1	2.10	0.51
9:N:128:HIS:CE1	9:N:135:PRO:HG2	2.45	0.51
1:A:1378:A:OP1	29:7:10:ARG:NH2	2.44	0.51
1:A:2894:G:N3	1:A:2894:G:H2'	2.26	0.51
1:A:188:G:H1	1:A:208:C:H42	1.59	0.51
1:A:458:G:O2'	29:7:39:ARG:HD3	2.11	0.51
1:A:1935:G:H1'	1:A:1964:G:N2	2.26	0.51
28:6:9:LEU:HD21	28:6:25:LYS:HB3	1.92	0.51
1:A:1547:C:H2'	1:A:1548:C:C6	2.46	0.51
1:A:1547:C:H2'	1:A:1548:C:H6	1.74	0.51
1:A:1379:A:H4'	1:A:1380:G:OP2	2.10	0.51
10:O:25:LEU:HD12	10:O:38:VAL:HG12	1.93	0.51
20:Y:43:ASN:OD1	20:Y:65:ALA:HB3	2.11	0.51
1:A:1143:A:OP1	9:N:25:ARG:NH2	2.44	0.51
1:A:2815:C:H2'	1:A:2816:C:H6	1.76	0.51
1:A:863:A:H2'	1:A:864:G:C8	2.46	0.51
2:B:77:U:OP1	21:Z:19:ARG:NH2	2.44	0.51
1:A:1614:A:C2	18:W:93:ALA:HB2	2.46	0.51
1:A:2408:U:OP2	34:A:4298:HOH:O	2.18	0.51
1:A:7:G:H2'	1:A:8:A:O4'	2.10	0.50
1:A:2126:A:H1'	1:A:2127:G:OP2	2.11	0.50
1:A:2108:C:H6	1:A:2108:C:H3'	1.76	0.50
6:G:58:GLN:HA	6:G:61:ALA:HB3	1.93	0.50
1:A:2124:G:H1	1:A:2174:C:N4	2.09	0.50
2:B:53:A:H5'	2:B:54:G:OP2	2.12	0.50
1:A:784:A:H3'	34:A:4103:HOH:O	2.11	0.50
15:T:84:GLN:HE21	15:T:85:LYS:HG2	1.76	0.50
1:A:1296:G:OP1	1:A:2709:G:O2'	2.24	0.50
1:A:1499:C:O2'	1:A:1500:G:H5'	2.11	0.50
8:I:83:ALA:HB2	8:I:88:ILE:HA	1.92	0.50
1:A:493:G:H2'	1:A:494:G:O4'	2.12	0.50
1:A:641:C:O2'	1:A:2350:C:OP1	2.21	0.50
17:V:58:VAL:HG12	17:V:97:LYS:HB2	1.92	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:1:23:LYS:HG2	23:1:29:GLY:HA3	1.93	0.50
1:A:83:G:N2	1:A:103:A:OP2	2.36	0.50
1:A:2158:A:O3'	1:A:2159:G:H8	1.94	0.50
1:A:1210:A:C8	1:A:1210:A:H5'	2.42	0.50
1:A:2206:G:H2'	1:A:2207:G:C2	2.47	0.50
1:A:2286:A:H4'	1:A:2287:A:O4'	2.12	0.50
7:H:86:GLU:HG2	7:H:132:ARG:HG3	1.93	0.50
1:A:247:G:H4'	1:A:386:G:C5	2.46	0.50
1:A:1298:C:H5''	1:A:1299:G:OP2	2.12	0.50
1:A:2713:A:OP1	13:R:14:SER:OG	2.26	0.50
15:T:55:ASN:N	15:T:59:THR:HG22	2.26	0.50
1:A:1514:U:H2'	1:A:1515:G:H8	1.77	0.50
1:A:748:G:C8	18:W:89:ALA:HB1	2.46	0.50
1:A:271(P):C:H2'	1:A:271(Q):G:H5'	1.94	0.50
1:A:760:G:H2'	1:A:761:A:O4'	2.12	0.50
6:G:166:ASP:O	6:G:170:ARG:N	2.34	0.50
1:A:122:G:N7	34:A:3877:HOH:O	2.35	0.50
21:Z:110:GLY:HA3	21:Z:174:VAL:HG11	1.92	0.50
1:A:2079:U:OP1	23:1:21:ARG:NH2	2.45	0.50
4:E:24:THR:HG22	4:E:186:GLY:O	2.12	0.50
21:Z:128:VAL:HG12	21:Z:129:SER:N	2.27	0.50
3:D:16:MET:HG3	3:D:206:LEU:O	2.12	0.50
8:I:5:LEU:HD21	8:I:12:LEU:HD13	1.93	0.50
8:I:86:THR:HG23	8:I:87:LYS:HB2	1.94	0.50
1:A:2298:A:H2'	1:A:2299:G:O4'	2.11	0.50
15:T:1:MET:HE2	15:T:3:ARG:HG2	1.92	0.50
1:A:2236:C:H2'	1:A:2237:G:H5'	1.93	0.50
1:A:2267:A:H2'	34:A:4797:HOH:O	2.11	0.50
5:F:184:TYR:CE2	5:F:188:ARG:HD2	2.46	0.49
1:A:1839:G:C8	1:A:1927:A:H1'	2.47	0.49
22:O:51:VAL:N	22:O:62:LEU:HD12	2.28	0.49
9:N:62:VAL:HG12	9:N:67:LEU:HD22	1.94	0.49
1:A:1945:G:H2'	1:A:1946:U:C6	2.47	0.49
3:D:12:SER:HB3	3:D:208:LYS:HB3	1.93	0.49
14:S:58:LEU:HB2	14:S:59:LYS:HB2	1.94	0.49
4:E:97:LYS:O	4:E:100:GLU:HG3	2.12	0.49
1:A:386:G:H4'	1:A:387:U:OP2	2.12	0.49
11:P:101:VAL:HA	11:P:106:LEU:O	2.13	0.49
1:A:271(M):G:O2'	1:A:271(N):U:H3'	2.11	0.49
26:4:16:CYS:HB3	26:4:20:ASN:O	2.13	0.49
24:2:29:LYS:HD3	24:2:57:ILE:HD13	1.94	0.49
15:T:118:ARG:HA	15:T:118:ARG:HH11	1.77	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2574:G:O2'	4:E:143:ASN:HB3	2.12	0.49
1:A:2818:G:O2'	1:A:2819:G:H5'	2.12	0.49
18:W:40:ASN:O	18:W:41:LYS:HG3	2.11	0.49
1:A:2019:A:N7	27:5:9:LYS:NZ	2.53	0.49
1:A:1745(A):C:H5'	1:A:1746:G:OP2	2.12	0.49
1:A:821:A:H2'	1:A:946:G:H5''	1.95	0.49
1:A:1971:A:OP2	3:D:242:ARG:NH2	2.45	0.49
1:A:1108:U:O2	1:A:1108:U:H2'	2.12	0.49
5:F:185:ASP:HA	5:F:188:ARG:HD3	1.94	0.49
18:W:86:LEU:HD12	18:W:87:PRO:HD2	1.93	0.49
4:E:52:LEU:O	4:E:75:VAL:HG22	2.12	0.49
3:D:172:TYR:CD1	3:D:186:HIS:HA	2.47	0.49
1:A:1914:C:OP2	1:A:1914:C:H6	1.94	0.49
1:A:1858:G:H2'	1:A:1883:G:H22	1.77	0.49
27:5:13:LYS:HB3	34:5:204:HOH:O	2.13	0.49
1:A:265:A:H1'	1:A:266:G:O4'	2.12	0.49
1:A:542:C:H2'	1:A:543:C:C6	2.48	0.49
1:A:1155:A:OP1	16:U:55:ARG:HD3	2.12	0.49
1:A:271(N):U:O2'	1:A:271(O):C:H5'	2.13	0.49
1:A:873:G:N2	1:A:905:U:C2	2.81	0.49
1:A:2572:A:N7	4:E:145:LYS:HB2	2.27	0.49
1:A:1962:C:O2'	1:A:1964:G:OP2	2.29	0.49
3:D:175:LEU:HD12	3:D:185:VAL:HG21	1.94	0.49
5:F:178:PRO:HG2	5:F:179:GLU:OE1	2.12	0.49
10:O:88:ASN:HD21	10:O:90:GLN:HB2	1.78	0.49
1:A:2171:A:H4'	1:A:2172:U:OP1	2.12	0.49
3:D:267:SER:C	3:D:269:PHE:H	2.16	0.49
1:A:1639:U:O2'	1:A:1640:C:H5''	2.12	0.49
1:A:1130:U:O2	4:E:149:ARG:NH2	2.45	0.49
1:A:196:A:O4'	11:P:46:LYS:HE2	2.13	0.49
22:0:11:ARG:O	22:0:14:ARG:NH2	2.44	0.49
1:A:2142:C:N3	1:A:2149:G:O6	2.45	0.49
1:A:9:U:O2'	1:A:10:G:OP1	2.29	0.49
1:A:902:C:H2'	1:A:903:C:H6	1.77	0.49
1:A:469:G:H2'	1:A:470:A:H5''	1.95	0.49
1:A:2406:U:C4	11:P:72:PRO:HD2	2.48	0.49
8:I:88:ILE:HG22	8:I:90:GLY:N	2.27	0.49
30:8:34:TRP:CE2	30:8:35:GLN:HG3	2.47	0.49
1:A:1721:G:N1	1:A:1739:U:OP2	2.45	0.49
21:Z:146:ILE:HA	21:Z:174:VAL:HG12	1.94	0.49
22:0:53:MET:HG3	22:0:59:LEU:CD2	2.43	0.49
21:Z:77:ASP:OD1	21:Z:80:ARG:HG2	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:7:G:H1	1:A:2896:C:H42	1.61	0.48
1:A:1359:A:N3	1:A:1359:A:O4'	2.46	0.48
1:A:856:C:O4'	22:0:27:GLU:HB3	2.12	0.48
1:A:2577:A:H5'	27:5:3:LYS:HD2	1.95	0.48
1:A:857:C:H4'	22:0:23:VAL:HG21	1.94	0.48
7:H:32:GLU:O	7:H:33:LEU:HD23	2.13	0.48
1:A:1441:G:H2'	1:A:1442:G:H8	1.78	0.48
1:A:64:A:O3'	19:X:71:GLY:HA3	2.13	0.48
29:7:47:ARG:HH11	29:7:47:ARG:HG3	1.78	0.48
1:A:27:G:H1	1:A:512:G:HO2'	1.60	0.48
1:A:1970:A:H4'	1:A:1971:A:OP1	2.13	0.48
7:H:5:GLY:HA2	7:H:69:ARG:HB3	1.96	0.48
9:N:42:TRP:CE3	16:U:63:VAL:HG11	2.48	0.48
18:W:60:ASN:HD22	18:W:60:ASN:H	1.58	0.48
1:A:903:C:H2'	1:A:904:C:C6	2.48	0.48
23:1:51:VAL:HG11	23:1:74:VAL:HG21	1.94	0.48
3:D:78:LYS:HE2	3:D:114:GLY:HA2	1.94	0.48
1:A:593:G:O6	34:A:3927:HOH:O	2.18	0.48
1:A:1876:A:H2'	1:A:1877:A:C8	2.48	0.48
1:A:1506:C:C2'	1:A:1507:A:H5'	2.42	0.48
1:A:708:C:H5'	1:A:709:U:OP2	2.13	0.48
10:O:59:LYS:HZ1	10:O:89:ASN:HD21	1.61	0.48
3:D:118:VAL:HG22	3:D:119:ALA:H	1.78	0.48
1:A:453:C:H5''	34:A:4375:HOH:O	2.13	0.48
1:A:2687:U:H2'	1:A:2688:U:O4'	2.12	0.48
6:G:102:PHE:CE2	6:G:141:PHE:HE1	2.31	0.48
1:A:2115:G:C2	1:A:2117:A:N7	2.82	0.48
1:A:639:U:O2'	1:A:640:C:H5'	2.13	0.48
8:I:61:ARG:HB3	8:I:133:HIS:CD2	2.47	0.48
1:A:2273:A:H2'	1:A:2274:A:C8	2.47	0.48
1:A:2080:G:P	23:1:35:THR:HG1	2.37	0.48
1:A:652(A):A:H4'	1:A:652(B):A:OP1	2.14	0.48
1:A:545:G:H4'	1:A:545:G:OP1	2.12	0.48
1:A:2646:C:H2'	1:A:2647:U:O4'	2.14	0.48
4:E:37:ARG:HA	4:E:42:ASP:OD2	2.13	0.48
4:E:179:GLU:HB3	4:E:181:LEU:HD22	1.95	0.48
24:2:22:GLU:OE2	24:2:68:ARG:NH2	2.46	0.48
1:A:2393:A:O2'	30:8:13:ARG:NH1	2.43	0.48
1:A:271(Y):U:O3'	1:A:271(Z):C:H6	1.96	0.48
1:A:2028:U:H2'	1:A:2029:G:O4'	2.13	0.48
18:W:83:LYS:O	18:W:84:ARG:HD3	2.12	0.48
1:A:1015:G:C2'	1:A:1016:G:H5'	2.43	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1025:G:C4	1:A:1135:C:H1'	2.49	0.48
1:A:997:G:OP1	16:U:92:ARG:HG2	2.14	0.48
7:H:69:ARG:HG3	7:H:70:THR:N	2.27	0.48
20:Y:28:LYS:HG2	20:Y:40:GLU:HG2	1.96	0.48
22:O:53:MET:HG3	22:O:59:LEU:HD23	1.96	0.48
1:A:2064:C:H2'	1:A:2065:C:C6	2.48	0.48
15:T:29:ARG:HB2	15:T:46:GLU:HB2	1.94	0.48
9:N:33:LEU:HD12	9:N:38:HIS:CE1	2.49	0.48
1:A:2371:G:HO2'	28:6:46:HIS:CE1	2.24	0.48
9:N:96:GLU:H	9:N:96:GLU:CD	2.17	0.48
12:Q:38:GLU:OE2	12:Q:128:LYS:N	2.33	0.48
30:8:32:LEU:O	30:8:36:LYS:HE3	2.13	0.48
1:A:154:G:H8	1:A:154:G:H5''	1.79	0.48
6:G:125:PHE:HB3	6:G:166:ASP:CG	2.34	0.48
1:A:2299:G:N7	34:A:4723:HOH:O	2.35	0.48
20:Y:99:CYS:HB3	20:Y:104:GLY:H	1.79	0.48
21:Z:5:LEU:HD22	21:Z:6:LYS:N	2.29	0.48
1:A:2311:A:O2'	1:A:2312:U:O4'	2.25	0.48
11:P:38:GLN:O	11:P:39:LYS:CB	2.62	0.48
1:A:2098:U:H2'	1:A:2099:U:O4'	2.12	0.48
21:Z:111:VAL:O	21:Z:113:ALA:N	2.47	0.48
1:A:2273:A:O2'	1:A:2274:A:H5'	2.13	0.48
21:Z:144:LEU:HD21	21:Z:150:LEU:HG	1.95	0.48
18:W:46:PHE:O	18:W:50:VAL:HG23	2.13	0.48
12:Q:7:MET:HE1	21:Z:193:GLU:CB	2.44	0.48
6:G:174:GLU:O	6:G:177:GLY:N	2.45	0.48
1:A:251:A:OP1	30:8:7:HIS:HE1	1.95	0.48
1:A:2748:A:OP1	7:H:70:THR:HG21	2.13	0.48
14:S:83:LYS:C	14:S:111:GLU:HG3	2.33	0.48
1:A:1138:G:H2'	9:N:106:MET:HE2	1.95	0.48
1:A:274:G:H2'	1:A:275:G:C8	2.48	0.48
28:6:11:LEU:HB3	28:6:49:HIS:HB3	1.95	0.48
11:P:39:LYS:CB	11:P:45:LEU:HG	2.37	0.48
1:A:271(L):U:C4'	1:A:271(M):G:OP1	2.61	0.48
23:1:3:LYS:HE3	23:1:3:LYS:HB3	1.51	0.48
2:B:91:C:OP1	12:Q:16:ARG:HG2	2.14	0.48
1:A:1769:G:O2'	1:A:1958:C:OP1	2.18	0.48
1:A:934:G:H2'	1:A:935:C:C6	2.48	0.48
1:A:2699:C:H2'	1:A:2700:C:O4'	2.13	0.48
2:B:2:C:H2'	2:B:3:C:C6	2.48	0.48
1:A:855:G:H2'	1:A:856:C:C6	2.49	0.47
2:B:8:U:O3'	14:S:25:ARG:NH2	2.47	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2784:C:H1'	4:E:37:ARG:NH1	2.28	0.47
1:A:1049:C:H2'	1:A:1050:A:C8	2.48	0.47
18:W:19:LEU:O	27:5:25:LEU:HD12	2.14	0.47
9:N:18:ALA:O	9:N:21:LYS:HB2	2.14	0.47
4:E:116:VAL:HG13	4:E:122:PHE:CG	2.47	0.47
2:B:28:C:OP1	14:S:36:TYR:OH	2.30	0.47
1:A:57:C:H2'	1:A:58:G:O4'	2.14	0.47
1:A:2304:G:O6	1:A:2312:U:O4	2.32	0.47
1:A:1568:G:H5''	3:D:61:LEU:HD22	1.96	0.47
8:I:79:ILE:O	8:I:144:VAL:HA	2.14	0.47
1:A:524:U:H2'	1:A:525:U:C6	2.49	0.47
6:G:47:LYS:HD3	6:G:81:LYS:CB	2.44	0.47
1:A:751:A:H5'	18:W:90:ARG:HA	1.97	0.47
1:A:2781:A:H5''	1:A:2782:G:H5'	1.96	0.47
1:A:2129:C:N3	1:A:2160:G:C6	2.83	0.47
1:A:2690:C:N4	1:A:2713:A:H1'	2.28	0.47
1:A:1211:U:H4'	1:A:1212:G:OP2	2.14	0.47
21:Z:111:VAL:HG12	21:Z:112:ARG:H	1.78	0.47
17:V:62:LEU:HD21	17:V:95:LEU:HB2	1.96	0.47
1:A:2286:A:OP1	28:6:29:ASN:ND2	2.48	0.47
4:E:21:VAL:HA	4:E:22:PRO:HD2	1.69	0.47
1:A:2850:A:OP2	1:A:2866:U:H5	1.97	0.47
1:A:1688:U:O2	1:A:1700:A:H5'	2.14	0.47
1:A:754:C:H2'	1:A:755:C:H6	1.78	0.47
26:4:16:CYS:HB2	26:4:36:CYS:SG	2.55	0.47
1:A:529:A:OP2	9:N:114:ARG:NH2	2.47	0.47
1:A:1413:G:O6	34:A:4496:HOH:O	2.19	0.47
1:A:1418:G:H8	1:A:1418:G:O5'	1.97	0.47
1:A:1992:G:C2	1:A:1997:G:C5	3.03	0.47
2:B:20:C:H2'	2:B:21:G:O4'	2.14	0.47
1:A:90:U:O2'	1:A:92:A:P	2.71	0.47
1:A:2845:G:O2'	1:A:2846:G:H5'	2.15	0.47
1:A:1036:G:H1	1:A:1119:C:N4	2.10	0.47
1:A:2206:G:H5'	1:A:2207:G:N7	2.29	0.47
15:T:97:ALA:O	15:T:98:LYS:HD2	2.14	0.47
1:A:1479:G:O2'	1:A:1558:A:H5'	2.14	0.47
14:S:10:ARG:O	14:S:14:VAL:HG13	2.14	0.47
14:S:10:ARG:NH2	14:S:91:PRO:HB2	2.28	0.47
1:A:1041:C:H5'	1:A:1042:G:OP2	2.14	0.47
1:A:1796:U:H4'	3:D:256:GLY:N	2.30	0.47
10:O:88:ASN:ND2	10:O:90:GLN:H	2.12	0.47
1:A:902:C:H2'	1:A:903:C:C6	2.50	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2334:G:O6	22:0:74:ARG:NH1	2.40	0.47
19:X:27:THR:HG23	19:X:80:ILE:HG13	1.97	0.47
1:A:362:U:O2'	1:A:363:G:H5''	2.15	0.47
5:F:108:LYS:O	5:F:112:MET:HG3	2.14	0.47
2:B:108:U:H2'	2:B:109:C:H5''	1.97	0.47
28:6:16:CYS:SG	28:6:18:ARG:HG3	2.55	0.47
1:A:244:A:C2	1:A:255:A:C4	3.03	0.47
11:P:63:PRO:HG2	30:8:25:MET:HB2	1.96	0.47
1:A:2439:A:H5'	1:A:2439:A:C8	2.50	0.47
6:G:16:ARG:NH2	6:G:28:VAL:O	2.48	0.47
1:A:278:A:H4'	1:A:279:C:OP1	2.14	0.47
1:A:2626:C:H2'	1:A:2627:G:O4'	2.15	0.47
1:A:1300:U:H4'	1:A:1301:A:H5''	1.97	0.47
1:A:1706:U:OP1	34:A:4145:HOH:O	2.20	0.47
1:A:2772:C:H2'	1:A:2773:C:C6	2.50	0.47
25:3:8:LEU:HD13	25:3:31:LEU:HA	1.96	0.47
1:A:1815:A:C5	1:A:1817:G:C6	3.03	0.47
23:1:86:SER:OG	23:1:89:GLU:HG2	2.15	0.47
1:A:1021:A:N6	1:A:1142(A):A:H61	2.12	0.47
1:A:1510:G:H2'	1:A:1511:C:C6	2.50	0.47
22:0:29:GLN:O	22:0:67:VAL:HG23	2.15	0.47
1:A:1514:U:H2'	1:A:1515:G:C8	2.50	0.47
1:A:1239:G:H2'	1:A:1240:U:O4'	2.14	0.47
17:V:21:ARG:HG3	17:V:93:GLU:HG3	1.96	0.47
19:X:52:VAL:HG12	19:X:82:GLN:HG2	1.97	0.47
1:A:1582:C:O2'	1:A:1586:A:N3	2.47	0.47
1:A:1652:A:C2'	1:A:1653:G:H5'	2.45	0.47
1:A:1493:C:C4	1:A:2206:G:H1'	2.50	0.47
5:F:158:THR:O	5:F:164:ARG:NH1	2.48	0.47
1:A:2734:A:H2'	1:A:2735:G:O4'	2.15	0.47
9:N:34:LEU:HD12	9:N:34:LEU:HA	1.72	0.47
1:A:1210:A:H4'	1:A:1211:U:O5'	2.14	0.46
1:A:529:A:H4'	34:A:4288:HOH:O	2.14	0.46
1:A:792:G:H5''	1:A:793:A:H5'	1.96	0.46
10:O:47:ILE:HB	10:O:48:PRO:HD2	1.97	0.46
8:I:140:LEU:HA	8:I:140:LEU:HD23	1.53	0.46
6:G:73:ALA:HB2	6:G:88:ILE:HD11	1.96	0.46
1:A:251:A:C5	1:A:252:G:H1'	2.49	0.46
21:Z:53:ILE:HG22	21:Z:71:VAL:O	2.15	0.46
1:A:911:A:H2'	12:Q:9:TYR:OH	2.15	0.46
3:D:76:PRO:HB2	3:D:116:GLN:HE21	1.80	0.46
1:A:2208:A:H1'	1:A:2219:G:C4	2.50	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:Y:32:PRO:O	20:Y:35:TYR:N	2.44	0.46
3:D:242:ARG:N	3:D:242:ARG:HD3	2.30	0.46
1:A:530:G:N1	34:A:4284:HOH:O	2.25	0.46
1:A:2146:C:H4'	1:A:2147:G:C8	2.50	0.46
1:A:1816:G:N1	3:D:35:LYS:HD3	2.30	0.46
1:A:83:G:OP1	20:Y:95:LYS:NZ	2.48	0.46
21:Z:144:LEU:CD2	21:Z:150:LEU:HG	2.45	0.46
1:A:2438:U:O2'	1:A:2440:C:OP1	2.24	0.46
11:P:84:ASN:HB3	11:P:117:GLU:O	2.16	0.46
14:S:96:GLY:HA3	14:S:98:VAL:N	2.31	0.46
4:E:71:GLY:HA2	4:E:72:VAL:O	2.16	0.46
1:A:2772:C:H2'	1:A:2773:C:H6	1.80	0.46
20:Y:35:TYR:CE2	20:Y:69:ALA:HB3	2.50	0.46
1:A:1810:A:H2'	1:A:1811:G:O4'	2.14	0.46
14:S:80:LEU:HD12	14:S:80:LEU:HA	1.72	0.46
1:A:2820:A:OP1	13:R:4:LEU:HD23	2.15	0.46
1:A:2833:G:H3'	1:A:2834:G:H5''	1.97	0.46
5:F:89:VAL:O	5:F:90:PHE:C	2.54	0.46
1:A:2427:C:H5''	1:A:2428:G:OP1	2.15	0.46
7:H:43:VAL:HG22	7:H:52:VAL:HG22	1.98	0.46
6:G:60:LEU:O	6:G:64:THR:N	2.38	0.46
14:S:11:LYS:HG3	14:S:91:PRO:HD3	1.96	0.46
1:A:2302:G:C6	1:A:2315:G:C6	3.04	0.46
22:O:26:TYR:O	22:O:29:GLN:HB2	2.15	0.46
7:H:33:LEU:HD21	7:H:136:ILE:HG13	1.98	0.46
20:Y:99:CYS:SG	20:Y:102:CYS:N	2.88	0.46
1:A:2262:U:O2'	1:A:2263:C:H5'	2.15	0.46
1:A:1425:G:H2'	1:A:1426:G:O4'	2.16	0.46
19:X:5:TYR:HD1	24:2:33:MET:HE2	1.81	0.46
2:B:14:U:OP2	2:B:70:C:O2'	2.30	0.46
28:6:34:LEU:HD22	28:6:36:LEU:HD11	1.98	0.46
1:A:723:G:H2'	1:A:724:U:O4'	2.16	0.46
9:N:128:HIS:HA	9:N:129:PRO:HD2	1.62	0.46
1:A:125:G:C6	29:7:10:ARG:HG3	2.51	0.46
21:Z:5:LEU:O	21:Z:59:LEU:HA	2.16	0.46
1:A:322:A:H5'	1:A:340:A:H1'	1.97	0.46
1:A:2191:G:H3'	1:A:2192:G:H8	1.81	0.46
1:A:950:G:C6	1:A:951:C:C4	3.04	0.46
1:A:2832:U:OP2	34:A:4206:HOH:O	2.20	0.46
24:2:69:ARG:O	24:2:70:GLN:HB2	2.15	0.46
4:E:201:THR:OG1	4:E:202:LYS:N	2.49	0.46
1:A:910:A:C5	12:Q:13:GLN:HG3	2.51	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:479:A:N3	1:A:481:G:H5''	2.30	0.46
1:A:2123:G:H1	1:A:2175:C:N4	2.14	0.46
1:A:92:A:C2'	1:A:93:G:H5'	2.45	0.46
1:A:1827:C:H5'	1:A:1971:A:H4'	1.98	0.46
1:A:2141:G:C6	1:A:2151:G:C6	3.03	0.46
1:A:330:A:H2	1:A:1210:A:HO2'	1.63	0.46
8:I:123:LEU:H	8:I:123:LEU:HD23	1.80	0.46
1:A:1529:G:C6	1:A:1530:C:C4	3.03	0.46
3:D:118:VAL:HG22	3:D:119:ALA:N	2.31	0.46
1:A:323:G:C8	5:F:171:PRO:HG3	2.51	0.46
12:Q:57:HIS:HD2	12:Q:117:ALA:HB2	1.80	0.46
1:A:1338:G:O2'	1:A:1393:A:N1	2.44	0.46
1:A:1779:U:C5	1:A:1784:A:N7	2.64	0.46
1:A:241:A:O4'	1:A:243:U:C6	2.69	0.46
1:A:686:G:O6	29:7:12:ARG:HD2	2.16	0.46
7:H:56:SER:OG	7:H:57:ASP:N	2.49	0.46
1:A:196:A:H2'	1:A:196:A:N3	2.31	0.46
21:Z:5:LEU:HD22	21:Z:6:LYS:H	1.81	0.46
7:H:94:TYR:CE2	7:H:107:VAL:HB	2.50	0.46
14:S:24:LEU:HD23	14:S:24:LEU:HA	1.77	0.46
21:Z:45:ASP:O	21:Z:49:ARG:HG3	2.16	0.46
18:W:41:LYS:HE3	27:5:25:LEU:HD21	1.96	0.46
2:B:117:G:H2'	2:B:118:G:O4'	2.16	0.46
1:A:271(S):G:C6	1:A:271(T):C:C4	3.05	0.45
5:F:7:TYR:N	5:F:22:ALA:HB3	2.29	0.45
1:A:1429:G:H2'	1:A:1430:C:C6	2.50	0.45
1:A:588:U:H1'	5:F:90:PHE:HB3	1.97	0.45
1:A:2313:C:H5''	6:G:91:ARG:HG3	1.98	0.45
30:8:62:LEU:HB3	30:8:65:GLU:HG2	1.97	0.45
1:A:2294:C:OP1	14:S:89:ARG:NH1	2.41	0.45
7:H:20:ALA:HB1	7:H:21:PRO:HD2	1.97	0.45
29:7:16:HIS:HB2	29:7:44:PRO:HG2	1.98	0.45
1:A:2312:U:H5'	6:G:88:ILE:HD12	1.97	0.45
9:N:112:LEU:O	9:N:115:ARG:N	2.46	0.45
1:A:1141:U:H4'	1:A:1142(A):A:O4'	2.16	0.45
21:Z:128:VAL:HG22	21:Z:161:VAL:H	1.81	0.45
6:G:137:GLU:HG3	6:G:152:LEU:HD21	1.98	0.45
8:I:133:HIS:ND1	8:I:134:PRO:O	2.43	0.45
4:E:116:VAL:HG13	4:E:122:PHE:HB2	1.98	0.45
30:8:29:LYS:HG2	30:8:44:LYS:HB3	1.98	0.45
9:N:99:LEU:O	9:N:103:VAL:HG23	2.16	0.45
21:Z:24:LEU:HB2	21:Z:41:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2170:A:H8	1:A:2170:A:OP2	1.99	0.45
1:A:1877:A:H5'	1:A:1878:G:OP2	2.17	0.45
21:Z:111:VAL:C	21:Z:113:ALA:N	2.69	0.45
1:A:916:G:O2'	1:A:917:A:O4'	2.33	0.45
21:Z:80:ARG:HG2	21:Z:80:ARG:H	1.62	0.45
20:Y:102:CYS:O	20:Y:104:GLY:N	2.48	0.45
12:Q:26:TYR:CD1	12:Q:28:ALA:HB2	2.51	0.45
25:3:4:LEU:O	25:3:36:VAL:HA	2.15	0.45
1:A:836:G:H5''	1:A:837:C:OP2	2.17	0.45
1:A:446:G:P	34:A:3953:HOH:O	2.67	0.45
1:A:271(H):G:O2'	1:A:271(I):G:OP2	2.28	0.45
2:B:49:C:OP1	14:S:96:GLY:HA2	2.17	0.45
1:A:1721:G:C2	1:A:1739:U:OP2	2.70	0.45
1:A:848:G:H2'	1:A:849:A:C8	2.52	0.45
1:A:415:A:H2'	1:A:416:C:C6	2.52	0.45
2:B:25:A:H2'	2:B:26:A:O4'	2.16	0.45
9:N:55:VAL:HG22	9:N:126:PRO:HA	1.99	0.45
1:A:2131:G:OP2	1:A:2131:G:H3'	2.17	0.45
1:A:2134:A:N3	1:A:2159:G:H1'	2.31	0.45
21:Z:30:ASN:HD22	21:Z:90:VAL:HB	1.82	0.45
1:A:1419:A:C8	1:A:1421:G:C6	3.05	0.45
1:A:375:C:H2'	1:A:376:C:C6	2.51	0.45
11:P:26:GLY:O	11:P:28:GLY:N	2.38	0.45
1:A:1697:G:OP2	1:A:1698:A:O2'	2.22	0.45
7:H:70:THR:HA	7:H:73:ALA:HB3	1.99	0.45
1:A:1180:C:H2'	1:A:1181:C:H6	1.80	0.45
26:4:40:HIS:HB3	26:4:43:TYR:HB3	1.97	0.45
1:A:2203:U:H4'	3:D:151:LYS:HG2	1.98	0.45
1:A:1529:G:H8	1:A:1529:G:O5'	1.99	0.45
3:D:71:ASP:HB3	3:D:103:ARG:NH2	2.32	0.45
4:E:112:GLY:O	4:E:159:HIS:HA	2.17	0.45
8:I:40:THR:O	8:I:44:LEU:HB2	2.17	0.45
24:2:1:MET:HG3	24:2:52:ASP:OD2	2.16	0.45
23:1:94:LEU:O	23:1:97:LEU:HB2	2.16	0.45
3:D:137:PRO:HB2	3:D:140:THR:HG23	1.99	0.45
1:A:828:U:H4'	1:A:831:G:N1	2.32	0.45
1:A:1575:C:H2'	1:A:1576:U:C6	2.51	0.45
1:A:252:G:P	11:P:50:ARG:HH11	2.38	0.45
1:A:1796:U:H4'	3:D:256:GLY:H	1.82	0.45
1:A:644:A:H4'	1:A:645:C:C5	2.51	0.45
9:N:54:VAL:HG11	9:N:99:LEU:HD12	1.97	0.45
15:T:23:ARG:HG3	15:T:120:ARG:CZ	2.46	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:359:A:H2'	1:A:360:G:O4'	2.17	0.45
1:A:1453:U:OP1	13:R:77:ARG:NH1	2.45	0.45
1:A:937:U:H2'	1:A:938:G:O4'	2.16	0.45
1:A:774:A:N3	1:A:774:A:H2'	2.31	0.45
1:A:620:G:N3	1:A:620:G:H5'	2.32	0.45
1:A:195:A:H4'	1:A:251:A:O2'	2.16	0.45
1:A:1047:G:H21	1:A:1111:A:N6	2.14	0.45
15:T:127:ALA:HA	15:T:129:ARG:N	2.32	0.45
1:A:923:C:C4'	22:O:29:GLN:HE21	2.29	0.45
8:I:44:LEU:HA	8:I:44:LEU:HD12	1.76	0.45
1:A:2199:A:OP2	1:A:2200:C:H5	1.99	0.45
3:D:237:GLU:OE1	34:D:404:HOH:O	2.21	0.45
2:B:59:A:H2'	2:B:60:C:C6	2.52	0.45
1:A:1493:C:N4	1:A:2206:G:H1'	2.32	0.45
1:A:2331:G:H4'	22:O:43:THR:H	1.82	0.45
11:P:97:PRO:HG3	11:P:112:LEU:HD12	1.99	0.45
24:2:64:LEU:HD21	24:2:68:ARG:HE	1.81	0.45
24:2:64:LEU:O	24:2:68:ARG:HG2	2.17	0.45
21:Z:104:PHE:HB3	21:Z:141:VAL:HG21	1.99	0.45
1:A:2313:C:H2'	1:A:2314:C:C6	2.51	0.45
1:A:2205:C:O2	1:A:2220:G:C2	2.70	0.45
7:H:71:LEU:HA	7:H:74:ASN:HB2	1.98	0.45
12:Q:16:ARG:O	12:Q:17:LEU:HD23	2.15	0.45
1:A:2591:C:OP1	3:D:239:ARG:HG2	2.17	0.45
5:F:65:TRP:HH2	5:F:72:ARG:HH21	1.64	0.45
8:I:1:MET:N	8:I:21:VAL:O	2.35	0.45
1:A:671:C:H2'	1:A:672:C:C6	2.52	0.45
1:A:1792:G:H2'	1:A:1793:C:H6	1.82	0.44
1:A:1108:U:O2'	1:A:1109:C:O4'	2.35	0.44
23:1:20:ARG:HH11	23:1:20:ARG:CG	2.27	0.44
21:Z:30:ASN:OD1	21:Z:32:HIS:N	2.47	0.44
30:8:34:TRP:O	30:8:36:LYS:N	2.50	0.44
6:G:121:ASN:HD21	6:G:123:ASN:HB2	1.82	0.44
17:V:52:VAL:HG22	17:V:55:ALA:HB3	1.99	0.44
1:A:764:A:N3	3:D:213:ARG:NH1	2.65	0.44
26:4:30:GLU:O	26:4:31:ILE:HG13	2.17	0.44
1:A:2833:G:O2'	1:A:2834:G:P	2.76	0.44
5:F:88:VAL:HG23	5:F:89:VAL:O	2.16	0.44
1:A:272(J):C:H2'	1:A:274:G:O4'	2.17	0.44
1:A:754:C:H2'	1:A:755:C:C6	2.52	0.44
1:A:1794:U:H2'	1:A:1795:C:H6	1.83	0.44
1:A:1794:U:H2'	1:A:1795:C:C6	2.52	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:R:21:TYR:OH	13:R:43:GLU:HG2	2.16	0.44
10:O:2:ILE:HG13	10:O:8:LEU:HD11	1.99	0.44
28:6:44:ARG:HH11	28:6:44:ARG:HB3	1.83	0.44
6:G:27:ASN:OD1	6:G:28:VAL:N	2.50	0.44
22:0:51:VAL:HG23	22:0:81:VAL:HG23	1.97	0.44
5:F:107:LYS:HE2	5:F:208:GLY:N	2.32	0.44
1:A:542:C:H2'	1:A:543:C:H6	1.83	0.44
1:A:1575:C:H2'	1:A:1576:U:H6	1.81	0.44
1:A:2454:G:H1'	34:A:4387:HOH:O	2.17	0.44
8:I:4:ILE:HG21	8:I:47:LEU:HD23	1.99	0.44
1:A:2787:C:H2'	1:A:2788:C:H6	1.82	0.44
9:N:58:ASP:N	9:N:58:ASP:OD1	2.46	0.44
3:D:38:LYS:HD2	3:D:39:LYS:N	2.32	0.44
1:A:271(Q):G:O2'	1:A:271(R):G:P	2.75	0.44
1:A:2140:C:H2'	1:A:2141:G:C8	2.53	0.44
1:A:1537:G:H2'	1:A:1538:G:H8	1.82	0.44
1:A:1537:G:H2'	1:A:1538:G:C8	2.52	0.44
9:N:42:TRP:CD1	9:N:48:MET:HE1	2.49	0.44
1:A:1592:C:H2'	1:A:1593:G:C8	2.53	0.44
3:D:17:THR:HG23	3:D:205:VAL:HB	1.98	0.44
6:G:41:GLN:O	6:G:89:GLY:HA2	2.18	0.44
1:A:934:G:H2'	1:A:935:C:H6	1.81	0.44
1:A:830:G:H4'	1:A:831:G:OP2	2.18	0.44
19:X:26:TYR:CE1	19:X:89:ILE:HG13	2.52	0.44
15:T:2:ASN:O	15:T:6:LEU:HD22	2.18	0.44
1:A:2416:C:O5'	1:A:2416:C:H6	2.00	0.44
1:A:1310:G:H1'	1:A:1611:C:H5'	1.99	0.44
2:B:32:C:N3	2:B:51:G:C2	2.85	0.44
1:A:1478:G:H2'	1:A:1479:G:H8	1.83	0.44
1:A:2834:G:N2	1:A:2882:A:N6	2.66	0.44
28:6:21:TYR:CE2	28:6:38:LYS:HG2	2.52	0.44
21:Z:98:MET:SD	21:Z:133:ILE:HD13	2.57	0.44
5:F:127:GLU:HA	5:F:196:LEU:HD12	1.98	0.44
1:A:574:C:OP1	34:A:3995:HOH:O	2.20	0.44
16:U:76:TYR:OH	16:U:92:ARG:NH1	2.50	0.44
1:A:92:A:O2'	1:A:93:G:H5'	2.17	0.44
1:A:2287:A:C4	1:A:2289:G:C8	3.04	0.44
1:A:2287:A:N3	1:A:2289:G:C8	2.86	0.44
1:A:2822:G:N7	34:A:4408:HOH:O	2.36	0.44
1:A:469:G:C2'	1:A:470:A:H5''	2.47	0.44
3:D:43:ARG:HG2	3:D:47:GLY:O	2.18	0.44
21:Z:151:HIS:C	21:Z:153:SER:H	2.21	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:H:169:VAL:HG12	7:H:170:ARG:N	2.33	0.44
21:Z:70:LEU:HD23	21:Z:70:LEU:HA	1.83	0.44
20:Y:67:LEU:HD23	20:Y:67:LEU:HA	1.61	0.44
1:A:2114:A:O2'	1:A:2167:U:H4'	2.17	0.44
1:A:2169:A:O2'	1:A:2170:A:H5'	2.18	0.44
1:A:639:U:H2'	1:A:640:C:H6	1.76	0.44
1:A:2315:G:C6	1:A:2316:C:N4	2.86	0.44
15:T:118:ARG:CG	15:T:118:ARG:HH11	2.31	0.44
1:A:1922:G:H2'	1:A:1923:U:O4'	2.18	0.44
16:U:104:GLN:CD	16:U:104:GLN:H	2.21	0.44
1:A:2602:A:H1'	1:A:2603:G:C5'	2.48	0.44
31:9:7:VAL:HA	31:9:34:GLN:OE1	2.18	0.44
5:F:22:ALA:HB1	5:F:24:LEU:HD22	1.99	0.44
1:A:1406:U:H2'	1:A:1407:C:C6	2.52	0.44
1:A:1529:G:O2'	1:A:1530:C:H5'	2.17	0.44
5:F:181:LEU:HA	5:F:181:LEU:HD12	1.84	0.44
1:A:1889:A:H2'	1:A:1890:A:C8	2.53	0.44
19:X:11:PRO:HD3	24:2:37:PHE:CE2	2.52	0.44
19:X:11:PRO:HD3	24:2:37:PHE:CZ	2.52	0.44
3:D:68:LYS:O	3:D:70:TRP:CD1	2.71	0.44
1:A:952:G:C6	1:A:953:A:N7	2.86	0.44
21:Z:183:LEU:HD23	21:Z:183:LEU:HA	1.84	0.44
15:T:35:LYS:HE2	15:T:35:LYS:HB3	1.74	0.44
1:A:1652:A:H2'	1:A:1653:G:H5'	2.00	0.44
1:A:1494:A:C6	1:A:1495:A:C6	3.06	0.44
20:Y:86:ARG:NH1	20:Y:100:ALA:HB1	2.33	0.44
3:D:101:GLU:OE1	3:D:103:ARG:HD3	2.17	0.44
1:A:1592:C:H2'	1:A:1593:G:H8	1.82	0.44
6:G:107:LEU:HD23	6:G:111:LEU:HD12	1.98	0.44
7:H:144:VAL:O	7:H:148:ILE:HG12	2.18	0.44
1:A:511:U:C5	1:A:512:G:C5	3.06	0.43
1:A:1106:G:N3	1:A:1106:G:H2'	2.33	0.43
1:A:639:U:H2'	1:A:640:C:C5	2.53	0.43
1:A:1858:G:H2'	1:A:1883:G:N2	2.33	0.43
1:A:125:G:H5''	29:7:19:ARG:HD3	1.99	0.43
1:A:2698:U:H2'	1:A:2699:C:C6	2.52	0.43
1:A:1329:U:H5''	1:A:1330:C:H5	1.83	0.43
8:I:130:TYR:HB3	8:I:138:ILE:HB	2.00	0.43
21:Z:166:SER:HA	21:Z:167:PRO:HD3	1.83	0.43
4:E:77:ILE:HD12	4:E:195:LEU:HD13	2.00	0.43
1:A:1202:C:N4	1:A:1203:G:C6	2.86	0.43
24:2:23:LYS:O	24:2:27:GLU:HG2	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:9:U:OP1	9:N:115:ARG:NH2	2.51	0.43
1:A:654:A:H2	1:A:655:A:C2	2.36	0.43
21:Z:14:LYS:HA	21:Z:15:PRO:HD3	1.91	0.43
1:A:1288:U:C2	1:A:1327:C:O2	2.71	0.43
14:S:49:VAL:HG12	14:S:73:LEU:HD12	2.00	0.43
1:A:1782:C:C4	1:A:2587:A:C2	3.06	0.43
26:4:15:ILE:HB	26:4:32:TYR:CE2	2.53	0.43
1:A:2146:C:H4'	1:A:2147:G:O4'	2.18	0.43
1:A:1885:A:H2'	1:A:1886:C:O4'	2.19	0.43
10:O:71:ARG:HB3	10:O:73:ASP:OD2	2.18	0.43
1:A:1711:C:H2'	1:A:1712:C:H6	1.83	0.43
1:A:2387:U:H4'	22:0:41:ARG:NH2	2.34	0.43
1:A:1545:A:H2'	1:A:1546:C:O4'	2.17	0.43
28:6:14:THR:HG21	28:6:48:VAL:HG13	2.00	0.43
10:O:4:PRO:O	10:O:5:GLN:HB2	2.17	0.43
1:A:2432:A:C6	23:1:33:LYS:HB3	2.54	0.43
1:A:354:G:H2'	1:A:355:G:C8	2.53	0.43
17:V:35:LEU:HB2	17:V:57:VAL:CG1	2.48	0.43
1:A:603:A:C8	1:A:655:A:C6	3.06	0.43
25:3:6:VAL:HG13	25:3:56:VAL:HG13	1.99	0.43
6:G:44:GLY:O	6:G:47:LYS:HG3	2.18	0.43
1:A:1501:C:O4'	3:D:100:GLY:HA2	2.17	0.43
1:A:448:U:O4	1:A:583:G:H1'	2.18	0.43
15:T:24:PRO:HA	15:T:49:VAL:O	2.17	0.43
17:V:22:VAL:HG23	17:V:23:GLU:O	2.18	0.43
1:A:1142(A):A:C4	1:A:1144:G:C8	3.07	0.43
1:A:1486:A:C4	1:A:1487:G:C8	3.06	0.43
1:A:922:U:H2'	1:A:923:C:C6	2.54	0.43
1:A:583:G:OP2	16:U:10:ARG:HD2	2.18	0.43
14:S:29:PHE:CD2	14:S:30:ARG:N	2.87	0.43
2:B:29:A:OP2	14:S:32:LEU:HD12	2.18	0.43
16:U:25:TRP:O	16:U:28:ARG:HB2	2.18	0.43
1:A:2304:G:H21	6:G:156:ASP:CG	2.22	0.43
1:A:139(A):G:N2	34:A:3817:HOH:O	2.50	0.43
1:A:2562:U:O2'	10:O:23:ARG:HD3	2.18	0.43
8:I:77:LEU:HD21	8:I:101:LEU:HA	2.00	0.43
15:T:118:ARG:NH1	15:T:118:ARG:HG3	2.30	0.43
1:A:2834:G:C8	1:A:2834:G:H5''	2.52	0.43
1:A:720:C:H2'	1:A:721:C:C6	2.54	0.43
1:A:901:A:H2'	1:A:902:C:C6	2.54	0.43
1:A:143:G:H2'	1:A:143(A):C:C6	2.54	0.43
1:A:819:A:H2'	1:A:820:A:H5'	2.01	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:R:103:ARG:HH12	13:R:110:PRO:HD3	1.84	0.43
1:A:1783:A:C2	1:A:2587:A:C5	3.06	0.43
1:A:2109:U:C6	1:A:2109:U:C3'	3.01	0.43
1:A:271(M):G:HO2'	1:A:271(N):U:H3'	1.84	0.43
1:A:2104:G:O6	1:A:2186:G:C4	2.72	0.43
26:4:15:ILE:O	26:4:33:VAL:N	2.49	0.43
2:B:33:G:C2	2:B:50:G:C2	3.06	0.43
8:I:61:ARG:HD2	8:I:61:ARG:N	2.34	0.43
14:S:56:LEU:HA	14:S:56:LEU:HD23	1.81	0.43
1:A:1639:U:H2'	1:A:1640:C:H5''	2.01	0.43
11:P:29:LYS:HB3	11:P:30:THR:H	1.60	0.43
21:Z:141:VAL:O	21:Z:144:LEU:HB2	2.19	0.43
28:6:11:LEU:HB2	28:6:21:TYR:HB2	1.99	0.43
6:G:176:LEU:HA	6:G:176:LEU:HD23	1.90	0.43
1:A:1779:U:C2	1:A:1783:A:N7	2.87	0.43
14:S:65:VAL:O	14:S:69:VAL:HG12	2.19	0.43
23:1:40:ARG:HB2	23:1:40:ARG:HE	1.57	0.43
6:G:7:LEU:HD11	6:G:107:LEU:HD12	1.99	0.43
1:A:2009:G:OP1	18:W:41:LYS:HE2	2.19	0.43
28:6:45:LYS:HG3	28:6:46:HIS:O	2.19	0.43
10:O:120:GLU:HG2	10:O:122:LEU:HG	2.00	0.43
1:A:2478:A:H5'	31:9:31:LYS:HE2	2.00	0.43
1:A:2281:C:O2'	1:A:2282:G:H5'	2.18	0.43
1:A:1165:U:H2'	1:A:1166:C:C6	2.54	0.43
1:A:2420:C:OP2	30:8:33:ASN:HB2	2.18	0.43
1:A:1783:A:OP1	34:A:3893:HOH:O	2.21	0.43
1:A:861:A:H2'	1:A:862:G:O4'	2.18	0.43
1:A:107:C:H2'	1:A:108:U:C6	2.53	0.43
1:A:1681:G:H1'	1:A:1762:A:H2'	2.01	0.43
4:E:181:LEU:HA	4:E:181:LEU:HD12	1.72	0.43
1:A:94:C:H5''	1:A:94(A):G:OP2	2.19	0.43
8:I:62:LYS:O	8:I:66:GLU:HG2	2.19	0.43
1:A:2747:G:O6	1:A:2755:C:H5''	2.17	0.43
1:A:2157:G:H2'	1:A:2158:A:C8	2.54	0.43
27:5:35:GLU:HG3	27:5:51:TYR:CB	2.49	0.43
5:F:106:ARG:HG2	5:F:106:ARG:H	1.50	0.43
2:B:66:A:H61	2:B:108:U:H2'	1.83	0.43
1:A:2191:G:H5'	1:A:2192:G:OP2	2.19	0.43
28:6:44:ARG:NH1	28:6:44:ARG:HB3	2.34	0.43
30:8:61:LEU:C	30:8:63:PRO:HD3	2.40	0.43
6:G:153:ARG:HB2	6:G:153:ARG:HE	1.51	0.43
1:A:89:G:OP2	1:A:90:U:H3'	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:26:LYS:HE2	3:D:28:GLU:O	2.19	0.42
1:A:1669:A:H5''	1:A:2550:G:OP1	2.20	0.42
2:B:50:G:H5''	14:S:61:ASN:ND2	2.33	0.42
9:N:42:TRP:HA	9:N:48:MET:SD	2.59	0.42
1:A:2287:A:O2'	1:A:2288:A:H3'	2.19	0.42
1:A:2275:C:H5'	1:A:2275:C:C6	2.53	0.42
1:A:2317:C:H2'	1:A:2318:G:C5'	2.49	0.42
1:A:729:G:C6	3:D:208:LYS:HB2	2.53	0.42
16:U:61:TRP:CH2	16:U:93:LYS:HB2	2.53	0.42
1:A:2378:A:H4'	14:S:23:ARG:NH1	2.33	0.42
1:A:634:C:H2'	1:A:635:C:C6	2.54	0.42
1:A:1685:C:H2'	1:A:1686:C:C6	2.54	0.42
5:F:149:ASP:OD2	5:F:149:ASP:N	2.40	0.42
8:I:35:LEU:N	8:I:35:LEU:HD23	2.34	0.42
1:A:2712:U:H1'	1:A:2712(A):A:C8	2.55	0.42
1:A:945:A:C2	1:A:2448:A:C4	3.08	0.42
5:F:32:LEU:HD12	5:F:32:LEU:HA	1.68	0.42
2:B:88:C:H2'	2:B:89:G:O4'	2.20	0.42
1:A:2111:C:C4	1:A:2145:C:C2	3.07	0.42
1:A:780:G:C2	1:A:782:A:C2	3.07	0.42
8:I:145:VAL:HG12	8:I:146:ALA:N	2.34	0.42
1:A:657:U:H2'	1:A:658:C:C6	2.54	0.42
1:A:1297:C:OP1	1:A:2710:C:H4'	2.19	0.42
1:A:548:A:H61	17:V:19:LYS:H	1.66	0.42
1:A:1187:G:H5''	17:V:81:TYR:CE2	2.55	0.42
8:I:98:ALA:O	8:I:101:LEU:N	2.52	0.42
2:B:32:C:N3	2:B:51:G:N2	2.67	0.42
12:Q:21:THR:O	21:Z:78:LYS:HD3	2.20	0.42
18:W:60:ASN:N	18:W:60:ASN:ND2	2.67	0.42
1:A:2292:C:P	14:S:17:ARG:HH22	2.41	0.42
1:A:2287:A:C4	1:A:2289:G:N7	2.87	0.42
19:X:53:LYS:HB3	19:X:82:GLN:HB3	2.01	0.42
19:X:5:TYR:HD1	24:2:33:MET:CE	2.32	0.42
1:A:2812:G:N2	1:A:2889:C:C2	2.86	0.42
1:A:2359:C:H2'	1:A:2360:A:O4'	2.19	0.42
1:A:601:C:O2	1:A:605:C:H4'	2.20	0.42
8:I:27:ARG:HD2	23:1:71:TYR:CE1	2.55	0.42
2:B:11:C:H3'	2:B:12:C:C6	2.54	0.42
15:T:50:ILE:HG22	15:T:102:ILE:HD11	2.01	0.42
22:O:17:GLN:OE1	22:O:17:GLN:HA	2.18	0.42
17:V:20:LEU:HD12	17:V:20:LEU:HA	1.79	0.42
1:A:1798:U:OP2	3:D:274:ARG:NH2	2.52	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:S:34:HIS:NE2	14:S:54:LEU:HD12	2.33	0.42
5:F:181:LEU:HB3	5:F:205:ARG:NH2	2.33	0.42
8:I:5:LEU:HD12	8:I:5:LEU:N	2.34	0.42
8:I:68:LEU:C	8:I:70:GLU:N	2.73	0.42
1:A:2095:C:H2'	1:A:2096:U:O4'	2.19	0.42
1:A:1367:A:N7	1:A:1368:G:H1'	2.35	0.42
1:A:649:G:H2'	1:A:650:C:O4'	2.18	0.42
1:A:2198:A:O5'	8:I:33:ARG:NH2	2.51	0.42
5:F:117:ARG:HA	5:F:117:ARG:HD3	1.87	0.42
16:U:106:PHE:O	16:U:110:VAL:HG23	2.20	0.42
1:A:1529:G:C5	1:A:1530:C:C4	3.08	0.42
12:Q:6:ARG:HG2	21:Z:194:PRO:HG2	2.01	0.42
1:A:2147:G:H2'	1:A:2148:G:O4'	2.20	0.42
2:B:82:G:C2'	2:B:83:G:H5'	2.49	0.42
15:T:19:LEU:HA	15:T:20:PRO:HD3	1.91	0.42
1:A:742:G:H2'	1:A:743:G:C8	2.55	0.42
1:A:2140:C:N3	1:A:2151:G:C6	2.88	0.42
13:R:67:LEU:HD13	13:R:67:LEU:HA	1.78	0.42
23:1:82:LEU:HD22	23:1:90:ILE:HG23	2.02	0.42
21:Z:48:PHE:CE2	21:Z:52:SER:HA	2.54	0.42
1:A:542:C:C6	1:A:542:C:H3'	2.55	0.42
25:3:4:LEU:HA	25:3:4:LEU:HD23	1.71	0.42
2:B:11:C:OP2	2:B:12:C:N4	2.36	0.42
6:G:96:ARG:O	6:G:99:MET:HB3	2.18	0.42
1:A:1601:G:O2'	1:A:1602:U:H5'	2.20	0.42
1:A:29:U:H2'	1:A:30:G:C8	2.54	0.42
1:A:866:A:C6	1:A:914:C:C5	3.08	0.42
1:A:1930:G:O2'	1:A:1931:U:P	2.78	0.42
1:A:1312:U:H4'	1:A:1313:U:O5'	2.19	0.42
1:A:2845:G:H5''	15:T:54:ARG:O	2.19	0.42
2:B:52:A:O2'	2:B:53:A:N3	2.52	0.42
1:A:2350:C:H2'	1:A:2351:G:O4'	2.20	0.42
1:A:255:A:H1'	1:A:384:U:C6	2.55	0.42
6:G:57:ALA:HB2	6:G:90:LEU:HD13	2.02	0.42
6:G:33:ARG:O	6:G:161:THR:HG22	2.19	0.42
1:A:664:C:H2'	1:A:665:C:H6	1.83	0.42
3:D:182:LEU:HA	3:D:182:LEU:HD23	1.73	0.42
1:A:2238:G:H2'	1:A:2238:G:N3	2.35	0.42
1:A:2322:A:H2'	1:A:2323:G:O4'	2.19	0.42
1:A:2820:A:C5	13:R:4:LEU:HD11	2.55	0.42
28:6:10:LEU:CD1	28:6:54:ILE:HA	2.46	0.42
1:A:2749:A:H5''	7:H:3:ARG:HH21	1.85	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1048:A:O2'	1:A:1049:C:P	2.77	0.42
1:A:2773:C:H5''	4:E:164:ARG:HG2	2.01	0.42
1:A:824:A:H1'	1:A:2358:G:N7	2.34	0.42
1:A:1911:U:C2	1:A:1918:A:C2	3.07	0.42
22:0:10:THR:HG22	22:0:12:ASN:H	1.84	0.42
6:G:86:MET:HA	6:G:87:PRO:HD3	1.84	0.42
1:A:1647:G:H3'	1:A:1647:G:OP2	2.20	0.42
1:A:2173:A:C6	1:A:2174:C:C2	3.07	0.42
1:A:271(F):C:C2	1:A:271(G):C:C6	3.08	0.42
2:B:52:A:O2'	2:B:53:A:H5''	2.20	0.42
8:I:112:LYS:C	8:I:114:LEU:N	2.70	0.42
1:A:861:A:N3	2:B:79:C:O2'	2.49	0.42
2:B:89:G:H8	2:B:89:G:OP2	2.02	0.42
1:A:903:C:H2'	1:A:904:C:H6	1.84	0.42
7:H:33:LEU:HD11	7:H:136:ILE:O	2.19	0.42
12:Q:7:MET:HE3	12:Q:7:MET:HB2	1.65	0.42
8:I:39:ALA:O	8:I:44:LEU:HD22	2.19	0.42
28:6:47:THR:HG22	28:6:48:VAL:N	2.35	0.42
16:U:58:ARG:HA	16:U:61:TRP:CE3	2.55	0.42
10:O:81:ASP:N	10:O:81:ASP:OD2	2.52	0.42
1:A:2093:G:H1	1:A:2196:C:H42	1.68	0.42
1:A:157:U:H4'	1:A:171:G:H21	1.85	0.42
1:A:2680:C:H5'	4:E:189:PRO:HA	2.02	0.42
16:U:29:SER:OG	16:U:30:LYS:NZ	2.48	0.42
4:E:93:VAL:HG12	4:E:182:LEU:HD12	2.01	0.42
2:B:46:A:C5	2:B:47:C:C4	3.08	0.42
1:A:2123:G:H2'	1:A:2124:G:C8	2.55	0.42
1:A:646:A:H5'	1:A:646:A:N3	2.34	0.42
1:A:857:C:H1'	22:0:26:TYR:CE2	2.55	0.42
1:A:1049:C:O2'	1:A:1050:A:OP1	2.37	0.42
1:A:2236:C:C2'	1:A:2237:G:H5'	2.50	0.42
2:B:2:C:H2'	2:B:3:C:H6	1.85	0.42
6:G:64:THR:OG1	6:G:65:GLY:N	2.51	0.42
1:A:1467:C:C2	1:A:1526:G:N2	2.88	0.42
1:A:2109:U:H3'	1:A:2109:U:C6	2.54	0.41
10:O:23:ARG:HG3	10:O:24:VAL:N	2.35	0.41
11:P:71:VAL:HG22	11:P:72:PRO:HA	2.02	0.41
28:6:6:ARG:NH1	28:6:26:ASN:HB2	2.35	0.41
1:A:725:G:C5	1:A:726:G:C6	3.08	0.41
1:A:864:G:C6	1:A:865:C:N4	2.87	0.41
9:N:28:THR:HG22	9:N:29:LYS:N	2.34	0.41
3:D:213:ARG:HA	3:D:213:ARG:HD2	1.65	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:656:G:H2'	1:A:657:U:O4'	2.20	0.41
1:A:880:G:N2	1:A:898:C:H1'	2.34	0.41
1:A:2836:U:H2'	1:A:2837:G:C8	2.55	0.41
1:A:536:A:H2'	1:A:537:C:C6	2.55	0.41
15:T:11:GLU:O	15:T:15:VAL:HG23	2.19	0.41
7:H:13:LYS:HA	7:H:14:GLY:HA2	1.56	0.41
14:S:41:ASP:OD1	14:S:43:GLU:HB2	2.20	0.41
1:A:2582:G:C2	1:A:2583:G:C8	3.08	0.41
16:U:17:ILE:HG23	16:U:39:LEU:HD12	2.00	0.41
19:X:57:LEU:HD13	19:X:78:LYS:HG2	2.01	0.41
5:F:123:LEU:HD12	5:F:124:LEU:N	2.35	0.41
5:F:133:ASN:HA	5:F:162:LEU:HD23	2.01	0.41
2:B:7:G:C2	2:B:115:G:C2	3.08	0.41
1:A:1985:G:OP2	34:A:3735:HOH:O	2.20	0.41
1:A:1045:A:N3	1:A:1045:A:C2'	2.82	0.41
3:D:172:TYR:HD1	3:D:185:VAL:C	2.23	0.41
1:A:1341:U:O2	19:X:80:ILE:HD13	2.20	0.41
1:A:2591:C:OP2	3:D:239:ARG:HB3	2.20	0.41
10:O:64:ARG:NH1	10:O:81:ASP:OD1	2.53	0.41
2:B:93:G:H2'	2:B:94:C:H6	1.85	0.41
21:Z:138:GLU:HB3	21:Z:156:LYS:NZ	2.35	0.41
12:Q:75:THR:HA	12:Q:89:ASN:O	2.20	0.41
1:A:823:G:C6	1:A:835:A:N1	2.88	0.41
1:A:2320:A:N3	1:A:2320:A:H2'	2.35	0.41
1:A:2108:C:C3'	1:A:2108:C:C6	3.04	0.41
1:A:1141:U:P	9:N:25:ARG:NH1	2.93	0.41
4:E:36:ARG:HG2	4:E:47:VAL:HG22	2.01	0.41
10:O:59:LYS:NZ	10:O:89:ASN:HD21	2.17	0.41
1:A:637:A:H8	11:P:117:GLU:HG3	1.86	0.41
30:8:29:LYS:HD3	30:8:44:LYS:C	2.40	0.41
1:A:1693:U:O2'	3:D:14:ARG:NH2	2.53	0.41
12:Q:35:VAL:CG1	12:Q:130:LYS:HB3	2.50	0.41
19:X:72:LYS:HB3	19:X:72:LYS:HE3	1.85	0.41
1:A:1107:G:H2'	1:A:1107:G:H8	1.42	0.41
1:A:907:U:H4'	12:Q:101:ARG:HH22	1.84	0.41
31:9:4:ARG:NH1	34:9:202:HOH:O	2.53	0.41
1:A:2259:G:H1'	1:A:2427:C:H2'	2.02	0.41
16:U:28:ARG:NH1	16:U:38:THR:OG1	2.45	0.41
2:B:103:G:O2'	21:Z:73:GLN:NE2	2.54	0.41
1:A:303:U:O4	34:A:4348:HOH:O	2.21	0.41
1:A:435:C:C5	1:A:436:C:C5	3.08	0.41
13:R:104:ARG:HG3	13:R:111:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2730:C:H4'	4:E:168:MET:O	2.21	0.41
5:F:101:LEU:HA	5:F:101:LEU:HD12	1.68	0.41
1:A:2778:A:H4'	1:A:2779:U:OP2	2.21	0.41
4:E:60:ASN:OD1	4:E:62:PRO:HD2	2.20	0.41
1:A:638:G:H2'	1:A:639:U:H6	1.85	0.41
26:4:15:ILE:HG13	26:4:21:VAL:HG22	2.01	0.41
11:P:121:LYS:HG3	11:P:122:PRO:HD2	2.01	0.41
3:D:108:PRO:HG2	3:D:111:LEU:HG	2.02	0.41
1:A:2316:C:H1'	6:G:128:ARG:NH2	2.35	0.41
14:S:56:LEU:O	14:S:58:LEU:HD23	2.21	0.41
1:A:2572:A:OP1	1:A:2574:G:O2'	2.35	0.41
1:A:900:A:C4	1:A:901:A:C8	3.09	0.41
1:A:866:A:C6	1:A:914:C:C6	3.08	0.41
1:A:2110:G:O2'	1:A:2120:G:H5'	2.21	0.41
1:A:685:A:C2	1:A:689:A:C6	3.09	0.41
11:P:27:HIS:O	11:P:31:ALA:HA	2.21	0.41
1:A:1497:U:H5''	1:A:1498:C:H5	1.85	0.41
24:2:3:LEU:HA	24:2:3:LEU:HD23	1.82	0.41
2:B:111:G:H2'	2:B:112:U:H6	1.86	0.41
20:Y:77:PRO:HD3	20:Y:106:LEU:HD23	2.02	0.41
1:A:805:G:H4'	11:P:38:GLN:HB3	2.01	0.41
31:9:32:HIS:O	31:9:34:GLN:HG3	2.20	0.41
1:A:191:A:H2'	1:A:192:C:C6	2.55	0.41
1:A:642:G:H21	1:A:646:A:H2	1.68	0.41
8:I:130:TYR:HA	8:I:130:TYR:HD1	1.70	0.41
1:A:332:A:H2'	34:A:4739:HOH:O	2.20	0.41
4:E:128:SER:OG	4:E:129:HIS:N	2.52	0.41
30:8:26:LYS:HZ2	30:8:26:LYS:HG2	1.70	0.41
1:A:580:C:H2'	1:A:581:C:C6	2.55	0.41
8:I:130:TYR:HD2	8:I:138:ILE:HD12	1.86	0.41
1:A:1526:G:C6	1:A:1527:G:C2	3.09	0.41
3:D:221:VAL:HG22	3:D:226:MET:CE	2.50	0.41
20:Y:76:CYS:HA	20:Y:77:PRO:HD3	1.88	0.41
1:A:2287:A:C5	1:A:2289:G:C5	3.09	0.41
1:A:384:U:H2'	1:A:385:C:H6	1.86	0.41
2:B:85:G:H2'	2:B:86:G:H5'	2.03	0.41
1:A:2337:G:C2	1:A:2338:G:C8	3.09	0.41
1:A:2526:G:H5'	1:A:2742:C:O2'	2.21	0.41
3:D:53:PHE:HB3	3:D:218:ARG:O	2.21	0.41
1:A:1759:A:H1'	1:A:2711:A:C2	2.56	0.41
13:R:54:LEU:HA	13:R:54:LEU:HD12	1.90	0.41
16:U:105:VAL:HG11	17:V:39:LEU:HD21	2.01	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
26:4:6:HIS:HA	26:4:7:PRO:HD2	1.76	0.41
1:A:10:G:H1'	1:A:2801(A):A:C2	2.56	0.41
1:A:2161:C:O2'	1:A:2162:G:H5'	2.20	0.41
1:A:2723:C:O3'	13:R:1:MET:HE3	2.21	0.41
1:A:2108:C:H2'	1:A:2109:U:C5'	2.50	0.41
1:A:1668:A:H4'	1:A:1669:A:O5'	2.21	0.41
8:I:72:LEU:HA	8:I:75:LEU:CD2	2.51	0.41
12:Q:32:TYR:CE2	12:Q:133:ARG:HG3	2.56	0.41
1:A:107:C:C2	1:A:108:U:C5	3.09	0.41
7:H:60:ARG:HB3	7:H:60:ARG:HE	1.74	0.41
1:A:2080:G:P	23:1:35:THR:OG1	2.78	0.41
4:E:116:VAL:HG13	4:E:122:PHE:CD2	2.56	0.41
8:I:79:ILE:HA	8:I:80:PRO:HD2	1.87	0.41
9:N:34:LEU:O	9:N:49:GLY:HA3	2.20	0.41
30:8:62:LEU:HB3	30:8:65:GLU:CG	2.51	0.41
1:A:819:A:C4	1:A:1189:A:C2	3.08	0.41
4:E:35:GLN:OE1	4:E:66:HIS:HE1	2.04	0.41
1:A:557:U:H2'	1:A:558:G:H8	1.86	0.41
5:F:168:ARG:HG2	5:F:175:THR:HG21	2.02	0.41
25:3:44:ARG:O	25:3:48:GLU:HG3	2.21	0.41
1:A:1541:G:H5''	1:A:1542:A:OP2	2.21	0.41
1:A:2884:U:O2	27:5:53:ALA:HB2	2.20	0.41
6:G:74:LYS:O	6:G:84:LYS:HG2	2.21	0.41
1:A:9:U:O4	1:A:2629:A:C2	2.73	0.41
1:A:2127:G:HO2'	1:A:2173:A:H2	1.64	0.41
26:4:14:ILE:HA	26:4:31:ILE:O	2.19	0.41
1:A:322:A:C5	1:A:340:A:C2	3.09	0.41
1:A:1711:C:H2'	1:A:1712:C:C6	2.55	0.41
3:D:218:ARG:HB3	3:D:219:PRO:HD2	2.03	0.41
6:G:24:GLY:O	6:G:26:GLN:NE2	2.54	0.41
1:A:127:A:H5''	1:A:128:C:O4'	2.20	0.41
10:O:104:ARG:NH1	15:T:34:VAL:HG21	2.36	0.41
5:F:140:LEU:HA	5:F:140:LEU:HD13	1.90	0.41
1:A:1106:G:H4'	1:A:1107:G:OP2	2.20	0.40
1:A:271(K):U:O2'	1:A:271(L):U:OP1	2.27	0.40
1:A:1364:G:N7	23:1:3:LYS:HD3	2.36	0.40
1:A:1538:G:O2'	1:A:1539:G:OP1	2.28	0.40
16:U:47:TYR:HA	16:U:50:ARG:NH2	2.36	0.40
5:F:150:GLY:HA2	5:F:172:TRP:CE3	2.57	0.40
1:A:2420:C:O5'	1:A:2420:C:H6	2.04	0.40
15:T:33:LYS:O	15:T:82:LEU:HD23	2.21	0.40
17:V:65:GLY:HA3	17:V:91:TYR:CZ	2.56	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
19:X:94:GLY:HA3	19:X:95:LEU:HA	1.63	0.40
6:G:103:LEU:HD23	6:G:103:LEU:HA	1.82	0.40
1:A:1047:G:H2'	1:A:1110:G:H22	1.84	0.40
1:A:271(H):G:C6	1:A:271(Q):G:C6	3.09	0.40
1:A:1568:G:H5'	3:D:60:ARG:HA	2.03	0.40
9:N:20:GLY:HA2	9:N:61:ARG:CG	2.49	0.40
26:4:42:PHE:CB	26:4:43:TYR:HB2	2.50	0.40
5:F:32:LEU:O	5:F:35:GLU:N	2.55	0.40
1:A:1636:C:H2'	1:A:1637:A:C8	2.56	0.40
1:A:1540:U:H2'	1:A:1541:G:O4'	2.21	0.40
1:A:1750:G:O2'	1:A:2860:A:N1	2.46	0.40
1:A:2473:U:H2'	1:A:2473:U:O2	2.20	0.40
9:N:5:VAL:HG12	9:N:5:VAL:O	2.21	0.40
1:A:1038:C:H6	1:A:1038:C:H5''	1.86	0.40
22:0:55:ARG:HB2	22:0:55:ARG:NH1	2.36	0.40
1:A:154(A):C:O2	1:A:154(A):C:H5''	2.22	0.40
15:T:84:GLN:NE2	15:T:85:LYS:HG2	2.35	0.40
1:A:479:A:H4'	1:A:480:A:OP1	2.21	0.40
1:A:1638:C:H4'	1:A:2710:C:O2	2.21	0.40
1:A:1246:A:OP1	34:A:4340:HOH:O	2.22	0.40
1:A:1260:G:C6	1:A:1261:C:C4	3.09	0.40
5:F:197:ASP:OD2	5:F:197:ASP:N	2.54	0.40
1:A:2319:G:C8	1:A:2320:A:C2	3.10	0.40
1:A:2174:C:H6	1:A:2174:C:O5'	2.04	0.40
1:A:811:U:H2'	11:P:21:ARG:HA	2.03	0.40
1:A:1212:G:N2	1:A:1236:G:O2'	2.52	0.40
1:A:862:G:P	34:A:4187:HOH:O	2.79	0.40
1:A:2854:G:H2'	1:A:2855:C:H6	1.85	0.40
1:A:2187:G:C6	1:A:2188:C:C2	3.09	0.40
10:O:2:ILE:HD12	10:O:6:THR:HG21	2.02	0.40
1:A:1615:C:C5	1:A:1617:C:C4	3.10	0.40
6:G:17:PRO:O	6:G:21:ARG:HB2	2.20	0.40
1:A:1436:G:H1'	1:A:1477:A:O2'	2.22	0.40
6:G:6:ALA:HB3	6:G:104:GLU:OE1	2.22	0.40
1:A:111:A:C2	1:A:112:U:C2	3.09	0.40
20:Y:106:LEU:O	20:Y:107:ASP:HB2	2.21	0.40
1:A:1528(A):A:N7	1:A:1529:G:C5	2.89	0.40
1:A:2315:G:H2'	1:A:2316:C:H6	1.86	0.40
1:A:2292:C:P	14:S:17:ARG:NH2	2.95	0.40
12:Q:119:ARG:HE	12:Q:119:ARG:HB3	1.65	0.40
27:5:29:THR:O	27:5:30:LEU:HD23	2.22	0.40
7:H:24:VAL:HG22	7:H:35:VAL:HB	2.03	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:10:THR:OG1	3:D:13:ARG:HB2	2.22	0.40
20:Y:65:ALA:HA	20:Y:66:PRO:HD3	1.91	0.40
1:A:460:A:C2	1:A:470:A:C4	3.10	0.40
1:A:1586:A:H2'	1:A:1587:A:H5'	2.03	0.40
15:T:99:LEU:O	15:T:102:ILE:HG12	2.21	0.40
12:Q:35:VAL:HG13	12:Q:130:LYS:HB3	2.04	0.40
10:O:42:SER:HB3	10:O:44:LYS:HE2	2.02	0.40
6:G:63:ILE:HD13	6:G:155:MET:HE1	2.03	0.40
6:G:105:LYS:NZ	26:4:25:TYR:O	2.54	0.40
6:G:105:LYS:HE2	6:G:105:LYS:HB2	1.90	0.40
1:A:2663:G:C5	1:A:2664:G:C5	3.09	0.40
1:A:745:G:C2'	1:A:746:A:H5'	2.51	0.40
1:A:484:C:H2'	1:A:485:C:C6	2.57	0.40
21:Z:63:ASP:OD1	21:Z:65:GLN:HB3	2.21	0.40

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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

All (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
30	8	35	GLN
9	N	5	VAL
7	H	65	HIS
8	I	85	GLU
9	N	4	TYR
9	N	19	GLU
7	H	92	ILE
29	7	46	VAL

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Mol	Chain	Res	Type
4	E	52	LEU
21	Z	193	GLU
4	E	72	VAL
3	D	3	VAL
14	S	85	VAL
21	Z	161	VAL
20	Y	3	VAL
21	Z	39	VAL
8	I	107	VAL

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

All (408) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	12	SER
3	D	13	ARG
3	D	25	THR
3	D	32	SER
3	D	35	LYS
3	D	37	LEU
3	D	39	LYS
3	D	61	LEU
3	D	89	SER
3	D	94	LEU
3	D	99	ASP
3	D	101	GLU
3	D	103	ARG
3	D	106	ILE
3	D	126	GLN
3	D	138	VAL
3	D	141	VAL
3	D	147	LEU
3	D	150	LYS
3	D	155	LEU
3	D	165	ILE
3	D	173	VAL

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Mol	Chain	Res	Type
3	D	192	THR
3	D	193	VAL
3	D	211	ARG
3	D	212	SER
3	D	217	ARG
3	D	221	VAL
3	D	229	VAL
3	D	242	ARG
3	D	257	LEU
3	D	259	THR
3	D	260	ARG
3	D	274	ARG
4	E	9	VAL
4	E	12	THR
4	E	21	VAL
4	E	24	THR
4	E	34	VAL
4	E	49	LEU
4	E	52	LEU
4	E	54	GLN
4	E	78	LEU
4	E	82	ARG
4	E	89	ASP
4	E	93	VAL
4	E	111	ARG
4	E	113	PHE
4	E	116	VAL
4	E	119	ARG
4	E	144	ARG
4	E	152	LYS
4	E	154	LYS
4	E	170	LEU
4	E	175	VAL
4	E	179	GLU
4	E	181	LEU
4	E	182	LEU
4	E	184	VAL
5	F	15	SER
5	F	18	ARG
5	F	20	LEU
5	F	24	LEU
5	F	33	LEU

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Mol	Chain	Res	Type
5	F	46	ARG
5	F	50	SER
5	F	53	THR
5	F	57	VAL
5	F	60	SER
5	F	74	ARG
5	F	77	ASP
5	F	82	ILE
5	F	88	VAL
5	F	96	ASP
5	F	106	ARG
5	F	110	LEU
5	F	133	ASN
5	F	135	LYS
5	F	140	LEU
5	F	158	THR
5	F	175	THR
5	F	183	VAL
5	F	192	LEU
5	F	197	ASP
5	F	201	VAL
6	G	3	LEU
6	G	13	GLU
6	G	20	ILE
6	G	21	ARG
6	G	31	VAL
6	G	33	ARG
6	G	43	LEU
6	G	88	ILE
6	G	96	ARG
6	G	117	PHE
6	G	135	LEU
6	G	138	GLN
6	G	143	GLU
6	G	145	THR
6	G	146	TYR
6	G	148	MET
6	G	149	VAL
6	G	150	ASP
6	G	153	ARG
6	G	159	VAL
6	G	161	THR

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Mol	Chain	Res	Type
6	G	170	ARG
7	H	7	LEU
7	H	15	VAL
7	H	16	SER
7	H	69	ARG
7	H	70	THR
7	H	88	LEU
7	H	98	LEU
7	H	106	THR
7	H	122	THR
7	H	129	THR
7	H	132	ARG
7	H	139	GLN
7	H	153	LYS
7	H	171	LEU
8	I	1	MET
8	I	7	GLU
8	I	9	LEU
8	I	12	LEU
8	I	15	VAL
8	I	44	LEU
8	I	47	LEU
8	I	54	GLN
8	I	61	ARG
8	I	68	LEU
8	I	75	LEU
8	I	77	LEU
8	I	85	GLU
8	I	92	VAL
8	I	93	THR
8	I	102	SER
8	I	108	THR
8	I	116	LEU
8	I	117	GLU
8	I	127	VAL
8	I	129	THR
8	I	130	TYR
8	I	140	LEU
8	I	142	VAL
9	N	2	LYS
9	N	9	VAL
9	N	12	ARG

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Mol	Chain	Res	Type
9	N	15	LEU
9	N	28	THR
9	N	33	LEU
9	N	34	LEU
9	N	43	THR
9	N	46	VAL
9	N	48	MET
9	N	55	VAL
9	N	58	ASP
9	N	62	VAL
9	N	63	THR
9	N	67	LEU
9	N	73	THR
9	N	87	LEU
9	N	93	THR
9	N	97	ARG
9	N	99	LEU
9	N	120	LEU
9	N	131	GLN
9	N	133	GLN
9	N	137	LYS
9	N	138	LEU
10	O	8	LEU
10	O	21	CYS
10	O	26	LYS
10	O	28	SER
10	O	42	SER
10	O	77	ILE
10	O	94	ARG
10	O	113	LYS
11	P	21	ARG
11	P	33	ARG
11	P	42	SER
11	P	45	LEU
11	P	55	ARG
11	P	59	LEU
11	P	64	LYS
11	P	70	GLN
11	P	86	LYS
11	P	98	GLU
11	P	106	LEU
11	P	112	LEU

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Mol	Chain	Res	Type
11	P	117	GLU
11	P	125	VAL
11	P	133	SER
11	P	147	LEU
12	Q	1	MET
12	Q	5	ARG
12	Q	7	MET
12	Q	8	LYS
12	Q	16	ARG
12	Q	21	THR
12	Q	25	ASP
12	Q	45	GLN
12	Q	55	VAL
12	Q	56	ARG
12	Q	75	THR
12	Q	79	LEU
12	Q	109	VAL
12	Q	119	ARG
12	Q	127	ILE
12	Q	138	ASP
13	R	6	SER
13	R	14	SER
13	R	18	LEU
13	R	28	LEU
13	R	29	LEU
13	R	33	ARG
13	R	36	THR
13	R	44	LEU
13	R	48	VAL
13	R	54	LEU
13	R	60	LEU
13	R	65	LEU
13	R	67	LEU
13	R	75	LEU
13	R	79	LEU
13	R	91	GLN
13	R	95	THR
13	R	100	LEU
13	R	111	LEU
14	S	3	ARG
14	S	11	LYS
14	S	14	VAL

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Mol	Chain	Res	Type
14	S	19	LYS
14	S	20	ARG
14	S	25	ARG
14	S	36	TYR
14	S	42	ASP
14	S	50	SER
14	S	54	LEU
14	S	67	ARG
14	S	69	VAL
14	S	98	VAL
14	S	110	LEU
14	S	111	GLU
15	T	1	MET
15	T	6	LEU
15	T	13	ARG
15	T	16	ARG
15	T	23	ARG
15	T	39	ARG
15	T	49	VAL
15	T	53	ARG
15	T	59	THR
15	T	74	ARG
15	T	82	LEU
15	T	93	ARG
15	T	96	ARG
15	T	107	ASP
15	T	118	ARG
16	U	8	VAL
16	U	31	SER
16	U	36	ARG
16	U	58	ARG
16	U	60	LEU
16	U	74	LEU
16	U	83	LEU
16	U	104	GLN
16	U	108	GLU
17	V	5	VAL
17	V	7	THR
17	V	18	LEU
17	V	28	GLU
17	V	33	VAL
17	V	35	LEU

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Mol	Chain	Res	Type
17	V	38	LEU
17	V	46	VAL
17	V	51	VAL
17	V	57	VAL
17	V	61	VAL
17	V	62	LEU
17	V	72	VAL
17	V	73	SER
17	V	79	VAL
17	V	89	GLN
17	V	95	LEU
18	W	11	ARG
18	W	15	ARG
18	W	17	VAL
18	W	23	LEU
18	W	27	LYS
18	W	51	LEU
18	W	60	ASN
18	W	67	ASP
18	W	98	LYS
18	W	100	THR
18	W	107	LEU
19	X	23	GLU
19	X	35	THR
19	X	45	THR
19	X	52	VAL
19	X	57	LEU
20	Y	2	ARG
20	Y	5	MET
20	Y	6	HIS
20	Y	7	VAL
20	Y	23	ARG
20	Y	31	LEU
20	Y	44	ILE
20	Y	55	TYR
20	Y	72	VAL
20	Y	85	VAL
20	Y	90	LEU
20	Y	92	ASN
20	Y	97	ARG
20	Y	99	CYS
21	Z	3	TYR

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Mol	Chain	Res	Type
21	Z	11	GLU
21	Z	19	ARG
21	Z	20	ARG
21	Z	31	ARG
21	Z	41	LEU
21	Z	42	VAL
21	Z	72	ARG
21	Z	76	LEU
21	Z	80	ARG
21	Z	86	VAL
21	Z	112	ARG
21	Z	126	VAL
21	Z	132	ASN
21	Z	133	ILE
21	Z	155	LEU
21	Z	156	LYS
21	Z	170	THR
22	0	20	ARG
22	0	43	THR
22	0	46	LYS
22	0	55	ARG
22	0	63	VAL
23	1	4	VAL
23	1	20	ARG
23	1	21	ARG
23	1	30	VAL
23	1	35	THR
23	1	40	ARG
23	1	58	ILE
23	1	59	THR
23	1	62	VAL
23	1	82	LEU
23	1	95	LEU
24	2	27	GLU
24	2	30	ARG
24	2	32	LEU
24	2	40	SER
24	2	53	LEU
24	2	55	ARG
25	3	6	VAL
25	3	8	LEU
25	3	23	LEU

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Mol	Chain	Res	Type
25	3	24	LYS
25	3	30	ARG
25	3	40	THR
26	4	14	ILE
26	4	16	CYS
26	4	18	CYS
26	4	20	ASN
26	4	34	GLU
26	4	35	VAL
26	4	37	SER
26	4	39	CYS
26	4	43	TYR
26	4	44	THR
27	5	16	ARG
27	5	29	THR
27	5	37	LYS
27	5	40	LYS
27	5	55	ARG
28	6	6	ARG
28	6	14	THR
28	6	18	ARG
28	6	23	THR
28	6	28	ARG
28	6	33	LYS
28	6	35	GLU
28	6	40	CYS
28	6	44	ARG
28	6	48	VAL
28	6	49	HIS
29	7	1	MET
29	7	4	THR
29	7	8	ASN
29	7	10	ARG
29	7	12	ARG
29	7	24	THR
29	7	32	LYS
29	7	43	THR
29	7	47	ARG
30	8	26	LYS
30	8	27	THR
30	8	29	LYS
30	8	30	ARG

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Mol	Chain	Res	Type
30	8	31	HIS
30	8	32	LEU
30	8	37	SER
30	8	58	ILE
30	8	59	LYS
31	9	17	ILE
31	9	25	VAL
31	9	26	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
5	F	69	HIS
6	G	123	ASN
6	G	138	GLN
8	I	105	HIS
9	N	133	GLN
10	O	89	ASN
15	T	84	GLN
16	U	72	HIS
18	W	60	ASN
18	W	61	ASN
19	X	31	HIS
21	Z	151	HIS
30	8	7	HIS
31	9	36	GLN

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%)

All (577) RNA backbone outliers are listed below:

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

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Mol	Chain	Res	Type
1	A	36	G
1	A	45	C
1	A	61	G
1	A	68	G
1	A	69	C
1	A	71	A
1	A	74	A
1	A	75	G
1	A	83	G
1	A	84	A
1	A	90	U
1	A	92	A
1	A	94	C
1	A	95	G
1	A	102	G
1	A	118	A
1	A	119	A
1	A	120	U
1	A	121	G
1	A	125	G
1	A	131	G
1	A	139(A)	G
1	A	141	A
1	A	154	G
1	A	154(A)	C
1	A	157	U
1	A	172	C
1	A	181	A
1	A	182	A
1	A	196	A
1	A	199	A
1	A	201	C
1	A	204	A
1	A	205	G
1	A	215	G
1	A	216	A
1	A	221	A
1	A	222	A
1	A	225	A
1	A	229	A
1	A	232	G
1	A	233	A

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Mol	Chain	Res	Type
1	A	248	G
1	A	250	G
1	A	271(I)	G
1	A	271(K)	U
1	A	271(L)	U
1	A	271(M)	G
1	A	271(N)	U
1	A	271(O)	C
1	A	271(P)	C
1	A	271(R)	G
1	A	272(B)	G
1	A	272(H)	C
1	A	272(I)	U
1	A	272(J)	C
1	A	277	C
1	A	278	A
1	A	279	C
1	A	294	A
1	A	311	A
1	A	329	G
1	A	330	A
1	A	332	A
1	A	352	G
1	A	363	G
1	A	363(F)	A
1	A	382	G
1	A	386	G
1	A	399	G
1	A	411	G
1	A	412	A
1	A	414	C
1	A	416	C
1	A	427	U
1	A	428	A
1	A	444	C
1	A	448	U
1	A	454	A
1	A	456	C
1	A	457	A
1	A	470	A
1	A	471	A
1	A	481	G

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Mol	Chain	Res	Type
1	A	504	U
1	A	505	A
1	A	509	C
1	A	510	C
1	A	512	G
1	A	513	A
1	A	530	G
1	A	531	C
1	A	532	A
1	A	533	G
1	A	543	C
1	A	545	G
1	A	546	C
1	A	547	A
1	A	548	A
1	A	563	G
1	A	571	A
1	A	573	G
1	A	574	C
1	A	575	A
1	A	584	C
1	A	588	U
1	A	603	A
1	A	604	G
1	A	606	U
1	A	607	U
1	A	614	U
1	A	614(A)	U
1	A	614(B)	G
1	A	615	G
1	A	619	G
1	A	627	A
1	A	637	A
1	A	644	A
1	A	645	C
1	A	646	A
1	A	647	G
1	A	652(B)	A
1	A	652(C)	G
1	A	652(D)	C
1	A	652(U)	G
1	A	656	G

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Mol	Chain	Res	Type
1	A	669	G
1	A	686	G
1	A	708	C
1	A	709	U
1	A	717	G
1	A	730	C
1	A	752	A
1	A	753	C
1	A	762	U
1	A	764	A
1	A	765	G
1	A	775	G
1	A	776	G
1	A	782	A
1	A	784	A
1	A	785	G
1	A	792	G
1	A	793	A
1	A	802	A
1	A	805	G
1	A	810	U
1	A	812	C
1	A	818	G
1	A	819	A
1	A	827	U
1	A	828	U
1	A	830	G
1	A	836	G
1	A	857	C
1	A	859	G
1	A	869	G
1	A	879	G
1	A	880	G
1	A	896	A
1	A	897	C
1	A	899	A
1	A	900	A
1	A	901	A
1	A	910	A
1	A	917	A
1	A	922	U
1	A	923	C

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Mol	Chain	Res	Type
1	A	932	G
1	A	934	G
1	A	938	G
1	A	941	A
1	A	945	A
1	A	946	G
1	A	958	U
1	A	959	A
1	A	961	C
1	A	968	G
1	A	974	G
1	A	975	C
1	A	975(A)	G
1	A	983	A
1	A	990	A
1	A	996	A
1	A	1012	U
1	A	1013	C
1	A	1016	G
1	A	1020	A
1	A	1022	G
1	A	1024	G
1	A	1025	G
1	A	1026	U
1	A	1027	A
1	A	1033	U
1	A	1034	G
1	A	1038	C
1	A	1041	C
1	A	1042	G
1	A	1044	G
1	A	1045	A
1	A	1046	A
1	A	1047	G
1	A	1048	A
1	A	1049	C
1	A	1050	A
1	A	1052	C
1	A	1107	G
1	A	1108	U
1	A	1109	C
1	A	1110	G

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Mol	Chain	Res	Type
1	A	1111	A
1	A	1112	G
1	A	1115	G
1	A	1129	A
1	A	1130	U
1	A	1135	C
1	A	1136	G
1	A	1139	G
1	A	1141	U
1	A	1142	U
1	A	1142(A)	A
1	A	1149	G
1	A	1155	A
1	A	1156	A
1	A	1164	G
1	A	1210	A
1	A	1211	U
1	A	1218	C
1	A	1224	C
1	A	1250	G
1	A	1253	A
1	A	1256	G
1	A	1267	U
1	A	1268	A
1	A	1271	G
1	A	1272	A
1	A	1273	U
1	A	1298	C
1	A	1300	U
1	A	1301	A
1	A	1305	C
1	A	1310	G
1	A	1313	U
1	A	1314	C
1	A	1329	U
1	A	1338	G
1	A	1352	U
1	A	1358	G
1	A	1365	A
1	A	1368	G
1	A	1370	C
1	A	1374	G

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Mol	Chain	Res	Type
1	A	1380	G
1	A	1384	A
1	A	1385	G
1	A	1391	U
1	A	1416	G
1	A	1417	C
1	A	1419	A
1	A	1420	U
1	A	1421	G
1	A	1427	A
1	A	1428	C
1	A	1429	G
1	A	1445	A
1	A	1449	A
1	A	1450	G
1	A	1459	G
1	A	1461	G
1	A	1467	C
1	A	1471	A
1	A	1472	A
1	A	1481	U
1	A	1482	G
1	A	1488	G
1	A	1490	A
1	A	1493	C
1	A	1497	U
1	A	1507	A
1	A	1508	A
1	A	1509	C
1	A	1509(A)	A
1	A	1518	U
1	A	1520	G
1	A	1531	C
1	A	1539	G
1	A	1542	A
1	A	1543	C
1	A	1554	A
1	A	1558	A
1	A	1559	G
1	A	1566	A
1	A	1569	A
1	A	1578	U

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Mol	Chain	Res	Type
1	A	1580	A
1	A	1582	C
1	A	1584	C
1	A	1586	A
1	A	1598	C
1	A	1608	A
1	A	1609	A
1	A	1610	A
1	A	1617	C
1	A	1625	C
1	A	1639	U
1	A	1640	C
1	A	1641	A
1	A	1648	C
1	A	1654	A
1	A	1674	G
1	A	1675	C
1	A	1696	G
1	A	1700	A
1	A	1701	A
1	A	1703	G
1	A	1722	A
1	A	1746	G
1	A	1750	G
1	A	1762	A
1	A	1763	G
1	A	1764	G
1	A	1773	A
1	A	1780	A
1	A	1781	C
1	A	1782	C
1	A	1791	A
1	A	1799	G
1	A	1800	C
1	A	1801	G
1	A	1816	G
1	A	1819	A
1	A	1820	U
1	A	1829	A
1	A	1834	U
1	A	1835	G
1	A	1836	C

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Mol	Chain	Res	Type
1	A	1847	A
1	A	1848	A
1	A	1858	G
1	A	1877	A
1	A	1878	G
1	A	1889	A
1	A	1900	A
1	A	1906	G
1	A	1913	A
1	A	1914	C
1	A	1929	G
1	A	1930	G
1	A	1934	C
1	A	1936	A
1	A	1938	A
1	A	1955	U
1	A	1962	C
1	A	1963	U
1	A	1967	C
1	A	1969	A
1	A	1970	A
1	A	1971	A
1	A	1972	A
1	A	1982	C
1	A	1991	U
1	A	1992	G
1	A	1993	U
1	A	1997	G
1	A	2023	G
1	A	2031	A
1	A	2032	G
1	A	2033	A
1	A	2036	C
1	A	2039	C
1	A	2043	C
1	A	2049	G
1	A	2055	C
1	A	2056	G
1	A	2060	A
1	A	2061	G
1	A	2062	A
1	A	2063	C

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Mol	Chain	Res	Type
1	A	2069	G
1	A	2093	G
1	A	2099	U
1	A	2103	C
1	A	2104	G
1	A	2105	C
1	A	2106	G
1	A	2108	C
1	A	2109	U
1	A	2110	G
1	A	2111	C
1	A	2116	G
1	A	2117	A
1	A	2118	U
1	A	2119	A
1	A	2126	A
1	A	2127	G
1	A	2131	G
1	A	2133	G
1	A	2134	A
1	A	2135	A
1	A	2143	C
1	A	2146	C
1	A	2147	G
1	A	2148	G
1	A	2159	G
1	A	2161	C
1	A	2170	A
1	A	2172	U
1	A	2173	A
1	A	2175	C
1	A	2176	A
1	A	2181	G
1	A	2185	C
1	A	2187	G
1	A	2188	C
1	A	2190	G
1	A	2191	G
1	A	2192	G
1	A	2198	A
1	A	2199	A
1	A	2200	C

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Mol	Chain	Res	Type
1	A	2206	G
1	A	2207	G
1	A	2208	A
1	A	2218	U
1	A	2225	A
1	A	2235	G
1	A	2238	G
1	A	2239	G
1	A	2240	C
1	A	2259	G
1	A	2268	A
1	A	2269	A
1	A	2273	A
1	A	2275	C
1	A	2280	G
1	A	2283	C
1	A	2287	A
1	A	2289	G
1	A	2304	G
1	A	2305	A
1	A	2306	C
1	A	2308	G
1	A	2309	A
1	A	2311	A
1	A	2316	C
1	A	2317	C
1	A	2318	G
1	A	2319	G
1	A	2320	A
1	A	2322	A
1	A	2325	G
1	A	2327	A
1	A	2334	G
1	A	2336	A
1	A	2347	C
1	A	2348	U
1	A	2350	C
1	A	2354	G
1	A	2371	G
1	A	2372	G
1	A	2383	G
1	A	2385	C

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Mol	Chain	Res	Type
1	A	2396	G
1	A	2405	G
1	A	2406	U
1	A	2410	G
1	A	2413	G
1	A	2414	G
1	A	2422	A
1	A	2423	U
1	A	2425	A
1	A	2429	G
1	A	2430	A
1	A	2435	A
1	A	2439	A
1	A	2440	C
1	A	2441	C
1	A	2448	A
1	A	2460	U
1	A	2461	C
1	A	2468	G
1	A	2469	A
1	A	2476	A
1	A	2478	A
1	A	2487	G
1	A	2494	G
1	A	2502	G
1	A	2505	G
1	A	2506	U
1	A	2518	A
1	A	2520	C
1	A	2525	G
1	A	2529	G
1	A	2535	G
1	A	2554	U
1	A	2566	A
1	A	2567	G
1	A	2569	G
1	A	2573	C
1	A	2584	U
1	A	2585	U
1	A	2586	C
1	A	2602	A
1	A	2603	G

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Mol	Chain	Res	Type
1	A	2608	G
1	A	2609	U
1	A	2610	C
1	A	2611	U
1	A	2612	C
1	A	2615	U
1	A	2629	A
1	A	2630	G
1	A	2632	A
1	A	2643	G
1	A	2663	G
1	A	2673	G
1	A	2690	C
1	A	2700	C
1	A	2702	U
1	A	2703	C
1	A	2707	G
1	A	2712	U
1	A	2712(A)	A
1	A	2713	A
1	A	2714	G
1	A	2726	U
1	A	2733	A
1	A	2758	A
1	A	2761	G
1	A	2762	G
1	A	2764	A
1	A	2765	A
1	A	2766	G
1	A	2769	C
1	A	2778	A
1	A	2791	C
1	A	2802	G
1	A	2803	C
1	A	2805	G
1	A	2808	U
1	A	2820	A
1	A	2821	A
1	A	2834	G
1	A	2835	A
1	A	2846	G
1	A	2851	A

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Mol	Chain	Res	Type
1	A	2872	G
1	A	2875	C
1	A	2880	C
1	A	2892	A
1	A	2893	G
1	A	2894	G
1	A	2895	U
2	B	8	U
2	B	9	G
2	B	12	C
2	B	13	A
2	B	17	C
2	B	24	G
2	B	25	A
2	B	29	A
2	B	32	C
2	B	40	U
2	B	44	G
2	B	53	A
2	B	54	G
2	B	56	G
2	B	72	G
2	B	73	A
2	B	84	C
2	B	87	G
2	B	88	C
2	B	106	G
2	B	110	G

All (62) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	9	U
1	A	90	U
1	A	196	A
1	A	221	A
1	A	249	C
1	A	271(K)	U
1	A	271(L)	U
1	A	271(M)	G
1	A	277	C
1	A	278	A

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Mol	Chain	Res	Type
1	A	363(E)	U
1	A	479	A
1	A	512	G
1	A	542	C
1	A	547	A
1	A	652(A)	A
1	A	669	G
1	A	746	A
1	A	752	A
1	A	764	A
1	A	774	A
1	A	776	G
1	A	827	U
1	A	856	C
1	A	896	A
1	A	900	A
1	A	974	G
1	A	1026	U
1	A	1033	U
1	A	1047	G
1	A	1048	A
1	A	1049	C
1	A	1106	G
1	A	1108	U
1	A	1210	A
1	A	1378	A
1	A	1379	A
1	A	1427	A
1	A	1507	A
1	A	1530	C
1	A	1538	G
1	A	1558	A
1	A	1608	A
1	A	1609	A
1	A	1617	C
1	A	1653	G
1	A	1799	G
1	A	1819	A
1	A	1992	G
1	A	2126	A
1	A	2171	A
1	A	2172	U

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Mol	Chain	Res	Type
1	A	2308	G
1	A	2318	G
1	A	2405	G
1	A	2439	A
1	A	2602	A
1	A	2610	C
1	A	2689	U
1	A	2712	U
1	A	2778	A
1	A	2802	G

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	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 ²)	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

All (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
9	N	8	GLN	4.9
1	A	2149	G	4.7
6	G	137	GLU	4.7
1	A	652(B)	A	4.6
1	A	2157	G	4.6
6	G	152	LEU	4.5
29	7	47	ARG	4.4
1	A	2133	G	4.2
6	G	74	LYS	4.2
1	A	405	U	4.1
11	P	149	GLU	4.1
1	A	1509	C	4.0
1	A	1847	A	3.9
1	A	2129	C	3.8
6	G	136	ARG	3.8
1	A	2790	A	3.8
1	A	2794	C	3.8
1	A	2180	U	3.7
1	A	2144	U	3.7
1	A	2150	U	3.6
5	F	208	GLY	3.6
1	A	2132	U	3.6
1	A	2110	G	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	157	U	3.5
1	A	2176	A	3.5
20	Y	1	MET	3.5
1	A	2173	A	3.4
1	A	2106	G	3.4
1	A	2159	G	3.4
1	A	2123	G	3.4
6	G	26	GLN	3.4
1	A	2112	G	3.3
20	Y	2	ARG	3.2
6	G	2	PRO	3.2
1	A	2124	G	3.2
1	A	2130	U	3.2
1	A	1963	U	3.2
1	A	2793	G	3.1
1	A	655	A	3.1
6	G	138	GLN	3.1
1	A	2125	G	3.1
1	A	2192	G	3.0
1	A	2161	C	3.0
1	A	652(A)	A	3.0
1	A	1574	C	3.0
12	Q	1	MET	3.0
1	A	2165	G	2.9
1	A	2174	C	2.9
1	A	1575	C	2.9
1	A	2140	C	2.8
7	H	98	LEU	2.8
1	A	2158	A	2.8
1	A	2122	U	2.8
22	0	17	GLN	2.7
6	G	33	ARG	2.7
7	H	116	GLU	2.7
24	2	8	LYS	2.6
6	G	87	PRO	2.6
21	Z	70	LEU	2.6
2	B	98	G	2.6
1	A	2146	C	2.6
1	A	2121	G	2.6
1	A	2191	G	2.6
1	A	1460	A	2.6
1	A	2164	C	2.6

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Mol	Chain	Res	Type	RSRZ
5	F	35	GLU	2.5
11	P	105	LEU	2.5
8	I	16	GLY	2.5
20	Y	85	VAL	2.5
20	Y	92	ASN	2.5
6	G	30	GLU	2.5
21	Z	72	ARG	2.4
4	E	55	ASN	2.4
11	P	92	GLU	2.4
1	A	1049	C	2.3
8	I	132	PRO	2.3
1	A	897	C	2.3
6	G	35	GLU	2.3
1	A	2145	C	2.3
11	P	93	GLY	2.3
11	P	117	GLU	2.3
1	A	896	A	2.3
1	A	1171	G	2.3
1	A	2160	G	2.2
1	A	272(A)	U	2.2
1	A	1917	U	2.2
1	A	2143	C	2.2
11	P	144	GLU	2.2
20	Y	34	LYS	2.2
6	G	160	VAL	2.2
8	I	117	GLU	2.1
8	I	37	VAL	2.1
11	P	146	VAL	2.1
24	2	70	GLN	2.1
6	G	139	LEU	2.1
11	P	135	LEU	2.1
30	8	65	GLU	2.1
20	Y	80	GLY	2.1
9	N	140	VAL	2.1
24	2	7	ARG	2.1
5	F	207	GLY	2.1
6	G	135	LEU	2.0
1	A	2170	A	2.0
7	H	119	GLU	2.0
8	I	64	GLU	2.0
1	A	529	A	2.0
1	A	548	A	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
32	MG	A	3504	1/1	0.10	-	61,61,61,61	0
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

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
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	0	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.