



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 04:42 am BST

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

<https://www.wwpdb.org/validation/2017/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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

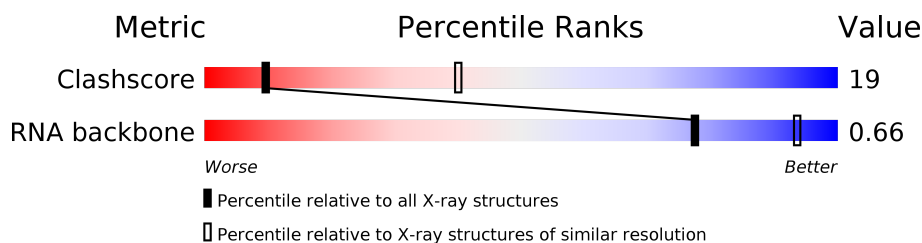
1 Overall quality at a glance

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	141614	1353 (3.70-3.50)
RNA backbone	3102	1017 (4.20-3.00)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	0	2880	
2	5	35	
3	K	141	
4	T	237	

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			

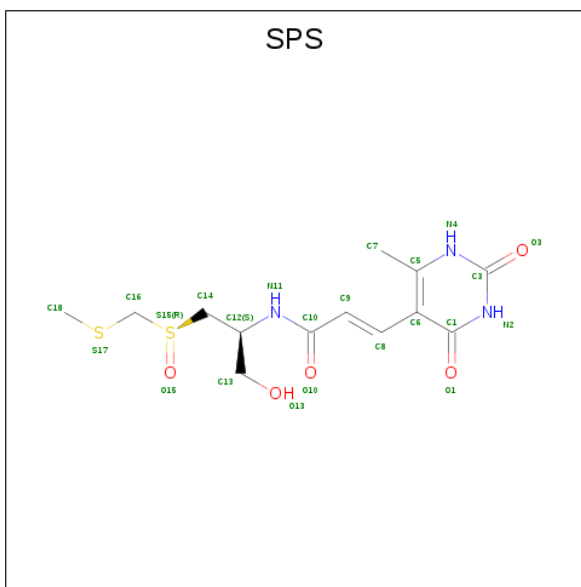
- Molecule 3 is a protein called 50S ribosomal protein L16.

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			

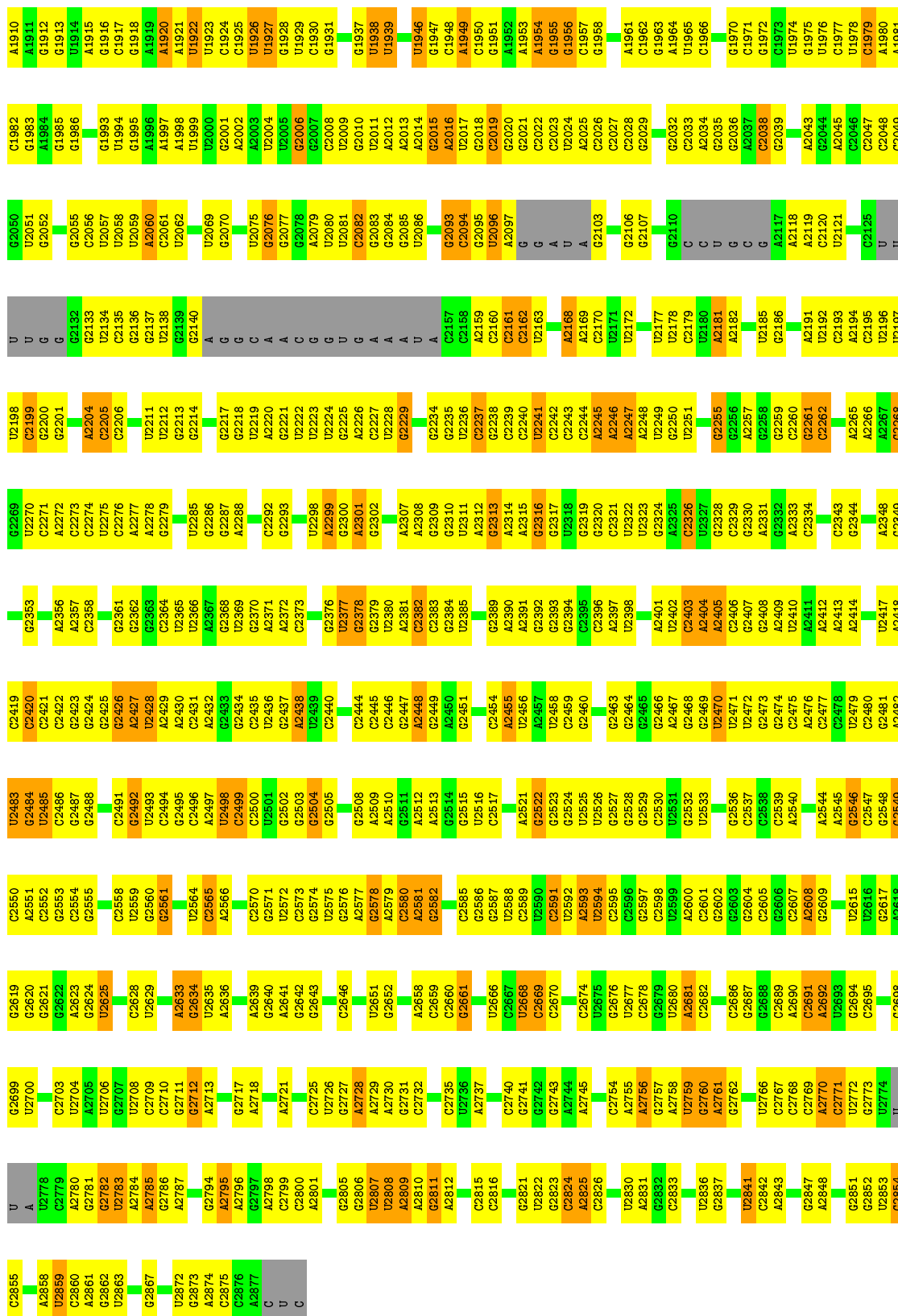
- Molecule 5 is SPARSOMYCIN (three-letter code: SPS) (formula: C₁₃H₁₉N₃O₅S₂).



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

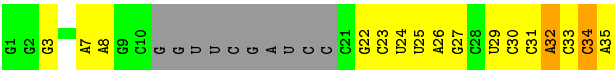


G1818	G1737	A1658	A1586	G1508	A1441	G1359	A1289	G1045	U978	C	U840	G778
U1819	G1742	G1650	A1587	A1509	C1442	U1365	A1290	U1046	A979	A911	G841	U779
G1820	G1743	G1660	G1443	A1510	G1443	U1366	G1291	G1047	G980	U1144	A842	U780
A1821	G1744	C1661	U1591	A1511	C1444	A1366	A1292		C981	U916	G843	G781
C1822	G1745	G1662	U1592	A1512	U1445	A1367	A1293			U917	G844	U782
	C1745	C1663	C1593	U1513	U1446	G1368		C1052	A884	U918	U845	G783
C1825	A1746	G1664	U1594	C1514	U1447	G1369	G1298	C1053		U919	U846	G784
U1826	G1747	C1665	A1595	U1515	A1448	U1370		C1054	A986	G920	A847	U785
	U1748	G1666	A1596	A1516	G1449	G1371	U1301	U1056	G987	A921	U786	U786
C1829	G1749	A1667	A1597	C1517	G1450	A1372		U1057	G988	A922	U852	
C1830	A1750	G1668	C1598	U1518	C1451	G1373	U1307	G1058		U925	C853	G788
G1831		A1669	G1599	G1519	U1452		C1308		A991	U926	G854	G789
	G1754	G1670	U1600	G1520	C1455	G1377	G1309	A1065		C926	G855	U790
C1835	G1755	A1671	U1601	U1521	C1456			U1066	A994	C927	G791	G791
C1836		A1672	G1602	C1522	C1457	C1380	G1311	G1067	A995	G928	U857	U792
G1837	G1760	A1603	A1603	A1523	C1458	G1381	G1312	A1068	C996	A929	G793	G793
C1838	G1761	C1677	A1604	C1524	U1459		U1313	G1069	C997	A930	U859	A794
A1839	C1762	G1678	A1605		U1459	A1386	A1344	G1070	C998	G931	U860	A795
A1840	G1763	U1679	C1606	A1532	U1467	G1387	A1315		A999	G932	G861	
G1841	A1764	U1680	A1607	G1527		C1388	A1316	G1073		G933		A796
	C1765	A1681	U1608	C1528	A1463	G1389	G1317	G1074	A1001	G934	C864	A797
G1850	U1766	A1682	G1609	U1530	G1465	G1390	A1318	C1075	A1002	C935	A865	G798
A1851		G1683	C1631	C1531	A1466	A1391	C1319	U1076	C1003	A936		U800
	G1770	G1684	U1611	A1532	U1467	U1392	A1320		A1004			
	A1771	A1685	U1612	G1533	U1468	G1393		A1081	U1005	C939	U868	C803
G1855		A1686	G1613		U1469		G1323		C1006	G940	C869	C804
U1856	A1772	C1687	C1614	U1539	G1470	A1397	G1324	A1084	A1007	U941	U871	G805
C1857	A1773	G1687	C1615	C1540	G1471	G1398	U1325	G1085	G1008	U942	G872	A806
A1858	A1775	G1688	C1616		C1472	C1399	U1326	C1086	C1009	U943	U873	A807
A1859	A1776	G1689	G1617	G1543	U1473		C1327	C1087		A944	A874	C808
G1860	A1777	C1692	U1618	A1544	A1474	G1402	U1328	C1088	U1014	G945	U875	C809
C1861	U1778	C1696	A1619	G1545	U1475	U1403	U1329	C1089	U1015		U876	U810
C1862	C1779	C1696	U1619	U1545	U1475	U1403	G1330	C1090	C1016	C948	G877	G811
	A1780	C1620	C1620			G1407	G1331	C1091	C1017	G949	C878	G812
C1865		C1703	G1621	C1552	U1478		G1332	C1092	C1018	G950	A879	A813
G1866	A1785	G1704	G1622	G1557	G1479	U1430	G1332	U1093	U1019	G951	C880	G814
	C1786		C1623	C1558	G1480	C1411	G1333		A1020	A952		A815
G1871	U1787	A1624	A1624		U1481	U1417	U1334	G1098	A1021	G953	G887	U816
	C1788	A1625	A1625	A1561	A1486	G1414	G1337	A1099	A1022	U954	G888	A817
G1880	U1789	A1626	A1626	G1562	A1487	C1415	G1338	G1100	U1023	G955	G889	G818
U1881	G1790	C1627	C1627	G1566	G1488	C1416	U1339	G1101	A1024	A956	U890	C819
G1882	C1791	G1628	G1628	G1567	G1489	C1417	G1340	A1114	A1025	G957	A891	U820
A1883	C1792	G1629	G1629	G1568	G1489	C1417	G1341		U1026	G958	G	A821
C1884	A1793	A1632		A1567	U1490	G1418	U1342	C1120	C1027	C959	G	G822
C1885	U1794	C1633	C1491	A1568	C1491	G1419	C1343	G1121	G1028	U960	G	U823
G1886		G1634	A1634		A1492	U1424	G1344	A1122	C1029	G961	U824	U824
C1887	A1717	G1635	G1635	G1571	A1493	G1425	G1345	G1127	A1030	A954	G	C825
A1888	U1723	C1636	A1636	G1572	A1494	U1426	G1346	C1127	A1032	G965	C	U826
G1889	G1722	A1643	G1643	G1573	G1495	U1427	C1347	C1128	C1031	A964	C	C827
C1890	C1724	G1644	G1644	C1575	G1496	G1428	G1348	G1129	U1038	G965	U	C828
				G1576	C1497	A1429	A1349	U1130	G1034	G967	A	C829
A1895	G1806			G1577	G1498	G1430	G1350	G1131	G1035	C	C	C830
A1896	C1807	C1648	C1648	U1578	A1499	U1431	G1351	G1132	U1036	U969	C	G831
	U1808	U1651	U1651	G1579	U1500	G1432	G1352	G1133	U1037	A970	A	A832
A1899	G1809	C1729	C1729	C1580	G1501	G1433	A1353	G1204	U1038	A971	C	A833
U1900	U1810	C1652	C1652	C1581	G1502	U1434	A1354	G1205	U1039	C972	C	A834
	A1811	C1653	C1653	C1582	G1503	G1435	A1355	A1137	A1040	U973	U	C972
U1906	U1812	U1732	U1732	A1582	G1504	G1436	A1356	A1138	G1041	U974	U	U837
C1907	U1813	U1733	U1733	A1583	G1504	G1437	U1357	A1139	U1044	C975	A	A838
	G1814	U1656	U1656	G1584	U1505		C1358	U1140			C	U839
U1909		C1736	A1657	A1585			G1358	U1141			C	U840

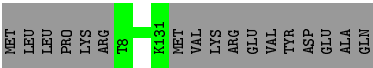
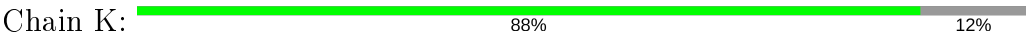


- Molecule 2: tRNA acceptor stem mimic

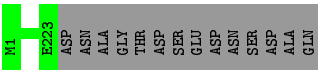




- Molecule 3: 50S ribosomal protein L16



- Molecule 4: GENERAL STRESS PROTEIN CTC



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore 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 [i](#)

5.1 Standard geometry [i](#)

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	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
1:0:1223:G:H21	1:0:1225:G:H21	0.92	0.90
1:0:929:A:H3'	1:0:930:A:H5''	1.52	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
1:0:2081:U:H2'	1:0:2082:C:H5''	1.62	0.81
1:0:109:A:H3'	1:0:110:U:H5''	1.61	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
1:0:2227:C:H2'	1:0:2228:U:H5'	1.66	0.78
1:0:2564:U:H5''	1:0:2565:C:H5'	1.65	0.78
2:5:3:G:H1	2:5:29:U:H3	1.32	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
1:0:1882:G:H21	1:0:1885:C:N4	1.86	0.72
1:0:471:A:H62	1:0:480:G:N2	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
1:0:1021:A:H1'	1:0:1164:C:H1'	1.71	0.72
1:0:2721:A:H62	1:0:2743:G:H21	1.37	0.72
1:0:1199:U:H3'	1:0:1200:G:C5'	2.20	0.72
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
1:0:795:A:H4'	1:0:796:A:N7	2.04	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
1:0:1196:G:H2'	1:0:1197:U:O4'	1.91	0.71
1:0:2691:C:H3'	1:0:2692:A:H5''	1.73	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)
1:0:1047:G:H1	1:0:1130:U:H3	1.37	0.71
1:0:1923:U:H4'	1:0:1948:C:H41	1.55	0.71
1:0:2380:U:H2'	1:0:2381:A:H5'	1.72	0.71
1:0:319:G:H21	1:0:340:G:H21	1.39	0.71
1:0:1373:G:H22	1:0:2192:U:H3	1.37	0.70
1:0:515:A:H2'	1:0:516:G:H5'	1.72	0.70
1:0:1621:C:H4'	1:0:1626:A:H61	1.56	0.70
1:0:1809:G:H2'	1:0:1810:U:O4'	1.91	0.70
1:0:1139:A:H1'	1:0:2496:C:H5'	1.72	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
1:0:1838:G:H2'	1:0:1839:A:H5'	1.75	0.69
1:0:800:U:H3'	1:0:804:C:N4	2.08	0.69
1:0:951:G:H2'	1:0:952:A:H5''	1.73	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
1:0:2607:C:H1'	1:0:2761:A:H2'	1.76	0.68
1:0:584:A:H4'	1:0:2479:U:H5'	1.74	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
1:0:2095:G:H2'	1:0:2096:U:H5''	1.74	0.67
1:0:2495:G:H2'	1:0:2496:C:C6	2.30	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
1:0:1181: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
1:0:813:A:O2'	1:0:815:A:H5'	1.94	0.67
1:0:588:G:H4'	1:0:2001:G:H5''	1.77	0.67
1:0:1915:A:H62	1:0:1951:G:N2	1.91	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
1:0:1749:G:O6	1:0:2674:C:H4'	1.94	0.67
1:0:2680:U:H3'	1:0:2681:A:H5'	1.76	0.67
1:0:2768:C:H2'	1:0:2769:C:O4'	1.94	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
1:0:1191:G:H2'	1:0:1192:A:H8	1.60	0.66
1:0:225:G:H3'	1:0:226:C:C5'	2.25	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
1:0:73:A:H4'	1:0:74:G:C1'	2.24	0.66
1:0:69:G:H4'	1:0:70:A:O5'	1.94	0.66
1:0:665:A:H3'	1:0:666:U:H5''	1.77	0.66
1:0:805:G:H5''	1:0:806:A:O5'	1.95	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
1:0:1487:C:H2'	1:0:1488:G:H8	1.60	0.66
1:0:538:A:H2'	1:0:539:A:H5''	1.77	0.66
1:0:66:U:H2'	1:0:67:G:N7	2.11	0.66
1:0:1312:G:H5'	1:0:1314:A:H1'	1.76	0.66
1:0:1352:G:H2'	1:0:1353:A:H8	1.60	0.66
1:0:652:C:H42	1:0:657:A:N6	1.94	0.66
1:0:1686:A:N3	1:0:1686:A:H2'	2.10	0.66
1:0:1033:G:H22	1:0:1150:C:H2'	1.61	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
1:0:805:G:H4'	1:0:806:A:OP2	1.96	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
1:0:1900:U:O2'	1:0:1946:U:H5'	1.96	0.65
1:0:777:A:N6	1:0:1766:U:H3	1.93	0.65
1:0:175:C:H1'	1:0:2413:A:H61	1.62	0.65
1:0:1679:U:C3'	1:0:1680:U:H5''	2.27	0.65
1:0:1679:U:H3'	1:0:1680:U:H5''	1.76	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
1:0:1938:U:O2'	1:0:1939:U:OP1	2.13	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2822:U:H2'	1:0:2823:G:O4'	1.97	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
1:0:1427:G:H2'	1:0:1428:G:H5'	1.80	0.64
1:0:2198:U:C3'	1:0:2199:C:H5''	2.28	0.64
1:0:2236:U:C3'	1:0:2237:C:H5''	2.27	0.64
1:0:2426:G:H22	1:0:2430:A:H62	1.45	0.64
1:0:317:U:H2'	1:0:318:G:H5''	1.78	0.64
1:0:2236:U:H2'	1:0:2237:C:H5''	1.77	0.64
1:0:1341:G:H22	1:0:1664:G:H1	1.46	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
1:0:83: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
1:0:1517:C:H2'	1:0:1518:C:C6	2.32	0.64
1:0:1807:A:H5'	1:0:1809:G:C1'	2.28	0.64
1:0:1580:C:H2'	1:0:1581:C:C6	2.32	0.63
1:0:73:A:H4'	1:0:74:G:H1'	1.80	0.63
1:0:974:U:H1'	1:0:2229:G:H21	1.60	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
1:0:1715:A:H1'	1:0:1717:A:O4'	1.99	0.63
1:0:927:C:H2'	1:0:928:G:O4'	1.98	0.63
1:0:952:A:O2'	1:0:1204:G:H4'	1.98	0.63
1:0:128:C:C2'	1:0:129:A:H5''	2.27	0.63
1:0:1428:G:H5''	1:0:1429:A:H5'	1.79	0.63
1:0:55:A:H2'	1:0:56:C:C6	2.34	0.63
1:0:653:G:N2	1:0:655:A:H1'	2.14	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
1:0:2570:C:H2'	1:0:2571:G:C8	2.34	0.62
1:0:998:C:H2'	1:0:999:A:O4'	1.98	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
1:0:2636:A:H62	1:0:2643:G:N2	1.90	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
1:0:1085:G:H2'	1:0:1086:C:C6	2.35	0.62
1:0:2015:G:O2'	1:0:2016:A:OP1	2.12	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
1:0:542:A:C2'	1:0:543:G:H5'	2.29	0.62
1:0:323:G:H5'	1:0:342:G:C6	2.35	0.62
1:0:831:G:H21	1:0:1203:A:N6	1.94	0.62
1:0:1354:A:H62	1:0:1407:G:H22	1.47	0.62
1:0:2755:A:O2'	1:0:2756:A:H5'	2.00	0.62
1:0:121:G:O2'	1:0:1389:C:H4'	2.00	0.62
1:0:2440:C:H1'	1:0:2471:U:H3	1.64	0.62
1:0:362:C:H2'	1:0:363:G:H4'	1.81	0.62
1:0:942:U:H2'	1:0:943:U:O4'	2.00	0.62
1:0:852:U:H3	1:0:950:G:H1	1.47	0.62
1:0:2035:G:H2'	1:0:2036:G:H8	1.64	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
1:0:73:A:H3'	1:0:73:A:N3	2.14	0.62
1:0:1807:A:H5'	1:0:1809:G:O4'	2.00	0.62
1:0:2268:G:H22	1:0:2323:U:H4'	1.65	0.62
1:0:858:G:H5''	1:0:859:U:H5'	1.80	0.62
1:0:1656:U:C2'	1:0:1657:A:H5''	2.29	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
1:0:81:C:H2'	1:0:82:G:O4'	2.00	0.61
1:0:878:C:H42	1:0:921:A:N6	1.97	0.61
1:0:1333:G:N2	1:0:1344:C:H41	1.96	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
1:0:940:G:C3'	1:0:941:U:H5''	2.14	0.61
1:0:1455:C:O2'	1:0:1644:G:H5''	2.00	0.61
1:0:2418:A:H4'	1:0:2420:C:OP2	1.99	0.61
1:0:2769:C:H2'	1:0:2770:A:H5'	1.83	0.61
1:0:1323:G:H2'	1:0:1324:G:H4'	1.82	0.61
1:0:860:U:C2'	1:0:861:G:H5'	2.31	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
1:0:871:U:H1'	1:0:2248:A:H5''	1.83	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
1:0:1426:U:H2'	1:0:1427:G:O4'	2.00	0.61
1:0:181:A:H4'	1:0:182:G:C5'	2.30	0.61
1:0:2045:A:H4'	1:0:2421:C:OP2	2.01	0.61
1:0:742:G:H2'	1:0:742:G:N3	2.14	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
1:0:800:U:H3'	1:0:804:C:H41	1.65	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
1:0:2549:G:H2'	1:0:2550:C:O4'	2.01	0.61
1:0:1871:G:N3	1:0:1871:G:H2'	2.16	0.61
1:0:2185:U:H2'	1:0:2186:G:C8	2.36	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
1:0:1713: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
1:0:2242:C:N4	1:0:2257:A:H61	1.99	0.60
1:0:2727:G:O2'	1:0:2728:A:H5''	2.02	0.60
1:0:1066:G:H2'	1:0:1067:G:H4'	1.84	0.60
1:0:2238:G:H2'	1:0:2239:C:C6	2.37	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
1:0:2058:U:H5'	1:0:2576:G:H1'	1.83	0.60
1:0:2858:A:H3'	1:0:2859:U:H5'	1.84	0.60
1:0:1625:A:H2'	1:0:1625:A:N3	2.16	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
1:0:1073: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
1:0:2377: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
1:0:357:A:H2'	1:0:358:C:H5'	1.84	0.59
1:0:1260:A:N6	1:0:1262:U:H1'	2.17	0.59
1:0:1298:G:N2	1:0:1341:G:H5''	2.17	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

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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
1:0:653:G:H4'	1:0:2328:G:H4'	1.83	0.59
1:0:2081:U:C2'	1:0:2082:C:H5''	2.32	0.59
1:0:2243:C:H2'	1:0:2244:C:O4'	2.02	0.59
1:0:69:G:H5''	1:0:70:A:OP1	2.02	0.59
1:0:1811:A:H1'	1:0:1813:A:C5	2.37	0.59
1:0:2770:A:H5'	1:0:2867:G:N2	2.17	0.59
1:0:1140:A:H61	1:0:2470:U:H6	1.50	0.59
1:0:1634:A:O2'	1:0:1635:G:OP1	2.16	0.59
1:0:1683:G:H2'	1:0:1684:G:O4'	2.03	0.59
1:0:2260:C:H4'	1:0:2368:G:H21	1.67	0.59
1:0:412:U:H2'	1:0:413:G:O4'	2.03	0.59
1:0:804:C:O2'	1:0:806:A:H4'	2.03	0.59
1:0:824:U:O2'	1:0:1264:C:H1'	2.02	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
1:0:1474:A:H3'	1:0:1474:A:N3	2.18	0.59
1:0:2205:C:H2'	1:0:2206:C:C6	2.38	0.59
1:0:368:A:H2'	1:0:369:C:O4'	2.03	0.59
1:0:459:A:H1'	1:0:466:A:N7	2.17	0.59
1:0:1354:A:H62	1:0:1407:G:N2	2.01	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
1:0:973:U:H2'	1:0:974:U:C6	2.37	0.59
1:0:17:G:H21	1:0:564:U:H5''	1.66	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
1:0:665:A:H3'	1:0:666:U:C5'	2.33	0.58
1:0:1181:C:C2'	1:0:1182:U:H5''	2.33	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
1:0:1918:G:H4'	1:0:1920:A:N3	2.18	0.58
1:0:1926:U:O2'	1:0:1928:G:H5'	2.03	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
1:0:2426:G:O6	1:0:2479:U:H2'	2.02	0.58
1:0:242:A:O2'	1:0:243:G:O4'	2.21	0.58
1:0:1567:A:H2'	1:0:1568:A:O4'	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1994:U:H2'	1:0:1995:G:O4'	2.04	0.58
1:0:2547:C:H2'	1:0:2548:G:C8	2.38	0.58
1:0:689:A:H2'	1:0:690:A:H5'	1.84	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
1:0:1474:A:C2'	1:0:1475:U:H5'	2.33	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
1:0:1180:A:H2'	1:0:1181:C:C6	2.39	0.58
1:0:2422:C:H2'	1:0:2423:G:C8	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
1:0:1301:U:H3	1:0:1339:U:H3	1.51	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
1:0:2691: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
1:0:521:U:H4'	1:0:1248:G:O2'	2.04	0.58
1:0:628:A:H2'	1:0:629:C:C6	2.39	0.58
1:0:632:A:H2'	1:0:633:G:H5'	1.85	0.58
1:0:766:A:H2'	1:0:767:G:C8	2.38	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
1:0:1712:G:H2'	1:0:1713:G:O4'	2.03	0.57
1:0:1916:G:H2'	1:0:1917:C:C6	2.39	0.57
1:0:2560:G:H4'	1:0:2561:G:N7	2.18	0.57
1:0:2579:A:H2'	1:0:2580:C:C5'	2.30	0.57
1:0:67:G:H22	1:0:72:A:H2'	1.68	0.57
1:0:2222:U:H2'	1:0:2223:U:C6	2.38	0.57
1:0:2794:G:H2'	1:0:2796:A:N7	2.20	0.57
1:0:1392:U:H2'	1:0:1393:G:H5'	1.87	0.57
1:0:2784:A:H3'	1:0:2785:A:H8	1.70	0.57
1:0:925:U:H4'	1:0:926:C:C5	2.40	0.57
1:0:873:U:P	1:0:928:G:H1	2.27	0.57
1:0:1514:C:H2'	1:0:1515:U:O4'	2.04	0.57
1:0:2236:U:H3'	1:0:2237:C:H5''	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1223:G:O2'	1:0:1224:A:OP2	2.21	0.57
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
1:0:1971:C:H2'	1:0:1972:G:H8	1.70	0.57
1:0:618:A:H2'	1:0:619:A:O4'	2.05	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
1:0:2437: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
1:0:1200: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
1:0:1087:C:H2'	1:0:1088:A:O4'	2.05	0.57
1:0:1472:C:C2'	1:0:1473:U:H5'	2.34	0.57
1:0:1947:G:OP1	1:0:1947:G:H3'	2.04	0.57
1:0:687:G:O2'	1:0:688:A:H5'	2.04	0.57
1:0:1220:G:H2'	1:0:1221:C:C6	2.40	0.56
1:0:2242:C:H42	1:0:2257:A:N6	2.03	0.56
1:0:2459:C:H2'	1:0:2460:G:H5'	1.87	0.56
1:0:1431:U:H2'	1:0:1432:G:O4'	2.06	0.56
1:0:2329:C:H2'	1:0:2330:G:H5'	1.87	0.56
1:0:2426:G:O2'	1:0:2427:A:OP2	2.19	0.56
1:0:2559:U:H2'	1:0:2560:G:H5'	1.88	0.56
1:0:73:A:H4'	1:0:74:G:O4'	2.05	0.56
1:0:1981:A:H4'	1:0:2704:U:O2'	2.05	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
1:0:2841:U:O2	1:0:2843:A:H1'	2.05	0.56
1:0:533:C:H2'	1:0:534:U:O4'	2.05	0.56
1:0:874:A:N6	1:0:928:G:H21	2.03	0.56
1:0:2494:C:H2'	1:0:2495:G:C8	2.40	0.56
1:0:2581:A:H2'	1:0:2582:G:H5''	1.86	0.56
1:0:2636:A:N6	1:0:2643:G:H21	1.93	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
1:0:804:C:O2	1:0:807:A:H5'	2.05	0.56
1:0:176:A:H5''	1:0:177:U:H5	1.71	0.56
1:0:2437:G:N2	1:0:2469:G:H2'	2.21	0.56
1:0:2552:C:H42	2:5:35:PPU:P	2.28	0.56
1:0:2564:U:C5'	1:0:2565:C:H5'	2.34	0.56
1:0:2641:A:H2'	1:0:2642:G:O4'	2.06	0.56
1:0:2668:U:C4'	1:0:2669:C:H5'	2.29	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:197:G:H22	1:0:440:U:H2'	1.70	0.56
1:0:103:U:H2'	1:0:104:C:C6	2.40	0.56
1:0:784:U:H2'	1:0:785:U:C6	2.41	0.56
1:0:876:A:H2'	1:0:877:G:C8	2.41	0.56
1:0:758:G:O2'	1:0:761:G:H1'	2.06	0.56
1:0:843:G:O2'	1:0:844:G:OP1	2.15	0.56
1:0:930:A:H4'	1:0:930:A:OP1	2.03	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
1:0:1337:G:H1'	1:0:1632:A:N6	2.21	0.55
1:0:1813:A:H2'	1:0:1814:G:C8	2.41	0.55
1:0:1923:U:H1'	1:0:1947:G:H4'	1.88	0.55
1:0:2018:G:H3'	1:0:2019:C:C5'	2.36	0.55
1:0:2270:U:H2'	1:0:2271:C:C6	2.42	0.55
1:0:2381:A:H4'	1:0:2382:C:H5	1.69	0.55
1:0:366:U:H2'	1:0:367:G:C8	2.41	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
1:0:775:U:O2	1:0:1445:A:H5''	2.06	0.55
1:0:1949:A:H1'	1:0:2572:U:C4'	2.37	0.55
1:0:2061:C:H1'	1:0:2413:A:H1'	1.89	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
1:0:2095:G:C2'	1:0:2096:U:H5''	2.36	0.55
1:0:1920:A:N6	1:0:1923:U:H6	2.05	0.55
1:0:2008:C:H2'	1:0:2009:U:C6	2.41	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
1:0:1669:A:H2'	1:0:1670:G:H4'	1.88	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
1:0:173:A:N3	1:0:173:A:H2'	2.22	0.55
1:0:2162:C:H2'	1:0:2163:U:C6	2.42	0.55
1:0:2321:C:H2'	1:0:2322:U:O4'	2.06	0.55
1:0:394:U:H2'	1:0:395:G:H8	1.71	0.55
1:0:879:A:H2'	1:0:879:A:N3	2.22	0.55
1:0:1181:C:H3'	1:0:1182:U:H5''	1.89	0.55
1:0:1429:A:H62	1:0:1601:U:H5''	1.72	0.55
1:0:1459:U:H2'	1:0:1475:U:O2'	2.07	0.55
1:0:1711:C:H4'	1:0:1712:G:C2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:162:C:H4'	1:0:195:A:O2'	2.07	0.55
1:0:2168:A:H2'	1:0:2169:A:H5'	1.89	0.55
1:0:2379:G:H2'	1:0:2380:U:O4'	2.06	0.55
1:0:583:C:H41	1:0:2017:U:H5	1.53	0.55
1:0:2204:A:O2'	1:0:2205:C:P	2.65	0.55
1:0:33:C:N4	1:0:466:A:H61	2.05	0.55
1:0:841:G:H3'	1:0:841:G:N3	2.21	0.55
1:0:114:C:O2'	1:0:124:A:H1'	2.07	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
1:0:951:G:C2'	1:0:952:A:H5''	2.36	0.55
1:0:831:G:N2	1:0:1203:A:H62	1.97	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
1:0:80:A:H2'	1:0:81:C:O4'	2.06	0.54
1:0:1141:U:H5'	1:0:2549:G:N2	2.22	0.54
1:0:1278:A:O2'	1:0:1279:G:P	2.65	0.54
1:0:1289:A:H62	1:0:1662:G:H1	1.55	0.54
1:0:67:G:H8	1:0:67:G:O5'	1.90	0.54
1:0:166:G:H21	1:0:184:A:N6	1.93	0.54
1:0:1982:C:H1'	1:0:2666:U:O2'	2.07	0.54
1:0:2854:G:H3'	1:0:2854:G:N3	2.22	0.54
1:0:791:G:H2'	1:0:792:U:C6	2.42	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
1:0:1925:C:H5''	2:5:30:C:H4'	1.88	0.54
1:0:1279:G:C2'	1:0:1280:U:OP2	2.56	0.54
1:0:1313:U:O2'	1:0:1314:A:P	2.66	0.54
1:0:1746:A:C2'	1:0:1747:G:H5'	2.37	0.54
1:0:1921:A:H2'	1:0:1922:U:H5''	1.90	0.54
1:0:1955:G:C2'	1:0:1956:G:H5'	2.37	0.54
1:0:2758:A:H5''	1:0:2759:U:H5	1.72	0.54
1:0:558:G:H5''	1:0:559:C:C5	2.42	0.54
1:0:646:C:H2'	1:0:647:G:O4'	2.07	0.54
1:0:69:G:H3'	1:0:111:G:O2'	2.08	0.54
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2426:G:N2	1:0:2430:A:H62	2.04	0.54
1:0:2516:U:H2'	1:0:2517:C:C6	2.42	0.54
1:0:564:U:H2'	1:0:565:A:C8	2.42	0.54
1:0:598:U:H2'	1:0:599:A:C8	2.42	0.54
1:0:1463:A:H2'	1:0:1464:A:C8	2.42	0.54
1:0:1356:G:H5'	1:0:1614:C:OP2	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
1:0:2249: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
1:0:2470:U:O2'	1:0:2471:U:H5'	2.08	0.54
1:0:468:A:H2'	1:0:469:G:H4'	1.90	0.54
1:0:67:G:N2	1:0:73:A:O5'	2.40	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
1:0:484:G:O2'	1:0:485:G:H5'	2.07	0.54
1:0:48:A:H4'	1:0:50:G:O4'	2.08	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
1:0:1789: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
1:0:929:A:H3'	1:0:930:A:C5'	2.33	0.54
1:0:1333:G:N2	1:0:1344:C:N4	2.55	0.53
1:0:216:U:H2'	1:0:217:U:O4'	2.08	0.53
1:0:242:A:O2'	1:0:243:G:O5'	2.26	0.53
1:0:2437:G:H2'	1:0:2469:G:C2	2.43	0.53
1:0:2572:U:H2'	1:0:2573:C:C6	2.43	0.53
1:0:2780:A:O2'	1:0:2781:G:H5'	2.08	0.53
1:0:878:C:N4	1:0:921:A:H62	2.04	0.53
1:0:1763:G:H2'	1:0:1764:A:H4'	1.89	0.53
1:0:317:U:C3'	1:0:318:G:H5''	2.39	0.53
1:0:597:U:H3	1:0:683:A:H2'	1.73	0.53
1:0:857:U:H2'	1:0:858:G:H5'	1.90	0.53
1:0:1358:C:H2'	1:0:1359:G:C5'	2.38	0.53
1:0:1497:C:O2'	1:0:1498:G:H5'	2.08	0.53
1:0:1528:C:C3'	1:0:1529:C:H5''	2.38	0.53
1:0:830:C:O2'	1:0:852:U:H5''	2.08	0.53
1:0:341:A:H1'	1:0:1223:G:O6	2.08	0.53
1:0:594:G:H21	1:0:1267:A:H62	1.57	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)
1:0:1414:G:H2'	1:0:1415:C:C6	2.43	0.53
1:0:1900:U:H4'	1:0:1946:U:O4'	2.09	0.53
1:0:1971:C:H2'	1:0:1972:G:C8	2.43	0.53
1:0:2321:C:O2'	1:0:2353:G:H5''	2.09	0.53
1:0:832:A:H2'	1:0:833:A:O4'	2.07	0.53
1:0:917:U:H2'	1:0:918:A:O4'	2.08	0.53
1:0:1301:U:H2'	1:0:1664:G:H21	1.73	0.53
1:0:173:A:O2'	1:0:174:A:OP1	2.20	0.53
1:0:1825:C:C2'	1:0:1826:U:H5'	2.38	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
1:0:2756:A:H1'	1:0:2758:A:N7	2.23	0.53
1:0:393:U:H2'	1:0:394:U:C6	2.43	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
1:0:918:A:C2'	1:0:919:U:H5''	2.36	0.53
1:0:1976:U:C2'	1:0:1977:C:H5'	2.37	0.53
1:0:665:A:OP2	1:0:666:U:H5'	2.09	0.53
1:0:1029:C:H2'	1:0:1030:U:H5''	1.91	0.53
1:0:1190:C:H2'	1:0:1191:G:C8	2.44	0.53
1:0:1326:U:H2'	1:0:1327:C:H5'	1.90	0.53
1:0:1576:G:H2'	1:0:1577:G:O4'	2.08	0.53
1:0:2498:U:H5''	1:0:2499:C:OP1	2.09	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
1:0:404:A:H2'	1:0:405:C:C6	2.43	0.53
1:0:1075:C:H2'	1:0:1076:U:O4'	2.09	0.53
1:0:757:U:O2'	1:0:758:G:H5'	2.09	0.53
1:0:874:A:H62	1:0:928:G:N2	2.07	0.53
1:0:939:C:H2'	1:0:940:G:C8	2.44	0.53
1:0:1745:C:H2'	1:0:1746:A:O4'	2.09	0.53
1:0:2312:A:H1'	1:0:2314:A:C8	2.44	0.53
1:0:486:U:H4'	1:0:520:C:H5'	1.90	0.53
1:0:658:G:H4'	1:0:2331:A:H5'	1.91	0.53
1:0:77:C:H2'	1:0:78:C:C6	2.44	0.53
1:0:960:U:H2'	1:0:961:G:C8	2.44	0.53
1:0:1775:A:H4'	1:0:1776:A:C8	2.44	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
1:0:541:C:N4	1:0:572:G:O4'	2.42	0.53
1:0:788:G:H5'	1:0:790:A:H1'	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:0:1502:G:O2'	1:0:1503:G:H5'	2.09	0.52
1:0:201:G:H2'	1:0:202:A:C8	2.44	0.52
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
1:0:1217:U:H2'	1:0:1218:C:C6	2.44	0.52
1:0:127:C:H2'	1:0:128:C:C6	2.44	0.52
1:0:1566:G:H4'	1:0:1733:U:O4	2.09	0.52
1:0:1938:U:C2'	1:0:1939:U:H5'	2.39	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
1:0:1365:U:H1'	1:0:1586:A:H2	1.74	0.52
1:0:1964:A:H5''	1:0:1965:U:OP2	2.08	0.52
1:0:870:C:H2'	1:0:871:U:C6	2.43	0.52
1:0:1313:U:O4	1:0:1651:U:H5'	2.09	0.52
1:0:1654:A:H2'	1:0:1655:C:C6	2.44	0.52
1:0:1286:U:H5''	1:0:1663:C:N4	2.24	0.52
1:0:167:A:H2'	1:0:168:A:C8	2.44	0.52
1:0:181:A:H4'	1:0:182:G:C4'	2.39	0.52
1:0:230:C:H2'	1:0:231:G:O4'	2.09	0.52
1:0:2401:A:H2'	1:0:2403:C:C5	2.44	0.52
1:0:688:A:O2'	1:0:2422:C:H4'	2.09	0.52
1:0:2809:A:C2'	1:0:2810:A:H5'	2.40	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
1:0:1970:G:H2'	1:0:1971:C:C6	2.44	0.52
1:0:2083:G:H2'	1:0:2084:G:O4'	2.10	0.52
1:0:212:U:H2'	1:0:213:C:C6	2.45	0.52
1:0:225:G:N2	1:0:2410:U:H1'	2.24	0.52
1:0:689:A:N3	1:0:689:A:H3'	2.24	0.52
1:0:9:U:H3	1:0:2608:A:N6	2.02	0.52
1:0:1234:C:H2'	1:0:1235: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
1:0:38:G:H2'	1:0:39:C:C6	2.44	0.52
1:0:446:C:H2'	1:0:447:U:C6	2.45	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
1:0:2059:U:H2'	1:0:2060:A:H5''	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2372:A:H2'	1:0:2373:C:C6	2.44	0.52
1:0:2757:G:OP2	1:0:2761:A:H4'	2.10	0.52
1:0:616:U:C2'	1:0:617:U:H5''	2.37	0.52
1:0:688:A:H1'	1:0:2423:G:H5'	1.92	0.52
1:0:1263:G:O2'	1:0:1264:C:OP1	2.27	0.52
1:0:2272:A:H2'	1:0:2273:C:C6	2.45	0.52
1:0:2440:C:H1'	1:0:2471:U:N3	2.25	0.52
1:0:317:U:C2'	1:0:318:G:H5''	2.39	0.52
1:0:476:G:H2'	1:0:477:A:C8	2.45	0.52
1:0:776:G:N3	1:0:776:G:H2'	2.25	0.52
1:0:795:A:H4'	1:0:796:A:C8	2.44	0.52
1:0:95:G:H2'	1:0:96:C:C6	2.45	0.52
2:5:33:C:H3'	2:5:34:C:H5'	1.92	0.52
1:0:168:A:H2'	1:0:169:C:C6	2.45	0.52
1:0:45:C:H5''	1:0:192:G:C8	2.44	0.52
1:0:2504:G:H2'	1:0:2505:G:C8	2.45	0.52
1:0:333:A:H1'	1:0:351:A:C4	2.44	0.52
1:0:215:G:O2'	1:0:617:U:H1'	2.09	0.52
1:0:980:G:H2'	1:0:981:C:C6	2.45	0.52
1:0:1597:A:H2'	1:0:1598:C:C6	2.45	0.52
1:0:2320:G:H2'	1:0:2321:C:O4'	2.09	0.52
1:0:2451:G:H2'	1:0:2508:G:N2	2.25	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
1:0:1677: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
1:0:491:A:N3	1:0:491:A:H2'	2.26	0.51
1:0:1358:C:H2'	1:0:1359:G:H5''	1.92	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
1:0:2623:A:H2'	1:0:2624:G:O4'	2.10	0.51
1:0:590:C:H2'	1:0:591:G:C8	2.45	0.51
1:0:826:U:H2'	1:0:827:C:C6	2.46	0.51
1:0:578:U:C1'	1:0:957:G:H21	2.22	0.51
1:0:959:C:H5''	1:0:972:C:O2'	2.11	0.51
1:0:1352:G:H2'	1:0:1353:A:C8	2.43	0.51
1:0:1661:C:O2'	1:0:1662:G:H5'	2.10	0.51
1:0:170:U:H2'	1:0:171:G:H8	1.75	0.51
1:0:1819:U:H5''	1:0:1954:A:O3'	2.11	0.51
1:0:2213:G:H2'	1:0:2214:G:C8	2.46	0.51
1:0:2660:C:O2'	1:0:2661:G:H5'	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:0:2426:G:O2'	1:0:2427:A:P	2.69	0.51
1:0:223:C:H4'	1:0:398:C:H1'	1.92	0.51
1:0:451:A:H2'	1:0:452:G:C8	2.45	0.51
1:0:2703:C:H2'	1:0:2704:U:C6	2.45	0.51
1:0:18:U:H2'	1:0:19:C:C6	2.45	0.51
1:0:2242:C:N4	1:0:2257:A:N6	2.58	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
1:0:1377:G:H4'	1:0:1800:A:H5'	1.93	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
1:0:838:A:H2'	1:0:839:U:C6	2.46	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
1:0:1881: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
1:0:868:U:H2'	1:0:869:C:C6	2.45	0.51
1:0:1067:G:H2'	1:0:1114:A:H61	1.76	0.51
1:0:1068:A:H2'	1:0:1069:G:C8	2.45	0.51
1:0:1092:U:H2'	1:0:1093:U:C6	2.45	0.51
1:0:1127:C:H2'	1:0:1128:G:H8	1.76	0.51
1:0:824:U:H1'	1:0:1264:C:H1'	1.92	0.51
1:0:1611:U:H2'	1:0:1612:U:O4'	2.11	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
1:0:2574:G:N7	1:0:2578:G:N2	2.59	0.51
1:0:2725:C:H2'	1:0:2726:U:C6	2.46	0.51
1:0:703:A:H2'	1:0:704:G:H8	1.76	0.51
1:0:689:A:N6	1:0:815:A:H61	2.05	0.51
1:0:941:U:H4'	1:0:941:U:OP1	2.10	0.51
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
1:0:114:C:H2'	1:0:115:G:O4'	2.11	0.50
1:0:1279:G:H1'	1:0:1280:U:H5	1.76	0.50
1:0:1626:A:OP2	1:0:1627:C:H5	1.95	0.50
1:0:2177:U:H2'	1:0:2178:U:C6	2.46	0.50
1:0:243:G:H2'	1:0:244:C:O4'	2.12	0.50
1:0:457:C:H2'	1:0:458:G:O4'	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:788:G:H5'	1:0:790:A:N3	2.26	0.50
1:0:1424:U:H2'	1:0:1425:G:C8	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
1:0:2397: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
1:0:2821:G:H2'	1:0:2822:U:C6	2.46	0.50
1:0:619:A:H2'	1:0:620:G:C8	2.46	0.50
1:0:116:A:N3	1:0:155:G:H1'	2.26	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
1:0:1747:G:C4'	1:0:1749:G:H1'	2.31	0.50
1:0:1857:G:H2'	1:0:1859:A:OP2	2.12	0.50
1:0:2023:C:H2'	1:0:2024:U:C6	2.46	0.50
1:0:2238:G:H2'	1:0:2239:C:H6	1.76	0.50
1:0:2329:C:C2'	1:0:2330:G:H5'	2.42	0.50
1:0:2726:U:H2'	1:0:2727:G:O4'	2.12	0.50
1:0:332:C:H2'	1:0:333:A:H5'	1.94	0.50
1:0:688:A:HO2'	1:0:2422:C:H4'	1.76	0.50
1:0:879:A:O2'	1:0:880:C:H5'	2.11	0.50
1:0:964:A:H2'	1:0:965:G:C8	2.46	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
1:0:1029:C:OP1	1:0:1047:G:H4'	2.11	0.50
1:0:1218:C:H2'	1:0:1219:C:C6	2.46	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
1:0:841:G:N1	1:0:2226:A:H4'	2.27	0.50
1:0:872:G:H2'	1:0:928:G:N1	2.27	0.50
1:0:1007:A:H2'	1:0:1008:G:C8	2.47	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
1:0:1259:A:H2'	1:0:1260:A:C8	2.47	0.50
1:0:1496:G:H5'	1:0:1575:C:N4	2.26	0.50
1:0:158:A:H2'	1:0:159:A:C8	2.47	0.50
1:0:1667:A:H2'	1:0:1668:G:H8	1.77	0.50
1:0:2010:G:H2'	1:0:2011:U:O4'	2.12	0.50
1:0:2082:C:H2'	1:0:2083:G:O4'	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2446:C:H2'	1:0:2447:G:C8	2.47	0.50
1:0:2754:C:H2'	1:0:2755:A:O4'	2.12	0.50
1:0:35:G:C1'	1:0:466:A:H1'	2.41	0.50
1:0:1895:A:H2'	1:0:1896:A:O4'	2.12	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
1:0:2079: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
1:0:599:A:H2'	1:0:600:G:H8	1.76	0.50
1:0:860:U:H2'	1:0:861:G:H5'	1.94	0.50
1:0:1016:C:H2'	1:0:1017:C:C6	2.47	0.49
1:0:1029:C:C3'	1:0:1030:U:H5''	2.42	0.49
1:0:1310:C:OP1	1:0:2689:C:H4'	2.12	0.49
1:0:991:A:H61	1:0:2020:G:H21	1.59	0.49
1:0:1055:A:N6	1:0:1122:A:H4'	2.27	0.49
1:0:1380:C:N4	1:0:1799:A:N1	2.61	0.49
1:0:1492:A:H2	1:0:1531:C:H41	1.58	0.49
1:0:1791:C:H2'	1:0:1792:C:H5''	1.94	0.49
1:0:338:G:O2'	1:0:339:U:H5'	2.13	0.49
1:0:597:U:N3	1:0:683:A:H2'	2.27	0.49
1:0:689:A:C2'	1:0:690:A:H5'	2.42	0.49
1:0:1312:G:H2'	1:0:1643:A:N6	2.27	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
1:0:190:A:H2'	1:0:191:G:C8	2.47	0.49
1:0:2313:G:H2'	1:0:2314:A:H5'	1.94	0.49
1:0:538:A:C2'	1:0:539:A:H5''	2.41	0.49
1:0:460:U:N3	1:0:592:G:H1'	2.22	0.49
1:0:831:G:C2'	1:0:832:A:H5''	2.42	0.49
1:0:1055:A:O2'	1:0:1058:G:H1'	2.13	0.49
1:0:1195:U:H2'	1:0:1196:G:H8	1.73	0.49
1:0:165:G:H2'	1:0:166:G:O4'	2.12	0.49
1:0:1889:G:H2'	1:0:1890:G:C8	2.48	0.49
1:0:1979:C:H42	1:0:2706:U:H6	1.60	0.49
1:0:579:G:H2'	1:0:2013:A:N6	2.27	0.49
1:0:2299:A:H2'	1:0:2299:A:N3	2.27	0.49
1:0:2532:G:H1'	1:0:2561:G:N3	2.28	0.49
1:0:2805:G:O2'	1:0:2806:G:H5'	2.12	0.49
1:0:441:A:H2'	1:0:442:A:O4'	2.11	0.49
1:0:810:U:H2'	1:0:811:G:C8	2.48	0.49
1:0:991:A:N6	1:0:2020:G:H21	2.11	0.49

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1038:U:H2'	1:0:1039:A:C8	2.48	0.49
1:0:1046:U:H2'	1:0:1047:G:C8	2.48	0.49
1:0:1141:U:O2'	1:0:1142:G:OP1	2.26	0.49
1:0:1182:U:C3'	1:0:1183:C:H5''	2.43	0.49
1:0:1272:G:H2'	1:0:1273:G:C8	2.48	0.49
1:0:1598:C:H2'	1:0:1599:G:O4'	2.13	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
1:0:632:A:C2'	1:0:633:G:H5'	2.43	0.49
1:0:476:G:H21	1:0:696:U:H1'	1.78	0.49
1:0:58:C:N4	1:0:73:A:C6	2.81	0.49
1:0:1040:A:H2'	1:0:1041:G:H5'	1.93	0.48
1:0:1349:A:H2'	1:0:1350:G:C8	2.48	0.48
1:0:1435:G:H21	1:0:1511:A:N6	2.12	0.48
1:0:2308:A:H2'	1:0:2309:G:C8	2.47	0.48
1:0:1937:G:N3	1:0:2530:C:H5'	2.28	0.48
1:0:2852:G:H2'	1:0:2853:U:O4'	2.13	0.48
1:0:790:A:H2'	1:0:791:G:C8	2.48	0.48
1:0:173:A:H61	1:0:844:G:H21	1.59	0.48
1:0:84:G:H2'	1:0:85:C:C6	2.48	0.48
1:0:109:A:C2'	1:0:110:U:H5''	2.43	0.48
1:0:1629:G:N1	1:0:1633:C:N4	2.61	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
1:0:2025:A:H2'	1:0:2026:C:H5''	1.94	0.48
1:0:521:U:H2'	1:0:522:G:H5'	1.95	0.48
1:0:565:A:H2'	1:0:566:U:C6	2.48	0.48
1:0:626:A:O2'	1:0:627:A:H5'	2.13	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
1:0:427:C:H2'	1:0:428:A:C8	2.49	0.48
1:0:864:C:H2'	1:0:865:A:C8	2.47	0.48
1:0:942:U:C2'	1:0:943:U:H5'	2.43	0.48
1:0:1033:G:H22	1:0:1150:C:C2'	2.26	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
1:0:1712:G:N3	1:0:1712:G:H3'	2.29	0.48
1:0:2093:G:O2'	1:0:2094:C:P	2.72	0.48
1:0:2301:A:H2'	1:0:2302:G:O4'	2.14	0.48
1:0:2343:C:H2'	1:0:2344:G:O4'	2.14	0.48
1:0:2780:A:H2'	1:0:2781:G:C8	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:367:G:C3'	1:0:368:A:H5''	2.43	0.48
1:0:429:C:H2'	1:0:430:C:O4'	2.13	0.48
1:0:756:C:H2'	1:0:757:U:C6	2.48	0.48
1:0:1678:G:H2'	1:0:1679:U:C6	2.48	0.48
1:0:1742:G:H2'	1:0:1743:C:C6	2.48	0.48
1:0:192:G:C4'	1:0:193:A:H4'	2.44	0.48
1:0:2059:U:H5	1:0:2575:U:N3	2.02	0.48
1:0:2483:U:H2'	1:0:2484:G:H5'	1.94	0.48
1:0:42:G:H2'	1:0:43:A:O4'	2.13	0.48
1:0:210:A:N6	1:0:442:A:H61	2.11	0.48
1:0:830:C:O2	1:0:852:U:H4'	2.13	0.48
1:0:1141:U:O2'	1:0:1142:G:P	2.72	0.48
1:0:1458:A:H3'	1:0:1459:U:H5'	1.96	0.48
1:0:1686:A:O2'	1:0:2528:G:H5'	2.14	0.48
1:0:181:A:H4'	1:0:182:G:O5'	2.12	0.48
1:0:2212:U:H2'	1:0:2213:G:C8	2.49	0.48
1:0:2721:A:N6	1:0:2743:G:H21	2.10	0.48
1:0:2815:C:H2'	1:0:2816:C:C6	2.49	0.48
1:0:477:A:H2'	1:0:478:G:O4'	2.14	0.48
1:0:548:G:H2'	1:0:549:G:C8	2.48	0.48
1:0:569:C:H2'	1:0:570:G:C8	2.49	0.48
1:0:635:C:H3'	1:0:636:G:H5''	1.95	0.48
1:0:71:A:O2'	1:0:72:A:OP1	2.21	0.48
1:0:742:G:N3	1:0:742:G:C2'	2.77	0.48
1:0:845:U:H2'	1:0:846:A:C8	2.49	0.48
1:0:1391:A:H2'	1:0:1392:U:C5	2.49	0.48
1:0:1684:G:H2'	1:0:1974:U:O4	2.14	0.48
1:0:2085:G:H2'	1:0:2086:U:C6	2.49	0.48
1:0:213:C:H42	1:0:238:G:H22	1.60	0.48
1:0:2503:G:H2'	1:0:2504:G:H5''	1.96	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
1:0:1429:A:H1'	1:0:1603:A:C6	2.49	0.48
1:0:1436:G:H2'	1:0:1437:A:C8	2.49	0.48
1:0:240:U:H4'	1:0:443:A:H5'	1.96	0.48
1:0:2580:C:N4	1:0:2582:G:O6	2.47	0.48
1:0:478:G:O2'	1:0:479:G:H5'	2.14	0.48
1:0:568:G:H5''	1:0:1019:U:H5'	1.96	0.48
1:0:1031:C:H1'	1:0:1151:U:O2	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1682:A:H2'	1:0:1683:G:C8	2.48	0.48
1:0:192:G:H4'	1:0:193:A:O5'	2.13	0.48
1:0:2316:G:H2'	1:0:2317:G:H8	1.78	0.48
1:0:2377:U:O2'	1:0:2378:G:P	2.72	0.48
1:0:323:G:H2'	1:0:324:C:C6	2.48	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
1:0:629: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
1:0:2220:A:H2'	1:0:2221:G:C8	2.49	0.48
1:0:2437:G:H4'	1:0:2438:A:N7	2.28	0.48
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
1:0:2424:G:H2'	1:0:2425:G:O4'	2.14	0.47
1:0:2483:U:H1'	1:0:2551:A:C2	2.49	0.47
1:0:1471:G:H1	1:0:2682:C:H42	1.61	0.47
1:0:2782:G:C2'	1:0:2783:U:OP1	2.62	0.47
1:0:664:C:H2'	1:0:665:A:C8	2.49	0.47
1:0:703:A:H2'	1:0:704:G:C8	2.49	0.47
1:0:941:U:H2'	1:0:942:U:C6	2.49	0.47
1:0:1793:A:H2'	1:0:1794:A:H8	1.79	0.47
1:0:1926:U:O2'	1:0:1927:U:H3'	2.14	0.47
1:0:204:A:H4'	1:0:205:A:N7	2.29	0.47
1:0:873:U:O2	1:0:2246:A:H5''	2.14	0.47
1:0:224:G:C5	1:0:226:C:H1'	2.48	0.47
1:0:2402:U:H5'	1:0:2404:A:N7	2.29	0.47
1:0:2830:U:H2'	1:0:2831:A:C8	2.49	0.47
1:0:780:U:H2'	1:0:781:G:H8	1.79	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
1:0:1016:C:H5''	1:0:1023:U:OP2	2.14	0.47
1:0:1147:G:H2'	1:0:1148:G:C8	2.50	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
1:0:2523: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
1:0:1226:A:C6	1:0:1250:A:H1'	2.49	0.47
1:0:1344:C:H2'	1:0:1346:C:OP1	2.14	0.47
1:0:1386:A:H2'	1:0:1387:G:O4'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:0:1993:G:H2'	1:0:1994:U:C6	2.50	0.47
1:0:2009:U:H2'	1:0:2010:G:C8	2.49	0.47
1:0:2204:A:H1'	1:0:2205:C:C5	2.49	0.47
1:0:2432:A:H4'	1:0:2551:A:O2'	2.15	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
1:0:108:G:H2'	1:0:109:A:C8	2.50	0.47
1:0:1316:G:H2'	1:0:1317:G:H8	1.79	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
1:0:1915:A:N6	1:0:1951:G:H21	1.99	0.47
1:0:2278:A:H2'	1:0:2279:G:C8	2.49	0.47
1:0:2393:G:H2'	1:0:2394:G:H8	1.80	0.47
1:0:2494:C:H2'	1:0:2495:G:H8	1.80	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
1:0:1028:G:H2'	1:0:1029:C:C6	2.50	0.47
1:0:1184:G:H2'	1:0:1185:C:H5'	1.97	0.47
1:0:1354:A:N6	1:0:1407:G:H22	2.11	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
1:0:2378:G:H2'	1:0:2379:G:H8	1.80	0.47
1:0:635:C:C3'	1:0:636:G:H5''	2.45	0.47
1:0:70:A:P	1:0:111:G:H4'	2.55	0.47
1:0:701:U:H1'	1:0:800:U:H5'	1.97	0.47
1:0:926:C:H2'	1:0:927:C:H5'	1.95	0.47
1:0:2021:G:H2'	1:0:2022:C:C6	2.50	0.47
1:0:2199:C:H2'	1:0:2200:G:C8	2.48	0.47
1:0:225:G:H21	1:0:2410:U:H1'	1.78	0.47
1:0:2307:A:H2'	1:0:2308:A:C8	2.50	0.47
1:0:2426:G:H5'	1:0:2480:C:N4	2.23	0.47
1:0:670:U:H2'	1:0:671:A:C8	2.49	0.47
1:0:2486:C:H4'	2:5:34:C:O2'	2.15	0.47
1:0:1269:G:H2'	1:0:1270:C:C6	2.50	0.47
1:0:1290:A:H2'	1:0:1291:G:C8	2.50	0.47
1:0:1418:C:H2'	1:0:1419:G:H8	1.79	0.47
1:0:1495:G:H2'	1:0:1496:G:C8	2.50	0.47
1:0:1578:U:H2'	1:0:1579:G:C8	2.50	0.47
1:0:1821:A:H3'	1:0:1822:C:H6	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2429:A:O2'	1:0:2430:A:H5'	2.14	0.47
1:0:2484:G:H21	1:0:2485:U:H5	1.63	0.47
1:0:2727:G:N1	1:0:2735:C:H5''	2.28	0.47
1:0:432:C:H2'	1:0:433:G:H8	1.80	0.47
1:0:556:A:H2'	1:0:557:U:H5'	1.97	0.47
1:0:643:A:H2'	1:0:644:A:C8	2.49	0.47
1:0:763:A:C2	1:0:765:C:H1'	2.49	0.47
1:0:819:C:H2'	1:0:820:U:C6	2.50	0.47
1:0:1039:A:H2'	1:0:1040:A:C8	2.49	0.47
1:0:1576:G:H5'	1:0:1576:G:H8	1.80	0.47
1:0:2211:U:H2'	1:0:2212:U:C6	2.50	0.47
1:0:2329:C:N4	1:0:2361:G:H22	2.13	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
1:0:1263:G:O2'	1:0:1264:C:P	2.73	0.47
1:0:2504:G:H2'	1:0:2505:G:H8	1.79	0.47
1:0:2559:U:C2'	1:0:2560:G:H5'	2.44	0.47
1:0:84:G:O2'	1:0:85:C:H5'	2.15	0.47
1:0:2276:C:O2	1:0:2301:A:H1'	2.15	0.46
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
1:0:771:C:H2'	1:0:772:G:H8	1.80	0.46
1:0:1480:G:H2'	1:0:1481:U:H5'	1.97	0.46
1:0:2137:G:H2'	1:0:2138:U:C6	2.50	0.46
1:0:2324:G:C4'	1:0:2326:C:H5''	2.43	0.46
1:0:2858:A:H3'	1:0:2859:U:C5'	2.44	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
1:0:173:A:N6	1:0:844:G:H21	2.14	0.46
1:0:864:C:H2'	1:0:865:A:H8	1.80	0.46
1:0:869:C:O2'	1:0:870:C:H5'	2.15	0.46
1:0:971:A:H2	1:0:2475:C:H1'	1.80	0.46
1:0:986:A:H2'	1:0:987:G:H5'	1.97	0.46
1:0:1014:G:O2'	1:0:1015:U:H5'	2.15	0.46
1:0:1223:G:H4'	1:0:1224:A:O5'	2.15	0.46
1:0:152:G:O2'	1:0:153:A:H5'	2.15	0.46
1:0:1829:C:C2'	1:0:1830:C:H5'	2.45	0.46
1:0:1975:G:H4'	1:0:1976:U:H5	1.80	0.46
1:0:2526:U:H2'	1:0:2527:G:C8	2.50	0.46
1:0:1949:A:H1'	1:0:2572:U:H4'	1.98	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
1:0:54:G:H2'	1:0:55:A:C8	2.50	0.46
1:0:878:C:O2'	1:0:879:A:P	2.72	0.46
1:0:1039:A:H2'	1:0:1040:A:H8	1.80	0.46
1:0:1301:U:H2'	1:0:1664:G:N2	2.30	0.46
1:0:760:U:O2	1:0:1997:A:H1'	2.16	0.46
1:0:2035:G:H2'	1:0:2036:G:C8	2.46	0.46
1:0:2372:A:H2'	1:0:2373:C:H6	1.79	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
1:0:387:A:H2'	1:0:388:G:O4'	2.15	0.46
1:0:546:A:H2'	1:0:547:U:C6	2.51	0.46
1:0:758:G:H2'	1:0:759:C:H5'	1.97	0.46
1:0:887:G:O2'	1:0:888:G:H5'	2.15	0.46
1:0:198:A:O2'	1:0:199:A:P	2.74	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
1:0:337:G:H2'	1:0:338:G:C8	2.51	0.46
1:0:738:G:H2'	1:0:739:G:O4'	2.14	0.46
1:0:1069:G:O2'	1:0:1070:G:H5'	2.16	0.46
1:0:108:G:H2'	1:0:109:A:H8	1.81	0.46
1:0:9:U:H2'	1:0:10:A:C8	2.51	0.46
1:0:1452:U:H5'	1:0:1532:A:O2'	2.15	0.46
1:0:1760:G:H2'	1:0:1761:G:C8	2.50	0.46
1:0:324:C:H2'	1:0:325:U:O4'	2.15	0.46
1:0:798:G:H2'	1:0:799:C:H5'	1.97	0.46
1:0:1029:C:H3'	1:0:1030:U:H5''	1.96	0.46
1:0:1279:G:H2'	1:0:1280:U:OP2	2.16	0.46
1:0:1572:C:C3'	1:0:1573:G:H5''	2.45	0.46
1:0:1836:C:H2'	1:0:1837:G:C8	2.50	0.46
1:0:1981:A:H2'	1:0:1982:C:C6	2.50	0.46
1:0:2459:C:C2'	1:0:2460:G:H5'	2.45	0.46
1:0:2475:C:H2'	1:0:2476:A:H5'	1.97	0.46
1:0:2499:C:N4	1:0:2521:A:H2	2.11	0.46
1:0:2800:C:H2'	1:0:2801:A:O4'	2.15	0.46
1:0:2807:U:C5	1:0:2859:U:H4'	2.51	0.46
1:0:584:A:H4'	1:0:2479:U:C5'	2.43	0.46
1:0:1962:C:O2'	1:0:1963:G:H5'	2.16	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
1:0:697:G:C2'	1:0:698:A:H5'	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:845:U:H2'	1:0:846:A:H8	1.80	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
1:0:777:A:H62	1:0:1766:U:H3	1.59	0.46
1:0:19:C:H2'	1:0:20:C:C6	2.49	0.46
1:0:2245:A:HO2'	1:0:2246:A:P	2.39	0.46
1:0:2698:G:H2'	1:0:2699:G:C8	2.51	0.46
1:0:462:G:H2'	1:0:463:C:H5'	1.98	0.46
1:0:85:C:O2'	1:0:86:U:H5'	2.16	0.46
1:0:918:A:H2'	1:0:919:U:C5'	2.42	0.46
1:0:932:G:H2'	1:0:933:G:C8	2.51	0.46
1:0:1331:G:H2'	1:0:1332:G:C8	2.51	0.46
1:0:1495:G:O2'	1:0:1496:G:P	2.73	0.46
1:0:161:U:H2'	1:0:162:C:C6	2.51	0.46
1:0:1703:C:H2'	1:0:1704:G:O4'	2.16	0.46
1:0:2161:C:H2'	1:0:2162:C:C6	2.50	0.46
1:0:2493:U:H2'	1:0:2494:C:C6	2.51	0.46
1:0:2488:G:N2	1:0:2559:U:H1'	2.31	0.46
1:0:2570:C:H2'	1:0:2571:G:H8	1.81	0.46
1:0:313:U:H2'	1:0:314:G:C8	2.50	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
2:5:26:A:H2'	2:5:27:G:H8	1.80	0.46
1:0:1380:C:C2'	1:0:1381:G:H5'	2.45	0.45
1:0:1677:C:H2'	1:0:1678:G:H8	1.81	0.45
1:0:1685:A:N6	1:0:1691:G:H1'	2.31	0.45
1:0:1835:C:H2'	1:0:1836:C:C6	2.51	0.45
1:0:207:U:H2'	1:0:208:C:C6	2.51	0.45
1:0:2093:G:H2'	1:0:2094:C:C5	2.51	0.45
1:0:2106:G:H2'	1:0:2107:G:C8	2.51	0.45
1:0:2193:C:H2'	1:0:2194:A:O4'	2.16	0.45
1:0:2333:A:H2'	1:0:2334:C:C6	2.52	0.45
1:0:2426:G:HO2'	1:0:2427:A:P	2.39	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
1:0:595:A:H2	1:0:822:G:N3	2.15	0.45
1:0:697:G:O2'	1:0:698:A:H5'	2.16	0.45
1:0:831:G:H5'	1:0:852:U:OP1	2.16	0.45
1:0:1068:A:H2'	1:0:1069:G:H8	1.81	0.45
1:0:1163:C:O2'	1:0:1164:C:H5'	2.15	0.45
1:0:1278:A:H4'	1:0:1279:G:O5'	2.17	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
1:0:1486: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
1:0:2017:U:O2'	1:0:2018:G:H5'	2.16	0.45
1:0:199:A:H61	1:0:209:G:H1'	1.81	0.45
1:0:2136:G:H2'	1:0:2137:G:C8	2.51	0.45
1:0:246:C:N3	1:0:247:A:N6	2.64	0.45
1:0:2560:G:N3	1:0:2560:G:H3'	2.31	0.45
1:0:2633:A:N6	1:0:2646:C:N4	2.63	0.45
1:0:2668:U:O2'	1:0:2669:C:P	2.74	0.45
1:0:1120:C:H2'	1:0:2731:G:N2	2.31	0.45
1:0:689:A:C8	1:0:2422:C:H1'	2.51	0.45
1:0:2120:C:H2'	1:0:2121:U:O4'	2.17	0.45
1:0:2474:G:O2'	1:0:2475:C:H5'	2.15	0.45
1:0:2628:C:H2'	1:0:2629:U:C6	2.52	0.45
1:0:2784:A:H3'	1:0:2785:A:C8	2.49	0.45
1:0:931:G:O2'	1:0:932:G:H5'	2.16	0.45
1:0:130:C:H2'	1:0:131:C:C6	2.51	0.45
1:0:1429:A:O2'	1:0:1430:G:H4'	2.17	0.45
1:0:1659:G:H2'	1:0:1660:G:C8	2.51	0.45
1:0:1886:G:H2'	1:0:1887:G:C8	2.51	0.45
1:0:2057:U:H2'	1:0:2058:U:C6	2.51	0.45
1:0:2259:G:H2'	1:0:2260:C:C6	2.52	0.45
1:0:2403:C:H2'	1:0:2408:G:O2'	2.17	0.45
1:0:2455:A:O2'	1:0:2456:U:H5'	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
1:0:2487:G:H4'	1:0:2533:U:O2'	2.15	0.45
1:0:1949:A:O2'	1:0:2572:U:H5'	2.17	0.45
1:0:2639:A:H2'	1:0:2640:G:O4'	2.16	0.45
1:0:2824:C:H1'	1:0:2843:A:C2	2.51	0.45
1:0:307:C:H2'	1:0:308:C:C6	2.52	0.45
1:0:317:U:H3'	1:0:318:G:H5''	1.97	0.45
1:0:40:U:H2'	1:0:41:G:C8	2.51	0.45
1:0:489:A:N6	1:0:491:A:H62	2.14	0.45
1:0:560:G:H2'	1:0:561:U:C6	2.51	0.45
1:0:2196:U:H2'	1:0:2197:U:C6	2.51	0.45
1:0:2278:A:H2'	1:0:2279:G:H8	1.82	0.45
1:0:2277:A:H2'	1:0:2278:A:O4'	2.16	0.45
1:0:2558:C:O2'	1:0:2559:U:H5'	2.17	0.45
1:0:2676:G:H2'	1:0:2677:U:C6	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:601:A:H3'	1:0:602:C:C5'	2.46	0.45
1:0:872:G:O2'	1:0:2247:A:N3	2.48	0.45
1:0:594:G:N2	1:0:1267:A:H62	2.14	0.45
1:0:1579:G:H2'	1:0:1580:C:C6	2.52	0.45
1:0:1586:A:H2'	1:0:1587:A:C8	2.52	0.45
1:0:1747:G:H1'	1:0:1749:G:C2	2.51	0.45
1:0:2552:C:OP1	1:0:2553:G:H5''	2.17	0.45
1:0:35:G:H1'	1:0:466:A:H1'	1.98	0.45
1:0:365:U:H2'	1:0:366:U:C6	2.52	0.45
1:0:421:G:H2'	1:0:422:C:C6	2.51	0.45
1:0:529:U:H2'	1:0:530:G:C8	2.51	0.45
1:0:675:C:H2'	1:0:676:G:C8	2.52	0.45
1:0:8:A:H2'	1:0:9:U:C6	2.51	0.45
1:0:1307:U:H2'	1:0:1308:C:O4'	2.17	0.45
1:0:1619:A:H3'	1:0:1619:A:N3	2.32	0.45
1:0:1777:A:H5'	1:0:1963:G:H21	1.82	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
1:0:1140:A:N6	1:0:2469:G:H5''	2.32	0.45
1:0:297:A:H2'	1:0:298:C:C6	2.51	0.45
2:5:30:C:H2'	2:5:31:C:H6	1.81	0.45
1:0:1223:G:O2'	1:0:1224:A:P	2.75	0.45
1:0:595:A:H62	1:0:1264:C:N4	2.14	0.45
1:0:13:A:H1'	1:0:536:A:H62	1.82	0.45
1:0:1452:U:H5''	1:0:1533:G:H5'	1.99	0.45
1:0:2022:C:H2'	1:0:2023:C:C6	2.52	0.45
1:0:2393:G:H2'	1:0:2394:G:C8	2.52	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
1:0:81:C:H4'	1:0:307:C:H5'	1.98	0.45
1:0:935:C:H2'	1:0:936:A:C8	2.51	0.45
1:0:1257:U:H2'	1:0:1258:G:C8	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
1:0:211:U:C2'	1:0:212:U:H5'	2.46	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
1:0:2600:A:H2'	1:0:2601:C:C6	2.52	0.45
1:0:916:U:H2'	1:0:917:U: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)
1:0:1608: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
1:0:1888:C:C4'	1:0:1889:G:H5''	2.47	0.45
1:0:1966:C:H4'	1:0:2585:C:H4'	1.97	0.45
1:0:2235:G:H2'	1:0:2236:U:H6	1.81	0.45
1:0:2512:A:H2'	1:0:2513:A:O4'	2.17	0.45
1:0:2572:U:C4	1:0:2573:C:N4	2.85	0.45
1:0:306:G:H2'	1:0:307:C:C6	2.52	0.45
1:0:342:G:O2'	1:0:343:A:OP1	2.34	0.45
1:0:1346:C:H2'	1:0:1347:C:C6	2.52	0.44
1:0:1367:A:H2'	1:0:1368:G:O4'	2.17	0.44
1:0:1628:C:H2'	1:0:1629:G:C8	2.52	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
1:0:2094:C:C4	1:0:2103:G:H1'	2.52	0.44
1:0:2377:U:O2'	1:0:2378:G:OP1	2.33	0.44
1:0:2619:G:H2'	1:0:2620:G:C8	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
1:0:91:A:H2'	1:0:92:U:C6	2.53	0.44
1:0:1130:U:H2'	1:0:1131:G:C8	2.53	0.44
1:0:1225:G:H2'	1:0:1249:G:H1	1.82	0.44
1:0:1921:A:C3'	1:0:1922:U:H5''	2.47	0.44
1:0:2240:C:H2'	1:0:2241:U:H5'	1.98	0.44
1:0:2370:G:HO2'	1:0:2371:A:H2	1.65	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
1:0:1204:G:H2'	1:0:1205:G:C8	2.52	0.44
1:0:1712:G:C2'	1:0:1713:G:H5'	2.46	0.44
1:0:1859:A:H2'	1:0:1860:A:C8	2.53	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
1:0:2426:G:H22	1:0:2431:C:N4	2.15	0.44
1:0:2809:A:N6	1:0:2854:G:H2'	2.32	0.44
1:0:2862:G:O2'	1:0:2863:U:H5'	2.17	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
1:0:644:A:H2'	1:0:645:G:H5'	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:788:G:C5'	1:0:790:A:H1'	2.47	0.44
1:0:987:G:H2'	1:0:988:G:H8	1.82	0.44
1:0:1251:G:H2'	1:0:1252:C:H6	1.80	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
1:0:2227:C:C2'	1:0:2228:U:H5'	2.41	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
1:0:351:A:H2'	1:0:352:G:O4'	2.18	0.44
1:0:653:G:H21	1:0:655:A:H1'	1.82	0.44
1:0:701:U:H2'	1:0:702:A:O4'	2.18	0.44
1:0:117:A:H4'	1:0:118:U:C6	2.53	0.44
1:0:1319:C:H2'	1:0:1320:A:H8	1.82	0.44
1:0:1518:C:C2'	1:0:1519:G:O5'	2.66	0.44
1:0:192:G:O2'	1:0:193:A:C5'	2.66	0.44
1:0:2709:C:H2'	1:0:2710:C:C6	2.52	0.44
1:0:2785:A:H2'	1:0:2786:G:O4'	2.17	0.44
1:0:520:C:O2'	1:0:1249:G:H5''	2.18	0.44
1:0:532:A:H2'	1:0:533:C:C6	2.53	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
1:0:716:U:H2'	1:0:717:G:O4'	2.18	0.44
1:0:837:U:H2'	1:0:838:A:C8	2.53	0.44
1:0:1002:C:H2'	1:0:1003:C:C6	2.53	0.44
1:0:2635:U:H2'	1:0:2636:A:C8	2.52	0.44
1:0:2668:U:C2'	1:0:2669:C:OP2	2.66	0.44
1:0:245:C:H5'	1:0:372:U:O2'	2.17	0.44
1:0:575:U:H2'	1:0:576:A:C8	2.53	0.44
1:0:604:U:H2'	1:0:605:G:H8	1.82	0.44
1:0:634:G:H2'	1:0:635:C:C6	2.52	0.44
1:0:925:U:H4'	1:0:926:C:C6	2.53	0.44
1:0:1840:A:H2'	1:0:1841:G:H5'	2.00	0.44
1:0:575:U:H4'	1:0:822:G:OP2	2.17	0.44
1:0:55:A:N6	1:0:69:G:O6	2.50	0.44
1:0:69:G:OP1	1:0:110:U:N3	2.51	0.44
1:0:1466:C:H2'	1:0:1467:U:O4'	2.17	0.44
1:0:147:G:C2	1:0:148:C:H1'	2.53	0.44
1:0:1821:A:H5''	1:0:1822:C:C5	2.52	0.44
1:0:1912:G:C2'	1:0:1912:G:N3	2.79	0.44
1:0:2492:G:H2'	1:0:2493:U:C6	2.53	0.44
1:0:2458:U:OP1	1:0:2516:U:H1'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:32:C:H2'	1:0:33:C:C6	2.53	0.44
1:0:508:G:H2'	1:0:509:U:C6	2.52	0.44
1:0:54:G:H2'	1:0:55:A:H8	1.83	0.44
1:0:694:G:H2'	1:0:695:G:C8	2.53	0.44
1:0:1031:C:H4'	1:0:1032:A:C8	2.53	0.44
1:0:1353:A:H1'	1:0:1619:A:O4'	2.17	0.44
1:0:2018:G:H3'	1:0:2019:C:H5'	2.00	0.44
1:0:2356:A:H2'	1:0:2357:A:C8	2.53	0.44
1:0:2668:U:HO2'	1:0:2669:C:P	2.41	0.44
1:0:2824:C:H2'	1:0:2825:A:OP2	2.17	0.44
1:0:1008:G:H2'	1:0:1009:C:C6	2.53	0.43
1:0:1055:A:H2	1:0:1121:G:H2'	1.83	0.43
1:0:1480:G:C2'	1:0:1481:U:H5'	2.47	0.43
1:0:1504:G:O2'	1:0:1505:U:H5'	2.18	0.43
1:0:1665:C:H2'	1:0:1666:G:C8	2.53	0.43
1:0:181:A:C4'	1:0:182:G:H4'	2.46	0.43
1:0:2276:C:O2'	1:0:2277:A:H5'	2.18	0.43
1:0:2436:U:H2'	1:0:2437:G:O4'	2.18	0.43
1:0:2712:G:H5'	1:0:2713:A:C8	2.53	0.43
1:0:2783:U:O2'	1:0:2784:A:H4'	2.18	0.43
1:0:415:A:C2'	1:0:416:U:H5'	2.47	0.43
1:0:543:G:H2'	1:0:544:U:C6	2.53	0.43
1:0:1155:G:H2'	1:0:1156:U:O4'	2.18	0.43
1:0:1274:C:O2'	1:0:1275:A:H5'	2.18	0.43
1:0:1291:G:H2'	1:0:1292:A:C8	2.53	0.43
1:0:1312:G:H5''	1:0:1313:U:C5'	2.36	0.43
1:0:168:A:H2'	1:0:169:C:H6	1.82	0.43
1:0:1750:A:H1'	1:0:2690:A:C2	2.52	0.43
1:0:1899:A:O2'	1:0:1946:U:H1'	2.18	0.43
1:0:2321:C:C2'	1:0:2322:U:H5'	2.47	0.43
1:0:2620:G:H2'	1:0:2621:G:H8	1.83	0.43
1:0:2772:U:H2'	1:0:2773:G:C8	2.53	0.43
1:0:437:G:O2'	1:0:438:G:H5'	2.17	0.43
1:0:457:C:O2'	1:0:458:G:H5'	2.18	0.43
1:0:715:U:H2'	1:0:716:U:C6	2.53	0.43
1:0:841:G:H4'	1:0:844:G:N1	2.33	0.43
1:0:859:U:H4'	1:0:860:U:C5	2.53	0.43
1:0:1227:A:H62	1:0:1248:G:H21	1.65	0.43
1:0:1518:C:O2'	1:0:1519:G:P	2.76	0.43
1:0:1561:A:H2'	1:0:1562:G:O4'	2.18	0.43
1:0:192:G:H4'	1:0:193:A:H4'	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:0:2485:U:O2'	1:0:2486:C:H5'	2.17	0.43
1:0:2510:A:N6	1:0:2641:A:H61	2.11	0.43
1:0:2680:U:H3'	1:0:2681:A:C5'	2.47	0.43
1:0:538:A:C3'	1:0:539:A:H5''	2.48	0.43
1:0:67:G:C4	1:0:73:A:C8	3.06	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
1:0:1605:A:H2'	1:0:1606:C:C6	2.54	0.43
1:0:242:A:O2'	1:0:243:G:OP2	2.37	0.43
1:0:420:C:H2'	1:0:421:G:C8	2.53	0.43
1:0:475:U:H2'	1:0:476:G:O4'	2.18	0.43
1:0:1614:C:H2'	1:0:1615:C:C6	2.53	0.43
1:0:173:A:N3	1:0:173:A:C2'	2.81	0.43
1:0:1938:U:H2'	1:0:1939:U:H5'	1.99	0.43
1:0:2497:A:O5'	1:0:2497:A:N3	2.52	0.43
1:0:1774:A:N1	1:0:2566:A:H2'	2.34	0.43
1:0:2780:A:H2'	1:0:2781:G:H8	1.83	0.43
1:0:2874:A:H2'	1:0:2875:C:C6	2.54	0.43
1:0:456:C:H2'	1:0:457:C:C6	2.54	0.43
1:0:871:U:H1'	1:0:2248:A:C5'	2.47	0.43
1:0:114:C:H4'	1:0:124:A:O2'	2.17	0.43
1:0:1478:U:H2'	1:0:1479:G:C8	2.53	0.43
1:0:1518:C:HO2'	1:0:1519:G:P	2.41	0.43
1:0:1975:G:H1'	1:0:1977:C:N4	2.33	0.43
1:0:2033:C:H2'	1:0:2034:A:O4'	2.18	0.43
1:0:810:U:H2'	1:0:811:G:H8	1.83	0.43
1:0:838:A:H4'	1:0:2407:G:C5	2.54	0.43
1:0:1075:C:H2'	1:0:1076:U:C6	2.54	0.43
1:0:109:A:H2'	1:0:110:U:H5''	2.00	0.43
1:0:1500:U:H2'	1:0:1501:C:C6	2.54	0.43
1:0:1518:C:H2'	1:0:1519:G:H8	1.84	0.43
1:0:192:G:O2'	1:0:193:A:P	2.76	0.43
1:0:1961:A:H2'	1:0:1962:C:O4'	2.18	0.43
1:0:215:G:H1'	1:0:617:U:O2	2.19	0.43
1:0:547:U:H2'	1:0:548:G:C8	2.53	0.43
1:0:88:G:H3'	1:0:89:A:C5'	2.42	0.43
1:0:959:C:H2'	1:0:960:U:C6	2.54	0.43
2:5:32:A:C5	2:5:33:C:H1'	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1033:G:N2	1:0:1150:C:H2'	2.29	0.43
1:0:1326:U:H4'	1:0:1345:G:H4'	2.01	0.43
1:0:2002:A:H61	1:0:2018:G:N2	2.16	0.43
1:0:201:G:H2'	1:0:202:A:H8	1.84	0.43
1:0:2056:C:H2'	1:0:2057:U:H6	1.84	0.43
1:0:2244:C:H1'	1:0:2255:G:N1	2.34	0.43
1:0:2265:A:H5''	1:0:2266:A:O4'	2.19	0.43
1:0:2602:G:OP1	1:0:2801:A:H1'	2.19	0.43
1:0:653:G:C2	1:0:655:A:H1'	2.53	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
1:0:967:G:H1'	1:0:970:A:N7	2.34	0.43
1:0:1455:C:HO2'	1:0:1644:G:H5''	1.84	0.43
1:0:1341:G:N2	1:0:1664:G:H1	2.15	0.43
1:0:1880:G:H2'	1:0:1881:U:C6	2.54	0.43
1:0:2213:G:H2'	1:0:2214:G:H8	1.84	0.43
1:0:2369:U:H2'	1:0:2370:G:C8	2.54	0.43
1:0:2586:G:H2'	1:0:2587:G:O4'	2.18	0.43
1:0:2785:A:O2'	1:0:2786:G:H5'	2.19	0.43
1:0:2795:A:N3	1:0:2795:A:H2'	2.32	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
1:0:814:G:H3'	1:0:815:A:C5'	2.49	0.43
1:0:878:C:HO2'	1:0:879:A:P	2.42	0.43
1:0:1194:U:H2'	1:0:1195:U:H6	1.79	0.43
1:0:121:G:H2'	1:0:122:G:O4'	2.19	0.43
1:0:762:A:H5'	1:0:1284:G:H1'	1.99	0.43
1:0:128:C:C3'	1:0:129:A:H5''	2.49	0.43
1:0:1604:A:H2'	1:0:1605:A:O4'	2.19	0.43
1:0:187:U:H2'	1:0:188:G:H8	1.83	0.43
1:0:1937:G:H4'	1:0:2529:G:H21	1.83	0.43
1:0:211:U:H2'	1:0:212:U:O4'	2.19	0.43
1:0:2310:G:H2'	1:0:2311:U:O4'	2.18	0.43
1:0:2311:U:HO2'	1:0:2312:A:H8	1.63	0.43
1:0:2034:A:N6	1:0:2593:A:N7	2.66	0.43
2:5:7:A:H2'	2:5:8:A:C8	2.54	0.43
1:0:1046:U:H2'	1:0:1047:G:H8	1.84	0.42
1:0:1193:G:O2'	1:0:1194:U:P	2.76	0.42
1:0:1591:U:H2'	1:0:1592:U:O4'	2.18	0.42
1:0:1917:C:H2'	1:0:1918:G:H5'	2.01	0.42
1:0:192:G:O2'	1:0:193:A:H5''	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2083:G:H22	1:0:2172:U:H3	1.66	0.42
1:0:242:A:N6	1:0:441:A:N7	2.66	0.42
1:0:2808:U:H3'	1:0:2809:A:C5'	2.47	0.42
1:0:539:A:N6	1:0:2024:U:H3	2.16	0.42
1:0:591:G:H2'	1:0:592:G:C8	2.54	0.42
1:0:628:A:H2'	1:0:629:C:H6	1.81	0.42
1:0:652:C:N4	1:0:657:A:H61	2.09	0.42
1:0:1743:C:H2'	1:0:1744:G:C8	2.54	0.42
1:0:172:A:N3	1:0:227:G:N2	2.65	0.42
1:0:2473:G:O2'	1:0:2474:G:H5'	2.19	0.42
1:0:2615:U:H3	1:0:2762:G:H1	1.66	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
1:0:81:C:O2'	1:0:82:G:H5'	2.19	0.42
1:0:820:U:H1'	1:0:2424:G:OP1	2.18	0.42
1:0:944:A:H2'	1:0:945:G:O4'	2.19	0.42
1:0:987:G:H2'	1:0:988:G:C8	2.54	0.42
1:0:1017:C:H2'	1:0:1018:C:O4'	2.18	0.42
1:0:1147:G:H2'	1:0:1148:G:H8	1.84	0.42
1:0:953:G:H4'	1:0:1203:A:O2'	2.19	0.42
1:0:1259:A:H2'	1:0:1260:A:H8	1.83	0.42
1:0:1489:C:H3'	1:0:1490:U:H5'	2.00	0.42
1:0:1532:A:H2'	1:0:1533:G:C8	2.53	0.42
1:0:181:A:C5'	1:0:182:G:OP1	2.62	0.42
1:0:2225:G:O2'	1:0:2226:A:H5'	2.20	0.42
1:0:2380:U:C2'	1:0:2381:A:H5'	2.44	0.42
1:0:2564:U:C4'	1:0:2565:C:H5'	2.49	0.42
1:0:2658:A:H2'	1:0:2659:C:H6	1.84	0.42
1:0:37:C:H2'	1:0:38:G:C8	2.54	0.42
1:0:1057:A:H3'	1:0:1058:G:H5'	2.00	0.42
1:0:1626:A:H5''	1:0:1627:C:OP2	2.20	0.42
1:0:2038:C:H5'	1:0:2039:G:C5'	2.49	0.42
1:0:2161:C:H2'	1:0:2162:C:C5	2.55	0.42
1:0:2261:G:H4'	1:0:2368:G:O2'	2.20	0.42
1:0:2426:G:H22	1:0:2431:C:H41	1.67	0.42
1:0:178:C:H4'	1:0:399:G:C2	2.54	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
1:0:1029:C:C2'	1:0:1030:U:H5''	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2204:A:HO2'	1:0:2205:C:H6	1.60	0.42
1:0:2757:G:H5'	1:0:2761:A:C1'	2.50	0.42
1:0:415:A:O2'	1:0:416:U:H5'	2.20	0.42
1:0:63:A:O2'	1:0:64:C:H5'	2.19	0.42
1:0:764:A:H3'	1:0:764:A:N3	2.35	0.42
2:5:33:C:H3'	2:5:34:C:C5'	2.48	0.42
1:0:1343:C:H2'	1:0:1344:C:C6	2.55	0.42
1:0:1489:C:H3'	1:0:1490:U:C5'	2.50	0.42
1:0:1762:C:H2'	1:0:1763:G:C8	2.54	0.42
1:0:1957:C:O2'	1:0:1958:G:H5'	2.19	0.42
1:0:2633:A:H4'	1:0:2634:G:C4'	2.40	0.42
1:0:3:U:H2'	1:0:4:C:C6	2.54	0.42
1:0:404:A:H1'	1:0:424:G:O2'	2.19	0.42
1:0:509:U:H2'	1:0:510:G:O4'	2.19	0.42
1:0:860:U:O2	1:0:860:U:H2'	2.19	0.42
1:0:984:A:H2'	1:0:1200:G:N2	2.33	0.42
1:0:1065:A:H2'	1:0:1066:G:C8	2.55	0.42
1:0:1187:A:HO2'	1:0:1188:A:P	2.41	0.42
1:0:1193:G:O2'	1:0:1194:U:OP1	2.36	0.42
1:0:119:G:H1'	1:0:129:A:N1	2.35	0.42
1:0:1281:A:N6	1:0:1995:G:O2'	2.52	0.42
1:0:1451:C:H2'	1:0:1452:U:C6	2.54	0.42
1:0:1566:G:H2'	1:0:1567:A:C8	2.55	0.42
1:0:1634:A:O2'	1:0:1635:G:H5'	2.19	0.42
1:0:1790:G:O3'	1:0:1791:C:H6	2.02	0.42
1:0:1836:C:H2'	1:0:1837:G:H8	1.84	0.42
1:0:2217:G:H5'	1:0:2219:U:O4	2.19	0.42
1:0:2555:G:C2'	1:0:2555:G:N3	2.83	0.42
1:0:354:C:H2'	1:0:355:G:O4'	2.20	0.42
1:0:644:A:H2'	1:0:645:G:O4'	2.19	0.42
1:0:646:C:O2'	1:0:650:U:H5''	2.19	0.42
1:0:649:G:H2'	1:0:650:U:C6	2.54	0.42
1:0:786:U:H2'	1:0:787:A:H5'	2.01	0.42
1:0:879:A:C2'	1:0:880:C:H5'	2.49	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
1:0:1671:A:C1'	1:0:2798:A:H5'	2.50	0.42
1:0:1926:U:O2'	1:0:1927:U:O5'	2.36	0.42
1:0:2133:G:H2'	1:0:2134:U:C6	2.55	0.42
1:0:2217:G:C2'	1:0:2217:G:N3	2.83	0.42
1:0:964:A:H1'	1:0:2245:A:OP2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:0:2824: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
1:0:562:G:H2'	1:0:563:U:O4'	2.20	0.42
1:0:1332:G:H2'	1:0:1333:G:O4'	2.20	0.42
1:0:1801:C:H3'	1:0:1802:A:H5'	2.02	0.42
1:0:198:A:O2'	1:0:199:A:OP2	2.30	0.42
1:0:2027:C:H2'	1:0:2028:C:C6	2.55	0.42
1:0:2500:C:H4'	1:0:2544:A:C4'	2.50	0.42
1:0:2633:A:H61	1:0:2646:C:N4	2.18	0.42
1:0:2766:U:O2'	1:0:2767:C:H5'	2.19	0.42
1:0:327:C:O2'	1:0:328:A:H5'	2.20	0.42
1:0:430:C:H2'	1:0:431:G:C8	2.54	0.42
1:0:617:U:H2'	1:0:618:A:O4'	2.20	0.42
1:0:669:G:H2'	1:0:670:U:H6	1.83	0.42
1:0:956:A:N3	1:0:956:A:H2'	2.34	0.42
1:0:1143:A:H2'	1:0:1144:U:C6	2.55	0.42
1:0:1479:G:H2'	1:0:1480:G:C8	2.54	0.42
1:0:1917:C:C2'	1:0:1918:G:H5'	2.49	0.42
1:0:2463:G:O2'	1:0:2464:G:H5'	2.20	0.42
1:0:2651:U:H2'	1:0:2652:G:H8	1.85	0.42
1:0:2784:A:C8	1:0:2785:A:C8	3.07	0.42
1:0:2836:U:H2'	1:0:2837:G:C8	2.55	0.42
1:0:520:C:H2'	1:0:521:U:O4'	2.20	0.42
1:0:878:C:O2'	1:0:879:A:OP1	2.35	0.42
1:0:1594:U:H2'	1:0:1595:A:C8	2.55	0.41
1:0:1962:C:H2'	1:0:1963:G:H8	1.85	0.41
1:0:2028:C:O2'	1:0:2029:G:H5'	2.20	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
1:0:2470:U:H1'	1:0:2548:G:O3'	2.20	0.41
1:0:1949:A:H1'	1:0:2572:U:H5'	2.01	0.41
1:0:2698:G:H2'	1:0:2699:G:O4'	2.19	0.41
1:0:314:G:H2'	1:0:315:G:H8	1.85	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
1:0:65:C:C3'	1:0:66:U:H5'	2.49	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
1:0:1938:U:O2'	1:0:1939:U:H5'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:873:U:C2	1:0:2246:A:H5''	2.55	0.41
1:0:1142:G:OP1	1:0:2494:C:H4'	2.20	0.41
1:0:2710:C:O2'	1:0:2711:G:H5'	2.20	0.41
1:0:319:G:H1'	1:0:511:A:H5'	2.02	0.41
1:0:438:G:H2'	1:0:439:C:C6	2.54	0.41
1:0:63:A:N6	1:0:89:A:N1	2.69	0.41
1:0:1177:U:H2'	1:0:1178:C:C6	2.55	0.41
1:0:1225:G:H2'	1:0:1249:G:N1	2.35	0.41
1:0:1231:A:H2'	1:0:1232:U:O4'	2.20	0.41
1:0:1807:A:O2'	1:0:1808:C:C4'	2.64	0.41
1:0:1829:C:O2'	1:0:1910:A:H1'	2.20	0.41
1:0:1888:C:H2'	1:0:1913:G:C6	2.55	0.41
1:0:579:G:H2'	1:0:2013:A:C5	2.55	0.41
1:0:2096:U:C2'	1:0:2097:A:H5''	2.44	0.41
1:0:871:U:O2	1:0:2247:A:H2'	2.20	0.41
1:0:2392:G:H2'	1:0:2393:G:H8	1.85	0.41
1:0:820:U:H5'	1:0:2424:G:H4'	2.01	0.41
1:0:2502:G:H2'	1:0:2503:G:H8	1.85	0.41
1:0:2564:U:H4'	1:0:2565:C:H5'	2.02	0.41
1:0:2640:G:H2'	1:0:2641:A:O4'	2.19	0.41
1:0:239:A:H5'	1:0:619:A:O2'	2.20	0.41
1:0:1172:U:H2'	1:0:1173:G: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
1:0:1495:G:O2'	1:0:1496:G:OP1	2.35	0.41
1:0:1671:A:H2'	1:0:1672:A:H8	1.86	0.41
1:0:1956:G:H2'	1:0:1957:C:O4'	2.20	0.41
1:0:2032:G:O2'	1:0:2033:C:H5'	2.20	0.41
1:0:2320:G:H2'	1:0:2321:C:C6	2.56	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
1:0:833:A:H2'	1:0:834:A:C8	2.55	0.41
1:0:1365:U:H5'	1:0:1587:A:H1'	2.03	0.41
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
1:0:159: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
1:0:2245:A:O2'	1:0:2246:A:P	2.78	0.41
1:0:317:U:H3'	1:0:318:G:C5'	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:853:C:H2'	1:0:854:G:C8	2.56	0.41
1:0:930:A:H3'	1:0:931:G:H8	1.85	0.41
1:0:1193:G:HO2'	1:0:1194:U:P	2.43	0.41
1:0:1329:U:H2'	1:0:1330:G:C8	2.56	0.41
1:0:1341:G:N2	1:0:1343:C:H1'	2.36	0.41
1:0:1415:C:O2'	1:0:1416:A:H5'	2.21	0.41
1:0:1464:A:H4'	1:0:1545:G:C4'	2.51	0.41
1:0:155:G:O2'	1:0:156:G:H5'	2.21	0.41
1:0:1774:A:H1'	1:0:2586:G:N2	2.31	0.41
1:0:2076:G:H2'	1:0:2077:G:C8	2.54	0.41
1:0:2134:U:H2'	1:0:2135:C:C6	2.55	0.41
1:0:2220:A:H2'	1:0:2221:G:H8	1.85	0.41
1:0:2348:A:H2'	1:0:2349:G:C8	2.55	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
1:0:2740:C:O2'	1:0:2741:G:H5'	2.20	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
1:0:639:G:O2'	1:0:640:C:H5'	2.21	0.41
1:0:769:C:H2'	1:0:770:U:O4'	2.20	0.41
1:0:857:U:C2'	1:0:858:G:H5'	2.50	0.41
1:0:1028:G:H2'	1:0:1029:C:H6	1.86	0.41
1:0:69:G:O3'	1:0:111:G:H4'	2.20	0.41
1:0:189:A:H2'	1:0:190:A:C8	2.55	0.41
1:0:2083:G:N2	1:0:2172:U:H3	2.18	0.41
1:0:307:C:H2'	1:0:308:C:H6	1.85	0.41
1:0:1286:U:H2'	1:0:2692:A:H2	1.85	0.41
1:0:139:A:H2'	1:0:140:G:C8	2.55	0.41
1:0:1521:U:H2'	1:0:1522:C:C6	2.56	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
1:0:1985:G:H2'	1:0:1986:G:C8	2.56	0.41
1:0:2011:U:H2'	1:0:2012:A:C8	2.56	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
1:0:488: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
1:0:691:C:H2'	1:0:692:C:C6	2.56	0.41
1:0:690:A:O2'	1:0:691:C:H5'	2.21	0.41
1:0:831:G:H2'	1:0:832:A:H5''	2.03	0.41
1:0:874:A:H2'	1:0:875:G:H5'	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:964:A:H2'	1:0:965:G:H8	1.85	0.41
1:0:1098:G:H21	1:0:1100:G:H4'	1.86	0.41
1:0:1221:C:H2'	1:0:1222:G:H8	1.85	0.41
1:0:1242:A:H2'	1:0:1243:G:C8	2.55	0.41
1:0:1594:U:H2'	1:0:1595:A:H8	1.85	0.41
1:0:1722:G:H2'	1:0:1723:U:C6	2.55	0.41
1:0:2200:G:H2'	1:0:2201:G:C8	2.56	0.41
1:0:2378:G:H2'	1:0:2379:G:C8	2.55	0.41
1:0:2383:C:H2'	1:0:2384:G:O4'	2.20	0.41
1:0:2404:A:OP1	1:0:2406:C:H5'	2.21	0.41
1:0:2448:A:C2'	1:0:2449:G:H5'	2.50	0.41
1:0:1084:A:H4'	1:0:2454:C:OP1	2.20	0.41
1:0:344:G:O2'	1:0:345:U:H5'	2.21	0.41
1:0:40:U:H2'	1:0:41:G:H8	1.86	0.41
1:0:925:U:H5''	1:0:926:C:OP1	2.21	0.41
1:0:1168:G:H2'	1:0:1169:C:C6	2.55	0.41
1:0:1352:G:N2	1:0:1619:A:H8	2.19	0.41
1:0:1586:A:H2'	1:0:1587:A:H8	1.86	0.41
1:0:1671:A:H1'	1:0:2798:A:H5'	2.02	0.41
1:0:1887:G:O2'	1:0:1888:C:H5'	2.21	0.41
1:0:1998:A:H2'	1:0:1999:U:H5'	2.02	0.41
1:0:2226:A:H2'	1:0:2227:C:H6	1.86	0.41
1:0:229:G:H2'	1:0:230:C:C6	2.56	0.41
1:0:2365:U:O2'	1:0:2366:U:H5'	2.21	0.41
1:0:2555:G:N3	1:0:2555:G:H2'	2.36	0.41
1:0:2560:G:H4'	1:0:2561:G:C8	2.56	0.41
1:0:305:A:H2'	1:0:306:G:O4'	2.21	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
1:0:1313:U:O2'	1:0:1314:A:OP2	2.39	0.41
1:0:1685:A:O2'	1:0:1686:A:O5'	2.39	0.41
1:0:2014:A:O5'	1:0:2014:A:H8	2.04	0.41
1:0:2056:C:H2'	1:0:2057:U:C6	2.56	0.41
1:0:218:A:H1'	1:0:220:U:C4	2.56	0.41
1:0:2390:A:H2'	1:0:2391:A:C8	2.56	0.41
1:0:24:G:H2'	1:0:25:U:C6	2.55	0.41
1:0:2548:G:H2'	1:0:2549:G:C5'	2.33	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
1:0:729:A:O2'	1:0:730:C:H5'	2.21	0.41
1:0:170:U:H5'	1:0:815:A:H2	1.86	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
1:0:2058:U:H3'	1:0:2217:G:N1	2.36	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
1:0:322:A:H1'	1:0:343:A:N7	2.36	0.40
1:0:322:A:H2	1:0:342:G:OP2	2.04	0.40
1:0:432:C:H2'	1:0:433:G:C8	2.57	0.40
1:0:82:G:O2'	1:0:83:A:H5'	2.21	0.40
1:0:1026:U:H2'	1:0:1027:C:C6	2.56	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
1:0:1850:G:H2'	1:0:1851:A:C8	2.55	0.40
1:0:1915:A:H2'	1:0:1916:G:O4'	2.21	0.40
1:0:2169:A:O2'	1:0:2170:C:H5'	2.21	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
1:0:2389:G:H2'	1:0:2390:A:O4'	2.21	0.40
1:0:2515:G:H2'	1:0:2516:U:C6	2.56	0.40
1:0:2824:C:C2'	1:0:2825:A:OP2	2.70	0.40
1:0:28:A:H2'	1:0:29:U:C6	2.56	0.40
1:0:44:G:N2	1:0:192:G:N2	2.69	0.40
1:0:477:A:H2'	1:0:478:G:H5'	2.02	0.40
1:0:607:C:H2'	1:0:608:G:C8	2.57	0.40
1:0:67:G:N2	1:0:73:A:O4'	2.54	0.40
1:0:747:A:H2'	1:0:748:A:H8	1.85	0.40
1:0:808:C:H2'	1:0:809:C:C6	2.57	0.40
2:5:22:G:H2'	2:5:23:C:C6	2.57	0.40
1:0:1040:A:C2'	1:0:1041:G:H5'	2.51	0.40
1:0:105:G:O2'	1:0:106:G:H5'	2.20	0.40
1:0:1162:A:H2'	1:0:1163:C:H6	1.87	0.40
1:0:1187:A:O2'	1:0:1188:A:P	2.79	0.40
1:0:1466:C:O2'	1:0:1467:U:H5'	2.21	0.40
1:0:1653:C:H2'	1:0:1654:A:C8	2.56	0.40
1:0:1696:C:H42	1:0:1755:G:H5''	1.87	0.40
1:0:185:C:H2'	1:0:186:C:C6	2.56	0.40
1:0:198:A:H4'	1:0:199:A:OP2	2.21	0.40
1:0:2081:U:H2'	1:0:2082:C:C5'	2.43	0.40
1:0:2234:G:H2'	1:0:2235:G:O4'	2.22	0.40
1:0:2241:U:H4'	1:0:2307:A:C2	2.56	0.40
1:0:2417:U:H4'	1:0:2419:C:OP1	2.22	0.40
1:0:2437:G:C2	1:0:2469:G:H2'	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2594:U:H2'	1:0:2595:C:C6	2.57	0.40
1:0:688:A:H1'	1:0:2422:C:O2'	2.21	0.40
1:0:854:G:H2'	1:0:855:G:C8	2.57	0.40
1:0:868:U:H2'	1:0:869:C:H6	1.86	0.40
1:0:890:U:H2'	1:0:891:A:C8	2.57	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
1:0:978:U:H2'	1:0:979:A:C8	2.56	0.40
1:0:1370:U:H2'	1:0:1371:G:O4'	2.22	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
1:0:1625:A:C4	1:0:1632:A:H1'	2.56	0.40
1:0:1736:C:H2'	1:0:1737:G:C8	2.57	0.40
1:0:1787:U:H2'	1:0:1788:C:C6	2.57	0.40
1:0:1982:C:H2'	1:0:1983:G:H8	1.86	0.40
1:0:579:G:H2'	1:0:2013:A:C6	2.56	0.40
1:0:2048:C:H2'	1:0:2049:C:H6	1.86	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
1:0:2383:C:C2'	1:0:2384:G:H5'	2.51	0.40
1:0:2553:G:H2'	1:0:2554:C:O4'	2.21	0.40
1:0:2418:A:N6	1:0:2581:A:OP1	2.54	0.40
1:0:2851:G:H2'	1:0:2852:G:C8	2.56	0.40
1:0:105:G:H21	1:0:357:A:N6	2.19	0.40
1:0:528:G:H2'	1:0:529:U:C6	2.57	0.40
1:0:550:C:H2'	1:0:551:A:H8	1.86	0.40
1:0:633:G:O2'	1:0:634:G:H5'	2.22	0.40
1:0:798:G:OP2	1:0:805:G:N7	2.54	0.40
1:0:1036:G:H1'	1:0:1145:C:H4'	2.03	0.40
1:0:1253:C:H2'	1:0:1254:G:O4'	2.21	0.40
1:0:1337:G:H1'	1:0:1632:A:C6	2.56	0.40
1:0:1358:C:C2'	1:0:1359:G:H5''	2.52	0.40
1:0:1369:G:H2'	1:0:1370:U:O4'	2.21	0.40
1:0:1398:G:H2'	1:0:1399:C:C6	2.56	0.40
1:0:1539:U:H2'	1:0:1540:C:C6	2.56	0.40
1:0:1806:G:O6	1:0:1807:A:N6	2.54	0.40
1:0:1918:G:H4'	1:0:1920:A:C2	2.57	0.40
1:0:2015:G:OP2	1:0:2434:G:H5'	2.22	0.40
1:0:2075:U:H1'	1:0:2204:A:C2	2.56	0.40
1:0:689:A:H8	1:0:2422:C:H1'	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2502:G:H2'	1:0:2503:G:C8	2.56	0.40
1:0:744:C:H2'	1:0:745:C:C6	2.56	0.40
1:0:948:C:H2'	1:0:949:G:C8	2.57	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	32,40,41	2.81	6 (18%)	33,57,60	0.98	3 (9%)

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	C-N3'	12.63	1.61	1.34
2	5	35	PPU	OC-CM	-4.96	1.27	1.42
2	5	35	PPU	C6-N1	3.86	1.38	1.33
2	5	35	PPU	CE1-CZ	3.70	1.46	1.38
2	5	35	PPU	CE2-CZ	2.70	1.44	1.38
2	5	35	PPU	CD2-CG	2.54	1.44	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	35	PPU	CM-OC-CZ	2.93	123.86	117.51
2	5	35	PPU	C9-N6-C6	2.23	126.26	119.51
2	5	35	PPU	C-CA-N	2.22	117.97	109.40

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	-	19,22,23	4.43	9 (47%)	17,28,30	4.15	8 (47%)

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	9/15/16/18	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	O10-C10	9.82	1.43	1.24
5	0	2881	SPS	C9-C8	8.40	1.54	1.33
5	0	2881	SPS	O1-C1	7.67	1.43	1.24
5	0	2881	SPS	C10-N11	6.56	1.50	1.34
5	0	2881	SPS	C5-N4	5.43	1.42	1.34
5	0	2881	SPS	C1-N2	5.39	1.42	1.33
5	0	2881	SPS	C6-C8	3.98	1.56	1.47
5	0	2881	SPS	C9-C10	2.96	1.54	1.48
5	0	2881	SPS	C7-C5	2.89	1.55	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	0	2881	SPS	C12-N11-C10	-7.47	112.03	122.57
5	0	2881	SPS	C1-N2-C3	6.40	120.55	115.14
5	0	2881	SPS	C8-C9-C10	-6.14	109.55	121.56
5	0	2881	SPS	C14-S15-C16	6.14	109.42	101.04
5	0	2881	SPS	O10-C10-C9	-5.96	109.44	123.03
5	0	2881	SPS	C6-C1-N2	-5.87	120.31	124.40
5	0	2881	SPS	C9-C10-N11	5.63	125.37	114.56
5	0	2881	SPS	O10-C10-N11	2.15	125.19	122.35

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	0	2881	SPS	C12

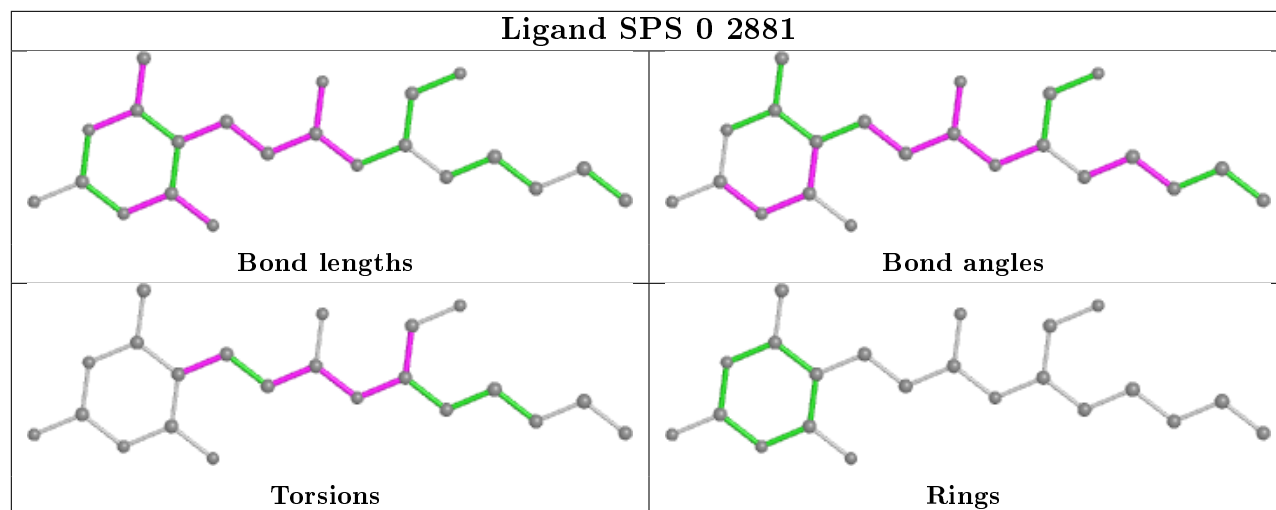
All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	0	2881	SPS	C1-C6-C8-C9
5	0	2881	SPS	C9-C10-N11-C12
5	0	2881	SPS	O10-C10-N11-C12
5	0	2881	SPS	C14-C12-C13-O13
5	0	2881	SPS	N11-C12-C13-O13
5	0	2881	SPS	C13-C12-N11-C10
5	0	2881	SPS	O10-C10-C9-C8
5	0	2881	SPS	N11-C10-C9-C8
5	0	2881	SPS	C14-C12-N11-C10

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.