



Full wwPDB EM Validation Report ⓘ

Nov 14, 2022 – 01:43 AM EST

PDB ID : 6WU9
EMDB ID : EMD-21907
Title : 50S subunit of 70S Ribosome Enterococcus faecalis MultiBody refinement
Authors : Jogl, G.; Khayat, R.
Deposited on : 2020-05-04
Resolution : 2.90 Å(reported)
Based on initial models : 5LI0, 4YBB

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

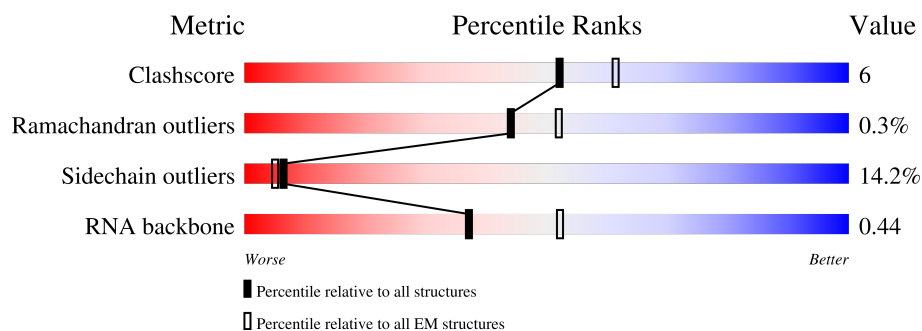
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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.














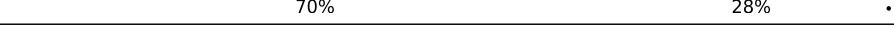

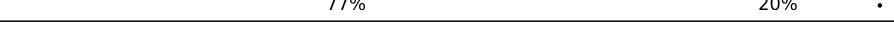






Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	2908	60% 26% 7% • 6%
2	B	116	48% 31% 19% •
3	D	207	66% 29% 5%
4	E	206	74% 21% 5%
5	F	177	53% 42% 5% •
6	G	176	62% 31% 7%
7	K	145	79% 17% •

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Mol	Chain	Length	Quality of chain
8	L	122	 78% 20% .
9	M	146	 81% 16% .
10	N	141	 69% 26% 5%
11	O	124	 69% 26% 5%
12	P	117	 70% 25% 5%
13	Q	114	 77% 19% .
14	R	118	 82% 16% .
15	S	102	 74% 25% .
16	T	112	 73% 22% .
17	U	89	 70% 25% 6%
18	V	101	 70% 23% 7%
19	X	76	 70% 28% .
20	Y	54	 74% 20% 6%
21	Z	61	 77% 20% .
22	0	58	 76% 24%
23	2	56	 82% 14% .
24	3	49	 67% 33%
25	4	44	 70% 27% .
26	5	64	 80% 17% .
27	6	38	 76% 16% 8%

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 82295 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2739	Total	C	N	O	P	0	0
			58793	26244	10818	18992	2739		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	116	Total	C	N	O	P	0	0
			2480	1106	444	814	116		

- Molecule 3 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	207	Total	C	N	O	S	0	0
			1579	994	292	289	4		

- Molecule 4 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	206	Total	C	N	O	S	0	0
			1574	984	290	298	2		

- Molecule 5 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	177	Total	C	N	O	S	0	0
			1392	887	239	260	6		

- Molecule 6 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	176	Total	C	N	O	S	0	0
			1345	842	244	255	4		

- Molecule 7 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	145	Total	C	N	O	S	0	0
			1130	714	205	207	4		

- Molecule 8 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	122	Total	C	N	O	S	0	0
			922	574	176	170	2		

- Molecule 9 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	146	Total	C	N	O	S	0	0
			1095	677	212	205	1		

- Molecule 10 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	141	Total	C	N	O	S	0	0
			1118	710	216	185	7		

- Molecule 11 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	O	124	Total	C	N	O	S	0	0
			991	612	191	185	3		

- Molecule 12 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	P	117	Total	C	N	O	S	0	0
			899	556	175	167	1		

- Molecule 13 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	Q	114	Total	C	N	O	0	0
			924	582	185	157		

- Molecule 14 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	R	118	Total	C	N	O	S	0	0
			950	602	184	160	4		

- Molecule 15 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	S	102	Total	C	N	O	S	0	0
			784	500	139	143	2		

- Molecule 16 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	112	Total	C	N	O	S	0	0
			849	532	156	159	2		

- Molecule 17 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	U	89	Total	C	N	O	S	0	0
			720	458	127	132	3		

- Molecule 18 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	V	101	Total	C	N	O	S	0	0
			763	486	135	140	2		

- Molecule 19 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	X	76	Total	C	N	O	0	0
			572	351	109	112		

- Molecule 20 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Y	54	Total	C	N	O	S	0	0
			425	265	86	72	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	51	ALA	THR	conflict	UNP A0A1B4XRZ8

- Molecule 21 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Z	61	Total	C	N	O	S	0	0
			504	314	94	95	1		

- Molecule 22 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	0	58	Total	C	N	O	S	0	0
			435	271	81	82	1		

- Molecule 23 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	2	56	Total	C	N	O	S	0	0
			429	262	88	73	6		

- Molecule 24 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	3	49	Total	C	N	O	S	0	0
			419	253	86	76	4		

- Molecule 25 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	4	44	Total	C	N	O	S	0	0
			374	227	91	54	2		

- Molecule 26 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	5	64	Total	C	N	O	S	0	0
			522	320	122	78	2		

- Molecule 27 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	6	38	Total	C	N	O	S	0	0
			304	188	66	44	6		

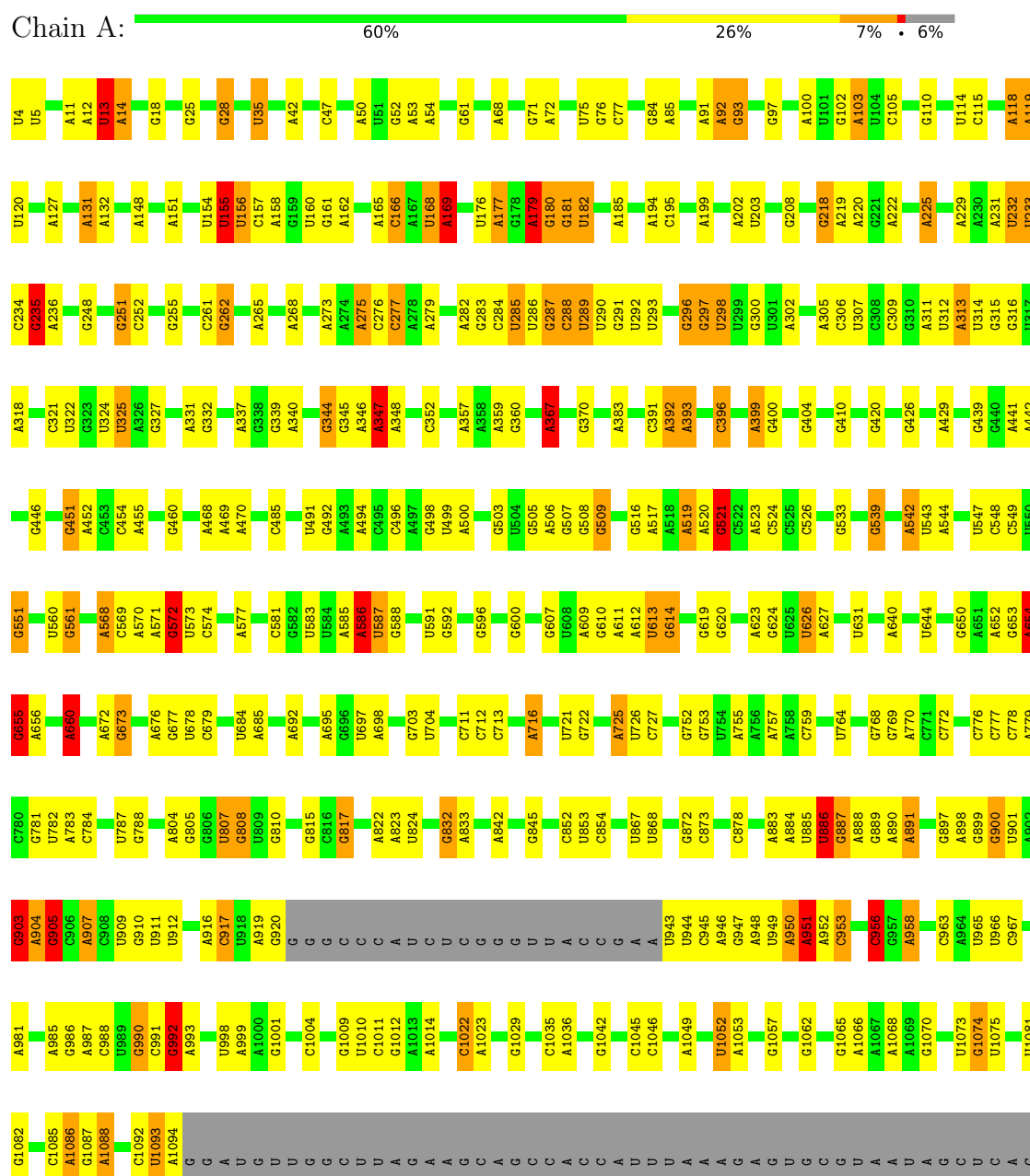
- Molecule 28 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
28	2	1	Total	Zn	0
			1	1	
28	3	1	Total	Zn	0
			1	1	
28	6	1	Total	Zn	0
			1	1	

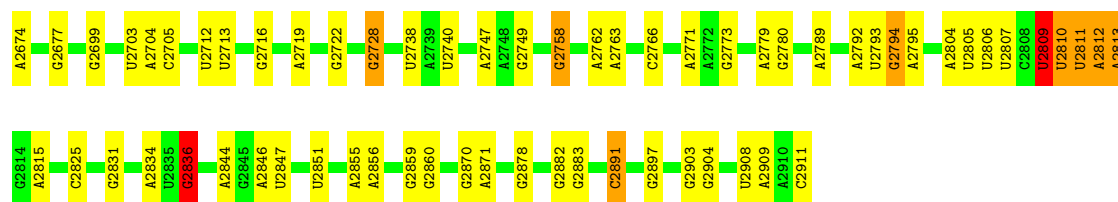
3 Residue-property plots

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

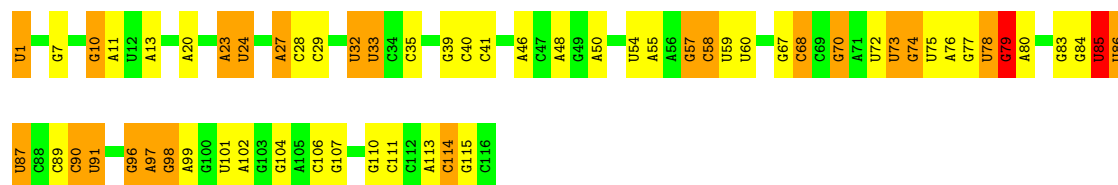
• Molecule 1: 23S rRNA



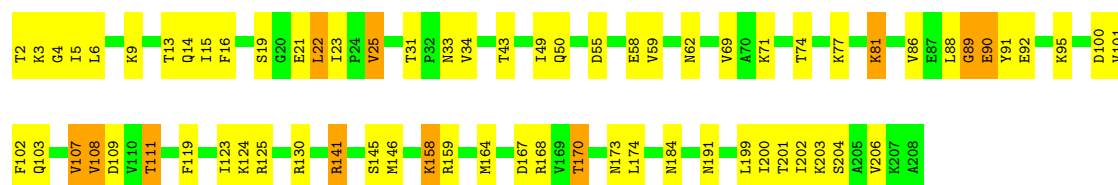
U551	A2444	G2335	C2228	U2100	G2006	G1886	A1787	G1644	G1548	G1456	G1360	C1238	U1237
C2552	U2445	A2336	G2238	G2101	U2007	G1887	G1790	U1645	C1548	A1457	U1365	U1239	G1236
A2556	A2449	G2339	G2239	A2102	C2008	A1890	U1793	U1551	U1551	C1459	U1365	A1241	U1235
G2563	A2453	U2340	C2240	U2106	A2011	U1894	U1796	A1652	A1552	A1460	G1373	U1247	G1234
U2566	C2454	A2341	A2241	G2107	C2020	C1895	C1796	A1653	A1559	A1461	U1376	G1256	U1236
G2570	C2455	A2342	G2252	A2108	U2021	C1896	A1798	A1658	G1560	U1462	U1376	A1257	G1237
C2571	G2458	G2344	G2253	G2109	C2022	G1897	A1799	C1658	C1567	C1470	G1379	G1262	G1235
C2572	A2461	G2345	G2264	U2110	G2035	A1898	A1800	G1669	U1570	G1471	U1380	G1263	U1236
A2575	U2462	G2348	G2267	U2113	U2036	G1902	C1804	A1673	G1570	G1474	U1388	A1264	G1235
A2580	U2463	A2349	C2272	G2114	C2038	A1910	A1805	G1674	G1571	U1475	A1389	G1275	G1235
C2581	A2464	A2360	C2277	U2115	C2039	U1908	G1807	G1686	A1572	A1486	G1390	G1278	G1235
G2587	U2474	C2361	G2277	U2116	G2041	G1920	C1809	A1689	U1576	G1488	C1393	C1278	G1235
C2588	A2475	U2371	A2280	U2117	A2043	A1927	C1814	C1690	A1577	C1489	G1394	A1284	G1235
G2592	C2476	G2365	A2281	U2118	G2045	U1928	A1815	C1691	A1578	U1491	G1397	U1286	G1235
G2596	U2477	A2366	A2282	U2119	A2047	A1930	A1816	A1591	A	C1492	C1398	G1287	G1235
G2597	A2478	G2367	A2283	U2120	U2048	U1931	A1817	C1699	U	C1493	G1400	A1288	G1235
U2598	C2481	U2371	A2284	U2121	G2049	A1932	A1823	U1700	G1583	G1494	A1401	A1290	G1235
A2601	A2482	A2371	A2285	U2122	C2050	C1934	A1824	A1708	G1584	U1495	G1404	G1293	G1235
G2602	U2483	G2379	C2289	U2123	A2051	G1935	G1825	C1713	U1585	U1497	G1405	A1299	G1235
G2605	A2484	U2387	G2293	U2124	G2052	G1936	G1826	G1717	G1589	G1498	A1406	U1300	G1235
G2606	U2485	A2387	C2294	U2125	U2053	G1943	A1830	G1725	G1590	A1500	G1407	C1301	G1235
G2613	C2486	G2395	C2295	U2126	A2054	G1960	A1843	C1726	A1591	U1501	A1408	G1194	G1235
A2616	U2487	G2396	C2296	U2127	C2055	C1961	G1837	G1730	U1594	C1505	G1411	G1197	G1235
C2624	A2488	U2403	G2297	U2128	G2056	U1969	U1841	C1734	G1600	U1507	A1420	G1202	G1235
U2627	U2489	G2405	C2307	U2129	A2057	U1970	G1856	G1746	A1604	G1508	A1421	U1206	G1235
A2628	C2490	A2406	A2314	U2130	G2070	C1976	G1860	A1764	A1606	C1510	A1423	A1207	G1235
U2629	U2491	U2416	U2315	U2131	A2073	C1977	A1861	C1755	A1612	G1514	G1428	A1209	G1235
G2632	U2492	C2417	C2316	U2132	G2074	G1978	A1862	U1756	U1615	U1518	A1429	C1210	G1235
G2637	U2493	G2418	C2317	U2133	G2075	C1981	G1863	U1757	A1615	G1519	U1430	C1211	G1235
G2638	U2494	C2419	U2318	U2134	C2076	C1982	G1864	C1758	U1624	G1520	A1431	A1212	G1235
U2639	U2495	C2420	U2319	U2135	C2077	A1984	A1867	G1759	U1624	G1521	U1432	U1213	G1235
G2645	U2496	G2421	G2322	U2136	C2078	A1985	A1868	G1760	U1624	U1525	G1434	U1214	G1235
U2650	U2497	C2422	A2323	U2137	C2079	G1986	G1871	C1762	G1628	G1526	A1434	G1216	G1235
C2664	U2498	U2436	U2326	U2138	G2083	G1989	G1872	G1764	G1629	U1527	G1446	G1217	G1235
G2672	U2499	G2437	C2327	U2139	A2085	G1994	A1873	U1764	G1630	U1528	U1447	U1336	G1235
G2673	U2500	U2438	G2328	U2140	C2086	A1995	A1874	G1770	A1631	U1532	U1448	A1337	G1235
G2674	U2501	C2439	U2329	U2141	C2087	U1996	G1875	A1776	A1633	U1535	U	U1349	G1235
G2675	U2502	U2440	C2331	U2142	U2088	G2001	G1876	G1777	C1635	A1536	U1451	C1350	G1235
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G2677	U2504	A2226	A2334	U2144	U2099	U2006	U1884	U1786	C1638	U1539	U1455	G1356	G1235
G2678	U2505	U2227	U2335	U2145	U2100	U2007	U1885	G1786	G1638	U1540	U1456	U1357	G1235
G2679	U2506	U2228	U2336	U2146	U2101	U2008	U1886	G1787	G1639	U1541	U1457	U1358	G1235
G2680	U2507	U2229	U2337	U2147	U2102	U2009	U1887	G1788	G1640	U1542	U1458	U1359	G1235
G2681	U2508	U2230	U2338	U2148	U2103	U2010	U1888	G1789	G1641	U1543	U1459	U1360	G1235
G2682	U2509	U2231	U2339	U2149	U2104	U2011	U1889	G1790	G1642	U1544	U1460	U1361	G1235
G2683	U2510	U2232	U2340	U2150	U2105	U2012	U1890	G1791	G1643	U1545	U1461	U1362	G1235
G2684	U2511	U2233	U2341	U2151	U2106	U2013	U1891	G1792	G1644	U1546	U1462	U1363	G1235
G2685	U2512	U2234	U2342	U2152	U2107	U2014	U1892	G1793	G1645	U1547	U1463	U1364	G1235
G2686	U2513	U2235	U2343	U2153	U2108	U2015	U1893	G1794	G1646	U1548	U1464	U1365	G1235
G2687	U2514	U2236	U2344	U2154	U2109	U2016	U1894	G1795	G1647	U1549	U1465	U1366	G1235
G2688	U2515	U2237	U2345	U2155	U2110	U2017	U1895	G1796	G1648	U1550	U1466	U1367	G1235
G2689	U2516	U2238	U2346	U2156	U2111	U2018	U1896	G1797	G1649	U1551	U1467	U1368	G1235
G2690	U2517	U2239	U2347	U2157	U2112	U2019	U1897	G1798	G1650	U1552	U1468	U1369	G1235
G2691	U2518	U2240	U2348	U2158	U2113	U2020	U1898	G1799	G1651	U1553	U1469	U1370	G1235
G2692	U2519	U2241	U2349	U2159	U2114	U2021	U1899	G1800	G1652	U1554	U1470	U1371	G1235
G2693	U2520	U2242	U2350	U2160	U2115	U2022	U1900	G1801	G1653	U1555	U1471	U1372	G1235
G2694	U2521	U2243	U2351	U2161	U2116	U2023	U1901	G1802	G1654	U1556	U1472	U1373	G1235
G2695	U2522	U2244	U2352	U2162	U2117	U2024	U1902	G1803	G1655	U1557	U1473	U1374	G1235
G2696	U2523	U2245	U2353	U2163	U2118	U2025	U1903	G1804	G1656	U1558	U1474	U1375	G1235
G2697	U2524	U2246	U2354	U2164	U2119	U2026	U1904	G1805	G1657	U1559	U1475	U1376	G1235
G2698	U2525	U2247	U2355	U2165	U2120	U2027	U1905	G1806	G1658	U1560	U1476	U1377	G1235
G2699	U2526	U2248	U2356	U2166	U2121	U2028	U1906	G1807	G1659	U1561	U1477	U1378	G1235
G2700	U2527	U2249	U2357	U2167	U2122	U2029	U1907	G1808	G1660	U1562	U1478	U1379	G1235
G2701	U2528	U2250	U2358	U2168	U2123	U2030	U1908	G1809	G1661	U1563	U1479	U1380	G1235
G2702	U2529	U2251	U2359	U2169	U2124	U2031	U1909	G1810	G1662	U1564	U1480	U1381	G1235
G2703	U2530	U2252	U2360	U2170	U2125	U2032	U1910	G1811	G1663	U1565	U1481	U1382	G1235
G2704	U2531	U2253	U2361	U2171	U2126	U2033	U1911	G1812	G1664	U1566	U1482	U1383	G1235
G2705	U2532	U2254	U2362	U2172	U2127	U2034	U1912	G1813	G1665	U1567	U1483	U1384	G1235
G2706	U2533	U2255	U2363	U2173	U2128	U2035	U1913	G1814	G1666	U1568	U1484	U1385	G1235
G2707	U2534	U2256	U2364	U2174	U2129	U2036	U1914	G1815	G1667	U1569	U1485	U1386	G1235
G2708	U2535	U2257	U2365	U2175	U2130	U2037	U1915	G1816	G1668	U1570	U1486	U1387	G1235
G2709	U2536	U2258	U2366	U2176	U2131	U2038	U1916	G1817	G1669	U1571	U1487	U1388	G1235
G2710	U2537	U2259	U2367	U2177	U2132	U2039	U1917	G1818	G1670	U1572	U1488	U1389	G1235
G2711	U2538	U2260	U2368	U2178	U2133	U2040	U1918	G1819	G1671	U1573	U1489	U1390	G1235
G2712	U2539	U2261	U2369	U2179	U2134	U2041	U1919	G1820	G1672	U1574	U1490	U1391	G1235
G2713	U2540	U2262	U2370	U2180	U2135	U2042	U1920	G1821	G1673	U1575	U1491	U1392	G1235
G2714	U2541	U2263	U2371	U2181	U2136	U2043	U1921	G1822	G1674	U1576	U1492	U1393	G1235
G2715	U2542	U2264	U2372	U2182	U2137	U2044	U1922	G1823	G1675	U1577	U1493	U1394	G1235
G2716	U2543	U2265	U2373	U2183	U2138	U2045	U1923	G1824	G1676	U1578	U1494	U1395	G1235
G2717	U2544	U2266	U2374	U2184	U2139	U2046	U1924	G1825	G1677	U1579	U1495	U1396	G1235
G2718	U2545	U2267	U2375	U2185	U2140	U2047	U1925	G1826	G1678	U1580	U1496	U1397	G1235
G2719	U2546	U2268	U2376	U2186	U2141	U2048	U1926	G1827	G1679	U1581	U1497	U1398	G1235
G2720	U2547	U2269	U2377	U2187	U2142	U2049	U1927	G1828	G1680	U1582	U1498	U1399	G1235
G2721	U2548	U2270	U2378	U2188	U2143	U2050	U1928	G1829	G1681	U1583	U1499	U1400	G1235
G2722	U2549	U2271	U2379	U2189	U2144	U2051	U1929	G1830	G1682	U1584	U1500	U1401	G1235
G2723	U2550	U2272	U2380	U2190	U2145	U2052	U1930	G1831	G1683	U1585	U1501	U1402	G1235
G2724	U2551	U2273	U2381	U2191	U2146	U2053	U1931	G1832	G1684	U1586	U1502	U1403	G1235
G2725	U2552	U2274	U2382	U2192	U2147	U2054	U1932	G1833	G1685	U1587	U1503	U1404	G1235
G2726	U2553	U2275	U2383	U2193	U2148	U2055	U1933	G1834	G1686	U1588	U1504	U1405	G1235
G2727	U2554	U2276	U2384	U									



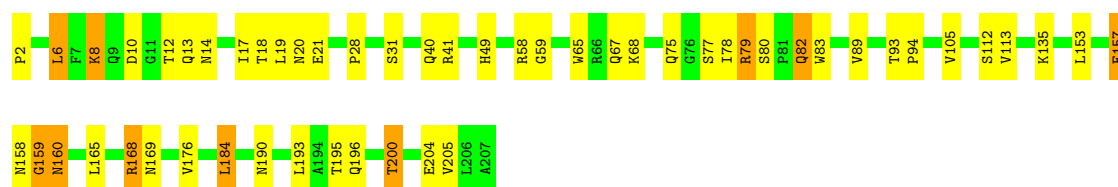
• Molecule 2: 5S rRNA



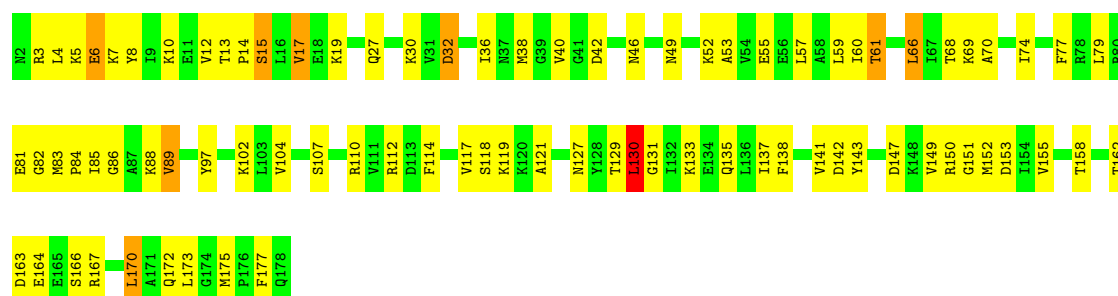
• Molecule 3: 50S ribosomal protein L3



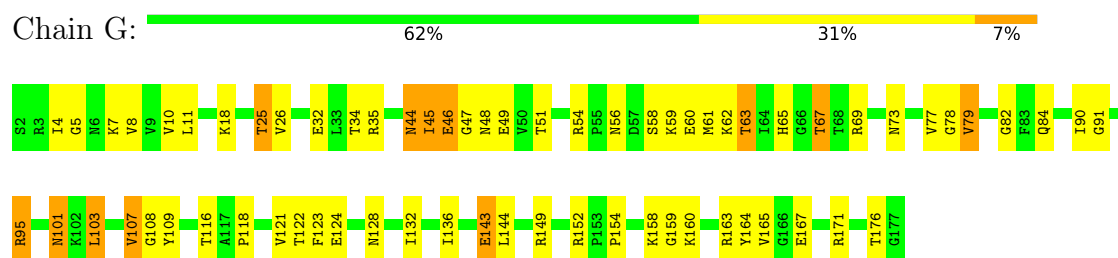
• Molecule 4: 50S ribosomal protein L4



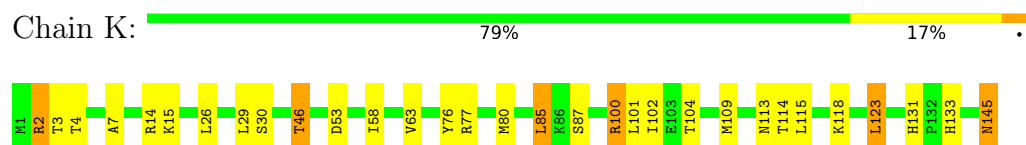
• Molecule 5: 50S ribosomal protein L5



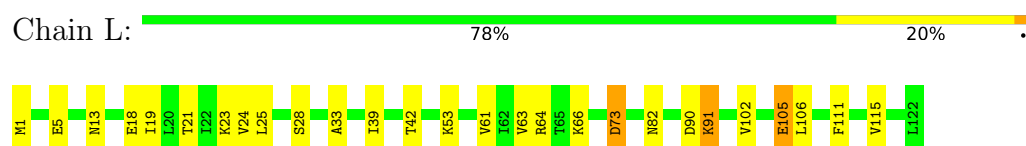
- Molecule 6: 50S ribosomal protein L6



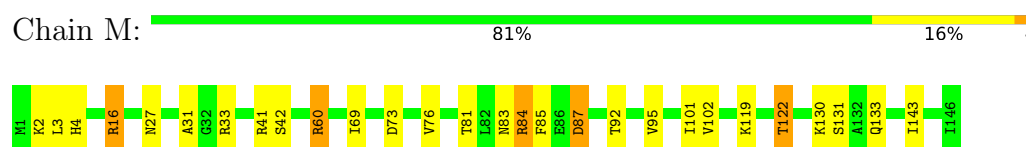
- Molecule 7: 50S ribosomal protein L13



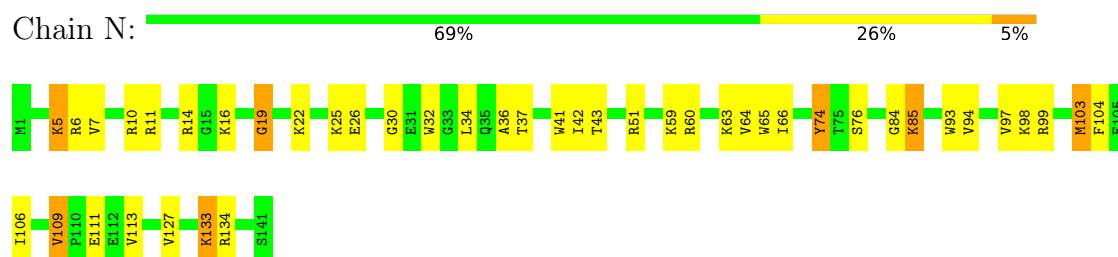
- Molecule 8: 50S ribosomal protein L14



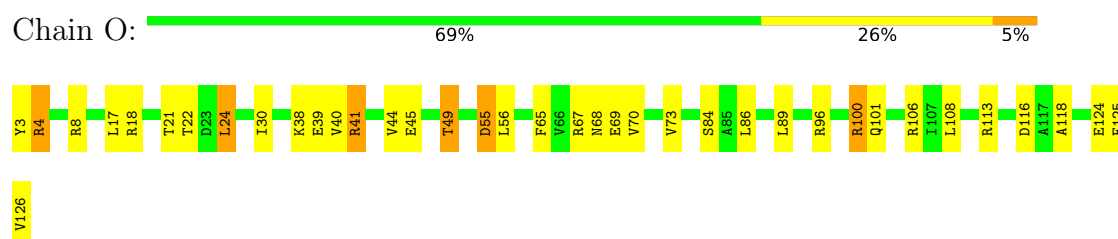
- Molecule 9: 50S ribosomal protein L15



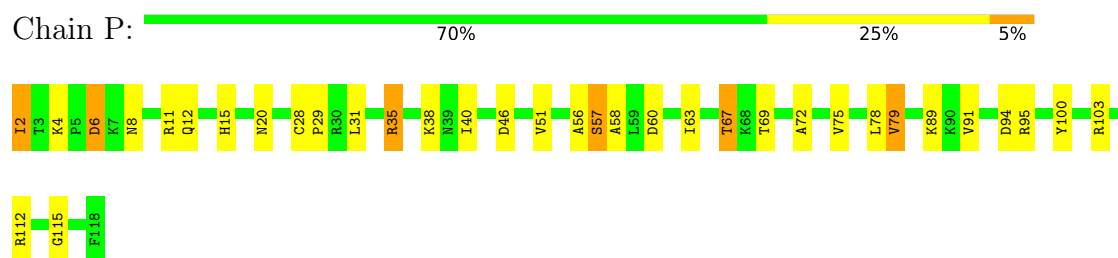
- Molecule 10: 50S ribosomal protein L16



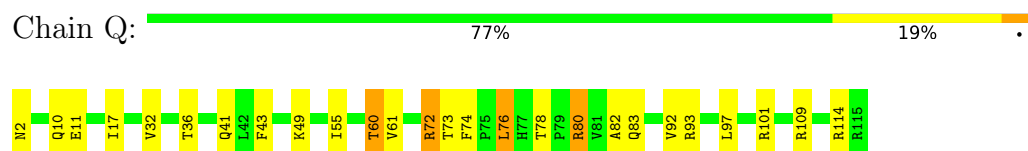
- Molecule 11: 50S ribosomal protein L17



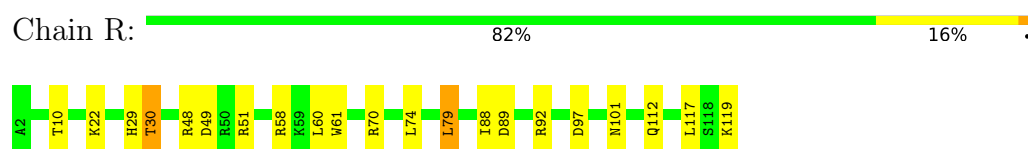
- Molecule 12: 50S ribosomal protein L18



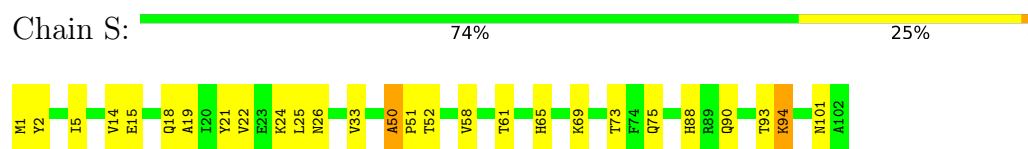
- Molecule 13: 50S ribosomal protein L19



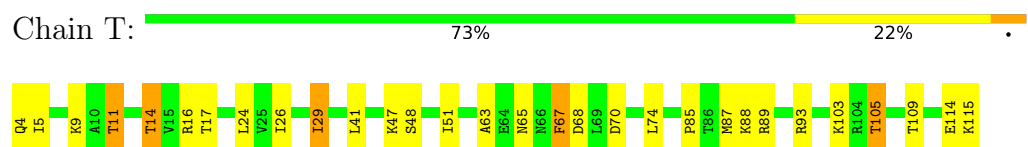
- Molecule 14: 50S ribosomal protein L20



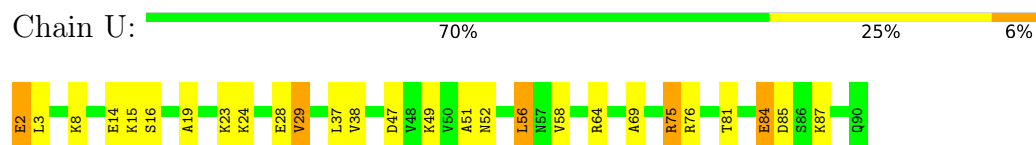
- Molecule 15: 50S ribosomal protein L21



- Molecule 16: 50S ribosomal protein L22



- Molecule 17: 50S ribosomal protein L23

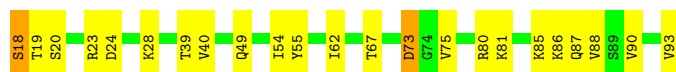


- Molecule 18: 50S ribosomal protein L24





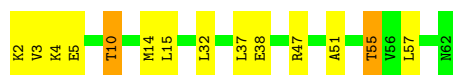
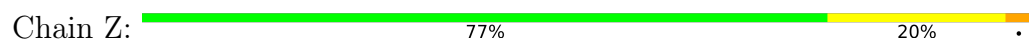
- Molecule 19: 50S ribosomal protein L27



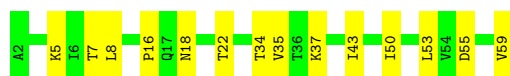
- Molecule 20: 50S ribosomal protein L28



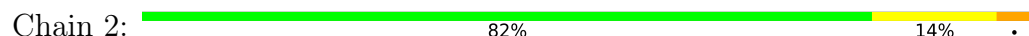
- Molecule 21: 50S ribosomal protein L29



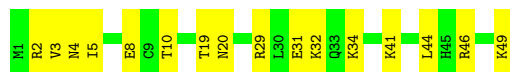
- Molecule 22: 50S ribosomal protein L30



- Molecule 23: 50S ribosomal protein L32



- Molecule 24: 50S ribosomal protein L33

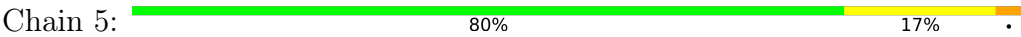


- Molecule 25: 50S ribosomal protein L34

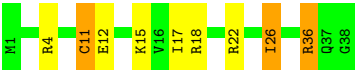




• Molecule 26: 50S ribosomal protein L35



• Molecule 27: 50S ribosomal protein L36



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	335675	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

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	1.21	32/65858 (0.0%)	1.30	435/102721 (0.4%)
2	B	0.97	1/2773 (0.0%)	1.23	23/4320 (0.5%)
3	D	0.54	0/1601	0.67	0/2150
4	E	0.52	0/1596	0.63	0/2159
5	F	0.36	0/1411	0.58	1/1897 (0.1%)
6	G	0.39	0/1365	0.57	0/1839
7	K	0.53	0/1151	0.68	2/1554 (0.1%)
8	L	0.51	0/929	0.65	1/1247 (0.1%)
9	M	0.52	1/1105 (0.1%)	0.64	0/1474
10	N	0.49	0/1141	0.61	0/1519
11	O	0.55	0/1000	0.71	1/1341 (0.1%)
12	P	0.47	0/908	0.64	0/1216
13	Q	0.56	0/938	0.63	0/1262
14	R	0.59	0/963	0.64	2/1280 (0.2%)
15	S	0.54	0/796	0.62	0/1068
16	T	0.49	0/858	0.64	1/1157 (0.1%)
17	U	0.50	0/727	0.65	1/972 (0.1%)
18	V	0.46	0/772	0.63	0/1035
19	X	0.56	0/578	0.61	0/773
20	Y	0.57	1/431 (0.2%)	0.60	0/574
21	Z	0.42	0/505	0.57	0/672
22	0	0.47	0/437	0.63	0/589
23	2	0.55	0/436	0.63	0/578
24	3	0.46	0/423	0.60	0/563
25	4	0.48	0/377	0.61	0/491
26	5	0.43	0/528	0.62	0/689
27	6	0.47	0/309	0.67	0/409
All	All	1.08	35/89916 (0.0%)	1.19	467/135549 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	D	0	1
10	N	0	2
11	O	0	2
15	S	0	1
16	T	0	1
18	V	0	1
All	All	0	8

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	903	G	C6-N1	-11.86	1.31	1.39
2	B	1	U	OP3-P	-10.45	1.48	1.61
1	A	769	G	N9-C4	-8.64	1.31	1.38
1	A	1492	G	N9-C4	-8.09	1.31	1.38
1	A	956	C	N3-C4	-7.24	1.28	1.33
1	A	2836	G	N9-C4	-7.18	1.32	1.38
20	Y	19	SER	CA-CB	-7.15	1.42	1.52
1	A	956	C	C4-N4	-7.06	1.27	1.33
9	M	60	ARG	C-N	-6.82	1.18	1.34
1	A	2444	A	N9-C4	-6.65	1.33	1.37
1	A	2044	A	N3-C4	-6.53	1.30	1.34
1	A	769	G	C2-N3	-6.40	1.27	1.32
1	A	1490	A	N9-C4	-6.38	1.34	1.37
1	A	769	G	N3-C4	-6.37	1.30	1.35
1	A	660	A	N9-C4	-6.22	1.34	1.37
1	A	660	A	N3-C4	-6.11	1.31	1.34
1	A	509	G	N9-C4	-5.91	1.33	1.38
1	A	1288	A	N3-C4	-5.89	1.31	1.34
1	A	2287	A	N3-C4	-5.86	1.31	1.34
1	A	903	G	C6-O6	-5.83	1.19	1.24
1	A	1571	G	N3-C4	-5.73	1.31	1.35
1	A	1337	A	N9-C4	-5.54	1.34	1.37
1	A	2606	G	C8-N7	-5.46	1.27	1.30
1	A	2007	U	C2-N3	-5.27	1.34	1.37
1	A	660	A	C5-C6	-5.26	1.36	1.41
1	A	2728	G	C8-N7	-5.21	1.27	1.30
1	A	539	G	N9-C4	-5.21	1.33	1.38
1	A	275	A	N9-C4	-5.18	1.34	1.37
1	A	2444	A	N3-C4	-5.18	1.31	1.34
1	A	903	G	C5-C6	-5.17	1.37	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1592	G	N9-C4	-5.13	1.33	1.38
1	A	1506	A	N9-C4	-5.11	1.34	1.37
1	A	2836	G	N3-C4	-5.08	1.31	1.35
1	A	1404	G	C6-N1	-5.07	1.36	1.39
1	A	2006	G	C8-N7	-5.00	1.27	1.30

All (467) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	956	C	N3-C4-N4	-30.89	96.38	118.00
1	A	956	C	C5-C4-N4	25.47	138.03	120.20
1	A	903	G	N1-C6-O6	-24.12	105.42	119.90
1	A	903	G	C5-C6-O6	22.01	141.81	128.60
1	A	1591	A	N1-C6-N6	-15.79	109.12	118.60
1	A	769	G	N3-C4-N9	-14.07	117.56	126.00
1	A	769	G	N3-C4-C5	13.80	135.50	128.60
1	A	1492	G	N3-C4-C5	13.01	135.10	128.60
1	A	2287	A	N7-C8-N9	12.67	120.14	113.80
1	A	769	G	C2-N3-C4	-12.50	105.65	111.90
1	A	1492	G	N3-C4-N9	-12.02	118.79	126.00
1	A	2287	A	C8-N9-C4	-10.74	101.50	105.80
2	B	85	U	C5-C6-N1	10.49	127.94	122.70
1	A	903	G	C4-C5-N7	10.31	114.92	110.80
1	A	2836	G	N3-C4-C5	10.05	133.62	128.60
1	A	2836	G	N3-C4-N9	-9.96	120.03	126.00
1	A	903	G	C4-N9-C1'	9.85	139.30	126.50
1	A	903	G	C8-N9-C1'	-9.71	114.38	127.00
1	A	956	C	C4-C5-C6	-9.64	112.58	117.40
1	A	1591	A	C2-N3-C4	9.62	115.41	110.60
1	A	2287	A	C5-N7-C8	-9.53	99.14	103.90
1	A	2420	C	O5'-P-OP2	-9.48	97.16	105.70
1	A	769	G	N3-C2-N2	-9.29	113.40	119.90
1	A	1505	C	N3-C2-O2	-9.22	115.44	121.90
1	A	956	C	N3-C4-C5	9.19	125.58	121.90
1	A	1592	G	N3-C4-C5	9.15	133.18	128.60
1	A	1551	U	C2-N1-C1'	9.11	128.63	117.70
1	A	903	G	N9-C4-C5	-9.05	101.78	105.40
1	A	1288	A	C2-N3-C4	-8.96	106.12	110.60
1	A	1167	A	C8-N9-C4	-8.94	102.22	105.80
1	A	2836	G	C5-N7-C8	-8.90	99.85	104.30
1	A	2454	C	O4'-C1'-N1	8.86	115.29	108.20
1	A	655	G	C8-N9-C4	8.84	109.94	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	551	G	O4'-C1'-N9	8.80	115.24	108.20
1	A	2287	A	C2-N3-C4	-8.56	106.32	110.60
1	A	2836	G	C2-N3-C4	-8.49	107.66	111.90
1	A	1592	G	N3-C4-N9	-8.33	121.00	126.00
1	A	1167	A	N7-C8-N9	8.25	117.92	113.80
1	A	509	G	C5-N7-C8	-8.17	100.21	104.30
1	A	1902	G	C8-N9-C4	-8.11	103.16	106.40
1	A	1571	G	N3-C2-N2	-8.08	114.24	119.90
1	A	2836	G	N7-C8-N9	7.98	117.09	113.10
1	A	344	G	C4-N9-C1'	7.97	136.86	126.50
1	A	1394	G	C4-C5-N7	7.96	113.98	110.80
1	A	1902	G	O4'-C1'-N9	7.82	114.46	108.20
1	A	208	G	O4'-C1'-N9	7.82	114.45	108.20
1	A	1434	C	C6-N1-C2	-7.81	117.18	120.30
1	A	2287	A	N1-C2-N3	7.81	133.20	129.30
1	A	1902	G	N7-C8-N9	7.80	117.00	113.10
1	A	1591	A	C5-C6-N6	7.78	129.92	123.70
1	A	660	A	N1-C6-N6	7.76	123.26	118.60
1	A	903	G	N3-C4-N9	7.75	130.65	126.00
1	A	344	G	N7-C8-N9	7.68	116.94	113.10
2	B	77	G	C4-C5-N7	7.60	113.84	110.80
1	A	711	C	C6-N1-C2	-7.56	117.28	120.30
2	B	96	G	C4-C5-N7	7.54	113.81	110.80
1	A	509	G	N7-C8-N9	7.48	116.84	113.10
1	A	275	A	N1-C2-N3	7.48	133.04	129.30
1	A	1492	G	C2-N3-C4	-7.47	108.16	111.90
1	A	1490	A	C2-N3-C4	-7.47	106.86	110.60
1	A	1497	U	N3-C2-O2	-7.46	116.97	122.20
1	A	586	A	N1-C6-N6	-7.44	114.14	118.60
1	A	769	G	C8-N9-C1'	7.38	136.59	127.00
1	A	2287	A	O4'-C1'-N9	7.37	114.09	108.20
1	A	992	G	C8-N9-C1'	-7.34	117.45	127.00
1	A	1175	C	C6-N1-C2	-7.34	117.37	120.30
1	A	1591	A	C6-C5-N7	7.31	137.42	132.30
1	A	2044	A	N7-C8-N9	7.29	117.45	113.80
1	A	1492	G	C4-N9-C1'	-7.24	117.08	126.50
2	B	96	G	C5-N7-C8	-7.23	100.69	104.30
1	A	235	G	N7-C8-N9	7.22	116.71	113.10
1	A	716	A	C2-N3-C4	-7.21	107.00	110.60
1	A	1489	C	C6-N1-C2	-7.20	117.42	120.30
1	A	2406	A	C2-N3-C4	-7.16	107.02	110.60
1	A	344	G	C6-C5-N7	-7.15	126.11	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2556	A	C8-N9-C4	-7.14	102.94	105.80
1	A	769	G	C4-N9-C1'	-7.13	117.23	126.50
1	A	951	A	O4'-C1'-N9	7.11	113.89	108.20
1	A	2226	A	C5-N7-C8	-7.08	100.36	103.90
1	A	235	G	C8-N9-C4	-7.07	103.57	106.40
1	A	1989	G	N7-C8-N9	7.07	116.63	113.10
1	A	1699	C	C6-N1-C2	-7.06	117.47	120.30
1	A	485	C	C6-N1-C2	-7.00	117.50	120.30
2	B	96	G	C6-C5-N7	-6.97	126.22	130.40
1	A	992	G	O4'-C1'-N9	6.97	113.77	108.20
1	A	1022	C	C2-N1-C1'	6.96	126.45	118.80
2	B	77	G	C5-N7-C8	-6.94	100.83	104.30
1	A	2226	A	N7-C8-N9	6.93	117.27	113.80
1	A	344	G	C8-N9-C1'	-6.93	118.00	127.00
1	A	1489	C	N3-C2-O2	-6.92	117.05	121.90
1	A	1994	G	N3-C4-C5	-6.89	125.15	128.60
2	B	77	G	N7-C8-N9	6.89	116.55	113.10
1	A	1505	C	C6-N1-C2	-6.89	117.55	120.30
1	A	1349	U	C2-N1-C1'	6.85	125.92	117.70
1	A	1394	G	C6-C5-N7	-6.80	126.32	130.40
1	A	1989	G	C4-C5-N7	6.79	113.52	110.80
1	A	903	G	C6-C5-N7	-6.75	126.35	130.40
1	A	509	G	C2-N3-C4	-6.74	108.53	111.90
2	B	77	G	C6-C5-N7	-6.74	126.36	130.40
1	A	344	G	C5-N7-C8	-6.72	100.94	104.30
1	A	509	G	N3-C4-C5	6.71	131.96	128.60
1	A	2441	C	C6-N1-C2	-6.70	117.62	120.30
1	A	903	G	C5-N7-C8	-6.67	100.96	104.30
2	B	96	G	N7-C8-N9	6.67	116.44	113.10
1	A	619	G	N3-C4-C5	-6.64	125.28	128.60
1	A	1492	G	C8-N9-C1'	6.62	135.61	127.00
1	A	298	U	O4'-C1'-N1	6.57	113.45	108.20
5	F	130	LEU	CA-CB-CG	6.56	130.39	115.30
1	A	1551	U	N1-C2-O2	6.54	127.38	122.80
1	A	1730	G	N3-C4-N9	6.54	129.93	126.00
1	A	1989	G	C5-N7-C8	-6.53	101.03	104.30
1	A	2044	A	C8-N9-C4	-6.53	103.19	105.80
1	A	2044	A	C5-N7-C8	-6.53	100.64	103.90
1	A	1234	C	C6-N1-C2	-6.51	117.70	120.30
1	A	1591	A	C5-C6-N1	6.50	120.95	117.70
1	A	2606	G	C4-N9-C1'	6.50	134.95	126.50
1	A	1713	C	C6-N1-C2	-6.50	117.70	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	725	A	C8-N9-C4	-6.49	103.21	105.80
1	A	509	G	N3-C4-N9	-6.48	122.11	126.00
1	A	344	G	C4-C5-N7	6.47	113.39	110.80
1	A	660	A	C5-N7-C8	-6.47	100.66	103.90
1	A	953	C	C6-N1-C2	-6.47	117.71	120.30
1	A	1229	G	N3-C4-N9	6.45	129.87	126.00
1	A	2588	G	C8-N9-C4	-6.44	103.82	106.40
1	A	344	G	O4'-C1'-N9	6.44	113.35	108.20
2	B	77	G	O4'-C1'-N9	6.43	113.34	108.20
1	A	1989	G	C6-C5-N7	-6.39	126.56	130.40
1	A	169	A	O4'-C1'-N9	6.39	113.31	108.20
1	A	2272	C	C6-N1-C2	-6.39	117.75	120.30
1	A	1996	U	C2-N1-C1'	6.37	125.35	117.70
2	B	68	C	C2-N1-C1'	6.37	125.81	118.80
1	A	1504	G	O4'-C1'-N9	6.37	113.30	108.20
1	A	1360	G	C8-N9-C4	-6.37	103.85	106.40
1	A	1551	U	C6-N1-C1'	-6.36	112.30	121.20
1	A	1388	U	N3-C2-O2	-6.33	117.77	122.20
1	A	275	A	C2-N3-C4	-6.33	107.44	110.60
1	A	583	U	C5-C4-O4	-6.33	122.10	125.90
1	A	776	C	C6-N1-C2	-6.33	117.77	120.30
1	A	331	A	O4'-C1'-N9	6.32	113.25	108.20
1	A	1364	G	C8-N9-C4	-6.31	103.88	106.40
1	A	992	G	C4-N9-C1'	6.30	134.69	126.50
1	A	2277	C	C6-N1-C2	-6.29	117.78	120.30
1	A	509	G	O4'-C1'-N9	6.28	113.22	108.20
1	A	2365	G	N3-C4-N9	6.27	129.76	126.00
1	A	1397	G	N3-C4-N9	6.25	129.75	126.00
1	A	28	G	O4'-C1'-N9	6.25	113.20	108.20
1	A	2241	A	C8-N9-C4	-6.24	103.30	105.80
1	A	905	G	N3-C4-C5	-6.22	125.49	128.60
1	A	1394	G	C5-N7-C8	-6.22	101.19	104.30
1	A	1493	C	C6-N1-C2	-6.21	117.82	120.30
1	A	261	C	C6-N1-C2	-6.21	117.82	120.30
1	A	2794	G	C4-N9-C1'	6.20	134.56	126.50
1	A	367	A	C5-N7-C8	-6.18	100.81	103.90
1	A	2226	A	C8-N9-C4	-6.17	103.33	105.80
1	A	1197	G	C4-N9-C1'	6.17	134.53	126.50
1	A	2039	C	C6-N1-C2	-6.17	117.83	120.30
1	A	235	G	O4'-C1'-N9	6.17	113.14	108.20
1	A	2049	G	N1-C6-O6	-6.16	116.20	119.90
1	A	1902	G	C5-N7-C8	-6.16	101.22	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	992	G	N3-C4-N9	6.15	129.69	126.00
1	A	716	A	C5-N7-C8	-6.12	100.84	103.90
1	A	655	G	N7-C8-N9	-6.11	110.05	113.10
1	A	2628	A	C8-N9-C4	-6.11	103.36	105.80
1	A	1350	C	C2-N1-C1'	6.10	125.51	118.80
1	A	2102	A	N1-C6-N6	-6.09	114.95	118.60
1	A	2296	G	N1-C6-O6	-6.08	116.25	119.90
1	A	1321	G	N1-C6-O6	-6.06	116.26	119.90
1	A	716	A	O4'-C1'-N9	6.06	113.05	108.20
1	A	1708	A	N1-C6-N6	-6.06	114.97	118.60
1	A	2834	A	N1-C6-N6	-6.05	114.97	118.60
1	A	1429	A	O4'-C1'-N9	6.04	113.04	108.20
1	A	1814	C	C6-N1-C2	-6.04	117.89	120.30
2	B	96	G	O4'-C1'-N9	6.03	113.03	108.20
1	A	1195	A	C8-N9-C4	-6.01	103.39	105.80
1	A	1490	A	C5-C6-N1	-6.00	114.70	117.70
1	A	155	U	O4'-C1'-N1	6.00	113.00	108.20
1	A	2588	G	N7-C8-N9	5.99	116.10	113.10
1	A	1591	A	N9-C4-C5	5.99	108.19	105.80
1	A	1487	U	O5'-P-OP2	-5.99	100.31	105.70
1	A	2062	G	N3-C4-N9	5.98	129.59	126.00
2	B	79	G	N7-C8-N9	5.98	116.09	113.10
2	B	96	G	C4-N9-C1'	5.98	134.27	126.50
1	A	235	G	C4-N9-C1'	5.97	134.26	126.50
1	A	2836	G	C8-N9-C4	-5.97	104.01	106.40
1	A	2606	G	C8-N9-C1'	-5.97	119.24	127.00
1	A	1800	A	O4'-C1'-N9	5.96	112.97	108.20
1	A	1571	G	N9-C4-C5	5.96	107.78	105.40
1	A	50	A	N1-C6-N6	-5.96	115.03	118.60
1	A	1506	A	C6-N1-C2	5.96	122.17	118.60
1	A	2367	G	N3-C4-C5	-5.96	125.62	128.60
1	A	262	G	N3-C4-N9	5.95	129.57	126.00
1	A	1804	C	C6-N1-C2	-5.95	117.92	120.30
1	A	2057	C	C2-N1-C1'	5.95	125.35	118.80
1	A	1490	A	C6-N1-C2	5.95	122.17	118.60
1	A	572	G	C2-N3-C4	5.94	114.87	111.90
1	A	712	C	C6-N1-C2	-5.94	117.92	120.30
1	A	360	G	C8-N9-C4	-5.93	104.03	106.40
1	A	903	G	N7-C8-N9	5.92	116.06	113.10
1	A	1337	A	C2-N3-C4	-5.92	107.64	110.60
1	A	2599	U	N3-C2-O2	-5.92	118.06	122.20
1	A	2602	G	C8-N9-C4	-5.90	104.04	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1288	A	C5-C6-N6	5.89	128.41	123.70
1	A	1989	G	O4'-C1'-N9	5.89	112.91	108.20
1	A	370	G	N3-C4-C5	-5.89	125.66	128.60
1	A	703	G	N1-C6-O6	-5.88	116.37	119.90
1	A	2307	C	C6-N1-C2	-5.88	117.95	120.30
1	A	1989	G	C2-N3-C4	-5.87	108.97	111.90
1	A	2809	U	C2-N1-C1'	5.87	124.74	117.70
1	A	1229	G	N3-C4-C5	-5.86	125.67	128.60
1	A	1224	G	N3-C4-N9	5.85	129.51	126.00
1	A	1011	C	C6-N1-C2	-5.83	117.97	120.30
1	A	654	A	O4'-C1'-N9	5.82	112.86	108.20
2	B	80	A	O4'-C1'-N9	5.81	112.85	108.20
16	T	24	LEU	CA-CB-CG	5.80	128.65	115.30
17	U	56	LEU	CA-CB-CG	5.80	128.64	115.30
1	A	509	G	C8-N9-C4	-5.79	104.08	106.40
1	A	2416	U	N3-C2-O2	-5.79	118.15	122.20
1	A	103	A	N7-C8-N9	5.79	116.69	113.80
1	A	1264	G	N3-C4-N9	5.79	129.47	126.00
1	A	1288	A	N1-C2-N3	5.78	132.19	129.30
1	A	886	U	N3-C2-O2	-5.78	118.16	122.20
1	A	396	C	C2-N1-C1'	5.78	125.16	118.80
1	A	990	G	C5-N7-C8	-5.78	101.41	104.30
1	A	2645	G	N1-C6-O6	-5.77	116.44	119.90
1	A	1885	C	N1-C2-O2	5.77	122.36	118.90
1	A	781	G	C8-N9-C4	-5.76	104.10	106.40
1	A	2365	G	C4-N9-C1'	5.76	133.98	126.50
1	A	1669	G	N1-C6-O6	-5.75	116.45	119.90
1	A	2049	G	C8-N9-C4	-5.75	104.10	106.40
1	A	1042	G	N1-C6-O6	-5.75	116.45	119.90
1	A	2287	A	C6-C5-N7	-5.73	128.29	132.30
1	A	2891	C	C6-N1-C2	-5.73	118.01	120.30
1	A	777	C	C6-N1-C2	-5.73	118.01	120.30
1	A	1012	G	N3-C4-N9	5.72	129.44	126.00
1	A	1471	G	N3-C4-N9	5.72	129.43	126.00
1	A	367	A	N7-C8-N9	5.72	116.66	113.80
1	A	2859	G	O4'-C1'-N9	5.72	112.77	108.20
1	A	1379	G	C4-N9-C1'	5.71	133.93	126.50
1	A	410	G	N3-C4-C5	-5.71	125.75	128.60
1	A	620	G	N3-C4-C5	-5.71	125.75	128.60
1	A	1337	A	N3-C4-N9	-5.71	122.83	127.40
1	A	1806	G	N1-C6-O6	-5.71	116.48	119.90
2	B	85	U	C4-C5-C6	-5.71	116.28	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	K	29	LEU	CA-CB-CG	5.71	128.42	115.30
1	A	103	A	C5-N7-C8	-5.70	101.05	103.90
1	A	248	G	N3-C4-N9	5.69	129.41	126.00
1	A	1492	G	O4'-C1'-N9	5.68	112.75	108.20
1	A	654	A	C8-N9-C4	5.68	108.07	105.80
1	A	817	G	N3-C4-C5	-5.68	125.76	128.60
1	A	823	A	N1-C6-N6	-5.68	115.19	118.60
1	A	367	A	C8-N9-C4	-5.67	103.53	105.80
1	A	2903	G	C2-N3-C4	-5.66	109.07	111.90
1	A	1604	A	P-O3'-C3'	5.66	126.49	119.70
1	A	35	U	C2-N1-C1'	5.65	124.48	117.70
1	A	18	G	N3-C4-N9	5.64	129.39	126.00
1	A	1996	U	N1-C2-O2	5.64	126.75	122.80
1	A	1434	C	C5-C6-N1	5.63	123.82	121.00
1	A	1197	G	C8-N9-C1'	-5.63	119.68	127.00
1	A	50	A	C5-C6-N6	5.62	128.20	123.70
1	A	2051	A	C2-N3-C4	5.62	113.41	110.60
1	A	655	G	C4-N9-C1'	-5.62	119.20	126.50
1	A	1551	U	C5-C6-N1	5.61	125.50	122.70
1	A	1337	A	N3-C4-C5	5.61	130.73	126.80
1	A	1717	G	N3-C4-C5	-5.61	125.80	128.60
1	A	1591	A	C4-C5-N7	-5.60	107.90	110.70
1	A	990	G	C4-C5-N7	5.60	113.04	110.80
1	A	644	U	N3-C2-O2	-5.60	118.28	122.20
14	R	117	LEU	CA-CB-CG	5.58	128.12	115.30
1	A	400	G	N3-C4-N9	5.57	129.34	126.00
1	A	904	A	O4'-C1'-N9	5.57	112.65	108.20
1	A	956	C	C5-C6-N1	5.56	123.78	121.00
1	A	2514	U	O4'-C1'-N1	5.56	112.65	108.20
1	A	2836	G	N3-C2-N2	-5.56	116.01	119.90
1	A	2537	G	N3-C4-N9	5.55	129.33	126.00
1	A	1717	G	C8-N9-C4	-5.55	104.18	106.40
1	A	1976	C	C6-N1-C2	-5.54	118.08	120.30
1	A	788	G	O4'-C1'-N9	5.54	112.63	108.20
1	A	1658	C	C6-N1-C2	-5.54	118.09	120.30
1	A	235	G	C5-N7-C8	-5.53	101.53	104.30
1	A	2613	G	N3-C4-C5	-5.53	125.83	128.60
1	A	2500	G	C8-N9-C4	-5.53	104.19	106.40
1	A	1397	G	C5-C6-O6	-5.53	125.28	128.60
1	A	2044	A	O4'-C1'-N9	5.53	112.62	108.20
1	A	963	C	C6-N1-C2	-5.52	118.09	120.30
1	A	2416	U	N1-C2-O2	5.52	126.66	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	222	A	C8-N9-C4	-5.51	103.60	105.80
1	A	1288	A	N3-C4-N9	-5.50	123.00	127.40
1	A	1605	C	P-O3'-C3'	5.50	126.30	119.70
1	A	905	G	N3-C4-N9	5.48	129.29	126.00
1	A	2455	C	N3-C2-O2	-5.48	118.06	121.90
1	A	769	G	C5-C6-N1	-5.47	108.77	111.50
1	A	619	G	N3-C4-N9	5.47	129.28	126.00
1	A	503	G	C6-C5-N7	5.46	133.68	130.40
1	A	1536	A	C8-N9-C4	-5.46	103.61	105.80
1	A	1996	U	N3-C2-O2	-5.46	118.38	122.20
1	A	1407	G	N1-C6-O6	-5.46	116.63	119.90
1	A	2287	A	C5-C6-N1	-5.45	114.97	117.70
1	A	1841	U	N3-C2-O2	-5.45	118.39	122.20
14	R	79	LEU	CA-CB-CG	5.44	127.82	115.30
1	A	47	C	C6-N1-C2	-5.43	118.13	120.30
1	A	494	A	N1-C6-N6	-5.43	115.34	118.60
1	A	2365	G	C8-N9-C1'	-5.42	119.95	127.00
1	A	2825	C	C6-N1-C2	-5.42	118.13	120.30
1	A	1571	G	N3-C4-N9	-5.42	122.75	126.00
1	A	2416	U	C2-N1-C1'	5.40	124.18	117.70
1	A	768	G	N3-C4-C5	-5.40	125.90	128.60
1	A	494	A	C5-C6-N6	5.39	128.02	123.70
1	A	2705	C	C6-N1-C2	-5.39	118.14	120.30
1	A	2728	G	C5-C6-O6	5.39	131.83	128.60
1	A	1950	A	N7-C8-N9	5.38	116.49	113.80
1	A	2903	G	N3-C4-C5	5.38	131.29	128.60
1	A	1203	G	C5-C6-N1	5.38	114.19	111.50
1	A	655	G	N3-C4-C5	5.38	131.29	128.60
1	A	1065	G	C8-N9-C4	-5.38	104.25	106.40
1	A	1394	G	O4'-C1'-N9	5.37	112.49	108.20
1	A	1989	G	C4-N9-C1'	5.37	133.48	126.50
1	A	2359	G	C8-N9-C4	-5.37	104.25	106.40
1	A	2639	G	N1-C6-O6	-5.37	116.68	119.90
2	B	77	G	C4-N9-C1'	5.36	133.47	126.50
1	A	229	A	C8-N9-C4	-5.36	103.66	105.80
1	A	2637	G	N3-C4-C5	-5.36	125.92	128.60
1	A	721	U	C6-N1-C2	-5.36	117.79	121.00
1	A	781	G	N3-C4-C5	-5.35	125.92	128.60
1	A	2084	G	N3-C4-C5	-5.35	125.92	128.60
1	A	2070	G	N3-C4-N9	5.35	129.21	126.00
1	A	2067	G	N3-C4-N9	5.35	129.21	126.00
1	A	549	C	C6-N1-C2	-5.35	118.16	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	80	A	N7-C8-N9	5.35	116.47	113.80
1	A	768	G	C8-N9-C4	-5.35	104.26	106.40
2	B	79	G	C8-N9-C4	-5.34	104.26	106.40
1	A	1994	G	C2-N3-C4	5.34	114.57	111.90
1	A	1490	A	N3-C4-C5	5.33	130.53	126.80
1	A	1673	A	N9-C4-C5	5.33	107.93	105.80
1	A	772	C	C6-N1-C2	-5.33	118.17	120.30
1	A	105	C	C6-N1-C2	-5.32	118.17	120.30
1	A	400	G	C4-N9-C1'	5.32	133.41	126.50
1	A	1216	G	C8-N9-C4	-5.32	104.27	106.40
1	A	2345	G	N1-C6-O6	-5.32	116.71	119.90
1	A	1644	G	N3-C4-N9	5.31	129.18	126.00
1	A	2405	G	O4'-C1'-N9	5.31	112.44	108.20
1	A	509	G	C4-C5-N7	5.30	112.92	110.80
1	A	1592	G	C2-N3-C4	-5.30	109.25	111.90
1	A	1776	A	O4'-C1'-N9	5.29	112.43	108.20
1	A	539	G	N3-C4-N9	-5.28	122.83	126.00
1	A	2794	G	C6-C5-N7	-5.28	127.23	130.40
1	A	400	G	C8-N9-C1'	-5.28	120.14	127.00
1	A	2067	G	N3-C4-C5	-5.27	125.96	128.60
1	A	1730	G	N3-C4-C5	-5.26	125.97	128.60
1	A	1288	A	N3-C4-C5	5.25	130.48	126.80
1	A	2073	A	O4'-C1'-N9	5.25	112.40	108.20
1	A	2062	G	N3-C4-C5	-5.25	125.97	128.60
1	A	179	A	N7-C8-N9	5.24	116.42	113.80
1	A	1978	G	N3-C4-C5	-5.24	125.98	128.60
1	A	807	U	O4'-C1'-N1	5.23	112.39	108.20
1	A	716	A	N7-C8-N9	5.23	116.41	113.80
1	A	2317	G	C4-N9-C1'	5.23	133.29	126.50
1	A	13	U	P-O3'-C3'	5.22	125.97	119.70
1	A	2360	A	N1-C6-N6	-5.22	115.47	118.60
1	A	347	A	O5'-P-OP1	-5.22	101.00	105.70
1	A	1491	U	O4'-C1'-N1	5.22	112.38	108.20
1	A	2208	C	C2-N1-C1'	5.22	124.54	118.80
1	A	367	A	C4-C5-N7	5.22	113.31	110.70
1	A	1203	G	N1-C6-O6	-5.21	116.78	119.90
1	A	1950	A	O4'-C1'-N9	5.21	112.37	108.20
1	A	1959	G	N3-C4-N9	5.21	129.12	126.00
1	A	992	G	N9-C1'-C2'	-5.21	106.27	112.00
1	A	1278	C	C6-N1-C2	-5.20	118.22	120.30
1	A	1431	A	C8-N9-C4	-5.20	103.72	105.80
1	A	660	A	C2-N3-C4	-5.20	108.00	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	521	G	N3-C4-C5	-5.20	126.00	128.60
1	A	2289	C	C6-N1-C2	-5.20	118.22	120.30
1	A	1360	G	O4'-C1'-N9	5.20	112.36	108.20
1	A	2794	G	C4-C5-N7	5.19	112.88	110.80
1	A	181	G	C2-N3-C4	5.19	114.50	111.90
1	A	460	G	N3-C4-C5	-5.18	126.01	128.60
1	A	907	A	C6-C5-N7	-5.18	128.67	132.30
1	A	1167	A	C6-C5-N7	-5.18	128.67	132.30
1	A	1349	U	N1-C2-O2	5.18	126.43	122.80
1	A	2592	G	N1-C6-O6	-5.18	116.79	119.90
1	A	660	A	N3-C4-C5	5.18	130.43	126.80
1	A	2020	C	C6-N1-C2	-5.18	118.23	120.30
1	A	1448	U	C5-C6-N1	5.18	125.29	122.70
1	A	2022	C	C6-N1-C2	-5.18	118.23	120.30
1	A	1193	C	C6-N1-C2	-5.17	118.23	120.30
1	A	1356	G	O4'-C1'-N9	5.17	112.33	108.20
1	A	181	G	C5-C6-N1	5.16	114.08	111.50
1	A	1397	G	N3-C4-C5	-5.16	126.02	128.60
1	A	1796	C	C6-N1-C2	-5.16	118.23	120.30
1	A	103	A	C8-N9-C4	-5.16	103.74	105.80
1	A	725	A	N9-C4-C5	5.16	107.86	105.80
1	A	460	G	C8-N9-C4	-5.15	104.34	106.40
2	B	80	A	C5-N7-C8	-5.15	101.32	103.90
1	A	990	G	N7-C8-N9	5.15	115.68	113.10
1	A	1590	A	P-O3'-C3'	5.15	125.88	119.70
1	A	2728	G	N1-C6-O6	-5.14	116.82	119.90
1	A	2057	C	C6-N1-C2	-5.13	118.25	120.30
1	A	2498	G	N3-C4-C5	-5.13	126.03	128.60
1	A	1074	G	N3-C4-C5	-5.13	126.03	128.60
1	A	2575	A	C5-C6-N1	5.13	120.27	117.70
8	L	91	LYS	C-N-CA	-5.13	108.88	121.70
1	A	2228	C	C6-N1-C2	-5.12	118.25	120.30
1	A	1431	A	N7-C8-N9	5.12	116.36	113.80
1	A	2794	G	N7-C8-N9	5.12	115.66	113.10
1	A	2794	G	C5-N7-C8	-5.12	101.74	104.30
1	A	1806	G	C5-C6-O6	5.11	131.67	128.60
1	A	451	G	N3-C4-C5	-5.11	126.05	128.60
1	A	1600	C	P-O3'-C3'	5.11	125.83	119.70
1	A	1730	G	C4-N9-C1'	5.10	133.14	126.50
1	A	468	A	O5'-P-OP2	-5.10	101.11	105.70
1	A	1491	U	N3-C2-O2	-5.10	118.63	122.20
1	A	1584	G	P-O3'-C3'	5.10	125.81	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1764	G	N1-C6-O6	-5.10	116.84	119.90
1	A	1011	C	C4-C5-C6	5.09	119.95	117.40
1	A	1571	G	N1-C2-N3	5.09	126.96	123.90
2	B	79	G	C5-N7-C8	-5.09	101.75	104.30
1	A	1645	U	O4'-C1'-N1	5.09	112.27	108.20
1	A	2322	G	C5-C6-O6	-5.09	125.55	128.60
1	A	2499	G	N1-C6-O6	-5.09	116.85	119.90
1	A	2556	A	N9-C4-C5	5.09	107.83	105.80
1	A	1216	G	N7-C8-N9	5.08	115.64	113.10
2	B	96	G	C8-N9-C1'	-5.08	120.40	127.00
1	A	644	U	N1-C2-N3	5.08	117.94	114.90
1	A	1645	U	N3-C2-O2	-5.08	118.65	122.20
1	A	568	A	N7-C8-N9	5.07	116.34	113.80
1	A	2596	G	C4-N9-C1'	5.07	133.09	126.50
1	A	2365	G	N3-C4-C5	-5.07	126.06	128.60
1	A	2521	C	N3-C2-O2	-5.07	118.35	121.90
1	A	2563	G	N3-C4-C5	-5.06	126.07	128.60
1	A	114	U	C2-N1-C1'	5.06	123.77	117.70
1	A	1364	G	N7-C8-N9	5.06	115.63	113.10
1	A	1605	C	O5'-P-OP1	-5.06	101.15	105.70
1	A	2628	A	N9-C4-C5	5.06	107.82	105.80
11	O	86	LEU	CA-CB-CG	5.06	126.93	115.30
1	A	1235	G	C2-N3-C4	5.05	114.43	111.90
1	A	2387	A	N1-C6-N6	-5.05	115.57	118.60
2	B	58	C	C2-N1-C1'	5.05	124.36	118.80
1	A	262	G	N3-C4-C5	-5.05	126.07	128.60
1	A	626	U	N3-C2-O2	-5.05	118.67	122.20
1	A	218	G	N3-C4-C5	-5.05	126.08	128.60
1	A	1022	C	C6-N1-C1'	-5.05	114.74	120.80
1	A	1505	C	N1-C2-O2	5.05	121.93	118.90
1	A	18	G	N3-C4-C5	-5.04	126.08	128.60
1	A	2722	G	C5-C6-O6	5.04	131.62	128.60
1	A	1167	A	C5-N7-C8	-5.04	101.38	103.90
1	A	25	G	C2-N3-C4	5.04	114.42	111.90
1	A	1730	G	C6-C5-N7	-5.04	127.38	130.40
1	A	2008	C	C6-N1-C2	-5.04	118.29	120.30
1	A	2041	G	C5-C6-N1	5.04	114.02	111.50
1	A	2317	G	N3-C4-N9	5.03	129.02	126.00
1	A	2794	G	C8-N9-C1'	-5.03	120.46	127.00
1	A	2632	G	N1-C6-O6	-5.03	116.88	119.90
1	A	2664	C	C6-N1-C2	-5.03	118.29	120.30
1	A	1293	G	C4-N9-C1'	5.02	133.03	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1786	G	N1-C6-O6	-5.02	116.89	119.90
1	A	1192	C	N3-C2-O2	-5.02	118.39	121.90
1	A	963	C	C2-N1-C1'	5.02	124.32	118.80
1	A	1717	G	C2-N3-C4	5.02	114.41	111.90
1	A	832	G	C8-N9-C4	-5.02	104.39	106.40
1	A	2444	A	N3-C4-N9	-5.01	123.39	127.40
1	A	1514	G	N1-C6-O6	-5.01	116.89	119.90
1	A	1959	G	N9-C4-C5	-5.01	103.39	105.40
1	A	2087	C	C6-N1-C2	-5.01	118.30	120.30
7	K	123	LEU	CA-CB-CG	5.01	126.82	115.30
1	A	561	G	N3-C4-N9	5.01	129.00	126.00
1	A	521	G	C5-C6-N1	5.00	114.00	111.50
1	A	905	G	N7-C8-N9	5.00	115.60	113.10
1	A	2371	U	C5-C6-N1	5.00	125.20	122.70

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	89	GLY	Peptide
10	N	16	LYS	Peptide
10	N	19	GLY	Peptide
11	O	4	ARG	Peptide
11	O	73	VAL	Peptide
15	S	50	ALA	Peptide
16	T	67	PHE	Peptide
18	V	87	ASP	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	58793	0	29547	404	0
2	B	2480	0	1249	42	0
3	D	1579	0	1661	31	0
4	E	1574	0	1621	28	0
5	F	1392	0	1454	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	G	1345	0	1375	36	0
7	K	1130	0	1169	16	0
8	L	922	0	985	14	0
9	M	1095	0	1148	15	0
10	N	1118	0	1180	25	0
11	O	991	0	1028	21	0
12	P	899	0	932	26	0
13	Q	924	0	979	9	0
14	R	950	0	1009	11	0
15	S	784	0	826	12	0
16	T	849	0	906	13	0
17	U	720	0	772	13	0
18	V	763	0	824	15	0
19	X	572	0	580	9	0
20	Y	425	0	460	4	0
21	Z	504	0	538	5	0
22	0	435	0	472	6	0
23	2	429	0	444	3	0
24	3	419	0	435	9	0
25	4	374	0	424	9	0
26	5	522	0	576	5	0
27	6	304	0	337	6	0
28	2	1	0	0	0	0
28	3	1	0	0	0	0
28	6	1	0	0	0	0
All	All	82295	0	52931	757	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (757) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1571:G:N2	1:A:1591:A:H62	1.58	1.01
1:A:275:A:H62	1:A:296:G:N2	1.67	0.93
1:A:1571:G:H22	1:A:1591:A:H62	0.94	0.92
1:A:1871:G:N2	1:A:1899:A:H62	1.69	0.91
1:A:1871:G:H21	1:A:1899:A:H62	0.92	0.90
1:A:2280:A:H62	1:A:2287:A:H2	1.19	0.86
1:A:1571:G:H22	1:A:1591:A:N6	1.73	0.85
10:N:51:ARG:HG3	10:N:66:ILE:HD11	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1004:C:HO2'	1:A:2287:A:H8	0.89	0.85
1:A:1871:G:H21	1:A:1899:A:N6	1.75	0.84
1:A:2704:A:N6	11:O:39:GLU:OE1	2.11	0.83
1:A:2406:A:H2	1:A:2438:C:H42	1.25	0.81
1:A:162:A:O2'	1:A:169:A:N6	2.14	0.81
1:A:500:A:H62	1:A:509:G:H8	1.28	0.81
12:P:6:ASP:OD1	12:P:6:ASP:N	2.09	0.81
6:G:44:ASN:ND2	6:G:51:THR:O	2.14	0.80
18:V:94:SER:OG	18:V:95:LYS:O	1.99	0.79
1:A:1868:A:H62	1:A:1902:G:H8	1.30	0.78
1:A:1004:C:O2'	1:A:2287:A:H8	1.67	0.78
6:G:54:ARG:NH1	6:G:56:ASN:OD1	2.17	0.78
1:A:904:A:HO2'	1:A:905:G:H8	1.31	0.77
1:A:347:A:O2'	1:A:348:A:H2'	1.85	0.77
1:A:1578:A:H2'	1:A:1579:U:C6	2.20	0.76
11:O:96:ARG:HH21	11:O:126:VAL:HG23	1.50	0.76
1:A:1151:A:H8	1:A:1152:G:H1'	1.49	0.76
5:F:40:VAL:HG12	5:F:42:ASP:H	1.49	0.76
1:A:85:A:O2'	1:A:100:A:N6	2.16	0.76
1:A:1488:G:O6	1:A:1508:G:O6	2.04	0.76
1:A:2454:C:O2'	1:A:2455:C:O5'	2.02	0.76
6:G:164:TYR:HB2	6:G:167:GLU:HG3	1.68	0.75
1:A:653:G:N1	1:A:655:G:OP2	2.19	0.74
1:A:287:G:N2	1:A:289:U:OP1	2.21	0.74
1:A:2348:G:O2'	12:P:20:ASN:ND2	2.21	0.73
1:A:84:G:H21	1:A:103:A:H2	1.34	0.73
5:F:36:ILE:HB	5:F:89:VAL:HG12	1.68	0.73
7:K:131:HIS:HD2	7:K:133:HIS:H	1.35	0.73
15:S:15:GLU:OE1	15:S:18:GLN:NE2	2.22	0.73
1:A:275:A:H62	1:A:296:G:H21	1.34	0.72
2:B:76:A:H62	2:B:96:G:H8	1.34	0.72
1:A:2811:U:H4'	1:A:2812:A:O5'	1.89	0.72
1:A:568:A:H2	1:A:2055:U:H3	1.37	0.72
1:A:716:A:H8	1:A:2083:G:H21	1.35	0.72
12:P:56:ALA:HB3	12:P:79:VAL:HG22	1.71	0.71
4:E:2:PRO:HD3	4:E:21:GLU:HG3	1.73	0.71
5:F:52:LYS:NZ	5:F:147:ASP:OD2	2.24	0.71
2:B:29:C:OP1	12:P:4:LYS:NZ	2.23	0.71
2:B:1:U:H3	2:B:115:G:H1	1.38	0.71
6:G:124:GLU:HB2	6:G:132:ILE:HB	1.71	0.71
1:A:951:A:O2'	1:A:952:A:N7	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:G:H1	25:4:37:LYS:HZ3	1.38	0.70
1:A:885:U:H2'	1:A:886:U:H4'	1.72	0.70
7:K:7:ALA:H	7:K:46:THR:HG21	1.55	0.70
1:A:2329:U:H2'	1:A:2330:U:C6	2.26	0.70
1:A:2673:G:OP2	6:G:158:LYS:NZ	2.22	0.70
1:A:2318:G:H22	1:A:2326:U:H3	1.38	0.70
13:Q:17:ILE:HD13	13:Q:76:LEU:HD22	1.72	0.70
1:A:899:G:OP2	19:X:86:LYS:NZ	2.24	0.69
1:A:2636:C:O2'	1:A:2836:G:N2	2.25	0.69
15:S:88:HIS:HE1	15:S:90:GLN:HG2	1.56	0.69
1:A:2856:A:H62	1:A:2882:G:H21	1.38	0.69
1:A:275:A:N6	1:A:296:G:H21	1.90	0.69
1:A:1756:U:O2'	1:A:1760:G:N2	2.25	0.69
3:D:123:ILE:HD12	3:D:141:ARG:HG3	1.75	0.69
2:B:78:U:H2'	2:B:79:G:H21	1.57	0.68
1:A:1629:A:H3'	1:A:1630:G:H5''	1.75	0.68
16:T:48:SER:HA	16:T:51:ILE:HD12	1.76	0.68
3:D:125:ARG:HG3	3:D:164:MET:HG3	1.76	0.68
4:E:10:ASP:OD1	4:E:10:ASP:N	2.23	0.68
2:B:97:A:O2'	2:B:98:G:OP1	2.10	0.68
5:F:130:LEU:HD13	5:F:131:GLY:H	1.58	0.67
5:F:170:LEU:HD22	5:F:175:MET:HG3	1.76	0.67
1:A:1504:G:O2'	1:A:1505:C:OP2	2.12	0.67
2:B:70:G:H8	2:B:102:A:H62	1.41	0.67
1:A:337:A:OP2	18:V:95:LYS:NZ	2.28	0.67
1:A:13:U:O2'	1:A:14:A:OP1	2.10	0.67
1:A:232:U:O2'	1:A:233:U:O5'	2.13	0.67
17:U:23:LYS:NZ	17:U:84:GLU:HA	2.10	0.67
17:U:29:VAL:HG21	17:U:38:VAL:HG22	1.78	0.66
24:3:31:GLU:HG2	24:3:46:ARG:HG2	1.77	0.66
1:A:154:U:HO2'	1:A:155:U:H6	1.41	0.66
1:A:1216:G:OP2	1:A:1217:G:N2	2.29	0.66
4:E:78:ILE:HG22	4:E:79:ARG:HD2	1.76	0.66
5:F:6:GLU:O	5:F:10:LYS:HB2	1.95	0.66
1:A:2328:A:H2'	1:A:2329:U:C6	2.30	0.66
1:A:533:G:H4'	16:T:11:THR:HG23	1.78	0.65
8:L:73:ASP:OD1	8:L:73:ASP:N	2.27	0.65
19:X:81:LYS:HB2	19:X:87:GLN:HG3	1.78	0.65
1:A:654:A:H1'	1:A:655:G:H2'	1.76	0.65
1:A:1585:U:H2'	1:A:1586:A:C8	2.32	0.65
1:A:1576:A:N1	1:A:1578:A:N6	2.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:6:17:ILE:HG22	27:6:18:ARG:H	1.61	0.65
1:A:1630:G:H1'	1:A:1631:A:C5	2.32	0.65
19:X:55:TYR:HE1	19:X:85:LYS:HD3	1.61	0.65
1:A:1167:A:C8	1:A:2532:A:H5''	2.33	0.64
1:A:2342:A:H2'	1:A:2343:A:C8	2.32	0.64
4:E:8:LYS:HD3	4:E:14:ASN:HD22	1.63	0.64
1:A:2453:A:H4'	1:A:2454:C:H3'	1.78	0.64
1:A:2520:U:H3	1:A:2597:G:H1	1.46	0.64
9:M:85:PHE:O	9:M:119:LYS:NZ	2.31	0.64
1:A:1216:G:H3'	1:A:1217:G:H5''	1.78	0.64
1:A:904:A:O2'	1:A:905:G:H8	1.80	0.64
1:A:623:A:H62	1:A:1288:A:H2	1.46	0.64
7:K:4:THR:HG21	14:R:61:TRP:HE1	1.62	0.64
1:A:508:G:H2'	1:A:509:G:H5'	1.80	0.63
1:A:1535:U:O2'	1:A:1536:A:OP1	2.14	0.63
1:A:1178:G:H21	7:K:109:MET:HE3	1.63	0.63
1:A:1074:G:O4'	27:6:18:ARG:NH1	2.31	0.63
18:V:97:THR:OG1	18:V:99:GLU:OE2	2.16	0.63
1:A:853:U:H2'	1:A:854:C:C6	2.34	0.63
1:A:1860:G:H2'	1:A:1861:A:C8	2.34	0.63
26:5:10:LEU:HB3	26:5:62:LEU:HD21	1.81	0.63
1:A:359:A:OP1	4:E:168:ARG:NH1	2.32	0.62
4:E:59:GLY:HA3	4:E:79:ARG:HD3	1.79	0.62
15:S:24:LYS:HA	15:S:93:THR:HG23	1.81	0.62
1:A:2333:A:H4'	1:A:2334:A:H5'	1.82	0.62
19:X:49:GLN:HE22	19:X:54:ILE:H	1.45	0.62
1:A:1570:G:H22	1:A:1592:G:H1	1.47	0.62
2:B:70:G:H8	2:B:102:A:N6	1.96	0.62
5:F:12:VAL:HG22	5:F:172:GLN:HG2	1.81	0.62
1:A:500:A:N6	1:A:509:G:H8	1.95	0.62
2:B:57:G:O2'	12:P:6:ASP:OD2	2.18	0.62
6:G:25:THR:HB	6:G:34:THR:HG22	1.82	0.62
10:N:43:THR:HG22	10:N:94:VAL:HG12	1.82	0.61
1:A:285:U:O2'	1:A:287:G:OP1	2.17	0.61
16:T:5:ILE:HD11	16:T:67:PHE:CG	2.35	0.61
1:A:539:G:N1	1:A:542:A:OP2	2.30	0.61
1:A:2280:A:N6	1:A:2287:A:H2	1.95	0.61
1:A:2329:U:H2'	1:A:2330:U:H6	1.65	0.61
1:A:2207:C:H2'	1:A:2208:C:O4'	2.00	0.61
1:A:2517:A:O2'	1:A:2519:G:OP2	2.18	0.61
1:A:891:A:O2'	22:0:22:THR:HG22	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1310:A:O2'	1:A:1689:A:N6	2.34	0.61
10:N:19:GLY:HA2	10:N:98:LYS:HD2	1.81	0.61
11:O:55:ASP:OD1	11:O:55:ASP:N	2.31	0.61
1:A:1194:G:OP2	14:R:58:ARG:NH1	2.34	0.61
1:A:626:U:H2'	1:A:627:A:H8	1.66	0.60
2:B:76:A:N6	2:B:96:G:H8	1.98	0.60
1:A:1994:G:O2'	1:A:1996:U:OP2	2.19	0.60
1:A:2514:U:O2	1:A:2518:U:N3	2.35	0.60
1:A:2771:A:N1	6:G:67:THR:HG21	2.15	0.60
1:A:1724:G:H21	1:A:1776:A:H3'	1.67	0.60
1:A:1756:U:O4	1:A:1758:C:H5''	2.01	0.60
1:A:626:U:H2'	1:A:627:A:C8	2.37	0.60
3:D:55:ASP:OD1	3:D:77:LYS:NZ	2.26	0.60
8:L:24:VAL:HG13	8:L:33:ALA:HB2	1.83	0.60
12:P:40:ILE:HD11	12:P:72:ALA:HA	1.82	0.60
14:R:97:ASP:OD1	14:R:101:ASN:ND2	2.35	0.60
1:A:1494:G:H1	1:A:1504:G:H21	1.50	0.60
5:F:166:SER:O	5:F:170:LEU:HB2	2.01	0.60
6:G:58:SER:O	6:G:61:MET:HG2	2.02	0.60
1:A:285:U:H2'	1:A:287:G:H8	1.66	0.59
7:K:63:VAL:HG21	7:K:102:ILE:HD11	1.83	0.59
1:A:262:G:H21	1:A:660:A:H8	1.51	0.59
1:A:2328:A:H2'	1:A:2329:U:H6	1.65	0.59
1:A:225:A:H62	1:A:235:G:H8	1.49	0.59
1:A:1323:A:H8	11:O:113:ARG:HD3	1.67	0.59
1:A:2341:A:H2'	1:A:2342:A:C8	2.36	0.59
10:N:41:TRP:HZ3	10:N:74:TYR:CE1	2.21	0.59
16:T:17:THR:HG22	16:T:47:LYS:HE3	1.84	0.59
21:Z:51:ALA:O	21:Z:55:THR:HG22	2.03	0.59
1:A:92:A:H2'	1:A:93:G:H5'	1.82	0.59
1:A:585:A:H4'	1:A:586:A:H5'	1.84	0.59
1:A:2810:U:C2	1:A:2811:U:H5	2.20	0.59
1:A:2758:G:N2	6:G:143:GLU:OE2	2.36	0.59
1:A:2361:C:OP1	24:3:34:LYS:NZ	2.34	0.58
1:A:2461:G:N2	1:A:2464:A:OP2	2.35	0.58
1:A:2856:A:H62	1:A:2882:G:N2	2.01	0.58
19:X:73:ASP:OD1	19:X:73:ASP:N	2.34	0.58
22:O:50:ILE:HG23	22:O:53:LEU:HD12	1.85	0.58
1:A:77:C:O2'	21:Z:55:THR:HG21	2.04	0.58
1:A:1376:U:OP1	17:U:15:LYS:NZ	2.37	0.58
1:A:1408:U:HO2'	1:A:2226:A:H8	1.49	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2454:C:HO2'	1:A:2455:C:P	2.27	0.58
1:A:1208:C:H2'	1:A:1209:A:C8	2.39	0.58
1:A:1861:A:O2'	1:A:1862:A:H8	1.87	0.58
12:P:15:HIS:HE1	12:P:94:ASP:OD2	1.87	0.58
7:K:145:ASN:OD1	7:K:145:ASN:N	2.36	0.58
1:A:586:A:O2'	1:A:587:U:H5''	2.04	0.58
5:F:53:ALA:HB2	5:F:150:ARG:HH12	1.68	0.58
6:G:4:ILE:O	6:G:69:ARG:HD3	2.04	0.58
24:3:29:ARG:NH1	24:3:49:LYS:HB2	2.19	0.58
5:F:42:ASP:O	5:F:49:ASN:ND2	2.37	0.57
19:X:55:TYR:CE1	19:X:85:LYS:HD3	2.38	0.57
5:F:38:MET:HE3	5:F:150:ARG:HH11	1.68	0.57
12:P:100:TYR:OH	12:P:112:ARG:NH2	2.37	0.57
1:A:1490:A:C2'	1:A:1491:U:H5'	2.34	0.57
1:A:607:G:H2'	1:A:2044:A:C2	2.40	0.57
12:P:40:ILE:H	12:P:58:ALA:HB2	1.69	0.57
3:D:9:LYS:HB2	3:D:200:ILE:HD11	1.86	0.57
5:F:46:ASN:O	5:F:49:ASN:ND2	2.37	0.57
25:4:34:ARG:NH1	25:4:41:VAL:O	2.37	0.57
1:A:1458:G:H1	1:A:1628:G:H21	1.53	0.57
9:M:101:ILE:HG22	9:M:102:VAL:HG23	1.85	0.57
1:A:1086:A:H2'	1:A:1086:A:N3	2.19	0.56
1:A:1585:U:H2'	1:A:1586:A:H8	1.69	0.56
15:S:50:ALA:O	15:S:52:THR:N	2.37	0.56
1:A:1633:A:O2'	1:A:1634:A:H5''	2.05	0.56
1:A:1793:U:H5	1:A:1798:A:N7	2.03	0.56
1:A:2219:A:H2'	1:A:2220:C:C6	2.41	0.56
10:N:41:TRP:HZ3	10:N:74:TYR:HE1	1.53	0.56
1:A:951:A:O2'	1:A:952:A:C8	2.56	0.56
1:A:905:G:H21	1:A:907:A:N6	2.03	0.56
1:A:160:U:H2'	1:A:161:G:O4'	2.06	0.56
1:A:2204:A:H2'	1:A:2205:A:C8	2.41	0.56
10:N:42:ILE:HD12	10:N:97:VAL:HG21	1.87	0.56
1:A:2085:A:H2'	1:A:2086:G:C8	2.41	0.56
5:F:138:PHE:HB2	5:F:141:VAL:HG23	1.88	0.56
8:L:63:VAL:HG11	8:L:102:VAL:HG22	1.88	0.56
1:A:344:G:H8	1:A:367:A:H61	1.53	0.55
1:A:916:A:H2'	1:A:917:C:O4'	2.07	0.55
1:A:1422:C:H2'	1:A:1423:A:C8	2.41	0.55
1:A:1571:G:N2	1:A:1591:A:N6	2.41	0.55
4:E:67:GLN:HG3	4:E:68:LYS:HG3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:158:ASN:O	4:E:160:ASN:N	2.33	0.55
6:G:95:ARG:HB3	6:G:128:ASN:HB3	1.87	0.55
1:A:2444:A:HO2'	1:A:2445:U:H6	1.54	0.55
1:A:1490:A:N1	1:A:1506:A:N1	2.54	0.55
1:A:1178:G:H21	7:K:109:MET:CE	2.19	0.55
5:F:129:THR:HG22	5:F:155:VAL:HG22	1.88	0.55
15:S:5:ILE:HD11	15:S:58:VAL:HG21	1.88	0.55
1:A:391:C:O2'	1:A:392:A:O5'	2.24	0.55
1:A:234:C:O2'	1:A:235:G:O4'	2.24	0.55
1:A:1583:A:N3	1:A:1583:A:H2'	2.20	0.55
5:F:60:ILE:HG22	5:F:61:THR:HG23	1.89	0.55
17:U:64:ARG:HG3	17:U:69:ALA:HB2	1.88	0.55
1:A:151:A:H61	1:A:179:A:H2	1.54	0.55
1:A:311:A:O2'	1:A:399:A:N1	2.39	0.55
1:A:1931:U:H2'	1:A:1932:A:O4'	2.07	0.55
6:G:26:VAL:HG12	6:G:79:VAL:HG11	1.88	0.55
1:A:367:A:H2	1:A:1247:U:HO2'	1.55	0.55
1:A:1394:G:H8	1:A:1409:A:H62	1.54	0.55
1:A:275:A:N6	1:A:296:G:N2	2.44	0.54
1:A:1208:C:H2'	1:A:1209:A:H8	1.72	0.54
3:D:89:GLY:O	3:D:91:TYR:N	2.40	0.54
1:A:2482:A:HO2'	1:A:2483:A:H8	1.55	0.54
2:B:68:C:H5	2:B:104:G:H22	1.56	0.54
1:A:2860:G:OP1	13:Q:93:ARG:NH1	2.40	0.54
2:B:39:G:OP1	2:B:41:C:N4	2.40	0.54
24:3:3:VAL:HG12	24:3:4:ASN:O	2.07	0.54
1:A:883:A:H2'	1:A:884:A:C8	2.43	0.54
1:A:1151:A:C8	1:A:1152:G:H1'	2.37	0.54
10:N:85:LYS:HG2	19:X:18:SER:N	2.22	0.54
1:A:950:A:H2'	1:A:953:C:C5	2.42	0.54
1:A:508:G:C2'	1:A:509:G:H5'	2.38	0.54
5:F:119:LYS:HB3	5:F:167:ARG:NH2	2.23	0.54
18:V:84:LYS:HB2	18:V:93:VAL:HG21	1.88	0.54
1:A:313:A:H2'	1:A:314:U:O4'	2.08	0.54
11:O:100:ARG:HG3	11:O:101:GLN:O	2.08	0.54
1:A:509:G:H1	25:4:37:LYS:NZ	2.06	0.54
5:F:5:LYS:HE3	5:F:97:TYR:HE2	1.73	0.54
8:L:102:VAL:HG13	8:L:106:LEU:HD12	1.90	0.53
1:A:1081:U:H2'	1:A:1082:G:H8	1.73	0.53
1:A:285:U:H2'	1:A:287:G:C8	2.43	0.53
1:A:1754:A:H2'	1:A:1755:C:O4'	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:P:75:VAL:O	12:P:79:VAL:HG23	2.09	0.53
1:A:904:A:H2'	10:N:22:LYS:HE3	1.89	0.53
1:A:1591:A:H2'	1:A:1592:G:C8	2.43	0.53
2:B:68:C:H5	2:B:104:G:H1	1.55	0.53
22:O:37:LYS:HB3	22:O:43:ILE:HD13	1.89	0.53
1:A:1202:G:O3'	15:S:24:LYS:NZ	2.42	0.53
1:A:2712:U:H2'	1:A:2713:U:C6	2.43	0.53
9:M:84:ARG:HH21	9:M:101:ILE:HD11	1.74	0.53
22:O:18:ASN:O	22:O:22:THR:HG23	2.09	0.53
1:A:1631:A:C4	1:A:1632:A:H2	2.27	0.53
1:A:118:A:OP2	1:A:119:A:H5''	2.09	0.53
16:T:16:ARG:NH1	16:T:103:LYS:HD3	2.23	0.53
18:V:87:ASP:O	18:V:89:LYS:N	2.36	0.53
1:A:292:U:H2'	1:A:293:U:C6	2.44	0.53
16:T:16:ARG:HH11	16:T:103:LYS:HD3	1.74	0.53
3:D:13:THR:OG1	3:D:14:GLN:N	2.42	0.53
17:U:23:LYS:HZ1	17:U:84:GLU:HA	1.73	0.53
1:A:1310:A:HO2'	1:A:1689:A:N6	2.07	0.52
1:A:2836:G:O5'	1:A:2836:G:H8	1.91	0.52
2:B:40:C:C5	5:F:66:LEU:HG	2.44	0.52
22:O:7:THR:HB	22:O:34:THR:HG22	1.90	0.52
25:4:8:ASN:HD22	25:4:11:LYS:H	1.57	0.52
1:A:2111:G:H2'	1:A:2112:U:C6	2.44	0.52
12:P:69:THR:HG22	12:P:103:ARG:HB3	1.91	0.52
1:A:899:G:N3	1:A:2282:A:H2'	2.24	0.52
1:A:2323:A:OP1	1:A:2323:A:H8	1.92	0.52
12:P:8:ASN:O	12:P:12:GLN:HG2	2.08	0.52
2:B:86:U:H4'	2:B:87:U:H5	1.74	0.52
8:L:28:SER:O	8:L:28:SER:OG	2.24	0.52
1:A:181:G:H2'	1:A:182:U:O4'	2.10	0.52
1:A:498:G:O6	4:E:58:ARG:HD3	2.08	0.52
1:A:1758:C:H2'	1:A:1759:G:C8	2.45	0.52
1:A:1872:G:H1'	1:A:1898:A:N6	2.23	0.52
2:B:48:A:OP1	12:P:69:THR:N	2.42	0.52
1:A:943:U:H2'	1:A:944:U:C6	2.45	0.52
1:A:945:C:H2'	1:A:946:A:O4'	2.10	0.52
5:F:40:VAL:HB	5:F:85:ILE:O	2.10	0.52
13:Q:60:THR:HB	13:Q:73:THR:HG22	1.92	0.52
1:A:1451:U:O2'	1:A:1452:G:OP2	2.27	0.52
3:D:107:VAL:HG23	3:D:173:ASN:HA	1.92	0.52
10:N:32:TRP:CZ3	10:N:133:LYS:HG2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:O:40:VAL:O	11:O:44:VAL:HG23	2.10	0.52
1:A:678:U:H2'	1:A:679:C:C6	2.45	0.51
1:A:1212:A:HO2'	1:A:1213:U:H6	1.53	0.51
1:A:1591:A:H3'	1:A:1591:A:N3	2.25	0.51
1:A:203:U:H4'	20:Y:22:MET:HB3	1.92	0.51
27:6:36:ARG:O	27:6:36:ARG:HG3	2.10	0.51
1:A:1330:C:H5'	11:O:69:GLU:O	2.09	0.51
6:G:103:LEU:HB2	6:G:123:PHE:CE2	2.46	0.51
17:U:58:VAL:HB	17:U:75:ARG:HB2	1.91	0.51
1:A:282:A:H2'	1:A:283:G:H8	1.74	0.51
1:A:1301:G:OP1	23:2:16:ARG:NH2	2.28	0.51
1:A:1867:A:H2'	1:A:1868:A:C8	2.46	0.51
6:G:10:VAL:HG22	6:G:49:GLU:HG3	1.93	0.51
2:B:50:A:C6	12:P:38:LYS:HE2	2.45	0.51
1:A:1491:U:O2'	1:A:1492:G:C8	2.59	0.51
1:A:92:A:C2'	1:A:93:G:H5'	2.41	0.51
1:A:154:U:O2'	1:A:155:U:H6	1.93	0.51
3:D:108:VAL:HG22	3:D:203:LYS:O	2.11	0.51
4:E:75:GLN:NE2	4:E:83:TRP:HE1	2.08	0.51
10:N:7:VAL:HG11	10:N:93:TRP:HH2	1.76	0.51
1:A:288:C:HO2'	1:A:289:U:H5	1.59	0.51
1:A:2481:C:H2'	1:A:2482:A:O4'	2.08	0.51
1:A:2672:C:H5''	6:G:158:LYS:HZ2	1.75	0.51
1:A:1046:C:H1'	7:K:109:MET:HE3	1.92	0.51
1:A:1572:A:H62	1:A:1589:G:H8	1.58	0.51
1:A:1593:U:H2'	1:A:1594:U:C6	2.46	0.51
1:A:2035:G:H2'	1:A:2035:G:N3	2.26	0.51
1:A:306:C:H2'	1:A:307:U:C6	2.45	0.50
1:A:2637:G:O5'	1:A:2836:G:N2	2.44	0.50
3:D:34:VAL:HG11	3:D:74:THR:HG21	1.93	0.50
10:N:109:VAL:HG13	10:N:113:VAL:HB	1.93	0.50
18:V:70:VAL:HG11	18:V:92:ARG:HH12	1.76	0.50
1:A:179:A:O3'	1:A:180:G:H8	1.94	0.50
1:A:1872:G:H1'	1:A:1898:A:H61	1.75	0.50
27:6:17:ILE:HD12	27:6:26:ILE:HD12	1.94	0.50
1:A:991:C:H2'	1:A:992:G:H5'	1.92	0.50
1:A:1206:U:H2'	1:A:1207:A:C8	2.46	0.50
2:B:39:G:P	2:B:41:C:H41	2.33	0.50
6:G:18:LYS:HB2	6:G:25:THR:HG23	1.93	0.50
1:A:1167:A:H8	1:A:2532:A:H5''	1.76	0.50
1:A:650:G:N2	1:A:654:A:H5'	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1816:A:H2'	1:A:1817:A:C8	2.46	0.50
1:A:2044:A:C8	1:A:2513:C:H5''	2.47	0.50
2:B:72:U:C2'	2:B:73:U:H5'	2.42	0.50
1:A:161:G:H2'	1:A:162:A:N3	2.26	0.50
1:A:454:C:H2'	1:A:455:A:C8	2.47	0.50
1:A:573:U:O2'	14:R:49:ASP:OD2	2.28	0.50
21:Z:14:MET:HG3	21:Z:57:LEU:HD21	1.94	0.50
1:A:897:G:H2'	1:A:898:A:C8	2.47	0.50
17:U:51:ALA:O	17:U:81:THR:HB	2.12	0.50
1:A:1207:A:H2'	1:A:1208:C:C6	2.47	0.49
1:A:2475:C:H2'	1:A:2476:U:C6	2.46	0.49
1:A:1399:C:O2'	1:A:1823:A:N3	2.40	0.49
10:N:59:LYS:O	10:N:60:ARG:HB2	2.13	0.49
11:O:17:LEU:O	11:O:21:THR:HG23	2.12	0.49
1:A:509:G:H22	25:4:37:LYS:HZ1	1.61	0.49
1:A:653:G:H2'	1:A:654:A:H5''	1.93	0.49
1:A:943:U:H2'	1:A:944:U:H6	1.77	0.49
1:A:1537:A:N3	1:A:1624:U:O2'	2.43	0.49
1:A:1624:U:OP2	1:A:1624:U:H6	1.96	0.49
1:A:1872:G:O2'	1:A:1898:A:N6	2.46	0.49
10:N:36:ALA:HB2	10:N:103:MET:SD	2.53	0.49
27:6:22:ARG:HH11	27:6:36:ARG:HD3	1.77	0.49
5:F:8:TYR:CE1	5:F:173:LEU:HD21	2.47	0.49
14:R:29:HIS:CD2	14:R:30:THR:HG23	2.48	0.49
1:A:1757:U:H4'	1:A:1757:U:OP2	2.13	0.49
18:V:73:PRO:HD3	18:V:101:LEU:HD22	1.95	0.49
1:A:161:G:N2	1:A:168:U:H5	2.11	0.49
1:A:1206:U:H2'	1:A:1207:A:H8	1.77	0.49
1:A:1315:A:H2'	1:A:1316:G:O4'	2.13	0.49
1:A:2551:U:H2'	1:A:2552:C:C6	2.48	0.49
1:A:1502:G:H5''	1:A:1503:U:H3'	1.95	0.49
2:B:84:G:C2	2:B:85:U:C2	3.01	0.49
1:A:2738:U:OP1	3:D:124:LYS:NZ	2.30	0.49
3:D:109:ASP:OD2	3:D:206:VAL:HG23	2.13	0.49
1:A:509:G:H22	25:4:37:LYS:NZ	2.10	0.49
1:A:2011:A:OP2	3:D:130:ARG:HD3	2.13	0.49
1:A:2674:A:OP1	6:G:176:THR:HB	2.13	0.49
7:K:100:ARG:O	7:K:104:THR:HG23	2.13	0.49
9:M:122:THR:O	9:M:122:THR:OG1	2.25	0.49
16:T:14:THR:HG22	16:T:105:THR:HG21	1.95	0.49
2:B:46:A:OP1	12:P:35:ARG:NH2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:78:U:H2'	2:B:79:G:N2	2.27	0.48
1:A:950:A:H2'	1:A:953:C:H5	1.77	0.48
1:A:1886:G:O2'	1:A:1887:G:OP2	2.24	0.48
1:A:1408:U:O2'	1:A:2226:A:H8	1.97	0.48
3:D:92:GLU:HG2	3:D:95:LYS:HE3	1.96	0.48
6:G:118:PRO:HD2	6:G:144:LEU:HD11	1.95	0.48
9:M:92:THR:H	9:M:95:VAL:HG12	1.78	0.48
12:P:29:PRO:HG2	12:P:91:VAL:HG12	1.94	0.48
1:A:273:A:OP2	1:A:297:G:N1	2.44	0.48
1:A:1453:U:C6	1:A:1628:G:H2'	2.48	0.48
1:A:2044:A:H8	1:A:2513:C:H5''	1.79	0.48
4:E:6:LEU:HG	4:E:17:ILE:HG13	1.95	0.48
11:O:68:ASN:O	11:O:70:VAL:N	2.40	0.48
1:A:912:U:OP1	10:N:5:LYS:N	2.44	0.48
1:A:1166:A:H8	1:A:1166:A:OP1	1.96	0.48
1:A:1256:G:OP1	14:R:22:LYS:NZ	2.47	0.48
5:F:70:ALA:HB3	5:F:82:GLY:H	1.78	0.48
16:T:87:MET:HB2	16:T:103:LYS:HB2	1.95	0.48
18:V:1:MET:SD	18:V:65:VAL:HG21	2.54	0.48
1:A:194:A:H2'	1:A:195:C:C6	2.49	0.48
11:O:45:GLU:O	11:O:49:THR:HG23	2.14	0.48
1:A:1009:G:H2'	1:A:1010:U:C6	2.49	0.48
1:A:290:U:H2'	1:A:291:G:O4'	2.14	0.47
5:F:164:GLU:HA	5:F:167:ARG:HG3	1.96	0.47
6:G:159:GLY:O	6:G:163:ARG:NH2	2.47	0.47
25:4:31:LEU:HD22	25:4:42:ILE:HD12	1.96	0.47
1:A:4:U:H2'	1:A:5:U:C6	2.49	0.47
1:A:519:A:N3	1:A:521:G:H5''	2.29	0.47
2:B:58:C:H2'	2:B:59:U:C6	2.49	0.47
5:F:3:ARG:O	5:F:7:LYS:HG3	2.14	0.47
1:A:392:A:H2'	1:A:393:A:C8	2.50	0.47
6:G:59:LYS:HG3	6:G:60:GLU:HG3	1.97	0.47
11:O:24:LEU:HB2	11:O:30:ILE:HD12	1.96	0.47
12:P:89:LYS:HG2	12:P:115:GLY:O	2.15	0.47
15:S:25:LEU:O	15:S:26:ASN:HB2	2.13	0.47
1:A:1535:U:HO2'	1:A:1536:A:P	2.33	0.47
1:A:2343:A:H2'	1:A:2344:G:C8	2.50	0.47
2:B:85:U:O4	2:B:86:U:N3	2.47	0.47
16:T:85:PRO:O	16:T:105:THR:OG1	2.31	0.47
1:A:900:G:O2'	1:A:901:U:OP2	2.32	0.47
2:B:59:U:H2'	2:B:60:U:C6	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:100:ASP:OD1	3:D:100:ASP:N	2.36	0.47
7:K:131:HIS:CD2	7:K:133:HIS:H	2.24	0.47
1:A:727:C:H1'	25:4:4:THR:HG22	1.95	0.47
1:A:1591:A:N3	1:A:1591:A:O5'	2.48	0.47
3:D:2:THR:OG1	3:D:3:LYS:N	2.47	0.47
6:G:48:ASN:O	6:G:49:GLU:HB2	2.14	0.47
15:S:19:ALA:HB1	15:S:94:LYS:HD3	1.96	0.47
17:U:8:LYS:HB2	17:U:28:GLU:O	2.14	0.47
1:A:11:A:H2'	1:A:12:A:C8	2.50	0.47
1:A:282:A:H2'	1:A:283:G:C8	2.49	0.47
1:A:2851:U:H5''	11:O:49:THR:HG21	1.96	0.47
1:A:1085:C:O2'	1:A:1086:A:OP1	2.29	0.47
1:A:1868:A:N6	1:A:1902:G:H8	2.06	0.47
1:A:1885:C:H41	1:A:1886:G:H21	1.62	0.47
2:B:32:U:O2'	2:B:33:U:O5'	2.32	0.47
3:D:19:SER:O	13:Q:80:ARG:NH2	2.36	0.47
5:F:70:ALA:HB3	5:F:82:GLY:N	2.30	0.47
1:A:526:C:O2'	16:T:65:ASN:ND2	2.48	0.47
1:A:1457:A:N1	1:A:1630:G:H4'	2.30	0.46
8:L:111:PHE:O	8:L:115:VAL:HG23	2.14	0.46
1:A:998:U:OP2	10:N:14:ARG:NH1	2.47	0.46
2:B:89:C:OP1	10:N:99:ARG:NH2	2.34	0.46
5:F:13:THR:O	5:F:17:VAL:HB	2.14	0.46
9:M:33:ARG:NH1	9:M:41:ARG:O	2.49	0.46
9:M:133:GLN:HG3	9:M:143:ILE:HG12	1.98	0.46
15:S:21:TYR:CE2	15:S:94:LYS:HG3	2.51	0.46
16:T:63:ALA:O	16:T:68:ASP:N	2.44	0.46
3:D:13:THR:HG23	3:D:25:VAL:HG12	1.97	0.46
4:E:41:ARG:HG2	4:E:41:ARG:HH11	1.80	0.46
1:A:654:A:H4'	1:A:655:G:C8	2.50	0.46
1:A:1490:A:H2'	1:A:1491:U:H5'	1.97	0.46
3:D:5:ILE:HG13	3:D:102:PHE:HE2	1.79	0.46
5:F:135:GLN:O	5:F:141:VAL:HG21	2.16	0.46
6:G:63:THR:O	6:G:67:THR:HG23	2.16	0.46
7:K:3:THR:O	7:K:3:THR:OG1	2.32	0.46
13:Q:32:VAL:HG21	13:Q:41:GLN:HE21	1.81	0.46
15:S:65:HIS:ND1	15:S:93:THR:HG22	2.31	0.46
21:Z:10:THR:O	21:Z:14:MET:HG2	2.15	0.46
1:A:61:G:OP1	21:Z:47:ARG:NH2	2.48	0.46
1:A:1088:A:H2'	1:A:1088:A:N3	2.31	0.46
1:A:1631:A:N3	1:A:1631:A:H2'	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2855:A:H2'	1:A:2856:A:C8	2.50	0.46
6:G:5:GLY:HA3	6:G:65:HIS:CD2	2.50	0.46
8:L:23:LYS:O	8:L:39:ILE:HG13	2.15	0.46
24:3:32:LYS:HA	24:3:32:LYS:HD3	1.74	0.46
1:A:492:G:C8	4:E:58:ARG:HD2	2.51	0.46
1:A:1492:G:N2	1:A:1504:G:H22	2.14	0.46
1:A:1692:G:O2'	11:O:116:ASP:OD1	2.32	0.46
2:B:90:C:HO2'	2:B:91:U:P	2.39	0.46
12:P:35:ARG:HA	12:P:40:ILE:HG22	1.97	0.46
1:A:1474:G:H2'	1:A:1475:U:C6	2.50	0.46
5:F:83:MET:O	5:F:85:ILE:HG13	2.16	0.46
18:V:47:PRO:HB3	18:V:52:PRO:O	2.15	0.46
1:A:782:U:H2'	1:A:783:A:C8	2.51	0.45
1:A:903:G:O6	1:A:956:C:N3	2.50	0.45
1:A:2314:A:H2'	1:A:2315:A:C8	2.51	0.45
5:F:4:LEU:HD22	5:F:7:LYS:HD2	1.98	0.45
5:F:55:GLU:O	5:F:59:LEU:HG	2.16	0.45
5:F:104:VAL:HG22	5:F:175:MET:H	1.80	0.45
1:A:1447:U:H2'	1:A:1448:U:O4'	2.16	0.45
1:A:469:A:H2'	1:A:470:A:C8	2.52	0.45
1:A:2763:A:H4'	6:G:62:LYS:HB2	1.97	0.45
24:3:41:LYS:HD3	24:3:41:LYS:HA	1.73	0.45
1:A:1167:A:N3	1:A:1167:A:H2'	2.31	0.45
1:A:2809:U:OP2	1:A:2810:U:N3	2.49	0.45
3:D:146:MET:HA	3:D:158:LYS:HE2	1.97	0.45
5:F:66:LEU:HD23	5:F:66:LEU:HA	1.73	0.45
15:S:88:HIS:CE1	15:S:90:GLN:HG2	2.44	0.45
1:A:251:G:O5'	1:A:252:C:H5''	2.17	0.45
1:A:1804:C:H2'	1:A:1805:A:C5	2.51	0.45
1:A:1861:A:H8	1:A:1861:A:OP2	1.99	0.45
1:A:2439:A:H5''	1:A:2441:C:O4'	2.17	0.45
1:A:2908:U:H2'	1:A:2909:A:O4'	2.15	0.45
5:F:117:VAL:HG12	5:F:118:SER:O	2.16	0.45
11:O:22:THR:HG21	11:O:67:ARG:HB2	1.99	0.45
5:F:68:THR:N	5:F:86:GLY:O	2.42	0.45
1:A:523:A:H5''	18:V:46:LYS:HG2	1.98	0.45
1:A:697:U:H2'	1:A:698:A:C8	2.52	0.45
1:A:2812:A:O2'	1:A:2813:A:OP1	2.20	0.45
11:O:96:ARG:HH21	11:O:126:VAL:CG2	2.25	0.45
15:S:69:LYS:HB3	15:S:69:LYS:HE2	1.67	0.45
26:5:32:ARG:H	26:5:32:ARG:HG3	1.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:U:H2'	1:A:325:U:O4'	2.17	0.45
1:A:613:U:H2'	1:A:614:G:C8	2.52	0.45
1:A:1390:A:H2'	1:A:1391:G:O4'	2.17	0.45
1:A:2264:G:N2	10:N:84:GLY:HA2	2.32	0.45
1:A:2359:G:N3	1:A:2395:C:H2'	2.31	0.45
9:M:83:ASN:O	9:M:119:LYS:NZ	2.47	0.45
17:U:19:ALA:HB1	17:U:24:LYS:HB2	1.99	0.45
1:A:1052:U:OP2	14:R:70:ARG:NH2	2.44	0.45
1:A:1453:U:H4'	1:A:1454:U:C6	2.52	0.45
5:F:117:VAL:HB	5:F:177:PHE:HD1	1.81	0.45
6:G:154:PRO:HA	6:G:160:LYS:O	2.17	0.45
9:M:2:LYS:HD3	9:M:4:HIS:CE1	2.52	0.45
1:A:1328:G:H2'	1:A:1329:U:C6	2.52	0.45
1:A:2458:G:OP2	4:E:68:LYS:NZ	2.38	0.45
18:V:41:VAL:O	18:V:58:GLU:HA	2.17	0.45
1:A:1451:U:P	1:A:1630:G:H22	2.40	0.44
1:A:2342:A:H2'	1:A:2343:A:H8	1.82	0.44
4:E:12:THR:O	4:E:14:ASN:N	2.50	0.44
6:G:10:VAL:HG13	6:G:48:ASN:O	2.17	0.44
12:P:40:ILE:O	12:P:58:ALA:HB2	2.18	0.44
23:2:23:THR:HG21	23:2:25:LYS:HE3	1.99	0.44
1:A:1499:G:H22	1:A:2716:G:H22	1.66	0.44
11:O:38:LYS:O	11:O:41:ARG:HG2	2.18	0.44
1:A:885:U:N3	1:A:886:U:H1'	2.32	0.44
1:A:1960:U:H2'	1:A:1961:C:C6	2.52	0.44
1:A:2078:C:H2'	1:A:2079:C:C6	2.53	0.44
1:A:2595:G:H2'	1:A:2595:G:N3	2.32	0.44
18:V:24:LEU:HD23	18:V:24:LEU:HA	1.66	0.44
1:A:900:G:N2	1:A:958:A:OP2	2.30	0.44
1:A:2494:C:H2'	1:A:2495:G:H5'	2.00	0.44
4:E:6:LEU:HD23	4:E:6:LEU:HA	1.74	0.44
1:A:1489:C:H3'	1:A:1490:A:C8	2.53	0.44
1:A:1584:G:H1'	1:A:1585:U:OP2	2.18	0.44
1:A:2605:C:H2'	1:A:2606:G:C8	2.52	0.44
4:E:28:PRO:HA	4:E:112:SER:HB2	1.98	0.44
5:F:69:LYS:HA	5:F:84:PRO:HA	1.98	0.44
6:G:90:ILE:HG22	6:G:91:GLY:H	1.82	0.44
1:A:2299:C:OP2	24:3:2:ARG:NH1	2.50	0.44
3:D:6:LEU:HD11	3:D:81:LYS:HB2	2.00	0.44
8:L:61:VAL:HG21	8:L:111:PHE:CE2	2.53	0.44
1:A:1240:A:H2'	1:A:1241:A:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:73:U:O2'	2:B:74:G:H8	2.00	0.44
3:D:33:ASN:N	3:D:33:ASN:HD22	2.16	0.44
5:F:14:PRO:O	5:F:17:VAL:HG12	2.18	0.44
1:A:283:G:N2	1:A:288:C:O2	2.37	0.44
2:B:27:A:H2'	2:B:28:C:C6	2.53	0.44
3:D:31:THR:HG22	3:D:184:ASN:HD22	1.83	0.44
6:G:45:ILE:HG22	6:G:46:GLU:H	1.82	0.44
1:A:162:A:N6	1:A:166:C:OP2	2.47	0.44
1:A:339:G:H2'	1:A:340:A:C8	2.53	0.44
1:A:516:G:N1	1:A:519:A:OP2	2.51	0.44
1:A:1823:A:H2'	1:A:1824:A:C8	2.52	0.44
1:A:2393:G:H2'	1:A:2394:U:C6	2.53	0.44
5:F:119:LYS:HB3	5:F:167:ARG:HH21	1.83	0.43
10:N:133:LYS:H	10:N:133:LYS:HG3	1.73	0.43
1:A:276:C:C2'	1:A:277:C:H5'	2.49	0.43
1:A:1068:A:N6	1:A:1165:G:H2'	2.32	0.43
5:F:102:LYS:O	5:F:107:SER:OG	2.24	0.43
6:G:7:LYS:HE3	6:G:7:LYS:HB2	1.85	0.43
13:Q:92:VAL:HG11	13:Q:97:LEU:HD21	2.01	0.43
18:V:1:MET:O	18:V:2:PHE:HD1	2.01	0.43
1:A:519:A:HO2'	1:A:521:G:H8	1.66	0.43
1:A:1393:C:H2'	1:A:1394:G:O4'	2.17	0.43
2:B:46:A:P	12:P:35:ARG:HH22	2.41	0.43
7:K:2:ARG:HD2	7:K:3:THR:HG23	1.99	0.43
1:A:499:U:H5''	25:4:40:LYS:HD3	2.00	0.43
1:A:1035:C:O2	7:K:4:THR:HG23	2.19	0.43
1:A:2571:G:H2'	1:A:2572:C:C6	2.53	0.43
1:A:1088:A:N1	1:A:1152:G:O2'	2.47	0.43
1:A:1167:A:O2'	1:A:1168:A:H5''	2.19	0.43
10:N:30:GLY:O	10:N:134:ARG:NH1	2.51	0.43
1:A:872:G:H2'	1:A:873:C:C6	2.53	0.43
4:E:135:LYS:HE2	4:E:135:LYS:HB2	1.79	0.43
16:T:74:LEU:HD23	16:T:114:GLU:HA	2.01	0.43
2:B:10:G:OP2	19:X:80:ARG:NH1	2.52	0.43
3:D:4:GLY:HA2	3:D:202:ILE:O	2.19	0.43
4:E:200:THR:O	4:E:204:GLU:HG3	2.19	0.43
6:G:149:ARG:O	6:G:149:ARG:HG2	2.18	0.43
9:M:73:ASP:OD1	9:M:73:ASP:N	2.51	0.43
3:D:107:VAL:HA	3:D:174:LEU:O	2.18	0.43
13:Q:43:PHE:HE2	13:Q:61:VAL:HB	1.84	0.43
1:A:1525:U:O2	1:A:1552:A:N6	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1725:A:H2'	1:A:1726:C:C6	2.53	0.43
2:B:1:U:O2	2:B:115:G:N2	2.39	0.43
3:D:111:THR:HG22	3:D:170:THR:HB	2.01	0.43
16:T:29:ILE:HD11	16:T:41:LEU:HG	1.99	0.43
17:U:29:VAL:HG21	17:U:38:VAL:CG2	2.47	0.43
1:A:345:G:H2'	1:A:346:A:C8	2.53	0.42
1:A:357:A:N3	4:E:169:ASN:ND2	2.66	0.42
1:A:854:C:H1'	1:A:1262:G:N2	2.34	0.42
1:A:2106:U:H4'	1:A:2107:G:H5''	2.00	0.42
1:A:2295:C:O2'	1:A:2296:G:H5'	2.19	0.42
1:A:2454:C:O2'	1:A:2455:C:O4'	2.37	0.42
3:D:123:ILE:HD13	3:D:130:ARG:HG3	2.01	0.42
3:D:159:ARG:HE	3:D:159:ARG:HB2	1.67	0.42
9:M:84:ARG:NH2	9:M:101:ILE:HD11	2.33	0.42
24:3:5:ILE:HG22	24:3:19:THR:HG23	2.01	0.42
26:5:54:ASP:O	26:5:58:ILE:HB	2.19	0.42
1:A:505:G:H2'	1:A:506:A:C8	2.54	0.42
1:A:1212:A:O2'	1:A:1213:U:H6	2.01	0.42
1:A:1216:G:N3	1:A:1216:G:H2'	2.34	0.42
5:F:15:SER:O	5:F:19:LYS:HG3	2.19	0.42
1:A:339:G:H2'	1:A:340:A:H8	1.85	0.42
1:A:1872:G:HO2'	1:A:1873:A:H8	1.65	0.42
1:A:2052:G:H2'	1:A:2053:G:O4'	2.19	0.42
1:A:2085:A:H2'	1:A:2086:G:H8	1.80	0.42
1:A:2855:A:H2'	1:A:2856:A:H8	1.84	0.42
5:F:74:ILE:O	5:F:79:LEU:HB2	2.18	0.42
17:U:2:GLU:CD	17:U:2:GLU:N	2.72	0.42
1:A:1447:U:N3	1:A:1448:U:C4	2.87	0.42
1:A:1489:C:H2'	1:A:1490:A:C8	2.54	0.42
1:A:1755:C:H2'	1:A:1756:U:H4'	2.01	0.42
1:A:2079:C:H2'	1:A:2080:C:H6	1.84	0.42
1:A:2099:U:H2'	1:A:2100:U:C6	2.54	0.42
12:P:67:THR:O	12:P:67:THR:OG1	2.32	0.42
14:R:119:LYS:HA	14:R:119:LYS:HD3	1.85	0.42
23:2:15:LYS:O	23:2:18:THR:HG23	2.19	0.42
1:A:1093:U:H2'	1:A:1094:A:O4'	2.20	0.42
1:A:1172:U:H5'	7:K:85:LEU:HD11	2.01	0.42
1:A:2317:G:O2'	5:F:121:ALA:HA	2.19	0.42
2:B:50:A:N6	12:P:38:LYS:HG2	2.35	0.42
2:B:97:A:HO2'	2:B:98:G:P	2.37	0.42
24:3:19:THR:OG1	24:3:20:ASN:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:A:H2'	1:A:132:A:C8	2.55	0.42
1:A:572:G:H2'	1:A:573:U:C6	2.54	0.42
1:A:672:A:H5''	1:A:673:G:OP2	2.19	0.42
1:A:1757:U:H2'	1:A:1758:C:C2	2.54	0.42
8:L:66:LYS:HE3	8:L:66:LYS:HB3	1.91	0.42
19:X:75:VAL:O	19:X:90:VAL:HA	2.20	0.42
20:Y:40:ILE:HD11	20:Y:45:LYS:HB2	2.01	0.42
1:A:156:U:H2'	1:A:157:C:C6	2.54	0.42
1:A:987:A:H2'	1:A:988:C:C6	2.54	0.42
1:A:1409:A:H5'	1:A:2226:A:O4'	2.20	0.42
1:A:2219:A:H2'	1:A:2220:C:H6	1.83	0.42
2:B:89:C:P	10:N:99:ARG:HH22	2.42	0.42
3:D:2:THR:OG1	3:D:204:SER:OG	2.37	0.42
4:E:2:PRO:HD2	4:E:19:LEU:O	2.20	0.42
4:E:59:GLY:HA2	4:E:79:ARG:HH11	1.84	0.42
10:N:64:VAL:HG22	10:N:106:ILE:HG12	2.02	0.42
14:R:48:ARG:HE	14:R:48:ARG:HB3	1.66	0.42
1:A:2319:U:N3	5:F:151:GLY:O	2.44	0.42
3:D:16:PHE:CE1	3:D:22:LEU:HG	2.55	0.42
10:N:66:ILE:HG12	10:N:104:PHE:CE1	2.55	0.42
1:A:454:C:H2'	1:A:455:A:H8	1.85	0.42
1:A:1699:C:H2'	1:A:1700:U:H6	1.85	0.42
8:L:91:LYS:HB3	8:L:111:PHE:CD2	2.55	0.42
12:P:57:SER:HB2	12:P:60:ASP:HB2	2.00	0.42
18:V:81:VAL:HG13	18:V:92:ARG:HB3	2.01	0.42
1:A:288:C:H1'	1:A:289:U:H5	1.85	0.42
1:A:1394:G:N1	1:A:1407:G:N7	2.68	0.42
1:A:2911:C:H6	1:A:2911:C:O5'	2.02	0.42
2:B:70:G:N3	2:B:70:G:O4'	2.52	0.42
2:B:72:U:H2'	2:B:73:U:H5'	2.02	0.42
11:O:18:ARG:HD3	11:O:65:PHE:HA	2.01	0.42
1:A:2429:G:H2'	1:A:2430:C:C6	2.55	0.41
1:A:312:U:O5'	1:A:312:U:H6	2.02	0.41
1:A:697:U:H2'	1:A:698:A:H8	1.85	0.41
1:A:1323:A:C8	11:O:113:ARG:HD3	2.51	0.41
1:A:1355:G:O2'	1:A:1356:G:H5'	2.20	0.41
1:A:1461:A:N3	1:A:1461:A:H2'	2.36	0.41
1:A:1808:U:H2'	1:A:1809:C:C6	2.55	0.41
1:A:2453:A:H4'	1:A:2454:C:C3'	2.47	0.41
5:F:32:ASP:OD2	12:P:2:ILE:HD12	2.21	0.41
7:K:76:TYR:CE1	7:K:87:SER:HB3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:C:HO2'	1:A:127:A:HO2'	1.59	0.41
1:A:154:U:O2'	1:A:155:U:H5'	2.20	0.41
1:A:1181:U:H4'	1:A:1182:A:O4'	2.20	0.41
1:A:2088:U:H2'	1:A:2089:U:C6	2.55	0.41
1:A:2420:C:C4	9:M:69:ILE:HD12	2.55	0.41
4:E:158:ASN:HB3	4:E:159:GLY:H	1.74	0.41
5:F:104:VAL:CG2	5:F:175:MET:H	2.33	0.41
6:G:18:LYS:HB2	6:G:25:THR:CG2	2.50	0.41
14:R:88:ILE:HD11	14:R:112:GLN:OE1	2.20	0.41
1:A:911:U:H5''	10:N:6:ARG:O	2.20	0.41
1:A:2419:G:O2'	1:A:2420:C:OP2	2.34	0.41
2:B:50:A:N1	12:P:38:LYS:HE2	2.35	0.41
4:E:157:GLU:H	4:E:157:GLU:HG3	1.56	0.41
5:F:163:ASP:O	5:F:167:ARG:HG3	2.21	0.41
6:G:107:VAL:O	6:G:109:TYR:N	2.54	0.41
12:P:63:ILE:HD11	12:P:78:LEU:HD12	2.01	0.41
14:R:70:ARG:HA	14:R:74:LEU:O	2.20	0.41
1:A:11:A:H2'	1:A:12:A:H8	1.86	0.41
1:A:1489:C:H3'	1:A:1490:A:H8	1.85	0.41
3:D:88:LEU:O	3:D:89:GLY:C	2.59	0.41
6:G:73:ASN:O	6:G:77:VAL:HG23	2.21	0.41
6:G:101:ASN:O	6:G:116:THR:HA	2.20	0.41
1:A:591:U:H2'	1:A:592:G:O4'	2.21	0.41
1:A:1492:G:H22	1:A:1504:G:N2	2.19	0.41
2:B:113:A:H2'	2:B:114:C:C6	2.55	0.41
4:E:40:GLN:OE1	4:E:184:LEU:HB2	2.20	0.41
10:N:32:TRP:CZ2	10:N:111:GLU:HG2	2.54	0.41
18:V:81:VAL:CG1	18:V:92:ARG:HB3	2.50	0.41
22:O:5:LYS:HB3	22:O:5:LYS:HE3	1.86	0.41
1:A:441:A:H2'	1:A:442:A:C8	2.56	0.41
1:A:853:U:H2'	1:A:854:C:H6	1.82	0.41
1:A:1518:U:O2'	1:A:1519:G:C8	2.73	0.41
1:A:1600:C:H6	1:A:1600:C:H2'	1.57	0.41
1:A:1699:C:H2'	1:A:1700:U:C6	2.56	0.41
5:F:40:VAL:HG22	5:F:150:ARG:NH1	2.35	0.41
5:F:164:GLU:HA	5:F:167:ARG:CG	2.50	0.41
10:N:63:LYS:HD2	10:N:65:TRP:CZ2	2.56	0.41
17:U:23:LYS:HZ3	17:U:84:GLU:HA	1.84	0.41
1:A:84:G:N2	1:A:103:A:H2	2.10	0.41
1:A:91:A:OP1	1:A:91:A:H8	2.04	0.41
6:G:163:ARG:HG3	6:G:164:TYR:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:15:LYS:O	7:K:53:ASP:HB3	2.20	0.41
9:M:130:LYS:HB2	9:M:130:LYS:HE2	1.88	0.41
27:6:11:CYS:SG	27:6:12:GLU:N	2.94	0.41
1:A:234:C:O2'	1:A:235:G:N3	2.46	0.41
1:A:716:A:H2	1:A:842:A:H61	1.69	0.41
1:A:1237:U:H2'	1:A:1238:C:C6	2.55	0.41
1:A:1518:U:O2'	1:A:1519:G:OP2	2.30	0.41
1:A:1538:A:H5''	1:A:1539:U:OP1	2.20	0.41
1:A:2379:G:N7	26:5:39:LYS:NZ	2.68	0.41
1:A:2575:A:O2'	8:L:23:LYS:HG3	2.20	0.41
1:A:2806:U:H2'	1:A:2807:U:C6	2.56	0.41
1:A:2809:U:O2	1:A:2809:U:H2'	2.20	0.41
3:D:5:ILE:HD11	3:D:101:VAL:HB	2.02	0.41
4:E:196:GLN:O	4:E:200:THR:HG23	2.21	0.41
9:M:27:ASN:O	9:M:31:ALA:HA	2.21	0.41
11:O:113:ARG:HD2	11:O:116:ASP:HB2	2.02	0.41
11:O:116:ASP:HB3	11:O:118:ALA:H	1.85	0.41
20:Y:6:TYR:CD2	20:Y:47:VAL:HG21	2.55	0.41
20:Y:19:SER:O	20:Y:19:SER:OG	2.33	0.41
1:A:807:U:O2'	1:A:808:G:OP2	2.38	0.41
1:A:2300:A:H4'	1:A:2301:A:O4'	2.20	0.41
2:B:23:A:H2'	2:B:24:U:C6	2.56	0.41
2:B:32:U:HO2'	2:B:33:U:P	2.44	0.41
1:A:176:U:H2'	1:A:177:A:C8	2.57	0.40
1:A:297:G:H5''	1:A:305:A:OP1	2.21	0.40
1:A:1824:A:H8	1:A:1824:A:O5'	2.04	0.40
1:A:1969:U:C4	1:A:2566:U:H1'	2.57	0.40
1:A:2318:G:O2'	5:F:153:ASP:OD1	2.33	0.40
1:A:53:A:H2'	1:A:54:A:C8	2.56	0.40
1:A:713:C:H4'	4:E:82:GLN:HE22	1.85	0.40
1:A:1631:A:N9	1:A:1632:A:H2	2.19	0.40
8:L:64:ARG:O	8:L:82:ASN:HA	2.21	0.40
11:O:4:ARG:HB2	11:O:39:GLU:OE2	2.21	0.40
1:A:288:C:H1'	1:A:289:U:C5	2.56	0.40
1:A:887:G:H5''	1:A:888:A:OP1	2.22	0.40
1:A:1213:U:H2'	1:A:1214:U:O4'	2.21	0.40
1:A:1492:G:N2	1:A:1504:G:N2	2.69	0.40
2:B:110:G:H2'	2:B:111:C:H6	1.87	0.40
8:L:63:VAL:HG22	8:L:106:LEU:HD11	2.03	0.40
8:L:105:GLU:H	8:L:105:GLU:HG2	1.64	0.40
1:A:897:G:H2'	1:A:898:A:H8	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1960:U:H2'	1:A:1961:C:H6	1.86	0.40
1:A:2454:C:H6	1:A:2454:C:H2'	1.70	0.40
4:E:158:ASN:C	4:E:160:ASN:H	2.23	0.40
6:G:78:GLY:HA2	6:G:82:GLY:H	1.87	0.40
9:M:87:ASP:OD1	9:M:119:LYS:HA	2.22	0.40
13:Q:72:ARG:HD3	13:Q:74:PHE:CZ	2.57	0.40
1:A:573:U:H2'	1:A:574:C:C6	2.56	0.40
5:F:30:LYS:O	5:F:158:THR:HB	2.22	0.40
13:Q:82:ALA:O	13:Q:83:GLN:HG2	2.21	0.40
17:U:23:LYS:HE2	17:U:85:ASP:H	1.87	0.40
26:5:14:VAL:HG13	26:5:22:LEU:HD22	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	205/207 (99%)	188 (92%)	16 (8%)	1 (0%)	29	61
4	E	204/206 (99%)	181 (89%)	21 (10%)	2 (1%)	15	45
5	F	175/177 (99%)	148 (85%)	27 (15%)	0	100	100
6	G	174/176 (99%)	145 (83%)	27 (16%)	2 (1%)	14	42
7	K	143/145 (99%)	133 (93%)	10 (7%)	0	100	100
8	L	120/122 (98%)	104 (87%)	15 (12%)	1 (1%)	19	51
9	M	144/146 (99%)	118 (82%)	25 (17%)	1 (1%)	22	54
10	N	139/141 (99%)	119 (86%)	20 (14%)	0	100	100
11	O	122/124 (98%)	102 (84%)	20 (16%)	0	100	100
12	P	115/117 (98%)	105 (91%)	10 (9%)	0	100	100
13	Q	112/114 (98%)	104 (93%)	8 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	R	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
15	S	100/102 (98%)	91 (91%)	8 (8%)	1 (1%)	15	45
16	T	110/112 (98%)	103 (94%)	7 (6%)	0	100	100
17	U	87/89 (98%)	73 (84%)	14 (16%)	0	100	100
18	V	99/101 (98%)	81 (82%)	18 (18%)	0	100	100
19	X	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
20	Y	52/54 (96%)	43 (83%)	8 (15%)	1 (2%)	8	28
21	Z	59/61 (97%)	57 (97%)	2 (3%)	0	100	100
22	0	56/58 (97%)	54 (96%)	2 (4%)	0	100	100
23	2	54/56 (96%)	46 (85%)	8 (15%)	0	100	100
24	3	47/49 (96%)	43 (92%)	4 (8%)	0	100	100
25	4	42/44 (96%)	42 (100%)	0	0	100	100
26	5	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
27	6	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
All	All	2647/2697 (98%)	2354 (89%)	284 (11%)	9 (0%)	44	71

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	90	GLU
9	M	16	ARG
4	E	13	GLN
8	L	25	LEU
20	Y	20	HIS
6	G	47	GLY
4	E	159	GLY
6	G	108	GLY
15	S	51	PRO

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 PDB entries followed by that with respect to all EM entries.

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	170/170 (100%)	140 (82%)	30 (18%)	2	5
4	E	172/172 (100%)	144 (84%)	28 (16%)	2	7
5	F	154/154 (100%)	129 (84%)	25 (16%)	2	7
6	G	146/146 (100%)	123 (84%)	23 (16%)	2	8
7	K	122/122 (100%)	105 (86%)	17 (14%)	3	10
8	L	98/98 (100%)	87 (89%)	11 (11%)	6	18
9	M	112/112 (100%)	102 (91%)	10 (9%)	9	29
10	N	112/112 (100%)	98 (88%)	14 (12%)	4	14
11	O	106/106 (100%)	92 (87%)	14 (13%)	4	12
12	P	91/91 (100%)	79 (87%)	12 (13%)	4	12
13	Q	97/97 (100%)	83 (86%)	14 (14%)	3	9
14	R	94/94 (100%)	87 (93%)	7 (7%)	13	38
15	S	83/83 (100%)	73 (88%)	10 (12%)	5	15
16	T	95/95 (100%)	82 (86%)	13 (14%)	3	11
17	U	80/80 (100%)	66 (82%)	14 (18%)	2	6
18	V	85/85 (100%)	71 (84%)	14 (16%)	2	7
19	X	61/61 (100%)	48 (79%)	13 (21%)	1	3
20	Y	47/47 (100%)	38 (81%)	9 (19%)	1	4
21	Z	55/55 (100%)	45 (82%)	10 (18%)	1	5
22	0	49/49 (100%)	44 (90%)	5 (10%)	7	22
23	2	46/46 (100%)	39 (85%)	7 (15%)	3	8
24	3	49/49 (100%)	46 (94%)	3 (6%)	18	48
25	4	39/39 (100%)	34 (87%)	5 (13%)	4	13
26	5	51/51 (100%)	44 (86%)	7 (14%)	3	11
27	6	35/35 (100%)	30 (86%)	5 (14%)	3	10
All	All	2249/2249 (100%)	1929 (86%)	320 (14%)	6	10

All (320) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	15	ILE
3	D	21	GLU
3	D	22	LEU
3	D	23	ILE

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Mol	Chain	Res	Type
3	D	25	VAL
3	D	43	THR
3	D	49	ILE
3	D	50	GLN
3	D	58	GLU
3	D	59	VAL
3	D	62	ASN
3	D	69	VAL
3	D	71	LYS
3	D	81	LYS
3	D	86	VAL
3	D	90	GLU
3	D	103	GLN
3	D	107	VAL
3	D	108	VAL
3	D	111	THR
3	D	119	PHE
3	D	141	ARG
3	D	145	SER
3	D	158	LYS
3	D	167	ASP
3	D	168	ARG
3	D	170	THR
3	D	191	ASN
3	D	199	LEU
3	D	201	THR
4	E	6	LEU
4	E	8	LYS
4	E	18	THR
4	E	20	ASN
4	E	31	SER
4	E	49	HIS
4	E	65	TRP
4	E	77	SER
4	E	79	ARG
4	E	80	SER
4	E	82	GLN
4	E	89	VAL
4	E	93	THR
4	E	94	PRO
4	E	105	VAL
4	E	113	VAL

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Mol	Chain	Res	Type
4	E	153	LEU
4	E	157	GLU
4	E	160	ASN
4	E	165	LEU
4	E	168	ARG
4	E	176	VAL
4	E	184	LEU
4	E	190	ASN
4	E	193	LEU
4	E	195	THR
4	E	200	THR
4	E	205	VAL
5	F	6	GLU
5	F	15	SER
5	F	17	VAL
5	F	27	GLN
5	F	32	ASP
5	F	57	LEU
5	F	61	THR
5	F	66	LEU
5	F	77	PHE
5	F	81	GLU
5	F	88	LYS
5	F	89	VAL
5	F	110	ARG
5	F	112	ARG
5	F	114	PHE
5	F	127	ASN
5	F	130	LEU
5	F	133	LYS
5	F	137	ILE
5	F	142	ASP
5	F	143	TYR
5	F	149	VAL
5	F	152	MET
5	F	162	THR
5	F	170	LEU
6	G	8	VAL
6	G	11	LEU
6	G	25	THR
6	G	32	GLU
6	G	35	ARG

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Mol	Chain	Res	Type
6	G	44	ASN
6	G	45	ILE
6	G	46	GLU
6	G	63	THR
6	G	67	THR
6	G	79	VAL
6	G	84	GLN
6	G	95	ARG
6	G	101	ASN
6	G	103	LEU
6	G	107	VAL
6	G	121	VAL
6	G	122	THR
6	G	136	ILE
6	G	143	GLU
6	G	152	ARG
6	G	165	VAL
6	G	171	ARG
7	K	2	ARG
7	K	14	ARG
7	K	26	LEU
7	K	30	SER
7	K	46	THR
7	K	58	ILE
7	K	77	ARG
7	K	80	MET
7	K	85	LEU
7	K	100	ARG
7	K	101	LEU
7	K	113	ASN
7	K	114	THR
7	K	115	LEU
7	K	118	LYS
7	K	123	LEU
7	K	145	ASN
8	L	1	MET
8	L	5	GLU
8	L	13	ASN
8	L	18	GLU
8	L	19	ILE
8	L	21	THR
8	L	42	THR

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Mol	Chain	Res	Type
8	L	53	LYS
8	L	73	ASP
8	L	90	ASP
8	L	105	GLU
9	M	3	LEU
9	M	16	ARG
9	M	42	SER
9	M	60	ARG
9	M	76	VAL
9	M	81	THR
9	M	84	ARG
9	M	87	ASP
9	M	122	THR
9	M	131	SER
10	N	5	LYS
10	N	10	ARG
10	N	11	ARG
10	N	25	LYS
10	N	26	GLU
10	N	34	LEU
10	N	37	THR
10	N	74	TYR
10	N	76	SER
10	N	85	LYS
10	N	103	MET
10	N	109	VAL
10	N	127	VAL
10	N	133	LYS
11	O	3	TYR
11	O	8	ARG
11	O	24	LEU
11	O	41	ARG
11	O	49	THR
11	O	55	ASP
11	O	56	LEU
11	O	84	SER
11	O	89	LEU
11	O	100	ARG
11	O	106	ARG
11	O	108	LEU
11	O	124	GLU
11	O	125	PHE

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Mol	Chain	Res	Type
12	P	2	ILE
12	P	6	ASP
12	P	11	ARG
12	P	28	CYS
12	P	31	LEU
12	P	35	ARG
12	P	46	ASP
12	P	51	VAL
12	P	57	SER
12	P	67	THR
12	P	79	VAL
12	P	95	ARG
13	Q	2	ASN
13	Q	10	GLN
13	Q	11	GLU
13	Q	36	THR
13	Q	49	LYS
13	Q	55	ILE
13	Q	60	THR
13	Q	72	ARG
13	Q	76	LEU
13	Q	78	THR
13	Q	80	ARG
13	Q	101	ARG
13	Q	109	ARG
13	Q	114	ARG
14	R	10	THR
14	R	30	THR
14	R	51	ARG
14	R	60	LEU
14	R	79	LEU
14	R	89	ASP
14	R	92	ARG
15	S	1	MET
15	S	2	TYR
15	S	14	VAL
15	S	22	VAL
15	S	33	VAL
15	S	61	THR
15	S	73	THR
15	S	75	GLN
15	S	94	LYS

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Mol	Chain	Res	Type
15	S	101	ASN
16	T	4	GLN
16	T	9	LYS
16	T	11	THR
16	T	14	THR
16	T	26	ILE
16	T	29	ILE
16	T	70	ASP
16	T	88	LYS
16	T	89	ARG
16	T	93	ARG
16	T	105	THR
16	T	109	THR
16	T	115	LYS
17	U	2	GLU
17	U	3	LEU
17	U	14	GLU
17	U	16	SER
17	U	29	VAL
17	U	37	LEU
17	U	47	ASP
17	U	49	LYS
17	U	52	ASN
17	U	56	LEU
17	U	75	ARG
17	U	76	ARG
17	U	84	GLU
17	U	87	LYS
18	V	1	MET
18	V	2	PHE
18	V	5	LYS
18	V	9	VAL
18	V	13	THR
18	V	17	LYS
18	V	29	LYS
18	V	41	VAL
18	V	58	GLU
18	V	59	VAL
18	V	68	VAL
18	V	69	MET
18	V	94	SER
18	V	99	GLU

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Mol	Chain	Res	Type
19	X	18	SER
19	X	19	THR
19	X	20	SER
19	X	23	ARG
19	X	24	ASP
19	X	28	LYS
19	X	39	THR
19	X	40	VAL
19	X	62	ILE
19	X	67	THR
19	X	73	ASP
19	X	88	VAL
19	X	93	VAL
20	Y	12	THR
20	Y	22	MET
20	Y	24	SER
20	Y	27	ARG
20	Y	28	THR
20	Y	32	ASN
20	Y	34	GLN
20	Y	36	VAL
20	Y	40	ILE
21	Z	2	LYS
21	Z	3	VAL
21	Z	4	LYS
21	Z	5	GLU
21	Z	10	THR
21	Z	15	LEU
21	Z	32	LEU
21	Z	37	LEU
21	Z	38	GLU
21	Z	55	THR
22	0	8	LEU
22	0	16	PRO
22	0	35	VAL
22	0	55	ASP
22	0	59	VAL
23	2	3	VAL
23	2	7	ARG
23	2	8	THR
23	2	18	THR
23	2	23	THR

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Mol	Chain	Res	Type
23	2	32	ASN
23	2	56	SER
24	3	8	GLU
24	3	10	THR
24	3	44	LEU
25	4	10	ARG
25	4	20	LYS
25	4	24	THR
25	4	34	ARG
25	4	43	SER
26	5	31	HIS
26	5	32	ARG
26	5	41	ARG
26	5	46	LYS
26	5	57	ARG
26	5	58	ILE
26	5	65	MET
27	6	4	ARG
27	6	11	CYS
27	6	15	LYS
27	6	26	ILE
27	6	36	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	37	GLN
3	D	62	ASN
3	D	68	HIS
4	E	13	GLN
4	E	14	ASN
4	E	49	HIS
4	E	75	GLN
4	E	82	GLN
4	E	141	GLN
4	E	196	GLN
5	F	37	ASN
5	F	49	ASN
7	K	48	HIS
7	K	59	ASN
7	K	113	ASN
7	K	131	HIS

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Mol	Chain	Res	Type
9	M	4	HIS
9	M	38	GLN
9	M	54	GLN
9	M	133	GLN
12	P	12	GLN
12	P	15	HIS
12	P	20	ASN
12	P	114	ASN
13	Q	41	GLN
14	R	101	ASN
15	S	18	GLN
15	S	83	HIS
15	S	86	GLN
15	S	88	HIS
16	T	4	GLN
16	T	46	ASN
16	T	65	ASN
19	X	49	GLN
20	Y	17	ASN
20	Y	23	ASN
20	Y	32	ASN
20	Y	34	GLN
21	Z	36	GLN
21	Z	48	GLN
22	0	40	ASN
23	2	40	HIS
25	4	8	ASN
26	5	4	GLN
26	5	31	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2733/2908 (93%)	536 (19%)	24 (0%)
2	B	115/116 (99%)	32 (27%)	3 (2%)
All	All	2848/3024 (94%)	568 (19%)	27 (0%)

All (568) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	13	U

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Mol	Chain	Res	Type
1	A	14	A
1	A	28	G
1	A	35	U
1	A	42	A
1	A	52	G
1	A	68	A
1	A	71	G
1	A	72	A
1	A	75	U
1	A	76	G
1	A	92	A
1	A	93	G
1	A	97	G
1	A	102	G
1	A	110	G
1	A	118	A
1	A	119	A
1	A	120	U
1	A	131	A
1	A	148	A
1	A	155	U
1	A	156	U
1	A	158	A
1	A	165	A
1	A	166	C
1	A	168	U
1	A	169	A
1	A	177	A
1	A	180	G
1	A	182	U
1	A	185	A
1	A	199	A
1	A	202	A
1	A	218	G
1	A	219	A
1	A	220	A
1	A	225	A
1	A	231	A
1	A	232	U
1	A	233	U
1	A	235	G
1	A	236	A

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Mol	Chain	Res	Type
1	A	251	G
1	A	255	G
1	A	265	A
1	A	268	A
1	A	277	C
1	A	279	A
1	A	284	C
1	A	285	U
1	A	286	U
1	A	287	G
1	A	288	C
1	A	289	U
1	A	296	G
1	A	297	G
1	A	298	U
1	A	300	G
1	A	302	A
1	A	309	C
1	A	313	A
1	A	315	G
1	A	316	G
1	A	318	A
1	A	321	C
1	A	322	U
1	A	325	U
1	A	327	G
1	A	332	G
1	A	347	A
1	A	352	C
1	A	367	A
1	A	383	A
1	A	392	A
1	A	393	A
1	A	396	C
1	A	399	A
1	A	404	G
1	A	420	G
1	A	426	G
1	A	429	A
1	A	439	G
1	A	446	G
1	A	451	G

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Mol	Chain	Res	Type
1	A	452	A
1	A	491	U
1	A	496	C
1	A	507	G
1	A	517	A
1	A	520	A
1	A	521	G
1	A	524	C
1	A	542	A
1	A	543	U
1	A	544	A
1	A	547	U
1	A	548	C
1	A	551	G
1	A	560	U
1	A	561	G
1	A	569	C
1	A	570	A
1	A	571	A
1	A	572	G
1	A	577	A
1	A	581	C
1	A	586	A
1	A	587	U
1	A	588	G
1	A	596	G
1	A	600	G
1	A	609	A
1	A	610	G
1	A	611	A
1	A	612	A
1	A	613	U
1	A	614	G
1	A	624	G
1	A	631	U
1	A	640	A
1	A	652	A
1	A	654	A
1	A	655	G
1	A	656	A
1	A	660	A
1	A	673	G

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Mol	Chain	Res	Type
1	A	676	A
1	A	677	G
1	A	684	U
1	A	685	A
1	A	692	A
1	A	695	A
1	A	704	U
1	A	722	G
1	A	726	U
1	A	752	G
1	A	753	G
1	A	755	A
1	A	757	A
1	A	759	C
1	A	764	U
1	A	770	A
1	A	778	C
1	A	779	A
1	A	784	C
1	A	787	U
1	A	804	A
1	A	805	G
1	A	808	G
1	A	810	G
1	A	815	G
1	A	817	G
1	A	822	A
1	A	824	U
1	A	832	G
1	A	833	A
1	A	845	G
1	A	852	C
1	A	867	U
1	A	868	U
1	A	878	C
1	A	886	U
1	A	887	G
1	A	889	G
1	A	890	A
1	A	891	A
1	A	900	G
1	A	903	G

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Mol	Chain	Res	Type
1	A	905	G
1	A	909	U
1	A	910	G
1	A	917	C
1	A	919	A
1	A	920	G
1	A	947	G
1	A	948	A
1	A	950	A
1	A	951	A
1	A	956	C
1	A	958	A
1	A	965	U
1	A	966	U
1	A	967	C
1	A	981	A
1	A	985	A
1	A	986	G
1	A	990	G
1	A	992	G
1	A	993	A
1	A	999	A
1	A	1001	G
1	A	1014	A
1	A	1023	A
1	A	1029	G
1	A	1036	A
1	A	1045	C
1	A	1049	A
1	A	1052	U
1	A	1053	A
1	A	1057	G
1	A	1062	G
1	A	1066	A
1	A	1070	G
1	A	1073	U
1	A	1075	U
1	A	1086	A
1	A	1087	G
1	A	1088	A
1	A	1092	C
1	A	1093	U

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Mol	Chain	Res	Type
1	A	1149	C
1	A	1150	G
1	A	1151	A
1	A	1152	G
1	A	1167	A
1	A	1168	A
1	A	1170	U
1	A	1172	U
1	A	1173	A
1	A	1174	C
1	A	1175	C
1	A	1179	G
1	A	1182	A
1	A	1188	A
1	A	1209	A
1	A	1210	C
1	A	1212	A
1	A	1215	A
1	A	1217	G
1	A	1224	G
1	A	1257	A
1	A	1275	G
1	A	1284	A
1	A	1285	G
1	A	1287	G
1	A	1290	A
1	A	1293	G
1	A	1299	A
1	A	1305	A
1	A	1308	G
1	A	1309	A
1	A	1310	A
1	A	1317	G
1	A	1320	A
1	A	1336	U
1	A	1337	A
1	A	1350	C
1	A	1365	U
1	A	1373	G
1	A	1380	U
1	A	1388	U
1	A	1397	G

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Mol	Chain	Res	Type
1	A	1398	C
1	A	1399	C
1	A	1401	A
1	A	1404	G
1	A	1406	C
1	A	1409	A
1	A	1411	G
1	A	1415	U
1	A	1420	A
1	A	1428	G
1	A	1429	A
1	A	1431	A
1	A	1432	U
1	A	1446	G
1	A	1447	U
1	A	1452	G
1	A	1453	U
1	A	1454	U
1	A	1455	U
1	A	1456	G
1	A	1457	A
1	A	1460	A
1	A	1461	A
1	A	1462	U
1	A	1469	A
1	A	1470	C
1	A	1471	G
1	A	1475	U
1	A	1487	U
1	A	1489	C
1	A	1491	U
1	A	1492	G
1	A	1493	C
1	A	1494	G
1	A	1495	A
1	A	1497	U
1	A	1501	A
1	A	1502	G
1	A	1503	U
1	A	1504	G
1	A	1505	C
1	A	1510	C

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Mol	Chain	Res	Type
1	A	1519	G
1	A	1521	G
1	A	1525	U
1	A	1527	A
1	A	1528	G
1	A	1532	A
1	A	1535	U
1	A	1536	A
1	A	1539	U
1	A	1548	C
1	A	1551	U
1	A	1552	A
1	A	1559	A
1	A	1560	G
1	A	1567	C
1	A	1568	G
1	A	1573	G
1	A	1577	A
1	A	1578	A
1	A	1584	G
1	A	1585	U
1	A	1586	A
1	A	1591	A
1	A	1593	U
1	A	1601	G
1	A	1605	C
1	A	1606	A
1	A	1612	A
1	A	1615	A
1	A	1624	U
1	A	1629	A
1	A	1630	G
1	A	1631	A
1	A	1632	A
1	A	1634	A
1	A	1635	C
1	A	1637	A
1	A	1638	C
1	A	1651	A
1	A	1653	A
1	A	1674	G
1	A	1686	G

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Mol	Chain	Res	Type
1	A	1689	A
1	A	1690	G
1	A	1691	C
1	A	1717	G
1	A	1730	G
1	A	1734	C
1	A	1746	G
1	A	1756	U
1	A	1757	U
1	A	1758	C
1	A	1759	G
1	A	1762	C
1	A	1770	G
1	A	1777	G
1	A	1778	G
1	A	1787	A
1	A	1790	G
1	A	1796	C
1	A	1798	A
1	A	1814	C
1	A	1815	A
1	A	1824	A
1	A	1826	A
1	A	1830	A
1	A	1837	G
1	A	1843	A
1	A	1853	G
1	A	1856	G
1	A	1861	A
1	A	1862	A
1	A	1864	G
1	A	1874	U
1	A	1876	G
1	A	1877	G
1	A	1884	U
1	A	1886	G
1	A	1887	G
1	A	1890	A
1	A	1894	U
1	A	1896	A
1	A	1910	A
1	A	1920	G

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Mol	Chain	Res	Type
1	A	1927	A
1	A	1928	C
1	A	1930	A
1	A	1934	C
1	A	1936	G
1	A	1943	G
1	A	1944	G
1	A	1950	A
1	A	1969	U
1	A	1970	U
1	A	1977	C
1	A	1981	C
1	A	1984	A
1	A	1985	A
1	A	1986	G
1	A	1996	U
1	A	2001	G
1	A	2005	U
1	A	2007	U
1	A	2035	G
1	A	2037	A
1	A	2044	A
1	A	2045	A
1	A	2046	G
1	A	2047	A
1	A	2050	C
1	A	2057	C
1	A	2065	A
1	A	2069	C
1	A	2070	G
1	A	2074	A
1	A	2075	G
1	A	2076	A
1	A	2080	C
1	A	2083	G
1	A	2107	G
1	A	2109	G
1	A	2112	U
1	A	2113	U
1	A	2208	C
1	A	2211	U
1	A	2212	A

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Mol	Chain	Res	Type
1	A	2213	A
1	A	2216	C
1	A	2217	G
1	A	2218	C
1	A	2238	G
1	A	2239	A
1	A	2252	G
1	A	2253	G
1	A	2267	G
1	A	2277	C
1	A	2283	A
1	A	2293	G
1	A	2296	G
1	A	2297	C
1	A	2301	A
1	A	2302	A
1	A	2303	G
1	A	2317	G
1	A	2319	U
1	A	2323	A
1	A	2331	C
1	A	2333	A
1	A	2334	A
1	A	2335	G
1	A	2336	A
1	A	2339	G
1	A	2340	U
1	A	2343	A
1	A	2348	G
1	A	2349	A
1	A	2361	C
1	A	2364	C
1	A	2393	G
1	A	2397	G
1	A	2399	C
1	A	2402	A
1	A	2404	U
1	A	2405	G
1	A	2416	U
1	A	2417	C
1	A	2418	C
1	A	2420	C

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Mol	Chain	Res	Type
1	A	2436	C
1	A	2437	U
1	A	2439	A
1	A	2443	G
1	A	2445	U
1	A	2449	A
1	A	2455	C
1	A	2462	A
1	A	2473	A
1	A	2488	C
1	A	2492	A
1	A	2505	U
1	A	2512	C
1	A	2517	A
1	A	2518	U
1	A	2519	G
1	A	2521	C
1	A	2522	G
1	A	2532	A
1	A	2534	C
1	A	2542	U
1	A	2543	G
1	A	2548	C
1	A	2570	C
1	A	2580	A
1	A	2581	G
1	A	2587	C
1	A	2597	G
1	A	2599	U
1	A	2600	C
1	A	2616	A
1	A	2624	C
1	A	2627	U
1	A	2629	U
1	A	2650	U
1	A	2677	G
1	A	2699	G
1	A	2703	U
1	A	2719	A
1	A	2728	G
1	A	2740	U
1	A	2747	A

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Mol	Chain	Res	Type
1	A	2749	G
1	A	2758	G
1	A	2762	A
1	A	2766	C
1	A	2773	G
1	A	2779	A
1	A	2780	G
1	A	2789	A
1	A	2792	A
1	A	2793	U
1	A	2794	G
1	A	2795	A
1	A	2804	A
1	A	2805	U
1	A	2809	U
1	A	2810	U
1	A	2812	A
1	A	2813	A
1	A	2815	A
1	A	2831	G
1	A	2836	G
1	A	2844	A
1	A	2846	A
1	A	2847	U
1	A	2870	G
1	A	2871	A
1	A	2878	G
1	A	2883	G
1	A	2891	C
1	A	2897	G
1	A	2904	G
2	B	7	G
2	B	10	G
2	B	11	A
2	B	13	A
2	B	20	A
2	B	23	A
2	B	24	U
2	B	27	A
2	B	33	U
2	B	35	C
2	B	54	U

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Mol	Chain	Res	Type
2	B	55	A
2	B	57	G
2	B	67	G
2	B	70	G
2	B	73	U
2	B	74	G
2	B	75	U
2	B	78	U
2	B	79	G
2	B	83	G
2	B	85	U
2	B	86	U
2	B	87	U
2	B	91	U
2	B	97	A
2	B	98	G
2	B	99	A
2	B	101	U
2	B	106	C
2	B	107	G
2	B	114	C

All (27) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	13	U
1	A	179	A
1	A	519	A
1	A	655	G
1	A	725	A
1	A	890	A
1	A	947	G
1	A	949	U
1	A	1022	C
1	A	1167	A
1	A	1431	A
1	A	1486	A
1	A	1584	G
1	A	1585	U
1	A	1590	A
1	A	1600	C
1	A	1604	A

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Mol	Chain	Res	Type
1	A	1605	C
1	A	1861	A
1	A	2419	G
1	A	2444	A
1	A	2532	A
1	A	2811	U
1	A	2812	A
2	B	32	U
2	B	90	C
2	B	97	A

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	M	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M	60:ARG	C	61:LEU	N	1.18

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-21907. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal surface views

This section was not generated.

6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.