



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 04:03 PM GMT

PDB ID : 3V2D
Title : Crystal structure of YfiA 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 : 2011-12-12
Resolution : 2.70 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>

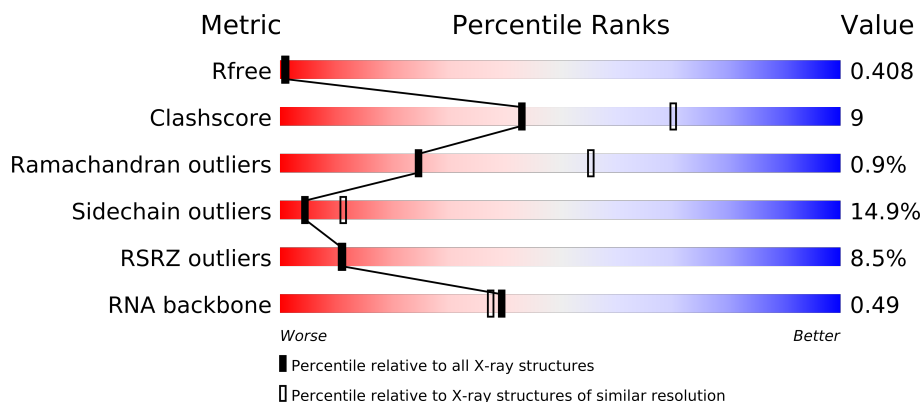
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.70 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	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)
RNA backbone	1838	1042 (3.20-2.20)

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 93185 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	2827	Total	C	N	O	P	0	0	0
			60898	27101	11400	19571	2826			

- 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
			1577	1004	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
			1043	672	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	101	Total	C	N	O	S		
			771	495	140	135	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	2	Total	Mg	0	0
			2	2		
32	B	19	Total	Mg	0	0
			19	19		
32	6	1	Total	Mg	0	0
			1	1		
32	W	1	Total	Mg	0	0
			1	1		
32	N	2	Total	Mg	0	0
			2	2		
32	2	2	Total	Mg	0	0
			2	2		
32	S	1	Total	Mg	0	0
			1	1		
32	E	6	Total	Mg	0	0
			6	6		
32	V	4	Total	Mg	0	0
			4	4		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	A	725	Total 725	Mg 725	0	0
32	R	5	Total 5	Mg 5	0	0
32	1	1	Total 1	Mg 1	0	0
32	D	6	Total 6	Mg 6	0	0
32	Z	2	Total 2	Mg 2	0	0
32	U	3	Total 3	Mg 3	0	0
32	9	3	Total 3	Mg 3	0	0
32	0	4	Total 4	Mg 4	0	0
32	G	1	Total 1	Mg 1	0	0
32	Q	5	Total 5	Mg 5	0	0
32	H	1	Total 1	Mg 1	0	0
32	7	1	Total 1	Mg 1	0	0
32	T	3	Total 3	Mg 3	0	0
32	8	1	Total 1	Mg 1	0	0
32	O	1	Total 1	Mg 1	0	0
32	Y	1	Total 1	Mg 1	0	0
32	3	2	Total 2	Mg 2	0	0
32	F	6	Total 6	Mg 6	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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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	1975	Total 1975	O 1975	0	0
34	B	45	Total 45	O 45	0	0
34	D	18	Total 18	O 18	0	0
34	E	16	Total 16	O 16	0	0
34	F	17	Total 17	O 17	0	0
34	G	2	Total 2	O 2	0	0
34	H	2	Total 2	O 2	0	0
34	N	7	Total 7	O 7	0	0
34	O	2	Total 2	O 2	0	0
34	P	21	Total 21	O 21	0	0
34	Q	8	Total 8	O 8	0	0
34	R	9	Total 9	O 9	0	0
34	S	2	Total 2	O 2	0	0
34	T	5	Total 5	O 5	0	0
34	U	7	Total 7	O 7	0	0

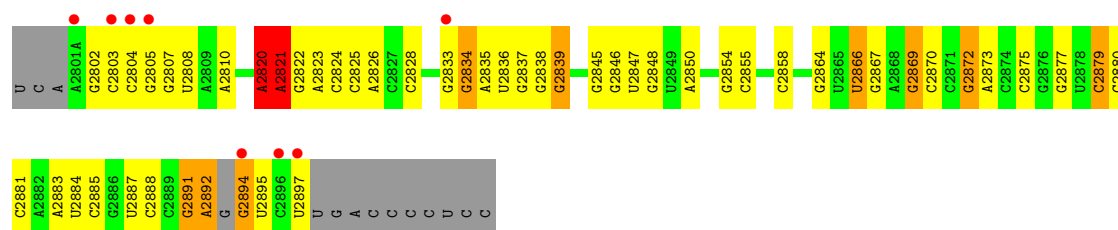
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	V	13	Total 13	O 13	0	0
34	W	6	Total 6	O 6	0	0
34	X	2	Total 2	O 2	0	0
34	Y	2	Total 2	O 2	0	0
34	Z	2	Total 2	O 2	0	0
34	0	6	Total 6	O 6	0	0
34	1	5	Total 5	O 5	0	0
34	3	5	Total 5	O 5	0	0
34	5	6	Total 6	O 6	0	0
34	6	1	Total 1	O 1	0	0
34	7	4	Total 4	O 4	0	0
34	8	9	Total 9	O 9	0	0
34	9	1	Total 1	O 1	0	0

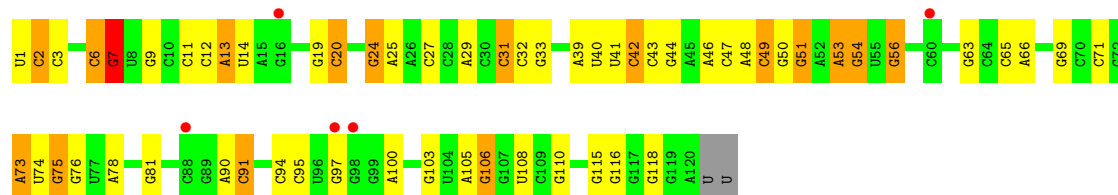


G2722	G2645	U2584	G2518	G2443	G2371	G2299	A2225	G2151	G2087	A2020	G1954	G1861	A1783	C1685
G2723	G2646	U2585	U2519	G2444	G2375	G2300	G2226	G2152	G2087	G2021	U1955	G1861	A1784	C1686
U2726	G2648	G2586	G2523	G2446	A2376	G2302	G2227	G2153	G2090	U2022	U1956	G1865	A1785	C1687
G2729	U2649	A2587	U2522	G2447	A2377	G2303	G2228	G2154	G2093	G2023	C1958	C1866	A1786	U1688
G2730	U2656	G2588	G2523	G2448	A2378	G2304	G2229	G2155	G2093	G2024	G1959	A1876	C1787	A1689
G2731	U2656	G2589	G2524	U2449	A2378	G2305	G2231	G2156	U2096	G2025	A1959	G1878	C1788	C1689
G2732	G2659	A2590	G2525	A2450	G2381	G2308	U2232	G2157	U2096	G2026	A1960	G1878	U1693	U1693
A2733	A2660	G2591	G2526	A2453	G2382	G2309	U2233	A2158	G2100	G2027	C1961	C1879	C1694	C1694
G2737	G2661	U2592	U2527	G2454	G2383	A2310	G2234	G2160	G2100	G2028	C1962	C1880	A1791	C1694
G2737	A2662	U2593	G2528	G2455	G2384	A2311	G2235	G2161	G2101	G2029	U1963	C1881	A1792	C1695
G2737	G2663	G2595	G2529	G2456	G2385	A2312	G2236	G2162	U2102	A2030	C1964	C1882	C1793	C1697
A2740	G2673	G2596	G2532	U2457	G2386	U2312	G2237	G2163	G2103	G2031	C1965	C1883	U1794	C1699
A2741	G2674	U2597	G2535	U2460	U2387	G2315	G2238	G2164	G2104	G2032	A1966	A1884	C1795	C1699
G2742	A2675	A2598	G2536	G2461	A2388	G2316	G2239	G2165	G2105	A2033	C1967	A1885	U1796	A1700
G2744	G2678	G2600	U2537	G2462	A2389	C2317	A2241	U2167	G2106	U2034	C1968	C1886	U1797	A1702
G2745	G2681	A2601	G2538	G2463	U2390	G2317	G2242	G2168	C2107	G2036	A1969	G1798	C1797	G1702
U2746	G2682	A	G2539	G2464	G2391	G2318	G2243	G2169	C2108	G2037	A1970	A1889	C1799	G1710
G2747	G2683	G2601	G2540	G2465	G2392	G2319	U2244	A2170	G2110	G2038	A1971	A1890	C1800	G1710
G2751	G2684	G2603	A2541	G2466	G2393	A2320	U2245	A2171	G2111	C2039	C1894	G1801	G1801	G1721
G2755	G2685	G2604	G2542	G2467	G2394	A2322	G2246	U2172	G2112	C2040	C1895	A1802	A1722	A1722
U2756	G2686	G2605	G2545	G2468	G2397	G2323	G2247	A2173	U2113	U2041	C1896	A1803	U1739	G1730
A2757	G2687	G2606	U2546	G2469	G2400	G2324	U2249	A2174	A2114	A2042	G1897	C1806	G1807	G1741
G2758	G2688	G2607	U2547	U2473	G2404	G2325	G2250	C2175	G2115	C2043	U1898	G1807	G1742	G1742
G2759	G2689	G2608	G2548	G2474	G2405	A2327	G2256	U2180	U2117	G2050	C1985	A1810	C1743	C1743
G2760	G2690	G2610	G2549	G2475	U2406	G2329	G2269	G2182	G2120	A2051	C1986	C1902	C1745	C1745
G2761	G2691	G2611	G2550	G2476	G2407	G2330	G2270	G2183	G2121	G2052	G1987	G1903	G1813	G1746
G2763	G2692	G2612	G2551	G2477	G2408	G2331	G2271	C2188	U2122	G2053	G1988	G1906	G1814	G1748
A2764	G2693	U2613	U2552	G2478	G2410	U2332	G2261	G2189	G2123	A2054	C1989	A1913	A1815	G1748
G2765	G2694	G2614	U2553	G2483	G2411	A2334	A2268	G2185	G2124	C2055	C1990	A1913	G1816	G1752
G2766	G2695	G2615	U2554	G2484	G2412	A2335	G2269	G2186	G2125	G2056	U1991	C1914	G1817	C1752
G2769	U2696	G2616	G2555	G2485	G2413	A2336	G2270	G2187	A2126	A2057	U1992	A1819	G1818	G1753
G2772	G2697	G2617	G2556	G2486	G2414	G2337	G2271	U2189	G2127	A2058	G1921	A1820	C1754	C1754
C2773	G2698	G2618	G2557	G2487	U2418	U2344	G2272	G2190	C2128	A2059	C1994	A1821	G1755	G1755
C2774	G2699	G2619	G2558	G2488	U2419	G2345	A2273	G2191	G2129	G2061	U1997	A1822	G1756	G1756
C2775	G2700	G2620	G2559	G2489	G2420	G2346	G2274	G2192	U2130	A2062	G1998	G1823	U1757	U1757
G2777	G2701	A2621	G2560	U2491	G2421	A2347	G2275	G2193	G2131	C2063	C1999	A1824	C1761	C1761
A2778	U2702	G2624	U2562	G2493	U2422	G2347	G2276	G2194	U2132	G2064	G2000	A1825	A1762	A1762
A2781	G2703	G2627	U2563	G2494	G2423	G2348	G2277	G2195	G2133	C2065	A2001	G1826	G1763	G1763
G2782	G2704	G2628	A2564	G2495	G2424	U2349	G2278	G2196	A2134	G2066	G2002	C1827	G1764	G1764
G2783	A2705	G2629	A2565	G2496	A2425	G2350	C2283	U2197	A2135	G2067	A1932	G1828	U1768	U1768
G2784	G2706	G2630	G2566	G2497	G2426	G2351	G2284	A2198	C2136	U2068	G1933	A1829	G1770	G1770
G2785	G2709	G2631	G2567	G2498	G2427	A2352	G2285	A2199	C2137	G2069	C1934	C1830	C1771	C1771
U2786	G2710	G2632	G2570	G2499	U2430	G2353	A2286	G2200	C2138	G2070	G1935	G1835	G1772	G1772
G2787	U2712	G2633	A2571	G2501	U2431	G2354	G2287	G2201	C2139	A2071	A1936	G1836	U1773	U1773
G2788	G2713	G2634	G2572	G2502	G2432	G2355	A2288	G2202	C2140	G2072	U1937	A1938	G1774	G1774
G2789	U2714	G2635	G2573	G2503	G2433	C2356	G2289	U2203	G2141	G2073	U1939	G1839	U1775	U1775
A2790	G2715	U2636	G2574	G2504	A2434	U2357	U2291	G2205	C2142	U2074	C1942	G1840	U1776	U1776
G2791	G2716	G2637	G2575	G2505	G2435	G2358	G2292	G2206	C2143	U2075	A2013	G1842	U1777	U1777
G2792	G2719	G2638	G2576	G2506	G2436	G2359	G2293	G2207	C2144	G2076	A2014	C1843	U1778	U1778
G2793	G2720	U2639	U2577	G2507	U2437	A2360	G2294	A2208	C2145	A2077	U1944	U1847	U1779	U1779
G2794	G2721	G2640	G2578	G2508	U2438	G2363	G2295	U2218	G2146	A2015	U1951	A1847	U1780	U1780
G	G2722	G2641	U2580	G2511	G2440	C2364	U2296	G2219	G2147	G2079	A1952	C1781	G1858	C1782
		G2642	G2581	G2512	G2442	G2365	A2298	G2220	U2150	G2080	A1953			



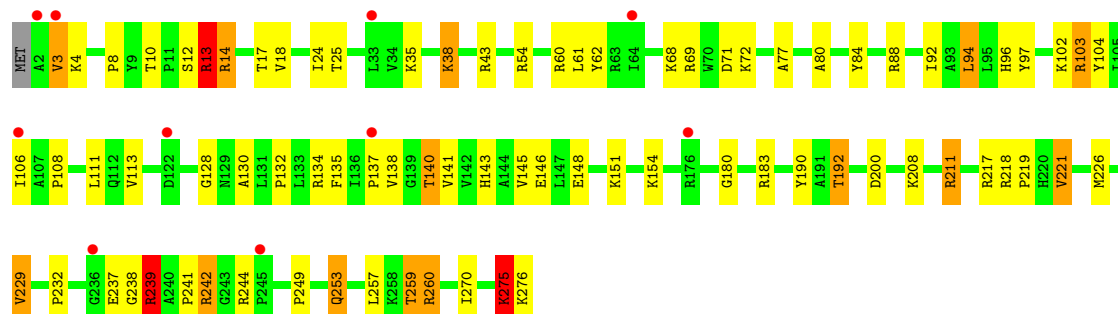
• Molecule 2: 5S Ribosomal RNA

Chain B:



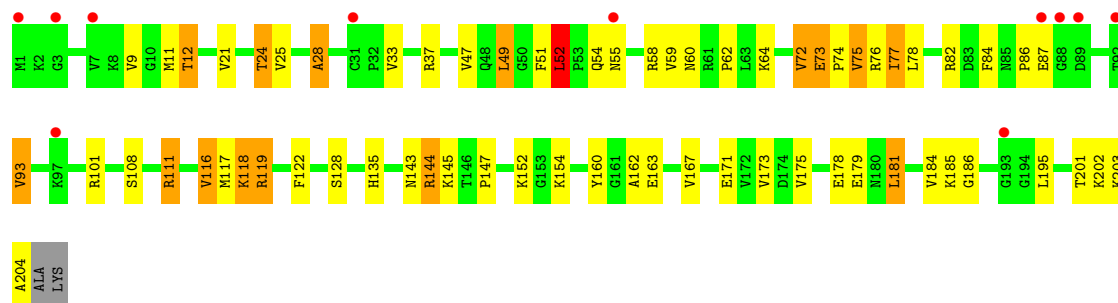
• Molecule 3: 50S Ribosomal Protein L2

Chain D:



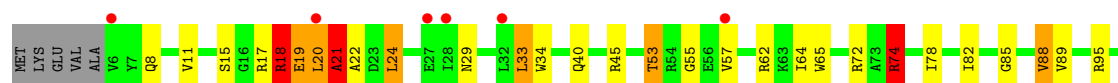
• Molecule 4: 50S Ribosomal Protein L3

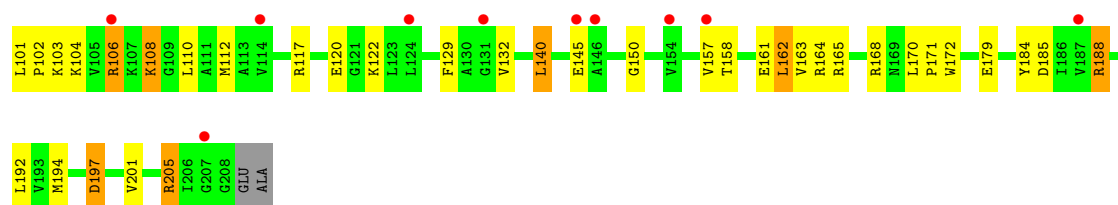
Chain E:



• Molecule 5: 50S Ribosomal Protein L4

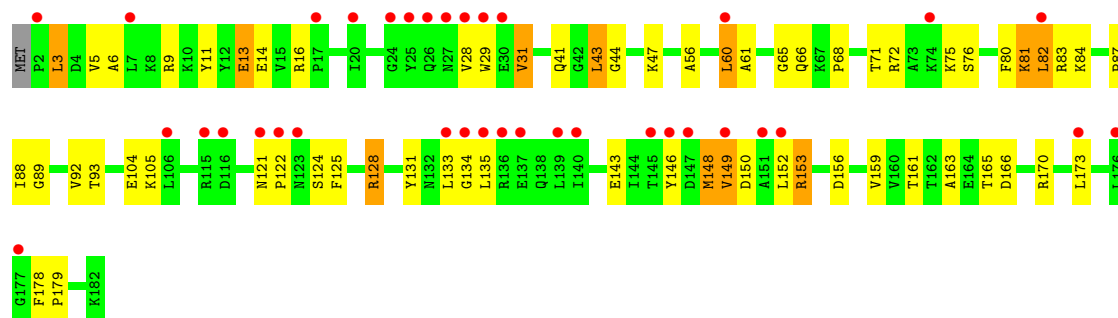
Chain F:





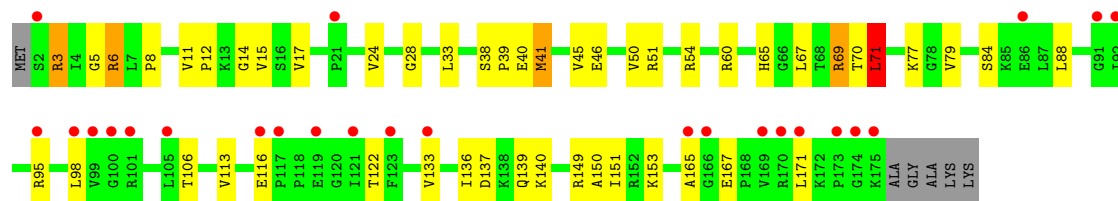
• Molecule 6: 50S Ribosomal Protein L5

Chain G:



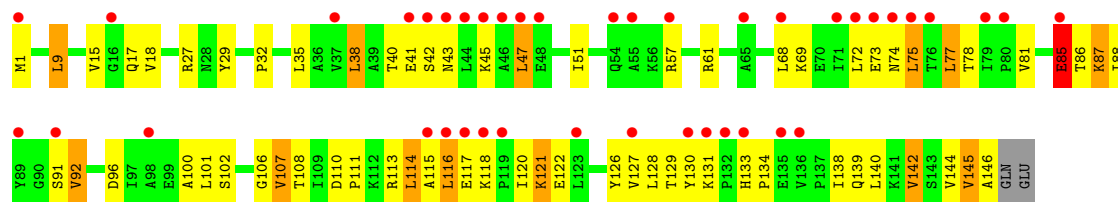
• Molecule 7: 50S Ribosomal Protein L6

Chain H:



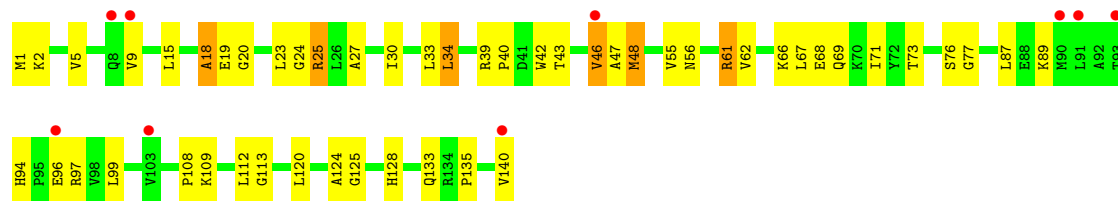
• Molecule 8: 50S Ribosomal Protein L9

Chain I:



• Molecule 9: 50S Ribosomal Protein L13

Chain N:



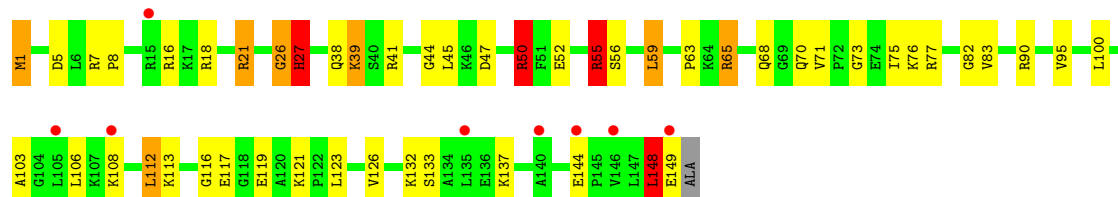
• Molecule 10: 50S Ribosomal Protein L14

Chain O:



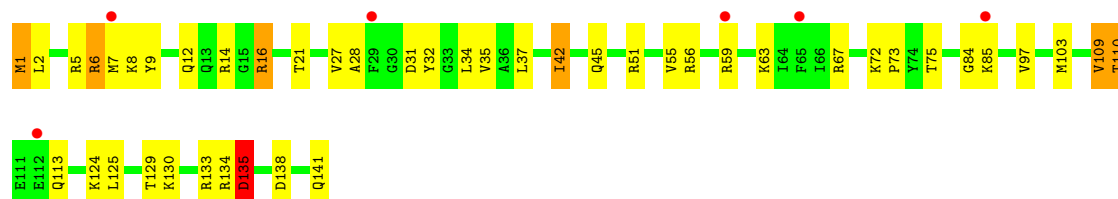
• Molecule 11: 50S Ribosomal Protein L15

Chain P:



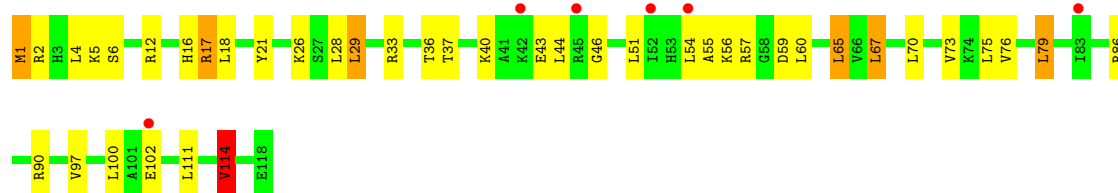
• Molecule 12: 50S Ribosomal Protein L16

Chain Q:



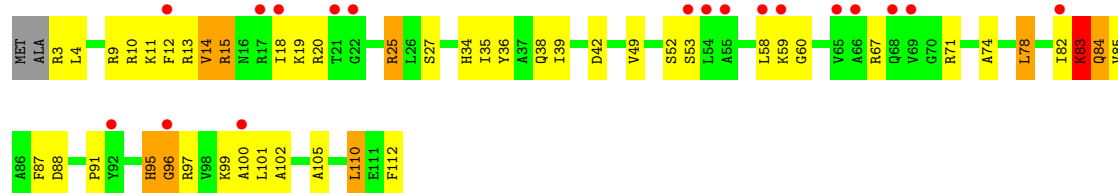
• Molecule 13: 50S Ribosomal Protein L17

Chain R:



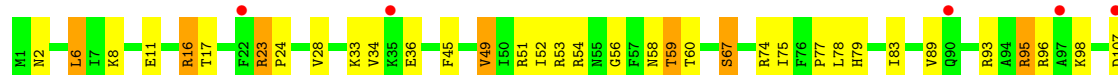
• Molecule 14: 50S Ribosomal Protein L18

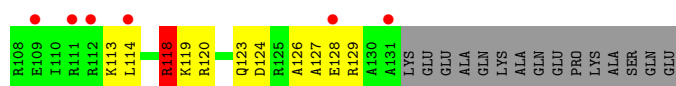
Chain S:



• Molecule 15: 50S Ribosomal Protein L19

Chain T:





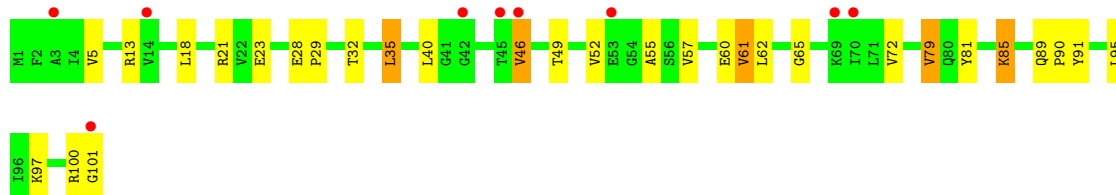
• Molecule 16: 50S Ribosomal Protein L20

Chain U:



• Molecule 17: 50S Ribosomal Protein L21

Chain V:



• Molecule 18: 50S Ribosomal Protein L22

Chain W:



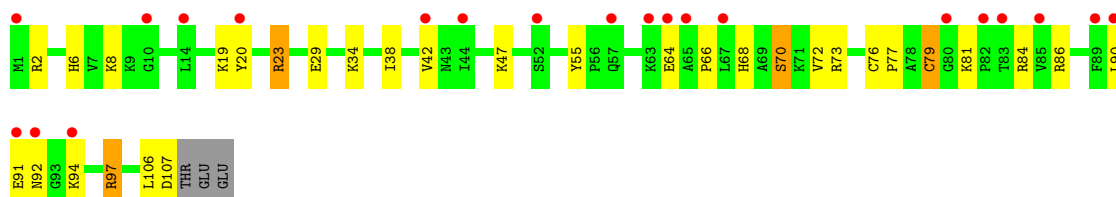
• Molecule 19: 50S Ribosomal Protein L23

Chain X:



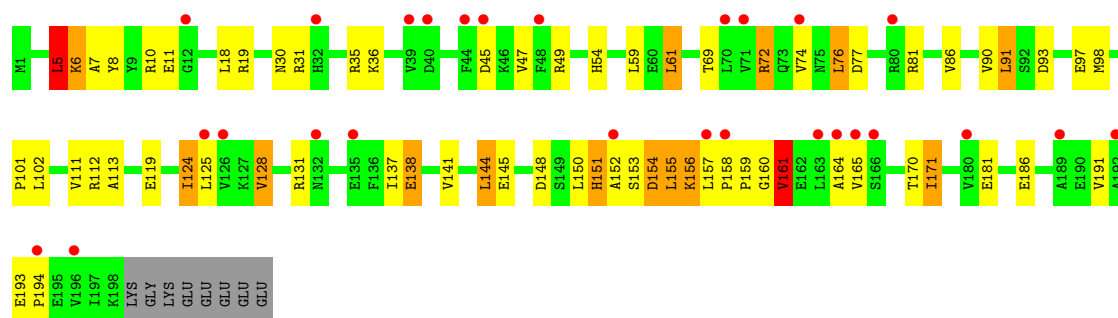
• Molecule 20: 50S Ribosomal Protein L24

Chain Y:



• Molecule 21: 50S Ribosomal Protein L25

Chain Z:



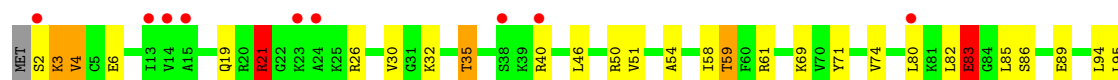
• Molecule 22: 50S Ribosomal Protein L27

Chain 0:



• Molecule 23: 50S Ribosomal Protein L28

Chain 1:



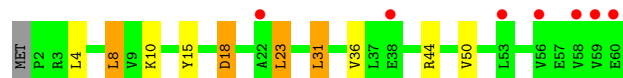
• Molecule 24: 50S Ribosomal Protein L29

Chain 2:



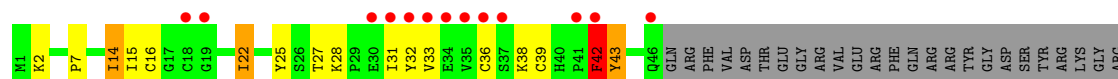
• Molecule 25: 50S Ribosomal Protein L30

Chain 3:



• Molecule 26: 50S Ribosomal Protein L31

Chain 4:



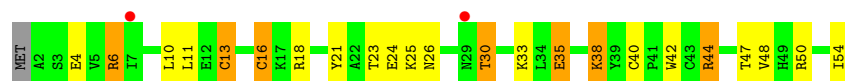
• Molecule 27: 50S Ribosomal Protein L32

Chain 5:



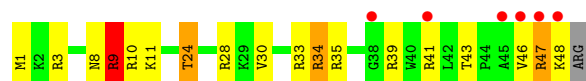
- Molecule 28: 50S Ribosomal Protein L33

Chain 6: 



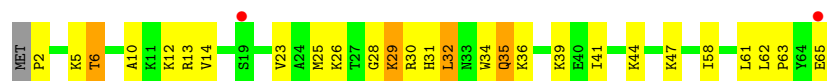
- Molecule 29: 50S Ribosomal Protein L34

Chain 7: 



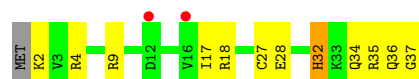
- Molecule 30: 50S Ribosomal Protein L35

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	209.63Å 449.30Å 620.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.71 – 2.70 49.71 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.4 (49.71-2.70) 98.4 (49.71-2.70)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.217 , 0.254 0.402 , 0.408	Depositor DCC
R_{free} test set	78243 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	55.6	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 26.4	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 1557851 reflections	Xtriage
F_o, F_c correlation	0.68	EDS
Total number of atoms	93185	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.42% 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	1.46	435/68200 (0.6%)	1.72	2119/106454 (2.0%)
2	B	1.09	2/2878 (0.1%)	1.48	44/4490 (1.0%)
3	D	0.90	1/2186 (0.0%)	1.02	8/2944 (0.3%)
4	E	0.89	0/1588	0.98	2/2145 (0.1%)
5	F	0.84	1/1612 (0.1%)	0.94	5/2184 (0.2%)
6	G	0.55	0/1393	0.78	0/1892
7	H	0.68	0/1343	0.80	0/1820
8	I	0.63	0/1058	0.84	0/1449
9	N	0.84	0/1139	0.96	4/1538 (0.3%)
10	O	0.86	0/933	0.92	2/1257 (0.2%)
11	P	0.85	0/1148	1.02	7/1529 (0.5%)
12	Q	0.85	0/1143	0.89	2/1527 (0.1%)
13	R	0.85	0/982	0.98	2/1312 (0.2%)
14	S	0.71	0/875	0.91	1/1168 (0.1%)
15	T	0.79	0/1077	0.98	2/1444 (0.1%)
16	U	0.89	0/977	0.95	4/1301 (0.3%)
17	V	0.85	0/782	0.92	0/1049
18	W	0.97	2/891 (0.2%)	0.97	3/1197 (0.3%)
19	X	0.88	0/756	0.90	1/1016 (0.1%)
20	Y	0.76	1/798 (0.1%)	1.04	4/1073 (0.4%)
21	Z	0.67	0/1555	0.85	4/2118 (0.2%)
22	0	0.78	0/602	0.94	3/804 (0.4%)
23	1	0.85	0/752	0.91	2/1003 (0.2%)
24	2	0.77	0/590	0.80	0/781
25	3	0.76	0/463	0.77	0/623
26	4	0.65	1/358 (0.3%)	0.82	1/487 (0.2%)
27	5	0.93	0/469	1.07	2/634 (0.3%)
28	6	0.89	1/456 (0.2%)	0.90	0/609
29	7	1.02	0/426	1.17	5/561 (0.9%)
30	8	0.92	0/516	0.98	1/679 (0.1%)
31	9	0.98	0/300	1.11	3/395 (0.8%)
All	All	1.30	444/98246 (0.5%)	1.55	2231/147483 (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
1	A	0	4
3	D	0	1
4	E	0	1
5	F	0	3
6	G	0	1
7	H	0	1
8	I	0	1
9	N	0	1
11	P	0	2
14	S	0	1
15	T	0	1
19	X	0	1
21	Z	0	1
23	1	0	1
26	4	0	1
27	5	0	1
All	All	0	22

All (444) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1021	A	N9-C4	-14.91	1.28	1.37
1	A	2287	A	N9-C4	-14.79	1.28	1.37
1	A	1142(A)	A	N9-C4	-14.66	1.29	1.37
1	A	945	A	N9-C4	-14.58	1.29	1.37
1	A	528	A	N9-C4	-13.49	1.29	1.37
1	A	2335	A	C6-N6	-12.44	1.24	1.33
1	A	2123	G	P-OP1	-12.01	1.28	1.49
1	A	2243	U	P-OP2	-11.95	1.28	1.49
1	A	788	A	P-OP2	-10.86	1.30	1.49
1	A	2589	A	P-O5'	-10.52	1.49	1.59
1	A	2057	A	P-OP2	-10.45	1.31	1.49
1	A	330	A	N9-C4	-10.35	1.31	1.37
1	A	933	A	N9-C4	-10.29	1.31	1.37
1	A	933	A	N3-C4	-10.00	1.28	1.34
1	A	679	C	P-OP2	-9.95	1.32	1.49
1	A	530	G	N9-C8	9.95	1.44	1.37
1	A	1026	U	P-OP2	-9.88	1.32	1.49
1	A	546	C	P-OP1	-9.68	1.32	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2445	G	P-OP1	-9.47	1.32	1.49
1	A	272(A)	U	C1'-N1	9.28	1.62	1.48
1	A	2296	U	C4-C5	9.11	1.51	1.43
1	A	2450	A	P-OP2	-9.10	1.33	1.49
1	A	1303	G	C6-N1	-9.06	1.33	1.39
1	A	945	A	C5-C6	-8.80	1.33	1.41
1	A	685	A	N9-C4	-8.79	1.32	1.37
1	A	945	A	N9-C8	8.78	1.44	1.37
1	A	945	A	N3-C4	-8.66	1.29	1.34
1	A	1762	A	P-OP1	-8.64	1.34	1.49
1	A	679	C	P-OP1	-8.58	1.34	1.49
1	A	2143	C	P-OP1	-8.49	1.34	1.49
2	B	27	C	P-OP1	-8.48	1.34	1.49
1	A	530	G	C2-N3	-8.42	1.26	1.32
1	A	2296	U	N1-C2	8.42	1.46	1.38
1	A	808	G	P-OP2	-8.40	1.34	1.49
1	A	2589	A	P-OP2	-8.40	1.34	1.49
1	A	2450	A	P-O5'	-8.36	1.51	1.59
1	A	1698	A	N9-C4	-8.35	1.32	1.37
1	A	2028	U	C2-N3	-8.29	1.31	1.37
1	A	2607	G	N7-C5	-8.29	1.34	1.39
1	A	788	A	P-O5'	-8.24	1.51	1.59
1	A	1274	A	N7-C5	-8.21	1.34	1.39
1	A	530	G	C8-N7	8.21	1.35	1.30
1	A	747	U	P-OP2	-8.18	1.35	1.49
1	A	1776	G	C8-N7	-8.15	1.26	1.30
1	A	2454	G	C6-N1	-8.15	1.33	1.39
1	A	1698	A	N9-C8	8.11	1.44	1.37
2	B	27	C	P-OP2	-8.08	1.35	1.49
1	A	809	G	P-OP2	-8.05	1.35	1.49
1	A	2444	G	O3'-P	-7.93	1.51	1.61
1	A	1190	G	N7-C5	-7.90	1.34	1.39
1	A	2143	C	P-OP2	-7.85	1.35	1.49
1	A	2035	G	P-OP1	-7.84	1.35	1.49
1	A	1762	A	P-OP2	-7.83	1.35	1.49
1	A	2450	A	P-OP1	-7.77	1.35	1.49
1	A	2502	G	N7-C5	-7.75	1.34	1.39
1	A	1045	A	N9-C4	7.70	1.42	1.37
1	A	2057	A	P-OP1	-7.67	1.35	1.49
1	A	2243	U	P-O5'	-7.67	1.52	1.59
1	A	278	A	C6-N1	7.60	1.40	1.35
1	A	808	G	N7-C5	-7.60	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2036	C	N1-C6	7.58	1.41	1.37
1	A	330	A	N9-C8	7.55	1.43	1.37
1	A	2572	A	C5-C4	-7.54	1.33	1.38
1	A	1026	U	P-OP1	-7.51	1.36	1.49
1	A	2055	C	P-OP1	-7.49	1.36	1.49
1	A	528	A	C5-C6	-7.48	1.34	1.41
1	A	809	G	P-OP1	-7.46	1.36	1.49
1	A	207	A	N9-C4	-7.45	1.33	1.37
1	A	2287	A	C5-C6	-7.43	1.34	1.41
1	A	685	A	N3-C4	-7.38	1.30	1.34
1	A	527	C	N3-C4	-7.37	1.28	1.33
1	A	1982	C	P-OP2	-7.33	1.36	1.49
1	A	2322	A	C8-N7	7.33	1.36	1.31
1	A	1770	G	C5-C4	-7.27	1.33	1.38
1	A	528	A	N9-C8	7.27	1.43	1.37
1	A	776	G	C6-N1	-7.24	1.34	1.39
1	A	945	A	N7-C5	-7.22	1.34	1.39
1	A	1982	C	P-OP1	-7.20	1.36	1.49
1	A	1653	G	N7-C5	-7.20	1.34	1.39
1	A	2057	A	P-O5'	-7.18	1.52	1.59
1	A	1981	A	O3'-P	-7.17	1.52	1.61
1	A	2449	U	O3'-P	-7.14	1.52	1.61
1	A	571	A	P-OP2	-7.13	1.36	1.49
1	A	1564	C	N3-C4	-7.10	1.28	1.33
1	A	679	C	P-O5'	-7.09	1.52	1.59
1	A	573	G	N7-C5	-7.08	1.35	1.39
1	A	2322	A	C6-N1	7.08	1.40	1.35
1	A	568	U	C4-O4	-7.06	1.18	1.23
1	A	2605	U	C2-N3	-7.05	1.32	1.37
1	A	2335	A	C5-C4	-7.05	1.33	1.38
1	A	751	A	N3-C4	-7.01	1.30	1.34
1	A	2393	A	C6-N1	-6.92	1.30	1.35
1	A	747	U	P-OP1	-6.92	1.37	1.49
1	A	1263	U	C4-O4	-6.92	1.18	1.23
1	A	528	A	C2-N3	-6.89	1.27	1.33
1	A	2019	A	C6-N1	-6.88	1.30	1.35
1	A	2437	U	C2-O2	-6.83	1.16	1.22
1	A	546	C	P-OP2	-6.78	1.37	1.49
1	A	1982	C	P-O5'	-6.76	1.52	1.59
1	A	1131	G	N1-C2	-6.76	1.32	1.37
1	A	2589	A	P-OP1	-6.75	1.37	1.49
1	A	2557	G	N1-C2	-6.75	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1324	G	N1-C2	-6.73	1.32	1.37
20	Y	79	CYS	CB-SG	-6.73	1.70	1.82
1	A	331	A	N9-C4	-6.72	1.33	1.37
1	A	53	A	N3-C4	-6.72	1.30	1.34
1	A	2454	G	N1-C2	-6.71	1.32	1.37
1	A	688	U	C2-O2	-6.70	1.16	1.22
1	A	1142(A)	A	N3-C4	-6.70	1.30	1.34
5	F	88	VAL	CB-CG1	-6.68	1.38	1.52
1	A	1204	A	N9-C4	-6.67	1.33	1.37
1	A	747	U	P-O5'	-6.63	1.53	1.59
1	A	450	G	N7-C5	-6.63	1.35	1.39
1	A	2505	G	N3-C4	-6.59	1.30	1.35
1	A	1611	C	N1-C6	-6.58	1.33	1.37
1	A	1698	A	C5-C4	6.57	1.43	1.38
1	A	787	U	O3'-P	-6.57	1.53	1.61
1	A	734	A	C6-N1	-6.54	1.30	1.35
1	A	1782	C	P-OP1	-6.52	1.37	1.49
1	A	2570	G	C5-C4	-6.52	1.33	1.38
1	A	2055	C	P-OP2	-6.50	1.37	1.49
1	A	1628	G	C8-N7	-6.49	1.27	1.30
1	A	328	U	C2-O2	-6.48	1.16	1.22
1	A	2032	G	N7-C5	-6.43	1.35	1.39
1	A	785	G	P-O5'	-6.42	1.53	1.59
1	A	2249	U	C4-O4	-6.41	1.18	1.23
1	A	2588	G	O3'-P	-6.40	1.53	1.61
26	4	16	CYS	CB-SG	-6.39	1.71	1.82
1	A	1764	G	N1-C2	-6.39	1.32	1.37
1	A	2065	C	N3-C4	-6.39	1.29	1.33
1	A	2442	C	C2-O2	-6.38	1.18	1.24
1	A	567	A	C6-N1	-6.38	1.31	1.35
1	A	2322	A	N9-C4	6.38	1.41	1.37
1	A	579	G	N9-C8	-6.37	1.33	1.37
1	A	265	A	N9-C4	-6.36	1.34	1.37
1	A	2035	G	P-O5'	-6.36	1.53	1.59
1	A	962	G	N9-C8	-6.34	1.33	1.37
1	A	808	G	P-O5'	-6.32	1.53	1.59
1	A	1366	A	C6-N1	-6.32	1.31	1.35
1	A	663	G	C6-N1	-6.31	1.35	1.39
1	A	2894	G	C5-C4	6.31	1.42	1.38
1	A	573	G	C8-N7	-6.30	1.27	1.30
1	A	2445	G	P-OP2	-6.29	1.38	1.49
1	A	808	G	P-OP1	-6.29	1.38	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1771	C	N3-C4	-6.29	1.29	1.33
1	A	2053	G	N9-C8	-6.28	1.33	1.37
1	A	1348	G	C5-C4	-6.28	1.33	1.38
1	A	2035	G	N7-C5	-6.27	1.35	1.39
1	A	1429	G	N1-C2	-6.26	1.32	1.37
1	A	530	G	N3-C4	-6.26	1.31	1.35
1	A	2067	G	N3-C4	-6.25	1.31	1.35
1	A	1200	C	N3-C4	-6.23	1.29	1.33
1	A	2546	U	C2-N3	-6.22	1.33	1.37
1	A	1826	G	C8-N7	6.22	1.34	1.30
1	A	12	U	N1-C2	6.22	1.44	1.38
1	A	795	C	C2-O2	-6.21	1.18	1.24
1	A	1558	A	N3-C4	-6.20	1.31	1.34
1	A	2823	A	N3-C4	-6.20	1.31	1.34
1	A	197	A	N3-C4	-6.18	1.31	1.34
1	A	802	A	C6-N1	-6.18	1.31	1.35
1	A	2689	U	C3'-O3'	6.18	1.50	1.42
1	A	512	G	C5-C4	-6.18	1.34	1.38
1	A	2028	U	C4-O4	-6.17	1.18	1.23
1	A	1247	A	N3-C4	-6.16	1.31	1.34
1	A	2497	A	C6-N1	-6.14	1.31	1.35
1	A	1842	G	N7-C5	-6.14	1.35	1.39
1	A	822	U	C2-O2	-6.13	1.16	1.22
1	A	1693	U	C4-O4	-6.13	1.18	1.23
1	A	362	U	C2-N3	6.11	1.42	1.37
1	A	1300	U	C3'-O3'	6.09	1.50	1.42
1	A	2286	A	N3-C4	-6.09	1.31	1.34
1	A	1021	A	N3-C4	-6.08	1.31	1.34
1	A	788	A	P-OP1	-6.06	1.38	1.49
1	A	945	A	C5-C4	6.06	1.43	1.38
1	A	608	A	N3-C4	-6.06	1.31	1.34
1	A	398	G	N7-C5	-6.05	1.35	1.39
1	A	330	A	N3-C4	-6.04	1.31	1.34
1	A	2065	C	N1-C6	-6.02	1.33	1.37
1	A	1764	G	C6-N1	-6.01	1.35	1.39
1	A	695	G	N1-C2	-6.01	1.32	1.37
1	A	1366	A	N3-C4	-6.01	1.31	1.34
1	A	584	C	N1-C6	-6.00	1.33	1.37
1	A	2032	G	C8-N7	-6.00	1.27	1.30
1	A	1187	G	N7-C5	-6.00	1.35	1.39
1	A	2599	G	N1-C2	-5.99	1.32	1.37
1	A	1698	A	N3-C4	-5.97	1.31	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2033	A	P-OP1	-5.97	1.38	1.49
1	A	2055	C	P-O5'	-5.97	1.53	1.59
1	A	69	C	N1-C6	-5.97	1.33	1.37
1	A	2641	G	N9-C8	-5.95	1.33	1.37
1	A	2432	A	N9-C4	-5.94	1.34	1.37
1	A	944	G	C6-N1	-5.92	1.35	1.39
1	A	2035	G	N9-C8	-5.91	1.33	1.37
1	A	2450	A	C6-N1	-5.90	1.31	1.35
1	A	1629	U	C4-O4	-5.89	1.19	1.23
1	A	525	U	N1-C2	-5.87	1.33	1.38
1	A	805	G	N1-C2	-5.85	1.33	1.37
1	A	1782	C	P-OP2	-5.85	1.39	1.49
1	A	2641	G	N7-C5	-5.85	1.35	1.39
1	A	2453	A	C6-N6	-5.85	1.29	1.33
1	A	972	G	C8-N7	-5.84	1.27	1.30
1	A	1287	A	C8-N7	-5.84	1.27	1.31
1	A	2764	A	N3-C4	-5.83	1.31	1.34
1	A	2445	G	P-O5'	-5.83	1.53	1.59
1	A	1210	A	N3-C4	-5.83	1.31	1.34
1	A	1753	G	N7-C5	-5.83	1.35	1.39
1	A	472	A	N3-C4	-5.82	1.31	1.34
1	A	1433	U	C2-N3	-5.82	1.33	1.37
1	A	608	A	C6-N1	-5.81	1.31	1.35
1	A	503	A	N3-C4	-5.80	1.31	1.34
1	A	2322	A	N7-C5	5.80	1.42	1.39
1	A	1393	A	N3-C4	-5.79	1.31	1.34
1	A	141	A	N9-C4	-5.78	1.34	1.37
1	A	2764	A	N9-C4	-5.78	1.34	1.37
1	A	1111	A	N9-C4	-5.78	1.34	1.37
1	A	2062	A	C5-C4	5.78	1.42	1.38
1	A	24	G	N1-C2	-5.76	1.33	1.37
1	A	113	G	N9-C4	-5.76	1.33	1.38
1	A	1107	G	N9-C4	5.76	1.42	1.38
1	A	510	C	N3-C4	-5.75	1.29	1.33
1	A	1021	A	C5-C6	-5.75	1.35	1.41
1	A	813	U	C2-N3	-5.75	1.33	1.37
1	A	197	A	C5-C6	-5.74	1.35	1.41
1	A	808	G	C8-N7	-5.74	1.27	1.30
1	A	1108	U	N1-C2	5.73	1.43	1.38
1	A	204	A	P-O5'	-5.73	1.54	1.59
1	A	1008	C	C4-C5	-5.73	1.38	1.43
1	A	2019	A	N7-C5	-5.73	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	831	G	C8-N7	-5.72	1.27	1.30
1	A	2090	G	C6-N1	-5.72	1.35	1.39
1	A	2286	A	C5-C4	5.72	1.42	1.38
1	A	196	A	C8-N7	-5.71	1.27	1.31
1	A	2346	A	N7-C5	-5.70	1.35	1.39
1	A	830	G	N7-C5	-5.69	1.35	1.39
1	A	997	G	C2-N3	-5.68	1.28	1.32
1	A	2434	A	C6-N1	-5.68	1.31	1.35
1	A	2570	G	C8-N7	-5.68	1.27	1.30
1	A	593	G	N1-C2	-5.68	1.33	1.37
1	A	2054	A	C5-C4	-5.67	1.34	1.38
1	A	90	U	C2-N3	5.67	1.41	1.37
1	A	780	G	P-OP2	-5.66	1.39	1.49
1	A	734	A	N9-C4	-5.66	1.34	1.37
1	A	2061	G	C8-N7	-5.65	1.27	1.30
1	A	2287	A	N3-C4	-5.64	1.31	1.34
1	A	1671	U	C4-O4	-5.64	1.19	1.23
1	A	675	A	N3-C4	-5.64	1.31	1.34
1	A	1782	C	P-O5'	-5.63	1.54	1.59
1	A	1773	A	C8-N7	-5.63	1.27	1.31
1	A	788	A	N7-C5	-5.62	1.35	1.39
1	A	2615	U	C2-N3	-5.62	1.33	1.37
1	A	2018	G	N1-C2	-5.62	1.33	1.37
1	A	2284	C	N1-C6	-5.62	1.33	1.37
1	A	197	A	C5-C4	-5.62	1.34	1.38
1	A	38	A	N7-C5	-5.61	1.35	1.39
1	A	1034	G	C5-C4	-5.60	1.34	1.38
1	A	208	C	N1-C6	-5.60	1.33	1.37
1	A	807	U	O3'-P	-5.59	1.54	1.61
1	A	745	G	P-OP2	-5.58	1.39	1.49
1	A	947	G	P-O5'	-5.58	1.54	1.59
1	A	2576	G	C2-N2	-5.58	1.28	1.34
1	A	2241	A	C6-N1	-5.58	1.31	1.35
1	A	429	A	C6-N1	-5.57	1.31	1.35
1	A	768	G	C6-N1	-5.57	1.35	1.39
1	A	278	A	N9-C4	5.56	1.41	1.37
1	A	1298	C	P-OP2	-5.55	1.39	1.49
1	A	2599	G	C6-N1	-5.55	1.35	1.39
1	A	105	C	N1-C6	5.55	1.40	1.37
1	A	1699	G	N1-C2	-5.55	1.33	1.37
1	A	829	A	N9-C4	-5.55	1.34	1.37
1	A	2066	C	N1-C6	-5.55	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1695	G	N7-C5	-5.54	1.35	1.39
1	A	1366	A	C5-C4	-5.53	1.34	1.38
1	A	1823	G	C6-N1	-5.51	1.35	1.39
1	A	571	A	P-OP1	-5.51	1.39	1.49
1	A	1992	G	C4'-C3'	-5.51	1.47	1.52
1	A	1027	A	N9-C8	-5.50	1.33	1.37
1	A	2207	G	N7-C5	-5.50	1.35	1.39
1	A	1160	G	N7-C5	-5.49	1.35	1.39
1	A	1122	G	N7-C5	-5.49	1.35	1.39
1	A	2249	U	C2-N3	-5.49	1.33	1.37
1	A	1256	G	P-O5'	-5.48	1.54	1.59
1	A	2286	A	N7-C5	-5.47	1.35	1.39
1	A	2612	C	P-OP1	-5.47	1.39	1.49
1	A	2621	A	N9-C4	-5.47	1.34	1.37
1	A	1954	G	N7-C5	-5.46	1.35	1.39
1	A	1672	C	N3-C4	-5.46	1.30	1.33
1	A	1786	A	C6-N1	-5.46	1.31	1.35
1	A	1971	A	C6-N1	-5.45	1.31	1.35
1	A	2335	A	C5-C6	-5.45	1.36	1.41
1	A	1649	G	C6-N1	-5.44	1.35	1.39
1	A	1762	A	C5'-C4'	-5.44	1.44	1.51
1	A	1675	C	N3-C4	-5.44	1.30	1.33
1	A	2059	A	N3-C4	-5.44	1.31	1.34
1	A	1427	A	N3-C4	5.43	1.38	1.34
1	A	2498	C	P-O5'	-5.43	1.54	1.59
1	A	2453	A	N7-C5	-5.43	1.35	1.39
1	A	135	G	C5-C4	-5.43	1.34	1.38
1	A	803	U	C2-N3	-5.43	1.33	1.37
1	A	1970	A	N3-C4	-5.43	1.31	1.34
1	A	265	A	N7-C5	-5.42	1.36	1.39
1	A	2065	C	C2-N3	-5.41	1.31	1.35
1	A	1971	A	C6-N6	-5.41	1.29	1.33
1	A	2377	A	N9-C4	-5.40	1.34	1.37
1	A	2826	A	N7-C5	-5.40	1.36	1.39
1	A	1393	A	N7-C5	-5.40	1.36	1.39
1	A	681	G	N9-C8	-5.40	1.34	1.37
1	A	775	G	N1-C2	-5.40	1.33	1.37
1	A	788	A	C8-N7	-5.39	1.27	1.31
1	A	677	A	N7-C5	-5.39	1.36	1.39
1	A	1650	G	C6-N1	-5.39	1.35	1.39
1	A	1990	C	N3-C4	-5.39	1.30	1.33
1	A	1575	C	N1-C6	-5.38	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2524	G	C6-N1	-5.38	1.35	1.39
1	A	776	G	N1-C2	-5.38	1.33	1.37
1	A	975	C	N3-C4	-5.38	1.30	1.33
1	A	27	G	N7-C5	-5.37	1.36	1.39
1	A	330	A	C5-C4	5.36	1.42	1.38
1	A	1295	C	C4-N4	-5.35	1.29	1.33
1	A	2545	G	N9-C8	-5.35	1.34	1.37
1	A	796	C	C2-O2	-5.35	1.19	1.24
1	A	489	G	C8-N7	-5.35	1.27	1.30
1	A	2740	A	C5-C4	-5.35	1.35	1.38
1	A	2542	A	C5-C6	-5.35	1.36	1.41
1	A	296	C	C2-N3	-5.35	1.31	1.35
1	A	561	G	N1-C2	-5.35	1.33	1.37
1	A	963	U	C2-N3	-5.35	1.34	1.37
1	A	1162	G	N9-C8	-5.34	1.34	1.37
1	A	1246	A	C5-C4	-5.34	1.35	1.38
1	A	2605	U	N3-C4	-5.34	1.33	1.38
1	A	2448	A	C6-N6	-5.33	1.29	1.33
1	A	2251	G	N9-C8	-5.33	1.34	1.37
1	A	2572	A	N9-C8	-5.32	1.33	1.37
1	A	517	C	C4-N4	-5.32	1.29	1.33
1	A	1985	G	C8-N7	-5.32	1.27	1.30
1	A	1977	A	N9-C8	-5.32	1.33	1.37
1	A	2508	G	P-O5'	-5.32	1.54	1.59
1	A	646	A	C5-C4	5.32	1.42	1.38
1	A	974	G	P-O5'	-5.31	1.54	1.59
1	A	2286	A	N9-C4	-5.30	1.34	1.37
1	A	1052	C	N1-C6	5.30	1.40	1.37
1	A	1204	A	C5-C4	5.30	1.42	1.38
1	A	2501	C	C2-N3	-5.30	1.31	1.35
1	A	255	A	C6-N1	-5.30	1.31	1.35
1	A	1367	A	C5-C4	-5.30	1.35	1.38
1	A	2304	G	C6-N1	5.30	1.43	1.39
1	A	2322	A	C5-C6	5.30	1.45	1.41
1	A	919	G	C2-N3	-5.29	1.28	1.32
1	A	513	A	N7-C5	-5.29	1.36	1.39
1	A	1030	G	C6-N1	-5.29	1.35	1.39
1	A	1260	G	C6-N1	-5.29	1.35	1.39
1	A	2438	U	N1-C2	-5.29	1.33	1.38
1	A	751	A	C6-N6	-5.28	1.29	1.33
1	A	1328	G	N7-C5	5.28	1.42	1.39
1	A	1611	C	N3-C4	-5.28	1.30	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	265	A	N3-C4	-5.28	1.31	1.34
1	A	2063	C	C2-O2	-5.28	1.19	1.24
1	A	271(M)	G	C2-N3	5.28	1.36	1.32
1	A	1278	A	N7-C5	-5.28	1.36	1.39
1	A	773	U	C4-O4	-5.27	1.19	1.23
1	A	1799	G	C3'-O3'	5.27	1.49	1.42
1	A	579	G	C8-N7	-5.26	1.27	1.30
1	A	1608	A	C5-C4	-5.25	1.35	1.38
1	A	1288	U	N3-C4	-5.25	1.33	1.38
1	A	1132	A	N7-C5	-5.25	1.36	1.39
1	A	808	G	O3'-P	-5.24	1.54	1.61
1	A	818	G	C6-N1	-5.24	1.35	1.39
1	A	1768	U	C2-N3	-5.23	1.34	1.37
1	A	331	A	N3-C4	-5.22	1.31	1.34
1	A	1641	A	N3-C4	-5.22	1.31	1.34
1	A	2061	G	P-OP2	-5.22	1.40	1.49
1	A	829	A	C8-N7	-5.21	1.27	1.31
1	A	330	A	C6-N1	-5.21	1.31	1.35
1	A	2641	G	C8-N7	-5.21	1.27	1.30
1	A	2581	G	P-OP1	-5.21	1.40	1.49
1	A	659	C	N1-C6	-5.21	1.34	1.37
1	A	1120	G	C6-N1	-5.20	1.35	1.39
3	D	237	GLU	CG-CD	5.20	1.59	1.51
1	A	2438	U	C4-O4	-5.19	1.19	1.23
1	A	1227	G	N1-C2	-5.19	1.33	1.37
1	A	219	G	N7-C5	-5.19	1.36	1.39
1	A	2434	A	N9-C8	-5.19	1.33	1.37
1	A	1142(A)	A	C2-N3	-5.17	1.28	1.33
1	A	573	G	C5-C4	-5.16	1.34	1.38
1	A	2442	C	C2-N3	-5.15	1.31	1.35
1	A	1352	U	C2-N3	-5.15	1.34	1.37
1	A	789	A	N7-C5	-5.14	1.36	1.39
1	A	1603	A	C8-N7	-5.14	1.27	1.31
1	A	2034	U	O3'-P	-5.14	1.54	1.61
1	A	1031	G	N1-C2	-5.13	1.33	1.37
1	A	1383	C	C2-N3	5.13	1.39	1.35
1	A	1268	A	N3-C4	-5.13	1.31	1.34
1	A	2032	G	C5-C4	-5.12	1.34	1.38
1	A	2505	G	C6-O6	-5.12	1.19	1.24
1	A	385	C	N1-C6	-5.12	1.34	1.37
1	A	752	A	C3'-O3'	5.12	1.49	1.42
1	A	1265	A	N3-C4	-5.12	1.31	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	684	G	C6-N1	-5.12	1.35	1.39
1	A	2007	C	P-O5'	-5.12	1.54	1.59
18	W	92	ARG	CZ-NH2	5.11	1.39	1.33
1	A	2791	C	N1-C2	5.11	1.45	1.40
1	A	383	U	C4-O4	5.11	1.27	1.23
1	A	393	C	C2-O2	-5.11	1.19	1.24
1	A	801	G	N9-C8	-5.11	1.34	1.37
1	A	1627	G	C8-N7	-5.11	1.27	1.30
28	6	16	CYS	CB-SG	-5.11	1.73	1.81
1	A	1046	A	N9-C4	5.10	1.41	1.37
1	A	775	G	C8-N7	-5.09	1.27	1.30
1	A	2547	U	N1-C2	-5.09	1.33	1.38
1	A	1031	G	C5-C4	-5.08	1.34	1.38
1	A	1045	A	N3-C4	5.08	1.38	1.34
1	A	532	A	C5-C6	-5.08	1.36	1.41
1	A	1013	C	C4-C5	-5.08	1.38	1.43
1	A	1770	G	N3-C4	-5.08	1.31	1.35
1	A	2454	G	C5-C4	-5.08	1.34	1.38
1	A	527	C	C2-O2	-5.07	1.19	1.24
1	A	229	A	N9-C4	5.06	1.40	1.37
1	A	1675	C	C4-C5	-5.05	1.39	1.43
1	A	2872	G	N1-C2	-5.05	1.33	1.37
1	A	1668	A	N3-C4	-5.05	1.31	1.34
1	A	1799	G	N9-C4	5.05	1.42	1.38
1	A	786	C	P-OP2	-5.05	1.40	1.49
1	A	1128	A	C8-N7	5.05	1.35	1.31
1	A	2274	A	C8-N7	-5.05	1.28	1.31
1	A	2599	G	C6-O6	-5.05	1.19	1.24
1	A	2007	C	N3-C4	-5.04	1.30	1.33
1	A	1890	A	N9-C4	-5.04	1.34	1.37
1	A	2729	G	C6-N1	-5.04	1.36	1.39
1	A	1266	G	C5-C6	-5.03	1.37	1.42
1	A	1676	A	N9-C4	-5.03	1.34	1.37
1	A	1649	G	N9-C8	-5.03	1.34	1.37
1	A	1696	G	P-O5'	-5.03	1.54	1.59
1	A	819	A	N9-C4	-5.03	1.34	1.37
1	A	85	G	C6-N1	-5.02	1.36	1.39
1	A	2054	A	C8-N7	-5.02	1.28	1.31
1	A	2598	A	N3-C4	-5.02	1.31	1.34
1	A	2242	G	O3'-P	-5.02	1.55	1.61
1	A	945	A	N1-C2	5.02	1.38	1.34
18	W	20	VAL	CB-CG2	-5.02	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	839	U	C2-N3	-5.02	1.34	1.37
1	A	182	A	P-O5'	-5.01	1.54	1.59
1	A	454	A	N7-C5	-5.01	1.36	1.39
1	A	2627	G	N7-C5	-5.00	1.36	1.39
1	A	1256	G	O3'-P	-5.00	1.55	1.61
1	A	2599	G	C5-C4	-5.00	1.34	1.38

All (2231) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2296	U	N3-C4-O4	-24.74	102.08	119.40
1	A	1021	A	C2-N3-C4	-23.74	98.73	110.60
1	A	2296	U	C2-N3-C4	-23.58	112.85	127.00
1	A	945	A	C5-N7-C8	-23.44	92.18	103.90
1	A	2335	A	C5-C6-N1	22.23	128.81	117.70
1	A	2287	A	C2-N3-C4	-20.28	100.46	110.60
1	A	2296	U	C5-C6-N1	-19.95	112.72	122.70
1	A	528	A	C2-N3-C4	-18.89	101.16	110.60
1	A	945	A	C4-C5-N7	18.60	120.00	110.70
1	A	330	A	C2-N3-C4	-18.41	101.39	110.60
1	A	528	A	N3-C4-C5	18.06	139.44	126.80
1	A	1653	G	C8-N9-C4	-17.58	99.37	106.40
1	A	945	A	C2-N3-C4	-17.43	101.89	110.60
1	A	1142(A)	A	C2-N3-C4	-17.22	101.99	110.60
1	A	2322	A	C6-N1-C2	-16.87	108.48	118.60
1	A	528	A	N3-C4-N9	-16.19	114.45	127.40
1	A	945	A	N7-C8-N9	16.04	121.82	113.80
1	A	2296	U	N1-C2-N3	15.85	124.41	114.90
1	A	2296	U	C5-C4-O4	15.84	135.40	125.90
1	A	2322	A	C5-C6-N1	15.84	125.62	117.70
1	A	933	A	C5-N7-C8	-15.26	96.27	103.90
1	A	2296	U	C2-N1-C1'	-15.05	99.64	117.70
1	A	2286	A	N7-C8-N9	14.71	121.15	113.80
1	A	2296	U	N3-C2-O2	-14.70	111.91	122.20
1	A	141	A	N7-C8-N9	14.69	121.14	113.80
1	A	2286	A	C8-N9-C4	-14.50	100.00	105.80
1	A	2287	A	N3-C4-C5	14.48	136.94	126.80
1	A	141	A	C5-N7-C8	-14.37	96.72	103.90
1	A	945	A	N1-C6-N6	14.22	127.13	118.60
1	A	1021	A	N3-C4-C5	13.88	136.52	126.80
1	A	933	A	N7-C8-N9	13.73	120.67	113.80
1	A	1698	A	C5-N7-C8	-13.69	97.06	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	568	U	C5-C4-O4	-13.63	117.72	125.90
1	A	856	C	C6-N1-C2	-13.47	114.91	120.30
1	A	1142(A)	A	C5-N7-C8	-13.46	97.17	103.90
1	A	961	C	C2-N3-C4	-13.23	113.28	119.90
1	A	2296	U	N3-C4-C5	13.18	122.51	114.60
1	A	945	A	C6-C5-N7	-13.14	123.10	132.30
1	A	1142(A)	A	N3-C4-N9	-13.11	116.92	127.40
1	A	1142(A)	A	N3-C4-C5	13.04	135.93	126.80
1	A	2312	U	N3-C2-O2	-13.00	113.10	122.20
1	A	1204	A	C2-N3-C4	-12.98	104.11	110.60
1	A	1372	U	C5-C4-O4	-12.80	118.22	125.90
1	A	1204	A	C5-N7-C8	-12.70	97.55	103.90
1	A	2286	A	C5-N7-C8	-12.69	97.56	103.90
1	A	2335	A	C6-N1-C2	-12.68	110.99	118.60
1	A	1021	A	C5-N7-C8	-12.66	97.57	103.90
1	A	528	A	C5-N7-C8	-12.65	97.58	103.90
1	A	1021	A	C5-C6-N1	-12.54	111.43	117.70
1	A	1698	A	C2-N3-C4	-12.41	104.39	110.60
1	A	1142(A)	A	C5-C6-N1	-12.39	111.50	117.70
1	A	2866	U	C5-C6-N1	-12.38	116.51	122.70
1	A	1021	A	N3-C4-N9	-12.36	117.51	127.40
1	A	847	U	C5-C6-N1	-12.35	116.53	122.70
1	A	278	A	C6-N1-C2	-12.35	111.19	118.60
1	A	2322	A	N1-C6-N6	-12.31	111.22	118.60
1	A	141	A	C8-N9-C4	-12.26	100.90	105.80
1	A	568	U	N3-C4-C5	12.24	121.94	114.60
1	A	2286	A	C2-N3-C4	-12.18	104.51	110.60
20	Y	2	ARG	NE-CZ-NH2	-12.13	114.24	120.30
1	A	1140	C	C6-N1-C2	-12.04	115.48	120.30
1	A	265	A	C5-N7-C8	-11.90	97.95	103.90
1	A	330	A	N1-C2-N3	11.82	135.21	129.30
1	A	966	G	C5-C6-O6	11.74	135.65	128.60
1	A	945	A	C8-N9-C4	-11.71	101.11	105.80
1	A	530	G	C5-N7-C8	-11.65	98.48	104.30
1	A	527	C	N1-C2-N3	11.63	127.34	119.20
1	A	1653	G	N9-C4-C5	11.56	110.02	105.40
1	A	2287	A	N3-C4-N9	-11.54	118.17	127.40
1	A	330	A	C5-N7-C8	-11.51	98.14	103.90
1	A	1698	A	N7-C8-N9	11.48	119.54	113.80
1	A	530	G	N3-C4-N9	-11.47	119.11	126.00
1	A	2335	A	C5-C6-N6	-11.41	114.57	123.70
1	A	945	A	N3-C4-C5	11.40	134.78	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2454	G	N1-C6-O6	-11.37	113.08	119.90
1	A	1203	G	C8-N9-C4	-11.31	101.88	106.40
1	A	2866	U	C5-C4-O4	11.26	132.66	125.90
1	A	528	A	C6-N1-C2	11.21	125.33	118.60
1	A	568	U	C2-N3-C4	-11.17	120.30	127.00
1	A	527	C	C5-C4-N4	11.16	128.01	120.20
1	A	2286	A	N1-C2-N3	10.95	134.77	129.30
1	A	2296	U	C6-N1-C1'	10.93	136.50	121.20
1	A	527	C	C4-C5-C6	10.88	122.84	117.40
1	A	847	U	C2-N1-C1'	-10.87	104.65	117.70
5	F	74	ARG	NE-CZ-NH1	10.85	125.72	120.30
1	A	729	G	C8-N9-C4	-10.81	102.08	106.40
1	A	1383	C	N1-C2-O2	-10.78	112.43	118.90
1	A	265	A	N7-C8-N9	10.76	119.18	113.80
1	A	2065	C	N3-C2-O2	-10.74	114.38	121.90
1	A	1939	U	N3-C4-C5	10.73	121.04	114.60
1	A	966	G	N1-C6-O6	-10.68	113.49	119.90
1	A	1653	G	N7-C8-N9	10.68	118.44	113.10
1	A	1108	U	N3-C2-O2	-10.59	114.79	122.20
1	A	2312	U	C6-N1-C2	-10.54	114.67	121.00
1	A	1698	A	C8-N9-C4	-10.53	101.59	105.80
1	A	933	A	C8-N9-C4	-10.49	101.60	105.80
1	A	1108	U	N1-C2-O2	10.42	130.09	122.80
1	A	265	A	C8-N9-C4	-10.29	101.69	105.80
1	A	1021	A	N1-C2-N3	10.24	134.42	129.30
1	A	530	G	N3-C4-C5	10.23	133.71	128.60
1	A	2866	U	N3-C4-O4	-10.19	112.26	119.40
1	A	1695	G	C8-N9-C4	-10.17	102.33	106.40
1	A	2495	G	C5-C6-N1	-10.17	106.42	111.50
1	A	2287	A	C5-C6-N1	-10.16	112.62	117.70
1	A	1678	G	N3-C4-C5	-10.13	123.54	128.60
1	A	2497	A	N1-C6-N6	-10.10	112.54	118.60
1	A	2700	C	C6-N1-C2	10.09	124.34	120.30
1	A	528	A	C4-C5-C6	-10.06	111.97	117.00
1	A	1204	A	N7-C8-N9	10.06	118.83	113.80
1	A	1300	U	N3-C2-O2	-10.04	115.17	122.20
1	A	2322	A	C2-N3-C4	10.02	115.61	110.60
1	A	1303	G	N1-C6-O6	-10.00	113.90	119.90
1	A	1204	A	C6-C5-N7	-9.99	125.31	132.30
1	A	265	A	C2-N3-C4	-9.99	105.61	110.60
1	A	2233	U	N1-C2-N3	9.96	120.88	114.90
1	A	1303	G	C5-C6-O6	9.95	134.57	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	330	A	N3-C4-N9	-9.94	119.45	127.40
1	A	1253	A	C2-N3-C4	9.92	115.56	110.60
1	A	1204	A	C4-C5-N7	9.90	115.65	110.70
1	A	1939	U	C4-C5-C6	-9.89	113.76	119.70
1	A	1782	C	C6-N1-C2	9.87	124.25	120.30
1	A	2286	A	C6-C5-N7	-9.87	125.39	132.30
1	A	530	G	C4-C5-N7	9.86	114.74	110.80
1	A	1254	A	C8-N9-C4	-9.83	101.87	105.80
1	A	1142(A)	A	N7-C8-N9	9.81	118.71	113.80
1	A	2226	C	C6-N1-C2	9.79	124.22	120.30
1	A	2287	A	C5-N7-C8	-9.79	99.01	103.90
1	A	330	A	N3-C4-C5	9.78	133.65	126.80
1	A	1678	G	C6-N1-C2	-9.75	119.25	125.10
1	A	1934	C	C5-C6-N1	-9.74	116.13	121.00
1	A	961	C	N1-C2-O2	-9.71	113.08	118.90
1	A	915	C	N3-C2-O2	-9.70	115.11	121.90
1	A	1372	U	N3-C4-O4	9.69	126.19	119.40
1	A	2027	G	C2-N3-C4	9.68	116.74	111.90
1	A	1204	A	N1-C2-N3	9.67	134.14	129.30
1	A	530	G	C8-N9-C4	-9.67	102.53	106.40
1	A	2105	C	C6-N1-C2	-9.64	116.44	120.30
1	A	565	C	C6-N1-C2	-9.61	116.45	120.30
1	A	2006	C	C6-N1-C2	-9.56	116.48	120.30
1	A	528	A	C5-C6-N1	-9.55	112.93	117.70
1	A	328	U	N3-C2-O2	-9.52	115.53	122.20
1	A	2036	C	N1-C2-O2	-9.51	113.19	118.90
1	A	223	A	C8-N9-C4	-9.51	102.00	105.80
1	A	1305	C	N3-C2-O2	-9.49	115.25	121.90
1	A	528	A	C4-C5-N7	9.45	115.42	110.70
1	A	481	G	C8-N9-C4	-9.41	102.64	106.40
1	A	1678	G	N9-C4-C5	9.39	109.15	105.40
1	A	2137	C	N3-C2-O2	-9.38	115.33	121.90
5	F	74	ARG	NE-CZ-NH2	-9.38	115.61	120.30
1	A	2437	U	N3-C2-O2	-9.38	115.64	122.20
1	A	2312	U	N1-C2-O2	9.32	129.33	122.80
1	A	1698	A	N3-C4-N9	-9.29	119.97	127.40
1	A	2609	U	C2-N3-C4	-9.29	121.43	127.00
1	A	847	U	N1-C2-N3	9.23	120.44	114.90
20	Y	2	ARG	NE-CZ-NH1	9.23	124.91	120.30
1	A	1200	C	C5-C6-N1	-9.22	116.39	121.00
1	A	2137	C	N1-C2-O2	9.13	124.38	118.90
1	A	1678	G	C8-N9-C4	-9.12	102.75	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	614	U	N3-C2-O2	-9.07	115.85	122.20
1	A	271(M)	G	N3-C4-N9	9.03	131.42	126.00
1	A	1963	U	C2-N1-C1'	9.01	128.51	117.70
1	A	2028	U	C6-N1-C2	9.00	126.40	121.00
1	A	944	G	C5-C6-O6	9.00	134.00	128.60
1	A	915	C	N1-C2-O2	8.96	124.28	118.90
1	A	943	U	C5-C4-O4	8.95	131.27	125.90
1	A	1346	G	N1-C6-O6	-8.95	114.53	119.90
1	A	2322	A	N9-C4-C5	8.93	109.37	105.80
1	A	2440	C	C6-N1-C2	8.92	123.87	120.30
1	A	2430	A	C8-N9-C4	-8.92	102.23	105.80
1	A	1383	C	N3-C2-O2	8.91	128.13	121.90
1	A	1618	A	N9-C4-C5	8.91	109.36	105.80
1	A	1223	G	N1-C6-O6	-8.90	114.56	119.90
1	A	803	U	N3-C2-O2	-8.88	115.99	122.20
1	A	1305	C	N1-C2-O2	8.88	124.23	118.90
1	A	1107	G	N3-C4-N9	8.84	131.30	126.00
1	A	1678	G	C4-C5-N7	-8.82	107.27	110.80
1	A	2453	A	C2-N3-C4	8.82	115.01	110.60
1	A	622	G	N1-C6-O6	-8.81	114.61	119.90
1	A	139(A)	G	C5-C6-O6	-8.81	123.32	128.60
1	A	622	G	C5-C6-O6	8.80	133.88	128.60
1	A	1203	G	N9-C4-C5	8.80	108.92	105.40
1	A	933	A	C2-N3-C4	-8.79	106.21	110.60
1	A	2318	G	C5-N7-C8	8.78	108.69	104.30
1	A	582	G	N1-C6-O6	-8.77	114.64	119.90
1	A	1962	C	C5-C6-N1	8.77	125.38	121.00
1	A	1359	A	C2-N3-C4	8.76	114.98	110.60
1	A	1944	U	C2-N3-C4	-8.76	121.74	127.00
2	B	91	C	C6-N1-C2	8.74	123.80	120.30
1	A	753	C	N1-C2-O2	8.72	124.13	118.90
1	A	933	A	C4-C5-N7	8.69	115.04	110.70
1	A	1359	A	N1-C2-N3	-8.68	124.96	129.30
1	A	945	A	N3-C4-N9	-8.67	120.46	127.40
1	A	479	A	N1-C6-N6	-8.67	113.40	118.60
1	A	1295	C	N3-C4-C5	8.66	125.36	121.90
1	A	1254	A	N7-C8-N9	8.65	118.12	113.80
1	A	1956	U	C2-N3-C4	-8.64	121.82	127.00
1	A	508	G	N1-C6-O6	8.63	125.08	119.90
1	A	1649	G	N1-C6-O6	-8.60	114.74	119.90
1	A	2304	G	C5-C6-N1	8.60	115.80	111.50
1	A	961	C	N3-C4-C5	8.58	125.33	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1698	A	N3-C4-C5	8.57	132.80	126.80
1	A	1049	C	C5-C6-N1	8.55	125.28	121.00
1	A	1678	G	N1-C2-N3	8.55	129.03	123.90
1	A	141	A	C4-C5-N7	8.55	114.97	110.70
1	A	139	G	C2-N3-C4	8.54	116.17	111.90
1	A	1928	A	C8-N9-C4	-8.54	102.39	105.80
1	A	1188	U	N3-C4-O4	-8.53	113.43	119.40
1	A	2388	A	C8-N9-C4	-8.53	102.39	105.80
1	A	205	G	C8-N9-C4	8.52	109.81	106.40
1	A	1248	G	C4-C5-N7	8.50	114.20	110.80
1	A	915	C	C6-N1-C2	-8.49	116.90	120.30
1	A	565	C	N3-C4-C5	-8.49	118.50	121.90
1	A	587	C	C6-N1-C2	-8.47	116.91	120.30
1	A	1107	G	C4-N9-C1'	8.46	137.50	126.50
1	A	2103	C	C2-N3-C4	8.46	124.13	119.90
1	A	1801	G	N1-C6-O6	8.46	124.97	119.90
1	A	265	A	C4-C5-N7	8.45	114.93	110.70
1	A	1609	A	N7-C8-N9	-8.45	109.58	113.80
1	A	1653	G	N3-C4-C5	-8.44	124.38	128.60
1	A	774	A	C2-N3-C4	8.43	114.82	110.60
1	A	527	C	N3-C2-O2	-8.41	116.01	121.90
1	A	1558	A	C2-N3-C4	-8.41	106.39	110.60
1	A	635	C	C6-N1-C2	-8.38	116.95	120.30
1	A	2206	G	N3-C4-C5	8.36	132.78	128.60
1	A	278	A	C5-C6-N6	-8.35	117.02	123.70
1	A	298	G	C5-C6-O6	8.33	133.60	128.60
1	A	2287	A	N1-C6-N6	8.33	123.59	118.60
1	A	1743	C	N1-C2-O2	-8.32	113.91	118.90
1	A	1021	A	N7-C8-N9	8.32	117.96	113.80
1	A	2312	U	C2-N1-C1'	8.32	127.68	117.70
1	A	2503	A	N1-C2-N3	-8.32	125.14	129.30
1	A	673	C	N3-C4-C5	8.32	125.23	121.90
1	A	1346	G	C5-C6-O6	8.31	133.59	128.60
1	A	330	A	N7-C8-N9	8.31	117.96	113.80
1	A	1672	C	C5-C6-N1	-8.30	116.85	121.00
1	A	527	C	C5-C6-N1	-8.30	116.85	121.00
1	A	1107	G	N3-C4-C5	-8.30	124.45	128.60
1	A	584	C	C5-C4-N4	-8.29	114.40	120.20
1	A	530	G	C4-C5-C6	-8.28	113.83	118.80
1	A	139(A)	G	N7-C8-N9	8.28	117.24	113.10
1	A	2335	A	C4-C5-C6	-8.27	112.86	117.00
1	A	1814	G	N1-C6-O6	-8.27	114.94	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2501	C	C5-C6-N1	-8.26	116.87	121.00
1	A	528	A	C8-N9-C1'	8.26	142.57	127.70
1	A	2825	C	C5-C6-N1	-8.25	116.87	121.00
1	A	822	U	N3-C2-O2	-8.23	116.44	122.20
1	A	981	A	C2-N3-C4	8.22	114.71	110.60
1	A	531	C	C2-N3-C4	-8.22	115.79	119.90
1	A	565	C	C4-C5-C6	8.22	121.51	117.40
2	B	20	C	C5-C4-N4	-8.21	114.45	120.20
1	A	2074	U	N1-C2-N3	8.20	119.82	114.90
1	A	2246	G	C5-C6-N1	8.20	115.60	111.50
1	A	847	U	C6-N1-C1'	8.19	132.66	121.20
1	A	2613	U	N3-C4-C5	8.19	119.51	114.60
1	A	2304	G	N9-C4-C5	8.18	108.67	105.40
1	A	2078	C	C6-N1-C2	-8.16	117.03	120.30
1	A	1203	G	C5-C6-O6	8.16	133.50	128.60
1	A	195	A	C5-N7-C8	8.15	107.97	103.90
1	A	362	U	C2-N3-C4	-8.14	122.12	127.00
1	A	732	C	C6-N1-C2	-8.13	117.05	120.30
1	A	1698	A	C5-C6-N1	-8.13	113.63	117.70
1	A	1618	A	N1-C6-N6	-8.13	113.72	118.60
1	A	1573	G	C8-N9-C4	8.12	109.65	106.40
1	A	2200	C	N3-C2-O2	-8.11	116.23	121.90
1	A	527	C	C6-N1-C2	-8.10	117.06	120.30
1	A	2230	G	N3-C2-N2	-8.10	114.23	119.90
1	A	933	A	C5-C6-N1	-8.10	113.65	117.70
1	A	585	G	C6-N1-C2	-8.09	120.25	125.10
1	A	1428	C	N1-C2-O2	-8.07	114.06	118.90
1	A	2236	C	C5-C6-N1	-8.07	116.96	121.00
1	A	1200	C	N3-C4-N4	-8.06	112.36	118.00
1	A	650	C	C6-N1-C2	-8.06	117.08	120.30
1	A	1782	C	C5-C6-N1	-8.06	116.97	121.00
1	A	2318	G	C4-C5-N7	-8.05	107.58	110.80
1	A	2609	U	C5-C6-N1	-8.05	118.67	122.70
1	A	646	A	C8-N9-C4	-8.05	102.58	105.80
1	A	933	A	C6-C5-N7	-8.05	126.67	132.30
1	A	1962	C	C4-C5-C6	-8.05	113.38	117.40
1	A	1111	A	N1-C6-N6	8.04	123.42	118.60
1	A	1045	A	C2-N3-C4	8.02	114.61	110.60
1	A	139(A)	G	C4-C5-N7	8.01	114.00	110.80
1	A	2015	A	C8-N9-C4	8.01	109.00	105.80
1	A	1311	G	N1-C6-O6	-8.01	115.10	119.90
23	1	21	ARG	NE-CZ-NH1	8.00	124.30	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2028	U	N3-C4-C5	8.00	119.40	114.60
1	A	2335	A	C4-C5-N7	7.99	114.69	110.70
1	A	2558	C	N3-C4-C5	7.99	125.09	121.90
1	A	2319	G	N7-C8-N9	7.98	117.09	113.10
1	A	847	U	C2-N3-C4	-7.95	122.23	127.00
1	A	2593	U	N3-C2-O2	-7.95	116.64	122.20
1	A	2287	A	C4-C5-N7	7.94	114.67	110.70
1	A	2825	C	C4-C5-C6	7.92	121.36	117.40
1	A	571	A	N9-C4-C5	-7.92	102.63	105.80
1	A	2713	A	C2-N3-C4	7.91	114.56	110.60
1	A	2065	C	N1-C2-O2	7.91	123.65	118.90
1	A	2237	G	N1-C2-N2	-7.91	109.08	116.20
1	A	1035	U	C5-C6-N1	-7.91	118.75	122.70
1	A	2304	G	C6-N1-C2	-7.90	120.36	125.10
1	A	2303	G	C4-C5-N7	-7.90	107.64	110.80
1	A	944	G	C8-N9-C4	-7.90	103.24	106.40
1	A	2206	G	C8-N9-C4	7.90	109.56	106.40
1	A	2585	U	C2-N1-C1'	7.90	127.18	117.70
1	A	961	C	C5-C4-N4	-7.88	114.69	120.20
1	A	429	A	N1-C6-N6	-7.87	113.88	118.60
1	A	2454	G	C5-C6-N1	7.87	115.43	111.50
1	A	1678	G	N3-C2-N2	-7.86	114.40	119.90
1	A	970	C	N1-C2-O2	-7.86	114.18	118.90
1	A	1998	G	C5-C6-O6	7.86	133.32	128.60
1	A	298	G	N1-C6-O6	-7.86	115.19	119.90
1	A	2319	G	C8-N9-C4	-7.85	103.26	106.40
1	A	986	C	N1-C2-O2	-7.85	114.19	118.90
1	A	530	G	N7-C8-N9	7.83	117.02	113.10
1	A	847	U	C5-C4-O4	7.83	130.60	125.90
1	A	944	G	N1-C6-O6	-7.83	115.20	119.90
1	A	1586	A	N1-C6-N6	-7.83	113.90	118.60
1	A	2491	U	N3-C4-C5	7.83	119.30	114.60
1	A	1187	G	N3-C2-N2	7.83	125.38	119.90
1	A	2879	C	N1-C2-O2	-7.83	114.20	118.90
1	A	2312	U	C5-C6-N1	7.82	126.61	122.70
1	A	2200	C	N1-C2-O2	7.81	123.59	118.90
1	A	1764	G	C5-C6-O6	7.81	133.29	128.60
1	A	90	U	C5-C6-N1	7.79	126.60	122.70
1	A	677	A	C5-C6-N6	7.79	129.93	123.70
1	A	2545	G	C5-C6-O6	-7.78	123.93	128.60
1	A	1934	C	C6-N1-C2	7.77	123.41	120.30
1	A	1992	G	C8-N9-C4	-7.77	103.29	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	G	N1-C6-O6	-7.77	115.24	119.90
1	A	1698	A	C4-C5-N7	7.76	114.58	110.70
1	A	2645	G	N3-C4-N9	-7.76	121.34	126.00
1	A	1672	C	C2-N3-C4	-7.75	116.02	119.90
1	A	729	G	N7-C8-N9	7.75	116.98	113.10
1	A	614	U	C5-C4-O4	7.75	130.55	125.90
1	A	1223	G	C5-C6-O6	7.75	133.25	128.60
1	A	132	G	C4-C5-N7	-7.74	107.70	110.80
1	A	649	G	N1-C6-O6	-7.72	115.27	119.90
1	A	2585	U	C6-N1-C1'	-7.71	110.40	121.20
1	A	271(M)	G	C4-N9-C1'	7.71	136.52	126.50
1	A	1126	A	N1-C6-N6	7.69	123.21	118.60
1	A	2303	G	N9-C4-C5	7.68	108.47	105.40
1	A	2512	C	C2-N3-C4	-7.67	116.06	119.90
1	A	2552	U	N1-C2-O2	-7.67	117.43	122.80
1	A	847	U	N3-C4-O4	-7.67	114.03	119.40
1	A	943	U	N3-C2-O2	-7.67	116.83	122.20
1	A	1200	C	C2-N3-C4	-7.66	116.07	119.90
1	A	2249	U	N3-C4-C5	7.66	119.20	114.60
1	A	1050	A	C8-N9-C4	-7.66	102.73	105.80
1	A	2791	C	C2-N1-C1'	7.66	127.22	118.80
1	A	2609	U	N1-C2-N3	7.65	119.49	114.90
1	A	204	A	C2-N3-C4	7.65	114.42	110.60
1	A	944	G	N7-C8-N9	7.65	116.92	113.10
1	A	1230	C	C5-C6-N1	-7.65	117.18	121.00
1	A	1878	G	N1-C6-O6	7.65	124.49	119.90
1	A	2319	G	C5-N7-C8	-7.63	100.48	104.30
29	7	39	ARG	NE-CZ-NH2	-7.63	116.48	120.30
1	A	2228	G	N1-C6-O6	-7.63	115.32	119.90
1	A	571	A	N1-C2-N3	-7.62	125.49	129.30
1	A	2062	A	C5-C6-N1	-7.61	113.89	117.70
1	A	420	C	N3-C4-N4	-7.61	112.67	118.00
1	A	2866	U	C4-C5-C6	7.60	124.26	119.70
1	A	1109	C	C4-C5-C6	7.60	121.20	117.40
1	A	1776	G	N3-C4-N9	7.60	130.56	126.00
14	S	96	GLY	N-CA-C	-7.58	94.14	113.10
1	A	271(M)	G	C8-N9-C1'	-7.58	117.15	127.00
1	A	2322	A	C4-C5-N7	-7.57	106.91	110.70
1	A	1757	U	C5-C6-N1	-7.57	118.92	122.70
1	A	2646	C	C6-N1-C2	7.57	123.33	120.30
1	A	2033	A	N1-C6-N6	-7.55	114.07	118.60
1	A	1109	C	N3-C4-C5	-7.55	118.88	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1123	C	N3-C4-C5	7.54	124.92	121.90
1	A	1475	G	N3-C4-N9	-7.54	121.48	126.00
1	A	141	A	C6-C5-N7	-7.53	127.03	132.30
1	A	614	U	N1-C2-N3	7.53	119.42	114.90
1	A	1488	G	C8-N9-C4	-7.52	103.39	106.40
1	A	205	G	N9-C4-C5	-7.52	102.39	105.40
1	A	527	C	N3-C4-C5	-7.52	118.89	121.90
1	A	113	G	N3-C4-N9	-7.52	121.49	126.00
1	A	1959	G	C8-N9-C4	-7.51	103.39	106.40
1	A	2286	A	C4-C5-C6	7.51	120.75	117.00
1	A	1108	U	C2-N1-C1'	7.50	126.70	117.70
1	A	1261	C	C2-N3-C4	-7.50	116.15	119.90
1	A	2056	G	N9-C4-C5	-7.50	102.40	105.40
1	A	2040	C	C6-N1-C2	7.50	123.30	120.30
1	A	2051	A	C5-N7-C8	7.49	107.65	103.90
1	A	278	A	N1-C2-N3	7.49	133.04	129.30
1	A	746	A	C2-N3-C4	7.49	114.34	110.60
1	A	2270	G	C5-C6-O6	-7.47	124.12	128.60
1	A	139(A)	G	C5-C6-N1	7.46	115.23	111.50
1	A	208	C	C5-C4-N4	-7.45	114.98	120.20
1	A	1695	G	N7-C8-N9	7.45	116.83	113.10
1	A	1764	G	N1-C6-O6	-7.44	115.44	119.90
1	A	652(H)	C	C5-C6-N1	7.44	124.72	121.00
1	A	1745	C	N3-C2-O2	7.43	127.10	121.90
1	A	278	A	C5-C6-N1	7.43	121.42	117.70
1	A	565	C	N1-C2-N3	7.43	124.40	119.20
1	A	2191	G	N1-C6-O6	7.42	124.36	119.90
1	A	1347	G	C8-N9-C4	-7.42	103.43	106.40
1	A	2375	G	C5-C6-O6	-7.41	124.15	128.60
1	A	681	G	C4-C5-N7	-7.41	107.84	110.80
1	A	1801	G	C5-C6-O6	-7.40	124.16	128.60
1	A	330	A	C8-N9-C4	-7.39	102.84	105.80
1	A	409	C	C6-N1-C2	7.38	123.25	120.30
1	A	776	G	C8-N9-C4	-7.36	103.45	106.40
1	A	481	G	N3-C4-C5	-7.36	124.92	128.60
1	A	1934	C	C4-C5-C6	7.36	121.08	117.40
1	A	508	G	C5-C6-O6	-7.35	124.19	128.60
1	A	1524	G	C6-C5-N7	7.34	134.81	130.40
1	A	141	A	C2-N3-C4	-7.34	106.93	110.60
1	A	139(A)	G	N3-C4-N9	7.34	130.40	126.00
1	A	253	C	N3-C2-O2	-7.33	116.77	121.90
1	A	746	A	N1-C2-N3	-7.33	125.64	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1142(A)	A	C6-N1-C2	7.33	123.00	118.60
1	A	313	C	N1-C2-O2	-7.30	114.52	118.90
1	A	2322	A	C6-C5-N7	7.30	137.41	132.30
1	A	563	G	C5-C6-O6	-7.30	124.22	128.60
1	A	2701	C	N1-C2-O2	-7.29	114.52	118.90
1	A	839	U	C5-C4-O4	7.29	130.27	125.90
1	A	1475	G	N3-C2-N2	-7.29	114.80	119.90
1	A	1021	A	N1-C6-N6	7.29	122.97	118.60
1	A	2000	G	C8-N9-C4	-7.28	103.49	106.40
1	A	2510	C	C6-N1-C2	-7.28	117.39	120.30
1	A	763	G	N3-C2-N2	7.28	125.00	119.90
1	A	236	C	C6-N1-C2	7.28	123.21	120.30
1	A	583	G	N3-C2-N2	7.27	124.99	119.90
1	A	2074	U	N1-C2-O2	-7.27	117.71	122.80
1	A	2866	U	C2-N3-C4	-7.26	122.64	127.00
1	A	1792	G	C2-N3-C4	-7.26	108.27	111.90
1	A	2493	U	N3-C4-C5	7.26	118.95	114.60
1	A	539	G	N1-C6-O6	-7.25	115.55	119.90
1	A	2028	U	C5-C6-N1	-7.24	119.08	122.70
1	A	2745	C	C6-N1-C2	-7.24	117.40	120.30
1	A	2714	G	C5-C6-O6	-7.23	124.26	128.60
1	A	2137	C	C6-N1-C2	-7.22	117.41	120.30
1	A	2461	C	C6-N1-C2	-7.22	117.41	120.30
1	A	1266	G	C4-C5-N7	7.22	113.69	110.80
1	A	1774	C	N1-C2-O2	-7.22	114.57	118.90
1	A	72	U	C5-C4-O4	-7.21	121.58	125.90
1	A	745	G	N3-C2-N2	-7.21	114.85	119.90
1	A	1787	A	N9-C4-C5	-7.21	102.92	105.80
1	A	139(A)	G	C2-N3-C4	7.21	115.50	111.90
1	A	1261	C	C5-C6-N1	-7.21	117.40	121.00
1	A	1212	G	N1-C6-O6	7.21	124.22	119.90
1	A	236	C	N3-C4-C5	7.20	124.78	121.90
1	A	193	U	N1-C2-O2	-7.20	117.76	122.80
1	A	1558	A	N1-C2-N3	7.20	132.90	129.30
1	A	2430	A	N7-C8-N9	7.20	117.40	113.80
1	A	2872	G	C5-C6-O6	7.20	132.92	128.60
1	A	1131	G	N3-C2-N2	7.19	124.94	119.90
1	A	2467	C	C6-N1-C2	-7.19	117.42	120.30
1	A	1142(A)	A	C8-N9-C4	-7.18	102.93	105.80
1	A	1792	G	C5-C6-O6	7.18	132.91	128.60
1	A	1992	G	P-O3'-C3'	7.18	128.31	119.70
1	A	793	A	N1-C2-N3	-7.17	125.71	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2017	U	N3-C2-O2	-7.17	117.18	122.20
1	A	462	C	C6-N1-C2	-7.16	117.44	120.30
1	A	1343	G	N1-C6-O6	-7.16	115.60	119.90
1	A	1107	G	C8-N9-C1'	-7.16	117.69	127.00
1	A	1939	U	N3-C4-O4	-7.15	114.40	119.40
1	A	2579	C	N3-C4-C5	7.15	124.76	121.90
1	A	2286	A	C5-C6-N1	-7.14	114.13	117.70
1	A	1162	G	C4-C5-N7	-7.14	107.94	110.80
1	A	2437	U	N1-C2-N3	7.14	119.19	114.90
1	A	2371	G	C5-C6-N1	7.14	115.07	111.50
1	A	546	C	C2-N1-C1'	7.13	126.65	118.80
1	A	1650	G	N1-C6-O6	-7.13	115.62	119.90
1	A	460	A	C2-N3-C4	7.12	114.16	110.60
1	A	803	U	N3-C4-O4	-7.12	114.41	119.40
1	A	2699	C	N1-C2-O2	-7.12	114.63	118.90
1	A	1170	G	C8-N9-C4	-7.12	103.55	106.40
1	A	1612	C	C4-C5-C6	7.12	120.96	117.40
1	A	933	A	N1-C6-N6	7.11	122.87	118.60
1	A	1985	G	C8-N9-C4	7.11	109.25	106.40
1	A	139(A)	G	C5-N7-C8	-7.10	100.75	104.30
1	A	2041	U	C2-N3-C4	-7.09	122.74	127.00
1	A	2371	G	N9-C4-C5	-7.09	102.56	105.40
1	A	262	A	C6-N1-C2	-7.09	114.35	118.60
1	A	571	A	C8-N9-C4	7.08	108.63	105.80
1	A	2371	G	C8-N9-C4	7.08	109.23	106.40
1	A	1753	G	C4-C5-N7	7.08	113.63	110.80
1	A	2875	C	C5-C6-N1	-7.08	117.46	121.00
1	A	1488	G	N7-C8-N9	7.07	116.64	113.10
1	A	1813	G	N1-C6-O6	7.06	124.14	119.90
1	A	1575	C	C2-N3-C4	-7.06	116.37	119.90
1	A	856	C	C5-C6-N1	7.06	124.53	121.00
1	A	1204	A	N1-C6-N6	7.05	122.83	118.60
1	A	2237	G	N3-C2-N2	7.05	124.83	119.90
1	A	527	C	N3-C4-N4	-7.03	113.08	118.00
1	A	1679	U	C4-C5-C6	7.03	123.92	119.70
1	A	139(A)	G	C4-N9-C1'	7.03	135.63	126.50
1	A	776	G	N1-C6-O6	-7.03	115.68	119.90
1	A	143	G	N3-C4-C5	7.02	132.11	128.60
1	A	1882	C	C2-N1-C1'	7.02	126.53	118.80
1	A	1973	G	C5-C6-O6	7.02	132.81	128.60
1	A	2161	C	C5-C4-N4	7.01	125.11	120.20
1	A	1311	G	C5-C6-O6	7.00	132.80	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	645	C	N1-C2-O2	7.00	123.10	118.90
1	A	1928	A	C2-N3-C4	7.00	114.10	110.60
1	A	1799	G	N3-C2-N2	6.99	124.80	119.90
1	A	463	G	C2-N3-C4	6.99	115.39	111.90
1	A	1021	A	C4-C5-N7	6.98	114.19	110.70
1	A	2073	C	C6-N1-C2	6.98	123.09	120.30
1	A	23	G	C4-C5-N7	-6.98	108.01	110.80
1	A	512	G	C2-N3-C4	6.98	115.39	111.90
1	A	528	A	C4-N9-C1'	-6.98	113.74	126.30
1	A	2318	G	N3-C4-C5	-6.98	125.11	128.60
1	A	1756	G	C2-N3-C4	6.98	115.39	111.90
1	A	1977	A	C8-N9-C4	6.98	108.59	105.80
1	A	2608	G	C6-N1-C2	-6.97	120.92	125.10
1	A	781	A	C6-N1-C2	-6.97	114.42	118.60
1	A	1819	A	C8-N9-C4	-6.96	103.02	105.80
1	A	1409	C	C6-N1-C2	6.96	123.08	120.30
1	A	2024	G	C8-N9-C4	6.96	109.18	106.40
1	A	2432	A	C2-N3-C4	-6.96	107.12	110.60
1	A	2576	G	C2-N3-C4	6.96	115.38	111.90
1	A	524	U	N3-C2-O2	-6.96	117.33	122.20
1	A	1017	G	C8-N9-C4	-6.96	103.62	106.40
1	A	2731	G	N1-C6-O6	6.95	124.07	119.90
1	A	981	A	N1-C2-N3	-6.94	125.83	129.30
1	A	1998	G	N1-C6-O6	-6.94	115.74	119.90
1	A	1037	G	N1-C6-O6	6.94	124.06	119.90
1	A	2354	G	C2-N3-C4	-6.93	108.43	111.90
1	A	208	C	N3-C4-N4	6.93	122.85	118.00
2	B	115	G	C8-N9-C4	6.93	109.17	106.40
1	A	370	G	N1-C6-O6	-6.93	115.74	119.90
1	A	1403	C	C2-N3-C4	-6.93	116.44	119.90
1	A	1807	G	C8-N9-C4	6.93	109.17	106.40
1	A	186	G	C4-C5-N7	-6.93	108.03	110.80
1	A	2894	G	C6-C5-N7	-6.92	126.25	130.40
1	A	2137	C	N3-C4-C5	-6.92	119.13	121.90
1	A	2464	C	C6-N1-C1'	-6.92	112.50	120.80
1	A	945	A	C5-C6-N1	-6.92	114.24	117.70
1	A	2623	G	C8-N9-C4	-6.91	103.64	106.40
11	P	148	LEU	CA-CB-CG	6.91	131.20	115.30
1	A	2304	G	C2-N3-C4	6.91	115.36	111.90
29	7	9	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	A	2154	G	C5-C6-O6	6.91	132.75	128.60
1	A	762	U	C5-C4-O4	-6.91	121.76	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1132	A	C8-N9-C4	-6.90	103.04	105.80
1	A	2504	U	N3-C4-O4	-6.90	114.57	119.40
1	A	2894	G	N7-C8-N9	6.90	116.55	113.10
1	A	330	A	C4-C5-N7	6.89	114.15	110.70
1	A	1612	C	C5-C6-N1	-6.89	117.56	121.00
1	A	1810	A	N1-C6-N6	-6.89	114.47	118.60
1	A	530	G	C8-N9-C1'	6.89	135.95	127.00
1	A	41	C	C5-C6-N1	-6.88	117.56	121.00
1	A	1140	C	N3-C4-C5	-6.88	119.15	121.90
1	A	1288	U	C5-C4-O4	6.88	130.03	125.90
1	A	130	C	N3-C4-C5	6.88	124.65	121.90
1	A	2073	C	C5-C6-N1	-6.88	117.56	121.00
1	A	2559	C	N3-C4-N4	-6.88	113.18	118.00
1	A	2864	G	C5-C6-O6	6.88	132.73	128.60
1	A	2574	G	C5-C6-N1	6.88	114.94	111.50
2	B	14	U	N3-C2-O2	-6.88	117.38	122.20
1	A	1524	G	N1-C6-O6	-6.88	115.77	119.90
1	A	2206	G	C4-N9-C1'	-6.88	117.56	126.50
2	B	71	C	C6-N1-C2	6.88	123.05	120.30
1	A	328	U	N1-C2-N3	6.87	119.02	114.90
1	A	1335	U	C2-N3-C4	-6.87	122.88	127.00
1	A	2595	G	N1-C6-O6	-6.87	115.78	119.90
1	A	1288	U	N3-C2-O2	-6.86	117.39	122.20
1	A	2154	G	C6-N1-C2	6.86	129.22	125.10
1	A	2239	G	C2-N3-C4	6.86	115.33	111.90
1	A	2848	G	N1-C6-O6	-6.86	115.78	119.90
1	A	2700	C	C5-C4-N4	-6.86	115.40	120.20
1	A	2615	U	C4-C5-C6	-6.85	115.59	119.70
1	A	2103	C	N1-C2-O2	6.85	123.01	118.90
1	A	1154	G	C5-C6-O6	-6.84	124.50	128.60
9	N	46	VAL	N-CA-C	6.84	129.46	111.00
1	A	734	A	C2-N3-C4	-6.83	107.18	110.60
1	A	2322	A	N3-C4-C5	-6.83	122.02	126.80
1	A	2581	G	N1-C6-O6	-6.83	115.80	119.90
1	A	2743	C	C5-C6-N1	-6.83	117.58	121.00
1	A	1609	A	C8-N9-C4	6.82	108.53	105.80
1	A	1049	C	C6-N1-C2	-6.82	117.57	120.30
1	A	741	G	C5-C6-O6	6.82	132.69	128.60
1	A	585	G	N3-C4-C5	-6.82	125.19	128.60
1	A	2352	A	C8-N9-C4	6.81	108.53	105.80
1	A	12	U	N3-C2-O2	-6.81	117.43	122.20
1	A	265	A	C6-C5-N7	-6.81	127.53	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2296	U	O4'-C1'-N1	6.81	113.65	108.20
1	A	1774	C	C6-N1-C2	-6.81	117.58	120.30
5	F	188	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	A	1819	A	N9-C4-C5	6.80	108.52	105.80
1	A	107	C	N3-C4-C5	6.80	124.62	121.90
1	A	1162	G	N1-C6-O6	-6.80	115.82	119.90
1	A	1899	G	C5-C6-O6	-6.80	124.52	128.60
1	A	565	C	N1-C2-O2	-6.80	114.82	118.90
1	A	1008	C	C6-N1-C2	-6.79	117.58	120.30
1	A	1223	G	N9-C4-C5	6.79	108.12	105.40
5	F	89	VAL	C-N-CA	-6.79	104.72	121.70
1	A	189	G	N1-C6-O6	6.79	123.97	119.90
1	A	571	A	N1-C6-N6	6.78	122.67	118.60
1	A	528	A	N7-C8-N9	6.78	117.19	113.80
1	A	2304	G	C8-N9-C1'	6.77	135.80	127.00
1	A	585	G	C5-C6-N1	6.76	114.88	111.50
1	A	702	G	C5-N7-C8	6.76	107.68	104.30
1	A	1649	G	C5-C6-O6	6.76	132.66	128.60
1	A	2218	U	N1-C2-O2	6.76	127.53	122.80
1	A	128	C	N1-C2-O2	-6.76	114.85	118.90
1	A	515	A	C6-N1-C2	-6.75	114.55	118.60
1	A	1200	C	N3-C2-O2	-6.74	117.18	121.90
1	A	469	G	N3-C4-C5	-6.74	125.23	128.60
1	A	2014	A	C2-N3-C4	-6.74	107.23	110.60
1	A	2016	U	C2-N3-C4	6.73	131.04	127.00
1	A	2287	A	C6-N1-C2	6.73	122.64	118.60
1	A	2289	G	C5-N7-C8	-6.72	100.94	104.30
1	A	546	C	N1-C2-O2	6.72	122.93	118.90
1	A	2324	C	C5-C4-N4	-6.72	115.49	120.20
1	A	1404	C	C6-N1-C2	-6.72	117.61	120.30
1	A	963	U	C5-C6-N1	-6.71	119.34	122.70
1	A	2304	G	C6-C5-N7	6.70	134.42	130.40
1	A	202	U	C5-C6-N1	-6.69	119.35	122.70
1	A	834	C	C2-N3-C4	-6.69	116.55	119.90
1	A	2848	G	C5-C6-O6	6.69	132.62	128.60
1	A	1792	G	C5-C6-N1	-6.69	108.16	111.50
1	A	1813	G	C8-N9-C4	6.69	109.07	106.40
1	A	1541	G	C8-N9-C4	-6.68	103.73	106.40
1	A	2549	G	C8-N9-C4	-6.68	103.73	106.40
1	A	139(A)	G	C8-N9-C4	-6.68	103.73	106.40
1	A	1471	A	C8-N9-C4	-6.68	103.13	105.80
1	A	720	C	C6-N1-C2	6.68	122.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2538	C	N3-C2-O2	-6.67	117.23	121.90
1	A	753	C	N3-C2-O2	-6.67	117.23	121.90
1	A	20	C	C2-N3-C4	-6.67	116.56	119.90
1	A	271(J)	C	N1-C2-O2	6.67	122.90	118.90
1	A	2778	A	C8-N9-C4	-6.67	103.13	105.80
1	A	809	G	C5-C6-O6	6.66	132.60	128.60
1	A	2296	U	C4-C5-C6	6.66	123.70	119.70
1	A	1475	G	N9-C4-C5	6.66	108.06	105.40
1	A	2740	A	C2-N3-C4	6.66	113.93	110.60
1	A	1894	C	C6-N1-C2	-6.66	117.64	120.30
3	D	239	ARG	NE-CZ-NH2	-6.66	116.97	120.30
2	B	73	A	C8-N9-C4	-6.65	103.14	105.80
9	N	25	ARG	NE-CZ-NH1	-6.65	116.97	120.30
1	A	1170	G	N7-C8-N9	6.65	116.42	113.10
1	A	1815	A	C8-N9-C4	6.65	108.46	105.80
1	A	1382	G	N1-C6-O6	6.64	123.89	119.90
1	A	2548	G	N3-C4-C5	-6.64	125.28	128.60
1	A	1229	G	C8-N9-C4	6.64	109.06	106.40
1	A	2597	G	C2-N3-C4	6.64	115.22	111.90
1	A	1142(A)	A	C4-C5-N7	6.64	114.02	110.70
1	A	1787	A	C8-N9-C4	6.63	108.45	105.80
1	A	2243	U	C5-C6-N1	6.63	126.02	122.70
1	A	1050	A	N7-C8-N9	6.63	117.11	113.80
1	A	793	A	C6-N1-C2	6.63	122.58	118.60
1	A	987	G	C8-N9-C4	-6.63	103.75	106.40
1	A	1930	G	N1-C2-N3	-6.63	119.92	123.90
1	A	2011	U	N1-C2-N3	6.63	118.88	114.90
1	A	582	G	C5-C6-O6	6.62	132.57	128.60
1	A	1031	G	C5-C6-N1	6.62	114.81	111.50
15	T	127	ALA	N-CA-C	-6.62	93.13	111.00
16	U	50	ARG	NE-CZ-NH2	6.62	123.61	120.30
1	A	1308	A	C5-N7-C8	6.61	107.21	103.90
1	A	486	C	C5-C6-N1	-6.61	117.69	121.00
1	A	1192	G	C8-N9-C4	6.61	109.04	106.40
1	A	2645	G	N3-C4-C5	6.61	131.91	128.60
3	D	13	ARG	NE-CZ-NH1	6.61	123.60	120.30
1	A	1127	A	N1-C2-N3	-6.61	126.00	129.30
1	A	2191	G	C6-C5-N7	-6.60	126.44	130.40
1	A	109	G	N1-C6-O6	-6.60	115.94	119.90
1	A	1748	G	C8-N9-C4	6.60	109.04	106.40
1	A	2877	G	C5-C6-N1	6.59	114.80	111.50
1	A	465	G	C8-N9-C4	-6.59	103.77	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1246	A	N7-C8-N9	-6.59	110.51	113.80
1	A	1429	G	N3-C2-N2	6.59	124.51	119.90
1	A	1878	G	C5-C6-N1	-6.59	108.21	111.50
1	A	1248	G	C5-N7-C8	-6.59	101.01	104.30
1	A	2456	C	C5-C6-N1	6.58	124.29	121.00
1	A	1761	C	C5-C4-N4	-6.58	115.59	120.20
1	A	1817	G	N9-C4-C5	-6.58	102.77	105.40
1	A	1248	G	N9-C4-C5	-6.58	102.77	105.40
1	A	1257	C	N3-C4-N4	-6.58	113.39	118.00
1	A	1942	C	C4-C5-C6	-6.58	114.11	117.40
1	A	1899	G	C4-C5-N7	6.58	113.43	110.80
1	A	2143	C	C5-C6-N1	6.58	124.29	121.00
1	A	250	G	C5-C6-N1	6.57	114.79	111.50
1	A	809	G	C6-N1-C2	6.57	129.04	125.10
18	W	92	ARG	NE-CZ-NH1	-6.57	117.01	120.30
1	A	295	G	C5-C6-O6	-6.57	124.66	128.60
1	A	1246	A	C5-N7-C8	6.57	107.19	103.90
1	A	2743	C	C2-N3-C4	-6.57	116.61	119.90
1	A	1120	G	C6-N1-C2	6.57	129.04	125.10
1	A	2045	C	C4-C5-C6	6.57	120.68	117.40
1	A	1796	U	C5-C6-N1	-6.56	119.42	122.70
1	A	2555	U	N1-C2-O2	-6.56	118.21	122.80
1	A	1180	C	C6-N1-C2	6.56	122.92	120.30
1	A	2539	C	N3-C4-C5	6.56	124.52	121.90
1	A	481	G	N9-C4-C5	6.56	108.02	105.40
1	A	701	G	N1-C6-O6	-6.56	115.97	119.90
1	A	2286	A	C4-N9-C1'	6.55	138.10	126.30
1	A	2503	A	C2-N3-C4	6.55	113.88	110.60
1	A	1431	U	C5-C6-N1	6.55	125.97	122.70
1	A	2336	A	N9-C4-C5	-6.55	103.18	105.80
1	A	732	C	N3-C4-C5	-6.54	119.28	121.90
1	A	2866	U	N1-C2-N3	6.54	118.83	114.90
1	A	271(M)	G	C6-C5-N7	-6.54	126.48	130.40
1	A	2062	A	C2-N3-C4	-6.54	107.33	110.60
1	A	1334	G	C8-N9-C4	-6.54	103.78	106.40
1	A	1790	C	C6-N1-C2	6.53	122.91	120.30
1	A	846	C	C5-C6-N1	-6.53	117.73	121.00
1	A	1343	G	C8-N9-C4	-6.53	103.79	106.40
1	A	351	G	C5-C6-O6	-6.52	124.69	128.60
1	A	588	U	C4-C5-C6	-6.52	115.79	119.70
1	A	1944	U	C5-C6-N1	-6.52	119.44	122.70
1	A	2700	C	C5-C6-N1	-6.52	117.74	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2866	U	N3-C2-O2	-6.52	117.63	122.20
1	A	34	C	N3-C4-C5	-6.52	119.29	121.90
1	A	1745	C	N1-C2-O2	-6.52	114.99	118.90
1	A	2605	U	N1-C2-O2	6.52	127.36	122.80
2	B	94	C	N3-C2-O2	-6.51	117.34	121.90
21	Z	5	LEU	CA-CB-CG	6.51	130.28	115.30
1	A	593	G	N9-C4-C5	6.51	108.00	105.40
1	A	2579	C	C5-C4-N4	-6.51	115.64	120.20
1	A	1018	C	C6-N1-C2	6.51	122.90	120.30
1	A	1997	G	C6-N1-C2	-6.51	121.19	125.10
1	A	1757	U	C6-N1-C2	6.50	124.90	121.00
1	A	1939	U	C2-N3-C4	-6.50	123.10	127.00
1	A	1254	A	N9-C4-C5	6.50	108.40	105.80
1	A	1366	A	N9-C4-C5	6.50	108.40	105.80
1	A	1586	A	C5-C6-N6	6.50	128.90	123.70
1	A	2016	U	C5-C4-O4	6.50	129.80	125.90
1	A	112	U	N3-C2-O2	-6.49	117.66	122.20
1	A	279	C	C6-N1-C2	-6.49	117.70	120.30
1	A	529	A	C5-N7-C8	-6.48	100.66	103.90
1	A	2570	G	C2-N3-C4	6.48	115.14	111.90
1	A	2593	U	N3-C4-O4	-6.48	114.86	119.40
1	A	2820	A	C2-N3-C4	-6.48	107.36	110.60
11	P	55	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	A	773	U	N3-C4-C5	6.48	118.49	114.60
1	A	2358	G	N1-C6-O6	-6.48	116.01	119.90
1	A	2791	C	C6-N1-C2	-6.47	117.71	120.30
1	A	593	G	C5-C6-O6	6.47	132.48	128.60
1	A	486	C	C6-N1-C2	6.47	122.89	120.30
1	A	571	A	C5-C6-N6	-6.47	118.52	123.70
1	A	688	U	N1-C2-N3	6.47	118.78	114.90
1	A	1564	C	C5-C4-N4	6.47	124.73	120.20
1	A	2071	A	N7-C8-N9	-6.47	110.57	113.80
1	A	454	A	C8-N9-C4	-6.46	103.21	105.80
1	A	1234	U	C5-C4-O4	-6.46	122.02	125.90
1	A	681	G	C5-N7-C8	6.46	107.53	104.30
1	A	959	A	N7-C8-N9	6.46	117.03	113.80
1	A	950	G	N1-C6-O6	-6.46	116.02	119.90
1	A	2028	U	N3-C4-O4	-6.46	114.88	119.40
3	D	13	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	A	132	G	N7-C8-N9	-6.46	109.87	113.10
1	A	670	A	C2-N3-C4	6.46	113.83	110.60
1	A	1135	C	N1-C2-O2	-6.46	115.03	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1457	A	N1-C6-N6	6.46	122.47	118.60
1	A	1700	A	N1-C6-N6	-6.46	114.73	118.60
1	A	2877	G	C8-N9-C4	6.46	108.98	106.40
1	A	2001	A	C5-N7-C8	6.46	107.13	103.90
1	A	1597	A	C5-N7-C8	6.45	107.12	103.90
1	A	562	U	N3-C2-O2	-6.45	117.69	122.20
1	A	2437	U	C5-C4-O4	6.45	129.77	125.90
1	A	271(H)	G	N3-C4-N9	6.45	129.87	126.00
1	A	298	G	N3-C4-C5	-6.45	125.38	128.60
1	A	2592	G	C8-N9-C4	-6.45	103.82	106.40
1	A	2182	G	N3-C4-N9	-6.44	122.13	126.00
1	A	139(A)	G	N3-C4-C5	-6.44	125.38	128.60
1	A	1785	A	C8-N9-C4	-6.44	103.22	105.80
1	A	803	U	C5-C6-N1	-6.44	119.48	122.70
1	A	2079	U	C4-C5-C6	6.44	123.56	119.70
1	A	1165	U	N3-C2-O2	-6.43	117.69	122.20
1	A	778	G	N3-C2-N2	6.43	124.40	119.90
1	A	1107	G	C2-N3-C4	6.42	115.11	111.90
1	A	2050	C	N1-C2-O2	-6.42	115.05	118.90
1	A	1301	A	N7-C8-N9	6.42	117.01	113.80
1	A	802	A	N1-C6-N6	-6.41	114.75	118.60
1	A	1037	G	C5-C6-O6	-6.41	124.75	128.60
1	A	945	A	N1-C2-N3	6.41	132.50	129.30
1	A	72	U	N1-C2-O2	-6.41	118.32	122.80
1	A	205	G	N3-C2-N2	6.41	124.38	119.90
1	A	125	G	C5-C6-O6	-6.40	124.76	128.60
1	A	2137	C	C2-N1-C1'	6.40	125.84	118.80
29	7	34	ARG	NE-CZ-NH2	6.40	123.50	120.30
1	A	2321	G	C8-N9-C4	-6.40	103.84	106.40
1	A	2605	U	N3-C2-O2	-6.39	117.72	122.20
1	A	1025	G	C8-N9-C4	-6.39	103.84	106.40
1	A	1298	C	N3-C4-N4	-6.39	113.53	118.00
1	A	672	C	C6-N1-C2	6.39	122.86	120.30
1	A	2233	U	N1-C2-O2	-6.39	118.33	122.80
1	A	2789	C	C6-N1-C2	6.38	122.85	120.30
1	A	20	C	C5-C6-N1	-6.38	117.81	121.00
1	A	2791	C	N1-C2-O2	6.38	122.73	118.90
1	A	2041	U	N1-C2-N3	6.37	118.72	114.90
1	A	2079	U	N1-C2-N3	6.37	118.72	114.90
1	A	1826	G	C8-N9-C4	-6.37	103.85	106.40
1	A	2196	C	C6-N1-C2	6.37	122.85	120.30
1	A	2449	U	N3-C2-O2	-6.37	117.74	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2525	G	N3-C2-N2	6.37	124.36	119.90
1	A	587	C	C5-C4-N4	6.36	124.65	120.20
1	A	1367	A	N7-C8-N9	-6.36	110.62	113.80
1	A	2620	C	N3-C4-N4	-6.36	113.55	118.00
1	A	478	A	C8-N9-C4	-6.36	103.25	105.80
1	A	645	C	C2-N1-C1'	6.36	125.80	118.80
1	A	2352	A	N9-C4-C5	-6.36	103.26	105.80
1	A	2608	G	N1-C2-N3	6.36	127.72	123.90
1	A	474	G	N1-C6-O6	-6.35	116.09	119.90
27	5	15	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	A	788	A	N1-C6-N6	6.35	122.41	118.60
1	A	830	G	C8-N9-C4	-6.35	103.86	106.40
1	A	2371	G	N3-C4-N9	6.35	129.81	126.00
1	A	827	U	N1-C2-O2	-6.35	118.36	122.80
1	A	945	A	C5-C6-N6	-6.35	118.62	123.70
1	A	40	C	C2-N3-C4	-6.35	116.72	119.90
1	A	2084	C	C6-N1-C2	6.35	122.84	120.30
1	A	2272	U	N3-C2-O2	-6.35	117.76	122.20
1	A	2501	C	C2-N3-C4	-6.35	116.73	119.90
1	A	2705	A	N1-C6-N6	6.35	122.41	118.60
1	A	709	U	C5-C6-N1	-6.34	119.53	122.70
19	X	57	LEU	CA-CB-CG	6.34	129.88	115.30
1	A	1597	A	C4-C5-N7	-6.34	107.53	110.70
1	A	193	U	N3-C4-C5	-6.33	110.80	114.60
1	A	1248	G	C6-C5-N7	-6.33	126.60	130.40
1	A	847	U	N1-C2-O2	-6.33	118.37	122.80
1	A	2619	C	C5-C6-N1	-6.33	117.83	121.00
1	A	1565	C	N1-C2-O2	-6.33	115.10	118.90
1	A	663	G	N1-C6-O6	-6.33	116.10	119.90
1	A	2041	U	C5-C4-O4	-6.33	122.10	125.90
1	A	2426	A	N1-C6-N6	6.33	122.40	118.60
1	A	121	G	C5-C6-O6	-6.32	124.81	128.60
1	A	463	G	N1-C6-O6	-6.32	116.11	119.90
1	A	2238	G	N9-C4-C5	-6.32	102.87	105.40
2	B	115	G	C5-C6-O6	-6.32	124.81	128.60
1	A	2286	A	C4-C5-N7	6.31	113.86	110.70
1	A	41	C	C2-N3-C4	-6.31	116.74	119.90
1	A	1110	G	N9-C4-C5	6.31	107.92	105.40
1	A	2322	A	N1-C2-N3	6.31	132.46	129.30
1	A	809	G	N1-C2-N3	-6.30	120.12	123.90
1	A	201	C	C2-N3-C4	-6.30	116.75	119.90
1	A	1440	G	C5-N7-C8	6.30	107.45	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1609	A	C5-N7-C8	6.30	107.05	103.90
1	A	2585	U	N1-C2-N3	-6.30	111.12	114.90
1	A	564	C	N1-C2-O2	-6.30	115.12	118.90
1	A	1799	G	N3-C4-C5	-6.30	125.45	128.60
1	A	752	A	C2-N3-C4	-6.29	107.45	110.60
1	A	652(T)	C	C2-N3-C4	6.29	123.05	119.90
1	A	1185	C	C6-N1-C2	-6.29	117.78	120.30
1	A	2296	U	C1'-O4'-C4'	-6.29	104.87	109.90
1	A	1663	C	C6-N1-C2	-6.29	117.78	120.30
1	A	887	A	C2-N3-C4	6.29	113.74	110.60
1	A	2678	C	C5-C4-N4	6.29	124.60	120.20
1	A	518	G	C5-C6-O6	6.28	132.37	128.60
1	A	1141	U	C2-N3-C4	-6.28	123.23	127.00
1	A	2057	A	N1-C2-N3	6.28	132.44	129.30
1	A	35	G	N1-C6-O6	-6.28	116.13	119.90
1	A	82	G	N1-C2-N2	-6.28	110.55	116.20
1	A	469	G	C6-N1-C2	-6.28	121.33	125.10
1	A	1126	A	N9-C4-C5	-6.28	103.29	105.80
1	A	2015	A	N7-C8-N9	-6.28	110.66	113.80
1	A	2613	U	C5-C4-O4	-6.28	122.13	125.90
1	A	2624	G	C8-N9-C4	6.28	108.91	106.40
1	A	2820	A	N1-C2-N3	6.28	132.44	129.30
1	A	683	C	N3-C4-C5	6.28	124.41	121.90
1	A	589	C	N3-C2-O2	-6.28	117.51	121.90
1	A	1142(A)	A	N1-C6-N6	6.28	122.37	118.60
1	A	223	A	N7-C8-N9	6.27	116.94	113.80
1	A	2443	C	C2-N3-C4	-6.27	116.76	119.90
2	B	97	G	N1-C2-N2	6.27	121.84	116.20
1	A	729	G	C4-N9-C1'	6.27	134.65	126.50
1	A	1811	G	C4-C5-N7	-6.27	108.29	110.80
1	A	1899	G	N3-C4-N9	6.27	129.76	126.00
1	A	2637	U	C2-N3-C4	-6.27	123.24	127.00
1	A	1788	C	N3-C4-C5	-6.26	119.39	121.90
1	A	1122	G	C5-C6-O6	-6.26	124.84	128.60
1	A	2071	A	C5-N7-C8	6.26	107.03	103.90
1	A	1573	G	N7-C8-N9	-6.26	109.97	113.10
1	A	1678	G	C4-C5-C6	6.26	122.55	118.80
1	A	1607	C	C5-C4-N4	-6.25	115.82	120.20
1	A	585	G	C4-C5-N7	-6.25	108.30	110.80
2	B	81	G	C6-C5-N7	-6.25	126.65	130.40
1	A	2066	C	C2-N3-C4	-6.25	116.77	119.90
1	A	1355	G	C5-C6-N1	6.25	114.62	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	588	U	C5-C6-N1	6.25	125.82	122.70
1	A	2519	U	N1-C2-O2	-6.25	118.43	122.80
1	A	2697	G	C5-N7-C8	6.25	107.42	104.30
1	A	2894	G	N1-C2-N2	-6.25	110.58	116.20
1	A	1396	U	N1-C2-N3	6.25	118.65	114.90
1	A	959	A	C8-N9-C4	-6.24	103.30	105.80
1	A	512	G	N3-C4-C5	-6.24	125.48	128.60
1	A	2636	U	C5-C4-O4	6.24	129.64	125.90
1	A	2881	C	C6-N1-C2	-6.24	117.81	120.30
1	A	1307	A	N7-C8-N9	-6.24	110.68	113.80
1	A	1433	U	C5-C4-O4	6.24	129.64	125.90
1	A	2235	G	N1-C2-N2	-6.24	110.59	116.20
1	A	2623	G	N9-C4-C5	6.23	107.89	105.40
1	A	2304	G	N1-C6-O6	-6.23	116.16	119.90
1	A	13	A	N1-C2-N3	6.23	132.41	129.30
1	A	870	A	C8-N9-C4	6.23	108.29	105.80
1	A	2500	U	N3-C2-O2	-6.23	117.84	122.20
1	A	40	C	N3-C4-C5	6.22	124.39	121.90
1	A	271(M)	G	N3-C4-C5	-6.22	125.49	128.60
1	A	1493	C	C2-N1-C1'	6.22	125.64	118.80
1	A	2574	G	C6-N1-C2	-6.22	121.37	125.10
1	A	461	C	C4-C5-C6	6.21	120.51	117.40
1	A	776	G	C5-C6-O6	6.21	132.33	128.60
1	A	193	U	N3-C4-O4	6.21	123.75	119.40
1	A	474	G	P-O3'-C3'	6.21	127.15	119.70
1	A	1203	G	C4-C5-N7	-6.21	108.32	110.80
1	A	256	A	C8-N9-C4	6.21	108.28	105.80
1	A	99	U	N3-C2-O2	-6.21	117.85	122.20
1	A	677	A	C5-C6-N1	-6.21	114.60	117.70
1	A	1290	C	C6-N1-C2	-6.21	117.82	120.30
1	A	2065	C	C4-C5-C6	6.21	120.50	117.40
1	A	470	A	N7-C8-N9	6.21	116.90	113.80
1	A	2207	G	N1-C6-O6	6.21	123.62	119.90
1	A	2524	G	N1-C6-O6	-6.21	116.18	119.90
1	A	119	A	N1-C2-N3	6.20	132.40	129.30
1	A	1288	U	N1-C2-N3	6.20	118.62	114.90
1	A	1557	C	N3-C4-C5	6.20	124.38	121.90
1	A	809	G	N1-C6-O6	-6.20	116.18	119.90
1	A	1792	G	C6-N1-C2	6.20	128.82	125.10
1	A	1998	G	C4-C5-N7	-6.20	108.32	110.80
1	A	2069	G	C4-C5-N7	-6.20	108.32	110.80
1	A	1963	U	N1-C2-O2	6.19	127.14	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	92	A	C8-N9-C4	-6.19	103.32	105.80
1	A	438	G	C8-N9-C4	-6.19	103.92	106.40
1	A	474	G	C8-N9-C4	-6.18	103.93	106.40
1	A	996	A	C2-N3-C4	6.18	113.69	110.60
1	A	829	A	C2-N3-C4	-6.18	107.51	110.60
1	A	518	G	N1-C6-O6	-6.18	116.19	119.90
1	A	2692	C	N3-C2-O2	-6.17	117.58	121.90
2	B	115	G	N1-C6-O6	6.17	123.61	119.90
1	A	104	U	C2-N3-C4	-6.17	123.30	127.00
1	A	649	G	C5-C6-O6	6.17	132.30	128.60
1	A	132	G	C5-N7-C8	6.17	107.38	104.30
1	A	395	U	N1-C2-O2	6.17	127.12	122.80
2	B	74	U	N1-C2-N3	6.17	118.60	114.90
1	A	512	G	O4'-C1'-N9	6.17	113.13	108.20
1	A	973	A	N7-C8-N9	6.16	116.88	113.80
1	A	1124	C	C5-C4-N4	-6.16	115.89	120.20
1	A	2872	G	C8-N9-C4	-6.16	103.94	106.40
1	A	1155	A	C2-N3-C4	6.16	113.68	110.60
1	A	2053	G	C5-C6-O6	-6.16	124.91	128.60
1	A	2032	G	C5-N7-C8	6.16	107.38	104.30
1	A	237	C	C5-C6-N1	-6.15	117.92	121.00
1	A	1779	U	C6-N1-C2	6.15	124.69	121.00
2	B	118	G	N3-C4-C5	6.15	131.68	128.60
1	A	2548	G	N1-C6-O6	-6.15	116.21	119.90
1	A	2545	G	N1-C6-O6	6.14	123.59	119.90
1	A	2894	G	C5-C6-N1	-6.14	108.43	111.50
1	A	116	C	C5-C6-N1	-6.14	117.93	121.00
1	A	998	C	N3-C2-O2	-6.14	117.60	121.90
1	A	1160	G	C8-N9-C4	-6.14	103.94	106.40
1	A	2606	C	C2-N3-C4	-6.14	116.83	119.90
1	A	2713	A	N1-C2-N3	-6.14	126.23	129.30
1	A	123	G	N7-C8-N9	-6.14	110.03	113.10
1	A	1697	G	C5-C6-O6	-6.14	124.92	128.60
1	A	1304	C	C6-N1-C2	6.14	122.75	120.30
1	A	2022	U	N1-C2-O2	-6.14	118.50	122.80
1	A	2524	G	C5-C6-N1	6.14	114.57	111.50
1	A	2807	G	C8-N9-C4	-6.14	103.94	106.40
1	A	214	G	C8-N9-C4	6.13	108.85	106.40
1	A	122	G	C5-C6-O6	-6.13	124.92	128.60
1	A	1551	C	C6-N1-C2	-6.13	117.85	120.30
1	A	2769	C	C5-C6-N1	-6.13	117.94	121.00
1	A	774	A	C8-N9-C4	-6.13	103.35	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	O	8	LEU	CA-CB-CG	6.13	129.39	115.30
1	A	2415	G	N3-C2-N2	-6.12	115.61	119.90
1	A	2053	G	C5-N7-C8	6.12	107.36	104.30
1	A	2061	G	N1-C6-O6	-6.12	116.22	119.90
1	A	2585	U	N1-C2-O2	6.12	127.09	122.80
1	A	143	G	N3-C4-N9	-6.12	122.33	126.00
1	A	706	A	C8-N9-C4	-6.12	103.35	105.80
1	A	745	G	C6-N1-C2	-6.12	121.43	125.10
1	A	195	A	N7-C8-N9	-6.12	110.74	113.80
1	A	987	G	N7-C8-N9	6.12	116.16	113.10
1	A	2103	C	N3-C4-C5	-6.12	119.45	121.90
1	A	1295	C	N3-C2-O2	-6.12	117.62	121.90
1	A	1602	U	C5-C6-N1	-6.12	119.64	122.70
1	A	1266	G	C5-C6-O6	-6.12	124.93	128.60
1	A	1638	C	C5-C6-N1	-6.12	117.94	121.00
1	A	2453	A	N1-C6-N6	-6.12	114.93	118.60
1	A	2554	U	N1-C2-O2	-6.11	118.52	122.80
1	A	690	G	C5-N7-C8	6.11	107.36	104.30
1	A	2288	A	C8-N9-C4	-6.11	103.36	105.80
1	A	1770	G	N1-C2-N3	-6.11	120.23	123.90
1	A	1580	A	N9-C4-C5	-6.11	103.36	105.80
1	A	1117	G	N1-C6-O6	6.10	123.56	119.90
1	A	2127	G	C6-N1-C2	6.10	128.76	125.10
1	A	116	C	N1-C2-N3	6.10	123.47	119.20
1	A	2891	G	C5-C6-O6	-6.10	124.94	128.60
1	A	805	G	N9-C4-C5	-6.10	102.96	105.40
1	A	2243	U	N3-C2-O2	6.09	126.46	122.20
1	A	752	A	N1-C2-N3	6.09	132.34	129.30
1	A	1650	G	C8-N9-C4	-6.09	103.97	106.40
1	A	2360	A	N1-C2-N3	6.09	132.34	129.30
1	A	206	U	C5-C6-N1	-6.09	119.66	122.70
1	A	1443	G	C8-N9-C4	-6.09	103.97	106.40
1	A	569	U	C5-C4-O4	-6.08	122.25	125.90
1	A	2681	C	C4-C5-C6	6.08	120.44	117.40
1	A	1188	U	C5-C4-O4	6.08	129.55	125.90
1	A	2714	G	C5-C6-N1	6.08	114.54	111.50
1	A	82	G	N3-C4-N9	6.08	129.65	126.00
1	A	262	A	N1-C2-N3	6.08	132.34	129.30
1	A	204	A	C5-C6-N1	6.07	120.74	117.70
1	A	474	G	N7-C8-N9	6.07	116.14	113.10
1	A	753	C	N3-C4-N4	-6.07	113.75	118.00
1	A	2226	C	C5-C6-N1	-6.07	117.96	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	U	10	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	A	1256	G	C8-N9-C4	6.07	108.83	106.40
1	A	1406	U	C6-N1-C2	-6.07	117.36	121.00
1	A	2303	G	N3-C2-N2	-6.07	115.65	119.90
1	A	2493	U	C2-N3-C4	-6.07	123.36	127.00
1	A	1825	A	C8-N9-C4	-6.07	103.37	105.80
1	A	71	A	N7-C8-N9	6.07	116.83	113.80
1	A	1307	A	C8-N9-C4	6.07	108.23	105.80
1	A	281	G	C8-N9-C4	6.07	108.83	106.40
1	A	2821	A	N1-C2-N3	6.06	132.33	129.30
1	A	846	C	C6-N1-C2	6.06	122.72	120.30
1	A	792	G	N3-C4-C5	-6.06	125.57	128.60
1	A	1780	A	N1-C2-N3	6.06	132.33	129.30
1	A	2454	G	C2-N3-C4	6.05	114.93	111.90
1	A	1698	A	C6-N1-C2	6.05	122.23	118.60
1	A	1021	A	C6-N1-C2	6.04	122.23	118.60
1	A	2331	G	N1-C6-O6	6.04	123.53	119.90
1	A	2892	A	C8-N9-C4	-6.04	103.38	105.80
1	A	212	G	N7-C8-N9	6.04	116.12	113.10
1	A	1194	A	N1-C2-N3	-6.04	126.28	129.30
1	A	893	C	C2-N1-C1'	6.04	125.44	118.80
1	A	1636	C	C4-C5-C6	6.04	120.42	117.40
1	A	2029	G	C2-N3-C4	6.03	114.92	111.90
1	A	1038	C	C5-C4-N4	-6.03	115.98	120.20
1	A	2553	G	N3-C2-N2	6.03	124.12	119.90
1	A	2601	C	C6-N1-C2	-6.03	117.89	120.30
1	A	90	U	C2-N3-C4	6.03	130.62	127.00
1	A	787	U	C6-N1-C2	-6.03	117.38	121.00
1	A	2041	U	N1-C2-O2	-6.03	118.58	122.80
1	A	298	G	C4-C5-N7	-6.03	108.39	110.80
1	A	552	G	C8-N9-C4	6.03	108.81	106.40
1	A	950	G	C5-C6-O6	6.03	132.22	128.60
1	A	1047	G	N3-C4-C5	-6.03	125.59	128.60
1	A	1257	C	C5-C4-N4	6.03	124.42	120.20
1	A	2270	G	N1-C6-O6	6.03	123.52	119.90
1	A	655	A	C8-N9-C4	-6.02	103.39	105.80
2	B	63	G	C8-N9-C4	6.02	108.81	106.40
1	A	242	G	N1-C6-O6	-6.02	116.29	119.90
1	A	803	U	C5-C4-O4	6.02	129.51	125.90
1	A	1157	G	C5-C6-O6	6.02	132.21	128.60
1	A	966	G	N3-C2-N2	6.02	124.11	119.90
1	A	1198	U	N1-C2-N3	6.02	118.51	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1308	A	C4-C5-N7	-6.01	107.69	110.70
1	A	1653	G	N3-C2-N2	-6.01	115.69	119.90
1	A	2233	U	C5-C4-O4	6.01	129.51	125.90
1	A	584	C	C2-N3-C4	-6.01	116.89	119.90
1	A	800	A	N7-C8-N9	-6.01	110.80	113.80
1	A	539	G	C5-C6-O6	6.01	132.21	128.60
1	A	1814	G	N1-C2-N2	-6.01	110.79	116.20
1	A	749	C	C2-N3-C4	-6.01	116.90	119.90
1	A	80	G	C5-C6-O6	6.00	132.20	128.60
1	A	1274	A	C8-N9-C4	-6.00	103.40	105.80
1	A	2610	C	C2-N3-C4	-6.00	116.90	119.90
1	A	196	A	C5-N7-C8	-6.00	100.90	103.90
1	A	1326	U	N1-C2-O2	5.99	127.00	122.80
1	A	2271	G	N3-C2-N2	5.99	124.09	119.90
1	A	2376	A	C6-N1-C2	-5.99	115.00	118.60
1	A	2238	G	N3-C4-N9	5.99	129.59	126.00
1	A	2319	G	C4-C5-N7	5.99	113.20	110.80
1	A	113	G	N3-C2-N2	-5.99	115.71	119.90
1	A	2161	C	N3-C4-N4	-5.99	113.81	118.00
1	A	125	G	C5-C6-N1	5.99	114.49	111.50
1	A	649	G	C8-N9-C4	-5.99	104.00	106.40
2	B	115	G	N9-C4-C5	-5.99	103.00	105.40
1	A	2335	A	N9-C4-C5	-5.98	103.41	105.80
1	A	1654	A	C5-N7-C8	5.98	106.89	103.90
1	A	690	G	N7-C8-N9	-5.98	110.11	113.10
1	A	2124	G	C6-N1-C2	5.98	128.69	125.10
1	A	1697	G	N1-C6-O6	5.98	123.49	119.90
1	A	470	A	C8-N9-C4	-5.98	103.41	105.80
1	A	531	C	N3-C4-C5	5.98	124.29	121.90
1	A	389	G	C8-N9-C4	5.97	108.79	106.40
1	A	2363	C	C2-N1-C1'	-5.97	112.23	118.80
1	A	1320	C	C5-C4-N4	5.97	124.38	120.20
1	A	2438	U	N3-C4-C5	5.97	118.18	114.60
1	A	80	G	N9-C4-C5	5.97	107.79	105.40
1	A	1683	C	N1-C2-O2	-5.97	115.32	118.90
1	A	1153	C	C6-N1-C2	-5.96	117.92	120.30
1	A	1323	U	C6-N1-C2	5.96	124.58	121.00
2	B	20	C	C2-N1-C1'	5.96	125.36	118.80
1	A	1710	C	N3-C4-C5	5.96	124.28	121.90
1	A	2869	G	C8-N9-C4	-5.96	104.02	106.40
1	A	2824	C	N3-C2-O2	-5.96	117.73	121.90
1	A	767	U	N3-C2-O2	-5.96	118.03	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1808	U	C5-C4-O4	5.96	129.47	125.90
1	A	114	U	C5-C4-O4	-5.95	122.33	125.90
1	A	517	C	N3-C4-C5	5.95	124.28	121.90
1	A	776	G	N9-C4-C5	5.95	107.78	105.40
1	A	1443	G	N7-C8-N9	5.95	116.08	113.10
2	B	56	G	C5-C6-O6	5.95	132.17	128.60
1	A	1440	G	C4-C5-N7	-5.95	108.42	110.80
1	A	1672	C	C4-C5-C6	5.95	120.37	117.40
1	A	451	C	N3-C2-O2	-5.94	117.74	121.90
1	A	772	C	C6-N1-C2	5.94	122.68	120.30
1	A	131	G	N3-C2-N2	5.94	124.06	119.90
1	A	1541	G	N9-C4-C5	5.94	107.78	105.40
1	A	2271	G	N1-C2-N2	-5.94	110.85	116.20
11	P	50	ARG	NE-CZ-NH2	5.94	123.27	120.30
1	A	2772	C	N3-C4-N4	-5.94	113.84	118.00
1	A	2595	G	N1-C2-N3	-5.94	120.34	123.90
1	A	2805	G	N3-C4-C5	-5.94	125.63	128.60
1	A	2557	G	N3-C2-N2	5.93	124.05	119.90
1	A	2715	C	C6-N1-C2	5.93	122.67	120.30
1	A	735	A	C4-C5-N7	-5.93	107.73	110.70
1	A	1570	A	C5-C6-N6	-5.93	118.95	123.70
1	A	2453	A	N1-C2-N3	-5.93	126.33	129.30
1	A	739	G	N3-C2-N2	-5.93	115.75	119.90
1	A	193	U	N3-C2-O2	5.93	126.35	122.20
1	A	196	A	N7-C8-N9	5.93	116.76	113.80
1	A	2877	G	C5-C6-O6	-5.93	125.04	128.60
1	A	119	A	N1-C6-N6	-5.92	115.05	118.60
1	A	752	A	N1-C6-N6	5.92	122.15	118.60
1	A	834	C	C5-C6-N1	-5.92	118.04	121.00
1	A	2820	A	N9-C4-C5	-5.92	103.43	105.80
2	B	51	G	N1-C6-O6	-5.92	116.35	119.90
1	A	1124	C	C2-N1-C1'	5.92	125.31	118.80
1	A	116	C	C4-C5-C6	5.92	120.36	117.40
1	A	188	G	N1-C6-O6	-5.92	116.35	119.90
1	A	951	C	N3-C4-N4	-5.92	113.86	118.00
1	A	2441	C	C5-C6-N1	-5.92	118.04	121.00
1	A	2074	U	C2-N3-C4	-5.91	123.45	127.00
1	A	1753	G	N3-C2-N2	5.91	124.04	119.90
1	A	90	U	C6-N1-C2	-5.91	117.45	121.00
1	A	187	G	C5-C6-O6	-5.91	125.05	128.60
1	A	944	G	C4-N9-C1'	5.91	134.18	126.50
1	A	1661	G	C5-C6-O6	5.91	132.15	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1799	G	P-O3'-C3'	5.91	126.79	119.70
1	A	141	A	N1-C6-N6	5.90	122.14	118.60
1	A	1438	U	C5-C4-O4	-5.90	122.36	125.90
1	A	681	G	C8-N9-C4	5.90	108.76	106.40
1	A	1899	G	N3-C4-C5	-5.90	125.65	128.60
3	D	239	ARG	N-CA-C	-5.90	95.06	111.00
1	A	1019	U	N1-C2-N3	5.90	118.44	114.90
1	A	1779	U	N3-C4-C5	5.90	118.14	114.60
1	A	1373	A	N7-C8-N9	-5.90	110.85	113.80
1	A	2354	G	N1-C6-O6	5.90	123.44	119.90
1	A	2559	C	C5-C4-N4	5.90	124.33	120.20
1	A	38	A	C8-N9-C4	-5.89	103.44	105.80
1	A	725	G	N3-C4-C5	-5.89	125.65	128.60
1	A	1313	U	C6-N1-C2	-5.89	117.47	121.00
1	A	49	A	C2-N3-C4	5.89	113.55	110.60
1	A	296	C	N3-C2-O2	-5.89	117.78	121.90
1	A	2430	A	C2-N3-C4	5.88	113.54	110.60
1	A	206	U	C2-N3-C4	-5.88	123.47	127.00
1	A	2230	G	N1-C2-N2	5.88	121.50	116.20
1	A	474	G	C5-C6-O6	5.88	132.13	128.60
1	A	526	A	C8-N9-C4	-5.88	103.45	105.80
1	A	535	C	N3-C4-C5	-5.88	119.55	121.90
1	A	587	C	N3-C4-C5	-5.88	119.55	121.90
1	A	766	C	C5-C6-N1	-5.88	118.06	121.00
1	A	66	C	C6-N1-C2	-5.88	117.95	120.30
1	A	1038	C	N3-C4-C5	5.88	124.25	121.90
2	B	65	C	N3-C4-C5	5.88	124.25	121.90
1	A	1963	U	C6-N1-C1'	-5.88	112.98	121.20
1	A	2469	A	C8-N9-C4	-5.88	103.45	105.80
1	A	72	U	N3-C2-O2	5.87	126.31	122.20
1	A	1298	C	N3-C4-C5	5.87	124.25	121.90
1	A	2824	C	N1-C2-O2	5.87	122.42	118.90
1	A	47	C	N3-C4-C5	5.87	124.25	121.90
1	A	2454	G	N3-C2-N2	5.87	124.01	119.90
1	A	2562	U	C2-N3-C4	-5.87	123.48	127.00
1	A	2706	G	C6-N1-C2	-5.87	121.58	125.10
2	B	56	G	N1-C6-O6	-5.87	116.38	119.90
1	A	758	C	N3-C4-N4	-5.86	113.90	118.00
1	A	2460	U	N1-C2-N3	5.86	118.42	114.90
1	A	143(A)	C	C2-N3-C4	-5.86	116.97	119.90
1	A	114	U	C2-N1-C1'	5.86	124.73	117.70
1	A	2013	A	N7-C8-N9	5.86	116.73	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	18	C	C6-N1-C2	-5.86	117.96	120.30
1	A	2700	C	N3-C4-C5	5.86	124.24	121.90
1	A	702	G	C4-C5-N7	-5.85	108.46	110.80
1	A	1300	U	N1-C2-N3	5.85	118.41	114.90
1	A	266	G	C8-N9-C4	5.85	108.74	106.40
1	A	822	U	N3-C4-O4	-5.85	115.30	119.40
1	A	2714	G	C4-C5-N7	5.85	113.14	110.80
1	A	2781	A	N1-C6-N6	-5.85	115.09	118.60
1	A	762	U	C2-N1-C1'	5.85	124.72	117.70
2	B	76	G	C8-N9-C4	5.85	108.74	106.40
1	A	1031	G	C6-N1-C2	-5.84	121.59	125.10
1	A	201	C	N3-C2-O2	-5.84	117.81	121.90
1	A	933	A	N3-C4-N9	-5.84	122.73	127.40
1	A	1288	U	C4-C5-C6	5.84	123.20	119.70
1	A	1260	G	C5-C6-O6	5.84	132.10	128.60
1	A	127	A	C5-C6-N1	5.83	120.62	117.70
1	A	652(J)	G	C8-N9-C4	-5.83	104.07	106.40
1	A	252	G	C8-N9-C4	-5.83	104.07	106.40
1	A	271(M)	G	N9-C4-C5	-5.83	103.07	105.40
1	A	2705	A	C5-C6-N6	-5.83	119.04	123.70
1	A	1347	G	N9-C4-C5	5.83	107.73	105.40
1	A	1373	A	N1-C2-N3	5.83	132.21	129.30
1	A	2105	C	N3-C4-C5	-5.83	119.57	121.90
1	A	2068	U	N1-C2-O2	-5.82	118.72	122.80
1	A	2233	U	N3-C4-O4	-5.82	115.32	119.40
1	A	2769	C	C2-N3-C4	-5.82	116.99	119.90
1	A	2431	U	C5-C6-N1	-5.82	119.79	122.70
1	A	2057	A	C4-C5-N7	-5.82	107.79	110.70
21	Z	77	ASP	CB-CG-OD1	5.82	123.53	118.30
1	A	701	G	C5-C6-O6	5.81	132.09	128.60
1	A	1757	U	C2-N3-C4	-5.81	123.51	127.00
1	A	2068	U	N1-C2-N3	5.81	118.39	114.90
1	A	272(H)	C	N3-C4-C5	5.81	124.22	121.90
1	A	1541	G	C4-C5-N7	-5.81	108.47	110.80
1	A	1880	C	N3-C2-O2	-5.81	117.83	121.90
1	A	2496	C	C2-N3-C4	-5.81	117.00	119.90
1	A	614	U	C6-N1-C2	-5.81	117.52	121.00
1	A	2556	C	N1-C2-O2	-5.81	115.42	118.90
1	A	481	G	C5-C6-N1	5.80	114.40	111.50
1	A	582	G	N3-C4-C5	-5.80	125.70	128.60
1	A	2497	A	C5-C6-N6	5.80	128.34	123.70
1	A	2606	C	C5-C6-N1	-5.80	118.10	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	645	C	C6-N1-C2	-5.80	117.98	120.30
1	A	1189	A	N9-C4-C5	-5.80	103.48	105.80
1	A	2161	C	C2-N3-C4	5.80	122.80	119.90
1	A	2371	G	N3-C2-N2	5.80	123.96	119.90
1	A	36	G	N1-C2-N3	5.80	127.38	123.90
1	A	681	G	N7-C8-N9	-5.80	110.20	113.10
1	A	527	C	C2-N3-C4	-5.80	117.00	119.90
3	D	43	ARG	NE-CZ-NH2	5.80	123.20	120.30
1	A	1204	A	C8-N9-C4	-5.79	103.48	105.80
1	A	1140	C	C5-C4-N4	5.79	124.26	120.20
1	A	1490	A	N7-C8-N9	-5.79	110.90	113.80
1	A	1362	C	C6-N1-C2	-5.79	117.98	120.30
1	A	1379	A	C8-N9-C4	5.79	108.12	105.80
22	0	77	ARG	NE-CZ-NH1	-5.79	117.41	120.30
1	A	1595	G	C8-N9-C4	-5.79	104.08	106.40
1	A	10	G	N1-C6-O6	-5.79	116.43	119.90
1	A	1170	G	C5-N7-C8	-5.79	101.41	104.30
1	A	2249	U	N1-C2-O2	5.79	126.85	122.80
1	A	1487	G	C8-N9-C4	-5.78	104.09	106.40
1	A	2564	A	C2-N3-C4	5.78	113.49	110.60
1	A	71	A	C8-N9-C4	-5.78	103.49	105.80
1	A	1817	G	C4-C5-N7	5.78	113.11	110.80
13	R	17	ARG	NE-CZ-NH1	-5.78	117.41	120.30
1	A	1475	G	C8-N9-C4	-5.78	104.09	106.40
1	A	1654	A	C4-C5-N7	-5.78	107.81	110.70
1	A	795	C	C5-C4-N4	5.78	124.24	120.20
1	A	2182	G	N9-C4-C5	5.78	107.71	105.40
1	A	2875	C	C2-N3-C4	-5.78	117.01	119.90
20	Y	79	CYS	CB-CA-C	-5.78	98.85	110.40
1	A	841	A	N1-C2-N3	5.77	132.19	129.30
1	A	998	C	N1-C2-O2	5.77	122.36	118.90
1	A	1653	G	C6-N1-C2	-5.77	121.64	125.10
1	A	933	A	N3-C4-C5	5.77	130.84	126.80
1	A	1204	A	C4-N9-C1'	5.77	136.69	126.30
1	A	2045	C	C5-C6-N1	-5.77	118.11	121.00
1	A	146	G	N3-C2-N2	5.77	123.94	119.90
1	A	200	U	C4-C5-C6	5.77	123.16	119.70
1	A	1110	G	N3-C2-N2	-5.77	115.86	119.90
1	A	2437	U	C4-C5-C6	5.77	123.16	119.70
1	A	1162	G	C5-N7-C8	5.77	107.18	104.30
1	A	28	A	N7-C8-N9	5.77	116.68	113.80
1	A	399	G	N1-C6-O6	5.77	123.36	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2552	U	N3-C2-O2	5.77	126.24	122.20
1	A	208	C	C6-N1-C2	5.76	122.61	120.30
1	A	295	G	N1-C6-O6	5.76	123.36	119.90
1	A	481	G	C2-N3-C4	5.76	114.78	111.90
1	A	1882	C	N1-C2-O2	5.76	122.36	118.90
1	A	139	G	C5-C6-N1	5.76	114.38	111.50
1	A	1575	C	C5-C4-N4	-5.76	116.17	120.20
1	A	650	C	N1-C2-O2	5.76	122.36	118.90
1	A	2410	G	C8-N9-C4	-5.75	104.10	106.40
1	A	451	C	C5-C6-N1	-5.75	118.12	121.00
1	A	1840	G	C5-C6-N1	5.75	114.38	111.50
1	A	2892	A	N7-C8-N9	5.75	116.67	113.80
1	A	1776	G	N9-C4-C5	-5.75	103.10	105.40
1	A	2191	G	C4-C5-N7	5.75	113.10	110.80
1	A	2445	G	N1-C6-O6	-5.75	116.45	119.90
29	7	34	ARG	NE-CZ-NH1	-5.75	117.43	120.30
1	A	1208	C	N1-C2-O2	-5.74	115.45	118.90
1	A	2251	G	C2-N3-C4	5.74	114.77	111.90
1	A	154(A)	C	N1-C2-O2	5.74	122.34	118.90
1	A	820	A	N1-C6-N6	-5.74	115.16	118.60
1	A	932	G	C5-C6-O6	5.74	132.04	128.60
1	A	2070	G	N3-C2-N2	5.74	123.92	119.90
13	R	114	VAL	CB-CA-C	-5.74	100.49	111.40
1	A	382	G	C5-N7-C8	5.74	107.17	104.30
1	A	1586	A	N9-C4-C5	5.74	108.09	105.80
1	A	2483	C	N3-C4-C5	-5.74	119.61	121.90
1	A	2491	U	C2-N3-C4	-5.74	123.56	127.00
1	A	735	A	C5-C6-N6	5.73	128.29	123.70
1	A	988	A	N9-C4-C5	-5.73	103.51	105.80
1	A	650	C	N3-C2-O2	-5.73	117.89	121.90
2	B	24	G	N1-C6-O6	5.73	123.34	119.90
1	A	1204	A	O4'-C1'-N9	5.73	112.78	108.20
1	A	1618	A	C4-C5-N7	-5.73	107.84	110.70
1	A	2261	C	C6-N1-C2	-5.73	118.01	120.30
1	A	2499	C	N3-C4-C5	-5.73	119.61	121.90
1	A	1900	A	C2-N3-C4	5.73	113.46	110.60
1	A	1164	G	C5-C6-O6	5.72	132.03	128.60
1	A	1221(A)	C	N3-C4-C5	5.72	124.19	121.90
1	A	1611	C	C4-C5-C6	5.72	120.26	117.40
2	B	75	G	C8-N9-C4	-5.72	104.11	106.40
20	Y	2	ARG	CD-NE-CZ	5.72	131.61	123.60
1	A	40	C	C5-C6-N1	-5.71	118.14	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2627	G	N9-C4-C5	-5.71	103.11	105.40
2	B	56	G	C8-N9-C4	-5.71	104.11	106.40
1	A	12	U	C6-N1-C2	-5.71	117.57	121.00
1	A	616	G	C5-C6-O6	5.71	132.03	128.60
1	A	646	A	N7-C8-N9	5.71	116.66	113.80
1	A	1396	U	C4-C5-C6	5.71	123.13	119.70
1	A	2233	U	C6-N1-C2	-5.71	117.57	121.00
1	A	1189	A	N1-C6-N6	5.71	122.03	118.60
1	A	2138	C	C2-N3-C4	5.71	122.75	119.90
1	A	2483	C	C6-N1-C2	-5.71	118.02	120.30
2	B	6	C	C6-N1-C2	5.71	122.58	120.30
1	A	1994	C	C5-C6-N1	-5.71	118.15	121.00
1	A	2525	G	C8-N9-C4	5.71	108.68	106.40
1	A	117	G	C2-N3-C4	5.70	114.75	111.90
1	A	2545	G	N3-C4-N9	5.70	129.42	126.00
1	A	1933	G	C4-C5-N7	-5.70	108.52	110.80
1	A	1043	C	N3-C4-C5	-5.70	119.62	121.90
1	A	2529	G	C5-C6-O6	-5.70	125.18	128.60
1	A	2435	A	C8-N9-C4	-5.70	103.52	105.80
1	A	135	G	C8-N9-C4	5.69	108.68	106.40
1	A	2053	G	C4-C5-N7	-5.69	108.52	110.80
1	A	41	C	C6-N1-C2	5.69	122.58	120.30
1	A	582	G	C5-N7-C8	5.69	107.14	104.30
1	A	582	G	C4-C5-N7	-5.69	108.52	110.80
1	A	479	A	C6-C5-N7	5.69	136.28	132.30
1	A	589	C	N1-C2-O2	5.69	122.31	118.90
1	A	1154	G	C6-N1-C2	-5.68	121.69	125.10
1	A	1813	G	N9-C4-C5	-5.68	103.13	105.40
1	A	1814	G	N3-C2-N2	5.68	123.88	119.90
1	A	1886	C	N1-C2-O2	-5.68	115.49	118.90
1	A	2318	G	N1-C6-O6	-5.68	116.49	119.90
1	A	1223	G	C6-C5-N7	5.68	133.81	130.40
1	A	677	A	N9-C4-C5	5.68	108.07	105.80
1	A	1653	G	C4-N9-C1'	5.68	133.88	126.50
31	9	35	ARG	NE-CZ-NH1	-5.68	117.46	120.30
1	A	461	C	C5-C6-N1	-5.67	118.16	121.00
1	A	1363	C	N3-C4-C5	5.67	124.17	121.90
1	A	1582	C	N3-C2-O2	-5.67	117.93	121.90
1	A	2356	C	N1-C2-O2	-5.67	115.50	118.90
1	A	131	G	C5-C6-N1	5.67	114.34	111.50
1	A	200	U	C5-C6-N1	-5.67	119.86	122.70
1	A	1327	C	C6-N1-C2	-5.67	118.03	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1527	G	N3-C2-N2	-5.67	115.93	119.90
1	A	426	C	N1-C2-O2	5.67	122.30	118.90
1	A	1379	A	N9-C4-C5	-5.67	103.53	105.80
1	A	2627	G	C8-N9-C4	5.67	108.67	106.40
1	A	658	C	C2-N3-C4	-5.67	117.07	119.90
1	A	1674	G	C4-N9-C1'	5.67	133.86	126.50
1	A	393	C	N1-C2-N3	5.66	123.17	119.20
1	A	652(S)	C	C2-N1-C1'	5.66	125.03	118.80
1	A	839	U	N1-C2-N3	5.66	118.30	114.90
1	A	1249	U	C5-C6-N1	-5.66	119.87	122.70
1	A	2078	C	N1-C2-N3	5.66	123.16	119.20
1	A	2869	G	N7-C8-N9	5.66	115.93	113.10
1	A	2363	C	N3-C4-N4	-5.66	114.04	118.00
1	A	271(J)	C	N3-C4-C5	5.66	124.16	121.90
1	A	737	C	C5-C6-N1	-5.66	118.17	121.00
1	A	935	C	N1-C2-O2	-5.66	115.50	118.90
1	A	1453	U	N1-C2-O2	-5.66	118.84	122.80
1	A	1826	G	N9-C4-C5	5.66	107.66	105.40
1	A	2617	C	N3-C4-N4	-5.66	114.04	118.00
1	A	1453	U	C2-N3-C4	-5.66	123.61	127.00
1	A	1459	G	N1-C2-N2	-5.66	111.11	116.20
1	A	2438	U	N1-C2-O2	-5.66	118.84	122.80
1	A	1189	A	C5-C6-N6	-5.65	119.18	123.70
1	A	546	C	C5-C6-N1	5.65	123.83	121.00
1	A	2079	U	C5-C6-N1	-5.65	119.87	122.70
1	A	475	U	C4-C5-C6	5.65	123.09	119.70
1	A	2457	U	N1-C2-O2	-5.65	118.84	122.80
1	A	1685	C	C5-C4-N4	-5.65	116.25	120.20
1	A	2584	U	C4-C5-C6	-5.65	116.31	119.70
1	A	1291	C	N3-C4-C5	-5.65	119.64	121.90
18	W	15	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	A	1260	G	C5-C6-N1	-5.65	108.68	111.50
1	A	2249	U	N3-C2-O2	-5.64	118.25	122.20
1	A	2335	A	N3-C4-N9	5.64	131.91	127.40
1	A	17	G	N3-C2-N2	-5.64	115.95	119.90
1	A	812	C	C5-C6-N1	5.64	123.82	121.00
1	A	823	G	N1-C6-O6	-5.64	116.51	119.90
1	A	2208	A	C8-N9-C4	-5.64	103.54	105.80
1	A	1200	C	N1-C2-N3	5.64	123.15	119.20
1	A	2586	C	N1-C2-O2	-5.64	115.52	118.90
2	B	49	C	C5-C6-N1	5.64	123.82	121.00
1	A	45	C	N3-C4-C5	5.63	124.15	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	578	A	N9-C4-C5	5.63	108.05	105.80
1	A	2377	A	C2-N3-C4	-5.63	107.78	110.60
1	A	2821	A	N9-C4-C5	-5.63	103.55	105.80
1	A	2066	C	N3-C2-O2	-5.63	117.96	121.90
1	A	123	G	C5-N7-C8	5.63	107.12	104.30
1	A	1377	G	N3-C4-C5	-5.62	125.79	128.60
1	A	1818	U	C5-C4-O4	-5.62	122.53	125.90
1	A	2456	C	C6-N1-C2	-5.62	118.05	120.30
1	A	192	C	C2-N1-C1'	-5.62	112.62	118.80
1	A	2426	A	C5-C6-N6	-5.62	119.20	123.70
1	A	778	G	N1-C6-O6	-5.62	116.53	119.90
1	A	962	G	C5-N7-C8	5.62	107.11	104.30
1	A	2475	C	C6-N1-C2	-5.62	118.05	120.30
11	P	27	HIS	CB-CA-C	-5.62	99.17	110.40
1	A	684	G	N7-C8-N9	5.62	115.91	113.10
1	A	732	C	N1-C2-O2	-5.61	115.53	118.90
1	A	684	G	C8-N9-C4	-5.61	104.16	106.40
1	A	271(H)	G	C8-N9-C1'	-5.61	119.71	127.00
1	A	1300	U	P-O3'-C3'	5.61	126.43	119.70
1	A	56	A	N1-C6-N6	-5.61	115.23	118.60
1	A	1997	G	C5-N7-C8	5.61	107.10	104.30
1	A	35	G	N3-C4-C5	-5.61	125.80	128.60
1	A	1126	A	C5-C6-N6	-5.61	119.22	123.70
1	A	1035	U	C2-N3-C4	-5.60	123.64	127.00
1	A	2611	U	N3-C4-C5	-5.60	111.24	114.60
1	A	671	C	C6-N1-C1'	5.60	127.52	120.80
1	A	2454	G	N3-C4-C5	-5.60	125.80	128.60
1	A	2495	G	C2-N3-C4	-5.60	109.10	111.90
1	A	2581	G	C5-C6-O6	5.60	131.96	128.60
1	A	545	G	C4-C5-N7	5.60	113.04	110.80
1	A	655	A	N7-C8-N9	5.60	116.60	113.80
1	A	1962	C	N3-C2-O2	5.60	125.82	121.90
2	B	7	G	C5-C6-O6	-5.59	125.24	128.60
21	Z	74	VAL	CB-CA-C	-5.59	100.77	111.40
31	9	32	HIS	ND1-CG-CD2	-5.59	98.17	106.00
1	A	1045	A	N1-C6-N6	-5.59	115.24	118.60
1	A	2629	A	C2-N3-C4	-5.59	107.80	110.60
1	A	347	A	C8-N9-C4	5.59	108.04	105.80
1	A	1842	G	C8-N9-C4	-5.59	104.16	106.40
1	A	1936	A	C5-N7-C8	-5.59	101.11	103.90
1	A	2642	G	N3-C2-N2	5.59	123.81	119.90
1	A	2041	U	N3-C4-O4	5.59	123.31	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	426	C	N3-C2-O2	-5.59	117.99	121.90
1	A	2072	G	C8-N9-C4	5.59	108.64	106.40
1	A	2506	U	N3-C4-O4	-5.59	115.49	119.40
2	B	20	C	N3-C4-N4	5.59	121.91	118.00
1	A	135	G	N7-C8-N9	-5.58	110.31	113.10
1	A	370	G	C2-N3-C4	5.58	114.69	111.90
1	A	741	G	N1-C6-O6	-5.58	116.55	119.90
2	B	24	G	C5-C6-O6	-5.58	125.25	128.60
1	A	1382	G	C5-C6-O6	-5.58	125.25	128.60
1	A	1609	A	C5-C6-N1	5.58	120.49	117.70
1	A	2549	G	N7-C8-N9	5.58	115.89	113.10
2	B	29	A	N1-C6-N6	5.58	121.95	118.60
1	A	244	A	C8-N9-C4	-5.58	103.57	105.80
1	A	1333	C	C5-C4-N4	-5.58	116.29	120.20
1	A	2066	C	N1-C2-N3	5.58	123.11	119.20
1	A	1977	A	N7-C8-N9	-5.58	111.01	113.80
1	A	529	A	C4-C5-N7	5.58	113.49	110.70
1	A	893	C	C6-N1-C1'	-5.58	114.11	120.80
1	A	1652	A	C5-C6-N1	-5.58	114.91	117.70
1	A	1122	G	C4-C5-N7	5.57	113.03	110.80
1	A	1328	G	N1-C2-N2	-5.57	111.19	116.20
1	A	1652	A	N1-C6-N6	5.57	121.94	118.60
1	A	2704	C	C6-N1-C2	-5.57	118.07	120.30
1	A	1681	G	C4-C5-N7	5.57	113.03	110.80
1	A	2182	G	C8-N9-C1'	5.57	134.24	127.00
1	A	777	A	N1-C2-N3	5.57	132.08	129.30
1	A	1721	G	N3-C2-N2	5.57	123.80	119.90
1	A	2037	G	C8-N9-C4	-5.57	104.17	106.40
1	A	2465	C	C5-C4-N4	-5.57	116.30	120.20
1	A	2567	G	N7-C8-N9	-5.57	110.32	113.10
1	A	2858	C	N3-C2-O2	5.57	125.80	121.90
1	A	2777	G	N7-C8-N9	-5.56	110.32	113.10
1	A	298	G	N1-C2-N2	-5.56	111.19	116.20
1	A	1261	C	N3-C4-C5	5.56	124.12	121.90
1	A	1578	U	N3-C2-O2	-5.56	118.31	122.20
1	A	883	G	C5-C6-O6	-5.56	125.26	128.60
1	A	2228	G	C5-C6-O6	5.56	131.94	128.60
1	A	1490	A	C8-N9-C4	5.56	108.02	105.80
1	A	1689	A	N1-C6-N6	-5.56	115.27	118.60
1	A	1650	G	N9-C4-C5	5.56	107.62	105.40
1	A	1279	G	N1-C6-O6	-5.56	116.57	119.90
1	A	65	C	C6-N1-C2	-5.55	118.08	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	669	G	C8-N9-C4	5.55	108.62	106.40
1	A	759	G	C2-N3-C4	5.55	114.68	111.90
1	A	1284	A	C2-N3-C4	-5.55	107.82	110.60
1	A	1326	U	N3-C2-O2	-5.55	118.31	122.20
1	A	1363	C	C2-N3-C4	-5.55	117.12	119.90
1	A	1610	A	C5-C6-N1	5.55	120.47	117.70
1	A	298	G	C5-N7-C8	5.55	107.07	104.30
1	A	575	A	N9-C4-C5	5.55	108.02	105.80
1	A	1343	G	C2-N3-C4	5.55	114.67	111.90
1	A	1627	G	N3-C2-N2	5.55	123.78	119.90
1	A	2444	G	N1-C6-O6	-5.55	116.57	119.90
11	P	103	ALA	N-CA-C	-5.54	96.03	111.00
1	A	1433	U	N3-C4-O4	-5.54	115.52	119.40
1	A	116	C	C5-C4-N4	5.54	124.08	120.20
1	A	975	C	N3-C4-C5	5.54	124.12	121.90
1	A	2304	G	C8-N9-C4	-5.54	104.18	106.40
1	A	516	C	C6-N1-C2	5.54	122.52	120.30
1	A	1541	G	C5-C6-O6	5.54	131.92	128.60
1	A	1595	G	N7-C8-N9	5.54	115.87	113.10
1	A	2591	C	C2-N3-C4	-5.54	117.13	119.90
1	A	1564	C	C2-N3-C4	5.53	122.67	119.90
1	A	265	A	N3-C4-C5	5.53	130.67	126.80
1	A	517	C	C5-C4-N4	-5.53	116.33	120.20
1	A	861	A	N1-C2-N3	-5.53	126.53	129.30
1	A	1260	G	C4-C5-N7	-5.53	108.59	110.80
1	A	1320	C	N3-C4-N4	-5.53	114.13	118.00
10	O	78	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	A	1835	G	N3-C4-N9	5.53	129.32	126.00
1	A	2512	C	N1-C2-O2	-5.53	115.58	118.90
1	A	132	G	C5-C6-N1	-5.52	108.74	111.50
1	A	788	A	C6-N1-C2	5.52	121.91	118.60
1	A	1256	G	N9-C4-C5	-5.52	103.19	105.40
30	8	30	ARG	NE-CZ-NH2	5.52	123.06	120.30
1	A	702	G	N7-C8-N9	-5.52	110.34	113.10
1	A	1140	C	N1-C2-N3	5.52	123.06	119.20
1	A	1963	U	N3-C2-O2	-5.52	118.33	122.20
1	A	2394	C	N1-C2-O2	-5.52	115.59	118.90
2	B	103	G	N1-C6-O6	5.52	123.21	119.90
1	A	562	U	C6-N1-C2	-5.52	117.69	121.00
1	A	1558	A	C8-N9-C4	-5.52	103.59	105.80
1	A	2296	U	C3'-C2'-C1'	-5.52	97.09	101.50
1	A	2304	G	C4-C5-N7	-5.52	108.59	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1788	C	C2-N3-C4	5.51	122.66	119.90
1	A	2207	G	C6-C5-N7	-5.51	127.09	130.40
1	A	53	A	C8-N9-C4	-5.51	103.59	105.80
1	A	834	C	N1-C2-O2	-5.51	115.59	118.90
1	A	1609	A	C2-N3-C4	5.51	113.36	110.60
1	A	1194	A	C4-C5-C6	-5.51	114.24	117.00
1	A	1237	A	C8-N9-C4	-5.51	103.59	105.80
1	A	1395	A	C2-N3-C4	5.51	113.36	110.60
1	A	1565	C	N3-C2-O2	5.51	125.76	121.90
1	A	1791	A	C8-N9-C4	-5.51	103.59	105.80
1	A	1835	G	C6-C5-N7	-5.51	127.09	130.40
1	A	1942	C	C5-C6-N1	5.51	123.75	121.00
1	A	211	A	C8-N9-C4	5.51	108.00	105.80
1	A	652(I)	C	C6-N1-C2	-5.51	118.10	120.30
1	A	1403	C	N1-C2-N3	5.51	123.06	119.20
1	A	2575	C	N3-C2-O2	-5.51	118.05	121.90
1	A	2522	U	N3-C4-O4	5.50	123.25	119.40
1	A	764	A	C6-N1-C2	-5.50	115.30	118.60
1	A	2615	U	N3-C4-O4	-5.50	115.55	119.40
1	A	187	G	C6-N1-C2	-5.50	121.80	125.10
1	A	829	A	N9-C4-C5	-5.50	103.60	105.80
1	A	2437	U	C5-C6-N1	-5.50	119.95	122.70
1	A	2512	C	C5-C4-N4	-5.50	116.35	120.20
1	A	1437	C	C6-N1-C2	-5.50	118.10	120.30
1	A	1558	A	C5-C6-N1	-5.50	114.95	117.70
1	A	1754	C	C2-N3-C4	-5.50	117.15	119.90
1	A	2006	C	C5-C6-N1	5.50	123.75	121.00
1	A	2318	G	N7-C8-N9	-5.50	110.35	113.10
1	A	951	C	N1-C2-O2	5.50	122.20	118.90
1	A	1401	G	N3-C4-N9	-5.50	122.70	126.00
1	A	2597	G	N3-C2-N2	-5.50	116.05	119.90
15	T	118	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	1391	U	N3-C2-O2	-5.50	118.35	122.20
1	A	1901	A	C2-N3-C4	5.50	113.35	110.60
1	A	2198	A	C2-N3-C4	5.49	113.35	110.60
1	A	102	G	P-O3'-C3'	5.49	126.29	119.70
1	A	194	G	N1-C2-N2	-5.49	111.26	116.20
1	A	2378	A	N1-C6-N6	5.49	121.89	118.60
1	A	2397	G	N3-C2-N2	-5.49	116.06	119.90
12	Q	135	ASP	CB-CA-C	-5.49	99.42	110.40
1	A	1274	A	C5-C6-N1	-5.49	114.96	117.70
1	A	735	A	C5-N7-C8	5.48	106.64	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2613	U	C4-C5-C6	-5.48	116.41	119.70
1	A	706	A	N7-C8-N9	5.48	116.54	113.80
1	A	805	G	C5-C6-N1	5.48	114.24	111.50
1	A	1813	G	N3-C2-N2	-5.48	116.06	119.90
1	A	584	C	N3-C4-N4	5.48	121.83	118.00
1	A	781	A	C2-N3-C4	5.48	113.34	110.60
1	A	1185	C	C5-C4-N4	5.47	124.03	120.20
1	A	2039	C	C5-C6-N1	5.47	123.74	121.00
1	A	1111	A	C8-N9-C4	5.47	107.99	105.80
1	A	2570	G	N1-C2-N3	-5.47	120.62	123.90
21	Z	151	HIS	N-CA-C	5.47	125.77	111.00
1	A	1266	G	N9-C4-C5	-5.47	103.21	105.40
1	A	1493	C	C6-N1-C1'	-5.47	114.23	120.80
1	A	838	C	C4-C5-C6	5.47	120.14	117.40
1	A	2588	G	N1-C2-N3	-5.47	120.62	123.90
1	A	107	C	C6-N1-C2	5.47	122.49	120.30
1	A	506	G	C8-N9-C4	-5.47	104.21	106.40
1	A	2500	U	N1-C2-O2	5.47	126.63	122.80
1	A	1799	G	N1-C2-N2	-5.46	111.28	116.20
1	A	2017	U	N1-C2-N3	5.46	118.18	114.90
1	A	325	G	C5-C6-N1	-5.46	108.77	111.50
1	A	1777	U	C5-C4-O4	5.46	129.18	125.90
1	A	672	C	N3-C4-C5	5.46	124.08	121.90
1	A	2574	G	C8-N9-C4	-5.46	104.22	106.40
1	A	217	G	N9-C4-C5	-5.46	103.22	105.40
1	A	362	U	N1-C2-O2	-5.46	118.98	122.80
1	A	2615	U	N1-C2-O2	5.46	126.62	122.80
1	A	1328	G	N1-C6-O6	-5.46	116.63	119.90
1	A	552	G	N7-C8-N9	-5.45	110.37	113.10
1	A	565	C	C5-C4-N4	5.45	124.02	120.20
1	A	1247	A	C8-N9-C4	5.45	107.98	105.80
2	B	97	G	N1-C6-O6	5.45	123.17	119.90
1	A	643	A	C8-N9-C4	-5.45	103.62	105.80
1	A	1339	G	C5-C6-O6	-5.45	125.33	128.60
1	A	2036	C	N3-C2-O2	5.45	125.72	121.90
1	A	1471	A	N7-C8-N9	5.45	116.53	113.80
1	A	79	G	C5-C6-O6	-5.45	125.33	128.60
1	A	822	U	C5-C6-N1	5.45	125.42	122.70
1	A	829	A	N1-C6-N6	5.45	121.87	118.60
1	A	1164	G	C4-C5-N7	-5.45	108.62	110.80
1	A	2894	G	C4-N9-C1'	5.45	133.58	126.50
1	A	1451	C	N3-C2-O2	-5.45	118.09	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1047	G	N3-C4-N9	5.44	129.26	126.00
4	E	78	LEU	CA-CB-CG	5.44	127.82	115.30
1	A	1800	C	C4-C5-C6	5.44	120.12	117.40
1	A	2628	C	N3-C4-C5	5.44	124.08	121.90
1	A	1582	C	N3-C4-N4	-5.44	114.19	118.00
1	A	1817	G	C8-N9-C4	5.44	108.58	106.40
1	A	1956	U	N3-C4-C5	5.44	117.86	114.60
1	A	2791	C	C5-C6-N1	5.44	123.72	121.00
2	B	103	G	C2-N3-C4	-5.44	109.18	111.90
1	A	1754	C	N1-C2-O2	-5.44	115.64	118.90
1	A	2249	U	N3-C4-O4	-5.44	115.59	119.40
1	A	2685	G	N1-C6-O6	-5.44	116.64	119.90
1	A	486	C	C4-C5-C6	5.43	120.12	117.40
1	A	691	C	C6-N1-C2	-5.43	118.13	120.30
1	A	781	A	C5-C6-N1	5.43	120.42	117.70
1	A	2597	G	C5-C6-O6	-5.43	125.34	128.60
1	A	792	G	C8-N9-C4	-5.43	104.23	106.40
1	A	1933	G	N9-C4-C5	5.43	107.57	105.40
1	A	2609	U	N1-C2-O2	-5.43	119.00	122.80
1	A	2303	G	C6-C5-N7	5.43	133.66	130.40
1	A	242	G	C5-C6-O6	5.43	131.86	128.60
1	A	1663	C	N3-C2-O2	-5.42	118.10	121.90
1	A	2044	C	C2-N3-C4	-5.42	117.19	119.90
1	A	2076	U	N1-C2-N3	5.42	118.16	114.90
31	9	9	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	2864	G	N1-C6-O6	-5.42	116.65	119.90
1	A	585	G	C2-N3-C4	5.42	114.61	111.90
1	A	395	U	C6-N1-C1'	-5.42	113.61	121.20
1	A	131	G	N1-C2-N2	-5.42	111.32	116.20
1	A	192	C	C4-C5-C6	5.42	120.11	117.40
1	A	1203	G	N1-C6-O6	-5.42	116.65	119.90
1	A	1256	G	N1-C6-O6	5.42	123.15	119.90
1	A	2438	U	C2-N3-C4	-5.42	123.75	127.00
1	A	2599	G	C5-C6-N1	5.42	114.21	111.50
1	A	362	U	N3-C4-C5	5.42	117.85	114.60
1	A	1155	A	N1-C6-N6	-5.42	115.35	118.60
1	A	1618	A	C5-C6-N6	5.42	128.03	123.70
1	A	2782	G	N3-C2-N2	5.42	123.69	119.90
1	A	28	A	C8-N9-C4	-5.42	103.63	105.80
1	A	179	G	N1-C6-O6	5.42	123.15	119.90
1	A	2512	C	N3-C4-C5	5.42	124.07	121.90
1	A	1311	G	N9-C4-C5	5.41	107.57	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2026	C	C6-N1-C2	5.41	122.47	120.30
1	A	2710	C	C5-C4-N4	-5.41	116.41	120.20
1	A	566	U	C2-N3-C4	5.41	130.25	127.00
1	A	1109	C	N1-C2-O2	-5.41	115.65	118.90
1	A	1367	A	C8-N9-C4	5.41	107.96	105.80
1	A	763	G	C2-N3-C4	5.41	114.60	111.90
1	A	13	A	C8-N9-C4	-5.41	103.64	105.80
1	A	326	G	N1-C2-N2	5.41	121.06	116.20
1	A	1188	U	N3-C2-O2	-5.41	118.42	122.20
1	A	1617	C	N1-C2-O2	-5.41	115.66	118.90
1	A	223	A	N9-C4-C5	5.40	107.96	105.80
1	A	809	G	C6-C5-N7	5.40	133.64	130.40
1	A	1047	G	C2-N3-C4	5.40	114.60	111.90
1	A	1943	U	C2-N3-C4	-5.40	123.76	127.00
1	A	2757	A	N7-C8-N9	5.40	116.50	113.80
1	A	265	A	N3-C4-N9	-5.40	123.08	127.40
1	A	598	G	N1-C6-O6	-5.40	116.66	119.90
1	A	2051	A	N7-C8-N9	-5.40	111.10	113.80
1	A	2237	G	N9-C4-C5	-5.40	103.24	105.40
1	A	481	G	N7-C8-N9	5.40	115.80	113.10
1	A	975	C	C2-N3-C4	-5.40	117.20	119.90
1	A	1459	G	N3-C2-N2	5.40	123.68	119.90
1	A	1988	C	C5-C6-N1	-5.40	118.30	121.00
1	A	2347	C	N3-C2-O2	-5.40	118.12	121.90
1	A	1899	G	C5-N7-C8	-5.40	101.60	104.30
1	A	2629	A	N1-C2-N3	5.40	132.00	129.30
1	A	279	C	C5-C6-N1	5.39	123.70	121.00
1	A	2615	U	N3-C4-C5	5.39	117.84	114.60
1	A	2710	C	C2-N3-C4	-5.39	117.20	119.90
1	A	2719	G	C5-C6-O6	-5.39	125.36	128.60
1	A	622	G	C4-C5-N7	-5.39	108.64	110.80
1	A	699	A	C6-N1-C2	-5.39	115.36	118.60
1	A	1582	C	C5-C4-N4	5.39	123.97	120.20
1	A	2656	U	C2-N1-C1'	5.39	124.17	117.70
2	B	24	G	N3-C4-N9	5.39	129.24	126.00
1	A	2199	A	C8-N9-C1'	-5.39	118.00	127.70
1	A	2686	G	N7-C8-N9	5.39	115.80	113.10
1	A	1930	G	C2-N3-C4	5.39	114.59	111.90
1	A	2611	U	C6-N1-C2	-5.39	117.77	121.00
1	A	271(J)	C	C6-N1-C2	5.38	122.45	120.30
1	A	1138	G	C5-C6-O6	-5.38	125.37	128.60
1	A	1618	A	C8-N9-C4	-5.38	103.65	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1752	C	C2-N1-C1'	-5.38	112.88	118.80
1	A	2549	G	C2-N3-C4	5.38	114.59	111.90
1	A	2363	C	C6-N1-C2	5.38	122.45	120.30
1	A	2039	C	C2-N3-C4	5.38	122.59	119.90
1	A	2465	C	N3-C4-C5	5.38	124.05	121.90
1	A	2733	A	N7-C8-N9	5.38	116.49	113.80
1	A	2249	U	C2-N3-C4	-5.38	123.78	127.00
9	N	76	SER	C-N-CA	-5.38	111.01	122.30
1	A	576	U	C5-C6-N1	5.37	125.39	122.70
1	A	1653	G	P-O3'-C3'	5.37	126.15	119.70
1	A	2821	A	C8-N9-C4	5.37	107.95	105.80
1	A	403	U	N3-C2-O2	-5.37	118.44	122.20
1	A	1609	A	N1-C6-N6	-5.37	115.38	118.60
1	A	2460	U	N3-C2-O2	-5.37	118.44	122.20
1	A	113	G	N1-C2-N2	5.37	121.03	116.20
1	A	203	C	N1-C2-O2	-5.37	115.68	118.90
1	A	212	G	C5-N7-C8	-5.37	101.62	104.30
1	A	325	G	C6-N1-C2	5.37	128.32	125.10
1	A	209	C	N3-C2-O2	-5.37	118.14	121.90
1	A	1438	U	C5-C6-N1	-5.37	120.02	122.70
1	A	1789	A	C5-N7-C8	5.37	106.58	103.90
1	A	23	G	C5-N7-C8	5.37	106.98	104.30
1	A	231	C	C4-C5-C6	5.37	120.08	117.40
1	A	370	G	N9-C4-C5	5.37	107.55	105.40
1	A	2560	C	C5-C4-N4	-5.37	116.44	120.20
2	B	31	C	C5-C4-N4	5.37	123.96	120.20
2	B	76	G	N3-C4-C5	5.37	131.28	128.60
1	A	229	A	C8-N9-C4	-5.36	103.66	105.80
1	A	351	G	N1-C6-O6	5.36	123.12	119.90
1	A	392	C	C6-N1-C2	5.36	122.44	120.30
1	A	1394	U	C5-C4-O4	-5.36	122.68	125.90
1	A	72	U	C2-N3-C4	-5.36	123.78	127.00
1	A	1633	G	C2-N3-C4	5.36	114.58	111.90
1	A	2586	C	N3-C2-O2	5.36	125.65	121.90
1	A	643	A	N1-C2-N3	5.36	131.98	129.30
1	A	1127	A	C6-N1-C2	5.36	121.81	118.60
1	A	2885	C	C5-C6-N1	5.36	123.68	121.00
1	A	964	C	N1-C2-O2	5.35	122.11	118.90
1	A	1442	G	C8-N9-C4	-5.35	104.26	106.40
1	A	113	G	N3-C4-C5	5.35	131.28	128.60
1	A	2003	G	C6-N1-C2	-5.35	121.89	125.10
1	A	2497	A	N1-C2-N3	5.35	131.98	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1567	A	C8-N9-C4	-5.35	103.66	105.80
1	A	2056	G	C4-C5-C6	-5.35	115.59	118.80
1	A	269	U	N1-C2-N3	-5.35	111.69	114.90
1	A	1305	C	C2-N1-C1'	5.35	124.68	118.80
1	A	2807	G	N3-C4-C5	-5.35	125.93	128.60
1	A	362	U	C5-C4-O4	-5.35	122.69	125.90
1	A	471	A	N7-C8-N9	5.35	116.47	113.80
1	A	1752	C	N3-C2-O2	5.35	125.64	121.90
1	A	2508	G	C2-N3-C4	5.35	114.57	111.90
1	A	2420	C	C6-N1-C2	5.34	122.44	120.30
11	P	50	ARG	NE-CZ-NH1	-5.34	117.63	120.30
1	A	434	U	N1-C2-N3	5.34	118.10	114.90
1	A	1124	C	N3-C4-N4	5.34	121.74	118.00
1	A	1260	G	N9-C4-C5	5.34	107.54	105.40
1	A	2371	G	N7-C8-N9	-5.34	110.43	113.10
1	A	692	C	N3-C4-C5	5.34	124.03	121.90
1	A	725	G	C8-N9-C4	-5.34	104.27	106.40
1	A	822	U	C6-N1-C2	-5.34	117.80	121.00
1	A	2105	C	C5-C6-N1	5.34	123.67	121.00
1	A	409	C	C4-C5-C6	-5.33	114.73	117.40
1	A	1339	G	C8-N9-C4	5.33	108.53	106.40
1	A	2542	A	N1-C6-N6	5.33	121.80	118.60
1	A	671	C	C5-C4-N4	5.33	123.93	120.20
1	A	1346	G	C2-N3-C4	5.33	114.56	111.90
1	A	1365	A	N1-C6-N6	5.33	121.80	118.60
1	A	53	A	N1-C2-N3	5.33	131.96	129.30
1	A	524	U	N1-C2-O2	5.33	126.53	122.80
1	A	1328	G	C5-C6-O6	5.33	131.79	128.60
1	A	2772	C	C5-C4-N4	5.33	123.93	120.20
1	A	201	C	N1-C2-N3	5.32	122.93	119.20
1	A	2382	G	C8-N9-C4	-5.32	104.27	106.40
1	A	2785	C	C5-C6-N1	5.32	123.66	121.00
1	A	640	C	C5-C6-N1	5.32	123.66	121.00
1	A	2701	C	C6-N1-C2	-5.32	118.17	120.30
1	A	798	G	N7-C8-N9	-5.32	110.44	113.10
22	0	25	ARG	NE-CZ-NH1	-5.32	117.64	120.30
1	A	416	C	N1-C2-O2	5.32	122.09	118.90
1	A	645	C	C5-C6-N1	5.32	123.66	121.00
1	A	743	G	C5-C6-O6	5.32	131.79	128.60
1	A	2347	C	N1-C2-O2	5.32	122.09	118.90
1	A	773	U	C2-N3-C4	-5.32	123.81	127.00
1	A	1111	A	N3-C4-C5	5.32	130.52	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2040	C	N3-C4-C5	5.32	124.03	121.90
1	A	377	C	C2-N3-C4	-5.31	117.24	119.90
1	A	2324	C	C4-C5-C6	-5.31	114.74	117.40
1	A	2689	U	N1-C2-O2	5.31	126.52	122.80
1	A	2869	G	N3-C2-N2	-5.31	116.18	119.90
1	A	579	G	C4-C5-N7	-5.31	108.68	110.80
1	A	1414	G	N1-C6-O6	5.31	123.09	119.90
1	A	1433	U	C5-C6-N1	-5.31	120.05	122.70
1	A	2107	C	C6-N1-C2	-5.31	118.18	120.30
1	A	202	U	C2-N3-C4	-5.31	123.81	127.00
1	A	746	A	C8-N9-C4	-5.31	103.68	105.80
1	A	1823	G	N1-C2-N2	-5.31	111.42	116.20
1	A	937	U	N3-C2-O2	5.31	125.91	122.20
1	A	92	A	N7-C8-N9	5.30	116.45	113.80
1	A	700	G	N1-C6-O6	-5.30	116.72	119.90
1	A	729	G	N9-C4-C5	5.30	107.52	105.40
1	A	822	U	N1-C2-O2	5.30	126.51	122.80
1	A	1153	C	C5-C6-N1	5.30	123.65	121.00
1	A	1530	C	C5-C4-N4	-5.30	116.49	120.20
1	A	2360	A	C4-C5-C6	5.30	119.65	117.00
1	A	2634	G	C5-C6-O6	-5.30	125.42	128.60
1	A	1250	G	N1-C2-N3	-5.30	120.72	123.90
1	A	2019	A	C8-N9-C4	-5.30	103.68	105.80
1	A	786	C	C6-N1-C2	5.30	122.42	120.30
1	A	2418	A	C6-N1-C2	-5.30	115.42	118.60
1	A	179	G	C5-C6-O6	-5.29	125.42	128.60
1	A	478	A	N7-C8-N9	5.29	116.45	113.80
1	A	585	G	C5-N7-C8	5.29	106.95	104.30
1	A	49	A	N1-C6-N6	-5.29	115.42	118.60
1	A	692	C	C4-C5-C6	-5.29	114.75	117.40
1	A	766	C	C6-N1-C2	5.29	122.42	120.30
1	A	1398	C	C2-N3-C4	-5.29	117.25	119.90
1	A	1957	C	N3-C4-N4	-5.29	114.30	118.00
1	A	2057	A	C5-N7-C8	5.29	106.55	103.90
1	A	2104	G	C4-N9-C1'	5.29	133.38	126.50
1	A	2392	A	C8-N9-C4	5.29	107.92	105.80
2	B	81	G	C5-C6-N1	-5.29	108.85	111.50
11	P	116	GLY	N-CA-C	5.29	126.33	113.10
1	A	271(E)	U	N3-C2-O2	-5.29	118.50	122.20
1	A	576	U	C4-C5-C6	-5.29	116.53	119.70
1	A	777	A	C4-C5-C6	5.29	119.65	117.00
1	A	1141	U	N1-C2-N3	5.29	118.08	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1401	G	N3-C4-C5	5.29	131.25	128.60
1	A	1774	C	N3-C4-C5	-5.29	119.78	121.90
1	A	186	G	C5-C6-O6	5.28	131.77	128.60
1	A	588	U	C2-N3-C4	5.28	130.17	127.00
1	A	607	U	N3-C4-O4	-5.28	115.70	119.40
1	A	1200	C	C5-C4-N4	5.28	123.90	120.20
1	A	1779	U	C5-C6-N1	-5.28	120.06	122.70
1	A	2003	G	N1-C2-N3	5.28	127.07	123.90
1	A	2548	G	C6-N1-C2	-5.28	121.93	125.10
1	A	795	C	N3-C4-N4	-5.28	114.30	118.00
1	A	1674	G	C6-C5-N7	-5.28	127.23	130.40
1	A	515	A	C5-C6-N1	5.28	120.34	117.70
1	A	2294	C	N3-C4-C5	5.28	124.01	121.90
1	A	2785	C	C6-N1-C2	-5.28	118.19	120.30
1	A	178	G	N9-C4-C5	5.27	107.51	105.40
1	A	788	A	N9-C4-C5	-5.27	103.69	105.80
1	A	1343	G	N3-C4-C5	-5.27	125.96	128.60
1	A	973	A	C8-N9-C4	-5.27	103.69	105.80
1	A	1114	G	N3-C2-N2	-5.27	116.21	119.90
1	A	827	U	N3-C4-O4	5.27	123.09	119.40
1	A	528	A	C8-N9-C4	-5.27	103.69	105.80
1	A	574	C	C2-N1-C1'	-5.27	113.01	118.80
1	A	420	C	C2-N3-C4	-5.27	117.27	119.90
1	A	768	G	N1-C6-O6	-5.27	116.74	119.90
1	A	12	U	C2-N1-C1'	5.26	124.02	117.70
1	A	444	C	C2-N1-C1'	-5.26	113.01	118.80
1	A	2087	G	C4-C5-N7	5.26	112.91	110.80
1	A	237	C	N3-C4-N4	-5.26	114.32	118.00
1	A	856	C	N1-C2-N3	5.26	122.88	119.20
1	A	2019	A	N1-C2-N3	5.26	131.93	129.30
1	A	2464	C	C2-N1-C1'	5.26	124.59	118.80
1	A	2525	G	N7-C8-N9	-5.26	110.47	113.10
1	A	1784	A	C8-N9-C4	5.26	107.90	105.80
9	N	23	LEU	C-N-CA	-5.26	111.26	122.30
16	U	10	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	535	C	C4-C5-C6	5.26	120.03	117.40
1	A	391	G	C4-C5-N7	5.25	112.90	110.80
1	A	2335	A	C5-N7-C8	-5.25	101.27	103.90
1	A	2560	C	C2-N3-C4	-5.25	117.27	119.90
1	A	1641	A	N1-C2-N3	5.25	131.93	129.30
1	A	1964	G	N3-C4-C5	-5.25	125.97	128.60
1	A	2548	G	C4-C5-N7	-5.25	108.70	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	A	N7-C8-N9	-5.25	111.17	113.80
1	A	135	G	C4-N9-C1'	-5.25	119.68	126.50
1	A	479	A	C5-N7-C8	5.25	106.52	103.90
1	A	2501	C	C6-N1-C2	5.25	122.40	120.30
1	A	984	A	P-O3'-C3'	5.25	126.00	119.70
1	A	2199	A	C4-N9-C1'	5.25	135.74	126.30
1	A	1992	G	C2'-C3'-O3'	5.24	122.09	113.70
1	A	2593	U	N1-C2-N3	5.24	118.05	114.90
1	A	231	C	C6-N1-C2	-5.24	118.20	120.30
1	A	408	G	C5-N7-C8	5.24	106.92	104.30
1	A	2303	G	C5-C6-O6	5.24	131.75	128.60
1	A	2627	G	N3-C4-C5	5.24	131.22	128.60
1	A	114	U	N3-C4-O4	5.24	123.07	119.40
1	A	648	G	N1-C6-O6	-5.24	116.76	119.90
1	A	652(J)	G	N3-C4-C5	-5.24	125.98	128.60
1	A	652(J)	G	N7-C8-N9	5.24	115.72	113.10
1	A	1192	G	C5-C6-N1	5.24	114.12	111.50
1	A	1942	C	N3-C4-C5	5.24	124.00	121.90
1	A	2035	G	N3-C2-N2	5.24	123.57	119.90
1	A	541	C	C6-N1-C2	-5.24	118.20	120.30
1	A	1531	C	C5-C6-N1	5.24	123.62	121.00
1	A	2567	G	C5-N7-C8	5.24	106.92	104.30
1	A	2606	C	N3-C4-N4	-5.24	114.33	118.00
1	A	474	G	N1-C2-N2	-5.24	111.49	116.20
1	A	82	G	N3-C2-N2	5.24	123.56	119.90
1	A	912	C	C6-N1-C2	-5.24	118.21	120.30
1	A	1287	A	C2-N3-C4	5.24	113.22	110.60
1	A	1111	A	N9-C4-C5	-5.23	103.71	105.80
1	A	1326	U	N3-C4-O4	-5.23	115.74	119.40
1	A	1369	G	C5-C6-O6	-5.23	125.46	128.60
1	A	199	A	C8-N9-C4	-5.23	103.71	105.80
1	A	363(E)	U	C5-C6-N1	5.23	125.31	122.70
1	A	1022	G	N3-C2-N2	-5.23	116.24	119.90
1	A	1558	A	N3-C4-N9	-5.23	123.22	127.40
1	A	1788	C	N3-C4-N4	5.23	121.66	118.00
1	A	2039	C	C6-N1-C2	-5.23	118.21	120.30
1	A	2709	G	C5-C6-O6	5.23	131.74	128.60
1	A	2729	G	C4-C5-N7	5.23	112.89	110.80
1	A	568	U	C4-C5-C6	-5.22	116.56	119.70
1	A	1883	G	N1-C6-O6	-5.22	116.77	119.90
2	B	73	A	N7-C8-N9	5.22	116.41	113.80
1	A	1570	A	N1-C6-N6	5.22	121.73	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2354	G	N3-C4-C5	5.22	131.21	128.60
1	A	1782	C	N3-C4-C5	5.22	123.99	121.90
1	A	652(S)	C	N1-C2-O2	5.22	122.03	118.90
1	A	2431	U	N1-C2-N3	5.22	118.03	114.90
2	B	41	U	C5-C4-O4	5.22	129.03	125.90
23	1	21	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	139(A)	G	C8-N9-C1'	-5.22	120.22	127.00
1	A	252	G	N9-C4-C5	5.22	107.49	105.40
1	A	2256	G	N7-C8-N9	5.22	115.71	113.10
1	A	2587	A	N1-C6-N6	-5.22	115.47	118.60
1	A	388	G	C2-N3-C4	5.22	114.51	111.90
1	A	2007	C	C6-N1-C2	-5.22	118.21	120.30
1	A	866	A	C4-N9-C1'	5.21	135.69	126.30
1	A	1288	U	C5-C6-N1	-5.21	120.09	122.70
1	A	2872	G	N1-C2-N2	-5.21	111.51	116.20
29	7	3	ARG	NE-CZ-NH2	5.21	122.91	120.30
1	A	677	A	N1-C6-N6	-5.21	115.47	118.60
1	A	1258	C	C6-N1-C2	5.21	122.39	120.30
1	A	2646	C	C5-C4-N4	-5.21	116.55	120.20
1	A	342	G	C8-N9-C4	-5.21	104.31	106.40
1	A	686	G	N1-C2-N2	-5.21	111.51	116.20
1	A	1111	A	C5-N7-C8	-5.21	101.29	103.90
1	A	1257	C	N3-C2-O2	-5.21	118.25	121.90
1	A	1625	C	N1-C2-O2	5.21	122.03	118.90
1	A	2233	U	C6-N1-C1'	5.21	128.50	121.20
1	A	2873	A	N7-C8-N9	5.21	116.41	113.80
1	A	1886	C	N3-C2-O2	5.21	125.55	121.90
1	A	2078	C	N3-C2-O2	-5.21	118.25	121.90
1	A	962	G	C4-C5-N7	-5.21	108.72	110.80
1	A	1323	U	C5-C4-O4	-5.21	122.78	125.90
1	A	2231	C	N1-C2-O2	-5.21	115.78	118.90
1	A	2506	U	C2-N1-C1'	-5.21	111.45	117.70
1	A	2518	A	C4-C5-C6	5.21	119.60	117.00
1	A	2105	C	C2-N3-C4	5.20	122.50	119.90
1	A	195	A	C4-C5-C6	5.20	119.60	117.00
1	A	847	U	C4-C5-C6	5.20	122.82	119.70
1	A	1797	C	C4-C5-C6	5.20	120.00	117.40
1	A	2465	C	C2-N3-C4	-5.20	117.30	119.90
1	A	2540	C	N1-C2-O2	-5.20	115.78	118.90
4	E	28	ALA	C-N-CA	-5.20	111.38	122.30
1	A	1008	C	C5-C6-N1	5.20	123.60	121.00
1	A	1988	C	C6-N1-C2	5.20	122.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	204	A	C5-C6-N6	-5.20	119.54	123.70
1	A	313	C	C6-N1-C2	-5.20	118.22	120.30
1	A	759	G	C4-C5-N7	-5.20	108.72	110.80
1	A	1558	A	N9-C4-C5	5.20	107.88	105.80
1	A	117	G	N3-C4-C5	-5.19	126.00	128.60
1	A	652(E)	G	C6-N1-C2	5.19	128.22	125.10
1	A	1527	G	C5-C6-N1	-5.19	108.90	111.50
1	A	34	C	C2-N3-C4	5.19	122.50	119.90
1	A	147	U	C2-N3-C4	-5.19	123.88	127.00
1	A	1818	U	N3-C4-O4	5.19	123.03	119.40
1	A	812	C	C6-N1-C2	-5.19	118.22	120.30
1	A	978	G	N7-C8-N9	-5.19	110.50	113.10
1	A	1311	G	C8-N9-C4	-5.19	104.32	106.40
1	A	1334	G	N9-C4-C5	5.19	107.48	105.40
1	A	1441	G	N7-C8-N9	-5.19	110.50	113.10
1	A	195	A	P-O3'-C3'	5.19	125.93	119.70
1	A	1524	G	C5-C6-O6	5.19	131.71	128.60
1	A	1926	U	C5-C4-O4	5.19	129.01	125.90
1	A	2382	G	N7-C8-N9	5.19	115.69	113.10
1	A	2593	U	C2-N3-C4	-5.19	123.89	127.00
1	A	2597	G	N9-C4-C5	5.19	107.47	105.40
1	A	2464	C	C5-C4-N4	-5.19	116.57	120.20
1	A	296	C	C5-C6-N1	-5.18	118.41	121.00
1	A	2241	A	N1-C6-N6	-5.18	115.49	118.60
2	B	41	U	C5-C6-N1	-5.18	120.11	122.70
2	B	81	G	N1-C6-O6	5.18	123.01	119.90
3	D	14	ARG	NE-CZ-NH1	-5.18	117.71	120.30
1	A	1023	U	N1-C2-N3	5.18	118.01	114.90
1	A	1865	G	N3-C4-N9	-5.18	122.89	126.00
1	A	1990	C	N3-C4-N4	-5.18	114.37	118.00
1	A	803	U	N1-C2-N3	5.18	118.00	114.90
1	A	214	G	C5-C6-O6	-5.17	125.50	128.60
1	A	673	C	C5-C4-N4	-5.17	116.58	120.20
1	A	1338	G	N3-C2-N2	5.17	123.52	119.90
1	A	1530	C	N3-C4-N4	5.17	121.62	118.00
1	A	1699	G	C5-C6-O6	5.17	131.71	128.60
1	A	2617	C	N1-C2-O2	5.17	122.00	118.90
1	A	2084	C	C5-C4-N4	-5.17	116.58	120.20
1	A	2440	C	C5-C6-N1	-5.17	118.41	121.00
1	A	1279	G	C8-N9-C4	-5.17	104.33	106.40
3	D	218	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	A	571	A	C4-C5-N7	5.17	113.28	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1338	G	N1-C6-O6	-5.17	116.80	119.90
1	A	34	C	C6-N1-C2	-5.17	118.23	120.30
1	A	1406	U	C5-C6-N1	5.17	125.28	122.70
1	A	2572	A	C6-N1-C2	-5.17	115.50	118.60
1	A	13	A	C6-N1-C2	-5.17	115.50	118.60
1	A	600	G	C5-C6-N1	-5.17	108.92	111.50
1	A	827	U	N3-C2-O2	5.17	125.82	122.20
1	A	1162	G	C5-C6-O6	5.17	131.70	128.60
1	A	2820	A	C8-N9-C4	5.17	107.87	105.80
27	5	15	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	A	665	C	N3-C4-C5	5.16	123.97	121.90
1	A	1106	G	C4-N9-C1'	5.16	133.21	126.50
1	A	2007	C	C4-C5-C6	5.16	119.98	117.40
1	A	2387	U	N1-C2-O2	-5.16	119.19	122.80
1	A	1295	C	C2-N3-C4	-5.16	117.32	119.90
1	A	11	G	C8-N9-C4	5.16	108.46	106.40
1	A	818	G	C5-C6-N1	5.16	114.08	111.50
1	A	1311	G	C4-C5-N7	-5.16	108.74	110.80
1	A	2353	G	C8-N9-C4	5.16	108.46	106.40
1	A	1131	G	C8-N9-C4	-5.16	104.34	106.40
1	A	2206	G	N9-C4-C5	-5.16	103.34	105.40
1	A	2694	G	N3-C4-N9	5.16	129.09	126.00
1	A	2713	A	N1-C6-N6	-5.16	115.51	118.60
1	A	608	A	C5-C6-N6	5.15	127.82	123.70
1	A	677	A	C8-N9-C4	-5.15	103.74	105.80
1	A	2006	C	N1-C2-O2	-5.15	115.81	118.90
1	A	2639	A	N9-C4-C5	-5.15	103.74	105.80
1	A	756	C	C5-C4-N4	5.15	123.81	120.20
1	A	861	A	C2-N3-C4	5.15	113.18	110.60
1	A	2737	G	C5-C6-N1	5.15	114.08	111.50
1	A	2751	G	N3-C4-C5	-5.15	126.02	128.60
1	A	364	C	C5-C6-N1	-5.15	118.42	121.00
1	A	690	G	C8-N9-C4	5.15	108.46	106.40
1	A	2346	A	C5-N7-C8	5.15	106.48	103.90
1	A	1236	G	C2-N3-C4	5.15	114.47	111.90
1	A	546	C	C6-N1-C1'	-5.15	114.62	120.80
1	A	706	A	C5-N7-C8	-5.15	101.33	103.90
1	A	104	U	N1-C2-O2	-5.15	119.20	122.80
1	A	143	G	C2-N3-C4	-5.15	109.33	111.90
1	A	1610	A	C6-N1-C2	-5.15	115.51	118.60
1	A	2730	C	C2-N3-C4	-5.15	117.33	119.90
1	A	130	C	C2-N3-C4	-5.14	117.33	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	231	C	N1-C2-N3	5.14	122.80	119.20
1	A	420	C	C5-C4-N4	5.14	123.80	120.20
1	A	771	G	C2-N3-C4	5.14	114.47	111.90
1	A	2070	G	N1-C2-N2	-5.14	111.57	116.20
18	W	92	ARG	NE-CZ-NH2	5.14	122.87	120.30
1	A	2259	G	C2-N3-C4	-5.14	109.33	111.90
1	A	2595	G	C5-C6-O6	5.14	131.68	128.60
1	A	271(H)	G	C5-C6-O6	-5.14	125.52	128.60
1	A	655	A	C5-N7-C8	-5.14	101.33	103.90
1	A	867	C	N1-C2-O2	-5.14	115.82	118.90
1	A	1052	C	N3-C2-O2	5.14	125.50	121.90
1	A	2633	G	C4-C5-N7	-5.14	108.74	110.80
1	A	1756	G	N1-C2-N3	-5.14	120.82	123.90
1	A	1897	G	C5-C6-O6	-5.14	125.52	128.60
1	A	605	C	N1-C2-O2	-5.14	115.82	118.90
1	A	1248	G	N7-C8-N9	5.14	115.67	113.10
1	A	762	U	C6-N1-C1'	-5.13	114.01	121.20
1	A	880	G	N1-C6-O6	5.13	122.98	119.90
1	A	955	C	C5-C4-N4	5.13	123.79	120.20
1	A	966	G	N1-C2-N2	-5.13	111.58	116.20
1	A	2233	U	C2-N3-C4	-5.13	123.92	127.00
1	A	2300	G	C8-N9-C4	-5.13	104.35	106.40
1	A	1674	G	N1-C6-O6	5.13	122.98	119.90
1	A	278	A	N3-C4-C5	-5.13	123.21	126.80
1	A	343	C	C5-C6-N1	-5.13	118.43	121.00
1	A	2769	C	C4-C5-C6	5.13	119.97	117.40
1	A	2825	C	C2-N3-C4	-5.13	117.33	119.90
1	A	1232	G	C4-C5-N7	-5.13	108.75	110.80
1	A	1300	U	N1-C2-O2	5.13	126.39	122.80
1	A	1679	U	N1-C2-N3	5.13	117.98	114.90
1	A	1899	G	C6-C5-N7	-5.13	127.32	130.40
1	A	2689	U	N3-C2-O2	-5.13	118.61	122.20
1	A	117	G	N3-C4-N9	5.13	129.08	126.00
1	A	1761	C	N3-C4-C5	5.13	123.95	121.90
1	A	1828	G	C8-N9-C4	5.13	108.45	106.40
1	A	503	A	N9-C4-C5	5.12	107.85	105.80
1	A	563	G	C5-C6-N1	5.12	114.06	111.50
1	A	2087	G	N3-C4-C5	5.12	131.16	128.60
5	F	62	ARG	NE-CZ-NH1	-5.12	117.74	120.30
1	A	2236	C	C6-N1-C2	5.12	122.35	120.30
1	A	2346	A	C4-C5-C6	5.12	119.56	117.00
1	A	2828	C	C6-N1-C2	5.12	122.35	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	598	G	C5-N7-C8	5.12	106.86	104.30
1	A	451	C	N1-C2-O2	5.12	121.97	118.90
1	A	481	G	N1-C6-O6	-5.12	116.83	119.90
12	Q	28	ALA	N-CA-C	5.12	124.82	111.00
1	A	398	G	C4-C5-N7	-5.12	108.75	110.80
1	A	2051	A	C4-C5-C6	5.12	119.56	117.00
1	A	460	A	N1-C2-N3	-5.12	126.74	129.30
1	A	1564	C	N3-C4-N4	-5.12	114.42	118.00
1	A	1674	G	C5-C6-O6	-5.12	125.53	128.60
2	B	91	C	N3-C4-C5	5.12	123.95	121.90
26	4	42	PHE	C-N-CA	5.12	134.49	121.70
1	A	1341	U	C5-C6-N1	-5.11	120.14	122.70
1	A	1961	C	N3-C2-O2	-5.11	118.32	121.90
1	A	2774	C	N3-C4-C5	-5.11	119.85	121.90
1	A	2872	G	N1-C6-O6	-5.11	116.83	119.90
1	A	870	A	N7-C8-N9	-5.11	111.24	113.80
1	A	1198	U	C6-N1-C2	-5.11	117.93	121.00
1	A	2588	G	N1-C6-O6	-5.11	116.83	119.90
1	A	1294	U	N1-C2-O2	-5.11	119.22	122.80
1	A	1959	G	N9-C4-C5	5.11	107.44	105.40
1	A	2716	U	N3-C2-O2	-5.11	118.62	122.20
1	A	1333	C	N1-C2-O2	-5.11	115.83	118.90
1	A	1435	G	C5-C6-O6	5.11	131.66	128.60
1	A	1806	C	N1-C2-O2	-5.11	115.83	118.90
1	A	1835	G	C4-N9-C1'	5.11	133.14	126.50
1	A	2250	G	N3-C4-C5	-5.11	126.05	128.60
1	A	475	U	N1-C2-N3	5.11	117.96	114.90
1	A	1195	G	C5-C6-N1	5.11	114.05	111.50
1	A	1997	G	N7-C8-N9	-5.11	110.55	113.10
1	A	214	G	C4-N9-C1'	-5.10	119.87	126.50
1	A	444	C	N1-C2-O2	-5.10	115.84	118.90
1	A	652(S)	C	C5-C6-N1	5.10	123.55	121.00
1	A	1541	G	N3-C4-C5	-5.10	126.05	128.60
1	A	1985	G	N3-C2-N2	-5.10	116.33	119.90
1	A	2538	C	N1-C2-O2	5.10	121.96	118.90
3	D	260	ARG	N-CA-CB	5.10	119.79	110.60
1	A	108	U	N3-C4-C5	5.10	117.66	114.60
1	A	123	G	C8-N9-C4	5.10	108.44	106.40
1	A	2111	C	C6-N1-C2	-5.10	118.26	120.30
1	A	2243	U	N1-C2-O2	-5.10	119.23	122.80
22	0	55	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	1204	A	C1'-O4'-C4'	-5.10	105.82	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1600	C	C4-C5-C6	5.10	119.95	117.40
1	A	1658	C	C4-C5-C6	5.10	119.95	117.40
1	A	2331	G	C5-C6-O6	-5.10	125.54	128.60
1	A	987	G	C5-N7-C8	-5.09	101.75	104.30
1	A	1823	G	N3-C2-N2	5.09	123.47	119.90
1	A	2062	A	N1-C6-N6	5.09	121.66	118.60
1	A	1985	G	N7-C8-N9	-5.09	110.55	113.10
1	A	1236	G	C5-C6-N1	5.09	114.05	111.50
1	A	1953	A	C5-C6-N6	-5.09	119.63	123.70
1	A	2335	A	C2-N3-C4	5.09	113.15	110.60
2	B	95	C	C2-N3-C4	-5.09	117.35	119.90
1	A	2035	G	O4'-C1'-N9	5.09	112.27	108.20
1	A	2409	G	C6-C5-N7	-5.09	127.35	130.40
1	A	2207	G	C4-N9-C1'	5.09	133.11	126.50
1	A	2637	U	N1-C2-N3	5.09	117.95	114.90
1	A	481	G	P-O3'-C3'	5.09	125.81	119.70
1	A	1323	U	C5-C6-N1	-5.09	120.16	122.70
1	A	2446	G	C8-N9-C4	-5.09	104.37	106.40
1	A	23	G	C5-C6-O6	5.08	131.65	128.60
16	U	52	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	A	242	G	C4-C5-N7	-5.08	108.77	110.80
1	A	338	G	N1-C6-O6	-5.08	116.85	119.90
1	A	692	C	C5-C6-N1	5.08	123.54	121.00
1	A	1212	G	C6-C5-N7	-5.08	127.35	130.40
1	A	2453	A	N3-C4-C5	-5.08	123.24	126.80
1	A	2490	G	N7-C8-N9	-5.08	110.56	113.10
1	A	2633	G	N1-C6-O6	-5.08	116.85	119.90
1	A	2699	C	C6-N1-C1'	5.08	126.90	120.80
1	A	1131	G	N1-C6-O6	-5.08	116.85	119.90
1	A	2438	U	N3-C2-O2	5.08	125.76	122.20
1	A	260	G	N9-C4-C5	5.08	107.43	105.40
1	A	753	C	C5-C4-N4	5.08	123.75	120.20
1	A	1968	G	C5-C6-O6	-5.08	125.55	128.60
1	A	1023	U	N3-C2-O2	-5.08	118.65	122.20
1	A	2207	G	C4-C5-C6	5.08	121.84	118.80
1	A	382	G	N7-C8-N9	-5.07	110.56	113.10
1	A	2073	C	C2-N3-C4	-5.07	117.36	119.90
1	A	2237	G	C8-N9-C4	5.07	108.43	106.40
1	A	671	C	C2-N1-C1'	-5.07	113.22	118.80
1	A	21	A	N1-C6-N6	5.07	121.64	118.60
1	A	2153	G	N3-C4-N9	-5.07	122.96	126.00
1	A	474	G	C5-N7-C8	-5.07	101.77	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2207	G	C8-N9-C1'	-5.07	120.41	127.00
1	A	1811	G	N9-C4-C5	5.07	107.43	105.40
1	A	2463	C	N1-C2-O2	-5.06	115.86	118.90
1	A	2751	G	C5-C6-O6	5.06	131.64	128.60
1	A	1699	G	N9-C4-C5	5.06	107.42	105.40
1	A	1885	A	N7-C8-N9	-5.06	111.27	113.80
1	A	526	A	N9-C4-C5	5.06	107.82	105.80
1	A	855	G	C5-C6-O6	5.06	131.64	128.60
1	A	431	U	N3-C2-O2	-5.06	118.66	122.20
1	A	1822	G	N9-C4-C5	5.06	107.42	105.40
1	A	2201	C	C6-N1-C2	5.06	122.32	120.30
1	A	2553	G	N1-C2-N2	-5.06	111.65	116.20
1	A	2683	C	N3-C4-N4	5.06	121.54	118.00
1	A	210	C	C2-N3-C4	-5.05	117.37	119.90
1	A	1772	G	N7-C8-N9	-5.05	110.57	113.10
1	A	2272	U	N1-C2-N3	5.05	117.93	114.90
1	A	2695	C	N3-C4-C5	5.05	123.92	121.90
1	A	967	C	N3-C4-C5	5.05	123.92	121.90
1	A	986	C	C6-N1-C2	-5.05	118.28	120.30
1	A	1344	G	N1-C2-N3	5.05	126.93	123.90
1	A	1451	C	N1-C2-O2	5.05	121.93	118.90
1	A	2375	G	C8-N9-C4	5.05	108.42	106.40
1	A	2588	G	N3-C2-N2	5.05	123.44	119.90
1	A	735	A	N1-C6-N6	-5.05	115.57	118.60
1	A	754	C	N3-C4-C5	5.05	123.92	121.90
1	A	1998	G	N9-C4-C5	5.05	107.42	105.40
1	A	2729	G	N9-C4-C5	-5.05	103.38	105.40
1	A	771	G	N3-C4-C5	-5.05	126.08	128.60
1	A	2242	G	P-O3'-C3'	5.05	125.76	119.70
1	A	2527	C	C2-N3-C4	5.05	122.42	119.90
1	A	1040	C	C2-N3-C4	-5.04	117.38	119.90
1	A	1359	A	C8-N9-C4	5.04	107.82	105.80
1	A	1043	C	C6-N1-C2	-5.04	118.28	120.30
1	A	1192	G	N7-C8-N9	-5.04	110.58	113.10
1	A	1475	G	N1-C2-N2	5.04	120.74	116.20
1	A	1427	A	P-O3'-C3'	5.04	125.75	119.70
1	A	1744	C	N3-C4-C5	5.04	123.92	121.90
1	A	2246	G	C2-N3-C4	5.04	114.42	111.90
1	A	2378	A	C5-C6-N6	-5.04	119.67	123.70
1	A	2589	A	C5-N7-C8	5.04	106.42	103.90
1	A	2056	G	N1-C6-O6	-5.04	116.88	119.90
1	A	2375	G	N1-C6-O6	5.04	122.92	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2074	U	C6-N1-C2	-5.04	117.98	121.00
1	A	2511	U	N1-C2-O2	-5.04	119.28	122.80
1	A	70	G	C5-C6-O6	5.03	131.62	128.60
1	A	395	U	C5-C4-O4	-5.03	122.88	125.90
1	A	456	C	C5-C4-N4	-5.03	116.68	120.20
1	A	1157	G	N1-C6-O6	-5.03	116.88	119.90
1	A	112	U	N1-C2-O2	5.03	126.32	122.80
1	A	1772	G	C8-N9-C4	5.03	108.41	106.40
1	A	2475	C	N3-C4-C5	-5.03	119.89	121.90
1	A	377	C	C5-C6-N1	-5.03	118.49	121.00
1	A	560	C	C6-N1-C2	5.03	122.31	120.30
1	A	812	C	C2-N1-C1'	5.03	124.33	118.80
1	A	1204	A	C3'-C2'-C1'	-5.03	97.48	101.50
1	A	1865	G	N3-C2-N2	-5.03	116.38	119.90
1	A	2686	G	C5-C6-N1	5.02	114.01	111.50
1	A	398	G	N9-C4-C5	5.02	107.41	105.40
1	A	1221(A)	C	C2-N3-C4	-5.02	117.39	119.90
1	A	1879	C	C6-N1-C2	-5.02	118.29	120.30
1	A	2008	C	C2-N3-C4	-5.02	117.39	119.90
1	A	686	G	C8-N9-C4	5.02	108.41	106.40
1	A	2628	C	C6-N1-C2	5.02	122.31	120.30
1	A	2388	A	N7-C8-N9	5.02	116.31	113.80
1	A	1124	C	N1-C2-O2	-5.02	115.89	118.90
1	A	1163	G	C8-N9-C4	5.02	108.41	106.40
1	A	2839	G	N1-C6-O6	-5.02	116.89	119.90
1	A	121	G	C5-C6-N1	5.01	114.01	111.50
1	A	272(H)	C	C2-N3-C4	-5.01	117.39	119.90
1	A	496	G	N3-C2-N2	5.01	123.41	119.90
1	A	1017	G	N7-C8-N9	5.01	115.61	113.10
1	A	2488	A	N1-C2-N3	5.01	131.81	129.30
1	A	2681	C	C5-C6-N1	-5.01	118.49	121.00
1	A	708	C	N3-C4-C5	5.01	123.91	121.90
1	A	2605	U	C5-C4-O4	5.01	128.91	125.90
2	B	31	C	C6-N1-C2	-5.01	118.30	120.30
1	A	126	A	C6-N1-C2	5.01	121.61	118.60
1	A	494	G	N1-C2-N3	5.01	126.91	123.90
1	A	535	C	C6-N1-C1'	5.01	126.81	120.80
1	A	840	C	N3-C4-C5	5.01	123.90	121.90
1	A	1235	G	C5-C6-O6	-5.01	125.59	128.60
1	A	1894	C	N3-C4-C5	-5.01	119.90	121.90
1	A	956	G	N9-C4-C5	-5.01	103.40	105.40
1	A	268	C	C6-N1-C2	-5.01	118.30	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1111	A	C4-C5-N7	5.01	113.20	110.70
1	A	1122	G	C6-C5-N7	-5.01	127.40	130.40
1	A	1230	C	C6-N1-C2	5.01	122.30	120.30
1	A	1301	A	C5-N7-C8	-5.01	101.40	103.90
1	A	1558	A	P-O3'-C3'	5.01	125.71	119.70
1	A	2609	U	C2-N1-C1'	-5.01	111.69	117.70
1	A	325	G	C8-N9-C4	5.00	108.40	106.40
1	A	615	G	C5-C6-O6	5.00	131.60	128.60
1	A	127	A	C5-C6-N6	-5.00	119.70	123.70
1	A	1343	G	N9-C4-C5	5.00	107.40	105.40
1	A	2250	G	N1-C6-O6	-5.00	116.90	119.90
1	A	319	C	N3-C2-O2	-5.00	118.40	121.90
1	A	1607	C	N3-C4-N4	5.00	121.50	118.00
1	A	1697	G	C4-C5-N7	5.00	112.80	110.80
1	A	2872	G	N3-C2-N2	5.00	123.40	119.90

There are no chirality outliers.

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
23	1	83	GLU	Peptide
26	4	42	PHE	Peptide
27	5	53	ALA	Peptide
1	A	2375	G	Sidechain
1	A	2464	C	Sidechain
1	A	271(Q)	G	Sidechain
1	A	512	G	Sidechain
3	D	275	LYS	Peptide
4	E	72	VAL	Peptide
5	F	20	LEU	Mainchain
5	F	21	ALA	Mainchain
5	F	85	GLY	Peptide
6	G	81	LYS	Peptide
7	H	70	THR	Peptide
8	I	85	GLU	Peptide
9	N	124	ALA	Peptide
11	P	26	GLY	Peptide
11	P	44	GLY	Peptide
14	S	83	LYS	Peptide
15	T	126	ALA	Peptide
19	X	23	GLU	Mainchain
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	60898	0	30697	757	0
2	B	2573	0	1306	27	0
3	D	2136	0	2218	55	0
4	E	1555	0	1607	41	0
5	F	1577	0	1612	44	0
6	G	1368	0	1324	37	0
7	H	1317	0	1376	23	0
8	I	1043	0	1054	39	0
9	N	1112	0	1180	25	0
10	O	923	0	981	11	0
11	P	1131	0	1201	39	0
12	Q	1122	0	1179	26	0
13	R	968	0	1033	24	0
14	S	865	0	905	38	0
15	T	1063	0	1103	26	0
16	U	959	0	1019	12	0
17	V	771	0	830	14	1
18	W	881	0	935	22	0
19	X	742	0	799	14	0
20	Y	785	0	828	16	0
21	Z	1522	0	1511	54	0
22	0	594	0	604	7	0
23	1	745	0	804	20	0
24	2	588	0	643	13	0
25	3	458	0	503	6	0
26	4	349	0	336	11	0
27	5	455	0	472	10	0
28	6	449	0	462	15	0
29	7	418	0	467	10	0
30	8	509	0	565	19	0
31	9	297	0	316	6	0
32	0	4	0	0	0	0
32	1	1	0	0	0	0
32	2	2	0	0	0	0
32	3	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	6	1	0	0	0	0
32	7	1	0	0	0	0
32	8	1	0	0	0	0
32	9	3	0	0	0	0
32	A	725	0	0	0	0
32	B	19	0	0	0	0
32	D	6	0	0	0	0
32	E	6	0	0	0	0
32	F	6	0	0	0	0
32	G	1	0	0	0	0
32	H	1	0	0	0	0
32	N	2	0	0	0	0
32	O	1	0	0	0	0
32	P	2	0	0	0	0
32	Q	5	0	0	0	0
32	R	5	0	0	0	0
32	S	1	0	0	0	0
32	T	3	0	0	0	0
32	U	3	0	0	0	0
32	V	4	0	0	0	0
32	W	1	0	0	0	0
32	Y	1	0	0	0	0
32	Z	2	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	1	5	0	0	0	0
34	3	5	0	0	0	0
34	5	6	0	0	0	0
34	6	1	0	0	0	0
34	7	4	0	0	2	0
34	8	9	0	0	0	0
34	9	1	0	0	0	0
34	A	1975	0	0	65	1
34	B	45	0	0	1	0
34	D	18	0	0	2	0
34	E	16	0	0	1	0
34	F	17	0	0	0	0
34	G	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	H	2	0	0	0	0
34	N	7	0	0	0	0
34	O	2	0	0	0	0
34	P	21	0	0	0	0
34	Q	8	0	0	0	0
34	R	9	0	0	0	1
34	S	2	0	0	0	0
34	T	5	0	0	0	0
34	U	7	0	0	0	0
34	V	13	0	0	1	1
34	W	6	0	0	0	0
34	X	2	0	0	0	0
34	Y	2	0	0	0	0
34	Z	2	0	0	0	0
All	All	93185	0	59870	1298	2

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 9.

All (1298) 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	1.59	1.34
1:A:885:C:N4	1:A:890:A:N6	1.97	1.13
1:A:2322:A:H61	1:A:2335:A:N6	1.48	1.11
1:A:885:C:H42	1:A:890:A:N6	1.50	1.03
1:A:1019:U:HO2'	1:A:1021:A:H2	1.01	0.99
23:1:21:ARG:HH11	23:1:21:ARG:HG2	1.28	0.99
19:X:31:HIS:HD2	19:X:33:LYS:H	1.10	0.98
1:A:1204:A:H2	1:A:1241:A:H62	1.08	0.96
1:A:975:C:O2	34:A:5558:HOH:O	1.83	0.96
1:A:2136:C:N4	1:A:2155:G:H1	1.64	0.95
1:A:2287:A:H62	1:A:2344:U:H3	1.14	0.94
1:A:1359:A:H61	1:A:1372:U:H3	1.10	0.94
4:E:47:VAL:HG21	4:E:86:PRO:HD2	1.50	0.94
22:0:11:ARG:O	22:0:14:ARG:NH2	2.00	0.93
15:T:16:ARG:NH2	15:T:83:ILE:O	2.02	0.93
1:A:1049:C:HO2'	1:A:1050:A:H8	0.97	0.90
1:A:1530:C:O2'	1:A:1531:C:O5'	1.88	0.90
1:A:1798:U:H5'	3:D:259:THR:HG22	1.56	0.88
15:T:54:ARG:HA	15:T:59:THR:HB	1.56	0.86
1:A:2304:G:H1	1:A:2312:U:H3	1.21	0.86
21:Z:160:GLY:HA2	21:Z:161:VAL:HB	1.55	0.85

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1689:A:H62	1:A:1698:A:H2	1.19	0.85
8:I:77:LEU:HB2	8:I:142:VAL:HG12	1.58	0.85
1:A:271(R):G:OP2	34:A:5363:HOH:O	1.94	0.85
1:A:1359:A:N6	1:A:1372:U:H3	1.75	0.85
1:A:2100:G:H1	1:A:2189:U:H3	1.21	0.85
1:A:2123:G:H1	1:A:2175:C:H42	1.24	0.84
1:A:2206:G:H5'	1:A:2207:G:N7	1.91	0.84
19:X:31:HIS:CD2	19:X:33:LYS:H	1.94	0.84
1:A:2733:A:OP1	34:A:5315:HOH:O	1.95	0.84
1:A:1741:A:N7	34:A:5427:HOH:O	2.10	0.83
1:A:885:C:N4	1:A:890:A:H61	1.75	0.83
1:A:571:A:H5'	1:A:2030:A:H62	1.44	0.82
1:A:2036:C:H6	1:A:2036:C:H5'	1.43	0.82
1:A:1890:A:OP2	34:A:5272:HOH:O	1.97	0.82
1:A:1047:G:H2'	1:A:1110:G:H22	1.45	0.82
1:A:587:C:OP2	11:P:21:ARG:NH2	2.13	0.81
1:A:1315:C:OP2	34:A:4699:HOH:O	1.98	0.81
1:A:2206:G:H3'	1:A:2207:G:C8	2.15	0.81
1:A:2322:A:N6	1:A:2335:A:N6	2.28	0.81
1:A:1506:C:H2'	1:A:1507:A:H5'	1.63	0.81
1:A:2268:A:OP1	34:A:5078:HOH:O	1.98	0.80
1:A:83:G:N2	1:A:103:A:OP2	2.12	0.80
15:T:118:ARG:HG3	15:T:118:ARG:HH11	1.46	0.80
8:I:107:VAL:HG12	8:I:108:THR:H	1.45	0.80
1:A:1581:G:OP2	34:A:5373:HOH:O	1.99	0.80
1:A:1364:G:OP2	23:1:3:LYS:HG2	1.82	0.79
1:A:956:G:OP2	12:Q:14:ARG:NH2	2.16	0.79
1:A:1762:A:H2'	34:A:5412:HOH:O	1.82	0.78
15:T:95:ARG:HG2	15:T:95:ARG:HH11	1.46	0.78
11:P:39:LYS:HB2	11:P:45:LEU:HG	1.66	0.78
20:Y:23:ARG:HG2	20:Y:42:VAL:HG22	1.65	0.78
1:A:1174:A:H5'	1:A:1177:A:H61	1.48	0.78
6:G:56:ALA:HB2	6:G:153:ARG:HE	1.49	0.77
1:A:1604:C:OP2	34:A:5249:HOH:O	2.01	0.77
1:A:1109:C:H5	1:A:1110:G:C6	2.02	0.77
18:W:14:PRO:HG2	18:W:78:GLU:HG2	1.66	0.77
1:A:2692:C:OP2	34:A:5348:HOH:O	2.00	0.77
1:A:999:U:OP2	34:A:4722:HOH:O	2.02	0.77
1:A:2721:A:N7	34:A:4319:HOH:O	2.17	0.76
1:A:2464:C:H1'	34:A:5214:HOH:O	1.85	0.76
23:1:82:LEU:HA	23:1:85:LEU:HD23	1.67	0.76
1:A:686:G:H5''	29:7:11:LYS:HE2	1.66	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:N:56:ASN:H	9:N:125:GLY:HA3	1.49	0.76
6:G:76:SER:HA	6:G:83:ARG:HA	1.68	0.76
1:A:1629:U:O4	34:A:4600:HOH:O	2.05	0.75
5:F:65:TRP:HH2	5:F:72:ARG:HH21	1.33	0.75
2:B:48:A:H4'	14:S:95:HIS:HD2	1.52	0.75
24:2:51:ARG:HA	24:2:54:LYS:HB2	1.69	0.75
1:A:1047:G:O2'	1:A:1048:A:O5'	2.05	0.74
1:A:1355:G:OP1	3:D:38:LYS:NZ	2.19	0.74
1:A:2285:C:OP2	28:6:6:ARG:NH1	2.21	0.74
1:A:570:G:O6	34:A:4363:HOH:O	2.04	0.74
2:B:6:C:H2'	2:B:7:G:H5''	1.67	0.74
1:A:1420:U:O2'	1:A:1421:G:OP1	2.06	0.74
6:G:11:TYR:CZ	6:G:16:ARG:HD3	2.23	0.74
11:P:100:LEU:HD12	11:P:112:LEU:HD11	1.69	0.74
1:A:213:A:OP2	34:A:5433:HOH:O	2.05	0.74
1:A:278:A:O2'	1:A:279:C:OP1	2.03	0.74
4:E:179:GLU:HB3	4:E:181:LEU:HD22	1.70	0.74
1:A:1427:A:H4'	1:A:1428:C:O5'	1.88	0.73
1:A:531:C:OP2	34:A:4820:HOH:O	2.05	0.73
23:1:54:ALA:HB1	23:1:83:GLU:HG3	1.70	0.73
12:Q:32:TYR:CE2	12:Q:133:ARG:HG3	2.23	0.73
1:A:652(I):C:H2'	1:A:652(J):G:C8	2.23	0.73
1:A:2226:C:OP2	34:A:5312:HOH:O	2.04	0.73
3:D:148:GLU:HB2	3:D:151:LYS:HD2	1.69	0.73
1:A:2318:G:O2'	1:A:2319:G:OP1	2.04	0.73
1:A:2789:C:O2'	1:A:2790:A:O2'	2.06	0.73
1:A:690:G:OP1	34:A:4099:HOH:O	2.07	0.73
2:B:66:A:H61	2:B:108:U:H2'	1.54	0.73
1:A:1048:A:OP2	1:A:1109:C:N4	2.22	0.72
5:F:53:THR:HG22	5:F:55:GLY:H	1.54	0.72
27:5:16:ARG:HH11	27:5:16:ARG:HG2	1.53	0.72
1:A:2820:A:OP2	13:R:2:ARG:NH2	2.21	0.72
1:A:2079:U:OP1	23:1:21:ARG:NH2	2.23	0.72
8:I:92:VAL:HG13	8:I:120:ILE:HB	1.72	0.72
9:N:24:GLY:HA2	9:N:27:ALA:HB3	1.72	0.72
1:A:2126:A:H4'	1:A:2127:G:O5'	1.88	0.71
25:3:8:LEU:HD13	25:3:31:LEU:HD23	1.72	0.71
4:E:111:ARG:HG3	4:E:160:TYR:CD1	2.26	0.71
30:8:62:LEU:HB3	30:8:65:GLU:HG2	1.71	0.71
3:D:238:GLY:O	3:D:239:ARG:HB2	1.89	0.71
1:A:2354:G:N7	34:A:5451:HOH:O	2.23	0.71
26:4:7:PRO:HB2	26:4:27:THR:HG21	1.73	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1359:A:N1	1:A:1372:U:O4	2.24	0.71
6:G:41:GLN:HB3	6:G:43:LEU:HD13	1.73	0.71
1:A:2144:U:HO2'	1:A:2147:G:H1	1.37	0.70
3:D:239:ARG:N	34:D:406:HOH:O	2.23	0.70
1:A:631:A:OP1	11:P:65:ARG:NH1	2.24	0.70
3:D:137:PRO:O	3:D:140:THR:HG23	1.91	0.70
7:H:33:LEU:HD21	7:H:136:ILE:HG13	1.73	0.70
1:A:2012:G:OP1	18:W:11:ARG:NH2	2.25	0.70
1:A:71:A:OP2	1:A:71:A:H3'	1.91	0.70
1:A:652(R):C:O2'	1:A:652(S):C:OP2	2.09	0.70
1:A:833:U:O2	11:P:55:ARG:NH2	2.25	0.70
21:Z:160:GLY:HA2	21:Z:161:VAL:CB	2.21	0.69
13:R:55:ALA:HB2	13:R:79:LEU:HD13	1.73	0.69
1:A:2145:C:O2'	1:A:2147:G:N2	2.25	0.69
1:A:2104:G:N2	1:A:2105:C:O2	2.25	0.69
1:A:1495:A:H2'	1:A:1496:A:C8	2.27	0.69
1:A:2207:G:O2'	1:A:2208:A:OP1	2.07	0.69
1:A:1798:U:C5'	3:D:259:THR:HG22	2.22	0.69
22:O:10:THR:HG22	22:O:12:ASN:H	1.57	0.69
6:G:72:ARG:HH12	6:G:87:PRO:HG3	1.56	0.69
1:A:641:C:O2'	1:A:2350:C:OP1	2.08	0.69
1:A:1783:A:OP1	34:A:4038:HOH:O	2.10	0.69
10:O:98:VAL:HG13	10:O:117:LEU:HB3	1.75	0.68
19:X:35:THR:HG22	19:X:38:GLU:H	1.58	0.68
2:B:106:G:H5'	21:Z:31:ARG:HG2	1.75	0.68
1:A:2140:C:H2'	1:A:2141:G:H8	1.59	0.68
1:A:2659:G:O6	34:A:5457:HOH:O	2.09	0.68
1:A:927:G:N7	34:A:5186:HOH:O	2.25	0.68
1:A:1507:A:O2'	1:A:1508:A:O5'	2.12	0.68
1:A:2448:A:OP1	34:A:4363:HOH:O	2.11	0.68
1:A:2127:G:O6	1:A:2161:C:N3	2.26	0.68
1:A:1403:C:H5''	1:A:1471:A:H1'	1.74	0.68
1:A:2845:G:O2'	1:A:2846:G:H5'	1.94	0.68
1:A:2523:G:N7	34:A:4565:HOH:O	2.26	0.68
21:Z:158:PRO:O	21:Z:161:VAL:HG11	1.94	0.68
1:A:2114:A:O2'	1:A:2167:U:O3'	2.11	0.68
1:A:1176:G:H1'	1:A:1177:A:OP1	1.94	0.68
1:A:2319:G:H22	14:S:3:ARG:HE	1.39	0.68
1:A:1332:G:OP1	34:A:4699:HOH:O	2.11	0.67
1:A:2763:G:OP2	34:A:4984:HOH:O	2.10	0.67
1:A:2123:G:H1	1:A:2175:C:N4	1.91	0.67
6:G:44:GLY:HA2	6:G:88:ILE:HG22	1.75	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1803:A:O2'	3:D:259:THR:HG21	1.94	0.67
7:H:3:ARG:HD3	7:H:54:ARG:HH12	1.59	0.67
11:P:59:LEU:HD11	30:8:10:ALA:HB2	1.74	0.67
14:S:25:ARG:NH1	14:S:42:ASP:OD2	2.28	0.67
14:S:58:LEU:HB2	14:S:59:LYS:HB2	1.76	0.67
4:E:54:GLN:HB2	4:E:76:ARG:HB3	1.76	0.67
1:A:1174:A:H4'	1:A:1175:U:OP1	1.94	0.67
1:A:203:C:H3'	1:A:204:A:H5''	1.76	0.66
15:T:95:ARG:HG2	15:T:95:ARG:NH1	2.10	0.66
1:A:2166:G:N2	1:A:2172:U:O4	2.28	0.66
1:A:2822:G:OP2	34:A:4877:HOH:O	2.12	0.66
1:A:2136:C:H42	1:A:2155:G:H1	1.41	0.66
4:E:24:THR:HG22	4:E:186:GLY:O	1.96	0.66
23:1:21:ARG:NH1	23:1:21:ARG:HG2	2.00	0.66
1:A:301:G:OP2	20:Y:84:ARG:NH2	2.28	0.66
1:A:271(M):G:O2'	1:A:271(N):U:O5'	2.13	0.66
1:A:948:G:OP1	34:A:5110:HOH:O	2.14	0.66
1:A:2839:G:H5'	13:R:46:GLY:HA2	1.78	0.65
1:A:2646:C:OP1	34:A:5315:HOH:O	2.13	0.65
1:A:1486:A:H2'	1:A:1487:G:H8	1.60	0.65
1:A:1484:G:O6	34:A:4413:HOH:O	2.11	0.65
20:Y:92:ASN:OD1	20:Y:94:LYS:HG3	1.96	0.65
1:A:62:C:OP1	34:A:3863:HOH:O	2.13	0.65
1:A:2042:A:OP1	34:A:4644:HOH:O	2.13	0.65
1:A:330:A:H2	1:A:1210:A:HO2'	1.44	0.65
1:A:1991:U:H2'	1:A:1992:G:H5''	1.78	0.65
1:A:530:G:N3	1:A:530:G:O4'	2.27	0.65
14:S:15:ARG:O	14:S:19:LYS:HG2	1.97	0.65
1:A:2127:G:N1	1:A:2161:C:O2	2.30	0.65
1:A:1040:C:H2'	1:A:1041:C:O4'	1.97	0.65
14:S:102:ALA:HA	14:S:105:ALA:HB3	1.79	0.65
14:S:14:VAL:O	14:S:18:ILE:HG12	1.97	0.65
1:A:2646:C:OP2	1:A:2732:G:O2'	2.14	0.65
9:N:47:ALA:HB2	9:N:112:LEU:HD11	1.79	0.64
5:F:53:THR:CG2	5:F:55:GLY:H	2.10	0.64
27:5:16:ARG:NH1	27:5:17:ASP:OD1	2.30	0.64
1:A:2206:G:O2'	1:A:2207:G:OP1	2.16	0.64
1:A:2349:G:H5'	1:A:2350:C:OP2	1.96	0.64
1:A:1434:A:H61	1:A:1558:A:H62	1.43	0.64
1:A:1153:C:OP2	34:A:4722:HOH:O	2.15	0.64
1:A:2114:A:H1'	1:A:2168:G:H5'	1.78	0.64
1:A:1796:U:H2'	1:A:1797:C:C6	2.32	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1896:G:N7	34:A:5330:HOH:O	2.30	0.64
15:T:24:PRO:HA	15:T:49:VAL:HG22	1.80	0.64
1:A:2304:G:H21	6:G:156:ASP:CG	2.01	0.64
1:A:1689:A:N6	1:A:1698:A:H2	1.95	0.64
1:A:2337:G:OP1	34:A:4348:HOH:O	2.15	0.64
1:A:380:U:OP1	34:A:4608:HOH:O	2.15	0.63
1:A:885:C:H3'	1:A:886:C:H5''	1.80	0.63
1:A:1420:U:HO2'	1:A:1421:G:P	2.21	0.63
11:P:38:GLN:HA	11:P:41:ARG:HG2	1.80	0.63
1:A:1300:U:H4'	1:A:1301:A:H5'	1.81	0.63
6:G:82:LEU:H	6:G:82:LEU:HD12	1.63	0.63
22:O:27:GLU:HG3	22:O:68:GLU:HA	1.80	0.63
1:A:607:U:OP1	5:F:102:PRO:HA	1.99	0.63
1:A:668:G:H5'	1:A:669:G:OP2	1.99	0.63
4:E:47:VAL:HG12	4:E:49:LEU:HD13	1.81	0.62
1:A:1360:A:OP2	34:A:5226:HOH:O	2.16	0.62
4:E:77:ILE:HD12	4:E:195:LEU:HD13	1.79	0.62
5:F:185:ASP:HA	5:F:188:ARG:HD3	1.82	0.62
30:8:23:VAL:HG11	30:8:47:LYS:HD3	1.81	0.62
18:W:18:ARG:NH1	18:W:76:VAL:O	2.32	0.62
1:A:1310:G:OP2	29:7:9:ARG:NH1	2.32	0.62
1:A:2128:C:H42	1:A:2160:G:H1	1.46	0.62
1:A:2136:C:N4	1:A:2155:G:N1	2.45	0.62
1:A:1109:C:C5	1:A:1110:G:C6	2.87	0.62
1:A:2894:G:H8	1:A:2894:G:O5'	1.83	0.62
1:A:2113:U:H2'	1:A:2114:A:O4'	1.99	0.62
1:A:1877:A:H5'	1:A:1878:G:OP2	1.98	0.62
1:A:251:A:C5	1:A:252:G:H1'	2.34	0.62
1:A:1693:U:O2'	3:D:14:ARG:NH2	2.32	0.62
10:O:2:ILE:HD12	10:O:6:THR:HG21	1.80	0.62
2:B:66:A:N6	2:B:108:U:H2'	2.13	0.62
1:A:1266:G:O5'	18:W:15:ARG:NH2	2.32	0.62
16:U:76:TYR:OH	16:U:92:ARG:NH1	2.32	0.62
1:A:2122:U:H2'	1:A:2123:G:H8	1.65	0.62
1:A:2349:G:H3'	1:A:2350:C:H5''	1.82	0.62
3:D:8:PRO:HB3	3:D:14:ARG:HB2	1.81	0.61
1:A:1531:C:H42	1:A:1538:G:H1	1.47	0.61
1:A:2142:C:H2'	1:A:2143:C:C6	2.35	0.61
1:A:1778:U:H2'	1:A:1784:A:N6	2.15	0.61
1:A:2810:A:N6	1:A:2891:G:O2'	2.32	0.61
1:A:2577:A:H5'	27:5:3:LYS:HD2	1.82	0.61
20:Y:68:HIS:ND1	20:Y:70:SER:HB3	2.16	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1047:G:H2'	1:A:1110:G:N2	2.15	0.61
1:A:2821:A:OP2	34:A:4877:HOH:O	2.16	0.61
8:I:38:LEU:HB3	8:I:40:THR:HG23	1.80	0.61
3:D:71:ASP:OD2	3:D:103:ARG:NH2	2.32	0.61
4:E:152:LYS:HD2	9:N:77:GLY:HA3	1.83	0.61
1:A:1045:A:H1'	1:A:1047:G:C2	2.36	0.61
21:Z:69:THR:HG22	21:Z:90:VAL:HA	1.83	0.61
1:A:1429:G:H2'	1:A:1430:C:C6	2.36	0.61
1:A:2332:U:O2'	1:A:2335:A:N3	2.28	0.61
21:Z:158:PRO:HD2	21:Z:161:VAL:HG21	1.83	0.61
1:A:1721:G:H5'	1:A:1722:A:OP2	2.01	0.61
1:A:2327:A:H2'	1:A:2328:A:C8	2.35	0.60
6:G:16:ARG:HG3	6:G:16:ARG:HH11	1.66	0.60
13:R:102:GLU:OE2	18:W:37:ARG:NH1	2.29	0.60
3:D:108:PRO:HB3	3:D:143:HIS:CE1	2.36	0.60
1:A:2014:A:OP1	34:A:4137:HOH:O	2.16	0.60
1:A:2208:A:H1'	1:A:2219:G:C4	2.36	0.60
1:A:639:U:H2'	1:A:640:C:C6	2.36	0.60
12:Q:37:LEU:HD21	12:Q:130:LYS:HE2	1.83	0.60
1:A:2162:G:O3'	1:A:2172:U:O2'	2.14	0.60
1:A:1250:G:N7	11:P:18:ARG:NH2	2.49	0.60
1:A:662:G:H5''	11:P:16:ARG:HG2	1.83	0.60
1:A:517:C:OP1	27:5:16:ARG:NH2	2.34	0.60
1:A:1153:C:OP1	16:U:92:ARG:NH1	2.31	0.60
8:I:27:ARG:HD2	23:1:71:TYR:CE1	2.37	0.60
1:A:2023:G:H5'	1:A:2617:C:H4'	1.82	0.60
1:A:2887:U:H2'	1:A:2888:C:C6	2.36	0.60
34:A:4864:HOH:O	4:E:135:HIS:NE2	2.31	0.60
1:A:2134:A:H1'	1:A:2159:G:H1'	1.83	0.60
1:A:1021:A:H3'	1:A:1021:A:C8	2.37	0.60
1:A:1174:A:H1'	1:A:1175:U:H5''	1.83	0.60
1:A:2777:G:H5''	1:A:2778:A:H5'	1.84	0.60
20:Y:90:LEU:HB3	20:Y:92:ASN:H	1.66	0.59
3:D:145:VAL:HG12	3:D:146:GLU:O	2.02	0.59
15:T:118:ARG:NH1	15:T:118:ARG:HG3	2.14	0.59
1:A:2833:G:H3'	1:A:2834:G:H5''	1.85	0.59
15:T:51:ARG:HG3	15:T:98:LYS:HE3	1.83	0.59
1:A:250:G:OP2	30:8:13:ARG:NH2	2.36	0.59
1:A:1047:G:H2'	1:A:1110:G:H1	1.66	0.59
5:F:197:ASP:OD2	5:F:197:ASP:N	2.33	0.59
1:A:1619:G:N7	34:A:5529:HOH:O	2.32	0.59
11:P:38:GLN:O	11:P:39:LYS:CB	2.51	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2577:A:O4'	27:5:3:LYS:HB2	2.03	0.59
8:I:145:VAL:HG12	8:I:146:ALA:H	1.67	0.59
1:A:588:U:H2'	1:A:589:C:C6	2.37	0.59
8:I:133:HIS:ND1	8:I:134:PRO:O	2.35	0.59
13:R:67:LEU:HD13	13:R:76:VAL:HG21	1.85	0.59
1:A:1025:G:C4	1:A:1135:C:H1'	2.37	0.59
1:A:1951:U:O4	34:A:4242:HOH:O	2.14	0.59
1:A:11:G:H2'	1:A:12:U:H5'	1.84	0.59
2:B:11:C:H3'	2:B:12:C:C6	2.38	0.59
1:A:1882:C:H5'	1:A:1883:G:OP2	2.02	0.59
1:A:886:C:H2'	1:A:887:A:H5''	1.85	0.59
5:F:101:LEU:O	5:F:106:ARG:NH1	2.33	0.59
1:A:139(A):G:N2	19:X:44:GLU:OE1	2.36	0.59
1:A:271(E):U:H2'	1:A:271(F):C:C6	2.38	0.59
12:Q:51:ARG:NH2	21:Z:186:GLU:OE1	2.35	0.59
11:P:63:PRO:HG2	30:8:25:MET:HB2	1.85	0.59
1:A:392:C:OP1	34:A:4205:HOH:O	2.17	0.58
1:A:2295:C:C2'	1:A:2296:U:H5'	2.32	0.58
1:A:1448:G:H4'	1:A:1542:A:OP1	2.03	0.58
1:A:2572:A:N7	4:E:144:ARG:HD2	2.18	0.58
1:A:7:G:H2'	1:A:8:A:O4'	2.03	0.58
19:X:31:HIS:HD2	19:X:33:LYS:N	1.93	0.58
1:A:1430:C:H2'	1:A:1431:U:C6	2.38	0.58
14:S:96:GLY:N	14:S:99:LYS:H	2.02	0.58
14:S:11:LYS:O	14:S:15:ARG:HB2	2.03	0.58
30:8:23:VAL:CG1	30:8:47:LYS:HD3	2.34	0.58
23:1:50:ARG:HG2	23:1:59:THR:HG22	1.86	0.58
1:A:84:A:H5''	20:Y:8:LYS:HE3	1.85	0.58
1:A:2137:C:O2	1:A:2137:C:H2'	2.02	0.58
1:A:2243:U:H2'	1:A:2244:U:C6	2.38	0.58
4:E:118:LYS:O	34:E:405:HOH:O	2.16	0.58
12:Q:135:ASP:OD2	21:Z:49:ARG:NH2	2.37	0.58
10:O:16:ALA:HB2	10:O:52:VAL:HG21	1.86	0.58
1:A:1379:A:H4'	1:A:1380:G:OP2	2.02	0.58
21:Z:161:VAL:O	21:Z:161:VAL:HG13	2.04	0.57
1:A:642:G:H21	1:A:646:A:H2	1.52	0.57
1:A:1405:U:H2'	1:A:1406:U:C6	2.39	0.57
1:A:2287:A:N6	1:A:2344:U:H3	1.95	0.57
1:A:911:A:H2'	12:Q:9:TYR:OH	2.05	0.57
11:P:126:VAL:HG12	11:P:148:LEU:HD22	1.86	0.57
1:A:621:A:OP2	11:P:108:LYS:NZ	2.36	0.57
4:E:143:ASN:HD22	4:E:147:PRO:HD3	1.70	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:E:201:THR:OG1	4:E:202:LYS:N	2.38	0.57
1:A:2114:A:H3'	1:A:2115:G:C8	2.38	0.57
21:Z:124:ILE:HG13	21:Z:125:LEU:H	1.69	0.57
1:A:1540:U:C2'	1:A:1541:G:H5'	2.34	0.57
1:A:1385:G:N7	34:A:5331:HOH:O	2.32	0.57
28:6:18:ARG:HG3	28:6:42:TRP:CD1	2.40	0.57
16:U:92:ARG:HA	16:U:95:LEU:HB2	1.85	0.57
1:A:652(G):G:H2'	1:A:652(H):C:C6	2.40	0.57
25:3:23:LEU:HD13	25:3:50:VAL:HG11	1.87	0.57
2:B:7:G:N7	34:B:337:HOH:O	2.33	0.57
1:A:2130:U:H1'	1:A:2158:A:N1	2.19	0.57
1:A:729:G:C6	3:D:208:LYS:HB2	2.40	0.57
1:A:1106:G:H4'	1:A:1107:G:OP2	2.05	0.57
30:8:34:TRP:CG	30:8:35:GLN:N	2.73	0.57
4:E:116:VAL:HG13	4:E:122:PHE:HB2	1.87	0.57
1:A:2532:G:O6	34:A:5005:HOH:O	2.15	0.57
1:A:1173:G:O2'	1:A:1174:A:O4'	2.22	0.56
1:A:12:U:H2'	1:A:12:U:O2	2.04	0.56
1:A:1929:G:H4'	1:A:1930:G:OP1	2.04	0.56
3:D:275:LYS:HG3	3:D:276:LYS:HB2	1.86	0.56
1:A:2319:G:H22	14:S:3:ARG:NE	2.04	0.56
1:A:2168:G:H22	1:A:2171:A:H2'	1.70	0.56
1:A:1486:A:H2'	1:A:1487:G:C8	2.40	0.56
12:Q:110:THR:HG23	12:Q:113:GLN:OE1	2.06	0.56
7:H:12:PRO:O	7:H:14:GLY:HA2	2.05	0.56
12:Q:12:GLN:HG2	12:Q:73:PRO:HD2	1.87	0.56
1:A:1218:C:H5''	1:A:1218:C:H6	1.70	0.56
1:A:2328:A:H2'	1:A:2329:G:C8	2.40	0.56
30:8:29:LYS:HG2	30:8:44:LYS:HB3	1.85	0.56
1:A:2115:G:O2'	1:A:2166:G:N2	2.38	0.56
28:6:16:CYS:SG	28:6:18:ARG:HG2	2.46	0.56
10:O:23:ARG:HG3	10:O:24:VAL:N	2.21	0.56
2:B:31:C:O2'	2:B:53:A:N6	2.39	0.56
1:A:2526:G:H21	31:9:2:LYS:HD2	1.70	0.56
1:A:2584:U:H2'	1:A:2585:U:H2'	1.88	0.56
1:A:657:U:H2'	1:A:658:C:C6	2.41	0.56
1:A:2131:G:OP1	1:A:2132:U:H3'	2.05	0.56
1:A:997:G:OP1	16:U:92:ARG:HG2	2.05	0.56
4:E:28:ALA:HB3	4:E:93:VAL:HG13	1.88	0.56
1:A:141:A:H8	1:A:1408:C:HO2'	1.50	0.56
1:A:2130:U:O2'	1:A:2133:G:O2'	2.24	0.56
1:A:644:A:H4'	1:A:645:C:C5	2.40	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
29:7:33:ARG:NH2	34:7:202:HOH:O	2.38	0.56
1:A:2850:A:OP2	1:A:2866:U:H5	1.89	0.56
1:A:2473:U:H2'	1:A:2473:U:O2	2.06	0.56
1:A:1178:C:H2'	1:A:1179:C:C6	2.42	0.55
14:S:11:LYS:HG3	14:S:91:PRO:HD3	1.88	0.55
27:5:51:TYR:CE1	27:5:56:LYS:HG2	2.42	0.55
2:B:2:C:H2'	2:B:3:C:C6	2.41	0.55
17:V:49:THR:HG22	17:V:49:THR:O	2.06	0.55
1:A:2152:G:H2'	1:A:2153:G:C8	2.40	0.55
26:4:15:ILE:O	26:4:32:TYR:HA	2.06	0.55
18:W:4:LYS:HE2	18:W:6:ILE:HD11	1.88	0.55
28:6:35:GLU:HG3	28:6:50:ARG:HG3	1.88	0.55
1:A:2439:A:H5'	1:A:2439:A:C8	2.42	0.55
1:A:1488:G:H5''	1:A:1488:G:H8	1.72	0.55
1:A:889:C:O2'	1:A:890:A:H8	1.90	0.55
7:H:28:GLY:HA3	7:H:79:VAL:HB	1.87	0.55
7:H:149:ARG:NH1	7:H:167:GLU:OE1	2.40	0.55
21:Z:138:GLU:H	21:Z:156:LYS:NZ	2.04	0.55
1:A:994:C:OP1	16:U:53:ARG:NH2	2.38	0.55
15:T:60:THR:HG22	15:T:77:PRO:HA	1.89	0.55
1:A:1204:A:H61	1:A:1240:U:H2'	1.70	0.55
9:N:56:ASN:HA	9:N:125:GLY:H	1.72	0.55
6:G:82:LEU:H	6:G:82:LEU:CD1	2.18	0.55
24:2:45:SER:O	24:2:46:GLN:HB2	2.06	0.55
12:Q:138:ASP:OD2	21:Z:81:ARG:NH1	2.39	0.55
1:A:652(C):G:N2	1:A:652(V):C:O2	2.35	0.55
20:Y:23:ARG:HB2	20:Y:23:ARG:NH1	2.22	0.55
1:A:1688:U:H1'	1:A:1701:A:C6	2.42	0.55
14:S:96:GLY:HA2	14:S:97:ARG:C	2.27	0.55
14:S:102:ALA:HB1	14:S:112:PHE:HZ	1.72	0.55
8:I:111:PRO:C	8:I:113:ARG:H	2.08	0.55
1:A:1654:A:OP1	13:R:1:MET:HA	2.07	0.55
4:E:203:LYS:CB	4:E:204:ALA:HA	2.35	0.55
1:A:1288:U:H2'	34:A:3915:HOH:O	2.06	0.55
5:F:120:GLU:HB2	5:F:122:LYS:HG2	1.89	0.55
11:P:59:LEU:HD21	30:8:10:ALA:HA	1.89	0.55
19:X:41:ASN:O	19:X:45:THR:HG23	2.06	0.55
1:A:359:A:H2'	1:A:360:G:O4'	2.07	0.55
1:A:1903:G:OP1	3:D:241:PRO:HB2	2.07	0.55
28:6:13:CYS:SG	28:6:47:THR:HG21	2.46	0.55
1:A:2879:C:O2'	34:A:4916:HOH:O	2.18	0.55
1:A:2322:A:H2'	1:A:2323:G:O4'	2.06	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
21:Z:81:ARG:HH21	21:Z:81:ARG:HG2	1.71	0.55
1:A:307:G:H21	1:A:330:A:H62	1.55	0.54
1:A:2469:A:H4'	12:Q:56:ARG:HG2	1.88	0.54
1:A:2506:U:OP1	4:E:144:ARG:NH2	2.41	0.54
3:D:242:ARG:N	3:D:242:ARG:HD3	2.22	0.54
1:A:77:C:OP1	24:2:59:ARG:HD3	2.08	0.54
1:A:1019:U:H3	1:A:1142(A):A:H62	1.56	0.54
8:I:106:GLY:HA2	8:I:107:VAL:HB	1.89	0.54
5:F:157:VAL:HB	5:F:194:MET:HG2	1.90	0.54
21:Z:152:ALA:HA	21:Z:155:LEU:HD13	1.89	0.54
8:I:29:TYR:O	8:I:32:PRO:HD2	2.08	0.54
21:Z:154:ASP:OD1	21:Z:154:ASP:N	2.40	0.54
3:D:275:LYS:HG3	3:D:276:LYS:N	2.22	0.54
14:S:95:HIS:C	14:S:99:LYS:HB3	2.27	0.54
4:E:11:MET:HG2	4:E:24:THR:HB	1.89	0.54
21:Z:138:GLU:H	21:Z:156:LYS:HZ1	1.53	0.54
18:W:40:ASN:O	18:W:41:LYS:HG3	2.08	0.54
1:A:1187:G:H5''	17:V:81:TYR:CE2	2.42	0.54
1:A:1932:A:H2'	1:A:1933:G:O4'	2.07	0.54
7:H:67:LEU:O	7:H:71:LEU:HB2	2.08	0.54
7:H:137:ASP:HB3	7:H:140:LYS:HB3	1.89	0.54
1:A:2304:G:O6	1:A:2312:U:O4	2.26	0.54
14:S:34:HIS:ND1	14:S:53:SER:OG	2.36	0.54
1:A:300:A:OP2	20:Y:86:ARG:NH2	2.41	0.54
1:A:2867:G:OP2	15:T:119:LYS:NZ	2.41	0.54
1:A:2198:A:H4'	1:A:2199:A:OP1	2.08	0.54
1:A:1359:A:H5'	1:A:1359:A:N3	2.23	0.53
1:A:1364:G:OP1	23:1:2:SER:HA	2.08	0.53
1:A:1540:U:O2'	1:A:1541:G:H5'	2.08	0.53
29:7:34:ARG:NH1	29:7:41:ARG:O	2.41	0.53
6:G:75:LYS:HA	6:G:84:LYS:HE2	1.90	0.53
1:A:2464:C:O2'	1:A:2465:C:H5''	2.09	0.53
5:F:101:LEU:HD12	5:F:102:PRO:HD2	1.89	0.53
1:A:1429:G:O2'	1:A:1430:C:H5'	2.09	0.53
1:A:2627:G:O2'	1:A:2781:A:N1	2.36	0.53
2:B:90:A:N7	2:B:91:C:H1'	2.22	0.53
4:E:55:ASN:HB3	4:E:58:ARG:HG3	1.90	0.53
1:A:1587:A:H2'	1:A:1588:C:C6	2.42	0.53
8:I:81:VAL:HG21	8:I:88:ILE:HD13	1.89	0.53
3:D:96:HIS:CD2	3:D:102:LYS:HD3	2.44	0.53
9:N:56:ASN:H	9:N:125:GLY:CA	2.19	0.53
5:F:17:ARG:O	5:F:18:ARG:HB2	2.08	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:O:63:VAL:HG12	10:O:106:LEU:HD11	1.89	0.53
21:Z:124:ILE:HG13	21:Z:125:LEU:N	2.23	0.53
1:A:1817:G:OP1	3:D:88:ARG:NH2	2.41	0.53
1:A:1021:A:H3'	1:A:1021:A:H8	1.73	0.53
8:I:77:LEU:CB	8:I:142:VAL:HG12	2.34	0.53
1:A:271(Q):G:O2'	1:A:271(R):G:H8	1.90	0.53
1:A:2171:A:H4'	1:A:2172:U:OP1	2.09	0.53
5:F:184:TYR:CD2	5:F:188:ARG:HD2	2.44	0.53
29:7:48:LYS:NZ	34:7:204:HOH:O	2.21	0.53
1:A:1047:G:C2'	1:A:1110:G:H22	2.15	0.53
1:A:1173:G:N2	1:A:1176:G:OP2	2.42	0.53
3:D:71:ASP:HB3	3:D:103:ARG:HH22	1.74	0.53
1:A:652(Q):G:H2'	1:A:652(R):C:H5'	1.90	0.53
1:A:1106:G:OP2	1:A:1106:G:H8	1.91	0.53
1:A:2126:A:H1'	1:A:2127:G:OP2	2.09	0.53
7:H:150:ALA:HA	7:H:153:LYS:HD2	1.89	0.53
1:A:1507:A:O2'	1:A:1508:A:H8	1.92	0.53
1:A:1178:C:H2'	1:A:1179:C:H6	1.73	0.53
1:A:652(D):C:H2'	1:A:652(E):G:O4'	2.09	0.53
1:A:2183:C:H2'	1:A:2184:G:C8	2.44	0.53
1:A:2483:C:N3	12:Q:124:LYS:NZ	2.55	0.53
1:A:2186:G:H2'	1:A:2186:G:N3	2.24	0.52
1:A:562:U:C4	1:A:2036:C:O4'	2.62	0.52
8:I:133:HIS:HD1	8:I:134:PRO:N	2.07	0.52
26:4:42:PHE:HB3	26:4:43:TYR:HB2	1.90	0.52
9:N:96:GLU:H	9:N:96:GLU:CD	2.11	0.52
5:F:184:TYR:CE2	5:F:188:ARG:HD2	2.45	0.52
1:A:2365:G:O6	30:8:39:LYS:HE3	2.09	0.52
1:A:218:A:C2	1:A:235:U:H4'	2.44	0.52
9:N:15:LEU:HB2	9:N:135:PRO:HB2	1.90	0.52
1:A:2080:G:OP1	23:1:35:THR:HG21	2.09	0.52
1:A:2377:A:H2'	1:A:2378:A:C8	2.45	0.52
1:A:674:G:H1'	5:F:74:ARG:HD3	1.91	0.52
1:A:952:G:OP1	12:Q:16:ARG:NH2	2.42	0.52
1:A:2317:C:C4	1:A:2318:G:N7	2.77	0.52
1:A:372:G:OP2	23:1:69:LYS:NZ	2.29	0.52
21:Z:54:HIS:ND1	21:Z:101:PRO:HG3	2.25	0.52
11:P:38:GLN:O	11:P:39:LYS:HB3	2.10	0.52
28:6:6:ARG:NH1	28:6:26:ASN:HB2	2.24	0.52
1:A:2319:G:N1	14:S:3:ARG:HA	2.25	0.52
21:Z:137:ILE:HG23	21:Z:156:LYS:HD2	1.91	0.52
1:A:1810:A:H2'	1:A:1811:G:O4'	2.09	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:Q:6:ARG:HB3	21:Z:194:PRO:HG2	1.90	0.52
3:D:3:VAL:HG13	3:D:17:THR:HB	1.92	0.52
1:A:1038:C:H42	1:A:1117:G:H1	1.56	0.52
1:A:1176:G:H21	1:A:1178:C:P	2.32	0.52
1:A:90:U:O2'	1:A:92:A:C8	2.62	0.52
1:A:141:A:H8	1:A:1408:C:O2'	1.93	0.52
1:A:1243:G:O2'	11:P:7:ARG:NH2	2.43	0.52
17:V:23:GLU:OE1	34:V:305:HOH:O	2.19	0.52
1:A:813:U:H2'	1:A:814:C:C6	2.45	0.52
1:A:207:A:H2'	1:A:208:C:O4'	2.08	0.52
21:Z:72:ARG:NH2	21:Z:97:GLU:O	2.43	0.52
8:I:96:ASP:O	8:I:100:ALA:N	2.39	0.52
1:A:1021:A:H8	1:A:1022:G:H5''	1.75	0.51
1:A:271(Q):G:O2'	1:A:271(R):G:C8	2.62	0.51
1:A:528:A:C2	1:A:2043:C:H4'	2.45	0.51
1:A:2134:A:N3	1:A:2159:G:O2'	2.40	0.51
8:I:107:VAL:HG12	8:I:108:THR:N	2.22	0.51
1:A:2463:C:O2'	1:A:2464:C:H5'	2.11	0.51
27:5:16:ARG:HG2	27:5:16:ARG:NH1	2.25	0.51
1:A:2125:G:N2	1:A:2172:U:H3'	2.25	0.51
14:S:101:LEU:O	14:S:102:ALA:HB3	2.10	0.51
14:S:10:ARG:O	14:S:14:VAL:HG13	2.10	0.51
1:A:141:A:C8	1:A:1408:C:O2'	2.61	0.51
5:F:11:VAL:HB	5:F:18:ARG:HB3	1.92	0.51
30:8:32:LEU:O	30:8:36:LYS:HE3	2.10	0.51
1:A:2147:G:H2'	1:A:2148:G:O4'	2.10	0.51
18:W:45:TYR:CZ	18:W:49:LYS:HE3	2.46	0.51
1:A:1329:U:H5''	1:A:1330:C:H5	1.76	0.51
8:I:110:ASP:N	8:I:130:TYR:OH	2.40	0.51
2:B:105:A:OP1	21:Z:72:ARG:NH1	2.42	0.51
23:1:6:GLU:HG3	23:1:61:ARG:O	2.11	0.51
18:W:66:GLU:HA	18:W:69:LEU:HD12	1.91	0.51
1:A:2357:U:OP1	22:0:20:ARG:HD3	2.10	0.51
2:B:6:C:C2'	2:B:7:G:H5''	2.39	0.51
10:O:98:VAL:HG22	10:O:118:ALA:HA	1.92	0.51
1:A:330:A:H2	1:A:1210:A:H2'	1.75	0.51
1:A:330:A:H2	1:A:1210:A:O2'	1.92	0.51
1:A:1914:C:H2'	1:A:1915:U:C6	2.45	0.51
1:A:2136:C:N3	1:A:2155:G:N2	2.46	0.51
1:A:1109:C:H5	1:A:1110:G:N1	2.08	0.51
1:A:1721:G:H2'	1:A:1740:G:O6	2.11	0.51
1:A:2022:U:O2'	1:A:2617:C:H5'	2.10	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:652(Q):G:C2'	1:A:652(R):C:H5'	2.41	0.51
14:S:82:ILE:HA	14:S:83:LYS:CB	2.40	0.51
1:A:2784:C:H1'	4:E:37:ARG:HH12	1.75	0.51
15:T:24:PRO:HD3	15:T:52:ILE:HD12	1.93	0.51
19:X:54:VAL:HG13	19:X:81:VAL:HG12	1.93	0.51
21:Z:128:VAL:HG23	21:Z:161:VAL:H	1.76	0.51
1:A:2166:G:H2'	1:A:2167:U:O4'	2.10	0.51
1:A:616:G:H5'	5:F:205:ARG:HD2	1.92	0.51
19:X:53:LYS:HB3	19:X:82:GLN:HB3	1.93	0.51
1:A:2611:U:OP2	1:A:2611:U:H3'	2.10	0.51
21:Z:111:VAL:C	21:Z:113:ALA:H	2.14	0.51
1:A:1658:C:OP1	34:A:4864:HOH:O	2.19	0.51
1:A:300:A:P	20:Y:86:ARG:HH22	2.34	0.50
1:A:2689:U:H4'	1:A:2690:C:H5'	1.93	0.50
1:A:602:G:O2'	1:A:655:A:N6	2.44	0.50
2:B:11:C:H3'	2:B:12:C:H6	1.76	0.50
1:A:185:U:H4'	1:A:218:A:H4'	1.93	0.50
18:W:65:LEU:HD12	18:W:68:ARG:HE	1.77	0.50
1:A:2104:G:N7	1:A:2186:G:N2	2.58	0.50
7:H:41:MET:HE3	7:H:54:ARG:HA	1.94	0.50
1:A:1406:U:H2'	1:A:1407:C:C6	2.46	0.50
1:A:1815:A:OP2	3:D:54:ARG:NH2	2.44	0.50
1:A:2205:C:O2	1:A:2220:G:C2	2.64	0.50
8:I:126:TYR:HB2	8:I:142:VAL:HG23	1.93	0.50
1:A:330:A:HO2'	1:A:331:A:H8	1.57	0.50
1:A:2203:U:O2'	1:A:2205:C:H5'	2.11	0.50
1:A:322:A:OP1	5:F:168:ARG:HD2	2.12	0.50
1:A:1358:G:OP2	34:A:4970:HOH:O	2.18	0.50
14:S:96:GLY:HA2	14:S:100:ALA:H	1.76	0.50
1:A:2317:C:C2	1:A:2318:G:N7	2.80	0.50
1:A:2000:G:OP1	13:R:5:LYS:NZ	2.39	0.50
1:A:1794:U:H2'	1:A:1795:C:C6	2.47	0.50
17:V:35:LEU:HB2	17:V:57:VAL:HG22	1.92	0.50
1:A:1371:G:HO2'	1:A:1372:U:H5	1.58	0.50
1:A:1530:C:H1'	1:A:1531:C:OP1	2.12	0.50
1:A:154:G:H5'	1:A:154(A):C:OP2	2.12	0.50
1:A:2052:G:H4'	4:E:143:ASN:O	2.11	0.50
28:6:10:LEU:HG	28:6:54:ILE:HG13	1.92	0.50
1:A:1049:C:O2'	1:A:1050:A:H8	1.78	0.50
1:A:2839:G:C5'	13:R:46:GLY:HA2	2.42	0.50
3:D:60:ARG:NH1	34:D:415:HOH:O	2.27	0.50
1:A:1045:A:N3	1:A:1045:A:H2'	2.26	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2125:G:H21	1:A:2126:A:N6	2.10	0.50
1:A:1980:G:O2'	1:A:1982:C:OP2	2.25	0.50
1:A:245:G:O5'	11:P:73:GLY:HA2	2.11	0.50
11:P:82:GLY:HA2	11:P:113:LYS:O	2.12	0.50
3:D:69:ARG:NH2	3:D:128:GLY:O	2.38	0.50
1:A:2031:A:C6	1:A:2498:C:H1'	2.47	0.50
1:A:821:A:H2'	1:A:946:G:H5''	1.93	0.50
1:A:2336:A:H61	22:O:43:THR:HG22	1.76	0.50
1:A:886:C:OP1	1:A:886:C:H4'	2.12	0.50
1:A:1403:C:C5'	1:A:1471:A:H1'	2.41	0.50
1:A:2158:A:H4'	1:A:2159:G:H5'	1.93	0.50
1:A:1417:C:H2'	1:A:1418:G:O4'	2.11	0.50
17:V:40:LEU:HB2	17:V:46:VAL:HG13	1.94	0.50
1:A:1529:G:C6	1:A:1530:C:N4	2.80	0.49
4:E:9:VAL:HG13	4:E:25:VAL:O	2.11	0.49
11:P:121:LYS:HD3	11:P:123:LEU:HD11	1.93	0.49
1:A:2036:C:C6	1:A:2036:C:H5'	2.35	0.49
1:A:1300:U:H4'	1:A:1301:A:C5'	2.41	0.49
5:F:184:TYR:O	5:F:188:ARG:HG3	2.12	0.49
1:A:2537:U:H2'	1:A:2538:C:C6	2.48	0.49
7:H:88:LEU:CD2	7:H:165:ALA:HA	2.42	0.49
1:A:1652:A:O2'	1:A:1653:G:H5'	2.12	0.49
1:A:2305:A:H5''	6:G:134:GLY:HA3	1.94	0.49
1:A:1721:G:N1	1:A:1739:U:OP2	2.45	0.49
1:A:2463:C:C2'	1:A:2464:C:H5'	2.42	0.49
2:B:49:C:OP1	14:S:97:ARG:N	2.44	0.49
1:A:1503:U:H2'	1:A:1504:C:C6	2.47	0.49
1:A:1963:U:H4'	1:A:1964:G:OP1	2.12	0.49
10:O:19:ILE:HG22	10:O:43:VAL:HG22	1.94	0.49
1:A:796:C:H2'	1:A:797:C:C6	2.47	0.49
1:A:243:U:OP1	30:8:6:THR:OG1	2.27	0.49
1:A:620:G:H5'	1:A:620:G:N3	2.27	0.49
1:A:2648:C:H2'	1:A:2649:U:C6	2.47	0.49
9:N:18:ALA:O	9:N:19:GLU:HB3	2.11	0.49
1:A:1185:C:H5''	1:A:1186:G:OP1	2.12	0.49
4:E:12:THR:HG21	15:T:11:GLU:OE2	2.12	0.49
4:E:12:THR:HG22	15:T:58:ASN:OD1	2.13	0.49
2:B:53:A:H2'	2:B:54:G:O4'	2.12	0.49
21:Z:150:LEU:O	21:Z:171:ILE:HG13	2.12	0.49
7:H:40:GLU:OE1	7:H:60:ARG:NH1	2.45	0.49
1:A:1268:A:H2'	1:A:1269:A:O4'	2.12	0.49
1:A:848:G:C4	1:A:933:A:H8	2.30	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:O:101:PRO:HG3	15:T:67:SER:OG	2.12	0.49
20:Y:23:ARG:HH11	20:Y:23:ARG:HB2	1.78	0.49
1:A:330:A:H2	1:A:1210:A:C2'	2.26	0.49
3:D:71:ASP:HB3	3:D:103:ARG:NH2	2.27	0.49
15:T:51:ARG:HG3	15:T:98:LYS:CE	2.42	0.49
1:A:910:A:N1	1:A:2277:G:H1'	2.28	0.49
3:D:77:ALA:HB2	3:D:97:TYR:CD2	2.48	0.49
21:Z:10:ARG:HG3	21:Z:36:LYS:HB3	1.94	0.49
1:A:271(Q):G:O2'	1:A:271(R):G:P	2.70	0.49
14:S:35:ILE:HD13	14:S:101:LEU:HD12	1.95	0.49
1:A:2001:A:H2'	1:A:2002:G:C8	2.48	0.49
1:A:2109:U:H2'	1:A:2110:G:C8	2.48	0.49
1:A:1545:A:H2'	1:A:1546:C:O4'	2.13	0.49
12:Q:34:LEU:HD11	12:Q:129:THR:HB	1.95	0.49
1:A:2122:U:H2'	1:A:2123:G:C8	2.48	0.49
1:A:2464:C:HO2'	1:A:2465:C:H5''	1.77	0.49
1:A:847:U:H5	1:A:933:A:H62	1.57	0.49
26:4:14:ILE:HD12	26:4:22:ILE:HD12	1.93	0.49
23:1:94:LEU:O	23:1:97:LEU:HB2	2.13	0.49
1:A:864:G:N2	1:A:913:U:C2	2.81	0.49
1:A:1021:A:H62	1:A:1141:U:H3	1.61	0.49
1:A:1506:C:C2'	1:A:1507:A:H5'	2.39	0.49
1:A:2319:G:N2	14:S:3:ARG:HB2	2.28	0.49
21:Z:93:ASP:HB2	21:Z:131:ARG:HH22	1.77	0.49
1:A:2563:U:O2	1:A:2565:A:H8	1.96	0.49
1:A:774:A:HO2'	1:A:775:G:H8	1.58	0.49
1:A:2138:C:H2'	1:A:2139:C:C6	2.48	0.49
1:A:1113:U:H2'	1:A:1114:G:C8	2.48	0.49
1:A:2321:G:H5''	1:A:2322:A:OP2	2.13	0.48
2:B:44:G:C2	2:B:48:A:C2	3.01	0.48
1:A:90:U:O2'	1:A:92:A:O4'	2.30	0.48
24:2:4:SER:HA	24:2:7:ARG:NH1	2.28	0.48
1:A:839:U:H2'	1:A:840:C:C6	2.48	0.48
1:A:2296:U:OP2	14:S:9:ARG:NH2	2.39	0.48
6:G:43:LEU:HB2	6:G:89:GLY:HA2	1.94	0.48
31:9:27:CYS:SG	31:9:28:GLU:N	2.86	0.48
11:P:26:GLY:O	11:P:27:HIS:CD2	2.66	0.48
6:G:16:ARG:HE	6:G:31:VAL:HG21	1.77	0.48
1:A:647:G:O5'	1:A:647:G:H8	1.96	0.48
9:N:108:PRO:O	9:N:113:GLY:HA3	2.13	0.48
21:Z:7:ALA:HB3	21:Z:61:LEU:HD12	1.94	0.48
6:G:60:LEU:HB3	6:G:68:PRO:HG3	1.95	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
15:T:2:ASN:O	15:T:6:LEU:HD22	2.13	0.48
1:A:811:U:O2'	11:P:21:ARG:HG3	2.13	0.48
1:A:1430:C:H2'	1:A:1431:U:H6	1.77	0.48
1:A:11:G:C2'	1:A:12:U:H5'	2.43	0.48
2:B:2:C:H2'	2:B:3:C:H6	1.79	0.48
6:G:179:PRO:HG3	26:4:43:TYR:OH	2.13	0.48
30:8:28:GLY:O	30:8:36:LYS:NZ	2.46	0.48
1:A:784:A:C8	1:A:792:G:C5	3.01	0.48
1:A:27:G:O6	34:A:4062:HOH:O	2.18	0.48
1:A:1858:G:H1'	1:A:1884:A:N6	2.28	0.48
1:A:2320:A:N3	1:A:2320:A:H2'	2.28	0.48
1:A:2130:U:O2'	1:A:2158:A:N6	2.45	0.48
1:A:764:A:H2	3:D:219:PRO:HG3	1.78	0.48
2:B:42:C:O2	6:G:92:VAL:HA	2.14	0.48
1:A:1239:G:H2'	1:A:1240:U:O4'	2.14	0.48
1:A:1604:C:H5'	34:A:3861:HOH:O	2.12	0.48
1:A:528:A:N1	1:A:2042:A:H2'	2.27	0.48
1:A:1210:A:H5''	1:A:1212:G:O4'	2.14	0.48
1:A:185:U:H2'	1:A:186:G:C8	2.49	0.48
21:Z:111:VAL:HG12	21:Z:112:ARG:N	2.28	0.48
22:0:72:ARG:HB2	22:0:75:LEU:HB2	1.96	0.48
23:1:82:LEU:HA	23:1:85:LEU:CD2	2.40	0.48
1:A:2820:A:OP1	13:R:4:LEU:HD23	2.14	0.48
1:A:2869:G:H2'	1:A:2870:C:O4'	2.14	0.48
1:A:664:C:H4'	1:A:941:A:OP1	2.14	0.48
1:A:484:C:H2'	1:A:485:C:C6	2.48	0.48
21:Z:45:ASP:OD2	21:Z:49:ARG:NH1	2.46	0.48
17:V:52:VAL:HG22	17:V:55:ALA:HB3	1.96	0.48
1:A:1031:G:H21	31:9:36:GLN:HE22	1.61	0.48
1:A:375:C:H2'	1:A:376:C:C6	2.49	0.48
1:A:1378:A:OP1	29:7:10:ARG:NH2	2.47	0.48
9:N:56:ASN:N	9:N:125:GLY:HA3	2.25	0.48
9:N:24:GLY:HA2	9:N:27:ALA:CB	2.42	0.48
1:A:1652:A:C2'	1:A:1653:G:H5'	2.43	0.48
28:6:21:TYR:CE2	28:6:38:LYS:HG2	2.49	0.48
1:A:2165:G:H2'	1:A:2166:G:C8	2.48	0.47
21:Z:125:LEU:HG	21:Z:164:ALA:HB3	1.96	0.47
1:A:1588:C:H2'	1:A:1589:C:H6	1.79	0.47
12:Q:5:ARG:O	21:Z:194:PRO:HD2	2.14	0.47
1:A:2193:G:H2'	1:A:2194:G:C8	2.49	0.47
1:A:1252:G:O4'	16:U:33:ARG:HD2	2.14	0.47
1:A:1165:U:H2'	1:A:1166:C:C6	2.48	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:Y:38:ILE:HD11	20:Y:66:PRO:HG3	1.95	0.47
1:A:284:U:H2'	1:A:285:C:C6	2.49	0.47
1:A:1593:G:H2'	1:A:1594:G:C8	2.49	0.47
1:A:2317:C:N3	1:A:2318:G:N7	2.61	0.47
25:3:8:LEU:HD13	25:3:31:LEU:CD2	2.42	0.47
1:A:2040:C:H2'	1:A:2041:U:O4'	2.14	0.47
5:F:150:GLY:HA2	5:F:172:TRP:CD2	2.49	0.47
2:B:13:A:N1	2:B:69:G:O2'	2.38	0.47
1:A:1530:C:O2'	1:A:1531:C:P	2.73	0.47
1:A:2111:C:H42	1:A:2147:G:N2	2.12	0.47
15:T:120:ARG:HA	15:T:123:GLN:HG2	1.95	0.47
1:A:2101:G:H2'	1:A:2102:U:O4'	2.13	0.47
1:A:1174:A:H1'	1:A:1175:U:C5'	2.45	0.47
1:A:1494:A:H2'	1:A:1495:A:C8	2.49	0.47
2:B:78:A:C2	2:B:100:A:C4	3.02	0.47
3:D:108:PRO:HB3	3:D:143:HIS:HE1	1.78	0.47
1:A:2303:G:O6	34:A:4025:HOH:O	2.17	0.47
3:D:180:GLY:HA3	3:D:275:LYS:HD3	1.96	0.47
8:I:129:THR:HG22	8:I:139:GLN:OE1	2.14	0.47
13:R:37:THR:OG1	13:R:40:LYS:HG3	2.15	0.47
1:A:2747:G:O6	1:A:2755:C:H5''	2.13	0.47
4:E:178:GLU:OE2	4:E:178:GLU:N	2.41	0.47
1:A:1047:G:H2'	1:A:1110:G:N1	2.30	0.47
1:A:652(I):C:H2'	1:A:652(J):G:N7	2.28	0.47
1:A:90:U:HO2'	1:A:92:A:H8	1.57	0.47
1:A:2128:C:N4	1:A:2160:G:H1	2.12	0.47
1:A:2134:A:H62	1:A:2157:G:H5'	1.79	0.47
1:A:2134:A:N6	1:A:2157:G:H5'	2.30	0.47
1:A:848:G:N9	1:A:933:A:H8	2.13	0.47
1:A:1268:A:C2	1:A:2013:A:C4	3.03	0.47
1:A:2169:A:H2'	1:A:2170:A:C8	2.49	0.47
1:A:1170:G:H5''	1:A:1170:G:H8	1.80	0.47
1:A:2134:A:C2	1:A:2159:G:H4'	2.50	0.47
28:6:16:CYS:HB2	28:6:18:ARG:NH1	2.30	0.47
1:A:1914:C:H2'	1:A:1915:U:H6	1.80	0.47
1:A:2690:C:H6	1:A:2690:C:OP2	1.97	0.47
26:4:14:ILE:HG23	26:4:31:ILE:HB	1.97	0.47
1:A:2601:C:H3'	34:A:5509:HOH:O	2.13	0.47
1:A:1580:A:H8	1:A:1580:A:OP2	1.97	0.47
21:Z:128:VAL:HG23	21:Z:161:VAL:N	2.30	0.47
1:A:1171:G:H3'	1:A:1173:G:H5'	1.96	0.47
1:A:92:A:H2'	1:A:93:G:O4'	2.15	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:747:U:O2	1:A:2014:A:H1'	2.14	0.47
1:A:2137:C:C2	1:A:2154:G:N2	2.83	0.47
1:A:1176:G:N2	1:A:1178:C:OP2	2.46	0.47
1:A:2224:G:H4'	1:A:2226:C:C2	2.50	0.47
1:A:2074:U:H2'	1:A:2075:U:C6	2.50	0.47
24:2:16:LEU:O	24:2:67:LYS:NZ	2.48	0.47
1:A:263:C:H2'	1:A:264:C:O4'	2.15	0.47
1:A:459:U:OP2	1:A:469:G:N1	2.39	0.47
1:A:1783:A:H5'	1:A:2608:G:H4'	1.97	0.46
4:E:51:PHE:CD1	4:E:52:LEU:HD22	2.50	0.46
1:A:2887:U:H2'	1:A:2888:C:H6	1.79	0.46
18:W:79:GLY:HA3	18:W:100:THR:HG22	1.97	0.46
1:A:1292:U:H2'	1:A:1293:C:C6	2.50	0.46
1:A:2884:U:H1'	27:5:53:ALA:HB2	1.97	0.46
1:A:2297:C:H1'	1:A:2322:A:C2	2.50	0.46
1:A:2115:G:H21	1:A:2171:A:N6	2.12	0.46
1:A:1494:A:O2'	1:A:1495:A:H5'	2.15	0.46
6:G:121:ASN:HA	6:G:122:PRO:HD3	1.78	0.46
1:A:1607:C:H4'	1:A:1608:A:O5'	2.15	0.46
1:A:2173:A:H2'	1:A:2174:C:H5'	1.97	0.46
1:A:883:G:H1	1:A:893:C:H42	1.63	0.46
1:A:539:G:H2'	1:A:540:C:C6	2.51	0.46
1:A:646:A:H2'	1:A:647:G:O4'	2.16	0.46
11:P:126:VAL:HG11	11:P:148:LEU:HD13	1.97	0.46
1:A:1816:G:H8	3:D:62:TYR:CZ	2.33	0.46
1:A:2836:U:C4	1:A:2883:A:N6	2.84	0.46
27:5:11:THR:HG23	27:5:15:ARG:HB3	1.97	0.46
23:1:3:LYS:HB3	23:1:4:VAL:H	1.50	0.46
1:A:95:G:O2'	24:2:46:GLN:HA	2.15	0.46
6:G:3:LEU:HD13	26:4:25:TYR:CE1	2.50	0.46
2:B:32:C:C2	2:B:51:G:N2	2.83	0.46
1:A:2295:C:O2'	1:A:2296:U:H5'	2.15	0.46
1:A:271(N):U:O2'	1:A:271(O):C:H5'	2.15	0.46
1:A:910:A:H62	12:Q:12:GLN:HA	1.80	0.46
25:3:10:LYS:NZ	25:3:15:TYR:OH	2.48	0.46
23:1:51:VAL:HG11	23:1:74:VAL:HG21	1.98	0.46
1:A:1274:A:N3	1:A:1297:C:H1'	2.31	0.46
1:A:1314:C:H6	1:A:1314:C:H5'	1.81	0.46
1:A:443:A:H1'	1:A:1201:C:O4'	2.15	0.46
7:H:113:VAL:HG11	7:H:151:ILE:HD13	1.98	0.46
20:Y:97:ARG:HH11	20:Y:107:ASP:C	2.19	0.46
8:I:77:LEU:HA	8:I:77:LEU:HD23	1.74	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:414:C:O2'	1:A:415:A:H5'	2.16	0.46
1:A:1143:A:OP1	9:N:25:ARG:NH2	2.49	0.46
1:A:362:U:O2'	1:A:363:G:H5''	2.16	0.46
1:A:30:G:OP2	16:U:5:LYS:HE2	2.15	0.46
1:A:1668:A:H4'	1:A:1669:A:O5'	2.16	0.46
2:B:39:A:O2'	2:B:46:A:N1	2.34	0.46
14:S:74:ALA:HA	14:S:110:LEU:HD22	1.98	0.46
5:F:179:GLU:CD	5:F:179:GLU:H	2.19	0.46
1:A:1701:A:H5''	1:A:1702:G:OP2	2.16	0.46
21:Z:144:LEU:HD12	21:Z:148:ASP:HB3	1.97	0.46
1:A:181:A:H1'	1:A:435:C:H5'	1.98	0.46
4:E:60:ASN:OD1	4:E:62:PRO:HD2	2.16	0.46
27:5:36:CYS:O	27:5:37:LYS:HD3	2.15	0.46
9:N:1:MET:O	9:N:2:LYS:HB2	2.16	0.46
17:V:29:PRO:HA	17:V:61:VAL:HG22	1.98	0.46
13:R:65:LEU:HD12	13:R:65:LEU:HA	1.77	0.46
1:A:2136:C:C4	1:A:2137:C:H5	2.34	0.46
11:P:59:LEU:HG	30:8:58:ILE:HD13	1.97	0.46
1:A:2133:G:C2	1:A:2157:G:H2'	2.51	0.46
1:A:2244:U:O2'	34:A:5428:HOH:O	2.19	0.46
1:A:645:C:H2'	1:A:645:C:O2	2.14	0.46
1:A:185:U:H2'	1:A:186:G:H8	1.80	0.46
1:A:993:G:OP1	16:U:50:ARG:NH2	2.46	0.46
13:R:97:VAL:HG22	13:R:114:VAL:HG13	1.97	0.46
1:A:1173:G:O2'	1:A:1174:A:O5'	2.34	0.45
14:S:34:HIS:O	14:S:97:ARG:NH2	2.49	0.45
1:A:1494:A:C6	1:A:1495:A:C6	3.04	0.45
14:S:101:LEU:HD23	14:S:102:ALA:H	1.81	0.45
21:Z:125:LEU:HB3	21:Z:165:VAL:HG12	1.98	0.45
1:A:774:A:N3	1:A:774:A:H2'	2.31	0.45
6:G:149:VAL:HG22	6:G:150:ASP:O	2.17	0.45
8:I:9:LEU:HD21	8:I:35:LEU:HD13	1.98	0.45
1:A:1020:A:N1	1:A:1141:U:O2'	2.43	0.45
1:A:236:C:H2'	1:A:237:C:C6	2.51	0.45
5:F:22:ALA:HB1	5:F:24:LEU:HD22	1.98	0.45
1:A:866:A:O2'	1:A:867:C:H5'	2.17	0.45
1:A:1551:C:OP2	34:A:5547:HOH:O	2.21	0.45
1:A:667:U:O2	30:8:2:PRO:HD2	2.16	0.45
3:D:10:THR:OG1	3:D:13:ARG:HB2	2.16	0.45
21:Z:35:ARG:HA	21:Z:35:ARG:HD2	1.79	0.45
15:T:119:LYS:O	15:T:123:GLN:HG2	2.17	0.45
1:A:604:G:OP2	11:P:90:ARG:NH1	2.50	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:615:G:OP1	5:F:40:GLN:NE2	2.47	0.45
29:7:24:THR:O	29:7:28:ARG:HG3	2.16	0.45
1:A:671:C:H2'	1:A:672:C:C6	2.51	0.45
8:I:47:LEU:HA	8:I:47:LEU:HD23	1.76	0.45
1:A:1175:U:H4'	1:A:1176:G:OP1	2.16	0.45
1:A:1177:A:OP1	1:A:1177:A:H3'	2.17	0.45
1:A:2789:C:O3'	1:A:2790:A:H4'	2.17	0.45
1:A:1588:C:H2'	1:A:1589:C:C6	2.51	0.45
8:I:130:TYR:HB3	8:I:138:ILE:HB	1.99	0.45
5:F:8:GLN:HB3	5:F:19:GLU:CG	2.47	0.45
5:F:20:LEU:O	5:F:21:ALA:O	2.34	0.45
1:A:708:C:C6	1:A:708:C:H5''	2.51	0.45
1:A:9:U:O2'	1:A:10:G:OP1	2.31	0.45
3:D:134:ARG:HD3	3:D:135:PHE:CZ	2.52	0.45
1:A:2683:C:O2	10:O:70:LYS:NZ	2.31	0.45
1:A:2208:A:H1'	1:A:2219:G:C5	2.52	0.45
1:A:83:G:N2	1:A:102:G:H1'	2.31	0.45
1:A:2115:G:H21	1:A:2171:A:H61	1.64	0.45
4:E:75:VAL:HG13	4:E:77:ILE:H	1.82	0.45
1:A:171:G:H2'	1:A:172:C:C6	2.50	0.45
1:A:481:G:C4	1:A:507:A:C2	3.04	0.45
1:A:1581:G:H2'	1:A:1582:C:O4'	2.17	0.45
1:A:2319:G:C2	14:S:3:ARG:HA	2.51	0.45
1:A:414:C:H2'	1:A:415:A:C8	2.51	0.45
1:A:244:A:C2	1:A:255:A:C4	3.05	0.45
30:8:61:LEU:C	30:8:63:PRO:HD3	2.37	0.45
1:A:2291:U:H2'	1:A:2292:C:C6	2.52	0.45
1:A:1047:G:HO2'	1:A:1048:A:P	2.37	0.45
1:A:2110:G:OP1	1:A:2118:U:N3	2.49	0.45
1:A:1149:G:H2'	1:A:1150:C:C6	2.52	0.45
12:Q:1:MET:HG2	12:Q:2:LEU:H	1.82	0.45
1:A:1125:G:H5'	31:9:37:GLY:HA2	1.97	0.45
1:A:2687:U:H2'	1:A:2688:U:O4'	2.15	0.45
1:A:2152:G:H2'	1:A:2153:G:H8	1.82	0.45
1:A:2172:U:H4'	1:A:2173:A:OP2	2.16	0.45
1:A:2104:G:N2	1:A:2105:C:C2	2.85	0.45
8:I:17:GLN:HG2	8:I:18:VAL:N	2.32	0.45
6:G:13:GLU:H	6:G:13:GLU:HG3	1.55	0.45
1:A:1204:A:N6	1:A:1240:U:H2'	2.32	0.45
1:A:1049:C:O2'	1:A:1050:A:P	2.75	0.45
1:A:1540:U:H2'	1:A:1541:G:O4'	2.16	0.45
21:Z:151:HIS:C	21:Z:153:SER:H	2.20	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2564:A:C2	1:A:2647:U:H4'	2.51	0.45
26:4:36:CYS:SG	26:4:38:LYS:O	2.75	0.45
1:A:2772:C:H2'	1:A:2773:C:C6	2.51	0.45
1:A:1021:A:C3'	1:A:1021:A:C8	3.00	0.45
12:Q:109:VAL:HG13	12:Q:113:GLN:HB2	1.98	0.45
12:Q:134:ARG:O	12:Q:138:ASP:HB2	2.17	0.45
21:Z:111:VAL:HG12	21:Z:112:ARG:H	1.82	0.45
1:A:1669:A:H5''	1:A:2550:G:OP1	2.17	0.45
1:A:615:G:OP1	5:F:40:GLN:HG2	2.17	0.45
5:F:140:LEU:HA	5:F:140:LEU:HD13	1.85	0.45
1:A:1019:U:O2'	1:A:1021:A:H2	1.80	0.44
1:A:1497:U:H5''	1:A:1498:C:H5	1.82	0.44
1:A:2064:C:H2'	1:A:2065:C:C6	2.52	0.44
1:A:945:A:H2	34:A:4175:HOH:O	1.98	0.44
1:A:892:G:H8	1:A:892:G:O5'	2.00	0.44
1:A:897:C:H6	1:A:897:C:O5'	2.01	0.44
1:A:958:U:H5''	12:Q:14:ARG:HD3	1.98	0.44
23:1:85:LEU:HB3	23:1:89:GLU:HG3	1.98	0.44
1:A:2147:G:H2'	1:A:2148:G:C4'	2.47	0.44
14:S:59:LYS:HE2	14:S:60:GLY:HA2	1.98	0.44
1:A:252:G:P	11:P:50:ARG:HH12	2.40	0.44
1:A:184:C:H2'	1:A:185:U:C6	2.53	0.44
21:Z:144:LEU:HD21	21:Z:150:LEU:HG	1.99	0.44
1:A:848:G:H2'	1:A:849:A:C8	2.52	0.44
1:A:1638:C:H4'	1:A:2710:C:O2	2.17	0.44
13:R:26:LYS:HE2	13:R:70:LEU:O	2.17	0.44
1:A:247:G:H4'	1:A:386:G:C5	2.53	0.44
20:Y:76:CYS:HA	20:Y:77:PRO:HD3	1.90	0.44
1:A:2713:A:H2'	1:A:2713:A:N3	2.31	0.44
1:A:1803:A:H4'	3:D:259:THR:HG23	1.98	0.44
1:A:958:U:O2'	1:A:959:A:OP2	2.35	0.44
1:A:1866:C:H2'	1:A:1876:A:O4'	2.17	0.44
1:A:2674:G:H2'	1:A:2675:A:C8	2.52	0.44
1:A:2308:G:O2'	1:A:2310:A:N7	2.50	0.44
1:A:1530:C:H2'	1:A:1530:C:H6	1.60	0.44
1:A:1700:A:H2'	1:A:1701:A:O5'	2.17	0.44
1:A:2009:G:OP1	18:W:41:LYS:HE2	2.18	0.44
1:A:2722:G:H2'	1:A:2723:C:C6	2.53	0.44
13:R:21:TYR:OH	13:R:43:GLU:HG2	2.17	0.44
18:W:83:LYS:O	18:W:84:ARG:HD3	2.17	0.44
5:F:129:PHE:HB2	5:F:132:VAL:HG22	1.99	0.44
13:R:51:LEU:HA	13:R:51:LEU:HD23	1.81	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
16:U:92:ARG:HG2	16:U:92:ARG:H	1.74	0.44
24:2:50:ILE:O	24:2:51:ARG:HB3	2.17	0.44
1:A:2172:U:H1'	1:A:2173:A:OP1	2.18	0.44
1:A:1794:U:H2'	1:A:1795:C:H6	1.82	0.44
10:O:115:VAL:HG13	10:O:121:VAL:HG21	2.00	0.44
1:A:2793:G:H2'	1:A:2794:C:O4'	2.17	0.44
1:A:1488:G:H5''	1:A:1488:G:C8	2.51	0.44
5:F:11:VAL:HB	5:F:18:ARG:CB	2.48	0.44
1:A:2096:U:H3	1:A:2193:G:H1	1.66	0.44
12:Q:27:VAL:O	12:Q:67:ARG:NH1	2.51	0.44
8:I:116:LEU:HD22	8:I:118:LYS:O	2.18	0.44
4:E:173:VAL:CG2	4:E:185:LYS:HB2	2.48	0.44
8:I:72:LEU:O	8:I:74:ASN:N	2.51	0.44
4:E:59:VAL:O	4:E:64:LYS:HE3	2.18	0.44
1:A:740:U:H2'	1:A:741:G:C8	2.52	0.44
7:H:3:ARG:HG2	7:H:6:ARG:HG2	1.99	0.44
1:A:1503:U:H2'	1:A:1504:C:H6	1.83	0.44
1:A:1379:A:O5'	1:A:1379:A:H8	2.01	0.44
1:A:1297:C:OP1	1:A:2710:C:H4'	2.18	0.44
13:R:70:LEU:HA	13:R:70:LEU:HD23	1.72	0.44
1:A:1939:U:OP1	1:A:2604:U:O2'	2.31	0.44
21:Z:6:LYS:HD3	21:Z:8:TYR:OH	2.17	0.44
1:A:579:G:H2'	1:A:580:C:C6	2.53	0.44
1:A:2275:C:H5'	1:A:2275:C:H6	1.81	0.44
1:A:887:A:H1'	1:A:889:C:OP2	2.18	0.44
1:A:832:G:OP1	11:P:38:GLN:O	2.36	0.44
4:E:119:ARG:HG2	4:E:160:TYR:CG	2.53	0.44
1:A:2143:C:N3	1:A:2148:G:O6	2.50	0.44
8:I:81:VAL:O	8:I:146:ALA:HA	2.17	0.44
11:P:126:VAL:CG1	11:P:148:LEU:HD13	2.48	0.44
1:A:1188:U:H4'	17:V:79:VAL:HG22	1.99	0.44
3:D:132:PRO:HD3	3:D:190:TYR:CZ	2.53	0.44
4:E:108:SER:O	4:E:162:ALA:HA	2.17	0.44
1:A:2347:C:H2'	1:A:2348:U:C6	2.53	0.44
1:A:1495:A:H2'	1:A:1496:A:H8	1.78	0.44
1:A:2630:G:H2'	1:A:2631:G:O4'	2.17	0.44
4:E:73:GLU:HA	4:E:74:PRO:HD3	1.63	0.44
1:A:590:A:H2'	1:A:591:C:O4'	2.18	0.44
1:A:1482:G:C6	1:A:1507:A:C6	3.06	0.43
20:Y:20:TYR:CD2	20:Y:42:VAL:HG13	2.52	0.43
14:S:87:PHE:CE1	14:S:102:ALA:HB2	2.53	0.43
21:Z:151:HIS:O	21:Z:152:ALA:HB3	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:234:C:H2'	1:A:235:U:H6	1.83	0.43
21:Z:141:VAL:O	21:Z:144:LEU:HB2	2.18	0.43
8:I:85:GLU:O	8:I:86:THR:OG1	2.31	0.43
1:A:2389:G:H5''	1:A:2390:U:O4'	2.18	0.43
1:A:861:A:C2	1:A:917:A:C4	3.06	0.43
1:A:922:U:H2'	1:A:923:C:C6	2.53	0.43
1:A:1825:A:OP1	3:D:249:PRO:HD3	2.18	0.43
12:Q:141:GLN:NE2	21:Z:76:LEU:HD22	2.32	0.43
8:I:106:GLY:HA2	8:I:107:VAL:CB	2.47	0.43
1:A:2317:C:N4	1:A:2318:G:O6	2.51	0.43
1:A:2778:A:O2'	1:A:2781:A:H5'	2.18	0.43
1:A:2275:C:H5'	1:A:2275:C:C6	2.53	0.43
1:A:478:A:N1	1:A:500:G:H4'	2.33	0.43
7:H:84:SER:HA	7:H:133:VAL:O	2.18	0.43
1:A:601:C:O2'	1:A:605:C:H5''	2.17	0.43
6:G:125:PHE:HB3	6:G:166:ASP:OD2	2.19	0.43
24:2:60:LEU:HA	24:2:60:LEU:HD23	1.81	0.43
18:W:20:VAL:O	18:W:23:LEU:HB2	2.17	0.43
1:A:2318:G:O2'	1:A:2319:G:H5''	2.19	0.43
1:A:2125:G:H22	1:A:2172:U:H5''	1.82	0.43
1:A:2111:C:H42	1:A:2147:G:H22	1.66	0.43
1:A:1539:G:H2'	1:A:1540:U:O4'	2.19	0.43
14:S:78:LEU:HA	14:S:82:ILE:O	2.18	0.43
6:G:148:MET:O	6:G:149:VAL:HB	2.19	0.43
1:A:1162:G:O2'	17:V:90:PRO:HG2	2.18	0.43
15:T:113:LYS:O	15:T:114:LEU:HD23	2.19	0.43
1:A:2576:G:H1'	34:A:5399:HOH:O	2.18	0.43
1:A:2854:G:H2'	1:A:2855:C:C6	2.52	0.43
5:F:108:LYS:O	5:F:112:MET:HG3	2.18	0.43
14:S:84:GLN:HG2	14:S:84:GLN:H	1.48	0.43
1:A:103:A:H8	1:A:103:A:O5'	2.02	0.43
1:A:11:G:H2'	1:A:12:U:C5'	2.48	0.43
1:A:784:A:C5	3:D:229:VAL:HG21	2.53	0.43
5:F:129:PHE:CD2	5:F:163:VAL:HG21	2.53	0.43
1:A:601:C:O2	1:A:605:C:H4'	2.18	0.43
1:A:637:A:OP1	11:P:133:SER:OG	2.30	0.43
1:A:2406:U:OP1	34:A:4753:HOH:O	2.21	0.43
1:A:1485:G:O2'	1:A:1486:A:H5'	2.17	0.43
4:E:101:ARG:CZ	4:E:171:GLU:HB2	2.48	0.43
10:O:70:LYS:HB3	10:O:70:LYS:HE2	1.72	0.43
19:X:26:TYR:CE1	19:X:89:ILE:HG13	2.53	0.43
1:A:297:C:H2'	1:A:298:G:O4'	2.17	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1796:U:H2'	1:A:1797:C:H6	1.79	0.43
1:A:708:C:H6	1:A:708:C:H5''	1.83	0.43
7:H:17:VAL:HG21	7:H:50:VAL:HG21	1.99	0.43
1:A:229:A:H3'	1:A:229:A:C8	2.54	0.43
1:A:2153:G:H2'	1:A:2154:G:C8	2.53	0.43
1:A:2207:G:HO2'	1:A:2208:A:P	2.33	0.43
1:A:2464:C:O2'	1:A:2465:C:P	2.76	0.43
6:G:82:LEU:HB3	6:G:83:ARG:H	1.65	0.43
1:A:2125:G:H21	1:A:2126:A:H62	1.66	0.43
21:Z:30:ASN:ND2	21:Z:90:VAL:HB	2.34	0.43
21:Z:98:MET:O	21:Z:125:LEU:HD12	2.18	0.43
3:D:17:THR:O	3:D:211:ARG:NH2	2.50	0.43
5:F:165:ARG:HG2	5:F:168:ARG:HH21	1.84	0.43
1:A:637:A:H8	11:P:117:GLU:HG3	1.84	0.43
9:N:42:TRP:HD1	9:N:48:MET:HE1	1.84	0.43
18:W:12:ILE:HD13	18:W:17:VAL:HG13	2.01	0.43
25:3:18:ASP:OD1	25:3:18:ASP:N	2.44	0.43
1:A:2123:G:N2	1:A:2175:C:N3	2.60	0.43
1:A:2316:C:H2'	1:A:2317:C:C6	2.53	0.43
1:A:2318:G:O2'	1:A:2319:G:P	2.77	0.43
3:D:238:GLY:O	3:D:239:ARG:CB	2.59	0.43
1:A:1823:G:OP1	3:D:54:ARG:NH1	2.51	0.43
1:A:1816:G:O6	3:D:35:LYS:NZ	2.36	0.43
1:A:708:C:H5'	1:A:709:U:OP2	2.18	0.43
1:A:2793:G:N2	1:A:2804:C:H1'	2.33	0.43
8:I:86:THR:O	8:I:87:LYS:HB2	2.19	0.43
11:P:133:SER:O	11:P:137:LYS:HG3	2.19	0.43
15:T:33:LYS:HG2	15:T:34:VAL:N	2.33	0.43
1:A:1744:C:O2'	1:A:1745:C:H5'	2.18	0.43
6:G:6:ALA:HB3	6:G:104:GLU:OE1	2.19	0.43
2:B:33:G:C2	2:B:50:G:C2	3.06	0.43
1:A:746:A:H2'	1:A:2612:C:H5''	2.00	0.43
9:N:109:LYS:HD2	9:N:109:LYS:N	2.33	0.43
18:W:14:PRO:HG2	18:W:78:GLU:CG	2.44	0.43
13:R:2:ARG:NH1	13:R:5:LYS:O	2.48	0.43
21:Z:31:ARG:H	21:Z:31:ARG:HG3	1.36	0.43
1:A:2364:C:H2'	1:A:2365:G:O4'	2.18	0.43
1:A:792:G:H5''	1:A:793:A:H5'	1.99	0.43
14:S:27:SER:HA	14:S:88:ASP:HB3	2.01	0.43
1:A:476:G:H4'	1:A:502:A:N1	2.34	0.43
1:A:2238:G:H2'	1:A:2238:G:N3	2.32	0.43
14:S:3:ARG:HG3	14:S:4:LEU:N	2.27	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1557:C:H5''	1:A:1558:A:OP2	2.19	0.43
28:6:35:GLU:OE2	28:6:50:ARG:HD3	2.19	0.43
1:A:226:G:H21	1:A:228:A:H62	1.67	0.43
1:A:455:C:N3	1:A:473:G:H5'	2.34	0.43
1:A:1048:A:O2'	1:A:1049:C:H5''	2.19	0.42
1:A:1003:G:N2	1:A:1153:C:C2	2.87	0.42
3:D:8:PRO:CB	3:D:14:ARG:HB2	2.47	0.42
1:A:1651:G:OP1	13:R:40:LYS:HE3	2.18	0.42
1:A:1140:C:O3'	9:N:25:ARG:NH1	2.52	0.42
17:V:60:GLU:HB2	17:V:97:LYS:HE2	2.01	0.42
1:A:1987:G:H2'	1:A:1988:C:H6	1.84	0.42
1:A:2552:U:C2	1:A:2554:U:H5'	2.54	0.42
1:A:1843:C:H5'	3:D:253:GLN:NE2	2.33	0.42
1:A:2430:A:N3	1:A:2430:A:H2'	2.34	0.42
5:F:33:LEU:HD12	5:F:33:LEU:HA	1.81	0.42
13:R:59:ASP:OD2	13:R:59:ASP:N	2.48	0.42
6:G:66:GLN:HE21	6:G:66:GLN:HB3	1.64	0.42
16:U:105:VAL:O	16:U:108:GLU:HB2	2.18	0.42
1:A:1176:G:H1'	1:A:1177:A:P	2.60	0.42
1:A:963:U:OP2	34:A:5110:HOH:O	2.20	0.42
18:W:37:ARG:HD3	18:W:38:TYR:CE2	2.54	0.42
13:R:12:ARG:HG2	13:R:16:HIS:ND1	2.33	0.42
11:P:1:MET:HE2	11:P:5:ASP:HB2	2.01	0.42
1:A:751:A:H5'	18:W:90:ARG:HA	2.00	0.42
1:A:2693:A:H2'	1:A:2694:G:H8	1.85	0.42
1:A:139(A):G:H22	19:X:44:GLU:CD	2.22	0.42
1:A:2784:C:H1'	4:E:37:ARG:NH1	2.34	0.42
3:D:68:LYS:O	3:D:69:ARG:HB2	2.19	0.42
5:F:104:LYS:O	5:F:108:LYS:HB2	2.18	0.42
1:A:1321:A:H2'	1:A:1322:A:O4'	2.19	0.42
17:V:65:GLY:HA3	17:V:91:TYR:CZ	2.54	0.42
1:A:305:U:H2'	1:A:306:U:C6	2.54	0.42
3:D:80:ALA:HB3	3:D:94:LEU:HD13	2.02	0.42
1:A:2300:G:C6	1:A:2301:C:C4	3.07	0.42
8:I:128:LEU:HA	8:I:128:LEU:HD23	1.90	0.42
1:A:1531:C:N4	1:A:1538:G:H1	2.15	0.42
1:A:587:C:P	11:P:21:ARG:HH22	2.39	0.42
1:A:2173:A:C3'	1:A:2174:C:H5'	2.49	0.42
1:A:652(S):C:H3'	1:A:652(T):C:C6	2.55	0.42
1:A:2104:G:N3	1:A:2104:G:H2'	2.34	0.42
14:S:102:ALA:HA	14:S:105:ALA:CB	2.49	0.42
26:4:15:ILE:HB	26:4:32:TYR:CD2	2.54	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:P:1:MET:CE	11:P:5:ASP:HB2	2.49	0.42
1:A:323:G:C8	5:F:171:PRO:HG3	2.54	0.42
1:A:717:G:H2'	1:A:718:A:O4'	2.19	0.42
1:A:1507:A:O2'	1:A:1508:A:C8	2.70	0.42
1:A:271(P):C:OP1	8:I:45:LYS:HD3	2.19	0.42
29:7:30:VAL:O	29:7:34:ARG:HG3	2.18	0.42
28:6:11:LEU:HB2	28:6:21:TYR:HB2	2.00	0.42
6:G:146:TYR:O	6:G:149:VAL:HG12	2.19	0.42
7:H:11:VAL:HG21	7:H:50:VAL:HG23	2.01	0.42
1:A:253:C:OP2	30:8:5:LYS:NZ	2.40	0.42
24:2:65:ASN:OD1	24:2:69:ARG:NH1	2.51	0.42
6:G:173:LEU:O	6:G:178:PHE:HB2	2.20	0.42
13:R:56:LYS:NZ	13:R:90:ARG:O	2.52	0.42
18:W:88:ARG:HG3	18:W:92:ARG:HH21	1.84	0.42
1:A:1639:U:H4'	1:A:2699:C:H4'	2.01	0.42
1:A:64:A:O3'	19:X:71:GLY:HA3	2.20	0.42
1:A:1027:A:C6	1:A:1126:A:C4	3.07	0.42
28:6:44:ARG:HH11	28:6:44:ARG:HB3	1.84	0.42
1:A:1179:C:O2'	1:A:1180:C:H5'	2.19	0.42
6:G:43:LEU:HA	6:G:43:LEU:HD12	1.83	0.42
1:A:1405:U:H2'	1:A:1406:U:H6	1.85	0.42
1:A:234:C:H2'	1:A:235:U:C6	2.55	0.42
18:W:66:GLU:HA	18:W:69:LEU:CD1	2.50	0.42
1:A:1858:G:OP2	1:A:1858:G:H8	2.03	0.42
2:B:42:C:O2	6:G:93:THR:N	2.45	0.42
1:A:484:C:H2'	1:A:485:C:H6	1.84	0.42
1:A:1247:A:OP1	5:F:95:ARG:NH2	2.48	0.42
6:G:161:THR:HG22	6:G:163:ALA:H	1.84	0.42
21:Z:5:LEU:O	21:Z:59:LEU:HA	2.20	0.42
1:A:1022:G:N7	9:N:66:LYS:HE2	2.35	0.42
1:A:2153:G:H2'	1:A:2154:G:H8	1.84	0.42
1:A:1496:A:H5''	1:A:1497:U:OP1	2.20	0.42
1:A:2158:A:H1'	1:A:2159:G:C8	2.54	0.42
8:I:133:HIS:HA	8:I:134:PRO:HD2	1.83	0.42
1:A:2787:C:H1'	4:E:62:PRO:HG3	2.02	0.42
1:A:54:G:O2'	29:7:35:ARG:HD3	2.20	0.42
7:H:46:GLU:OE1	7:H:51:ARG:NH2	2.42	0.42
29:7:47:ARG:HH11	29:7:47:ARG:HG3	1.84	0.42
6:G:124:SER:HB2	6:G:131:TYR:CE1	2.55	0.42
1:A:1529:G:O2'	1:A:1530:C:H5'	2.20	0.42
1:A:1482:G:O6	1:A:1507:A:N6	2.53	0.42
8:I:27:ARG:HD2	23:1:71:TYR:CZ	2.54	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:E:144:ARG:HB3	4:E:145:LYS:H	1.44	0.42
1:A:729:G:C5	3:D:208:LYS:HB2	2.55	0.42
21:Z:93:ASP:HB2	21:Z:131:ARG:NH2	2.34	0.42
1:A:546:C:H6	1:A:548:A:OP1	2.03	0.42
1:A:127:A:H5''	1:A:128:C:C6	2.55	0.42
6:G:16:ARG:HE	6:G:31:VAL:CG2	2.32	0.42
1:A:1784:A:H4'	1:A:1785:A:O5'	2.20	0.42
4:E:101:ARG:O	4:E:201:THR:HG22	2.19	0.42
1:A:1971:A:OP2	3:D:242:ARG:NH2	2.53	0.42
23:1:19:GLN:CB	23:1:35:THR:HG22	2.50	0.42
1:A:1858:G:H1'	1:A:1884:A:H62	1.83	0.42
1:A:590:A:OP1	5:F:95:ARG:NH1	2.53	0.42
3:D:25:THR:HG21	3:D:113:VAL:HG11	2.01	0.42
8:I:114:LEU:HD12	8:I:115:ALA:H	1.85	0.42
12:Q:84:GLY:O	12:Q:85:LYS:HB2	2.20	0.42
1:A:1224:C:O2'	17:V:85:LYS:HA	2.20	0.42
16:U:76:TYR:HH	16:U:92:ARG:NH1	2.16	0.42
11:P:100:LEU:HD23	11:P:100:LEU:HA	1.80	0.42
1:A:2406:U:H2'	1:A:2406:U:OP2	2.19	0.42
1:A:2660:A:H2'	1:A:2661:G:O4'	2.20	0.42
1:A:862:G:H2'	1:A:863:A:O4'	2.20	0.42
1:A:35:G:H2'	1:A:36:G:O4'	2.19	0.42
1:A:825:C:OP1	34:A:4648:HOH:O	2.22	0.42
1:A:1899:G:N3	1:A:1899:G:H2'	2.34	0.42
1:A:71:A:N7	19:X:31:HIS:HE1	2.18	0.41
1:A:89:G:H3'	1:A:90:U:H5''	2.03	0.41
7:H:71:LEU:HD12	7:H:71:LEU:HA	1.74	0.41
21:Z:101:PRO:O	21:Z:102:LEU:HD12	2.20	0.41
8:I:69:LYS:HG3	8:I:138:ILE:HG12	2.02	0.41
1:A:361:G:O2'	1:A:362:U:H5'	2.20	0.41
1:A:1999:C:H4'	1:A:2723:C:O2	2.20	0.41
1:A:2554:U:H2'	1:A:2555:U:C6	2.55	0.41
25:3:4:LEU:O	25:3:36:VAL:HA	2.19	0.41
1:A:1561:G:OP2	34:A:4629:HOH:O	2.21	0.41
31:9:17:ILE:HA	31:9:17:ILE:HD12	1.77	0.41
1:A:783:A:H2'	1:A:783:A:N3	2.35	0.41
14:S:96:GLY:N	14:S:99:LYS:HB3	2.34	0.41
1:A:2315:G:C6	1:A:2316:C:C4	3.09	0.41
1:A:271(O):C:H2'	1:A:271(P):C:C6	2.55	0.41
18:W:58:ALA:HB1	18:W:64:MET:HB2	2.01	0.41
1:A:2549:G:H8	1:A:2549:G:H5''	1.85	0.41
24:2:28:LYS:HE3	24:2:56:GLN:OE1	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:F:164:ARG:O	5:F:168:ARG:HB2	2.21	0.41
1:A:2836:U:H2'	1:A:2837:G:C8	2.55	0.41
6:G:105:LYS:NZ	26:4:25:TYR:O	2.49	0.41
21:Z:5:LEU:HD23	21:Z:47:VAL:HG21	2.03	0.41
3:D:92:ILE:HD12	3:D:104:TYR:CD2	2.56	0.41
5:F:34:TRP:CE2	11:P:8:PRO:HD3	2.55	0.41
3:D:130:ALA:HA	3:D:192:THR:HA	2.02	0.41
1:A:1745(A):C:H5'	1:A:1746:G:OP2	2.20	0.41
2:B:1:U:H2'	2:B:1:U:O2	2.20	0.41
1:A:2173:A:N6	1:A:2174:C:O2	2.53	0.41
13:R:29:LEU:HD23	13:R:70:LEU:HD11	2.02	0.41
19:X:5:TYR:CZ	24:2:30:ARG:HB2	2.56	0.41
31:9:32:HIS:O	31:9:34:GLN:HG3	2.19	0.41
1:A:438:G:H2'	1:A:440:G:C8	2.55	0.41
1:A:634:C:H2'	1:A:635:C:C6	2.55	0.41
8:I:51:ILE:HD13	8:I:51:ILE:HA	1.79	0.41
4:E:47:VAL:HG23	4:E:84:PHE:O	2.20	0.41
1:A:1354:A:H2'	1:A:1355:G:O4'	2.20	0.41
12:Q:72:LYS:HA	12:Q:73:PRO:HD3	1.87	0.41
2:B:31:C:H4'	6:G:29:TRP:CH2	2.55	0.41
28:6:35:GLU:CD	28:6:50:ARG:HH11	2.23	0.41
28:6:23:THR:OG1	28:6:24:GLU:N	2.54	0.41
28:6:25:LYS:HE3	28:6:30:THR:O	2.21	0.41
1:A:1489:U:HO2'	1:A:1490:A:H8	1.68	0.41
1:A:118:A:N3	1:A:178:G:H1'	2.35	0.41
1:A:690:G:H2'	1:A:691:C:C6	2.56	0.41
1:A:2103:C:N3	1:A:2104:G:N7	2.68	0.41
7:H:140:LYS:HB2	7:H:140:LYS:HE3	1.81	0.41
5:F:150:GLY:HA2	5:F:172:TRP:CE3	2.56	0.41
1:A:1510:G:H2'	1:A:1511:C:C6	2.55	0.41
7:H:38:SER:HA	7:H:39:PRO:HD3	1.84	0.41
20:Y:79:CYS:HB2	20:Y:81:LYS:H	1.86	0.41
7:H:8:PRO:O	7:H:69:ARG:NH1	2.53	0.41
21:Z:91:LEU:HA	21:Z:91:LEU:HD12	1.84	0.41
1:A:569:U:C4	1:A:570:G:C6	3.09	0.41
1:A:2171:A:H1'	1:A:2172:U:C6	2.55	0.41
15:T:23:ARG:HG3	15:T:120:ARG:NH1	2.34	0.41
1:A:1987:G:H2'	1:A:1988:C:C6	2.55	0.41
7:H:5:GLY:HA2	7:H:69:ARG:HB3	2.03	0.41
1:A:2273:A:H2'	1:A:2274:A:C8	2.56	0.41
1:A:2404:C:O3'	11:P:77:ARG:NH2	2.53	0.41
6:G:61:ALA:O	6:G:65:GLY:N	2.47	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:N:69:GLN:O	9:N:71:ILE:HD12	2.21	0.41
15:T:56:GLY:O	15:T:59:THR:HG23	2.20	0.41
13:R:67:LEU:HD13	13:R:67:LEU:HA	1.87	0.41
1:A:2682:U:O2'	15:T:58:ASN:ND2	2.53	0.41
21:Z:145:GLU:H	21:Z:148:ASP:HB2	1.85	0.41
1:A:362:U:H2'	1:A:362:U:H6	1.54	0.41
1:A:2250:G:OP2	1:A:2275:C:H2'	2.20	0.41
21:Z:76:LEU:HD12	21:Z:76:LEU:HA	1.83	0.41
1:A:242:G:C8	30:8:5:LYS:HG2	2.56	0.41
1:A:2712:U:OP1	1:A:2714:G:H4'	2.21	0.41
11:P:68:GLN:HG3	30:8:12:LYS:HG2	2.03	0.41
8:I:91:SER:HB3	8:I:121:LYS:HD3	2.02	0.41
1:A:287:C:H2'	1:A:288:C:H6	1.86	0.41
1:A:748:G:C8	18:W:89:ALA:HB1	2.55	0.41
2:B:43:C:OP1	26:4:2:LYS:HB2	2.20	0.41
1:A:1022:G:H22	1:A:1142(A):A:H2	1.55	0.41
1:A:1177:A:H2'	1:A:1177:A:OP2	2.21	0.41
1:A:2464:C:O2'	1:A:2465:C:H6	2.03	0.41
24:2:51:ARG:O	24:2:55:ARG:HD2	2.21	0.41
1:A:2838:G:C6	1:A:2839:G:C5	3.09	0.41
1:A:330:A:O2'	1:A:331:A:H8	2.03	0.41
5:F:103:LYS:HA	5:F:106:ARG:HG2	2.03	0.41
1:A:1429:G:HO2'	1:A:1430:C:H5'	1.86	0.41
1:A:695:G:OP1	1:A:1380:G:O2'	2.28	0.41
1:A:2118:U:O2'	1:A:2119:A:H5''	2.21	0.41
1:A:1028:A:N6	1:A:1125:G:H2'	2.35	0.41
5:F:64:ILE:HG21	5:F:78:ILE:HG23	2.03	0.41
9:N:30:ILE:HG22	9:N:34:LEU:HD22	2.02	0.41
1:A:2093:G:C6	1:A:2225:A:C8	3.08	0.41
3:D:183:ARG:HG3	3:D:270:ILE:HG12	2.03	0.41
15:T:45:PHE:CE1	15:T:74:ARG:HG3	2.56	0.41
1:A:2637:U:C2'	1:A:2638:G:H5'	2.51	0.41
3:D:24:ILE:HD13	3:D:84:TYR:HB2	2.03	0.41
1:A:271(K):U:H4'	1:A:271(L):U:OP2	2.15	0.41
1:A:1686:C:C2'	1:A:1687:G:H5'	2.51	0.41
1:A:2497:A:H5''	34:A:4007:HOH:O	2.21	0.41
13:R:17:ARG:HD2	13:R:17:ARG:HH11	1.63	0.41
1:A:2103:C:O2	1:A:2187:G:C2	2.73	0.41
11:P:47:ASP:OD2	11:P:50:ARG:NH2	2.53	0.41
1:A:2134:A:HO2'	1:A:2159:G:N2	2.19	0.41
1:A:30:G:H2'	1:A:31:C:C6	2.56	0.41
9:N:48:MET:HG3	9:N:48:MET:H	1.58	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:Q:103:MET:CE	12:Q:125:LEU:HD13	2.51	0.41
1:A:720:C:H2'	1:A:721:C:C6	2.55	0.41
1:A:857:C:H4'	22:0:23:VAL:HG21	2.01	0.41
16:U:58:ARG:HA	16:U:61:TRP:CE3	2.56	0.41
6:G:128:ARG:HE	6:G:128:ARG:HB2	1.57	0.41
4:E:52:LEU:O	4:E:76:ARG:N	2.45	0.40
4:E:117:MET:O	4:E:118:LYS:HB3	2.21	0.40
9:N:20:GLY:HA2	9:N:61:ARG:HD3	2.04	0.40
1:A:2492:U:H2'	1:A:2493:U:H6	1.86	0.40
1:A:1290:C:H2'	1:A:1291:C:H6	1.85	0.40
14:S:67:ARG:O	14:S:71:ARG:HG3	2.21	0.40
1:A:2705:A:H2'	1:A:2706:G:O4'	2.21	0.40
1:A:2345:G:N3	1:A:2381:C:H2'	2.36	0.40
21:Z:160:GLY:CA	21:Z:161:VAL:HB	2.38	0.40
23:1:86:SER:O	23:1:89:GLU:HG2	2.20	0.40
11:P:52:GLU:HB3	11:P:55:ARG:HD2	2.03	0.40
7:H:54:ARG:HD3	7:H:65:HIS:ND1	2.35	0.40
1:A:1558:A:N3	1:A:1558:A:O4'	2.54	0.40
1:A:1701:A:OP2	34:A:5539:HOH:O	2.22	0.40
1:A:300:A:P	20:Y:86:ARG:NH2	2.94	0.40
17:V:61:VAL:HG22	17:V:61:VAL:O	2.21	0.40
5:F:29:ASN:H	5:F:112:MET:CE	2.34	0.40
14:S:39:ILE:HD12	14:S:85:VAL:HG21	2.02	0.40
1:A:225:A:O2'	1:A:257:A:H4'	2.22	0.40
1:A:2298:A:H2'	1:A:2299:G:O4'	2.22	0.40
1:A:265:A:H1'	1:A:266:G:O4'	2.21	0.40
3:D:221:VAL:HG22	3:D:226:MET:CE	2.51	0.40
3:D:232:PRO:HB3	3:D:244:ARG:CZ	2.51	0.40
9:N:128:HIS:CD2	9:N:128:HIS:H	2.39	0.40
24:2:3:LEU:HA	24:2:3:LEU:HD23	1.87	0.40
1:A:1173:G:H2'	1:A:1173:G:OP2	2.21	0.40
1:A:2526:G:H5'	1:A:2742:C:O2'	2.21	0.40
17:V:5:VAL:HG11	17:V:57:VAL:HG21	2.04	0.40
1:A:1164:G:H2'	1:A:1165:U:C6	2.57	0.40
3:D:4:LYS:HG2	3:D:18:VAL:CG2	2.51	0.40
1:A:2061:G:H5''	1:A:2503:A:C2	2.57	0.40
5:F:162:LEU:HD12	5:F:162:LEU:HA	1.93	0.40
1:A:271(Q):G:O2'	1:A:271(R):G:OP2	2.39	0.40
1:A:1721:G:H8	1:A:1741:A:H62	1.70	0.40
1:A:1174:A:H5'	1:A:1177:A:N6	2.26	0.40
1:A:856:C:HO2'	1:A:857:C:P	2.44	0.40
15:T:128:GLU:O	15:T:129:ARG:C	2.59	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:Q:42:ILE:HD13	12:Q:97:VAL:HG21	2.04	0.40
1:A:776:G:H4'	1:A:777:A:O5'	2.21	0.40
9:N:39:ARG:HA	9:N:40:PRO:HD3	1.96	0.40
1:A:1575:C:H2'	1:A:1576:U:C6	2.56	0.40
19:X:33:LYS:HA	19:X:33:LYS:HD3	1.88	0.40
15:T:16:ARG:HB2	15:T:79:HIS:ND1	2.36	0.40
1:A:1889:A:H2'	1:A:1890:A:C8	2.56	0.40
1:A:2318:G:N3	1:A:2318:G:H2'	2.36	0.40
1:A:2114:A:H3'	1:A:2115:G:H8	1.84	0.40
1:A:2833:G:O2'	1:A:2834:G:P	2.80	0.40
8:I:131:LYS:C	8:I:133:HIS:H	2.25	0.40
1:A:2850:A:OP2	1:A:2866:U:C5	2.72	0.40
1:A:443:A:N7	5:F:45:ARG:HG2	2.37	0.40
8:I:86:THR:HG22	8:I:122:GLU:OE2	2.21	0.40
1:A:2637:U:O2'	1:A:2638:G:H5'	2.21	0.40
9:N:94:HIS:HB3	9:N:97:ARG:HD3	2.03	0.40
1:A:614:U:H2'	1:A:614(A):U:O4'	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
34:R:309:HOH:O	34:V:310:HOH:O[4.445]	2.03	0.17
17:V:101:GLY:O	34:A:5726:HOH:O[4.545]	2.17	0.03

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%)	262 (96%)	8 (3%)	3 (1%)	21 49
4	E	202/206 (98%)	191 (95%)	8 (4%)	3 (2%)	15 38
5	F	201/210 (96%)	189 (94%)	10 (5%)	2 (1%)	22 51
6	G	179/182 (98%)	149 (83%)	26 (14%)	4 (2%)	10 25
7	H	172/180 (96%)	161 (94%)	10 (6%)	1 (1%)	33 66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	I	144/148 (97%)	116 (81%)	24 (17%)	4 (3%)	8	18
9	N	138/140 (99%)	125 (91%)	11 (8%)	2 (1%)	16	41
10	O	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
11	P	147/150 (98%)	132 (90%)	13 (9%)	2 (1%)	16	41
12	Q	139/141 (99%)	132 (95%)	6 (4%)	1 (1%)	30	62
13	R	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
14	S	108/112 (96%)	99 (92%)	8 (7%)	1 (1%)	25	55
15	T	129/146 (88%)	125 (97%)	4 (3%)	0	100	100
16	U	114/118 (97%)	114 (100%)	0	0	100	100
17	V	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
18	W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
19	X	93/96 (97%)	85 (91%)	8 (9%)	0	100	100
20	Y	105/110 (96%)	93 (89%)	12 (11%)	0	100	100
21	Z	196/206 (95%)	178 (91%)	14 (7%)	4 (2%)	11	28
22	0	74/85 (87%)	72 (97%)	2 (3%)	0	100	100
23	1	95/98 (97%)	92 (97%)	1 (1%)	2 (2%)	11	27
24	2	68/72 (94%)	64 (94%)	4 (6%)	0	100	100
25	3	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
26	4	44/71 (62%)	35 (80%)	8 (18%)	1 (2%)	10	24
27	5	57/60 (95%)	53 (93%)	4 (7%)	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	25
30	8	62/65 (95%)	60 (97%)	1 (2%)	1 (2%)	14	35
31	9	34/37 (92%)	34 (100%)	0	0	100	100
All	All	3373/3526 (96%)	3144 (93%)	197 (6%)	32 (1%)	25	55

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	F	21	ALA
6	G	82	LEU
8	I	107	VAL
11	P	27	HIS
21	Z	161	VAL

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Mol	Chain	Res	Type
3	D	239	ARG
5	F	18	ARG
6	G	149	VAL
7	H	71	LEU
23	1	3	LYS
4	E	118	LYS
6	G	81	LYS
21	Z	193	GLU
3	D	275	LYS
4	E	52	LEU
8	I	75	LEU
8	I	87	LYS
9	N	18	ALA
11	P	39	LYS
12	Q	135	ASP
14	S	83	LYS
29	7	46	VAL
23	1	83	GLU
26	4	28	LYS
30	8	35	GLN
6	G	14	GLU
8	I	73	GLU
9	N	5	VAL
21	Z	191	VAL
3	D	3	VAL
4	E	72	VAL
21	Z	157	LEU

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%)	191 (89%)	24 (11%)	9	20
4	E	163/166 (98%)	140 (86%)	23 (14%)	5	12
5	F	158/166 (95%)	134 (85%)	24 (15%)	4	10
6	G	128/156 (82%)	107 (84%)	21 (16%)	3	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	H	141/148 (95%)	125 (89%)	16 (11%)	9	19
8	I	100/124 (81%)	73 (73%)	27 (27%)	1	2
9	N	117/119 (98%)	99 (85%)	18 (15%)	4	10
10	O	98/100 (98%)	89 (91%)	9 (9%)	13	29
11	P	114/116 (98%)	94 (82%)	20 (18%)	3	7
12	Q	111/111 (100%)	94 (85%)	17 (15%)	4	10
13	R	101/101 (100%)	81 (80%)	20 (20%)	2	5
14	S	84/88 (96%)	70 (83%)	14 (17%)	3	8
15	T	110/127 (87%)	90 (82%)	20 (18%)	2	6
16	U	93/94 (99%)	80 (86%)	13 (14%)	5	12
17	V	80/82 (98%)	65 (81%)	15 (19%)	2	6
18	W	89/92 (97%)	77 (86%)	12 (14%)	6	13
19	X	75/78 (96%)	66 (88%)	9 (12%)	7	17
20	Y	80/91 (88%)	66 (82%)	14 (18%)	3	7
21	Z	159/179 (89%)	137 (86%)	22 (14%)	5	13
22	0	59/67 (88%)	52 (88%)	7 (12%)	8	18
23	1	78/83 (94%)	65 (83%)	13 (17%)	3	8
24	2	65/67 (97%)	57 (88%)	8 (12%)	7	17
25	3	49/52 (94%)	44 (90%)	5 (10%)	11	24
26	4	39/63 (62%)	34 (87%)	5 (13%)	6	15
27	5	50/52 (96%)	43 (86%)	7 (14%)	5	12
28	6	50/52 (96%)	40 (80%)	10 (20%)	2	5
29	7	41/42 (98%)	35 (85%)	6 (15%)	5	11
30	8	52/55 (94%)	45 (86%)	7 (14%)	6	13
31	9	32/34 (94%)	30 (94%)	2 (6%)	25	53
All	All	2731/2923 (93%)	2323 (85%)	408 (15%)	4	11

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	38	LYS

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Mol	Chain	Res	Type
3	D	61	LEU
3	D	72	LYS
3	D	94	LEU
3	D	103	ARG
3	D	106	ILE
3	D	111	LEU
3	D	138	VAL
3	D	140	THR
3	D	141	VAL
3	D	154	LYS
3	D	192	THR
3	D	200	ASP
3	D	211	ARG
3	D	217	ARG
3	D	221	VAL
3	D	229	VAL
3	D	242	ARG
3	D	253	GLN
3	D	257	LEU
3	D	259	THR
3	D	260	ARG
4	E	12	THR
4	E	21	VAL
4	E	24	THR
4	E	33	VAL
4	E	49	LEU
4	E	52	LEU
4	E	73	GLU
4	E	75	VAL
4	E	77	ILE
4	E	82	ARG
4	E	87	GLU
4	E	93	VAL
4	E	111	ARG
4	E	116	VAL
4	E	119	ARG
4	E	128	SER
4	E	144	ARG
4	E	154	LYS
4	E	163	GLU
4	E	167	VAL
4	E	175	VAL

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Mol	Chain	Res	Type
4	E	181	LEU
4	E	184	VAL
5	F	15	SER
5	F	18	ARG
5	F	19	GLU
5	F	24	LEU
5	F	33	LEU
5	F	53	THR
5	F	57	VAL
5	F	74	ARG
5	F	82	ILE
5	F	88	VAL
5	F	106	ARG
5	F	108	LYS
5	F	110	LEU
5	F	117	ARG
5	F	140	LEU
5	F	145	GLU
5	F	158	THR
5	F	161	GLU
5	F	162	LEU
5	F	170	LEU
5	F	192	LEU
5	F	197	ASP
5	F	201	VAL
5	F	205	ARG
6	G	3	LEU
6	G	5	VAL
6	G	9	ARG
6	G	13	GLU
6	G	28	VAL
6	G	31	VAL
6	G	43	LEU
6	G	47	LYS
6	G	60	LEU
6	G	71	THR
6	G	80	PHE
6	G	128	ARG
6	G	133	LEU
6	G	135	LEU
6	G	143	GLU
6	G	148	MET

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Mol	Chain	Res	Type
6	G	152	LEU
6	G	153	ARG
6	G	159	VAL
6	G	165	THR
6	G	170	ARG
7	H	3	ARG
7	H	6	ARG
7	H	15	VAL
7	H	24	VAL
7	H	41	MET
7	H	45	VAL
7	H	69	ARG
7	H	71	LEU
7	H	77	LYS
7	H	95	ARG
7	H	98	LEU
7	H	106	THR
7	H	116	GLU
7	H	122	THR
7	H	139	GLN
7	H	171	LEU
8	I	1	MET
8	I	9	LEU
8	I	15	VAL
8	I	38	LEU
8	I	41	GLU
8	I	42	SER
8	I	43	ASN
8	I	47	LEU
8	I	57	ARG
8	I	61	ARG
8	I	68	LEU
8	I	75	LEU
8	I	77	LEU
8	I	78	THR
8	I	85	GLU
8	I	92	VAL
8	I	101	LEU
8	I	102	SER
8	I	114	LEU
8	I	116	LEU
8	I	117	GLU

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Mol	Chain	Res	Type
8	I	121	LYS
8	I	127	VAL
8	I	140	LEU
8	I	142	VAL
8	I	144	VAL
8	I	145	VAL
9	N	9	VAL
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	61	ARG
9	N	62	VAL
9	N	67	LEU
9	N	68	GLU
9	N	73	THR
9	N	87	LEU
9	N	89	LYS
9	N	99	LEU
9	N	120	LEU
9	N	133	GLN
9	N	140	VAL
10	O	10	VAL
10	O	17	ARG
10	O	20	MET
10	O	24	VAL
10	O	35	VAL
10	O	53	LYS
10	O	94	ARG
10	O	97	ARG
10	O	113	LYS
11	P	1	MET
11	P	21	ARG
11	P	50	ARG
11	P	55	ARG
11	P	56	SER
11	P	59	LEU
11	P	65	ARG
11	P	70	GLN
11	P	71	VAL

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Mol	Chain	Res	Type
11	P	75	ILE
11	P	76	LYS
11	P	83	VAL
11	P	95	VAL
11	P	106	LEU
11	P	112	LEU
11	P	119	GLU
11	P	132	LYS
11	P	144	GLU
11	P	148	LEU
11	P	149	GLU
12	Q	1	MET
12	Q	6	ARG
12	Q	7	MET
12	Q	8	LYS
12	Q	16	ARG
12	Q	21	THR
12	Q	31	ASP
12	Q	35	VAL
12	Q	42	ILE
12	Q	45	GLN
12	Q	55	VAL
12	Q	59	ARG
12	Q	63	LYS
12	Q	75	THR
12	Q	109	VAL
12	Q	110	THR
12	Q	135	ASP
13	R	1	MET
13	R	6	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	54	LEU
13	R	57	ARG
13	R	60	LEU
13	R	65	LEU
13	R	67	LEU
13	R	73	VAL

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Mol	Chain	Res	Type
13	R	75	LEU
13	R	79	LEU
13	R	86	ARG
13	R	100	LEU
13	R	111	LEU
13	R	114	VAL
14	S	12	PHE
14	S	13	ARG
14	S	14	VAL
14	S	15	ARG
14	S	20	ARG
14	S	25	ARG
14	S	36	TYR
14	S	38	GLN
14	S	49	VAL
14	S	52	SER
14	S	78	LEU
14	S	84	GLN
14	S	95	HIS
14	S	110	LEU
15	T	6	LEU
15	T	8	LYS
15	T	16	ARG
15	T	17	THR
15	T	23	ARG
15	T	28	VAL
15	T	36	GLU
15	T	49	VAL
15	T	53	ARG
15	T	59	THR
15	T	67	SER
15	T	75	ILE
15	T	78	LEU
15	T	89	VAL
15	T	93	ARG
15	T	95	ARG
15	T	96	ARG
15	T	107	ASP
15	T	118	ARG
15	T	124	ASP
16	U	8	VAL
16	U	19	LYS

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Mol	Chain	Res	Type
16	U	27	LEU
16	U	31	SER
16	U	36	ARG
16	U	52	ARG
16	U	59	ARG
16	U	60	LEU
16	U	74	LEU
16	U	83	LEU
16	U	92	ARG
16	U	104	GLN
16	U	108	GLU
17	V	13	ARG
17	V	18	LEU
17	V	21	ARG
17	V	28	GLU
17	V	32	THR
17	V	35	LEU
17	V	46	VAL
17	V	61	VAL
17	V	62	LEU
17	V	72	VAL
17	V	79	VAL
17	V	85	LYS
17	V	89	GLN
17	V	95	LEU
17	V	100	ARG
18	W	11	ARG
18	W	15	ARG
18	W	17	VAL
18	W	19	LEU
18	W	23	LEU
18	W	27	LYS
18	W	51	LEU
18	W	68	ARG
18	W	83	LYS
18	W	96	ILE
18	W	100	THR
18	W	107	LEU
19	X	35	THR
19	X	45	THR
19	X	52	VAL
19	X	54	VAL

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Mol	Chain	Res	Type
19	X	57	LEU
19	X	60	ARG
19	X	66	LEU
19	X	68	ARG
19	X	92	LEU
20	Y	6	HIS
20	Y	19	LYS
20	Y	23	ARG
20	Y	29	GLU
20	Y	34	LYS
20	Y	47	LYS
20	Y	55	TYR
20	Y	64	GLU
20	Y	70	SER
20	Y	72	VAL
20	Y	73	ARG
20	Y	91	GLU
20	Y	97	ARG
20	Y	106	LEU
21	Z	5	LEU
21	Z	6	LYS
21	Z	11	GLU
21	Z	18	LEU
21	Z	19	ARG
21	Z	61	LEU
21	Z	72	ARG
21	Z	76	LEU
21	Z	86	VAL
21	Z	91	LEU
21	Z	119	GLU
21	Z	124	ILE
21	Z	128	VAL
21	Z	138	GLU
21	Z	144	LEU
21	Z	154	ASP
21	Z	155	LEU
21	Z	156	LYS
21	Z	161	VAL
21	Z	170	THR
21	Z	171	ILE
21	Z	181	GLU
22	0	9	SER

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Mol	Chain	Res	Type
22	0	19	LYS
22	0	20	ARG
22	0	32	ARG
22	0	53	MET
22	0	55	ARG
22	0	74	ARG
23	1	4	VAL
23	1	21	ARG
23	1	26	ARG
23	1	30	VAL
23	1	32	LYS
23	1	35	THR
23	1	40	ARG
23	1	46	LEU
23	1	58	ILE
23	1	59	THR
23	1	80	LEU
23	1	83	GLU
23	1	95	LEU
24	2	28	LYS
24	2	30	ARG
24	2	32	LEU
24	2	52	ASP
24	2	53	LEU
24	2	55	ARG
24	2	64	LEU
24	2	68	ARG
25	3	8	LEU
25	3	18	ASP
25	3	23	LEU
25	3	31	LEU
25	3	44	ARG
26	4	14	ILE
26	4	22	ILE
26	4	33	VAL
26	4	39	CYS
26	4	43	TYR
27	5	9	LYS
27	5	15	ARG
27	5	16	ARG
27	5	29	THR
27	5	37	LYS

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Mol	Chain	Res	Type
27	5	40	LYS
27	5	55	ARG
28	6	4	GLU
28	6	6	ARG
28	6	13	CYS
28	6	30	THR
28	6	33	LYS
28	6	35	GLU
28	6	38	LYS
28	6	40	CYS
28	6	44	ARG
28	6	48	VAL
29	7	1	MET
29	7	8	ASN
29	7	9	ARG
29	7	24	THR
29	7	43	THR
29	7	47	ARG
30	8	6	THR
30	8	14	VAL
30	8	26	LYS
30	8	29	LYS
30	8	31	HIS
30	8	32	LEU
30	8	41	ILE
31	9	4	ARG
31	9	18	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	253	GLN
4	E	143	ASN
5	F	169	ASN
6	G	40	ASN
9	N	133	GLN
11	P	38	GLN
11	P	70	GLN
15	T	58	ASN
19	X	31	HIS
19	X	82	GLN
21	Z	34	ASN

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Mol	Chain	Res	Type
31	9	36	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2819/2915 (96%)	514 (18%)	72 (2%)
2	B	119/122 (97%)	19 (15%)	0
All	All	2938/3037 (96%)	533 (18%)	72 (2%)

All (533) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	G
1	A	15	G
1	A	34	C
1	A	45	C
1	A	69	C
1	A	71	A
1	A	72	U
1	A	74	A
1	A	75	G
1	A	84	A
1	A	90	U
1	A	99	U
1	A	102	G
1	A	103	A
1	A	118	A
1	A	119	A
1	A	120	U
1	A	139(A)	G
1	A	141	A
1	A	154	G
1	A	154(A)	C
1	A	173	G
1	A	181	A
1	A	182	A
1	A	196	A
1	A	199	A
1	A	200	U
1	A	204	A
1	A	205	G

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Mol	Chain	Res	Type
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	233	A
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(R)	G
1	A	272(B)	G
1	A	275	G
1	A	279	C
1	A	286	C
1	A	311	A
1	A	329	G
1	A	330	A
1	A	332	A
1	A	333	G
1	A	342	G
1	A	352	G
1	A	363	G
1	A	363(F)	A
1	A	386	G
1	A	396	G
1	A	405	U
1	A	406	G
1	A	411	G
1	A	412	A
1	A	415	A
1	A	422	A
1	A	427	U
1	A	428	A
1	A	444	C
1	A	448	U
1	A	454	A

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Mol	Chain	Res	Type
1	A	456	C
1	A	470	A
1	A	475	U
1	A	480	A
1	A	481	G
1	A	482	A
1	A	504	U
1	A	505	A
1	A	509	C
1	A	529	A
1	A	530	G
1	A	531	C
1	A	532	A
1	A	533	G
1	A	545	G
1	A	546	C
1	A	549	G
1	A	563	G
1	A	573	G
1	A	575	A
1	A	586	A
1	A	587	C
1	A	588	U
1	A	603	A
1	A	604	G
1	A	606	U
1	A	607	U
1	A	614(B)	G
1	A	615	G
1	A	619	G
1	A	627	A
1	A	634	C
1	A	637	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(E)	G
1	A	652(F)	G
1	A	652(G)	G
1	A	652(P)	G

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Mol	Chain	Res	Type
1	A	652(Q)	G
1	A	652(R)	C
1	A	652(T)	C
1	A	652(U)	G
1	A	669	G
1	A	686	G
1	A	707	G
1	A	708	C
1	A	730	C
1	A	752	A
1	A	753	C
1	A	764	A
1	A	765	G
1	A	774	A
1	A	775	G
1	A	776	G
1	A	782	A
1	A	784	A
1	A	785	G
1	A	790	C
1	A	792	G
1	A	805	G
1	A	812	C
1	A	819	A
1	A	827	U
1	A	828	U
1	A	830	G
1	A	857	C
1	A	859	G
1	A	866	A
1	A	880	G
1	A	884	C
1	A	885	C
1	A	886	C
1	A	888	C
1	A	889	C
1	A	890	A
1	A	896	A
1	A	897	C
1	A	899	A
1	A	900	A
1	A	901	A

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Mol	Chain	Res	Type
1	A	910	A
1	A	916	G
1	A	917	A
1	A	932	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	974	G
1	A	975	C
1	A	983	A
1	A	994	C
1	A	996	A
1	A	1005	C
1	A	1012	U
1	A	1013	C
1	A	1022	G
1	A	1026	U
1	A	1027	A
1	A	1033	U
1	A	1038	C
1	A	1039	G
1	A	1042	G
1	A	1043	C
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
1	A	1111	A
1	A	1112	G
1	A	1128	A

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Mol	Chain	Res	Type
1	A	1129	A
1	A	1130	U
1	A	1135	C
1	A	1136	G
1	A	1139	G
1	A	1144	G
1	A	1155	A
1	A	1156	A
1	A	1171	G
1	A	1173	G
1	A	1174	A
1	A	1175	U
1	A	1176	G
1	A	1177	A
1	A	1178	C
1	A	1210	A
1	A	1211	U
1	A	1219	G
1	A	1220	A
1	A	1253	A
1	A	1256	G
1	A	1271	G
1	A	1272	A
1	A	1273	U
1	A	1300	U
1	A	1301	A
1	A	1303	G
1	A	1305	C
1	A	1308	A
1	A	1314	C
1	A	1321	A
1	A	1329	U
1	A	1345	C
1	A	1352	U
1	A	1359	A
1	A	1360	A
1	A	1365	A
1	A	1370	C
1	A	1373	A
1	A	1380	G
1	A	1384	A
1	A	1385	G

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Mol	Chain	Res	Type
1	A	1386	C
1	A	1404	C
1	A	1416	G
1	A	1417	C
1	A	1419	A
1	A	1421	G
1	A	1427	A
1	A	1428	C
1	A	1430	C
1	A	1436	G
1	A	1437	C
1	A	1445	A
1	A	1449	A
1	A	1450	G
1	A	1452	A
1	A	1459	G
1	A	1467	C
1	A	1471	A
1	A	1472	A
1	A	1482	G
1	A	1487	G
1	A	1488	G
1	A	1489	U
1	A	1493	C
1	A	1496	A
1	A	1497	U
1	A	1507	A
1	A	1508	A
1	A	1509	C
1	A	1509(A)	A
1	A	1525	G
1	A	1531	C
1	A	1541	G
1	A	1542	A
1	A	1543	C
1	A	1545	A
1	A	1558	A
1	A	1559	G
1	A	1566	A
1	A	1569	A
1	A	1578	U
1	A	1580	A

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Mol	Chain	Res	Type
1	A	1581	G
1	A	1582	C
1	A	1584	C
1	A	1586	A
1	A	1588	C
1	A	1598	C
1	A	1608	A
1	A	1609	A
1	A	1610	A
1	A	1617	C
1	A	1631	C
1	A	1640	C
1	A	1647	G
1	A	1648	C
1	A	1653	G
1	A	1654	A
1	A	1674	G
1	A	1696	G
1	A	1700	A
1	A	1701	A
1	A	1721	G
1	A	1722	A
1	A	1739	U
1	A	1740	G
1	A	1742	G
1	A	1746	G
1	A	1756	G
1	A	1762	A
1	A	1763	G
1	A	1764	G
1	A	1769	G
1	A	1773	A
1	A	1780	A
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	1820	U
1	A	1829	A
1	A	1830	C

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Mol	Chain	Res	Type
1	A	1835	G
1	A	1839	G
1	A	1847	A
1	A	1858	G
1	A	1861	G
1	A	1877	A
1	A	1878	G
1	A	1881	C
1	A	1882	C
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	1937	A
1	A	1938	A
1	A	1955	U
1	A	1963	U
1	A	1965	C
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	2020	A
1	A	2023	G
1	A	2031	A
1	A	2033	A
1	A	2036	C
1	A	2043	C
1	A	2055	C
1	A	2056	G
1	A	2060	A

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Mol	Chain	Res	Type
1	A	2061	G
1	A	2062	A
1	A	2069	G
1	A	2102	U
1	A	2103	C
1	A	2105	C
1	A	2107	C
1	A	2108	C
1	A	2113	U
1	A	2116	G
1	A	2117	A
1	A	2118	U
1	A	2120	G
1	A	2123	G
1	A	2126	A
1	A	2127	G
1	A	2131	G
1	A	2133	G
1	A	2134	A
1	A	2138	C
1	A	2142	C
1	A	2144	U
1	A	2145	C
1	A	2146	C
1	A	2147	G
1	A	2148	G
1	A	2154	G
1	A	2159	G
1	A	2160	G
1	A	2165	G
1	A	2166	G
1	A	2172	U
1	A	2173	A
1	A	2174	C
1	A	2184	G
1	A	2185	C
1	A	2186	G
1	A	2187	G
1	A	2190	G
1	A	2191	G
1	A	2192	G
1	A	2193	G

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Mol	Chain	Res	Type
1	A	2198	A
1	A	2199	A
1	A	2200	C
1	A	2206	G
1	A	2207	G
1	A	2208	A
1	A	2218	U
1	A	2219	G
1	A	2225	A
1	A	2238	G
1	A	2239	G
1	A	2268	A
1	A	2275	C
1	A	2283	C
1	A	2287	A
1	A	2289	G
1	A	2296	U
1	A	2297	C
1	A	2305	A
1	A	2311	A
1	A	2318	G
1	A	2319	G
1	A	2320	A
1	A	2321	G
1	A	2325	G
1	A	2327	A
1	A	2334	G
1	A	2347	C
1	A	2350	C
1	A	2383	G
1	A	2385	C
1	A	2393	A
1	A	2400	G
1	A	2406	U
1	A	2410	G
1	A	2414	G
1	A	2419	U
1	A	2422	A
1	A	2423	U
1	A	2425	A
1	A	2429	G
1	A	2430	A

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Mol	Chain	Res	Type
1	A	2431	U
1	A	2435	A
1	A	2439	A
1	A	2441	C
1	A	2448	A
1	A	2465	C
1	A	2469	A
1	A	2474	C
1	A	2476	A
1	A	2478	A
1	A	2498	C
1	A	2502	G
1	A	2505	G
1	A	2506	U
1	A	2518	A
1	A	2525	G
1	A	2529	G
1	A	2535	G
1	A	2549	G
1	A	2554	U
1	A	2555	U
1	A	2566	A
1	A	2567	G
1	A	2573	C
1	A	2609	U
1	A	2611	U
1	A	2612	C
1	A	2615	U
1	A	2629	A
1	A	2630	G
1	A	2663	G
1	A	2673	G
1	A	2675	A
1	A	2689	U
1	A	2690	C
1	A	2691	C
1	A	2702	U
1	A	2703	C
1	A	2712(A)	A
1	A	2713	A
1	A	2714	G
1	A	2726	U

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Mol	Chain	Res	Type
1	A	2733	A
1	A	2757	A
1	A	2758	A
1	A	2760	C
1	A	2765	A
1	A	2766	G
1	A	2778	A
1	A	2789	C
1	A	2790	A
1	A	2791	C
1	A	2802	G
1	A	2803	C
1	A	2808	U
1	A	2820	A
1	A	2821	A
1	A	2834	G
1	A	2835	A
1	A	2847	U
1	A	2872	G
1	A	2880	C
1	A	2892	A
1	A	2895	U
1	A	2897	U
2	B	2	C
2	B	7	G
2	B	9	G
2	B	13	A
2	B	19	G
2	B	20	C
2	B	24	G
2	B	25	A
2	B	40	U
2	B	42	C
2	B	47	C
2	B	53	A
2	B	54	G
2	B	56	G
2	B	73	A
2	B	75	G
2	B	106	G
2	B	110	G
2	B	116	G

All (72) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	9	U
1	A	71	A
1	A	102	G
1	A	196	A
1	A	199	A
1	A	215	G
1	A	249	C
1	A	271(K)	U
1	A	271(M)	G
1	A	278	A
1	A	363(E)	U
1	A	405	U
1	A	474	G
1	A	481	G
1	A	587	C
1	A	669	G
1	A	685	A
1	A	686	G
1	A	746	A
1	A	752	A
1	A	764	A
1	A	774	A
1	A	827	U
1	A	856	C
1	A	900	A
1	A	945	A
1	A	958	U
1	A	974	G
1	A	1026	U
1	A	1047	G
1	A	1049	C
1	A	1106	G
1	A	1108	U
1	A	1142(A)	A
1	A	1155	A
1	A	1174	A
1	A	1175	U
1	A	1176	G
1	A	1210	A
1	A	1300	U
1	A	1379	A
1	A	1420	U

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Mol	Chain	Res	Type
1	A	1427	A
1	A	1507	A
1	A	1530	C
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	1800	C
1	A	1819	A
1	A	1992	G
1	A	2122	U
1	A	2126	A
1	A	2171	A
1	A	2172	U
1	A	2207	G
1	A	2275	C
1	A	2288	A
1	A	2318	G
1	A	2406	U
1	A	2422	A
1	A	2430	A
1	A	2439	A
1	A	2689	U
1	A	2726	U
1	A	2756	U
1	A	2778	A
1	A	2789	C
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 814 ligands modelled in this entry, 814 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	2827/2915 (96%)	0.29	186 (6%) 18 20	24, 40, 120, 169	0
2	B	120/122 (98%)	0.42	5 (4%) 35 39	39, 65, 76, 119	0
3	D	275/276 (99%)	0.35	10 (3%) 41 46	24, 39, 51, 79	0
4	E	204/206 (99%)	0.24	11 (5%) 25 27	24, 44, 64, 81	0
5	F	203/210 (96%)	0.61	16 (7%) 13 13	25, 49, 82, 113	0
6	G	181/182 (99%)	1.02	36 (19%) 2 2	64, 83, 108, 138	0
7	H	174/180 (96%)	0.74	25 (14%) 3 4	49, 64, 80, 92	0
8	I	146/148 (98%)	1.41	41 (28%) 1 1	46, 75, 91, 98	0
9	N	140/140 (100%)	0.32	9 (6%) 19 21	30, 44, 66, 83	0
10	O	122/122 (100%)	0.10	2 (1%) 68 74	34, 43, 62, 65	0
11	P	149/150 (99%)	0.50	8 (5%) 25 27	25, 51, 77, 96	0
12	Q	141/141 (100%)	0.36	6 (4%) 34 38	31, 47, 59, 74	0
13	R	118/118 (100%)	0.41	6 (5%) 27 30	30, 39, 51, 62	0
14	S	110/112 (98%)	1.02	18 (16%) 2 3	48, 62, 77, 85	0
15	T	131/146 (89%)	0.50	11 (8%) 11 12	38, 46, 76, 103	0
16	U	116/118 (98%)	0.13	3 (2%) 53 59	28, 38, 53, 70	0
17	V	101/101 (100%)	0.45	9 (8%) 10 10	27, 48, 67, 83	0
18	W	112/113 (99%)	0.13	5 (4%) 32 36	28, 35, 52, 92	0
19	X	95/96 (98%)	0.27	1 (1%) 77 82	33, 43, 65, 84	0
20	Y	107/110 (97%)	1.01	21 (19%) 2 2	44, 55, 77, 88	0
21	Z	198/206 (96%)	0.65	27 (13%) 4 4	48, 68, 91, 103	0
22	0	76/85 (89%)	0.54	5 (6%) 18 20	37, 44, 57, 75	0
23	1	97/98 (98%)	0.52	9 (9%) 9 9	31, 44, 74, 82	0
24	2	70/72 (97%)	1.43	23 (32%) 1 1	42, 56, 67, 93	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	3	59/60 (98%)	0.71	7 (11%) 5 5	33, 42, 66, 84	0
26	4	46/71 (64%)	1.17	13 (28%) 1 1	73, 96, 111, 116	0
27	5	59/60 (98%)	0.07	0 100 100	23, 38, 56, 68	0
28	6	53/54 (98%)	0.45	2 (3%) 38 43	40, 46, 59, 66	0
29	7	48/49 (97%)	0.48	6 (12%) 5 5	26, 30, 51, 71	0
30	8	64/65 (98%)	0.25	2 (3%) 47 52	34, 38, 45, 57	0
31	9	36/37 (97%)	0.78	2 (5%) 24 25	38, 46, 57, 69	0
All	All	6378/6563 (97%)	0.44	525 (8%) 11 12	23, 45, 93, 169	0

All (525) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2133	G	13.9
1	A	2108	C	11.6
1	A	2132	U	11.6
1	A	652(B)	A	10.4
1	A	2790	A	10.4
1	A	2131	G	9.5
6	G	152	LEU	8.8
1	A	2169	A	8.3
6	G	147	ASP	8.2
1	A	2157	G	8.2
1	A	2160	G	7.9
1	A	2146	C	7.9
21	Z	164	ALA	7.5
1	A	2129	C	7.4
8	I	132	PRO	7.4
1	A	2116	G	7.3
1	A	1509	C	7.3
3	D	2	ALA	7.2
20	Y	92	ASN	7.0
1	A	2161	C	6.8
8	I	133	HIS	6.4
20	Y	1	MET	6.3
1	A	897	C	6.3
6	G	136	ARG	6.2
7	H	171	LEU	6.2
8	I	68	LEU	6.2
1	A	2149	G	6.1
6	G	28	VAL	6.1

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Mol	Chain	Res	Type	RSRZ
8	I	79	ILE	6.0
1	A	271(N)	U	5.9
7	H	98	LEU	5.9
1	A	2123	G	5.9
1	A	2130	U	5.9
6	G	24	GLY	5.9
8	I	117	GLU	5.7
6	G	137	GLU	5.7
8	I	41	GLU	5.7
1	A	2134	A	5.5
1	A	888	C	5.5
20	Y	91	GLU	5.5
1	A	2158	A	5.4
1	A	171	G	5.4
8	I	127	VAL	5.4
15	T	131	ALA	5.4
14	S	65	VAL	5.3
1	A	2897	U	5.3
1	A	1176	G	5.2
26	4	34	GLU	5.2
6	G	26	GLN	5.2
1	A	2112	G	5.2
8	I	65	ALA	5.2
1	A	878	A	5.1
1	A	645	C	5.1
22	0	17	GLN	5.1
21	Z	70	LEU	5.1
1	A	2107	C	5.0
1	A	1107	G	5.0
1	A	1460	A	4.9
1	A	652(H)	C	4.9
7	H	133	VAL	4.9
23	1	14	VAL	4.9
1	A	652(J)	G	4.9
22	0	42	GLY	4.8
1	A	652(C)	G	4.8
1	A	900	A	4.8
1	A	2125	G	4.8
1	A	2182	G	4.8
1	A	2145	C	4.8
21	Z	163	LEU	4.8
1	A	2792	G	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	1847	A	4.7
1	A	2109	U	4.7
1	A	2173	A	4.7
1	A	894	C	4.7
6	G	146	TYR	4.6
15	T	35	LYS	4.6
7	H	119	GLU	4.6
31	9	12	ASP	4.6
6	G	122	PRO	4.6
9	N	8	GLN	4.5
1	A	1045	A	4.5
1	A	2896	C	4.5
1	A	652(I)	C	4.5
1	A	2804	C	4.5
20	Y	10	GLY	4.5
1	A	2191	G	4.4
1	A	883	G	4.4
8	I	73	GLU	4.4
11	P	105	LEU	4.4
1	A	2793	G	4.4
6	G	145	THR	4.4
1	A	2150	U	4.4
1	A	2117	A	4.4
9	N	140	VAL	4.4
8	I	116	LEU	4.4
1	A	1913	A	4.3
14	S	55	ALA	4.3
21	Z	157	LEU	4.3
6	G	74	LYS	4.3
8	I	57	ARG	4.2
4	E	87	GLU	4.2
21	Z	194	PRO	4.2
1	A	2122	U	4.2
1	A	2162	G	4.2
7	H	21	PRO	4.2
15	T	128	GLU	4.2
1	A	2147	G	4.1
6	G	151	ALA	4.1
1	A	2794	C	4.1
20	Y	80	GLY	4.1
24	2	60	LEU	4.1
6	G	177	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
17	V	42	GLY	4.1
8	I	131	LYS	4.1
1	A	2128	C	4.1
1	A	2175	C	4.0
23	1	40	ARG	4.0
6	G	139	LEU	4.0
26	4	37	SER	4.0
1	A	2159	G	4.0
24	2	11	GLU	4.0
1	A	1543	C	4.0
1	A	2110	G	4.0
25	3	59	VAL	3.9
24	2	48	HIS	3.9
1	A	1117	G	3.9
6	G	30	GLU	3.9
7	H	174	GLY	3.9
1	A	2124	G	3.9
21	Z	45	ASP	3.9
1	A	652(G)	G	3.9
1	A	2168	G	3.9
13	R	102	GLU	3.9
18	W	112	GLY	3.8
4	E	92	THR	3.8
1	A	2166	G	3.8
1	A	2141	G	3.8
1	A	2167	U	3.8
8	I	42	SER	3.8
1	A	1168	G	3.8
1	A	2165	G	3.8
10	O	91	LEU	3.8
14	S	21	THR	3.8
25	3	60	GLU	3.7
1	A	1046	A	3.7
21	Z	12	GLY	3.7
12	Q	59	ARG	3.7
29	7	47	ARG	3.7
1	A	886	C	3.7
6	G	121	ASN	3.7
18	W	86	LEU	3.7
15	T	97	ALA	3.7
1	A	893	C	3.7
1	A	2164	C	3.7

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Mol	Chain	Res	Type	RSRZ
6	G	29	TRP	3.7
24	2	13	ALA	3.6
6	G	176	LEU	3.6
8	I	75	LEU	3.6
24	2	24	LEU	3.6
1	A	652(A)	A	3.6
1	A	885	C	3.6
8	I	71	ILE	3.6
1	A	172	C	3.6
4	E	89	ASP	3.6
21	Z	126	VAL	3.6
1	A	2176	A	3.6
1	A	405	U	3.5
1	A	652(D)	C	3.5
17	V	101	GLY	3.5
24	2	56	GLN	3.5
5	F	32	LEU	3.5
1	A	6	A	3.5
1	A	1108	U	3.5
15	T	111	ARG	3.5
11	P	108	LYS	3.5
21	Z	158	PRO	3.5
21	Z	165	VAL	3.5
1	A	880	G	3.4
24	2	46	GLN	3.4
1	A	2894	G	3.4
1	A	2144	U	3.4
24	2	70	GLN	3.4
1	A	652(Q)	G	3.4
1	A	1042	G	3.4
1	A	2174	C	3.4
18	W	1	MET	3.4
29	7	45	ALA	3.3
8	I	54	GLN	3.3
1	A	229	A	3.3
21	Z	192	ALA	3.3
1	A	271(K)	U	3.3
8	I	76	THR	3.3
20	Y	89	PHE	3.3
3	D	122	ASP	3.3
7	H	99	VAL	3.3
1	A	2135	A	3.3

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Mol	Chain	Res	Type	RSRZ
20	Y	82	PRO	3.3
20	Y	85	VAL	3.3
1	A	1169	G	3.3
6	G	115	ARG	3.3
20	Y	90	LEU	3.2
24	2	49	LYS	3.2
8	I	37	VAL	3.2
4	E	193	GLY	3.2
5	F	146	ALA	3.2
11	P	149	GLU	3.2
24	2	15	LYS	3.2
25	3	38	GLU	3.2
5	F	131	GLY	3.2
15	T	90	GLN	3.1
21	Z	196	VAL	3.1
8	I	115	ALA	3.1
7	H	92	ILE	3.1
26	4	18	CYS	3.1
1	A	2140	C	3.1
14	S	59	LYS	3.1
6	G	2	PRO	3.1
9	N	93	THR	3.1
1	A	1026	U	3.1
20	Y	83	THR	3.1
7	H	175	LYS	3.1
8	I	80	PRO	3.1
21	Z	125	LEU	3.1
7	H	100	GLY	3.1
1	A	2153	G	3.1
1	A	2805	G	3.1
8	I	16	GLY	3.0
14	S	53	SER	3.0
28	6	29	ASN	3.0
1	A	1040	C	3.0
1	A	1171	G	3.0
26	4	36	CYS	3.0
4	E	88	GLY	3.0
14	S	58	LEU	3.0
23	1	23	LYS	3.0
1	A	271(M)	G	3.0
29	7	46	VAL	3.0
1	A	2127	G	3.0

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Mol	Chain	Res	Type	RSRZ
4	E	31	CYS	3.0
1	A	1047	G	2.9
1	A	2148	G	2.9
20	Y	57	GLN	2.9
3	D	176	ARG	2.9
1	A	271(V)	G	2.9
5	F	207	GLY	2.9
14	S	22	GLY	2.9
24	2	10	LEU	2.9
1	A	357	A	2.9
21	Z	71	VAL	2.9
7	H	121	ILE	2.9
25	3	53	LEU	2.9
21	Z	166	SER	2.9
6	G	27	ASN	2.9
16	U	104	GLN	2.9
8	I	44	LEU	2.9
21	Z	135	GLU	2.9
25	3	58	VAL	2.9
1	A	272(A)	U	2.9
1	A	278	A	2.9
14	S	69	VAL	2.9
1	A	652(P)	G	2.9
1	A	1115	G	2.9
1	A	2833	G	2.9
1	A	546	C	2.9
15	T	109	GLU	2.9
1	A	882	G	2.8
4	E	97	LYS	2.8
26	4	19	GLY	2.8
29	7	48	LYS	2.8
30	8	65	GLU	2.8
1	A	1963	U	2.8
1	A	34	C	2.8
6	G	25	TYR	2.8
14	S	12	PHE	2.8
8	I	85	GLU	2.8
1	A	361	G	2.8
24	2	5	GLU	2.8
1	A	715	G	2.8
8	I	89	TYR	2.8
22	0	11	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
30	8	19	SER	2.8
8	I	130	TYR	2.8
8	I	48	GLU	2.8
23	1	15	ALA	2.8
13	R	42	LYS	2.8
7	H	105	LEU	2.8
17	V	45	THR	2.8
26	4	32	TYR	2.8
29	7	38	GLY	2.7
11	P	135	LEU	2.7
1	A	262	A	2.7
1	A	614(A)	U	2.7
17	V	14	VAL	2.7
25	3	56	VAL	2.7
1	A	889	C	2.7
1	A	1532	C	2.7
4	E	1	MET	2.7
1	A	1509(A)	A	2.7
21	Z	40	ASP	2.7
3	D	64	ILE	2.7
7	H	86	GLU	2.7
1	A	2170	A	2.7
6	G	123	ASN	2.7
7	H	170	ARG	2.7
26	4	33	VAL	2.7
2	B	88	C	2.7
8	I	136	VAL	2.7
4	E	55	ASN	2.6
3	D	106	ILE	2.6
1	A	2154	G	2.6
24	2	12	GLU	2.6
8	I	47	LEU	2.6
24	2	18	PRO	2.6
7	H	166	GLY	2.6
14	S	100	ALA	2.6
1	A	473	G	2.6
2	B	98	G	2.6
21	Z	180	VAL	2.6
7	H	91	GLY	2.6
24	2	47	ASN	2.6
20	Y	52	SER	2.6
21	Z	44	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	1175	U	2.6
1	A	1450	G	2.6
26	4	41	PRO	2.6
1	A	627	A	2.6
22	0	43	THR	2.6
1	A	1745(A)	C	2.6
20	Y	94	LYS	2.6
1	A	879	G	2.6
6	G	133	LEU	2.5
8	I	72	LEU	2.5
14	S	82	ILE	2.5
26	4	31	ILE	2.5
9	N	46	VAL	2.5
23	1	2	SER	2.5
8	I	45	LYS	2.5
16	U	85	LYS	2.5
20	Y	44	ILE	2.5
21	Z	74	VAL	2.5
26	4	35	VAL	2.5
6	G	60	LEU	2.5
1	A	11	G	2.5
1	A	1921	G	2.5
14	S	66	ALA	2.5
6	G	7	LEU	2.5
6	G	149	VAL	2.5
12	Q	7	MET	2.5
1	A	887	A	2.5
17	V	70	ILE	2.5
28	6	7	ILE	2.5
1	A	32	C	2.5
1	A	272(J)	C	2.5
5	F	57	VAL	2.5
13	R	83	ILE	2.5
21	Z	80	ARG	2.5
2	B	60	C	2.5
6	G	140	ILE	2.5
1	A	1421	G	2.4
8	I	118	LYS	2.4
5	F	28	ILE	2.4
1	A	2163	C	2.4
1	A	890	A	2.4
1	A	1877	A	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	2106	G	2.4
1	A	2181	G	2.4
1	A	2603	G	2.4
3	D	245	PRO	2.4
1	A	1592	C	2.4
6	G	82	LEU	2.4
8	I	46	ALA	2.4
11	P	146	VAL	2.4
31	9	16	VAL	2.4
24	2	51	ARG	2.4
1	A	1116	C	2.4
1	A	2136	C	2.4
7	H	2	SER	2.4
7	H	116	GLU	2.4
3	D	137	PRO	2.4
7	H	95	ARG	2.4
19	X	43	VAL	2.4
21	Z	189	ALA	2.4
6	G	17	PRO	2.4
17	V	46	VAL	2.4
18	W	11	ARG	2.4
1	A	1049	C	2.4
1	A	2803	C	2.4
8	I	43	ASN	2.4
8	I	135	GLU	2.3
12	Q	85	LYS	2.3
1	A	2180	U	2.3
5	F	106	ARG	2.3
1	A	1531	C	2.3
1	A	1575	C	2.3
20	Y	14	LEU	2.3
21	Z	152	ALA	2.3
12	Q	112	GLU	2.3
5	F	20	LEU	2.3
26	4	30	GLU	2.3
5	F	187	VAL	2.3
9	N	9	VAL	2.3
20	Y	42	VAL	2.3
1	A	1530	C	2.3
11	P	15	ARG	2.3
1	A	716	A	2.3
24	2	8	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
24	2	16	LEU	2.3
6	G	20	ILE	2.3
13	R	45	ARG	2.3
8	I	74	ASN	2.3
1	A	1041	C	2.3
5	F	114	VAL	2.3
8	I	55	ALA	2.3
1	A	896	A	2.3
24	2	52	ASP	2.3
1	A	2152	G	2.3
1	A	2190	G	2.3
2	B	16	G	2.3
1	A	652(T)	C	2.3
6	G	106	LEU	2.3
15	T	114	LEU	2.3
16	U	98	LEU	2.3
8	I	98	ALA	2.3
13	R	52	ILE	2.3
8	I	1	MET	2.3
3	D	33	LEU	2.3
29	7	41	ARG	2.3
1	A	10	G	2.3
18	W	3	ALA	2.3
6	G	134	GLY	2.3
5	F	154	VAL	2.2
7	H	169	VAL	2.2
11	P	144	GLU	2.2
6	G	116	ASP	2.2
1	A	548	A	2.2
1	A	2801(A)	A	2.2
22	0	44	ARG	2.2
1	A	236	C	2.2
1	A	2139	C	2.2
1	A	2142	C	2.2
1	A	701	G	2.2
5	F	6	VAL	2.2
24	2	67	LYS	2.2
1	A	1167	U	2.2
23	1	13	ILE	2.2
5	F	145	GLU	2.2
9	N	96	GLU	2.2
6	G	135	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
23	1	24	ALA	2.2
1	A	238	C	2.2
1	A	355	G	2.2
1	A	881	G	2.2
1	A	1173	G	2.2
7	H	173	PRO	2.2
12	Q	65	PHE	2.2
23	1	38	SER	2.2
7	H	101	ARG	2.2
20	Y	65	ALA	2.2
20	Y	63	LYS	2.2
15	T	22	PHE	2.2
9	N	91	LEU	2.2
20	Y	67	LEU	2.2
1	A	2156	G	2.2
14	S	18	ILE	2.2
17	V	69	LYS	2.2
21	Z	32	HIS	2.1
1	A	271(C)	C	2.1
1	A	2183	C	2.1
5	F	157	VAL	2.1
15	T	107	ASP	2.1
3	D	236	GLY	2.1
14	S	68	GLN	2.1
7	H	117	PRO	2.1
10	O	38	VAL	2.1
26	4	42	PHE	2.1
26	4	46	GLN	2.1
1	A	356	G	2.1
1	A	2194	G	2.1
4	E	7	VAL	2.1
21	Z	48	PHE	2.1
8	I	123	LEU	2.1
1	A	529	A	2.1
1	A	1866	C	2.1
11	P	140	ALA	2.1
14	S	17	ARG	2.1
17	V	3	ALA	2.1
9	N	103	VAL	2.1
1	A	1044	G	2.1
23	1	80	LEU	2.1
7	H	165	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	652(O)	C	2.1
14	S	92	TYR	2.1
4	E	3	GLY	2.1
5	F	124	LEU	2.1
13	R	54	LEU	2.1
17	V	53	GLU	2.1
20	Y	64	GLU	2.1
25	3	22	ALA	2.1
6	G	173	LEU	2.1
1	A	895	U	2.1
12	Q	29	PHE	2.1
15	T	112	ARG	2.1
24	2	7	ARG	2.1
24	2	14	ARG	2.1
14	S	54	LEU	2.1
1	A	1383	C	2.0
1	A	2137	C	2.0
8	I	119	PRO	2.0
7	H	123	PHE	2.0
14	S	96	GLY	2.0
1	A	360	G	2.0
1	A	549	G	2.0
3	D	3	VAL	2.0
21	Z	39	VAL	2.0
1	A	901	A	2.0
1	A	1445	A	2.0
9	N	90	MET	2.0
20	Y	20	TYR	2.0
24	2	9	GLN	2.0
8	I	91	SER	2.0
2	B	97	G	2.0
21	Z	132	ASN	2.0
1	A	655	A	2.0
5	F	27	GLU	2.0
1	A	272(I)	U	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	3697	1/1	0.23	-	66,66,66,66	0
32	MG	A	3003	1/1	0.25	-	23,23,23,23	0
32	MG	A	3657	1/1	0.12	-	26,26,26,26	0
32	MG	A	3277	1/1	0.08	-	29,29,29,29	0
32	MG	A	3611	1/1	0.16	-	26,26,26,26	0
32	MG	A	3513	1/1	0.13	-	28,28,28,28	0
32	MG	Q	204	1/1	0.19	-	46,46,46,46	0
32	MG	A	3485	1/1	0.51	-	74,74,74,74	0
32	MG	Z	302	1/1	0.14	-	45,45,45,45	0
32	MG	A	3499	1/1	0.15	-	53,53,53,53	0
32	MG	A	3005	1/1	0.18	-	47,47,47,47	0
32	MG	A	3564	1/1	0.43	-	67,67,67,67	0
32	MG	A	3324	1/1	0.09	-	30,30,30,30	0
32	MG	A	3581	1/1	0.14	-	39,39,39,39	0
32	MG	A	3025	1/1	0.23	-	66,66,66,66	0
32	MG	A	3376	1/1	0.06	-	41,41,41,41	0
32	MG	A	3347	1/1	0.06	-	37,37,37,37	0
32	MG	A	3146	1/1	0.34	-	48,48,48,48	0
32	MG	B	219	1/1	0.14	-	54,54,54,54	0
32	MG	A	3169	1/1	0.07	-	31,31,31,31	0
32	MG	A	3360	1/1	0.09	-	33,33,33,33	0
32	MG	A	3268	1/1	0.40	-	60,60,60,60	0
32	MG	A	3053	1/1	0.49	-	54,54,54,54	0
32	MG	A	3568	1/1	0.23	-	54,54,54,54	0
32	MG	A	3468	1/1	0.19	-	54,54,54,54	0
32	MG	A	3041	1/1	0.54	-	30,30,30,30	0
32	MG	A	3059	1/1	0.43	-	36,36,36,36	0
32	MG	G	201	1/1	0.06	-	56,56,56,56	0
32	MG	A	3229	1/1	0.11	-	45,45,45,45	0
32	MG	A	3071	1/1	0.24	-	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3293	1/1	0.08	-	43,43,43,43	0
32	MG	9	103	1/1	0.42	-	52,52,52,52	0
32	MG	A	3084	1/1	0.28	-	30,30,30,30	0
32	MG	A	3261	1/1	0.58	-	66,66,66,66	0
32	MG	A	3212	1/1	0.19	-	56,56,56,56	0
32	MG	A	3642	1/1	0.18	-	59,59,59,59	0
32	MG	A	3447	1/1	0.66	-	54,54,54,54	0
32	MG	A	3032	1/1	0.16	-	34,34,34,34	0
32	MG	A	3415	1/1	0.10	-	23,23,23,23	0
32	MG	A	3251	1/1	0.15	-	38,38,38,38	0
32	MG	A	3246	1/1	0.09	-	24,24,24,24	0
32	MG	A	3407	1/1	0.11	-	19,19,19,19	0
32	MG	A	3645	1/1	0.32	-	53,53,53,53	0
32	MG	A	3652	1/1	0.49	-	91,91,91,91	0
32	MG	A	3016	1/1	0.59	-	38,38,38,38	0
32	MG	A	3538	1/1	0.16	-	29,29,29,29	0
32	MG	A	3465	1/1	0.08	-	33,33,33,33	0
32	MG	A	3638	1/1	0.66	-	28,28,28,28	0
32	MG	A	3011	1/1	0.07	-	27,27,27,27	0
32	MG	A	3466	1/1	0.20	-	50,50,50,50	0
32	MG	B	206	1/1	0.22	-	34,34,34,34	0
32	MG	A	3520	1/1	0.25	-	47,47,47,47	0
32	MG	A	3194	1/1	0.06	-	24,24,24,24	0
32	MG	A	3290	1/1	0.11	-	52,52,52,52	0
32	MG	A	3007	1/1	0.19	-	24,24,24,24	0
32	MG	T	201	1/1	0.72	-	49,49,49,49	0
32	MG	A	3671	1/1	0.38	-	46,46,46,46	0
32	MG	A	3316	1/1	0.18	-	77,77,77,77	0
32	MG	A	3712	1/1	0.21	-	45,45,45,45	0
32	MG	A	3063	1/1	0.12	-	42,42,42,42	0
32	MG	A	3272	1/1	0.18	-	32,32,32,32	0
32	MG	A	3692	1/1	0.07	-	27,27,27,27	0
32	MG	B	212	1/1	0.10	-	49,49,49,49	0
32	MG	A	3039	1/1	0.48	-	35,35,35,35	0
32	MG	A	3515	1/1	0.17	-	29,29,29,29	0
32	MG	B	202	1/1	0.22	-	45,45,45,45	0
32	MG	B	201	1/1	0.57	-	67,67,67,67	0
32	MG	A	3099	1/1	0.21	-	44,44,44,44	0
32	MG	D	302	1/1	0.24	-	33,33,33,33	0
32	MG	B	209	1/1	0.10	-	45,45,45,45	0
32	MG	A	3286	1/1	0.15	-	68,68,68,68	0
32	MG	6	102	1/1	0.11	-	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3197	1/1	0.20	-	39,39,39,39	0
32	MG	A	3605	1/1	0.08	-	36,36,36,36	0
32	MG	A	3576	1/1	0.53	-	42,42,42,42	0
32	MG	A	3387	1/1	0.15	-	29,29,29,29	0
32	MG	A	3548	1/1	0.16	-	27,27,27,27	0
32	MG	A	3370	1/1	0.26	-	61,61,61,61	0
32	MG	A	3673	1/1	0.12	-	47,47,47,47	0
32	MG	A	3620	1/1	0.24	-	52,52,52,52	0
32	MG	A	3151	1/1	0.10	-	36,36,36,36	0
32	MG	U	202	1/1	0.14	-	34,34,34,34	0
32	MG	A	3566	1/1	0.21	-	74,74,74,74	0
32	MG	A	3377	1/1	0.28	-	39,39,39,39	0
32	MG	A	3097	1/1	0.15	-	33,33,33,33	0
32	MG	A	3451	1/1	0.11	-	37,37,37,37	0
32	MG	A	3074	1/1	0.34	-	42,42,42,42	0
32	MG	A	3557	1/1	0.15	-	34,34,34,34	0
32	MG	A	3115	1/1	0.30	-	26,26,26,26	0
32	MG	A	3539	1/1	0.22	-	60,60,60,60	0
32	MG	A	3457	1/1	0.23	-	36,36,36,36	0
32	MG	A	3014	1/1	0.17	-	69,69,69,69	0
32	MG	A	3574	1/1	0.32	-	57,57,57,57	0
32	MG	A	3183	1/1	0.11	-	71,71,71,71	0
32	MG	A	3505	1/1	0.44	-	77,77,77,77	0
32	MG	A	3267	1/1	0.13	-	40,40,40,40	0
32	MG	A	3313	1/1	0.17	-	64,64,64,64	0
32	MG	A	3300	1/1	0.09	-	67,67,67,67	0
32	MG	A	3687	1/1	0.39	-	38,38,38,38	0
32	MG	A	3028	1/1	0.15	-	40,40,40,40	0
32	MG	A	3291	1/1	0.20	-	40,40,40,40	0
32	MG	A	3446	1/1	0.05	-	49,49,49,49	0
32	MG	A	3615	1/1	0.14	-	40,40,40,40	0
32	MG	9	104	1/1	0.14	-	52,52,52,52	0
32	MG	A	3533	1/1	0.07	-	55,55,55,55	0
32	MG	A	3250	1/1	0.11	-	25,25,25,25	0
32	MG	A	3179	1/1	0.08	-	44,44,44,44	0
32	MG	A	3201	1/1	0.09	-	57,57,57,57	0
32	MG	A	3001	1/1	0.13	-	41,41,41,41	0
32	MG	A	3238	1/1	0.11	-	49,49,49,49	0
32	MG	A	3724	1/1	0.12	-	47,47,47,47	0
32	MG	A	3462	1/1	0.09	-	63,63,63,63	0
32	MG	A	3436	1/1	0.22	-	58,58,58,58	0
32	MG	A	3330	1/1	0.44	-	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3035	1/1	0.14	-	29,29,29,29	0
32	MG	A	3022	1/1	0.18	-	34,34,34,34	0
33	ZN	6	101	1/1	0.03	-	42,42,42,42	0
32	MG	B	215	1/1	0.12	-	57,57,57,57	0
32	MG	A	3066	1/1	0.16	-	48,48,48,48	0
32	MG	A	3177	1/1	0.20	-	37,37,37,37	0
32	MG	A	3666	1/1	0.16	-	50,50,50,50	0
32	MG	A	3126	1/1	0.12	-	45,45,45,45	0
32	MG	A	3508	1/1	0.16	-	46,46,46,46	0
32	MG	A	3367	1/1	0.17	-	32,32,32,32	0
32	MG	N	201	1/1	0.17	-	57,57,57,57	0
32	MG	A	3215	1/1	0.36	-	51,51,51,51	0
32	MG	A	3494	1/1	0.50	-	35,35,35,35	0
32	MG	A	3110	1/1	0.13	-	50,50,50,50	0
32	MG	B	205	1/1	0.11	-	48,48,48,48	0
32	MG	A	3283	1/1	0.30	-	44,44,44,44	0
32	MG	A	3480	1/1	0.12	-	31,31,31,31	0
32	MG	A	3072	1/1	0.47	-	45,45,45,45	0
32	MG	A	3154	1/1	0.06	-	32,32,32,32	0
32	MG	A	3258	1/1	0.09	-	63,63,63,63	0
32	MG	A	3191	1/1	0.27	-	58,58,58,58	0
32	MG	A	3701	1/1	0.06	-	44,44,44,44	0
32	MG	A	3134	1/1	0.34	-	44,44,44,44	0
32	MG	A	3098	1/1	0.17	-	27,27,27,27	0
32	MG	A	3653	1/1	0.13	-	61,61,61,61	0
32	MG	A	3048	1/1	0.41	-	31,31,31,31	0
32	MG	A	3717	1/1	0.17	-	71,71,71,71	0
32	MG	A	3679	1/1	0.34	-	64,64,64,64	0
32	MG	A	3403	1/1	0.09	-	24,24,24,24	0
32	MG	A	3351	1/1	0.27	-	55,55,55,55	0
32	MG	A	3241	1/1	0.21	-	45,45,45,45	0
32	MG	A	3328	1/1	0.13	-	54,54,54,54	0
32	MG	A	3209	1/1	0.12	-	41,41,41,41	0
32	MG	A	3006	1/1	0.11	-	37,37,37,37	0
32	MG	A	3713	1/1	0.12	-	49,49,49,49	0
32	MG	A	3686	1/1	0.14	-	57,57,57,57	0
32	MG	A	3289	1/1	0.18	-	32,32,32,32	0
32	MG	A	3185	1/1	0.27	-	43,43,43,43	0
32	MG	A	3663	1/1	0.34	-	60,60,60,60	0
32	MG	A	3404	1/1	0.11	-	26,26,26,26	0
32	MG	A	3113	1/1	0.17	-	57,57,57,57	0
32	MG	A	3149	1/1	0.25	-	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	3546	1/1	0.08	-	60,60,60,60	0
32	MG	A	3455	1/1	0.20	-	51,51,51,51	0
32	MG	F	304	1/1	0.44	-	47,47,47,47	0
32	MG	A	3226	1/1	0.10	-	24,24,24,24	0
32	MG	A	3089	1/1	0.38	-	39,39,39,39	0
32	MG	A	3545	1/1	0.24	-	50,50,50,50	0
32	MG	A	3507	1/1	0.55	-	71,71,71,71	0
32	MG	A	3650	1/1	0.65	-	68,68,68,68	0
32	MG	A	3309	1/1	0.25	-	39,39,39,39	0
32	MG	A	3391	1/1	0.11	-	39,39,39,39	0
32	MG	A	3382	1/1	0.14	-	27,27,27,27	0
32	MG	A	3417	1/1	0.10	-	33,33,33,33	0
32	MG	A	3688	1/1	0.08	-	36,36,36,36	0
32	MG	9	102	1/1	0.21	-	29,29,29,29	0
32	MG	A	3140	1/1	0.13	-	34,34,34,34	0
32	MG	A	3056	1/1	0.18	-	32,32,32,32	0
32	MG	F	302	1/1	0.20	-	31,31,31,31	0
32	MG	A	3256	1/1	0.12	-	21,21,21,21	0
32	MG	A	3013	1/1	0.19	-	23,23,23,23	0
32	MG	A	3361	1/1	0.12	-	36,36,36,36	0
32	MG	A	3326	1/1	0.15	-	47,47,47,47	0
32	MG	A	3296	1/1	0.14	-	61,61,61,61	0
32	MG	A	3352	1/1	0.14	-	40,40,40,40	0
32	MG	A	3704	1/1	0.16	-	47,47,47,47	0
32	MG	A	3282	1/1	0.16	-	44,44,44,44	0
32	MG	A	3239	1/1	0.07	-	29,29,29,29	0
32	MG	A	3244	1/1	0.25	-	39,39,39,39	0
32	MG	B	213	1/1	0.39	-	46,46,46,46	0
32	MG	A	3329	1/1	0.18	-	39,39,39,39	0
32	MG	0	101	1/1	0.41	-	40,40,40,40	0
32	MG	F	305	1/1	0.21	-	29,29,29,29	0
32	MG	F	303	1/1	0.24	-	43,43,43,43	0
32	MG	A	3152	1/1	0.18	-	22,22,22,22	0
32	MG	A	3540	1/1	0.22	-	63,63,63,63	0
32	MG	A	3675	1/1	0.09	-	37,37,37,37	0
32	MG	A	3243	1/1	0.12	-	20,20,20,20	0
32	MG	A	3559	1/1	0.09	-	67,67,67,67	0
32	MG	A	3554	1/1	0.09	-	56,56,56,56	0
32	MG	A	3178	1/1	0.13	-	37,37,37,37	0
32	MG	A	3401	1/1	0.12	-	25,25,25,25	0
32	MG	A	3189	1/1	0.10	-	46,46,46,46	0
32	MG	A	3472	1/1	0.07	-	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3131	1/1	0.39	-	45,45,45,45	0
32	MG	A	3148	1/1	0.15	-	47,47,47,47	0
32	MG	A	3223	1/1	0.16	-	61,61,61,61	0
32	MG	A	3060	1/1	0.37	-	41,41,41,41	0
32	MG	A	3398	1/1	0.20	-	35,35,35,35	0
32	MG	A	3112	1/1	0.30	-	59,59,59,59	0
32	MG	A	3054	1/1	0.18	-	49,49,49,49	0
32	MG	A	3235	1/1	0.16	-	56,56,56,56	0
32	MG	A	3037	1/1	0.20	-	30,30,30,30	0
32	MG	A	3563	1/1	0.13	-	35,35,35,35	0
32	MG	A	3609	1/1	0.10	-	47,47,47,47	0
32	MG	A	3363	1/1	0.06	-	27,27,27,27	0
32	MG	A	3558	1/1	0.15	-	59,59,59,59	0
32	MG	A	3710	1/1	0.31	-	88,88,88,88	0
32	MG	A	3487	1/1	0.28	-	57,57,57,57	0
32	MG	A	3637	1/1	0.21	-	46,46,46,46	0
32	MG	A	3274	1/1	0.08	-	38,38,38,38	0
32	MG	A	3042	1/1	0.19	-	35,35,35,35	0
32	MG	A	3368	1/1	0.26	-	46,46,46,46	0
32	MG	A	3087	1/1	0.12	-	28,28,28,28	0
32	MG	A	3690	1/1	0.16	-	52,52,52,52	0
32	MG	S	201	1/1	0.16	-	63,63,63,63	0
32	MG	A	3664	1/1	0.17	-	44,44,44,44	0
32	MG	A	3409	1/1	0.15	-	23,23,23,23	0
32	MG	A	3021	1/1	0.40	-	32,32,32,32	0
32	MG	A	3525	1/1	0.39	-	95,95,95,95	0
32	MG	A	3603	1/1	0.10	-	21,21,21,21	0
32	MG	A	3706	1/1	0.09	-	52,52,52,52	0
32	MG	A	3308	1/1	0.09	-	23,23,23,23	0
32	MG	A	3082	1/1	0.10	-	42,42,42,42	0
32	MG	A	3273	1/1	0.21	-	39,39,39,39	0
32	MG	A	3218	1/1	0.09	-	28,28,28,28	0
32	MG	A	3216	1/1	0.10	-	34,34,34,34	0
32	MG	A	3253	1/1	0.06	-	18,18,18,18	0
32	MG	B	207	1/1	0.17	-	49,49,49,49	0
32	MG	E	303	1/1	0.41	-	47,47,47,47	0
32	MG	A	3585	1/1	0.36	-	77,77,77,77	0
32	MG	A	3137	1/1	0.08	-	23,23,23,23	0
32	MG	O	104	1/1	0.23	-	49,49,49,49	0
32	MG	A	3214	1/1	0.13	-	62,62,62,62	0
32	MG	A	3509	1/1	0.06	-	29,29,29,29	0
32	MG	A	3500	1/1	0.24	-	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3358	1/1	0.11	-	48,48,48,48	0
32	MG	A	3477	1/1	0.19	-	21,21,21,21	0
32	MG	A	3591	1/1	0.41	-	59,59,59,59	0
32	MG	A	3454	1/1	0.13	-	57,57,57,57	0
32	MG	A	3495	1/1	0.15	-	68,68,68,68	0
32	MG	A	3265	1/1	0.09	-	51,51,51,51	0
32	MG	A	3681	1/1	0.13	-	43,43,43,43	0
32	MG	T	203	1/1	0.20	-	51,51,51,51	0
32	MG	A	3294	1/1	0.15	-	44,44,44,44	0
32	MG	A	3383	1/1	0.07	-	20,20,20,20	0
32	MG	P	201	1/1	0.23	-	44,44,44,44	0
32	MG	A	3133	1/1	0.41	-	55,55,55,55	0
32	MG	R	201	1/1	0.35	-	39,39,39,39	0
32	MG	A	3339	1/1	0.12	-	41,41,41,41	0
32	MG	A	3075	1/1	0.46	-	38,38,38,38	0
32	MG	A	3047	1/1	0.38	-	33,33,33,33	0
32	MG	A	3392	1/1	0.08	-	36,36,36,36	0
32	MG	Y	202	1/1	0.29	-	49,49,49,49	0
32	MG	A	3437	1/1	0.22	-	24,24,24,24	0
32	MG	D	303	1/1	0.11	-	19,19,19,19	0
32	MG	A	3064	1/1	0.30	-	39,39,39,39	0
32	MG	A	3544	1/1	0.14	-	22,22,22,22	0
32	MG	A	3624	1/1	0.50	-	34,34,34,34	0
32	MG	A	3305	1/1	0.13	-	19,19,19,19	0
32	MG	A	3236	1/1	0.06	-	45,45,45,45	0
32	MG	A	3430	1/1	0.16	-	40,40,40,40	0
32	MG	A	3049	1/1	0.33	-	44,44,44,44	0
32	MG	A	3397	1/1	0.15	-	31,31,31,31	0
32	MG	A	3602	1/1	0.22	-	76,76,76,76	0
32	MG	A	3366	1/1	0.14	-	26,26,26,26	0
32	MG	A	3696	1/1	0.13	-	34,34,34,34	0
32	MG	A	3224	1/1	0.09	-	29,29,29,29	0
32	MG	A	3629	1/1	0.05	-	63,63,63,63	0
32	MG	A	3255	1/1	0.25	-	31,31,31,31	0
32	MG	A	3168	1/1	0.91	-	73,73,73,73	0
32	MG	A	3711	1/1	0.15	-	54,54,54,54	0
32	MG	A	3656	1/1	0.20	-	40,40,40,40	0
32	MG	A	3618	1/1	0.29	-	85,85,85,85	0
32	MG	A	3317	1/1	0.12	-	54,54,54,54	0
32	MG	A	3434	1/1	0.08	-	30,30,30,30	0
32	MG	A	3725	1/1	0.37	-	42,42,42,42	0
32	MG	A	3348	1/1	0.12	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3396	1/1	0.13	-	34,34,34,34	0
32	MG	A	3138	1/1	0.09	-	51,51,51,51	0
32	MG	A	3432	1/1	0.09	-	28,28,28,28	0
32	MG	B	217	1/1	0.28	-	66,66,66,66	0
32	MG	A	3208	1/1	0.07	-	39,39,39,39	0
32	MG	R	202	1/1	0.09	-	35,35,35,35	0
32	MG	A	3187	1/1	0.16	-	46,46,46,46	0
32	MG	A	3315	1/1	0.11	-	42,42,42,42	0
32	MG	A	3171	1/1	0.10	-	41,41,41,41	0
32	MG	A	3406	1/1	0.14	-	24,24,24,24	0
32	MG	A	3393	1/1	0.23	-	30,30,30,30	0
32	MG	A	3172	1/1	0.21	-	23,23,23,23	0
32	MG	Z	301	1/1	0.36	-	61,61,61,61	0
32	MG	A	3526	1/1	0.06	-	25,25,25,25	0
32	MG	A	3143	1/1	0.09	-	24,24,24,24	0
32	MG	E	301	1/1	0.26	-	43,43,43,43	0
32	MG	A	3584	1/1	0.23	-	41,41,41,41	0
32	MG	A	3350	1/1	0.09	-	51,51,51,51	0
32	MG	A	3278	1/1	0.20	-	36,36,36,36	0
32	MG	A	3590	1/1	0.09	-	78,78,78,78	0
32	MG	A	3373	1/1	0.08	-	24,24,24,24	0
32	MG	A	3689	1/1	0.09	-	21,21,21,21	0
32	MG	A	3184	1/1	0.11	-	36,36,36,36	0
32	MG	A	3680	1/1	0.57	-	69,69,69,69	0
32	MG	A	3206	1/1	0.17	-	52,52,52,52	0
32	MG	A	3257	1/1	0.06	-	51,51,51,51	0
32	MG	A	3411	1/1	0.10	-	22,22,22,22	0
32	MG	A	3484	1/1	0.19	-	57,57,57,57	0
32	MG	A	3297	1/1	0.22	-	47,47,47,47	0
32	MG	A	3553	1/1	0.11	-	60,60,60,60	0
32	MG	A	3062	1/1	0.22	-	40,40,40,40	0
32	MG	A	3280	1/1	0.45	-	96,96,96,96	0
32	MG	A	3181	1/1	0.55	-	69,69,69,69	0
32	MG	A	3464	1/1	0.20	-	65,65,65,65	0
32	MG	D	305	1/1	0.14	-	30,30,30,30	0
32	MG	A	3320	1/1	0.22	-	28,28,28,28	0
32	MG	A	3162	1/1	0.17	-	68,68,68,68	0
32	MG	A	3078	1/1	0.23	-	43,43,43,43	0
32	MG	A	3102	1/1	0.47	-	51,51,51,51	0
32	MG	A	3489	1/1	0.58	-	52,52,52,52	0
32	MG	A	3065	1/1	0.18	-	46,46,46,46	0
32	MG	A	3196	1/1	0.16	-	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	U	201	1/1	0.31	-	30,30,30,30	0
32	MG	A	3722	1/1	0.12	-	73,73,73,73	0
32	MG	A	3378	1/1	0.07	-	26,26,26,26	0
32	MG	V	203	1/1	0.18	-	56,56,56,56	0
32	MG	A	3453	1/1	0.13	-	45,45,45,45	0
32	MG	2	101	1/1	0.14	-	46,46,46,46	0
33	ZN	9	101	1/1	0.04	-	49,49,49,49	0
32	MG	A	3720	1/1	0.75	-	97,97,97,97	0
32	MG	A	3672	1/1	1.06	-	72,72,72,72	0
32	MG	A	3055	1/1	0.18	-	44,44,44,44	0
32	MG	A	3395	1/1	0.09	-	39,39,39,39	0
32	MG	A	3332	1/1	0.10	-	27,27,27,27	0
32	MG	A	3046	1/1	0.36	-	38,38,38,38	0
32	MG	A	3225	1/1	0.22	-	35,35,35,35	0
32	MG	R	204	1/1	0.16	-	49,49,49,49	0
32	MG	A	3587	1/1	0.28	-	62,62,62,62	0
32	MG	A	3355	1/1	0.11	-	41,41,41,41	0
32	MG	A	3551	1/1	0.22	-	52,52,52,52	0
32	MG	A	3237	1/1	0.18	-	31,31,31,31	0
32	MG	A	3443	1/1	0.05	-	46,46,46,46	0
32	MG	A	3512	1/1	0.13	-	91,91,91,91	0
32	MG	A	3593	1/1	0.10	-	34,34,34,34	0
32	MG	A	3372	1/1	0.15	-	44,44,44,44	0
32	MG	Q	203	1/1	0.06	-	38,38,38,38	0
32	MG	A	3607	1/1	0.32	-	58,58,58,58	0
32	MG	A	3285	1/1	0.10	-	27,27,27,27	0
32	MG	A	3130	1/1	0.07	-	24,24,24,24	0
32	MG	A	3292	1/1	0.54	-	52,52,52,52	0
32	MG	A	3307	1/1	0.08	-	32,32,32,32	0
32	MG	A	3429	1/1	0.14	-	56,56,56,56	0
32	MG	A	3561	1/1	0.18	-	48,48,48,48	0
32	MG	A	3420	1/1	0.10	-	38,38,38,38	0
32	MG	A	3549	1/1	0.15	-	41,41,41,41	0
32	MG	A	3572	1/1	0.09	-	59,59,59,59	0
32	MG	B	218	1/1	0.10	-	69,69,69,69	0
32	MG	T	202	1/1	0.20	-	52,52,52,52	0
32	MG	A	3045	1/1	0.30	-	33,33,33,33	0
32	MG	A	3619	1/1	0.24	-	36,36,36,36	0
32	MG	A	3414	1/1	0.15	-	29,29,29,29	0
32	MG	A	3271	1/1	0.13	-	47,47,47,47	0
32	MG	A	3668	1/1	0.22	-	69,69,69,69	0
32	MG	A	3068	1/1	0.20	-	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3705	1/1	0.18	-	63,63,63,63	0
32	MG	A	3027	1/1	0.15	-	31,31,31,31	0
32	MG	A	3542	1/1	0.15	-	33,33,33,33	0
32	MG	A	3067	1/1	0.22	-	74,74,74,74	0
32	MG	A	3488	1/1	0.12	-	65,65,65,65	0
32	MG	A	3252	1/1	0.15	-	21,21,21,21	0
32	MG	A	3678	1/1	0.35	-	95,95,95,95	0
32	MG	A	3150	1/1	0.14	-	28,28,28,28	0
32	MG	A	3219	1/1	0.06	-	19,19,19,19	0
32	MG	A	3597	1/1	0.08	-	43,43,43,43	0
32	MG	A	3496	1/1	0.23	-	51,51,51,51	0
32	MG	A	3413	1/1	0.16	-	28,28,28,28	0
32	MG	A	3050	1/1	0.18	-	32,32,32,32	0
32	MG	A	3478	1/1	0.16	-	31,31,31,31	0
32	MG	A	3408	1/1	0.12	-	24,24,24,24	0
32	MG	A	3384	1/1	0.17	-	30,30,30,30	0
32	MG	A	3118	1/1	0.11	-	24,24,24,24	0
32	MG	A	3092	1/1	0.17	-	39,39,39,39	0
32	MG	A	3721	1/1	0.10	-	57,57,57,57	0
32	MG	A	3433	1/1	0.30	-	31,31,31,31	0
32	MG	A	3193	1/1	0.14	-	46,46,46,46	0
32	MG	Q	202	1/1	0.12	-	47,47,47,47	0
32	MG	A	3052	1/1	0.33	-	57,57,57,57	0
32	MG	A	3589	1/1	0.30	-	56,56,56,56	0
32	MG	A	3288	1/1	0.21	-	36,36,36,36	0
32	MG	A	3474	1/1	0.43	-	77,77,77,77	0
32	MG	A	3633	1/1	0.33	-	82,82,82,82	0
32	MG	A	3560	1/1	0.17	-	57,57,57,57	0
32	MG	A	3644	1/1	0.08	-	30,30,30,30	0
32	MG	A	3318	1/1	0.07	-	57,57,57,57	0
32	MG	A	3301	1/1	0.41	-	61,61,61,61	0
32	MG	O	201	1/1	0.17	-	53,53,53,53	0
32	MG	D	304	1/1	0.17	-	46,46,46,46	0
32	MG	A	3604	1/1	0.06	-	37,37,37,37	0
32	MG	A	3135	1/1	0.17	-	67,67,67,67	0
32	MG	A	3635	1/1	0.33	-	55,55,55,55	0
32	MG	A	3337	1/1	0.07	-	43,43,43,43	0
32	MG	A	3502	1/1	0.38	-	67,67,67,67	0
32	MG	A	3306	1/1	0.12	-	34,34,34,34	0
32	MG	A	3425	1/1	0.17	-	27,27,27,27	0
32	MG	A	3431	1/1	0.12	-	41,41,41,41	0
32	MG	A	3569	1/1	0.30	-	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3058	1/1	0.93	-	54,54,54,54	0
32	MG	A	3156	1/1	0.14	-	22,22,22,22	0
32	MG	A	3030	1/1	0.20	-	41,41,41,41	0
32	MG	A	3295	1/1	0.45	-	54,54,54,54	0
32	MG	Q	201	1/1	0.35	-	61,61,61,61	0
32	MG	A	3595	1/1	0.22	-	58,58,58,58	0
33	ZN	4	101	1/1	0.05	-	117,117,117,117	0
32	MG	A	3676	1/1	0.09	-	31,31,31,31	0
32	MG	B	214	1/1	0.12	-	38,38,38,38	0
32	MG	A	3002	1/1	0.23	-	20,20,20,20	0
32	MG	A	3207	1/1	0.14	-	28,28,28,28	0
32	MG	A	3210	1/1	0.35	-	64,64,64,64	0
32	MG	A	3141	1/1	0.18	-	33,33,33,33	0
32	MG	A	3640	1/1	0.17	-	59,59,59,59	0
32	MG	A	3364	1/1	0.05	-	27,27,27,27	0
32	MG	B	204	1/1	0.21	-	47,47,47,47	0
32	MG	A	3547	1/1	0.10	-	26,26,26,26	0
32	MG	A	3482	1/1	0.19	-	49,49,49,49	0
32	MG	A	3412	1/1	0.10	-	25,25,25,25	0
32	MG	A	3577	1/1	0.19	-	66,66,66,66	0
32	MG	A	3647	1/1	0.17	-	51,51,51,51	0
32	MG	A	3444	1/1	0.13	-	40,40,40,40	0
33	ZN	Y	201	1/1	0.04	-	54,54,54,54	0
32	MG	A	3435	1/1	0.14	-	50,50,50,50	0
32	MG	A	3270	1/1	0.06	-	31,31,31,31	0
32	MG	A	3069	1/1	0.19	-	36,36,36,36	0
32	MG	A	3517	1/1	0.25	-	53,53,53,53	0
32	MG	A	3450	1/1	0.15	-	41,41,41,41	0
32	MG	A	3565	1/1	0.46	-	50,50,50,50	0
32	MG	A	3259	1/1	0.14	-	86,86,86,86	0
32	MG	A	3015	1/1	0.29	-	67,67,67,67	0
32	MG	A	3660	1/1	0.23	-	72,72,72,72	0
32	MG	A	3490	1/1	0.26	-	57,57,57,57	0
32	MG	A	3170	1/1	0.16	-	27,27,27,27	0
32	MG	A	3331	1/1	0.29	-	71,71,71,71	0
32	MG	A	3452	1/1	0.21	-	53,53,53,53	0
32	MG	A	3094	1/1	0.24	-	41,41,41,41	0
32	MG	A	3158	1/1	0.08	-	39,39,39,39	0
32	MG	A	3527	1/1	0.09	-	31,31,31,31	0
32	MG	A	3161	1/1	0.19	-	45,45,45,45	0
32	MG	E	304	1/1	0.16	-	53,53,53,53	0
32	MG	R	203	1/1	0.54	-	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3612	1/1	0.20	-	44,44,44,44	0
32	MG	A	3153	1/1	0.13	-	44,44,44,44	0
32	MG	A	3375	1/1	0.19	-	37,37,37,37	0
32	MG	A	3626	1/1	0.27	-	35,35,35,35	0
32	MG	A	3245	1/1	0.30	-	49,49,49,49	0
32	MG	A	3323	1/1	0.26	-	49,49,49,49	0
32	MG	A	3123	1/1	0.32	-	69,69,69,69	0
32	MG	A	3031	1/1	0.13	-	33,33,33,33	0
32	MG	A	3335	1/1	0.12	-	38,38,38,38	0
32	MG	A	3504	1/1	0.48	-	77,77,77,77	0
32	MG	A	3018	1/1	0.20	-	44,44,44,44	0
32	MG	A	3677	1/1	0.32	-	55,55,55,55	0
32	MG	A	3634	1/1	0.72	-	56,56,56,56	0
32	MG	A	3503	1/1	0.06	-	33,33,33,33	0
32	MG	A	3390	1/1	0.08	-	37,37,37,37	0
32	MG	A	3623	1/1	0.16	-	46,46,46,46	0
32	MG	A	3103	1/1	0.70	-	37,37,37,37	0
32	MG	A	3009	1/1	0.29	-	32,32,32,32	0
32	MG	A	3497	1/1	0.09	-	34,34,34,34	0
32	MG	V	201	1/1	0.54	-	30,30,30,30	0
32	MG	A	3104	1/1	0.50	-	60,60,60,60	0
32	MG	A	3088	1/1	0.71	-	33,33,33,33	0
32	MG	A	3248	1/1	0.09	-	39,39,39,39	0
32	MG	A	3669	1/1	0.22	-	62,62,62,62	0
32	MG	A	3531	1/1	0.77	-	54,54,54,54	0
32	MG	A	3144	1/1	0.15	-	70,70,70,70	0
32	MG	A	3311	1/1	0.12	-	43,43,43,43	0
32	MG	A	3567	1/1	0.26	-	44,44,44,44	0
32	MG	A	3362	1/1	0.18	-	34,34,34,34	0
32	MG	A	3709	1/1	0.19	-	47,47,47,47	0
32	MG	A	3422	1/1	0.06	-	28,28,28,28	0
32	MG	A	3190	1/1	0.27	-	52,52,52,52	0
32	MG	D	301	1/1	0.26	-	37,37,37,37	0
32	MG	A	3043	1/1	0.25	-	26,26,26,26	0
32	MG	A	3648	1/1	0.12	-	58,58,58,58	0
32	MG	A	3299	1/1	0.07	-	33,33,33,33	0
32	MG	A	3100	1/1	0.16	-	48,48,48,48	0
32	MG	A	3079	1/1	0.12	-	23,23,23,23	0
32	MG	A	3230	1/1	0.22	-	27,27,27,27	0
32	MG	A	3024	1/1	0.47	-	44,44,44,44	0
32	MG	A	3475	1/1	0.38	-	58,58,58,58	0
32	MG	A	3442	1/1	0.19	-	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	3606	1/1	0.09	-	32,32,32,32	0
32	MG	A	3263	1/1	0.06	-	52,52,52,52	0
32	MG	A	3132	1/1	0.16	-	64,64,64,64	0
32	MG	A	3232	1/1	0.14	-	39,39,39,39	0
32	MG	A	3038	1/1	0.28	-	53,53,53,53	0
32	MG	A	3354	1/1	0.15	-	19,19,19,19	0
32	MG	A	3445	1/1	0.07	-	24,24,24,24	0
32	MG	A	3388	1/1	0.11	-	29,29,29,29	0
32	MG	A	3632	1/1	1.26	-	81,81,81,81	0
32	MG	A	3522	1/1	0.62	-	51,51,51,51	0
32	MG	A	3227	1/1	0.14	-	53,53,53,53	0
32	MG	A	3369	1/1	0.10	-	27,27,27,27	0
32	MG	A	3469	1/1	0.20	-	63,63,63,63	0
32	MG	A	3026	1/1	0.21	-	25,25,25,25	0
32	MG	A	3186	1/1	0.12	-	62,62,62,62	0
32	MG	A	3017	1/1	0.15	-	43,43,43,43	0
32	MG	A	3155	1/1	0.17	-	20,20,20,20	0
32	MG	A	3661	1/1	0.30	-	78,78,78,78	0
32	MG	V	204	1/1	0.24	-	67,67,67,67	0
32	MG	A	3613	1/1	0.24	-	67,67,67,67	0
32	MG	A	3655	1/1	0.08	-	39,39,39,39	0
32	MG	A	3473	1/1	0.39	-	50,50,50,50	0
32	MG	A	3518	1/1	0.10	-	43,43,43,43	0
32	MG	A	3163	1/1	0.23	-	60,60,60,60	0
32	MG	A	3374	1/1	0.13	-	30,30,30,30	0
32	MG	A	3389	1/1	0.07	-	27,27,27,27	0
32	MG	A	3061	1/1	0.46	-	55,55,55,55	0
32	MG	A	3723	1/1	0.30	-	94,94,94,94	0
32	MG	A	3122	1/1	0.20	-	63,63,63,63	0
32	MG	3	101	1/1	0.16	-	52,52,52,52	0
32	MG	A	3594	1/1	0.24	-	63,63,63,63	0
32	MG	F	301	1/1	0.36	-	40,40,40,40	0
32	MG	A	3298	1/1	0.12	-	40,40,40,40	0
32	MG	A	3628	1/1	0.09	-	25,25,25,25	0
32	MG	A	3106	1/1	0.43	-	52,52,52,52	0
32	MG	A	3394	1/1	0.09	-	42,42,42,42	0
32	MG	A	3344	1/1	0.18	-	30,30,30,30	0
32	MG	A	3402	1/1	0.07	-	24,24,24,24	0
32	MG	A	3242	1/1	0.14	-	30,30,30,30	0
32	MG	A	3479	1/1	0.17	-	41,41,41,41	0
32	MG	A	3670	1/1	0.19	-	48,48,48,48	0
32	MG	A	3534	1/1	0.19	-	58,58,58,58	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	0.10	-	42,42,42,42	0
32	MG	A	3254	1/1	0.13	-	20,20,20,20	0
32	MG	A	3703	1/1	0.13	-	49,49,49,49	0
32	MG	A	3128	1/1	0.11	-	50,50,50,50	0
32	MG	A	3200	1/1	0.27	-	67,67,67,67	0
32	MG	A	3459	1/1	0.16	-	28,28,28,28	0
32	MG	A	3699	1/1	0.49	-	70,70,70,70	0
32	MG	A	3222	1/1	0.17	-	44,44,44,44	0
32	MG	A	3175	1/1	0.15	-	41,41,41,41	0
32	MG	A	3524	1/1	0.28	-	52,52,52,52	0
32	MG	A	3266	1/1	0.33	-	66,66,66,66	0
32	MG	Q	205	1/1	0.10	-	42,42,42,42	0
32	MG	A	3423	1/1	0.16	-	23,23,23,23	0
32	MG	A	3506	1/1	0.12	-	72,72,72,72	0
32	MG	A	3349	1/1	0.16	-	24,24,24,24	0
32	MG	A	3492	1/1	0.08	-	29,29,29,29	0
32	MG	A	3662	1/1	0.10	-	22,22,22,22	0
32	MG	O	103	1/1	0.14	-	71,71,71,71	0
32	MG	A	3080	1/1	0.15	-	21,21,21,21	0
32	MG	A	3036	1/1	0.21	-	27,27,27,27	0
32	MG	A	3685	1/1	0.05	-	42,42,42,42	0
32	MG	A	3691	1/1	0.11	-	38,38,38,38	0
32	MG	A	3610	1/1	0.53	-	60,60,60,60	0
32	MG	A	3076	1/1	0.17	-	26,26,26,26	0
32	MG	A	3198	1/1	0.16	-	47,47,47,47	0
32	MG	A	3481	1/1	0.08	-	25,25,25,25	0
32	MG	A	3336	1/1	0.09	-	44,44,44,44	0
32	MG	A	3221	1/1	0.15	-	55,55,55,55	0
32	MG	A	3599	1/1	0.41	-	43,43,43,43	0
32	MG	A	3114	1/1	0.10	-	54,54,54,54	0
32	MG	A	3627	1/1	0.26	-	29,29,29,29	0
32	MG	A	3467	1/1	0.22	-	34,34,34,34	0
32	MG	A	3470	1/1	0.11	-	45,45,45,45	0
32	MG	A	3321	1/1	0.17	-	46,46,46,46	0
32	MG	A	3051	1/1	0.14	-	29,29,29,29	0
32	MG	A	3204	1/1	0.20	-	58,58,58,58	0
32	MG	A	3582	1/1	0.09	-	60,60,60,60	0
32	MG	A	3276	1/1	0.16	-	43,43,43,43	0
32	MG	A	3643	1/1	0.10	-	42,42,42,42	0
32	MG	A	3202	1/1	0.17	-	57,57,57,57	0
32	MG	A	3124	1/1	0.12	-	79,79,79,79	0
32	MG	A	3501	1/1	0.06	-	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	D	306	1/1	0.32	-	65,65,65,65	0
32	MG	A	3535	1/1	0.10	-	64,64,64,64	0
32	MG	A	3580	1/1	0.30	-	65,65,65,65	0
32	MG	A	3516	1/1	0.12	-	35,35,35,35	0
32	MG	A	3410	1/1	0.15	-	26,26,26,26	0
32	MG	A	3614	1/1	0.16	-	75,75,75,75	0
32	MG	A	3164	1/1	0.11	-	38,38,38,38	0
32	MG	A	3659	1/1	0.14	-	56,56,56,56	0
32	MG	A	3541	1/1	0.10	-	46,46,46,46	0
32	MG	A	3646	1/1	0.31	-	34,34,34,34	0
32	MG	A	3579	1/1	0.22	-	48,48,48,48	0
32	MG	A	3174	1/1	0.39	-	42,42,42,42	0
32	MG	P	202	1/1	0.48	-	54,54,54,54	0
32	MG	A	3107	1/1	0.62	-	48,48,48,48	0
32	MG	A	3718	1/1	0.16	-	70,70,70,70	0
32	MG	A	3233	1/1	0.30	-	63,63,63,63	0
32	MG	A	3033	1/1	0.78	-	58,58,58,58	0
32	MG	A	3708	1/1	0.17	-	35,35,35,35	0
32	MG	B	210	1/1	0.16	-	62,62,62,62	0
32	MG	A	3338	1/1	0.17	-	48,48,48,48	0
32	MG	A	3203	1/1	0.11	-	19,19,19,19	0
32	MG	A	3260	1/1	0.17	-	69,69,69,69	0
32	MG	A	3279	1/1	0.12	-	37,37,37,37	0
32	MG	A	3034	1/1	0.29	-	52,52,52,52	0
32	MG	A	3192	1/1	0.21	-	35,35,35,35	0
32	MG	A	3129	1/1	0.10	-	50,50,50,50	0
32	MG	A	3333	1/1	0.10	-	49,49,49,49	0
32	MG	A	3029	1/1	0.26	-	23,23,23,23	0
32	MG	B	216	1/1	0.48	-	59,59,59,59	0
32	MG	A	3008	1/1	0.89	-	61,61,61,61	0
32	MG	A	3714	1/1	0.20	-	83,83,83,83	0
32	MG	E	306	1/1	0.10	-	24,24,24,24	0
32	MG	A	3552	1/1	0.15	-	25,25,25,25	0
32	MG	A	3111	1/1	0.45	-	67,67,67,67	0
32	MG	A	3532	1/1	0.34	-	66,66,66,66	0
32	MG	A	3188	1/1	0.19	-	52,52,52,52	0
32	MG	A	3105	1/1	0.77	-	67,67,67,67	0
32	MG	A	3399	1/1	0.08	-	27,27,27,27	0
32	MG	A	3220	1/1	0.10	-	49,49,49,49	0
32	MG	A	3588	1/1	0.16	-	34,34,34,34	0
32	MG	A	3716	1/1	0.18	-	53,53,53,53	0
32	MG	A	3249	1/1	0.15	-	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	3651	1/1	0.19	-	50,50,50,50	0
32	MG	A	3616	1/1	0.15	-	35,35,35,35	0
32	MG	A	3240	1/1	0.17	-	46,46,46,46	0
32	MG	A	3180	1/1	0.12	-	30,30,30,30	0
32	MG	A	3529	1/1	0.35	-	69,69,69,69	0
32	MG	A	3514	1/1	0.09	-	26,26,26,26	0
32	MG	A	3302	1/1	0.23	-	46,46,46,46	0
32	MG	A	3142	1/1	0.19	-	21,21,21,21	0
32	MG	A	3456	1/1	0.09	-	62,62,62,62	0
32	MG	A	3428	1/1	0.23	-	31,31,31,31	0
32	MG	A	3601	1/1	0.27	-	63,63,63,63	0
32	MG	1	101	1/1	0.23	-	40,40,40,40	0
32	MG	A	3658	1/1	0.11	-	53,53,53,53	0
32	MG	A	3228	1/1	0.14	-	61,61,61,61	0
32	MG	A	3573	1/1	0.16	-	49,49,49,49	0
32	MG	A	3073	1/1	0.57	-	45,45,45,45	0
32	MG	A	3682	1/1	0.14	-	53,53,53,53	0
32	MG	A	3101	1/1	0.23	-	47,47,47,47	0
32	MG	A	3093	1/1	0.33	-	47,47,47,47	0
32	MG	A	3695	1/1	0.09	-	41,41,41,41	0
32	MG	R	205	1/1	0.13	-	45,45,45,45	0
32	MG	A	3145	1/1	0.19	-	34,34,34,34	0
32	MG	A	3641	1/1	0.10	-	38,38,38,38	0
32	MG	A	3694	1/1	0.14	-	43,43,43,43	0
32	MG	A	3310	1/1	0.30	-	63,63,63,63	0
32	MG	N	202	1/1	0.07	-	57,57,57,57	0
32	MG	A	3707	1/1	0.52	-	49,49,49,49	0
32	MG	A	3586	1/1	0.59	-	104,104,104,104	0
32	MG	A	3121	1/1	0.10	-	30,30,30,30	0
32	MG	A	3571	1/1	0.17	-	55,55,55,55	0
32	MG	A	3139	1/1	0.07	-	33,33,33,33	0
32	MG	A	3698	1/1	0.13	-	26,26,26,26	0
32	MG	A	3493	1/1	0.16	-	45,45,45,45	0
32	MG	A	3312	1/1	0.53	-	69,69,69,69	0
32	MG	A	3578	1/1	0.21	-	63,63,63,63	0
32	MG	A	3012	1/1	0.28	-	52,52,52,52	0
32	MG	A	3385	1/1	0.24	-	33,33,33,33	0
32	MG	A	3319	1/1	0.06	-	48,48,48,48	0
32	MG	A	3157	1/1	0.23	-	30,30,30,30	0
32	MG	A	3380	1/1	0.15	-	31,31,31,31	0
32	MG	A	3166	1/1	0.24	-	65,65,65,65	0
32	MG	A	3471	1/1	0.17	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3715	1/1	0.12	-	64,64,64,64	0
32	MG	U	203	1/1	0.18	-	31,31,31,31	0
32	MG	A	3086	1/1	0.35	-	40,40,40,40	0
32	MG	A	3523	1/1	0.15	-	27,27,27,27	0
32	MG	A	3418	1/1	0.17	-	46,46,46,46	0
32	MG	A	3550	1/1	0.11	-	23,23,23,23	0
32	MG	A	3303	1/1	0.36	-	51,51,51,51	0
32	MG	A	3345	1/1	0.14	-	28,28,28,28	0
32	MG	A	3649	1/1	0.17	-	27,27,27,27	0
32	MG	A	3536	1/1	0.09	-	21,21,21,21	0
32	MG	A	3108	1/1	0.11	-	39,39,39,39	0
32	MG	A	3004	1/1	0.21	-	27,27,27,27	0
32	MG	A	3342	1/1	0.22	-	44,44,44,44	0
32	MG	A	3199	1/1	0.80	-	67,67,67,67	0
32	MG	A	3461	1/1	0.27	-	78,78,78,78	0
32	MG	A	3359	1/1	0.06	-	24,24,24,24	0
32	MG	A	3631	1/1	0.46	-	25,25,25,25	0
32	MG	A	3269	1/1	0.10	-	48,48,48,48	0
32	MG	W	201	1/1	0.22	-	44,44,44,44	0
32	MG	A	3356	1/1	0.14	-	30,30,30,30	0
32	MG	A	3116	1/1	0.09	-	46,46,46,46	0
32	MG	A	3090	1/1	0.14	-	36,36,36,36	0
32	MG	A	3127	1/1	0.32	-	30,30,30,30	0
32	MG	A	3556	1/1	0.29	-	46,46,46,46	0
32	MG	8	101	1/1	0.21	-	45,45,45,45	0
32	MG	A	3521	1/1	0.15	-	55,55,55,55	0
32	MG	A	3346	1/1	0.26	-	49,49,49,49	0
32	MG	A	3460	1/1	0.14	-	24,24,24,24	0
32	MG	A	3096	1/1	0.13	-	33,33,33,33	0
32	MG	A	3684	1/1	0.13	-	55,55,55,55	0
32	MG	A	3085	1/1	0.15	-	34,34,34,34	0
32	MG	V	202	1/1	0.33	-	83,83,83,83	0
32	MG	A	3334	1/1	0.09	-	34,34,34,34	0
32	MG	A	3438	1/1	0.15	-	31,31,31,31	0
32	MG	A	3284	1/1	0.20	-	58,58,58,58	0
32	MG	0	102	1/1	0.18	-	50,50,50,50	0
32	MG	A	3683	1/1	0.15	-	72,72,72,72	0
32	MG	A	3217	1/1	0.08	-	24,24,24,24	0
32	MG	B	211	1/1	0.25	-	61,61,61,61	0
32	MG	A	3070	1/1	0.48	-	58,58,58,58	0
32	MG	A	3234	1/1	0.53	-	66,66,66,66	0
32	MG	A	3592	1/1	0.16	-	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	3421	1/1	0.07	-	28,28,28,28	0
32	MG	A	3486	1/1	0.57	-	72,72,72,72	0
32	MG	A	3211	1/1	0.12	-	60,60,60,60	0
32	MG	E	302	1/1	0.14	-	29,29,29,29	0
32	MG	A	3275	1/1	0.69	-	57,57,57,57	0
32	MG	A	3159	1/1	0.21	-	41,41,41,41	0
32	MG	A	3621	1/1	0.19	-	68,68,68,68	0
32	MG	A	3674	1/1	0.38	-	80,80,80,80	0
32	MG	A	3441	1/1	0.20	-	42,42,42,42	0
32	MG	A	3040	1/1	0.18	-	35,35,35,35	0
32	MG	A	3205	1/1	0.27	-	49,49,49,49	0
32	MG	7	101	1/1	0.25	-	45,45,45,45	0
32	MG	A	3498	1/1	0.09	-	23,23,23,23	0
32	MG	A	3570	1/1	0.70	-	59,59,59,59	0
32	MG	F	306	1/1	0.14	-	61,61,61,61	0
32	MG	A	3483	1/1	0.14	-	20,20,20,20	0
32	MG	A	3125	1/1	0.09	-	28,28,28,28	0
32	MG	A	3596	1/1	0.19	-	43,43,43,43	0
32	MG	A	3327	1/1	0.08	-	37,37,37,37	0
32	MG	A	3562	1/1	0.70	-	66,66,66,66	0
32	MG	A	3165	1/1	0.23	-	49,49,49,49	0
32	MG	A	3530	1/1	0.10	-	58,58,58,58	0
32	MG	A	3176	1/1	0.11	-	30,30,30,30	0
32	MG	A	3019	1/1	0.15	-	34,34,34,34	0
32	MG	B	208	1/1	0.11	-	33,33,33,33	0
32	MG	A	3617	1/1	0.39	-	31,31,31,31	0
32	MG	A	3416	1/1	0.22	-	34,34,34,34	0
32	MG	A	3379	1/1	0.12	-	29,29,29,29	0
32	MG	A	3608	1/1	0.09	-	50,50,50,50	0
32	MG	A	3340	1/1	0.31	-	54,54,54,54	0
32	MG	A	3491	1/1	0.44	-	56,56,56,56	0
32	MG	A	3287	1/1	0.35	-	36,36,36,36	0
32	MG	A	3136	1/1	0.26	-	36,36,36,36	0
32	MG	A	3537	1/1	0.10	-	33,33,33,33	0
32	MG	H	201	1/1	0.17	-	60,60,60,60	0
32	MG	A	3304	1/1	0.50	-	69,69,69,69	0
32	MG	A	3636	1/1	0.40	-	47,47,47,47	0
32	MG	A	3528	1/1	0.18	-	24,24,24,24	0
32	MG	A	3583	1/1	0.43	-	55,55,55,55	0
32	MG	A	3057	1/1	0.18	-	31,31,31,31	0
32	MG	2	102	1/1	0.47	-	60,60,60,60	0
32	MG	A	3314	1/1	0.08	-	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3693	1/1	0.10	-	24,24,24,24	0
32	MG	A	3424	1/1	0.26	-	59,59,59,59	0
32	MG	A	3555	1/1	0.25	-	93,93,93,93	0
32	MG	A	3463	1/1	0.20	-	63,63,63,63	0
32	MG	A	3400	1/1	0.06	-	22,22,22,22	0
32	MG	A	3419	1/1	0.11	-	25,25,25,25	0
32	MG	A	3117	1/1	0.27	-	48,48,48,48	0
32	MG	A	3083	1/1	0.28	-	32,32,32,32	0
32	MG	A	3231	1/1	0.07	-	41,41,41,41	0
32	MG	A	3598	1/1	0.11	-	39,39,39,39	0
33	ZN	5	101	1/1	0.04	-	42,42,42,42	0
32	MG	A	3654	1/1	0.22	-	61,61,61,61	0
32	MG	A	3109	1/1	0.13	-	35,35,35,35	0
32	MG	A	3371	1/1	0.15	-	37,37,37,37	0
32	MG	A	3081	1/1	0.25	-	36,36,36,36	0
32	MG	A	3365	1/1	0.17	-	23,23,23,23	0
32	MG	A	3510	1/1	0.08	-	35,35,35,35	0
32	MG	A	3440	1/1	0.84	-	60,60,60,60	0
32	MG	A	3173	1/1	0.38	-	31,31,31,31	0
32	MG	A	3160	1/1	0.84	-	53,53,53,53	0
32	MG	A	3427	1/1	0.08	-	68,68,68,68	0
32	MG	A	3213	1/1	0.18	-	67,67,67,67	0
32	MG	A	3020	1/1	0.31	-	50,50,50,50	0
32	MG	A	3353	1/1	0.24	-	22,22,22,22	0
32	MG	A	3091	1/1	0.20	-	40,40,40,40	0
32	MG	A	3322	1/1	0.13	-	69,69,69,69	0
32	MG	A	3147	1/1	0.07	-	36,36,36,36	0
32	MG	A	3182	1/1	0.18	-	47,47,47,47	0
32	MG	A	3575	1/1	0.24	-	49,49,49,49	0
32	MG	A	3625	1/1	0.07	-	57,57,57,57	0
32	MG	A	3667	1/1	0.18	-	69,69,69,69	0
32	MG	A	3639	1/1	0.12	-	35,35,35,35	0
32	MG	A	3119	1/1	0.20	-	39,39,39,39	0
32	MG	A	3622	1/1	0.82	-	40,40,40,40	0
32	MG	A	3381	1/1	0.20	-	32,32,32,32	0
32	MG	A	3120	1/1	0.05	-	30,30,30,30	0
32	MG	A	3702	1/1	0.14	-	49,49,49,49	0
32	MG	A	3448	1/1	0.12	-	65,65,65,65	0
32	MG	A	3262	1/1	0.15	-	56,56,56,56	0
32	MG	B	203	1/1	0.47	-	48,48,48,48	0
32	MG	E	305	1/1	0.21	-	35,35,35,35	0
32	MG	A	3195	1/1	0.33	-	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	3095	1/1	0.34	-	37,37,37,37	0
32	MG	A	3665	1/1	0.21	-	65,65,65,65	0
32	MG	A	3511	1/1	0.13	-	54,54,54,54	0
32	MG	A	3325	1/1	0.52	-	45,45,45,45	0
32	MG	A	3600	1/1	0.87	-	89,89,89,89	0
32	MG	A	3023	1/1	0.23	-	38,38,38,38	0
32	MG	A	3476	1/1	0.09	-	22,22,22,22	0
32	MG	A	3543	1/1	0.10	-	32,32,32,32	0
32	MG	A	3458	1/1	0.18	-	38,38,38,38	0
32	MG	A	3341	1/1	0.36	-	43,43,43,43	0
32	MG	A	3439	1/1	0.16	-	50,50,50,50	0
32	MG	A	3630	1/1	0.34	-	72,72,72,72	0
32	MG	A	3357	1/1	0.07	-	30,30,30,30	0
32	MG	A	3077	1/1	0.11	-	32,32,32,32	0
32	MG	A	3386	1/1	0.10	-	24,24,24,24	0
32	MG	A	3449	1/1	0.10	-	55,55,55,55	0
32	MG	3	102	1/1	0.29	-	38,38,38,38	0
32	MG	A	3519	1/1	0.05	-	35,35,35,35	0
32	MG	A	3405	1/1	0.19	-	56,56,56,56	0
32	MG	A	3010	1/1	0.17	-	44,44,44,44	0
32	MG	A	3343	1/1	0.13	-	44,44,44,44	0
32	MG	A	3426	1/1	0.13	-	28,28,28,28	0
32	MG	A	3700	1/1	0.27	-	57,57,57,57	0
32	MG	A	3264	1/1	0.16	-	51,51,51,51	0
32	MG	A	3247	1/1	0.12	-	52,52,52,52	0
32	MG	A	3167	1/1	0.22	-	63,63,63,63	0
32	MG	A	3044	1/1	0.21	-	54,54,54,54	0
32	MG	A	3719	1/1	0.26	-	54,54,54,54	0

6.5 Other polymers ⓘ

There are no such residues in this entry.