



Full wwPDB X-ray Structure Validation Report

Nov 23, 2014 – 11:49 AM EST

PDB ID : 4W2D
Title : Crystal structure of the peptolide 12C bound to bacterial ribosome
Authors : Fagan, C.E.; Dunham, C.M.
Deposited on : 2014-03-24
Resolution : 3.60 Å(reported)

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

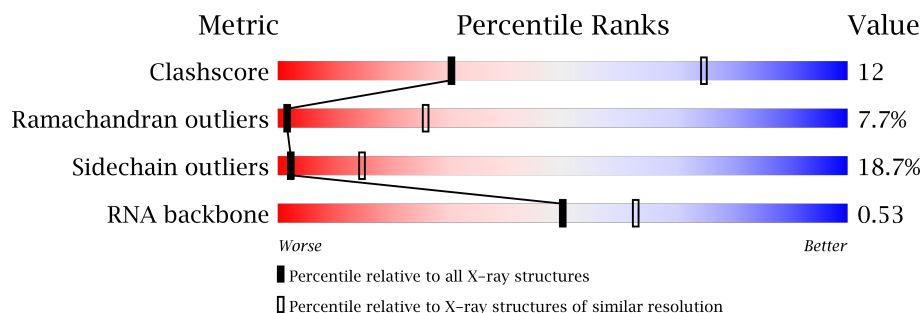
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable24195

1 Overall quality at a glance

The reported resolution of this entry is 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1155 (3.80-3.40)
Ramachandran outliers	78287	1109 (3.80-3.40)
Sidechain outliers	78261	1108 (3.80-3.40)
RNA backbone	1838	1012 (4.40-2.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	2915	
2	B	122	
3	C	276	
4	D	206	
5	E	210	
6	F	182	
7	G	180	
8	H	148	
9	I	140	
10	J	122	
11	K	150	
12	L	141	
13	M	118	
14	N	112	

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Mol	Chain	Length	Quality of chain
15	O	146	
16	P	118	
17	Q	101	
18	R	113	
19	S	96	
20	T	110	
21	U	206	
22	V	85	
23	W	98	
24	X	72	
25	Y	60	
26	Z	71	
27	a	60	
28	b	54	
29	c	49	
30	d	65	
31	e	37	
32	f	12	

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 92327 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2883	Total	C	N	O	P	0	0	0
			62091	27636	11613	19960	2882			

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

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

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			

- Molecule 12 is a protein called 50S ribosomal protein L16.

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

- Molecule 13 is a protein called 50S ribosomal protein L17.

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

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	N	111	Total	C	N	O	0	0	0
			882	556	176	150			

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	R	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	S	92	Total	C	N	O	0	0	0
			725	471	131	123			

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	102	Total	C	N	O	S	0	0	0
			785	505	150	125	5			

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	U	183	Total	C	N	O	S	0	0	0
			1461	933	260	265	3			

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	82	Total	C	N	O	S	0	0	0
			648	401	138	108	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	X	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	Y	59	Total	C	N	O	0	0	0
			469	298	90	81			

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	71	Total	C	N	O	S	0	0	0
			581	364	108	104	5			

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	a	57	Total	C	N	O	S	0	0	0
			442	278	88	71	5			

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	b	49	Total	C	N	O	S	0	0	0
			424	264	87	69	4			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	c	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	d	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	e	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 32 is a protein called T17-GLY-GLY-PRO-LYS-LYS-LYS-LYS-LYS-VAL-GLY-GLY.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
32	f	9	Total	C	N	O	0	0	0
			116	78	18	20			

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	D	2	Total	Mg	0	0
			2	2		
33	K	1	Total	Mg	0	0
			1	1		
33	B	4	Total	Mg	0	0
			4	4		
33	C	1	Total	Mg	0	0
			1	1		
33	c	1	Total	Mg	0	0
			1	1		
33	A	279	Total	Mg	0	0
			279	279		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	L	1	Total	Mg	0	0
			1	1		
33	S	1	Total	Mg	0	0
			1	1		

- Molecule 34 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	e	1	Total	Zn	0	0
			1	1		

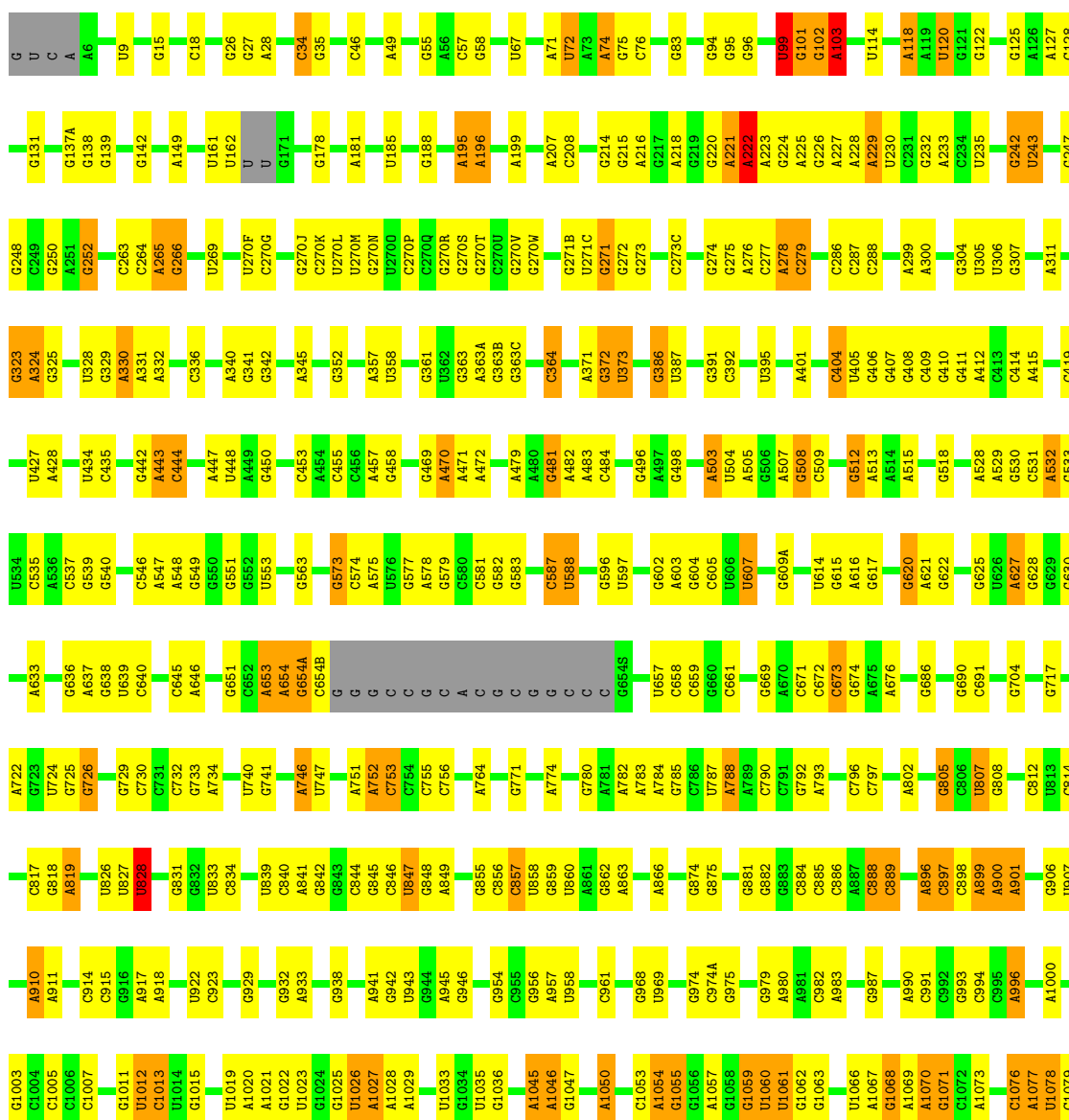
3 Residue-property plots

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

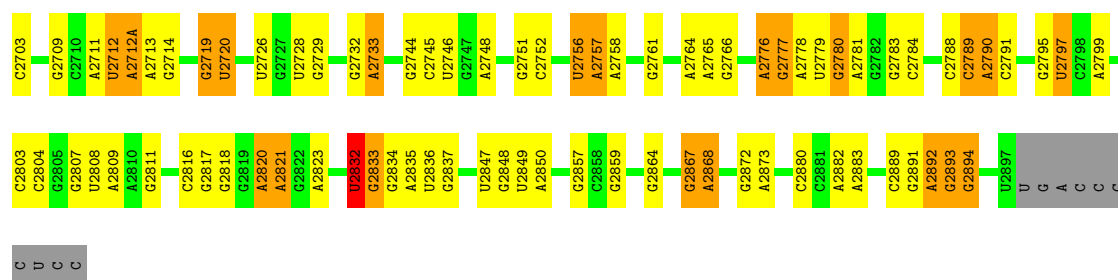
Note EDS was not executed.

• Molecule 1: 23S ribosomal RNA

Chain A:

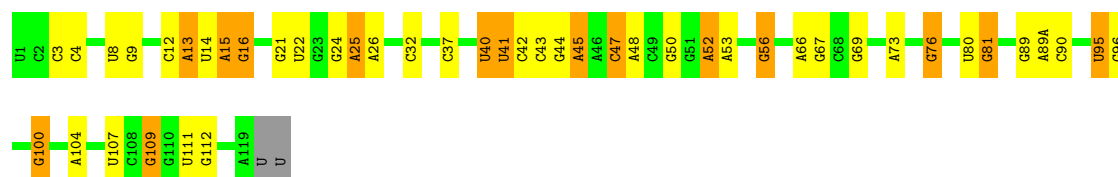


U2609	A2393	G2304	G2190	G2110	G1899	A1787	G1674	A1569	C1467	G1368	G1264	G1169	G1080
C2610	C2394	A2305	G2191	C2111	C1902	C1790	G1678	A1570	A1471	G1369	A1265	G1170	U1081
U2611	C2395	C2306	G2192	G2112	G1903	A1791	G1679	U1578	A1472	G1370	G1266	G1171	U1082
C2612	U2401	G2307	G2193	U2113	G1903	A1791	U1680	U1579	G1473	G1371	G1270	G1172	U1083
U2613	U2402	A2308	U2197	A2114	G1910	U1794	U1688	A1580	G1479	U1372	C1270	U1175	A1084
A2614	C2403	A2309	A2198	G2115	C1914	C1795	U1689	C1585	G1480	A1373	A1272	G1176	A1085
U2615	C2404	A2310	A2199	G2116	U1915	U1796	A1689	U1586	G1481	U1374	U1273	A1177	A1086
C2616	C2405	U2312	G2210	A2117	U1916	U1797	C1694	A1587	G1482	A1379	C1178	A1178	A1087
U2617	U2406	A2311	G2211	A2118	U1917	U1798	G1695	A1588	G1483	U1482	C1179	A1179	A1088
G2618	A2407	U2312	A2212	G2120	U1917	G1799	G1696	C1589	A1490	G1380	C1180	C1180	U1090
C2619	G2410	G2315	U2213	G2121	A1918	C1800	G1697	C1589	A1384	A1287	G1183	G1092	G1091
G2620	G2411	G2318	U2215	G2123	A1919	G1801	G1698	C1589	G1385	G1287	G1183	G1092	G1092
A2621	G2415	G2319	G2224	G2124	C1920	A1802	A1698	C1589	G1386	C1291	G1186	G1093	G1093
U2622	U2528	A2320	G2225	A2125	U1926	A1803	G1699	C1589	U1391	U1292	G1187	U1094	U1094
C2623	U2529	A2321	A2226	G2126	U1927	A1803	A1700	G1595	U1497	G1188	A1189	A1095	A1095
A2624	U2530	U2322	C2227	G2127	A1928	A1810	G1703	C1598	C1498	G1296	U1189	U1097	U1097
U2625	A2425	G2324	A2227	C2128	G1929	A1816	G1703	C1599	G1500	U1300	G1190	A1098	A1098
C2626	U2537	A2325	U2232	G2131	U1930	G1816	G1717	C1599	U1396	A1301	G1195	G1099	G1099
U2627	C2538	A2326	U2233	U2132	G1931	A1819	G1718	A1603	C1506	G1195	G1195	G1100	G1100
A2628	U2542	A2327	U2234	G2133	A1932	U1820	G1725	C1607	A1507	G1311	C1201	U1101	U1101
G2629	G2543	G2330	G2238	G2134	U1933	U1821	G1726	A1608	A1508	U1312	G1202	A1103	A1103
C2630	A2434	U2331	G2239	G2135	U1934	A1822	U1730	A1609	C1509	U1313	G1203	A1104	A1104
U2631	A2435	G2332	U2243	C2136	A1937	A1823	G1728	A1610	A1510	U1314	G1204	U1105	U1105
A2632	U2554	A2333	U2244	C2137	A1938	A1824	U1729	A1611	A1511	U1315	A1205	G1106	G1106
C2633	U2555	A2334	U2245	G2138	U1939	A1825	U1730	A1612	U1512	U1316	G1206	G1107	G1107
G2634	C2556	A2335	U2246	G2139	A1940	A1826	G1731	A1613	A1513	A1317	G1207	G1108	G1108
U2635	U2557	A2336	G2247	G2140	U1941	A1827	U1732	A1614	U1514	A1318	G1208	G1109	G1109
C2636	C2558	A2337	U2248	G2141	U1942	A1828	U1733	A1615	U1515	A1319	G1209	G1110	G1110
U2637	U2559	A2338	U2249	G2142	U1943	A1829	G1734	A1616	U1516	U1320	G1210	A1111	A1111
G2638	U2560	A2339	U2250	G2143	U1944	A1830	U1735	A1617	G1522	U1321	U1211	G1112	G1112
U2639	U2561	A2340	G2251	G2144	U1945	A1831	G1736	A1618	G1416	U1322	G1212	G1113	G1113
C2640	U2562	A2341	G2252	G2145	U1946	A1832	U1737	A1619	A1528	A1323	A1220	G1114	G1114
U2641	U2563	A2342	G2253	G2146	U1947	A1833	U1738	A1620	A1529	G1332	G1223	G1122	G1122
G2642	U2564	A2343	U2254	G2147	U1948	A1834	U1739	A1621	A1530	G1333	G1224	G1123	G1123
C2643	U2565	A2344	U2255	G2148	U1949	A1835	U1740	A1622	G1533	G1334	G1225	G1124	G1124
U2644	U2566	A2345	U2256	G2149	U1950	A1836	U1741	A1623	G1534	U1341	G1226	U1130	U1130
G2645	U2567	A2346	U2257	G2150	U1951	A1837	U1742	A1624	A1535	A1342	A1227	G1131	G1131
C2646	U2568	A2347	U2258	G2151	U1952	A1838	U1743	A1625	A1536	G1343	G1231	G1132	G1132
U2647	U2569	A2348	U2259	G2152	U1953	A1839	U1744	A1626	A1537	G1344	G1232	G1133	G1133
G2648	U2570	A2349	U2260	G2153	U1954	A1840	U1745	A1627	G1538	G1345	G1233	G1134	G1134
U2649	U2571	A2350	U2261	G2154	U1955	A1841	U1746	A1628	U1541	G1346	G1234	G1135	G1135
C2649	U2572	A2351	U2262	G2155	U1956	A1842	U1747	A1629	A1542	U1347	G1235	G1136	G1136
G2650	U2573	A2352	U2263	G2156	U1957	A1843	U1748	A1630	A1543	U1348	G1236	G1137	G1137
U2651	U2574	A2353	U2264	G2157	U1958	A1844	U1749	A1631	A1544	G1349	G1237	G1138	G1138
C2652	U2575	A2354	U2265	G2158	U1959	A1845	U1750	A1632	A1545	U1350	G1238	G1139	G1139
U2653	U2576	A2355	U2266	G2159	U1960	A1846	U1751	A1633	G1546	U1351	G1239	G1140	G1140
G2654	U2577	A2356	U2267	G2160	U1961	A1847	U1752	A1634	U1547	G1352	G1240	U1141	U1141
U2655	U2578	A2357	U2268	G2161	U1962	A1848	U1753	A1635	G1548	U1353	G1241	U1142	U1142
C2656	U2579	A2358	U2269	G2162	U1963	A1849	U1754	A1636	U1549	G1354	G1242	A1142A	A1142A
U2657	U2580	A2359	U2270	G2163	U1964	A1850	U1755	A1637	G1550	U1355	G1243	G1149	G1149
G2658	U2581	A2360	U2271	G2164	U1965	A1851	U1756	A1638	A1551	G1356	G1244	G1150	G1150
C2659	U2582	A2361	U2272	G2165	U1966	A1852	U1757	A1639	A1552	U1357	G1245	G1151	G1151
U2660	U2583	A2362	U2273	G2166	U1967	A1853	U1758	A1640	A1553	G1358	G1246	G1152	G1152
G2661	U2584	A2363	U2274	G2167	U1968	A1854	U1759	A1641	A1554	U1359	G1247	G1153	G1153
U2662	U2585	A2364	U2275	G2168	U1969	A1855	U1760	A1642	A1555	U1360	G1248	G1154	G1154
C2663	U2586	A2365	U2276	G2169	U1970	A1856	U1761	A1643	A1556	U1361	G1249	G1155	G1155
U2664	U2587	A2366	U2277	G2170	U1971	A1857	U1762	A1644	A1557	U1362	G1250	G1156	G1156
G2665	U2588	A2367	U2278	G2171	U1972	A1858	U1763	A1645	A1558	U1363	G1251	G1157	G1157
U2666	U2589	A2368	U2279	G2172	U1973	A1859	U1764	A1646	A1559	U1364	G1252	G1158	G1158
C2667	U2590	A2369	U2280	G2173	U1974	A1860	U1765	A1647	A1560	U1365	G1253	G1159	G1159
U2668	U2591	A2370	U2281	G2174	U1975	A1861	U1766	A1648	A1561	G1366	G1254	G1160	G1160
G2669	U2592	A2371	U2282	G2175	U1976	A1862	U1767	A1649	A1562	U1367	G1255	G1161	G1161
U2670	U2593	A2372	U2283	G2176	U1977	A1863	U1768	A1650	A1563	G1368	G1256	G1162	G1162
C2671	U2594	A2373	U2284	G2177	U1978	A1864	U1769	A1651	A1564	U1369	G1257	G1163	G1163
U2672	U2595	A2374	U2285	G2178	U1979	A1865	U1770	A1652	A1565	U1370	G1258	G1164	G1164
G2673	U2596	A2375	U2286	G2179	U1980	A1866	U1771	A1653	A1566	U1371	G1259	G1165	G1165
U2674	U2597	A2376	U2287	G2180	U1981	A1867	U1772	A1654	A1567	U1372	G1260	G1166	G1166
C2675	U2598	A2377	U2288	G2181	U1982	A1868	U1773	A1655	A1568	U1373	G1261	G1167	G1167
U2676	U2599	A2378	U2289	G2182	U1983	A1869	U1774	A1656	A1569	U1374	G1262	G1168	G1168
G2677	U2600	A2379	U2290	G2183	U1984	A1870	U1775	A1657	A1570	U1375	G1263	G1169	G1169
C2678	U2601	A2380	U2291	G2184	U1985	A1871	U1776	A1658	A1571	U1376	G1264	G1170	G1170
U2679	U2602	A2381	U2292	G2185	U1986	A1872	U1777	A1659	A1572	U1377	G1265	G1171	G1171
G2680	U2603	A2382	U2293	G2186	U1987	A1873	U1778	A1660	A1573	U1378	G1266	G1172	G1172
C2681	U2604	A2383	U2294	G2187	U1988	A1874	U1779	A1661	A1574	U1379	G1267	G1173	G1173
U2682	U2605	A2384	U2295	G2188	U1989	A1875	U1780	A1662	A1575	U1380	G1268	G1174	G1174
G2683	U2606	A2385	U2296	G2189	U1990	A1876	U1781	A1663	A1576	U1381	G1269	G1175	G1175
U2684	U2607	A2386	U2297	G2190	U1991	A1877	U1782	A1664	A1577	U1382	G1270	G1176	G1176
C2685	U2608	A2387	U2298	G2191	U1992	A1878	U1783	A1665	A1578	U1383	G1271	G1177	G1177
U2686	U2609	A2388	U2299	G2192	U1993	A1879	U1784	A1666	A1579	U1384	G1272	G1178	G1178
G2687	U2610	A2389	U2300	G2193	U1994	A1880	U1785	A1667	A1580	U1385	G1273	G1179	G1179
U2688	U2611	A2390	U2301	G2194	U1995	A1881	U1786	A1668	A1581	U1386	G1274	G1180	G1180
C2689	U2612	A2391	U2302	G2195	U1996	A1882	U1787	A1669	A1582	U1387	G1275	G1181	G1181
U2690	U2613	A2392	U2303	G2196	U1997	A1883	U1788	A1670	A1583	U1388	G1276	G1182	G1182
G2691	U2614	A2393	U2304	G2197	U1998	A1884	U1789	A1671	A1584	U1389	G1277	G1183	G1183
U2692	U2615	A2394	U2305	G2198	U1999	A1885	U1790	A1672	A1585	U1390	G1278	G1184	G1184
C2693	U2616	A2395	U2306	G2199	U2000	A1886	U1791	A1673	A1586	U1391	G1279	G1185	G1185
U2694	U2617	A2396	U2307	G2200	U2001	A1887	U1792	A1674	A1587	U1392	G1280	G1186	G1186
G2695	U2618	A2397	U2308	G2201	U2002	A1888	U1793	A1675	A1588	U1393	G1281	G1187	G1187
U2696	U2619	A2398	U2309	G2202	U2003	A1889	U1794	A1676	A1589	U1394	G1282	G1188	G1188
C2697	U2620	A2399	U2310	G2203	U2004	A1890	U1795						



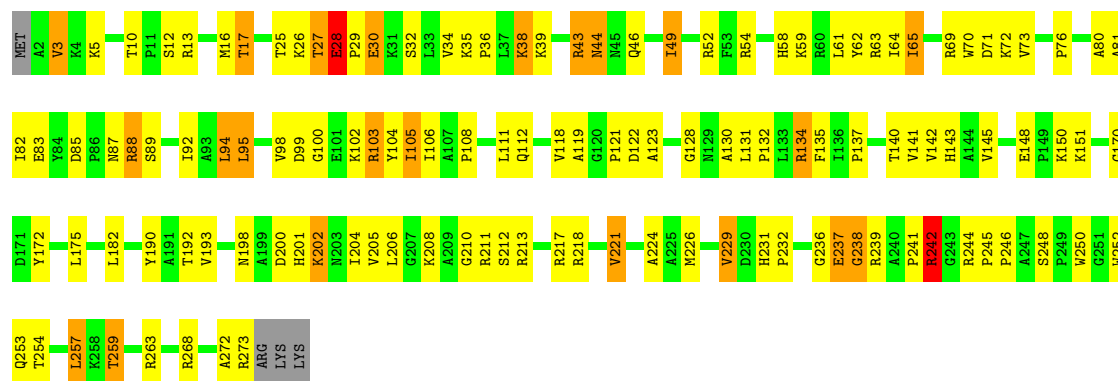
• Molecule 2: 5S ribosomal RNA

Chain B:



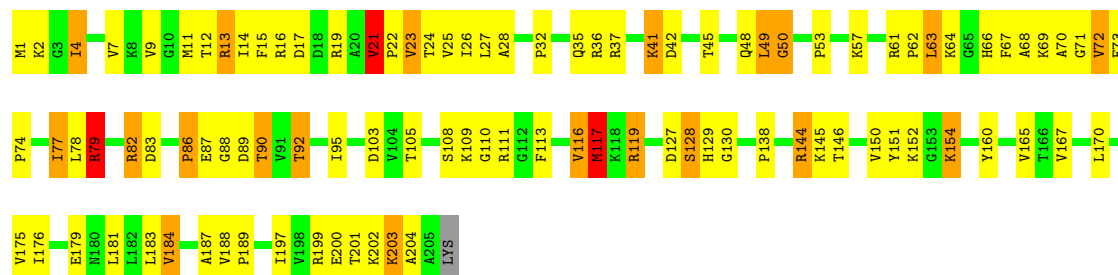
• Molecule 3: 50S ribosomal protein L2

Chain C:



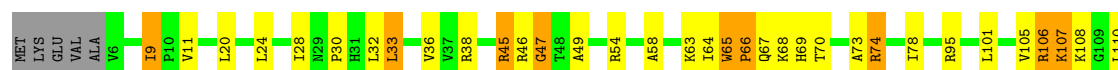
• Molecule 4: 50S ribosomal protein L3

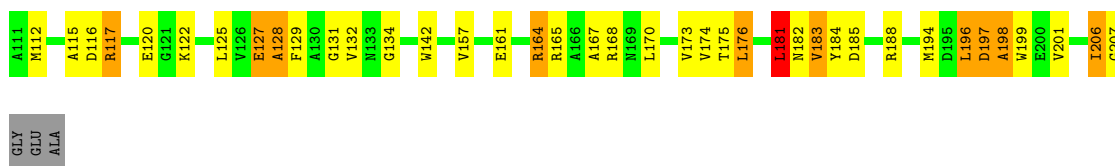
Chain D:



• Molecule 5: 50S ribosomal protein L4

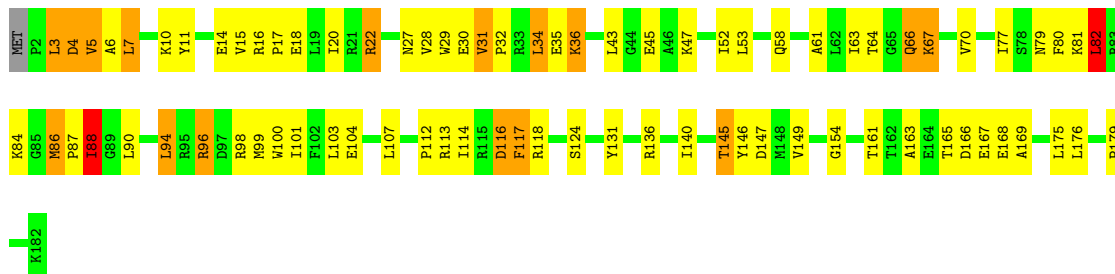
Chain E:





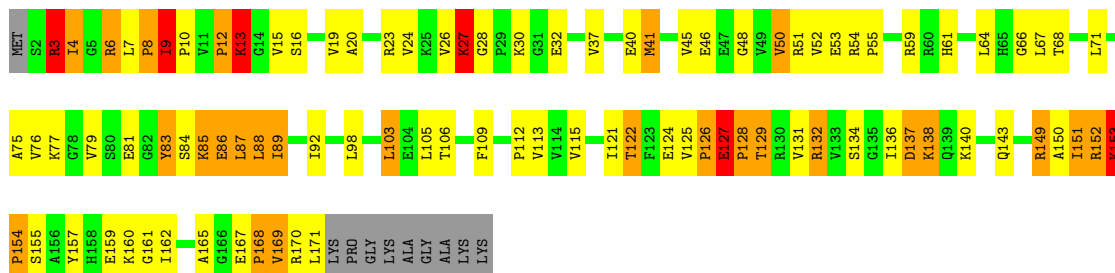
• Molecule 6: 50S ribosomal protein L5

Chain F:



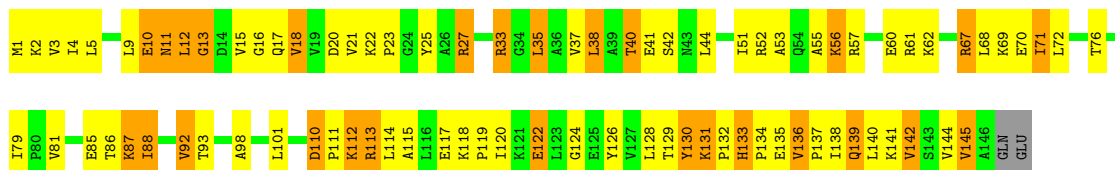
• Molecule 7: 50S ribosomal protein L6

Chain G:



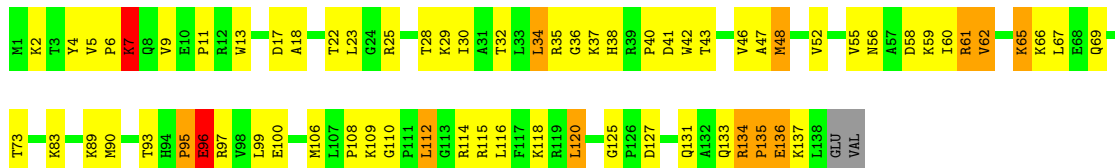
• Molecule 8: 50S ribosomal protein L9

Chain H:



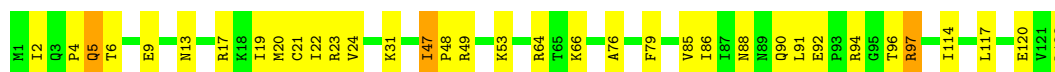
• Molecule 9: 50S ribosomal protein L13

Chain I:



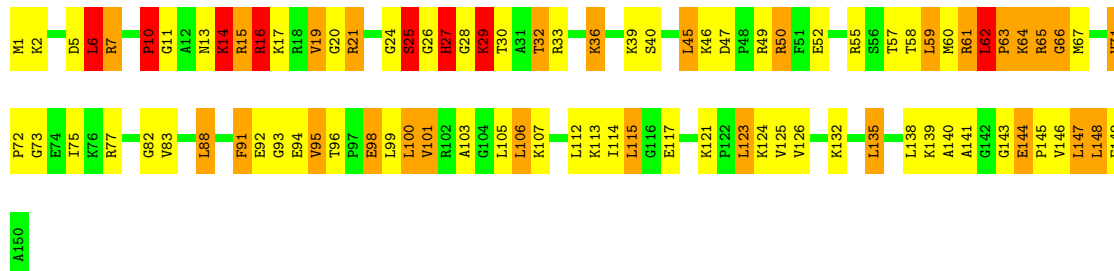
• Molecule 10: 50S ribosomal protein L14

Chain J:



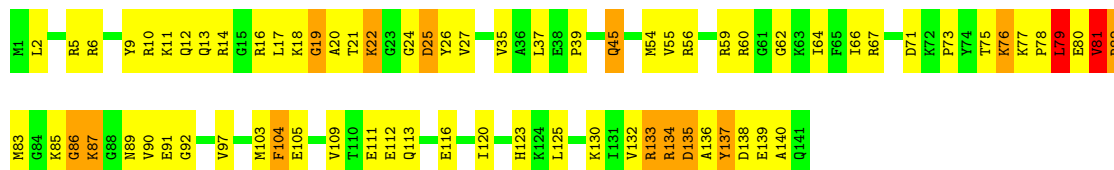
- Molecule 11: 50S ribosomal protein L15

Chain K:



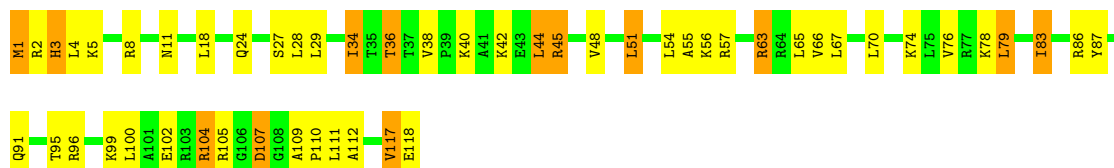
- Molecule 12: 50S ribosomal protein L16

Chain L:



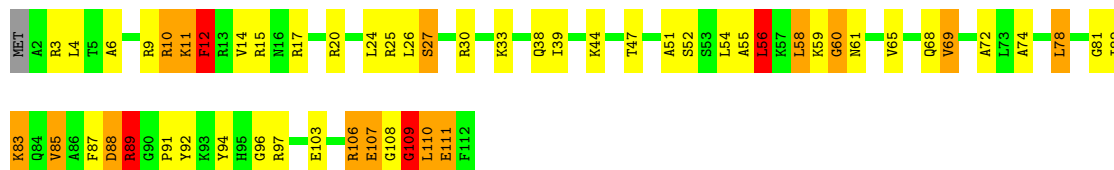
- Molecule 13: 50S ribosomal protein L17

Chain M:



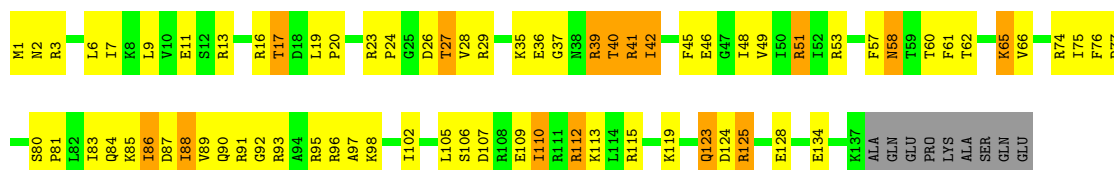
- Molecule 14: 50S ribosomal protein L18

Chain N:



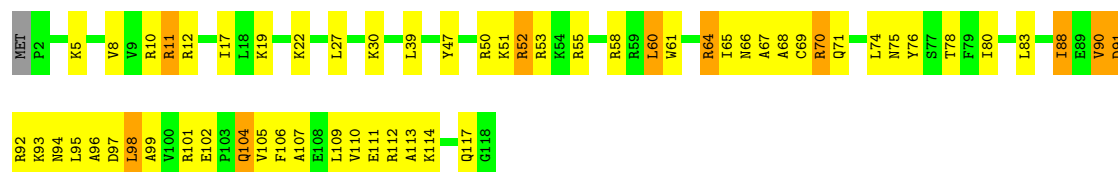
- Molecule 15: 50S ribosomal protein L19

Chain O:



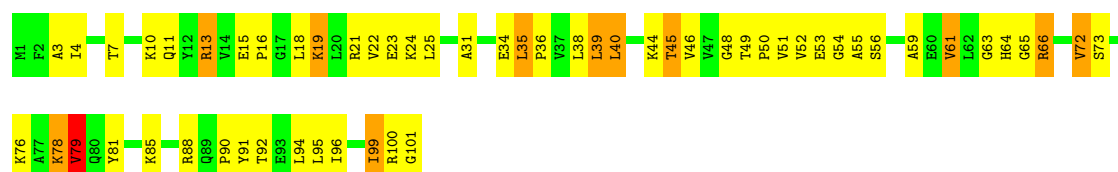
- Molecule 16: 50S ribosomal protein L20

Chain P: 



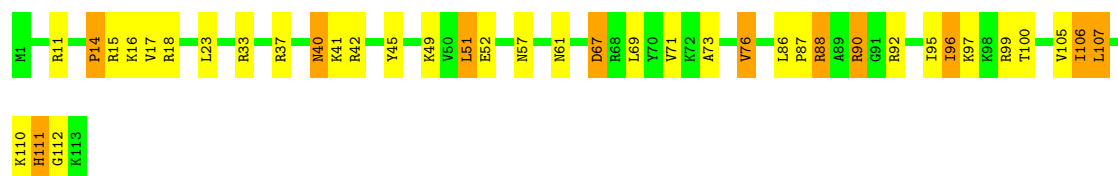
- Molecule 17: 50S ribosomal protein L21

Chain Q: 



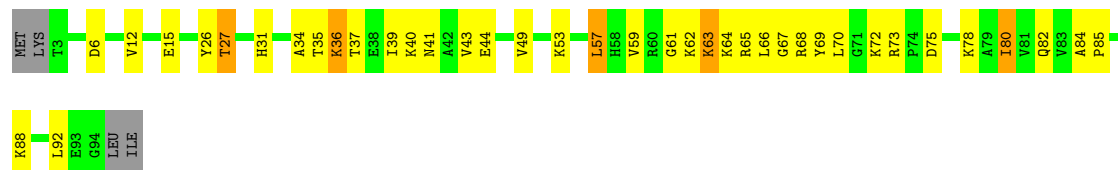
- Molecule 18: 50S ribosomal protein L22

Chain R: 



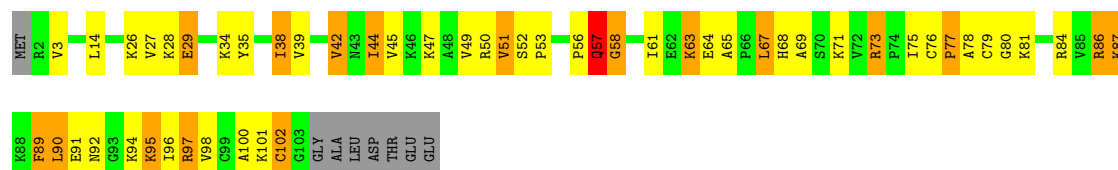
- Molecule 19: 50S ribosomal protein L23

Chain S: 



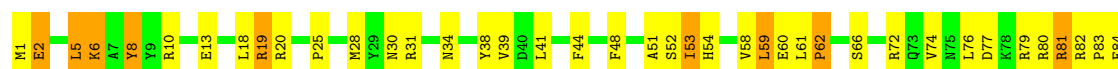
- Molecule 20: 50S ribosomal protein L24

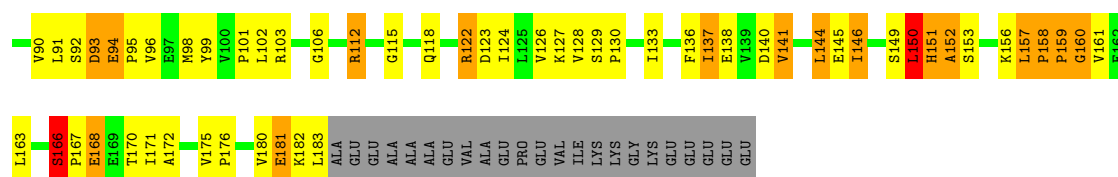
Chain T: 



- Molecule 21: 50S ribosomal protein L25

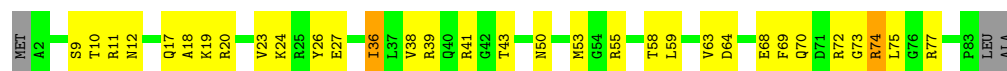
Chain U: 





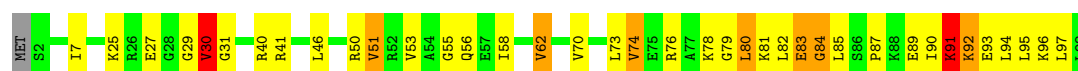
- Molecule 22: 50S ribosomal protein L27

Chain V:



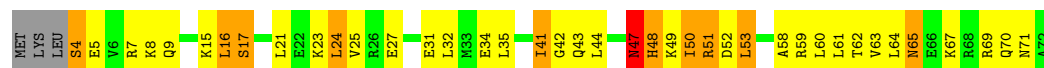
- Molecule 23: 50S ribosomal protein L28

Chain W:



- Molecule 24: 50S ribosomal protein L29

Chain X:



- Molecule 25: 50S ribosomal protein L30

Chain Y:



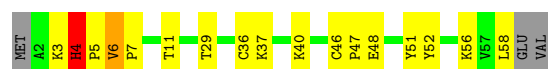
- Molecule 26: 50S ribosomal protein L31

Chain Z:



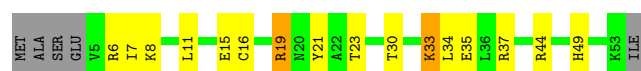
- Molecule 27: 50S ribosomal protein L32

Chain a:



- Molecule 28: 50S ribosomal protein L33

Chain b:



- Molecule 29: 50S ribosomal protein L34

Chain c: 



- Molecule 30: 50S ribosomal protein L35

Chain d: 



- Molecule 31: 50S ribosomal protein L36

Chain e: 



- Molecule 32: T17-GLY-GLY-PRO-LYS-LYS-LYS-LYS-LYS-VAL-GLY-GLY

Chain f: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.24Å 443.46Å 618.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.79 – 3.60	Depositor
% Data completeness (in resolution range)	98.1 (49.79-3.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PHENIX (phenix.refine: 1.8.3_1479)	Depositor
R, R_{free}	0.222 , 0.254	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	92327	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, T17, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.29	0/69543	0.83	41/108563 (0.0%)
2	B	0.29	0/2878	0.91	11/4490 (0.2%)
3	C	0.57	0/2165	0.77	1/2919 (0.0%)
4	D	0.48	1/1601 (0.1%)	0.74	2/2160 (0.1%)
5	E	0.48	0/1620	0.71	1/2194 (0.0%)
6	F	0.40	0/1499	0.60	0/2016
7	G	0.50	1/1332 (0.1%)	0.76	2/1802 (0.1%)
8	H	0.38	0/1151	0.66	0/1558
9	I	0.43	0/1131	0.64	0/1525
10	J	0.50	0/943	0.65	0/1269
11	K	0.55	2/1162 (0.2%)	0.93	4/1544 (0.3%)
12	L	0.56	0/1143	0.78	0/1527
13	M	0.45	0/982	0.73	0/1312
14	N	0.39	0/892	0.71	0/1187
15	O	0.44	0/1155	0.67	0/1542
16	P	0.50	0/982	0.69	0/1306
17	Q	0.46	0/790	0.73	1/1057 (0.1%)
18	R	0.45	0/911	0.68	0/1220
19	S	0.50	0/739	0.66	0/993
20	T	0.45	0/798	0.69	0/1064
21	U	0.45	2/1493 (0.1%)	0.68	4/2026 (0.2%)
22	V	0.48	0/657	0.69	0/874
23	W	0.46	0/770	0.69	0/1022
24	X	0.52	0/583	0.73	0/771
25	Y	0.41	0/474	0.59	0/635
26	Z	0.37	0/594	0.69	0/795
27	a	0.68	3/456 (0.7%)	0.89	3/617 (0.5%)
28	b	0.37	0/431	0.68	0/575
29	c	0.57	0/438	0.71	0/575
30	d	0.58	0/525	0.82	0/691
31	e	0.32	0/310	0.48	0/407
32	f	0.25	0/56	0.45	0/70

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.35	9/100204 (0.0%)	0.80	70/150306 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	E	0	1
7	G	0	1
14	N	0	1
21	U	0	1
24	X	0	1
30	d	0	2
All	All	0	7

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	63	PRO	N-CD	6.16	1.56	1.47
21	U	159	PRO	N-CD	5.60	1.55	1.47
27	a	5	PRO	N-CD	5.52	1.55	1.47
11	K	10	PRO	N-CD	5.41	1.55	1.47
4	D	22	PRO	N-CD	5.35	1.55	1.47
21	U	158	PRO	N-CD	5.34	1.55	1.47
27	a	47	PRO	N-CD	5.31	1.55	1.47
7	G	154	PRO	N-CD	5.28	1.55	1.47
27	a	7	PRO	N-CD	5.09	1.54	1.47

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	771	G	C2-N3-C4	-10.26	106.77	111.90
1	A	771	G	N9-C4-C5	-8.13	102.15	105.40
1	A	673	C	C2-N3-C4	-7.98	115.91	119.90
2	B	81	G	C5-C6-O6	-7.36	124.18	128.60
1	A	1950	G	N3-C4-N9	6.93	130.16	126.00
1	A	807	U	C2-N3-C4	-6.93	122.84	127.00
1	A	1950	G	O4'-C1'-N9	6.46	113.37	108.20
2	B	81	G	N3-C4-N9	6.37	129.82	126.00
1	A	828	U	C2-N1-C1'	6.32	125.28	117.70
1	A	771	G	C8-N9-C4	6.31	108.92	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	81	G	C4-N9-C1'	6.31	134.70	126.50
2	B	81	G	C6-C5-N7	-6.27	126.64	130.40
1	A	103	A	N1-C6-N6	6.26	122.36	118.60
1	A	2335	A	O4'-C1'-N9	6.20	113.16	108.20
2	B	81	G	C8-N9-C1'	-6.13	119.03	127.00
1	A	906	G	C5-C6-O6	6.08	132.25	128.60
2	B	95	U	C5-C4-O4	6.02	129.51	125.90
17	Q	35	LEU	CA-CB-CG	5.99	129.08	115.30
5	E	74	ARG	NE-CZ-NH1	5.87	123.24	120.30
7	G	9	ILE	C-N-CD	5.87	140.72	128.40
27	a	6	VAL	C-N-CD	5.84	140.66	128.40
1	A	103	A	C4-C5-C6	5.82	119.91	117.00
2	B	76	G	N3-C2-N2	-5.82	115.83	119.90
1	A	828	U	N1-C2-O2	5.77	126.84	122.80
2	B	76	G	C6-N1-C2	-5.77	121.64	125.10
1	A	1130	U	P-O3'-C3'	5.70	126.54	119.70
27	a	46	CYS	C-N-CD	5.69	140.35	128.40
1	A	2506	U	C2-N1-C1'	5.67	124.50	117.70
1	A	669	G	C4-N9-C1'	5.66	133.86	126.50
11	K	59	LEU	CA-CB-CG	5.66	128.31	115.30
11	K	10	PRO	CA-N-CD	-5.58	103.68	111.50
1	A	673	C	N3-C4-C5	5.58	124.13	121.90
1	A	2447	G	C6-N1-C2	-5.58	121.75	125.10
3	C	229	VAL	CB-CA-C	-5.56	100.84	111.40
1	A	828	U	N3-C2-O2	-5.56	118.31	122.20
1	A	771	G	C4-C5-N7	5.53	113.01	110.80
1	A	99	U	P-O3'-C3'	5.52	126.32	119.70
7	G	153	LYS	C-N-CD	5.51	139.98	128.40
4	D	21	VAL	C-N-CD	5.50	139.96	128.40
1	A	771	G	N3-C4-C5	5.46	131.33	128.60
1	A	99	U	OP2-P-O3'	5.41	117.10	105.20
1	A	1313	U	C2-N1-C1'	5.38	124.16	117.70
1	A	1950	G	C8-N9-C1'	-5.37	120.02	127.00
2	B	100	G	C8-N9-C1'	5.37	133.97	127.00
21	U	115	GLY	N-CA-C	-5.36	99.71	113.10
21	U	158	PRO	C-N-CD	5.32	139.57	128.40
11	K	25	SER	N-CA-C	-5.29	96.71	111.00
21	U	157	LEU	C-N-CD	5.27	139.46	128.40
1	A	503	A	P-O3'-C3'	5.26	126.01	119.70
1	A	2378	A	N1-C6-N6	5.26	121.75	118.60
11	K	62	LEU	C-N-CD	5.24	139.41	128.40
1	A	1950	G	C4-N9-C1'	5.23	133.30	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1779	U	C2-N1-C1'	5.22	123.96	117.70
1	A	1372	U	C5-C4-O4	-5.16	122.81	125.90
2	B	81	G	O4'-C1'-N9	5.14	112.31	108.20
2	B	81	G	N1-C6-O6	5.11	122.97	119.90
1	A	2832	U	P-O3'-C3'	5.11	125.83	119.70
1	A	222	A	P-O3'-C3'	5.10	125.82	119.70
1	A	2053	G	C5-N7-C8	-5.10	101.75	104.30
1	A	669	G	C8-N9-C1'	-5.09	120.38	127.00
1	A	1396	U	N1-C2-O2	5.09	126.36	122.80
1	A	807	U	C5-C4-O4	-5.05	122.87	125.90
1	A	1141	U	C2-N3-C4	-5.05	123.97	127.00
1	A	1992	G	P-O3'-C3'	5.04	125.75	119.70
4	D	117	MET	CA-CB-CG	5.04	121.87	113.30
27	a	4	HIS	C-N-CD	5.03	138.97	128.40
1	A	404	C	P-O3'-C3'	5.03	125.74	119.70
21	U	150	LEU	CA-CB-CG	5.03	126.86	115.30
1	A	2681	C	P-O3'-C3'	5.02	125.73	119.70
1	A	1558	A	P-O3'-C3'	5.01	125.71	119.70

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	E	47	GLY	Peptide
7	G	127	GLU	Peptide
14	N	109	GLY	Peptide
21	U	181	GLU	Peptide
24	X	17	SER	Peptide
30	d	30	ARG	Peptide
30	d	51	ALA	Peptide

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	62091	0	31294	688	0
2	B	2573	0	1306	35	0
3	C	2115	0	2195	128	0
4	D	1568	0	1634	78	0
5	E	1585	0	1632	63	0
6	F	1474	0	1535	54	0
7	G	1307	0	1382	89	0
8	H	1136	0	1223	48	0
9	I	1104	0	1180	50	0
10	J	933	0	996	19	0
11	K	1145	0	1228	83	0
12	L	1122	0	1178	50	0
13	M	968	0	1033	33	0
14	N	882	0	943	45	0
15	O	1141	0	1202	50	0
16	P	964	0	1022	52	0
17	Q	779	0	852	43	0
18	R	900	0	964	26	0
19	S	725	0	778	21	0
20	T	785	0	878	40	0
21	U	1461	0	1493	80	0
22	V	648	0	672	29	0
23	W	763	0	848	28	0
24	X	581	0	629	23	0
25	Y	469	0	518	15	0
26	Z	581	0	574	47	0
27	a	442	0	465	0	0
28	b	424	0	450	0	0
29	c	430	0	480	0	0
30	d	517	0	582	0	0
31	e	307	0	336	0	0
32	f	116	0	67	0	0
33	A	279	0	0	0	0
33	B	4	0	0	0	0
33	C	1	0	0	0	0
33	D	2	0	0	0	0
33	K	1	0	0	0	0
33	L	1	0	0	0	0
33	S	1	0	0	0	0
33	c	1	0	0	0	0
34	e	1	0	0	0	0
All	All	92327	0	61569	1694	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including

hydrogens) of the entry. The overall clashscore for this entry is 12.

All (1694) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:L:134:ARG:CZ	21:U:122:ARG:HH21	1.34	1.39
4:D:14:ILE:HG22	4:D:21:VAL:CG2	1.56	1.35
3:C:121:PRO:HB3	3:C:135:PHE:CE2	1.64	1.31
4:D:14:ILE:CG2	4:D:21:VAL:HG23	1.62	1.29
21:U:93:ASP:O	21:U:94:GLU:HG2	1.10	1.24
3:C:121:PRO:CB	3:C:135:PHE:HE2	1.55	1.18
3:C:121:PRO:CB	3:C:135:PHE:CE2	2.34	1.09
12:L:134:ARG:CZ	21:U:122:ARG:NH2	2.16	1.09
8:H:53:ALA:O	8:H:57:ARG:HG3	1.52	1.08
1:A:1169:G:H1	1:A:1180:C:N4	1.52	1.07
7:G:10:PRO:HG2	7:G:50:VAL:HG13	1.32	1.06
21:U:93:ASP:O	21:U:94:GLU:CG	2.03	1.05
21:U:91:LEU:HG	21:U:130:PRO:HB3	1.41	1.03
1:A:1359:A:N6	1:A:1372:U:N3	2.07	1.02
4:D:24:THR:HG21	4:D:188:VAL:HG11	1.37	1.02
7:G:10:PRO:CG	7:G:50:VAL:HG13	1.91	0.99
1:A:2099:U:H3	1:A:2190:G:H1	1.05	0.98
1:A:2287:A:H62	1:A:2344:U:H3	1.04	0.98
4:D:14:ILE:CG2	4:D:21:VAL:CG2	2.29	0.98
1:A:2701:C:H3'	1:A:2702:U:H5''	1.43	0.97
14:N:59:LYS:HD3	14:N:60:GLY:N	1.80	0.97
4:D:24:THR:HG21	4:D:188:VAL:CG1	1.97	0.95
5:E:68:LYS:HG2	5:E:69:HIS:CE1	2.02	0.94
3:C:121:PRO:CA	3:C:135:PHE:CE2	2.50	0.94
5:E:68:LYS:HG2	5:E:69:HIS:ND1	1.83	0.94
1:A:896:A:H1'	21:U:176:PRO:HB3	1.50	0.94
21:U:95:PRO:HG2	21:U:127:LYS:HD3	1.48	0.94
1:A:1533:C:H42	1:A:1538:G:H1	1.01	0.93
3:C:121:PRO:HA	3:C:135:PHE:CE2	2.03	0.93
3:C:121:PRO:CA	3:C:135:PHE:HE2	1.82	0.92
3:C:121:PRO:HA	3:C:135:PHE:CD2	2.05	0.92
14:N:59:LYS:HD3	14:N:60:GLY:H	1.34	0.91
1:A:49:A:N7	1:A:120:U:C4	2.38	0.91
8:H:52:ARG:O	8:H:56:LYS:HB3	1.71	0.91
1:A:993:G:OP1	16:P:50:ARG:NH2	2.04	0.91
1:A:1338:G:N7	19:S:62:LYS:NZ	2.20	0.90
21:U:151:HIS:HB3	21:U:170:THR:HA	1.54	0.90
1:A:1359:A:N6	1:A:1372:U:H3	1.71	0.89
4:D:50:GLY:HA2	4:D:77:ILE:HA	1.53	0.89
12:L:134:ARG:NH1	21:U:122:ARG:HH21	1.69	0.89

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:T:79:CYS:SG	20:T:80:GLY:N	2.45	0.88
7:G:152:ARG:HG3	7:G:153:LYS:HD2	1.53	0.88
7:G:10:PRO:HD3	7:G:50:VAL:O	1.73	0.87
7:G:109:PHE:CZ	7:G:152:ARG:HD3	2.09	0.87
1:A:847:U:O4	1:A:933:A:N1	2.08	0.87
20:T:76:CYS:HB3	20:T:96:ILE:HD13	1.57	0.87
1:A:1533:C:N4	1:A:1538:G:H1	1.73	0.86
1:A:1138:G:H21	9:I:106:MET:HE3	1.41	0.86
18:R:18:ARG:HG3	18:R:76:VAL:HG13	1.58	0.85
11:K:58:THR:O	11:K:61:ARG:NE	2.09	0.84
15:O:26:ASP:HB3	15:O:92:GLY:H	1.42	0.84
9:I:4:TYR:O	16:P:64:ARG:NH1	2.10	0.84
1:A:67:U:H3	1:A:74:A:H2	1.25	0.84
21:U:145:GLU:HG3	21:U:146:ILE:HG12	1.59	0.83
1:A:2098:U:H3	1:A:2191:G:H1	1.26	0.83
7:G:12:PRO:HD3	7:G:48:GLY:O	1.77	0.83
1:A:483:A:H4'	20:T:49:VAL:HA	1.59	0.83
6:F:27:ASN:HB3	6:F:30:GLU:HG3	1.60	0.83
11:K:19:VAL:HG13	11:K:21:ARG:H	1.41	0.83
16:P:90:VAL:O	16:P:92:ARG:N	2.11	0.82
1:A:1021:A:H61	1:A:1142(A):A:H61	1.22	0.82
1:A:620:G:H4'	1:A:621:A:H5''	1.60	0.82
18:R:90:ARG:HG3	18:R:90:ARG:HH11	1.45	0.82
23:W:7:ILE:HD12	23:W:62:VAL:HG11	1.62	0.81
1:A:265:A:N6	1:A:427:U:O2'	2.13	0.81
1:A:1664:A:H61	1:A:1996:C:H42	1.29	0.81
9:I:4:TYR:OH	9:I:7:LYS:NZ	2.14	0.81
24:X:47:ASN:O	24:X:49:LYS:N	2.12	0.81
7:G:10:PRO:CD	7:G:50:VAL:O	2.29	0.80
1:A:1824:G:OP1	3:C:52:ARG:NH1	2.14	0.80
8:H:92:VAL:HG13	8:H:120:ILE:HG23	1.64	0.80
1:A:956:G:H5''	12:L:77:LYS:HE2	1.64	0.80
8:H:130:TYR:HB3	8:H:136:VAL:HG13	1.62	0.80
20:T:76:CYS:SG	20:T:77:PRO:HD2	2.22	0.80
1:A:1359:A:N6	1:A:1372:U:C4	2.50	0.80
1:A:2580:U:H4'	4:D:130:GLY:HA3	1.65	0.79
1:A:1169:G:N2	1:A:1180:C:N3	2.30	0.79
19:S:67:GLY:O	19:S:69:TYR:N	2.15	0.79
7:G:10:PRO:CD	7:G:50:VAL:HG13	2.13	0.79
21:U:182:LYS:HG3	21:U:183:LEU:HD23	1.62	0.79
1:A:780:G:H21	1:A:783:A:H62	1.30	0.79
11:K:62:LEU:H	11:K:62:LEU:HD23	1.46	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
21:U:144:LEU:HD11	21:U:149:SER:HA	1.63	0.79
3:C:121:PRO:HB3	3:C:135:PHE:CZ	2.19	0.78
26:Z:1:MET:SD	26:Z:6:HIS:NE2	2.56	0.78
1:A:847:U:C4	1:A:933:A:N1	2.51	0.78
3:C:248:SER:CB	3:C:252:TRP:CE2	2.66	0.78
7:G:10:PRO:HG2	7:G:50:VAL:CG1	2.13	0.78
10:J:88:ASN:HD21	10:J:92:GLU:HB2	1.47	0.77
3:C:69:ARG:NH2	3:C:128:GLY:O	2.17	0.77
9:I:95:PRO:O	9:I:97:ARG:N	2.18	0.77
1:A:2068:U:H3	1:A:2430:A:H2	1.32	0.77
11:K:47:ASP:OD2	11:K:50:ARG:NH2	2.17	0.77
18:R:90:ARG:HG3	18:R:90:ARG:NH1	2.00	0.76
1:A:2287:A:N6	1:A:2344:U:H3	1.82	0.76
1:A:49:A:N7	1:A:120:U:O4	2.18	0.76
5:E:197:ASP:O	5:E:199:TRP:N	2.19	0.76
13:M:74:LYS:O	13:M:76:VAL:N	2.18	0.76
1:A:1169:G:H1	1:A:1180:C:H42	0.77	0.75
1:A:1607:C:N4	1:A:1622:G:OP2	2.19	0.75
1:A:2051:A:C2	1:A:2052:G:O6	2.40	0.75
21:U:54:HIS:O	21:U:98:MET:CE	2.35	0.75
1:A:67:U:N3	1:A:74:A:C2	2.53	0.75
15:O:57:PHE:O	15:O:58:ASN:ND2	2.20	0.75
15:O:27:THR:HG23	15:O:90:GLN:HB3	1.67	0.75
16:P:92:ARG:O	16:P:94:ASN:N	2.20	0.75
1:A:888:C:H3'	1:A:889:C:H4'	1.69	0.75
9:I:13:TRP:HB2	9:I:133:GLN:HG3	1.69	0.74
17:Q:24:LYS:HA	17:Q:92:THR:HG23	1.68	0.74
14:N:78:LEU:HD21	14:N:108:GLY:HA3	1.68	0.74
15:O:51:ARG:HG2	15:O:98:LYS:HG3	1.70	0.74
21:U:30:ASN:HD22	21:U:90:VAL:HB	1.51	0.74
4:D:24:THR:CG2	4:D:188:VAL:HG11	2.16	0.74
6:F:161:THR:HG22	6:F:163:ALA:H	1.53	0.74
7:G:15:VAL:HG21	7:G:76:VAL:HG13	1.68	0.74
14:N:56:LEU:HB3	14:N:58:LEU:HD22	1.69	0.74
21:U:95:PRO:CG	21:U:127:LYS:HD3	2.18	0.74
19:S:27:THR:HB	19:S:80:ILE:HB	1.69	0.73
26:Z:9:LEU:H	26:Z:27:THR:HG23	1.53	0.73
1:A:2030:A:H4'	1:A:2031:A:H8	1.52	0.73
11:K:14:LYS:O	11:K:16:ARG:N	2.22	0.73
1:A:676:A:H8	1:A:2069:G:H21	1.33	0.73
1:A:483:A:H5'	20:T:49:VAL:HG22	1.69	0.73
21:U:158:PRO:O	21:U:160:GLY:N	2.22	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:G:86:GLU:HG3	7:G:165:ALA:H	1.53	0.73
12:L:24:GLY:O	12:L:26:TYR:N	2.19	0.73
12:L:111:GLU:OE1	12:L:133:ARG:NH2	2.22	0.73
12:L:104:PHE:HE2	12:L:125:LEU:HD11	1.54	0.73
1:A:1509:C:H3'	1:A:1510:A:H5''	1.71	0.72
1:A:587:C:OP2	11:K:21:ARG:NH2	2.21	0.72
1:A:2701:C:H3'	1:A:2702:U:C5'	2.19	0.72
26:Z:48:ARG:HH12	26:Z:52:THR:HG22	1.54	0.72
8:H:144:VAL:HG13	8:H:145:VAL:HG13	1.70	0.72
6:F:64:THR:HG23	6:F:66:GLN:H	1.55	0.72
20:T:51:VAL:HG13	20:T:52:SER:H	1.54	0.72
1:A:1190:G:OP1	11:K:30:THR:OG1	2.06	0.72
6:F:6:ALA:H	26:Z:23:GLU:HG2	1.54	0.72
3:C:35:LYS:HD2	3:C:104:TYR:CE1	2.25	0.72
21:U:91:LEU:CD1	21:U:96:VAL:HG21	2.20	0.72
7:G:129:THR:OG1	7:G:129:THR:O	2.08	0.72
10:J:47:ILE:HG13	10:J:48:PRO:HD2	1.72	0.72
21:U:96:VAL:HG12	21:U:128:VAL:O	1.89	0.72
24:X:42:GLY:O	24:X:44:LEU:N	2.20	0.72
21:U:103:ARG:HB2	21:U:138:GLU:HG2	1.72	0.71
7:G:153:LYS:HG2	7:G:162:ILE:HG13	1.72	0.71
4:D:170:LEU:HD21	4:D:187:ALA:HB3	1.72	0.71
14:N:24:LEU:HB2	14:N:85:VAL:HG12	1.70	0.71
21:U:102:LEU:HG	21:U:123:ASP:HA	1.72	0.71
1:A:2315:G:OP1	6:F:36:LYS:NZ	2.24	0.71
9:I:89:LYS:O	9:I:93:THR:HG22	1.90	0.71
15:O:77:PRO:HB2	15:O:80:SER:HB2	1.72	0.71
14:N:106:ARG:HA	14:N:110:LEU:HD21	1.73	0.71
20:T:42:VAL:HG12	20:T:65:ALA:HB3	1.71	0.71
10:J:2:ILE:HD12	10:J:6:THR:HG21	1.72	0.71
20:T:29:GLU:HB3	20:T:38:ILE:HG23	1.70	0.70
1:A:2287:A:N6	1:A:2344:U:N3	2.37	0.70
3:C:43:ARG:HB3	3:C:54:ARG:HB2	1.74	0.70
6:F:47:LYS:HD3	6:F:81:LYS:HB2	1.73	0.70
1:A:602:G:HO2'	1:A:604:G:HO2'	1.34	0.70
11:K:62:LEU:HD23	11:K:62:LEU:N	2.05	0.70
18:R:17:VAL:HG12	18:R:76:VAL:HG11	1.72	0.70
21:U:54:HIS:O	21:U:98:MET:HE1	1.91	0.70
1:A:1667:G:O2'	1:A:1991:U:O4	2.09	0.70
5:E:185:ASP:HA	5:E:188:ARG:HD3	1.72	0.70
1:A:2245:U:H5'	1:A:2246:G:H5'	1.73	0.70
1:A:498:G:N3	20:T:47:LYS:NZ	2.37	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:250:G:OP2	4:D:13:ARG:NH2	117.96	0.70
21:U:80:ARG:HH21	21:U:82:ARG:HH22	1.40	0.69
1:A:1045:A:C6	1:A:1111:A:N7	2.59	0.69
1:A:1899:G:H21	1:A:1902:C:N4	1.89	0.69
1:A:270(T):G:H5''	23:W:97:LEU:HD22	1.73	0.69
5:E:182:ASN:ND2	5:E:185:ASP:OD2	2.19	0.69
1:A:372:G:N2	1:A:401:A:OP2	2.22	0.69
3:C:182:LEU:H	3:C:272:ALA:HB3	1.56	0.69
1:A:482:A:H4'	20:T:47:LYS:HD2	1.73	0.69
21:U:95:PRO:HB2	21:U:127:LYS:HG2	1.73	0.69
26:Z:56:VAL:HA	26:Z:60:GLN:HB2	1.73	0.69
3:C:71:ASP:HB2	3:C:103:ARG:HH22	1.58	0.69
5:E:184:TYR:O	5:E:188:ARG:HG3	1.93	0.69
1:A:956:G:OP2	12:L:14:ARG:NH2	2.24	0.69
1:A:1980:G:O2'	1:A:1982:C:OP2	2.09	0.69
5:E:110:LEU:HD11	5:E:181:LEU:HD13	1.74	0.69
4:D:128:SER:OG	4:D:129:HIS:N	2.24	0.69
21:U:141:VAL:HG23	21:U:144:LEU:HB2	1.74	0.68
5:E:157:VAL:HB	5:E:194:MET:HB3	1.76	0.68
3:C:25:THR:O	3:C:27:THR:N	2.26	0.68
15:O:123:GLN:O	15:O:125:ARG:N	2.26	0.68
1:A:1728:G:N1	1:A:1730:U:OP2	2.27	0.68
1:A:2123:G:H1	1:A:2175:C:H42	1.42	0.68
1:A:910:A:H62	12:L:12:GLN:HA	1.57	0.68
23:W:73:LEU:HD13	23:W:90:ILE:HG22	1.76	0.68
1:A:2576:G:O2'	1:A:2579:C:OP2	2.12	0.68
11:K:64:LYS:C	11:K:66:GLY:H	1.95	0.68
4:D:95:ILE:H	4:D:95:ILE:HD12	1.59	0.68
1:A:2306:C:H3'	1:A:2307:G:H5''	1.75	0.68
3:C:142:VAL:HG23	3:C:193:VAL:HA	1.75	0.68
7:G:15:VAL:HG11	7:G:79:VAL:HG23	1.75	0.68
9:I:133:GLN:HB2	9:I:135:PRO:HD3	1.76	0.68
12:L:37:LEU:HD21	12:L:130:LYS:HE3	1.74	0.68
1:A:573:G:OP2	17:Q:78:LYS:NZ	2.27	0.68
3:C:248:SER:OG	3:C:252:TRP:CE2	2.46	0.68
3:C:248:SER:OG	3:C:252:TRP:NE1	2.25	0.68
11:K:39:LYS:HG3	11:K:45:LEU:HD22	1.75	0.68
1:A:1509:C:N3	1:A:1511:A:N6	2.41	0.67
2:B:24:G:O6	2:B:56:G:O2'	2.09	0.67
1:A:1021:A:OP2	9:I:65:LYS:NZ	2.27	0.67
12:L:134:ARG:NH1	21:U:122:ARG:NH2	2.34	0.67
1:A:1479:G:N7	1:A:1510:A:N6	2.41	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2308:G:H1	1:A:2311:A:H2	1.38	0.67
1:A:67:U:N3	1:A:74:A:H2	1.92	0.67
4:D:1:MET:N	4:D:83:ASP:O	2.28	0.67
7:G:137:ASP:OD1	7:G:138:LYS:N	2.27	0.67
1:A:2168:G:N2	1:A:2170:A:N7	2.42	0.67
12:L:89:ASN:O	12:L:92:GLY:N	2.18	0.67
3:C:35:LYS:HG2	3:C:64:ILE:H	1.59	0.67
1:A:1490:A:O2'	3:C:99:ASP:OD1	2.12	0.67
1:A:443:A:H3'	5:E:45:ARG:HH12	1.60	0.67
11:K:64:LYS:C	11:K:66:GLY:N	2.48	0.67
2:B:44:G:H1'	2:B:47:C:N4	2.09	0.67
15:O:16:ARG:NH2	15:O:83:ILE:O	2.27	0.67
8:H:5:LEU:HD21	8:H:12:LEU:HB3	1.76	0.67
13:M:78:LYS:HE2	13:M:83:ILE:HD11	1.77	0.67
17:Q:52:VAL:HG21	17:Q:55:ALA:HB3	1.76	0.67
1:A:1057:A:H62	1:A:1086:A:H2'	1.59	0.67
1:A:2849:U:H5	15:O:93:ARG:HH12	1.42	0.67
1:A:2444:G:OP2	5:E:68:LYS:HE3	1.94	0.66
8:H:4:ILE:HG12	8:H:18:VAL:HG22	1.76	0.66
1:A:581:C:H2'	1:A:582:G:H8	1.60	0.66
7:G:86:GLU:HG3	7:G:165:ALA:N	2.10	0.66
1:A:674:G:H1'	5:E:74:ARG:HD3	1.77	0.66
18:R:45:TYR:CZ	18:R:49:LYS:HD2	2.30	0.66
20:T:49:VAL:O	20:T:51:VAL:N	2.29	0.66
1:A:1407:C:H42	1:A:1595:G:H1	1.43	0.66
12:L:137:TYR:CE1	21:U:83:PRO:HG3	2.31	0.66
20:T:97:ARG:HE	20:T:98:VAL:HB	1.61	0.66
1:A:2343:C:O2'	1:A:2373:G:O2'	2.14	0.66
1:A:2470:G:H5'	12:L:56:ARG:HH22	1.61	0.66
21:U:182:LYS:HG3	21:U:183:LEU:HA	1.78	0.66
21:U:60:GLU:HA	21:U:66:SER:HA	1.77	0.66
1:A:1013:C:H42	1:A:1149:G:H1	1.43	0.66
1:A:780:G:N2	1:A:783:A:H62	1.94	0.66
9:I:35:ARG:O	9:I:37:LYS:N	2.29	0.66
11:K:105:LEU:O	11:K:106:LEU:HB2	1.95	0.66
14:N:55:ALA:O	14:N:56:LEU:HB2	1.96	0.66
21:U:128:VAL:HB	21:U:161:VAL:HG13	1.77	0.66
1:A:2848:G:O2'	1:A:2867:G:N2	2.28	0.66
17:Q:21:ARG:HD2	17:Q:91:TYR:CD1	2.31	0.66
1:A:2051:A:H2	1:A:2052:G:O6	1.76	0.65
7:G:153:LYS:HB3	7:G:162:ILE:H	1.61	0.65
15:O:16:ARG:HD3	15:O:19:LEU:HD11	1.77	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:G:10:PRO:HD2	7:G:50:VAL:HG13	1.78	0.65
23:W:29:GLY:O	23:W:31:GLY:N	2.30	0.65
1:A:1568:G:H4'	3:C:59:LYS:HB3	1.78	0.65
1:A:443:A:H3'	5:E:45:ARG:NH1	2.11	0.65
1:A:1077:A:H5'	1:A:1078:U:H5''	1.77	0.65
1:A:2023:G:H5'	1:A:2617:C:H4'	1.78	0.65
4:D:13:ARG:HD2	11:K:61:ARG:HD3	123.04	0.65
16:P:8:VAL:HG23	16:P:11:ARG:HH21	1.62	0.65
1:A:793:A:OP2	1:A:2071:A:O2'	2.15	0.65
1:A:1754:C:OP1	15:O:96:ARG:NH1	2.29	0.65
24:X:50:ILE:HD12	24:X:51:ARG:H	1.62	0.65
1:A:2502:G:H5''	1:A:2503:A:H5''	1.79	0.65
7:G:20:ALA:HB3	7:G:23:ARG:HG2	1.77	0.65
22:V:10:THR:HG22	22:V:12:ASN:H	1.62	0.65
8:H:40:THR:O	8:H:44:LEU:HB2	1.97	0.65
3:C:30:GLU:HG3	3:C:63:ARG:NH2	2.12	0.65
3:C:80:ALA:HB3	3:C:94:LEU:HD13	1.79	0.65
1:A:855:G:O2'	22:V:27:GLU:OE2	2.10	0.65
1:A:607:U:H3	1:A:621:A:H2	1.42	0.64
5:E:107:LYS:HD2	5:E:207:GLY:H	1.62	0.64
1:A:2404:C:O3'	11:K:77:ARG:NH2	2.29	0.64
1:A:819:A:OP2	1:A:1187:G:N2	2.23	0.64
3:C:44:ASN:HB3	3:C:49:ILE:HA	1.78	0.64
1:A:1055:G:H1	1:A:1104:C:H42	1.44	0.64
12:L:78:PRO:O	12:L:79:LEU:HB2	1.97	0.64
14:N:58:LEU:H	14:N:58:LEU:CD2	2.10	0.64
1:A:690:G:O2'	3:C:43:ARG:NH2	2.30	0.64
16:P:88:ILE:HG22	16:P:90:VAL:HG23	1.79	0.64
21:U:91:LEU:HD11	21:U:96:VAL:HG21	1.79	0.64
21:U:93:ASP:C	21:U:94:GLU:HG2	2.10	0.64
13:M:51:LEU:HD13	13:M:66:VAL:HG13	1.79	0.64
2:B:52:A:H62	14:N:33:LYS:HG3	1.63	0.64
15:O:36:GLU:HG3	15:O:41:ARG:HE	1.62	0.64
1:A:2111:C:N3	1:A:2118:U:O2'	2.30	0.64
1:A:581:C:H2'	1:A:582:G:C8	2.33	0.64
3:C:35:LYS:NZ	3:C:64:ILE:O	2.31	0.64
1:A:2406:U:N3	11:K:73:GLY:O	2.24	0.64
6:F:112:PRO:HB3	26:Z:37:SER:HB2	1.80	0.63
24:X:41:ILE:HD11	24:X:44:LEU:HG	1.80	0.63
3:C:35:LYS:HG2	3:C:64:ILE:N	2.13	0.63
20:T:91:GLU:HG3	20:T:92:ASN:H	1.63	0.63
26:Z:48:ARG:O	26:Z:50:VAL:N	2.31	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2126:A:N6	1:A:2163:C:O2'	2.31	0.63
1:A:224:G:O6	1:A:419:C:O2'	2.17	0.63
3:C:25:THR:HG23	3:C:27:THR:HB	1.80	0.63
7:G:12:PRO:O	7:G:13:LYS:HB2	1.97	0.63
11:K:13:ASN:O	11:K:15:ARG:N	2.32	0.63
1:A:1918:A:O2'	1:A:1920:C:N4	2.32	0.63
1:A:2415:G:H4'	11:K:67:MET:N	2.14	0.63
7:G:153:LYS:HG3	7:G:161:GLY:HA2	1.80	0.63
7:G:83:TYR:CZ	7:G:138:LYS:HD2	2.34	0.63
8:H:56:LYS:HG3	8:H:57:ARG:N	2.13	0.63
10:J:13:ASN:ND2	10:J:96:THR:O	2.30	0.63
1:A:2394:C:OP1	11:K:63:PRO:HD2	1.99	0.63
16:P:83:LEU:HD12	16:P:113:ALA:HB2	1.79	0.63
26:Z:23:GLU:O	26:Z:25:TYR:N	2.31	0.63
1:A:2310:A:N6	6:F:79:ASN:HB2	2.13	0.63
1:A:2789:C:H1'	1:A:2892:A:H2	1.64	0.62
7:G:26:VAL:HG11	7:G:75:ALA:HB1	1.81	0.62
1:A:1296:G:OP1	1:A:2709:G:O2'	2.13	0.62
1:A:1833:U:O2'	1:A:1969:A:N1	2.29	0.62
8:H:124:GLY:H	8:H:142:VAL:HG23	1.63	0.62
15:O:1:MET:O	15:O:3:ARG:N	2.29	0.62
3:C:248:SER:CB	3:C:252:TRP:CZ2	2.83	0.62
5:E:46:ARG:HH11	5:E:46:ARG:HG2	1.65	0.62
6:F:3:LEU:HD12	6:F:4:ASP:H	1.64	0.62
4:D:23:VAL:HG12	4:D:184:VAL:O	2.00	0.62
1:A:263:C:H2'	1:A:264:C:O4'	2.00	0.62
8:H:81:VAL:HG21	8:H:88:ILE:HD12	1.80	0.62
1:A:1728:G:H8	1:A:1732:A:H62	1.48	0.62
1:A:1754:C:P	15:O:96:ARG:HH12	2.21	0.62
1:A:1798:U:C5'	3:C:259:THR:HG22	2.29	0.62
22:V:27:GLU:HG3	22:V:68:GLU:HA	1.82	0.62
26:Z:37:SER:HB3	26:Z:42:PHE:CD1	2.35	0.62
3:C:248:SER:HB3	3:C:252:TRP:CE2	2.34	0.61
16:P:92:ARG:HD2	17:Q:11:GLN:HB2	1.82	0.61
5:E:197:ASP:OD1	5:E:197:ASP:N	2.33	0.61
14:N:83:LYS:C	14:N:109:GLY:HA3	2.21	0.61
1:A:2030:A:H4'	1:A:2031:A:C8	2.36	0.61
1:A:392:C:H5''	1:A:409:C:H5''	1.81	0.61
1:A:1045:A:C8	1:A:1111:A:N6	2.68	0.61
1:A:2099:U:O4	1:A:2190:G:O6	2.18	0.61
12:L:134:ARG:NE	21:U:122:ARG:NH2	2.49	0.61
1:A:573:G:N1	1:A:2031:A:OP2	2.20	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:G:113:VAL:HG11	7:G:151:ILE:HD12	1.83	0.61
23:W:83:GLU:O	23:W:85:LEU:N	2.34	0.61
1:A:2864:G:OP1	15:O:119:LYS:HD2	2.01	0.61
3:C:108:PRO:HB3	3:C:143:HIS:CE1	2.35	0.61
16:P:52:ARG:HA	16:P:55:ARG:HG3	1.83	0.61
1:A:2692:C:O2	1:A:2847:U:O2'	2.18	0.60
3:C:72:LYS:NZ	3:C:99:ASP:OD2	2.33	0.60
21:U:58:VAL:O	21:U:60:GLU:N	2.34	0.60
1:A:774:A:H2	1:A:787:U:HO2'	1.48	0.60
12:L:35:VAL:HG13	12:L:130:LYS:HB3	1.83	0.60
1:A:2469:A:O2'	12:L:56:ARG:HG2	2.01	0.60
7:G:150:ALA:O	7:G:152:ARG:N	2.34	0.60
1:A:1203:G:H3'	1:A:1204:A:H5''	1.83	0.60
1:A:1652:A:OP1	13:M:8:ARG:NH1	2.33	0.60
11:K:95:VAL:HG13	11:K:100:LEU:HD21	1.83	0.60
1:A:2131:G:H4'	1:A:2132:U:H4'	1.84	0.60
3:C:35:LYS:HD2	3:C:104:TYR:CD1	2.35	0.60
4:D:9:VAL:HB	4:D:25:VAL:HG23	1.83	0.60
4:D:25:VAL:HG12	4:D:183:LEU:HG	1.84	0.60
10:J:96:THR:O	10:J:97:ARG:HB3	2.01	0.60
1:A:252:G:OP2	11:K:50:ARG:NH1	2.35	0.60
15:O:84:GLN:OE1	15:O:85:LYS:NZ	2.34	0.60
1:A:530:G:O2'	1:A:532:A:N7	2.35	0.60
6:F:28:VAL:HG23	6:F:29:TRP:CD1	2.36	0.60
7:G:152:ARG:CG	7:G:153:LYS:HD2	2.28	0.60
7:G:4:ILE:HB	7:G:6:ARG:HG2	1.82	0.60
1:A:2335:A:O2'	1:A:2336:A:O5'	2.15	0.60
1:A:2377:A:H2'	1:A:2378:A:C8	2.37	0.60
8:H:21:VAL:HG21	8:H:25:TYR:HD2	1.66	0.60
11:K:147:LEU:O	11:K:148:LEU:HB2	2.02	0.60
21:U:54:HIS:O	21:U:98:MET:HE2	2.00	0.60
1:A:137(A):G:H1'	19:S:41:ASN:ND2	2.16	0.60
4:D:14:ILE:HG22	4:D:21:VAL:HG23	0.69	0.59
13:M:42:LYS:HA	13:M:45:ARG:HD2	1.84	0.59
1:A:2298:A:H62	1:A:2318:G:H8	1.50	0.59
2:B:40:U:O2'	2:B:45:A:N6	2.32	0.59
7:G:98:LEU:HD22	7:G:125:VAL:HB	1.83	0.59
8:H:129:THR:HG22	8:H:137:PRO:HB3	1.84	0.59
18:R:86:LEU:HD12	18:R:87:PRO:HD2	1.83	0.59
18:R:90:ARG:CG	18:R:90:ARG:HH11	2.14	0.59
2:B:44:G:H1'	2:B:47:C:H42	1.67	0.59
4:D:36:ARG:HH21	4:D:88:GLY:HA2	1.68	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
25:Y:6:VAL:HG13	25:Y:56:VAL:HG13	1.84	0.59
1:A:49:A:N7	1:A:120:U:C5	2.70	0.59
1:A:2126:A:H4'	1:A:2127:G:O5'	2.03	0.59
1:A:855:G:H1	1:A:922:U:H3	1.51	0.59
1:A:27:G:H1'	1:A:513:A:N6	2.17	0.59
18:R:111:HIS:CD2	18:R:112:GLY:H	2.20	0.59
1:A:330:A:HO2'	1:A:331:A:H8	1.51	0.59
8:H:67:ARG:HH21	8:H:68:LEU:HB2	1.68	0.59
11:K:26:GLY:O	11:K:28:GLY:N	2.35	0.59
2:B:44:G:OP1	26:Z:1:MET:N	2.36	0.59
7:G:6:ARG:NH2	7:G:54:ARG:HH22	2.01	0.59
1:A:2636:U:OP1	4:D:79:ARG:HA	2.03	0.59
1:A:2646:C:OP2	1:A:2732:G:O2'	2.15	0.59
14:N:26:LEU:HB3	14:N:87:PHE:HA	1.85	0.59
3:C:28:GLU:OE1	3:C:29:PRO:HD2	2.03	0.58
6:F:136:ARG:O	6:F:154:GLY:HA2	2.02	0.58
7:G:15:VAL:HG12	7:G:28:GLY:HA3	1.83	0.58
9:I:40:PRO:HB3	16:P:68:ALA:HB2	1.85	0.58
1:A:2581:G:N2	1:A:2581:G:OP2	2.36	0.58
13:M:67:LEU:HD13	13:M:76:VAL:HG21	1.84	0.58
14:N:106:ARG:HA	14:N:110:LEU:HD11	1.86	0.58
19:S:61:GLY:N	19:S:75:ASP:OD1	2.36	0.58
11:K:58:THR:HG22	11:K:61:ARG:HG3	1.85	0.58
17:Q:44:LYS:O	17:Q:46:VAL:N	2.36	0.58
23:W:51:VAL:HG11	23:W:74:VAL:HG21	1.84	0.58
1:A:1664:A:H61	1:A:1996:C:N4	1.98	0.58
1:A:2292:C:P	14:N:17:ARG:HH22	2.26	0.58
26:Z:42:PHE:O	26:Z:44:THR:N	2.36	0.58
2:B:15:A:H5'	2:B:16:G:C8	2.39	0.58
5:E:127:GLU:O	5:E:129:PHE:N	2.32	0.58
21:U:5:LEU:HD11	21:U:39:VAL:HB	1.85	0.58
21:U:146:ILE:HG22	21:U:176:PRO:HD3	1.84	0.58
10:J:64:ARG:HG2	10:J:79:PHE:CG	2.38	0.58
1:A:1068:G:O2'	1:A:1096:A:N3	2.37	0.58
8:H:56:LYS:HE3	8:H:57:ARG:HA	1.84	0.58
13:M:27:SER:HB3	13:M:34:ILE:HD11	1.84	0.58
1:A:221:A:H4'	1:A:222:A:O5'	2.04	0.57
5:E:28:ILE:HG22	5:E:112:MET:HB3	1.85	0.57
6:F:98:ARG:NH1	26:Z:1:MET:SD	2.77	0.57
13:M:117:VAL:HG22	13:M:118:GLU:H	1.68	0.57
15:O:24:PRO:HA	15:O:49:VAL:HG13	1.85	0.57
6:F:67:LYS:HE2	26:Z:6:HIS:CE1	2.38	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1403:C:H5''	1:A:1471:A:H1'	1.85	0.57
4:D:35:GLN:HB3	4:D:48:GLN:HB2	1.86	0.57
13:M:24:GLN:OE1	13:M:36:THR:HG21	2.04	0.57
14:N:10:ARG:NH2	14:N:91:PRO:O	2.36	0.57
18:R:73:ALA:HB3	18:R:106:ILE:HD13	1.84	0.57
1:A:1899:G:H21	1:A:1902:C:H41	1.51	0.57
16:P:92:ARG:HD3	16:P:94:ASN:HB3	1.85	0.57
22:V:50:ASN:HB3	22:V:63:VAL:HG22	1.86	0.57
1:A:247:G:H4'	1:A:386:G:C5	2.39	0.57
12:L:116:GLU:O	12:L:120:ILE:HG12	2.05	0.57
1:A:1428:C:N4	1:A:1570:A:OP2	2.36	0.57
1:A:2133:G:H1'	1:A:2158:A:H61	1.70	0.57
11:K:135:LEU:O	11:K:139:LYS:HB2	2.04	0.57
12:L:66:ILE:HA	12:L:104:PHE:HA	1.85	0.57
3:C:65:ILE:H	3:C:65:ILE:HD13	1.68	0.57
4:D:11:MET:HG2	4:D:24:THR:OG1	2.04	0.57
1:A:138:G:N2	19:S:44:GLU:OE2	2.29	0.57
21:U:91:LEU:HG	21:U:130:PRO:CB	2.26	0.57
7:G:149:ARG:HG3	7:G:162:ILE:O	2.05	0.57
14:N:52:SER:O	14:N:55:ALA:O	2.21	0.57
6:F:98:ARG:HH12	26:Z:1:MET:HB3	1.69	0.57
1:A:1534:G:N2	1:A:1537:C:O2	2.38	0.57
3:C:71:ASP:CB	3:C:103:ARG:HH22	2.18	0.57
1:A:1094:U:O2'	1:A:1096:A:OP1	2.19	0.57
10:J:85:VAL:HG11	10:J:114:ILE:HD11	1.87	0.57
1:A:857:C:OP2	22:V:77:ARG:NH2	2.37	0.57
1:A:2632:A:HO2'	1:A:2811:G:HO2'	1.51	0.56
2:B:12:C:H2'	22:V:73:GLY:HA3	1.87	0.56
5:E:107:LYS:HD2	5:E:206:ILE:HA	1.86	0.56
8:H:33:ARG:HB3	8:H:35:LEU:HG	1.86	0.56
12:L:85:LYS:O	12:L:87:LYS:N	2.38	0.56
21:U:77:ASP:OD2	21:U:80:ARG:HD3	2.05	0.56
1:A:1664:A:N6	1:A:1996:C:H42	2.00	0.56
26:Z:71:ARG:HB2	26:Z:71:ARG:HH11	1.68	0.56
1:A:1798:U:H5''	3:C:259:THR:HG22	1.87	0.56
6:F:81:LYS:O	6:F:82:LEU:HB2	2.04	0.56
21:U:19:ARG:NH1	21:U:84:GLU:O	2.35	0.56
1:A:1204:A:H1'	1:A:1206:G:C8	2.40	0.56
1:A:1464:C:HO2'	1:A:1528:A:H8	1.51	0.56
1:A:1991:U:H2'	1:A:1992:G:H5''	1.87	0.56
11:K:101:VAL:HG23	11:K:106:LEU:HB3	1.88	0.56
2:B:50:G:OP1	14:N:61:ASN:ND2	2.38	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
15:O:60:THR:HG22	15:O:77:PRO:HA	1.86	0.56
17:Q:59:ALA:HB2	17:Q:96:ILE:HD13	1.88	0.56
18:R:71:VAL:HA	18:R:107:LEU:HD12	1.87	0.56
3:C:121:PRO:HA	3:C:135:PHE:HD2	1.62	0.56
8:H:79:ILE:HB	8:H:142:VAL:HA	1.88	0.56
21:U:152:ALA:HB2	21:U:168:GLU:HA	1.87	0.56
6:F:67:LYS:HZ1	26:Z:6:HIS:CD2	2.23	0.56
12:L:20:ALA:HB3	21:U:79:ARG:CZ	2.35	0.56
1:A:2689:U:OP2	1:A:2719:G:N2	2.33	0.56
2:B:24:G:H1'	2:B:26:A:H62	1.70	0.56
7:G:153:LYS:HA	7:G:153:LYS:NZ	2.21	0.56
17:Q:66:ARG:HH11	17:Q:88:ARG:HD3	1.71	0.56
1:A:1266:G:O5'	18:R:15:ARG:NH2	2.38	0.56
1:A:2820:A:C8	4:D:109:LYS:HE2	2.40	0.56
7:G:92:ILE:HD12	7:G:92:ILE:H	1.71	0.56
1:A:2109:U:H3	1:A:2180:U:H3	1.54	0.56
10:J:97:ARG:HA	10:J:117:LEU:HD22	1.88	0.56
3:C:43:ARG:NH1	3:C:44:ASN:OD1	2.39	0.56
7:G:10:PRO:HD2	7:G:50:VAL:CG1	2.35	0.56
9:I:56:ASN:N	9:I:125:GLY:O	2.22	0.56
1:A:2849:U:OP2	15:O:95:ARG:NH1	2.39	0.56
20:T:95:LYS:HB3	20:T:100:ALA:HA	1.87	0.56
1:A:2335:A:O2'	1:A:2336:A:H2'	2.05	0.56
1:A:2340:G:H2'	1:A:2341:G:H8	1.70	0.56
1:A:1266:G:O2'	1:A:2012:G:O6	2.16	0.55
9:I:40:PRO:O	16:P:64:ARG:HD2	2.06	0.55
14:N:58:LEU:HD23	14:N:58:LEU:H	1.70	0.55
15:O:29:ARG:HB2	15:O:46:GLU:HG3	1.88	0.55
3:C:232:PRO:HB3	3:C:244:ARG:NH1	2.21	0.55
11:K:52:GLU:HG3	11:K:57:THR:HG22	1.88	0.55
15:O:39:ARG:HG2	15:O:40:THR:H	1.72	0.55
17:Q:38:LEU:H	17:Q:51:VAL:HG13	1.70	0.55
12:L:20:ALA:HB3	21:U:79:ARG:NH2	2.21	0.55
1:A:922:U:H2'	1:A:923:C:C6	2.42	0.55
5:E:101:LEU:O	5:E:106:ARG:NH1	2.40	0.55
7:G:121:ILE:HG12	7:G:140:LYS:HD2	1.89	0.55
1:A:1416:G:H2'	1:A:1417:C:C6	2.42	0.55
1:A:2096:U:H3	1:A:2193:G:H1	1.54	0.55
1:A:2688:U:H5	1:A:2720:U:OP2	1.89	0.55
1:A:1826:G:OP1	3:C:224:ALA:N	2.39	0.55
1:A:273(C):C:H42	1:A:363(C):G:H1	1.52	0.55
2:B:13:A:N1	2:B:69:G:O2'	2.28	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:14:ILE:CG2	4:D:21:VAL:HG21	2.34	0.55
4:D:63:LEU:HD12	4:D:64:LYS:N	2.22	0.55
8:H:129:THR:HA	8:H:137:PRO:HA	1.88	0.55
15:O:3:ARG:HG3	15:O:7:ILE:HG12	1.88	0.55
1:A:2438:U:O3'	1:A:2439:A:H3'	2.07	0.55
1:A:458:G:O2'	1:A:469:G:O6	2.19	0.55
1:A:574:C:N3	4:D:145:LYS:NZ	2.50	0.55
5:E:68:LYS:O	5:E:69:HIS:HB2	2.07	0.55
7:G:157:TYR:HA	7:G:171:LEU:O	2.06	0.55
7:G:41:MET:HE1	7:G:64:LEU:HB3	1.87	0.55
1:A:1062:G:H2'	1:A:1063:G:C8	2.42	0.55
17:Q:61:VAL:HG23	17:Q:63:GLY:H	1.71	0.55
22:V:27:GLU:HB2	22:V:69:PHE:HD1	1.72	0.55
1:A:1178:C:H2'	1:A:1179:C:C6	2.41	0.55
1:A:1359:A:H61	1:A:1372:U:H3	1.39	0.55
8:H:3:VAL:HG12	8:H:38:LEU:HA	1.87	0.55
11:K:71:VAL:HG13	11:K:72:PRO:HD3	1.88	0.55
15:O:26:ASP:O	15:O:49:VAL:HG12	2.07	0.55
17:Q:34:GLU:O	17:Q:36:PRO:HD3	2.06	0.55
18:R:14:PRO:O	18:R:17:VAL:N	2.40	0.55
5:E:116:ASP:OD2	11:K:1:MET:N	2.26	0.55
15:O:62:THR:HG22	15:O:75:ILE:HG12	1.89	0.55
21:U:48:PHE:CE1	21:U:52:SER:HA	2.42	0.54
1:A:270(R):G:H2'	1:A:270(S):G:H8	1.73	0.54
1:A:34:C:H41	1:A:447:A:H61	1.55	0.54
1:A:764:A:N3	3:C:213:ARG:NH1	2.55	0.54
1:A:898:C:H2'	1:A:899:A:H5'	1.88	0.54
3:C:12:SER:O	3:C:16:MET:HB2	2.08	0.54
1:A:2346:A:H8	4:D:35:GLN:NE2	135.62	0.54
9:I:42:TRP:O	16:P:64:ARG:NH2	2.41	0.54
1:A:1187:G:H5''	17:Q:81:TYR:CE1	2.43	0.54
21:U:5:LEU:HD21	21:U:44:PHE:HA	1.89	0.54
1:A:587:C:H4'	1:A:588:U:O5'	2.07	0.54
13:M:55:ALA:HB2	13:M:79:LEU:HD13	1.89	0.54
13:M:56:LYS:NZ	13:M:87:TYR:O	2.40	0.54
1:A:27:G:N2	1:A:513:A:OP2	2.40	0.54
1:A:900:A:H3'	1:A:901:A:H8	1.73	0.54
11:K:64:LYS:O	11:K:66:GLY:N	2.41	0.54
12:L:109:VAL:HG13	12:L:113:GLN:HB3	1.89	0.54
1:A:1798:U:H5'	3:C:259:THR:HG22	1.90	0.54
24:X:35:LEU:HD12	24:X:53:LEU:HD12	1.89	0.54
1:A:99:U:H4'	1:A:101:G:H5''	1.89	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2573:C:OP1	1:A:2574:G:OP1	2.25	0.54
2:B:43:C:H5'	26:Z:1:MET:HA	1.89	0.54
9:I:35:ARG:HB2	9:I:42:TRP:CH2	2.42	0.54
22:V:20:ARG:O	22:V:24:LYS:NZ	2.39	0.54
1:A:444:C:H4'	5:E:49:ALA:HB2	1.89	0.54
1:A:2061:G:OP1	5:E:68:LYS:NZ	2.41	0.54
16:P:76:TYR:CZ	16:P:80:ILE:HG13	2.43	0.54
26:Z:55:ARG:HG3	26:Z:59:PHE:HD2	1.72	0.54
1:A:1790:C:H2'	1:A:1791:A:C5	2.42	0.54
6:F:15:VAL:HG21	6:F:176:LEU:HD23	1.90	0.54
4:D:111:ARG:HD2	4:D:160:TYR:CD2	2.42	0.54
7:G:12:PRO:CD	7:G:48:GLY:O	2.55	0.54
21:U:149:SER:HB2	21:U:172:ALA:O	2.07	0.54
1:A:528:A:C2	1:A:2042:A:H2'	2.42	0.54
3:C:70:TRP:CH2	3:C:150:LYS:HA	2.43	0.54
8:H:79:ILE:N	8:H:141:LYS:O	2.40	0.54
21:U:82:ARG:HG3	21:U:83:PRO:HD2	1.90	0.54
1:A:2849:U:P	15:O:95:ARG:HH12	2.31	0.53
3:C:43:ARG:CB	3:C:54:ARG:HB2	2.38	0.53
1:A:2680:C:H5'	4:D:189:PRO:HA	1.90	0.53
4:D:78:LEU:HG	4:D:79:ARG:NE	2.23	0.53
1:A:1341:U:OP2	1:A:1394:U:O2'	2.19	0.53
8:H:62:LYS:HE3	8:H:134:PRO:HG2	1.90	0.53
9:I:6:PRO:HG3	9:I:41:ASP:HB2	1.89	0.53
24:X:15:LYS:H	24:X:67:LYS:HE2	1.73	0.53
1:A:1641:A:H2'	1:A:1642:G:O4'	2.08	0.53
3:C:244:ARG:HB2	3:C:245:PRO:HD2	1.90	0.53
9:I:30:ILE:HG23	9:I:52:VAL:HG11	1.91	0.53
11:K:88:LEU:HD12	11:K:95:VAL:HG11	1.90	0.53
17:Q:66:ARG:NH1	17:Q:88:ARG:HD3	2.23	0.53
1:A:2286:A:H4'	1:A:2287:A:O4'	2.09	0.53
1:A:2304:G:H22	1:A:2312:U:H3	1.57	0.53
3:C:30:GLU:HG3	3:C:63:ARG:HH21	1.72	0.53
14:N:58:LEU:O	14:N:58:LEU:HD23	2.08	0.53
15:O:112:ARG:NE	15:O:112:ARG:O	2.39	0.53
15:O:51:ARG:CG	15:O:98:LYS:HG3	2.38	0.53
1:A:1826:G:H4'	3:C:242:ARG:CZ	2.39	0.53
1:A:2114:A:N6	1:A:2119:A:N7	2.56	0.53
12:L:12:GLN:HG2	12:L:73:PRO:HD2	1.90	0.53
1:A:673:C:OP1	5:E:54:ARG:NH1	2.37	0.53
3:C:206:LEU:O	3:C:211:ARG:HD3	2.09	0.53
8:H:93:THR:HG22	8:H:119:PRO:HB3	1.91	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
15:O:105:LEU:O	15:O:107:ASP:N	2.42	0.53
1:A:28:A:N6	1:A:512:G:H1'	2.23	0.53
1:A:862:G:H2'	1:A:863:A:O4'	2.08	0.53
9:I:13:TRP:O	9:I:135:PRO:HD2	2.08	0.53
9:I:96:GLU:HG2	9:I:97:ARG:N	2.23	0.53
11:K:92:GLU:HA	11:K:123:LEU:HD23	1.89	0.53
15:O:16:ARG:HE	15:O:19:LEU:HD21	1.73	0.53
16:P:102:GLU:OE1	17:Q:13:ARG:NH2	2.41	0.53
1:A:1790:C:H5''	1:A:1791:A:OP1	2.08	0.53
1:A:2496:C:P	12:L:81:VAL:HG12	2.48	0.53
1:A:918:A:N3	2:B:80:U:O2'	2.38	0.53
1:A:2154:G:H2'	1:A:2155:G:H8	1.73	0.53
1:A:27:G:N2	1:A:512:G:H2'	2.24	0.53
3:C:85:ASP:OD2	3:C:88:ARG:HD2	2.08	0.53
1:A:2392:A:C8	11:K:60:MET:HG2	2.44	0.53
14:N:10:ARG:O	14:N:12:PHE:N	2.42	0.53
6:F:179:PRO:HG3	26:Z:38:LYS:NZ	2.24	0.53
1:A:996:A:OP2	16:P:92:ARG:NH2	2.42	0.53
7:G:149:ARG:NH1	7:G:167:GLU:OE1	2.42	0.53
1:A:1209:G:H21	1:A:1210:A:H62	1.56	0.52
1:A:287:C:H2'	1:A:288:C:C6	2.43	0.52
1:A:605:C:O2	1:A:657:U:O2'	2.27	0.52
1:A:1359:A:N6	1:A:1373:A:C5	2.77	0.52
3:C:132:PRO:HD3	3:C:190:TYR:CZ	2.44	0.52
20:T:35:TYR:CE2	20:T:69:ALA:HB3	2.44	0.52
1:A:2683:C:OP1	15:O:53:ARG:NH2	2.38	0.52
2:B:104:A:H5'	21:U:72:ARG:HD3	1.90	0.52
6:F:96:ARG:O	6:F:98:ARG:N	2.42	0.52
9:I:110:GLY:O	9:I:114:ARG:HG3	2.09	0.52
1:A:1426:G:OP2	1:A:1427:A:O2'	2.28	0.52
1:A:1407:C:N4	1:A:1595:G:H1	2.08	0.52
1:A:551:G:H5'	1:A:1220:A:H1'	1.91	0.52
1:A:828:U:H4'	1:A:831:G:N1	2.24	0.52
14:N:6:ALA:O	14:N:10:ARG:HD3	2.09	0.52
26:Z:54:GLY:O	26:Z:59:PHE:HB2	2.09	0.52
5:E:24:LEU:HD23	5:E:115:ALA:HA	1.91	0.52
11:K:20:GLY:HA2	11:K:27:HIS:O	2.10	0.52
1:A:2022:U:O2'	1:A:2617:C:H5'	2.08	0.52
5:E:63:LYS:HE2	5:E:67:GLN:HB2	1.91	0.52
6:F:88:ILE:O	6:F:88:ILE:HD13	2.09	0.52
1:A:958:U:OP2	12:L:14:ARG:NH1	2.42	0.52
25:Y:40:THR:HB	25:Y:43:ILE:HG12	1.92	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1316:U:H2'	1:A:1317:A:C8	2.44	0.52
7:G:152:ARG:HG3	7:G:153:LYS:N	2.25	0.52
1:A:2334:G:H5'	14:N:9:ARG:HG2	1.91	0.52
23:W:83:GLU:HG2	23:W:84:GLY:N	2.24	0.52
24:X:58:ALA:O	24:X:62:THR:HG23	2.10	0.52
1:A:1071:G:O6	1:A:1091:G:O6	2.28	0.52
1:A:49:A:C8	1:A:120:U:C5	2.98	0.52
1:A:1533:C:N3	1:A:1538:G:N2	2.46	0.52
11:K:62:LEU:CD2	11:K:62:LEU:N	2.72	0.52
1:A:443:A:H5''	1:A:444:C:OP1	2.10	0.51
3:C:248:SER:HB3	3:C:252:TRP:CZ2	2.43	0.51
6:F:77:ILE:HD13	6:F:82:LEU:HD12	1.92	0.51
7:G:88:LEU:H	7:G:88:LEU:HD22	1.75	0.51
15:O:88:ILE:HD12	15:O:90:GLN:N	2.25	0.51
1:A:874:G:H5''	21:U:175:VAL:HG11	1.92	0.51
3:C:250:TRP:HE3	3:C:252:TRP:HE1	1.58	0.51
7:G:26:VAL:HG13	7:G:27:LYS:H	1.76	0.51
16:P:107:ALA:O	16:P:110:VAL:HB	2.10	0.51
18:R:40:ASN:O	18:R:41:LYS:HG2	2.10	0.51
3:C:148:GLU:HB2	3:C:151:LYS:HD2	1.92	0.51
1:A:2224:G:OP1	3:C:268:ARG:HD3	2.11	0.51
8:H:110:ASP:N	8:H:130:TYR:OH	2.43	0.51
13:M:83:ILE:HG22	13:M:87:TYR:HE2	1.76	0.51
9:I:38:HIS:O	16:P:67:ALA:HB1	2.10	0.51
17:Q:25:LEU:H	17:Q:92:THR:HG21	1.74	0.51
21:U:124:ILE:HG22	21:U:126:VAL:HG13	1.92	0.51
23:W:70:VAL:O	23:W:74:VAL:HG23	2.10	0.51
1:A:1093:G:H5'	7:G:170:ARG:NH1	2.26	0.51
1:A:1972:A:H2'	1:A:1973:G:H8	1.74	0.51
1:A:2298:A:H2'	1:A:2299:G:O4'	2.11	0.51
1:A:2469:A:H5''	1:A:2470:G:C8	2.46	0.51
6:F:16:ARG:O	6:F:20:ILE:HG12	2.10	0.51
8:H:41:GLU:HG2	8:H:42:SER:N	2.24	0.51
11:K:96:THR:HG22	11:K:126:VAL:HB	1.93	0.51
1:A:2250:G:C4	12:L:82:ARG:HG3	2.46	0.51
17:Q:65:GLY:HA3	17:Q:91:TYR:CZ	2.46	0.51
24:X:24:LEU:HD13	24:X:60:LEU:HD11	1.92	0.51
5:E:127:GLU:OE1	5:E:196:LEU:HB2	2.11	0.51
1:A:2011:U:OP1	18:R:42:ARG:NH1	2.44	0.51
24:X:65:ASN:HB3	24:X:69:ARG:NH2	2.26	0.51
4:D:62:PRO:O	4:D:64:LYS:N	2.43	0.51
1:A:2377:A:O2'	14:N:111:GLU:O	2.18	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:N:11:LYS:HB2	14:N:91:PRO:HB3	1.93	0.51
15:O:109:GLU:O	15:O:113:LYS:HB2	2.11	0.51
16:P:47:TYR:HA	16:P:50:ARG:NH2	2.26	0.51
18:R:106:ILE:O	18:R:106:ILE:HG12	2.07	0.51
1:A:142:G:H1'	19:S:37:THR:HG21	1.93	0.51
1:A:414:C:O2	1:A:1864:U:O2'	2.25	0.51
2:B:44:G:H5''	2:B:45:A:OP1	2.11	0.51
3:C:35:LYS:NZ	3:C:104:TYR:HB2	2.26	0.51
1:A:1820:U:C2	3:C:202:LYS:HB3	2.46	0.51
7:G:6:ARG:NE	7:G:54:ARG:HH12	2.09	0.51
8:H:11:ASN:O	8:H:12:LEU:HB2	2.11	0.51
16:P:92:ARG:NH1	17:Q:11:GLN:O	2.44	0.51
12:L:134:ARG:NH2	21:U:122:ARG:HH21	1.98	0.51
1:A:2850:A:N7	1:A:2868:A:O2'	2.37	0.51
13:M:104:ARG:HD3	13:M:111:LEU:HD21	1.92	0.51
25:Y:43:ILE:O	25:Y:47:VAL:HG23	2.10	0.51
1:A:2115:G:N2	1:A:2165:G:N7	2.49	0.51
1:A:2347:C:H2'	1:A:2348:U:C6	2.46	0.51
7:G:89:ILE:O	7:G:89:ILE:HG12	2.10	0.51
12:L:2:LEU:H	12:L:2:LEU:HD23	1.76	0.51
20:T:81:LYS:HG2	20:T:97:ARG:HD3	1.93	0.51
1:A:1050:A:H8	1:A:2751:G:HO2'	1.58	0.51
1:A:639:U:H2'	1:A:640:C:C6	2.46	0.51
1:A:625:G:O6	11:K:107:LYS:HE2	2.11	0.51
1:A:1649:G:O2'	13:M:107:ASP:OD2	2.20	0.51
1:A:1210:A:H5''	1:A:1212:G:O4'	2.11	0.50
4:D:111:ARG:HA	13:M:1:MET:CG	2.40	0.50
12:L:66:ILE:O	12:L:104:PHE:N	2.39	0.50
18:R:57:ASN:O	18:R:61:ASN:HB2	2.10	0.50
26:Z:10:VAL:HG22	26:Z:11:PRO:HD2	1.93	0.50
1:A:2610:C:H4'	1:A:2611:U:OP2	2.10	0.50
12:L:89:ASN:O	12:L:91:GLU:N	2.44	0.50
14:N:30:ARG:HG3	14:N:97:ARG:NH2	2.26	0.50
1:A:910:A:N3	1:A:2264:C:O2'	2.39	0.50
6:F:5:VAL:HG11	6:F:100:TRP:HB3	1.93	0.50
7:G:10:PRO:CG	7:G:50:VAL:CG1	2.76	0.50
17:Q:52:VAL:HG23	17:Q:55:ALA:H	1.76	0.50
1:A:1061:U:H3'	1:A:1062:G:H5''	1.93	0.50
1:A:1264:G:H3'	1:A:1265:A:H5''	1.94	0.50
1:A:470:A:H2'	1:A:471:A:O4'	2.11	0.50
5:E:167:ALA:HB1	5:E:173:VAL:HG11	1.93	0.50
8:H:13:GLY:HA3	8:H:17:GLN:OE1	2.12	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:J:120:GLU:HG2	10:J:122:LEU:HG	1.94	0.50
5:E:65:TRP:O	5:E:67:GLN:N	2.43	0.50
7:G:84:SER:O	7:G:85:LYS:HB2	2.11	0.50
11:K:36:LYS:HB3	11:K:40:SER:HB3	1.94	0.50
1:A:1278:A:H4'	13:M:34:ILE:HD12	1.94	0.50
1:A:1109:C:O2'	1:A:1110:G:OP1	2.30	0.50
1:A:2319:G:N7	14:N:3:ARG:HB3	2.27	0.50
7:G:4:ILE:HG13	7:G:6:ARG:NE	2.26	0.50
17:Q:61:VAL:HA	17:Q:94:LEU:HD23	1.93	0.50
1:A:1069:A:H4'	1:A:1070:A:H5''	1.93	0.50
1:A:2071:A:H2'	1:A:2072:G:H8	1.76	0.50
1:A:1803:A:H4'	3:C:259:THR:HG23	1.93	0.50
5:E:108:LYS:O	5:E:112:MET:HG3	2.12	0.50
9:I:58:ASP:OD1	9:I:58:ASP:N	2.45	0.50
12:L:66:ILE:HG13	12:L:67:ARG:N	2.27	0.50
1:A:1689:A:H62	1:A:1698:A:H2	1.58	0.49
1:A:2340:G:H2'	1:A:2341:G:C8	2.47	0.49
4:D:103:ASP:OD1	4:D:201:THR:HG23	2.12	0.49
1:A:1012:U:O4	9:I:25:ARG:HA	2.12	0.49
16:P:83:LEU:HG	16:P:88:ILE:HG13	1.93	0.49
20:T:97:ARG:HH21	20:T:98:VAL:HB	1.76	0.49
1:A:278:A:H2'	1:A:279:C:C6	2.47	0.49
4:D:35:GLN:HG2	4:D:37:ARG:HE	1.77	0.49
9:I:7:LYS:N	9:I:7:LYS:HD2	2.27	0.49
11:K:126:VAL:HG13	11:K:145:PRO:HB2	1.94	0.49
22:V:70:GLN:OE1	22:V:72:ARG:HD3	2.12	0.49
1:A:102:G:H4'	1:A:103:A:O5'	2.11	0.49
1:A:2795:G:H3'	1:A:2797:U:C5'	2.42	0.49
4:D:73:GLU:HG3	4:D:74:PRO:HD2	1.92	0.49
1:A:1081:U:H3'	1:A:1082:U:H4'	1.94	0.49
1:A:340:A:H2'	1:A:341:G:O4'	2.12	0.49
2:B:41:U:C4	6:F:70:VAL:HG23	2.48	0.49
16:P:61:TRP:CD2	16:P:94:ASN:HA	2.47	0.49
26:Z:15:ILE:H	26:Z:15:ILE:HD13	1.76	0.49
1:A:1348:G:H2'	1:A:1349:A:H5''	1.94	0.49
1:A:888:C:H3'	1:A:889:C:C4'	2.40	0.49
3:C:76:PRO:HG2	3:C:98:VAL:HG21	1.93	0.49
9:I:34:LEU:HD21	9:I:120:LEU:HB2	1.94	0.49
9:I:17:ASP:O	9:I:56:ASN:HB2	2.12	0.49
19:S:53:LYS:HB3	19:S:82:GLN:HB3	1.93	0.49
1:A:1858:G:O2'	1:A:1884:A:N6	2.44	0.49
1:A:807:U:H2'	1:A:808:G:C8	2.47	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:27:THR:HG21	3:C:83:GLU:HG2	1.94	0.49
1:A:691:C:O4'	3:C:43:ARG:NH2	2.46	0.49
16:P:95:LEU:HD22	17:Q:4:ILE:HD12	1.93	0.49
19:S:57:LEU:HD11	19:S:78:LYS:HD2	1.94	0.49
6:F:67:LYS:HZ1	26:Z:1:MET:HB2	1.78	0.49
1:A:2071:A:H2'	1:A:2072:G:C8	2.48	0.49
1:A:583:G:OP2	16:P:10:ARG:HD2	2.13	0.49
4:D:179:GLU:HB3	4:D:181:LEU:HD23	1.94	0.49
6:F:94:LEU:HD12	6:F:99:MET:HA	1.95	0.49
1:A:2232:U:P	23:W:40:ARG:HH12	2.35	0.49
1:A:943:U:OP2	11:K:36:LYS:NZ	2.42	0.49
7:G:98:LEU:HD13	7:G:125:VAL:HB	1.94	0.49
1:A:1754:C:P	15:O:96:ARG:NH1	2.86	0.49
1:A:573:G:O2'	1:A:574:C:H3'	2.13	0.49
3:C:170:GLY:C	3:C:172:TYR:H	2.16	0.49
4:D:24:THR:O	4:D:24:THR:HG22	2.13	0.49
20:T:86:ARG:HB2	20:T:95:LYS:HD2	1.94	0.49
1:A:1311:G:N2	1:A:1603:A:H62	2.11	0.49
1:A:1384:A:N3	1:A:1405:U:H1'	2.27	0.49
1:A:1427:A:H4'	1:A:1428:C:O5'	2.12	0.49
5:E:185:ASP:OD1	5:E:188:ARG:NH1	2.35	0.49
8:H:76:THR:OG1	8:H:139:GLN:OE1	2.31	0.49
10:J:4:PRO:O	10:J:5:GLN:HB2	2.11	0.49
16:P:98:LEU:O	16:P:102:GLU:N	2.37	0.49
22:V:53:MET:HA	22:V:58:THR:O	2.13	0.49
1:A:1045:A:O2'	1:A:1046:A:OP2	2.28	0.48
1:A:2776:A:H4'	1:A:2777:G:O5'	2.12	0.48
1:A:654(A):G:H8	1:A:654(A):G:OP2	1.96	0.48
3:C:248:SER:OG	3:C:252:TRP:CD1	2.57	0.48
3:C:61:LEU:O	3:C:63:ARG:NH1	2.45	0.48
5:E:176:LEU:HD21	5:E:181:LEU:HA	1.94	0.48
7:G:55:PRO:HG2	7:G:61:HIS:CE1	2.48	0.48
12:L:104:PHE:CE2	12:L:125:LEU:HD11	2.41	0.48
1:A:2693:A:H2'	1:A:2694:G:H8	1.78	0.48
1:A:671:C:H2'	1:A:672:C:H6	1.78	0.48
1:A:2227:A:H5''	3:C:263:ARG:NH1	2.29	0.48
3:C:35:LYS:HD3	3:C:63:ARG:CB	2.43	0.48
6:F:166:ASP:HA	6:F:169:ALA:HB3	1.95	0.48
10:J:76:ALA:HB3	15:O:75:ILE:HD12	1.95	0.48
1:A:954:G:H5''	12:L:13:GLN:HB3	1.94	0.48
15:O:107:ASP:H	15:O:110:ILE:HG22	1.78	0.48
18:R:51:LEU:HD23	18:R:105:VAL:HG11	1.94	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:W:41:ARG:HG3	23:W:41:ARG:HH11	1.78	0.48
1:A:1026:U:H1'	1:A:1027:A:O5'	2.12	0.48
1:A:1085:A:O2'	1:A:1086:A:OP1	2.27	0.48
1:A:1408:C:H2'	1:A:1409:C:C6	2.48	0.48
1:A:2335:A:HO2'	1:A:2336:A:P	2.35	0.48
1:A:220:G:O2'	1:A:233:A:N3	2.42	0.48
1:A:2641:G:P	9:I:83:LYS:HE3	2.53	0.48
7:G:137:ASP:HB3	7:G:140:LYS:HB3	1.94	0.48
11:K:82:GLY:HA2	11:K:113:LYS:O	2.12	0.48
11:K:135:LEU:HD13	11:K:139:LYS:HE2	1.94	0.48
4:D:111:ARG:HG2	13:M:1:MET:SD	2.53	0.48
11:K:46:LYS:HB3	11:K:46:LYS:HE3	1.54	0.48
17:Q:15:GLU:O	17:Q:18:LEU:HB2	2.14	0.48
1:A:2712:U:O2'	1:A:2712(A):A:H8	1.96	0.48
1:A:278:A:O2'	1:A:279:C:O4'	2.20	0.48
11:K:5:ASP:O	11:K:6:LEU:O	2.31	0.48
15:O:102:ILE:HB	15:O:110:ILE:HD13	1.95	0.48
16:P:60:LEU:O	16:P:60:LEU:HD22	2.14	0.48
19:S:63:LYS:O	19:S:64:LYS:HD2	2.14	0.48
2:B:12:C:C2'	22:V:73:GLY:HA3	2.43	0.48
1:A:1819:A:H4'	1:A:1820:U:O5'	2.13	0.48
1:A:2081:C:H2'	1:A:2082:A:H8	1.79	0.48
1:A:676:A:N1	1:A:802:A:N1	2.61	0.48
11:K:52:GLU:O	11:K:55:ARG:HG2	2.14	0.48
1:A:1045:A:C5	1:A:1111:A:N7	2.81	0.48
1:A:1220:A:OP2	16:P:19:LYS:NZ	2.33	0.48
11:K:14:LYS:O	11:K:16:ARG:HG2	2.13	0.48
16:P:97:ASP:OD2	16:P:101:ARG:NH1	2.46	0.48
16:P:90:VAL:HG22	17:Q:39:LEU:HB3	1.96	0.48
1:A:874:G:H4'	21:U:118:GLN:OE1	2.13	0.48
1:A:1101:U:H2'	1:A:1102:C:C6	2.49	0.48
1:A:1287:A:N7	13:M:107:ASP:HB2	2.28	0.48
1:A:1508:A:O2'	1:A:1509:C:O4'	2.25	0.48
1:A:1537:C:H2'	1:A:1538:G:C8	2.48	0.48
1:A:207:A:H2'	1:A:208:C:O4'	2.14	0.48
1:A:2212:A:H1'	1:A:2215:G:C5	2.48	0.48
1:A:28:A:H61	1:A:512:G:H1'	1.78	0.48
3:C:35:LYS:HZ1	3:C:104:TYR:HB2	1.79	0.48
3:C:254:THR:O	3:C:254:THR:OG1	2.30	0.48
14:N:58:LEU:HD12	14:N:68:GLN:OE1	2.14	0.48
17:Q:76:LYS:HB2	17:Q:81:TYR:HB3	1.95	0.48
18:R:67:ASP:OD1	18:R:67:ASP:N	2.46	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:T:44:ILE:HG13	20:T:45:VAL:N	2.28	0.48
1:A:270(T):G:OP1	23:W:97:LEU:HD13	2.13	0.48
14:N:74:ALA:HB1	14:N:107:GLU:HB3	1.96	0.48
1:A:2146:C:H4'	1:A:2147:G:C8	2.49	0.48
1:A:270(F):U:H2'	1:A:270(G):C:C6	2.49	0.48
1:A:2780:G:OP2	9:I:118:LYS:HE2	2.14	0.48
1:A:450:G:O6	1:A:453:C:OP1	2.32	0.48
1:A:817:C:H2'	1:A:818:G:O4'	2.14	0.48
16:P:92:ARG:CZ	17:Q:11:GLN:H	2.26	0.48
20:T:35:TYR:CD2	20:T:69:ALA:HB3	2.49	0.48
1:A:1053:C:H42	1:A:1106:G:H1	1.60	0.47
1:A:1357:U:H2'	1:A:1358:G:O4'	2.13	0.47
1:A:1910:G:H1	1:A:1920:C:H42	1.62	0.47
1:A:2291:U:H2'	1:A:2292:C:C6	2.48	0.47
1:A:2777:G:OP2	1:A:2781:A:O2'	2.20	0.47
1:A:729:G:C6	3:C:208:LYS:HB2	2.49	0.47
3:C:28:GLU:HB2	3:C:29:PRO:CD	2.44	0.47
5:E:36:VAL:HG11	5:E:183:VAL:HG11	1.95	0.47
8:H:69:LYS:HG3	8:H:136:VAL:HB	1.96	0.47
9:I:134:ARG:N	9:I:135:PRO:HD3	2.29	0.47
11:K:98:GLU:HA	11:K:101:VAL:HB	1.96	0.47
14:N:65:VAL:O	14:N:69:VAL:HG12	2.14	0.47
17:Q:44:LYS:O	17:Q:46:VAL:HG12	2.13	0.47
1:A:99:U:H1'	1:A:101:G:OP2	2.14	0.47
1:A:1103:A:H5'	1:A:1104:C:H5	1.79	0.47
1:A:1013:C:N4	1:A:1149:G:H1	2.11	0.47
1:A:2511:U:O4	1:A:2575:C:N3	2.46	0.47
1:A:807:U:H2'	1:A:808:G:H8	1.78	0.47
7:G:6:ARG:HA	7:G:66:GLY:HA2	1.95	0.47
1:A:2210:G:H5'	1:A:2211:G:C5	2.49	0.47
1:A:2590:A:OP2	3:C:238:GLY:HA2	2.15	0.47
1:A:72:U:N3	24:X:62:THR:HG22	2.30	0.47
12:L:21:THR:HB	12:L:22:LYS:H	1.40	0.47
23:W:91:LYS:HB3	23:W:92:LYS:H	1.44	0.47
1:A:740:U:H5''	1:A:1784:A:H3'	1.95	0.47
1:A:242:G:H4'	1:A:243:U:O5'	2.14	0.47
1:A:2789:C:H1'	1:A:2892:A:C2	2.46	0.47
1:A:764:A:H5'	3:C:210:GLY:HA2	1.95	0.47
3:C:71:ASP:HB2	3:C:103:ARG:NH2	2.27	0.47
11:K:144:GLU:N	11:K:144:GLU:OE1	2.40	0.47
24:X:59:ARG:O	24:X:63:VAL:HG23	2.15	0.47
1:A:2154:G:H2'	1:A:2155:G:C8	2.48	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:G:153:LYS:HB3	7:G:154:PRO:HD3	1.96	0.47
18:R:110:LYS:HG3	18:R:111:HIS:H	1.80	0.47
1:A:137(A):G:H1'	19:S:41:ASN:HD22	1.76	0.47
1:A:2182:G:H2'	1:A:2183:C:C6	2.50	0.47
1:A:2287:A:N6	1:A:2344:U:C2	2.83	0.47
1:A:2732:G:H3'	1:A:2733:A:O4'	2.14	0.47
1:A:479:A:N3	1:A:481:G:H5''	2.30	0.47
1:A:498:G:H1'	20:T:47:LYS:HZ3	1.79	0.47
2:B:37:C:N3	2:B:48:A:O2'	2.41	0.47
5:E:164:ARG:HG3	5:E:175:THR:OG1	2.15	0.47
15:O:11:GLU:OE1	15:O:11:GLU:N	2.43	0.47
20:T:73:ARG:HE	20:T:73:ARG:HB3	1.47	0.47
21:U:182:LYS:CG	21:U:183:LEU:HA	2.44	0.47
22:V:19:LYS:HD3	22:V:19:LYS:HA	1.66	0.47
23:W:53:VAL:HG22	23:W:74:VAL:HG13	1.96	0.47
1:A:1454:U:H5'	13:M:63:ARG:HE	1.79	0.47
1:A:26:G:H1'	1:A:515:A:H61	1.79	0.47
6:F:28:VAL:O	6:F:31:VAL:HG13	2.14	0.47
9:I:30:ILE:HG22	9:I:34:LEU:HD22	1.96	0.47
1:A:2308:G:N1	1:A:2311:A:C2	2.61	0.47
1:A:2867:G:O2'	1:A:2868:A:P	2.73	0.47
1:A:372:G:H1'	1:A:373:U:H5	1.80	0.47
3:C:237:GLU:O	3:C:239:ARG:N	2.47	0.47
5:E:129:PHE:HA	5:E:142:TRP:NE1	2.29	0.47
5:E:182:ASN:HD21	5:E:185:ASP:CG	2.14	0.47
6:F:113:ARG:HG2	26:Z:34:GLU:OE2	2.14	0.47
6:F:34:LEU:HD22	6:F:35:GLU:N	2.30	0.47
1:A:1316:U:H2'	1:A:1317:A:H8	1.79	0.47
1:A:587:C:N3	11:K:33:ARG:NH1	2.62	0.47
1:A:896:A:H61	21:U:112:ARG:NH1	2.12	0.47
1:A:443:A:N7	5:E:45:ARG:HD2	2.30	0.47
6:F:114:ILE:HD13	6:F:140:ILE:HG21	1.96	0.47
7:G:122:THR:HG22	7:G:134:SER:HB2	1.96	0.47
7:G:4:ILE:HB	7:G:6:ARG:CG	2.43	0.47
7:G:4:ILE:HG13	7:G:6:ARG:CZ	2.44	0.47
11:K:19:VAL:HG13	11:K:21:ARG:N	2.20	0.47
12:L:81:VAL:O	12:L:82:ARG:NE	2.48	0.47
1:A:577:G:O2'	1:A:1254:A:OP1	2.29	0.47
1:A:1360:A:C6	1:A:1372:U:C4	3.03	0.47
1:A:1697:G:H5''	1:A:1698:A:H3'	1.96	0.47
5:E:9:ILE:HG23	5:E:20:LEU:O	2.15	0.47
14:N:52:SER:HB2	14:N:55:ALA:H	1.80	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1472:A:H2'	1:A:1473:G:O4'	2.15	0.47
1:A:2243:U:H2'	1:A:2244:U:C6	2.50	0.47
1:A:2401:U:H2'	1:A:2402:C:H5''	1.97	0.47
1:A:270(R):G:H2'	1:A:270(S):G:C8	2.50	0.47
3:C:17:THR:CG2	3:C:205:VAL:H	2.28	0.47
4:D:116:VAL:HG11	4:D:138:PRO:HB3	1.97	0.47
4:D:150:VAL:HG13	4:D:154:LYS:HG3	1.96	0.47
6:F:11:TYR:HA	6:F:15:VAL:HB	1.95	0.47
8:H:144:VAL:HG22	8:H:145:VAL:H	1.80	0.47
11:K:29:LYS:HD2	11:K:30:THR:HG23	1.97	0.47
26:Z:38:LYS:HD3	26:Z:42:PHE:HE1	1.80	0.47
1:A:2527:C:H5''	5:E:30:PRO:HB2	121.43	0.46
5:E:108:LYS:HB3	5:E:108:LYS:NZ	2.31	0.46
11:K:88:LEU:HB2	11:K:91:PHE:HE1	1.80	0.46
14:N:27:SER:HA	14:N:88:ASP:HB2	1.96	0.46
20:T:87:LYS:HD3	20:T:92:ASN:HB3	1.98	0.46
25:Y:23:LEU:HD13	25:Y:50:VAL:HG11	1.96	0.46
1:A:1035:U:H2'	1:A:1036:G:C8	2.50	0.46
1:A:1270:C:H5''	1:A:1271:G:H5'	1.97	0.46
1:A:1434:A:H61	1:A:1558:A:H62	1.62	0.46
1:A:1639:U:H2'	1:A:1640:C:H5''	1.96	0.46
1:A:1796:U:H2'	1:A:1797:C:C6	2.49	0.46
1:A:2031:A:N3	1:A:2455:G:O2'	2.39	0.46
1:A:957:A:N1	1:A:2458:G:H4'	2.30	0.46
1:A:2543:G:H2'	1:A:2544:G:C8	2.49	0.46
1:A:2728:U:H2'	1:A:2729:G:C8	2.51	0.46
5:E:127:GLU:OE2	5:E:128:ALA:N	2.47	0.46
8:H:68:LEU:HA	8:H:71:ILE:HG22	1.97	0.46
11:K:96:THR:O	11:K:99:LEU:HB3	2.15	0.46
1:A:2277:G:OP2	22:V:10:THR:HG21	2.15	0.46
1:A:1087:G:C5	1:A:1089:G:H1'	2.50	0.46
1:A:407:G:H2'	1:A:408:G:H8	1.80	0.46
1:A:483:A:H3'	1:A:484:C:H6	1.81	0.46
3:C:94:LEU:HD22	3:C:95:LEU:N	2.31	0.46
9:I:114:ARG:O	9:I:115:ARG:HB3	2.15	0.46
22:V:17:GLN:O	22:V:19:LYS:HE3	2.14	0.46
1:A:1055:G:H1	1:A:1104:C:N4	2.11	0.46
1:A:2334:G:C6	22:V:75:LEU:HD21	2.51	0.46
2:B:89(A):A:C5	2:B:90:C:H1'	2.51	0.46
3:C:206:LEU:HA	3:C:206:LEU:HD23	1.51	0.46
3:C:25:THR:CG2	3:C:82:ILE:H	2.27	0.46
4:D:176:ILE:HB	4:D:181:LEU:HB2	1.97	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:K:121:LYS:HE2	11:K:121:LYS:HB2	1.74	0.46
24:X:47:ASN:HB2	24:X:48:HIS:H	1.50	0.46
25:Y:8:LEU:HD22	25:Y:31:LEU:HD22	1.96	0.46
1:A:1113:U:H2'	1:A:1114:G:C8	2.50	0.46
1:A:1579:A:H2'	1:A:1580:A:C8	2.50	0.46
1:A:2324:C:H5''	1:A:2325:G:H5'	1.97	0.46
1:A:304:G:H2'	1:A:305:U:C6	2.51	0.46
4:D:36:ARG:NH2	4:D:88:GLY:HA2	2.29	0.46
7:G:16:SER:O	7:G:26:VAL:O	2.33	0.46
16:P:75:ASN:HB3	16:P:78:THR:H	1.81	0.46
26:Z:55:ARG:HG3	26:Z:59:PHE:CD2	2.49	0.46
1:A:195:A:H5''	1:A:196:A:O5'	2.16	0.46
3:C:118:VAL:HG22	3:C:119:ALA:N	2.31	0.46
3:C:35:LYS:HB3	3:C:63:ARG:HA	1.98	0.46
7:G:152:ARG:HG3	7:G:153:LYS:CD	2.35	0.46
8:H:3:VAL:O	8:H:18:VAL:HA	2.15	0.46
20:T:94:LYS:HD2	20:T:101:LYS:HZ3	1.81	0.46
1:A:1154:G:OP2	16:P:58:ARG:NH1	2.48	0.46
1:A:1203:G:O6	1:A:1204:A:N6	2.48	0.46
1:A:137(A):G:H2'	1:A:139:G:N7	2.31	0.46
3:C:35:LYS:HE3	3:C:63:ARG:C	2.36	0.46
6:F:34:LEU:HD12	6:F:100:TRP:CH2	2.50	0.46
12:L:136:ALA:O	12:L:138:ASP:N	2.40	0.46
13:M:109:ALA:HA	13:M:110:PRO:HD2	1.77	0.46
1:A:2882:A:OP1	13:M:96:ARG:NH1	2.48	0.46
23:W:96:LYS:H	23:W:97:LEU:HD12	1.81	0.46
26:Z:2:LYS:HA	26:Z:2:LYS:HD2	1.67	0.46
1:A:1059:G:H3'	1:A:1060:U:H5''	1.97	0.46
1:A:2197:U:H1'	1:A:2198:A:C8	2.50	0.46
1:A:2331:G:H4'	22:V:43:THR:H	1.80	0.46
1:A:2790:A:O2'	1:A:2893:G:N3	2.48	0.46
3:C:121:PRO:CA	3:C:135:PHE:CD2	2.81	0.46
7:G:167:GLU:HA	7:G:168:PRO:HD3	1.79	0.46
11:K:135:LEU:HD23	11:K:135:LEU:HA	1.74	0.46
1:A:661:C:H5''	11:K:15:ARG:NH2	2.30	0.46
1:A:2023:G:H4'	1:A:2617:C:O3'	2.16	0.46
1:A:2699:C:H2'	1:A:2700:C:O4'	2.16	0.46
1:A:2836:U:H2'	1:A:2837:G:C8	2.51	0.46
1:A:578:A:OP1	1:A:1255:U:O2'	2.21	0.46
1:A:740:U:H2'	1:A:741:G:C8	2.51	0.46
4:D:116:VAL:O	4:D:117:MET:HB3	2.16	0.46
5:E:129:PHE:O	5:E:142:TRP:CD1	2.69	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:G:15:VAL:CG1	7:G:79:VAL:HG23	2.44	0.46
4:D:13:ARG:HB3	11:K:63:PRO:CA	125.54	0.46
12:L:135:ASP:OD1	12:L:135:ASP:N	2.48	0.46
18:R:110:LYS:HG3	18:R:111:HIS:ND1	2.31	0.46
20:T:84:ARG:HB3	20:T:95:LYS:HD3	1.97	0.46
23:W:80:LEU:HB2	23:W:81:LYS:H	1.61	0.46
1:A:755:C:H2'	1:A:756:C:C6	2.51	0.46
2:B:111:U:H2'	2:B:112:G:H8	1.80	0.46
1:A:2599:G:OP2	3:C:236:GLY:HA2	2.15	0.46
4:D:70:ALA:O	4:D:72:VAL:N	2.49	0.46
7:G:103:LEU:HD23	7:G:115:VAL:HB	1.97	0.46
11:K:138:LEU:C	11:K:140:ALA:H	2.18	0.46
17:Q:19:LYS:HA	17:Q:94:LEU:O	2.15	0.46
1:A:229:A:OP1	1:A:229:A:H4'	2.16	0.45
1:A:2867:G:O2'	1:A:2868:A:C8	2.69	0.45
1:A:755:C:H2'	1:A:756:C:H6	1.81	0.45
3:C:10:THR:OG1	3:C:13:ARG:HB2	2.16	0.45
4:D:108:SER:HB3	4:D:165:VAL:HG21	1.99	0.45
5:E:129:PHE:C	5:E:131:GLY:H	2.18	0.45
7:G:106:THR:HG22	7:G:112:PRO:HB3	1.97	0.45
11:K:58:THR:O	11:K:61:ARG:CZ	2.65	0.45
20:T:51:VAL:HG13	20:T:52:SER:N	2.28	0.45
1:A:2788:C:O2'	1:A:2809:A:N3	2.40	0.45
3:C:137:PRO:O	3:C:140:THR:HG23	2.16	0.45
5:E:11:VAL:HA	5:E:125:LEU:O	2.16	0.45
13:M:24:GLN:HE21	13:M:44:LEU:HG	1.81	0.45
13:M:78:LYS:O	13:M:83:ILE:HG12	2.16	0.45
14:N:58:LEU:N	14:N:58:LEU:CD2	2.73	0.45
23:W:58:ILE:N	23:W:58:ILE:HD12	2.30	0.45
23:W:91:LYS:HA	23:W:91:LYS:HE3	1.98	0.45
24:X:4:SER:OG	24:X:5:GLU:OE1	2.23	0.45
6:F:6:ALA:N	26:Z:23:GLU:HG2	2.28	0.45
1:A:83:G:N2	1:A:103:A:OP2	2.45	0.45
1:A:2159:G:H2'	1:A:2160:G:H8	1.81	0.45
1:A:2712:U:HO2'	1:A:2712(A):A:P	2.38	0.45
1:A:2817:G:OP1	13:M:99:LYS:NZ	2.44	0.45
1:A:844:C:H2'	1:A:845:G:O4'	2.16	0.45
7:G:109:PHE:CE1	7:G:152:ARG:HD3	2.51	0.45
7:G:86:GLU:O	7:G:87:LEU:HB2	2.16	0.45
8:H:131:LYS:HB3	8:H:132:PRO:HA	1.98	0.45
8:H:51:ILE:O	8:H:55:ALA:N	2.31	0.45
11:K:27:HIS:ND1	11:K:27:HIS:N	2.64	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:M:51:LEU:HD12	13:M:70:LEU:HG	1.97	0.45
16:P:66:ASN:O	16:P:70:ARG:HB2	2.17	0.45
16:P:68:ALA:O	16:P:71:GLN:HB2	2.16	0.45
1:A:336:C:HO2'	20:T:35:TYR:HH	1.65	0.45
20:T:87:LYS:HA	20:T:92:ASN:HB3	1.98	0.45
1:A:1678:G:N2	1:A:1989:G:H22	2.14	0.45
1:A:2591:C:H2'	1:A:2592:G:C8	2.51	0.45
11:K:124:LYS:HA	11:K:143:GLY:O	2.16	0.45
1:A:1454:U:H5'	13:M:63:ARG:NE	2.32	0.45
1:A:2847:U:P	15:O:98:LYS:HZ3	2.39	0.45
16:P:58:ARG:HA	16:P:61:TRP:CE3	2.52	0.45
1:A:1113:U:H2'	1:A:1114:G:H8	1.81	0.45
1:A:1020:A:N1	1:A:1141:U:H2'	2.32	0.45
1:A:1533:C:H2'	1:A:1534:G:N7	2.31	0.45
1:A:807:U:O2'	1:A:2060:A:N1	2.46	0.45
1:A:2086:U:H2'	1:A:2087:G:C8	2.51	0.45
1:A:2537:U:H2'	1:A:2538:C:C6	2.51	0.45
1:A:306:U:H2'	1:A:307:G:O4'	2.17	0.45
17:Q:36:PRO:HA	17:Q:56:SER:OG	2.16	0.45
20:T:56:PRO:O	20:T:58:GLY:N	2.49	0.45
24:X:24:LEU:HD23	24:X:24:LEU:HA	1.67	0.45
1:A:1045:A:N3	1:A:1047:G:N2	2.65	0.45
1:A:1061:U:H5'	1:A:1070:A:O2'	2.16	0.45
1:A:1069:A:H2'	1:A:1073:A:N7	2.31	0.45
1:A:2022:U:O2'	1:A:2616:C:O2'	2.22	0.45
1:A:2693:A:H2'	1:A:2694:G:C8	2.51	0.45
1:A:848:G:H2'	1:A:849:A:C8	2.52	0.45
1:A:1142(A):A:H4'	9:I:25:ARG:HH22	1.80	0.45
15:O:6:LEU:HA	15:O:9:LEU:HB2	1.99	0.45
17:Q:19:LYS:HG3	17:Q:95:LEU:HD23	1.98	0.45
20:T:101:LYS:HG2	20:T:102:CYS:H	1.81	0.45
22:V:23:VAL:HA	22:V:38:VAL:HA	1.99	0.45
1:A:122:G:OP1	1:A:149:A:O2'	2.27	0.45
1:A:2123:G:H1	1:A:2175:C:N4	2.11	0.45
1:A:407:G:H2'	1:A:408:G:C8	2.52	0.45
3:C:44:ASN:N	3:C:44:ASN:ND2	2.64	0.45
6:F:146:TYR:O	6:F:149:VAL:HG22	2.16	0.45
24:X:21:LEU:O	24:X:25:VAL:HG23	2.17	0.45
1:A:1028:A:N6	1:A:1125:G:H2'	2.32	0.45
1:A:2636:U:OP2	4:D:79:ARG:NH1	2.49	0.45
1:A:27:G:H22	1:A:512:G:H2'	1.80	0.45
1:A:286:C:H2'	1:A:287:C:C6	2.52	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:874:G:H2'	1:A:875:G:H8	1.81	0.45
4:D:67:PHE:O	4:D:69:LYS:N	2.49	0.45
7:G:85:LYS:HA	7:G:85:LYS:HD2	1.89	0.45
15:O:102:ILE:HA	15:O:105:LEU:CD2	2.47	0.45
2:B:12:C:O2	22:V:74:ARG:HD2	2.17	0.45
23:W:79:GLY:N	23:W:80:LEU:HD23	2.32	0.45
25:Y:31:LEU:O	25:Y:32:GLN:HB2	2.17	0.45
26:Z:22:ILE:HG22	26:Z:23:GLU:H	1.82	0.45
26:Z:16:CYS:HB3	26:Z:33:VAL:HB	1.98	0.45
1:A:1021:A:H61	1:A:1142(A):A:N6	2.01	0.45
1:A:1231:G:H2'	1:A:1232:G:H8	1.82	0.45
1:A:1380:G:O2'	1:A:1569:A:N6	2.50	0.45
1:A:1534:G:N3	1:A:1534:G:H2'	2.32	0.45
1:A:548:A:H8	1:A:548:A:O5'	2.00	0.45
1:A:1500:G:O2'	3:C:100:GLY:O	2.24	0.45
7:G:45:VAL:O	7:G:45:VAL:HG13	2.17	0.45
8:H:120:ILE:HD11	8:H:126:TYR:CZ	2.52	0.45
8:H:88:ILE:HG12	8:H:122:GLU:N	2.31	0.45
1:A:2025:C:H2'	1:A:2026:C:C6	2.52	0.45
1:A:2346:A:H8	4:D:35:GLN:HE21	136.01	0.45
1:A:2630:G:O4'	1:A:2894:G:H1'	2.17	0.45
1:A:2689:U:H4'	1:A:2690:C:O5'	2.15	0.45
7:G:153:LYS:CB	7:G:154:PRO:HD3	2.47	0.45
7:G:3:ARG:NE	7:G:3:ARG:HA	2.32	0.45
11:K:126:VAL:HG12	11:K:147:LEU:HD22	1.99	0.45
2:B:50:G:H5''	14:N:61:ASN:ND2	2.32	0.45
18:R:97:LYS:HE2	18:R:99:ARG:NH2	2.32	0.45
21:U:82:ARG:HG3	21:U:83:PRO:CD	2.47	0.45
21:U:94:GLU:HB2	21:U:95:PRO:HA	1.99	0.45
1:A:2395:C:O2'	23:W:30:VAL:HG12	2.17	0.45
1:A:1984:G:H2'	1:A:1985:G:H8	1.82	0.44
1:A:270(J):G:H2'	1:A:270(K):C:O4'	2.18	0.44
3:C:39:LYS:HB2	3:C:62:TYR:HB2	1.98	0.44
4:D:13:ARG:HD2	11:K:61:ARG:CD	122.20	0.44
4:D:167:VAL:HG21	4:D:187:ALA:CB	2.47	0.44
10:J:86:ILE:HG22	10:J:94:ARG:HD3	1.99	0.44
23:W:53:VAL:HB	23:W:58:ILE:HD13	1.98	0.44
1:A:1717:G:H1	1:A:1742:C:H42	1.65	0.44
1:A:833:U:H2'	1:A:834:C:C6	2.52	0.44
1:A:841:A:H2'	1:A:842:G:C8	2.52	0.44
18:R:33:ARG:NH2	18:R:52:GLU:OE1	2.50	0.44
19:S:35:THR:O	19:S:39:ILE:HG13	2.16	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
21:U:19:ARG:NH1	21:U:84:GLU:HB2	2.32	0.44
24:X:41:ILE:HD11	24:X:44:LEU:CG	2.48	0.44
1:A:1165:U:H2'	1:A:1166:C:C6	2.53	0.44
1:A:2356:C:H2'	1:A:2357:U:O4'	2.18	0.44
1:A:2470:G:H5'	12:L:56:ARG:NH2	2.30	0.44
1:A:279:C:H42	1:A:361:G:H1	1.65	0.44
1:A:858:U:H1'	1:A:2268:A:H2'	2.00	0.44
2:B:15:A:H5'	2:B:16:G:H8	1.82	0.44
1:A:2784:C:O2'	4:D:37:ARG:NH1	2.50	0.44
6:F:114:ILE:HB	6:F:117:PHE:HB2	1.99	0.44
7:G:52:VAL:HG21	7:G:68:THR:HG22	2.00	0.44
9:I:62:VAL:HG12	9:I:66:LYS:HD2	1.98	0.44
10:J:17:ARG:NH2	10:J:47:ILE:HD13	2.33	0.44
16:P:104:GLN:OE1	16:P:105:VAL:HG23	2.18	0.44
16:P:66:ASN:HB2	16:P:76:TYR:HB2	1.99	0.44
17:Q:99:ILE:HD13	17:Q:99:ILE:H	1.82	0.44
1:A:1087:G:C4	1:A:1089:G:H1'	2.52	0.44
1:A:1981:A:H5''	1:A:1982:C:OP2	2.17	0.44
3:C:248:SER:HB2	3:C:252:TRP:CZ2	2.51	0.44
5:E:63:LYS:HE3	5:E:65:TRP:O	2.18	0.44
9:I:134:ARG:O	9:I:136:GLU:N	2.50	0.44
1:A:2293:C:OP1	14:N:89:ARG:NH1	2.51	0.44
1:A:1021:A:N6	1:A:1142(A):A:H61	2.03	0.44
1:A:1434:A:H61	1:A:1558:A:N6	2.15	0.44
1:A:1543:A:O2'	1:A:1544:C:OP2	2.31	0.44
1:A:2667:C:H1'	7:G:109:PHE:HD1	1.82	0.44
5:E:47:GLY:HA3	5:E:95:ARG:O	2.18	0.44
15:O:61:PHE:CE1	15:O:76:PHE:HB2	2.53	0.44
15:O:42:ILE:HG21	15:O:84:GLN:NE2	2.32	0.44
16:P:88:ILE:HG12	16:P:88:ILE:H	1.49	0.44
20:T:51:VAL:O	20:T:56:PRO:HA	2.18	0.44
21:U:19:ARG:HD3	21:U:25:PRO:HD2	1.99	0.44
1:A:1019:U:HO2'	1:A:1021:A:H2	1.60	0.44
1:A:1332:G:H2'	1:A:1332:G:H8	1.67	0.44
1:A:1535:U:H5''	1:A:1537:C:C4	2.52	0.44
1:A:2756:U:H1'	1:A:2757:A:H5''	2.00	0.44
1:A:2627:G:O2'	1:A:2781:A:N1	2.41	0.44
1:A:2811:G:H1	1:A:2889:C:H42	1.65	0.44
1:A:455:C:HO2'	1:A:472:A:H2	1.64	0.44
1:A:653:A:H4'	1:A:654:A:OP2	2.18	0.44
1:A:839:U:H2'	1:A:840:C:C6	2.53	0.44
2:B:3:C:H2'	2:B:4:C:C6	2.52	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:85:ASP:HB2	3:C:92:ILE:HD13	1.99	0.44
6:F:98:ARG:O	6:F:101:ILE:HG13	2.17	0.44
6:F:47:LYS:HE3	6:F:47:LYS:HB2	1.73	0.44
7:G:124:GLU:HB3	7:G:132:ARG:HG3	1.99	0.44
17:Q:15:GLU:HG3	17:Q:16:PRO:HD2	1.99	0.44
19:S:70:LEU:HD23	19:S:70:LEU:H	1.83	0.44
21:U:80:ARG:NH2	21:U:82:ARG:HH22	2.12	0.44
24:X:17:SER:CB	24:X:67:LYS:HE3	2.47	0.44
1:A:1183:G:H4'	25:Y:29:ARG:HH22	1.82	0.44
1:A:1608:A:H1'	1:A:1610:A:OP2	2.17	0.44
1:A:1914:C:H2'	1:A:1915:U:O4'	2.18	0.44
1:A:2347:C:H2'	1:A:2348:U:H6	1.83	0.44
1:A:627:A:H4'	1:A:628:G:H5'	1.99	0.44
2:B:24:G:H5''	2:B:25:A:OP1	2.17	0.44
8:H:88:ILE:HG12	8:H:122:GLU:H	1.83	0.44
15:O:48:ILE:H	15:O:48:ILE:HD12	1.83	0.44
21:U:52:SER:O	21:U:54:HIS:N	2.50	0.44
26:Z:35:VAL:C	26:Z:37:SER:H	2.20	0.44
1:A:2619:C:H5''	4:D:152:LYS:HA	1.99	0.44
1:A:18:C:O2'	1:A:553:U:OP1	2.35	0.44
2:B:80:U:O2'	2:B:81:G:H5'	2.18	0.44
4:D:37:ARG:O	4:D:45:THR:HA	2.18	0.44
21:U:166:SER:HB2	21:U:167:PRO:C	2.39	0.44
22:V:43:THR:O	22:V:43:THR:HG23	2.17	0.44
24:X:31:GLU:HB2	24:X:53:LEU:HD11	2.00	0.44
1:A:2114:A:N3	1:A:2114:A:H3'	2.32	0.44
1:A:414:C:H2'	1:A:415:A:C8	2.53	0.44
4:D:105:THR:OG1	4:D:199:ARG:NH1	2.50	0.44
5:E:184:TYR:CE2	5:E:188:ARG:HD2	2.52	0.44
7:G:4:ILE:H	7:G:4:ILE:HG12	1.59	0.44
23:W:70:VAL:O	23:W:73:LEU:HB2	2.18	0.44
26:Z:48:ARG:CZ	26:Z:51:ASP:HA	2.47	0.44
26:Z:60:GLN:HB3	26:Z:61:ARG:H	1.55	0.44
1:A:2271:G:OP1	22:V:18:ALA:HB1	2.17	0.43
1:A:2556:C:H2'	1:A:2557:G:O4'	2.17	0.43
1:A:2566:A:H4'	1:A:2567:G:O5'	2.18	0.43
1:A:1050:A:H8	1:A:2751:G:O2'	2.01	0.43
3:C:250:TRP:HE3	3:C:252:TRP:NE1	2.16	0.43
3:C:61:LEU:HD13	3:C:61:LEU:HA	1.92	0.43
4:D:188:VAL:O	4:D:188:VAL:HG13	2.18	0.43
5:E:66:PRO:O	5:E:68:LYS:N	2.51	0.43
6:F:10:LYS:HE2	6:F:175:LEU:O	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:F:67:LYS:O	6:F:67:LYS:HD2	2.17	0.43
2:B:41:U:O4	6:F:70:VAL:HG23	2.17	0.43
7:G:15:VAL:HG23	7:G:15:VAL:O	2.17	0.43
13:M:38:VAL:HG22	13:M:112:ALA:HB2	1.99	0.43
11:K:126:VAL:HG12	11:K:147:LEU:CD2	2.48	0.43
13:M:34:ILE:HA	13:M:34:ILE:HD13	1.71	0.43
15:O:35:LYS:HD2	15:O:35:LYS:H	1.83	0.43
17:Q:52:VAL:O	17:Q:54:GLY:N	2.51	0.43
1:A:2328:A:H2'	1:A:2329:G:C8	2.53	0.43
1:A:898:C:C2'	1:A:899:A:H5'	2.48	0.43
7:G:67:LEU:O	7:G:71:LEU:HB2	2.17	0.43
8:H:130:TYR:N	8:H:136:VAL:O	2.51	0.43
13:M:70:LEU:HD23	13:M:70:LEU:HA	1.84	0.43
1:A:1173:G:H4'	1:A:1174:A:N7	2.33	0.43
1:A:1694:C:H4'	1:A:1695:G:O5'	2.18	0.43
3:C:92:ILE:HD12	3:C:104:TYR:CD2	2.54	0.43
4:D:87:GLU:O	4:D:89:ASP:N	2.50	0.43
5:E:33:LEU:HD12	5:E:33:LEU:HA	1.87	0.43
5:E:64:ILE:HG23	5:E:65:TRP:CD1	2.53	0.43
10:J:88:ASN:OD1	10:J:90:GLN:HB2	2.19	0.43
11:K:83:VAL:O	11:K:114:ILE:HA	2.19	0.43
19:S:72:LYS:HG2	19:S:73:ARG:O	2.18	0.43
23:W:25:LYS:C	23:W:27:GLU:H	2.22	0.43
24:X:15:LYS:H	24:X:67:LYS:CE	2.32	0.43
1:A:1223:C:OP2	17:Q:88:ARG:NH1	2.51	0.43
1:A:1530:G:O6	1:A:1542:G:N2	2.52	0.43
1:A:1680:U:O2	1:A:1763:G:H3'	2.18	0.43
1:A:826:U:OP1	1:A:2429:G:OP1	2.36	0.43
2:B:15:A:H1'	2:B:109:G:C4	2.53	0.43
8:H:110:ASP:HB3	8:H:112:LYS:N	2.33	0.43
9:I:112:LEU:O	9:I:112:LEU:HG	2.17	0.43
10:J:64:ARG:HG2	10:J:79:PHE:CD1	2.54	0.43
21:U:5:LEU:HB3	21:U:59:LEU:HA	2.00	0.43
25:Y:51:ALA:HA	25:Y:54:VAL:HG12	2.00	0.43
1:A:1054:A:H5'	1:A:1055:G:OP2	2.18	0.43
1:A:1359:A:N6	1:A:1373:A:C4	2.87	0.43
1:A:1870:C:H2'	1:A:1871:A:O4'	2.18	0.43
1:A:1903:G:OP2	3:C:241:PRO:HB2	2.19	0.43
1:A:1916:A:H2'	1:A:1917:U:O4'	2.18	0.43
1:A:1910:G:H1	1:A:1920:C:N4	2.15	0.43
1:A:2308:G:H22	1:A:2311:A:H2	1.66	0.43
1:A:582:G:H2'	1:A:583:G:C8	2.54	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:67:U:C2	1:A:74:A:H2	2.35	0.43
3:C:132:PRO:HG3	3:C:190:TYR:CE1	2.54	0.43
11:K:126:VAL:HG22	11:K:145:PRO:HG2	2.00	0.43
20:T:67:LEU:HD12	20:T:67:LEU:HA	1.78	0.43
20:T:80:GLY:O	20:T:81:LYS:HG3	2.18	0.43
21:U:52:SER:O	21:U:52:SER:OG	2.30	0.43
23:W:94:LEU:HA	23:W:94:LEU:HD23	1.82	0.43
26:Z:43:TYR:CD1	26:Z:43:TYR:C	2.92	0.43
1:A:226:G:H2'	1:A:227:A:C8	2.54	0.43
1:A:265:A:O2'	1:A:266:G:H4'	2.18	0.43
1:A:363(A):A:H2'	1:A:363(B):G:C8	2.54	0.43
1:A:273(C):C:N4	1:A:363(C):G:H1	2.15	0.43
4:D:119:ARG:HG2	4:D:160:TYR:HB2	2.00	0.43
4:D:14:ILE:HG23	4:D:15:PHE:N	2.34	0.43
7:G:152:ARG:O	7:G:153:LYS:HB2	2.19	0.43
1:A:1952:A:C5	10:J:22:ILE:HD12	2.54	0.43
14:N:39:ILE:HD12	14:N:85:VAL:HG11	2.00	0.43
17:Q:55:ALA:HB2	17:Q:101:GLY:HA2	2.00	0.43
21:U:52:SER:C	21:U:54:HIS:H	2.22	0.43
26:Z:55:ARG:C	26:Z:59:PHE:HB3	2.39	0.43
1:A:1231:G:H2'	1:A:1232:G:C8	2.54	0.43
1:A:1607:C:H5''	1:A:1608:A:H5'	2.01	0.43
1:A:1799:G:H4'	1:A:1800:C:O5'	2.18	0.43
1:A:2780:G:P	9:I:118:LYS:HE2	2.58	0.43
4:D:4:ILE:HD12	4:D:28:ALA:HB1	2.01	0.43
6:F:145:THR:O	6:F:147:ASP:N	2.44	0.43
6:F:31:VAL:HA	6:F:32:PRO:HD3	1.83	0.43
11:K:15:ARG:O	11:K:17:LYS:HG3	2.19	0.43
11:K:30:THR:O	11:K:33:ARG:HB2	2.18	0.43
1:A:1190:G:H5'	11:K:32:THR:HA	2.01	0.43
11:K:5:ASP:O	11:K:6:LEU:C	2.57	0.43
20:T:87:LYS:HB2	20:T:87:LYS:NZ	2.34	0.43
2:B:12:C:O2'	22:V:74:ARG:HG3	2.19	0.43
26:Z:6:HIS:HA	26:Z:7:PRO:HD2	1.82	0.43
1:A:118:A:N3	1:A:178:G:H1'	2.34	0.43
1:A:579:G:O2'	1:A:2019:A:OP1	2.29	0.43
1:A:242:G:H1'	1:A:243:U:OP2	2.18	0.43
1:A:746:A:C6	1:A:2611:U:H5''	2.54	0.43
1:A:363(B):G:H2'	1:A:363(C):G:C8	2.54	0.43
1:A:507:A:H5''	1:A:508:G:H5'	2.01	0.43
4:D:201:THR:HG22	4:D:203:LYS:H	1.83	0.43
6:F:103:LEU:HA	6:F:103:LEU:HD23	1.83	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:K:113:LYS:HG2	11:K:115:LEU:HD23	2.01	0.43
15:O:80:SER:HA	15:O:81:PRO:HD3	1.89	0.43
19:S:53:LYS:H	19:S:82:GLN:HB3	1.83	0.43
1:A:857:C:H1'	22:V:26:TYR:CE1	2.54	0.43
24:X:61:LEU:HD23	24:X:61:LEU:HA	1.85	0.43
24:X:17:SER:HB3	24:X:67:LYS:HE3	2.00	0.43
1:A:1373:A:C6	1:A:1374:G:C4	3.07	0.43
1:A:1952:A:N3	1:A:2560:C:O2'	2.49	0.43
1:A:630:G:N2	1:A:633:A:OP2	2.45	0.43
1:A:897:C:H4'	21:U:182:LYS:HD2	2.01	0.43
3:C:134:ARG:HD3	3:C:135:PHE:CE1	2.54	0.43
4:D:111:ARG:HD2	4:D:160:TYR:CE2	2.54	0.43
4:D:36:ARG:HH21	4:D:88:GLY:CA	2.32	0.43
12:L:45:GLN:H	12:L:45:GLN:CD	2.22	0.43
14:N:30:ARG:NH2	14:N:92:TYR:CD1	2.87	0.43
1:A:751:A:H5'	18:R:90:ARG:HA	1.99	0.43
1:A:1342:A:OP1	19:S:36:LYS:NZ	2.52	0.43
23:W:58:ILE:HG23	23:W:87:PRO:HG3	2.01	0.43
25:Y:7:LYS:HE2	25:Y:32:GLN:O	2.19	0.43
26:Z:14:ILE:HG13	26:Z:31:ILE:HB	1.99	0.43
1:A:1291:C:H2'	1:A:1292:U:C6	2.54	0.42
1:A:1354:A:OP1	3:C:38:LYS:HE2	2.18	0.42
1:A:1794:U:H2'	1:A:1795:C:C6	2.53	0.42
1:A:2364:C:H2'	1:A:2365:G:O4'	2.18	0.42
1:A:2564:A:C2	1:A:2647:U:H4'	2.53	0.42
1:A:2783:G:H2'	1:A:2784:C:C6	2.54	0.42
1:A:277:C:H3'	1:A:278:A:C5'	2.49	0.42
1:A:443:A:H1'	1:A:1201:C:O4'	2.19	0.42
1:A:512:G:OP1	1:A:1234:U:O2'	2.33	0.42
2:B:81:G:O6	2:B:95:U:C2	2.72	0.42
3:C:248:SER:HB3	3:C:252:TRP:CD2	2.54	0.42
7:G:126:PRO:HB2	7:G:127:GLU:H	1.59	0.42
9:I:134:ARG:H	9:I:135:PRO:HD3	1.83	0.42
10:J:88:ASN:ND2	10:J:92:GLU:HB2	2.23	0.42
17:Q:64:HIS:ND1	17:Q:92:THR:HG22	2.34	0.42
1:A:1063:G:H22	1:A:1076:C:H1'	1.84	0.42
1:A:323:G:H1'	1:A:1205:U:O2	2.19	0.42
1:A:2336:A:H61	22:V:43:THR:HG21	1.84	0.42
1:A:2448:A:OP2	1:A:2499:C:OP2	2.36	0.42
1:A:278:A:H4'	1:A:279:C:OP1	2.19	0.42
1:A:372:G:O2'	1:A:373:U:P	2.77	0.42
1:A:845:G:H8	1:A:845:G:OP2	2.02	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:K:125:VAL:CG1	11:K:138:LEU:HD21	2.49	0.42
21:U:8:TYR:HA	21:U:62:PRO:HD3	2.00	0.42
24:X:8:LYS:HB2	24:X:8:LYS:HE3	1.83	0.42
1:A:71:A:H62	1:A:114:U:H1'	1.84	0.42
1:A:1567:A:H5'	3:C:58:HIS:CG	2.54	0.42
1:A:2392:A:H2	1:A:2424:C:H42	1.68	0.42
1:A:2629:A:O2'	1:A:2630:G:H5''	2.19	0.42
1:A:305:U:H2'	1:A:306:U:C6	2.54	0.42
1:A:391:G:O2'	1:A:410:G:OP1	2.30	0.42
1:A:740:U:H2'	1:A:741:G:H8	1.84	0.42
4:D:201:THR:HG22	4:D:203:LYS:N	2.34	0.42
6:F:64:THR:CG2	6:F:66:GLN:H	2.28	0.42
7:G:126:PRO:HG2	7:G:128:PRO:HA	2.00	0.42
9:I:96:GLU:HG2	9:I:97:ARG:H	1.84	0.42
11:K:39:LYS:HG3	11:K:45:LEU:CD2	2.45	0.42
15:O:45:PHE:CE1	15:O:65:LYS:HE3	2.55	0.42
15:O:58:ASN:HD22	15:O:58:ASN:C	2.23	0.42
21:U:6:LYS:HB2	21:U:6:LYS:HE3	1.88	0.42
25:Y:4:LEU:HD22	25:Y:56:VAL:HG12	2.01	0.42
1:A:1926:U:O2'	1:A:1928:A:N7	2.46	0.42
1:A:2563:U:H1'	1:A:2566:A:N6	2.34	0.42
1:A:2655:G:O2'	1:A:2656:U:P	2.77	0.42
1:A:2712:U:O2'	1:A:2712(A):A:C8	2.73	0.42
1:A:434:U:H1'	1:A:435:C:H5	1.84	0.42
1:A:94:G:H2'	1:A:95:G:O4'	2.19	0.42
2:B:14:U:O3'	2:B:107:U:O2'	2.35	0.42
3:C:36:PRO:CB	3:C:61:LEU:HB3	2.50	0.42
6:F:16:ARG:N	6:F:17:PRO:HD2	2.34	0.42
7:G:15:VAL:HG11	7:G:79:VAL:CG2	2.45	0.42
7:G:159:GLU:O	7:G:160:LYS:HG2	2.19	0.42
11:K:1:MET:HB3	11:K:2:LYS:H	1.61	0.42
12:L:39:PRO:HA	12:L:97:VAL:O	2.20	0.42
12:L:76:LYS:HG3	12:L:77:LYS:N	2.35	0.42
14:N:81:GLY:O	14:N:83:LYS:N	2.53	0.42
18:R:86:LEU:HD22	18:R:96:ILE:HD12	2.01	0.42
25:Y:8:LEU:HB3	25:Y:31:LEU:HA	2.01	0.42
1:A:1179:C:H2'	1:A:1180:C:O4'	2.20	0.42
1:A:1497:U:H5''	1:A:1498:C:H5	1.83	0.42
1:A:1803:A:O2'	3:C:259:THR:HG21	2.18	0.42
1:A:2052:G:C4	1:A:2053:G:C8	3.07	0.42
1:A:2647:U:H2'	1:A:2648:C:C6	2.55	0.42
3:C:25:THR:HG22	3:C:82:ILE:H	1.84	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:35:LYS:HE3	3:C:64:ILE:N	2.35	0.42
4:D:57:LYS:HD2	4:D:57:LYS:HA	1.87	0.42
5:E:45:ARG:HH11	5:E:45:ARG:CG	2.33	0.42
1:A:911:A:H2'	12:L:9:TYR:OH	2.20	0.42
1:A:71:A:N6	1:A:114:U:H1'	2.34	0.42
1:A:127:A:H5''	1:A:128:C:C6	2.54	0.42
1:A:1747:G:H2'	1:A:1748:G:H8	1.84	0.42
1:A:1838:C:H4'	1:A:1839:G:H8	1.84	0.42
1:A:2667:C:H1'	7:G:109:PHE:CD1	2.55	0.42
1:A:2816:C:O2	1:A:2883:A:O2'	2.36	0.42
1:A:787:U:H5''	1:A:788:A:H5'	2.02	0.42
14:N:106:ARG:HA	14:N:110:LEU:CD2	2.47	0.42
14:N:83:LYS:NZ	14:N:109:GLY:HA2	2.33	0.42
17:Q:65:GLY:O	17:Q:90:PRO:HA	2.20	0.42
22:V:53:MET:CB	22:V:59:LEU:HD23	2.50	0.42
1:A:1265:A:H8	1:A:1265:A:OP1	2.01	0.42
1:A:2124:G:H2'	1:A:2125:G:O4'	2.19	0.42
1:A:2378:A:O5'	1:A:2378:A:H8	2.01	0.42
1:A:2821:A:OP1	4:D:110:GLY:N	2.40	0.42
1:A:328:U:H4'	20:T:68:HIS:CD2	2.55	0.42
1:A:704:G:H2'	1:A:726:G:H22	1.85	0.42
3:C:25:THR:HG21	3:C:81:ALA:HA	2.02	0.42
9:I:46:VAL:HG13	9:I:48:MET:HG3	2.02	0.42
10:J:21:CYS:O	10:J:22:ILE:HD13	2.20	0.42
11:K:36:LYS:HB3	11:K:40:SER:CB	2.49	0.42
14:N:60:GLY:O	14:N:61:ASN:HB3	2.18	0.42
15:O:26:ASP:HB2	15:O:91:ARG:HA	2.00	0.42
1:A:994:C:OP1	16:P:53:ARG:NH2	2.52	0.42
20:T:51:VAL:HG23	20:T:57:GLN:N	2.35	0.42
22:V:27:GLU:HB2	22:V:69:PHE:CD1	2.53	0.42
1:A:2168:G:N3	1:A:2168:G:H2'	2.34	0.42
1:A:2378:A:C5	1:A:2379:G:H1'	2.55	0.42
1:A:2698:U:H2'	1:A:2699:C:C6	2.55	0.42
1:A:247:G:H4'	1:A:386:G:C4	2.55	0.42
1:A:671:C:H2'	1:A:672:C:C6	2.53	0.42
11:K:29:LYS:HD2	11:K:30:THR:CG2	2.50	0.42
1:A:2467:C:H4'	12:L:123:HIS:CD2	2.54	0.42
21:U:182:LYS:HE3	21:U:182:LYS:HB2	1.69	0.42
21:U:54:HIS:ND1	21:U:99:TYR:O	2.47	0.42
1:A:1078:U:HO2'	1:A:1088:A:H2	1.63	0.42
1:A:1094:U:O2	1:A:1096:A:H5'	2.20	0.42
1:A:814:C:O2'	1:A:1225:C:N3	2.50	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1224:G:N2	1:A:1227:A:OP2	2.32	0.42
1:A:1794:U:H2'	1:A:1795:C:H6	1.85	0.42
1:A:2389:G:H5''	1:A:2390:U:O4'	2.19	0.42
1:A:2393:A:H5'	11:K:62:LEU:HB3	2.01	0.42
1:A:2695:C:H2'	1:A:2696:U:C6	2.55	0.42
1:A:307:G:H21	1:A:330:A:N6	2.17	0.42
1:A:483:A:H3'	1:A:484:C:C6	2.55	0.42
1:A:958:U:O2	2:B:89(A):A:H4'	2.20	0.42
3:C:135:PHE:CD1	3:C:135:PHE:N	2.85	0.42
3:C:34:VAL:HG22	3:C:35:LYS:HG3	2.00	0.42
1:A:2788:C:OP1	4:D:61:ARG:NH1	2.53	0.42
14:N:38:GLN:HG3	14:N:47:THR:HG21	2.02	0.42
20:T:63:LYS:HA	20:T:63:LYS:HD2	1.86	0.42
1:A:987:G:O2'	1:A:1000:A:N3	2.42	0.42
1:A:1239:G:H2'	1:A:1240:U:O4'	2.20	0.42
1:A:1598:C:H5'	19:S:36:LYS:CB	2.48	0.42
1:A:1972:A:H2'	1:A:1973:G:C8	2.55	0.42
1:A:2655:G:O2'	1:A:2656:U:OP2	2.38	0.42
3:C:221:VAL:HG22	3:C:226:MET:CE	2.49	0.42
3:C:245:PRO:HA	3:C:246:PRO:HD3	1.87	0.42
3:C:89:SER:O	3:C:198:ASN:ND2	2.52	0.42
8:H:98:ALA:HB2	8:H:111:PRO:HB3	2.01	0.42
9:I:35:ARG:HB2	9:I:42:TRP:CZ3	2.55	0.42
9:I:59:LYS:HE3	9:I:61:ARG:HH22	1.84	0.42
19:S:84:ALA:HB1	19:S:85:PRO:HD2	2.02	0.42
20:T:96:ILE:HG13	20:T:98:VAL:H	1.85	0.42
21:U:1:MET:HG2	21:U:2:GLU:H	1.85	0.42
22:V:53:MET:HB3	22:V:59:LEU:HD23	2.01	0.42
25:Y:35:ARG:HB3	25:Y:37:LEU:HD21	2.01	0.42
26:Z:16:CYS:SG	26:Z:36:CYS:HB3	2.59	0.42
26:Z:39:CYS:O	26:Z:40:HIS:HB2	2.20	0.42
26:Z:37:SER:HB3	26:Z:42:PHE:HB3	2.00	0.42
1:A:1336:A:H2'	1:A:1337:G:C8	2.55	0.41
1:A:1499:C:H2'	1:A:1500:G:H8	1.84	0.41
1:A:1614:A:N6	18:R:88:ARG:H	2.18	0.41
1:A:2610:C:H4'	1:A:2611:U:H5'	2.02	0.41
1:A:2832:U:H4'	1:A:2833:G:C5'	2.49	0.41
3:C:232:PRO:HB3	3:C:244:ARG:CZ	2.50	0.41
4:D:167:VAL:HG21	4:D:187:ALA:HB1	2.01	0.41
6:F:165:THR:OG1	6:F:168:GLU:HG3	2.20	0.41
6:F:86:MET:HA	6:F:87:PRO:HD2	1.95	0.41
7:G:30:LYS:HE2	7:G:81:GLU:H	1.85	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:H:56:LYS:HZ1	8:H:60:GLU:HG2	1.85	0.41
9:I:137:LYS:HA	9:I:137:LYS:HD2	1.77	0.41
9:I:7:LYS:H	9:I:7:LYS:HD2	1.84	0.41
12:L:54:MET:HB3	12:L:64:ILE:HD13	2.01	0.41
12:L:85:LYS:O	12:L:86:GLY:C	2.58	0.41
13:M:3:HIS:O	13:M:5:LYS:N	2.53	0.41
21:U:157:LEU:HD22	21:U:161:VAL:HB	2.02	0.41
26:Z:24:THR:OG1	26:Z:25:TYR:N	2.53	0.41
26:Z:68:ARG:HB2	26:Z:69:LYS:H	1.51	0.41
1:A:1188:U:H4'	17:Q:79:VAL:HG22	2.01	0.41
1:A:2059:A:H5'	1:A:2060:A:OP2	2.20	0.41
1:A:2619:C:H4'	4:D:151:TYR:O	2.20	0.41
1:A:2745:C:C4	1:A:2746:U:C4	3.08	0.41
2:B:95:U:H2'	2:B:96:G:C8	2.54	0.41
5:E:107:LYS:CD	5:E:207:GLY:H	2.30	0.41
9:I:29:LYS:H	9:I:29:LYS:HG2	1.53	0.41
9:I:65:LYS:O	9:I:69:GLN:HG2	2.20	0.41
11:K:82:GLY:HA3	11:K:115:LEU:HD21	2.01	0.41
13:M:2:ARG:HG2	13:M:5:LYS:NZ	2.35	0.41
14:N:51:ALA:HB1	14:N:69:VAL:HG23	2.02	0.41
16:P:109:LEU:HA	16:P:109:LEU:HD23	1.89	0.41
16:P:30:LYS:HA	16:P:30:LYS:HD3	1.90	0.41
19:S:26:TYR:HB3	19:S:92:LEU:HD12	2.02	0.41
22:V:36:ILE:HD11	22:V:39:ARG:HG2	2.02	0.41
22:V:41:ARG:NE	22:V:41:ARG:HA	2.34	0.41
23:W:76:ARG:HD2	23:W:76:ARG:H	1.84	0.41
1:A:1825:A:OP1	3:C:231:HIS:NE2	2.53	0.41
1:A:2081:C:H2'	1:A:2082:A:C8	2.55	0.41
1:A:2267:A:H5''	1:A:2268:A:H5'	2.02	0.41
1:A:2593:U:H2'	1:A:2594:C:C6	2.55	0.41
1:A:2857:G:N2	1:A:2859:G:H3'	2.36	0.41
3:C:105:ILE:HA	3:C:105:ILE:HD12	1.55	0.41
5:E:117:ARG:HD2	5:E:120:GLU:OE2	2.20	0.41
7:G:8:PRO:HB2	7:G:9:ILE:H	1.71	0.41
8:H:133:HIS:HB2	8:H:134:PRO:CD	2.50	0.41
8:H:67:ARG:NH2	8:H:68:LEU:HB2	2.33	0.41
9:I:18:ALA:HB3	9:I:55:VAL:O	2.19	0.41
17:Q:72:VAL:HG13	17:Q:85:LYS:HG2	2.01	0.41
20:T:84:ARG:O	20:T:95:LYS:HD3	2.20	0.41
21:U:150:LEU:HD22	21:U:171:ILE:HB	2.02	0.41
23:W:89:GLU:HA	23:W:93:GLU:HB2	2.02	0.41
1:A:1153:C:H2'	1:A:1154:G:O4'	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:270(V):G:H2'	1:A:270(W):G:H8	1.84	0.41
1:A:2849:U:H5	15:O:93:ARG:NH1	2.14	0.41
1:A:724:U:H2'	1:A:725:G:O4'	2.20	0.41
1:A:636:G:OP1	11:K:132:LYS:HB2	2.20	0.41
12:L:19:GLY:O	12:L:21:THR:OG1	2.23	0.41
14:N:56:LEU:HD12	14:N:56:LEU:HA	1.76	0.41
17:Q:22:VAL:HG12	17:Q:23:GLU:H	1.85	0.41
17:Q:38:LEU:O	17:Q:51:VAL:HA	2.20	0.41
22:V:72:ARG:HB2	22:V:75:LEU:HB2	2.02	0.41
1:A:1541:U:H2'	1:A:1542:G:O4'	2.20	0.41
1:A:1588:C:H2'	1:A:1589:C:H6	1.85	0.41
1:A:1667:G:OP2	1:A:1667:G:H8	2.03	0.41
1:A:185:U:H4'	1:A:218:A:H4'	2.01	0.41
1:A:752:A:H4'	1:A:753:C:H5'	2.03	0.41
4:D:181:LEU:HA	4:D:181:LEU:HD13	1.85	0.41
6:F:166:ASP:OD1	6:F:166:ASP:N	2.54	0.41
1:A:1007:C:H4'	9:I:108:PRO:HD3	2.02	0.41
14:N:88:ASP:O	14:N:89:ARG:HB3	2.21	0.41
16:P:69:CYS:HB3	16:P:106:PHE:CZ	2.56	0.41
17:Q:72:VAL:CG1	17:Q:85:LYS:HG2	2.50	0.41
26:Z:48:ARG:NH1	26:Z:52:THR:H	2.19	0.41
1:A:1103:A:H5'	1:A:1104:C:C5	2.55	0.41
1:A:2308:G:HO2'	1:A:2310:A:H2	1.68	0.41
1:A:1759:A:H1'	1:A:2711:A:C2	2.55	0.41
2:B:76:G:N2	2:B:100:G:O6	2.51	0.41
4:D:144:ARG:HB3	4:D:145:LYS:H	1.45	0.41
4:D:25:VAL:HG11	15:O:11:GLU:HG2	2.01	0.41
5:E:125:LEU:HA	5:E:194:MET:O	2.20	0.41
7:G:19:VAL:HG22	7:G:24:VAL:HG12	2.03	0.41
8:H:57:ARG:O	8:H:61:ARG:HG2	2.20	0.41
21:U:106:GLY:O	21:U:141:VAL:HG13	2.20	0.41
1:A:1506:C:H3'	1:A:1507:A:H5''	2.01	0.41
1:A:1773:A:H2'	1:A:1774:C:O4'	2.19	0.41
1:A:1929:G:H4'	1:A:1930:G:OP1	2.21	0.41
1:A:2455:G:H2'	1:A:2456:C:C6	2.55	0.41
1:A:658:C:H2'	1:A:659:C:C6	2.56	0.41
1:A:979:G:H2'	1:A:982:C:N4	2.36	0.41
2:B:40:U:H3	2:B:43:C:H5''	1.86	0.41
5:E:9:ILE:HD11	5:E:125:LEU:HG	2.03	0.41
11:K:101:VAL:C	11:K:103:ALA:H	2.23	0.41
14:N:107:GLU:N	14:N:110:LEU:HD11	2.36	0.41
16:P:98:LEU:HD23	16:P:99:ALA:N	2.36	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
21:U:5:LEU:HB3	21:U:6:LYS:H	1.65	0.41
1:A:1093:G:H4'	7:G:170:ARG:NH2	2.35	0.41
1:A:1364:G:N2	1:A:1367:A:OP2	2.33	0.41
1:A:2301:C:H2'	1:A:2302:G:C8	2.56	0.41
1:A:27:G:HO2'	1:A:28:A:H8	1.64	0.41
1:A:273:G:H1	1:A:364:C:H42	1.67	0.41
1:A:732:C:H2'	1:A:733:G:O4'	2.21	0.41
1:A:76:C:H1'	24:X:62:THR:HG21	2.02	0.41
3:C:36:PRO:HB3	3:C:61:LEU:HB3	2.03	0.41
4:D:41:LYS:HA	4:D:41:LYS:HE2	2.02	0.41
4:D:64:LYS:C	4:D:66:HIS:H	2.24	0.41
4:D:86:PRO:HB2	4:D:87:GLU:H	1.67	0.41
5:E:68:LYS:O	5:E:69:HIS:CB	2.68	0.41
6:F:103:LEU:O	6:F:107:LEU:HG	2.21	0.41
11:K:59:LEU:HA	11:K:61:ARG:NH2	2.36	0.41
13:M:44:LEU:HD22	13:M:48:VAL:HG23	2.02	0.41
16:P:17:ILE:HG23	16:P:39:LEU:HD12	2.02	0.41
16:P:8:VAL:O	16:P:12:ARG:HG3	2.20	0.41
21:U:136:PHE:CD1	21:U:138:GLU:HG3	2.56	0.41
21:U:5:LEU:HA	21:U:5:LEU:HD22	1.86	0.41
1:A:1344:G:H4'	1:A:1384:A:C5	2.55	0.41
1:A:1359:A:N7	1:A:1373:A:C6	2.89	0.41
1:A:1810:A:H8	1:A:1810:A:O5'	2.04	0.41
1:A:2335:A:HO2'	1:A:2336:A:C5'	2.31	0.41
1:A:774:A:H2	1:A:787:U:O2'	2.03	0.41
1:A:814:C:H41	11:K:25:SER:HA	1.84	0.41
1:A:848:G:O6	1:A:929:G:H2'	2.20	0.41
1:A:968:G:H2'	1:A:969:U:O4'	2.21	0.41
3:C:102:LYS:C	3:C:103:ARG:HG2	2.40	0.41
3:C:130:ALA:C	3:C:131:LEU:HD12	2.42	0.41
3:C:3:VAL:HG13	3:C:17:THR:HG23	2.03	0.41
6:F:61:ALA:HA	6:F:64:THR:HG22	2.02	0.41
7:G:153:LYS:HZ2	7:G:153:LYS:HA	1.84	0.41
8:H:21:VAL:HG22	8:H:22:LYS:H	1.85	0.41
8:H:37:VAL:HG12	8:H:38:LEU:H	1.84	0.41
9:I:96:GLU:O	9:I:100:GLU:HG3	2.20	0.41
12:L:16:ARG:HB3	12:L:17:LEU:H	1.76	0.41
12:L:80:GLU:HB2	12:L:81:VAL:H	1.69	0.41
21:U:182:LYS:CB	21:U:183:LEU:HA	2.51	0.41
23:W:83:GLU:C	23:W:85:LEU:H	2.24	0.41
1:A:1007:C:OP1	9:I:35:ARG:NH1	2.52	0.41
1:A:1026:U:H4'	1:A:1027:A:OP1	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1029:A:H8	1:A:1029:A:O5'	2.04	0.41
1:A:1385:G:H1'	1:A:1386:C:C6	2.56	0.41
1:A:1657:C:H2'	1:A:1658:C:C6	2.55	0.41
1:A:83:G:H21	1:A:103:A:H62	1.69	0.41
3:C:145:VAL:HG11	3:C:175:LEU:HD11	2.02	0.41
3:C:35:LYS:HZ1	3:C:65:ILE:HA	1.85	0.41
6:F:124:SER:HB2	6:F:131:TYR:CE1	2.56	0.41
6:F:18:GLU:OE1	6:F:22:ARG:NH1	2.49	0.41
16:P:92:ARG:HD2	16:P:95:LEU:HD12	2.02	0.41
16:P:92:ARG:NH2	17:Q:11:GLN:H	2.18	0.41
19:S:31:HIS:HB3	19:S:34:ALA:HB2	2.03	0.41
21:U:8:TYR:HD2	21:U:38:TYR:CZ	2.39	0.41
26:Z:43:TYR:O	26:Z:46:GLN:HA	2.20	0.41
26:Z:55:ARG:HG2	26:Z:55:ARG:O	2.21	0.41
1:A:1061:U:H4'	1:A:1070:A:H1'	2.01	0.41
1:A:1578:U:C2'	1:A:1579:A:H5'	2.51	0.41
1:A:2098:U:O2	1:A:2191:G:N2	2.45	0.41
1:A:2185:C:H2'	1:A:2186:G:C8	2.56	0.41
1:A:2712:U:O2'	1:A:2712(A):A:P	2.79	0.41
1:A:2867:G:HO2'	1:A:2868:A:H8	1.65	0.41
1:A:596:G:H2'	1:A:597:U:O4'	2.21	0.41
3:C:201:HIS:O	3:C:204:ILE:HG12	2.21	0.41
3:C:62:TYR:HA	3:C:87:ASN:OD1	2.21	0.41
4:D:32:PRO:HA	4:D:90:THR:HA	2.03	0.41
5:E:67:GLN:O	5:E:67:GLN:HG3	2.21	0.41
6:F:7:LEU:HD12	6:F:104:GLU:HA	2.03	0.41
7:G:125:VAL:HG22	7:G:131:VAL:HG13	2.02	0.41
7:G:152:ARG:NE	7:G:153:LYS:NZ	2.68	0.41
8:H:115:ALA:HB3	8:H:128:LEU:HD12	2.02	0.41
9:I:7:LYS:NZ	9:I:7:LYS:H	2.18	0.41
11:K:106:LEU:O	11:K:107:LYS:HB2	2.20	0.41
26:Z:48:ARG:HH12	26:Z:52:THR:H	1.68	0.41
1:A:1341:U:O4'	19:S:57:LEU:HD23	2.21	0.40
1:A:1520:U:H2'	1:A:1521:G:O4'	2.21	0.40
1:A:1651:G:N7	13:M:11:ASN:ND2	2.60	0.40
1:A:218:A:C2	1:A:235:U:H4'	2.57	0.40
1:A:2803:C:H2'	1:A:2804:C:C6	2.56	0.40
1:A:2867:G:O2'	1:A:2868:A:H8	2.03	0.40
1:A:324:A:H2'	1:A:325:G:O4'	2.21	0.40
1:A:796:C:H2'	1:A:797:C:C6	2.56	0.40
1:A:874:G:H2'	1:A:875:G:C8	2.56	0.40
4:D:95:ILE:CD1	4:D:95:ILE:H	2.31	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:H:23:PRO:O	8:H:27:ARG:HG2	2.21	0.40
10:J:4:PRO:O	10:J:5:GLN:CB	2.69	0.40
11:K:29:LYS:HB3	11:K:30:THR:H	1.59	0.40
16:P:96:ALA:HA	16:P:98:LEU:HD23	2.03	0.40
21:U:28:MET:O	21:U:34:ASN:HA	2.22	0.40
1:A:1797:C:H4'	3:C:257:LEU:O	2.21	0.40
1:A:1826:G:H4'	3:C:242:ARG:NH2	2.36	0.40
1:A:1869:G:H5'	1:A:1870:C:OP2	2.20	0.40
1:A:2334:G:H4'	1:A:2335:A:OP2	2.21	0.40
1:A:2633:G:H2'	1:A:2634:G:O4'	2.21	0.40
1:A:271:G:H2'	1:A:272:G:H8	1.86	0.40
1:A:196:A:O2'	1:A:805:G:O6	2.34	0.40
1:A:1843:C:H5'	3:C:253:GLN:OE1	2.21	0.40
5:E:28:ILE:HG13	5:E:28:ILE:H	1.68	0.40
7:G:15:VAL:HG21	7:G:76:VAL:CG1	2.44	0.40
1:A:1688:U:O2	1:A:1700:A:H5''	2.21	0.40
1:A:1754:C:H2'	1:A:1755:A:O4'	2.21	0.40
1:A:1930:G:H2'	1:A:1968:G:N1	2.36	0.40
1:A:357:A:H2'	1:A:358:U:C6	2.57	0.40
4:D:49:LEU:HD12	4:D:49:LEU:HA	1.72	0.40
5:E:64:ILE:HA	5:E:64:ILE:HD12	1.80	0.40
8:H:38:LEU:H	8:H:38:LEU:HD12	1.86	0.40
9:I:65:LYS:H	9:I:65:LYS:HG2	1.60	0.40
14:N:69:VAL:HA	14:N:72:ALA:HB3	2.03	0.40
16:P:19:LYS:O	16:P:22:LYS:HB2	2.21	0.40
21:U:96:VAL:CG1	21:U:128:VAL:O	2.66	0.40
26:Z:14:ILE:O	26:Z:14:ILE:HG23	2.21	0.40
1:A:1186:G:H2'	1:A:1187:G:O4'	2.20	0.40
1:A:1329:U:H5''	1:A:1330:C:H5	1.86	0.40
1:A:2010:G:H5''	18:R:42:ARG:HB2	2.03	0.40
1:A:2579:C:H2'	1:A:2580:U:O4'	2.21	0.40
1:A:2776:A:OP1	1:A:2776:A:H3'	2.21	0.40
1:A:900:A:H3'	1:A:901:A:C8	2.54	0.40
5:E:168:ARG:HG3	5:E:175:THR:HG21	2.02	0.40
5:E:125:LEU:HD21	5:E:199:TRP:CE3	2.57	0.40
7:G:46:GLU:OE1	7:G:51:ARG:NH1	2.54	0.40
16:P:61:TRP:O	16:P:65:ILE:HG13	2.22	0.40
17:Q:21:ARG:HD2	17:Q:91:TYR:CE1	2.56	0.40
20:T:89:PHE:C	20:T:90:LEU:HD13	2.42	0.40
25:Y:12:PRO:O	25:Y:14:GLY:N	2.55	0.40
1:A:942:G:O2'	1:A:1189:A:N3	2.49	0.40
1:A:1417:C:H2'	1:A:1418:G:O4'	2.21	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1782:C:H1'	1:A:2609:U:H5''	2.03	0.40
1:A:1932:A:H2'	1:A:1933:G:O4'	2.21	0.40
1:A:2577:A:H2'	1:A:2614:A:N6	2.36	0.40
1:A:535:C:O3'	16:P:53:ARG:NH1	2.54	0.40
1:A:57:C:H2'	1:A:58:G:O4'	2.21	0.40
3:C:150:LYS:HA	3:C:150:LYS:HD3	1.94	0.40
3:C:237:GLU:O	3:C:238:GLY:C	2.59	0.40
5:E:122:LYS:HD3	5:E:122:LYS:HA	1.86	0.40
5:E:198:ALA:HA	5:E:201:VAL:HG12	2.03	0.40
15:O:19:LEU:HA	15:O:20:PRO:HD3	1.91	0.40
16:P:17:ILE:HD13	16:P:17:ILE:HA	1.92	0.40
17:Q:3:ALA:HA	17:Q:40:LEU:O	2.21	0.40
21:U:136:PHE:C	21:U:137:ILE:HG12	2.41	0.40
23:W:87:PRO:O	23:W:91:LYS:HB2	2.20	0.40
25:Y:52:HIS:CD2	25:Y:53:LEU:HG	2.57	0.40
25:Y:5:LYS:HE3	25:Y:34:GLU:OE2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	270/276 (98%)	228 (84%)	33 (12%)	9 (3%)	6	55
4	D	203/206 (98%)	144 (71%)	42 (21%)	17 (8%)	1	23
5	E	200/210 (95%)	168 (84%)	24 (12%)	8 (4%)	5	48
6	F	179/182 (98%)	142 (79%)	25 (14%)	12 (7%)	2	31
7	G	168/180 (93%)	124 (74%)	23 (14%)	21 (12%)	1	12
8	H	144/148 (97%)	107 (74%)	20 (14%)	17 (12%)	1	13
9	I	136/140 (97%)	105 (77%)	17 (12%)	14 (10%)	1	16
10	J	120/122 (98%)	108 (90%)	10 (8%)	2 (2%)	14	70

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	K	148/150 (99%)	108 (73%)	22 (15%)	18 (12%)	1	12
12	L	139/141 (99%)	98 (70%)	22 (16%)	19 (14%)	0	9
13	M	116/118 (98%)	99 (85%)	11 (10%)	6 (5%)	3	39
14	N	109/112 (97%)	79 (72%)	17 (16%)	13 (12%)	1	12
15	O	135/146 (92%)	108 (80%)	17 (13%)	10 (7%)	2	28
16	P	115/118 (98%)	102 (89%)	9 (8%)	4 (4%)	6	53
17	Q	99/101 (98%)	79 (80%)	12 (12%)	8 (8%)	1	24
18	R	111/113 (98%)	100 (90%)	9 (8%)	2 (2%)	13	68
19	S	90/96 (94%)	82 (91%)	6 (7%)	2 (2%)	10	64
20	T	100/110 (91%)	70 (70%)	18 (18%)	12 (12%)	1	12
21	U	181/206 (88%)	125 (69%)	38 (21%)	18 (10%)	1	18
22	V	80/85 (94%)	73 (91%)	7 (9%)	0	100	100
23	W	95/98 (97%)	72 (76%)	17 (18%)	6 (6%)	2	33
24	X	67/72 (93%)	55 (82%)	6 (9%)	6 (9%)	1	21
25	Y	57/60 (95%)	52 (91%)	4 (7%)	1 (2%)	13	68
26	Z	69/71 (97%)	35 (51%)	15 (22%)	19 (28%)	0	1
27	a	55/60 (92%)	45 (82%)	9 (16%)	1 (2%)	13	68
28	b	47/54 (87%)	22 (47%)	17 (36%)	8 (17%)	0	5
29	c	47/49 (96%)	43 (92%)	3 (6%)	1 (2%)	11	65
30	d	62/65 (95%)	48 (77%)	10 (16%)	4 (6%)	2	32
31	e	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
32	f	7/12 (58%)	3 (43%)	3 (43%)	1 (14%)	0	8
All	All	3384/3538 (96%)	2655 (78%)	470 (14%)	259 (8%)	1	26

All (259) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	26	LYS
3	C	28	GLU
3	C	122	ASP
3	C	123	ALA
4	D	2	LYS
4	D	19	ARG
4	D	53	PRO

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Mol	Chain	Res	Type
4	D	63	LEU
4	D	71	GLY
5	E	73	ALA
5	E	134	GLY
6	F	96	ARG
7	G	3	ARG
7	G	12	PRO
7	G	86	GLU
7	G	126	PRO
7	G	127	GLU
7	G	128	PRO
7	G	153	LYS
7	G	155	SER
7	G	168	PRO
7	G	169	VAL
8	H	133	HIS
8	H	145	VAL
9	I	9	VAL
9	I	22	THR
9	I	36	GLY
11	K	6	LEU
11	K	10	PRO
11	K	14	LYS
11	K	15	ARG
11	K	25	SER
11	K	27	HIS
11	K	95	VAL
11	K	106	LEU
11	K	148	LEU
12	L	18	LYS
12	L	22	LYS
12	L	25	ASP
12	L	79	LEU
12	L	86	GLY
12	L	90	VAL
12	L	134	ARG
13	M	3	HIS
14	N	82	ILE
14	N	88	ASP
14	N	107	GLU
15	O	2	ASN
15	O	123	GLN

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Mol	Chain	Res	Type
15	O	124	ASP
16	P	90	VAL
16	P	91	ASP
16	P	93	LYS
17	Q	45	THR
19	S	68	ARG
20	T	50	ARG
20	T	57	GLN
20	T	77	PRO
20	T	78	ALA
21	U	6	LYS
21	U	53	ILE
21	U	146	ILE
21	U	152	ALA
21	U	159	PRO
23	W	30	VAL
23	W	84	GLY
23	W	91	LYS
23	W	95	LEU
24	X	16	LEU
24	X	43	GLN
24	X	47	ASN
24	X	48	HIS
26	Z	24	THR
26	Z	40	HIS
26	Z	49	PHE
27	a	4	HIS
28	b	15	GLU
29	c	48	LYS
30	d	52	LYS
30	d	62	LEU
3	C	238	GLY
3	C	242	ARG
4	D	7	VAL
4	D	204	ALA
5	E	128	ALA
5	E	132	VAL
5	E	181	LEU
6	F	4	ASP
6	F	36	LYS
7	G	13	LYS
7	G	27	LYS

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Mol	Chain	Res	Type
7	G	50	VAL
7	G	85	LYS
9	I	23	LEU
9	I	96	GLU
10	J	5	GLN
11	K	65	ARG
11	K	66	GLY
11	K	93	GLY
11	K	141	ALA
12	L	6	ARG
12	L	60	ARG
12	L	137	TYR
13	M	4	LEU
13	M	45	ARG
13	M	107	ASP
14	N	12	PHE
14	N	56	LEU
14	N	109	GLY
15	O	13	ARG
15	O	39	ARG
15	O	106	SER
17	Q	31	ALA
17	Q	48	GLY
17	Q	79	VAL
18	R	111	HIS
20	T	58	GLY
20	T	102	CYS
21	U	13	GLU
21	U	81	ARG
24	X	70	GLN
24	X	71	ASN
26	Z	5	ILE
26	Z	18	CYS
26	Z	22	ILE
26	Z	37	SER
26	Z	43	TYR
26	Z	50	VAL
28	b	7	ILE
28	b	16	CYS
28	b	33	LYS
3	C	32	SER
4	D	50	GLY

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Mol	Chain	Res	Type
4	D	79	ARG
4	D	90	THR
4	D	92	THR
4	D	117	MET
4	D	184	VAL
5	E	198	ALA
7	G	87	LEU
7	G	137	ASP
7	G	138	LYS
7	G	151	ILE
8	H	11	ASN
8	H	12	LEU
8	H	72	LEU
8	H	113	ARG
8	H	122	GLU
9	I	7	LYS
9	I	131	GLN
11	K	16	ARG
11	K	29	LYS
12	L	19	GLY
12	L	105	GLU
12	L	133	ARG
13	M	86	ARG
14	N	4	LEU
14	N	11	LYS
14	N	60	GLY
15	O	97	ALA
17	Q	49	THR
17	Q	53	GLU
17	Q	100	ARG
20	T	42	VAL
20	T	63	LYS
21	U	59	LEU
21	U	92	SER
21	U	160	GLY
21	U	166	SER
25	Y	3	ARG
26	Z	23	GLU
26	Z	30	GLU
26	Z	34	GLU
26	Z	66	SER
28	b	19	ARG

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Mol	Chain	Res	Type
28	b	49	HIS
30	d	30	ARG
30	d	34	TRP
32	f	2	GLY
6	F	14	GLU
6	F	82	LEU
6	F	86	MET
6	F	116	ASP
7	G	8	PRO
7	G	83	TYR
8	H	10	GLU
8	H	87	LYS
8	H	114	LEU
9	I	11	PRO
9	I	28	THR
9	I	47	ALA
12	L	104	PHE
12	L	140	ALA
14	N	89	ARG
14	N	96	GLY
15	O	17	THR
19	S	40	LYS
20	T	51	VAL
20	T	53	PRO
26	Z	9	LEU
26	Z	16	CYS
26	Z	25	TYR
26	Z	54	GLY
28	b	35	GLU
3	C	3	VAL
3	C	46	GLN
4	D	68	ALA
4	D	82	ARG
4	D	86	PRO
6	F	5	VAL
6	F	53	LEU
6	F	117	PHE
8	H	18	VAL
8	H	71	ILE
8	H	117	GLU
8	H	118	LYS
9	I	95	PRO

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Mol	Chain	Res	Type
9	I	134	ARG
9	I	135	PRO
11	K	11	GLY
11	K	24	GLY
12	L	11	LYS
12	L	27	VAL
14	N	94	TYR
14	N	110	LEU
15	O	86	ILE
16	P	117	GLN
17	Q	50	PRO
20	T	3	VAL
20	T	39	VAL
21	U	51	ALA
21	U	61	LEU
21	U	62	PRO
21	U	168	GLU
21	U	181	GLU
23	W	74	VAL
26	Z	14	ILE
28	b	21	TYR
4	D	72	VAL
5	E	58	ALA
9	I	127	ASP
10	J	97	ARG
11	K	7	ARG
12	L	62	GLY
23	W	55	GLY
26	Z	60	GLN
8	H	15	VAL
12	L	81	VAL
5	E	66	PRO
8	H	16	GLY
15	O	37	GLY
18	R	14	PRO
21	U	101	PRO
8	H	13	GLY
6	F	52	ILE
6	F	88	ILE
7	G	7	LEU
13	M	117	VAL
21	U	94	GLU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	214/218 (98%)	180 (84%)	34 (16%)	4	24
4	D	165/166 (99%)	135 (82%)	30 (18%)	2	16
5	E	161/166 (97%)	137 (85%)	24 (15%)	4	27
6	F	155/156 (99%)	134 (86%)	21 (14%)	6	32
7	G	142/148 (96%)	116 (82%)	26 (18%)	2	16
8	H	122/124 (98%)	92 (75%)	30 (25%)	1	7
9	I	117/119 (98%)	96 (82%)	21 (18%)	2	17
10	J	100/100 (100%)	89 (89%)	11 (11%)	9	44
11	K	116/116 (100%)	81 (70%)	35 (30%)	0	4
12	L	111/111 (100%)	92 (83%)	19 (17%)	3	20
13	M	101/101 (100%)	80 (79%)	21 (21%)	2	11
14	N	87/88 (99%)	68 (78%)	19 (22%)	1	9
15	O	120/127 (94%)	98 (82%)	22 (18%)	2	16
16	P	93/94 (99%)	77 (83%)	16 (17%)	3	19
17	Q	82/82 (100%)	67 (82%)	15 (18%)	2	16
18	R	92/92 (100%)	75 (82%)	17 (18%)	2	15
19	S	74/78 (95%)	60 (81%)	14 (19%)	2	14
20	T	85/91 (93%)	64 (75%)	21 (25%)	1	7
21	U	162/179 (90%)	133 (82%)	29 (18%)	2	17
22	V	65/67 (97%)	59 (91%)	6 (9%)	13	55
23	W	82/83 (99%)	70 (85%)	12 (15%)	5	28
24	X	64/67 (96%)	47 (73%)	17 (27%)	1	6
25	Y	51/52 (98%)	43 (84%)	8 (16%)	4	25
26	Z	63/63 (100%)	43 (68%)	20 (32%)	0	3
27	a	49/52 (94%)	36 (74%)	13 (26%)	1	6
28	b	48/52 (92%)	38 (79%)	10 (21%)	2	11
29	c	42/42 (100%)	35 (83%)	7 (17%)	3	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	d	54/55 (98%)	41 (76%)	13 (24%)	1	7
31	e	34/34 (100%)	32 (94%)	2 (6%)	28	76
32	f	5/7 (71%)	4 (80%)	1 (20%)	2	12
All	All	2856/2930 (98%)	2322 (81%)	534 (19%)	2	15

All (534) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	5	LYS
3	C	17	THR
3	C	27	THR
3	C	28	GLU
3	C	30	GLU
3	C	38	LYS
3	C	43	ARG
3	C	44	ASN
3	C	49	ILE
3	C	65	ILE
3	C	73	VAL
3	C	88	ARG
3	C	94	LEU
3	C	95	LEU
3	C	103	ARG
3	C	105	ILE
3	C	106	ILE
3	C	111	LEU
3	C	112	GLN
3	C	134	ARG
3	C	141	VAL
3	C	192	THR
3	C	200	ASP
3	C	202	LYS
3	C	212	SER
3	C	217	ARG
3	C	218	ARG
3	C	221	VAL
3	C	229	VAL
3	C	237	GLU
3	C	242	ARG
3	C	257	LEU
3	C	259	THR

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Mol	Chain	Res	Type
3	C	273	ARG
4	D	4	ILE
4	D	12	THR
4	D	13	ARG
4	D	16	ARG
4	D	17	ASP
4	D	21	VAL
4	D	23	VAL
4	D	26	ILE
4	D	27	LEU
4	D	41	LYS
4	D	42	ASP
4	D	49	LEU
4	D	77	ILE
4	D	79	ARG
4	D	82	ARG
4	D	92	THR
4	D	113	PHE
4	D	116	VAL
4	D	117	MET
4	D	119	ARG
4	D	127	ASP
4	D	128	SER
4	D	144	ARG
4	D	146	THR
4	D	154	LYS
4	D	175	VAL
4	D	197	ILE
4	D	200	GLU
4	D	202	LYS
4	D	203	LYS
5	E	9	ILE
5	E	32	LEU
5	E	33	LEU
5	E	38	ARG
5	E	45	ARG
5	E	65	TRP
5	E	70	THR
5	E	78	ILE
5	E	105	VAL
5	E	106	ARG
5	E	107	LYS

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Mol	Chain	Res	Type
5	E	117	ARG
5	E	127	GLU
5	E	161	GLU
5	E	164	ARG
5	E	165	ARG
5	E	170	LEU
5	E	174	VAL
5	E	176	LEU
5	E	181	LEU
5	E	183	VAL
5	E	196	LEU
5	E	197	ASP
5	E	206	ILE
6	F	3	LEU
6	F	7	LEU
6	F	22	ARG
6	F	31	VAL
6	F	34	LEU
6	F	43	LEU
6	F	45	GLU
6	F	58	GLN
6	F	63	ILE
6	F	66	GLN
6	F	67	LYS
6	F	80	PHE
6	F	82	LEU
6	F	84	LYS
6	F	88	ILE
6	F	90	LEU
6	F	94	LEU
6	F	116	ASP
6	F	118	ARG
6	F	145	THR
6	F	167	GLU
7	G	3	ARG
7	G	4	ILE
7	G	6	ARG
7	G	9	ILE
7	G	13	LYS
7	G	27	LYS
7	G	32	GLU
7	G	37	VAL

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Mol	Chain	Res	Type
7	G	40	GLU
7	G	41	MET
7	G	53	GLU
7	G	59	ARG
7	G	77	LYS
7	G	88	LEU
7	G	89	ILE
7	G	103	LEU
7	G	105	LEU
7	G	122	THR
7	G	129	THR
7	G	132	ARG
7	G	136	ILE
7	G	143	GLN
7	G	149	ARG
7	G	152	ARG
7	G	153	LYS
7	G	169	VAL
8	H	1	MET
8	H	2	LYS
8	H	9	LEU
8	H	10	GLU
8	H	20	ASP
8	H	27	ARG
8	H	33	ARG
8	H	35	LEU
8	H	38	LEU
8	H	40	THR
8	H	56	LYS
8	H	67	ARG
8	H	70	GLU
8	H	85	GLU
8	H	86	THR
8	H	87	LYS
8	H	88	ILE
8	H	92	VAL
8	H	101	LEU
8	H	110	ASP
8	H	112	LYS
8	H	113	ARG
8	H	130	TYR
8	H	131	LYS

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Mol	Chain	Res	Type
8	H	135	GLU
8	H	136	VAL
8	H	138	ILE
8	H	139	GLN
8	H	140	LEU
8	H	142	VAL
9	I	2	LYS
9	I	5	VAL
9	I	7	LYS
9	I	32	THR
9	I	34	LEU
9	I	43	THR
9	I	48	MET
9	I	60	ILE
9	I	61	ARG
9	I	62	VAL
9	I	65	LYS
9	I	67	LEU
9	I	73	THR
9	I	90	MET
9	I	96	GLU
9	I	99	LEU
9	I	109	LYS
9	I	112	LEU
9	I	116	LEU
9	I	120	LEU
9	I	136	GLU
10	J	9	GLU
10	J	19	ILE
10	J	20	MET
10	J	23	ARG
10	J	24	VAL
10	J	31	LYS
10	J	47	ILE
10	J	49	ARG
10	J	53	LYS
10	J	66	LYS
10	J	91	LEU
11	K	6	LEU
11	K	7	ARG
11	K	10	PRO
11	K	14	LYS

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Mol	Chain	Res	Type
11	K	16	ARG
11	K	19	VAL
11	K	21	ARG
11	K	27	HIS
11	K	29	LYS
11	K	32	THR
11	K	36	LYS
11	K	45	LEU
11	K	49	ARG
11	K	50	ARG
11	K	61	ARG
11	K	62	LEU
11	K	64	LYS
11	K	65	ARG
11	K	71	VAL
11	K	75	ILE
11	K	88	LEU
11	K	91	PHE
11	K	94	GLU
11	K	98	GLU
11	K	100	LEU
11	K	101	VAL
11	K	112	LEU
11	K	115	LEU
11	K	117	GLU
11	K	123	LEU
11	K	135	LEU
11	K	144	GLU
11	K	146	VAL
11	K	147	LEU
11	K	149	GLU
12	L	5	ARG
12	L	10	ARG
12	L	25	ASP
12	L	45	GLN
12	L	55	VAL
12	L	59	ARG
12	L	71	ASP
12	L	75	THR
12	L	76	LYS
12	L	79	LEU
12	L	81	VAL

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Mol	Chain	Res	Type
12	L	82	ARG
12	L	83	MET
12	L	87	LYS
12	L	103	MET
12	L	112	GLU
12	L	132	VAL
12	L	135	ASP
12	L	139	GLU
13	M	1	MET
13	M	18	LEU
13	M	28	LEU
13	M	29	LEU
13	M	34	ILE
13	M	36	THR
13	M	40	LYS
13	M	44	LEU
13	M	51	LEU
13	M	54	LEU
13	M	57	ARG
13	M	63	ARG
13	M	65	LEU
13	M	79	LEU
13	M	83	ILE
13	M	91	GLN
13	M	95	THR
13	M	100	LEU
13	M	102	GLU
13	M	104	ARG
13	M	105	ARG
14	N	10	ARG
14	N	12	PHE
14	N	14	VAL
14	N	15	ARG
14	N	20	ARG
14	N	25	ARG
14	N	27	SER
14	N	44	LYS
14	N	54	LEU
14	N	56	LEU
14	N	58	LEU
14	N	69	VAL
14	N	78	LEU

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Mol	Chain	Res	Type
14	N	83	LYS
14	N	85	VAL
14	N	89	ARG
14	N	103	GLU
14	N	106	ARG
14	N	111	GLU
15	O	17	THR
15	O	23	ARG
15	O	27	THR
15	O	28	VAL
15	O	40	THR
15	O	41	ARG
15	O	42	ILE
15	O	51	ARG
15	O	58	ASN
15	O	65	LYS
15	O	66	VAL
15	O	74	ARG
15	O	86	ILE
15	O	87	ASP
15	O	88	ILE
15	O	89	VAL
15	O	110	ILE
15	O	112	ARG
15	O	115	ARG
15	O	125	ARG
15	O	128	GLU
15	O	134	GLU
16	P	5	LYS
16	P	11	ARG
16	P	27	LEU
16	P	51	LYS
16	P	52	ARG
16	P	60	LEU
16	P	64	ARG
16	P	70	ARG
16	P	74	LEU
16	P	88	ILE
16	P	91	ASP
16	P	98	LEU
16	P	104	GLN
16	P	111	GLU

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Mol	Chain	Res	Type
16	P	112	ARG
16	P	114	LYS
17	Q	7	THR
17	Q	10	LYS
17	Q	13	ARG
17	Q	19	LYS
17	Q	35	LEU
17	Q	39	LEU
17	Q	40	LEU
17	Q	45	THR
17	Q	61	VAL
17	Q	66	ARG
17	Q	72	VAL
17	Q	73	SER
17	Q	78	LYS
17	Q	79	VAL
17	Q	99	ILE
18	R	11	ARG
18	R	16	LYS
18	R	23	LEU
18	R	37	ARG
18	R	40	ASN
18	R	51	LEU
18	R	67	ASP
18	R	69	LEU
18	R	76	VAL
18	R	88	ARG
18	R	90	ARG
18	R	92	ARG
18	R	95	ILE
18	R	96	ILE
18	R	100	THR
18	R	106	ILE
18	R	107	LEU
19	S	6	ASP
19	S	12	VAL
19	S	15	GLU
19	S	27	THR
19	S	36	LYS
19	S	43	VAL
19	S	49	VAL
19	S	57	LEU

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Mol	Chain	Res	Type
19	S	59	VAL
19	S	63	LYS
19	S	65	ARG
19	S	66	LEU
19	S	80	ILE
19	S	88	LYS
20	T	14	LEU
20	T	26	LYS
20	T	27	VAL
20	T	28	LYS
20	T	29	GLU
20	T	34	LYS
20	T	38	ILE
20	T	44	ILE
20	T	57	GLN
20	T	61	ILE
20	T	64	GLU
20	T	67	LEU
20	T	71	LYS
20	T	73	ARG
20	T	75	ILE
20	T	86	ARG
20	T	87	LYS
20	T	89	PHE
20	T	90	LEU
20	T	95	LYS
20	T	97	ARG
21	U	2	GLU
21	U	5	LEU
21	U	8	TYR
21	U	10	ARG
21	U	18	LEU
21	U	19	ARG
21	U	20	ARG
21	U	31	ARG
21	U	41	LEU
21	U	53	ILE
21	U	74	VAL
21	U	76	LEU
21	U	81	ARG
21	U	93	ASP
21	U	112	ARG

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Mol	Chain	Res	Type
21	U	122	ARG
21	U	129	SER
21	U	133	ILE
21	U	137	ILE
21	U	140	ASP
21	U	141	VAL
21	U	144	LEU
21	U	150	LEU
21	U	151	HIS
21	U	153	SER
21	U	156	LYS
21	U	163	LEU
21	U	166	SER
21	U	180	VAL
22	V	9	SER
22	V	11	ARG
22	V	36	ILE
22	V	55	ARG
22	V	64	ASP
22	V	74	ARG
23	W	30	VAL
23	W	46	LEU
23	W	50	ARG
23	W	51	VAL
23	W	56	GLN
23	W	62	VAL
23	W	78	LYS
23	W	80	LEU
23	W	82	LEU
23	W	83	GLU
23	W	91	LYS
23	W	92	LYS
24	X	4	SER
24	X	7	ARG
24	X	9	GLN
24	X	16	LEU
24	X	23	LYS
24	X	24	LEU
24	X	27	GLU
24	X	32	LEU
24	X	34	GLU
24	X	41	ILE

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Mol	Chain	Res	Type
24	X	47	ASN
24	X	50	ILE
24	X	51	ARG
24	X	52	ASP
24	X	53	LEU
24	X	64	LEU
24	X	65	ASN
25	Y	6	VAL
25	Y	8	LEU
25	Y	23	LEU
25	Y	30	ARG
25	Y	31	LEU
25	Y	36	VAL
25	Y	37	LEU
25	Y	56	VAL
26	Z	6	HIS
26	Z	10	VAL
26	Z	15	ILE
26	Z	16	CYS
26	Z	22	ILE
26	Z	27	THR
26	Z	34	GLU
26	Z	39	CYS
26	Z	42	PHE
26	Z	43	TYR
26	Z	48	ARG
26	Z	49	PHE
26	Z	53	GLU
26	Z	57	GLU
26	Z	58	ARG
26	Z	61	ARG
26	Z	63	TYR
26	Z	67	TYR
26	Z	68	ARG
26	Z	71	ARG
27	a	3	LYS
27	a	4	HIS
27	a	6	VAL
27	a	11	THR
27	a	29	THR
27	a	36	CYS
27	a	37	LYS

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Mol	Chain	Res	Type
27	a	40	LYS
27	a	48	GLU
27	a	51	TYR
27	a	52	TYR
27	a	56	LYS
27	a	58	LEU
28	b	6	ARG
28	b	8	LYS
28	b	11	LEU
28	b	19	ARG
28	b	23	THR
28	b	30	THR
28	b	33	LYS
28	b	34	LEU
28	b	37	ARG
28	b	44	ARG
29	c	1	MET
29	c	4	THR
29	c	8	ASN
29	c	9	ARG
29	c	10	ARG
29	c	14	LYS
29	c	47	ARG
30	d	13	ARG
30	d	14	VAL
30	d	15	LYS
30	d	29	LYS
30	d	30	ARG
30	d	34	TRP
30	d	43	GLN
30	d	44	LYS
30	d	47	LYS
30	d	56	GLU
30	d	58	ILE
30	d	64	TYR
30	d	65	GLU
31	e	1	MET
31	e	17	ILE
32	f	7	LYS

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

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2880/2915 (98%)	563 (19%)	57 (1%)
2	B	119/122 (97%)	21 (17%)	1 (0%)
All	All	2999/3037 (98%)	584 (19%)	58 (1%)

All (584) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	U
1	A	15	G
1	A	34	C
1	A	35	G
1	A	46	C
1	A	55	G
1	A	72	U
1	A	74	A
1	A	75	G
1	A	96	G
1	A	101	G
1	A	102	G
1	A	103	A
1	A	118	A
1	A	120	U
1	A	125	G
1	A	131	G
1	A	161	U
1	A	162	U
1	A	181	A
1	A	188	G
1	A	196	A
1	A	199	A
1	A	214	G
1	A	215	G
1	A	216	A
1	A	221	A
1	A	222	A
1	A	223	A
1	A	225	A
1	A	228	A
1	A	229	A
1	A	230	U
1	A	232	G

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Mol	Chain	Res	Type
1	A	242	G
1	A	243	U
1	A	248	G
1	A	252	G
1	A	265	A
1	A	266	G
1	A	269	U
1	A	270(L)	U
1	A	270(M)	U
1	A	270(N)	G
1	A	270(P)	C
1	A	271(B)	G
1	A	271(C)	U
1	A	271	G
1	A	274	G
1	A	275	G
1	A	276	A
1	A	278	A
1	A	279	C
1	A	299	A
1	A	300	A
1	A	311	A
1	A	323	G
1	A	324	A
1	A	329	G
1	A	330	A
1	A	332	A
1	A	342	G
1	A	345	A
1	A	352	G
1	A	363	G
1	A	364	C
1	A	371	A
1	A	372	G
1	A	373	U
1	A	386	G
1	A	387	U
1	A	395	U
1	A	405	U
1	A	406	G
1	A	411	G
1	A	412	A

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Mol	Chain	Res	Type
1	A	428	A
1	A	442	G
1	A	443	A
1	A	444	C
1	A	448	U
1	A	457	A
1	A	470	A
1	A	481	G
1	A	496	G
1	A	504	U
1	A	505	A
1	A	509	C
1	A	512	G
1	A	518	G
1	A	529	A
1	A	531	C
1	A	532	A
1	A	533	G
1	A	537	C
1	A	539	G
1	A	540	G
1	A	546	C
1	A	547	A
1	A	549	G
1	A	563	G
1	A	573	G
1	A	575	A
1	A	588	U
1	A	603	A
1	A	607	U
1	A	609(A)	G
1	A	614	U
1	A	615	G
1	A	616	A
1	A	617	G
1	A	620	G
1	A	622	G
1	A	627	A
1	A	637	A
1	A	638	G
1	A	645	C
1	A	646	A

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Mol	Chain	Res	Type
1	A	651	G
1	A	654	A
1	A	654(A)	G
1	A	654(B)	C
1	A	686	G
1	A	717	G
1	A	722	A
1	A	726	G
1	A	730	C
1	A	734	A
1	A	746	A
1	A	747	U
1	A	753	C
1	A	782	A
1	A	784	A
1	A	785	G
1	A	788	A
1	A	790	C
1	A	792	G
1	A	805	G
1	A	812	C
1	A	819	A
1	A	827	U
1	A	828	U
1	A	847	U
1	A	856	C
1	A	857	C
1	A	859	G
1	A	860	U
1	A	866	A
1	A	881	G
1	A	882	G
1	A	884	C
1	A	885	C
1	A	886	C
1	A	888	C
1	A	889	C
1	A	896	A
1	A	897	C
1	A	899	A
1	A	900	A
1	A	901	A

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Mol	Chain	Res	Type
1	A	907	U
1	A	910	A
1	A	914	C
1	A	915	C
1	A	917	A
1	A	932	G
1	A	938	G
1	A	941	A
1	A	945	A
1	A	946	G
1	A	961	C
1	A	974	G
1	A	974(A)	C
1	A	975	G
1	A	980	A
1	A	983	A
1	A	990	A
1	A	991	C
1	A	996	A
1	A	1003	G
1	A	1005	C
1	A	1011	G
1	A	1012	U
1	A	1013	C
1	A	1015	G
1	A	1022	G
1	A	1023	U
1	A	1025	G
1	A	1026	U
1	A	1027	A
1	A	1033	U
1	A	1045	A
1	A	1046	A
1	A	1050	A
1	A	1054	A
1	A	1055	G
1	A	1059	G
1	A	1060	U
1	A	1061	U
1	A	1066	U
1	A	1067	A
1	A	1068	G

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Mol	Chain	Res	Type
1	A	1070	A
1	A	1071	G
1	A	1076	C
1	A	1077	A
1	A	1078	U
1	A	1079	C
1	A	1082	U
1	A	1083	U
1	A	1084	A
1	A	1085	A
1	A	1086	A
1	A	1088	A
1	A	1089	G
1	A	1095	A
1	A	1096	A
1	A	1097	U
1	A	1099	G
1	A	1103	A
1	A	1104	C
1	A	1110	G
1	A	1111	A
1	A	1122	G
1	A	1131	G
1	A	1135	C
1	A	1136	G
1	A	1139	G
1	A	1142	U
1	A	1142(A)	A
1	A	1170	G
1	A	1173	G
1	A	1174	A
1	A	1175	U
1	A	1176	G
1	A	1178	C
1	A	1179	C
1	A	1180	C
1	A	1195	G
1	A	1204	A
1	A	1205	U
1	A	1210	A
1	A	1211	U
1	A	1220	A

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Mol	Chain	Res	Type
1	A	1236	G
1	A	1238	G
1	A	1248	G
1	A	1253	A
1	A	1256	G
1	A	1265	A
1	A	1271	G
1	A	1272	A
1	A	1273	U
1	A	1300	U
1	A	1301	A
1	A	1321	A
1	A	1329	U
1	A	1349	A
1	A	1352	U
1	A	1365	A
1	A	1368	G
1	A	1370	C
1	A	1379	A
1	A	1384	A
1	A	1385	G
1	A	1386	C
1	A	1391	U
1	A	1407	C
1	A	1411	C
1	A	1416	G
1	A	1419	A
1	A	1420	U
1	A	1421	G
1	A	1428	C
1	A	1444(A)	A
1	A	1445	C
1	A	1449	A
1	A	1449(A)	G
1	A	1455	G
1	A	1458	C
1	A	1460	A
1	A	1461	G
1	A	1467	C
1	A	1471	A
1	A	1482	U
1	A	1483	G

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Mol	Chain	Res	Type
1	A	1493	C
1	A	1497	U
1	A	1506	C
1	A	1507	A
1	A	1508	A
1	A	1510	A
1	A	1511	A
1	A	1514	U
1	A	1522	G
1	A	1534	G
1	A	1535	U
1	A	1536	A
1	A	1537	C
1	A	1543	A
1	A	1544	C
1	A	1545	A
1	A	1547	C
1	A	1554	A
1	A	1558	A
1	A	1559	G
1	A	1566	A
1	A	1569	A
1	A	1578	U
1	A	1579	A
1	A	1580	A
1	A	1585	C
1	A	1586	A
1	A	1592	C
1	A	1598	C
1	A	1599	C
1	A	1608	A
1	A	1609	A
1	A	1616	A
1	A	1617	C
1	A	1618	A
1	A	1640	C
1	A	1646	C
1	A	1648	C
1	A	1654	A
1	A	1660	C
1	A	1664	A
1	A	1668	A

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Mol	Chain	Res	Type
1	A	1674	G
1	A	1695	G
1	A	1698	A
1	A	1699	G
1	A	1700	A
1	A	1703	G
1	A	1725	G
1	A	1728	G
1	A	1729	A
1	A	1731	G
1	A	1733	G
1	A	1742	C
1	A	1743	G
1	A	1750	G
1	A	1754	C
1	A	1756	G
1	A	1762	A
1	A	1763	G
1	A	1764	G
1	A	1773	A
1	A	1776	G
1	A	1780	A
1	A	1781	C
1	A	1787	A
1	A	1791	A
1	A	1799	G
1	A	1800	C
1	A	1801	G
1	A	1816	G
1	A	1820	U
1	A	1829	A
1	A	1835	G
1	A	1847	A
1	A	1850	G
1	A	1858	G
1	A	1869	G
1	A	1870	C
1	A	1872	A
1	A	1878	G
1	A	1882	C
1	A	1888	G
1	A	1889	A

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Mol	Chain	Res	Type
1	A	1896	G
1	A	1903	G
1	A	1919	A
1	A	1930	G
1	A	1931	U
1	A	1937	A
1	A	1939	U
1	A	1955	U
1	A	1956	U
1	A	1963	U
1	A	1964	G
1	A	1967	C
1	A	1969	A
1	A	1971	A
1	A	1972	A
1	A	1981	A
1	A	1982	C
1	A	1991	U
1	A	1992	G
1	A	1993	U
1	A	2020	A
1	A	2023	G
1	A	2031	A
1	A	2033	A
1	A	2039	C
1	A	2043	C
1	A	2049	G
1	A	2052	G
1	A	2055	C
1	A	2056	G
1	A	2059	A
1	A	2060	A
1	A	2061	G
1	A	2062	A
1	A	2063	C
1	A	2069	G
1	A	2093	G
1	A	2099	U
1	A	2100	G
1	A	2111	C
1	A	2112	G
1	A	2113	U

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Mol	Chain	Res	Type
1	A	2114	A
1	A	2115	G
1	A	2116	G
1	A	2117	A
1	A	2119	A
1	A	2120	G
1	A	2126	A
1	A	2127	G
1	A	2128	C
1	A	2131	G
1	A	2132	U
1	A	2133	G
1	A	2136	C
1	A	2146	C
1	A	2148	G
1	A	2158	A
1	A	2166	G
1	A	2168	G
1	A	2173	A
1	A	2176	A
1	A	2178	C
1	A	2190	G
1	A	2192	G
1	A	2198	A
1	A	2210	G
1	A	2211	G
1	A	2212	A
1	A	2213	U
1	A	2215	G
1	A	2225	A
1	A	2238	G
1	A	2239	G
1	A	2243	U
1	A	2246	G
1	A	2275	C
1	A	2280	G
1	A	2283	C
1	A	2287	A
1	A	2288	A
1	A	2305	A
1	A	2307	G
1	A	2308	G

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Mol	Chain	Res	Type
1	A	2311	A
1	A	2319	G
1	A	2320	A
1	A	2325	G
1	A	2334	G
1	A	2336	A
1	A	2342	C
1	A	2346	A
1	A	2347	C
1	A	2350	C
1	A	2377	A
1	A	2383	G
1	A	2385	C
1	A	2392	A
1	A	2402	C
1	A	2403	C
1	A	2406	U
1	A	2410	G
1	A	2423	U
1	A	2425	A
1	A	2429	G
1	A	2430	A
1	A	2434	A
1	A	2435	A
1	A	2439	A
1	A	2440	C
1	A	2441	C
1	A	2448	A
1	A	2450	A
1	A	2469	A
1	A	2470	G
1	A	2471	C
1	A	2474	C
1	A	2475	C
1	A	2476	A
1	A	2484	G
1	A	2494	G
1	A	2498	C
1	A	2502	G
1	A	2505	G
1	A	2518	A
1	A	2524	G

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Mol	Chain	Res	Type
1	A	2529	G
1	A	2542	A
1	A	2543	G
1	A	2554	U
1	A	2562	U
1	A	2566	A
1	A	2567	G
1	A	2586	C
1	A	2602	A
1	A	2609	U
1	A	2611	U
1	A	2612	C
1	A	2621	A
1	A	2629	A
1	A	2632	A
1	A	2655	G
1	A	2656	U
1	A	2665	A
1	A	2673	G
1	A	2682	U
1	A	2689	U
1	A	2690	C
1	A	2702	U
1	A	2703	C
1	A	2712	U
1	A	2712(A)	A
1	A	2713	A
1	A	2714	G
1	A	2720	U
1	A	2726	U
1	A	2733	A
1	A	2744	G
1	A	2748	A
1	A	2752	C
1	A	2757	A
1	A	2758	A
1	A	2761	G
1	A	2764	A
1	A	2765	A
1	A	2766	G
1	A	2777	G
1	A	2778	A

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Mol	Chain	Res	Type
1	A	2779	U
1	A	2780	G
1	A	2789	C
1	A	2790	A
1	A	2791	C
1	A	2797	U
1	A	2799	A
1	A	2807	G
1	A	2808	U
1	A	2818	G
1	A	2820	A
1	A	2821	A
1	A	2823	A
1	A	2833	G
1	A	2834	G
1	A	2835	A
1	A	2867	G
1	A	2868	A
1	A	2872	G
1	A	2873	A
1	A	2880	C
1	A	2891	G
1	A	2892	A
1	A	2893	G
1	A	2894	G
2	B	8	U
2	B	9	G
2	B	13	A
2	B	15	A
2	B	16	G
2	B	21	G
2	B	22	U
2	B	25	A
2	B	32	C
2	B	40	U
2	B	41	U
2	B	42	C
2	B	45	A
2	B	47	C
2	B	52	A
2	B	53	A
2	B	56	G

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Mol	Chain	Res	Type
2	B	67	G
2	B	73	A
2	B	89	G
2	B	109	G

All (58) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	99	U
1	A	102	G
1	A	195	A
1	A	221	A
1	A	222	A
1	A	229	A
1	A	242	G
1	A	271(B)	G
1	A	278	A
1	A	372	G
1	A	404	C
1	A	503	A
1	A	508	G
1	A	587	C
1	A	637	A
1	A	653	A
1	A	654	A
1	A	752	A
1	A	846	C
1	A	856	C
1	A	859	G
1	A	896	A
1	A	974(A)	C
1	A	1012	U
1	A	1022	G
1	A	1026	U
1	A	1045	A
1	A	1078	U
1	A	1085	A
1	A	1109	C
1	A	1130	U
1	A	1178	C
1	A	1210	A
1	A	1427	A

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Mol	Chain	Res	Type
1	A	1558	A
1	A	1653	G
1	A	1694	C
1	A	1698	A
1	A	1799	G
1	A	1819	A
1	A	1929	G
1	A	1930	G
1	A	1955	U
1	A	1992	G
1	A	2126	A
1	A	2439	A
1	A	2566	A
1	A	2610	C
1	A	2655	G
1	A	2681	C
1	A	2689	U
1	A	2712	U
1	A	2719	G
1	A	2756	U
1	A	2776	A
1	A	2832	U
1	A	2867	G
2	B	66	A

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 291 ligands modelled in this entry, 291 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.