



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 22, 2024 – 05:32 AM EDT

PDB ID : 4IOA  
Title : Crystal structure of compound 4e bound to large ribosomal subunit (50S) from *Deinococcus radiodurans*  
Authors : Han, S.; Marr, E.S.  
Deposited on : 2013-01-07  
Resolution : 3.20 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](mailto: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 types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

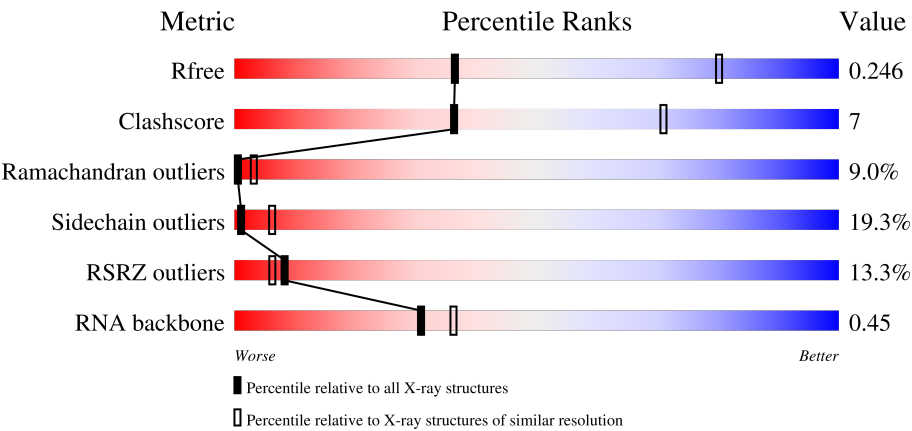
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	164625	1370 (3.20-3.20)
Clashscore	180529	1497 (3.20-3.20)
Ramachandran outliers	177936	1479 (3.20-3.20)
Sidechain outliers	177891	1478 (3.20-3.20)
RSRZ outliers	164620	1371 (3.20-3.20)
RNA backbone	3690	1111 (3.50-2.90)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	X	2880	<div><div>4%</div><div>36%</div><div>34%</div><div>19%</div><div>7%</div></div>
2	Y	123	<div><div>7%</div><div>40%</div><div>42%</div><div>15%</div><div></div></div>
3	A	274	<div><div>18%</div><div>48%</div><div>30%</div><div>8%</div><div>12%</div></div>
4	B	211	<div><div>5%</div><div>67%</div><div>21%</div><div>9%</div><div></div></div>

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Mol	Chain	Length	Quality of chain
5	C	205	
6	D	180	
7	E	185	
8	F	144	
9	G	174	
10	H	134	
11	I	156	
12	J	141	
13	K	116	
14	L	114	
15	M	166	
16	N	118	
17	O	100	
18	P	134	
19	Q	95	
20	R	115	
21	S	237	
22	T	91	
23	U	81	
24	V	67	
25	W	55	
26	Z	60	
27	1	55	
28	2	47	
29	3	66	

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Mol	Chain	Length	Quality of chain
30	4	37	<div> <div>84%</div> <div>73%</div> <div>24%</div> </div>

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
31	MG	X	2904	-	-	-	X
31	MG	X	2922	-	-	-	X
31	MG	X	2930	-	-	-	X

## 2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 83879 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	X	2686	Total	C	N	O	P	0	0	0
			57651	25718	10642	18606	2685			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	122	Total	C	N	O	P	0	0	0
			2598	1161	476	840	121			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	240	Total	C	N	O	S	0	0	0
			1826	1137	366	321	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	205	Total	C	N	O	S	0	0	0
			1539	965	295	271	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	197	Total	C	N	O	S	0	0	0
			1506	935	287	282	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	177	Total	C	N	O	S	0	0	0
			1400	892	247	254	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	171	Total	C	N	O	S	0	0	0
			1286	812	237	236	1			

- Molecule 8 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	71	Total	C	N	O	S	0	0	0
			503	310	91	99	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	G	142	Total	C	N	O	S	0	0	0
			1114	704	209	198	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	H	134	Total	C	N	O	S	0	0	0
			997	614	198	180	5			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	I	141	Total	C	N	O	0	0	0
			1067	655	216	196			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	J	136	Total	C	N	O	S	0	0	0
			1090	696	202	185	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	113	Total	C	N	O	S	0	0	0
			878	541	178	157	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	L	104	Total	C	N	O	0	0	0
			779	476	161	142			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	M	108	Total	C	N	O	0	0	0
			871	543	172	156			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	N	117	Total	C	N	O	S	0	0	0
			978	608	210	159	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	O	94	Total	C	N	O	0	0	0
			741	465	139	137			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	P	127	Total	C	N	O	S	0	0	0
			1014	639	199	174	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Q	93	Total	C	N	O	S	0	0	0
			726	458	136	130	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	110	Total	C	N	O	S	0	0	0
			825	513	160	151	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	S	175	Total	C	N	O	S	0	0	0
			1345	849	236	254	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	T	84	Total	C	N	O	S	0	0	0
			625	393	122	109	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	U	72	Total	C	N	O		0	0	0
			552	341	116	95				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	V	66	Total	C	N	O	S	0	0	0
			533	327	107	96	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	W	55	Total	C	N	O	S	0	0	0
			424	264	82	76	2			

- Molecule 26 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	58	Total	C	N	O	S	0	0	0
			457	281	94	77	5			

- Molecule 27 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
27	1	53	Total C	0	0	53
			53 53			

- Molecule 28 is a protein called 50S ribosomal protein L34.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
28	2	46	Total C 46 46	0	0	46

- Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
29	3	63	Total C 63 63	0	0	63

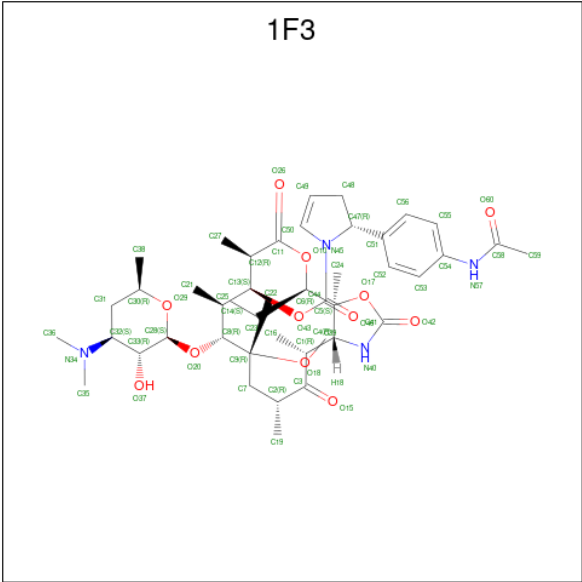
- Molecule 30 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
30	4	37	Total C N O S 297 179 66 47 5	0	0	0

- Molecule 31 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	X	30	Total Mg 30 30	0	0
31	Y	5	Total Mg 5 5	0	0

- Molecule 32 is (3aS,4R,7R,8S,9S,10R,11R,13R,15R,15aR)-4-ethyl-11-methoxy-3a,7,9,11,13,15-hexamethyl-2,6,14-trioxo-10-{[3,4,6-trideoxy-3-(dimethylamino)-beta-D-xylo-hexopyranosyl]oxy}tetradecahydro-2H-oxacyclotetradecino[4,3-d][1,3]oxazol-8-yl (2R)-2-[4-(acetylamino)phenyl]-2,3-dihydro-1H-pyrrole-1-carboxylate (three-letter code: 1F3) (formula: C<sub>44</sub>H<sub>66</sub>N<sub>4</sub>O<sub>12</sub>).

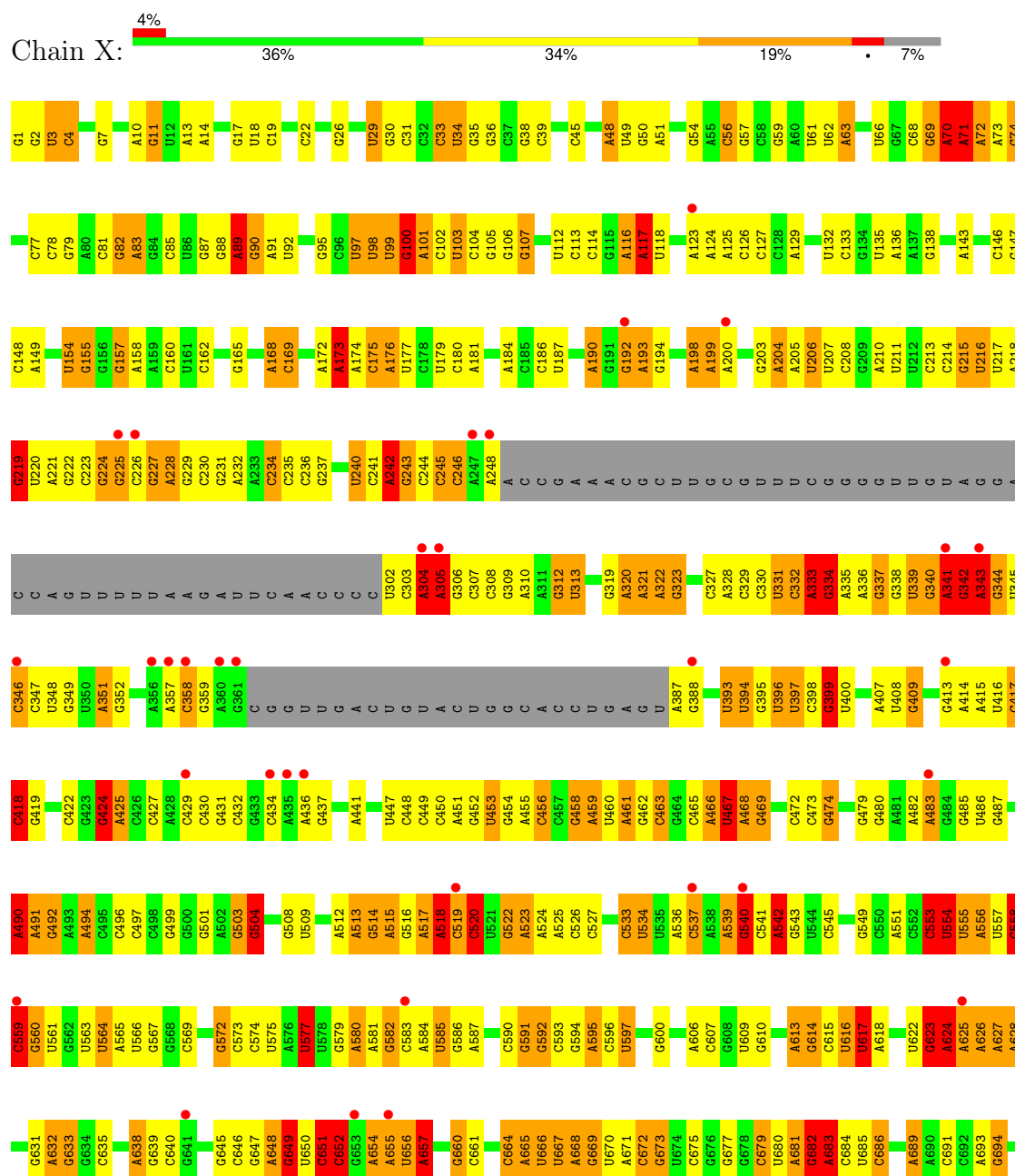


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	X	1	Total	C	N	O	0	0
			60	44	4	12		

### 3 Residue-property plots

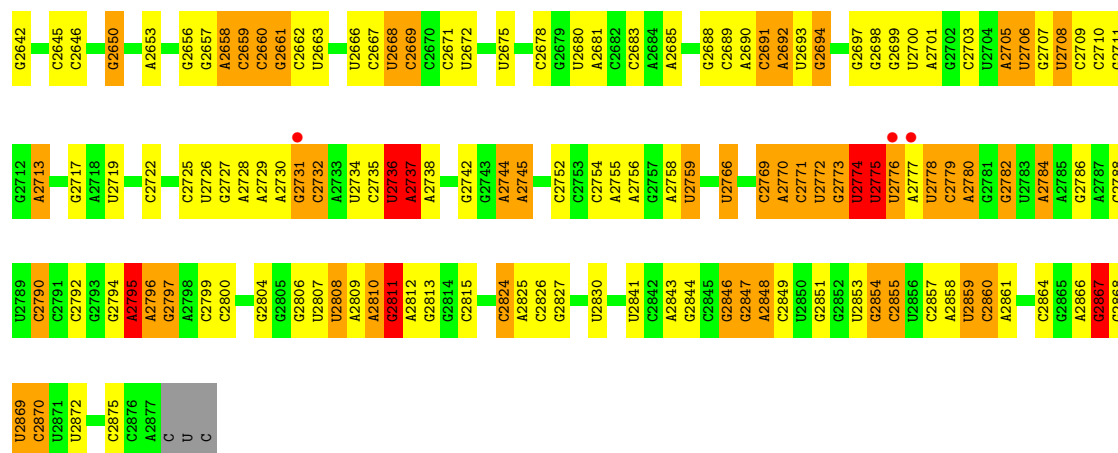
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

#### • Molecule 1: 23S ribosomal RNA

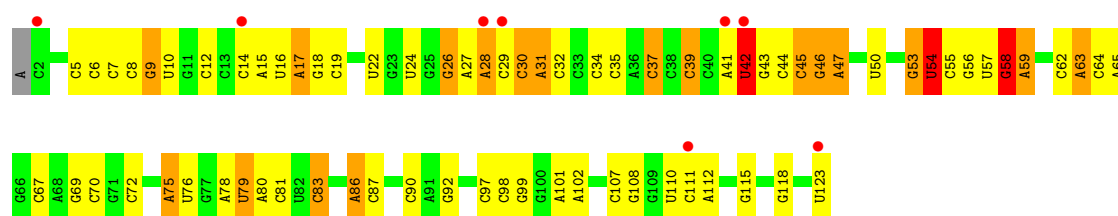


U1647	U1648	U1651	U1652	C1655	U1656	C1657	C1658	U1659	C1660	C1661	G1662	C1663	C1664	C1665	C1666	C1667	G1668	A1669	G1670	A1671	A1672	C1673	C1674	C1675	U1680	G1683	C1684	A1685	C1686	C1687	U1688	U1689	C1621	G1622	C1623	A1624	A1625	A1626	C1627	C1628	A1629	C1630	C1631	A1632	C1633	A1634	G1635	G1636	G1637	G1638	G1639	A1640	G1641	G1642	U1403	C1404	A1405	A1406	U1407	U1408	A1409	U1410	C1411	C1412	U1413	U1414	C1415	A1416	C1417	C1418	U1419	A1493	U1494	G1564	U1565	G1566	G1567	U1568	G1569	U1570	U1571	U1572	U1573	U1574	U1575	U1576	U1577	U1578	U1579	C1580	C1581	A1582	A1583	G1584	A1585	A1586	A1587	A1588	G1589	C1590	U1600	U1601	G1602	A1603	U1604	U1605	U1606	U1607	U1608	G1613	U1617	U1618	C1619	G1620	G1621	G1622	G1623	G1624	G1625	G1626	G1627	G1628	G1629	G1630	G1631	G1632	G1633	G1634	G1635	G1636	G1637	G1638	G1639	G1640	G1641	G1642	G1643	G1644	G1645	G1646	G1496	C1497	U1498	A1499	U1500	U1505	U1506	C1507	U1508	A1509	A1510	U1513	U1514	U1515	U1516	G1519	U1520	U1521	C1522	A1523	C1524	A1525	U1526	G1527	C1528	U1529	A1530	U1531	A1532	G1533	A1534	C1535	U1539	C1540	G1541	G1542	G1543	A1544	G1545	G1546	U1547	U1548	C1549	C1550	U1551	U1552	G1553	G1554	U1559	A1560	A1561	G1562	G1563	G1564	G1565	G1566	G1567	G1568	G1569	G1570	G1571	G1572	G1573	G1574	G1575	G1576	G1577	G1578	G1579	G1580	G1581	G1582	G1583	G1584	G1585	G1586	G1587	G1588	G1589	G1590	G1591	G1592	G1593	G1594	G1595	G1596	G1597	G1598	G1599	G1600	G1601	G1602	G1603	G1604	G1605	G1606	G1607	G1608	G1609	G1610	G1611	G1612	G1613	G1614	G1615	G1616	G1617	G1618	G1619	G1620	G1621	G1622	G1623	G1624	G1625	G1626	G1627	G1628	G1629	G1630	G1631	G1632	G1633	G1634	G1635	G1636	G1637	G1638	G1639	G1640	G1641	G1642	G1643	G1644	G1645	G1646	G1422	C1423	U1424	U1425	U1426	U1427	U1428	U1429	U1430	U1431	U1432	U1433	U1434	U1435	U1436	U1437	U1438	A1441	A1442	G1443	G1444	A1445	U1446	U1447	U1448	G1451	U1454	U1458	U1459	G1460	C1461	G1465	G1466	U1467	U1468	U1469	G1470	G1471	G1472	G1473	U1474	U1475	G1476	C1477	U1478	U1482	G1483	C1487	G1488	C1489	U1490	C1491	A1492	A1493	U1494	G1495	G1429	U1430	U1431	U1432	U1433	U1434	U1435	U1436	U1437	U1438	U1439	U1440	U1441	U1442	U1443	U1444	U1445	U1446	U1447	U1448	U1449	U1450	U1451	U1452	U1453	U1454	U1455	U1456	U1457	U1458	U1459	U1460	U1461	U1462	U1463	U1464	U1465	U1466	U1467	U1468	U1469	U1470	U1471	U1472	U1473	U1474	U1475	U1476	U1477	U1478	U1479	U1480	U1481	U1482	U1483	U1484	U1485	U1486	U1487	U1488	U1489	U1490	U1491	U1492	U1493	U1494	U1495	U1496	U1497	U1498	U1499	U1500	U1501	U1502	U1503	U1504	U1505	U1506	U1507	U1508	U1509	U1510	U1511	U1512	U1513	U1514	U1515	U1516	U1517	U1518	U1519	U1520	U1521	U1522	U1523	U1524	U1525	U1526	U1527	U1528	U1529	U1530	U1531	U1532	U1533	U1534	U1535	U1536	U1537	U1538	U1539	U1540	U1541	U1542	U1543	U1544	U1545	U1546	U1547	U1548	U1549	U1550	U1551	U1552	U1553	U1554	U1555	U1556	U1557	U1558	U1559	U1560	U1561	U1562	U1563	U1564	U1565	U1566	U1567	U1568	U1569	U1570	U1571	U1572	U1573	U1574	U1575	U1576	U1577	U1578	U1579	U1580	U1581	U1582	U1583	U1584	U1585	U1586	U1587	U1588	U1589	U1590	U1591	U1592	U1593	U1594	U1595	U1596	U1597	U1598	U1599	U1600	U1601	U1602	U1603	U1604	U1605	U1606	U1607	U1608	U1609	U1610	U1611	U1612	U1613	U1614	U1615	U1616	U1617	U1618	U1619	U1620	U1621	U1622	U1623	U1624	U1625	U1626	U1627	U1628	U1629	U1630	U1631	U1632	U1633	U1634	U1635	U1636	U1637	U1638	U1639	U1640	U1641	U1642	U1643	U1644	U1645	U1646	U1647	U1648	U1649	U1650	U1651	U1652	U1653	U1654	U1655	U1656	U1657	U1658	U1659	U1660	U1661	U1662	U1663	U1664	U1665	U1666	U1667	U1668	U1669	U1670	U1671	U1672	U1673	U1674	U1675	U1676	U1677	U1678	U1679	U1680	U1681	U1682	U1683	U1684	U1685	U1686	U1687	U1688	U1689	U1690	U1691	U1692	U1693	U1694	U1695	U1696	U1697	U1698	U1699	U1700	U1701	U1702	U1703	U1704	U1705	U1706	U1707	U1708	U1709	U1710	U1711	U1712	U1713	U1714	U1715	U1716	U1717	U1718	U1719	U1720	U1721	U1722	U1723	U1724	U1725	U1726	U1727	U1728	U1729	U1730	U1731	U1732	U1733	U1734	U1735	U1736	U1737	U1738	U1739	U1740	U1741	U1742	U1743	U1744	U1745	U1746	U1747	U1748	U1749	U1750	U1751	U1752	U1753	U1754	U1755	U1756	U1757	U1758	U1759	U1760	U1761	U1762	U1763	U1764	U1765	U1766	U1767	U1768	U1769	U1770	U1771	U1772	U1773	U1774	U1775	U1776	U1777	U1778	U1779	U1780	U1781	U1782	U1783	U1784	U1785	U1786	U1787	U1788	U1789	U1790	U1791	U1792	U1793	U1794	U1795	U1796	U1797	U1798	U1799	U1800	U1801	U1802	U1803	U1804	U1805	U1806	U1807	U1808	U1809	U1810	U1811	U1812	U1813	U1814	U1815	U1816	U1817	U1818	U1819	U1820	U1821	U1822	U1823	U1824	U1825	U1826	U1827	U1828	U1829	U1830	U1831	U1832	U1833	U1834	U1835	U1836	U1837	U1838	U1839	U1840	U1841	U1842	U1843	U1844	U1845	U1846	U1847	U1848	U1849	U1850	U1851	U1852	U1853	U1854	U1855	U1856	U1857	U1858	U1859	U1860	U1861	U1862	U1863	U1864	U1865	U1866	U1867	U1868	U1869	U1870	U1871	U1872	U1873	U1874	U1875	U1876	U1877	U1878	U1879	U1880	U1881	U1882	U1883	U1884	U1885	U1886	U1887	U1888	U1889	U1890	U1891	U1892	U1893	U1894	U1895	U1896	U1897	U1898	U1899	U1900	U1901	U1902	U1903	U1904	U1905	U1906	U1907	U1908	U1909	U1910	U1911	U1912	U1913	U1914	U1915	U1916	U1917	U1918	U1919	U1920	U1921	U1922	U1923	U1924	U1925	U1926	U1927	U1928	U1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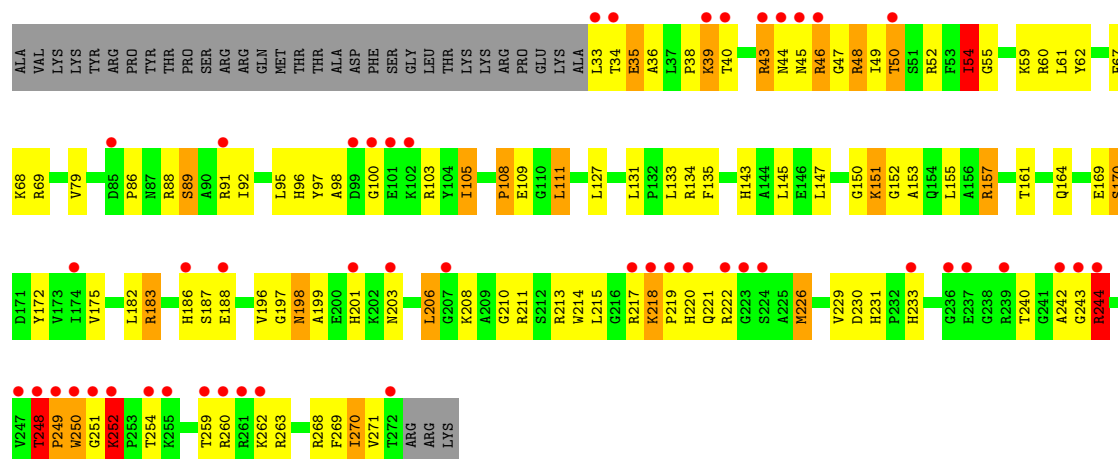
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U2441	A2371	G2299	G2299	G2230	C	U2016	C1945	G1806	G1807	G1735
U2442	A2372	G2300	G2300	G2231	C	U2017	G1946	U1807	U1736	
U2443	C2373	A2301	A2301	G2232	C	G2018	G1947	C1808	G1737	
U2444	C2374	G2302	G2302	G2232	C	C2019	C1947	U1809	G1737	
U2445	G2375	G2303	G2303	G2236	C	A2020	C1950	U1810	G1741	
U2446	G2376	G2304	G2304	G2237	C	A2025	G1951	U1811	G1742	
U2447	U2377	C2305	C2305	G2238	C	C2026	A1952	U1812		
U2448	U2377	A2306	A2306	G2239	C	A2031	A1953	A1813	C1746	
U2449	U2380	A2307	A2307	G2239	C	G2034	A1954	G1814	A1746	
U2452	A2381	G2308	G2308	U2241	C	G2035	G1955	G1815	U1747	
U2455	C2382	G2309	G2309	U2241	C	A2036	G1958	G1816	U1748	
U2456	G2383	G2310	G2310	U2242	C	G2037		U1817	G1749	
U2456	G2384	A2311	A2311	U2243	C	A2037	C1962	U1818	U1752	
U2456	U2385	G2312	G2312	U2243	C	G2038	G1963	U1819	A1753	
U2456	G2386	A2313	A2313	U2247	C	G2039	A1964	G1820	G1754	
U2463	U2387	A2314	A2314	U2251	C		U1965	A1821	G1755	
U2464	G2388	A2315	A2315	U2251	C	A2042	C1971	G1823		
U2470	G2389	U2318	U2318	U2254	C	A2043	G1972	C1824	C1758	
U2471	G2392	C2321	C2321	G2255	C	G2044	G1973	C1825		
U2472	G2393	U2322	U2322	G2256	C	A2045	U1974	U1826	C1762	
U2473	G2394	U2323	U2323	A2257	C	G2046	G1975	G1827	G1763	
U2474	C2395	G2324	G2324	G2258	C	C2047	U1976	C1828	A1764	
U2475	C2396	A2325	A2325	G2261	C	G2048	U1977	C1829	C1765	
U2476	A2397	U2326	U2326	G2262	C	C2049	C1977	C1830	U1766	
U2477	U2398	G2327	G2327	G2263	C	U2051	U1978	G1831	G1767	
U2478	G2401	G2328	G2328	C2264	C	G2052	C1979	G1832	U1768	
U2479	U2402	C2329	C2329	A2265	C	U2062	A1980	U1833	U1769	
U2480	C2403	G2330	G2330	G2266	C	A2063	A1981	G1834	U1770	
U2481	A2404	C2334	C2334	A2267	C	U2064	C1982	A1771	A1771	
U2482	A2405	U2335	U2335	U2270	C	U2067	G1983	C1772	C1772	
U2484	C2406	G2336	G2336	G2271	C		A1984	C1773	C1773	
U2485	G2407	G2339	G2339	A2272	C	G2070	G1985	A1910	A1774	
U2486	G2408	C2340	C2340	G2273	C	G2071	G1986	G1841	A1775	
U2487	A2409	G2343	G2343	G2274	C	G2072	G1987	G1842	A1776	
U2488	U2410	U2344	U2344	U2275	C	G2073	A1988	U1843	A1777	
U2489	A2414	G2344	G2344	G2276	C	U2074	U1989	C1844	U1778	
U2491	G2415	C2347	C2347	G2279	C	U2075	C1991	A1845	C1779	
U2492	U2416	A2348	A2348	G2280	C	G2076	G1992	G1850	C1781	
U2493	U2417	G2349	G2349	G2281	C		G1993	C1853	A1785	
U2494	A2418	G2350	G2350	G2282	C	A2079	U1994	G1854	C1786	
U2495	C2419	G2351	G2351	G2283	C	U2081	G1995	U1922	U1787	
A2641	C2496			U2284	C		G1996	C1858	C1788	
					C		A1997	A1859	U1789	



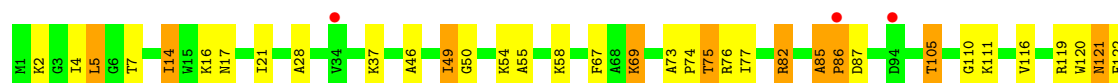
• Molecule 2: 5S ribosomal RNA



• Molecule 3: 50S ribosomal protein L2

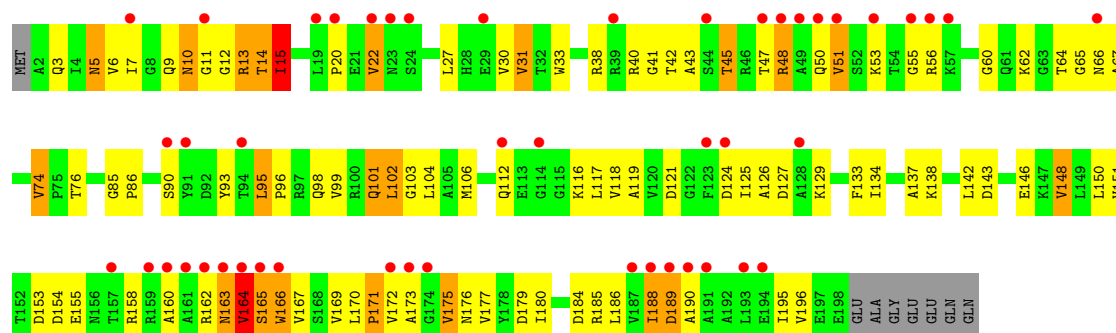


• Molecule 4: 50S ribosomal protein L3

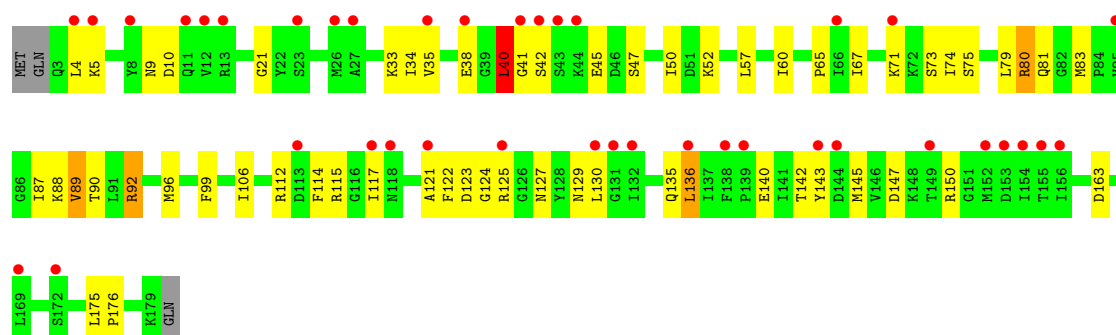




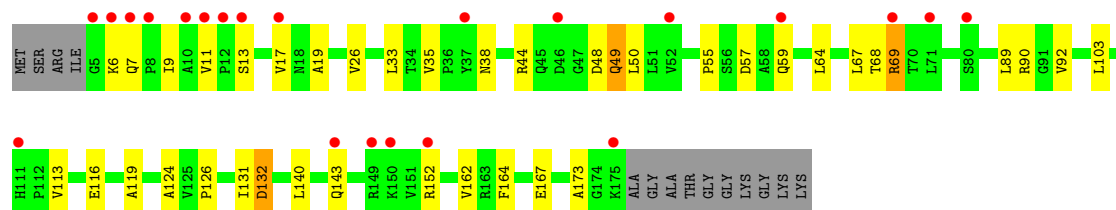
• Molecule 5: 50S ribosomal protein L4



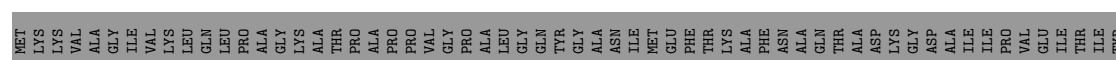
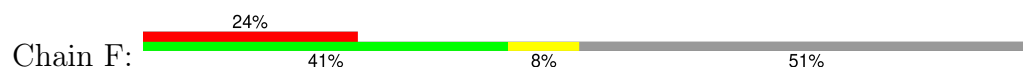
• Molecule 6: 50S ribosomal protein L5

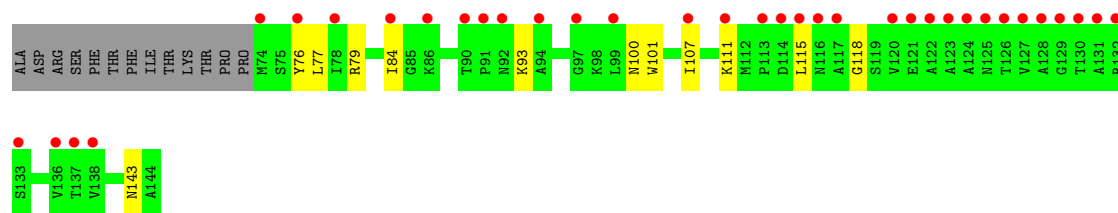


• Molecule 7: 50S ribosomal protein L6

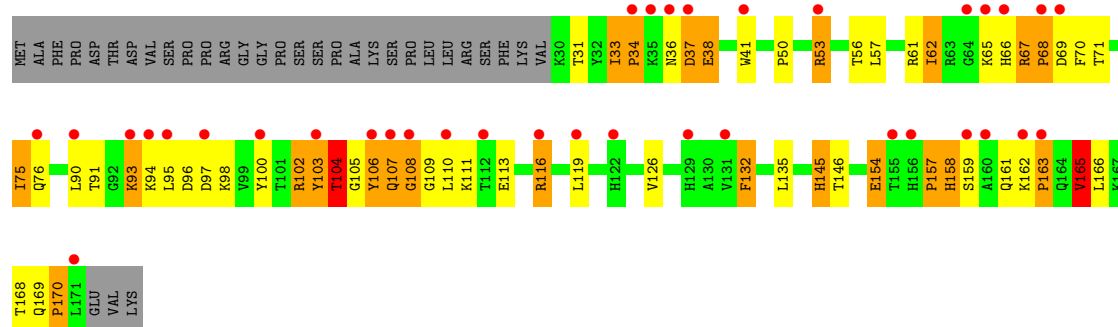


• Molecule 8: 50S ribosomal protein L11

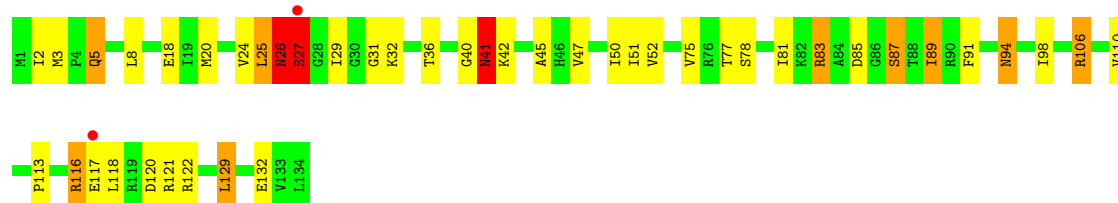




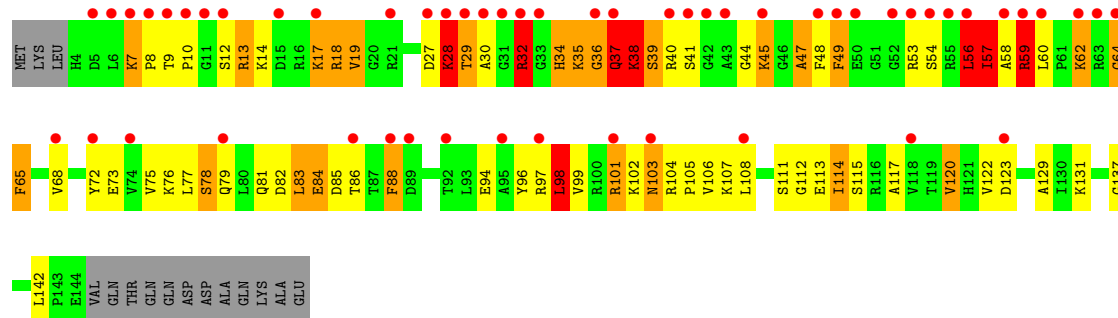
• Molecule 9: 50S ribosomal protein L13



• Molecule 10: 50S ribosomal protein L14



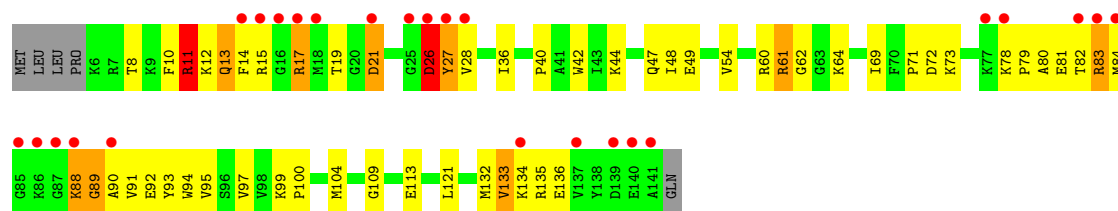
• Molecule 11: 50S ribosomal protein L15



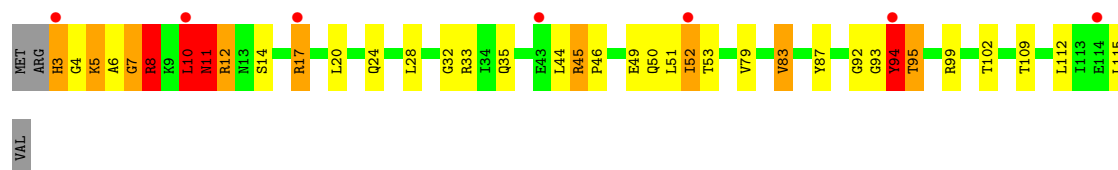
• Molecule 12: 50S ribosomal protein L16



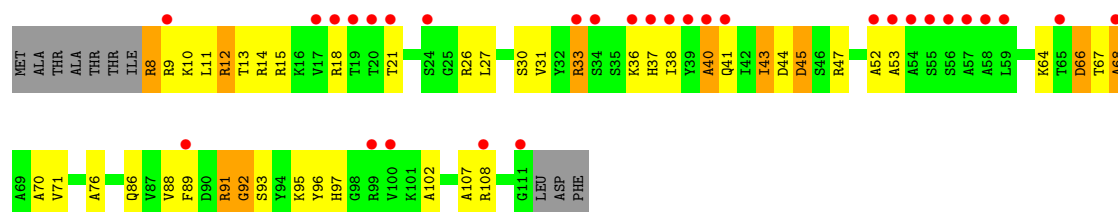




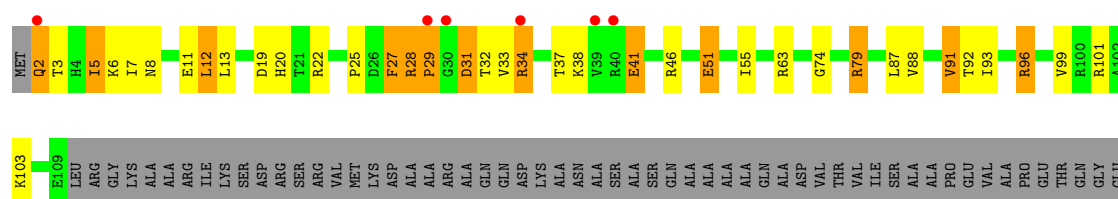
• Molecule 13: 50S ribosomal protein L17



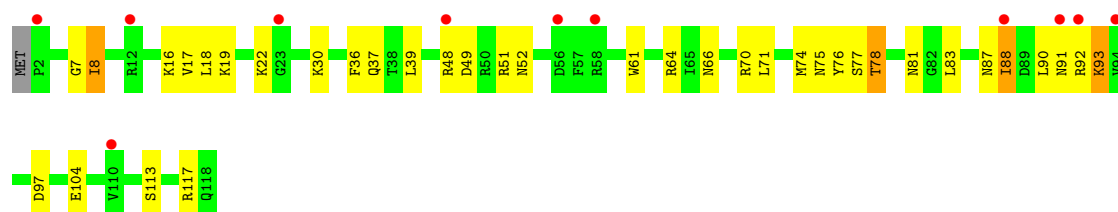
• Molecule 14: 50S ribosomal protein L18



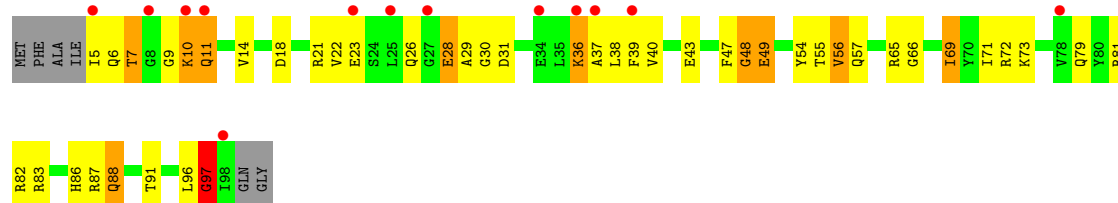
• Molecule 15: 50S ribosomal protein L19



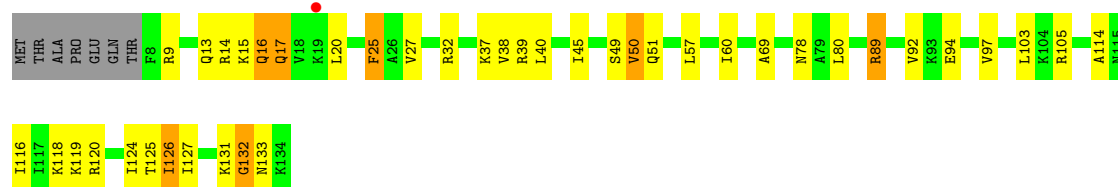
• Molecule 16: 50S ribosomal protein L20



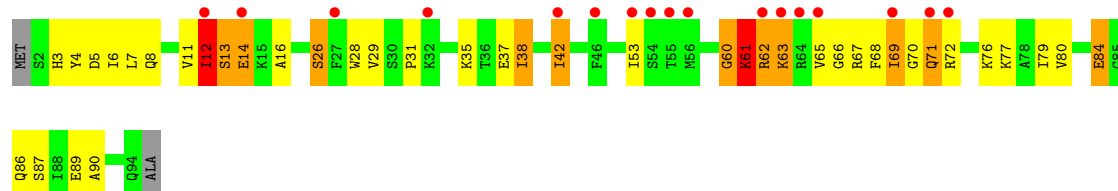
• Molecule 17: 50S ribosomal protein L21



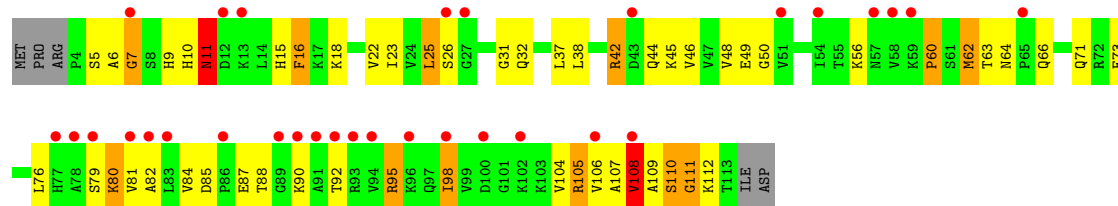
- Molecule 18: 50S ribosomal protein L22



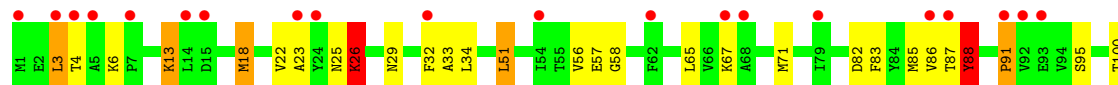
- Molecule 19: 50S ribosomal protein L23

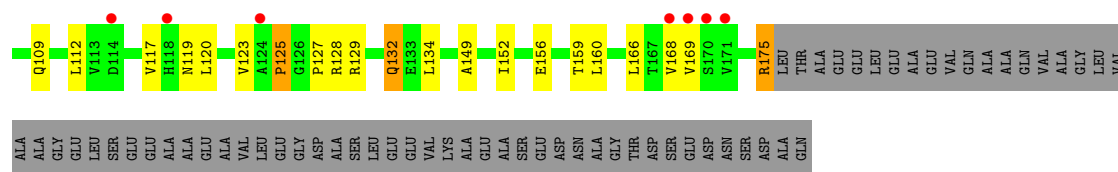


- Molecule 20: 50S ribosomal protein L24



- Molecule 21: 50S ribosomal protein L25

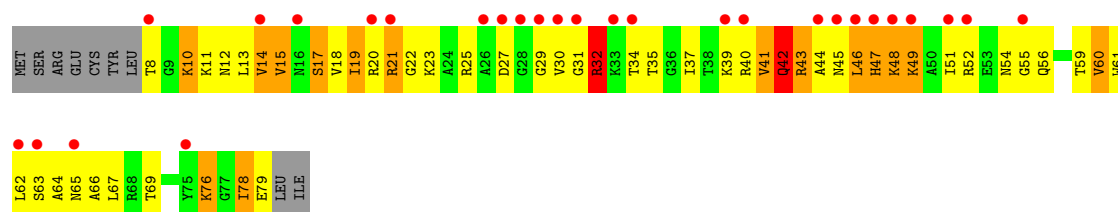
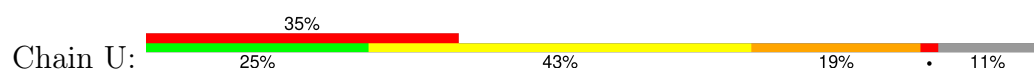




- Molecule 22: 50S ribosomal protein L27



- Molecule 23: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L29



- Molecule 25: 50S ribosomal protein L30

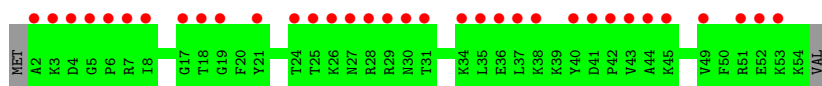


- Molecule 26: 50S ribosomal protein L32

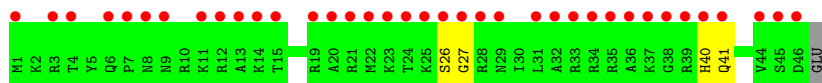
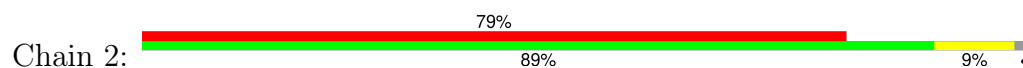


- Molecule 27: 50S ribosomal protein L33

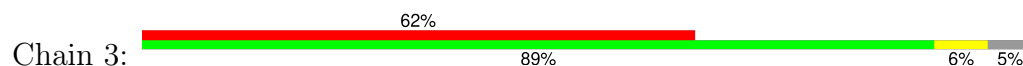




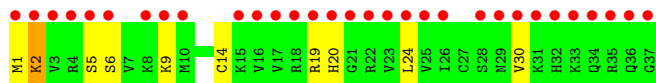
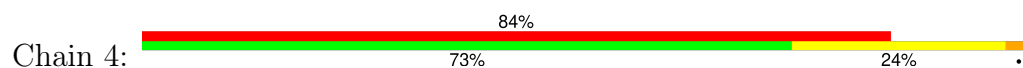
- Molecule 28: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L36



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	169.77Å 406.66Å 696.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.20 30.00 – 3.23	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-3.20) 89.7 (30.00-3.23)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.51 (at 3.24Å)	Xtriage
Refinement program	autoBUSTER	Depositor
R, $R_{free}$	0.197 , 0.230 0.210 , 0.246	Depositor DCC
$R_{free}$ test set	17364 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	80.0	Xtriage
Anisotropy	0.713	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 84.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	83879	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1F3, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	X	1.00	38/64561 (0.1%)	1.86	1965/100708 (2.0%)
2	Y	1.02	0/2904	1.68	66/4525 (1.5%)
3	A	0.62	0/1862	0.96	2/2510 (0.1%)
4	B	0.60	0/1567	0.96	2/2105 (0.1%)
5	C	0.63	0/1529	0.95	1/2070 (0.0%)
6	D	0.47	0/1419	0.67	0/1903
7	E	0.44	0/1308	0.68	0/1771
8	F	0.47	0/508	0.64	0/683
9	G	0.64	0/1138	1.01	4/1539 (0.3%)
10	H	0.55	0/1007	0.84	1/1352 (0.1%)
11	I	0.73	0/1081	1.11	8/1448 (0.6%)
12	J	0.65	0/1113	0.92	2/1486 (0.1%)
13	K	0.80	2/886 (0.2%)	0.99	3/1188 (0.3%)
14	L	0.57	0/785	0.95	1/1048 (0.1%)
15	M	0.65	1/884 (0.1%)	0.98	2/1186 (0.2%)
16	N	0.51	0/994	0.78	0/1323
17	O	0.56	0/750	0.96	1/1000 (0.1%)
18	P	0.56	0/1027	0.82	0/1373
19	Q	0.62	0/737	1.04	4/988 (0.4%)
20	R	0.64	0/835	0.99	0/1121
21	S	0.49	0/1370	0.73	0/1862
22	T	0.53	0/633	0.85	0/838
23	U	0.75	0/556	1.12	2/741 (0.3%)
24	V	0.47	0/537	0.69	0/714
25	W	0.46	0/426	0.79	0/568
26	Z	0.65	0/469	0.97	0/629
30	4	0.48	0/298	0.72	0/390
All	All	0.91	41/91184 (0.0%)	1.68	2064/137069 (1.5%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	X	0	6

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	540	G	C2-N3	9.96	1.40	1.32
1	X	774	A	C5-C4	9.11	1.45	1.38
1	X	774	A	N7-C5	-7.92	1.34	1.39
1	X	2018	G	N9-C8	7.57	1.43	1.37
1	X	542	A	N7-C5	-7.47	1.34	1.39
1	X	1333	G	N9-C4	-6.86	1.32	1.38
1	X	537	C	N1-C2	6.71	1.46	1.40
1	X	774	A	N1-C2	6.70	1.40	1.34
1	X	540	G	N3-C4	6.67	1.40	1.35
1	X	1946	U	C1'-N1	6.67	1.58	1.48
1	X	774	A	N3-C4	6.56	1.38	1.34
13	K	3	HIS	CA-C	6.52	1.70	1.52
1	X	1980	A	N7-C5	-6.30	1.35	1.39
13	K	52	ILE	CG1-CD1	6.21	1.93	1.50
1	X	699	G	N9-C4	-6.18	1.33	1.38
15	M	29	PRO	CA-C	5.88	1.64	1.52
1	X	462	G	C6-O6	5.86	1.29	1.24
1	X	1468	A	N9-C4	5.79	1.41	1.37
1	X	343	A	N9-C4	5.76	1.41	1.37
1	X	796	A	N9-C4	-5.72	1.34	1.37
1	X	1467	U	C1'-N1	5.72	1.57	1.48
1	X	1288	A	C4'-C3'	-5.64	1.47	1.52
1	X	2485	U	N1-C2	5.64	1.43	1.38
1	X	434	C	C1'-N1	5.62	1.57	1.48
1	X	1688	U	C2-N3	5.54	1.41	1.37
1	X	2321	C	C1'-N1	5.41	1.56	1.48
1	X	540	G	C3'-O3'	5.38	1.49	1.42
1	X	537	C	C4-C5	5.34	1.47	1.43
1	X	868	U	C1'-N1	5.33	1.56	1.48
1	X	1223	G	C2-N3	5.30	1.36	1.32
1	X	2482	A	N3-C4	5.27	1.38	1.34
1	X	1688	U	N3-C4	5.25	1.43	1.38
1	X	327	C	C1'-N1	5.24	1.56	1.48
1	X	2485	U	C1'-N1	5.22	1.56	1.48
1	X	78	C	C1'-N1	5.21	1.56	1.48
1	X	358	C	C1'-N1	5.21	1.56	1.48

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	2795	A	N3-C4	5.19	1.38	1.34
1	X	1522	C	C1'-N1	5.09	1.56	1.48
1	X	1688	U	C4-O4	5.05	1.27	1.23
1	X	559	C	C3'-O3'	5.03	1.49	1.42
1	X	2072	C	C1'-N1	5.03	1.56	1.48

All (2064) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1288	A	C1'-O4'-C4'	-38.76	78.89	109.90
1	X	1288	A	C5'-C4'-O4'	20.93	134.22	109.10
1	X	1716	G	P-O3'-C3'	19.09	142.60	119.70
1	X	1288	A	C4'-C3'-C2'	-19.04	83.56	102.60
1	X	2808	U	O4'-C1'-N1	17.91	122.53	108.20
1	X	1775	A	P-O3'-C3'	17.83	141.10	119.70
1	X	1333	G	N3-C4-N9	-17.19	115.69	126.00
1	X	774	A	N7-C8-N9	16.88	122.24	113.80
1	X	540	G	P-O3'-C3'	16.87	139.94	119.70
1	X	1631	C	O4'-C1'-N1	16.27	121.21	108.20
1	X	537	C	O4'-C1'-N1	16.23	121.18	108.20
1	X	1333	G	O4'-C1'-N9	15.97	120.98	108.20
1	X	1288	A	O4'-C1'-N9	15.69	120.75	108.20
1	X	2497	A	P-O3'-C3'	15.66	138.49	119.70
1	X	1473	U	P-O3'-C3'	15.41	138.20	119.70
1	X	1631	C	P-O3'-C3'	15.28	138.03	119.70
1	X	2705	A	P-O3'-C3'	15.27	138.03	119.70
1	X	774	A	N1-C6-N6	15.10	127.66	118.60
1	X	1475	U	P-O3'-C3'	14.90	137.59	119.70
1	X	994	A	P-O3'-C3'	14.88	137.56	119.70
1	X	343	A	O4'-C1'-N9	14.77	120.02	108.20
1	X	1278	A	O4'-C1'-N9	14.74	120.00	108.20
1	X	777	A	P-O3'-C3'	14.73	137.37	119.70
1	X	2014	A	P-O3'-C3'	14.71	137.36	119.70
1	X	2706	U	P-O3'-C3'	14.71	137.35	119.70
1	X	399	G	P-O3'-C3'	14.67	137.30	119.70
1	X	774	A	C5-N7-C8	-14.57	96.61	103.90
1	X	1812	U	C1'-O4'-C4'	-14.53	98.27	109.90
1	X	540	G	N3-C4-N9	14.43	134.66	126.00
1	X	1249	G	P-O3'-C3'	14.41	136.99	119.70
1	X	1482	U	O4'-C1'-N1	14.39	119.71	108.20
1	X	802	A	P-O3'-C3'	14.30	136.86	119.70
1	X	100	G	P-O3'-C3'	13.66	136.10	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1409	U	P-O3'-C3'	13.51	135.91	119.70
1	X	176	A	P-O3'-C3'	13.47	135.86	119.70
1	X	2564	U	P-O3'-C3'	13.40	135.78	119.70
1	X	98	U	P-O3'-C3'	13.38	135.75	119.70
1	X	1570	C	O4'-C1'-N1	13.37	118.90	108.20
1	X	2736	U	P-O3'-C3'	13.23	135.58	119.70
1	X	774	A	C8-N9-C4	-13.23	100.51	105.80
1	X	774	A	C6-C5-N7	-13.06	123.16	132.30
1	X	1019	U	P-O3'-C3'	12.92	135.21	119.70
1	X	2404	A	P-O3'-C3'	12.91	135.20	119.70
1	X	1811	A	P-O3'-C3'	12.85	135.11	119.70
1	X	1820	G	P-O3'-C3'	12.84	135.11	119.70
1	X	1037	U	C1'-O4'-C4'	-12.83	99.63	109.90
1	X	1333	G	N3-C4-C5	12.79	135.00	128.60
1	X	540	G	N3-C2-N2	12.78	128.84	119.90
1	X	540	G	C4-C5-N7	12.77	115.91	110.80
1	X	1152	C	P-O3'-C3'	12.75	135.00	119.70
1	X	33	C	P-O3'-C3'	12.69	134.92	119.70
1	X	2018	G	P-O3'-C3'	12.67	134.91	119.70
1	X	1938	U	P-O3'-C3'	12.59	134.81	119.70
1	X	1561	A	P-O3'-C3'	12.59	134.80	119.70
1	X	1037	U	O4'-C1'-N1	12.53	118.22	108.20
1	X	2706	U	O4'-C1'-N1	12.51	118.21	108.20
1	X	1233	A	P-O3'-C3'	12.46	134.65	119.70
1	X	334	G	P-O3'-C3'	12.35	134.52	119.70
1	X	2371	A	O4'-C1'-N9	12.29	118.04	108.20
1	X	1467	U	P-O3'-C3'	-12.28	104.96	119.70
1	X	1963	G	P-O3'-C3'	12.27	134.42	119.70
1	X	469	G	O4'-C1'-N9	12.21	117.97	108.20
1	X	1055	A	P-O3'-C3'	12.18	134.31	119.70
1	X	467	U	C1'-O4'-C4'	-12.17	100.16	109.90
1	X	554	U	O4'-C1'-N1	12.06	117.84	108.20
1	X	1468	A	O4'-C1'-N9	12.06	117.84	108.20
1	X	1283	C	P-O3'-C3'	11.99	134.09	119.70
1	X	2770	A	P-O3'-C3'	11.98	134.07	119.70
1	X	683	A	P-O3'-C3'	11.94	134.03	119.70
1	X	1468	A	C8-N9-C4	-11.93	101.03	105.80
1	X	2608	A	P-O3'-C3'	11.85	133.92	119.70
1	X	2204	A	P-O3'-C3'	11.75	133.81	119.70
1	X	99	U	P-O3'-C3'	11.75	133.80	119.70
1	X	2312	A	P-O3'-C3'	11.72	133.77	119.70
1	X	1031	C	P-O3'-C3'	11.72	133.76	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1467	U	C5-C6-N1	11.71	128.56	122.70
1	X	774	A	C4-C5-N7	11.67	116.53	110.70
1	X	48	A	P-O3'-C3'	11.63	133.66	119.70
1	X	969	U	P-O3'-C3'	11.57	133.58	119.70
1	X	780	U	P-O3'-C3'	11.54	133.54	119.70
1	X	594	G	P-O3'-C3'	11.50	133.50	119.70
1	X	1790	G	P-O3'-C3'	11.48	133.48	119.70
2	Y	16	U	P-O3'-C3'	11.39	133.37	119.70
1	X	2589	C	P-O3'-C3'	11.37	133.34	119.70
1	X	1468	A	O4'-C1'-C2'	-11.17	94.63	105.80
1	X	2298	U	P-O3'-C3'	11.10	133.01	119.70
1	X	1975	G	P-O3'-C3'	11.09	133.01	119.70
1	X	2088	U	P-O3'-C3'	11.08	133.00	119.70
1	X	2498	U	P-O3'-C3'	11.08	132.99	119.70
1	X	1574	A	C4'-C3'-C2'	-11.06	91.54	102.60
1	X	514	G	P-O3'-C3'	11.05	132.96	119.70
1	X	537	C	N3-C2-O2	-11.05	114.17	121.90
1	X	2261	G	P-O3'-C3'	10.97	132.86	119.70
1	X	1333	G	C8-N9-C1'	10.96	141.25	127.00
1	X	1096	A	P-O3'-C3'	10.93	132.82	119.70
1	X	1574	A	O4'-C1'-N9	10.80	116.84	108.20
1	X	1669	A	O4'-C4'-C3'	-10.80	93.20	104.00
1	X	540	G	C6-C5-N7	-10.78	123.93	130.40
1	X	2596	C	O4'-C1'-N1	10.78	116.83	108.20
1	X	1186	G	P-O3'-C3'	10.71	132.55	119.70
1	X	656	U	O4'-C1'-N1	10.61	116.69	108.20
1	X	825	C	P-O3'-C3'	-10.58	107.01	119.70
1	X	1194	U	P-O3'-C3'	10.55	132.36	119.70
1	X	540	G	C5-C6-O6	-10.52	122.29	128.60
1	X	1688	U	N3-C4-O4	10.51	126.76	119.40
1	X	553	C	P-O3'-C3'	10.50	132.30	119.70
1	X	71	A	P-O3'-C3'	10.50	132.30	119.70
1	X	1850	G	P-O3'-C3'	10.48	132.28	119.70
1	X	664	C	P-O3'-C3'	10.47	132.27	119.70
1	X	1333	G	N3-C2-N2	-10.46	112.58	119.90
1	X	699	G	C5-N7-C8	-10.42	99.09	104.30
1	X	540	G	N3-C4-C5	-10.41	123.39	128.60
1	X	2551	A	P-O3'-C3'	10.37	132.15	119.70
1	X	342	G	P-O3'-C3'	10.37	132.14	119.70
1	X	537	C	C1'-O4'-C4'	-10.36	101.61	109.90
1	X	2769	C	C1'-O4'-C4'	-10.35	101.62	109.90
1	X	540	G	C5-C6-N1	10.34	116.67	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1496	G	P-O3'-C3'	10.31	132.07	119.70
1	X	458	G	P-O3'-C3'	10.29	132.05	119.70
1	X	939	C	C5'-C4'-O4'	10.29	121.45	109.10
1	X	518	A	P-O3'-C3'	10.27	132.02	119.70
1	X	814	G	O4'-C1'-N9	-10.25	100.00	108.20
1	X	1033	G	P-O3'-C3'	10.25	132.00	119.70
1	X	1053	G	P-O3'-C3'	10.19	131.93	119.70
1	X	542	A	C8-N9-C4	-10.17	101.73	105.80
1	X	540	G	C3'-C2'-C1'	10.15	109.62	101.50
1	X	1139	A	C1'-O4'-C4'	-10.13	101.80	109.90
1	X	803	C	P-O3'-C3'	10.09	131.81	119.70
1	X	83	A	P-O3'-C3'	10.08	131.79	119.70
1	X	2426	G	P-O3'-C3'	10.06	131.78	119.70
1	X	554	U	P-O3'-C3'	10.05	131.76	119.70
1	X	1632	A	P-O3'-C3'	10.01	131.71	119.70
1	X	2795	A	P-O3'-C3'	9.97	131.67	119.70
1	X	175	C	P-O3'-C3'	9.97	131.66	119.70
1	X	805	G	O4'-C1'-N9	-9.96	100.23	108.20
1	X	632	A	O4'-C1'-N9	9.93	116.14	108.20
1	X	2769	C	O4'-C1'-N1	9.90	116.12	108.20
1	X	1552	C	P-O3'-C3'	9.89	131.56	119.70
1	X	655	A	P-O3'-C3'	9.85	131.52	119.70
1	X	480	G	C5-C6-O6	-9.83	122.70	128.60
1	X	1812	U	O4'-C1'-N1	9.79	116.03	108.20
1	X	2418	A	P-O3'-C3'	9.78	131.43	119.70
1	X	1333	G	N9-C4-C5	9.76	109.31	105.40
1	X	1482	U	C1'-O4'-C4'	-9.76	102.09	109.90
1	X	814	G	P-O3'-C3'	9.75	131.40	119.70
1	X	2330	G	P-O3'-C3'	9.73	131.38	119.70
1	X	1442	C	P-O3'-C3'	9.72	131.36	119.70
1	X	2633	A	P-O3'-C3'	9.71	131.35	119.70
1	X	666	U	O4'-C1'-N1	9.67	115.94	108.20
1	X	558	G	P-O3'-C3'	9.66	131.30	119.70
1	X	73	A	P-O3'-C3'	9.66	131.29	119.70
1	X	2691	C	O4'-C1'-C2'	-9.66	96.14	105.80
1	X	1182	U	P-O3'-C3'	9.65	131.29	119.70
1	X	699	G	N3-C4-C5	9.63	133.42	128.60
1	X	759	C	C5-C6-N1	9.62	125.81	121.00
1	X	689	A	C5-N7-C8	-9.61	99.09	103.90
1	X	554	U	C1'-O4'-C4'	-9.61	102.22	109.90
1	X	1575	C	P-O3'-C3'	9.58	131.19	119.70
1	X	689	A	O4'-C1'-N9	9.56	115.85	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	3	U	P-O3'-C3'	9.55	131.16	119.70
1	X	542	A	C3'-C2'-C1'	9.55	109.14	101.50
1	X	1613	G	C1'-O4'-C4'	-9.54	102.27	109.90
1	X	691	C	O4'-C1'-N1	9.49	115.79	108.20
1	X	1333	G	C4-N9-C1'	-9.49	114.17	126.50
1	X	169	C	O4'-C1'-N1	9.48	115.79	108.20
1	X	542	A	N7-C8-N9	9.45	118.53	113.80
2	Y	26	G	P-O3'-C3'	9.43	131.02	119.70
1	X	1288	A	C3'-C2'-C1'	-9.40	93.98	101.50
1	X	841	G	O4'-C1'-N9	9.39	115.72	108.20
1	X	540	G	N7-C8-N9	9.39	117.79	113.10
1	X	2229	G	P-O3'-C3'	9.38	130.96	119.70
1	X	1288	A	O4'-C4'-C3'	-9.36	94.64	104.00
1	X	1664	G	O5'-P-OP2	9.35	121.92	110.70
1	X	1601	U	P-O3'-C3'	9.35	130.92	119.70
1	X	1975	G	C2'-C3'-O3'	9.35	130.07	109.50
1	X	1633	C	O4'-C1'-N1	9.28	115.63	108.20
1	X	1412	C	C3'-C2'-C1'	-9.28	94.08	101.50
1	X	2051	U	O4'-C1'-N1	9.23	115.58	108.20
1	X	1086	C	P-O3'-C3'	9.22	130.76	119.70
1	X	540	G	C5-N7-C8	-9.21	99.70	104.30
1	X	2669	C	N1-C2-O2	9.17	124.40	118.90
1	X	638	A	P-O3'-C3'	9.13	130.66	119.70
1	X	1689	U	O4'-C1'-N1	9.12	115.50	108.20
1	X	1345	G	P-O3'-C3'	9.12	130.64	119.70
1	X	2703	C	O4'-C1'-N1	9.10	115.48	108.20
1	X	699	G	N3-C4-N9	-9.09	120.55	126.00
1	X	1754	G	P-O3'-C3'	9.07	130.58	119.70
1	X	763	A	P-O3'-C3'	9.07	130.58	119.70
1	X	1459	U	P-O3'-C3'	9.06	130.58	119.70
1	X	467	U	O4'-C1'-N1	9.06	115.45	108.20
1	X	789	G	P-O3'-C3'	9.06	130.57	119.70
1	X	1574	A	C1'-O4'-C4'	-9.06	102.66	109.90
1	X	3	U	C3'-C2'-C1'	-9.03	94.27	101.50
1	X	2554	C	O4'-C1'-N1	9.01	115.41	108.20
1	X	666	U	C1'-O4'-C4'	-9.01	102.69	109.90
1	X	198	A	P-O3'-C3'	8.99	130.48	119.70
1	X	537	C	N1-C2-O2	8.99	124.29	118.90
1	X	1799	A	C1'-O4'-C4'	-8.97	102.72	109.90
1	X	1154	A	P-O3'-C3'	8.96	130.45	119.70
1	X	483	A	P-O3'-C3'	-8.95	108.96	119.70
1	X	2018	G	N3-C4-N9	-8.93	120.64	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2672	U	O4'-C1'-N1	8.93	115.34	108.20
1	X	796	A	C5-N7-C8	-8.92	99.44	103.90
1	X	1184	G	P-O3'-C3'	8.91	130.39	119.70
1	X	515	A	P-O3'-C3'	8.89	130.37	119.70
1	X	1137	A	P-O3'-C3'	8.89	130.37	119.70
1	X	2222	U	O4'-C1'-N1	8.89	115.31	108.20
1	X	2018	G	N9-C1'-C2'	8.86	125.52	114.00
1	X	341	A	P-O3'-C3'	8.84	130.31	119.70
1	X	2475	C	O4'-C1'-N1	8.82	115.26	108.20
1	X	574	C	O4'-C1'-N1	8.82	115.26	108.20
1	X	1830	C	P-O3'-C3'	8.82	130.28	119.70
1	X	2671	C	O4'-C1'-N1	8.82	115.25	108.20
1	X	689	A	N7-C8-N9	8.81	118.20	113.80
1	X	559	C	N1-C1'-C2'	8.80	125.44	114.00
1	X	2706	U	C4'-C3'-C2'	8.78	111.38	102.60
1	X	1746	A	O4'-C1'-N9	8.78	115.23	108.20
1	X	2689	C	P-O3'-C3'	8.78	130.24	119.70
1	X	418	C	C1'-O4'-C4'	-8.75	102.90	109.90
1	X	774	A	C5-C6-N1	-8.74	113.33	117.70
1	X	841	G	C8-N9-C4	-8.74	102.90	106.40
1	X	1812	U	N1-C1'-C2'	8.73	125.34	114.00
1	X	1509	A	O4'-C1'-N9	8.72	115.17	108.20
1	X	1265	G	O4'-C1'-N9	-8.70	101.24	108.20
1	X	2782	G	C5-C6-O6	-8.70	123.38	128.60
1	X	686	C	O4'-C1'-N1	8.70	115.16	108.20
1	X	483	A	O4'-C1'-N9	8.68	115.14	108.20
1	X	1278	A	C3'-C2'-C1'	-8.65	94.58	101.50
1	X	540	G	N9-C4-C5	-8.65	101.94	105.40
1	X	625	A	P-O3'-C3'	8.64	130.07	119.70
1	X	1656	U	O4'-C1'-N1	8.64	115.11	108.20
1	X	1468	A	P-O3'-C3'	8.62	130.04	119.70
1	X	566	U	O4'-C1'-N1	8.61	115.08	108.20
1	X	758	G	C2'-C3'-O3'	8.60	128.43	109.50
1	X	540	G	N1-C2-N2	-8.59	108.47	116.20
1	X	953	G	O4'-C1'-N9	8.59	115.07	108.20
1	X	804	C	O4'-C1'-N1	8.58	115.07	108.20
1	X	2691	C	P-O3'-C3'	8.58	130.00	119.70
1	X	656	U	P-O3'-C3'	8.58	130.00	119.70
1	X	1938	U	C4'-C3'-C2'	8.58	111.18	102.60
1	X	216	U	O4'-C1'-N1	8.58	115.06	108.20
1	X	467	U	P-O3'-C3'	8.57	129.98	119.70
1	X	490	A	O4'-C1'-N9	8.56	115.05	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	54	U	O4'-C1'-N1	8.56	115.05	108.20
1	X	204	A	P-O3'-C3'	8.55	129.96	119.70
1	X	242	A	C4'-C3'-C2'	-8.55	94.05	102.60
1	X	788	G	P-O3'-C3'	8.53	129.93	119.70
1	X	1223	G	C3'-C2'-C1'	8.52	108.31	101.50
1	X	1399	C	O4'-C1'-N1	8.51	115.01	108.20
1	X	181	A	P-O3'-C3'	8.50	129.90	119.70
1	X	1974	U	O4'-C1'-N1	8.49	115.00	108.20
1	X	2594	U	C5-C6-N1	8.45	126.93	122.70
1	X	1602	G	P-O3'-C3'	8.45	129.84	119.70
1	X	1467	U	C4-C5-C6	-8.44	114.64	119.70
1	X	1278	A	C1'-O4'-C4'	-8.43	103.16	109.90
1	X	939	C	C1'-O4'-C4'	-8.42	103.16	109.90
1	X	1581	C	P-O3'-C3'	8.42	129.80	119.70
1	X	343	A	C8-N9-C4	-8.41	102.44	105.80
1	X	31	C	O4'-C1'-N1	8.40	114.92	108.20
1	X	2426	G	O4'-C1'-N9	8.40	114.92	108.20
1	X	537	C	N3-C4-N4	-8.38	112.13	118.00
1	X	1716	G	C4'-C3'-C2'	8.38	110.98	102.60
1	X	1441	A	P-O3'-C3'	8.37	129.75	119.70
1	X	2778	U	P-O3'-C3'	8.37	129.74	119.70
1	X	1469	U	N1-C1'-C2'	8.34	124.85	114.00
1	X	1574	A	C5'-C4'-O4'	8.34	119.11	109.10
1	X	2189	A	P-O3'-C3'	8.33	129.69	119.70
1	X	1953	A	P-O5'-C5'	-8.32	107.58	120.90
1	X	2018	G	C5'-C4'-C3'	-8.32	102.69	116.00
1	X	2685	A	N1-C6-N6	-8.32	113.61	118.60
1	X	1539	U	O4'-C1'-N1	8.31	114.85	108.20
1	X	1753	A	O4'-C1'-N9	8.30	114.84	108.20
1	X	2408	G	P-O5'-C5'	-8.30	107.62	120.90
1	X	2018	G	N3-C4-C5	8.30	132.75	128.60
1	X	2745	A	P-O3'-C3'	8.29	129.65	119.70
1	X	346	C	C6-N1-C2	-8.29	116.98	120.30
1	X	2191	A	O4'-C1'-N9	8.28	114.83	108.20
1	X	2867	G	N7-C8-N9	8.28	117.24	113.10
1	X	809	C	O4'-C1'-N1	8.27	114.82	108.20
1	X	2867	G	C5-N7-C8	-8.27	100.17	104.30
1	X	841	G	N7-C8-N9	8.26	117.23	113.10
1	X	358	C	O4'-C1'-N1	8.26	114.81	108.20
1	X	631	G	P-O5'-C5'	-8.25	107.70	120.90
1	X	346	C	O4'-C1'-N1	8.24	114.79	108.20
1	X	467	U	C2-N1-C1'	8.21	127.56	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	490	A	P-O3'-C3'	8.21	129.55	119.70
1	X	731	A	P-O3'-C3'	8.20	129.54	119.70
1	X	2710	C	P-O3'-C3'	-8.20	109.86	119.70
1	X	1523	A	P-O3'-C3'	8.20	129.53	119.70
1	X	1765	C	N1-C2-O2	8.19	123.81	118.90
1	X	1251	G	O4'-C1'-N9	8.18	114.75	108.20
1	X	2824	C	P-O3'-C3'	8.18	129.51	119.70
1	X	2491	C	O5'-P-OP2	-8.18	98.34	105.70
1	X	847	C	O4'-C1'-N1	8.17	114.74	108.20
1	X	593	C	O4'-C1'-N1	8.15	114.72	108.20
1	X	661	C	N1-C2-O2	8.15	123.79	118.90
1	X	2857	C	O4'-C1'-N1	8.12	114.69	108.20
1	X	469	G	P-O3'-C3'	8.12	129.44	119.70
1	X	2034	A	P-O3'-C3'	8.11	129.44	119.70
1	X	2867	G	C4-C5-N7	8.11	114.04	110.80
1	X	2487	G	O4'-C1'-N9	8.10	114.68	108.20
1	X	2730	A	P-O3'-C3'	8.10	129.42	119.70
1	X	1188	A	P-O3'-C3'	8.09	129.41	119.70
1	X	2298	U	O4'-C1'-N1	8.09	114.67	108.20
1	X	751	G	O4'-C4'-C3'	-8.08	95.92	104.00
1	X	597	U	O4'-C4'-C3'	-8.07	95.93	104.00
1	X	1232	U	O4'-C1'-N1	8.07	114.66	108.20
1	X	1712	G	N3-C2-N2	8.06	125.54	119.90
1	X	758	G	C3'-C2'-C1'	-8.06	95.05	101.50
1	X	1310	C	O4'-C1'-N1	8.05	114.64	108.20
1	X	1962	C	C3'-C2'-C1'	-8.05	95.06	101.50
1	X	99	U	O4'-C1'-N1	8.05	114.64	108.20
1	X	813	A	P-O3'-C3'	8.05	129.36	119.70
1	X	859	U	O4'-C1'-N1	8.05	114.64	108.20
1	X	526	C	O4'-C1'-N1	8.04	114.64	108.20
1	X	580	A	P-O3'-C3'	8.04	129.35	119.70
1	X	39	C	O4'-C1'-N1	8.03	114.62	108.20
1	X	1524	C	P-O3'-C3'	8.02	129.32	119.70
1	X	2667	C	P-O3'-C3'	8.02	129.32	119.70
1	X	739	G	O4'-C1'-N9	8.01	114.61	108.20
1	X	74	G	O4'-C4'-C3'	-8.00	96.00	104.00
1	X	542	A	N1-C2-N3	8.00	133.30	129.30
1	X	1468	A	C5-C6-N1	7.99	121.70	117.70
1	X	1710	U	P-O3'-C3'	7.99	129.29	119.70
1	X	117	A	P-O3'-C3'	7.99	129.28	119.70
1	X	313	U	O4'-C1'-N1	7.96	114.57	108.20
1	X	2854	G	C1'-O4'-C4'	-7.96	103.53	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2854	G	P-O3'-C3'	7.96	129.25	119.70
1	X	2859	U	O4'-C1'-N1	7.95	114.56	108.20
1	X	579	G	C4-C5-N7	-7.94	107.62	110.80
1	X	1314	A	P-O3'-C3'	7.94	129.22	119.70
1	X	542	A	C6-N1-C2	-7.93	113.84	118.60
1	X	1673	C	O4'-C1'-N1	7.93	114.54	108.20
1	X	2492	G	O4'-C1'-N9	7.93	114.54	108.20
1	X	1469	U	P-O3'-C3'	7.91	129.19	119.70
1	X	796	A	N1-C6-N6	7.91	123.35	118.60
1	X	841	G	N9-C1'-C2'	7.91	124.28	114.00
1	X	685	U	O4'-C1'-N1	7.90	114.52	108.20
1	X	165	G	O4'-C1'-N9	7.90	114.52	108.20
1	X	1139	A	O4'-C1'-N9	7.89	114.52	108.20
1	X	631	G	P-O3'-C3'	7.89	129.17	119.70
1	X	467	U	C4'-C3'-C2'	-7.89	94.71	102.60
1	X	699	G	N7-C8-N9	7.88	117.04	113.10
1	X	236	C	O4'-C1'-N1	7.88	114.50	108.20
1	X	2018	G	O4'-C1'-N9	7.87	114.50	108.20
1	X	100	G	O4'-C1'-N9	7.87	114.49	108.20
1	X	2258	G	C1'-O4'-C4'	-7.86	103.61	109.90
1	X	1679	U	N3-C2-O2	-7.85	116.70	122.20
1	X	307	C	O4'-C1'-N1	7.85	114.48	108.20
1	X	2009	U	O4'-C1'-N1	7.84	114.48	108.20
1	X	2810	A	P-O3'-C3'	7.84	129.11	119.70
1	X	554	U	N1-C1'-C2'	7.84	124.19	114.00
2	Y	42	U	O4'-C1'-N1	7.84	114.47	108.20
1	X	774	A	C5-C6-N6	-7.83	117.43	123.70
1	X	1775	A	C2'-C3'-O3'	7.83	126.73	109.50
1	X	1770	U	O4'-C4'-C3'	-7.83	96.17	104.00
1	X	1526	U	O4'-C1'-N1	7.82	114.46	108.20
1	X	2854	G	N9-C1'-C2'	7.82	124.16	114.00
1	X	868	U	O4'-C1'-N1	7.81	114.45	108.20
1	X	308	C	O4'-C1'-N1	7.81	114.45	108.20
1	X	864	C	O4'-C1'-N1	7.81	114.45	108.20
1	X	1161	U	O4'-C1'-N1	7.80	114.44	108.20
1	X	672	C	O4'-C4'-C3'	-7.80	96.20	104.00
1	X	1688	U	N3-C4-C5	-7.80	109.92	114.60
13	K	94	TYR	C-N-CA	7.79	141.19	121.70
1	X	2597	G	O4'-C1'-N9	7.78	114.42	108.20
1	X	2489	C	O4'-C1'-N1	7.78	114.42	108.20
1	X	2275	U	P-O3'-C3'	7.77	129.02	119.70
1	X	577	U	N3-C4-C5	-7.77	109.94	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1496	G	C3'-C2'-C1'	-7.76	95.29	101.50
1	X	2299	A	P-O3'-C3'	7.76	129.02	119.70
1	X	956	A	N1-C6-N6	7.75	123.25	118.60
1	X	1467	U	N1-C2-N3	-7.74	110.26	114.90
1	X	2043	A	O4'-C1'-N9	7.73	114.39	108.20
1	X	242	A	C1'-O4'-C4'	-7.73	103.72	109.90
1	X	312	G	P-O3'-C3'	7.72	128.97	119.70
1	X	526	C	C3'-C2'-C1'	-7.72	95.32	101.50
1	X	1829	C	O4'-C1'-N1	7.71	114.37	108.20
1	X	927	C	O4'-C1'-N1	7.70	114.36	108.20
1	X	1844	C	O4'-C1'-N1	7.68	114.35	108.20
1	X	1947	G	P-O3'-C3'	7.67	128.91	119.70
1	X	2813	G	O4'-C1'-N9	7.67	114.34	108.20
1	X	2062	U	O4'-C1'-N1	7.67	114.33	108.20
1	X	1561	A	C3'-C2'-C1'	-7.66	95.37	101.50
1	X	841	G	O4'-C4'-C3'	-7.66	96.34	104.00
1	X	462	G	C5-C6-N1	-7.66	107.67	111.50
1	X	1663	C	N1-C2-O2	7.64	123.49	118.90
1	X	1141	U	C2'-C3'-O3'	7.64	126.31	109.50
1	X	1674	C	O4'-C1'-N1	7.64	114.31	108.20
1	X	2501	U	C5'-C4'-C3'	-7.63	103.80	116.00
1	X	2018	G	C5-N7-C8	-7.62	100.49	104.30
1	X	2756	A	P-O3'-C3'	7.62	128.85	119.70
1	X	537	C	P-O3'-C3'	7.61	128.83	119.70
1	X	1976	U	P-O5'-C5'	-7.60	108.73	120.90
19	Q	60	GLY	C-N-CA	7.60	140.70	121.70
1	X	480	G	C4-C5-N7	7.59	113.84	110.80
1	X	1392	U	P-O3'-C3'	7.59	128.81	119.70
1	X	1468	A	C3'-C2'-C1'	-7.59	95.43	101.50
1	X	2000	U	O5'-P-OP2	-7.59	98.87	105.70
1	X	1279	G	C5-C6-O6	-7.58	124.05	128.60
1	X	2808	U	C1'-O4'-C4'	-7.57	103.84	109.90
1	X	2016	A	P-O3'-C3'	7.57	128.78	119.70
1	X	768	U	O4'-C1'-N1	7.57	114.25	108.20
1	X	1333	G	C8-N9-C4	-7.56	103.38	106.40
1	X	1607	A	P-O3'-C3'	7.56	128.77	119.70
1	X	1364	C	O4'-C1'-N1	7.55	114.24	108.20
1	X	699	G	C4-C5-N7	7.55	113.82	110.80
1	X	796	A	N7-C8-N9	7.55	117.58	113.80
1	X	2005	U	O4'-C1'-N1	7.54	114.24	108.20
1	X	1072	U	P-O3'-C3'	7.54	128.75	119.70
1	X	312	G	C1'-O4'-C4'	-7.54	103.87	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	246	C	O4'-C1'-N1	7.54	114.23	108.20
2	Y	30	C	O4'-C1'-N1	7.54	114.23	108.20
1	X	1963	G	C2'-C3'-O3'	7.53	126.08	109.50
1	X	2550	C	O4'-C1'-N1	7.53	114.22	108.20
1	X	1562	G	O4'-C1'-N9	7.51	114.21	108.20
1	X	520	C	P-O3'-C3'	7.51	128.71	119.70
1	X	2477	C	C5'-C4'-O4'	-7.50	100.10	109.10
1	X	759	C	C6-N1-C2	-7.49	117.31	120.30
1	X	2824	C	C2'-C3'-O3'	7.49	125.97	109.50
1	X	1466	C	C4'-C3'-C2'	-7.48	95.12	102.60
1	X	2370	G	C1'-O4'-C4'	-7.48	103.92	109.90
1	X	3	U	C2'-C3'-O3'	7.48	125.95	109.50
1	X	456	C	O4'-C1'-N1	7.48	114.18	108.20
1	X	774	A	C2-N3-C4	-7.48	106.86	110.60
1	X	1306	U	O4'-C1'-N1	7.48	114.18	108.20
1	X	418	C	C5'-C4'-O4'	7.46	118.05	109.10
1	X	1128	G	P-O3'-C3'	7.45	128.64	119.70
1	X	2031	A	O4'-C1'-N9	7.44	114.16	108.20
1	X	661	C	C4'-C3'-C2'	-7.44	95.16	102.60
1	X	1467	U	N1-C2-O2	7.44	128.01	122.80
1	X	408	U	P-O3'-C3'	7.43	128.62	119.70
1	X	394	U	O4'-C1'-N1	7.42	114.14	108.20
1	X	218	A	P-O3'-C3'	7.42	128.61	119.70
1	X	939	C	O4'-C1'-N1	7.41	114.13	108.20
1	X	2206	C	O4'-C1'-N1	7.41	114.13	108.20
1	X	346	C	N1-C1'-C2'	7.41	123.63	114.00
1	X	1917	C	O4'-C1'-N1	7.41	114.13	108.20
1	X	1770	U	N3-C2-O2	-7.41	117.02	122.20
1	X	1429	A	C1'-O4'-C4'	-7.39	103.98	109.90
1	X	1988	A	P-O3'-C3'	7.39	128.57	119.70
1	X	503	G	O4'-C4'-C3'	-7.39	96.61	104.00
1	X	509	U	O4'-C1'-N1	7.38	114.11	108.20
1	X	796	A	C2-N3-C4	-7.38	106.91	110.60
1	X	537	C	C5-C6-N1	-7.38	117.31	121.00
1	X	429	C	O4'-C1'-N1	7.37	114.09	108.20
1	X	2193	C	O4'-C1'-N1	7.36	114.09	108.20
1	X	357	A	P-O3'-C3'	7.36	128.53	119.70
1	X	2392	G	O4'-C1'-N9	7.36	114.08	108.20
1	X	938	G	O4'-C1'-N9	7.35	114.08	108.20
1	X	1034	U	O4'-C1'-N1	7.35	114.08	108.20
1	X	826	U	O4'-C1'-N1	7.34	114.07	108.20
1	X	1265	G	P-O5'-C5'	7.34	132.64	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1656	U	P-O3'-C3'	7.34	128.50	119.70
1	X	68	C	O4'-C1'-N1	7.33	114.07	108.20
1	X	1336	G	C5-C6-O6	-7.33	124.20	128.60
1	X	192	G	P-O3'-C3'	7.33	128.50	119.70
1	X	838	A	OP1-P-O3'	7.33	121.31	105.20
1	X	89	A	P-O3'-C3'	7.32	128.49	119.70
1	X	765	C	P-O3'-C3'	7.32	128.48	119.70
1	X	2270	U	O4'-C1'-N1	7.32	114.06	108.20
2	Y	81	C	O4'-C1'-N1	7.32	114.05	108.20
1	X	174	A	P-O3'-C3'	7.31	128.48	119.70
1	X	2395	C	O4'-C1'-N1	7.30	114.04	108.20
1	X	777	A	C2'-C3'-O3'	7.29	125.53	109.50
1	X	1593	C	O4'-C1'-N1	7.29	114.03	108.20
1	X	2752	C	O4'-C1'-N1	7.29	114.03	108.20
1	X	1068	A	P-O3'-C3'	7.28	128.44	119.70
1	X	1470	G	P-O3'-C3'	-7.28	110.97	119.70
1	X	1044	U	P-O3'-C3'	7.27	128.43	119.70
1	X	661	C	O4'-C1'-N1	7.26	114.01	108.20
1	X	1339	U	O4'-C1'-N1	7.26	114.01	108.20
1	X	661	C	N3-C2-O2	-7.26	116.82	121.90
1	X	926	C	O4'-C1'-N1	7.25	114.00	108.20
1	X	1334	A	O4'-C4'-C3'	-7.25	96.75	104.00
1	X	343	A	N7-C8-N9	7.24	117.42	113.80
1	X	2589	C	O4'-C1'-N1	-7.24	102.41	108.20
1	X	1770	U	C5-C6-N1	-7.24	119.08	122.70
1	X	59	G	P-O3'-C3'	7.23	128.37	119.70
1	X	742	G	P-O3'-C3'	7.22	128.37	119.70
1	X	1670	G	P-O3'-C3'	7.22	128.37	119.70
1	X	418	C	O4'-C1'-N1	7.22	113.98	108.20
1	X	2185	U	O4'-C1'-N1	7.22	113.97	108.20
1	X	2853	U	O4'-C1'-N1	7.21	113.97	108.20
1	X	1680	U	O4'-C4'-C3'	-7.21	96.79	104.00
1	X	882	C	O4'-C1'-N1	7.21	113.97	108.20
1	X	947	C	O4'-C1'-N1	7.21	113.96	108.20
1	X	1447	U	O4'-C1'-N1	7.20	113.96	108.20
1	X	2408	G	C5'-C4'-C3'	-7.20	104.47	116.00
1	X	843	G	P-O3'-C3'	7.20	128.34	119.70
1	X	518	A	N9-C1'-C2'	7.19	123.35	114.00
1	X	1333	G	C2-N3-C4	-7.19	108.31	111.90
1	X	1474	A	P-O3'-C3'	7.17	128.31	119.70
1	X	525	A	O4'-C1'-N9	7.17	113.94	108.20
1	X	1812	U	P-O3'-C3'	7.17	128.31	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	387	A	P-O3'-C3'	7.17	128.31	119.70
1	X	824	U	N1-C1'-C2'	7.16	123.31	114.00
1	X	2782	G	N1-C6-O6	7.16	124.19	119.90
1	X	1277	G	O4'-C1'-N9	7.15	113.92	108.20
1	X	514	G	O4'-C1'-N9	-7.14	102.48	108.20
1	X	2731	G	P-O3'-C3'	7.14	128.27	119.70
1	X	2668	U	C5-C4-O4	7.14	130.18	125.90
1	X	242	A	O4'-C4'-C3'	-7.14	96.86	104.00
1	X	517	A	P-O3'-C3'	7.14	128.26	119.70
1	X	1664	G	O5'-P-OP1	-7.14	99.28	105.70
1	X	2708	U	O4'-C1'-N1	7.14	113.91	108.20
1	X	1570	C	C1'-O4'-C4'	-7.13	104.19	109.90
1	X	714	G	O4'-C4'-C3'	-7.13	96.87	104.00
1	X	801	A	P-O3'-C3'	7.13	128.25	119.70
1	X	2217	G	P-O3'-C3'	7.13	128.25	119.70
1	X	2615	U	O4'-C1'-N1	7.13	113.90	108.20
1	X	1266	G	P-O3'-C3'	7.12	128.25	119.70
1	X	2744	A	O4'-C1'-N9	7.12	113.90	108.20
1	X	1467	U	C4'-C3'-O3'	7.12	127.24	113.00
1	X	540	G	C4-N9-C1'	7.12	135.75	126.50
1	X	542	A	C6-C5-N7	-7.12	127.32	132.30
1	X	1679	U	O4'-C4'-C3'	-7.12	96.88	104.00
1	X	1355	A	P-O3'-C3'	7.12	128.24	119.70
1	X	2408	G	C4'-C3'-C2'	7.12	109.72	102.60
1	X	617	U	N3-C2-O2	-7.10	117.23	122.20
1	X	2553	G	C5-C6-O6	-7.10	124.34	128.60
1	X	2808	U	C3'-C2'-C1'	-7.09	95.83	101.50
1	X	780	U	O4'-C1'-N1	7.09	113.87	108.20
1	X	1442	C	N1-C2-O2	7.09	123.15	118.90
1	X	494	A	N9-C1'-C2'	-7.08	104.21	112.00
1	X	1594	U	O4'-C1'-N1	7.07	113.86	108.20
1	X	1652	G	O4'-C1'-N9	-7.07	102.54	108.20
1	X	2485	U	O4'-C1'-N1	7.07	113.86	108.20
2	Y	17	A	O4'-C1'-N9	7.07	113.86	108.20
1	X	491	A	O4'-C1'-N9	-7.07	102.55	108.20
1	X	2872	U	O4'-C1'-N1	7.06	113.85	108.20
1	X	2808	U	C5'-C4'-O4'	7.06	117.57	109.10
1	X	1333	G	N1-C2-N2	7.06	122.55	116.20
1	X	537	C	C5'-C4'-O4'	7.06	117.57	109.10
1	X	2722	C	O4'-C1'-N1	7.05	113.84	108.20
1	X	1221	C	O4'-C1'-N1	7.05	113.84	108.20
1	X	666	U	P-O3'-C3'	7.05	128.16	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	711	C	O4'-C1'-N1	7.05	113.84	108.20
1	X	1742	G	P-O3'-C3'	-7.05	111.24	119.70
1	X	1986	G	P-O3'-C3'	-7.04	111.25	119.70
1	X	2626	U	O4'-C1'-N1	7.04	113.84	108.20
1	X	2830	U	O4'-C1'-N1	7.04	113.83	108.20
1	X	1200	G	O4'-C1'-N9	7.04	113.83	108.20
1	X	1634	A	P-O3'-C3'	7.04	128.15	119.70
1	X	1651	U	O4'-C1'-N1	7.04	113.83	108.20
1	X	1935	A	P-O3'-C3'	7.04	128.15	119.70
1	X	845	U	O4'-C1'-N1	7.03	113.82	108.20
1	X	1302	C	O4'-C1'-N1	7.03	113.82	108.20
1	X	453	U	O4'-C1'-N1	7.02	113.82	108.20
1	X	761	G	C1'-O4'-C4'	-7.02	104.28	109.90
1	X	937	C	O4'-C1'-N1	7.02	113.82	108.20
1	X	227	G	O4'-C1'-N9	7.02	113.81	108.20
1	X	469	G	N3-C4-C5	-7.02	125.09	128.60
1	X	1071	U	P-O3'-C3'	7.01	128.11	119.70
1	X	2864	C	O4'-C1'-N1	7.01	113.81	108.20
1	X	1776	A	P-O3'-C3'	7.00	128.10	119.70
1	X	2669	C	O4'-C1'-C2'	-7.00	98.81	105.80
1	X	1946	U	N3-C2-O2	-6.99	117.31	122.20
1	X	1434	U	P-O3'-C3'	6.99	128.09	119.70
1	X	2039	G	C8-N9-C4	-6.97	103.61	106.40
1	X	592	G	O4'-C1'-N9	6.97	113.78	108.20
1	X	117	A	C1'-O4'-C4'	-6.97	104.33	109.90
1	X	474	G	O4'-C1'-N9	6.96	113.77	108.20
1	X	485	G	P-O3'-C3'	6.96	128.06	119.70
1	X	2698	G	C4'-C3'-C2'	-6.96	95.64	102.60
1	X	459	A	P-O3'-C3'	6.95	128.04	119.70
1	X	1434	U	C1'-O4'-C4'	-6.95	104.34	109.90
1	X	304	A	P-O5'-C5'	6.94	132.01	120.90
1	X	1550	C	O4'-C1'-N1	6.94	113.75	108.20
1	X	1997	A	N1-C6-N6	6.93	122.76	118.60
1	X	1434	U	O4'-C1'-N1	6.93	113.75	108.20
1	X	1663	C	OP1-P-O3'	6.93	120.45	105.20
1	X	835	U	N3-C2-O2	-6.93	117.35	122.20
1	X	2347	C	O4'-C1'-N1	6.93	113.74	108.20
1	X	2788	C	O4'-C1'-N1	6.92	113.74	108.20
1	X	751	G	C2'-C3'-O3'	6.92	124.78	113.70
1	X	1412	C	P-O3'-C3'	6.92	128.00	119.70
1	X	594	G	O4'-C1'-N9	6.92	113.73	108.20
1	X	1094	C	O4'-C1'-N1	6.91	113.73	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2581	A	P-O3'-C3'	6.91	127.99	119.70
1	X	467	U	C6-N1-C1'	-6.91	111.53	121.20
2	Y	37	C	O4'-C1'-N1	6.91	113.72	108.20
1	X	526	C	O5'-P-OP2	-6.90	99.49	105.70
1	X	1712	G	N3-C4-N9	6.90	130.14	126.00
1	X	308	C	P-O5'-C5'	6.90	131.94	120.90
1	X	2660	C	O4'-C1'-N1	6.90	113.72	108.20
1	X	2088	U	O4'-C1'-N1	6.90	113.72	108.20
1	X	1984	A	P-O5'-C5'	-6.89	109.87	120.90
1	X	2018	G	P-O5'-C5'	-6.89	109.87	120.90
1	X	585	U	O4'-C1'-N1	6.89	113.71	108.20
1	X	190	A	O4'-C1'-N9	6.89	113.71	108.20
1	X	305	A	O4'-C1'-N9	6.89	113.71	108.20
1	X	206	U	O4'-C1'-N1	6.88	113.71	108.20
13	K	7	GLY	C-N-CA	6.88	138.91	121.70
1	X	1865	C	O4'-C1'-N1	6.88	113.70	108.20
1	X	2043	A	P-O3'-C3'	6.88	127.95	119.70
1	X	2067	U	O4'-C1'-N1	6.87	113.70	108.20
1	X	413	G	C8-N9-C4	-6.86	103.66	106.40
1	X	650	U	O4'-C1'-N1	6.86	113.69	108.20
9	G	106	TYR	N-CA-CB	6.85	122.94	110.60
1	X	2075	U	P-O3'-C3'	6.85	127.92	119.70
1	X	469	G	C1'-O4'-C4'	-6.85	104.42	109.90
1	X	2523	G	O4'-C1'-N9	6.84	113.67	108.20
1	X	1432	G	O4'-C1'-N9	6.84	113.67	108.20
1	X	1249	G	C4'-C3'-C2'	6.84	109.44	102.60
1	X	334	G	C1'-O4'-C4'	-6.84	104.43	109.90
1	X	430	C	O4'-C1'-N1	6.84	113.67	108.20
1	X	2407	G	P-O3'-C3'	6.83	127.90	119.70
1	X	2423	G	O5'-P-OP2	-6.83	99.55	105.70
1	X	1680	U	O5'-P-OP2	-6.81	99.57	105.70
1	X	840	U	O4'-C1'-N1	6.81	113.65	108.20
1	X	796	A	C4-C5-N7	6.81	114.10	110.70
1	X	2208	U	O4'-C1'-N1	6.80	113.64	108.20
1	X	2799	C	O4'-C1'-N1	6.80	113.64	108.20
1	X	2082	C	O4'-C1'-N1	6.80	113.64	108.20
1	X	92	U	O4'-C1'-N1	6.79	113.63	108.20
1	X	2774	U	O4'-C1'-N1	6.79	113.63	108.20
1	X	539	A	C1'-O4'-C4'	-6.79	104.47	109.90
1	X	556	A	P-O3'-C3'	6.79	127.84	119.70
1	X	1787	U	O4'-C1'-N1	6.78	113.63	108.20
1	X	689	A	C2-N3-C4	-6.78	107.21	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	689	A	C4-C5-N7	6.78	114.09	110.70
2	Y	57	U	O4'-C1'-N1	6.78	113.62	108.20
1	X	1223	G	C6-C5-N7	-6.78	126.33	130.40
1	X	1771	A	P-O3'-C3'	6.77	127.83	119.70
1	X	2236	U	O4'-C1'-N1	6.77	113.62	108.20
1	X	1093	U	O4'-C1'-N1	6.77	113.61	108.20
1	X	1010	U	P-O5'-C5'	6.76	131.72	120.90
1	X	2671	C	O5'-P-OP2	-6.75	99.62	105.70
1	X	333	A	P-O3'-C3'	6.75	127.80	119.70
1	X	1279	G	C4-C5-N7	6.75	113.50	110.80
1	X	2038	C	OP2-P-O3'	6.75	120.05	105.20
1	X	2456	U	O4'-C1'-N1	6.75	113.60	108.20
1	X	759	C	C4'-C3'-C2'	6.75	109.34	102.60
1	X	730	C	P-O3'-C3'	6.74	127.79	119.70
1	X	1344	C	N1-C2-O2	6.74	122.94	118.90
1	X	943	U	O4'-C1'-N1	6.74	113.59	108.20
2	Y	55	C	O4'-C1'-N1	6.74	113.59	108.20
1	X	2408	G	C8-N9-C4	-6.74	103.70	106.40
1	X	1946	U	N1-C2-O2	6.73	127.51	122.80
1	X	981	C	O4'-C1'-N1	6.73	113.58	108.20
1	X	995	A	O4'-C1'-N9	6.73	113.58	108.20
1	X	1922	U	P-O3'-C3'	6.73	127.77	119.70
1	X	1664	G	P-O5'-C5'	6.73	131.66	120.90
1	X	1862	C	O4'-C1'-N1	6.73	113.58	108.20
1	X	1958	G	O4'-C4'-C3'	-6.71	97.29	104.00
1	X	1947	G	O4'-C1'-N9	-6.71	102.83	108.20
2	Y	16	U	N1-C1'-C2'	6.71	122.72	114.00
1	X	1522	C	C3'-C2'-C1'	-6.71	96.14	101.50
1	X	866	U	O4'-C1'-N1	6.70	113.56	108.20
1	X	1314	A	C4'-C3'-O3'	-6.70	95.33	109.40
1	X	1731	C	O4'-C1'-N1	6.70	113.56	108.20
1	X	2373	C	O4'-C1'-N1	6.70	113.56	108.20
1	X	418	C	C4'-C3'-C2'	-6.70	95.90	102.60
1	X	519	C	C6-N1-C2	-6.70	117.62	120.30
1	X	774	A	C6-N1-C2	6.70	122.62	118.60
1	X	1712	G	O4'-C1'-N9	6.69	113.55	108.20
1	X	632	A	P-O3'-C3'	6.69	127.73	119.70
1	X	1319	C	O4'-C1'-N1	6.69	113.55	108.20
1	X	1662	G	P-O3'-C3'	6.69	127.72	119.70
1	X	2478	C	O4'-C1'-N1	6.69	113.55	108.20
1	X	948	C	P-O3'-C3'	-6.68	111.68	119.70
1	X	951	G	C3'-C2'-C1'	-6.68	96.15	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1804	U	O4'-C1'-N1	6.67	113.54	108.20
1	X	564	U	O4'-C1'-N1	6.67	113.54	108.20
1	X	1183	C	O4'-C1'-N1	6.67	113.53	108.20
1	X	2480	C	O4'-C1'-N1	6.67	113.53	108.20
1	X	533	C	O4'-C1'-N1	6.65	113.52	108.20
1	X	343	A	N9-C1'-C2'	6.65	122.65	114.00
1	X	1468	A	N7-C8-N9	6.65	117.13	113.80
1	X	2189	A	C8-N9-C4	-6.64	103.14	105.80
1	X	928	G	C5-C6-O6	-6.64	124.61	128.60
1	X	494	A	C3'-C2'-C1'	6.64	106.81	101.50
1	X	2501	U	O4'-C1'-N1	6.64	113.51	108.20
1	X	646	C	O4'-C1'-N1	6.64	113.51	108.20
1	X	1980	A	C5'-C4'-O4'	6.63	117.06	109.10
1	X	1712	G	N1-C2-N2	-6.63	110.24	116.20
1	X	1725	C	O4'-C1'-N1	6.62	113.50	108.20
1	X	35	G	O4'-C1'-N9	6.62	113.50	108.20
1	X	689	A	C1'-O4'-C4'	-6.62	104.60	109.90
1	X	1938	U	N1-C1'-C2'	6.62	122.60	114.00
1	X	2697	G	C2-N3-C4	6.62	115.21	111.90
1	X	989	G	O4'-C1'-N9	6.61	113.49	108.20
1	X	2735	C	O4'-C1'-N1	6.61	113.49	108.20
1	X	613	A	P-O3'-C3'	6.61	127.63	119.70
1	X	677	G	C4'-C3'-C2'	-6.61	95.99	102.60
1	X	725	C	O4'-C1'-N1	6.61	113.49	108.20
1	X	1288	A	C8-N9-C1'	-6.60	115.82	127.70
1	X	1469	U	N3-C2-O2	-6.60	117.58	122.20
1	X	1467	U	C4'-C3'-C2'	6.59	109.19	102.60
1	X	2181	A	C1'-O4'-C4'	-6.59	104.62	109.90
1	X	1120	C	P-O3'-C3'	6.59	127.61	119.70
1	X	2841	U	O4'-C1'-N1	6.59	113.47	108.20
1	X	2274	C	O4'-C1'-N1	6.59	113.47	108.20
1	X	2734	U	O4'-C1'-N1	6.59	113.47	108.20
1	X	1325	U	P-O3'-C3'	6.58	127.60	119.70
1	X	1292	A	O4'-C1'-N9	6.58	113.46	108.20
1	X	2383	C	O4'-C1'-N1	6.58	113.46	108.20
1	X	467	U	O4'-C4'-C3'	-6.57	97.43	104.00
1	X	651	C	O4'-C1'-N1	6.57	113.46	108.20
1	X	97	U	O4'-C1'-N1	6.57	113.45	108.20
1	X	1683	G	O4'-C1'-N9	6.57	113.45	108.20
1	X	2431	C	O4'-C1'-N1	6.56	113.45	108.20
1	X	617	U	O4'-C1'-N1	6.56	113.45	108.20
1	X	1696	C	O4'-C1'-N1	6.56	113.45	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	788	G	C2'-C3'-O3'	6.56	124.19	113.70
1	X	1549	C	O4'-C1'-N1	6.55	113.44	108.20
1	X	1882	G	C3'-C2'-C1'	6.55	106.74	101.50
1	X	1412	C	C2'-C3'-O3'	6.54	124.17	113.70
1	X	575	U	O4'-C1'-N1	6.54	113.43	108.20
1	X	2239	C	O4'-C1'-N1	6.54	113.43	108.20
1	X	2708	U	P-O3'-C3'	-6.54	111.86	119.70
1	X	2860	C	O4'-C1'-N1	6.53	113.43	108.20
1	X	1411	C	O4'-C1'-N1	6.53	113.42	108.20
1	X	819	C	O5'-P-OP2	-6.53	99.82	105.70
1	X	1909	U	C2-N1-C1'	6.53	125.53	117.70
1	X	1403	U	P-O3'-C3'	6.53	127.53	119.70
1	X	1989	C	C1'-O4'-C4'	6.53	115.12	109.90
1	X	2804	G	C5-C6-N1	6.52	114.76	111.50
1	X	738	G	N7-C8-N9	6.52	116.36	113.10
1	X	2628	C	C3'-C2'-C1'	-6.52	96.29	101.50
1	X	527	C	N1-C2-O2	6.51	122.81	118.90
1	X	955	G	N9-C1'-C2'	6.51	122.47	114.00
1	X	2553	G	C5-N7-C8	-6.51	101.05	104.30
1	X	2482	A	C5'-C4'-O4'	6.50	116.90	109.10
1	X	746	G	N3-C4-C5	-6.50	125.35	128.60
1	X	1032	A	C5-N7-C8	-6.50	100.65	103.90
1	X	1992	G	OP1-P-OP2	-6.50	109.86	119.60
1	X	2797	G	N3-C4-N9	6.50	129.90	126.00
2	Y	54	U	P-O5'-C5'	6.49	131.29	120.90
1	X	2691	C	O4'-C1'-N1	6.49	113.39	108.20
1	X	2553	G	C4-C5-N7	6.48	113.39	110.80
1	X	2656	G	O4'-C1'-N9	6.48	113.38	108.20
1	X	114	C	O4'-C1'-N1	6.48	113.38	108.20
1	X	243	G	P-O5'-C5'	6.47	131.25	120.90
1	X	540	G	C4'-C3'-C2'	-6.47	96.13	102.60
1	X	234	C	O4'-C1'-N1	6.47	113.38	108.20
1	X	467	U	C3'-C2'-C1'	-6.47	96.33	101.50
1	X	591	G	O4'-C1'-N9	6.47	113.38	108.20
1	X	1752	U	O4'-C1'-N1	6.47	113.38	108.20
1	X	2591	C	O4'-C1'-N1	6.47	113.38	108.20
1	X	549	G	O4'-C1'-N9	6.47	113.37	108.20
1	X	2437	G	O4'-C1'-N9	6.47	113.37	108.20
1	X	19	C	O4'-C1'-N1	6.46	113.37	108.20
1	X	569	C	P-O3'-C3'	-6.46	111.94	119.70
1	X	796	A	C6-C5-N7	-6.46	127.78	132.30
1	X	1663	C	P-O3'-C3'	6.46	127.45	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1223	G	C4-C5-N7	6.46	113.38	110.80
1	X	160	C	O4'-C1'-N1	6.46	113.37	108.20
1	X	648	A	P-O3'-C3'	6.46	127.45	119.70
1	X	483	A	C3'-C2'-C1'	-6.46	96.33	101.50
1	X	879	A	O4'-C1'-N9	-6.46	103.03	108.20
2	Y	70	C	O4'-C1'-N1	6.46	113.36	108.20
1	X	759	C	C5'-C4'-C3'	-6.45	105.68	116.00
1	X	1825	C	O4'-C1'-N1	6.45	113.36	108.20
1	X	649	G	O4'-C1'-N9	6.45	113.36	108.20
1	X	689	A	C8-N9-C4	-6.45	103.22	105.80
1	X	2815	C	O4'-C1'-N1	6.45	113.36	108.20
1	X	22	C	P-O3'-C3'	6.45	127.44	119.70
1	X	1811	A	C2'-C3'-O3'	6.45	124.01	113.70
1	X	1313	U	C1'-O4'-C4'	-6.44	104.75	109.90
1	X	1749	G	P-O3'-C3'	6.44	127.43	119.70
1	X	606	A	O4'-C4'-C3'	-6.43	97.57	104.00
1	X	1044	U	O4'-C1'-N1	6.43	113.34	108.20
1	X	2726	U	O4'-C1'-N1	6.43	113.34	108.20
1	X	1388	C	O4'-C1'-N1	6.43	113.34	108.20
1	X	1413	U	O4'-C1'-N1	6.43	113.34	108.20
1	X	2262	C	O4'-C1'-N1	6.43	113.34	108.20
1	X	2591	C	C5-C6-N1	6.43	124.21	121.00
1	X	496	C	P-O3'-C3'	-6.42	111.99	119.70
1	X	2019	C	O4'-C1'-N1	6.42	113.34	108.20
1	X	774	A	C4-C5-C6	6.42	120.21	117.00
1	X	2530	C	O5'-P-OP2	-6.42	99.92	105.70
1	X	2426	G	C5'-C4'-C3'	-6.42	105.74	116.00
1	X	784	U	O4'-C1'-N1	6.41	113.33	108.20
1	X	665	A	O4'-C1'-N9	6.41	113.33	108.20
1	X	1570	C	N1-C2-O2	6.41	122.74	118.90
1	X	2782	G	C6-C5-N7	-6.41	126.56	130.40
1	X	1249	G	C2'-C3'-O3'	6.41	123.95	113.70
1	X	1561	A	C4'-C3'-O3'	6.41	125.81	113.00
1	X	1943	A	C4'-C3'-C2'	6.40	109.00	102.60
1	X	1768	U	N1-C2-O2	6.40	127.28	122.80
1	X	2675	U	O4'-C1'-N1	6.40	113.32	108.20
1	X	71	A	C4'-C3'-C2'	6.40	109.00	102.60
1	X	758	G	P-O3'-C3'	6.39	127.37	119.70
1	X	2452	U	O4'-C1'-N1	6.39	113.32	108.20
1	X	774	A	C5'-C4'-O4'	6.39	116.77	109.10
1	X	890	U	O4'-C1'-N1	6.39	113.31	108.20
1	X	2256	G	C8-N9-C4	-6.38	103.85	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	173	A	O4'-C1'-N9	6.37	113.30	108.20
1	X	1489	C	O4'-C1'-N1	6.37	113.30	108.20
1	X	1770	U	C1'-O4'-C4'	-6.37	104.80	109.90
1	X	2782	G	C4-C5-N7	6.37	113.35	110.80
1	X	2439	U	O4'-C1'-N1	6.37	113.29	108.20
1	X	841	G	C1'-O4'-C4'	-6.37	104.81	109.90
1	X	738	G	C8-N9-C4	-6.36	103.86	106.40
1	X	220	U	O4'-C1'-N1	6.36	113.29	108.20
1	X	483	A	C4'-C3'-C2'	6.36	108.96	102.60
1	X	504	G	O4'-C4'-C3'	-6.36	97.64	104.00
1	X	542	A	C5-N7-C8	-6.36	100.72	103.90
1	X	1468	A	N3-C4-C5	-6.36	122.35	126.80
1	X	2291	U	O4'-C1'-N1	6.35	113.28	108.20
1	X	869	C	O4'-C1'-N1	6.34	113.27	108.20
1	X	1764	A	N1-C6-N6	6.34	122.40	118.60
1	X	522	G	O4'-C1'-N9	6.33	113.27	108.20
1	X	1122	A	O4'-C1'-N9	6.33	113.26	108.20
1	X	1334	A	C3'-C2'-C1'	-6.33	96.44	101.50
1	X	2678	C	O4'-C1'-N1	6.32	113.26	108.20
1	X	66	U	O4'-C1'-N1	6.32	113.26	108.20
1	X	539	A	O4'-C1'-N9	6.32	113.26	108.20
1	X	858	G	O4'-C1'-N9	6.32	113.26	108.20
1	X	501	G	O4'-C1'-N9	6.32	113.25	108.20
1	X	540	G	C2-N3-C4	6.32	115.06	111.90
1	X	1831	G	C8-N9-C4	-6.31	103.87	106.40
1	X	1144	U	O4'-C1'-N1	6.31	113.25	108.20
11	I	28	LYS	C-N-CA	6.31	137.47	121.70
1	X	2500	C	O4'-C1'-N1	6.31	113.25	108.20
1	X	2795	A	O4'-C1'-N9	-6.30	103.16	108.20
1	X	537	C	C2-N3-C4	-6.30	116.75	119.90
1	X	656	U	P-O5'-C5'	6.30	130.98	120.90
1	X	2189	A	N7-C8-N9	6.30	116.95	113.80
1	X	1407	G	N9-C1'-C2'	6.29	122.18	114.00
1	X	399	G	C2'-C3'-O3'	6.29	123.76	113.70
1	X	579	G	O4'-C1'-N9	6.29	113.23	108.20
1	X	1278	A	N9-C1'-C2'	6.29	122.17	114.00
1	X	432	C	O4'-C1'-N1	6.28	113.23	108.20
1	X	1997	A	P-O3'-C3'	6.28	127.24	119.70
1	X	1247	U	O4'-C1'-N1	6.28	113.22	108.20
1	X	2482	A	N1-C2-N3	-6.28	126.16	129.30
1	X	2540	A	O4'-C1'-N9	6.28	113.22	108.20
1	X	878	C	N1-C2-O2	6.28	122.67	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	467	U	N1-C1'-C2'	6.28	122.16	114.00
1	X	2318	U	O4'-C1'-N1	6.28	113.22	108.20
1	X	2074	U	O4'-C1'-N1	6.27	113.22	108.20
1	X	1314	A	N9-C1'-C2'	6.26	122.14	114.00
1	X	1963	G	N3-C4-C5	-6.26	125.47	128.60
1	X	657	A	C3'-C2'-C1'	-6.26	96.49	101.50
1	X	434	C	P-O3'-C3'	6.26	127.21	119.70
1	X	729	A	P-O3'-C3'	6.25	127.21	119.70
1	X	2639	A	P-O3'-C3'	-6.25	112.19	119.70
1	X	237	G	O4'-C1'-N9	6.25	113.20	108.20
1	X	413	G	N7-C8-N9	6.25	116.23	113.10
1	X	559	C	C2'-C3'-O3'	6.25	123.69	113.70
1	X	2393	G	O4'-C1'-N9	6.25	113.20	108.20
1	X	2705	A	C4'-C3'-C2'	6.25	108.85	102.60
1	X	332	C	O4'-C1'-N1	6.25	113.20	108.20
1	X	1990	U	N3-C2-O2	-6.25	117.83	122.20
1	X	1001	A	O4'-C1'-N9	6.24	113.19	108.20
1	X	1111	C	O4'-C1'-N1	6.24	113.19	108.20
1	X	879	A	C4'-C3'-C2'	6.24	108.84	102.60
1	X	1051	U	O4'-C1'-N1	6.24	113.19	108.20
1	X	187	U	O4'-C1'-N1	6.24	113.19	108.20
1	X	1598	C	O4'-C1'-N1	6.24	113.19	108.20
1	X	2081	U	O4'-C1'-N1	6.24	113.19	108.20
1	X	2594	U	C4-C5-C6	-6.24	115.96	119.70
1	X	2359	U	O4'-C1'-N1	6.23	113.19	108.20
1	X	780	U	C3'-C2'-C1'	-6.23	96.52	101.50
1	X	675	C	O4'-C1'-N1	6.22	113.18	108.20
1	X	2800	C	O4'-C1'-N1	6.22	113.18	108.20
1	X	1909	U	N1-C1'-C2'	6.22	122.08	114.00
1	X	1341	G	P-O3'-C3'	-6.21	112.25	119.70
1	X	2692	A	O5'-P-OP1	6.21	118.16	110.70
2	Y	83	C	N1-C2-O2	6.21	122.63	118.90
1	X	683	A	N9-C1'-C2'	6.21	122.07	114.00
1	X	1669	A	P-O5'-C5'	6.21	130.83	120.90
1	X	148	C	O4'-C1'-N1	6.21	113.17	108.20
1	X	1353	A	P-O3'-C3'	6.20	127.14	119.70
1	X	1373	G	O4'-C1'-N9	6.20	113.16	108.20
1	X	2181	A	O4'-C1'-N9	6.20	113.16	108.20
1	X	1991	C	P-O3'-C3'	-6.20	112.26	119.70
1	X	1624	A	C1'-O4'-C4'	-6.20	104.94	109.90
2	Y	45	C	N1-C2-O2	6.20	122.62	118.90
1	X	236	C	N1-C2-O2	6.19	122.62	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1621	C	O4'-C1'-N1	6.19	113.16	108.20
1	X	1288	A	N9-C1'-C2'	6.19	122.05	114.00
1	X	1819	U	O4'-C1'-N1	6.19	113.15	108.20
1	X	1882	G	P-O3'-C3'	6.19	127.13	119.70
1	X	2627	G	N1-C6-O6	6.19	123.61	119.90
1	X	595	A	O4'-C1'-N9	6.18	113.15	108.20
1	X	1953	A	C5'-C4'-O4'	6.18	116.52	109.10
1	X	956	A	C5-C6-N6	-6.18	118.75	123.70
1	X	346	C	C5-C6-N1	6.18	124.09	121.00
1	X	1075	C	O4'-C1'-N1	6.18	113.14	108.20
1	X	1288	A	C5'-C4'-C3'	6.18	125.89	116.00
1	X	857	U	O4'-C1'-N1	6.18	113.14	108.20
1	X	995	A	C3'-C2'-C1'	-6.18	96.56	101.50
1	X	1059	A	P-O3'-C3'	6.17	127.11	119.70
1	X	1467	U	N1-C1'-C2'	6.17	122.03	114.00
1	X	1983	G	P-O3'-C3'	6.17	127.11	119.70
1	X	2408	G	P-O3'-C3'	-6.17	112.30	119.70
1	X	2867	G	C6-C5-N7	-6.17	126.70	130.40
1	X	780	U	C2'-C3'-O3'	6.17	123.57	113.70
2	Y	87	C	O4'-C1'-N1	6.17	113.14	108.20
1	X	323	G	P-O5'-C5'	-6.17	111.03	120.90
1	X	2627	G	C5-C6-O6	-6.17	124.90	128.60
1	X	1505	U	O4'-C1'-N1	6.16	113.13	108.20
1	X	1579	G	O4'-C1'-N9	6.16	113.13	108.20
1	X	1006	C	P-O3'-C3'	6.16	127.09	119.70
1	X	169	C	N1-C2-O2	6.16	122.60	118.90
1	X	322	A	P-O3'-C3'	6.16	127.09	119.70
1	X	1338	G	C5-C6-O6	-6.16	124.90	128.60
1	X	1417	C	O4'-C1'-N1	6.16	113.13	108.20
1	X	1850	G	O4'-C1'-N9	6.16	113.13	108.20
1	X	1647	U	O4'-C1'-N1	6.16	113.12	108.20
1	X	393	U	O4'-C1'-N1	6.15	113.12	108.20
1	X	682	G	P-O3'-C3'	6.15	127.08	119.70
1	X	1398	G	O4'-C1'-N9	6.15	113.12	108.20
1	X	358	C	C6-N1-C2	-6.15	117.84	120.30
1	X	859	U	C5'-C4'-O4'	6.15	116.48	109.10
1	X	917	U	O4'-C1'-N1	6.15	113.12	108.20
1	X	1142	G	C1'-O4'-C4'	-6.14	104.98	109.90
1	X	796	A	C5-C6-N1	-6.14	114.63	117.70
1	X	1234	C	N1-C2-O2	6.14	122.58	118.90
1	X	542	A	C4-C5-C6	6.14	120.07	117.00
1	X	516	G	O4'-C1'-N9	6.14	113.11	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1981	A	O5'-P-OP2	-6.14	100.17	105.70
1	X	466	A	P-O3'-C3'	6.14	127.06	119.70
1	X	1032	A	N7-C8-N9	6.14	116.87	113.80
2	Y	32	C	C6-N1-C2	-6.14	117.84	120.30
1	X	193	A	O4'-C1'-N9	6.13	113.11	108.20
1	X	1467	U	C5-C4-O4	-6.13	122.22	125.90
2	Y	110	U	O4'-C1'-N1	6.13	113.11	108.20
1	X	2238	G	O4'-C1'-N9	6.13	113.11	108.20
1	X	2492	G	C8-N9-C4	-6.13	103.95	106.40
23	U	18	VAL	C-N-CA	6.13	137.03	121.70
1	X	387	A	C5'-C4'-O4'	6.13	116.45	109.10
1	X	982	C	O4'-C1'-N1	6.13	113.10	108.20
1	X	1496	G	C2'-C3'-O3'	6.13	123.50	113.70
1	X	2636	A	O4'-C1'-N9	6.13	113.10	108.20
1	X	321	A	P-O3'-C3'	6.12	127.05	119.70
1	X	1788	C	O4'-C1'-N1	6.12	113.10	108.20
1	X	1336	G	C5-C6-N1	6.12	114.56	111.50
1	X	244	C	O4'-C1'-N1	6.12	113.09	108.20
1	X	1468	A	N9-C1'-C2'	6.12	121.95	114.00
1	X	1792	C	P-O3'-C3'	6.12	127.04	119.70
1	X	2229	G	C8-N9-C4	-6.12	103.95	106.40
1	X	2809	A	P-O3'-C3'	6.12	127.04	119.70
1	X	2711	G	C5-C6-O6	-6.11	124.93	128.60
1	X	30	G	C8-N9-C4	-6.11	103.95	106.40
1	X	1017	C	O4'-C1'-N1	6.11	113.09	108.20
1	X	2312	A	O4'-C1'-N9	6.11	113.09	108.20
1	X	422	C	O4'-C1'-N1	6.11	113.08	108.20
1	X	29	U	O4'-C1'-N1	6.10	113.08	108.20
1	X	1380	C	O4'-C1'-N1	6.10	113.08	108.20
1	X	2844	G	O4'-C1'-N9	6.10	113.08	108.20
1	X	668	A	P-O3'-C3'	6.09	127.01	119.70
1	X	162	C	O4'-C1'-N1	6.09	113.07	108.20
19	Q	61	LYS	N-CA-C	6.09	127.45	111.00
1	X	707	U	O4'-C1'-N1	6.09	113.07	108.20
1	X	1181	C	O4'-C1'-N1	6.09	113.07	108.20
1	X	700	C	O4'-C1'-N1	6.09	113.07	108.20
1	X	1515	U	O4'-C1'-N1	6.09	113.07	108.20
9	G	103	TYR	C-N-CA	6.09	136.92	121.70
1	X	358	C	P-O5'-C5'	6.08	130.64	120.90
1	X	596	C	P-O5'-C5'	-6.08	111.17	120.90
1	X	2018	G	C1'-O4'-C4'	-6.08	105.03	109.90
1	X	396	U	C1'-O4'-C4'	-6.08	105.03	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	399	G	C4'-C3'-C2'	6.08	108.68	102.60
1	X	1540	C	O4'-C1'-N1	6.08	113.06	108.20
1	X	1142	G	O4'-C1'-C2'	-6.08	99.72	105.80
1	X	776	G	N9-C1'-C2'	6.08	121.90	114.00
1	X	1149	G	P-O3'-C3'	6.08	127.00	119.70
1	X	1233	A	C2'-C3'-O3'	6.08	123.43	113.70
1	X	1522	C	N1-C2-O2	6.08	122.55	118.90
1	X	135	U	O4'-C1'-N1	6.08	113.06	108.20
1	X	2554	C	N1-C2-O2	6.07	122.54	118.90
1	X	1466	C	O4'-C1'-N1	6.07	113.06	108.20
1	X	2414	A	P-O5'-C5'	6.07	130.61	120.90
1	X	618	A	O4'-C1'-N9	6.07	113.05	108.20
1	X	331	U	O4'-C1'-N1	6.06	113.05	108.20
1	X	113	C	O4'-C1'-N1	6.06	113.05	108.20
1	X	1060	C	O4'-C1'-N1	6.06	113.05	108.20
1	X	1758	C	O4'-C1'-N1	6.06	113.05	108.20
1	X	2039	G	C5-C6-O6	-6.06	124.97	128.60
1	X	2184	C	O4'-C1'-N1	6.06	113.05	108.20
1	X	346	C	N3-C4-C5	-6.06	119.48	121.90
1	X	1006	C	N1-C1'-C2'	6.05	121.87	114.00
1	X	2336	G	O5'-P-OP2	-6.05	100.25	105.70
11	I	36	GLY	C-N-CA	6.05	136.83	121.70
1	X	1149	G	O4'-C1'-N9	6.05	113.04	108.20
1	X	1843	U	O4'-C1'-N1	6.05	113.04	108.20
1	X	1287	A	N1-C6-N6	-6.05	114.97	118.60
1	X	1353	A	O4'-C1'-N9	6.05	113.04	108.20
1	X	2661	G	O4'-C1'-N9	6.05	113.04	108.20
1	X	2685	A	C5-C6-N1	6.05	120.72	117.70
1	X	2281	C	O4'-C1'-N1	6.04	113.04	108.20
1	X	219	G	N9-C1'-C2'	6.04	121.85	114.00
1	X	90	G	N3-C4-C5	-6.04	125.58	128.60
1	X	473	C	OP2-P-O3'	6.04	118.48	105.20
1	X	1732	U	P-O3'-C3'	6.04	126.95	119.70
1	X	2295	C	O4'-C1'-N1	6.03	113.03	108.20
1	X	2799	C	C5-C4-N4	-6.03	115.98	120.20
1	X	1182	U	C2'-C3'-O3'	6.03	123.35	113.70
1	X	2264	C	O4'-C1'-N1	6.03	113.02	108.20
1	X	393	U	N3-C4-O4	6.03	123.62	119.40
1	X	833	A	N1-C6-N6	6.03	122.22	118.60
1	X	1333	G	C6-C5-N7	6.03	134.02	130.40
2	Y	54	U	C4'-C3'-C2'	-6.02	96.58	102.60
1	X	957	G	P-O3'-C3'	6.02	126.93	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2548	G	O4'-C4'-C3'	-6.02	97.98	104.00
1	X	1976	U	O4'-C1'-N1	6.02	113.01	108.20
1	X	2443	C	O4'-C1'-N1	6.01	113.01	108.20
1	X	2325	A	P-O3'-C3'	6.01	126.91	119.70
1	X	2558	C	O4'-C1'-N1	6.01	113.01	108.20
1	X	1655	C	O4'-C1'-N1	6.01	113.01	108.20
1	X	1913	G	P-O3'-C3'	6.01	126.91	119.70
1	X	2363	G	O4'-C1'-N9	6.01	113.01	108.20
1	X	724	C	O4'-C1'-N1	6.00	113.00	108.20
1	X	1324	G	O4'-C1'-N9	6.00	113.00	108.20
1	X	577	U	O4'-C1'-N1	6.00	113.00	108.20
1	X	2608	A	C1'-O4'-C4'	-6.00	105.10	109.90
2	Y	50	U	O4'-C1'-N1	6.00	113.00	108.20
1	X	1548	U	O4'-C1'-N1	5.99	112.99	108.20
2	Y	7	C	O4'-C1'-N1	5.99	112.99	108.20
1	X	413	G	N3-C4-C5	-5.99	125.61	128.60
1	X	1946	U	C2-N1-C1'	5.99	124.89	117.70
1	X	1099	A	P-O3'-C3'	5.99	126.88	119.70
1	X	338	G	C8-N9-C4	-5.99	104.01	106.40
1	X	1541	G	C4'-C3'-C2'	-5.99	96.61	102.60
1	X	2408	G	OP1-P-OP2	-5.99	110.62	119.60
1	X	2645	C	N1-C2-O2	5.99	122.49	118.90
11	I	41	SER	N-CA-C	5.99	127.16	111.00
1	X	221	A	O4'-C1'-N9	5.98	112.99	108.20
1	X	1573	G	P-O3'-C3'	5.98	126.88	119.70
1	X	302	U	O4'-C1'-N1	5.98	112.98	108.20
1	X	1461	C	O4'-C1'-N1	5.98	112.98	108.20
1	X	2371	A	C8-N9-C4	-5.98	103.41	105.80
1	X	779	U	O4'-C1'-N1	5.97	112.98	108.20
1	X	2193	C	O4'-C4'-C3'	-5.97	98.03	104.00
11	I	38	LYS	C-N-CA	5.97	136.63	121.70
1	X	223	C	O4'-C1'-N1	5.97	112.98	108.20
1	X	714	G	C3'-C2'-C1'	-5.97	96.72	101.50
1	X	2194	A	P-O3'-C3'	5.97	126.86	119.70
1	X	2775	U	O4'-C1'-N1	5.97	112.97	108.20
1	X	946	U	O4'-C1'-N1	5.97	112.97	108.20
1	X	1345	G	O5'-P-OP2	-5.97	100.33	105.70
1	X	2482	A	C2-N3-C4	5.97	113.58	110.60
1	X	2561	G	C4-C5-N7	5.96	113.19	110.80
1	X	1002	C	C6-N1-C2	-5.96	117.92	120.30
1	X	822	G	C4'-C3'-C2'	-5.96	96.64	102.60
1	X	1142	G	C3'-C2'-C1'	-5.96	96.73	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1030	U	O4'-C1'-N1	5.96	112.97	108.20
1	X	2719	U	O4'-C1'-N1	5.96	112.97	108.20
1	X	559	C	P-O3'-C3'	5.96	126.85	119.70
1	X	1950	C	O4'-C1'-N1	5.96	112.97	108.20
1	X	2683	C	O4'-C1'-N1	5.96	112.96	108.20
1	X	2408	G	N3-C4-C5	-5.95	125.62	128.60
1	X	2324	G	P-O3'-C3'	5.94	126.83	119.70
1	X	224	G	C5'-C4'-O4'	5.94	116.23	109.10
1	X	2258	G	C4'-C3'-C2'	-5.94	96.66	102.60
1	X	2858	A	O4'-C1'-N9	5.94	112.95	108.20
1	X	1336	G	C4-C5-N7	5.94	113.17	110.80
1	X	1530	U	O4'-C1'-N1	5.94	112.95	108.20
1	X	656	U	C1'-O4'-C4'	-5.94	105.15	109.90
1	X	2681	A	C5-C6-N1	5.94	120.67	117.70
15	M	28	ARG	N-CA-C	-5.93	94.98	111.00
1	X	1338	G	N3-C4-C5	-5.93	125.64	128.60
1	X	1350	G	C5-C6-O6	-5.93	125.04	128.60
2	Y	58	G	C3'-C2'-C1'	5.93	106.24	101.50
1	X	979	A	O4'-C1'-N9	5.93	112.94	108.20
1	X	2478	C	C6-N1-C2	-5.93	117.93	120.30
1	X	2552	C	C4'-C3'-C2'	-5.93	96.67	102.60
1	X	2576	G	O4'-C1'-N9	-5.93	103.46	108.20
1	X	1311	C	O4'-C1'-N1	5.92	112.94	108.20
2	Y	24	U	O4'-C1'-N1	5.92	112.94	108.20
1	X	2699	G	P-O3'-C3'	5.92	126.81	119.70
1	X	520	C	C4'-C3'-C2'	-5.92	96.68	102.60
1	X	2257	A	P-O5'-C5'	5.92	130.37	120.90
1	X	68	C	N1-C2-O2	5.92	122.45	118.90
1	X	2354	G	O4'-C4'-C3'	-5.92	98.08	104.00
1	X	242	A	P-O5'-C5'	5.92	130.36	120.90
1	X	567	G	O4'-C1'-N9	5.91	112.93	108.20
1	X	1468	A	C6-N1-C2	-5.91	115.05	118.60
1	X	1805	G	O4'-C1'-N9	5.91	112.93	108.20
1	X	841	G	C5-N7-C8	-5.91	101.35	104.30
1	X	1754	G	P-O5'-C5'	5.91	130.35	120.90
1	X	2406	C	P-O5'-C5'	5.91	130.35	120.90
1	X	2690	A	O4'-C1'-N9	5.91	112.93	108.20
1	X	865	A	O4'-C1'-N9	5.91	112.93	108.20
1	X	2382	C	C6-N1-C2	-5.91	117.94	120.30
1	X	825	C	P-O5'-C5'	5.91	130.35	120.90
1	X	1304	U	O4'-C1'-N1	5.91	112.92	108.20
1	X	1412	C	O4'-C4'-C3'	-5.91	98.09	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1667	A	O4'-C1'-N9	5.90	112.92	108.20
1	X	2578	G	P-O5'-C5'	5.90	130.35	120.90
1	X	2267	A	P-O3'-C3'	5.90	126.78	119.70
1	X	2854	G	O4'-C1'-C2'	-5.90	99.90	105.80
1	X	2045	A	C3'-C2'-C1'	5.90	106.22	101.50
1	X	2560	G	N3-C4-C5	-5.90	125.65	128.60
1	X	2593	A	P-O3'-C3'	5.90	126.78	119.70
1	X	1064	C	O4'-C1'-N1	5.90	112.92	108.20
1	X	154	U	O4'-C1'-N1	5.90	112.92	108.20
1	X	811	G	N1-C6-O6	-5.90	116.36	119.90
1	X	1454	U	N3-C4-O4	5.90	123.53	119.40
1	X	622	U	O4'-C1'-N1	5.89	112.91	108.20
1	X	2847	G	C8-N9-C4	-5.89	104.04	106.40
1	X	338	G	O4'-C1'-N9	5.89	112.91	108.20
1	X	1313	U	O4'-C1'-N1	5.89	112.91	108.20
1	X	2560	G	C5-C6-O6	-5.89	125.07	128.60
2	Y	22	U	O4'-C1'-N1	5.89	112.91	108.20
1	X	2692	A	P-O3'-C3'	5.88	126.76	119.70
1	X	466	A	P-O5'-C5'	5.88	130.31	120.90
1	X	681	A	C8-N9-C4	-5.88	103.45	105.80
1	X	2366	U	O4'-C1'-N1	5.88	112.91	108.20
1	X	2484	G	C8-N9-C4	-5.88	104.05	106.40
1	X	983	G	P-O3'-C3'	5.88	126.75	119.70
1	X	430	C	C5-C6-N1	5.88	123.94	121.00
1	X	1265	G	O5'-P-OP2	-5.87	100.42	105.70
1	X	955	G	N3-C4-C5	-5.87	125.67	128.60
1	X	1090	C	O4'-C1'-N1	5.87	112.89	108.20
1	X	2229	G	C5'-C4'-O4'	5.87	116.14	109.10
1	X	320	A	C2-N3-C4	5.87	113.53	110.60
1	X	431	G	O4'-C1'-N9	5.87	112.89	108.20
1	X	1338	G	N3-C4-N9	5.87	129.52	126.00
1	X	1468	A	C2-N3-C4	5.86	113.53	110.60
1	X	2018	G	N7-C8-N9	5.86	116.03	113.10
1	X	791	G	P-O3'-C3'	5.86	126.73	119.70
1	X	1922	U	N3-C2-O2	-5.86	118.10	122.20
1	X	2826	C	C4'-C3'-C2'	-5.86	96.75	102.60
1	X	2587	G	O4'-C1'-N9	5.85	112.88	108.20
1	X	1775	A	C4'-C3'-O3'	-5.85	97.11	109.40
1	X	2875	C	O4'-C1'-N1	5.85	112.88	108.20
1	X	679	C	O4'-C1'-N1	5.84	112.87	108.20
1	X	2478	C	P-O3'-C3'	-5.84	112.69	119.70
2	Y	81	C	C5-C6-N1	5.84	123.92	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2258	G	O4'-C1'-N9	5.84	112.87	108.20
1	X	309	G	N7-C8-N9	5.84	116.02	113.10
1	X	515	A	O4'-C1'-N9	5.84	112.87	108.20
1	X	651	C	P-O3'-C3'	5.83	126.70	119.70
1	X	731	A	O4'-C1'-N9	5.83	112.87	108.20
1	X	1087	C	P-O5'-C5'	5.83	130.23	120.90
1	X	2025	A	O4'-C1'-N9	5.83	112.86	108.20
1	X	1472	C	O4'-C1'-N1	5.83	112.86	108.20
1	X	1514	C	O4'-C1'-N1	5.83	112.86	108.20
1	X	1243	G	O4'-C1'-N9	5.82	112.86	108.20
1	X	2422	C	O4'-C1'-N1	5.82	112.86	108.20
1	X	1288	A	N9-C4-C5	-5.82	103.47	105.80
1	X	1695	U	C5'-C4'-O4'	5.82	116.08	109.10
1	X	1703	C	C3'-C2'-C1'	-5.82	96.85	101.50
1	X	1115	C	O4'-C1'-N1	5.81	112.85	108.20
1	X	757	U	OP2-P-O3'	5.81	117.98	105.20
2	Y	67	C	P-O3'-C3'	5.81	126.67	119.70
1	X	424	G	P-O3'-C3'	5.81	126.67	119.70
1	X	2806	G	O4'-C1'-N9	5.81	112.85	108.20
1	X	1367	A	O4'-C1'-N9	5.81	112.84	108.20
1	X	1328	C	O4'-C1'-N1	5.80	112.84	108.20
1	X	1407	G	P-O3'-C3'	5.80	126.67	119.70
1	X	1344	C	N3-C4-C5	5.80	124.22	121.90
1	X	1244	U	O4'-C1'-N1	5.80	112.84	108.20
1	X	2303	C	N1-C2-O2	5.80	122.38	118.90
1	X	747	A	P-O3'-C3'	-5.80	112.74	119.70
1	X	2321	C	C6-N1-C2	-5.80	117.98	120.30
1	X	1781	C	C5'-C4'-O4'	5.79	116.06	109.10
1	X	1288	A	N1-C6-N6	5.79	122.07	118.60
1	X	1506	C	O4'-C1'-N1	5.79	112.83	108.20
1	X	1831	G	N7-C8-N9	5.79	116.00	113.10
1	X	2075	U	C1'-O4'-C4'	-5.79	105.27	109.90
1	X	2485	U	C2-N1-C1'	5.79	124.65	117.70
1	X	1286	U	P-O5'-C5'	5.78	130.15	120.90
1	X	1680	U	C2'-C3'-O3'	5.78	122.95	113.70
1	X	2315	A	P-O5'-C5'	5.78	130.15	120.90
1	X	437	G	O4'-C1'-N9	5.78	112.82	108.20
1	X	1469	U	C5'-C4'-O4'	5.78	116.04	109.10
1	X	2006	G	O5'-P-OP1	-5.78	100.50	105.70
1	X	2541	U	N3-C2-O2	-5.78	118.15	122.20
1	X	559	C	N1-C2-O2	5.78	122.37	118.90
1	X	2406	C	O4'-C1'-N1	5.78	112.82	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	952	A	P-O5'-C5'	5.78	130.15	120.90
1	X	1097	A	P-O3'-C3'	5.78	126.63	119.70
1	X	2616	U	O4'-C1'-N1	5.78	112.82	108.20
1	X	2619	G	N7-C8-N9	5.78	115.99	113.10
1	X	1546	C	O4'-C1'-N1	5.78	112.82	108.20
1	X	873	U	O4'-C1'-N1	5.77	112.82	108.20
1	X	648	A	C1'-O4'-C4'	-5.77	105.28	109.90
1	X	683	A	C2'-C3'-O3'	5.77	122.94	113.70
1	X	1086	C	C3'-C2'-C1'	5.77	106.12	101.50
1	X	327	C	O4'-C1'-N1	5.77	112.81	108.20
1	X	508	G	O4'-C1'-N9	5.77	112.82	108.20
1	X	1092	U	O4'-C1'-N1	5.77	112.82	108.20
1	X	2795	A	C3'-C2'-C1'	5.77	106.11	101.50
1	X	2697	G	P-O3'-C3'	-5.77	112.78	119.70
1	X	2371	A	N7-C8-N9	5.76	116.68	113.80
1	X	1191	G	P-O3'-C3'	5.76	126.61	119.70
1	X	199	A	P-O3'-C3'	5.75	126.61	119.70
1	X	2668	U	N3-C4-O4	-5.75	115.37	119.40
14	L	88	VAL	C-N-CA	5.75	136.08	121.70
1	X	1363	C	O4'-C1'-N1	5.75	112.80	108.20
1	X	1806	G	C8-N9-C4	-5.75	104.10	106.40
1	X	2370	G	O4'-C1'-N9	5.75	112.80	108.20
1	X	1964	A	O4'-C1'-N9	5.75	112.80	108.20
1	X	3	U	O4'-C4'-C3'	-5.74	98.26	104.00
1	X	1010	U	N3-C2-O2	-5.74	118.18	122.20
1	X	1145	C	P-O3'-C3'	5.74	126.59	119.70
1	X	1712	G	C6-C5-N7	-5.74	126.95	130.40
1	X	2587	G	C5-C6-O6	-5.74	125.15	128.60
1	X	2869	U	O4'-C1'-N1	5.74	112.79	108.20
1	X	2256	G	O4'-C1'-N9	5.74	112.79	108.20
1	X	1265	G	P-O3'-C3'	5.74	126.58	119.70
1	X	1762	C	O4'-C1'-N1	5.74	112.79	108.20
1	X	2811	G	O4'-C1'-N9	5.74	112.79	108.20
1	X	1561	A	O4'-C4'-C3'	-5.73	98.27	104.00
1	X	339	U	P-O3'-C3'	5.73	126.58	119.70
9	G	108	GLY	N-CA-C	-5.73	98.78	113.10
1	X	322	A	O4'-C1'-N9	5.73	112.78	108.20
1	X	2329	C	O4'-C1'-N1	5.73	112.78	108.20
1	X	467	U	C5-C4-O4	-5.73	122.46	125.90
1	X	767	G	O4'-C1'-N9	5.72	112.78	108.20
1	X	955	G	N3-C4-N9	5.72	129.43	126.00
1	X	1575	C	C4'-C3'-C2'	5.72	108.32	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1467	U	C5'-C4'-O4'	-5.71	102.24	109.10
1	X	480	G	C5-C6-N1	5.71	114.36	111.50
1	X	537	C	N3-C4-C5	5.71	124.19	121.90
1	X	2230	G	C5-C6-O6	-5.71	125.17	128.60
1	X	2535	C	C5'-C4'-C3'	-5.71	106.86	116.00
1	X	777	A	C4'-C3'-C2'	5.71	108.31	102.60
1	X	2694	G	C5'-C4'-O4'	-5.71	102.25	109.10
1	X	2086	U	O4'-C1'-N1	5.70	112.76	108.20
1	X	2668	U	C5-C6-N1	-5.70	119.85	122.70
1	X	322	A	N9-C1'-C2'	5.70	121.41	114.00
1	X	1662	G	N9-C1'-C2'	5.70	121.41	114.00
1	X	660	G	C3'-C2'-C1'	-5.70	96.94	101.50
1	X	519	C	C5'-C4'-O4'	-5.70	102.26	109.10
1	X	1795	C	O4'-C1'-N1	5.70	112.76	108.20
2	Y	32	C	C5-C6-N1	5.70	123.85	121.00
1	X	1141	U	P-O3'-C3'	5.69	126.53	119.70
1	X	1631	C	N1-C1'-C2'	5.69	121.40	114.00
1	X	1828	C	O4'-C1'-N1	5.69	112.75	108.20
2	Y	111	C	P-O3'-C3'	5.69	126.53	119.70
2	Y	50	U	C3'-C2'-C1'	-5.69	96.95	101.50
1	X	1253	C	P-O3'-C3'	-5.69	112.88	119.70
1	X	1831	G	O4'-C1'-N9	5.69	112.75	108.20
1	X	1091	C	O4'-C1'-N1	5.69	112.75	108.20
1	X	1281	A	P-O3'-C3'	5.68	126.52	119.70
1	X	2495	G	O4'-C1'-N9	5.68	112.75	108.20
1	X	889	C	O4'-C1'-N1	5.68	112.75	108.20
1	X	955	G	N1-C2-N2	-5.68	111.09	116.20
1	X	1531	C	C1'-O4'-C4'	-5.68	105.36	109.90
1	X	2463	G	C5'-C4'-O4'	5.68	115.92	109.10
1	X	2552	C	N1-C1'-C2'	5.68	121.38	114.00
1	X	1063	C	O4'-C1'-N1	5.67	112.74	108.20
1	X	1182	U	O4'-C1'-N1	5.67	112.74	108.20
1	X	1105	U	O4'-C1'-N1	5.67	112.73	108.20
1	X	2528	G	OP1-P-O3'	5.67	117.67	105.20
1	X	1663	C	N3-C2-O2	-5.67	117.93	121.90
1	X	1824	C	C3'-C2'-C1'	-5.67	96.97	101.50
1	X	2080	U	O4'-C1'-N1	5.67	112.73	108.20
1	X	827	C	O4'-C1'-N1	5.67	112.73	108.20
1	X	2591	C	N1-C2-O2	5.67	122.30	118.90
1	X	2444	C	O4'-C1'-N1	5.66	112.73	108.20
1	X	816	U	O4'-C1'-N1	5.66	112.73	108.20
1	X	1076	U	O4'-C1'-N1	5.66	112.73	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2198	U	P-O3'-C3'	5.66	126.49	119.70
1	X	224	G	O4'-C1'-N9	5.66	112.72	108.20
1	X	975	C	O4'-C1'-N1	5.65	112.72	108.20
1	X	1531	C	O4'-C1'-N1	5.65	112.72	108.20
1	X	660	G	N3-C2-N2	-5.65	115.94	119.90
1	X	450	C	O4'-C1'-N1	5.65	112.72	108.20
1	X	545	C	C3'-C2'-C1'	-5.65	96.98	101.50
1	X	2745	A	C2-N3-C4	5.65	113.42	110.60
1	X	483	A	C5'-C4'-O4'	5.65	115.88	109.10
1	X	675	C	C3'-C2'-C1'	-5.65	96.98	101.50
1	X	1820	G	C4'-C3'-C2'	5.65	108.25	102.60
1	X	1347	C	OP2-P-O3'	5.65	117.62	105.20
2	Y	34	C	O4'-C1'-N1	5.65	112.72	108.20
2	Y	75	A	P-O3'-C3'	5.64	126.47	119.70
1	X	534	U	O4'-C1'-N1	5.64	112.71	108.20
1	X	702	A	O3'-P-O5'	-5.64	93.29	104.00
1	X	2485	U	N3-C2-O2	-5.64	118.25	122.20
1	X	332	C	P-O3'-C3'	5.64	126.47	119.70
1	X	1487	C	O4'-C1'-N1	5.63	112.71	108.20
1	X	540	G	C8-N9-C1'	-5.63	119.68	127.00
1	X	858	G	C3'-C2'-C1'	5.63	106.00	101.50
1	X	2481	G	O3'-P-O5'	-5.63	93.30	104.00
1	X	750	C	O4'-C1'-N1	5.63	112.70	108.20
1	X	1415	C	O4'-C1'-N1	5.63	112.70	108.20
1	X	219	G	O4'-C1'-C2'	-5.62	100.17	105.80
1	X	455	A	P-O3'-C3'	5.62	126.45	119.70
1	X	2479	U	C4'-C3'-C2'	-5.62	96.98	102.60
1	X	1241	G	O4'-C1'-N9	5.62	112.69	108.20
1	X	1567	A	O4'-C1'-N9	5.62	112.69	108.20
1	X	33	C	C4'-C3'-C2'	5.62	108.22	102.60
1	X	648	A	N9-C1'-C2'	5.62	121.30	114.00
1	X	2609	G	N3-C4-C5	-5.61	125.79	128.60
1	X	2417	U	P-O3'-C3'	5.61	126.44	119.70
1	X	1277	G	N3-C4-C5	-5.61	125.80	128.60
1	X	1266	G	N9-C1'-C2'	5.61	121.29	114.00
1	X	1925	C	O4'-C1'-N1	5.61	112.69	108.20
1	X	1833	U	O4'-C1'-N1	5.61	112.69	108.20
1	X	553	C	N1-C2-O2	5.61	122.26	118.90
1	X	827	C	P-O5'-C5'	5.61	129.87	120.90
1	X	879	A	C5'-C4'-C3'	-5.61	107.03	116.00
1	X	1249	G	N1-C6-O6	-5.61	116.54	119.90
1	X	1689	U	P-O3'-C3'	5.61	126.43	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1983	G	C4'-C3'-C2'	-5.61	97.00	102.60
1	X	2398	U	O4'-C1'-N1	5.60	112.68	108.20
1	X	1341	G	P-O5'-C5'	5.60	129.86	120.90
1	X	1547	U	O4'-C1'-N1	5.60	112.68	108.20
1	X	1570	C	C2-N1-C1'	5.60	124.96	118.80
1	X	2049	C	O4'-C1'-N1	5.60	112.68	108.20
1	X	623	G	O4'-C1'-N9	5.60	112.68	108.20
1	X	208	C	O4'-C1'-N1	5.60	112.68	108.20
1	X	699	G	C8-N9-C4	-5.60	104.16	106.40
1	X	1298	G	OP2-P-O3'	5.60	117.52	105.20
1	X	1734	C	N1-C2-O2	5.60	122.26	118.90
1	X	995	A	N9-C1'-C2'	5.60	121.28	114.00
1	X	1031	C	N1-C2-O2	5.59	122.26	118.90
1	X	2237	C	P-O3'-C3'	5.59	126.41	119.70
1	X	36	G	C8-N9-C4	-5.59	104.16	106.40
1	X	1344	C	O4'-C4'-C3'	-5.59	98.41	104.00
1	X	1882	G	P-O5'-C5'	5.59	129.85	120.90
1	X	558	G	O4'-C1'-N9	5.59	112.67	108.20
12	J	88	LYS	C-N-CA	5.59	134.04	122.30
1	X	1224	A	P-O3'-C3'	5.59	126.40	119.70
1	X	1971	C	O4'-C1'-N1	5.59	112.67	108.20
1	X	81	C	O4'-C1'-N1	5.58	112.67	108.20
1	X	1570	C	C3'-C2'-C1'	-5.58	97.03	101.50
1	X	2018	G	C4-C5-C6	-5.58	115.45	118.80
1	X	1993	G	O4'-C1'-N9	5.58	112.67	108.20
1	X	2528	G	C8-N9-C4	-5.58	104.17	106.40
1	X	215	G	O4'-C1'-N9	5.58	112.66	108.20
1	X	1776	A	C2-N3-C4	5.58	113.39	110.60
1	X	2273	C	O4'-C1'-N1	5.58	112.66	108.20
1	X	2046	C	O4'-C1'-N1	5.58	112.66	108.20
1	X	753	U	C5'-C4'-O4'	-5.58	102.41	109.10
1	X	1333	G	C5-N7-C8	-5.57	101.51	104.30
1	X	2447	G	P-O3'-C3'	5.57	126.38	119.70
1	X	2675	U	N3-C2-O2	-5.57	118.30	122.20
1	X	337	G	C8-N9-C4	-5.57	104.17	106.40
1	X	820	U	P-O3'-C3'	-5.57	113.02	119.70
1	X	978	U	O4'-C1'-N1	5.57	112.65	108.20
1	X	607	C	O4'-C4'-C3'	-5.56	98.44	104.00
1	X	681	A	N7-C8-N9	5.56	116.58	113.80
1	X	479	G	C5-C6-O6	-5.56	125.27	128.60
1	X	770	U	C5-C4-O4	-5.56	122.56	125.90
1	X	1013	G	C8-N9-C4	-5.56	104.18	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1031	C	C4'-C3'-C2'	5.56	108.16	102.60
1	X	175	C	C6-N1-C2	-5.56	118.08	120.30
1	X	2314	A	P-O3'-C3'	5.56	126.37	119.70
1	X	838	A	C2-N3-C4	5.56	113.38	110.60
1	X	1033	G	C2'-C3'-O3'	5.56	122.59	113.70
1	X	1333	G	C4-C5-C6	-5.55	115.47	118.80
1	X	1	G	P-O3'-C3'	5.55	126.36	119.70
1	X	828	C	O4'-C1'-N1	5.55	112.64	108.20
1	X	840	U	O5'-P-OP2	-5.55	100.70	105.70
1	X	418	C	C5'-C4'-C3'	5.55	124.88	116.00
1	X	876	A	O4'-C1'-N9	5.55	112.64	108.20
1	X	2504	G	O4'-C1'-N9	5.55	112.64	108.20
2	Y	72	C	O4'-C1'-N1	5.55	112.64	108.20
1	X	359	G	O4'-C1'-N9	5.55	112.64	108.20
1	X	449	C	O4'-C1'-N1	5.55	112.64	108.20
1	X	1623	C	N1-C2-O2	5.55	122.23	118.90
1	X	2759	U	P-O3'-C3'	5.55	126.36	119.70
1	X	647	G	P-O3'-C3'	5.54	126.35	119.70
1	X	1544	A	P-O3'-C3'	5.54	126.35	119.70
1	X	1700	C	P-O3'-C3'	-5.54	113.05	119.70
1	X	2575	U	C5-C4-O4	-5.54	122.57	125.90
1	X	2742	G	O4'-C1'-N9	5.54	112.64	108.20
1	X	2229	G	P-O5'-C5'	-5.54	112.03	120.90
19	Q	62	ARG	C-N-CA	5.54	135.55	121.70
1	X	1143	A	C1'-O4'-C4'	-5.54	105.47	109.90
1	X	1814	G	O4'-C1'-N9	5.54	112.63	108.20
1	X	1108	U	O4'-C1'-N1	5.54	112.63	108.20
1	X	1389	C	O4'-C1'-N1	5.54	112.63	108.20
1	X	1570	C	C6-N1-C1'	-5.54	114.16	120.80
1	X	168	A	O4'-C1'-N9	5.54	112.63	108.20
1	X	462	G	C4-C5-C6	5.54	122.12	118.80
1	X	985	G	C5-N7-C8	-5.53	101.53	104.30
1	X	1201	G	N3-C2-N2	-5.53	116.03	119.90
1	X	2591	C	C2-N3-C4	5.53	122.67	119.90
1	X	1016	C	O4'-C1'-N1	5.53	112.63	108.20
1	X	1469	U	O3'-P-O5'	5.53	114.51	104.00
1	X	99	U	C2-N1-C1'	5.53	124.34	117.70
1	X	211	U	O4'-C1'-N1	5.53	112.62	108.20
1	X	467	U	N3-C4-O4	5.53	123.27	119.40
1	X	1252	C	O4'-C1'-N1	5.53	112.62	108.20
1	X	972	C	C1'-O4'-C4'	-5.53	105.48	109.90
2	Y	6	C	O4'-C1'-N1	5.53	112.62	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2490	U	O4'-C1'-N1	5.53	112.62	108.20
1	X	990	A	O4'-C4'-C3'	-5.53	98.47	104.00
1	X	1963	G	C3'-C2'-C1'	5.53	105.92	101.50
1	X	2870	C	O4'-C1'-N1	5.52	112.62	108.20
1	X	22	C	O4'-C1'-N1	5.52	112.62	108.20
1	X	689	A	N1-C6-N6	5.52	121.91	118.60
1	X	796	A	C8-N9-C4	-5.52	103.59	105.80
1	X	823	U	C2'-C3'-O3'	5.52	122.53	113.70
1	X	2708	U	C5'-C4'-C3'	-5.52	107.16	116.00
17	O	97	GLY	N-CA-C	5.52	126.90	113.10
1	X	1699	A	C5-C6-N1	-5.52	114.94	117.70
1	X	2771	C	O4'-C1'-N1	5.52	112.61	108.20
1	X	447	U	P-O3'-C3'	5.52	126.32	119.70
1	X	1630	A	O3'-P-O5'	-5.52	93.52	104.00
1	X	2797	G	C6-C5-N7	-5.52	127.09	130.40
1	X	998	C	O4'-C1'-N1	5.51	112.61	108.20
1	X	2190	A	C5'-C4'-C3'	5.51	124.82	116.00
1	X	2199	C	N1-C1'-C2'	5.51	121.17	114.00
1	X	2560	G	C6-N1-C2	-5.51	121.79	125.10
1	X	652	C	P-O5'-C5'	-5.51	112.08	120.90
1	X	155	G	O4'-C1'-N9	5.51	112.61	108.20
1	X	448	C	N1-C2-O2	5.51	122.21	118.90
2	Y	19	C	N1-C2-O2	5.51	122.20	118.90
1	X	580	A	N9-C1'-C2'	5.51	121.16	114.00
1	X	2285	U	O4'-C1'-N1	5.51	112.61	108.20
1	X	2646	C	C6-N1-C2	-5.51	118.10	120.30
1	X	186	C	N1-C2-O2	5.51	122.20	118.90
1	X	555	U	P-O3'-C3'	5.51	126.31	119.70
1	X	1089	C	P-O3'-C3'	5.51	126.31	119.70
1	X	2255	G	C5-C6-O6	-5.51	125.30	128.60
2	Y	9	G	C3'-C2'-C1'	-5.50	97.10	101.50
1	X	309	G	C8-N9-C4	-5.50	104.20	106.40
1	X	1250	A	C5'-C4'-O4'	5.50	115.70	109.10
1	X	1337	G	O4'-C1'-N9	5.50	112.60	108.20
1	X	1442	C	C4'-C3'-C2'	5.50	108.10	102.60
1	X	303	C	O4'-C1'-N1	5.50	112.60	108.20
1	X	1280	U	C5-C6-N1	5.50	125.45	122.70
1	X	2772	U	O4'-C1'-N1	5.50	112.60	108.20
1	X	942	U	N3-C2-O2	-5.50	118.35	122.20
2	Y	30	C	P-O5'-C5'	5.50	129.70	120.90
1	X	63	A	C2-N3-C4	5.50	113.35	110.60
1	X	2619	G	C5-N7-C8	-5.49	101.55	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	7	G	C5'-C4'-C3'	-5.49	107.22	116.00
1	X	2018	G	C8-N9-C4	-5.49	104.20	106.40
2	Y	79	U	O4'-C1'-N1	5.49	112.59	108.20
1	X	180	C	O4'-C1'-N1	5.49	112.59	108.20
1	X	1169	C	O4'-C1'-N1	5.49	112.59	108.20
1	X	1513	U	O4'-C1'-N1	5.49	112.59	108.20
1	X	2222	U	N3-C2-O2	-5.49	118.36	122.20
1	X	2485	U	N1-C2-O2	5.48	126.64	122.80
1	X	2769	C	C5'-C4'-C3'	-5.48	107.23	116.00
2	Y	31	A	O4'-C1'-N9	5.48	112.59	108.20
19	Q	60	GLY	N-CA-C	5.48	126.80	113.10
1	X	2540	A	O4'-C4'-C3'	-5.48	98.52	104.00
1	X	1422	C	O4'-C1'-N1	5.48	112.58	108.20
1	X	1629	G	C4'-C3'-C2'	-5.48	97.12	102.60
1	X	2808	U	P-O5'-C5'	5.48	129.66	120.90
1	X	2867	G	C8-N9-C4	-5.48	104.21	106.40
1	X	1979	C	P-O3'-C3'	5.48	126.27	119.70
1	X	669	G	O4'-C4'-C3'	-5.47	98.53	104.00
1	X	2484	G	C2-N3-C4	5.47	114.64	111.90
1	X	103	U	O4'-C1'-N1	5.47	112.58	108.20
1	X	1009	C	N1-C2-O2	5.47	122.18	118.90
1	X	1055	A	O4'-C1'-N9	5.47	112.58	108.20
1	X	1410	U	O4'-C1'-N1	5.47	112.58	108.20
1	X	1977	C	O4'-C1'-N1	5.47	112.58	108.20
1	X	2409	A	N9-C1'-C2'	5.47	121.11	114.00
1	X	753	U	O4'-C1'-N1	5.47	112.58	108.20
1	X	1939	U	O4'-C1'-N1	5.47	112.58	108.20
1	X	2533	U	C5-C6-N1	5.47	125.43	122.70
1	X	344	G	N9-C1'-C2'	5.46	121.10	114.00
1	X	761	G	P-O5'-C5'	-5.46	112.16	120.90
1	X	1713	G	P-O5'-C5'	5.46	129.64	120.90
1	X	126	C	O4'-C1'-N1	5.46	112.57	108.20
1	X	2782	G	C3'-C2'-C1'	-5.46	97.13	101.50
1	X	1745	C	C6-N1-C2	-5.46	118.12	120.30
1	X	542	A	C1'-O4'-C4'	5.46	114.27	109.90
1	X	1132	C	O4'-C1'-N1	5.46	112.57	108.20
1	X	112	U	N1-C1'-C2'	5.46	121.09	114.00
1	X	1870	U	O4'-C1'-N1	5.46	112.56	108.20
1	X	63	A	N1-C2-N3	-5.46	126.57	129.30
1	X	802	A	C4'-C3'-C2'	5.46	108.06	102.60
1	X	1943	A	C5'-C4'-C3'	-5.46	107.27	116.00
1	X	214	C	O4'-C1'-N1	5.45	112.56	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	773	G	OP1-P-O3'	5.45	117.20	105.20
1	X	1223	G	N3-C4-N9	5.45	129.27	126.00
1	X	615	C	O4'-C1'-N1	5.45	112.56	108.20
1	X	2709	C	O4'-C1'-N1	5.45	112.56	108.20
1	X	545	C	O4'-C1'-N1	5.45	112.56	108.20
1	X	11	G	N7-C8-N9	5.45	115.82	113.10
1	X	774	A	N9-C4-C5	-5.45	103.62	105.80
1	X	1678	G	P-O3'-C3'	-5.45	113.16	119.70
1	X	1164	C	O4'-C1'-N1	5.45	112.56	108.20
1	X	2440	C	O4'-C1'-N1	5.45	112.56	108.20
1	X	398	C	O4'-C1'-N1	5.44	112.56	108.20
1	X	1412	C	O4'-C1'-N1	5.44	112.55	108.20
1	X	56	C	O4'-C1'-N1	5.44	112.55	108.20
1	X	1635	G	C8-N9-C4	-5.44	104.22	106.40
1	X	1938	U	P-O5'-C5'	5.44	129.60	120.90
1	X	1963	G	O4'-C1'-N9	5.44	112.55	108.20
2	Y	5	C	N1-C2-O2	5.44	122.16	118.90
1	X	1500	U	O4'-C1'-N1	5.44	112.55	108.20
1	X	1935	A	P-O5'-C5'	-5.44	112.20	120.90
1	X	1421	U	O4'-C1'-N1	5.43	112.55	108.20
2	Y	32	C	O4'-C1'-N1	5.43	112.55	108.20
1	X	1286	U	O4'-C1'-N1	5.43	112.54	108.20
1	X	1975	G	N9-C1'-C2'	5.43	121.06	114.00
1	X	851	C	O4'-C1'-N1	5.43	112.54	108.20
1	X	1660	G	C4'-C3'-C2'	-5.43	97.17	102.60
1	X	2659	C	O4'-C1'-N1	5.42	112.54	108.20
1	X	242	A	C5'-C4'-C3'	5.42	124.68	116.00
1	X	1617	G	C5-C6-N1	5.42	114.21	111.50
1	X	2172	U	O4'-C1'-N1	5.42	112.54	108.20
1	X	1608	U	O4'-C1'-N1	5.42	112.54	108.20
1	X	2792	C	O4'-C1'-N1	5.42	112.54	108.20
2	Y	58	G	P-O3'-C3'	5.42	126.20	119.70
1	X	79	G	C8-N9-C4	-5.42	104.23	106.40
1	X	1821	A	O4'-C4'-C3'	-5.42	98.58	104.00
1	X	1695	U	O4'-C1'-N1	5.42	112.53	108.20
1	X	1927	U	P-O3'-C3'	5.42	126.20	119.70
1	X	2484	G	P-O5'-C5'	5.42	129.57	120.90
1	X	673	G	C4'-C3'-C2'	5.42	108.02	102.60
1	X	806	A	O4'-C1'-N9	-5.41	103.87	108.20
1	X	976	C	O4'-C1'-N1	5.41	112.53	108.20
1	X	1043	A	O4'-C1'-N9	5.41	112.53	108.20
1	X	1937	G	P-O3'-C3'	5.41	126.19	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	798	G	P-O3'-C3'	5.41	126.19	119.70
1	X	959	C	P-O3'-C3'	-5.41	113.21	119.70
1	X	2499	C	O4'-C1'-N1	5.41	112.53	108.20
1	X	11	G	C8-N9-C4	-5.41	104.24	106.40
1	X	923	A	N1-C6-N6	5.41	121.84	118.60
1	X	1077	U	P-O3'-C3'	5.41	126.19	119.70
1	X	2042	A	C4'-C3'-C2'	-5.41	97.19	102.60
2	Y	118	G	O4'-C1'-N9	5.41	112.53	108.20
1	X	1909	U	N1-C2-O2	5.40	126.58	122.80
1	X	2075	U	O4'-C1'-N1	5.40	112.52	108.20
1	X	2854	G	N7-C8-N9	5.40	115.80	113.10
1	X	479	G	N1-C6-O6	5.40	123.14	119.90
1	X	2323	U	P-O3'-C3'	5.40	126.18	119.70
1	X	2694	G	C5-C6-O6	-5.40	125.36	128.60
2	Y	17	A	P-O3'-C3'	5.39	126.17	119.70
1	X	157	G	C5'-C4'-C3'	-5.39	107.38	116.00
1	X	749	C	O4'-C1'-N1	5.39	112.51	108.20
2	Y	90	C	N1-C2-O2	5.39	122.13	118.90
1	X	430	C	C6-N1-C2	-5.38	118.15	120.30
1	X	1712	G	C4-N9-C1'	5.38	133.50	126.50
1	X	1986	G	N3-C4-C5	-5.38	125.91	128.60
1	X	2570	C	O4'-C1'-N1	5.38	112.51	108.20
1	X	175	C	C5-C6-N1	5.38	123.69	121.00
1	X	246	C	N1-C2-O2	5.38	122.13	118.90
1	X	1014	G	N3-C4-C5	-5.38	125.91	128.60
1	X	1490	U	O4'-C1'-N1	5.38	112.50	108.20
1	X	1385	C	N1-C2-O2	5.38	122.13	118.90
1	X	2015	G	N9-C1'-C2'	5.38	120.99	114.00
1	X	793	G	N1-C6-O6	-5.38	116.67	119.90
1	X	1036	G	P-O3'-C3'	5.38	126.15	119.70
1	X	2072	C	O4'-C1'-N1	5.38	112.50	108.20
1	X	2089	C	O4'-C1'-N1	5.38	112.50	108.20
1	X	941	U	O4'-C1'-N1	5.38	112.50	108.20
1	X	2492	G	N3-C4-C5	-5.38	125.91	128.60
1	X	184	A	O4'-C1'-N9	5.37	112.50	108.20
1	X	542	A	P-O3'-C3'	5.37	126.15	119.70
1	X	1139	A	O4'-C1'-C2'	-5.37	100.43	105.80
1	X	1467	U	O4'-C4'-C3'	-5.37	98.63	104.00
1	X	1685	A	P-O5'-C5'	5.37	129.50	120.90
2	Y	92	G	C3'-C2'-C1'	-5.37	97.20	101.50
1	X	467	U	C5'-C4'-C3'	5.37	124.59	116.00
1	X	1858	C	N1-C2-O2	5.37	122.12	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2403	C	N1-C2-O2	5.37	122.12	118.90
1	X	2717	G	O4'-C1'-N9	5.37	112.50	108.20
2	Y	29	C	O4'-C1'-N1	5.37	112.49	108.20
1	X	751	G	O5'-P-OP2	-5.37	100.87	105.70
1	X	1339	U	OP2-P-O3'	5.37	117.01	105.20
1	X	1715	A	P-O3'-C3'	5.37	126.14	119.70
1	X	2658	A	O5'-P-OP2	-5.37	100.87	105.70
1	X	213	C	O4'-C1'-N1	5.36	112.49	108.20
1	X	863	C	O4'-C1'-N1	5.36	112.49	108.20
1	X	99	U	N3-C2-O2	-5.36	118.45	122.20
1	X	682	G	C3'-C2'-C1'	5.36	105.79	101.50
1	X	2232	G	C5-C6-O6	-5.36	125.38	128.60
1	X	2691	C	N3-C2-O2	-5.36	118.15	121.90
1	X	308	C	P-O3'-C3'	-5.36	113.27	119.70
1	X	1497	C	C6-N1-C2	-5.36	118.16	120.30
1	X	1840	A	O4'-C1'-N9	5.36	112.48	108.20
1	X	235	C	N1-C2-O2	5.36	122.11	118.90
1	X	513	A	C1'-O4'-C4'	-5.36	105.61	109.90
1	X	2666	U	C3'-C2'-C1'	5.36	105.78	101.50
1	X	472	C	O4'-C1'-N1	5.35	112.48	108.20
1	X	1219	C	O4'-C1'-N1	5.35	112.48	108.20
1	X	1222	G	P-O3'-C3'	5.35	126.12	119.70
1	X	1491	C	O4'-C1'-N1	5.35	112.48	108.20
1	X	319	G	C5-C6-O6	-5.35	125.39	128.60
1	X	814	G	N9-C1'-C2'	5.35	120.95	114.00
1	X	1199	U	O4'-C1'-N1	5.35	112.48	108.20
1	X	1390	G	N3-C4-C5	-5.35	125.93	128.60
1	X	2483	U	O4'-C1'-N1	5.35	112.48	108.20
1	X	2870	C	C6-N1-C2	-5.35	118.16	120.30
1	X	1803	G	O4'-C1'-N9	5.34	112.48	108.20
1	X	1622	G	N3-C4-C5	-5.34	125.93	128.60
1	X	417	C	N1-C2-O2	5.34	122.10	118.90
1	X	2410	U	OP2-P-O3'	5.34	116.95	105.20
1	X	2688	G	P-O3'-C3'	-5.34	113.29	119.70
1	X	1172	U	O4'-C1'-N1	5.34	112.47	108.20
1	X	1496	G	O4'-C1'-N9	5.34	112.47	108.20
1	X	1753	A	C8-N9-C4	-5.34	103.67	105.80
1	X	2553	G	N7-C8-N9	5.34	115.77	113.10
1	X	2700	U	OP1-P-O3'	5.34	116.94	105.20
1	X	458	G	C3'-C2'-C1'	5.33	105.77	101.50
1	X	694	G	O4'-C1'-N9	5.33	112.47	108.20
1	X	1283	C	N3-C4-C5	-5.33	119.77	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1711	C	P-O3'-C3'	5.33	126.10	119.70
1	X	1278	A	C5-N7-C8	-5.33	101.23	103.90
1	X	1882	G	O4'-C1'-N9	5.33	112.47	108.20
1	X	2535	C	N1-C2-O2	5.33	122.10	118.90
2	Y	101	A	C3'-C2'-C1'	-5.33	97.24	101.50
1	X	70	A	P-O5'-C5'	-5.33	112.38	120.90
1	X	1790	G	C2'-C3'-O3'	5.33	122.22	113.70
1	X	2774	U	P-O3'-C3'	5.33	126.09	119.70
2	Y	10	U	O4'-C4'-C3'	-5.33	98.67	104.00
11	I	44	GLY	N-CA-C	5.33	126.42	113.10
1	X	757	U	P-O3'-C3'	5.33	126.09	119.70
1	X	1720	G	P-O3'-C3'	-5.33	113.31	119.70
1	X	1301	U	N3-C2-O2	-5.33	118.47	122.20
1	X	2429	A	P-O3'-C3'	-5.33	113.31	119.70
2	Y	12	C	O4'-C4'-C3'	-5.33	98.67	104.00
1	X	973	U	O3'-P-O5'	-5.32	93.89	104.00
1	X	1722	G	O4'-C1'-N9	5.32	112.46	108.20
1	X	61	U	C1'-O4'-C4'	-5.32	105.65	109.90
1	X	1225	G	N9-C1'-C2'	5.32	120.91	114.00
1	X	1785	A	O4'-C1'-N9	5.32	112.45	108.20
2	Y	55	C	P-O3'-C3'	5.32	126.08	119.70
1	X	858	G	P-O3'-C3'	5.32	126.08	119.70
1	X	1202	U	O4'-C1'-N1	5.32	112.45	108.20
1	X	2375	G	O4'-C4'-C3'	-5.32	98.69	104.00
1	X	2732	C	N1-C2-O2	5.32	122.09	118.90
23	U	32	ARG	N-CA-C	-5.31	96.65	111.00
1	X	1716	G	C1'-O4'-C4'	5.31	114.15	109.90
1	X	2015	G	C5-C6-N1	5.31	114.16	111.50
1	X	1238	A	O4'-C1'-N9	5.31	112.45	108.20
1	X	1725	C	P-O3'-C3'	5.31	126.07	119.70
1	X	524	A	O4'-C4'-C3'	-5.31	98.69	104.00
1	X	146	C	O4'-C1'-N1	5.30	112.44	108.20
1	X	2275	U	P-O5'-C5'	5.30	129.39	120.90
1	X	536	A	C3'-C2'-C1'	5.30	105.74	101.50
1	X	1056	U	P-O3'-C3'	5.30	126.06	119.70
1	X	1248	G	O3'-P-O5'	-5.30	93.93	104.00
1	X	876	A	P-O3'-C3'	5.30	126.06	119.70
1	X	1210	C	O4'-C1'-N1	5.30	112.44	108.20
1	X	2691	C	N1-C2-O2	5.30	122.08	118.90
1	X	418	C	P-O5'-C5'	5.30	129.37	120.90
1	X	1661	C	C4'-C3'-C2'	-5.30	97.30	102.60
1	X	2071	G	O4'-C1'-N9	5.30	112.44	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2568	A	O4'-C1'-N9	5.30	112.44	108.20
1	X	33	C	N1-C2-O2	5.29	122.08	118.90
1	X	1988	A	C5-N7-C8	-5.29	101.25	103.90
1	X	179	U	O4'-C1'-N1	5.29	112.44	108.20
1	X	723	C	O4'-C1'-N1	5.29	112.43	108.20
1	X	2256	G	N7-C8-N9	5.29	115.75	113.10
2	Y	90	C	O4'-C1'-N1	5.29	112.43	108.20
1	X	817	A	O4'-C1'-N9	5.29	112.43	108.20
1	X	2321	C	O4'-C1'-N1	5.29	112.43	108.20
1	X	2551	A	OP1-P-O3'	5.29	116.84	105.20
1	X	851	C	C3'-C2'-C1'	-5.29	97.27	101.50
1	X	2567	G	N3-C4-C5	-5.29	125.96	128.60
1	X	2804	G	C5-C6-O6	-5.29	125.43	128.60
1	X	2229	G	C2-N3-C4	5.29	114.54	111.90
1	X	98	U	O4'-C1'-N1	5.29	112.43	108.20
1	X	427	C	O4'-C1'-N1	5.29	112.43	108.20
1	X	1154	A	C4'-C3'-C2'	5.29	107.89	102.60
1	X	2667	C	N1-C2-O2	5.29	122.07	118.90
1	X	329	C	O4'-C1'-N1	5.28	112.43	108.20
1	X	554	U	C3'-C2'-C1'	-5.28	97.27	101.50
1	X	1054	C	O4'-C1'-N1	5.28	112.43	108.20
1	X	1496	G	C4'-C3'-O3'	5.28	123.57	113.00
1	X	2418	A	C3'-C2'-C1'	5.28	105.73	101.50
1	X	2854	G	C5-N7-C8	-5.28	101.66	104.30
1	X	969	U	C4'-C3'-C2'	5.28	107.88	102.60
1	X	1746	A	N1-C6-N6	-5.28	115.43	118.60
1	X	2464	G	C3'-C2'-C1'	-5.28	97.28	101.50
1	X	337	G	N7-C8-N9	5.28	115.74	113.10
1	X	4	C	O4'-C1'-N1	5.28	112.42	108.20
1	X	664	C	O4'-C1'-N1	5.28	112.42	108.20
1	X	1741	G	C8-N9-C4	-5.28	104.29	106.40
1	X	1987	G	N3-C4-C5	-5.28	125.96	128.60
1	X	2276	C	O4'-C1'-N1	5.28	112.42	108.20
2	Y	86	A	N1-C6-N6	5.28	121.77	118.60
1	X	1863	U	O4'-C1'-N1	5.27	112.42	108.20
1	X	346	C	C2-N3-C4	5.27	122.54	119.90
1	X	1841	G	C8-N9-C4	-5.27	104.29	106.40
1	X	78	C	C6-N1-C2	-5.27	118.19	120.30
1	X	352	G	P-O5'-C5'	5.27	129.33	120.90
1	X	1326	U	C2-N1-C1'	5.27	124.02	117.70
1	X	1341	G	C5-C6-N1	5.27	114.14	111.50
1	X	746	G	N3-C4-N9	5.27	129.16	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1263	G	P-O3'-C3'	5.27	126.02	119.70
1	X	1873	A	O4'-C1'-N9	5.27	112.41	108.20
1	X	2568	A	O4'-C4'-C3'	-5.27	98.73	104.00
2	Y	107	C	N1-C2-O2	5.27	122.06	118.90
1	X	927	C	N1-C2-O2	5.26	122.06	118.90
1	X	1980	A	C4-C5-C6	5.26	119.63	117.00
2	Y	97	C	O4'-C1'-N1	5.26	112.41	108.20
1	X	358	C	C5-C6-N1	5.26	123.63	121.00
1	X	1478	U	N3-C2-O2	-5.26	118.52	122.20
1	X	1755	G	O5'-P-OP2	-5.26	100.97	105.70
1	X	2047	C	O4'-C1'-N1	5.26	112.41	108.20
1	X	1194	U	C2'-C3'-O3'	5.26	122.11	113.70
1	X	2479	U	O4'-C1'-N1	5.26	112.41	108.20
1	X	2564	U	O4'-C1'-N1	5.26	112.41	108.20
1	X	617	U	C2-N1-C1'	5.26	124.01	117.70
1	X	1657	A	C5'-C4'-O4'	-5.26	102.79	109.10
1	X	2000	U	O4'-C1'-N1	5.26	112.41	108.20
1	X	765	C	N1-C2-O2	5.25	122.05	118.90
1	X	1703	C	O4'-C1'-N1	5.25	112.40	108.20
1	X	1923	U	P-O3'-C3'	5.25	126.00	119.70
1	X	2380	U	O4'-C1'-N1	5.25	112.40	108.20
1	X	940	G	O4'-C1'-N9	5.25	112.40	108.20
1	X	954	U	C5-C4-O4	-5.25	122.75	125.90
1	X	1687	C	P-O3'-C3'	5.25	126.00	119.70
1	X	2524	G	C8-N9-C4	-5.25	104.30	106.40
1	X	320	A	O4'-C1'-N9	5.25	112.40	108.20
1	X	1458	A	P-O3'-C3'	5.25	126.00	119.70
2	Y	41	A	P-O3'-C3'	5.25	126.00	119.70
13	K	11	ASN	C-N-CA	5.25	134.81	121.70
1	X	949	G	C3'-C2'-C1'	-5.24	97.31	101.50
1	X	1432	G	C1'-O4'-C4'	-5.24	105.70	109.90
1	X	2826	C	P-O3'-C3'	5.24	125.99	119.70
1	X	133	C	N1-C2-O2	5.24	122.05	118.90
1	X	2481	G	P-O3'-C3'	5.24	125.99	119.70
1	X	1201	G	P-O3'-C3'	5.24	125.99	119.70
1	X	2422	C	N3-C4-C5	5.24	124.00	121.90
1	X	1830	C	N1-C1'-C2'	5.24	120.81	114.00
1	X	2773	G	P-O3'-C3'	5.24	125.98	119.70
1	X	884	C	O4'-C1'-N1	5.24	112.39	108.20
1	X	1765	C	N3-C2-O2	-5.24	118.23	121.90
15	M	29	PRO	N-CA-C	5.24	125.72	112.10
1	X	1231	A	O4'-C1'-N9	5.24	112.39	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1273	G	C5-C6-O6	-5.24	125.46	128.60
1	X	1278	A	N7-C8-N9	5.24	116.42	113.80
1	X	1663	C	O3'-P-O5'	-5.24	94.05	104.00
1	X	2014	A	C4'-C3'-C2'	5.24	107.84	102.60
1	X	2848	A	C1'-O4'-C4'	-5.24	105.71	109.90
1	X	1811	A	C4'-C3'-C2'	5.23	107.83	102.60
1	X	2039	G	N3-C2-N2	-5.23	116.24	119.90
1	X	169	C	O5'-P-OP2	-5.23	100.99	105.70
1	X	1338	G	C2-N3-C4	5.23	114.51	111.90
1	X	1326	U	N1-C2-O2	5.22	126.46	122.80
1	X	2662	C	N1-C2-O2	5.22	122.03	118.90
2	Y	63	A	O4'-C1'-N9	5.22	112.38	108.20
4	B	162	MET	CB-CA-C	5.22	120.84	110.40
1	X	985	G	N7-C8-N9	5.22	115.71	113.10
1	X	542	A	N1-C6-N6	5.22	121.73	118.60
1	X	967	G	P-O5'-C5'	5.22	129.25	120.90
1	X	1446	U	O4'-C1'-N1	5.22	112.38	108.20
1	X	1764	A	C5-C6-N6	-5.22	119.53	123.70
1	X	2209	G	C8-N9-C4	-5.22	104.31	106.40
1	X	1235	C	C6-N1-C2	-5.22	118.21	120.30
1	X	2619	G	C8-N9-C4	-5.22	104.31	106.40
1	X	245	C	N1-C2-O2	5.21	122.03	118.90
1	X	480	G	C6-C5-N7	-5.21	127.27	130.40
1	X	559	C	C5'-C4'-O4'	5.21	115.36	109.10
1	X	825	C	C5'-C4'-O4'	5.21	115.36	109.10
1	X	2190	A	C4'-C3'-C2'	-5.21	97.39	102.60
1	X	2488	G	C5-C6-N1	5.21	114.11	111.50
1	X	468	A	P-O3'-C3'	5.21	125.95	119.70
1	X	617	U	N1-C2-O2	5.21	126.45	122.80
1	X	2243	C	O4'-C1'-N1	5.21	112.37	108.20
1	X	483	A	O5'-C5'-C4'	5.21	121.60	111.70
1	X	1637	U	O4'-C1'-N1	5.21	112.37	108.20
1	X	2473	G	N3-C4-C5	-5.21	125.99	128.60
1	X	2605	C	O4'-C1'-N1	5.21	112.37	108.20
1	X	1885	C	O4'-C1'-N1	5.21	112.37	108.20
1	X	542	A	C5-C6-N6	-5.21	119.53	123.70
1	X	799	C	P-O3'-C3'	5.21	125.95	119.70
1	X	1877	C	O4'-C1'-N1	5.21	112.36	108.20
1	X	2284	U	O4'-C1'-N1	5.21	112.36	108.20
1	X	2448	A	O4'-C1'-N9	5.21	112.37	108.20
2	Y	41	A	O4'-C1'-N9	5.21	112.36	108.20
1	X	1729	C	O4'-C1'-N1	5.21	112.36	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2349	G	C3'-C2'-C1'	-5.21	97.34	101.50
1	X	945	G	C8-N9-C4	-5.20	104.32	106.40
1	X	1631	C	C4'-C3'-C2'	-5.20	97.40	102.60
1	X	593	C	P-O5'-C5'	5.20	129.22	120.90
1	X	1629	G	P-O3'-C3'	5.20	125.94	119.70
2	Y	53	G	C8-N9-C4	-5.20	104.32	106.40
1	X	542	A	C5'-C4'-O4'	5.20	115.34	109.10
1	X	560	G	P-O3'-C3'	-5.20	113.46	119.70
1	X	2441	U	O4'-C1'-N1	5.20	112.36	108.20
1	X	2697	G	C5-C6-O6	-5.20	125.48	128.60
1	X	2018	G	O4'-C1'-C2'	-5.20	100.60	105.80
1	X	2408	G	C2'-C3'-O3'	5.20	122.02	113.70
1	X	2013	A	C1'-O4'-C4'	-5.20	105.74	109.90
1	X	349	G	P-O5'-C5'	5.20	129.21	120.90
1	X	1142	G	C5-C6-O6	-5.20	125.48	128.60
1	X	1336	G	N9-C4-C5	-5.20	103.32	105.40
1	X	1699	A	O4'-C1'-N9	-5.20	104.04	108.20
1	X	1747	G	N9-C1'-C2'	5.20	120.75	114.00
1	X	1963	G	C8-N9-C4	-5.20	104.32	106.40
1	X	2471	U	O4'-C1'-N1	5.20	112.36	108.20
1	X	2573	C	O4'-C1'-N1	5.20	112.36	108.20
1	X	2854	G	P-O5'-C5'	5.20	129.21	120.90
1	X	596	C	P-O3'-C3'	5.19	125.93	119.70
1	X	2810	A	C1'-O4'-C4'	-5.19	105.74	109.90
1	X	1613	G	O4'-C1'-N9	5.19	112.35	108.20
2	Y	54	U	C5'-C4'-O4'	5.19	115.33	109.10
1	X	874	A	O4'-C1'-N9	5.19	112.35	108.20
1	X	2560	G	C8-N9-C4	-5.19	104.32	106.40
1	X	499	G	O4'-C1'-N9	5.19	112.35	108.20
1	X	956	A	C5'-C4'-O4'	5.19	115.33	109.10
1	X	1626	A	N1-C2-N3	-5.19	126.71	129.30
1	X	2377	U	O4'-C1'-N1	5.19	112.35	108.20
1	X	18	U	P-O3'-C3'	-5.19	113.48	119.70
1	X	786	U	O4'-C1'-N1	5.19	112.35	108.20
1	X	97	U	C5'-C4'-C3'	-5.18	107.70	116.00
1	X	2489	C	P-O3'-C3'	-5.18	113.48	119.70
1	X	2799	C	N3-C4-C5	5.18	123.97	121.90
1	X	78	C	C5-C6-N1	5.18	123.59	121.00
1	X	422	C	C6-N1-C2	-5.18	118.23	120.30
1	X	1496	G	C8-N9-C4	-5.18	104.33	106.40
11	I	35	LYS	N-CA-C	-5.18	97.02	111.00
1	X	2858	A	P-O5'-C5'	5.18	129.19	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	646	C	C6-N1-C2	-5.18	118.23	120.30
1	X	751	G	C3'-C2'-C1'	-5.18	97.36	101.50
11	I	64	GLY	N-CA-C	5.18	126.04	113.10
1	X	230	C	O4'-C1'-N1	5.17	112.34	108.20
1	X	1396	C	O4'-C1'-N1	5.17	112.34	108.20
1	X	246	C	N3-C2-O2	-5.17	118.28	121.90
1	X	309	G	C5-C6-O6	-5.17	125.50	128.60
1	X	330	C	N1-C2-O2	5.17	122.00	118.90
1	X	2543	A	O4'-C1'-N9	5.17	112.34	108.20
1	X	341	A	C3'-C2'-C1'	5.17	105.64	101.50
1	X	1170	U	O4'-C1'-N1	5.17	112.33	108.20
1	X	2790	C	O4'-C1'-N1	5.17	112.33	108.20
1	X	1038	U	O4'-C1'-N1	5.17	112.33	108.20
1	X	1112	U	O4'-C1'-N1	5.17	112.33	108.20
1	X	1150	C	O4'-C1'-N1	5.17	112.33	108.20
1	X	1825	C	C3'-C2'-C1'	-5.17	97.37	101.50
1	X	351	A	C3'-C2'-C1'	-5.16	97.37	101.50
1	X	1717	A	C5-C6-N1	5.16	120.28	117.70
1	X	2237	C	O4'-C1'-N1	5.16	112.33	108.20
1	X	2385	U	O4'-C1'-N1	5.16	112.33	108.20
1	X	2493	U	O4'-C1'-N1	5.16	112.33	108.20
1	X	2705	A	C4'-C3'-O3'	5.16	123.33	113.00
1	X	2855	C	O4'-C1'-N1	5.16	112.33	108.20
1	X	454	G	P-O3'-C3'	5.16	125.89	119.70
1	X	1711	C	P-O5'-C5'	5.16	129.16	120.90
1	X	2776	U	P-O3'-C3'	5.16	125.89	119.70
1	X	200	A	P-O3'-C3'	5.16	125.89	119.70
1	X	1014	G	C2-N3-C4	5.16	114.48	111.90
1	X	1281	A	OP2-P-O3'	5.16	116.55	105.20
1	X	823	U	O4'-C1'-N1	5.16	112.33	108.20
1	X	2650	G	C4'-C3'-C2'	5.16	107.76	102.60
1	X	2766	U	O4'-C1'-N1	5.16	112.33	108.20
1	X	2786	G	O4'-C1'-N9	5.16	112.32	108.20
1	X	951	G	O4'-C4'-C3'	-5.15	98.85	104.00
1	X	1124	U	O4'-C1'-N1	5.15	112.32	108.20
1	X	1623	C	P-O3'-C3'	5.15	125.88	119.70
1	X	2593	A	O3'-P-O5'	-5.15	94.21	104.00
1	X	730	C	O4'-C1'-N1	5.15	112.32	108.20
1	X	1469	U	N1-C2-N3	5.15	117.99	114.90
1	X	1265	G	O5'-P-OP1	5.15	116.88	110.70
3	A	248	THR	CB-CA-C	5.15	125.50	111.60
1	X	72	A	O4'-C1'-N9	5.15	112.32	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1390	G	C8-N9-C4	-5.15	104.34	106.40
1	X	1987	G	C8-N9-C4	-5.15	104.34	106.40
1	X	1250	A	P-O3'-C3'	5.14	125.87	119.70
1	X	1622	G	P-O3'-C3'	5.14	125.87	119.70
1	X	1940	C	O4'-C1'-N1	5.14	112.32	108.20
1	X	1429	A	N9-C1'-C2'	5.14	120.68	114.00
1	X	1912	G	P-O3'-C3'	5.14	125.87	119.70
1	X	2039	G	N7-C8-N9	5.14	115.67	113.10
2	Y	53	G	N3-C4-C5	-5.14	126.03	128.60
1	X	70	A	C5'-C4'-C3'	-5.14	107.77	116.00
1	X	2561	G	C5-C6-O6	-5.14	125.52	128.60
1	X	1648	C	N1-C2-O2	5.14	121.98	118.90
1	X	2274	C	C6-N1-C2	-5.14	118.24	120.30
1	X	1790	G	C4'-C3'-C2'	5.14	107.74	102.60
1	X	2663	U	P-O3'-C3'	-5.14	113.53	119.70
1	X	1014	G	C8-N9-C4	-5.14	104.35	106.40
1	X	1167	A	O4'-C1'-N9	-5.14	104.09	108.20
9	G	106	TYR	CA-C-N	-5.14	105.90	117.20
1	X	582	G	P-O3'-C3'	5.13	125.86	119.70
1	X	771	C	N1-C2-O2	5.13	121.98	118.90
1	X	955	G	C4-N9-C1'	5.13	133.18	126.50
1	X	1248	G	OP1-P-O3'	5.13	116.49	105.20
11	I	32	ARG	N-CA-C	-5.13	97.14	111.00
1	X	626	A	P-O3'-C3'	5.13	125.86	119.70
1	X	2298	U	C4'-C3'-C2'	5.13	107.73	102.60
1	X	1975	G	C2-N3-C4	5.13	114.47	111.90
1	X	2697	G	N3-C4-C5	-5.13	126.04	128.60
1	X	2855	C	C6-N1-C2	-5.13	118.25	120.30
1	X	2176	U	O4'-C1'-N1	5.13	112.30	108.20
1	X	2279	G	C8-N9-C4	-5.13	104.35	106.40
2	Y	10	U	O4'-C1'-N1	5.12	112.30	108.20
1	X	1432	G	P-O3'-C3'	5.12	125.85	119.70
1	X	240	U	O4'-C4'-C3'	-5.12	98.88	104.00
1	X	984	A	P-O3'-C3'	5.12	125.84	119.70
1	X	2681	A	C4'-C3'-C2'	-5.12	97.48	102.60
1	X	820	U	O4'-C1'-N1	5.12	112.30	108.20
1	X	1409	U	C1'-O4'-C4'	-5.12	105.81	109.90
1	X	2011	U	C5-C4-O4	-5.12	122.83	125.90
1	X	2619	G	C5'-C4'-C3'	-5.12	107.81	116.00
1	X	2846	G	O5'-P-OP2	-5.12	101.09	105.70
1	X	2296	U	O4'-C1'-N1	5.12	112.29	108.20
1	X	2804	G	C6-N1-C2	-5.12	122.03	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1279	G	C1'-O4'-C4'	-5.12	105.81	109.90
1	X	577	U	C2-N3-C4	5.11	130.07	127.00
1	X	2867	G	C3'-C2'-C1'	5.11	105.59	101.50
2	Y	8	C	O4'-C1'-N1	5.11	112.29	108.20
1	X	1351	G	C3'-C2'-C1'	5.11	105.59	101.50
1	X	660	G	C8-N9-C4	-5.11	104.36	106.40
1	X	2006	G	C5'-C4'-O4'	5.11	115.23	109.10
10	H	26	ASN	C-N-CA	5.11	134.47	121.70
12	J	88	LYS	N-CA-C	5.11	124.80	111.00
1	X	1559	G	P-O3'-C3'	5.11	125.83	119.70
1	X	1712	G	C8-N9-C1'	-5.11	120.36	127.00
1	X	225	G	O4'-C1'-N9	5.11	112.28	108.20
1	X	1407	G	C4-N9-C1'	5.11	133.14	126.50
1	X	1627	C	O4'-C1'-N1	5.11	112.28	108.20
1	X	1853	C	O4'-C1'-N1	5.11	112.28	108.20
4	B	132	LYS	C-N-CA	5.11	134.46	121.70
1	X	1244	U	C5-C6-N1	5.10	125.25	122.70
1	X	1218	C	O4'-C1'-N1	5.10	112.28	108.20
1	X	1468	A	N1-C6-N6	-5.10	115.54	118.60
1	X	327	C	N1-C2-O2	5.10	121.96	118.90
1	X	334	G	C2-N3-C4	5.10	114.45	111.90
1	X	519	C	C5-C6-N1	5.10	123.55	121.00
1	X	1142	G	P-O3'-C3'	5.10	125.82	119.70
1	X	1245	G	O4'-C1'-N9	5.10	112.28	108.20
1	X	1733	U	O4'-C1'-N1	5.10	112.28	108.20
1	X	1679	U	N1-C2-N3	5.10	117.96	114.90
1	X	2196	U	O4'-C1'-N1	5.10	112.28	108.20
1	X	579	G	C5-N7-C8	5.10	106.85	104.30
1	X	1340	C	O3'-P-O5'	-5.10	94.32	104.00
1	X	561	U	C3'-C2'-C1'	-5.09	97.42	101.50
1	X	1120	C	C3'-C2'-C1'	5.09	105.58	101.50
1	X	2659	C	P-O5'-C5'	5.09	129.05	120.90
1	X	132	U	O4'-C1'-N1	5.09	112.28	108.20
1	X	34	U	C5'-C4'-O4'	5.09	115.21	109.10
1	X	485	G	P-O5'-C5'	5.09	129.04	120.90
1	X	523	A	N9-C1'-C2'	5.09	120.62	114.00
1	X	1237	G	O4'-C1'-N9	5.09	112.27	108.20
1	X	2396	C	P-O5'-C5'	-5.09	112.76	120.90
1	X	2476	A	P-O3'-C3'	5.09	125.81	119.70
1	X	2650	G	N3-C4-C5	-5.09	126.06	128.60
1	X	345	U	P-O5'-C5'	5.09	129.04	120.90
1	X	206	U	N1-C2-O2	5.09	126.36	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	759	C	O5'-C5'-C4'	5.09	121.37	111.70
1	X	993	C	P-O3'-C3'	-5.09	113.60	119.70
1	X	1497	C	C5-C6-N1	5.09	123.54	121.00
1	X	2680	U	O4'-C1'-N1	5.09	112.27	108.20
1	X	2784	A	O4'-C1'-N9	-5.08	104.13	108.20
1	X	2794	G	P-O5'-C5'	-5.08	112.76	120.90
3	A	242	ALA	N-CA-C	5.08	124.73	111.00
1	X	2416	U	C3'-C2'-C1'	-5.08	97.43	101.50
1	X	2827	G	N3-C4-C5	-5.08	126.06	128.60
1	X	2867	G	C5'-C4'-O4'	5.08	115.20	109.10
2	Y	28	A	C2-N3-C4	5.08	113.14	110.60
1	X	1944	C	N1-C2-O2	5.08	121.95	118.90
1	X	1994	U	O4'-C1'-N1	5.08	112.27	108.20
1	X	2487	G	C8-N9-C4	-5.08	104.37	106.40
1	X	2620	G	C5-C6-O6	-5.08	125.55	128.60
1	X	551	A	C3'-C2'-C1'	-5.08	97.44	101.50
1	X	639	G	C5-C6-O6	-5.08	125.55	128.60
1	X	811	G	O4'-C1'-N9	5.08	112.26	108.20
1	X	2299	A	N9-C1'-C2'	5.08	120.60	114.00
1	X	2314	A	P-O5'-C5'	5.08	129.03	120.90
1	X	2632	U	P-O3'-C3'	5.08	125.79	119.70
1	X	1994	U	OP1-P-O3'	5.08	116.36	105.20
1	X	71	A	P-O5'-C5'	5.07	129.02	120.90
1	X	812	G	C8-N9-C4	-5.07	104.37	106.40
1	X	1695	U	N3-C2-O2	-5.07	118.65	122.20
1	X	2229	G	N9-C4-C5	5.07	107.43	105.40
1	X	70	A	P-O3'-C3'	5.07	125.78	119.70
1	X	777	A	C5'-C4'-C3'	-5.07	107.89	116.00
1	X	773	G	O4'-C1'-N9	5.07	112.25	108.20
1	X	1753	A	N7-C8-N9	5.07	116.33	113.80
1	X	1264	C	N1-C2-O2	5.07	121.94	118.90
1	X	1509	A	P-O5'-C5'	5.07	129.01	120.90
1	X	69	G	O4'-C1'-N9	5.07	112.25	108.20
1	X	1973	C	O4'-C1'-N1	5.07	112.25	108.20
1	X	2681	A	C6-N1-C2	-5.07	115.56	118.60
1	X	1099	A	C3'-C2'-C1'	5.06	105.55	101.50
1	X	1528	C	C5-C6-N1	5.06	123.53	121.00
1	X	1223	G	C5-C6-O6	-5.06	125.56	128.60
1	X	2251	U	P-O3'-C3'	5.06	125.77	119.70
1	X	2487	G	C5-C6-N1	5.06	114.03	111.50
1	X	1524	C	O4'-C1'-N1	5.06	112.25	108.20
1	X	1928	G	P-O5'-C5'	5.06	128.99	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2324	G	N3-C4-C5	-5.06	126.07	128.60
5	C	163	ASN	C-N-CA	5.06	134.34	121.70
1	X	664	C	N1-C2-O2	5.06	121.93	118.90
1	X	2485	U	P-O3'-C3'	5.06	125.77	119.70
1	X	2731	G	O4'-C1'-N9	5.06	112.25	108.20
1	X	26	G	C5-C6-O6	-5.05	125.57	128.60
1	X	559	C	N3-C2-O2	-5.05	118.36	121.90
1	X	1451	C	C5'-C4'-O4'	5.05	115.16	109.10
1	X	1674	C	C5'-C4'-O4'	-5.05	103.04	109.10
1	X	1796	A	C2-N3-C4	5.05	113.13	110.60
1	X	1799	A	C5'-C4'-O4'	5.05	115.16	109.10
1	X	2744	A	P-O3'-C3'	5.05	125.76	119.70
1	X	624	A	O4'-C1'-N9	5.05	112.24	108.20
1	X	1250	A	O4'-C1'-N9	-5.05	104.16	108.20
1	X	1666	G	O4'-C4'-C3'	-5.05	98.95	104.00
1	X	2064	U	O4'-C1'-N1	5.05	112.24	108.20
1	X	2288	A	P-O3'-C3'	5.05	125.76	119.70
1	X	2426	G	C1'-O4'-C4'	-5.05	105.86	109.90
1	X	461	A	C2-N3-C4	5.05	113.12	110.60
1	X	536	A	N1-C6-N6	5.05	121.63	118.60
1	X	635	C	C6-N1-C2	-5.05	118.28	120.30
1	X	1986	G	N1-C6-O6	-5.05	116.87	119.90
1	X	1665	C	O5'-P-OP2	-5.05	101.16	105.70
1	X	2507	U	P-O3'-C3'	5.05	125.75	119.70
1	X	1426	U	O4'-C1'-N1	5.04	112.24	108.20
1	X	1497	C	O4'-C1'-N1	5.04	112.23	108.20
1	X	1535	C	O4'-C1'-N1	5.04	112.23	108.20
1	X	1282	A	C5'-C4'-C3'	-5.04	107.93	116.00
1	X	1980	A	O4'-C1'-N9	5.04	112.23	108.20
1	X	2729	A	O4'-C1'-N9	5.04	112.23	108.20
1	X	1284	G	N7-C8-N9	5.04	115.62	113.10
1	X	769	C	O4'-C1'-N1	5.04	112.23	108.20
1	X	1199	U	OP2-P-O3'	5.04	116.28	105.20
1	X	1467	U	C1'-O4'-C4'	5.04	113.93	109.90
1	X	1838	G	P-O3'-C3'	5.04	125.75	119.70
1	X	337	G	C5-C6-O6	-5.04	125.58	128.60
1	X	407	A	O4'-C1'-N9	5.04	112.23	108.20
1	X	753	U	P-O3'-C3'	5.04	125.74	119.70
1	X	2745	A	N1-C2-N3	-5.04	126.78	129.30
1	X	107	G	C5'-C4'-C3'	-5.04	107.94	116.00
1	X	1872	A	C4'-C3'-C2'	-5.04	97.56	102.60
1	X	349	G	N3-C4-C5	-5.03	126.08	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	964	A	C5'-C4'-O4'	5.03	115.14	109.10
1	X	1291	G	O4'-C4'-C3'	-5.03	98.97	104.00
1	X	465	C	P-O5'-C5'	-5.03	112.85	120.90
1	X	1229	C	O4'-C1'-N1	5.03	112.22	108.20
1	X	2691	C	O3'-P-O5'	-5.03	94.44	104.00
1	X	17	G	P-O3'-C3'	-5.03	113.67	119.70
1	X	467	U	C5'-C4'-O4'	5.03	115.14	109.10
1	X	2228	U	N3-C4-O4	5.03	122.92	119.40
1	X	228	A	OP1-P-O3'	5.03	116.26	105.20
1	X	616	U	C5'-C4'-C3'	-5.03	107.96	116.00
1	X	1000	G	O4'-C1'-N9	5.03	112.22	108.20
1	X	1033	G	C5'-C4'-O4'	-5.03	103.07	109.10
1	X	1669	A	C3'-C2'-C1'	-5.03	97.48	101.50
1	X	1766	U	C5-C4-O4	-5.03	122.88	125.90
1	X	190	A	C1'-O4'-C4'	-5.03	105.88	109.90
1	X	560	G	C4'-C3'-C2'	5.03	107.63	102.60
1	X	633	G	P-O5'-C5'	5.03	128.94	120.90
1	X	1174	G	O4'-C1'-N9	5.03	112.22	108.20
1	X	1812	U	P-O5'-C5'	5.03	128.94	120.90
1	X	2503	G	C5-C6-N1	5.03	114.01	111.50
1	X	2567	G	C6-N1-C2	-5.03	122.08	125.10
1	X	2598	C	N3-C4-C5	5.03	123.91	121.90
1	X	2620	G	C4'-C3'-C2'	-5.03	97.57	102.60
1	X	767	G	P-O5'-C5'	5.02	128.94	120.90
1	X	1541	G	O4'-C1'-N9	5.02	112.22	108.20
1	X	2701	A	P-O3'-C3'	-5.02	113.67	119.70
1	X	2727	G	O4'-C1'-N9	5.02	112.22	108.20
1	X	1222	G	N3-C4-N9	5.02	129.01	126.00
1	X	1777	A	C1'-O4'-C4'	-5.02	105.88	109.90
1	X	2737	A	C5'-C4'-C3'	-5.02	107.97	116.00
2	Y	35	C	O4'-C1'-N1	5.02	112.22	108.20
1	X	232	A	P-O5'-C5'	5.02	128.93	120.90
1	X	344	G	C8-N9-C4	-5.02	104.39	106.40
1	X	480	G	N1-C6-O6	5.02	122.91	119.90
1	X	537	C	C3'-C2'-C1'	-5.01	97.49	101.50
1	X	573	C	N1-C2-O2	5.01	121.91	118.90
1	X	1049	C	O4'-C1'-N1	5.01	112.21	108.20
1	X	1669	A	C1'-O4'-C4'	-5.01	105.89	109.90
2	Y	54	U	C1'-O4'-C4'	-5.01	105.89	109.90
1	X	845	U	N3-C2-O2	-5.01	118.69	122.20
1	X	2261	G	C4'-C3'-C2'	5.01	107.61	102.60
1	X	73	A	N9-C1'-C2'	5.01	120.51	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	610	G	O3'-P-O5'	-5.01	94.48	104.00
1	X	1234	C	O4'-C1'-N1	5.01	112.21	108.20
1	X	1770	U	C4-C5-C6	5.01	122.71	119.70
1	X	1418	C	N1-C2-O2	5.01	121.91	118.90
1	X	497	C	C3'-C2'-C1'	-5.01	97.50	101.50
1	X	2340	C	OP1-P-OP2	5.01	127.11	119.60
1	X	1280	U	N1-C1'-C2'	5.00	120.51	114.00
1	X	1812	U	C2-N1-C1'	5.00	123.71	117.70
1	X	2347	C	C3'-C2'-C1'	-5.00	97.50	101.50
2	Y	45	C	N3-C2-O2	-5.00	118.40	121.90
1	X	1075	C	C3'-C2'-C1'	5.00	105.50	101.50
1	X	1671	A	OP1-P-OP2	5.00	127.10	119.60
1	X	1822	C	C3'-C2'-C1'	-5.00	97.50	101.50
1	X	2292	C	O4'-C1'-N1	5.00	112.20	108.20
1	X	2298	U	C2-N1-C1'	5.00	123.70	117.70

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	1288	A	Sidechain
1	X	1684	G	Sidechain
1	X	219	G	Sidechain
1	X	474	G	Sidechain
1	X	683	A	Sidechain
1	X	739	G	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	X	57651	0	29049	431	0
2	Y	2598	0	1328	17	0
3	A	1826	0	1885	62	0
4	B	1539	0	1600	62	0
5	C	1506	0	1525	57	0
6	D	1400	0	1481	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	E	1286	0	1336	9	0
8	F	503	0	520	3	0
9	G	1114	0	1144	63	0
10	H	997	0	1046	24	0
11	I	1067	0	1103	48	0
12	J	1090	0	1125	32	0
13	K	878	0	930	28	0
14	L	779	0	820	17	0
15	M	871	0	894	29	0
16	N	978	0	1020	25	0
17	O	741	0	756	30	0
18	P	1014	0	1096	20	0
19	Q	726	0	753	23	0
20	R	825	0	881	28	0
21	S	1345	0	1372	21	0
22	T	625	0	655	11	0
23	U	552	0	604	28	0
24	V	533	0	558	4	0
25	W	424	0	470	9	0
26	Z	457	0	462	16	0
27	1	53	0	0	0	0
28	2	46	0	0	2	0
29	3	63	0	0	2	0
30	4	297	0	330	5	0
31	X	30	0	0	0	0
31	Y	5	0	0	0	0
32	X	60	0	66	2	0
All	All	83879	0	54809	969	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 7.

All (969) 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)
13:K:52:ILE:CD1	13:K:52:ILE:CG1	1.93	1.47
11:I:62:LYS:NZ	11:I:64:GLY:HA2	1.60	1.15
1:X:1333:G:N2	1:X:1344:C:H41	1.44	1.12
15:M:79:ARG:HG3	15:M:79:ARG:HH11	1.03	1.10
19:Q:29:VAL:HG11	19:Q:38:ILE:HD11	1.35	1.09
1:X:759:C:H6	1:X:759:C:H5''	1.07	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:542:A:C2	1:X:2004:U:H2'	1.93	1.03
11:I:62:LYS:HZ1	11:I:64:GLY:HA2	1.24	1.02
1:X:542:A:H2	1:X:2004:U:H2'	1.24	1.00
4:B:152:LYS:HB2	9:G:106:TYR:HB3	1.39	1.00
1:X:759:C:H5''	1:X:759:C:C6	1.98	0.98
1:X:617:U:H5	1:X:632:A:C2	1.82	0.96
1:X:1919:A:H2	1:X:1926:U:H3	0.99	0.95
1:X:1333:G:H22	1:X:1344:C:N4	1.62	0.95
1:X:1448:A:H61	1:X:1574:A:H61	0.97	0.94
1:X:1466:C:H2'	1:X:1467:U:O4'	1.69	0.91
16:N:93:LYS:HE3	17:O:5:ILE:HD13	1.52	0.91
1:X:2042:A:H5''	5:C:65:GLY:HA2	1.53	0.91
1:X:1333:G:H22	1:X:1344:C:H41	0.94	0.91
1:X:2371:A:H2	1:X:2403:C:H42	1.15	0.91
15:M:79:ARG:HG3	15:M:79:ARG:NH1	1.80	0.91
1:X:787:A:H2	1:X:800:U:HO2'	1.16	0.90
9:G:33:ILE:HB	9:G:34:PRO:HD3	1.53	0.89
1:X:617:U:H5	1:X:632:A:H2	1.16	0.89
1:X:1277:G:OP1	26:Z:19:ARG:NH2	2.04	0.89
17:O:5:ILE:HD12	17:O:6:GLN:H	1.35	0.88
1:X:1468:A:H5'	1:X:1472:C:N4	1.87	0.88
1:X:1919:A:H2	1:X:1926:U:N3	1.70	0.88
1:X:1542:G:H22	1:X:1562:G:H1	1.15	0.88
1:X:1770:U:H5	1:X:1775:A:N7	1.73	0.87
26:Z:4:HIS:HB3	26:Z:5:PRO:HD3	1.56	0.86
1:X:617:U:C5	1:X:632:A:C2	2.64	0.86
4:B:152:LYS:CB	9:G:106:TYR:HB3	2.07	0.85
9:G:67:ARG:HG2	9:G:70:PHE:HA	1.56	0.85
1:X:542:A:H2	1:X:2004:U:C2'	1.88	0.85
5:C:43:ALA:HB1	5:C:86:PRO:HB2	1.59	0.83
23:U:48:LYS:HG2	23:U:49:LYS:H	1.42	0.82
1:X:1882:G:N2	1:X:1885:C:H41	1.77	0.82
4:B:131:SER:O	4:B:132:LYS:HG3	1.78	0.81
4:B:54:LYS:HB2	4:B:75:THR:O	1.81	0.81
1:X:971:A:H61	12:J:83:ARG:HH22	1.27	0.81
1:X:1266:G:N7	11:I:32:ARG:NH1	2.29	0.81
1:X:1811:A:H4'	1:X:1812:U:H5''	1.62	0.80
11:I:62:LYS:HZ3	11:I:64:GLY:HA2	1.45	0.80
1:X:1173:G:H21	17:O:88:GLN:HE22	1.29	0.80
9:G:132:PHE:CZ	9:G:145:HIS:HB2	2.16	0.80
1:X:70:A:H5'	1:X:71:A:H3'	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:137:ALA:HB1	5:C:142:LEU:HB2	1.63	0.79
1:X:689:A:H8	1:X:2052:G:H21	1.31	0.79
11:I:58:ALA:O	11:I:59:ARG:HB2	1.80	0.79
1:X:482:A:H2'	1:X:483:A:O4'	1.83	0.78
1:X:320:A:N3	1:X:340:G:O2'	2.15	0.78
9:G:33:ILE:HB	9:G:34:PRO:CD	2.13	0.78
1:X:215:G:H21	1:X:632:A:H8	1.33	0.77
23:U:22:GLY:HA3	23:U:39:LYS:HD2	1.66	0.77
9:G:100:TYR:HB2	9:G:116:ARG:NH1	1.99	0.77
19:Q:61:LYS:H	19:Q:72:ARG:HA	1.50	0.77
1:X:1448:A:N6	1:X:1574:A:H61	1.79	0.76
1:X:1673:C:H5''	4:B:136:ARG:CD	2.15	0.76
1:X:1333:G:N2	1:X:1344:C:N4	2.25	0.76
1:X:463:C:H42	1:X:467:U:H5	1.30	0.76
1:X:1963:G:O2'	1:X:1965:U:OP2	2.03	0.76
4:B:116:VAL:HG22	4:B:136:ARG:HE	1.50	0.76
4:B:50:GLY:HA3	4:B:75:THR:HG21	1.67	0.75
16:N:66:ASN:ND2	16:N:70:ARG:HH12	1.84	0.75
15:M:79:ARG:HH11	15:M:79:ARG:CG	1.92	0.75
5:C:48:ARG:HB2	5:C:51:VAL:HG22	1.69	0.75
1:X:2617:G:P	4:B:82:ARG:HH22	2.10	0.74
2:Y:46:G:H5'	6:D:92:ARG:HH12	1.53	0.74
13:K:17:ARG:NH1	13:K:20:LEU:HD23	2.01	0.74
1:X:2551:A:N7	4:B:145:LYS:HB2	2.04	0.73
1:X:1054:C:H42	1:X:1123:G:H1	1.37	0.73
17:O:10:LYS:HG3	17:O:11:GLN:HG2	1.70	0.72
1:X:1811:A:H5''	3:A:161:THR:HG21	1.71	0.72
3:A:210:GLY:HA2	3:A:213:ARG:HB2	1.71	0.72
3:A:231:HIS:HD2	3:A:233:HIS:H	1.35	0.72
1:X:759:C:H6	1:X:759:C:C5'	1.95	0.71
1:X:1673:C:C5'	4:B:136:ARG:HD2	2.19	0.71
1:X:2042:A:H5''	5:C:65:GLY:CA	2.19	0.71
1:X:2266:A:H2	1:X:2325:A:H62	1.38	0.71
25:W:12:ARG:CG	25:W:12:ARG:HH11	2.02	0.71
25:W:12:ARG:HH11	25:W:12:ARG:HG2	1.56	0.71
3:A:231:HIS:CD2	3:A:233:HIS:H	2.08	0.71
1:X:1675:C:OP1	4:B:134:TRP:NE1	2.24	0.71
1:X:2653:A:O2'	10:H:41:ASN:ND2	2.24	0.71
4:B:116:VAL:HG22	4:B:136:ARG:NE	2.05	0.70
1:X:304:A:H2'	1:X:305:A:H5''	1.71	0.70
18:P:92:VAL:HG13	18:P:126:ILE:HD13	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:U:17:SER:HB2	23:U:44:ALA:HA	1.74	0.70
23:U:48:LYS:CG	23:U:49:LYS:H	2.04	0.70
13:K:79:VAL:HA	13:K:83:VAL:HG13	1.74	0.70
1:X:640:C:H4'	1:X:660:G:H21	1.54	0.70
1:X:1030:U:H3	1:X:1153:A:H62	1.38	0.70
1:X:2772:U:H3	1:X:2780:A:H61	1.39	0.70
5:C:38:ARG:HH12	5:C:176:ASN:HD21	1.40	0.69
4:B:16:LYS:HB2	4:B:21:ILE:HD11	1.73	0.69
3:A:36:ALA:HB1	3:A:62:TYR:O	1.91	0.69
9:G:100:TYR:HB2	9:G:116:ARG:HH11	1.58	0.69
1:X:1673:C:H5''	4:B:136:ARG:HD2	1.75	0.69
17:O:66:GLY:O	17:O:87:ARG:NH1	2.26	0.69
23:U:32:ARG:H	23:U:32:ARG:HE	1.41	0.69
1:X:2779:C:H2'	1:X:2780:A:C8	2.28	0.69
1:X:415:A:H61	1:X:436:A:H61	1.41	0.68
1:X:797:A:C5	3:A:229:VAL:HG21	2.28	0.68
4:B:7:THR:HG21	15:M:5:ILE:HD11	1.75	0.68
13:K:11:ASN:OD1	13:K:11:ASN:N	2.26	0.68
1:X:1753:A:O5'	1:X:1753:A:H8	1.76	0.68
1:X:1238:A:H4'	17:O:83:ARG:HG2	1.76	0.68
1:X:1675:C:OP1	4:B:134:TRP:CE2	2.47	0.68
15:M:34:ARG:NH2	15:M:88:VAL:HG13	2.09	0.68
1:X:797:A:N7	3:A:229:VAL:HG21	2.08	0.67
1:X:2501:U:H5''	1:X:2501:U:H6	1.59	0.67
15:M:27:PHE:HA	15:M:96:ARG:HH21	1.59	0.67
10:H:98:ILE:HG22	10:H:106:ARG:HG3	1.76	0.67
11:I:76:LYS:HB2	11:I:79:GLN:HG2	1.76	0.67
16:N:83:LEU:HD12	16:N:113:SER:HB2	1.77	0.67
16:N:88:ILE:HG13	17:O:49:GLU:HB2	1.76	0.67
1:X:841:G:H2'	1:X:842:A:C8	2.30	0.66
23:U:47:HIS:CD2	23:U:48:LYS:H	2.13	0.66
1:X:38:G:H1	1:X:453:U:H3	1.43	0.66
1:X:652:C:H42	1:X:657:A:H61	1.42	0.66
23:U:48:LYS:HG2	23:U:49:LYS:N	2.10	0.66
1:X:1586:A:H5'	3:A:38:PRO:HG3	1.76	0.66
1:X:1816:G:O2'	3:A:252:LYS:HG2	1.95	0.66
1:X:1468:A:H5'	1:X:1472:C:H41	1.56	0.66
3:A:89:SER:HB2	3:A:201:HIS:CE1	2.30	0.66
12:J:14:PHE:HE1	12:J:90:ALA:HA	1.59	0.65
1:X:219:G:N2	1:X:231:G:H2'	2.12	0.65
1:X:1467:U:H2'	1:X:1468:A:OP1	1.94	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:4:HIS:HB3	26:Z:5:PRO:CD	2.24	0.65
1:X:1770:U:C5	1:X:1775:A:N7	2.61	0.65
9:G:70:PHE:CB	16:N:64:ARG:HG2	2.27	0.65
1:X:2266:A:H62	1:X:2323:U:H3	1.43	0.65
1:X:1466:C:C2'	1:X:1467:U:O4'	2.44	0.65
6:D:80:ARG:HD3	6:D:83:MET:HB2	1.78	0.65
11:I:28:LYS:HE3	11:I:36:GLY:HA3	1.79	0.65
12:J:40:PRO:HB3	12:J:99:LYS:HD2	1.78	0.65
19:Q:60:GLY:H	19:Q:72:ARG:HD3	1.62	0.64
20:R:92:THR:HB	20:R:95:ARG:HH22	1.60	0.64
2:Y:45:C:H2'	6:D:92:ARG:NH1	2.12	0.64
3:A:183:ARG:HH11	3:A:183:ARG:HB3	1.62	0.64
23:U:22:GLY:HA3	23:U:39:LYS:CD	2.27	0.64
3:A:96:HIS:HE1	3:A:100:GLY:HA2	1.62	0.64
11:I:30:ALA:HB3	11:I:34:HIS:CE1	2.32	0.64
1:X:1584:G:H4'	3:A:59:LYS:HB3	1.80	0.64
1:X:2222:U:H2'	1:X:2223:U:C6	2.32	0.64
3:A:172:TYR:HA	3:A:186:HIS:HA	1.80	0.64
1:X:1033:G:N2	1:X:1153:A:C2	2.66	0.63
20:R:105:ARG:HH12	20:R:112:LYS:HA	1.63	0.63
13:K:17:ARG:HH11	13:K:20:LEU:HD23	1.60	0.63
9:G:61:ARG:HH11	9:G:66:HIS:H	1.44	0.63
1:X:1673:C:H5''	4:B:136:ARG:HD3	1.79	0.63
1:X:2545:A:H61	10:H:40:GLY:HA3	1.63	0.63
9:G:70:PHE:HB3	16:N:64:ARG:HG2	1.81	0.63
11:I:28:LYS:HZ1	11:I:37:GLN:H	1.47	0.63
1:X:203:G:H1'	1:X:205:A:H61	1.64	0.63
1:X:1803:G:H21	3:A:46:ARG:HD2	1.64	0.63
15:M:25:PRO:HD2	15:M:91:VAL:HG12	1.81	0.63
5:C:133:PHE:HB2	5:C:160:ALA:HB1	1.81	0.62
9:G:161:GLN:HG2	9:G:165:VAL:HG11	1.80	0.62
1:X:564:U:H2'	1:X:565:A:C8	2.33	0.62
3:A:244:ARG:HB3	3:A:252:LYS:NZ	2.13	0.62
4:B:55:ALA:HB3	4:B:58:LYS:HG3	1.81	0.62
1:X:2790:C:O2'	26:Z:43:HIS:HD2	1.82	0.62
11:I:73:GLU:OE1	11:I:101:ARG:HB2	1.98	0.62
1:X:1007:A:H4'	16:N:93:LYS:HB3	1.81	0.62
16:N:66:ASN:HB3	16:N:76:TYR:H	1.64	0.62
1:X:82:G:H1	1:X:100:G:H2'	1.64	0.62
13:K:24:GLN:HB3	13:K:44:LEU:HD22	1.82	0.62
20:R:22:VAL:HG11	20:R:80:LYS:HZ3	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1033:G:H4'	1:X:1034:U:H5'	1.82	0.62
32:X:2931:1F3:H20	32:X:2931:1F3:H61	1.81	0.61
11:I:32:ARG:HD2	17:O:79:GLN:NE2	2.15	0.61
20:R:46:VAL:HG11	20:R:80:LYS:HD3	1.81	0.61
1:X:617:U:C5	1:X:632:A:H2	2.06	0.61
20:R:92:THR:HB	20:R:95:ARG:NH2	2.16	0.61
5:C:164:VAL:C	5:C:166:TRP:H	2.04	0.61
1:X:346:C:H2'	1:X:347:C:C6	2.36	0.61
1:X:224:G:OP2	1:X:226:C:N4	2.31	0.60
1:X:2037:A:H2'	26:Z:8:LYS:HE3	1.82	0.60
1:X:971:A:N6	12:J:83:ARG:HH22	1.99	0.60
1:X:774:A:O5'	1:X:774:A:H8	1.85	0.60
1:X:649:G:H1	1:X:660:G:H1	1.49	0.60
1:X:2197:U:H2'	1:X:2198:U:C6	2.37	0.60
4:B:116:VAL:H	4:B:136:ARG:HE	1.49	0.60
1:X:540:G:O6	1:X:2006:G:OP1	2.18	0.60
10:H:85:ASP:HB3	15:M:87:LEU:HD12	1.83	0.60
9:G:62:ILE:HG22	9:G:135:LEU:HD21	1.84	0.60
9:G:67:ARG:CG	9:G:70:PHE:HA	2.29	0.60
13:K:11:ASN:OD1	13:K:17:ARG:NH2	2.33	0.60
16:N:66:ASN:HD22	16:N:70:ARG:HH12	1.49	0.60
1:X:2334:C:H1'	22:T:39:ARG:HH21	1.65	0.60
17:O:5:ILE:HD12	17:O:6:GLN:N	2.12	0.60
1:X:2551:A:C8	4:B:144:ARG:HD3	2.37	0.60
1:X:946:U:H2'	1:X:947:C:H6	1.67	0.59
1:X:2362:G:H2'	1:X:2363:G:C8	2.37	0.59
17:O:11:GLN:HE22	17:O:38:LEU:HB3	1.65	0.59
16:N:66:ASN:HB3	16:N:76:TYR:N	2.18	0.59
1:X:2597:G:H21	4:B:150:VAL:HG11	1.66	0.59
5:C:3:GLN:HG2	5:C:116:LYS:HD2	1.84	0.59
20:R:10:HIS:O	20:R:11:ASN:HB2	2.02	0.59
1:X:504:G:H21	18:P:78:ASN:HD21	1.51	0.59
1:X:2713:A:H61	4:B:203:LYS:HG2	1.68	0.59
1:X:760:U:C6	26:Z:3:LYS:HG3	2.38	0.59
1:X:512:A:H4'	18:P:15:LYS:HB3	1.84	0.59
4:B:152:LYS:HD2	9:G:106:TYR:H	1.68	0.59
12:J:92:GLU:HG3	12:J:93:TYR:HD2	1.67	0.58
1:X:827:C:H2'	1:X:828:C:H6	1.68	0.58
1:X:597:U:O4	1:X:683:A:H1'	2.03	0.58
25:W:4:LYS:HG2	25:W:52:GLU:HB3	1.85	0.58
1:X:946:U:H2'	1:X:947:C:C6	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:78:SER:HA	10:H:91:PHE:O	2.04	0.58
1:X:2371:A:H8	11:I:59:ARG:HG3	1.69	0.58
11:I:81:GLN:HG2	11:I:114:ILE:HG22	1.86	0.58
18:P:13:GLN:O	18:P:16:GLN:HG2	2.02	0.58
29:3:10:ALA:CA	29:3:12:ARG:CA	2.82	0.58
1:X:1050:G:H1	1:X:1127:C:H42	1.51	0.58
1:X:2617:G:P	4:B:82:ARG:NH2	2.76	0.58
1:X:451:A:H2'	1:X:452:G:C8	2.39	0.58
1:X:1468:A:H5'	1:X:1472:C:H42	1.68	0.58
3:A:91:ARG:HG3	3:A:198:ASN:H	1.69	0.58
9:G:61:ARG:NH1	9:G:66:HIS:H	2.02	0.58
3:A:39:LYS:HB2	3:A:62:TYR:HB2	1.86	0.58
4:B:120:TRP:HB3	4:B:155:ARG:HH11	1.69	0.58
20:R:16:PHE:HZ	20:R:46:VAL:HG22	1.69	0.58
1:X:623:G:H3'	1:X:624:A:H5''	1.86	0.57
1:X:1773:C:H1'	1:X:2588:U:H5''	1.85	0.57
1:X:1962:C:H2'	1:X:1963:G:H5'	1.85	0.57
5:C:43:ALA:CB	5:C:86:PRO:HB2	2.32	0.57
5:C:48:ARG:C	5:C:50:GLN:H	2.07	0.57
5:C:27:LEU:O	5:C:31:VAL:HG23	2.05	0.57
15:M:32:THR:CG2	15:M:91:VAL:HG22	2.34	0.57
18:P:40:LEU:HB3	26:Z:25:LEU:HD13	1.86	0.57
1:X:759:C:C6	1:X:759:C:C5'	2.78	0.57
1:X:1287:A:H2'	1:X:1288:A:H5''	1.86	0.57
12:J:99:LYS:HG3	12:J:100:PRO:HD2	1.87	0.57
1:X:1918:G:H1'	1:X:1947:G:N2	2.20	0.57
9:G:102:ARG:HH11	9:G:102:ARG:HB3	1.70	0.57
11:I:17:LYS:O	11:I:18:ARG:HB2	2.03	0.57
16:N:88:ILE:HG23	17:O:48:GLY:HA3	1.86	0.57
1:X:787:A:H2	1:X:800:U:O2'	1.84	0.57
1:X:1811:A:H4'	1:X:1812:U:C5'	2.32	0.57
4:B:131:SER:O	4:B:132:LYS:CG	2.52	0.57
1:X:558:G:O3'	1:X:559:C:H4'	2.03	0.57
1:X:504:G:H4'	18:P:27:VAL:HG13	1.87	0.57
1:X:1882:G:H22	1:X:1885:C:H41	1.49	0.57
18:P:105:ARG:HD3	18:P:119:LYS:HE3	1.86	0.57
9:G:69:ASP:H	9:G:76:GLN:HE21	1.51	0.56
13:K:10:LEU:HA	13:K:17:ARG:HG2	1.86	0.56
1:X:670:U:H2'	1:X:671:A:C8	2.40	0.56
1:X:954:U:OP2	11:I:38:LYS:HG2	2.04	0.56
2:Y:45:C:H2'	6:D:92:ARG:HH11	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:16:LYS:HB2	4:B:21:ILE:CD1	2.35	0.56
1:X:673:G:H5'	5:C:93:TYR:CD1	2.41	0.56
6:D:47:SER:HA	6:D:50:ILE:HD12	1.87	0.56
13:K:3:HIS:CG	13:K:5:LYS:HZ3	2.23	0.56
15:M:31:ASP:OD2	15:M:31:ASP:N	2.31	0.56
1:X:1030:U:HO2'	1:X:1032:A:H2	1.52	0.56
1:X:1033:G:H22	1:X:1153:A:H2	1.49	0.56
17:O:36:LYS:HZ1	17:O:54:TYR:HB3	1.70	0.56
1:X:1113:C:H2'	1:X:1114:A:H8	1.70	0.56
9:G:105:GLY:O	9:G:106:TYR:C	2.42	0.56
17:O:10:LYS:HD2	17:O:37:ALA:HB3	1.88	0.56
1:X:760:U:O2	1:X:1997:A:H1'	2.06	0.56
5:C:48:ARG:C	5:C:50:GLN:N	2.58	0.56
5:C:176:ASN:HD22	5:C:179:ASP:H	1.54	0.56
16:N:66:ASN:HB3	16:N:76:TYR:HB2	1.87	0.56
1:X:172:A:H61	1:X:175:C:H3'	1.71	0.56
1:X:334:G:H3'	5:C:162:ARG:HE	1.70	0.56
11:I:32:ARG:HD2	17:O:79:GLN:HE22	1.70	0.56
5:C:30:VAL:HG11	5:C:177:VAL:HG21	1.88	0.55
21:S:149:ALA:HA	21:S:152:ILE:HD12	1.87	0.55
4:B:134:TRP:HD1	4:B:134:TRP:H	1.53	0.55
9:G:116:ARG:HD2	9:G:119:LEU:HD12	1.89	0.55
11:I:75:VAL:HG22	11:I:99:VAL:HG11	1.88	0.55
13:K:87:TYR:HE1	13:K:94:TYR:HD2	1.54	0.55
1:X:1032:A:H8	1:X:1033:G:H5''	1.71	0.55
5:C:95:LEU:HD23	5:C:96:PRO:HD2	1.88	0.55
1:X:1673:C:H5'	4:B:136:ARG:HD2	1.88	0.55
11:I:94:GLU:HA	11:I:97:ARG:HE	1.71	0.55
13:K:7:GLY:O	13:K:8:ARG:HG2	2.06	0.55
13:K:33:ARG:HD3	13:K:112:LEU:HD22	1.89	0.55
20:R:90:LYS:HB2	20:R:108:VAL:HG11	1.88	0.55
23:U:48:LYS:CG	23:U:49:LYS:N	2.70	0.55
1:X:1278:A:H2	1:X:1997:A:H62	1.54	0.55
7:E:164:PHE:HB2	7:E:167:GLU:HB2	1.88	0.55
1:X:2387:U:H2'	1:X:2388:G:H8	1.71	0.55
3:A:218:LYS:HE3	3:A:221:GLN:HB2	1.89	0.55
12:J:44:LYS:HD3	12:J:47:GLN:HE22	1.71	0.55
1:X:1373:G:H22	1:X:2192:U:H3	1.54	0.55
1:X:1448:A:H61	1:X:1574:A:N6	1.82	0.55
1:X:746:G:N7	1:X:774:A:C6	2.75	0.54
18:P:14:ARG:HA	18:P:17:GLN:HG2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1473:U:OP2	1:X:1473:U:H6	1.90	0.54
1:X:2797:G:OP2	13:K:3:HIS:NE2	2.40	0.54
3:A:89:SER:HB2	3:A:201:HIS:HE1	1.72	0.54
3:A:96:HIS:HE1	3:A:100:GLY:CA	2.20	0.54
9:G:104:THR:OG1	9:G:110:LEU:HB3	2.07	0.54
19:Q:38:ILE:O	19:Q:42:ILE:HG22	2.07	0.54
21:S:25:ASN:HB3	21:S:85:MET:HB2	1.88	0.54
1:X:2617:G:OP2	4:B:82:ARG:NH2	2.40	0.54
12:J:109:GLY:HA3	21:S:112:LEU:HD21	1.90	0.54
18:P:57:LEU:HA	18:P:60:ILE:HD12	1.89	0.54
2:Y:62:C:H2'	2:Y:63:A:C8	2.42	0.54
12:J:12:LYS:O	12:J:13:GLN:HB2	2.08	0.54
16:N:81:ASN:HD22	16:N:117:ARG:HH21	1.56	0.54
1:X:1790:G:H5'	1:X:1811:A:H61	1.73	0.54
5:C:146:GLU:HG3	5:C:185:ARG:HH11	1.72	0.54
1:X:2371:A:C8	11:I:59:ARG:HG3	2.41	0.54
11:I:10:PRO:HA	11:I:14:LYS:HB2	1.89	0.54
1:X:1810:U:H2'	3:A:157:ARG:HD3	1.90	0.54
1:X:2790:C:O2'	26:Z:43:HIS:CD2	2.61	0.53
4:B:147:PRO:C	4:B:149:ARG:H	2.11	0.53
6:D:92:ARG:HH21	6:D:92:ARG:HB2	1.72	0.53
13:K:3:HIS:HB3	13:K:5:LYS:CE	2.39	0.53
1:X:346:C:H2'	1:X:347:C:H6	1.73	0.53
11:I:117:ALA:HA	11:I:137:GLY:O	2.08	0.53
18:P:57:LEU:HD13	18:P:69:ALA:HA	1.91	0.53
1:X:748:A:H3'	1:X:749:C:H6	1.73	0.53
1:X:2196:U:H2'	1:X:2197:U:O4'	2.08	0.53
2:Y:42:U:H1'	2:Y:47:A:H61	1.73	0.53
10:H:116:ARG:HG3	15:M:38:LYS:HZ3	1.73	0.53
25:W:1:MET:HB3	25:W:34:VAL:HG12	1.90	0.53
1:X:1976:U:H4'	4:B:128:SER:OG	2.08	0.53
2:Y:9:G:O2'	14:L:41:GLN:NE2	2.41	0.53
5:C:98:GLN:HA	5:C:101:GLN:HG3	1.90	0.53
10:H:116:ARG:HG3	15:M:38:LYS:NZ	2.22	0.53
15:M:28:ARG:H	15:M:96:ARG:NH2	2.06	0.53
1:X:2306:A:H2'	1:X:2307:A:C8	2.43	0.53
1:X:1467:U:H6	1:X:1467:U:H3'	1.74	0.53
6:D:75:SER:HB2	6:D:79:LEU:HD13	1.90	0.53
9:G:158:HIS:HA	9:G:161:GLN:CD	2.29	0.53
1:X:77:C:H42	1:X:106:G:H1	1.55	0.53
1:X:490:A:N3	1:X:492:G:H5''	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:206:LEU:HA	3:A:211:ARG:HG2	1.90	0.53
23:U:49:LYS:HB2	23:U:61:TRP:HA	1.91	0.53
1:X:2766:U:OP1	4:B:69:LYS:HE2	2.09	0.53
2:Y:83:C:N4	2:Y:98:C:N3	2.57	0.53
5:C:148:VAL:HG13	5:C:185:ARG:HB2	1.91	0.53
1:X:172:A:H5''	1:X:173:A:OP2	2.09	0.53
4:B:149:ARG:CZ	9:G:106:TYR:HD1	2.22	0.53
6:D:38:GLU:HB3	6:D:87:ILE:HB	1.91	0.53
7:E:89:LEU:HD23	7:E:162:VAL:HG22	1.91	0.53
9:G:61:ARG:HH11	9:G:65:LYS:HB3	1.73	0.53
9:G:67:ARG:NE	9:G:70:PHE:O	2.40	0.53
15:M:27:PHE:HB3	15:M:93:ILE:HD12	1.89	0.53
1:X:870:C:H4'	22:T:23:VAL:HG21	1.90	0.52
1:X:1519:G:H2'	1:X:1520:G:H8	1.73	0.52
1:X:1943:A:H8	1:X:1943:A:H5''	1.74	0.52
1:X:2272:A:H5''	14:L:15:ARG:HH21	1.73	0.52
1:X:2811:G:H2'	1:X:2812:A:C8	2.45	0.52
5:C:14:THR:HG22	5:C:15:ILE:H	1.74	0.52
13:K:32:GLY:HA2	13:K:115:LEU:HD12	1.91	0.52
20:R:22:VAL:HG11	20:R:80:LYS:HD2	1.91	0.52
1:X:2241:U:H5	22:T:17:ASN:OD1	1.92	0.52
1:X:2659:C:H5'	4:B:189:PRO:HA	1.91	0.52
3:A:145:LEU:HD23	3:A:155:LEU:HD12	1.92	0.52
9:G:67:ARG:HB3	9:G:70:PHE:HA	1.90	0.52
9:G:103:TYR:CE2	9:G:111:LYS:HB2	2.44	0.52
1:X:793:G:H21	1:X:796:A:H62	1.57	0.52
1:X:823:U:OP1	11:I:32:ARG:NH1	2.42	0.52
20:R:16:PHE:CE2	20:R:80:LYS:HE2	2.43	0.52
1:X:2505:G:H1'	30:4:1:MET:HB2	1.91	0.52
10:H:41:ASN:ND2	10:H:41:ASN:H	2.07	0.52
9:G:68:PRO:HD2	9:G:76:GLN:HB3	1.92	0.52
12:J:62:GLY:H	21:S:175:ARG:H	1.57	0.52
21:S:3:LEU:HD11	21:S:33:ALA:H	1.75	0.52
1:X:2484:G:C2	32:X:2931:1F3:H7	2.45	0.52
19:Q:66:GLY:C	19:Q:68:PHE:H	2.13	0.52
19:Q:68:PHE:O	19:Q:70:GLY:N	2.42	0.52
20:R:60:PRO:HD2	20:R:62:MET:HB2	1.91	0.52
21:S:3:LEU:HD22	21:S:34:LEU:HB3	1.92	0.52
1:X:666:U:O2'	1:X:667:U:H5''	2.10	0.52
1:X:760:U:C5	26:Z:3:LYS:HG3	2.44	0.52
3:A:226:MET:HG2	3:A:230:ASP:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:553:C:H42	1:X:559:C:N4	2.08	0.52
1:X:1850:G:H1'	1:X:1867:A:N6	2.25	0.52
1:X:1909:U:H5'	1:X:1911:A:OP2	2.09	0.52
3:A:108:PRO:HB3	3:A:143:HIS:CE1	2.45	0.51
11:I:97:ARG:O	11:I:98:LEU:HB2	2.10	0.51
23:U:41:VAL:HG23	23:U:42:GLN:H	1.74	0.51
12:J:79:PRO:HD2	12:J:88:LYS:HD2	1.90	0.51
15:M:34:ARG:HB2	15:M:91:VAL:HG23	1.91	0.51
1:X:2387:U:H2'	1:X:2388:G:C8	2.46	0.51
11:I:28:LYS:CE	11:I:36:GLY:HA3	2.40	0.51
26:Z:16:ARG:HD3	26:Z:20:ARG:CZ	2.40	0.51
1:X:1805:G:H1'	3:A:50:THR:HG21	1.92	0.51
1:X:1673:C:C5'	4:B:136:ARG:CD	2.80	0.51
1:X:1071:U:H4'	1:X:1072:U:H3'	1.92	0.51
23:U:49:LYS:HB3	23:U:61:TRP:CE3	2.46	0.51
3:A:244:ARG:HB3	3:A:252:LYS:HZ1	1.76	0.51
4:B:46:ALA:HB2	4:B:82:ARG:HG2	1.92	0.51
4:B:110:GLY:O	13:K:3:HIS:CD2	2.64	0.51
19:Q:31:PRO:HA	19:Q:76:LYS:HD2	1.92	0.51
1:X:168:A:H2'	1:X:169:C:C6	2.45	0.51
7:E:6:LYS:HB3	7:E:69:ARG:HD2	1.92	0.51
19:Q:12:ILE:HG12	19:Q:13:SER:H	1.74	0.51
1:X:2867:G:O5'	1:X:2867:G:H8	1.93	0.51
11:I:108:LEU:HD23	11:I:129:ALA:HB1	1.93	0.51
14:L:76:ALA:HB2	14:L:107:ALA:HA	1.91	0.51
1:X:686:C:H5''	5:C:74:VAL:HB	1.93	0.51
1:X:2725:C:H1'	7:E:143:GLN:HG3	1.91	0.51
9:G:100:TYR:CB	9:G:116:ARG:NH1	2.72	0.51
13:K:45:ARG:HB3	13:K:46:PRO:HD3	1.91	0.51
1:X:1134:C:H2'	1:X:1135:C:H6	1.76	0.50
1:X:1685:A:H5''	10:H:5:GLN:HG2	1.92	0.50
17:O:57:GLN:H	17:O:97:GLY:CA	2.25	0.50
21:S:3:LEU:HD21	21:S:32:PHE:HB3	1.93	0.50
12:J:78:LYS:HA	12:J:88:LYS:NZ	2.26	0.50
1:X:553:C:H42	1:X:559:C:H42	1.58	0.50
24:V:23:LYS:O	24:V:27:GLU:HG2	2.10	0.50
1:X:2406:C:H5''	1:X:2408:G:OP1	2.11	0.50
1:X:2542:U:O2	1:X:2544:A:H8	1.95	0.50
13:K:49:GLU:O	13:K:52:ILE:HG12	2.12	0.50
1:X:1142:G:H5''	9:G:111:LYS:HD2	1.93	0.50
1:X:2355:A:H61	14:L:91:ARG:CZ	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2543:A:H5'	1:X:2627:G:H4'	1.93	0.50
9:G:103:TYR:CG	9:G:111:LYS:HA	2.46	0.50
1:X:1699:A:H61	1:X:1723:U:H3	1.58	0.50
3:A:79:VAL:HG21	3:A:111:LEU:HD22	1.94	0.50
13:K:10:LEU:CD2	13:K:17:ARG:HB2	2.42	0.50
17:O:88:GLN:HE21	17:O:88:GLN:HA	1.76	0.50
1:X:1467:U:C2'	1:X:1468:A:OP1	2.58	0.50
1:X:1827:G:H1'	1:X:1914:U:C2	2.47	0.50
2:Y:62:C:H2'	2:Y:63:A:H8	1.76	0.50
4:B:116:VAL:HG13	4:B:136:ARG:HH21	1.75	0.50
5:C:96:PRO:HB2	5:C:99:VAL:HG23	1.93	0.50
5:C:151:VAL:HG11	5:C:175:VAL:HG22	1.93	0.50
10:H:75:VAL:HG12	10:H:118:LEU:HD11	1.94	0.50
1:X:2006:G:H5'	1:X:2596:C:H4'	1.93	0.50
4:B:147:PRO:C	4:B:149:ARG:N	2.65	0.50
9:G:154:GLU:O	9:G:157:PRO:HD2	2.11	0.50
1:X:1006:C:O2	16:N:61:TRP:HZ2	1.95	0.50
1:X:1032:A:C8	1:X:1033:G:H5''	2.47	0.50
9:G:103:TYR:CZ	9:G:111:LYS:HB2	2.46	0.50
9:G:104:THR:OG1	9:G:105:GLY:N	2.44	0.50
1:X:347:C:H4'	20:R:15:HIS:CD2	2.48	0.49
11:I:108:LEU:HD13	11:I:120:VAL:HG11	1.94	0.49
1:X:2423:G:P	5:C:62:LYS:HD2	2.52	0.49
11:I:77:LEU:HB2	11:I:111:SER:H	1.77	0.49
1:X:341:A:H2	1:X:1223:G:H2'	1.77	0.49
1:X:1033:G:H5'	9:G:93:LYS:NZ	2.26	0.49
1:X:1805:G:H1'	3:A:50:THR:CG2	2.43	0.49
6:D:33:LYS:HB3	6:D:92:ARG:HG2	1.94	0.49
12:J:15:ARG:HB3	12:J:73:LYS:HZ2	1.78	0.49
18:P:103:LEU:HB2	18:P:119:LYS:HB2	1.95	0.49
1:X:494:A:C8	20:R:56:LYS:HD2	2.48	0.49
1:X:1443:G:H2'	1:X:1444:C:C6	2.47	0.49
1:X:2657:G:H2'	1:X:2658:A:O4'	2.13	0.49
18:P:49:SER:O	18:P:51:GLN:N	2.45	0.49
1:X:1219:C:H5''	11:I:7:LYS:HE2	1.93	0.49
1:X:2490:U:H2'	1:X:2491:C:O4'	2.13	0.49
5:C:22:VAL:HG13	5:C:106:MET:HG2	1.93	0.49
9:G:106:TYR:O	9:G:110:LEU:HD12	2.12	0.49
11:I:47:ALA:O	11:I:49:PHE:N	2.41	0.49
16:N:17:VAL:HG11	16:N:36:PHE:HB2	1.94	0.49
17:O:38:LEU:HD23	17:O:47:PHE:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:16:ARG:HD3	26:Z:20:ARG:NH1	2.28	0.49
1:X:418:C:H4'	1:X:418:C:OP2	2.13	0.49
1:X:746:G:N7	1:X:774:A:C5	2.81	0.49
1:X:2178:U:H2'	1:X:2179:C:C6	2.48	0.49
11:I:62:LYS:HZ3	11:I:64:GLY:CA	2.21	0.49
13:K:3:HIS:CG	13:K:5:LYS:NZ	2.80	0.49
16:N:75:ASN:ND2	16:N:78:THR:H	2.10	0.49
1:X:1674:C:H2'	1:X:1675:C:H6	1.78	0.49
3:A:150:GLY:O	3:A:152:GLY:N	2.46	0.49
3:A:161:THR:O	3:A:196:VAL:HG23	2.13	0.49
10:H:83:ARG:NE	10:H:89:ILE:HD11	2.28	0.49
13:K:10:LEU:HD23	13:K:17:ARG:HB2	1.95	0.49
18:P:38:VAL:HG12	18:P:97:VAL:HG21	1.95	0.49
19:Q:71:GLN:HG2	19:Q:72:ARG:N	2.27	0.49
1:X:827:C:H2'	1:X:828:C:C6	2.48	0.48
1:X:969:U:C4	12:J:17:ARG:HB2	2.48	0.48
4:B:2:LYS:HB2	4:B:200:SER:HB3	1.95	0.48
5:C:45:THR:HG21	5:C:85:GLY:HA3	1.94	0.48
1:X:2212:U:H2'	1:X:2213:G:C8	2.48	0.48
14:L:27:LEU:HD23	14:L:44:ASP:HA	1.95	0.48
1:X:224:G:H4'	1:X:399:G:C5	2.48	0.48
14:L:8:ARG:HG3	14:L:9:ARG:H	1.77	0.48
14:L:68:ALA:HB1	14:L:102:ALA:HB3	1.95	0.48
16:N:49:ASP:HA	16:N:52:ASN:HB2	1.95	0.48
24:V:25:LEU:HD21	24:V:47:ARG:HG2	1.95	0.48
1:X:609:U:H5'	11:I:18:ARG:HD3	1.94	0.48
1:X:1329:U:H2'	1:X:1330:G:C8	2.48	0.48
21:S:132:GLN:HE21	21:S:132:GLN:H	1.61	0.48
1:X:791:G:H5'	3:A:48:ARG:HH21	1.77	0.48
10:H:110:VAL:HG23	10:H:129:LEU:HD12	1.94	0.48
15:M:5:ILE:HB	15:M:7:ILE:HG12	1.95	0.48
1:X:517:A:H5''	1:X:518:A:H5'	1.96	0.48
1:X:1833:U:H2'	1:X:1834:G:C8	2.48	0.48
1:X:2362:G:H2'	1:X:2363:G:H8	1.77	0.48
6:D:123:ASP:HB3	6:D:127:ASN:HB2	1.96	0.48
7:E:9:ILE:HD11	7:E:69:ARG:HG2	1.95	0.48
14:L:30:SER:O	14:L:40:ALA:HA	2.13	0.48
14:L:30:SER:HB2	14:L:43:ILE:HD11	1.96	0.48
1:X:2209:G:H4'	23:U:46:LEU:HB2	1.96	0.48
9:G:70:PHE:HB2	16:N:64:ARG:HG2	1.94	0.48
9:G:96:ASP:O	9:G:98:LYS:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:13:ARG:H	11:I:13:ARG:HE	1.62	0.48
14:L:8:ARG:HG3	14:L:9:ARG:N	2.29	0.48
1:X:879:A:H2'	1:X:879:A:N3	2.29	0.48
1:X:1922:U:OP1	1:X:2583:U:O2'	2.29	0.48
20:R:95:ARG:HH12	20:R:107:ALA:H	1.61	0.48
1:X:2307:A:H2'	1:X:2308:A:C8	2.49	0.48
1:X:572:G:N3	16:N:37:GLN:NE2	2.60	0.48
1:X:1753:A:O5'	1:X:1753:A:C8	2.63	0.48
1:X:1777:A:H1'	1:X:1921:A:N6	2.29	0.48
1:X:2522:G:H2'	1:X:2523:G:C8	2.49	0.48
21:S:91:PRO:HG2	21:S:125:PRO:HD2	1.96	0.48
1:X:1169:C:H4'	25:W:28:ILE:O	2.14	0.47
1:X:1468:A:O5'	1:X:1468:A:H8	1.97	0.47
1:X:2774:U:O2'	1:X:2775:U:H5''	2.14	0.47
13:K:3:HIS:HB3	13:K:5:LYS:HE2	1.96	0.47
20:R:25:LEU:HD12	20:R:81:VAL:HB	1.96	0.47
1:X:88:G:OP2	1:X:89:A:H3'	2.14	0.47
14:L:12:ARG:HA	14:L:92:GLY:O	2.14	0.47
21:S:117:VAL:HB	21:S:168:VAL:HG13	1.97	0.47
1:X:1257:U:H5''	11:I:17:LYS:HG3	1.95	0.47
1:X:1582:A:OP1	3:A:211:ARG:NE	2.43	0.47
1:X:1685:A:N6	1:X:1693:A:H61	2.12	0.47
1:X:2516:U:H2'	1:X:2517:C:C6	2.49	0.47
21:S:3:LEU:HD13	21:S:4:THR:H	1.78	0.47
1:X:1998:A:N3	26:Z:6:VAL:HG23	2.29	0.47
1:X:2779:C:H2'	1:X:2780:A:H8	1.79	0.47
23:U:43:ARG:HG2	23:U:44:ALA:N	2.30	0.47
3:A:43:ARG:HH21	3:A:54:ILE:HG13	1.80	0.47
5:C:186:LEU:HG	5:C:188:ILE:HG12	1.95	0.47
9:G:132:PHE:HB2	9:G:145:HIS:CE1	2.49	0.47
17:O:11:GLN:NE2	17:O:38:LEU:HB3	2.30	0.47
1:X:503:G:H2'	1:X:504:G:O4'	2.15	0.47
1:X:681:A:H5''	1:X:681:A:H8	1.79	0.47
5:C:3:GLN:O	5:C:12:GLY:HA3	2.15	0.47
11:I:78:SER:HB3	11:I:112:GLY:HA3	1.96	0.47
1:X:1173:G:H1'	17:O:21:ARG:HD2	1.97	0.47
1:X:2860:C:H2'	1:X:2861:A:O4'	2.14	0.47
2:Y:64:C:H2'	2:Y:65:A:H8	1.79	0.47
3:A:244:ARG:HB3	3:A:252:LYS:HZ2	1.80	0.47
20:R:105:ARG:HH22	20:R:112:LYS:CA	2.28	0.47
1:X:922:A:H2'	1:X:923:A:C8	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1662:G:H5''	1:X:1663:C:H5'	1.96	0.47
1:X:1787:U:H2'	1:X:1788:C:C6	2.50	0.47
1:X:1854:G:H1	1:X:1863:U:H3	1.62	0.47
1:X:2498:U:H4'	1:X:2499:C:OP1	2.14	0.47
13:K:11:ASN:ND2	13:K:12:ARG:HE	2.12	0.47
26:Z:16:ARG:O	26:Z:20:ARG:HD2	2.14	0.47
1:X:203:G:H5'	1:X:234:C:H4'	1.97	0.47
1:X:241:C:H2'	1:X:242:A:H5''	1.96	0.47
1:X:1287:A:C2'	1:X:1288:A:H5''	2.45	0.47
1:X:1342:U:H5''	1:X:1343:C:H5	1.80	0.47
1:X:2343:C:H2'	1:X:2344:G:O4'	2.15	0.47
5:C:112:GLN:HA	5:C:116:LYS:HD3	1.96	0.47
17:O:57:GLN:H	17:O:97:GLY:HA2	1.79	0.47
20:R:22:VAL:HG13	20:R:81:VAL:O	2.14	0.47
22:T:14:ARG:HG3	22:T:15:ASP:H	1.80	0.47
30:4:2:LYS:HA	30:4:2:LYS:HE2	1.97	0.47
9:G:75:ILE:H	9:G:75:ILE:HG13	1.58	0.47
1:X:341:A:C2	1:X:1223:G:H2'	2.50	0.46
1:X:1367:A:H2'	1:X:1368:G:O4'	2.16	0.46
1:X:1509:A:H8	1:X:1510:A:C8	2.33	0.46
1:X:1788:C:H2'	1:X:1789:U:H6	1.81	0.46
4:B:195:LEU:H	15:M:2:GLN:HG2	1.79	0.46
7:E:17:VAL:HG13	7:E:26:VAL:HG22	1.97	0.46
8:F:77:LEU:HD13	8:F:107:ILE:HG23	1.96	0.46
3:A:67:PHE:HD2	3:A:153:ALA:HB3	1.79	0.46
5:C:158:ARG:HA	5:C:169:VAL:HG21	1.96	0.46
12:J:69:ILE:HG23	12:J:104:MET:HA	1.97	0.46
23:U:47:HIS:HD2	23:U:48:LYS:O	1.97	0.46
1:X:341:A:HO2'	1:X:342:G:H8	1.63	0.46
4:B:120:TRP:O	4:B:121:ASN:HB2	2.14	0.46
20:R:15:HIS:O	20:R:16:PHE:HB3	2.15	0.46
1:X:651:C:H2'	1:X:652:C:H5''	1.98	0.46
1:X:1278:A:H61	1:X:1996:A:H5''	1.80	0.46
1:X:2661:G:O6	1:X:2708:U:H1'	2.16	0.46
3:A:243:GLY:C	3:A:244:ARG:HD3	2.36	0.46
14:L:10:LYS:O	14:L:14:ARG:HB2	2.16	0.46
1:X:240:U:H2'	1:X:241:C:O4'	2.15	0.46
1:X:956:A:C4	1:X:2427:A:C2	3.03	0.46
3:A:43:ARG:N	3:A:43:ARG:HD2	2.31	0.46
4:B:131:SER:O	4:B:132:LYS:CB	2.64	0.46
4:B:133:LYS:HB3	4:B:133:LYS:HE2	1.61	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:176:ASN:HB3	5:C:179:ASP:HB2	1.96	0.46
7:E:124:ALA:HB3	7:E:132:ASP:HB2	1.97	0.46
9:G:108:GLY:H	9:G:110:LEU:HG	1.79	0.46
26:Z:33:CYS:SG	26:Z:46:CYS:SG	3.11	0.46
30:4:19:ARG:HB2	30:4:24:LEU:HD13	1.98	0.46
1:X:590:C:H2'	1:X:591:G:C8	2.51	0.46
3:A:252:LYS:HE3	3:A:252:LYS:H	1.80	0.46
5:C:5:ASN:HB2	5:C:10:ASN:HA	1.98	0.46
9:G:36:ASN:O	9:G:38:GLU:N	2.34	0.46
15:M:27:PHE:HB3	15:M:93:ILE:CD1	2.45	0.46
21:S:87:THR:O	21:S:88:TYR:HB3	2.16	0.46
1:X:1845:A:N1	1:X:2070:G:H1'	2.30	0.46
1:X:2266:A:N6	1:X:2323:U:H3	2.13	0.46
9:G:90:LEU:HD23	9:G:94:LYS:HA	1.98	0.46
14:L:66:ASP:C	14:L:68:ALA:H	2.19	0.46
16:N:74:MET:HB3	16:N:75:ASN:H	1.63	0.46
1:X:627:A:H2'	1:X:628:A:C8	2.50	0.46
1:X:1882:G:H21	1:X:1885:C:H41	1.62	0.46
3:A:67:PHE:HB3	3:A:153:ALA:H	1.81	0.46
9:G:162:LYS:N	9:G:163:PRO:HD2	2.31	0.46
10:H:24:VAL:HA	10:H:51:ILE:HG22	1.98	0.46
10:H:27:SER:HB2	10:H:121:ARG:HH22	1.81	0.46
12:J:73:LYS:HB3	12:J:95:VAL:HG12	1.97	0.46
20:R:25:LEU:H	20:R:80:LYS:HA	1.81	0.46
23:U:10:LYS:HD3	23:U:60:VAL:HG21	1.97	0.46
1:X:331:U:H1'	5:C:162:ARG:NH1	2.31	0.46
1:X:1630:A:C2	18:P:114:ALA:HB2	2.51	0.46
1:X:2167:A:H2'	1:X:2168:A:H8	1.80	0.46
11:I:57:ILE:HD13	11:I:57:ILE:HA	1.93	0.46
4:B:181:LEU:HD11	15:M:12:LEU:HD23	1.98	0.46
11:I:30:ALA:HB3	11:I:34:HIS:HE1	1.78	0.46
21:S:127:PRO:C	21:S:129:ARG:H	2.19	0.46
30:4:19:ARG:HD2	30:4:24:LEU:HD22	1.98	0.46
1:X:2795:A:H4'	13:K:5:LYS:HG2	1.97	0.45
5:C:45:THR:HB	5:C:86:PRO:O	2.15	0.45
5:C:119:ALA:H	5:C:189:ASP:HA	1.81	0.45
9:G:57:LEU:HD22	9:G:170:PRO:HA	1.98	0.45
12:J:14:PHE:CE1	12:J:90:ALA:HA	2.46	0.45
1:X:2324:G:N3	1:X:2360:C:H2'	2.32	0.45
1:X:2754:C:H2'	1:X:2755:A:O4'	2.17	0.45
3:A:95:LEU:HD12	3:A:105:ILE:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:108:PRO:HB3	3:A:143:HIS:HE1	1.81	0.45
10:H:26:ASN:HD22	10:H:26:ASN:HA	1.41	0.45
1:X:1142:G:OP1	9:G:107:GLN:HB3	2.16	0.45
1:X:1466:C:H2'	1:X:1467:U:C1'	2.46	0.45
1:X:1817:U:O4'	3:A:252:LYS:HD3	2.16	0.45
1:X:2477:C:H6	1:X:2477:C:H5'	1.81	0.45
2:Y:54:U:H4'	2:Y:54:U:OP1	2.17	0.45
5:C:164:VAL:HB	5:C:165:SER:H	1.57	0.45
9:G:67:ARG:CB	9:G:70:PHE:HA	2.47	0.45
9:G:157:PRO:C	9:G:159:SER:H	2.20	0.45
12:J:28:VAL:HG21	12:J:135:ARG:HA	1.98	0.45
18:P:94:GLU:HG3	18:P:127:ILE:HB	1.99	0.45
1:X:29:U:O5'	1:X:29:U:H6	2.00	0.45
1:X:1468:A:O5'	1:X:1468:A:C8	2.70	0.45
1:X:2397:A:H2'	1:X:2398:U:O4'	2.17	0.45
1:X:2772:U:H2'	1:X:2773:G:C8	2.52	0.45
4:B:14:ILE:HG13	15:M:20:HIS:CE1	2.52	0.45
5:C:102:LEU:O	5:C:106:MET:HB2	2.17	0.45
6:D:40:LEU:HD21	6:D:87:ILE:HD12	1.98	0.45
11:I:108:LEU:HB2	11:I:122:VAL:HG11	1.98	0.45
19:Q:11:VAL:HB	19:Q:26:SER:HB2	1.99	0.45
1:X:227:G:H2'	1:X:228:A:C8	2.52	0.45
1:X:336:A:H2'	1:X:337:G:C8	2.52	0.45
1:X:1467:U:C6	1:X:1467:U:C5'	3.00	0.45
1:X:2074:U:H1'	23:U:48:LYS:HE3	1.97	0.45
20:R:48:VAL:HG12	20:R:50:GLY:H	1.80	0.45
1:X:1187:A:H2'	1:X:1188:A:C8	2.52	0.45
1:X:1268:U:C2	5:C:66:ASN:HA	2.52	0.45
9:G:132:PHE:CE2	9:G:145:HIS:HB2	2.51	0.45
1:X:1218:C:O4'	11:I:13:ARG:HD3	2.16	0.45
1:X:1467:U:H5	1:X:1468:A:O4'	2.00	0.45
5:C:43:ALA:HB1	5:C:86:PRO:CB	2.41	0.45
6:D:136:LEU:HD11	6:D:143:TYR:HB2	1.99	0.45
8:F:93:LYS:HA	21:S:109:GLN:HG3	1.98	0.45
10:H:2:ILE:HB	10:H:45:ALA:HB3	1.99	0.45
13:K:17:ARG:NH1	13:K:20:LEU:CD2	2.77	0.45
17:O:69:ILE:HG22	17:O:86:HIS:HB3	1.98	0.45
1:X:231:G:H4'	1:X:397:U:H5''	1.98	0.45
1:X:1373:G:H1	1:X:2192:U:H3	1.64	0.45
1:X:2797:G:OP2	13:K:3:HIS:CD2	2.69	0.45
3:A:250:TRP:HB3	3:A:251:GLY:H	1.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:146:THR:OG1	4:B:147:PRO:HD3	2.17	0.45
5:C:45:THR:HG22	5:C:47:THR:OG1	2.17	0.45
23:U:29:GLY:C	23:U:31:GLY:H	2.16	0.45
1:X:1467:U:C5	1:X:1468:A:O4'	2.70	0.45
1:X:1919:A:C2	1:X:1926:U:N3	2.62	0.45
1:X:1022:A:H5''	16:N:77:SER:HB2	2.00	0.44
1:X:1234:C:H2'	1:X:1235:C:H6	1.82	0.44
1:X:1437:A:H2'	1:X:1438:G:H8	1.82	0.44
25:W:3:ILE:HD12	25:W:51:LEU:HD13	1.99	0.44
5:C:146:GLU:HG3	5:C:185:ARG:NH1	2.32	0.44
8:F:79:ARG:HG2	8:F:84:ILE:HB	1.99	0.44
1:X:424:G:H4'	1:X:425:A:O5'	2.18	0.44
1:X:800:U:H5''	1:X:801:A:H5'	1.99	0.44
1:X:814:G:OP1	5:C:50:GLN:HB2	2.18	0.44
1:X:1675:C:OP1	4:B:134:TRP:CD1	2.69	0.44
3:A:147:LEU:HD22	3:A:183:ARG:HH22	1.81	0.44
10:H:116:ARG:HG3	15:M:38:LYS:CE	2.47	0.44
19:Q:29:VAL:HG21	19:Q:38:ILE:HG13	1.98	0.44
23:U:22:GLY:N	23:U:39:LYS:HB2	2.32	0.44
9:G:132:PHE:CE1	9:G:145:HIS:HB2	2.52	0.44
15:M:28:ARG:O	15:M:96:ARG:NH2	2.50	0.44
20:R:45:LYS:HA	20:R:76:LEU:O	2.16	0.44
1:X:2545:A:N6	10:H:40:GLY:HA3	2.31	0.44
7:E:103:LEU:HD11	7:E:131:ILE:HG12	1.99	0.44
12:J:61:ARG:HG2	21:S:175:ARG:HG3	2.00	0.44
13:K:3:HIS:CE1	13:K:5:LYS:HZ3	2.34	0.44
1:X:341:A:O2'	1:X:342:G:H8	2.01	0.44
1:X:553:C:H4'	1:X:554:U:OP1	2.17	0.44
1:X:1190:C:H2'	1:X:1191:G:H8	1.82	0.44
3:A:248:THR:HB	3:A:249:PRO:HD2	2.00	0.44
5:C:74:VAL:HG23	5:C:76:THR:H	1.83	0.44
12:J:11:ARG:HH12	12:J:72:ASP:HB2	1.83	0.44
12:J:92:GLU:HG3	12:J:93:TYR:CD2	2.51	0.44
13:K:46:PRO:O	13:K:50:GLN:HG3	2.18	0.44
1:X:689:A:H8	1:X:2052:G:N2	2.06	0.44
1:X:1030:U:O2'	1:X:1032:A:H2	1.99	0.44
1:X:585:U:H2'	1:X:586:G:C8	2.52	0.44
1:X:673:G:H5'	5:C:93:TYR:CE1	2.52	0.44
1:X:712:A:H2'	1:X:713:G:O4'	2.18	0.44
1:X:1012:A:H2'	1:X:1013:G:O4'	2.17	0.44
1:X:1255:A:H2'	1:X:1256:C:C6	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:23:GLU:HB2	17:O:91:THR:HG21	1.99	0.44
17:O:72:ARG:HD2	17:O:83:ARG:HH11	1.82	0.44
19:Q:60:GLY:H	19:Q:72:ARG:HH11	1.66	0.44
28:2:26:SER:CA	28:2:27:GLY:CA	2.95	0.44
1:X:649:G:H22	1:X:660:G:N2	2.16	0.44
1:X:1273:G:H2'	1:X:1274:C:O4'	2.18	0.44
1:X:1405:A:N6	19:Q:14:GLU:HG2	2.32	0.44
1:X:2339:A:H4'	11:I:56:LEU:HD21	2.00	0.44
11:I:45:LYS:HD3	11:I:45:LYS:H	1.82	0.44
1:X:1421:U:H2'	1:X:1422:C:O4'	2.18	0.43
1:X:1547:U:H2'	1:X:1548:U:C6	2.53	0.43
1:X:1674:C:H2'	1:X:1675:C:C6	2.53	0.43
1:X:1979:C:H4'	1:X:1980:A:OP1	2.18	0.43
15:M:41:GLU:HG3	15:M:46:ARG:HD2	2.00	0.43
16:N:17:VAL:HG13	16:N:39:LEU:HD12	1.98	0.43
19:Q:62:ARG:O	19:Q:70:GLY:HA3	2.18	0.43
24:V:21:ARG:HG3	24:V:46:LEU:HD22	2.00	0.43
1:X:38:G:H21	5:C:42:THR:HG21	1.83	0.43
1:X:116:A:C8	1:X:117:A:C8	3.06	0.43
1:X:875:G:O2'	2:Y:80:A:N3	2.44	0.43
2:Y:39:C:H2'	14:L:97:HIS:HE1	1.83	0.43
3:A:97:TYR:HE2	3:A:103:ARG:HB2	1.83	0.43
15:M:33:VAL:HG22	15:M:51:GLU:HB2	2.00	0.43
23:U:25:ARG:O	23:U:32:ARG:HD2	2.18	0.43
1:X:748:A:H5''	1:X:749:C:H5	1.84	0.43
1:X:748:A:H5'	1:X:749:C:OP2	2.19	0.43
1:X:1307:U:H5''	1:X:1307:U:H6	1.83	0.43
1:X:2485:U:O2	1:X:2485:U:H2'	2.17	0.43
5:C:6:VAL:HG12	5:C:7:ILE:HG12	1.99	0.43
6:D:35:VAL:HG22	6:D:90:THR:HG23	1.99	0.43
22:T:25:LYS:HB2	22:T:37:LEU:HB3	2.00	0.43
1:X:2310:G:H4'	22:T:43:THR:H	1.83	0.43
18:P:39:ARG:HG3	18:P:97:VAL:HB	2.00	0.43
23:U:64:ALA:C	23:U:66:ALA:H	2.21	0.43
3:A:188:GLU:H	3:A:188:GLU:HG2	1.54	0.43
5:C:118:VAL:HG22	5:C:188:ILE:HD12	2.00	0.43
9:G:103:TYR:O	9:G:107:GLN:NE2	2.51	0.43
1:X:336:A:H2'	1:X:337:G:H8	1.83	0.43
1:X:1765:C:H6	1:X:1765:C:O5'	2.01	0.43
6:D:60:ILE:HB	6:D:99:PHE:HE1	1.83	0.43
1:X:577:U:O5'	1:X:956:A:N6	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1574:A:O2'	1:X:1575:C:H3'	2.18	0.43
1:X:2186:G:H2'	1:X:2187:A:C8	2.54	0.43
1:X:2556:A:H5''	1:X:2557:G:H5'	2.00	0.43
11:I:28:LYS:NZ	11:I:36:GLY:CA	2.81	0.43
19:Q:35:LYS:HA	19:Q:38:ILE:HG22	2.00	0.43
1:X:517:A:C5'	1:X:518:A:H5'	2.48	0.43
1:X:1859:A:H2'	1:X:1860:A:C8	2.54	0.43
1:X:2270:U:H2'	1:X:2271:C:C6	2.53	0.43
2:Y:30:C:H2'	2:Y:31:A:H8	1.84	0.43
4:B:77:ILE:HD13	15:M:3:THR:HG22	2.00	0.43
6:D:65:PRO:HA	6:D:89:VAL:HG13	2.01	0.43
19:Q:28:TRP:CZ3	19:Q:77:LYS:HB2	2.53	0.43
28:2:40:HIS:CA	28:2:41:GLN:CA	2.97	0.43
1:X:890:U:H2'	1:X:891:A:H3'	2.00	0.43
1:X:1329:U:H2'	1:X:1330:G:H8	1.84	0.43
4:B:105:THR:HB	4:B:166:THR:HA	2.01	0.43
10:H:116:ARG:HG3	15:M:38:LYS:HE2	2.01	0.43
20:R:9:HIS:CD2	20:R:9:HIS:H	2.37	0.43
21:S:51:LEU:HD13	21:S:86:VAL:HG21	2.00	0.43
1:X:460:U:O4	1:X:592:G:H1'	2.18	0.43
1:X:651:C:C2'	1:X:652:C:H5''	2.49	0.43
3:A:108:PRO:HD2	3:A:111:LEU:HB2	2.01	0.43
10:H:113:PRO:HB3	10:H:132:GLU:HB3	2.01	0.43
11:I:102:LYS:O	11:I:104:ARG:N	2.52	0.43
23:U:51:ILE:HG12	23:U:59:THR:HB	2.00	0.43
1:X:590:C:H2'	1:X:591:G:H8	1.84	0.42
1:X:614:G:C8	11:I:98:LEU:HD21	2.53	0.42
1:X:719:A:H2'	1:X:720:A:O4'	2.18	0.42
2:Y:46:G:H4'	6:D:92:ARG:HH12	1.84	0.42
5:C:170:LEU:HA	5:C:171:PRO:HD3	1.84	0.42
1:X:748:A:H3'	1:X:749:C:C6	2.53	0.42
1:X:1583:A:H3'	3:A:86:PRO:HG3	2.01	0.42
6:D:73:SER:O	6:D:79:LEU:HB3	2.19	0.42
9:G:102:ARG:O	9:G:102:ARG:HG2	2.19	0.42
23:U:78:ILE:HG12	23:U:79:GLU:H	1.85	0.42
1:X:216:U:H2'	1:X:217:U:C6	2.55	0.42
1:X:333:A:O4'	1:X:351:A:H1'	2.19	0.42
1:X:533:C:H1'	1:X:563:U:O2'	2.19	0.42
1:X:873:U:H1'	1:X:2247:A:H5''	2.00	0.42
1:X:1193:G:H2'	1:X:1194:U:C6	2.54	0.42
11:I:83:LEU:HD23	11:I:84:GLU:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:26:ASP:HB3	12:J:27:TYR:H	1.61	0.42
12:J:78:LYS:HA	12:J:88:LYS:HZ3	1.84	0.42
17:O:36:LYS:NZ	17:O:54:TYR:HB3	2.35	0.42
1:X:103:U:H2'	1:X:104:C:H6	1.82	0.42
1:X:394:U:H2'	1:X:395:G:C8	2.54	0.42
1:X:771:C:O2	1:X:1964:A:H2	2.03	0.42
1:X:1336:G:OP1	18:P:105:ARG:HD2	2.20	0.42
1:X:1483:G:N2	1:X:1541:G:H1'	2.35	0.42
1:X:1779:C:OP1	3:A:222:ARG:NH1	2.52	0.42
1:X:1790:G:H5'	1:X:1811:A:N6	2.34	0.42
1:X:1974:U:H2'	1:X:1975:G:H5''	2.00	0.42
2:Y:78:A:H2'	2:Y:79:U:O4'	2.18	0.42
3:A:231:HIS:HD2	3:A:233:HIS:N	2.11	0.42
19:Q:66:GLY:O	19:Q:68:PHE:N	2.52	0.42
19:Q:68:PHE:C	19:Q:70:GLY:H	2.21	0.42
1:X:409:G:H1'	23:U:45:ASN:HD22	1.83	0.42
1:X:1339:U:H5''	1:X:1994:U:H1'	2.01	0.42
1:X:1493:A:H2'	1:X:1494:G:O4'	2.19	0.42
1:X:2015:G:O2'	4:B:145:LYS:HE2	2.20	0.42
9:G:107:GLN:C	9:G:109:GLY:N	2.72	0.42
10:H:77:THR:HA	10:H:94:ASN:HB3	2.00	0.42
22:T:23:VAL:HA	22:T:38:VAL:HG23	2.01	0.42
1:X:1384:G:N2	1:X:1385:C:H41	2.17	0.42
1:X:1687:C:O5'	1:X:1687:C:H6	2.01	0.42
1:X:2784:A:C6	1:X:2866:A:C8	3.07	0.42
3:A:182:LEU:HB2	3:A:268:ARG:O	2.19	0.42
1:X:954:U:P	11:I:38:LYS:HG2	2.59	0.42
9:G:98:LYS:HB3	9:G:116:ARG:HB2	2.01	0.42
9:G:107:GLN:C	9:G:109:GLY:H	2.23	0.42
15:M:33:VAL:HA	15:M:51:GLU:HB2	2.01	0.42
18:P:89:ARG:CZ	18:P:132:GLY:H	2.32	0.42
19:Q:53:ILE:HD13	19:Q:80:VAL:HG13	2.01	0.42
1:X:520:C:O2	1:X:520:C:H2'	2.18	0.42
1:X:542:A:H2	1:X:2004:U:O2'	2.01	0.42
1:X:852:U:H2'	1:X:853:C:C6	2.55	0.42
1:X:1563:U:H2'	1:X:1564:U:C6	2.54	0.42
1:X:1736:C:H2'	1:X:1737:G:H8	1.84	0.42
1:X:2238:G:O4'	1:X:2406:C:H2'	2.20	0.42
3:A:96:HIS:CE1	3:A:100:GLY:HA2	2.47	0.42
10:H:85:ASP:OD2	10:H:87:SER:HB3	2.20	0.42
16:N:88:ILE:CG1	17:O:49:GLU:HB2	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:S:3:LEU:HB3	21:S:56:VAL:HA	2.02	0.42
21:S:23:ALA:HA	21:S:83:PHE:O	2.19	0.42
1:X:56:C:H2'	1:X:57:G:O4'	2.19	0.42
1:X:347:C:H2'	1:X:348:U:C6	2.54	0.42
1:X:616:U:H5'	1:X:617:U:OP2	2.20	0.42
1:X:689:A:H2	1:X:815:A:H61	1.64	0.42
1:X:693:A:H2'	1:X:694:G:C8	2.54	0.42
1:X:830:C:O2'	1:X:852:U:H5''	2.19	0.42
1:X:1441:A:H4'	1:X:1442:C:O5'	2.20	0.42
1:X:2237:C:O2'	1:X:2406:C:OP2	2.37	0.42
12:J:48:ILE:HD12	12:J:71:PRO:HG3	2.01	0.42
23:U:52:ARG:HD3	23:U:62:LEU:HD22	2.01	0.42
1:X:101:A:H5''	1:X:102:C:H5	1.85	0.42
1:X:487:G:H4'	1:X:512:A:N1	2.34	0.42
1:X:1033:G:N2	1:X:1153:A:H2	2.10	0.42
1:X:1128:G:H3'	1:X:1129:A:H5''	2.01	0.42
3:A:43:ARG:N	3:A:43:ARG:CD	2.83	0.42
4:B:177:ALA:C	4:B:179:GLU:H	2.24	0.42
9:G:33:ILE:O	9:G:69:ASP:OD1	2.38	0.42
12:J:82:THR:HB	12:J:83:ARG:H	1.76	0.42
12:J:88:LYS:HB3	12:J:89:GLY:H	1.59	0.42
19:Q:35:LYS:O	19:Q:38:ILE:HG22	2.20	0.42
1:X:339:U:O4	1:X:343:A:C8	2.73	0.41
1:X:649:G:N2	1:X:660:G:N2	2.68	0.41
1:X:1219:C:H2'	1:X:1220:G:O4'	2.20	0.41
1:X:1644:G:H2'	1:X:1645:U:H6	1.85	0.41
1:X:2445:C:H5''	30:4:6:SER:HB3	2.01	0.41
1:X:2621:G:OP1	9:G:110:LEU:HD22	2.20	0.41
4:B:85:ALA:H	4:B:86:PRO:HD2	1.85	0.41
9:G:106:TYR:O	9:G:108:GLY:N	2.48	0.41
10:H:25:LEU:HD11	10:H:52:VAL:HG23	2.01	0.41
1:X:534:U:H4'	1:X:564:U:H4'	2.01	0.41
1:X:679:C:H2'	1:X:680:U:C6	2.55	0.41
3:A:88:ARG:O	3:A:89:SER:CB	2.68	0.41
4:B:5:LEU:HG	4:B:195:LEU:HD11	2.02	0.41
5:C:33:TRP:CD1	5:C:95:LEU:HB2	2.55	0.41
6:D:40:LEU:HB2	6:D:41:GLY:H	1.70	0.41
20:R:10:HIS:O	20:R:11:ASN:CB	2.68	0.41
1:X:1276:U:H1'	26:Z:10:LYS:HG3	2.03	0.41
1:X:2226:A:H2'	1:X:2227:C:C6	2.55	0.41
1:X:2851:G:H4'	15:M:8:ASN:ND2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:34:ILE:HG12	6:D:96:MET:HG3	2.02	0.41
21:S:25:ASN:O	21:S:26:LYS:HB3	2.20	0.41
29:3:31:HIS:CA	29:3:32:GLN:CA	2.98	0.41
1:X:85:C:H5''	20:R:42:ARG:HH21	1.85	0.41
1:X:1117:G:H2'	1:X:1118:G:H8	1.85	0.41
1:X:1437:A:H2'	1:X:1438:G:C8	2.55	0.41
1:X:1542:G:N2	1:X:1562:G:H1	1.99	0.41
1:X:2796:A:H2'	1:X:2797:G:C8	2.55	0.41
3:A:67:PHE:CD2	3:A:153:ALA:HB3	2.56	0.41
15:M:55:ILE:O	15:M:103:LYS:O	2.38	0.41
17:O:56:VAL:HG12	17:O:97:GLY:HA3	2.02	0.41
25:W:45:LYS:O	25:W:48:LYS:HB2	2.19	0.41
1:X:71:A:C5	24:V:54:ASN:HB3	2.55	0.41
1:X:922:A:N1	1:X:2256:G:H1'	2.34	0.41
1:X:1658:A:H2'	1:X:1659:G:O4'	2.21	0.41
1:X:1672:A:H3'	1:X:1673:C:C6	2.55	0.41
1:X:2266:A:C2	1:X:2325:A:N6	2.81	0.41
1:X:2736:U:H1'	1:X:2737:A:H5''	2.02	0.41
5:C:164:VAL:C	5:C:166:TRP:N	2.72	0.41
6:D:114:PHE:HZ	6:D:176:PRO:HG2	1.84	0.41
9:G:50:PRO:HG2	9:G:53:ARG:HG3	2.02	0.41
11:I:62:LYS:CE	11:I:64:GLY:HA2	2.45	0.41
12:J:42:TRP:CD1	12:J:97:VAL:HG12	2.56	0.41
14:L:26:ARG:HG2	14:L:86:GLN:HB3	2.02	0.41
16:N:93:LYS:CE	17:O:5:ILE:HD13	2.37	0.41
17:O:73:LYS:HB2	17:O:82:ARG:HB2	2.03	0.41
1:X:203:G:H1'	1:X:205:A:N6	2.32	0.41
1:X:572:G:H22	1:X:587:A:H2	1.68	0.41
1:X:2292:C:H5''	6:D:88:LYS:HD3	2.01	0.41
4:B:4:ILE:HD13	4:B:28:ALA:HB1	2.02	0.41
4:B:149:ARG:CZ	9:G:106:TYR:CD1	3.02	0.41
1:X:829:C:H2'	1:X:830:C:H6	1.86	0.41
1:X:2035:G:N2	4:B:148:GLY:O	2.48	0.41
3:A:169:GLU:HB3	3:A:170:SER:H	1.63	0.41
12:J:36:ILE:HD12	12:J:133:VAL:HG21	2.02	0.41
17:O:5:ILE:CD1	17:O:6:GLN:H	2.19	0.41
1:X:2508:G:H5''	1:X:2509:A:H5''	2.01	0.41
3:A:134:ARG:HG3	3:A:135:PHE:HD2	1.86	0.41
6:D:92:ARG:HB2	6:D:92:ARG:NH2	2.36	0.41
12:J:14:PHE:HE1	12:J:90:ALA:CA	2.28	0.41
20:R:84:VAL:HG23	20:R:88:THR:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:110:SER:OG	20:R:111:GLY:N	2.52	0.41
22:T:59:LEU:HD12	22:T:79:ILE:HD12	2.02	0.41
25:W:12:ARG:HG3	25:W:50:LEU:HD21	2.03	0.41
1:X:1378:A:H2'	1:X:1378:A:N3	2.36	0.41
1:X:2206:C:H1'	3:A:262:LYS:HE3	2.02	0.41
1:X:2552:C:H5''	1:X:2553:G:H5''	2.03	0.41
4:B:5:LEU:HD22	4:B:49:ILE:HG22	2.02	0.41
4:B:149:ARG:NH1	9:G:106:TYR:HB2	2.36	0.41
7:E:48:ASP:HB3	7:E:49:GLN:HE21	1.86	0.41
11:I:28:LYS:HZ2	11:I:36:GLY:HA2	1.86	0.41
18:P:25:PHE:CD2	18:P:25:PHE:C	2.94	0.41
19:Q:12:ILE:O	19:Q:16:ALA:HB3	2.20	0.41
20:R:7:GLY:HA3	20:R:42:ARG:O	2.20	0.41
21:S:13:LYS:HB2	21:S:18:MET:HB2	2.03	0.41
22:T:14:ARG:HG3	22:T:15:ASP:N	2.36	0.41
22:T:48:GLY:H	22:T:51:VAL:HB	1.86	0.41
23:U:22:GLY:H	23:U:39:LYS:HB2	1.85	0.41
1:X:986:A:O3'	16:N:48:ARG:NH1	2.54	0.41
1:X:1443:G:H2'	1:X:1444:C:H6	1.86	0.41
1:X:1582:A:OP1	3:A:211:ARG:NH2	2.48	0.41
1:X:1997:A:H2'	1:X:1998:A:C8	2.56	0.41
1:X:2407:G:H5''	1:X:2408:G:OP1	2.21	0.41
1:X:2869:U:H2'	1:X:2870:C:C6	2.56	0.41
4:B:67:PHE:CE1	4:B:75:THR:HG22	2.56	0.41
5:C:3:GLN:CG	5:C:116:LYS:HD2	2.51	0.41
5:C:146:GLU:HB3	5:C:184:ASP:HB2	2.03	0.41
10:H:27:SER:HA	10:H:50:ILE:HD12	2.02	0.41
1:X:654:A:H2'	1:X:654:A:N3	2.36	0.40
4:B:14:ILE:HG22	4:B:21:ILE:HB	2.04	0.40
26:Z:51:TYR:HA	26:Z:55:ARG:HA	2.03	0.40
1:X:88:G:H3'	1:X:89:A:H5''	2.04	0.40
1:X:1623:C:H4'	1:X:1624:A:O5'	2.21	0.40
1:X:2561:G:H5'	1:X:2561:G:H8	1.86	0.40
5:C:166:TRP:HB3	5:C:167:VAL:H	1.63	0.40
22:T:14:ARG:CG	22:T:15:ASP:H	2.34	0.40
23:U:14:VAL:O	23:U:15:VAL:HG22	2.21	0.40
1:X:10:A:H2'	1:X:11:G:C8	2.56	0.40
1:X:70:A:H5'	1:X:71:A:C3'	2.44	0.40
1:X:1337:G:OP2	18:P:105:ARG:NH1	2.54	0.40
2:Y:58:G:H4'	2:Y:59:A:H5''	2.04	0.40
2:Y:64:C:H2'	2:Y:65:A:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:162:LYS:N	9:G:163:PRO:CD	2.85	0.40
12:J:79:PRO:CD	12:J:88:LYS:HD2	2.50	0.40
19:Q:68:PHE:C	19:Q:70:GLY:N	2.75	0.40
19:Q:89:GLU:HB3	19:Q:90:ALA:H	1.51	0.40
20:R:108:VAL:HB	20:R:109:ALA:H	1.49	0.40
21:S:95:SER:HB3	21:S:119:ASN:HD22	1.86	0.40
23:U:21:ARG:HG2	23:U:40:ARG:HG2	2.04	0.40
1:X:463:C:N4	1:X:467:U:H5	2.08	0.40
1:X:923:A:C5	12:J:12:LYS:HE3	2.57	0.40
5:C:188:ILE:H	5:C:188:ILE:HG13	1.42	0.40
1:X:682:G:N3	1:X:682:G:C2'	2.83	0.40
1:X:811:G:OP2	5:C:56:ARG:HG3	2.21	0.40
1:X:1004:A:H5'	17:O:71:ILE:HD11	2.04	0.40
1:X:1016:C:O2'	9:G:56:THR:HG21	2.21	0.40
1:X:1467:U:H3'	1:X:1467:U:C6	2.54	0.40
11:I:72:TYR:CE2	11:I:105:PRO:HB2	2.57	0.40
12:J:54:VAL:CG1	12:J:121:LEU:HB3	2.52	0.40
14:L:15:ARG:HD3	14:L:15:ARG:HA	1.93	0.40
14:L:67:THR:O	14:L:70:ALA:HB3	2.22	0.40
25:W:3:ILE:O	25:W:31:SER:HA	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	238/274 (87%)	170 (71%)	39 (16%)	29 (12%)	0	1
4	B	203/211 (96%)	172 (85%)	17 (8%)	14 (7%)	1	7
5	C	195/205 (95%)	131 (67%)	37 (19%)	27 (14%)	0	1
6	D	175/180 (97%)	136 (78%)	26 (15%)	13 (7%)	1	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	E	169/185 (91%)	132 (78%)	29 (17%)	8 (5%)	2	14
8	F	69/144 (48%)	59 (86%)	8 (12%)	2 (3%)	3	24
9	G	140/174 (80%)	103 (74%)	23 (16%)	14 (10%)	0	2
10	H	132/134 (98%)	117 (89%)	9 (7%)	6 (4%)	2	15
11	I	139/156 (89%)	79 (57%)	34 (24%)	26 (19%)	0	0
12	J	134/141 (95%)	97 (72%)	26 (19%)	11 (8%)	1	4
13	K	111/116 (96%)	96 (86%)	7 (6%)	8 (7%)	1	6
14	L	102/114 (90%)	72 (71%)	20 (20%)	10 (10%)	0	3
15	M	106/166 (64%)	95 (90%)	7 (7%)	4 (4%)	2	18
16	N	115/118 (98%)	101 (88%)	10 (9%)	4 (4%)	3	20
17	O	92/100 (92%)	66 (72%)	13 (14%)	13 (14%)	0	1
18	P	125/134 (93%)	114 (91%)	5 (4%)	6 (5%)	2	14
19	Q	91/95 (96%)	59 (65%)	19 (21%)	13 (14%)	0	1
20	R	108/115 (94%)	66 (61%)	23 (21%)	19 (18%)	0	0
21	S	173/237 (73%)	145 (84%)	20 (12%)	8 (5%)	2	15
22	T	82/91 (90%)	64 (78%)	9 (11%)	9 (11%)	0	2
23	U	70/81 (86%)	39 (56%)	17 (24%)	14 (20%)	0	0
24	V	64/67 (96%)	57 (89%)	3 (5%)	4 (6%)	1	8
25	W	53/55 (96%)	49 (92%)	4 (8%)	0	100	100
26	Z	56/60 (93%)	47 (84%)	5 (9%)	4 (7%)	1	6
30	4	35/37 (95%)	28 (80%)	5 (14%)	2 (6%)	1	11
All	All	2977/3390 (88%)	2294 (77%)	415 (14%)	268 (9%)	0	3

All (268) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	60	ARG
3	A	151	LYS
3	A	170	SER
3	A	187	SER
3	A	199	ALA
3	A	248	THR
3	A	250	TRP
3	A	271	VAL
4	B	76	ARG

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Mol	Chain	Res	Type
4	B	86	PRO
4	B	122	PHE
5	C	20	PRO
5	C	64	THR
5	C	67	ALA
5	C	129	LYS
5	C	163	ASN
5	C	164	VAL
5	C	172	VAL
7	E	126	PRO
9	G	33	ILE
9	G	37	ASP
9	G	67	ARG
9	G	91	THR
9	G	97	ASP
9	G	104	THR
9	G	107	GLN
9	G	158	HIS
9	G	170	PRO
10	H	27	SER
10	H	29	ILE
11	I	17	LYS
11	I	18	ARG
11	I	37	GLN
11	I	39	SER
11	I	48	PHE
11	I	56	LEU
11	I	59	ARG
11	I	62	LYS
11	I	86	THR
11	I	98	LEU
11	I	103	ASN
12	J	13	GLN
12	J	26	ASP
12	J	83	ARG
12	J	89	GLY
12	J	136	GLU
13	K	6	ALA
13	K	8	ARG
13	K	95	THR
14	L	21	THR
14	L	40	ALA

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Mol	Chain	Res	Type
14	L	68	ALA
14	L	95	LYS
15	M	27	PHE
15	M	29	PRO
16	N	7	GLY
16	N	8	ILE
16	N	92	ARG
17	O	10	LYS
17	O	31	ASP
17	O	97	GLY
18	P	9	ARG
18	P	50	VAL
19	Q	12	ILE
19	Q	13	SER
19	Q	67	ARG
19	Q	69	ILE
19	Q	84	GLU
20	R	11	ASN
20	R	62	MET
20	R	66	GLN
20	R	82	ALA
20	R	98	ILE
20	R	108	VAL
21	S	26	LYS
21	S	156	GLU
22	T	15	ASP
22	T	19	LYS
23	U	15	VAL
23	U	27	ASP
23	U	47	HIS
23	U	48	LYS
23	U	60	VAL
24	V	2	LYS
26	Z	4	HIS
3	A	54	ILE
3	A	98	ALA
3	A	197	GLY
3	A	198	ASN
3	A	220	HIS
4	B	121	ASN
4	B	123	ALA
4	B	132	LYS

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Mol	Chain	Res	Type
4	B	135	HIS
4	B	146	THR
5	C	9	GLN
5	C	22	VAL
5	C	55	GLY
5	C	60	GLY
5	C	121	ASP
5	C	125	ILE
5	C	127	ASP
5	C	165	SER
5	C	195	ILE
6	D	4	LEU
6	D	9	ASN
6	D	121	ALA
6	D	124	GLY
7	E	19	ALA
10	H	31	GLY
11	I	19	VAL
11	I	47	ALA
11	I	49	PHE
12	J	17	ARG
12	J	21	ASP
12	J	60	ARG
12	J	80	ALA
13	K	14	SER
13	K	92	GLY
14	L	45	ASP
14	L	92	GLY
15	M	41	GLU
16	N	87	ASN
17	O	30	GLY
17	O	48	GLY
19	Q	6	ILE
19	Q	63	LYS
20	R	5	SER
20	R	6	ALA
20	R	7	GLY
20	R	60	PRO
21	S	57	GLU
21	S	88	TYR
21	S	91	PRO
22	T	5	LYS

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Mol	Chain	Res	Type
22	T	14	ARG
23	U	19	ILE
23	U	30	VAL
23	U	41	VAL
23	U	55	GLY
23	U	78	ILE
26	Z	36	CYS
26	Z	37	HIS
30	4	20	HIS
3	A	109	GLU
3	A	206	LEU
3	A	219	PRO
3	A	249	PRO
3	A	263	ARG
4	B	73	ALA
4	B	74	PRO
5	C	15	ILE
5	C	173	ALA
5	C	189	ASP
5	C	190	ALA
6	D	5	LYS
6	D	122	PHE
7	E	55	PRO
7	E	119	ALA
7	E	173	ALA
9	G	34	PRO
9	G	68	PRO
10	H	41	ASN
11	I	54	SER
11	I	65	PHE
11	I	82	ASP
13	K	93	GLY
14	L	52	ALA
14	L	96	TYR
17	O	43	GLU
18	P	20	LEU
18	P	80	LEU
18	P	131	LYS
19	Q	61	LYS
19	Q	86	GLN
19	Q	87	SER
20	R	49	GLU

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Mol	Chain	Res	Type
20	R	85	ASP
20	R	87	GLU
20	R	110	SER
24	V	3	PRO
24	V	10	GLN
26	Z	53	ASP
3	A	35	GLU
3	A	45	ASN
3	A	89	SER
3	A	127	LEU
3	A	254	THR
3	A	269	PHE
4	B	85	ALA
4	B	137	ARG
5	C	13	ARG
6	D	10	ASP
6	D	40	LEU
6	D	52	LYS
7	E	7	GLN
7	E	13	SER
10	H	5	GLN
11	I	28	LYS
11	I	88	PHE
11	I	115	SER
13	K	4	GLY
14	L	53	ALA
17	O	9	GLY
17	O	28	GLU
17	O	29	ALA
17	O	49	GLU
19	Q	3	HIS
19	Q	4	TYR
20	R	16	PHE
20	R	63	THR
21	S	58	GLY
21	S	125	PRO
22	T	74	LYS
23	U	34	THR
23	U	42	GLN
23	U	76	LYS
3	A	55	GLY
3	A	244	ARG

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Mol	Chain	Res	Type
3	A	270	ILE
5	C	196	VAL
6	D	21	GLY
6	D	42	SER
6	D	71	LYS
6	D	81	GLN
7	E	59	GLN
9	G	165	VAL
10	H	42	LYS
11	I	8	PRO
11	I	9	THR
11	I	131	LYS
12	J	11	ARG
12	J	84	MET
13	K	10	LEU
14	L	33	ARG
17	O	7	THR
17	O	36	LYS
19	Q	5	ASP
20	R	31	GLY
20	R	111	GLY
22	T	7	VAL
23	U	12	ASN
4	B	17	ASN
4	B	75	THR
5	C	11	GLY
5	C	126	ALA
8	F	143	ASN
11	I	29	THR
17	O	11	GLN
21	S	6	LYS
30	4	5	SER
9	G	163	PRO
11	I	68	VAL
24	V	64	GLY
3	A	47	GLY
3	A	252	LYS
5	C	41	GLY
5	C	103	GLY
8	F	118	GLY
18	P	132	GLY
20	R	64	ASN

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Mol	Chain	Res	Type
22	T	13	GLY
22	T	73	GLY
5	C	171	PRO
9	G	157	PRO
11	I	57	ILE
15	M	74	GLY
22	T	27	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	185/215 (86%)	144 (78%)	41 (22%)	1	4
4	B	155/157 (99%)	135 (87%)	20 (13%)	3	17
5	C	157/163 (96%)	125 (80%)	32 (20%)	1	5
6	D	153/156 (98%)	129 (84%)	24 (16%)	2	10
7	E	136/144 (94%)	117 (86%)	19 (14%)	3	14
8	F	51/107 (48%)	46 (90%)	5 (10%)	6	27
9	G	118/146 (81%)	95 (80%)	23 (20%)	1	6
10	H	103/103 (100%)	81 (79%)	22 (21%)	1	5
11	I	108/121 (89%)	72 (67%)	36 (33%)	0	0
12	J	110/115 (96%)	93 (84%)	17 (16%)	2	10
13	K	90/93 (97%)	73 (81%)	17 (19%)	1	6
14	L	74/82 (90%)	54 (73%)	20 (27%)	0	1
15	M	94/134 (70%)	75 (80%)	19 (20%)	1	5
16	N	96/97 (99%)	81 (84%)	15 (16%)	2	10
17	O	75/79 (95%)	60 (80%)	15 (20%)	1	5
18	P	109/115 (95%)	94 (86%)	15 (14%)	3	14
19	Q	75/76 (99%)	60 (80%)	15 (20%)	1	5
20	R	91/96 (95%)	71 (78%)	20 (22%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	S	149/192 (78%)	126 (85%)	23 (15%)	2	11
22	T	62/67 (92%)	53 (86%)	9 (14%)	2	13
23	U	57/66 (86%)	33 (58%)	24 (42%)	0	0
24	V	54/55 (98%)	44 (82%)	10 (18%)	1	7
25	W	48/48 (100%)	38 (79%)	10 (21%)	1	5
26	Z	51/53 (96%)	37 (72%)	14 (28%)	0	1
30	4	35/35 (100%)	31 (89%)	4 (11%)	4	21
All	All	2436/2715 (90%)	1967 (81%)	469 (19%)	1	6

All (469) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	33	LEU
3	A	34	THR
3	A	35	GLU
3	A	39	LYS
3	A	40	THR
3	A	43	ARG
3	A	44	ASN
3	A	46	ARG
3	A	48	ARG
3	A	49	ILE
3	A	50	THR
3	A	52	ARG
3	A	54	ILE
3	A	61	LEU
3	A	68	LYS
3	A	69	ARG
3	A	92	ILE
3	A	105	ILE
3	A	108	PRO
3	A	111	LEU
3	A	131	LEU
3	A	133	LEU
3	A	151	LYS
3	A	157	ARG
3	A	164	GLN
3	A	175	VAL
3	A	183	ARG
3	A	203	ASN

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Mol	Chain	Res	Type
3	A	208	LYS
3	A	214	TRP
3	A	215	LEU
3	A	217	ARG
3	A	218	LYS
3	A	226	MET
3	A	240	THR
3	A	244	ARG
3	A	248	THR
3	A	252	LYS
3	A	259	THR
3	A	260	ARG
3	A	270	ILE
4	B	5	LEU
4	B	14	ILE
4	B	37	LYS
4	B	49	ILE
4	B	69	LYS
4	B	82	ARG
4	B	87	ASP
4	B	105	THR
4	B	111	LYS
4	B	119	ARG
4	B	131	SER
4	B	133	LYS
4	B	134	TRP
4	B	137	ARG
4	B	149	ARG
4	B	150	VAL
4	B	168	GLN
4	B	179	GLU
4	B	184	VAL
4	B	203	LYS
5	C	5	ASN
5	C	10	ASN
5	C	13	ARG
5	C	14	THR
5	C	15	ILE
5	C	31	VAL
5	C	40	ARG
5	C	45	THR
5	C	48	ARG

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Mol	Chain	Res	Type
5	C	51	VAL
5	C	53	LYS
5	C	74	VAL
5	C	90	SER
5	C	95	LEU
5	C	101	GLN
5	C	102	LEU
5	C	104	LEU
5	C	117	LEU
5	C	124	ASP
5	C	134	ILE
5	C	138	LYS
5	C	143	ASP
5	C	148	VAL
5	C	150	LEU
5	C	153	ASP
5	C	154	ASP
5	C	155	GLU
5	C	164	VAL
5	C	166	TRP
5	C	175	VAL
5	C	180	ILE
5	C	188	ILE
6	D	40	LEU
6	D	45	GLU
6	D	57	LEU
6	D	67	ILE
6	D	74	ILE
6	D	80	ARG
6	D	89	VAL
6	D	92	ARG
6	D	106	ILE
6	D	112	ARG
6	D	115	ARG
6	D	117	ILE
6	D	125	ARG
6	D	129	ASN
6	D	130	LEU
6	D	135	GLN
6	D	136	LEU
6	D	140	GLU
6	D	142	THR

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Mol	Chain	Res	Type
6	D	145	MET
6	D	147	ASP
6	D	150	ARG
6	D	163	ASP
6	D	175	LEU
7	E	11	VAL
7	E	33	LEU
7	E	35	VAL
7	E	38	ASN
7	E	44	ARG
7	E	49	GLN
7	E	50	LEU
7	E	57	ASP
7	E	64	LEU
7	E	67	LEU
7	E	68	THR
7	E	69	ARG
7	E	90	ARG
7	E	92	VAL
7	E	113	VAL
7	E	116	GLU
7	E	132	ASP
7	E	140	LEU
7	E	152	ARG
8	F	76	TYR
8	F	100	ASN
8	F	101	TRP
8	F	111	LYS
8	F	115	LEU
9	G	31	THR
9	G	37	ASP
9	G	38	GLU
9	G	41	TRP
9	G	53	ARG
9	G	62	ILE
9	G	71	THR
9	G	75	ILE
9	G	93	LYS
9	G	95	LEU
9	G	102	ARG
9	G	104	THR
9	G	113	GLU

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Mol	Chain	Res	Type
9	G	116	ARG
9	G	126	VAL
9	G	132	PHE
9	G	145	HIS
9	G	146	THR
9	G	154	GLU
9	G	165	VAL
9	G	166	LEU
9	G	168	THR
9	G	169	GLN
10	H	3	MET
10	H	8	LEU
10	H	18	GLU
10	H	20	MET
10	H	25	LEU
10	H	26	ASN
10	H	27	SER
10	H	32	LYS
10	H	36	THR
10	H	41	ASN
10	H	47	VAL
10	H	81	ILE
10	H	83	ARG
10	H	87	SER
10	H	89	ILE
10	H	94	ASN
10	H	106	ARG
10	H	116	ARG
10	H	117	GLU
10	H	120	ASP
10	H	122	ARG
10	H	129	LEU
11	I	7	LYS
11	I	12	SER
11	I	13	ARG
11	I	19	VAL
11	I	27	ASP
11	I	29	THR
11	I	32	ARG
11	I	34	HIS
11	I	35	LYS
11	I	37	GLN

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Mol	Chain	Res	Type
11	I	38	LYS
11	I	39	SER
11	I	40	ARG
11	I	45	LYS
11	I	53	ARG
11	I	56	LEU
11	I	57	ILE
11	I	59	ARG
11	I	60	LEU
11	I	65	PHE
11	I	78	SER
11	I	83	LEU
11	I	84	GLU
11	I	85	ASP
11	I	88	PHE
11	I	96	TYR
11	I	98	LEU
11	I	101	ARG
11	I	103	ASN
11	I	106	VAL
11	I	107	LYS
11	I	113	GLU
11	I	114	ILE
11	I	120	VAL
11	I	123	ASP
11	I	142	LEU
12	J	8	THR
12	J	10	PHE
12	J	11	ARG
12	J	19	THR
12	J	21	ASP
12	J	26	ASP
12	J	27	TYR
12	J	49	GLU
12	J	61	ARG
12	J	64	LYS
12	J	81	GLU
12	J	91	VAL
12	J	94	TRP
12	J	113	GLU
12	J	132	MET
12	J	133	VAL

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Mol	Chain	Res	Type
12	J	134	LYS
13	K	5	LYS
13	K	8	ARG
13	K	10	LEU
13	K	11	ASN
13	K	12	ARG
13	K	17	ARG
13	K	28	LEU
13	K	35	GLN
13	K	45	ARG
13	K	51	LEU
13	K	53	THR
13	K	83	VAL
13	K	94	TYR
13	K	95	THR
13	K	99	ARG
13	K	102	THR
13	K	109	THR
14	L	8	ARG
14	L	11	LEU
14	L	12	ARG
14	L	13	THR
14	L	18	ARG
14	L	31	VAL
14	L	33	ARG
14	L	36	LYS
14	L	37	HIS
14	L	38	ILE
14	L	43	ILE
14	L	45	ASP
14	L	47	ARG
14	L	64	LYS
14	L	66	ASP
14	L	71	VAL
14	L	89	PHE
14	L	91	ARG
14	L	93	SER
14	L	108	ARG
15	M	2	GLN
15	M	5	ILE
15	M	6	LYS
15	M	11	GLU

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Mol	Chain	Res	Type
15	M	12	LEU
15	M	13	LEU
15	M	19	ASP
15	M	22	ARG
15	M	31	ASP
15	M	34	ARG
15	M	37	THR
15	M	51	GLU
15	M	63	ARG
15	M	79	ARG
15	M	91	VAL
15	M	92	THR
15	M	96	ARG
15	M	99	VAL
15	M	101	ARG
16	N	8	ILE
16	N	16	LYS
16	N	18	LEU
16	N	19	LYS
16	N	22	LYS
16	N	30	LYS
16	N	51	ARG
16	N	71	LEU
16	N	78	THR
16	N	88	ILE
16	N	90	LEU
16	N	91	ASN
16	N	93	LYS
16	N	97	ASP
16	N	104	GLU
17	O	7	THR
17	O	14	VAL
17	O	18	ASP
17	O	22	VAL
17	O	26	GLN
17	O	28	GLU
17	O	39	PHE
17	O	40	VAL
17	O	55	THR
17	O	56	VAL
17	O	65	ARG
17	O	69	ILE

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Mol	Chain	Res	Type
17	O	81	ARG
17	O	88	GLN
17	O	96	LEU
18	P	16	GLN
18	P	17	GLN
18	P	25	PHE
18	P	32	ARG
18	P	37	LYS
18	P	45	ILE
18	P	50	VAL
18	P	89	ARG
18	P	116	ILE
18	P	118	LYS
18	P	120	ARG
18	P	124	ILE
18	P	125	THR
18	P	126	ILE
18	P	133	ASN
19	Q	7	LEU
19	Q	8	GLN
19	Q	12	ILE
19	Q	14	GLU
19	Q	26	SER
19	Q	37	GLU
19	Q	38	ILE
19	Q	42	ILE
19	Q	61	LYS
19	Q	63	LYS
19	Q	65	VAL
19	Q	69	ILE
19	Q	71	GLN
19	Q	79	ILE
19	Q	84	GLU
20	R	11	ASN
20	R	18	LYS
20	R	23	ILE
20	R	25	LEU
20	R	26	SER
20	R	32	GLN
20	R	37	LEU
20	R	38	LEU
20	R	42	ARG

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Mol	Chain	Res	Type
20	R	44	GLN
20	R	71	GLN
20	R	73	GLU
20	R	79	SER
20	R	80	LYS
20	R	95	ARG
20	R	98	ILE
20	R	104	VAL
20	R	105	ARG
20	R	106	VAL
20	R	108	VAL
21	S	3	LEU
21	S	13	LYS
21	S	18	MET
21	S	22	VAL
21	S	26	LYS
21	S	29	ASN
21	S	51	LEU
21	S	65	LEU
21	S	67	LYS
21	S	71	MET
21	S	82	ASP
21	S	88	TYR
21	S	100	THR
21	S	120	LEU
21	S	123	VAL
21	S	128	ARG
21	S	132	GLN
21	S	134	LEU
21	S	159	THR
21	S	160	LEU
21	S	166	LEU
21	S	169	VAL
21	S	175	ARG
22	T	5	LYS
22	T	16	SER
22	T	17	ASN
22	T	37	LEU
22	T	38	VAL
22	T	62	LEU
22	T	63	SER
22	T	64	ASP

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Mol	Chain	Res	Type
22	T	85	GLN
23	U	8	THR
23	U	10	LYS
23	U	11	LYS
23	U	13	LEU
23	U	14	VAL
23	U	17	SER
23	U	19	ILE
23	U	20	ARG
23	U	21	ARG
23	U	23	LYS
23	U	32	ARG
23	U	35	THR
23	U	37	ILE
23	U	42	GLN
23	U	43	ARG
23	U	46	LEU
23	U	49	LYS
23	U	54	ASN
23	U	56	GLN
23	U	63	SER
23	U	65	ASN
23	U	67	LEU
23	U	69	THR
23	U	76	LYS
24	V	1	MET
24	V	7	ARG
24	V	13	ASP
24	V	14	PHE
24	V	19	ASP
24	V	21	ARG
24	V	25	LEU
24	V	41	HIS
24	V	49	GLU
24	V	65	GLU
25	W	2	LYS
25	W	4	LYS
25	W	9	VAL
25	W	10	ILE
25	W	12	ARG
25	W	15	ASN
25	W	30	ASP

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Mol	Chain	Res	Type
25	W	32	ARG
25	W	34	VAL
25	W	36	ASP
26	Z	3	LYS
26	Z	4	HIS
26	Z	6	VAL
26	Z	8	LYS
26	Z	18	MET
26	Z	19	ARG
26	Z	31	THR
26	Z	35	GLN
26	Z	40	LYS
26	Z	41	LEU
26	Z	53	ASP
26	Z	55	ARG
26	Z	57	VAL
26	Z	58	LEU
30	4	2	LYS
30	4	9	LYS
30	4	14	CYS
30	4	30	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	96	HIS
3	A	201	HIS
3	A	231	HIS
4	B	129	HIS
4	B	180	ASN
5	C	5	ASN
5	C	61	GLN
5	C	66	ASN
5	C	176	ASN
6	D	9	ASN
7	E	38	ASN
7	E	49	GLN
7	E	106	ASN
7	E	143	GLN
9	G	76	GLN
10	H	26	ASN
10	H	41	ASN

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Mol	Chain	Res	Type
11	I	37	GLN
14	L	41	GLN
14	L	49	GLN
14	L	97	HIS
15	M	20	HIS
15	M	48	GLN
16	N	31	GLN
16	N	66	ASN
16	N	75	ASN
16	N	81	ASN
16	N	91	ASN
17	O	11	GLN
17	O	79	GLN
17	O	88	GLN
18	P	13	GLN
18	P	16	GLN
18	P	17	GLN
18	P	78	ASN
18	P	81	HIS
18	P	115	ASN
19	Q	71	GLN
20	R	15	HIS
20	R	69	GLN
21	S	80	HIS
21	S	119	ASN
21	S	132	GLN
22	T	17	ASN
22	T	35	ASN
23	U	42	GLN
23	U	47	HIS
24	V	41	HIS
25	W	49	HIS
26	Z	43	HIS
26	Z	44	HIS
30	4	36	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2681/2880 (93%)	638 (23%)	238 (8%)
2	Y	121/123 (98%)	28 (23%)	5 (4%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	2802/3003 (93%)	666 (23%)	243 (8%)

All (666) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	2	G
1	X	3	U
1	X	4	C
1	X	13	A
1	X	14	A
1	X	33	C
1	X	34	U
1	X	45	C
1	X	48	A
1	X	49	U
1	X	50	G
1	X	51	A
1	X	54	G
1	X	63	A
1	X	69	G
1	X	70	A
1	X	71	A
1	X	72	A
1	X	74	G
1	X	82	G
1	X	83	A
1	X	87	G
1	X	89	A
1	X	90	G
1	X	91	A
1	X	95	G
1	X	97	U
1	X	98	U
1	X	99	U
1	X	100	G
1	X	101	A
1	X	105	G
1	X	107	G
1	X	116	A
1	X	117	A
1	X	118	U
1	X	123	A

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Mol	Chain	Res	Type
1	X	124	A
1	X	125	A
1	X	127	C
1	X	129	A
1	X	136	A
1	X	138	G
1	X	143	A
1	X	147	G
1	X	149	A
1	X	154	U
1	X	155	G
1	X	157	G
1	X	158	A
1	X	173	A
1	X	176	A
1	X	177	U
1	X	192	G
1	X	193	A
1	X	194	G
1	X	199	A
1	X	204	A
1	X	206	U
1	X	207	U
1	X	210	A
1	X	222	G
1	X	225	G
1	X	229	G
1	X	242	A
1	X	243	G
1	X	245	C
1	X	246	C
1	X	248	A
1	X	304	A
1	X	305	A
1	X	306	G
1	X	310	A
1	X	312	G
1	X	313	U
1	X	321	A
1	X	322	A
1	X	323	G
1	X	328	A

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Mol	Chain	Res	Type
1	X	333	A
1	X	335	A
1	X	340	G
1	X	341	A
1	X	342	G
1	X	343	A
1	X	344	G
1	X	358	C
1	X	388	G
1	X	393	U
1	X	397	U
1	X	399	G
1	X	400	U
1	X	409	G
1	X	414	A
1	X	418	C
1	X	419	G
1	X	424	G
1	X	425	A
1	X	441	A
1	X	456	C
1	X	459	A
1	X	461	A
1	X	463	C
1	X	466	A
1	X	467	U
1	X	468	A
1	X	469	G
1	X	486	U
1	X	491	A
1	X	492	G
1	X	504	G
1	X	513	A
1	X	514	G
1	X	515	A
1	X	518	A
1	X	519	C
1	X	520	C
1	X	523	A
1	X	539	A
1	X	540	G
1	X	541	C

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Mol	Chain	Res	Type
1	X	542	A
1	X	543	G
1	X	554	U
1	X	555	U
1	X	556	A
1	X	558	G
1	X	559	C
1	X	560	G
1	X	572	G
1	X	577	U
1	X	580	A
1	X	581	A
1	X	582	G
1	X	583	C
1	X	584	A
1	X	595	A
1	X	600	G
1	X	613	A
1	X	614	G
1	X	617	U
1	X	623	G
1	X	624	A
1	X	625	A
1	X	626	A
1	X	627	A
1	X	628	A
1	X	633	G
1	X	638	A
1	X	645	G
1	X	648	A
1	X	649	G
1	X	651	C
1	X	652	C
1	X	654	A
1	X	655	A
1	X	656	U
1	X	657	A
1	X	664	C
1	X	665	A
1	X	667	U
1	X	669	G
1	X	682	G

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Mol	Chain	Res	Type
1	X	683	A
1	X	684	C
1	X	698	A
1	X	699	G
1	X	700	C
1	X	728	G
1	X	729	A
1	X	730	C
1	X	731	A
1	X	732	G
1	X	736	G
1	X	743	A
1	X	747	A
1	X	751	G
1	X	752	G
1	X	753	U
1	X	758	G
1	X	759	C
1	X	760	U
1	X	777	A
1	X	778	G
1	X	780	U
1	X	781	G
1	X	788	G
1	X	789	G
1	X	790	A
1	X	795	A
1	X	797	A
1	X	798	G
1	X	802	A
1	X	803	C
1	X	804	C
1	X	805	G
1	X	806	A
1	X	814	G
1	X	815	A
1	X	818	G
1	X	825	C
1	X	832	A
1	X	840	U
1	X	841	G
1	X	858	G

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Mol	Chain	Res	Type
1	X	859	U
1	X	872	G
1	X	879	A
1	X	880	C
1	X	922	A
1	X	926	C
1	X	931	G
1	X	938	G
1	X	939	C
1	X	940	G
1	X	944	A
1	X	952	A
1	X	955	G
1	X	956	A
1	X	957	G
1	X	969	U
1	X	970	A
1	X	972	C
1	X	973	U
1	X	985	G
1	X	994	A
1	X	995	A
1	X	1000	G
1	X	1001	A
1	X	1006	C
1	X	1007	A
1	X	1014	G
1	X	1016	C
1	X	1022	A
1	X	1023	U
1	X	1024	G
1	X	1028	G
1	X	1031	C
1	X	1032	A
1	X	1033	G
1	X	1034	U
1	X	1036	G
1	X	1037	U
1	X	1038	U
1	X	1044	U
1	X	1051	U
1	X	1053	G

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Mol	Chain	Res	Type
1	X	1054	C
1	X	1055	A
1	X	1056	U
1	X	1057	A
1	X	1058	G
1	X	1060	C
1	X	1068	A
1	X	1073	G
1	X	1077	U
1	X	1078	A
1	X	1081	A
1	X	1082	G
1	X	1086	C
1	X	1087	C
1	X	1090	C
1	X	1094	C
1	X	1097	A
1	X	1098	G
1	X	1099	A
1	X	1100	G
1	X	1108	U
1	X	1115	C
1	X	1121	G
1	X	1122	A
1	X	1123	G
1	X	1128	G
1	X	1129	A
1	X	1130	U
1	X	1139	A
1	X	1140	A
1	X	1141	U
1	X	1142	G
1	X	1143	A
1	X	1145	C
1	X	1146	G
1	X	1152	C
1	X	1153	A
1	X	1154	A
1	X	1155	G
1	X	1161	U
1	X	1183	C
1	X	1185	C

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Mol	Chain	Res	Type
1	X	1187	A
1	X	1188	A
1	X	1189	G
1	X	1191	G
1	X	1192	A
1	X	1194	U
1	X	1195	U
1	X	1223	G
1	X	1224	A
1	X	1233	A
1	X	1234	C
1	X	1240	G
1	X	1250	A
1	X	1251	G
1	X	1265	G
1	X	1266	G
1	X	1269	G
1	X	1275	A
1	X	1281	A
1	X	1284	G
1	X	1285	A
1	X	1286	U
1	X	1288	A
1	X	1289	A
1	X	1297	A
1	X	1299	A
1	X	1300	A
1	X	1302	C
1	X	1307	U
1	X	1313	U
1	X	1314	A
1	X	1315	A
1	X	1319	C
1	X	1334	A
1	X	1339	U
1	X	1341	G
1	X	1342	U
1	X	1358	C
1	X	1365	U
1	X	1378	A
1	X	1381	G
1	X	1392	U

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Mol	Chain	Res	Type
1	X	1399	C
1	X	1404	C
1	X	1410	U
1	X	1412	C
1	X	1413	U
1	X	1428	G
1	X	1429	A
1	X	1430	G
1	X	1432	G
1	X	1433	A
1	X	1434	U
1	X	1441	A
1	X	1442	C
1	X	1443	G
1	X	1451	C
1	X	1460	G
1	X	1465	G
1	X	1467	U
1	X	1468	A
1	X	1469	U
1	X	1470	G
1	X	1473	U
1	X	1474	A
1	X	1475	U
1	X	1476	G
1	X	1482	U
1	X	1490	U
1	X	1497	C
1	X	1498	G
1	X	1505	U
1	X	1506	C
1	X	1508	G
1	X	1509	A
1	X	1513	U
1	X	1514	C
1	X	1523	A
1	X	1524	C
1	X	1525	A
1	X	1528	C
1	X	1531	C
1	X	1532	A
1	X	1533	G

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Mol	Chain	Res	Type
1	X	1545	G
1	X	1551	U
1	X	1552	C
1	X	1553	G
1	X	1554	G
1	X	1562	G
1	X	1563	U
1	X	1571	G
1	X	1574	A
1	X	1575	C
1	X	1576	G
1	X	1583	A
1	X	1584	G
1	X	1585	A
1	X	1594	U
1	X	1600	U
1	X	1601	U
1	X	1602	G
1	X	1603	A
1	X	1608	U
1	X	1613	G
1	X	1624	A
1	X	1625	A
1	X	1626	A
1	X	1631	C
1	X	1632	A
1	X	1634	A
1	X	1648	C
1	X	1657	A
1	X	1665	C
1	X	1669	A
1	X	1691	G
1	X	1710	U
1	X	1711	C
1	X	1712	G
1	X	1713	G
1	X	1716	G
1	X	1717	A
1	X	1732	U
1	X	1733	U
1	X	1734	C
1	X	1747	G

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Mol	Chain	Res	Type
1	X	1754	G
1	X	1755	G
1	X	1764	A
1	X	1773	C
1	X	1776	A
1	X	1790	G
1	X	1791	C
1	X	1792	C
1	X	1793	A
1	X	1799	A
1	X	1806	G
1	X	1807	A
1	X	1808	C
1	X	1812	U
1	X	1813	A
1	X	1820	G
1	X	1821	A
1	X	1825	C
1	X	1831	G
1	X	1840	A
1	X	1850	G
1	X	1861	G
1	X	1863	U
1	X	1867	A
1	X	1874	G
1	X	1882	G
1	X	1883	A
1	X	1886	G
1	X	1910	A
1	X	1912	G
1	X	1913	G
1	X	1919	A
1	X	1920	A
1	X	1921	A
1	X	1923	U
1	X	1939	U
1	X	1943	A
1	X	1947	G
1	X	1950	C
1	X	1953	A
1	X	1954	A
1	X	1955	G

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Mol	Chain	Res	Type
1	X	1958	G
1	X	1963	G
1	X	1964	A
1	X	1965	U
1	X	1975	G
1	X	1976	U
1	X	1980	A
1	X	2006	G
1	X	2010	G
1	X	2014	A
1	X	2015	G
1	X	2018	G
1	X	2019	C
1	X	2026	C
1	X	2035	G
1	X	2038	C
1	X	2039	G
1	X	2044	G
1	X	2045	A
1	X	2046	C
1	X	2052	G
1	X	2076	G
1	X	2079	A
1	X	2088	U
1	X	2089	C
1	X	2171	U
1	X	2180	U
1	X	2181	A
1	X	2189	A
1	X	2190	A
1	X	2191	A
1	X	2195	C
1	X	2196	U
1	X	2197	U
1	X	2198	U
1	X	2199	C
1	X	2204	A
1	X	2205	C
1	X	2217	G
1	X	2218	G
1	X	2222	U
1	X	2247	A

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Mol	Chain	Res	Type
1	X	2262	C
1	X	2265	A
1	X	2266	A
1	X	2283	G
1	X	2284	U
1	X	2285	U
1	X	2286	G
1	X	2287	G
1	X	2288	A
1	X	2291	U
1	X	2294	U
1	X	2295	C
1	X	2298	U
1	X	2299	A
1	X	2300	G
1	X	2301	A
1	X	2306	A
1	X	2313	G
1	X	2314	A
1	X	2315	A
1	X	2324	G
1	X	2325	A
1	X	2326	C
1	X	2329	C
1	X	2339	A
1	X	2351	G
1	X	2355	A
1	X	2358	C
1	X	2362	G
1	X	2363	G
1	X	2364	C
1	X	2370	G
1	X	2371	A
1	X	2375	G
1	X	2381	A
1	X	2382	C
1	X	2385	U
1	X	2389	G
1	X	2396	C
1	X	2401	A
1	X	2402	U
1	X	2404	A

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Mol	Chain	Res	Type
1	X	2405	A
1	X	2408	G
1	X	2409	A
1	X	2410	U
1	X	2420	C
1	X	2426	G
1	X	2427	A
1	X	2448	A
1	X	2449	G
1	X	2452	U
1	X	2455	A
1	X	2463	G
1	X	2470	U
1	X	2475	C
1	X	2477	C
1	X	2480	C
1	X	2481	G
1	X	2482	A
1	X	2483	U
1	X	2484	G
1	X	2485	U
1	X	2498	U
1	X	2499	C
1	X	2501	U
1	X	2504	G
1	X	2508	G
1	X	2514	G
1	X	2543	A
1	X	2545	A
1	X	2546	G
1	X	2548	G
1	X	2552	C
1	X	2553	G
1	X	2557	G
1	X	2561	G
1	X	2565	C
1	X	2580	C
1	X	2581	A
1	X	2582	G
1	X	2588	U
1	X	2589	C
1	X	2591	C

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Mol	Chain	Res	Type
1	X	2594	U
1	X	2600	A
1	X	2609	G
1	X	2611	A
1	X	2613	A
1	X	2615	U
1	X	2620	G
1	X	2633	A
1	X	2640	G
1	X	2642	G
1	X	2650	G
1	X	2668	U
1	X	2692	A
1	X	2693	U
1	X	2694	G
1	X	2705	A
1	X	2706	U
1	X	2707	G
1	X	2713	A
1	X	2728	A
1	X	2731	G
1	X	2732	C
1	X	2736	U
1	X	2737	A
1	X	2738	A
1	X	2744	A
1	X	2745	A
1	X	2758	A
1	X	2759	U
1	X	2770	A
1	X	2771	C
1	X	2774	U
1	X	2775	U
1	X	2776	U
1	X	2777	A
1	X	2778	U
1	X	2779	C
1	X	2780	A
1	X	2782	G
1	X	2795	A
1	X	2796	A
1	X	2808	U

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Mol	Chain	Res	Type
1	X	2810	A
1	X	2811	G
1	X	2824	C
1	X	2825	A
1	X	2843	A
1	X	2846	G
1	X	2847	G
1	X	2848	A
1	X	2849	C
1	X	2854	G
1	X	2855	C
1	X	2859	U
1	X	2868	G
2	Y	14	C
2	Y	15	A
2	Y	17	A
2	Y	18	G
2	Y	26	G
2	Y	27	A
2	Y	28	A
2	Y	37	C
2	Y	39	C
2	Y	42	U
2	Y	43	G
2	Y	44	C
2	Y	46	G
2	Y	47	A
2	Y	53	G
2	Y	54	U
2	Y	56	G
2	Y	58	G
2	Y	59	A
2	Y	69	G
2	Y	75	A
2	Y	76	U
2	Y	99	G
2	Y	102	A
2	Y	108	G
2	Y	112	A
2	Y	115	G
2	Y	123	U

All (243) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	3	U
1	X	13	A
1	X	33	C
1	X	48	A
1	X	50	G
1	X	62	U
1	X	70	A
1	X	71	A
1	X	74	G
1	X	82	G
1	X	83	A
1	X	89	A
1	X	98	U
1	X	99	U
1	X	100	G
1	X	117	A
1	X	124	A
1	X	154	U
1	X	176	A
1	X	190	A
1	X	198	A
1	X	199	A
1	X	242	A
1	X	312	G
1	X	321	A
1	X	322	A
1	X	328	A
1	X	332	C
1	X	334	G
1	X	341	A
1	X	342	G
1	X	343	A
1	X	396	U
1	X	399	G
1	X	416	U
1	X	417	C
1	X	418	C
1	X	458	G
1	X	466	A
1	X	467	U
1	X	469	G
1	X	490	A
1	X	504	G

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Mol	Chain	Res	Type
1	X	513	A
1	X	522	G
1	X	537	C
1	X	539	A
1	X	542	A
1	X	553	C
1	X	554	U
1	X	557	U
1	X	558	G
1	X	559	C
1	X	580	A
1	X	583	C
1	X	648	A
1	X	655	A
1	X	664	C
1	X	668	A
1	X	672	C
1	X	682	G
1	X	683	A
1	X	698	A
1	X	751	G
1	X	758	G
1	X	759	C
1	X	761	G
1	X	777	A
1	X	780	U
1	X	788	G
1	X	789	G
1	X	796	A
1	X	802	A
1	X	803	C
1	X	806	A
1	X	813	A
1	X	814	G
1	X	824	U
1	X	841	G
1	X	842	A
1	X	858	G
1	X	859	U
1	X	872	G
1	X	878	C
1	X	879	A

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Mol	Chain	Res	Type
1	X	939	C
1	X	940	G
1	X	955	G
1	X	969	U
1	X	972	C
1	X	994	A
1	X	1000	G
1	X	1031	C
1	X	1033	G
1	X	1037	U
1	X	1053	G
1	X	1055	A
1	X	1056	U
1	X	1072	U
1	X	1081	A
1	X	1086	C
1	X	1096	A
1	X	1099	A
1	X	1120	C
1	X	1121	G
1	X	1139	A
1	X	1141	U
1	X	1152	C
1	X	1154	A
1	X	1182	U
1	X	1186	G
1	X	1191	G
1	X	1194	U
1	X	1223	G
1	X	1233	A
1	X	1249	G
1	X	1288	A
1	X	1299	A
1	X	1313	U
1	X	1314	A
1	X	1353	A
1	X	1357	U
1	X	1378	A
1	X	1409	U
1	X	1410	U
1	X	1412	C
1	X	1432	G

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Mol	Chain	Res	Type
1	X	1433	A
1	X	1441	A
1	X	1442	C
1	X	1459	U
1	X	1473	U
1	X	1475	U
1	X	1496	G
1	X	1505	U
1	X	1513	U
1	X	1531	C
1	X	1541	G
1	X	1552	C
1	X	1561	A
1	X	1562	G
1	X	1574	A
1	X	1575	C
1	X	1581	C
1	X	1583	A
1	X	1601	U
1	X	1607	A
1	X	1618	U
1	X	1624	A
1	X	1625	A
1	X	1631	C
1	X	1680	U
1	X	1710	U
1	X	1711	C
1	X	1716	G
1	X	1732	U
1	X	1775	A
1	X	1777	A
1	X	1790	G
1	X	1791	C
1	X	1799	A
1	X	1800	A
1	X	1807	A
1	X	1810	U
1	X	1811	A
1	X	1812	U
1	X	1820	G
1	X	1865	C
1	X	1872	A

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Mol	Chain	Res	Type
1	X	1882	G
1	X	1883	A
1	X	1909	U
1	X	1920	A
1	X	1921	A
1	X	1938	U
1	X	1953	A
1	X	1963	G
1	X	1975	G
1	X	1980	A
1	X	2014	A
1	X	2018	G
1	X	2075	U
1	X	2083	G
1	X	2088	U
1	X	2180	U
1	X	2181	A
1	X	2189	A
1	X	2198	U
1	X	2204	A
1	X	2217	G
1	X	2228	U
1	X	2254	C
1	X	2258	G
1	X	2261	G
1	X	2298	U
1	X	2299	A
1	X	2305	C
1	X	2312	A
1	X	2314	A
1	X	2324	G
1	X	2354	G
1	X	2361	G
1	X	2370	G
1	X	2381	A
1	X	2401	A
1	X	2404	A
1	X	2409	A
1	X	2447	G
1	X	2477	C
1	X	2482	A
1	X	2497	A

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Mol	Chain	Res	Type
1	X	2498	U
1	X	2560	G
1	X	2564	U
1	X	2580	C
1	X	2608	A
1	X	2615	U
1	X	2624	G
1	X	2660	C
1	X	2669	C
1	X	2691	C
1	X	2705	A
1	X	2706	U
1	X	2731	G
1	X	2736	U
1	X	2744	A
1	X	2758	A
1	X	2769	C
1	X	2770	A
1	X	2778	U
1	X	2807	U
1	X	2808	U
1	X	2810	A
1	X	2824	C
1	X	2846	G
1	X	2848	A
1	X	2854	G
1	X	2867	G
2	Y	26	G
2	Y	46	G
2	Y	54	U
2	Y	58	G
2	Y	86	A

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 36 ligands modelled in this entry, 35 are monoatomic - leaving 1 for Mogul analysis.

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
32	1F3	X	2931	-	63,64,64	1.32	7 (11%)	83,96,96	1.87	19 (22%)

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
32	1F3	X	2931	-	-	9/78/119/119	0/5/5/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	X	2931	1F3	C50-C49	4.20	1.50	1.34
32	X	2931	1F3	C48-C47	-4.14	1.51	1.54
32	X	2931	1F3	C50-N45	3.34	1.44	1.38
32	X	2931	1F3	O17-C5	-3.08	1.43	1.47
32	X	2931	1F3	C47-N45	-2.63	1.43	1.47
32	X	2931	1F3	C41-N40	2.53	1.37	1.33
32	X	2931	1F3	C51-C47	-2.02	1.48	1.51

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	X	2931	1F3	C59-C58-N57	-5.48	106.72	114.95
32	X	2931	1F3	C28-O20-C8	-4.96	107.83	116.26
32	X	2931	1F3	C23-C6-C5	-4.94	108.42	115.23
32	X	2931	1F3	O60-C58-N57	3.83	128.31	123.06
32	X	2931	1F3	C47-N45-C50	3.52	113.23	109.61
32	X	2931	1F3	O29-C30-C38	-3.41	100.49	106.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	X	2931	1F3	C48-C47-N45	3.02	105.56	103.17
32	X	2931	1F3	C27-C12-C13	-3.00	106.28	113.00
32	X	2931	1F3	C48-C47-C51	-2.89	108.03	113.91
32	X	2931	1F3	C4-N40-C41	-2.66	108.91	112.39
32	X	2931	1F3	C30-C31-C32	-2.62	105.99	110.46
32	X	2931	1F3	C47-C48-C49	2.36	107.55	103.04
32	X	2931	1F3	O43-C13-C12	-2.35	103.66	107.84
32	X	2931	1F3	C9-C7-C2	2.30	119.85	116.10
32	X	2931	1F3	O10-C6-C23	2.30	111.63	107.36
32	X	2931	1F3	C52-C51-C47	-2.27	116.42	120.76
32	X	2931	1F3	O10-C11-O26	2.25	128.02	123.95
32	X	2931	1F3	C48-C49-C50	-2.17	106.31	111.47
32	X	2931	1F3	C16-C1-C3	-2.10	104.41	108.09

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	X	2931	1F3	C59-C58-N57-C54
32	X	2931	1F3	O60-C58-N57-C54
32	X	2931	1F3	C16-C1-C4-N40
32	X	2931	1F3	O20-C8-C9-C7
32	X	2931	1F3	C3-C2-C7-C9
32	X	2931	1F3	C14-C8-C9-C7
32	X	2931	1F3	O20-C8-C9-C22
32	X	2931	1F3	C3-C1-C4-N40
32	X	2931	1F3	C16-C1-C4-C5

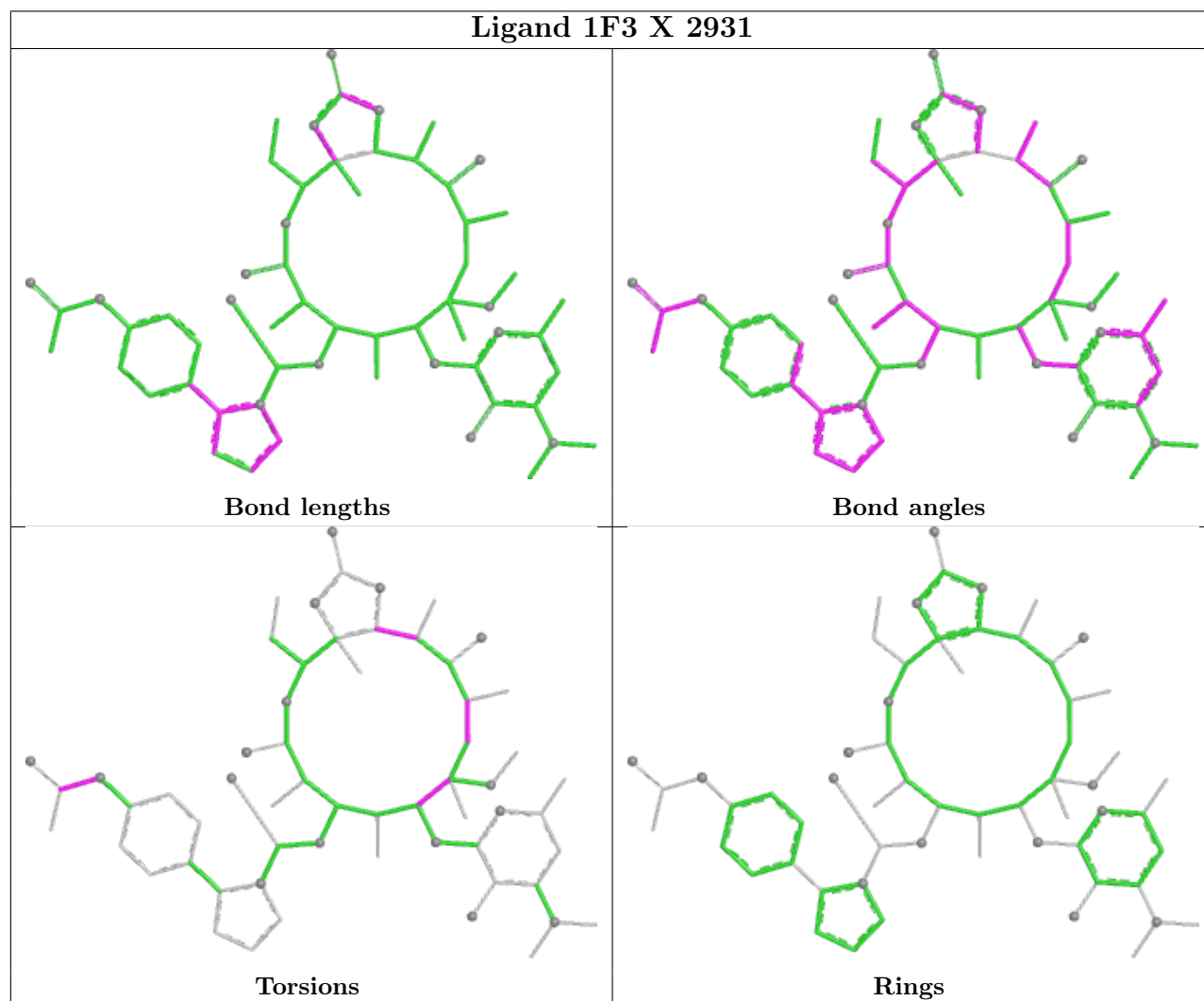
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	X	2931	1F3	2	0

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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	X	2686/2880 (93%)	0.16	127 (4%) 37 25	43, 87, 194, 279	0
2	Y	122/123 (99%)	0.62	8 (6%) 26 17	82, 129, 165, 187	0
3	A	240/274 (87%)	1.19	48 (20%) 3 3	63, 107, 137, 156	0
4	B	205/211 (97%)	0.15	10 (4%) 36 25	38, 68, 99, 145	0
5	C	197/205 (96%)	1.26	47 (23%) 2 2	55, 107, 150, 178	0
6	D	177/180 (98%)	1.17	39 (22%) 3 2	148, 178, 210, 216	0
7	E	171/185 (92%)	0.82	22 (12%) 9 6	98, 139, 178, 188	0
8	F	71/144 (49%)	2.40	35 (49%) 0 1	221, 234, 251, 259	0
9	G	142/174 (81%)	1.18	36 (25%) 2 2	65, 89, 137, 149	0
10	H	134/134 (100%)	-0.10	2 (1%) 71 56	49, 62, 88, 110	0
11	I	141/156 (90%)	2.11	54 (38%) 1 1	54, 120, 171, 195	0
12	J	136/141 (96%)	0.90	25 (18%) 4 3	83, 106, 147, 172	0
13	K	113/116 (97%)	0.01	7 (6%) 28 18	37, 53, 71, 99	0
14	L	104/114 (91%)	1.41	30 (28%) 1 1	91, 122, 149, 166	0
15	M	108/166 (65%)	0.13	6 (5%) 31 20	44, 64, 106, 128	0
16	N	117/118 (99%)	0.54	11 (9%) 15 11	54, 86, 124, 152	0
17	O	94/100 (94%)	0.80	13 (13%) 8 5	67, 106, 146, 160	0
18	P	127/134 (94%)	-0.15	1 (0%) 82 70	48, 64, 103, 143	0
19	Q	93/95 (97%)	1.00	17 (18%) 4 3	69, 101, 156, 193	0
20	R	110/115 (95%)	1.46	31 (28%) 1 1	84, 113, 170, 173	0
21	S	175/237 (73%)	0.93	27 (15%) 6 5	119, 154, 178, 190	0
22	T	84/91 (92%)	1.05	16 (19%) 4 3	72, 103, 176, 195	0
23	U	72/81 (88%)	1.96	28 (38%) 1 1	86, 122, 146, 182	0
24	V	66/67 (98%)	0.70	8 (12%) 10 7	88, 128, 213, 230	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9	
25	W	55/55 (100%)	0.14	0	100	100	76, 96, 123, 161	0
26	Z	58/60 (96%)	0.46	4 (6%)	24	17	47, 64, 96, 108	0
27	1	53/55 (96%)	5.65	34 (64%)	0	1	6, 28, 62, 73	0
28	2	46/47 (97%)	5.12	37 (80%)	0	0	3, 10, 27, 42	0
29	3	63/66 (95%)	5.52	41 (65%)	0	1	3, 18, 41, 84	0
30	4	37/37 (100%)	5.53	31 (83%)	0	0	191, 239, 247, 252	0
All	All	5997/6561 (91%)	0.71	795 (13%)	8	6	3, 96, 193, 279	0

All (795) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
27	1	7	ARG	51.0
27	1	4	ASP	44.3
29	3	60	LEU	38.8
28	2	46	ASP	21.7
27	1	3	LYS	19.3
29	3	41	ILE	19.2
29	3	20	GLY	18.8
29	3	28	GLY	16.5
27	1	44	ALA	15.1
29	3	33	ASN	14.6
9	G	97	ASP	13.8
30	4	20	HIS	13.4
30	4	24	LEU	12.0
28	2	7	PRO	11.8
11	I	52	GLY	11.6
27	1	21	TYR	11.5
27	1	2	ALA	11.4
28	2	34	ARG	11.2
29	3	38	GLY	11.1
29	3	56	ALA	11.1
29	3	2	PRO	11.0
23	U	16	ASN	11.0
29	3	11	LYS	10.8
27	1	40	TYR	10.6
29	3	43	GLY	10.4
28	2	35	ARG	10.1
29	3	19	THR	10.0
29	3	14	ILE	9.9
11	I	29	THR	9.8

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Mol	Chain	Res	Type	RSRZ
29	3	62	LEU	9.8
26	Z	2	ALA	9.7
29	3	51	ALA	9.7
12	J	84	MET	9.6
27	1	24	THR	9.5
27	1	41	ASP	9.5
11	I	9	THR	9.4
30	4	17	VAL	9.4
11	I	48	PHE	9.3
27	1	43	VAL	9.2
3	A	203	ASN	9.1
8	F	127	VAL	9.1
29	3	30	ARG	8.9
30	4	19	ARG	8.9
29	3	39	ASP	8.8
30	4	21	GLY	8.7
30	4	36	GLN	8.6
1	X	248	A	8.6
30	4	31	LYS	8.5
27	1	19	GLY	8.5
30	4	23	VAL	8.5
29	3	17	THR	8.4
28	2	36	ALA	8.4
24	V	2	LYS	8.3
19	Q	64	ARG	8.3
28	2	21	ARG	8.1
28	2	38	GLY	8.1
11	I	63	ARG	8.1
8	F	115	LEU	7.8
28	2	31	LEU	7.7
28	2	27	GLY	7.6
8	F	126	THR	7.5
30	4	5	SER	7.5
30	4	30	VAL	7.4
29	3	37	SER	7.3
27	1	5	GLY	7.3
14	L	34	SER	7.3
30	4	35	ARG	7.2
19	Q	69	ILE	7.2
3	A	220	HIS	7.0
28	2	3	ARG	6.9
28	2	11	LYS	6.9

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Mol	Chain	Res	Type	RSRZ
28	2	37	LYS	6.9
29	3	35	GLY	6.8
30	4	37	GLY	6.8
8	F	123	ALA	6.7
11	I	8	PRO	6.7
30	4	4	ARG	6.7
20	R	77	HIS	6.6
3	A	85	ASP	6.6
20	R	82	ALA	6.5
28	2	1	MET	6.5
28	2	20	ALA	6.4
30	4	16	VAL	6.4
17	O	5	ILE	6.4
3	A	219	PRO	6.3
23	U	27	ASP	6.3
30	4	22	ARG	6.2
1	X	731	A	6.2
29	3	4	MET	6.2
5	C	189	ASP	6.2
4	B	135	HIS	6.2
11	I	36	GLY	6.2
22	T	9	SER	6.2
28	2	15	THR	6.1
30	4	26	ILE	6.1
1	X	1069	G	6.1
28	2	6	GLN	6.1
7	E	5	GLY	6.0
20	R	78	ALA	6.0
5	C	165	SER	6.0
30	4	33	LYS	5.9
5	C	47	THR	5.9
11	I	31	GLY	5.9
28	2	41	GLN	5.9
8	F	129	GLY	5.9
11	I	53	ARG	5.8
28	2	4	THR	5.8
28	2	23	LYS	5.8
9	G	129	HIS	5.8
29	3	34	THR	5.8
8	F	136	VAL	5.8
30	4	3	VAL	5.8
9	G	103	TYR	5.7

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Mol	Chain	Res	Type	RSRZ
5	C	193	LEU	5.7
30	4	1	MET	5.7
20	R	58	VAL	5.7
29	3	63	PRO	5.6
28	2	8	ASN	5.6
30	4	18	ARG	5.6
5	C	91	TYR	5.6
1	X	1082	G	5.5
11	I	50	GLU	5.4
28	2	9	ASN	5.4
27	1	29	ARG	5.4
28	2	28	ARG	5.4
1	X	1091	C	5.4
3	A	260	ARG	5.4
30	4	29	ASN	5.4
5	C	190	ALA	5.3
29	3	55	TRP	5.3
3	A	46	ARG	5.3
27	1	36	GLU	5.3
3	A	250	TRP	5.3
22	T	10	SER	5.3
9	G	106	TYR	5.3
14	L	33	ARG	5.3
9	G	110	LEU	5.3
14	L	40	ALA	5.3
22	T	15	ASP	5.2
8	F	99	LEU	5.2
7	E	37	TYR	5.2
5	C	174	GLY	5.2
1	X	2327	U	5.2
22	T	11	LYS	5.2
16	N	48	ARG	5.2
8	F	137	THR	5.1
5	C	44	SER	5.1
14	L	36	LYS	5.1
6	D	42	SER	5.1
5	C	48	ARG	5.0
11	I	33	GLY	5.0
23	U	47	HIS	5.0
17	O	39	PHE	5.0
29	3	18	GLY	5.0
27	1	34	LYS	4.9

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Mol	Chain	Res	Type	RSRZ
17	O	23	GLU	4.9
29	3	8	LYS	4.9
1	X	413	G	4.9
30	4	2	LYS	4.9
27	1	30	ASN	4.8
12	J	14	PHE	4.8
5	C	49	ALA	4.8
1	X	225	G	4.8
1	X	483	A	4.8
29	3	9	MET	4.8
2	Y	123	U	4.8
7	E	6	LYS	4.8
14	L	57	ALA	4.8
8	F	114	ASP	4.8
20	R	81	VAL	4.8
30	4	32	HIS	4.8
29	3	32	GLN	4.7
23	U	52	ARG	4.7
21	S	24	TYR	4.7
11	I	10	PRO	4.7
11	I	30	ALA	4.7
16	N	94	VAL	4.7
22	T	7	VAL	4.7
5	C	57	LYS	4.7
14	L	39	TYR	4.7
12	J	18	MET	4.6
1	X	1083	C	4.6
11	I	32	ARG	4.6
8	F	125	ASN	4.6
29	3	42	ARG	4.6
1	X	2326	C	4.6
29	3	40	GLU	4.5
20	R	91	ALA	4.5
6	D	43	SER	4.5
21	S	67	LYS	4.5
9	G	171	LEU	4.5
21	S	114	ASP	4.4
11	I	64	GLY	4.4
5	C	66	ASN	4.4
16	N	91	ASN	4.4
23	U	21	ARG	4.4
19	Q	65	VAL	4.4

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Mol	Chain	Res	Type	RSRZ
5	C	55	GLY	4.4
11	I	54	SER	4.4
27	1	18	THR	4.4
23	U	39	LYS	4.3
3	A	43	ARG	4.3
7	E	143	GLN	4.3
8	F	130	THR	4.3
20	R	92	THR	4.3
8	F	124	ALA	4.3
20	R	7	GLY	4.3
27	1	27	ASN	4.3
3	A	239	ARG	4.2
30	4	28	SER	4.2
20	R	100	ASP	4.2
3	A	102	LYS	4.2
23	U	34	THR	4.2
1	X	1086	C	4.2
29	3	58	MET	4.2
12	J	141	ALA	4.2
28	2	32	ALA	4.2
20	R	79	SER	4.2
28	2	14	LYS	4.2
5	C	161	ALA	4.2
1	X	1913	G	4.2
14	L	21	THR	4.2
30	4	8	LYS	4.2
27	1	17	GLY	4.2
21	S	1	MET	4.2
1	X	774	A	4.2
28	2	39	ARG	4.2
1	X	2328	G	4.1
12	J	140	GLU	4.1
14	L	20	THR	4.1
6	D	153	ASP	4.1
24	V	6	MET	4.1
22	T	12	ASN	4.1
1	X	356	A	4.1
28	2	24	THR	4.1
20	R	102	LYS	4.1
9	G	156	HIS	4.1
3	A	249	PRO	4.0
21	S	91	PRO	4.0

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Mol	Chain	Res	Type	RSRZ
19	Q	56	MET	4.0
1	X	434	C	4.0
12	J	86	LYS	4.0
12	J	82	THR	4.0
23	U	46	LEU	4.0
12	J	27	TYR	4.0
20	R	43	ASP	4.0
28	2	40	HIS	4.0
11	I	28	LYS	3.9
12	J	17	ARG	3.9
30	4	25	VAL	3.9
13	K	17	ARG	3.9
24	V	1	MET	3.9
14	L	111	GLY	3.9
1	X	1068	A	3.9
1	X	1429	A	3.9
11	I	60	LEU	3.9
19	Q	42	ILE	3.9
19	Q	62	ARG	3.9
28	2	44	VAL	3.9
13	K	3	HIS	3.9
12	J	88	LYS	3.9
11	I	103	ASN	3.8
1	X	1428	G	3.8
9	G	65	LYS	3.8
28	2	12	ARG	3.8
11	I	97	ARG	3.8
29	3	7	HIS	3.8
11	I	37	GLN	3.8
8	F	128	ALA	3.8
11	I	58	ALA	3.8
22	T	13	GLY	3.8
1	X	1070	G	3.7
6	D	8	TYR	3.7
29	3	29	LYS	3.7
1	X	435	A	3.7
1	X	1085	G	3.7
17	O	34	GLU	3.7
14	L	53	ALA	3.7
3	A	186	HIS	3.7
19	Q	55	THR	3.7
23	U	65	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
3	A	101	GLU	3.7
6	D	130	LEU	3.7
21	S	92	VAL	3.7
1	X	1037	U	3.6
8	F	131	ALA	3.6
1	X	358	C	3.6
27	1	31	THR	3.6
3	A	242	ALA	3.6
1	X	2280	A	3.6
11	I	56	LEU	3.6
17	O	36	LYS	3.6
7	E	52	VAL	3.6
1	X	123	A	3.6
19	Q	72	ARG	3.5
11	I	15	ASP	3.5
21	S	14	LEU	3.5
11	I	88	PHE	3.5
3	A	259	THR	3.5
1	X	1117	G	3.5
9	G	163	PRO	3.5
11	I	6	LEU	3.5
22	T	8	GLY	3.5
20	R	94	VAL	3.5
3	A	248	THR	3.5
12	J	90	ALA	3.5
24	V	48	ARG	3.5
26	Z	56	GLN	3.5
1	X	1100	G	3.5
1	X	1092	U	3.5
1	X	1089	C	3.4
1	X	1524	C	3.4
27	1	52	GLU	3.4
14	L	58	ALA	3.4
11	I	86	THR	3.4
8	F	111	LYS	3.4
12	J	16	GLY	3.4
23	U	49	LYS	3.4
6	D	154	ILE	3.4
5	C	194	GLU	3.4
17	O	37	ALA	3.4
3	A	39	LYS	3.4
27	1	28	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
11	I	95	ALA	3.4
21	S	7	PRO	3.4
4	B	94	ASP	3.4
9	G	37	ASP	3.4
15	M	34	ARG	3.4
15	M	40	ARG	3.4
27	1	51	ARG	3.4
11	I	41	SER	3.4
29	3	31	HIS	3.4
11	I	5	ASP	3.4
1	X	1084	A	3.4
3	A	272	THR	3.4
20	R	26	SER	3.4
23	U	63	SER	3.4
30	4	6	SER	3.4
11	I	45	LYS	3.3
6	D	85	VAL	3.3
8	F	120	VAL	3.3
9	G	160	ALA	3.3
9	G	119	LEU	3.3
28	2	45	SER	3.3
29	3	24	ALA	3.3
21	S	15	ASP	3.3
3	A	224	SER	3.3
27	1	49	VAL	3.3
22	T	19	LYS	3.3
12	J	21	ASP	3.3
11	I	59	ARG	3.3
17	O	8	GLY	3.3
20	R	83	LEU	3.3
18	P	19	LYS	3.3
3	A	254	THR	3.3
21	S	87	THR	3.3
23	U	62	LEU	3.3
29	3	3	LYS	3.2
1	X	304	A	3.2
11	I	74	VAL	3.2
12	J	28	VAL	3.2
5	C	19	LEU	3.2
9	G	162	LYS	3.2
20	R	90	LYS	3.2
22	T	6	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
16	N	92	ARG	3.2
1	X	2323	U	3.2
6	D	149	THR	3.2
1	X	1090	C	3.2
17	O	11	GLN	3.2
24	V	19	ASP	3.2
1	X	1067	G	3.2
20	R	27	GLY	3.2
11	I	55	ARG	3.2
14	L	18	ARG	3.2
20	R	93	ARG	3.2
1	X	2776	U	3.2
23	U	45	ASN	3.2
3	A	237	GLU	3.2
1	X	2330	G	3.2
27	1	45	LYS	3.2
3	A	261	ARG	3.1
23	U	28	GLY	3.1
11	I	27	ASP	3.1
4	B	205	SER	3.1
3	A	188	GLU	3.1
1	X	2329	C	3.1
1	X	2288	A	3.1
6	D	131	GLY	3.1
23	U	31	GLY	3.1
6	D	12	VAL	3.1
9	G	36	ASN	3.1
19	Q	14	GLU	3.1
27	1	8	ILE	3.1
22	T	14	ARG	3.1
1	X	346	C	3.1
1	X	1888	C	3.1
8	F	86	LYS	3.1
27	1	53	LYS	3.1
23	U	44	ALA	3.1
17	O	98	ILE	3.1
2	Y	28	A	3.1
5	C	160	ALA	3.1
9	G	155	THR	3.1
23	U	55	GLY	3.1
27	1	25	THR	3.1
11	I	62	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
6	D	138	PHE	3.1
13	K	94	TYR	3.1
16	N	56	ASP	3.0
3	A	252	LYS	3.0
1	X	1093	U	3.0
1	X	361	G	3.0
3	A	243	GLY	3.0
1	X	1095	A	3.0
1	X	1523	A	3.0
23	U	8	THR	3.0
23	U	51	ILE	3.0
27	1	26	LYS	3.0
8	F	121	GLU	3.0
10	H	117	GLU	3.0
1	X	1951	G	3.0
19	Q	54	SER	3.0
7	E	69	ARG	3.0
20	R	96	LYS	3.0
28	2	19	ARG	3.0
3	A	34	THR	3.0
3	A	50	THR	3.0
1	X	1432	G	3.0
29	3	5	LYS	3.0
3	A	244	ARG	3.0
4	B	136	ARG	3.0
7	E	10	ALA	3.0
8	F	107	ILE	3.0
7	E	59	GLN	2.9
19	Q	71	GLN	2.9
1	X	357	A	2.9
6	D	156	ILE	2.9
6	D	44	LYS	2.9
6	D	118	ASN	2.9
20	R	57	ASN	2.9
11	I	21	ARG	2.9
3	A	218	LYS	2.9
6	D	121	ALA	2.9
21	S	124	ALA	2.9
3	A	44	ASN	2.9
6	D	152	MET	2.9
19	Q	63	LYS	2.9
14	L	38	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	X	2385	U	2.9
8	F	92	ASN	2.9
20	R	89	GLY	2.9
16	N	88	ILE	2.9
3	A	40	THR	2.9
6	D	4	LEU	2.9
12	J	87	GLY	2.9
1	X	1734	C	2.9
8	F	78	ILE	2.9
1	X	540	G	2.8
13	K	43	GLU	2.8
4	B	202	ALA	2.8
11	I	43	ALA	2.8
3	A	91	ARG	2.8
5	C	124	ASP	2.8
7	E	17	VAL	2.8
29	3	21	LYS	2.8
11	I	11	GLY	2.8
29	3	27	SER	2.8
1	X	655	A	2.8
1	X	1522	C	2.8
1	X	1872	A	2.8
2	Y	2	C	2.8
30	4	34	GLN	2.8
3	A	201	HIS	2.8
5	C	90	SER	2.8
5	C	188	ILE	2.8
8	F	84	ILE	2.8
3	A	33	LEU	2.8
30	4	15	LYS	2.8
5	C	112	GLN	2.8
11	I	79	GLN	2.8
7	E	12	PRO	2.8
9	G	69	ASP	2.8
19	Q	27	PHE	2.8
28	2	26	SER	2.8
13	K	10	LEU	2.8
1	X	1467	U	2.8
9	G	76	GLN	2.8
9	G	107	GLN	2.8
4	B	86	PRO	2.8
21	S	54	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	X	1753	A	2.8
1	X	2290	A	2.8
1	X	537	C	2.8
28	2	33	ARG	2.8
7	E	80	SER	2.8
3	A	223	GLY	2.8
19	Q	53	ILE	2.8
7	E	150	LYS	2.7
26	Z	3	LYS	2.7
1	X	247	A	2.7
1	X	1071	U	2.7
1	X	1112	U	2.7
9	G	122	HIS	2.7
24	V	3	PRO	2.7
7	E	46	ASP	2.7
14	L	55	SER	2.7
1	X	1121	G	2.7
21	S	93	GLU	2.7
1	X	1078	A	2.7
1	X	1468	A	2.7
7	E	8	PRO	2.7
30	4	9	LYS	2.7
6	D	169	LEU	2.7
27	1	37	LEU	2.7
6	D	26	MET	2.7
9	G	100	TYR	2.7
11	I	89	ASP	2.7
1	X	1887	G	2.7
7	E	111	HIS	2.7
20	R	106	VAL	2.7
1	X	559	C	2.7
5	C	159	ARG	2.7
16	N	58	ARG	2.7
3	A	100	GLY	2.6
9	G	159	SER	2.6
12	J	25	GLY	2.6
12	J	139	ASP	2.6
23	U	48	LYS	2.6
4	B	204	ALA	2.6
6	D	139	PRO	2.6
5	C	94	THR	2.6
5	C	191	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
14	L	37	HIS	2.6
11	I	101	ARG	2.6
22	T	20	TYR	2.6
1	X	1393	G	2.6
1	X	2283	G	2.6
1	X	436	A	2.6
12	J	85	GLY	2.6
1	X	1120	C	2.6
15	M	29	PRO	2.6
9	G	66	HIS	2.6
5	C	39	ARG	2.6
5	C	166	TRP	2.6
8	F	117	ALA	2.6
1	X	1104	G	2.6
8	F	122	ALA	2.6
1	X	2265	A	2.6
1	X	730	C	2.6
1	X	1912	G	2.6
3	A	251	GLY	2.6
14	L	99	ARG	2.6
6	D	23	SER	2.6
6	D	172	SER	2.6
20	R	51	VAL	2.6
20	R	98	ILE	2.5
24	V	36	GLN	2.5
1	X	2581	A	2.5
2	Y	41	A	2.5
8	F	76	TYR	2.5
14	L	59	LEU	2.5
27	1	6	PRO	2.5
9	G	94	LYS	2.5
21	S	86	VAL	2.5
11	I	72	TYR	2.5
8	F	132	ARG	2.5
16	N	12	ARG	2.5
6	D	5	LYS	2.5
28	2	25	LYS	2.5
11	I	68	VAL	2.5
3	A	174	ILE	2.5
1	X	1553	G	2.5
3	A	99	ASP	2.5
11	I	49	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
12	J	26	ASP	2.5
21	S	62	PHE	2.5
9	G	108	GLY	2.5
2	Y	111	C	2.5
11	I	12	SER	2.5
1	X	1881	U	2.5
21	S	68	ALA	2.5
1	X	641	G	2.5
5	C	29	GLU	2.5
6	D	132	ILE	2.5
14	L	19	THR	2.5
1	X	1059	A	2.5
12	J	134	LYS	2.5
26	Z	8	LYS	2.5
8	F	116	ASN	2.5
8	F	94	ALA	2.5
1	X	519	C	2.5
15	M	39	VAL	2.5
19	Q	12	ILE	2.4
5	C	162	ARG	2.4
8	F	133	SER	2.4
21	S	170	SER	2.4
1	X	1188	A	2.4
6	D	117	ILE	2.4
22	T	36	ILE	2.4
5	C	56	ARG	2.4
6	D	41	GLY	2.4
5	C	51	VAL	2.4
14	L	56	SER	2.4
21	S	168	VAL	2.4
28	2	29	ASN	2.4
23	U	40	ARG	2.4
1	X	343	A	2.4
1	X	1954	A	2.4
2	Y	42	U	2.4
1	X	583	C	2.4
1	X	2195	C	2.4
2	Y	14	C	2.4
4	B	134	TRP	2.4
4	B	146	THR	2.4
8	F	113	PRO	2.4
7	E	71	LEU	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
9	G	90	LEU	2.4
27	1	35	LEU	2.4
3	A	262	LYS	2.4
12	J	77	LYS	2.4
1	X	1189	G	2.4
14	L	68	ALA	2.4
1	X	2281	C	2.4
14	L	9	ARG	2.4
20	R	65	PRO	2.4
11	I	17	LYS	2.4
4	B	34	VAL	2.4
6	D	35	VAL	2.4
14	L	100	VAL	2.4
1	X	843	G	2.4
1	X	1355	A	2.4
5	C	20	PRO	2.3
8	F	91	PRO	2.3
17	O	25	LEU	2.3
5	C	22	VAL	2.3
8	F	138	VAL	2.3
11	I	40	ARG	2.3
12	J	83	ARG	2.3
5	C	7	ILE	2.3
16	N	2	PRO	2.3
1	X	360	A	2.3
5	C	123	PHE	2.3
5	C	24	SER	2.3
20	R	12	ASP	2.3
9	G	53	ARG	2.3
11	I	118	VAL	2.3
21	S	171	VAL	2.3
17	O	10	LYS	2.3
14	L	24	SER	2.3
1	X	305	A	2.3
1	X	625	A	2.3
6	D	38	GLU	2.3
7	E	152	ARG	2.3
9	G	131	VAL	2.3
16	N	110	VAL	2.3
23	U	26	ALA	2.3
1	X	1223	G	2.3
1	X	2084	G	2.3

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Mol	Chain	Res	Type	RSRZ
3	A	233	HIS	2.3
29	3	36	LYS	2.3
8	F	90	THR	2.3
15	M	2	GLN	2.3
20	R	86	PRO	2.3
27	1	42	PRO	2.3
3	A	247	VAL	2.3
12	J	137	VAL	2.3
27	1	38	LYS	2.3
9	G	41	TRP	2.3
21	S	4	THR	2.3
20	R	59	LYS	2.3
5	C	128	ALA	2.3
28	2	13	ALA	2.3
6	D	136	LEU	2.3
24	V	53	LEU	2.3
6	D	66	ILE	2.2
20	R	54	ILE	2.2
9	G	34	PRO	2.2
19	Q	46	PHE	2.2
23	U	75	TYR	2.2
9	G	93	LYS	2.2
23	U	33	LYS	2.2
20	R	108	VAL	2.2
21	S	79	ILE	2.2
5	C	23	ASN	2.2
29	3	6	THR	2.2
9	G	116	ARG	2.2
1	X	1525	A	2.2
14	L	52	ALA	2.2
5	C	163	ASN	2.2
6	D	144	ASP	2.2
21	S	32	PHE	2.2
22	T	17	ASN	2.2
6	D	13	ARG	2.2
1	X	1562	G	2.2
14	L	65	THR	2.2
5	C	164	VAL	2.2
23	U	14	VAL	2.2
1	X	2284	U	2.2
1	X	200	A	2.2
1	X	2777	A	2.2

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Mol	Chain	Res	Type	RSRZ
14	L	108	ARG	2.2
7	E	175	LYS	2.2
8	F	74	MET	2.2
30	4	10	MET	2.2
1	X	1094	C	2.2
6	D	27	ALA	2.2
1	X	192	G	2.2
1	X	2731	G	2.2
1	X	1099	A	2.2
1	X	1516	A	2.2
1	X	2189	A	2.2
6	D	113	ASP	2.2
7	E	11	VAL	2.2
11	I	92	THR	2.2
11	I	123	ASP	2.2
8	F	97	GLY	2.1
13	K	52	ILE	2.1
2	Y	29	C	2.1
3	A	255	LYS	2.1
1	X	2198	U	2.1
1	X	2286	G	2.1
9	G	95	LEU	2.1
14	L	54	ALA	2.1
11	I	42	GLY	2.1
3	A	222	ARG	2.1
17	O	78	VAL	2.1
3	A	45	ASN	2.1
3	A	217	ARG	2.1
6	D	125	ARG	2.1
9	G	35	LYS	2.1
19	Q	32	LYS	2.1
20	R	13	LYS	2.1
1	X	1109	A	2.1
21	S	169	VAL	2.1
5	C	173	ALA	2.1
21	S	5	ALA	2.1
10	H	27	SER	2.1
3	A	207	GLY	2.1
7	E	7	GLN	2.1
14	L	41	GLN	2.1
1	X	732	G	2.1
9	G	68	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	X	1588	A	2.1
11	I	7	LYS	2.1
12	J	15	ARG	2.1
5	C	157	THR	2.1
6	D	155	THR	2.1
7	E	13	SER	2.1
6	D	11	GLN	2.1
1	X	1552	C	2.1
1	X	1812	U	2.1
5	C	187	VAL	2.1
23	U	30	VAL	2.1
22	T	24	LYS	2.0
22	T	74	LYS	2.0
29	3	53	ALA	2.0
1	X	2427	A	2.0
1	X	653	G	2.0
1	X	1073	G	2.0
1	X	2076	G	2.0
9	G	64	GLY	2.0
23	U	29	GLY	2.0
6	D	143	TYR	2.0
5	C	50	GLN	2.0
14	L	89	PHE	2.0
28	2	22	MET	2.0
5	C	172	VAL	2.0
14	L	17	VAL	2.0
1	X	429	C	2.0
1	X	1183	C	2.0
21	S	118	HIS	2.0
5	C	53	LYS	2.0
6	D	71	LYS	2.0
7	E	149	ARG	2.0
12	J	78	LYS	2.0
23	U	20	ARG	2.0
3	A	236	GLY	2.0
5	C	114	GLY	2.0
15	M	30	GLY	2.0
9	G	112	THR	2.0
1	X	341	A	2.0
11	I	108	LEU	2.0
21	S	3	LEU	2.0
1	X	388	G	2.0

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Mol	Chain	Res	Type	RSRZ
1	X	2085	G	2.0
1	X	2324	G	2.0
13	K	114	GLU	2.0
1	X	1365	U	2.0
21	S	23	ALA	2.0
1	X	226	C	2.0
1	X	1190	C	2.0
5	C	11	GLY	2.0
16	N	23	GLY	2.0
17	O	27	GLY	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
31	MG	X	2922	1/1	0.53	0.83	81,81,81,81	0
31	MG	X	2904	1/1	0.61	0.87	90,90,90,90	0
31	MG	X	2930	1/1	0.80	1.19	71,71,71,71	0
31	MG	X	2910	1/1	0.82	0.43	85,85,85,85	0
31	MG	X	2912	1/1	0.84	0.31	60,60,60,60	0
31	MG	Y	205	1/1	0.84	0.12	77,77,77,77	0
31	MG	X	2906	1/1	0.86	0.85	79,79,79,79	0
31	MG	X	2901	1/1	0.86	0.62	110,110,110,110	0
31	MG	X	2929	1/1	0.87	0.35	77,77,77,77	0
31	MG	X	2907	1/1	0.87	0.38	53,53,53,53	0
31	MG	X	2911	1/1	0.87	0.34	35,35,35,35	0
31	MG	X	2926	1/1	0.88	0.51	56,56,56,56	0
31	MG	X	2908	1/1	0.89	0.39	49,49,49,49	0

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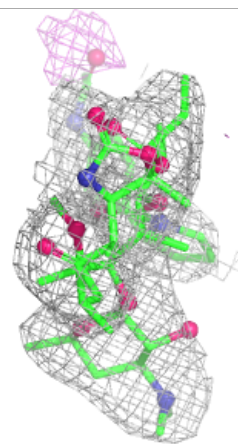
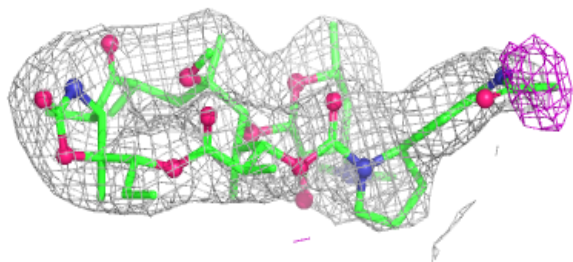
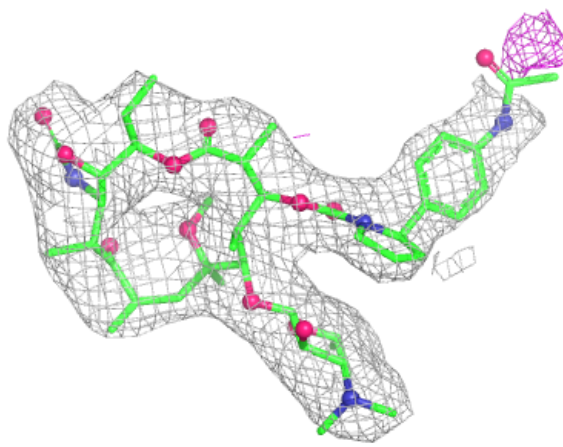
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
31	MG	Y	201	1/1	0.89	0.63	82,82,82,82	0
31	MG	X	2925	1/1	0.89	0.49	39,39,39,39	0
31	MG	X	2913	1/1	0.91	0.45	66,66,66,66	0
31	MG	X	2905	1/1	0.92	0.22	104,104,104,104	0
31	MG	Y	203	1/1	0.92	0.47	87,87,87,87	0
31	MG	Y	204	1/1	0.92	0.16	67,67,67,67	0
31	MG	X	2923	1/1	0.92	0.63	74,74,74,74	0
31	MG	X	2916	1/1	0.93	0.50	53,53,53,53	0
31	MG	X	2903	1/1	0.93	0.17	82,82,82,82	0
31	MG	Y	202	1/1	0.93	0.34	54,54,54,54	0
31	MG	X	2920	1/1	0.94	0.56	38,38,38,38	0
31	MG	X	2927	1/1	0.94	0.20	106,106,106,106	0
31	MG	X	2919	1/1	0.94	0.60	56,56,56,56	0
31	MG	X	2924	1/1	0.95	0.42	39,39,39,39	0
32	1F3	X	2931	60/60	0.95	0.10	38,60,90,99	0
31	MG	X	2917	1/1	0.96	0.47	37,37,37,37	0
31	MG	X	2902	1/1	0.97	0.63	45,45,45,45	0
31	MG	X	2915	1/1	0.97	0.26	24,24,24,24	0
31	MG	X	2914	1/1	0.98	0.54	51,51,51,51	0
31	MG	X	2918	1/1	0.98	0.48	32,32,32,32	0
31	MG	X	2921	1/1	0.98	0.38	18,18,18,18	0
31	MG	X	2928	1/1	0.98	0.58	42,42,42,42	0
31	MG	X	2909	1/1	0.99	0.45	37,37,37,37	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around 1F3 X 2931:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.