



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:08 PM GMT

PDB ID : 1NJM
Title : The crystal structure of the 50S Large ribosomal subunit from *Deinococcus radiodurans* complexed with a tRNA acceptor stem mimic (ASM) and the antibiotic sparsomycin
Authors : Bashan, A.; Agmon, I.; Zarivatch, R.; Schlutzen, F.; Harms, J.M.; Berisio, R.; Bartels, H.; Hansen, H.A.; Yonath, A.
Deposited on : 2003-01-02
Resolution : 3.60 Å(reported)

This is a Full wwPDB X-ray Structure 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/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

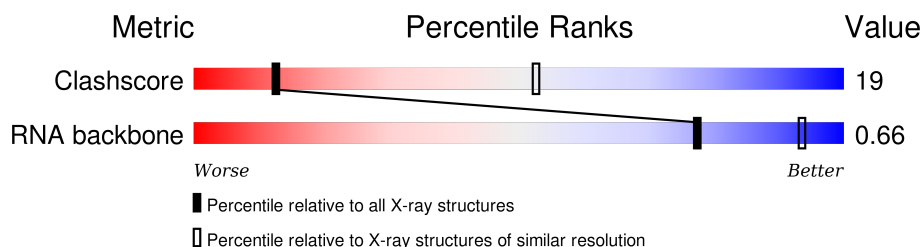
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

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	102246	1010 (3.74-3.46)
RNA backbone	2183	1058 (4.40-2.80)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	0	2880	 33% 51% 11% .
2	5	35	 26% 40% 6% 29%
3	K	141	 88% 12%
4	T	237	 94% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SPS	0	2881	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 60271 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	0	2766	Total	C	N	O	P	0	0	0
			59359	26479	10949	19166	2765			

- Molecule 2 is a RNA chain called tRNA acceptor stem mimic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	5	25	Total	C	N	O	P	0	0	0
			543	249	97	173	24			

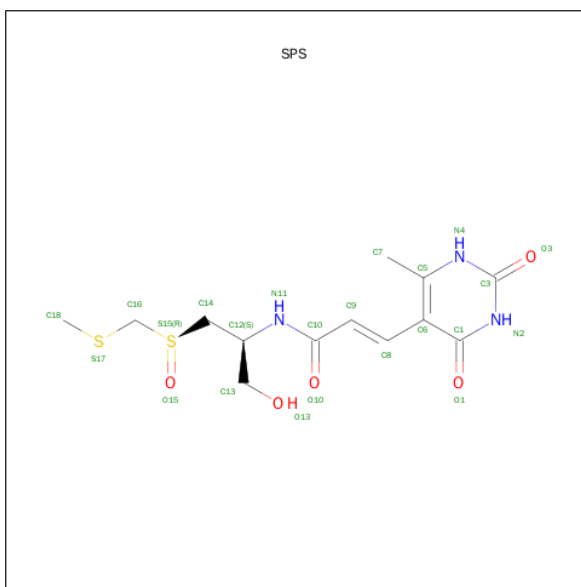
- Molecule 3 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
3	K	124	Total	C	0	0	124
			124	124			

- Molecule 4 is a protein called GENERAL STRESS PROTEIN CTC.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
4	T	223	Total	C	0	0	223
			223	223			

- Molecule 5 is SPARSOMYCIN (three-letter code: SPS) (formula: C₁₃H₁₉N₃O₅S₂).



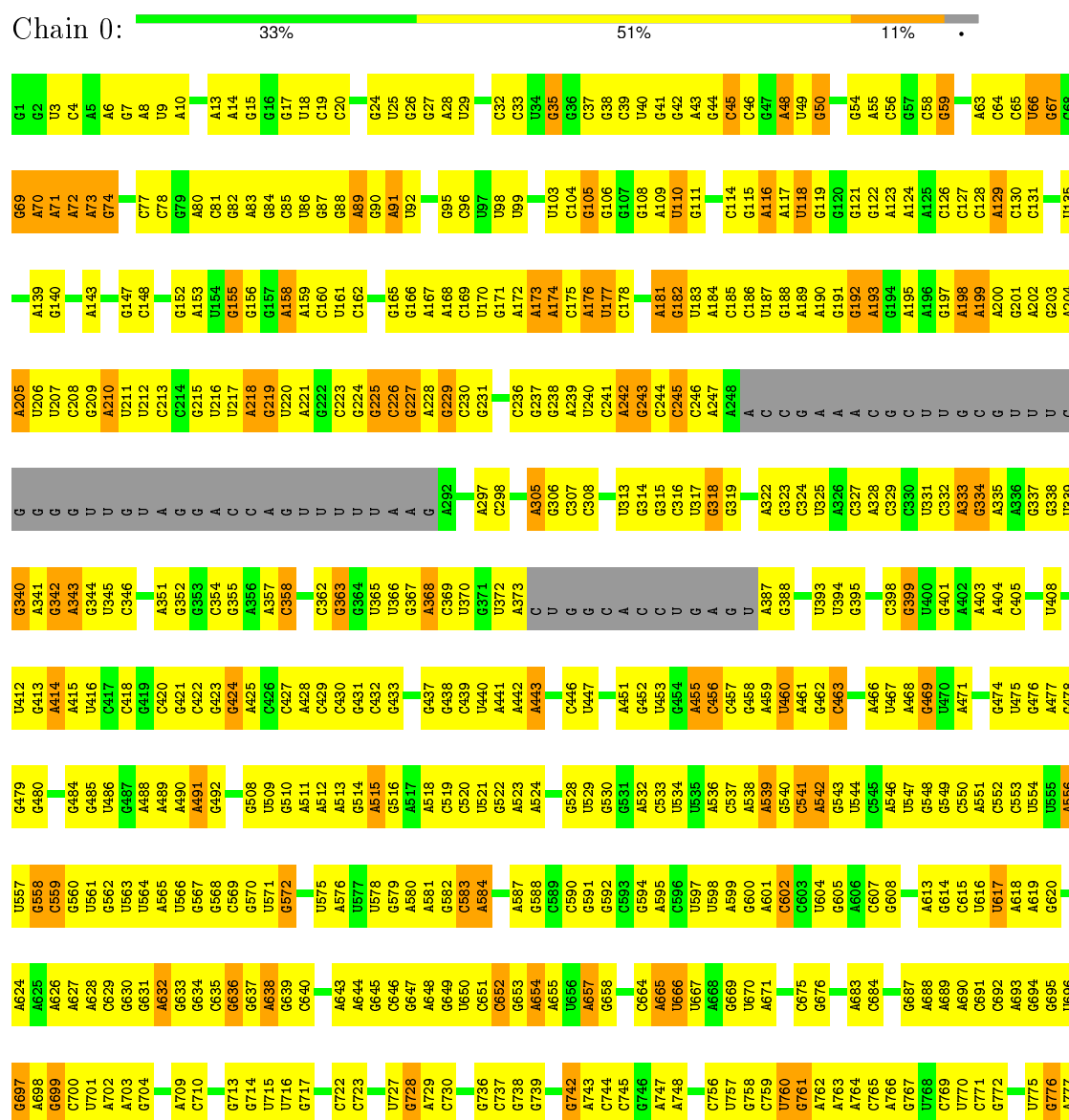
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	0	1	Total	C	N	O	S	0	0
			22	13	3	4	2		

3 Residue-property plots

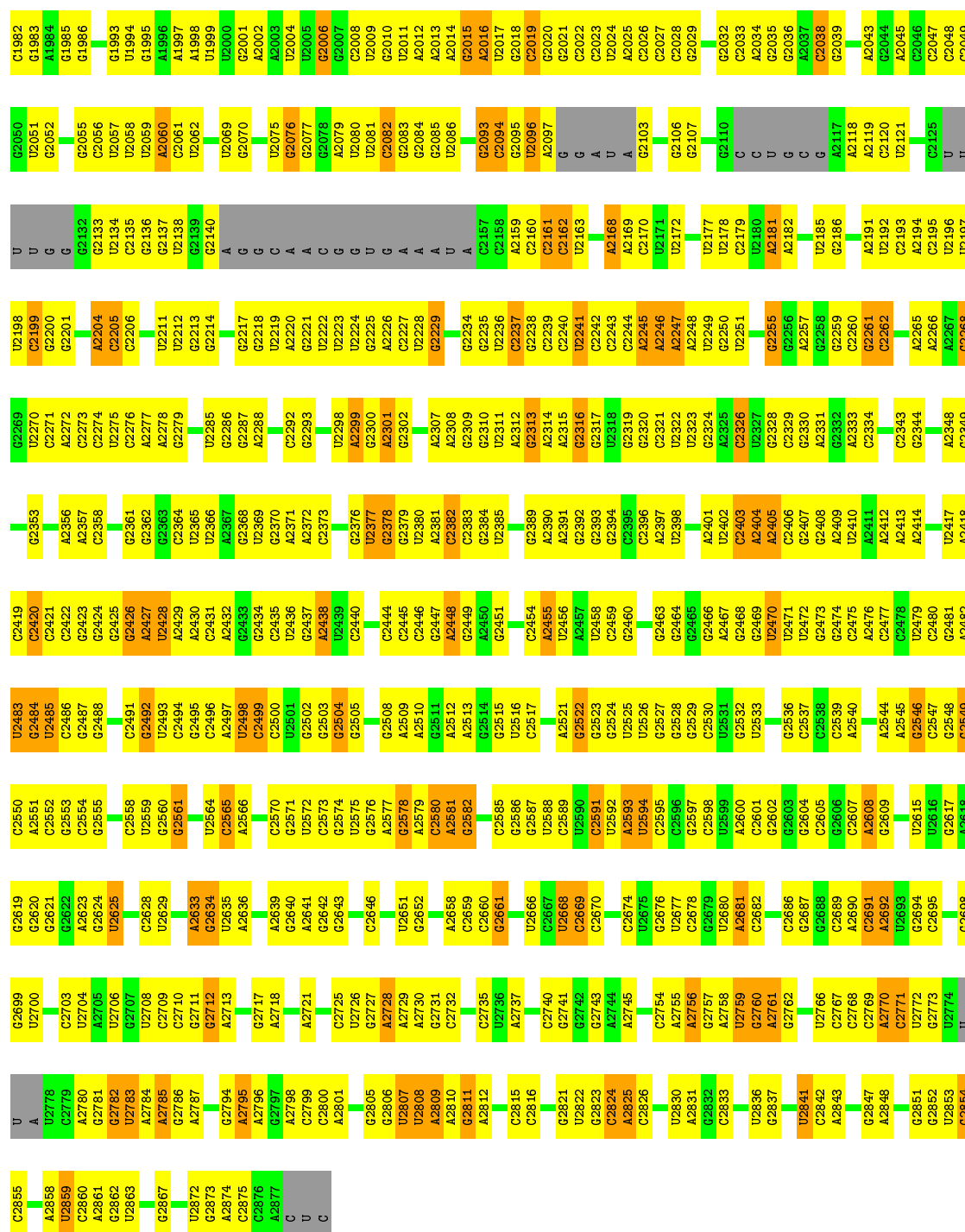
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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

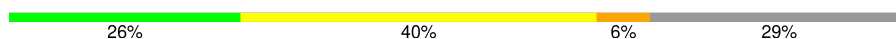


A1910	G1818	G1737	A1658	A1586	G1508	A1441	G1369	A1289	G1217	G1142	G1045	U978	C	U840	G778
A1911	U1819	G1742	G1659	A1587	A1509	C1442	U1365	A1290	U1218	A1143	U1046	A979	A911	G841	U779
G1912	G1820	G1743	G1660	U1591	A1510	G1443	U1366	G1291	C1219	U1144	G1047	G980	U916	G842	U780
G1913	A1821	G1745	G1661	U1592	A1511	C1444	A1366	A1292	C1220	G1145	C1052	C981	U917	G843	G781
U1914	C1822	G1746	G1662	U1593	A1512	U1445	A1367	A1293	C1221	G1146	G1053	A984	U918	G844	U782
A1915	C1825	A1745	G1663	U1594	U1513	U1446	G1368	G1298	C1222	G1147	G1054	G985	U919	U845	G783
G1916	U1826	G1747	G1664	U1595	C1514	U1447	G1369	U1308	G1223	G1148	G1055	A986	U920	A846	U784
C1917	G1836	G1748	G1665	A1596	U1515	U1448	U1370	U1301	A1224	G1149	U1056	G987	A921	C847	U785
A1919	C1830	G1749	G1667	U1597	A1516	C1449	G1371	U1307	G1225	C1150	A1057	G988	A922	U852	U786
U1920	A1830	A1750	G1668	C1598	C1518	C1451	G1372	U1308	A1226	G1151	G1058	U991	U925	C853	G788
G1921	G1831	U1754	U1669	G1599	G1519	U1452	G1373	C1309	A1227	A1154	U1059	A994	U926	G854	G789
U1922	G1835	G1755	A1670	U1601	G1520	U1455	G1377	G1310	A1231	A1155	A1065	A994	G927	G855	A790
U1923	C1836	U1672	A1671	G1602	U1521	C1456	U1377	C1311	U1232	U1156	G1066	A995	G928	A856	G791
C1924	G1837	G1760	A1672	A1603	C1522	C1457	C1380	G1312	A1233	A1162	G1067	A996	G929	U857	U792
U1926	G1838	G1761	C1677	A1604	A1523	U1458	G1381	U1313	C1234	C1163	A1068	G997	A930	G858	G793
U1927	A1839	C1762	G1678	A1605	C1524	U1459	A1366	U1314	C1235	C1164	G1069	G998	A931	U859	A794
G1928	A1840	G1763	U1679	C1606	G1527	U1460	G1387	A1315	A1242	G1165	G1070	A999	G932	U860	A795
U1929	G1841	A1764	U1680	A1607	C1528	A1463	C1388	G1316	A1243	A1166	G1073	G1000	G933	G861	A796
U1930	C1842	C1765	A1681	U1608	C1529	A1464	C1389	G1317	G1244	A1167	G1074	A1001	G934	C864	A797
G1931	A1851	U1766	G1682	G1609	U1530	C1465	G1390	A1318	G1248	G1168	U1075	C1002	A935	A865	C799
U1932	G1852	U1767	G1683	A1610	C1531	C1466	C1391	C1319	U1249	C1169	U1076	C1003	A936	U868	U800
G1933	G1853	U1770	G1684	U1611	A1532	U1467	U1392	A1320	G1250	U1172	A1081	U1004	C939	C869	C803
U1934	U1855	A1771	A1685	U1612	G1533	U1468	G1393	G1323	G1251	G1173	C1082	C1006	G940	C870	C804
U1935	U1856	A1772	C1687	G1613	U1539	U1469	A1397	G1324	C1252	U1177	A1084	A1007	U941	U871	G805
G1936	C1857	A1773	G1688	C1614	C1540	G1470	G1398	C1325	C1253	U1178	G1085	G1008	U942	G872	A806
U1946	G1858	A1774	G1689	C1615	U1541	C1471	C1399	U1326	G1254	C1178	C1086	C1009	U943	U873	A807
G1947	A1859	A1775	G1691	C1616	G1543	C1472	G1402	C1327	U1257	A1179	C1087	A944	U944	A874	C808
C1948	A1860	A1776	C1692	U1617	A1544	U1473	U1403	G1328	C1258	A1180	C1088	U1015	G945	G875	C809
A1949	G1861	U1777	G1693	U1618	G1545	U1474	U1404	U1329	A1259	C1181	C1089	U1016	C948	A876	U810
C1950	C1862	C1779	U1696	A1619	G1546	U1475	U1405	G1330	G1260	C1182	C1090	C1017	G949	G877	U811
G1951	U1863	U1780	C1697	C1620	C1552	U1476	G1407	G1331	U1261	G1183	C1091	C1018	G950	C878	G812
U1952	G1864	G1703	G1704	C1621	C1553	U1477	U1410	G1332	U1262	C1184	U1093	U1019	G951	A879	A813
A1953	C1865	C1705	U1706	C1622	G1557	U1478	U1411	G1333	G1263	G1185	G1098	A1020	A952	C880	G814
A1954	G1866	A1785	C1707	C1623	C1558	U1479	C1412	A1334	C1264	A1187	C1099	A1021	G953	G887	A815
G1955	U1867	C1786	G1708	A1624	G1561	U1480	G1413	G1337	G1265	A1188	A1022	U954	G954	G888	U816
G1956	C1868	U1787	U1709	A1625	G1562	U1481	U1414	G1338	G1266	G1189	G1100	U1023	G955	C889	G818
C1957	A1869	C1788	U1710	C1626	U1563	U1482	A1415	U1339	A1267	C1190	C1024	G1024	A956	U890	C819
U1958	G1871	U1789	G1711	A1627	G1566	C1487	C1416	G1340	U1268	G1191	A1114	A1025	G957	A891	U820
G1959	C1883	C1792	G1713	C1628	G1567	U1488	C1417	G1341	G1269	A1192	C1026	U1026	G958	G	A821
A1961	A1884	A1793	A1714	G1629	A1567	C1489	C1418	U1342	C1270	G1193	C1027	C1027	C959	G	G822
C1962	C1885	U1794	U1715	A1632	A1568	U1490	G1419	C1343	C1271	U1194	G1028	U1029	G961	G	U824
G1963	G1886	A1799	G1716	C1633	G1571	U1491	U1424	G1344	G1272	U1195	A1122	U1030	A964	G	G825
A1964	C1887	A1800	A1717	A1634	C1572	U1492	G1425	G1345	G1273	G1196	C1127	C1031	A965	G	C826
U1965	G1888	C1801	G1722	G1635	G1573	G1493	U1426	C1346	C1274	U1197	G1128	A1032	G966	C	C827
C1966	A1889	A1802	U1723	G1643	A1574	G1495	G1427	C1347	A1275	C1198	A1129	G1033	A967	C	C828
G1970	G1890	G1806	C1724	G1644	C1575	G1496	G1428	C1348	U1278	U1199	U1130	U1034	G967	A	G829
C1971	A1895	A1807	U1725	U1645	G1576	C1497	A1429	G1349	G1279	G1200	G1131	G1035	G968	C	C830
G1972	U1896	C1727	C1728	C1648	G1577	U1498	G1430	G1350	G1280	A1203	C1132	G1036	U969	C	G831
U1974	C1897	A1808	U1729	U1651	U1578	A1499	U1431	G1351	A1281	G1204	G1133	U1037	A970	A	A832
G1975	G1899	C1730	G1652	G1652	G1579	U1500	G1432	G1352	U1282	G1205	C1134	A1038	G971	C	A833
U1976	U1900	A1810	C1653	C1581	C1580	G1501	A1433	A1353	A1284	A1137	U1138	U1039	G972	C	A834
C1977	A1811	C1731	U1731	G1502	C1581	G1503	U1434	A1354	A1285	C1210	A1139	A1040	U973	U	U837
U1978	U1812	U1732	U1732	A1654	A1582	U1504	G1435	A1355	A1286	G1211	A1140	G1041	C975	A	A838
C1979	C1907	U1733	U1733	C1655	A1583	G1504	G1436	C1356	A1287	U1141	U1044	U1044	U974	U	U839
A1980	U1908	A1814	C1736	U1656	A1584	U1505	A1437	U1357	A1288	C1214				C	
A1981	U1909			A1657	A1585			C1358							



- Molecule 2: tRNA acceptor stem mimic

Chain 5:

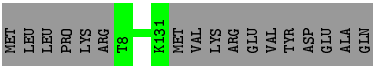


- Molecule 3: 50S ribosomal protein L16

Chain K:

88%

12%

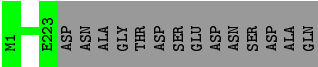


- Molecule 4: GENERAL STRESS PROTEIN CTC

Chain T:

94%

6%



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	169.60 Å 409.40 Å 695.10 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.60	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-3.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.284 , 0.308	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	60271	wwPDB-VP
Average B, all atoms (Å ²)	74.0	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: SPS, PPU

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	0	0.14	0/66467	0.63	0/103673
2	5	0.16	0/563	0.63	0/873
All	All	0.14	0/67030	0.63	0/104546

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	873	U	Sidechain

5.2 Too-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 hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59359	0	29917	1742	0
2	5	543	0	290	16	0
3	K	124	0	0	0	0
4	T	223	0	0	0	0
5	0	22	0	19	0	0
All	All	60271	0	30226	1754	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (1754) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:940:G:H3'	1:0:941:U:H5''	1.22	1.14
1:0:1141:U:H3	1:0:2008:C:H5''	1.20	1.05
1:0:1073:G:H2'	1:0:1074:G:H4'	1.40	1.00
1:0:2548:G:H2'	1:0:2549:G:H5''	1.44	1.00
1:0:2769:C:H2'	1:0:2867:G:H22	1.22	0.98
1:0:58:C:H3'	1:0:59:G:H5''	1.42	0.97
1:0:688:A:H62	1:0:816:U:H3	1.09	0.97
1:0:2668:U:H4'	1:0:2669:C:H5'	1.46	0.97
1:0:1252:C:H2'	1:0:1253:C:H5''	1.47	0.97
1:0:2636:A:H62	1:0:2643:G:H21	1.12	0.96
1:0:1086:C:H2'	1:0:1087:C:H5''	1.49	0.95
1:0:1182:U:H2'	1:0:1183:C:H5''	1.47	0.95
1:0:1496:G:H1	1:0:1527:G:H1	1.14	0.94
1:0:471:A:H62	1:0:480:G:H21	1.12	0.94
1:0:221:A:H62	1:0:231:G:H21	1.14	0.94
1:0:1572:C:H2'	1:0:1573:G:H5''	1.48	0.94
1:0:1747:G:H4'	1:0:1749:G:H1'	1.48	0.94
1:0:2579:A:H2'	1:0:2580:C:H5''	1.49	0.94
1:0:225:G:H3'	1:0:226:C:H5'	1.48	0.93
1:0:1953:A:H1'	1:0:1955:G:H1'	1.52	0.92
1:0:1312:G:H5''	1:0:1313:U:H5'	1.53	0.91
1:0:847:C:H41	1:0:955:G:H21	1.18	0.91
1:0:166:G:H21	1:0:184:A:H62	1.12	0.91
1:0:929:A:H3'	1:0:930:A:H5''	1.52	0.90
1:0:1223:G:H21	1:0:1225:G:H21	0.92	0.90
2:5:31:C:H3'	2:5:32:A:H5''	1.54	0.90
1:0:1199:U:H3'	1:0:1200:G:H5''	1.52	0.90
1:0:831:G:H21	1:0:1203:A:H62	1.17	0.89
1:0:1915:A:H62	1:0:1951:G:H21	1.19	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:789:G:H21	1:0:806:A:H62	1.14	0.89
1:0:1656:U:H2'	1:0:1657:A:H5''	1.56	0.88
1:0:104:C:H2'	1:0:105:G:H5''	1.56	0.88
1:0:2633:A:H4'	1:0:2634:G:H4'	1.56	0.87
1:0:2059:U:H5	1:0:2575:U:H3	1.23	0.87
1:0:367:G:H2'	1:0:368:A:H5''	1.55	0.87
1:0:403:A:H4'	1:0:425:A:H5'	1.57	0.86
1:0:128:C:H2'	1:0:129:A:H5''	1.58	0.86
1:0:1223:G:H21	1:0:1225:G:N2	1.74	0.86
1:0:1964:A:H3'	1:0:1965:U:H5'	1.60	0.84
1:0:1034:U:H1'	1:0:1133:G:H5''	1.59	0.84
1:0:2047:C:H42	1:0:2425:G:H1	1.24	0.83
1:0:1436:G:H1'	1:0:1508:G:H21	1.41	0.83
1:0:2607:C:H3'	1:0:2608:A:H5'	1.58	0.82
1:0:2794:G:H3'	1:0:2796:A:H62	1.43	0.82
1:0:109:A:H3'	1:0:110:U:H5''	1.61	0.81
1:0:2081:U:H2'	1:0:2082:C:H5''	1.62	0.81
1:0:2806:G:H1'	1:0:2858:A:H2'	1.63	0.81
1:0:2198:U:H3'	1:0:2199:C:H5''	1.62	0.81
1:0:88:G:H3'	1:0:89:A:H5''	1.61	0.81
1:0:940:G:H3'	1:0:941:U:C5'	2.09	0.81
1:0:2491:C:H2'	1:0:2492:G:H5''	1.63	0.81
1:0:26:G:H21	1:0:524:A:H62	1.25	0.81
1:0:2522:G:H21	1:0:2625:U:H5''	1.45	0.80
1:0:2700:U:H3	1:0:2848:A:N6	1.79	0.80
1:0:9:U:H3	1:0:2608:A:H62	1.29	0.80
1:0:2426:G:H5'	1:0:2480:C:H41	1.47	0.80
1:0:1223:G:N2	1:0:1225:G:H21	1.76	0.79
1:0:542:A:H2'	1:0:543:G:H5'	1.65	0.79
1:0:1141:U:N3	1:0:2008:C:H5''	1.97	0.79
1:0:2769:C:H2'	1:0:2867:G:N2	1.97	0.79
1:0:460:U:H3	1:0:592:G:H1'	1.46	0.79
1:0:2548:G:C2'	1:0:2549:G:H5''	2.10	0.79
1:0:918:A:H2'	1:0:919:U:H5''	1.64	0.79
1:0:176:A:H1'	1:0:2221:G:H21	1.48	0.78
2:5:3:G:H1	2:5:29:U:H3	1.32	0.78
1:0:2564:U:H5''	1:0:2565:C:H5'	1.65	0.78
1:0:2227:C:H2'	1:0:2228:U:H5'	1.66	0.78
1:0:1811:A:O2'	1:0:1812:U:H5''	1.83	0.78
1:0:70:A:O3'	1:0:71:A:H3'	1.84	0.78
1:0:689:A:H61	1:0:815:A:H61	1.30	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:26:G:N2	1:0:524:A:H62	1.83	0.77
1:0:1432:G:H21	1:0:1596:A:H62	1.28	0.77
1:0:1188:A:H62	1:0:1189:G:H21	1.31	0.77
1:0:59:G:H1'	1:0:73:A:N1	2.01	0.76
1:0:181:A:H5''	1:0:182:G:OP1	1.84	0.76
1:0:2261:G:H4'	1:0:2262:C:OP2	1.86	0.76
1:0:652:C:H42	1:0:657:A:H61	1.31	0.76
1:0:2770:A:H5'	1:0:2867:G:H22	1.50	0.76
1:0:2624:G:H4'	1:0:2712:G:H2'	1.69	0.75
1:0:2096:U:H2'	1:0:2097:A:H5''	1.69	0.75
1:0:688:A:N6	1:0:816:U:H3	1.85	0.75
1:0:2503:G:H3'	1:0:2504:G:H5''	1.69	0.74
1:0:2700:U:H3	1:0:2848:A:H62	1.35	0.74
1:0:616:U:H2'	1:0:617:U:H5''	1.69	0.74
1:0:1252:C:C2'	1:0:1253:C:H5''	2.18	0.74
1:0:1473:U:H4'	1:0:1474:A:C8	2.23	0.73
1:0:218:A:O2'	1:0:219:G:H4'	1.87	0.73
1:0:67:G:N2	1:0:72:A:H2'	2.04	0.73
1:0:1182:U:C2'	1:0:1183:C:H5''	2.17	0.73
1:0:109:A:C3'	1:0:110:U:H5''	2.19	0.72
1:0:2241:U:H1'	1:0:2307:A:H1'	1.70	0.72
1:0:471:A:H62	1:0:480:G:N2	1.86	0.72
1:0:1882:G:H21	1:0:1885:C:N4	1.86	0.72
1:0:1572:C:C2'	1:0:1573:G:H5''	2.18	0.72
1:0:878:C:H42	1:0:921:A:H62	1.36	0.72
1:0:2721:A:H62	1:0:2743:G:H21	1.37	0.72
1:0:1021:A:H1'	1:0:1164:C:H1'	1.71	0.72
1:0:1199:U:H3'	1:0:1200:G:C5'	2.20	0.72
1:0:795:A:H4'	1:0:796:A:N7	2.04	0.71
1:0:1908:C:H2'	1:0:1909:U:H4'	1.72	0.71
1:0:202:A:H2'	1:0:203:G:O4'	1.88	0.71
1:0:1528:C:H2'	1:0:1529:C:H5''	1.71	0.71
1:0:1479:G:N2	1:0:1543:G:H21	1.87	0.71
1:0:2691:C:H3'	1:0:2692:A:H5''	1.73	0.71
1:0:1196:G:H2'	1:0:1197:U:O4'	1.91	0.71
1:0:58:C:H3'	1:0:59:G:C5'	2.19	0.71
1:0:2503:G:C3'	1:0:2504:G:H5''	2.21	0.71
1:0:1001:A:H62	1:0:1200:G:H1'	1.55	0.71
1:0:1807:A:O2'	1:0:1808:C:H4'	1.90	0.71
1:0:33:C:H42	1:0:466:A:H61	1.38	0.71
1:0:65:C:H2'	1:0:66:U:H5'	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1923:U:H4'	1:0:1948:C:H41	1.55	0.71
1:0:1047:G:H1	1:0:1130:U:H3	1.37	0.71
1:0:319:G:H21	1:0:340:G:H21	1.39	0.71
1:0:2380:U:H2'	1:0:2381:A:H5'	1.72	0.71
1:0:515:A:H2'	1:0:516:G:H5'	1.72	0.70
1:0:1373:G:H22	1:0:2192:U:H3	1.37	0.70
1:0:1139:A:H1'	1:0:2496:C:H5'	1.72	0.70
1:0:1809:G:H2'	1:0:1810:U:O4'	1.91	0.70
1:0:1621:C:H4'	1:0:1626:A:H61	1.56	0.70
1:0:514:G:N3	1:0:514:G:H2'	2.06	0.70
1:0:181:A:H4'	1:0:182:G:H4'	1.74	0.70
1:0:1529:C:H2'	1:0:1530:U:O4'	1.92	0.70
1:0:2759:U:H4'	1:0:2760:G:OP2	1.90	0.70
1:0:1023:U:H1'	1:0:1154:A:N7	2.06	0.69
1:0:2522:G:N2	1:0:2625:U:H5''	2.06	0.69
1:0:2510:A:H61	1:0:2641:A:H61	1.40	0.69
1:0:2510:A:H61	1:0:2641:A:N6	1.90	0.69
1:0:2808:U:H3'	1:0:2809:A:H5'	1.74	0.69
1:0:951:G:H2'	1:0:952:A:H5''	1.73	0.69
1:0:800:U:H3'	1:0:804:C:N4	2.08	0.69
1:0:1838:G:H2'	1:0:1839:A:H5'	1.75	0.69
1:0:65:C:C2'	1:0:66:U:H5'	2.23	0.69
1:0:2727:G:H1	1:0:2735:C:H5''	1.58	0.68
1:0:1188:A:N6	1:0:1189:G:H21	1.90	0.68
1:0:584:A:H4'	1:0:2479:U:H5'	1.74	0.68
1:0:2607:C:H1'	1:0:2761:A:H2'	1.76	0.68
1:0:653:G:H2'	1:0:654:A:H4'	1.75	0.68
1:0:1978:U:H3'	1:0:1979:C:H5''	1.74	0.68
1:0:576:A:H2	1:0:580:A:H62	1.42	0.68
1:0:1955:G:H2'	1:0:1956:G:H5'	1.75	0.68
1:0:941:U:H2'	1:0:942:U:O4'	1.94	0.68
1:0:1791:C:O2'	1:0:1793:A:H5'	1.94	0.67
1:0:2495:G:H2'	1:0:2496:C:C6	2.30	0.67
1:0:2095:G:H2'	1:0:2096:U:H5''	1.74	0.67
1:0:583:C:N3	1:0:2016:A:H4'	2.09	0.67
1:0:2491:C:C2'	1:0:2492:G:H5''	2.24	0.67
1:0:813:A:O2'	1:0:815:A:H5'	1.94	0.67
1:0:1181:C:H2'	1:0:1182:U:H5''	1.76	0.67
1:0:367:G:C2'	1:0:368:A:H5''	2.24	0.67
1:0:588:G:H4'	1:0:2001:G:H5''	1.77	0.67
1:0:1749:G:O6	1:0:2674:C:H4'	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1953:A:H1'	1:0:1955:G:C1'	2.21	0.67
1:0:1915:A:H62	1:0:1951:G:N2	1.91	0.67
1:0:2768:C:H2'	1:0:2769:C:O4'	1.94	0.67
1:0:2680:U:H3'	1:0:2681:A:H5'	1.76	0.67
1:0:1086:C:C2'	1:0:1087:C:H5''	2.23	0.67
1:0:1500:U:H3	1:0:1520:G:H22	1.43	0.67
1:0:225:G:H3'	1:0:226:C:C5'	2.25	0.66
1:0:1191:G:H2'	1:0:1192:A:H8	1.60	0.66
1:0:73:A:H4'	1:0:74:G:C1'	2.24	0.66
1:0:1474:A:H2'	1:0:1475:U:H5'	1.77	0.66
1:0:1685:A:H1'	1:0:1686:A:C5	2.30	0.66
1:0:69:G:H4'	1:0:70:A:O5'	1.94	0.66
1:0:805:G:H5''	1:0:806:A:O5'	1.95	0.66
1:0:665:A:H3'	1:0:666:U:H5''	1.77	0.66
1:0:1746:A:H2'	1:0:1747:G:H5'	1.77	0.66
1:0:1923:U:H4'	1:0:1948:C:N4	2.11	0.66
1:0:1774:A:H1'	1:0:2586:G:H21	1.61	0.66
1:0:45:C:H5''	1:0:192:G:N7	2.10	0.66
1:0:66:U:H2'	1:0:67:G:N7	2.11	0.66
1:0:538:A:H2'	1:0:539:A:H5''	1.77	0.66
1:0:1487:C:H2'	1:0:1488:G:H8	1.60	0.66
1:0:1312:G:H5'	1:0:1314:A:H1'	1.76	0.66
1:0:652:C:H42	1:0:657:A:N6	1.94	0.66
1:0:1352:G:H2'	1:0:1353:A:H8	1.60	0.66
1:0:1686:A:N3	1:0:1686:A:H2'	2.10	0.66
1:0:805:G:H4'	1:0:806:A:OP2	1.96	0.65
1:0:1188:A:H62	1:0:1189:G:N2	1.93	0.65
1:0:651:C:H2'	1:0:652:C:H5''	1.77	0.65
1:0:1033:G:H22	1:0:1150:C:H2'	1.61	0.65
1:0:2324:G:H4'	1:0:2326:C:H5''	1.79	0.65
1:0:1888:C:H5''	1:0:1889:G:H5''	1.79	0.65
1:0:777:A:N6	1:0:1766:U:H3	1.93	0.65
1:0:1900:U:O2'	1:0:1946:U:H5'	1.96	0.65
1:0:175:C:H1'	1:0:2413:A:H61	1.62	0.65
1:0:1679:U:H3'	1:0:1680:U:H5''	1.76	0.65
1:0:1679:U:C3'	1:0:1680:U:H5''	2.27	0.65
1:0:2499:C:H41	1:0:2521:A:H2	1.42	0.65
1:0:1195:U:H2'	1:0:1196:G:C8	2.32	0.65
1:0:13:A:H1'	1:0:536:A:N6	2.12	0.65
1:0:727:U:H2'	1:0:728:G:H5''	1.79	0.65
1:0:2822:U:H2'	1:0:2823:G:O4'	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1938:U:O2'	1:0:1939:U:OP1	2.13	0.65
1:0:236:C:H1'	1:0:632:A:O2'	1.96	0.65
1:0:104:C:C2'	1:0:105:G:H5''	2.27	0.64
1:0:2312:A:H4'	1:0:2313:G:N7	2.12	0.64
1:0:2426:G:H22	1:0:2430:A:H62	1.45	0.64
1:0:2198:U:C3'	1:0:2199:C:H5''	2.28	0.64
1:0:317:U:H2'	1:0:318:G:H5''	1.78	0.64
1:0:1427:G:H2'	1:0:1428:G:H5'	1.80	0.64
1:0:2236:U:C3'	1:0:2237:C:H5''	2.27	0.64
1:0:2236:U:H2'	1:0:2237:C:H5''	1.77	0.64
1:0:2245:A:H4'	1:0:2246:A:C8	2.32	0.64
1:0:2404:A:O2'	1:0:2405:A:OP2	2.15	0.64
1:0:1341:G:H22	1:0:1664:G:H1	1.46	0.64
1:0:83:A:H4'	1:0:84:G:O4'	1.97	0.64
1:0:1194:U:H2'	1:0:1195:U:C6	2.32	0.64
1:0:2690:A:OP2	1:0:2694:G:H5'	1.97	0.64
1:0:614:G:H2'	1:0:615:C:C6	2.32	0.64
1:0:571:U:H2'	1:0:581:A:H1'	1.79	0.64
1:0:2080:U:H2'	1:0:2081:U:C6	2.33	0.64
1:0:1807:A:H5'	1:0:1809:G:C1'	2.28	0.64
1:0:1517:C:H2'	1:0:1518:C:C6	2.32	0.64
1:0:1580:C:H2'	1:0:1581:C:C6	2.32	0.63
1:0:974:U:H1'	1:0:2229:G:H21	1.60	0.63
1:0:73:A:H4'	1:0:74:G:H1'	1.80	0.63
2:5:29:U:H2'	2:5:30:C:C6	2.33	0.63
1:0:1250:A:O2'	1:0:1251:G:H4'	1.98	0.63
1:0:927:C:H2'	1:0:928:G:O4'	1.98	0.63
1:0:1715:A:H1'	1:0:1717:A:O4'	1.99	0.63
1:0:952:A:O2'	1:0:1204:G:H4'	1.98	0.63
1:0:55:A:H2'	1:0:56:C:C6	2.34	0.63
1:0:128:C:C2'	1:0:129:A:H5''	2.27	0.63
1:0:653:G:N2	1:0:655:A:H1'	2.14	0.63
1:0:1428:G:H5''	1:0:1429:A:H5'	1.79	0.63
1:0:221:A:H62	1:0:231:G:N2	1.91	0.63
1:0:2261:G:H5''	1:0:2262:C:O5'	1.98	0.63
1:0:167:A:H62	1:0:183:U:H3	1.47	0.63
1:0:998:C:H2'	1:0:999:A:O4'	1.98	0.62
1:0:2570:C:H2'	1:0:2571:G:C8	2.34	0.62
1:0:2636:A:H62	1:0:2643:G:N2	1.90	0.62
1:0:1181:C:C3'	1:0:1182:U:H5''	2.29	0.62
1:0:2508:G:H5''	1:0:2509:A:H5''	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2422:C:H2'	1:0:2423:G:H8	1.64	0.62
1:0:2617:G:H22	1:0:2755:A:H2'	1.65	0.62
1:0:2015:G:O2'	1:0:2016:A:OP1	2.12	0.62
1:0:1085:G:H2'	1:0:1086:C:C6	2.35	0.62
1:0:542:A:C2'	1:0:543:G:H5'	2.29	0.62
1:0:2381:A:H4'	1:0:2382:C:C5	2.34	0.62
1:0:439:C:H2'	1:0:440:U:O4'	1.99	0.62
1:0:831:G:H21	1:0:1203:A:N6	1.94	0.62
1:0:323:G:H5'	1:0:342:G:C6	2.35	0.62
1:0:2755:A:O2'	1:0:2756:A:H5'	2.00	0.62
1:0:1354:A:H62	1:0:1407:G:H22	1.47	0.62
1:0:942:U:H2'	1:0:943:U:O4'	2.00	0.62
1:0:2440:C:H1'	1:0:2471:U:H3	1.64	0.62
1:0:852:U:H3	1:0:950:G:H1	1.47	0.62
1:0:362:C:H2'	1:0:363:G:H4'	1.81	0.62
1:0:121:G:O2'	1:0:1389:C:H4'	2.00	0.62
1:0:73:A:H3'	1:0:73:A:N3	2.14	0.62
1:0:2721:A:H62	1:0:2743:G:N2	1.98	0.62
1:0:414:A:H2'	1:0:415:A:O4'	1.99	0.62
1:0:2035:G:H2'	1:0:2036:G:H8	1.64	0.62
1:0:1807:A:H5'	1:0:1809:G:O4'	2.00	0.62
1:0:858:G:H5''	1:0:859:U:H5'	1.80	0.62
1:0:2268:G:H22	1:0:2323:U:H4'	1.65	0.62
1:0:2246:A:H2'	1:0:2246:A:N3	2.15	0.62
1:0:2472:U:H5''	2:5:33:C:O2'	2.00	0.62
1:0:1656:U:C2'	1:0:1657:A:H5''	2.29	0.62
1:0:878:C:H42	1:0:921:A:N6	1.97	0.61
1:0:81:C:H2'	1:0:82:G:O4'	2.00	0.61
1:0:940:G:C3'	1:0:941:U:H5''	2.14	0.61
1:0:974:U:H1'	1:0:2229:G:N2	2.15	0.61
1:0:814:G:H3'	1:0:815:A:H5'	1.82	0.61
1:0:1333:G:N2	1:0:1344:C:H41	1.96	0.61
1:0:2769:C:H2'	1:0:2770:A:H5'	1.83	0.61
1:0:2418:A:H4'	1:0:2420:C:OP2	1.99	0.61
1:0:1455:C:O2'	1:0:1644:G:H5''	2.00	0.61
1:0:860:U:C2'	1:0:861:G:H5'	2.31	0.61
1:0:1323:G:H2'	1:0:1324:G:H4'	1.82	0.61
1:0:871:U:H1'	1:0:2248:A:H5''	1.83	0.61
1:0:1976:U:H2'	1:0:1977:C:H5'	1.82	0.61
1:0:669:G:H2'	1:0:670:U:C6	2.36	0.61
1:0:1198:C:H5''	1:0:1199:U:H5''	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1286:U:H5''	1:0:1663:C:H42	1.65	0.61
1:0:2045:A:H4'	1:0:2421:C:OP2	2.01	0.61
1:0:181:A:H4'	1:0:182:G:C5'	2.30	0.61
1:0:742:G:N3	1:0:742:G:H2'	2.14	0.61
1:0:1426:U:H2'	1:0:1427:G:O4'	2.00	0.61
1:0:800:U:H3'	1:0:804:C:H41	1.65	0.61
1:0:455:A:H4'	1:0:1214:C:O2'	2.00	0.61
1:0:1380:C:H2'	1:0:1381:G:H5'	1.81	0.61
1:0:2549:G:H2'	1:0:2550:C:O4'	2.01	0.61
1:0:1188:A:H2'	1:0:1189:G:O4'	2.01	0.61
1:0:2223:U:H2'	1:0:2224:U:O4'	2.00	0.61
1:0:2357:A:H2'	1:0:2358:C:O4'	2.01	0.61
1:0:2544:A:H2'	1:0:2545:A:H4'	1.83	0.61
1:0:2185:U:H2'	1:0:2186:G:C8	2.36	0.61
1:0:1871:G:N3	1:0:1871:G:H2'	2.16	0.61
1:0:1713:G:H2'	1:0:1714:A:O4'	2.00	0.60
1:0:2012:A:N7	1:0:2014:A:H5'	2.16	0.60
1:0:2727:G:O2'	1:0:2728:A:H5''	2.02	0.60
1:0:2242:C:N4	1:0:2257:A:H61	1.99	0.60
1:0:2238:G:H2'	1:0:2239:C:C6	2.37	0.60
1:0:1066:G:H2'	1:0:1067:G:H4'	1.84	0.60
1:0:1458:A:H3'	1:0:1459:U:C5'	2.32	0.60
1:0:2322:U:O2'	1:0:2323:U:H5'	2.00	0.60
1:0:471:A:N6	1:0:480:G:H21	1.93	0.60
1:0:2858:A:H3'	1:0:2859:U:H5'	1.84	0.60
1:0:2058:U:H5'	1:0:2576:G:H1'	1.83	0.60
1:0:2009:U:H3	1:0:2020:G:H1	1.50	0.60
1:0:2402:U:H5'	1:0:2404:A:C5	2.37	0.60
1:0:1625:A:H2'	1:0:1625:A:N3	2.16	0.60
1:0:1073:G:C2'	1:0:1074:G:H4'	2.26	0.60
1:0:1289:A:O2'	1:0:1290:A:H5'	2.02	0.60
1:0:191:G:O2'	1:0:192:G:H5'	2.02	0.60
1:0:192:G:O2'	1:0:193:A:OP2	2.18	0.60
1:0:1088:A:H2'	1:0:1089:C:O4'	2.02	0.59
1:0:357:A:H2'	1:0:358:C:H5'	1.84	0.59
1:0:2377:U:H2'	1:0:2378:G:C8	2.37	0.59
1:0:2759:U:H5''	1:0:2760:G:O5'	2.02	0.59
1:0:2426:G:C5'	1:0:2480:C:H41	2.14	0.59
1:0:2491:C:C3'	1:0:2492:G:H5''	2.32	0.59
1:0:653:G:H4'	1:0:2328:G:H4'	1.83	0.59
1:0:1298:G:N2	1:0:1341:G:H5''	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2604:G:H2'	1:0:2605:C:C6	2.37	0.59
1:0:1260:A:N6	1:0:1262:U:H1'	2.17	0.59
1:0:69:G:H5''	1:0:70:A:OP1	2.02	0.59
1:0:2243:C:H2'	1:0:2244:C:O4'	2.02	0.59
1:0:2081:U:C2'	1:0:2082:C:H5''	2.32	0.59
1:0:2770:A:H5'	1:0:2867:G:N2	2.17	0.59
1:0:1811:A:H1'	1:0:1813:A:C5	2.37	0.59
1:0:1140:A:H61	1:0:2470:U:H6	1.50	0.59
1:0:804:C:O2'	1:0:806:A:H4'	2.03	0.59
1:0:2260:C:H4'	1:0:2368:G:H21	1.67	0.59
1:0:824:U:O2'	1:0:1264:C:H1'	2.02	0.59
1:0:1683:G:H2'	1:0:1684:G:O4'	2.03	0.59
1:0:412:U:H2'	1:0:413:G:O4'	2.03	0.59
1:0:1634:A:O2'	1:0:1635:G:OP1	2.16	0.59
1:0:1747:G:H1'	1:0:1749:G:N3	2.18	0.59
1:0:2368:G:H5''	1:0:2369:U:O4'	2.02	0.59
1:0:2547:C:H2'	1:0:2548:G:H8	1.68	0.59
1:0:366:U:H2'	1:0:367:G:H8	1.67	0.59
1:0:368:A:H2'	1:0:369:C:O4'	2.03	0.59
1:0:1474:A:N3	1:0:1474:A:H3'	2.18	0.59
1:0:459:A:H1'	1:0:466:A:N7	2.17	0.59
1:0:2205:C:H2'	1:0:2206:C:C6	2.38	0.59
1:0:1354:A:H62	1:0:1407:G:N2	2.01	0.59
1:0:973:U:H2'	1:0:974:U:C6	2.37	0.59
1:0:1472:C:H2'	1:0:1473:U:H5'	1.84	0.59
1:0:513:A:H4'	1:0:515:A:H5'	1.83	0.59
1:0:552:C:H2'	1:0:553:C:H4'	1.85	0.59
1:0:665:A:H3'	1:0:666:U:C5'	2.33	0.58
1:0:2236:U:C2'	1:0:2237:C:H5''	2.33	0.58
1:0:242:A:O2'	1:0:243:G:P	2.61	0.58
1:0:17:G:H21	1:0:564:U:H5''	1.66	0.58
1:0:1181:C:C2'	1:0:1182:U:H5''	2.33	0.58
1:0:1918:G:H4'	1:0:1920:A:N3	2.18	0.58
1:0:1528:C:C2'	1:0:1529:C:H5''	2.33	0.58
1:0:1664:G:O5'	1:0:1665:C:OP1	2.21	0.58
1:0:1926:U:O2'	1:0:1928:G:H5'	2.03	0.58
1:0:2426:G:O6	1:0:2479:U:H2'	2.02	0.58
1:0:1354:A:O2'	1:0:1355:A:OP1	2.19	0.58
1:0:1730:G:H2'	1:0:1731:C:C6	2.38	0.58
1:0:242:A:O2'	1:0:243:G:O4'	2.21	0.58
1:0:2547:C:H2'	1:0:2548:G:C8	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:689:A:H2'	1:0:690:A:H5'	1.84	0.58
1:0:1994:U:H2'	1:0:1995:G:O4'	2.04	0.58
1:0:1567:A:H2'	1:0:1568:A:O4'	2.04	0.58
1:0:1251:G:H2'	1:0:1252:C:C6	2.38	0.58
1:0:874:A:H62	1:0:928:G:H21	1.51	0.58
1:0:931:G:N2	1:0:2247:A:H5''	2.18	0.58
1:0:984:A:H2'	1:0:1200:G:H22	1.68	0.58
1:0:2677:U:H2'	1:0:2678:C:C6	2.39	0.58
1:0:404:A:H5'	1:0:425:A:H4'	1.85	0.58
1:0:1474:A:C2'	1:0:1475:U:H5'	2.33	0.58
1:0:2422:C:H2'	1:0:2423:G:C8	2.39	0.58
1:0:1180:A:H2'	1:0:1181:C:C6	2.39	0.58
1:0:2579:A:C2'	1:0:2580:C:H5''	2.27	0.58
1:0:929:A:H2'	1:0:930:A:H4'	1.85	0.58
1:0:605:G:H4'	1:0:949:G:O2'	2.03	0.58
1:0:2607:C:H3'	1:0:2608:A:C5'	2.31	0.58
1:0:839:U:H2'	1:0:841:G:O4'	2.03	0.58
1:0:521:U:H4'	1:0:1248:G:O2'	2.04	0.58
1:0:2691:C:H3'	1:0:2692:A:C5'	2.33	0.58
1:0:490:A:O2'	1:0:491:A:H5'	2.03	0.58
1:0:632:A:H2'	1:0:633:G:H5'	1.85	0.58
1:0:1301:U:H3	1:0:1339:U:H3	1.51	0.58
1:0:766:A:H2'	1:0:767:G:C8	2.38	0.58
1:0:1779:C:H2'	1:0:1780:A:O4'	2.04	0.58
1:0:2274:C:H2'	1:0:2275:U:H5'	1.86	0.58
1:0:628:A:H2'	1:0:629:C:C6	2.39	0.58
1:0:118:U:H1'	1:0:143:A:C8	2.39	0.57
1:0:1615:C:H2'	1:0:1616:C:C6	2.39	0.57
1:0:67:G:H22	1:0:72:A:H2'	1.68	0.57
1:0:2579:A:H2'	1:0:2580:C:C5'	2.30	0.57
1:0:1916:G:H2'	1:0:1917:C:C6	2.39	0.57
1:0:1712:G:H2'	1:0:1713:G:O4'	2.03	0.57
1:0:2560:G:H4'	1:0:2561:G:N7	2.18	0.57
1:0:2794:G:H2'	1:0:2796:A:N7	2.20	0.57
1:0:2222:U:H2'	1:0:2223:U:C6	2.38	0.57
1:0:873:U:P	1:0:928:G:H1	2.27	0.57
1:0:925:U:H4'	1:0:926:C:C5	2.40	0.57
1:0:2784:A:H3'	1:0:2785:A:H8	1.70	0.57
1:0:1392:U:H2'	1:0:1393:G:H5'	1.87	0.57
1:0:2236:U:H3'	1:0:2237:C:H5''	1.85	0.57
1:0:1514:C:H2'	1:0:1515:U:O4'	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:541:C:H2'	1:0:2002:A:N1	2.20	0.57
1:0:2581:A:H2'	1:0:2582:G:C5'	2.34	0.57
1:0:1223:G:O2'	1:0:1224:A:OP2	2.21	0.57
1:0:618:A:H2'	1:0:619:A:O4'	2.05	0.57
1:0:1971:C:H2'	1:0:1972:G:H8	1.70	0.57
1:0:2437:G:H2'	1:0:2469:G:N2	2.20	0.57
1:0:587:A:H2'	1:0:588:G:H5''	1.87	0.57
1:0:1137:A:H5''	1:0:1138:A:H5''	1.86	0.57
1:0:1464:A:H4'	1:0:1545:G:H4'	1.86	0.57
1:0:1200:G:O4'	1:0:1200:G:OP1	2.22	0.57
1:0:319:G:H21	1:0:340:G:N2	2.03	0.57
1:0:687:G:O2'	1:0:688:A:H5'	2.04	0.57
1:0:1087:C:H2'	1:0:1088:A:O4'	2.05	0.57
1:0:1947:G:OP1	1:0:1947:G:H3'	2.04	0.57
1:0:1472:C:C2'	1:0:1473:U:H5'	2.34	0.57
1:0:2242:C:H42	1:0:2257:A:N6	2.03	0.56
1:0:1220:G:H2'	1:0:1221:C:C6	2.40	0.56
1:0:2459:C:H2'	1:0:2460:G:H5'	1.87	0.56
1:0:2426:G:O2'	1:0:2427:A:OP2	2.19	0.56
1:0:73:A:H4'	1:0:74:G:O4'	2.05	0.56
1:0:1431:U:H2'	1:0:1432:G:O4'	2.06	0.56
1:0:2559:U:H2'	1:0:2560:G:H5'	1.88	0.56
1:0:2329:C:H2'	1:0:2330:G:H5'	1.87	0.56
1:0:874:A:N6	1:0:928:G:H21	2.03	0.56
1:0:369:C:H2'	1:0:370:U:O4'	2.05	0.56
1:0:217:U:H5'	1:0:633:G:O2'	2.06	0.56
1:0:533:C:H2'	1:0:534:U:O4'	2.05	0.56
1:0:1981:A:H4'	1:0:2704:U:O2'	2.05	0.56
1:0:2841:U:O2	1:0:2843:A:H1'	2.05	0.56
1:0:2494:C:H2'	1:0:2495:G:C8	2.40	0.56
1:0:2636:A:N6	1:0:2643:G:H21	1.93	0.56
1:0:2581:A:H2'	1:0:2582:G:H5''	1.86	0.56
1:0:804:C:O2	1:0:807:A:H5'	2.05	0.56
1:0:1280:U:O2'	1:0:1281:A:H5'	2.06	0.56
1:0:197:G:N2	1:0:440:U:H2'	2.21	0.56
1:0:2437:G:N2	1:0:2469:G:H2'	2.21	0.56
1:0:2668:U:C4'	1:0:2669:C:H5'	2.29	0.56
1:0:2641:A:H2'	1:0:2642:G:O4'	2.06	0.56
1:0:176:A:H5''	1:0:177:U:H5	1.71	0.56
1:0:2564:U:C5'	1:0:2565:C:H5'	2.34	0.56
1:0:197:G:H22	1:0:440:U:H2'	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2552:C:H42	2:5:35:PPU:P	2.28	0.56
1:0:103:U:H2'	1:0:104:C:C6	2.40	0.56
1:0:876:A:H2'	1:0:877:G:C8	2.41	0.56
1:0:784:U:H2'	1:0:785:U:C6	2.41	0.56
1:0:930:A:H4'	1:0:930:A:OP1	2.03	0.56
1:0:843:G:O2'	1:0:844:G:OP1	2.15	0.56
1:0:758:G:O2'	1:0:761:G:H1'	2.06	0.56
1:0:2492:G:H2'	1:0:2493:U:O4'	2.05	0.56
1:0:1191:G:H2'	1:0:1192:A:C8	2.40	0.56
1:0:1356:G:H1'	1:0:1613:G:C2	2.40	0.56
1:0:2018:G:H3'	1:0:2019:C:C5'	2.36	0.55
1:0:1923:U:H1'	1:0:1947:G:H4'	1.88	0.55
1:0:366:U:H2'	1:0:367:G:C8	2.41	0.55
1:0:1813:A:H2'	1:0:1814:G:C8	2.41	0.55
1:0:2381:A:H4'	1:0:2382:C:H5	1.69	0.55
1:0:1337:G:H1'	1:0:1632:A:N6	2.21	0.55
1:0:2270:U:H2'	1:0:2271:C:C6	2.42	0.55
1:0:1258:G:H2'	1:0:1259:A:C8	2.42	0.55
1:0:1273:G:H2'	1:0:1274:C:C6	2.42	0.55
1:0:2061:C:H1'	1:0:2413:A:H1'	1.89	0.55
1:0:1949:A:H1'	1:0:2572:U:C4'	2.37	0.55
1:0:241:C:O2'	1:0:242:A:H5''	2.06	0.55
1:0:630:G:H2'	1:0:631:G:H5'	1.89	0.55
1:0:775:U:O2	1:0:1445:A:H5''	2.06	0.55
1:0:2095:G:C2'	1:0:2096:U:H5''	2.36	0.55
1:0:2008:C:H2'	1:0:2009:U:C6	2.41	0.55
1:0:1920:A:N6	1:0:1923:U:H6	2.05	0.55
1:0:515:A:C2'	1:0:516:G:H5'	2.37	0.55
1:0:604:U:H2'	1:0:605:G:C8	2.41	0.55
1:0:226:C:H4'	1:0:227:G:C8	2.41	0.55
1:0:839:U:H5''	1:0:2408:G:OP2	2.06	0.55
1:0:1669:A:H2'	1:0:1670:G:H4'	1.88	0.55
1:0:173:A:N3	1:0:173:A:H2'	2.22	0.55
1:0:879:A:H2'	1:0:879:A:N3	2.22	0.55
1:0:2321:C:H2'	1:0:2322:U:O4'	2.06	0.55
1:0:2162:C:H2'	1:0:2163:U:C6	2.42	0.55
1:0:394:U:H2'	1:0:395:G:H8	1.71	0.55
1:0:583:C:H41	1:0:2017:U:H5	1.53	0.55
1:0:1181:C:H3'	1:0:1182:U:H5''	1.89	0.55
1:0:1459:U:H2'	1:0:1475:U:O2'	2.07	0.55
1:0:2379:G:H2'	1:0:2380:U:O4'	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1429:A:H62	1:0:1601:U:H5''	1.72	0.55
1:0:1711:C:H4'	1:0:1712:G:C2	2.42	0.55
1:0:2168:A:H2'	1:0:2169:A:H5'	1.89	0.55
1:0:162:C:H4'	1:0:195:A:O2'	2.07	0.55
1:0:841:G:H3'	1:0:841:G:N3	2.21	0.55
1:0:33:C:N4	1:0:466:A:H61	2.05	0.55
1:0:2204:A:O2'	1:0:2205:C:P	2.65	0.55
1:0:951:G:C2'	1:0:952:A:H5''	2.36	0.55
1:0:1288:A:O2'	1:0:1289:A:H5'	2.07	0.55
1:0:1789:U:C2'	1:0:1790:G:H5'	2.37	0.55
1:0:1791:C:H1'	1:0:1793:A:O4'	2.06	0.55
1:0:775:U:H4'	1:0:776:G:C8	2.42	0.55
1:0:114:C:O2'	1:0:124:A:H1'	2.07	0.55
1:0:831:G:N2	1:0:1203:A:H62	1.97	0.54
1:0:80:A:H2'	1:0:81:C:O4'	2.06	0.54
1:0:1922:U:H1'	1:0:2570:C:O2'	2.06	0.54
1:0:2571:G:H2'	1:0:2572:U:C6	2.42	0.54
1:0:2783:U:OP1	1:0:2783:U:O4'	2.25	0.54
1:0:782:U:H2'	1:0:783:G:C8	2.42	0.54
1:0:1141:U:H5'	1:0:2549:G:N2	2.22	0.54
1:0:67:G:H8	1:0:67:G:O5'	1.90	0.54
1:0:1289:A:H62	1:0:1662:G:H1	1.55	0.54
1:0:1278:A:O2'	1:0:1279:G:P	2.65	0.54
1:0:166:G:H21	1:0:184:A:N6	1.93	0.54
1:0:2854:G:H3'	1:0:2854:G:N3	2.22	0.54
1:0:1982:C:H1'	1:0:2666:U:O2'	2.07	0.54
1:0:791:G:H2'	1:0:792:U:C6	2.42	0.54
1:0:1925:C:H5''	2:5:30:C:H4'	1.88	0.54
1:0:1004:A:H2'	1:0:1005:U:H5''	1.88	0.54
1:0:1829:C:H2'	1:0:1830:C:H5'	1.90	0.54
1:0:1746:A:C2'	1:0:1747:G:H5'	2.37	0.54
1:0:1955:G:C2'	1:0:1956:G:H5'	2.37	0.54
1:0:1313:U:O2'	1:0:1314:A:P	2.66	0.54
1:0:2758:A:H5''	1:0:2759:U:H5	1.72	0.54
1:0:1279:G:C2'	1:0:1280:U:OP2	2.56	0.54
1:0:1921:A:H2'	1:0:1922:U:H5''	1.90	0.54
1:0:646:C:H2'	1:0:647:G:O4'	2.07	0.54
1:0:558:G:H5''	1:0:559:C:C5	2.42	0.54
1:0:2426:G:N2	1:0:2430:A:H62	2.04	0.54
1:0:69:G:H3'	1:0:111:G:O2'	2.08	0.54
1:0:564:U:H2'	1:0:565:A:C8	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1210:C:H2'	1:0:1211:G:O4'	2.08	0.54
1:0:1818:G:H2'	1:0:1819:U:C6	2.42	0.54
1:0:598:U:H2'	1:0:599:A:C8	2.42	0.54
1:0:2516:U:H2'	1:0:2517:C:C6	2.42	0.54
1:0:2470:U:O2'	1:0:2471:U:H5'	2.08	0.54
1:0:798:G:O2'	1:0:1770:U:H4'	2.08	0.54
1:0:177:U:H2'	1:0:178:C:C6	2.43	0.54
1:0:1356:G:H5'	1:0:1614:C:OP2	2.08	0.54
1:0:1463:A:H2'	1:0:1464:A:C8	2.42	0.54
1:0:2249:U:H2'	1:0:2250:G:O4'	2.08	0.54
1:0:2466:G:H2'	1:0:2467:A:C8	2.43	0.54
1:0:67:G:N2	1:0:73:A:O5'	2.40	0.54
1:0:468:A:H2'	1:0:469:G:H4'	1.90	0.54
1:0:942:U:O2'	1:0:943:U:H5'	2.08	0.54
1:0:847:C:N4	1:0:955:G:H21	1.96	0.54
1:0:484:G:O2'	1:0:485:G:H5'	2.07	0.54
1:0:1664:G:H4'	1:0:1665:C:O5'	2.07	0.54
1:0:2319:G:H2'	1:0:2320:G:C8	2.43	0.54
1:0:2574:G:H1'	1:0:2576:G:O6	2.07	0.54
1:0:48:A:H4'	1:0:50:G:O4'	2.08	0.54
1:0:929:A:H3'	1:0:930:A:C5'	2.33	0.54
1:0:1789:U:O2'	1:0:1790:G:H5'	2.07	0.54
1:0:728:G:H2'	1:0:729:A:O4'	2.08	0.54
1:0:2437:G:H2'	1:0:2469:G:C2	2.43	0.53
1:0:878:C:N4	1:0:921:A:H62	2.04	0.53
1:0:216:U:H2'	1:0:217:U:O4'	2.08	0.53
1:0:1333:G:N2	1:0:1344:C:N4	2.55	0.53
1:0:2572:U:H2'	1:0:2573:C:C6	2.43	0.53
1:0:242:A:O2'	1:0:243:G:O5'	2.26	0.53
1:0:2780:A:O2'	1:0:2781:G:H5'	2.08	0.53
1:0:317:U:C3'	1:0:318:G:H5''	2.39	0.53
1:0:857:U:H2'	1:0:858:G:H5'	1.90	0.53
1:0:597:U:H3	1:0:683:A:H2'	1.73	0.53
1:0:1763:G:H2'	1:0:1764:A:H4'	1.89	0.53
1:0:830:C:O2'	1:0:852:U:H5''	2.08	0.53
1:0:1528:C:C3'	1:0:1529:C:H5''	2.38	0.53
1:0:1497:C:O2'	1:0:1498:G:H5'	2.08	0.53
1:0:1358:C:H2'	1:0:1359:G:C5'	2.38	0.53
1:0:341:A:H1'	1:0:1223:G:O6	2.08	0.53
1:0:832:A:H2'	1:0:833:A:O4'	2.07	0.53
1:0:126:C:H2'	1:0:127:C:C6	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:917:U:H2'	1:0:918:A:O4'	2.08	0.53
1:0:1900:U:H4'	1:0:1946:U:O4'	2.09	0.53
1:0:2321:C:O2'	1:0:2353:G:H5''	2.09	0.53
1:0:1971:C:H2'	1:0:1972:G:C8	2.43	0.53
1:0:1414:G:H2'	1:0:1415:C:C6	2.43	0.53
1:0:594:G:H21	1:0:1267:A:H62	1.57	0.53
1:0:918:A:C2'	1:0:919:U:H5''	2.36	0.53
1:0:173:A:O2'	1:0:174:A:OP1	2.20	0.53
1:0:2756:A:H1'	1:0:2758:A:N7	2.23	0.53
1:0:1838:G:C2'	1:0:1839:A:H5'	2.39	0.53
1:0:1974:U:H2'	1:0:1975:G:H5''	1.89	0.53
1:0:1301:U:H2'	1:0:1664:G:H21	1.73	0.53
1:0:393:U:H2'	1:0:394:U:C6	2.43	0.53
1:0:1825:C:C2'	1:0:1826:U:H5'	2.38	0.53
1:0:638:A:O2'	1:0:639:G:H5'	2.08	0.53
1:0:737:C:H2'	1:0:738:G:O4'	2.09	0.53
1:0:665:A:OP2	1:0:666:U:H5'	2.09	0.53
1:0:1976:U:C2'	1:0:1977:C:H5'	2.37	0.53
1:0:404:A:H2'	1:0:405:C:C6	2.43	0.53
1:0:26:G:H21	1:0:524:A:N6	2.03	0.53
1:0:2700:U:N3	1:0:2848:A:N6	2.55	0.53
1:0:1190:C:H2'	1:0:1191:G:C8	2.44	0.53
1:0:1029:C:H2'	1:0:1030:U:H5''	1.91	0.53
1:0:1326:U:H2'	1:0:1327:C:H5'	1.90	0.53
1:0:2498:U:H5''	1:0:2499:C:OP1	2.09	0.53
1:0:1576:G:H2'	1:0:1577:G:O4'	2.08	0.53
1:0:939:C:H2'	1:0:940:G:C8	2.44	0.53
1:0:874:A:H62	1:0:928:G:N2	2.07	0.53
1:0:757:U:O2'	1:0:758:G:H5'	2.09	0.53
1:0:1075:C:H2'	1:0:1076:U:O4'	2.09	0.53
1:0:1745:C:H2'	1:0:1746:A:O4'	2.09	0.53
1:0:486:U:H4'	1:0:520:C:H5'	1.90	0.53
1:0:2312:A:H1'	1:0:2314:A:C8	2.44	0.53
1:0:77:C:H2'	1:0:78:C:C6	2.44	0.53
1:0:658:G:H4'	1:0:2331:A:H5'	1.91	0.53
1:0:960:U:H2'	1:0:961:G:C8	2.44	0.53
1:0:541:C:N4	1:0:572:G:O4'	2.42	0.53
1:0:807:A:H2'	1:0:808:C:C6	2.44	0.53
1:0:843:G:O2'	1:0:844:G:H5'	2.09	0.53
1:0:2728:A:H2'	1:0:2729:A:O4'	2.09	0.53
1:0:394:U:H2'	1:0:395:G:C8	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:788:G:H5'	1:0:790:A:H1'	1.90	0.53
1:0:1775:A:H4'	1:0:1776:A:C8	2.44	0.53
1:0:2229:G:H2'	1:0:2475:C:OP1	2.09	0.52
1:0:2014:A:H62	1:0:2477:C:H1'	1.74	0.52
1:0:2483:U:H1'	1:0:2551:A:H2	1.74	0.52
1:0:201:G:H2'	1:0:202:A:C8	2.44	0.52
1:0:1502:G:O2'	1:0:1503:G:H5'	2.09	0.52
1:0:55:A:H2'	1:0:56:C:H6	1.75	0.52
2:5:31:C:H3'	2:5:32:A:C5'	2.34	0.52
1:0:127:C:H2'	1:0:128:C:C6	2.44	0.52
1:0:1938:U:C2'	1:0:1939:U:H5'	2.39	0.52
1:0:1566:G:H4'	1:0:1733:U:O4	2.09	0.52
1:0:1217:U:H2'	1:0:1218:C:C6	2.44	0.52
1:0:870:C:H2'	1:0:871:U:C6	2.43	0.52
1:0:1964:A:H5''	1:0:1965:U:OP2	2.08	0.52
1:0:1365:U:H1'	1:0:1586:A:H2	1.74	0.52
1:0:688:A:O2'	1:0:2422:C:H4'	2.09	0.52
1:0:230:C:H2'	1:0:231:G:O4'	2.09	0.52
1:0:1313:U:O4	1:0:1651:U:H5'	2.09	0.52
1:0:2401:A:H2'	1:0:2403:C:C5	2.44	0.52
1:0:181:A:H4'	1:0:182:G:C4'	2.39	0.52
1:0:1286:U:H5''	1:0:1663:C:N4	2.24	0.52
1:0:2809:A:C2'	1:0:2810:A:H5'	2.40	0.52
1:0:167:A:H2'	1:0:168:A:C8	2.44	0.52
1:0:597:U:H2'	1:0:598:U:C6	2.44	0.52
1:0:599:A:H2'	1:0:600:G:C8	2.44	0.52
1:0:1654:A:H2'	1:0:1655:C:C6	2.44	0.52
1:0:689:A:N3	1:0:689:A:H3'	2.24	0.52
1:0:225:G:N2	1:0:2410:U:H1'	2.24	0.52
1:0:9:U:H3	1:0:2608:A:N6	2.02	0.52
1:0:2083:G:H2'	1:0:2084:G:O4'	2.10	0.52
1:0:1970:G:H2'	1:0:1971:C:C6	2.44	0.52
1:0:212:U:H2'	1:0:213:C:C6	2.45	0.52
1:0:1312:G:C5'	1:0:1313:U:H5'	2.34	0.52
1:0:2057:U:O2'	1:0:2576:G:H1'	2.09	0.52
1:0:1234:C:H2'	1:0:1235:C:C6	2.45	0.52
1:0:446:C:H2'	1:0:447:U:C6	2.45	0.52
1:0:38:G:H2'	1:0:39:C:C6	2.44	0.52
1:0:688:A:H1'	1:0:2423:G:H5'	1.92	0.52
1:0:2059:U:H2'	1:0:2060:A:H5''	1.90	0.52
1:0:2757:G:OP2	1:0:2761:A:H4'	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:616:U:C2'	1:0:617:U:H5''	2.37	0.52
1:0:1162:A:H2'	1:0:1163:C:C6	2.44	0.52
1:0:1288:A:H2'	1:0:1289:A:O4'	2.09	0.52
1:0:2372:A:H2'	1:0:2373:C:C6	2.44	0.52
1:0:2440:C:H1'	1:0:2471:U:N3	2.25	0.52
2:5:33:C:H3'	2:5:34:C:H5'	1.92	0.52
1:0:795:A:H4'	1:0:796:A:C8	2.44	0.52
1:0:1263:G:O2'	1:0:1264:C:OP1	2.27	0.52
1:0:317:U:C2'	1:0:318:G:H5''	2.39	0.52
1:0:776:G:N3	1:0:776:G:H2'	2.25	0.52
1:0:95:G:H2'	1:0:96:C:C6	2.45	0.52
1:0:2272:A:H2'	1:0:2273:C:C6	2.45	0.52
1:0:476:G:H2'	1:0:477:A:C8	2.45	0.52
1:0:2504:G:H2'	1:0:2505:G:C8	2.45	0.52
1:0:215:G:O2'	1:0:617:U:H1'	2.09	0.52
1:0:45:C:H5''	1:0:192:G:C8	2.44	0.52
1:0:168:A:H2'	1:0:169:C:C6	2.45	0.52
1:0:980:G:H2'	1:0:981:C:C6	2.45	0.52
1:0:333:A:H1'	1:0:351:A:C4	2.44	0.52
1:0:2451:G:H2'	1:0:2508:G:N2	2.25	0.52
1:0:2320:G:H2'	1:0:2321:C:O4'	2.09	0.52
1:0:1597:A:H2'	1:0:1598:C:C6	2.45	0.52
1:0:129:A:H2'	1:0:130:C:C6	2.45	0.51
1:0:2756:A:H4'	1:0:2758:A:OP1	2.09	0.51
1:0:491:A:H2'	1:0:491:A:N3	2.26	0.51
1:0:1677:C:H2'	1:0:1678:G:C8	2.45	0.51
1:0:2536:G:H2'	1:0:2537:C:C6	2.45	0.51
1:0:590:C:H2'	1:0:591:G:C8	2.45	0.51
1:0:2623:A:H2'	1:0:2624:G:O4'	2.10	0.51
1:0:1788:C:H2'	1:0:1789:U:C6	2.46	0.51
1:0:2160:C:H2'	1:0:2161:C:C6	2.46	0.51
1:0:1358:C:H2'	1:0:1359:G:H5''	1.92	0.51
1:0:959:C:H5''	1:0:972:C:O2'	2.11	0.51
1:0:578:U:C1'	1:0:957:G:H21	2.22	0.51
1:0:826:U:H2'	1:0:827:C:C6	2.46	0.51
1:0:170:U:H2'	1:0:171:G:H8	1.75	0.51
1:0:1661:C:O2'	1:0:1662:G:H5'	2.10	0.51
1:0:1352:G:H2'	1:0:1353:A:C8	2.43	0.51
1:0:1819:U:H5''	1:0:1954:A:O3'	2.11	0.51
1:0:2660:C:O2'	1:0:2661:G:H5'	2.11	0.51
1:0:2213:G:H2'	1:0:2214:G:C8	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2426:G:O2'	1:0:2427:A:P	2.69	0.51
1:0:1018:C:H2'	1:0:1019:U:C5	2.45	0.51
1:0:1860:A:H2'	1:0:1861:G:O4'	2.11	0.51
1:0:1865:C:H2'	1:0:1866:G:O4'	2.10	0.51
1:0:451:A:H2'	1:0:452:G:C8	2.45	0.51
1:0:223:C:H4'	1:0:398:C:H1'	1.92	0.51
1:0:2703:C:H2'	1:0:2704:U:C6	2.45	0.51
1:0:2429:A:H5''	1:0:2476:A:C6	2.46	0.51
1:0:512:A:H2'	1:0:513:A:H5'	1.93	0.51
1:0:2242:C:N4	1:0:2257:A:N6	2.58	0.51
1:0:18:U:H2'	1:0:19:C:C6	2.45	0.51
1:0:838:A:H2'	1:0:839:U:C6	2.46	0.51
1:0:742:G:H2'	1:0:1766:U:H1'	1.93	0.51
1:0:422:C:H2'	1:0:423:G:H8	1.76	0.51
1:0:1377:G:H4'	1:0:1800:A:H5'	1.93	0.51
1:0:868:U:H2'	1:0:869:C:C6	2.45	0.51
1:0:1881:U:H2'	1:0:1882:G:H5'	1.93	0.51
1:0:1926:U:H1'	1:0:1928:G:H5'	1.93	0.51
1:0:158:A:H2'	1:0:159:A:O4'	2.10	0.51
1:0:1727:C:H4'	1:0:2833:C:O2	2.10	0.51
1:0:941:U:H4'	1:0:941:U:OP1	2.10	0.51
1:0:689:A:N6	1:0:815:A:H61	2.05	0.51
1:0:2725:C:H2'	1:0:2726:U:C6	2.46	0.51
1:0:824:U:H1'	1:0:1264:C:H1'	1.92	0.51
1:0:1067:G:H2'	1:0:1114:A:H61	1.76	0.51
1:0:2574:G:N7	1:0:2578:G:N2	2.59	0.51
1:0:210:A:N6	1:0:242:A:N7	2.59	0.51
1:0:1038:U:O2	1:0:2466:G:H4'	2.10	0.51
1:0:1127:C:H2'	1:0:1128:G:H8	1.76	0.51
1:0:1068:A:H2'	1:0:1069:G:C8	2.45	0.51
1:0:1611:U:H2'	1:0:1612:U:O4'	2.11	0.51
1:0:703:A:H2'	1:0:704:G:H8	1.76	0.51
1:0:1092:U:H2'	1:0:1093:U:C6	2.45	0.51
1:0:1626:A:OP2	1:0:1627:C:H5	1.95	0.50
1:0:1279:G:H1'	1:0:1280:U:H5	1.76	0.50
1:0:243:G:H2'	1:0:244:C:O4'	2.12	0.50
1:0:114:C:H2'	1:0:115:G:O4'	2.11	0.50
1:0:788:G:H5'	1:0:790:A:N3	2.26	0.50
1:0:2177:U:H2'	1:0:2178:U:C6	2.46	0.50
1:0:1052:C:H2'	1:0:1053:G:C8	2.45	0.50
1:0:1057:A:H3'	1:0:1058:G:C5'	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:457:C:H2'	1:0:458:G:O4'	2.11	0.50
1:0:619:A:H2'	1:0:620:G:C8	2.46	0.50
1:0:2821:G:H2'	1:0:2822:U:C6	2.46	0.50
1:0:14:A:H2	1:0:2604:G:HO2'	1.59	0.50
1:0:1861:G:O2'	1:0:1862:C:H5'	2.11	0.50
1:0:2178:U:H2'	1:0:2179:C:C6	2.46	0.50
1:0:1424:U:H2'	1:0:1425:G:C8	2.46	0.50
1:0:2397:A:H2'	1:0:2398:U:O4'	2.11	0.50
1:0:2771:C:H2'	1:0:2772:U:C6	2.46	0.50
1:0:1198:C:C5'	1:0:1199:U:H5''	2.42	0.50
1:0:2727:G:C2'	1:0:2728:A:H5''	2.41	0.50
1:0:534:U:H4'	1:0:564:U:O2'	2.12	0.50
1:0:116:A:N3	1:0:155:G:H1'	2.26	0.50
1:0:688:A:HO2'	1:0:2422:C:H4'	1.76	0.50
1:0:1747:G:C4'	1:0:1749:G:H1'	2.31	0.50
1:0:964:A:H2'	1:0:965:G:C8	2.46	0.50
1:0:2238:G:H2'	1:0:2239:C:H6	1.76	0.50
1:0:879:A:O2'	1:0:880:C:H5'	2.11	0.50
1:0:2726:U:H2'	1:0:2727:G:O4'	2.12	0.50
1:0:2023:C:H2'	1:0:2024:U:C6	2.46	0.50
1:0:2329:C:C2'	1:0:2330:G:H5'	2.42	0.50
1:0:332:C:H2'	1:0:333:A:H5'	1.94	0.50
1:0:1857:G:H2'	1:0:1859:A:OP2	2.12	0.50
1:0:1073:G:H2'	1:0:1074:G:C4'	2.29	0.50
1:0:2181:A:H2'	1:0:2182:A:H5'	1.92	0.50
1:0:872:G:H2'	1:0:928:G:N1	2.27	0.50
1:0:841:G:N1	1:0:2226:A:H4'	2.27	0.50
1:0:1029:C:OP1	1:0:1047:G:H4'	2.11	0.50
1:0:1683:G:C2'	1:0:1684:G:H5'	2.42	0.50
1:0:216:U:H5''	1:0:601:A:N6	2.27	0.50
1:0:316:C:H2'	1:0:317:U:C6	2.47	0.50
1:0:1218:C:H2'	1:0:1219:C:C6	2.46	0.50
1:0:2010:G:H2'	1:0:2011:U:O4'	2.12	0.50
1:0:1496:G:H5'	1:0:1575:C:N4	2.26	0.50
1:0:2082:C:H2'	1:0:2083:G:O4'	2.11	0.50
1:0:1164:C:H2'	1:0:1165:G:O4'	2.11	0.50
1:0:1194:U:O2'	1:0:1195:U:P	2.70	0.50
1:0:35:G:C1'	1:0:466:A:H1'	2.41	0.50
1:0:2754:C:H2'	1:0:2755:A:O4'	2.12	0.50
1:0:1259:A:H2'	1:0:1260:A:C8	2.47	0.50
1:0:158:A:H2'	1:0:159:A:C8	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1007:A:H2'	1:0:1008:G:C8	2.47	0.50
1:0:2446:C:H2'	1:0:2447:G:C8	2.47	0.50
1:0:1667:A:H2'	1:0:1668:G:H8	1.77	0.50
1:0:2435:C:H2'	1:0:2436:U:C6	2.47	0.50
1:0:236:C:O2	1:0:632:A:H1'	2.11	0.50
1:0:1895:A:H2'	1:0:1896:A:O4'	2.12	0.50
1:0:2079:A:H2'	1:0:2080:U:C6	2.47	0.50
1:0:2404:A:H5''	1:0:2405:A:H3'	1.94	0.50
1:0:860:U:H2'	1:0:861:G:H5'	1.94	0.50
1:0:599:A:H2'	1:0:600:G:H8	1.76	0.50
1:0:991:A:H61	1:0:2020:G:H21	1.59	0.49
1:0:1029:C:C3'	1:0:1030:U:H5''	2.42	0.49
1:0:1016:C:H2'	1:0:1017:C:C6	2.47	0.49
1:0:1310:C:OP1	1:0:2689:C:H4'	2.12	0.49
1:0:689:A:C2'	1:0:690:A:H5'	2.42	0.49
1:0:1791:C:H2'	1:0:1792:C:H5''	1.94	0.49
1:0:1380:C:N4	1:0:1799:A:N1	2.61	0.49
1:0:597:U:N3	1:0:683:A:H2'	2.27	0.49
1:0:1055:A:N6	1:0:1122:A:H4'	2.27	0.49
1:0:338:G:O2'	1:0:339:U:H5'	2.13	0.49
1:0:1492:A:H2	1:0:1531:C:H41	1.58	0.49
1:0:1312:G:H2'	1:0:1643:A:N6	2.27	0.49
1:0:831:G:C2'	1:0:832:A:H5''	2.42	0.49
1:0:460:U:N3	1:0:592:G:H1'	2.22	0.49
1:0:190:A:H2'	1:0:191:G:C8	2.47	0.49
1:0:538:A:C2'	1:0:539:A:H5''	2.41	0.49
1:0:2313:G:H2'	1:0:2314:A:H5'	1.94	0.49
1:0:1354:A:H3'	1:0:1410:U:O2	2.12	0.49
1:0:1820:G:O2'	1:0:1821:A:P	2.70	0.49
1:0:991:A:N6	1:0:2020:G:H21	2.11	0.49
1:0:165:G:H2'	1:0:166:G:O4'	2.12	0.49
1:0:2805:G:O2'	1:0:2806:G:H5'	2.12	0.49
1:0:1195:U:H2'	1:0:1196:G:H8	1.73	0.49
1:0:1979:C:H42	1:0:2706:U:H6	1.60	0.49
1:0:1889:G:H2'	1:0:1890:G:C8	2.48	0.49
1:0:441:A:H2'	1:0:442:A:O4'	2.11	0.49
1:0:2532:G:H1'	1:0:2561:G:N3	2.28	0.49
1:0:1055:A:O2'	1:0:1058:G:H1'	2.13	0.49
1:0:579:G:H2'	1:0:2013:A:N6	2.27	0.49
1:0:810:U:H2'	1:0:811:G:C8	2.48	0.49
1:0:2299:A:H2'	1:0:2299:A:N3	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:215:G:H4'	1:0:617:U:O2'	2.12	0.49
1:0:1685:A:H1'	1:0:1686:A:N7	2.28	0.49
1:0:1455:C:H2'	1:0:1456:C:C6	2.48	0.49
1:0:792:U:H2'	1:0:793:G:O4'	2.12	0.49
1:0:645:G:H2'	1:0:646:C:C6	2.48	0.49
1:0:693:A:H2'	1:0:694:G:C8	2.47	0.49
1:0:2244:C:N4	1:0:2245:A:N6	2.59	0.49
1:0:459:A:H62	1:0:484:G:H1'	1.78	0.49
1:0:1686:A:H2'	1:0:1687:C:H5'	1.94	0.49
1:0:1685:A:C6	1:0:1691:G:H1'	2.48	0.49
1:0:45:C:H2'	1:0:46:C:C6	2.47	0.49
1:0:2235:G:H2'	1:0:2236:U:C6	2.48	0.49
1:0:780:U:H2'	1:0:781:G:C8	2.48	0.49
1:0:431:G:H2'	1:0:432:C:C6	2.47	0.49
1:0:2428:U:O2'	1:0:2429:A:H5'	2.12	0.49
1:0:1793:A:H2'	1:0:1794:A:C8	2.48	0.49
1:0:2057:U:H1'	1:0:2577:A:H1'	1.93	0.49
1:0:1445:A:H2'	1:0:1446:U:O4'	2.13	0.49
1:0:2161:C:O2'	1:0:2162:C:P	2.71	0.49
1:0:338:G:H1	1:0:346:C:H42	1.60	0.49
1:0:2799:C:H2'	1:0:2800:C:O4'	2.12	0.49
1:0:1912:G:H2'	1:0:1912:G:N3	2.27	0.49
1:0:2794:G:H3'	1:0:2796:A:N6	2.20	0.49
1:0:1807:A:HO2'	1:0:1808:C:P	2.35	0.49
1:0:1679:U:H2'	1:0:1680:U:H5''	1.94	0.49
1:0:1665:C:N4	1:0:1993:G:H1	2.11	0.49
1:0:1259:A:H2'	1:0:1260:A:O4'	2.12	0.49
1:0:1785:A:H2'	1:0:1786:C:C6	2.47	0.49
1:0:2026:C:H2'	1:0:2027:C:C6	2.47	0.49
1:0:109:A:H3'	1:0:110:U:C5'	2.39	0.49
1:0:172:A:H4'	1:0:228:A:H4'	1.94	0.49
1:0:930:A:H5'	1:0:931:G:C8	2.47	0.49
1:0:951:G:C3'	1:0:952:A:H5''	2.43	0.49
1:0:2503:G:C2'	1:0:2504:G:H5''	2.43	0.49
1:0:203:G:O2'	1:0:204:A:H5'	2.13	0.49
1:0:83:A:C6	1:0:98:U:H1'	2.47	0.49
1:0:860:U:O2'	1:0:861:G:H5'	2.13	0.49
1:0:2574:G:H2'	1:0:2574:G:N3	2.28	0.49
1:0:1825:C:O2'	1:0:1826:U:H5'	2.13	0.49
1:0:211:U:O2'	1:0:212:U:H5'	2.13	0.49
1:0:2093:G:H2'	1:0:2094:C:C6	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1141:U:O2'	1:0:1142:G:OP1	2.26	0.49
1:0:58:C:N4	1:0:73:A:C6	2.81	0.49
1:0:1182:U:C3'	1:0:1183:C:H5''	2.43	0.49
1:0:1046:U:H2'	1:0:1047:G:C8	2.48	0.49
1:0:632:A:C2'	1:0:633:G:H5'	2.43	0.49
1:0:1729:C:H2'	1:0:1730:G:C8	2.48	0.49
1:0:2783:U:H2'	1:0:2784:A:O4'	2.12	0.49
1:0:1272:G:H2'	1:0:1273:G:C8	2.48	0.49
1:0:1038:U:H2'	1:0:1039:A:C8	2.48	0.49
1:0:476:G:H21	1:0:696:U:H1'	1.78	0.49
1:0:1598:C:H2'	1:0:1599:G:O4'	2.13	0.49
1:0:173:A:H61	1:0:844:G:H21	1.59	0.48
1:0:2308:A:H2'	1:0:2309:G:C8	2.47	0.48
1:0:84:G:H2'	1:0:85:C:C6	2.48	0.48
1:0:790:A:H2'	1:0:791:G:C8	2.48	0.48
1:0:1040:A:H2'	1:0:1041:G:H5'	1.93	0.48
1:0:1435:G:H21	1:0:1511:A:N6	2.12	0.48
1:0:1349:A:H2'	1:0:1350:G:C8	2.48	0.48
1:0:2852:G:H2'	1:0:2853:U:O4'	2.13	0.48
1:0:1937:G:N3	1:0:2530:C:H5'	2.28	0.48
1:0:109:A:C2'	1:0:110:U:H5''	2.43	0.48
1:0:521:U:H2'	1:0:522:G:H5'	1.95	0.48
1:0:1715:A:H1'	1:0:1717:A:C1'	2.42	0.48
1:0:1871:G:C2'	1:0:1871:G:N3	2.76	0.48
1:0:565:A:H2'	1:0:566:U:C6	2.48	0.48
1:0:2025:A:H2'	1:0:2026:C:H5''	1.94	0.48
1:0:1629:G:N1	1:0:1633:C:N4	2.61	0.48
1:0:626:A:O2'	1:0:627:A:H5'	2.13	0.48
1:0:942:U:C2'	1:0:943:U:H5'	2.43	0.48
1:0:864:C:H2'	1:0:865:A:C8	2.47	0.48
1:0:427:C:H2'	1:0:428:A:C8	2.49	0.48
1:0:1099:A:H5''	1:0:1100:G:N7	2.27	0.48
1:0:2872:U:H2'	1:0:2873:G:C8	2.49	0.48
1:0:1495:G:HO2'	1:0:1496:G:P	2.36	0.48
1:0:1571:G:H2'	1:0:1572:C:C6	2.48	0.48
1:0:367:G:C3'	1:0:368:A:H5''	2.43	0.48
1:0:1033:G:H22	1:0:1150:C:C2'	2.26	0.48
1:0:1712:G:N3	1:0:1712:G:H3'	2.29	0.48
1:0:756:C:H2'	1:0:757:U:C6	2.48	0.48
1:0:2780:A:H2'	1:0:2781:G:C8	2.48	0.48
1:0:429:C:H2'	1:0:430:C:O4'	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2093:G:O2'	1:0:2094:C:P	2.72	0.48
1:0:2343:C:H2'	1:0:2344:G:O4'	2.14	0.48
1:0:2301:A:H2'	1:0:2302:G:O4'	2.14	0.48
1:0:2483:U:H2'	1:0:2484:G:H5'	1.94	0.48
1:0:830:C:O2	1:0:852:U:H4'	2.13	0.48
1:0:2059:U:H5	1:0:2575:U:N3	2.02	0.48
1:0:192:G:C4'	1:0:193:A:H4'	2.44	0.48
1:0:1678:G:H2'	1:0:1679:U:C6	2.48	0.48
1:0:210:A:N6	1:0:442:A:H61	2.11	0.48
1:0:1742:G:H2'	1:0:1743:C:C6	2.48	0.48
1:0:42:G:H2'	1:0:43:A:O4'	2.13	0.48
1:0:1141:U:O2'	1:0:1142:G:P	2.72	0.48
1:0:71:A:O2'	1:0:72:A:OP1	2.21	0.48
1:0:181:A:H4'	1:0:182:G:O5'	2.12	0.48
1:0:1458:A:H3'	1:0:1459:U:H5'	1.96	0.48
1:0:2721:A:N6	1:0:2743:G:H21	2.10	0.48
1:0:1686:A:O2'	1:0:2528:G:H5'	2.14	0.48
1:0:742:G:N3	1:0:742:G:C2'	2.77	0.48
1:0:635:C:H3'	1:0:636:G:H5''	1.95	0.48
1:0:477:A:H2'	1:0:478:G:O4'	2.14	0.48
1:0:2212:U:H2'	1:0:2213:G:C8	2.49	0.48
1:0:2815:C:H2'	1:0:2816:C:C6	2.49	0.48
1:0:548:G:H2'	1:0:549:G:C8	2.48	0.48
1:0:845:U:H2'	1:0:846:A:C8	2.49	0.48
1:0:569:C:H2'	1:0:570:G:C8	2.49	0.48
1:0:583:C:O2'	1:0:584:A:OP2	2.31	0.48
1:0:64:C:H2'	1:0:65:C:C6	2.48	0.48
1:0:2503:G:H2'	1:0:2504:G:H5''	1.96	0.48
1:0:1684:G:H2'	1:0:1974:U:O4	2.14	0.48
1:0:1391:A:H2'	1:0:1392:U:C5	2.49	0.48
1:0:213:C:H42	1:0:238:G:H22	1.60	0.48
1:0:2085:G:H2'	1:0:2086:U:C6	2.49	0.48
1:0:2580:C:N4	1:0:2582:G:O6	2.47	0.48
1:0:1436:G:H2'	1:0:1437:A:C8	2.49	0.48
1:0:1429:A:H1'	1:0:1603:A:C6	2.49	0.48
1:0:478:G:O2'	1:0:479:G:H5'	2.14	0.48
1:0:240:U:H4'	1:0:443:A:H5'	1.96	0.48
1:0:582:G:H2'	1:0:583:C:H3'	1.96	0.48
1:0:583:C:O2'	1:0:584:A:P	2.71	0.48
1:0:239:A:H4'	1:0:620:G:H5'	1.95	0.48
1:0:2377:U:O2'	1:0:2378:G:P	2.72	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:568:G:H5''	1:0:1019:U:H5'	1.96	0.48
1:0:192:G:H4'	1:0:193:A:O5'	2.13	0.48
1:0:1682:A:H2'	1:0:1683:G:C8	2.48	0.48
1:0:323:G:H2'	1:0:324:C:C6	2.48	0.48
1:0:629:C:H2'	1:0:630:G:H5'	1.95	0.48
1:0:979:A:H2'	1:0:980:G:C8	2.49	0.48
1:0:1036:G:H1'	1:0:1145:C:C4'	2.44	0.48
1:0:1316:G:H2'	1:0:1317:G:C8	2.49	0.48
1:0:1031:C:H1'	1:0:1151:U:O2	2.14	0.48
1:0:2316:G:H2'	1:0:2317:G:H8	1.78	0.48
1:0:2437:G:H4'	1:0:2438:A:N7	2.28	0.48
1:0:2220:A:H2'	1:0:2221:G:C8	2.49	0.48
1:0:941:U:H2'	1:0:942:U:C6	2.49	0.47
1:0:2483:U:H1'	1:0:2551:A:C2	2.49	0.47
1:0:2424:G:H2'	1:0:2425:G:O4'	2.14	0.47
1:0:664:C:H2'	1:0:665:A:C8	2.49	0.47
1:0:1679:U:C2'	1:0:1680:U:H5''	2.44	0.47
1:0:2204:A:O2'	1:0:2205:C:OP2	2.32	0.47
1:0:2782:G:C2'	1:0:2783:U:OP1	2.62	0.47
1:0:703:A:H2'	1:0:704:G:C8	2.49	0.47
1:0:1471:G:H1	1:0:2682:C:H42	1.61	0.47
1:0:224:G:C5	1:0:226:C:H1'	2.48	0.47
1:0:873:U:O2	1:0:2246:A:H5''	2.14	0.47
1:0:204:A:H4'	1:0:205:A:N7	2.29	0.47
1:0:1793:A:H2'	1:0:1794:A:H8	1.79	0.47
1:0:2402:U:H5'	1:0:2404:A:N7	2.29	0.47
1:0:1926:U:O2'	1:0:1927:U:H3'	2.14	0.47
1:0:780:U:H2'	1:0:781:G:H8	1.79	0.47
1:0:2830:U:H2'	1:0:2831:A:C8	2.49	0.47
1:0:2168:A:C2'	1:0:2169:A:H5'	2.44	0.47
1:0:2448:A:H2'	1:0:2449:G:O4'	2.13	0.47
1:0:2651:U:H2'	1:0:2652:G:C8	2.49	0.47
1:0:2002:A:H61	1:0:2018:G:H21	1.62	0.47
1:0:2421:C:O2'	1:0:2422:C:H5'	2.13	0.47
1:0:1016:C:H5''	1:0:1023:U:OP2	2.14	0.47
1:0:2523:G:O2'	1:0:2524:G:H5'	2.14	0.47
1:0:2708:U:H2'	1:0:2709:C:C6	2.49	0.47
1:0:1147:G:H2'	1:0:1148:G:C8	2.50	0.47
1:0:2009:U:H2'	1:0:2010:G:C8	2.49	0.47
1:0:2434:G:H2'	1:0:2435:C:C6	2.50	0.47
1:0:974:U:H2'	1:0:975:C:C6	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1226:A:C6	1:0:1250:A:H1'	2.49	0.47
1:0:2432:A:H4'	1:0:2551:A:O2'	2.15	0.47
1:0:1436:G:C1'	1:0:1508:G:H21	2.21	0.47
1:0:1326:U:H1'	1:0:1626:A:N3	2.30	0.47
1:0:1344:C:H2'	1:0:1346:C:OP1	2.14	0.47
1:0:1993:G:H2'	1:0:1994:U:C6	2.50	0.47
1:0:2204:A:H1'	1:0:2205:C:C5	2.49	0.47
1:0:1386:A:H2'	1:0:1387:G:O4'	2.14	0.47
1:0:2494:C:H2'	1:0:2495:G:H8	1.80	0.47
1:0:108:G:H2'	1:0:109:A:C8	2.50	0.47
1:0:1915:A:N6	1:0:1951:G:H21	1.99	0.47
1:0:1436:G:H1'	1:0:1508:G:N2	2.18	0.47
1:0:1809:G:O2'	1:0:1810:U:H5'	2.14	0.47
1:0:2782:G:H2'	1:0:2783:U:OP1	2.15	0.47
1:0:452:G:H2'	1:0:453:U:O4'	2.15	0.47
1:0:2278:A:H2'	1:0:2279:G:C8	2.49	0.47
1:0:1316:G:H2'	1:0:1317:G:H8	1.79	0.47
1:0:2393:G:H2'	1:0:2394:G:H8	1.80	0.47
1:0:2426:G:H5'	1:0:2480:C:N4	2.23	0.47
1:0:70:A:P	1:0:111:G:H4'	2.55	0.47
1:0:225:G:H21	1:0:2410:U:H1'	1.78	0.47
1:0:926:C:H2'	1:0:927:C:H5'	1.95	0.47
1:0:2486:C:H4'	2:5:34:C:O2'	2.15	0.47
1:0:701:U:H1'	1:0:800:U:H5'	1.97	0.47
1:0:2199:C:H2'	1:0:2200:G:C8	2.48	0.47
1:0:2307:A:H2'	1:0:2308:A:C8	2.50	0.47
1:0:1028:G:H2'	1:0:1029:C:C6	2.50	0.47
1:0:2378:G:H2'	1:0:2379:G:H8	1.80	0.47
1:0:2021:G:H2'	1:0:2022:C:C6	2.50	0.47
1:0:635:C:C3'	1:0:636:G:H5''	2.45	0.47
1:0:1354:A:N6	1:0:1407:G:H22	2.11	0.47
1:0:670:U:H2'	1:0:671:A:C8	2.49	0.47
1:0:1821:A:H5''	1:0:1822:C:H5	1.80	0.47
1:0:2069:U:H2'	1:0:2070:G:C8	2.49	0.47
1:0:1184:G:H2'	1:0:1185:C:H5'	1.97	0.47
1:0:2429:A:O2'	1:0:2430:A:H5'	2.14	0.47
1:0:1495:G:H2'	1:0:1496:G:C8	2.50	0.47
1:0:2484:G:H21	1:0:2485:U:H5	1.63	0.47
1:0:819:C:H2'	1:0:820:U:C6	2.50	0.47
1:0:1290:A:H2'	1:0:1291:G:C8	2.50	0.47
1:0:2727:G:N1	1:0:2735:C:H5''	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1578:U:H2'	1:0:1579:G:C8	2.50	0.47
1:0:763:A:C2	1:0:765:C:H1'	2.49	0.47
1:0:643:A:H2'	1:0:644:A:C8	2.49	0.47
1:0:1821:A:H3'	1:0:1822:C:H6	1.80	0.47
1:0:432:C:H2'	1:0:433:G:H8	1.80	0.47
1:0:1418:C:H2'	1:0:1419:G:H8	1.79	0.47
1:0:1269:G:H2'	1:0:1270:C:C6	2.50	0.47
1:0:556:A:H2'	1:0:557:U:H5'	1.97	0.47
1:0:2329:C:N4	1:0:2361:G:H22	2.13	0.47
1:0:1039:A:H2'	1:0:1040:A:C8	2.49	0.47
1:0:1576:G:H8	1:0:1576:G:H5'	1.80	0.47
1:0:2211:U:H2'	1:0:2212:U:C6	2.50	0.47
1:0:2062:U:H4'	1:0:2412:A:H2	1.79	0.47
1:0:2658:A:H2'	1:0:2659:C:C6	2.50	0.47
1:0:2504:G:H2'	1:0:2505:G:H8	1.79	0.47
1:0:1263:G:O2'	1:0:1264:C:P	2.73	0.47
1:0:84:G:O2'	1:0:85:C:H5'	2.15	0.47
1:0:2559:U:C2'	1:0:2560:G:H5'	2.44	0.47
1:0:241:C:C2'	1:0:242:A:H5''	2.44	0.46
1:0:2444:C:O2'	1:0:2445:C:H5'	2.15	0.46
1:0:2276:C:O2	1:0:2301:A:H1'	2.15	0.46
1:0:771:C:H2'	1:0:772:G:H8	1.80	0.46
1:0:971:A:H2	1:0:2475:C:H1'	1.80	0.46
1:0:869:C:O2'	1:0:870:C:H5'	2.15	0.46
1:0:2858:A:H3'	1:0:2859:U:C5'	2.44	0.46
1:0:173:A:N6	1:0:844:G:H21	2.14	0.46
1:0:1480:G:H2'	1:0:1481:U:H5'	1.97	0.46
1:0:2324:G:C4'	1:0:2326:C:H5''	2.43	0.46
1:0:342:G:HO2'	1:0:343:A:P	2.38	0.46
1:0:758:G:N2	1:0:763:A:N1	2.62	0.46
1:0:776:G:N3	1:0:776:G:C2'	2.79	0.46
1:0:864:C:H2'	1:0:865:A:H8	1.80	0.46
1:0:986:A:H2'	1:0:987:G:H5'	1.97	0.46
1:0:2137:G:H2'	1:0:2138:U:C6	2.50	0.46
1:0:54:G:H2'	1:0:55:A:C8	2.50	0.46
1:0:1223:G:H4'	1:0:1224:A:O5'	2.15	0.46
1:0:878:C:O2'	1:0:879:A:P	2.72	0.46
1:0:1975:G:H4'	1:0:1976:U:H5	1.80	0.46
1:0:1949:A:H1'	1:0:2572:U:H4'	1.98	0.46
1:0:1829:C:C2'	1:0:1830:C:H5'	2.45	0.46
1:0:2526:U:H2'	1:0:2527:G:C8	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2717:G:H2'	1:0:2718:A:C8	2.51	0.46
1:0:152:G:O2'	1:0:153:A:H5'	2.15	0.46
1:0:1014:G:O2'	1:0:1015:U:H5'	2.15	0.46
1:0:2642:G:H2'	1:0:2643:G:O4'	2.16	0.46
1:0:2757:G:H5'	1:0:2761:A:H1'	1.97	0.46
1:0:1301:U:H2'	1:0:1664:G:N2	2.30	0.46
1:0:2035:G:H2'	1:0:2036:G:C8	2.46	0.46
1:0:758:G:H2'	1:0:759:C:H5'	1.97	0.46
1:0:1039:A:H2'	1:0:1040:A:H8	1.80	0.46
1:0:2372:A:H2'	1:0:2373:C:H6	1.79	0.46
1:0:546:A:H2'	1:0:547:U:C6	2.51	0.46
1:0:760:U:O2	1:0:1997:A:H1'	2.16	0.46
1:0:887:G:O2'	1:0:888:G:H5'	2.15	0.46
1:0:387:A:H2'	1:0:388:G:O4'	2.15	0.46
1:0:2809:A:H2'	1:0:2810:A:H5'	1.98	0.46
1:0:2825:A:H2'	1:0:2826:C:C6	2.50	0.46
1:0:738:G:H2'	1:0:739:G:O4'	2.14	0.46
1:0:337:G:H2'	1:0:338:G:C8	2.51	0.46
1:0:198:A:O2'	1:0:199:A:P	2.74	0.46
1:0:108:G:H2'	1:0:109:A:H8	1.81	0.46
1:0:798:G:H2'	1:0:799:C:H5'	1.97	0.46
1:0:9:U:H2'	1:0:10:A:C8	2.51	0.46
1:0:324:C:H2'	1:0:325:U:O4'	2.15	0.46
1:0:1069:G:O2'	1:0:1070:G:H5'	2.16	0.46
1:0:1760:G:H2'	1:0:1761:G:C8	2.50	0.46
1:0:1452:U:H5'	1:0:1532:A:O2'	2.15	0.46
1:0:2475:C:H2'	1:0:2476:A:H5'	1.97	0.46
1:0:584:A:H4'	1:0:2479:U:C5'	2.43	0.46
1:0:1572:C:C3'	1:0:1573:G:H5''	2.45	0.46
1:0:2807:U:C5	1:0:2859:U:H4'	2.51	0.46
1:0:1029:C:H3'	1:0:1030:U:H5''	1.96	0.46
1:0:2499:C:N4	1:0:2521:A:H2	2.11	0.46
1:0:1279:G:H2'	1:0:1280:U:OP2	2.16	0.46
1:0:2459:C:C2'	1:0:2460:G:H5'	2.45	0.46
1:0:1981:A:H2'	1:0:1982:C:C6	2.50	0.46
1:0:2800:C:H2'	1:0:2801:A:O4'	2.15	0.46
1:0:1836:C:H2'	1:0:1837:G:C8	2.50	0.46
1:0:636:G:H2'	1:0:637:G:H5'	1.97	0.46
1:0:694:G:H2'	1:0:695:G:H8	1.81	0.46
1:0:845:U:H2'	1:0:846:A:H8	1.80	0.46
1:0:1962:C:O2'	1:0:1963:G:H5'	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:697:G:C2'	1:0:698:A:H5'	2.46	0.46
1:0:2245:A:HO2'	1:0:2246:A:P	2.39	0.46
1:0:932:G:H2'	1:0:933:G:C8	2.51	0.46
1:0:918:A:H2'	1:0:919:U:C5'	2.42	0.46
1:0:777:A:H62	1:0:1766:U:H3	1.59	0.46
1:0:1427:G:C2'	1:0:1428:G:H5'	2.44	0.46
1:0:1429:A:N6	1:0:1602:G:H5'	2.31	0.46
1:0:85:C:O2'	1:0:86:U:H5'	2.16	0.46
1:0:19:C:H2'	1:0:20:C:C6	2.49	0.46
1:0:462:G:H2'	1:0:463:C:H5'	1.98	0.46
1:0:2698:G:H2'	1:0:2699:G:C8	2.51	0.46
1:0:2493:U:H2'	1:0:2494:C:C6	2.51	0.46
1:0:1495:G:O2'	1:0:1496:G:P	2.73	0.46
1:0:27:G:N2	1:0:522:G:HO2'	2.14	0.46
1:0:952:A:H2'	1:0:953:G:O4'	2.16	0.46
1:0:313:U:H2'	1:0:314:G:C8	2.50	0.46
1:0:1331:G:H2'	1:0:1332:G:C8	2.51	0.46
1:0:2570:C:H2'	1:0:2571:G:H8	1.81	0.46
1:0:2488:G:N2	1:0:2559:U:H1'	2.31	0.46
1:0:2161:C:H2'	1:0:2162:C:C6	2.50	0.46
1:0:161:U:H2'	1:0:162:C:C6	2.51	0.46
2:5:26:A:H2'	2:5:27:G:H8	1.80	0.46
1:0:1703:C:H2'	1:0:1704:G:O4'	2.16	0.46
1:0:2426:G:HO2'	1:0:2427:A:P	2.39	0.45
1:0:831:G:H5'	1:0:852:U:OP1	2.16	0.45
1:0:595:A:H2	1:0:822:G:N3	2.15	0.45
1:0:1685:A:N6	1:0:1691:G:H1'	2.31	0.45
1:0:1677:C:H2'	1:0:1678:G:H8	1.81	0.45
1:0:1380:C:C2'	1:0:1381:G:H5'	2.45	0.45
1:0:2574:G:N3	1:0:2574:G:C2'	2.79	0.45
1:0:331:U:H2'	1:0:332:C:H5''	1.97	0.45
1:0:2093:G:H2'	1:0:2094:C:C5	2.51	0.45
1:0:1835:C:H2'	1:0:1836:C:C6	2.51	0.45
1:0:697:G:O2'	1:0:698:A:H5'	2.16	0.45
1:0:207:U:H2'	1:0:208:C:C6	2.51	0.45
1:0:2333:A:H2'	1:0:2334:C:C6	2.52	0.45
1:0:2193:C:H2'	1:0:2194:A:O4'	2.16	0.45
1:0:2106:G:H2'	1:0:2107:G:C8	2.51	0.45
1:0:2017:U:O2'	1:0:2018:G:H5'	2.16	0.45
1:0:689:A:C8	1:0:2422:C:H1'	2.51	0.45
1:0:2668:U:O2'	1:0:2669:C:P	2.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1313:U:O2'	1:0:1314:A:O5'	2.32	0.45
1:0:2633:A:N6	1:0:2646:C:N4	2.63	0.45
1:0:1163:C:O2'	1:0:1164:C:H5'	2.15	0.45
1:0:1486:A:H2'	1:0:1487:C:C6	2.50	0.45
1:0:1888:C:H5''	1:0:1889:G:C5'	2.46	0.45
1:0:1278:A:H4'	1:0:1279:G:O5'	2.17	0.45
1:0:2560:G:N3	1:0:2560:G:H3'	2.31	0.45
1:0:1068:A:H2'	1:0:1069:G:H8	1.81	0.45
1:0:2136:G:H2'	1:0:2137:G:C8	2.51	0.45
1:0:199:A:H61	1:0:209:G:H1'	1.81	0.45
1:0:1120:C:H2'	1:0:2731:G:N2	2.31	0.45
1:0:246:C:N3	1:0:247:A:N6	2.64	0.45
1:0:2474:G:O2'	1:0:2475:C:H5'	2.15	0.45
1:0:931:G:O2'	1:0:932:G:H5'	2.16	0.45
1:0:2784:A:H3'	1:0:2785:A:C8	2.49	0.45
1:0:2628:C:H2'	1:0:2629:U:C6	2.52	0.45
1:0:2120:C:H2'	1:0:2121:U:O4'	2.17	0.45
1:0:2468:G:H2'	1:0:2469:G:O4'	2.17	0.45
1:0:2475:C:C2'	1:0:2476:A:H5'	2.46	0.45
1:0:2639:A:H2'	1:0:2640:G:O4'	2.16	0.45
1:0:130:C:H2'	1:0:131:C:C6	2.51	0.45
1:0:2403:C:H2'	1:0:2408:G:O2'	2.17	0.45
1:0:2259:G:H2'	1:0:2260:C:C6	2.52	0.45
1:0:489:A:N6	1:0:491:A:H62	2.14	0.45
1:0:1886:G:H2'	1:0:1887:G:C8	2.51	0.45
1:0:317:U:H3'	1:0:318:G:H5''	1.97	0.45
1:0:1429:A:O2'	1:0:1430:G:H4'	2.17	0.45
1:0:307:C:H2'	1:0:308:C:C6	2.52	0.45
1:0:1949:A:O2'	1:0:2572:U:H5'	2.17	0.45
1:0:2057:U:H2'	1:0:2058:U:C6	2.51	0.45
1:0:2824:C:H1'	1:0:2843:A:C2	2.51	0.45
1:0:2487:G:H4'	1:0:2533:U:O2'	2.15	0.45
1:0:2455:A:O2'	1:0:2456:U:H5'	2.17	0.45
1:0:560:G:H2'	1:0:561:U:C6	2.51	0.45
1:0:1659:G:H2'	1:0:1660:G:C8	2.51	0.45
1:0:40:U:H2'	1:0:41:G:C8	2.51	0.45
1:0:872:G:O2'	1:0:2247:A:N3	2.48	0.45
1:0:2676:G:H2'	1:0:2677:U:C6	2.51	0.45
1:0:601:A:H3'	1:0:602:C:C5'	2.46	0.45
1:0:2558:C:O2'	1:0:2559:U:H5'	2.17	0.45
1:0:2277:A:H2'	1:0:2278:A:O4'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2278:A:H2'	1:0:2279:G:H8	1.82	0.45
1:0:2196:U:H2'	1:0:2197:U:C6	2.51	0.45
1:0:1747:G:H1'	1:0:1749:G:C2	2.51	0.45
1:0:365:U:H2'	1:0:366:U:C6	2.52	0.45
1:0:8:A:H2'	1:0:9:U:C6	2.51	0.45
1:0:35:G:H1'	1:0:466:A:H1'	1.98	0.45
1:0:1579:G:H2'	1:0:1580:C:C6	2.52	0.45
1:0:2552:C:OP1	1:0:2553:G:H5''	2.17	0.45
1:0:594:G:N2	1:0:1267:A:H62	2.14	0.45
1:0:1586:A:H2'	1:0:1587:A:C8	2.52	0.45
1:0:421:G:H2'	1:0:422:C:C6	2.51	0.45
1:0:675:C:H2'	1:0:676:G:C8	2.52	0.45
1:0:529:U:H2'	1:0:530:G:C8	2.51	0.45
1:0:1140:A:N6	1:0:2469:G:H5''	2.32	0.45
2:5:30:C:H2'	2:5:31:C:H6	1.81	0.45
1:0:1619:A:H3'	1:0:1619:A:N3	2.32	0.45
1:0:2055:G:H2'	1:0:2056:C:C6	2.52	0.45
1:0:2205:C:H2'	1:0:2206:C:H6	1.80	0.45
1:0:1777:A:H5'	1:0:1963:G:H21	1.82	0.45
1:0:1307:U:H2'	1:0:1308:C:O4'	2.17	0.45
1:0:297:A:H2'	1:0:298:C:C6	2.51	0.45
1:0:1223:G:O2'	1:0:1224:A:P	2.75	0.45
1:0:340:G:H1'	1:0:488:A:C4	2.52	0.45
1:0:567:G:H2'	1:0:568:G:C8	2.52	0.45
1:0:595:A:H62	1:0:1264:C:N4	2.14	0.45
1:0:2022:C:H2'	1:0:2023:C:C6	2.52	0.45
1:0:13:A:H1'	1:0:536:A:H62	1.82	0.45
1:0:81:C:H4'	1:0:307:C:H5'	1.98	0.45
1:0:2393:G:H2'	1:0:2394:G:C8	2.52	0.45
1:0:1452:U:H5''	1:0:1533:G:H5'	1.99	0.45
1:0:935:C:H2'	1:0:936:A:C8	2.51	0.45
1:0:916:U:H2'	1:0:917:U:C6	2.52	0.45
1:0:2239:C:O2'	1:0:2240:C:H5'	2.17	0.45
1:0:2376:G:H2'	1:0:2377:U:C6	2.52	0.45
1:0:1886:G:H2'	1:0:1887:G:H8	1.82	0.45
1:0:1888:C:C5'	1:0:1889:G:H5''	2.45	0.45
1:0:1257:U:H2'	1:0:1258:G:C8	2.52	0.45
1:0:211:U:C2'	1:0:212:U:H5'	2.46	0.45
1:0:2600:A:H2'	1:0:2601:C:C6	2.52	0.45
1:0:968:C:H2'	1:0:970:A:OP1	2.17	0.45
1:0:1494:G:H2'	1:0:1495:G:C8	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1888:C:C4'	1:0:1889:G:H5''	2.47	0.45
1:0:2235:G:H2'	1:0:2236:U:H6	1.81	0.45
1:0:306:G:H2'	1:0:307:C:C6	2.52	0.45
1:0:2572:U:C4	1:0:2573:C:N4	2.85	0.45
1:0:342:G:O2'	1:0:343:A:OP1	2.34	0.45
1:0:2512:A:H2'	1:0:2513:A:O4'	2.17	0.45
1:0:1608:U:H2'	1:0:1609:G:C8	2.52	0.45
1:0:187:U:H2'	1:0:188:G:C8	2.52	0.45
1:0:1966:C:H4'	1:0:2585:C:H4'	1.97	0.45
1:0:2377:U:O2'	1:0:2378:G:OP1	2.33	0.44
1:0:1346:C:H2'	1:0:1347:C:C6	2.52	0.44
1:0:2694:G:H2'	1:0:2695:C:C6	2.52	0.44
1:0:736:G:H2'	1:0:737:C:O4'	2.16	0.44
1:0:811:G:O2'	1:0:812:G:H5'	2.18	0.44
1:0:2094:C:C4	1:0:2103:G:H1'	2.52	0.44
1:0:1628:C:H2'	1:0:1629:G:C8	2.52	0.44
1:0:2619:G:H2'	1:0:2620:G:C8	2.52	0.44
1:0:91:A:H2'	1:0:92:U:C6	2.53	0.44
1:0:1855:G:H4'	1:0:2390:A:H4'	1.99	0.44
1:0:1906:U:H2'	1:0:1907:C:C6	2.52	0.44
1:0:1367:A:H2'	1:0:1368:G:O4'	2.17	0.44
1:0:1225:G:H2'	1:0:1249:G:H1	1.82	0.44
1:0:2370:G:HO2'	1:0:2371:A:H2	1.65	0.44
1:0:2240:C:H2'	1:0:2241:U:H5'	1.98	0.44
1:0:1130:U:H2'	1:0:1131:G:C8	2.53	0.44
1:0:1921:A:C3'	1:0:1922:U:H5''	2.47	0.44
1:0:237:G:H2'	1:0:238:G:O4'	2.17	0.44
1:0:2524:G:H2'	1:0:2525:U:O4'	2.17	0.44
1:0:2591:C:O2'	1:0:2592:U:H5'	2.17	0.44
1:0:709:A:H2'	1:0:710:C:C6	2.53	0.44
1:0:2426:G:H22	1:0:2431:C:N4	2.15	0.44
1:0:1204:G:H2'	1:0:1205:G:C8	2.52	0.44
1:0:403:A:H4'	1:0:425:A:C5'	2.39	0.44
1:0:514:G:C2'	1:0:514:G:N3	2.79	0.44
1:0:2809:A:N6	1:0:2854:G:H2'	2.32	0.44
1:0:1712:G:C2'	1:0:1713:G:H5'	2.46	0.44
1:0:210:A:N6	1:0:442:A:N6	2.66	0.44
1:0:2159:A:H2'	1:0:2160:C:C6	2.52	0.44
1:0:788:G:C5'	1:0:790:A:H1'	2.47	0.44
1:0:644:A:H2'	1:0:645:G:H5'	1.99	0.44
1:0:1859:A:H2'	1:0:1860:A:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:987:G:H2'	1:0:988:G:H8	1.82	0.44
1:0:2862:G:O2'	1:0:2863:U:H5'	2.17	0.44
1:0:1251:G:H2'	1:0:1252:C:H6	1.80	0.44
1:0:701:U:H2'	1:0:702:A:O4'	2.18	0.44
1:0:2227:C:C2'	1:0:2228:U:H5'	2.41	0.44
1:0:1286:U:H4'	1:0:1288:A:OP1	2.17	0.44
1:0:1292:A:H2'	1:0:1293:A:H8	1.83	0.44
1:0:653:G:H21	1:0:655:A:H1'	1.82	0.44
1:0:351:A:H2'	1:0:352:G:O4'	2.18	0.44
1:0:2292:C:H2'	1:0:2293:G:C8	2.53	0.44
1:0:2860:C:H2'	1:0:2861:A:O4'	2.18	0.44
1:0:520:C:O2'	1:0:1249:G:H5''	2.18	0.44
1:0:837:U:H2'	1:0:838:A:C8	2.53	0.44
1:0:192:G:O2'	1:0:193:A:C5'	2.66	0.44
1:0:1518:C:C2'	1:0:1519:G:O5'	2.66	0.44
1:0:532:A:H2'	1:0:533:C:C6	2.53	0.44
1:0:117:A:H4'	1:0:118:U:C6	2.53	0.44
1:0:2785:A:H2'	1:0:2786:G:O4'	2.17	0.44
1:0:2709:C:H2'	1:0:2710:C:C6	2.52	0.44
1:0:1319:C:H2'	1:0:1320:A:H8	1.82	0.44
1:0:716:U:H2'	1:0:717:G:O4'	2.18	0.44
1:0:540:G:O6	1:0:2006:G:OP1	2.36	0.44
1:0:699:G:H3'	1:0:699:G:N3	2.33	0.44
1:0:2668:U:C2'	1:0:2669:C:OP2	2.66	0.44
1:0:2635:U:H2'	1:0:2636:A:C8	2.52	0.44
1:0:925:U:H4'	1:0:926:C:C6	2.53	0.44
1:0:575:U:H2'	1:0:576:A:C8	2.53	0.44
1:0:634:G:H2'	1:0:635:C:C6	2.52	0.44
1:0:604:U:H2'	1:0:605:G:H8	1.82	0.44
1:0:245:C:H5'	1:0:372:U:O2'	2.17	0.44
1:0:1002:C:H2'	1:0:1003:C:C6	2.53	0.44
1:0:55:A:N6	1:0:69:G:O6	2.50	0.44
1:0:575:U:H4'	1:0:822:G:OP2	2.17	0.44
1:0:1840:A:H2'	1:0:1841:G:H5'	2.00	0.44
1:0:2492:G:H2'	1:0:2493:U:C6	2.53	0.44
1:0:54:G:H2'	1:0:55:A:H8	1.83	0.44
1:0:69:G:OP1	1:0:110:U:N3	2.51	0.44
1:0:32:C:H2'	1:0:33:C:C6	2.53	0.44
1:0:2458:U:OP1	1:0:2516:U:H1'	2.18	0.44
1:0:1821:A:H5''	1:0:1822:C:C5	2.52	0.44
1:0:694:G:H2'	1:0:695:G:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1912:G:C2'	1:0:1912:G:N3	2.79	0.44
1:0:508:G:H2'	1:0:509:U:C6	2.52	0.44
1:0:147:G:C2	1:0:148:C:H1'	2.53	0.44
1:0:1466:C:H2'	1:0:1467:U:O4'	2.17	0.44
1:0:2018:G:H3'	1:0:2019:C:H5'	2.00	0.44
1:0:2668:U:HO2'	1:0:2669:C:P	2.41	0.44
1:0:1353:A:H1'	1:0:1619:A:O4'	2.17	0.44
1:0:2356:A:H2'	1:0:2357:A:C8	2.53	0.44
1:0:2824:C:H2'	1:0:2825:A:OP2	2.17	0.44
1:0:1031:C:H4'	1:0:1032:A:C8	2.53	0.44
1:0:2436:U:H2'	1:0:2437:G:O4'	2.18	0.43
1:0:543:G:H2'	1:0:544:U:C6	2.53	0.43
1:0:181:A:C4'	1:0:182:G:H4'	2.46	0.43
1:0:2712:G:H5'	1:0:2713:A:C8	2.53	0.43
1:0:1480:G:C2'	1:0:1481:U:H5'	2.47	0.43
1:0:1665:C:H2'	1:0:1666:G:C8	2.53	0.43
1:0:415:A:C2'	1:0:416:U:H5'	2.47	0.43
1:0:2783:U:O2'	1:0:2784:A:H4'	2.18	0.43
1:0:1055:A:H2	1:0:1121:G:H2'	1.83	0.43
1:0:1008:G:H2'	1:0:1009:C:C6	2.53	0.43
1:0:2276:C:O2'	1:0:2277:A:H5'	2.18	0.43
1:0:1504:G:O2'	1:0:1505:U:H5'	2.18	0.43
1:0:1312:G:H5''	1:0:1313:U:C5'	2.36	0.43
1:0:841:G:H4'	1:0:844:G:N1	2.33	0.43
1:0:1291:G:H2'	1:0:1292:A:C8	2.53	0.43
1:0:1899:A:O2'	1:0:1946:U:H1'	2.18	0.43
1:0:1750:A:H1'	1:0:2690:A:C2	2.52	0.43
1:0:168:A:H2'	1:0:169:C:H6	1.82	0.43
1:0:437:G:O2'	1:0:438:G:H5'	2.17	0.43
1:0:859:U:H4'	1:0:860:U:C5	2.53	0.43
1:0:2321:C:C2'	1:0:2322:U:H5'	2.47	0.43
1:0:1274:C:O2'	1:0:1275:A:H5'	2.18	0.43
1:0:457:C:O2'	1:0:458:G:H5'	2.18	0.43
1:0:2772:U:H2'	1:0:2773:G:C8	2.53	0.43
1:0:2620:G:H2'	1:0:2621:G:H8	1.83	0.43
1:0:715:U:H2'	1:0:716:U:C6	2.53	0.43
1:0:1155:G:H2'	1:0:1156:U:O4'	2.18	0.43
1:0:67:G:C4	1:0:73:A:C8	3.06	0.43
1:0:2510:A:N6	1:0:2641:A:H61	2.11	0.43
1:0:1227:A:H62	1:0:1248:G:H21	1.65	0.43
1:0:2485:U:O2'	1:0:2486:C:H5'	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2680:U:H3'	1:0:2681:A:C5'	2.47	0.43
1:0:192:G:H4'	1:0:193:A:H4'	1.99	0.43
1:0:538:A:C3'	1:0:539:A:H5''	2.48	0.43
1:0:1518:C:O2'	1:0:1519:G:P	2.76	0.43
1:0:2161:C:O2'	1:0:2162:C:OP1	2.34	0.43
1:0:2392:G:H2'	1:0:2393:G:C8	2.54	0.43
1:0:1561:A:H2'	1:0:1562:G:O4'	2.18	0.43
2:5:24:U:H2'	2:5:25:U:C6	2.54	0.43
1:0:1016:C:H2'	1:0:1017:C:H6	1.83	0.43
1:0:1278:A:O2'	1:0:1279:G:O5'	2.36	0.43
1:0:242:A:O2'	1:0:243:G:OP2	2.37	0.43
1:0:475:U:H2'	1:0:476:G:O4'	2.18	0.43
1:0:420:C:H2'	1:0:421:G:C8	2.53	0.43
1:0:1605:A:H2'	1:0:1606:C:C6	2.54	0.43
1:0:871:U:H1'	1:0:2248:A:C5'	2.47	0.43
1:0:173:A:N3	1:0:173:A:C2'	2.81	0.43
1:0:1774:A:N1	1:0:2566:A:H2'	2.34	0.43
1:0:1938:U:H2'	1:0:1939:U:H5'	1.99	0.43
1:0:1614:C:H2'	1:0:1615:C:C6	2.53	0.43
1:0:2780:A:H2'	1:0:2781:G:H8	1.83	0.43
1:0:456:C:H2'	1:0:457:C:C6	2.54	0.43
1:0:2497:A:N3	1:0:2497:A:O5'	2.52	0.43
1:0:2874:A:H2'	1:0:2875:C:C6	2.54	0.43
1:0:838:A:H4'	1:0:2407:G:C5	2.54	0.43
1:0:1478:U:H2'	1:0:1479:G:C8	2.53	0.43
1:0:1975:G:H1'	1:0:1977:C:N4	2.33	0.43
1:0:1518:C:HO2'	1:0:1519:G:P	2.41	0.43
1:0:114:C:H4'	1:0:124:A:O2'	2.17	0.43
1:0:810:U:H2'	1:0:811:G:H8	1.83	0.43
1:0:2033:C:H2'	1:0:2034:A:O4'	2.18	0.43
1:0:109:A:H2'	1:0:110:U:H5''	2.00	0.43
1:0:88:G:H3'	1:0:89:A:C5'	2.42	0.43
2:5:32:A:C5	2:5:33:C:H1'	2.54	0.43
1:0:215:G:H1'	1:0:617:U:O2	2.19	0.43
1:0:1500:U:H2'	1:0:1501:C:C6	2.54	0.43
1:0:192:G:O2'	1:0:193:A:P	2.76	0.43
1:0:1518:C:H2'	1:0:1519:G:H8	1.84	0.43
1:0:1075:C:H2'	1:0:1076:U:C6	2.54	0.43
1:0:959:C:H2'	1:0:960:U:C6	2.54	0.43
1:0:547:U:H2'	1:0:548:G:C8	2.53	0.43
1:0:1961:A:H2'	1:0:1962:C:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2002:A:H61	1:0:2018:G:N2	2.16	0.43
1:0:2244:C:H1'	1:0:2255:G:N1	2.34	0.43
1:0:820:U:H2'	1:0:821:A:C8	2.53	0.43
1:0:840:U:H4'	1:0:841:G:C2	2.53	0.43
1:0:201:G:H2'	1:0:202:A:H8	1.84	0.43
1:0:1326:U:H4'	1:0:1345:G:H4'	2.01	0.43
1:0:653:G:C2	1:0:655:A:H1'	2.53	0.43
1:0:1033:G:N2	1:0:1150:C:H2'	2.29	0.43
1:0:2056:C:H2'	1:0:2057:U:H6	1.84	0.43
1:0:2602:G:OP1	1:0:2801:A:H1'	2.19	0.43
1:0:967:G:H1'	1:0:970:A:N7	2.34	0.43
1:0:2265:A:H5''	1:0:2266:A:O4'	2.19	0.43
1:0:814:G:H3'	1:0:815:A:C5'	2.49	0.43
1:0:2369:U:H2'	1:0:2370:G:C8	2.54	0.43
1:0:1880:G:H2'	1:0:1881:U:C6	2.54	0.43
1:0:878:C:HO2'	1:0:879:A:P	2.42	0.43
1:0:2586:G:H2'	1:0:2587:G:O4'	2.18	0.43
1:0:1341:G:N2	1:0:1664:G:H1	2.15	0.43
1:0:1455:C:HO2'	1:0:1644:G:H5''	1.84	0.43
1:0:2785:A:O2'	1:0:2786:G:H5'	2.19	0.43
1:0:2213:G:H2'	1:0:2214:G:H8	1.84	0.43
1:0:338:G:H2'	1:0:339:U:O4'	2.19	0.43
1:0:722:C:H2'	1:0:723:C:C6	2.54	0.43
1:0:2795:A:N3	1:0:2795:A:H2'	2.32	0.43
1:0:128:C:C3'	1:0:129:A:H5''	2.49	0.43
1:0:1194:U:H2'	1:0:1195:U:H6	1.79	0.43
1:0:2311:U:HO2'	1:0:2312:A:H8	1.63	0.43
1:0:2310:G:H2'	1:0:2311:U:O4'	2.18	0.43
1:0:121:G:H2'	1:0:122:G:O4'	2.19	0.43
1:0:211:U:H2'	1:0:212:U:O4'	2.19	0.43
1:0:1937:G:H4'	1:0:2529:G:H21	1.83	0.43
1:0:187:U:H2'	1:0:188:G:H8	1.83	0.43
1:0:1604:A:H2'	1:0:1605:A:O4'	2.19	0.43
1:0:2034:A:N6	1:0:2593:A:N7	2.66	0.43
1:0:762:A:H5'	1:0:1284:G:H1'	1.99	0.43
2:5:7:A:H2'	2:5:8:A:C8	2.54	0.43
1:0:1917:C:H2'	1:0:1918:G:H5'	2.01	0.42
1:0:2083:G:H22	1:0:2172:U:H3	1.66	0.42
1:0:591:G:H2'	1:0:592:G:C8	2.54	0.42
1:0:652:C:N4	1:0:657:A:H61	2.09	0.42
1:0:1193:G:O2'	1:0:1194:U:P	2.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1046:U:H2'	1:0:1047:G:H8	1.84	0.42
1:0:2808:U:H3'	1:0:2809:A:C5'	2.47	0.42
1:0:192:G:O2'	1:0:193:A:H5''	2.19	0.42
1:0:539:A:N6	1:0:2024:U:H3	2.16	0.42
1:0:242:A:N6	1:0:441:A:N7	2.66	0.42
1:0:628:A:H2'	1:0:629:C:H6	1.81	0.42
1:0:1591:U:H2'	1:0:1592:U:O4'	2.18	0.42
1:0:2473:G:O2'	1:0:2474:G:H5'	2.19	0.42
1:0:172:A:N3	1:0:227:G:N2	2.65	0.42
1:0:820:U:H1'	1:0:2424:G:OP1	2.18	0.42
1:0:81:C:O2'	1:0:82:G:H5'	2.19	0.42
1:0:2786:G:H2'	1:0:2787:A:C8	2.54	0.42
1:0:758:G:N3	1:0:763:A:N6	2.64	0.42
1:0:1743:C:H2'	1:0:1744:G:C8	2.54	0.42
1:0:987:G:H2'	1:0:988:G:C8	2.54	0.42
1:0:944:A:H2'	1:0:945:G:O4'	2.19	0.42
1:0:2615:U:H3	1:0:2762:G:H1	1.66	0.42
1:0:953:G:H4'	1:0:1203:A:O2'	2.19	0.42
1:0:2564:U:C4'	1:0:2565:C:H5'	2.49	0.42
1:0:2225:G:O2'	1:0:2226:A:H5'	2.20	0.42
1:0:181:A:C5'	1:0:182:G:OP1	2.62	0.42
1:0:2380:U:C2'	1:0:2381:A:H5'	2.44	0.42
1:0:1017:C:H2'	1:0:1018:C:O4'	2.18	0.42
1:0:1259:A:H2'	1:0:1260:A:H8	1.83	0.42
1:0:37:C:H2'	1:0:38:G:C8	2.54	0.42
1:0:1147:G:H2'	1:0:1148:G:H8	1.84	0.42
1:0:2658:A:H2'	1:0:2659:C:H6	1.84	0.42
1:0:1532:A:H2'	1:0:1533:G:C8	2.53	0.42
1:0:1489:C:H3'	1:0:1490:U:H5'	2.00	0.42
1:0:2426:G:H22	1:0:2431:C:H41	1.67	0.42
1:0:541:C:H42	1:0:572:G:C1'	2.33	0.42
1:0:523:A:H2	1:0:591:G:H4'	1.83	0.42
1:0:178:C:H4'	1:0:399:G:C2	2.54	0.42
1:0:2261:G:H4'	1:0:2368:G:O2'	2.20	0.42
1:0:1626:A:H5''	1:0:1627:C:OP2	2.20	0.42
1:0:2161:C:H2'	1:0:2162:C:C5	2.55	0.42
1:0:1057:A:H3'	1:0:1058:G:H5'	2.00	0.42
1:0:2038:C:H5'	1:0:2039:G:C5'	2.49	0.42
1:0:63:A:O2'	1:0:64:C:H5'	2.19	0.42
2:5:33:C:H3'	2:5:34:C:C5'	2.48	0.42
1:0:2757:G:H5'	1:0:2761:A:C1'	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1029:C:C2'	1:0:1030:U:H5''	2.49	0.42
1:0:415:A:O2'	1:0:416:U:H5'	2.20	0.42
1:0:2204:A:HO2'	1:0:2205:C:H6	1.60	0.42
1:0:1358:C:H2'	1:0:1359:G:H5'	2.01	0.42
1:0:1708:C:H2'	1:0:1709:U:O4'	2.19	0.42
1:0:764:A:H3'	1:0:764:A:N3	2.35	0.42
1:0:1957:C:O2'	1:0:1958:G:H5'	2.19	0.42
1:0:984:A:H2'	1:0:1200:G:N2	2.33	0.42
1:0:2633:A:H4'	1:0:2634:G:C4'	2.40	0.42
1:0:404:A:H1'	1:0:424:G:O2'	2.19	0.42
1:0:1343:C:H2'	1:0:1344:C:C6	2.55	0.42
1:0:860:U:O2	1:0:860:U:H2'	2.19	0.42
1:0:1762:C:H2'	1:0:1763:G:C8	2.54	0.42
1:0:509:U:H2'	1:0:510:G:O4'	2.19	0.42
1:0:1489:C:H3'	1:0:1490:U:C5'	2.50	0.42
1:0:3:U:H2'	1:0:4:C:C6	2.54	0.42
1:0:119:G:H1'	1:0:129:A:N1	2.35	0.42
1:0:1187:A:HO2'	1:0:1188:A:P	2.41	0.42
1:0:879:A:C2'	1:0:880:C:H5'	2.49	0.42
1:0:1193:G:O2'	1:0:1194:U:OP1	2.36	0.42
1:0:1790:G:O3'	1:0:1791:C:H6	2.02	0.42
1:0:1281:A:N6	1:0:1995:G:O2'	2.52	0.42
1:0:1065:A:H2'	1:0:1066:G:C8	2.55	0.42
1:0:2217:G:H5'	1:0:2219:U:O4	2.19	0.42
1:0:1634:A:O2'	1:0:1635:G:H5'	2.19	0.42
1:0:1566:G:H2'	1:0:1567:A:C8	2.55	0.42
1:0:644:A:H2'	1:0:645:G:O4'	2.19	0.42
1:0:649:G:H2'	1:0:650:U:C6	2.54	0.42
1:0:646:C:O2'	1:0:650:U:H5''	2.19	0.42
1:0:1451:C:H2'	1:0:1452:U:C6	2.54	0.42
1:0:1836:C:H2'	1:0:1837:G:H8	1.84	0.42
1:0:786:U:H2'	1:0:787:A:H5'	2.01	0.42
1:0:354:C:H2'	1:0:355:G:O4'	2.20	0.42
1:0:2555:G:C2'	1:0:2555:G:N3	2.83	0.42
1:0:964:A:H1'	1:0:2245:A:OP2	2.19	0.42
1:0:2245:A:C2'	1:0:2246:A:OP2	2.67	0.42
1:0:2633:A:H5''	1:0:2634:G:OP1	2.20	0.42
1:0:1030:U:OP1	1:0:1046:U:H1'	2.20	0.42
1:0:1499:A:H2'	1:0:1500:U:C6	2.54	0.42
1:0:2217:G:C2'	1:0:2217:G:N3	2.83	0.42
1:0:1926:U:O2'	1:0:1927:U:O5'	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2824:C:HO2'	1:0:2825:A:P	2.42	0.42
1:0:48:A:O5'	1:0:50:G:H4'	2.20	0.42
1:0:1671:A:C1'	1:0:2798:A:H5'	2.50	0.42
1:0:562:G:H2'	1:0:563:U:O4'	2.20	0.42
1:0:2133:G:H2'	1:0:2134:U:C6	2.55	0.42
1:0:2633:A:H61	1:0:2646:C:N4	2.18	0.42
1:0:617:U:H2'	1:0:618:A:O4'	2.20	0.42
1:0:1332:G:H2'	1:0:1333:G:O4'	2.20	0.42
1:0:669:G:H2'	1:0:670:U:H6	1.83	0.42
1:0:2500:C:H4'	1:0:2544:A:C4'	2.50	0.42
1:0:430:C:H2'	1:0:431:G:C8	2.54	0.42
1:0:2027:C:H2'	1:0:2028:C:C6	2.55	0.42
1:0:198:A:O2'	1:0:199:A:OP2	2.30	0.42
1:0:327:C:O2'	1:0:328:A:H5'	2.20	0.42
1:0:1801:C:H3'	1:0:1802:A:H5'	2.02	0.42
1:0:2766:U:O2'	1:0:2767:C:H5'	2.19	0.42
1:0:956:A:N3	1:0:956:A:H2'	2.34	0.42
1:0:520:C:H2'	1:0:521:U:O4'	2.20	0.42
1:0:1917:C:C2'	1:0:1918:G:H5'	2.49	0.42
1:0:878:C:O2'	1:0:879:A:OP1	2.35	0.42
1:0:1479:G:H2'	1:0:1480:G:C8	2.54	0.42
1:0:2784:A:C8	1:0:2785:A:C8	3.07	0.42
1:0:2651:U:H2'	1:0:2652:G:H8	1.85	0.42
1:0:1143:A:H2'	1:0:1144:U:C6	2.55	0.42
1:0:2463:G:O2'	1:0:2464:G:H5'	2.20	0.42
1:0:2836:U:H2'	1:0:2837:G:C8	2.55	0.42
1:0:2470:U:H1'	1:0:2548:G:O3'	2.20	0.41
1:0:65:C:C3'	1:0:66:U:H5'	2.49	0.41
1:0:616:U:C3'	1:0:617:U:H5''	2.50	0.41
1:0:635:C:H2'	1:0:636:G:H5''	2.02	0.41
1:0:314:G:H2'	1:0:315:G:H8	1.85	0.41
1:0:1949:A:H1'	1:0:2572:U:H5'	2.01	0.41
1:0:2217:G:H4'	1:0:2219:U:C5	2.55	0.41
1:0:2250:G:O2'	1:0:2251:U:H5'	2.20	0.41
1:0:2028:C:O2'	1:0:2029:G:H5'	2.20	0.41
1:0:1962:C:H2'	1:0:1963:G:H8	1.85	0.41
1:0:2698:G:H2'	1:0:2699:G:O4'	2.19	0.41
1:0:1594:U:H2'	1:0:1595:A:C8	2.55	0.41
1:0:1142:G:OP1	1:0:2494:C:H4'	2.20	0.41
1:0:63:A:N6	1:0:89:A:N1	2.69	0.41
1:0:873:U:C2	1:0:2246:A:H5''	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:319:G:H1'	1:0:511:A:H5'	2.02	0.41
1:0:1938:U:O2'	1:0:1939:U:H5'	2.20	0.41
1:0:438:G:H2'	1:0:439:C:C6	2.54	0.41
1:0:2710:C:O2'	1:0:2711:G:H5'	2.20	0.41
1:0:1402:G:H2'	1:0:1403:U:O4'	2.21	0.41
1:0:1930:C:H2'	1:0:1931:G:C8	2.55	0.41
1:0:2640:G:H2'	1:0:2641:A:O4'	2.19	0.41
1:0:871:U:O2	1:0:2247:A:H2'	2.20	0.41
1:0:1225:G:H2'	1:0:1249:G:N1	2.35	0.41
1:0:820:U:H5'	1:0:2424:G:H4'	2.01	0.41
1:0:2564:U:H4'	1:0:2565:C:H5'	2.02	0.41
1:0:2096:U:C2'	1:0:2097:A:H5''	2.44	0.41
1:0:2502:G:H2'	1:0:2503:G:H8	1.85	0.41
1:0:239:A:H5'	1:0:619:A:O2'	2.20	0.41
1:0:1807:A:O2'	1:0:1808:C:C4'	2.64	0.41
1:0:1888:C:H2'	1:0:1913:G:C6	2.55	0.41
1:0:1829:C:O2'	1:0:1910:A:H1'	2.20	0.41
1:0:579:G:H2'	1:0:2013:A:C5	2.55	0.41
1:0:2392:G:H2'	1:0:2393:G:H8	1.85	0.41
1:0:1231:A:H2'	1:0:1232:U:O4'	2.20	0.41
1:0:1177:U:H2'	1:0:1178:C:C6	2.55	0.41
1:0:1495:G:O2'	1:0:1496:G:OP1	2.35	0.41
1:0:1956:G:H2'	1:0:1957:C:O4'	2.20	0.41
1:0:833:A:H2'	1:0:834:A:C8	2.55	0.41
1:0:1189:G:O2'	1:0:1190:C:H5'	2.21	0.41
1:0:1354:A:C2	1:0:1411:C:H4'	2.55	0.41
1:0:2320:G:H2'	1:0:2321:C:C6	2.56	0.41
1:0:2032:G:O2'	1:0:2033:C:H5'	2.20	0.41
1:0:1671:A:H2'	1:0:1672:A:H8	1.86	0.41
1:0:328:A:O2'	1:0:329:C:H5'	2.21	0.41
1:0:334:G:N3	1:0:344:G:H1'	2.36	0.41
1:0:1172:U:H2'	1:0:1173:G:C8	2.55	0.41
1:0:2245:A:O2'	1:0:2246:A:P	2.78	0.41
1:0:930:A:H3'	1:0:931:G:H8	1.85	0.41
1:0:317:U:H3'	1:0:318:G:C5'	2.51	0.41
1:0:1365:U:H5'	1:0:1587:A:H1'	2.03	0.41
1:0:474:G:N2	1:0:476:G:H3'	2.36	0.41
1:0:827:C:H2'	1:0:828:C:C6	2.55	0.41
1:0:159:A:H2'	1:0:160:C:H5'	2.02	0.41
1:0:2093:G:O2'	1:0:2094:C:OP1	2.34	0.41
1:0:853:C:H2'	1:0:854:G:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1448:A:H2'	1:0:1449:C:C6	2.55	0.41
1:0:1557:G:H2'	1:0:1558:C:C6	2.56	0.41
1:0:2546:G:H2'	1:0:2547:C:C6	2.56	0.41
1:0:1656:U:O2'	1:0:2678:C:H4'	2.21	0.41
1:0:2220:A:H2'	1:0:2221:G:H8	1.85	0.41
1:0:1193:G:HO2'	1:0:1194:U:P	2.43	0.41
1:0:1774:A:H1'	1:0:2586:G:N2	2.31	0.41
1:0:314:G:H2'	1:0:315:G:C8	2.54	0.41
1:0:315:G:H2'	1:0:316:C:C6	2.55	0.41
1:0:1341:G:N2	1:0:1343:C:H1'	2.36	0.41
1:0:857:U:C2'	1:0:858:G:H5'	2.50	0.41
1:0:1464:A:H4'	1:0:1545:G:C4'	2.51	0.41
1:0:1415:C:O2'	1:0:1416:A:H5'	2.21	0.41
1:0:639:G:O2'	1:0:640:C:H5'	2.21	0.41
1:0:155:G:O2'	1:0:156:G:H5'	2.21	0.41
1:0:2134:U:H2'	1:0:2135:C:C6	2.55	0.41
1:0:769:C:H2'	1:0:770:U:O4'	2.20	0.41
1:0:2348:A:H2'	1:0:2349:G:C8	2.55	0.41
1:0:2076:G:H2'	1:0:2077:G:C8	2.54	0.41
1:0:1329:U:H2'	1:0:1330:G:C8	2.56	0.41
1:0:2740:C:O2'	1:0:2741:G:H5'	2.20	0.41
1:0:69:G:O3'	1:0:111:G:H4'	2.20	0.41
1:0:2083:G:N2	1:0:2172:U:H3	2.18	0.41
1:0:1028:G:H2'	1:0:1029:C:H6	1.86	0.41
1:0:189:A:H2'	1:0:190:A:C8	2.55	0.41
1:0:307:C:H2'	1:0:308:C:H6	1.85	0.41
1:0:2011:U:H2'	1:0:2012:A:C8	2.56	0.41
1:0:690:A:O2'	1:0:691:C:H5'	2.21	0.41
1:0:691:C:H2'	1:0:692:C:C6	2.56	0.41
1:0:874:A:H2'	1:0:875:G:H5'	2.03	0.41
1:0:964:A:H2'	1:0:965:G:H8	1.85	0.41
1:0:831:G:H2'	1:0:832:A:H5''	2.03	0.41
1:0:1286:U:H2'	1:0:2692:A:H2	1.85	0.41
1:0:488:A:H2'	1:0:489:A:C8	2.55	0.41
1:0:513:A:C4'	1:0:515:A:H5'	2.48	0.41
1:0:1888:C:H4'	1:0:1889:G:H5''	2.02	0.41
1:0:1928:G:H2'	1:0:1929:U:C6	2.55	0.41
1:0:2445:C:H2'	1:0:2446:C:O4'	2.20	0.41
1:0:2795:A:N3	1:0:2795:A:C2'	2.84	0.41
1:0:139:A:H2'	1:0:140:G:C8	2.55	0.41
1:0:1985:G:H2'	1:0:1986:G:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1521:U:H2'	1:0:1522:C:C6	2.56	0.41
1:0:229:G:H2'	1:0:230:C:C6	2.56	0.41
1:0:925:U:H5''	1:0:926:C:OP1	2.21	0.41
1:0:2200:G:H2'	1:0:2201:G:C8	2.56	0.41
1:0:2226:A:H2'	1:0:2227:C:H6	1.86	0.41
1:0:2378:G:H2'	1:0:2379:G:C8	2.55	0.41
1:0:1352:G:N2	1:0:1619:A:H8	2.19	0.41
1:0:1887:G:O2'	1:0:1888:C:H5'	2.21	0.41
1:0:2404:A:OP1	1:0:2406:C:H5'	2.21	0.41
1:0:305:A:H2'	1:0:306:G:O4'	2.21	0.41
1:0:2560:G:H4'	1:0:2561:G:C8	2.56	0.41
1:0:1221:C:H2'	1:0:1222:G:H8	1.85	0.41
1:0:1586:A:H2'	1:0:1587:A:H8	1.86	0.41
1:0:1098:G:H21	1:0:1100:G:H4'	1.86	0.41
1:0:2448:A:C2'	1:0:2449:G:H5'	2.50	0.41
1:0:40:U:H2'	1:0:41:G:H8	1.86	0.41
1:0:2555:G:N3	1:0:2555:G:H2'	2.36	0.41
1:0:1671:A:H1'	1:0:2798:A:H5'	2.02	0.41
1:0:1594:U:H2'	1:0:1595:A:H8	1.85	0.41
1:0:344:G:O2'	1:0:345:U:H5'	2.21	0.41
1:0:1242:A:H2'	1:0:1243:G:C8	2.55	0.41
1:0:2383:C:H2'	1:0:2384:G:O4'	2.20	0.41
1:0:1084:A:H4'	1:0:2454:C:OP1	2.20	0.41
1:0:1722:G:H2'	1:0:1723:U:C6	2.55	0.41
1:0:2365:U:O2'	1:0:2366:U:H5'	2.21	0.41
1:0:1168:G:H2'	1:0:1169:C:C6	2.55	0.41
1:0:1998:A:H2'	1:0:1999:U:H5'	2.02	0.41
1:0:713:G:H2'	1:0:714:G:C8	2.56	0.41
1:0:6:A:H2'	1:0:7:G:C8	2.56	0.41
1:0:2014:A:O5'	1:0:2014:A:H8	2.04	0.41
1:0:2548:G:H2'	1:0:2549:G:C5'	2.33	0.41
1:0:170:U:H5'	1:0:815:A:H2	1.86	0.41
1:0:1313:U:O2'	1:0:1314:A:OP2	2.39	0.41
1:0:218:A:H1'	1:0:220:U:C4	2.56	0.41
1:0:1685:A:O2'	1:0:1686:A:O5'	2.39	0.41
1:0:729:A:O2'	1:0:730:C:H5'	2.21	0.41
1:0:2056:C:H2'	1:0:2057:U:C6	2.56	0.41
1:0:2390:A:H2'	1:0:2391:A:C8	2.56	0.41
1:0:2686:C:H2'	1:0:2687:G:H8	1.86	0.41
1:0:2811:G:H2'	1:0:2812:A:C8	2.56	0.41
1:0:24:G:H2'	1:0:25:U:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1686:A:C2'	1:0:1687:C:H5'	2.51	0.40
1:0:82:G:O2'	1:0:83:A:H5'	2.21	0.40
1:0:322:A:H2	1:0:342:G:OP2	2.04	0.40
1:0:322:A:H1'	1:0:343:A:N7	2.36	0.40
1:0:2058:U:H3'	1:0:2217:G:N1	2.36	0.40
1:0:432:C:H2'	1:0:433:G:C8	2.57	0.40
1:0:2539:C:H2'	1:0:2540:A:C8	2.56	0.40
1:0:2597:G:H2'	1:0:2598:C:C6	2.56	0.40
1:0:67:G:N2	1:0:73:A:O4'	2.54	0.40
1:0:1915:A:H2'	1:0:1916:G:O4'	2.21	0.40
1:0:808:C:H2'	1:0:809:C:C6	2.57	0.40
1:0:1528:C:H3'	1:0:1529:C:H5''	2.03	0.40
1:0:1621:C:C4'	1:0:1626:A:H61	2.31	0.40
1:0:44:G:N2	1:0:192:G:N2	2.69	0.40
1:0:2312:A:H1'	1:0:2314:A:N9	2.36	0.40
1:0:2329:C:H41	1:0:2361:G:N2	2.18	0.40
1:0:2824:C:C2'	1:0:2825:A:OP2	2.70	0.40
1:0:2169:A:O2'	1:0:2170:C:H5'	2.21	0.40
1:0:2515:G:H2'	1:0:2516:U:C6	2.56	0.40
1:0:477:A:H2'	1:0:478:G:H5'	2.02	0.40
1:0:2389:G:H2'	1:0:2390:A:O4'	2.21	0.40
1:0:1026:U:H2'	1:0:1027:C:C6	2.56	0.40
1:0:607:C:H2'	1:0:608:G:C8	2.57	0.40
1:0:747:A:H2'	1:0:748:A:H8	1.85	0.40
2:5:22:G:H2'	2:5:23:C:C6	2.57	0.40
1:0:28:A:H2'	1:0:29:U:C6	2.56	0.40
1:0:1850:G:H2'	1:0:1851:A:C8	2.55	0.40
1:0:2437:G:C2	1:0:2469:G:H2'	2.55	0.40
1:0:688:A:H1'	1:0:2422:C:O2'	2.21	0.40
1:0:868:U:H2'	1:0:869:C:H6	1.86	0.40
1:0:930:A:H5'	1:0:931:G:N7	2.37	0.40
1:0:931:G:H2'	1:0:932:G:O4'	2.21	0.40
1:0:953:G:H2'	1:0:954:U:O4'	2.21	0.40
1:0:105:G:O2'	1:0:106:G:H5'	2.20	0.40
1:0:2081:U:H2'	1:0:2082:C:C5'	2.43	0.40
1:0:1187:A:O2'	1:0:1188:A:P	2.79	0.40
1:0:2241:U:H4'	1:0:2307:A:C2	2.56	0.40
1:0:1162:A:H2'	1:0:1163:C:H6	1.87	0.40
1:0:2234:G:H2'	1:0:2235:G:O4'	2.22	0.40
1:0:1040:A:C2'	1:0:1041:G:H5'	2.51	0.40
1:0:1653:C:H2'	1:0:1654:A:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:978:U:H2'	1:0:979:A:C8	2.56	0.40
1:0:198:A:H4'	1:0:199:A:OP2	2.21	0.40
1:0:1466:C:O2'	1:0:1467:U:H5'	2.21	0.40
1:0:854:G:H2'	1:0:855:G:C8	2.57	0.40
1:0:1696:C:H42	1:0:1755:G:H5''	1.87	0.40
1:0:2594:U:H2'	1:0:2595:C:C6	2.57	0.40
1:0:890:U:H2'	1:0:891:A:C8	2.57	0.40
1:0:185:C:H2'	1:0:186:C:C6	2.56	0.40
1:0:2417:U:H4'	1:0:2419:C:OP1	2.22	0.40
1:0:2418:A:N6	1:0:2581:A:OP1	2.54	0.40
1:0:798:G:OP2	1:0:805:G:N7	2.54	0.40
1:0:105:G:H21	1:0:357:A:N6	2.19	0.40
1:0:204:A:HO2'	1:0:205:A:H8	1.67	0.40
1:0:2378:G:O2'	1:0:2379:G:H5'	2.21	0.40
1:0:1787:U:H2'	1:0:1788:C:C6	2.57	0.40
1:0:633:G:O2'	1:0:634:G:H5'	2.22	0.40
1:0:1625:A:C4	1:0:1632:A:H1'	2.56	0.40
1:0:1982:C:H2'	1:0:1983:G:H8	1.86	0.40
1:0:2553:G:H2'	1:0:2554:C:O4'	2.21	0.40
1:0:579:G:H2'	1:0:2013:A:C6	2.56	0.40
1:0:2851:G:H2'	1:0:2852:G:C8	2.56	0.40
1:0:1418:C:H2'	1:0:1419:G:C8	2.55	0.40
1:0:1532:A:H2'	1:0:1533:G:H8	1.86	0.40
1:0:528:G:H2'	1:0:529:U:C6	2.57	0.40
1:0:2383:C:C2'	1:0:2384:G:H5'	2.51	0.40
1:0:1736:C:H2'	1:0:1737:G:C8	2.57	0.40
1:0:550:C:H2'	1:0:551:A:H8	1.86	0.40
1:0:1370:U:H2'	1:0:1371:G:O4'	2.22	0.40
1:0:2048:C:H2'	1:0:2049:C:H6	1.86	0.40
1:0:2015:G:OP2	1:0:2434:G:H5'	2.22	0.40
1:0:689:A:H8	1:0:2422:C:H1'	1.86	0.40
1:0:1253:C:H2'	1:0:1254:G:O4'	2.21	0.40
1:0:1918:G:H4'	1:0:1920:A:C2	2.57	0.40
1:0:2502:G:H2'	1:0:2503:G:C8	2.56	0.40
1:0:1806:G:O6	1:0:1807:A:N6	2.54	0.40
1:0:1337:G:H1'	1:0:1632:A:C6	2.56	0.40
1:0:2075:U:H1'	1:0:2204:A:C2	2.56	0.40
1:0:948:C:H2'	1:0:949:G:C8	2.57	0.40
1:0:1358:C:C2'	1:0:1359:G:H5''	2.52	0.40
1:0:1036:G:H1'	1:0:1145:C:H4'	2.03	0.40
1:0:1369:G:H2'	1:0:1370:U:O4'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:744:C:H2'	1:0:745:C:C6	2.56	0.40
1:0:1539:U:H2'	1:0:1540:C:C6	2.56	0.40
1:0:1398:G:H2'	1:0:1399:C:C6	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2757/2880 (95%)	416 (15%)	44 (1%)
2	5	22/35 (62%)	2 (9%)	0
All	All	2779/2915 (95%)	418 (15%)	44 (1%)

All (418) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	15	G
1	0	35	G
1	0	45	C
1	0	48	A
1	0	49	U
1	0	50	G
1	0	59	G
1	0	66	U
1	0	67	G
1	0	70	A
1	0	71	A
1	0	72	A
1	0	74	G

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Mol	Chain	Res	Type
1	0	87	G
1	0	89	A
1	0	90	G
1	0	91	A
1	0	99	U
1	0	105	G
1	0	110	U
1	0	116	A
1	0	118	U
1	0	123	A
1	0	129	A
1	0	135	U
1	0	155	G
1	0	158	A
1	0	173	A
1	0	174	A
1	0	176	A
1	0	177	U
1	0	181	A
1	0	182	G
1	0	193	A
1	0	199	A
1	0	200	A
1	0	205	A
1	0	206	U
1	0	210	A
1	0	218	A
1	0	219	G
1	0	225	G
1	0	226	C
1	0	227	G
1	0	229	G
1	0	242	A
1	0	243	G
1	0	245	C
1	0	305	A
1	0	318	G
1	0	333	A
1	0	334	G
1	0	335	A
1	0	340	G
1	0	342	G

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Mol	Chain	Res	Type
1	0	343	A
1	0	358	C
1	0	363	G
1	0	368	A
1	0	373	A
1	0	399	G
1	0	401	G
1	0	408	U
1	0	414	A
1	0	418	C
1	0	424	G
1	0	443	A
1	0	455	A
1	0	456	C
1	0	460	U
1	0	461	A
1	0	463	C
1	0	467	U
1	0	469	G
1	0	491	A
1	0	492	G
1	0	515	A
1	0	518	A
1	0	519	C
1	0	537	C
1	0	539	A
1	0	541	C
1	0	542	A
1	0	554	U
1	0	556	A
1	0	558	G
1	0	559	C
1	0	572	G
1	0	584	A
1	0	602	C
1	0	613	A
1	0	617	U
1	0	624	A
1	0	632	A
1	0	636	G
1	0	638	A
1	0	648	A

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Mol	Chain	Res	Type
1	0	652	C
1	0	654	A
1	0	657	A
1	0	665	A
1	0	666	U
1	0	667	U
1	0	684	C
1	0	697	G
1	0	699	G
1	0	700	C
1	0	728	G
1	0	742	G
1	0	743	A
1	0	760	U
1	0	761	G
1	0	776	G
1	0	778	G
1	0	789	G
1	0	794	A
1	0	796	A
1	0	797	A
1	0	798	G
1	0	803	C
1	0	806	A
1	0	813	A
1	0	818	G
1	0	825	C
1	0	832	A
1	0	840	U
1	0	841	G
1	0	844	G
1	0	860	U
1	0	873	U
1	0	879	A
1	0	919	U
1	0	922	A
1	0	926	C
1	0	930	A
1	0	931	G
1	0	941	U
1	0	944	A
1	0	952	A

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Mol	Chain	Res	Type
1	0	957	G
1	0	969	U
1	0	970	A
1	0	972	C
1	0	973	U
1	0	984	A
1	0	994	A
1	0	996	C
1	0	1005	U
1	0	1006	C
1	0	1023	U
1	0	1024	G
1	0	1030	U
1	0	1032	A
1	0	1033	G
1	0	1036	G
1	0	1037	U
1	0	1044	U
1	0	1055	A
1	0	1056	U
1	0	1057	A
1	0	1067	G
1	0	1073	G
1	0	1074	G
1	0	1075	C
1	0	1081	A
1	0	1087	C
1	0	1090	C
1	0	1099	A
1	0	1122	A
1	0	1137	A
1	0	1138	A
1	0	1142	G
1	0	1145	C
1	0	1146	G
1	0	1155	G
1	0	1167	A
1	0	1182	U
1	0	1183	C
1	0	1185	C
1	0	1188	A
1	0	1194	U

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Mol	Chain	Res	Type
1	0	1195	U
1	0	1199	U
1	0	1200	G
1	0	1224	A
1	0	1253	C
1	0	1262	U
1	0	1264	C
1	0	1266	G
1	0	1269	G
1	0	1278	A
1	0	1279	G
1	0	1280	U
1	0	1284	G
1	0	1285	A
1	0	1288	A
1	0	1314	A
1	0	1324	G
1	0	1334	A
1	0	1338	G
1	0	1342	U
1	0	1343	C
1	0	1355	A
1	0	1356	G
1	0	1359	G
1	0	1391	A
1	0	1392	U
1	0	1397	A
1	0	1398	G
1	0	1433	A
1	0	1441	A
1	0	1442	C
1	0	1443	G
1	0	1459	U
1	0	1465	G
1	0	1468	A
1	0	1469	U
1	0	1470	G
1	0	1475	U
1	0	1482	U
1	0	1490	U
1	0	1496	G
1	0	1505	U

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Mol	Chain	Res	Type
1	0	1508	G
1	0	1509	A
1	0	1513	U
1	0	1519	G
1	0	1524	C
1	0	1529	C
1	0	1552	C
1	0	1571	G
1	0	1573	G
1	0	1574	A
1	0	1576	G
1	0	1582	A
1	0	1583	A
1	0	1585	A
1	0	1618	U
1	0	1623	C
1	0	1624	A
1	0	1625	A
1	0	1632	A
1	0	1633	C
1	0	1634	A
1	0	1635	G
1	0	1648	C
1	0	1651	U
1	0	1657	A
1	0	1664	G
1	0	1665	C
1	0	1670	G
1	0	1671	A
1	0	1680	U
1	0	1685	A
1	0	1691	G
1	0	1692	C
1	0	1710	U
1	0	1712	G
1	0	1715	A
1	0	1717	A
1	0	1724	C
1	0	1733	U
1	0	1748	U
1	0	1749	G
1	0	1750	A

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Mol	Chain	Res	Type
1	0	1754	G
1	0	1755	G
1	0	1764	A
1	0	1771	A
1	0	1778	U
1	0	1800	A
1	0	1801	C
1	0	1802	A
1	0	1807	A
1	0	1808	C
1	0	1821	A
1	0	1831	G
1	0	1884	A
1	0	1889	G
1	0	1920	A
1	0	1922	U
1	0	1924	C
1	0	1926	U
1	0	1927	U
1	0	1938	U
1	0	1939	U
1	0	1946	U
1	0	1949	A
1	0	1950	C
1	0	1954	A
1	0	1955	G
1	0	1956	G
1	0	1979	C
1	0	1980	A
1	0	2004	U
1	0	2006	G
1	0	2015	G
1	0	2016	A
1	0	2019	C
1	0	2038	C
1	0	2043	A
1	0	2051	U
1	0	2052	G
1	0	2060	A
1	0	2076	G
1	0	2082	C
1	0	2094	C

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Mol	Chain	Res	Type
1	0	2096	U
1	0	2118	A
1	0	2119	A
1	0	2140	G
1	0	2162	C
1	0	2168	A
1	0	2181	A
1	0	2191	A
1	0	2195	C
1	0	2199	C
1	0	2205	C
1	0	2218	G
1	0	2229	G
1	0	2237	C
1	0	2241	U
1	0	2245	A
1	0	2246	A
1	0	2247	A
1	0	2255	G
1	0	2262	C
1	0	2268	G
1	0	2285	U
1	0	2286	G
1	0	2287	G
1	0	2288	A
1	0	2298	U
1	0	2299	A
1	0	2300	G
1	0	2301	A
1	0	2313	G
1	0	2315	A
1	0	2316	G
1	0	2326	C
1	0	2362	G
1	0	2364	C
1	0	2378	G
1	0	2382	C
1	0	2385	U
1	0	2396	C
1	0	2403	C
1	0	2405	A
1	0	2409	A

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Mol	Chain	Res	Type
1	0	2414	A
1	0	2420	C
1	0	2427	A
1	0	2428	U
1	0	2438	A
1	0	2448	A
1	0	2455	A
1	0	2470	U
1	0	2481	G
1	0	2482	A
1	0	2483	U
1	0	2484	G
1	0	2485	U
1	0	2492	G
1	0	2498	U
1	0	2499	C
1	0	2504	G
1	0	2522	G
1	0	2546	G
1	0	2549	G
1	0	2561	G
1	0	2565	C
1	0	2578	G
1	0	2580	C
1	0	2581	A
1	0	2582	G
1	0	2588	U
1	0	2589	C
1	0	2591	C
1	0	2593	A
1	0	2594	U
1	0	2608	A
1	0	2609	G
1	0	2625	U
1	0	2633	A
1	0	2634	G
1	0	2661	G
1	0	2669	C
1	0	2670	C
1	0	2681	A
1	0	2691	C
1	0	2692	A

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Mol	Chain	Res	Type
1	0	2712	G
1	0	2728	A
1	0	2730	A
1	0	2732	C
1	0	2737	A
1	0	2745	A
1	0	2756	A
1	0	2760	G
1	0	2761	A
1	0	2770	A
1	0	2771	C
1	0	2783	U
1	0	2785	A
1	0	2795	A
1	0	2807	U
1	0	2808	U
1	0	2809	A
1	0	2811	G
1	0	2825	A
1	0	2841	U
1	0	2842	C
1	0	2847	G
1	0	2854	G
1	0	2855	C
1	0	2859	U
2	5	32	A
2	5	34	C

All (44) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	69	G
1	0	71	A
1	0	73	A
1	0	173	A
1	0	181	A
1	0	192	G
1	0	198	A
1	0	242	A
1	0	342	G
1	0	583	C
1	0	805	G

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Mol	Chain	Res	Type
1	0	843	G
1	0	878	C
1	0	1074	G
1	0	1141	U
1	0	1187	A
1	0	1193	G
1	0	1194	U
1	0	1223	G
1	0	1263	G
1	0	1278	A
1	0	1279	G
1	0	1313	U
1	0	1354	A
1	0	1495	G
1	0	1518	C
1	0	1634	A
1	0	1664	G
1	0	1807	A
1	0	1820	G
1	0	1938	U
1	0	2015	G
1	0	2093	G
1	0	2161	C
1	0	2204	A
1	0	2245	A
1	0	2261	G
1	0	2377	U
1	0	2404	A
1	0	2426	G
1	0	2668	U
1	0	2759	U
1	0	2782	G
1	0	2824	C

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PPU	5	35	1,2	30,40,41	2.78	6 (20%)	37,57,60	1.32	6 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PPU	5	35	1,2	-	0/21/43/44	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	35	PPU	OC-CM	-4.92	1.27	1.42
2	5	35	PPU	CD2-CG	2.59	1.44	1.38
2	5	35	PPU	CE2-CZ	2.68	1.44	1.38
2	5	35	PPU	C6-N1	3.40	1.38	1.34
2	5	35	PPU	CE1-CZ	3.67	1.46	1.38
2	5	35	PPU	C-N3'	12.05	1.61	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	35	PPU	C4'-C3'-N3'	-3.41	106.49	113.61
2	5	35	PPU	C1'-N9-C4	-2.03	123.88	126.94
2	5	35	PPU	C-CA-N	2.08	117.97	108.73
2	5	35	PPU	C9-N6-C6	2.15	126.26	119.48
2	5	35	PPU	CM-OC-CZ	2.71	123.86	117.51
2	5	35	PPU	C2-N1-C6	3.93	119.79	111.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	5	35	PPU	1	0

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	SPS	0	2881	-	17,22,23	4.47	9 (52%)	16,28,30	4.26	8 (50%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SPS	0	2881	-	1/1/2/6	2/15/16/18	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	0	2881	SPS	C7-C5	2.47	1.55	1.50
5	0	2881	SPS	C9-C10	3.09	1.54	1.48
5	0	2881	SPS	C6-C8	3.94	1.56	1.47
5	0	2881	SPS	C1-N2	5.02	1.42	1.33
5	0	2881	SPS	C10-N11	5.14	1.50	1.34
5	0	2881	SPS	C5-N4	5.35	1.42	1.34
5	0	2881	SPS	C9-C8	7.90	1.54	1.32
5	0	2881	SPS	O1-C1	8.00	1.43	1.24
5	0	2881	SPS	O10-C10	9.59	1.43	1.24

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	0	2881	SPS	C12-N11-C10	-7.86	112.03	122.58
5	0	2881	SPS	O10-C10-C9	-7.05	109.44	123.01
5	0	2881	SPS	C8-C9-C10	-5.54	109.55	121.63
5	0	2881	SPS	C6-C8-C9	-5.05	110.36	127.09
5	0	2881	SPS	C7-C5-C6	-2.02	121.24	123.69
5	0	2881	SPS	C9-C10-N11	5.11	125.37	114.12
5	0	2881	SPS	C1-N2-C3	6.13	120.55	115.25
5	0	2881	SPS	C14-S15-C16	6.36	109.42	100.97

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	0	2881	SPS	C12

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	0	2881	SPS	C9-C10-N11-C12
5	0	2881	SPS	O10-C10-N11-C12

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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.