Full wwPDB X-ray Structure Validation Report ⓘ

Feb 11, 2024 – 09:17 AM EST

PDB ID	:	3CCE
Title	:	Structure of Anisomycin resistant 50S Ribosomal Subunit: 23S rRNA mutation U2535A
Authors	:	Blaha, G.; Gurel, G.
Deposited on	:	2008-02-25
Resolution	:	2.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

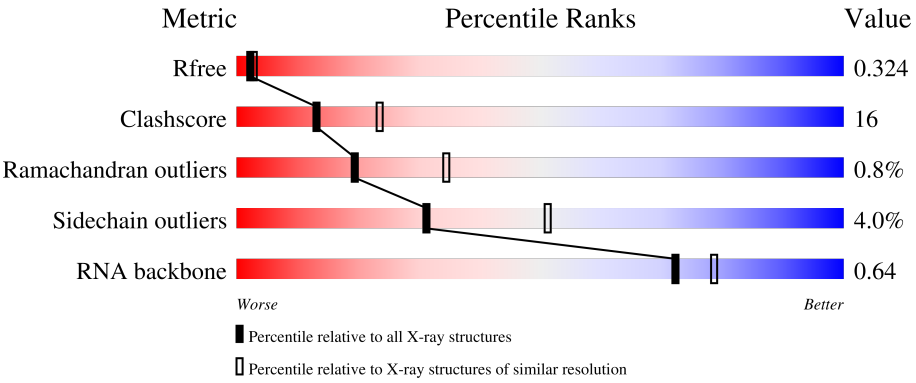
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.75 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_{free}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RNA backbone	3102	1060 (3.02-2.50)

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 >=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 <=5%

Mol	Chain	Length	Quality of chain
1	A	240	65% 30%
2	B	338	62% 34%
3	C	246	67% 30%
4	D	177	41% 37% 21%
5	E	178	67% 29%
6	F	120	74% 25%

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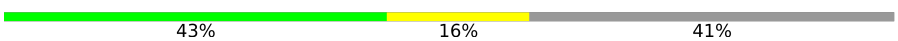
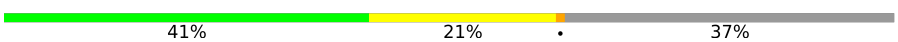
Mol	Chain	Length	Quality of chain
7	G	348	
8	H	177	
9	I	162	
10	J	145	
11	K	132	
12	L	165	
13	M	196	
14	N	187	
15	O	116	
16	P	149	
17	Q	96	
18	R	155	
19	S	85	
20	T	120	
21	U	67	
22	V	71	
23	W	154	
24	X	92	
25	Y	241	
26	Z	116	
27	1	57	
28	2	50	
29	3	92	
30	0	2923	
31	9	122	

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
33	CL	J	8801	-	-	X	-
33	CL	J	8802	-	-	X	-

2 Entry composition (i)

There are 38 unique types of molecules in this entry. The entry contains 99124 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 protein called 50S ribosomal protein L2P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	237	1753	1072	352	324	5	0	0	0

- Molecule 2 is a protein called 50S ribosomal protein L3P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	337	2625	1616	493	511	5	0	0	0

- Molecule 3 is a protein called 50S ribosomal protein L4P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	246	1860	1130	345	384	1	0	0	0

- Molecule 4 is a protein called 50S ribosomal protein L5P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	140	1094	685	195	210	4	0	0	0

- Molecule 5 is a protein called 50S ribosomal protein L6P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	172	1357	840	224	289	4	0	0	0

- Molecule 6 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	119	890	551	141	197	1	0	0	0

- Molecule 7 is a protein called 50S ribosomal protein L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	29	Total	C	N	O	S	0	0	0
			240	149	39	51	1			

- Molecule 8 is a protein called 50S ribosomal protein L10e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	160	Total	C	N	O	S	0	0	0
			1282	798	240	238	6			

- Molecule 9 is a protein called 50S ribosomal protein L11P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	70	Total	C	N	O	S	0	0	0
			519	323	81	114	1			

- Molecule 10 is a protein called 50S ribosomal protein L13P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	142	Total	C	N	O	S	0	0	0
			1120	696	199	222	3			

- Molecule 11 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	132	Total	C	N	O	S	0	0	0
			994	609	189	192	4			

- Molecule 12 is a protein called 50S ribosomal protein L15P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	L	145	Total	C	N	O	0	0	0
			1118	670	222	226			

- Molecule 13 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	194	Total	C	N	O	S	0	0	0
			1558	943	333	281	1			

- Molecule 14 is a protein called 50S ribosomal protein L18P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	186	Total	C	N	O	S	0	0	0
			1445	895	262	286	2			

- Molecule 15 is a protein called 50S ribosomal protein L18e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	O	115	Total	C	N	O	0	0	0
			865	529	161	175			

- Molecule 16 is a protein called 50S ribosomal protein L19e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	P	143	Total	C	N	O	0	0	0
			1136	683	229	224			

- Molecule 17 is a protein called 50S ribosomal protein L21e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	Q	95	Total	C	N	O	0	0	0
			735	450	141	144			

- Molecule 18 is a protein called 50S ribosomal protein L22P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	R	150	Total	C	N	O	S	0	0	0
			1149	713	209	223	4			

- Molecule 19 is a protein called 50S ribosomal protein L23P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	81	Total	C	N	O	S	0	0	0
			641	389	111	138	3			

- Molecule 20 is a protein called 50S ribosomal protein L24P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	T	119	Total	C	N	O	0	0	0
			950	568	180	202			

- Molecule 21 is a protein called 50S ribosomal protein L24e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	U	53	Total	C	N	O	S	0	0	0
			410	244	75	86	5			

- Molecule 22 is a protein called 50S ribosomal protein L29P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	65	Total	C	N	O	S	0	0	0
			499	304	94	100	1			

- Molecule 23 is a protein called 50S ribosomal protein L30P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	154	Total	C	N	O	S	0	0	0
			1196	737	209	244	6			

- Molecule 24 is a protein called 50S ribosomal protein L31e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	X	82	Total	C	N	O	S	0	0	0
			654	402	129	122	1			

- Molecule 25 is a protein called 50S ribosomal protein L32e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	Y	142	Total	C	N	O	0	0	0
			1130	686	228	216			

- Molecule 26 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	73	Total	C	N	O	S	0	0	0
			573	343	113	112	5			

- Molecule 27 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 28 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 29 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 30 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	0	2754	Total	C	N	O	P	0	0	0
			59022	26350	10876	19051	2745			

- Molecule 31 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	9	122	Total	C	N	O	P	0	0	0
			2599	1160	471	847	121			

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	A	2	Total	Mg	0	0
			2	2		
32	B	1	Total	Mg	0	0
			1	1		
32	K	1	Total	Mg	0	0
			1	1		
32	T	1	Total	Mg	0	0
			1	1		
32	Y	1	Total	Mg	0	0
			1	1		
32	0	86	Total	Mg	0	0
			86	86		
32	9	1	Total	Mg	0	0
			1	1		

- Molecule 33 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	A	1	Total Cl 1 1	0	0
33	B	1	Total Cl 1 1	0	0
33	J	3	Total Cl 3 3	0	0
33	L	1	Total Cl 1 1	0	0
33	M	1	Total Cl 1 1	0	0
33	N	1	Total Cl 1 1	0	0
33	O	1	Total Cl 1 1	0	0
33	Q	1	Total Cl 1 1	0	0
33	R	1	Total Cl 1 1	0	0
33	3	1	Total Cl 1 1	0	0
33	0	10	Total Cl 10 10	0	0

- Molecule 34 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	A	3	Total Sr 3 3	0	0
34	B	2	Total Sr 2 2	0	0
34	F	1	Total Sr 1 1	0	0
34	R	1	Total Sr 1 1	0	0
34	S	1	Total Sr 1 1	0	0
34	1	2	Total Sr 2 2	0	0
34	3	2	Total Sr 2 2	0	0
34	0	92	Total Sr 92 92	0	0
34	9	4	Total Sr 4 4	0	0

- Molecule 35 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	C	1	Total Na 1 1	0	0
35	J	1	Total Na 1 1	0	0
35	M	1	Total Na 1 1	0	0
35	Q	1	Total Na 1 1	0	0
35	R	1	Total Na 1 1	0	0
35	S	1	Total Na 1 1	0	0
35	0	67	Total Na 67 67	0	0
35	9	2	Total Na 2 2	0	0

- Molecule 36 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	O	1	Total Cd 1 1	0	0
36	U	1	Total Cd 1 1	0	0
36	Z	1	Total Cd 1 1	0	0
36	1	1	Total Cd 1 1	0	0
36	3	1	Total Cd 1 1	0	0

- Molecule 37 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	0	2	Total K 2 2	0	0

- Molecule 38 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	A	118	Total O 118 118	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	B	144	Total O 144 144	0	0
38	C	179	Total O 179 179	0	0
38	D	46	Total O 46 46	0	0
38	E	40	Total O 40 40	0	0
38	F	27	Total O 27 27	0	0
38	G	19	Total O 19 19	0	0
38	H	68	Total O 68 68	0	0
38	I	5	Total O 5 5	0	0
38	J	55	Total O 55 55	0	0
38	K	52	Total O 52 52	0	0
38	L	84	Total O 84 84	0	0
38	M	127	Total O 127 127	0	0
38	N	63	Total O 63 63	0	0
38	O	40	Total O 40 40	0	0
38	P	61	Total O 61 61	0	0
38	Q	43	Total O 43 43	0	0
38	R	84	Total O 84 84	0	0
38	S	33	Total O 33 33	0	0
38	T	33	Total O 33 33	0	0
38	U	28	Total O 28 28	0	0
38	V	14	Total O 14 14	0	0

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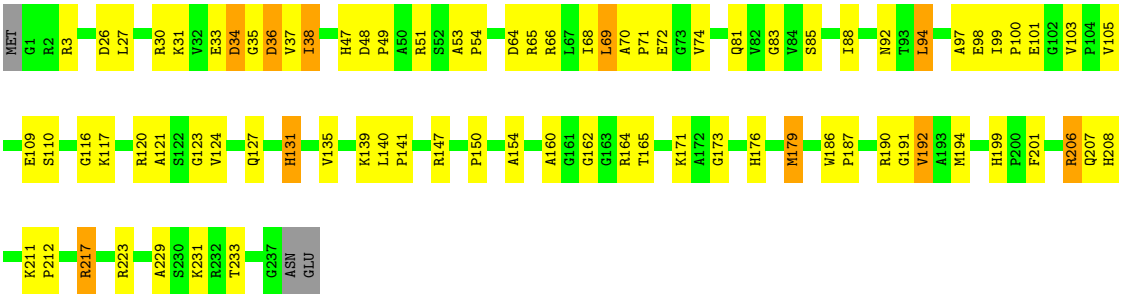
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	W	67	Total O 67 67	0	0
38	X	30	Total O 30 30	0	0
38	Y	100	Total O 100 100	0	0
38	Z	32	Total O 32 32	0	0
38	1	55	Total O 55 55	0	0
38	2	42	Total O 42 42	0	0
38	3	63	Total O 63 63	0	0
38	0	5927	Total O 5927 5927	0	0
38	9	144	Total O 144 144	0	0

3 Residue-property plots (i)

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

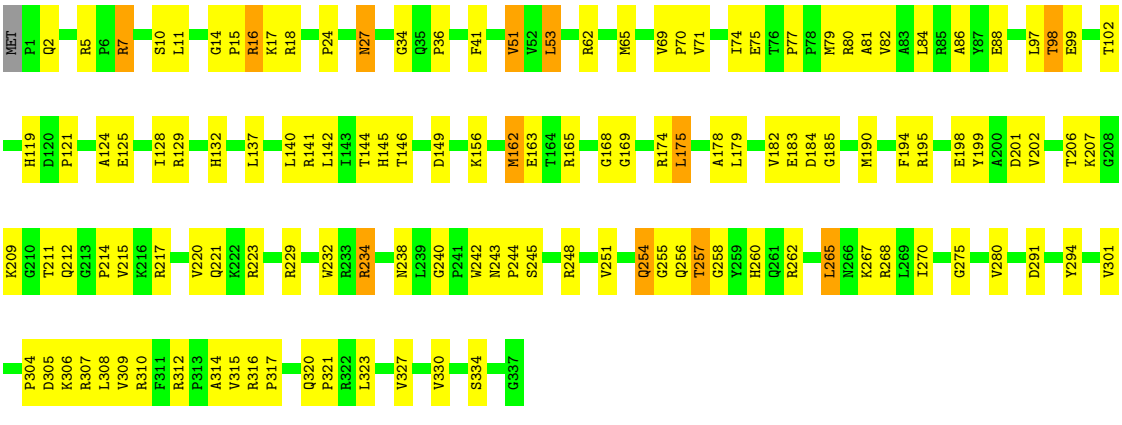
- Molecule 1: 50S ribosomal protein L2P

Chain A:



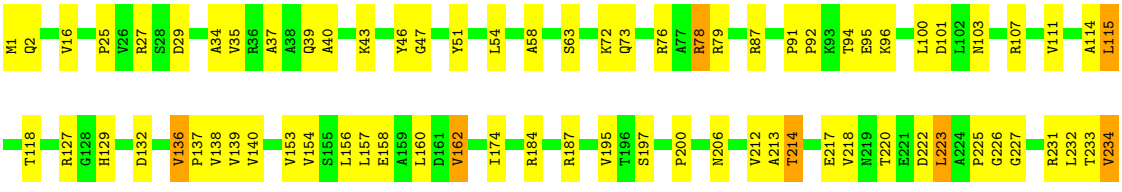
- Molecule 2: 50S ribosomal protein L3P

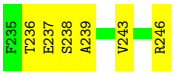
Chain B:



- Molecule 3: 50S ribosomal protein L4P

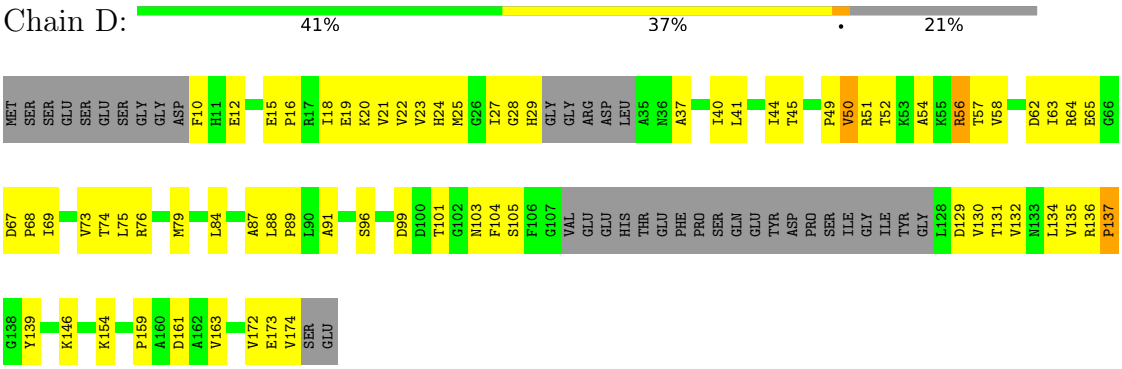
Chain C:





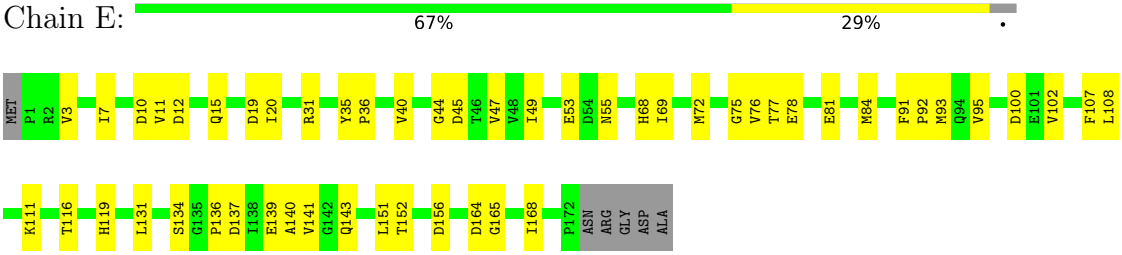
• Molecule 4: 50S ribosomal protein L5P

Chain D:



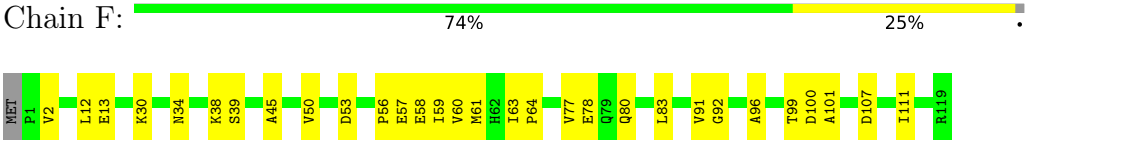
• Molecule 5: 50S ribosomal protein L6P

Chain E:



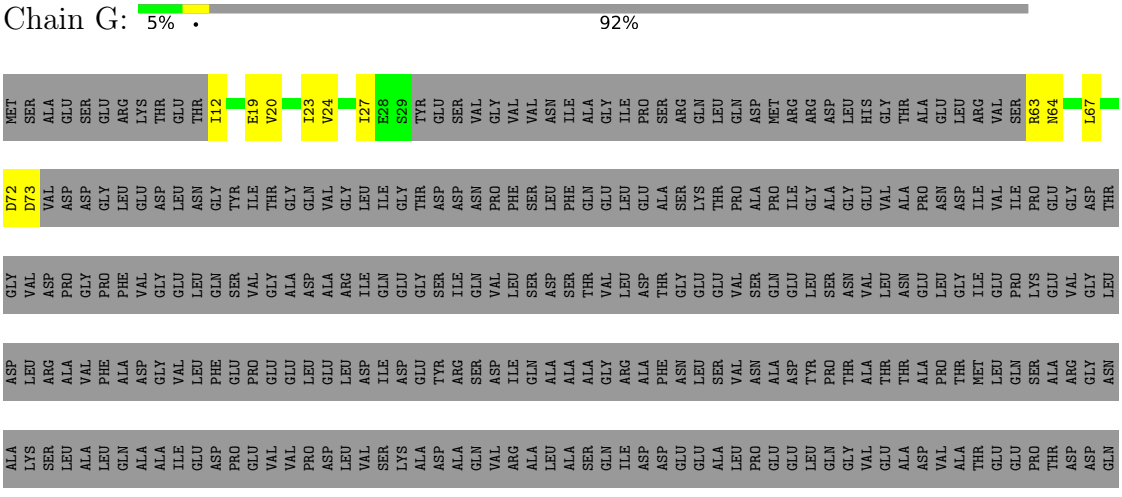
• Molecule 6: 50S ribosomal protein L7Ae

Chain F:



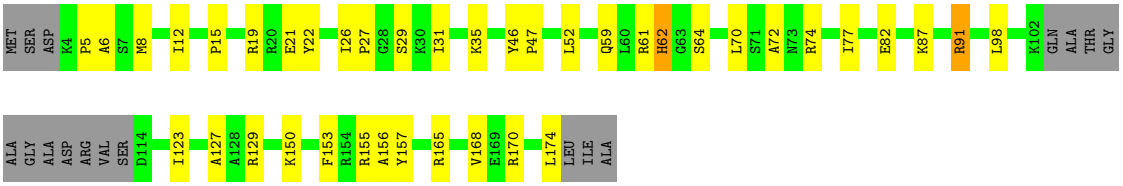
• Molecule 7: 50S ribosomal protein L10E

Chain G:



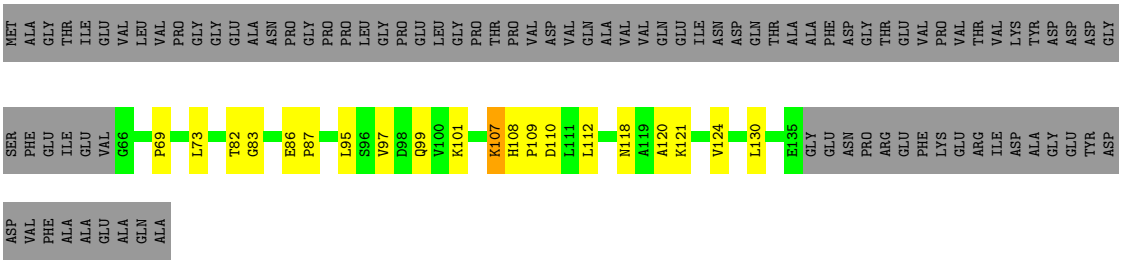
• Molecule 8: 50S ribosomal protein L10e

Chain H:



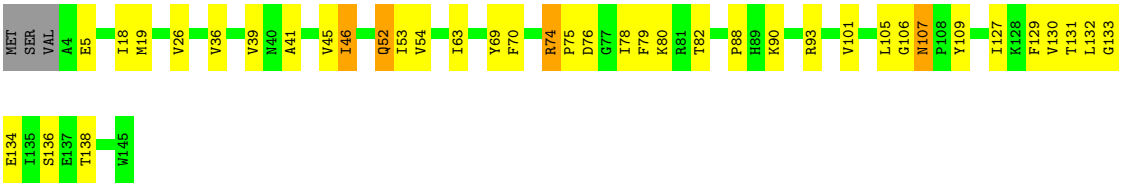
• Molecule 9: 50S ribosomal protein L11P

Chain I:



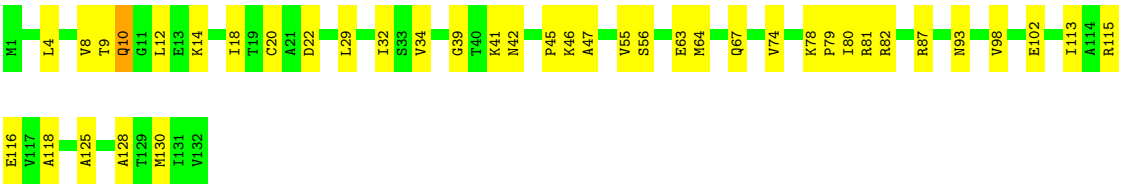
• Molecule 10: 50S ribosomal protein L13P

Chain J:



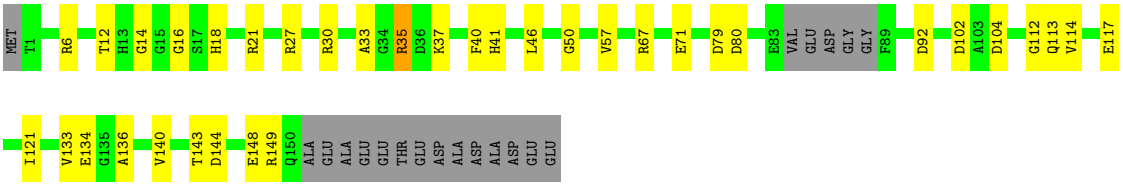
• Molecule 11: 50S ribosomal protein L14P

Chain K:



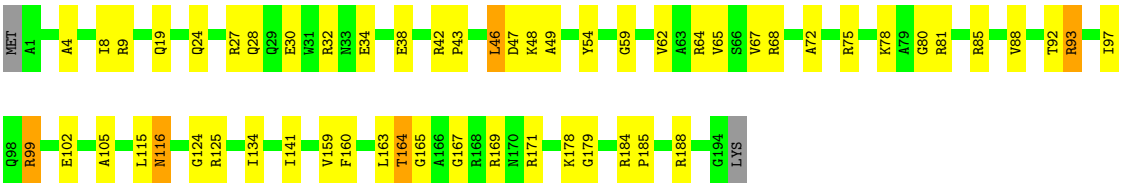
• Molecule 12: 50S ribosomal protein L15P

Chain L:



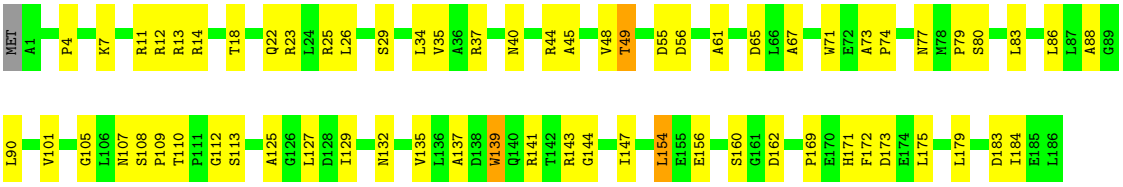
• Molecule 13: 50S ribosomal protein L15e

Chain M:



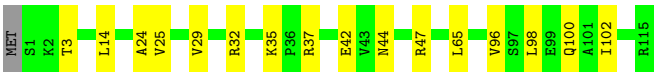
• Molecule 14: 50S ribosomal protein L18P

Chain N:



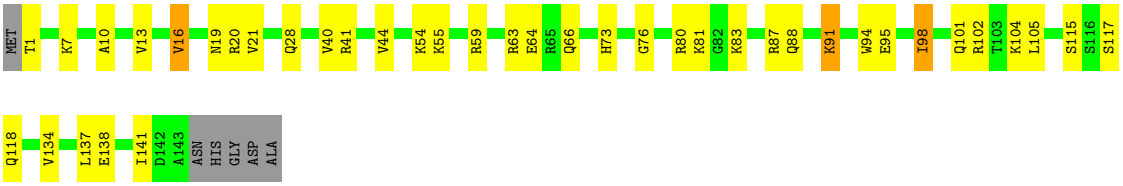
• Molecule 15: 50S ribosomal protein L18e

Chain O:



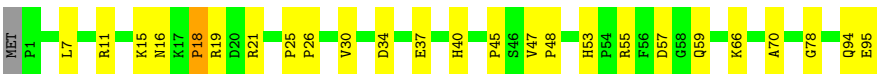
• Molecule 16: 50S ribosomal protein L19e

Chain P:



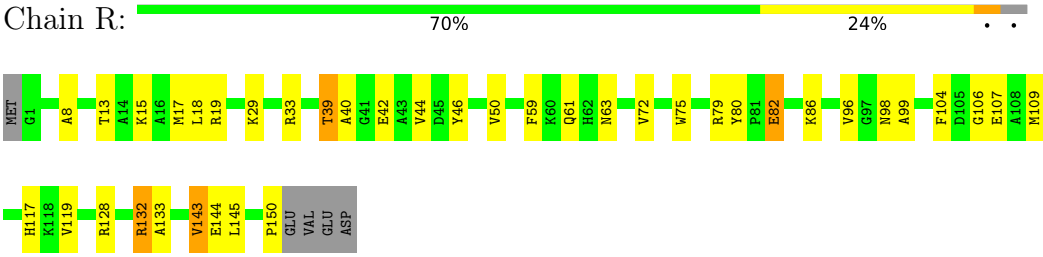
• Molecule 17: 50S ribosomal protein L21e

Chain Q:



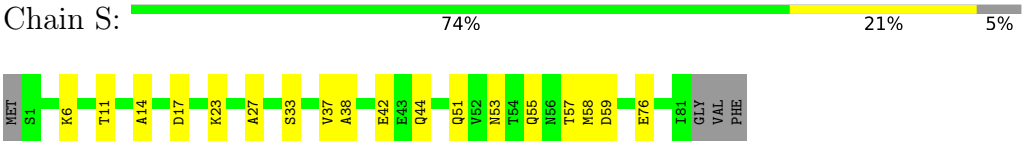
• Molecule 18: 50S ribosomal protein L22P

Chain R:



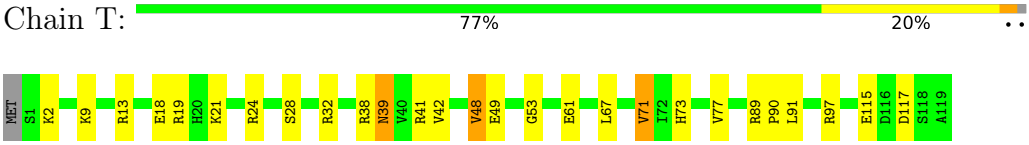
• Molecule 19: 50S ribosomal protein L23P

Chain S:



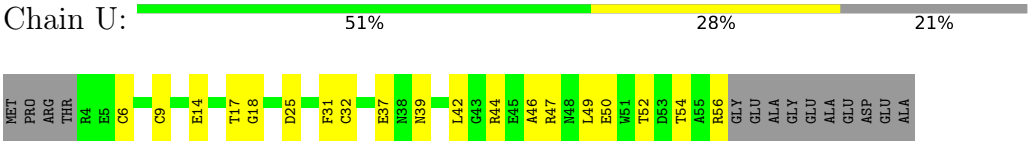
• Molecule 20: 50S ribosomal protein L24P

Chain T:



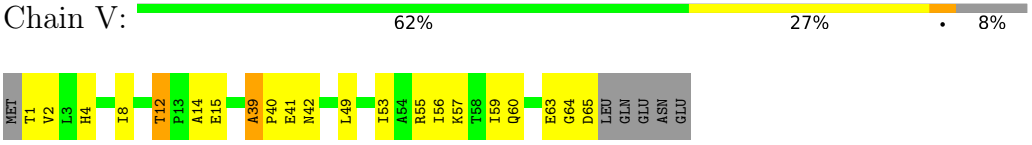
• Molecule 21: 50S ribosomal protein L24e

Chain U:



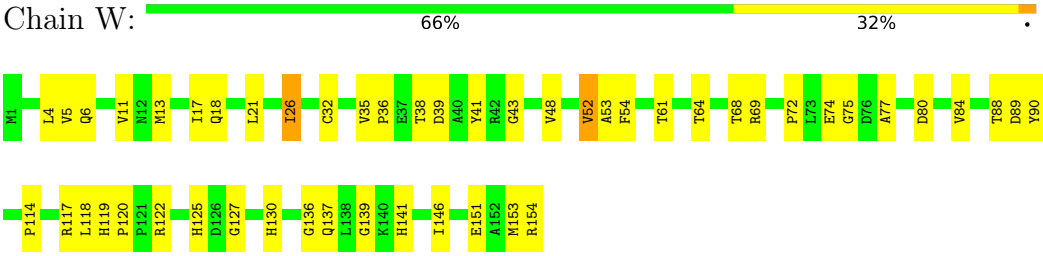
• Molecule 22: 50S ribosomal protein L29P

Chain V:



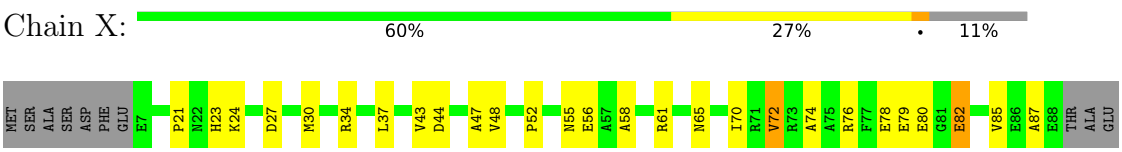
• Molecule 23: 50S ribosomal protein L30P

Chain W:



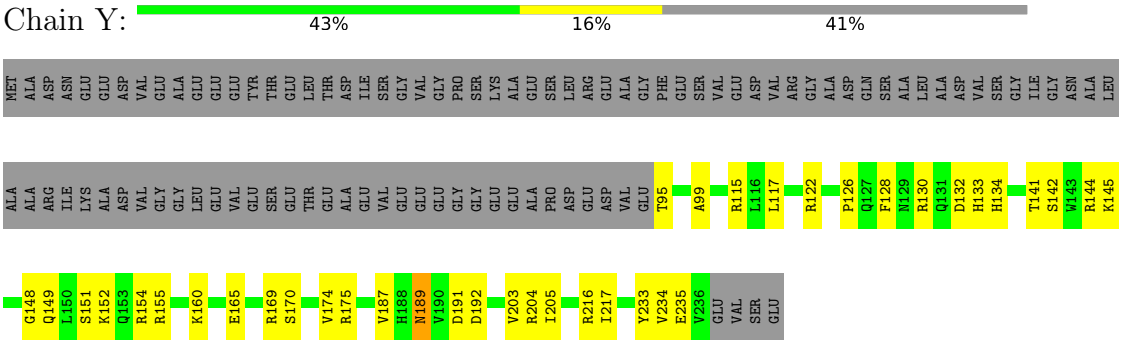
• Molecule 24: 50S ribosomal protein L31e

Chain X:



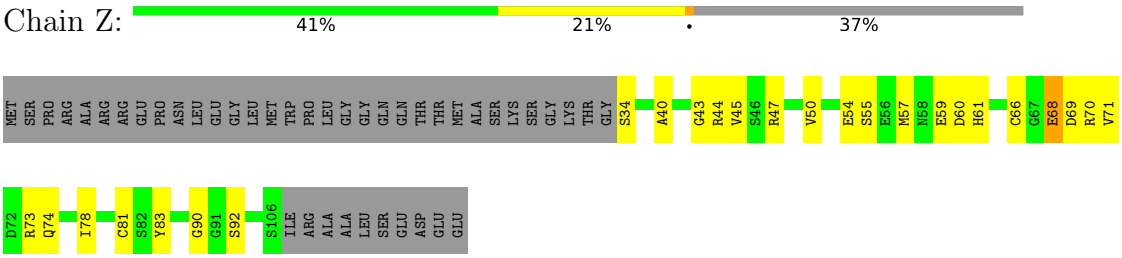
• Molecule 25: 50S ribosomal protein L32e

Chain Y:



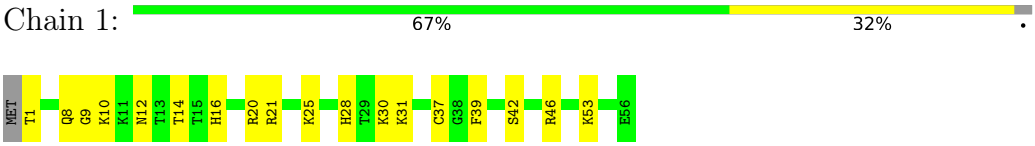
• Molecule 26: 50S ribosomal protein L37Ae

Chain Z:



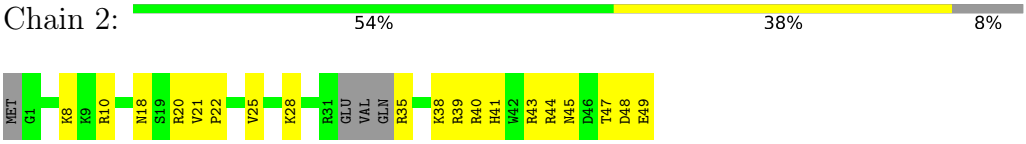
• Molecule 27: 50S ribosomal protein L37e

Chain 1:



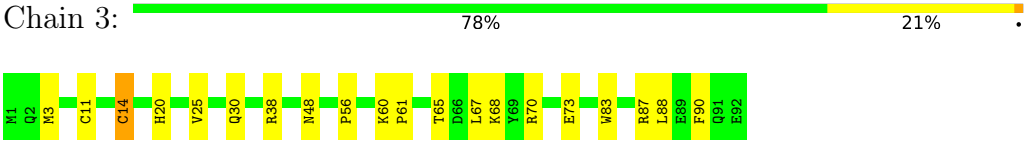
• Molecule 28: 50S ribosomal protein L39e

Chain 2:



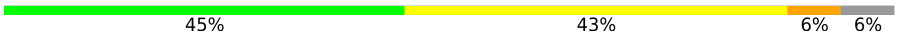
• Molecule 29: 50S ribosomal protein L44E

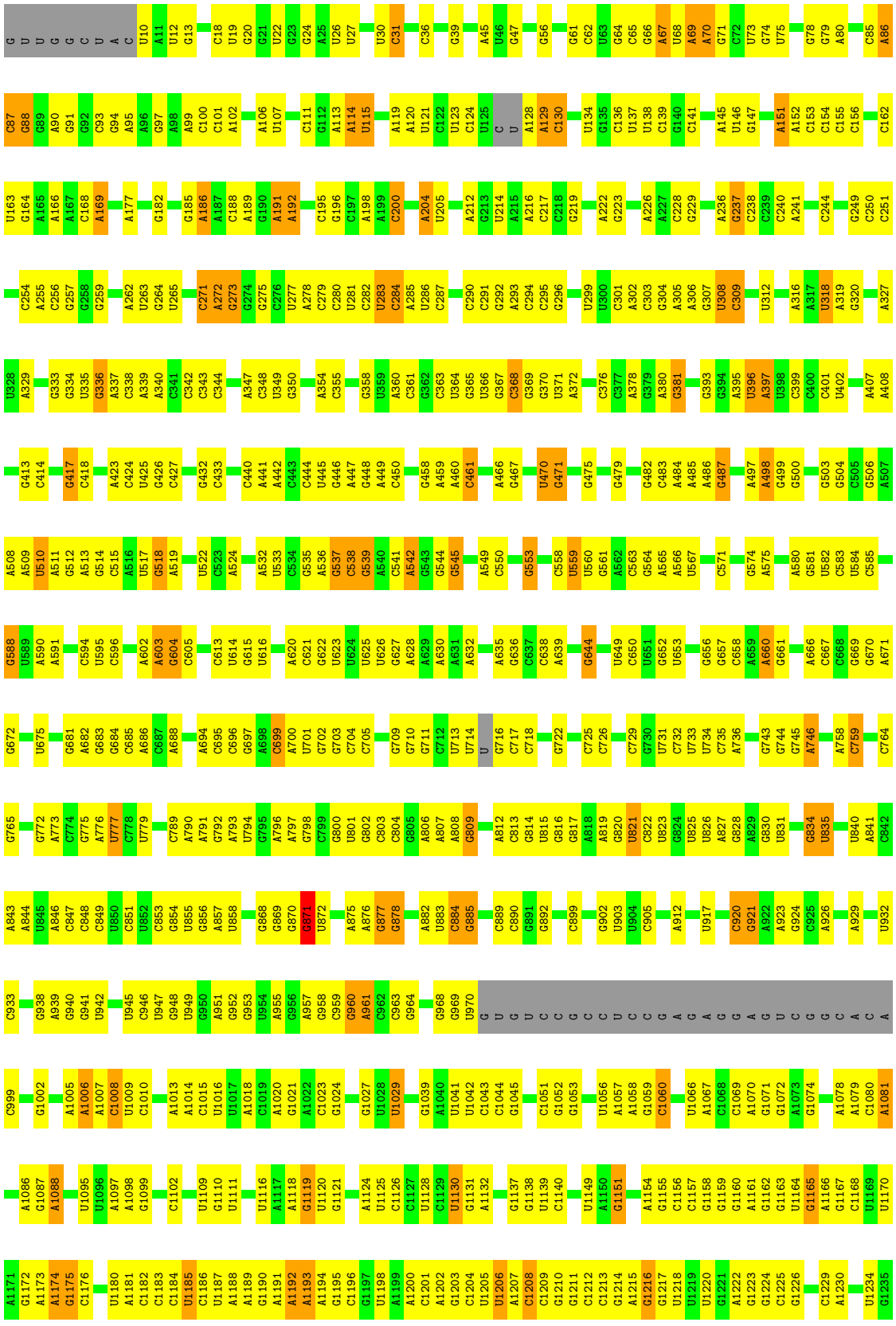
Chain 3:

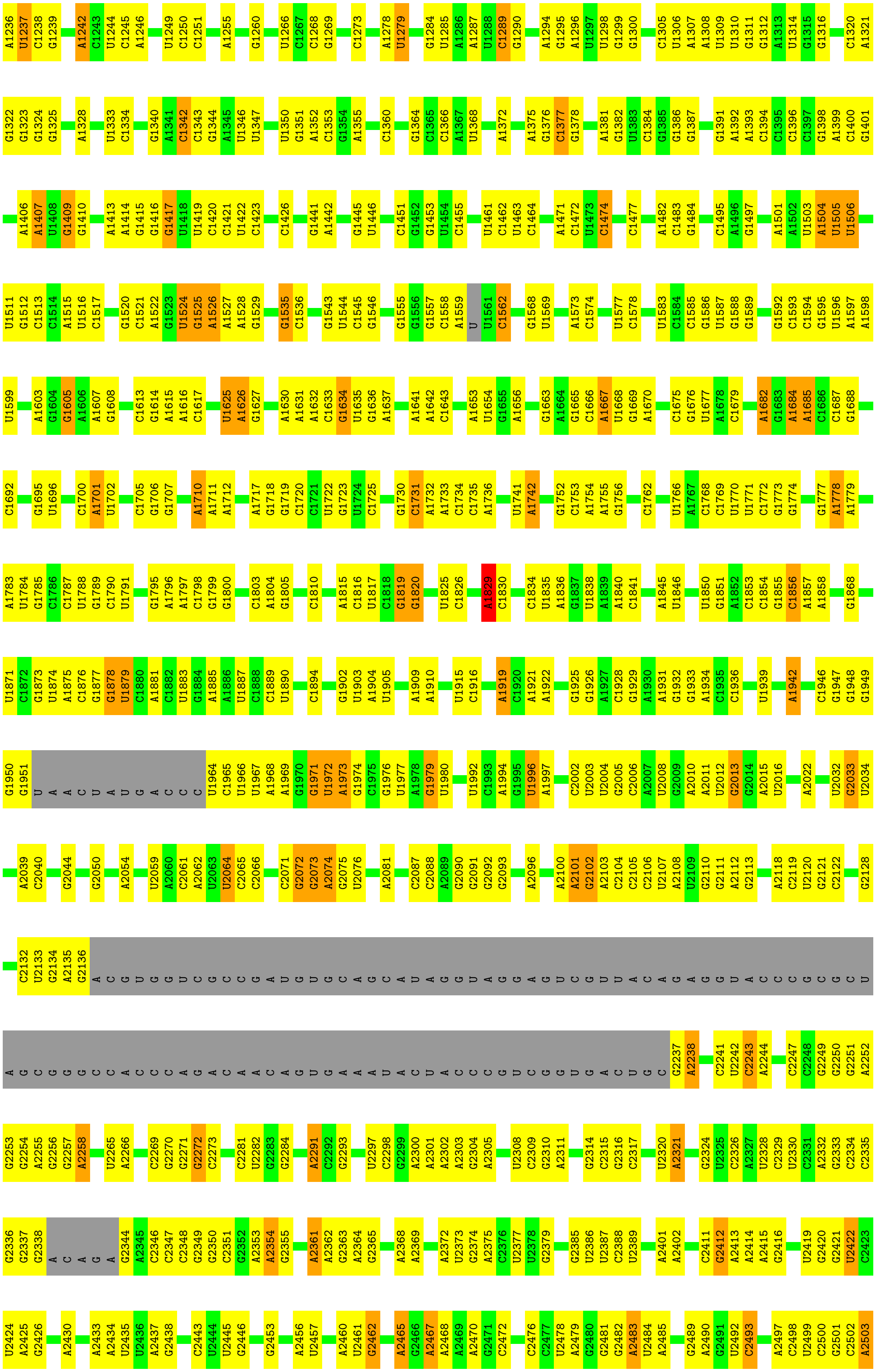


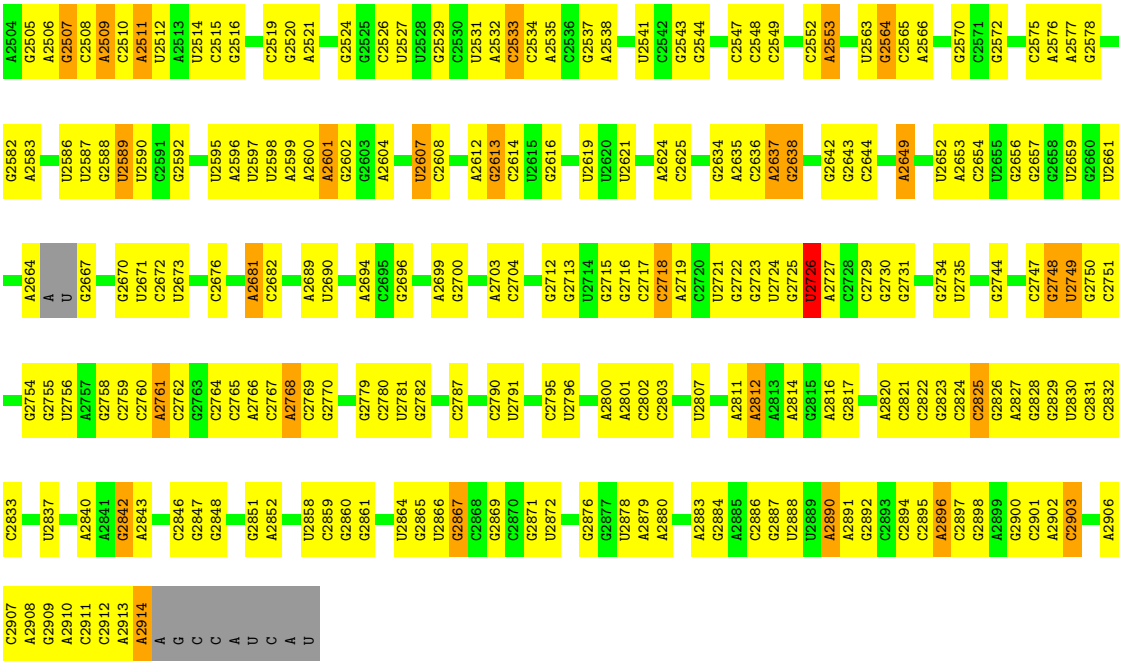
• Molecule 30: 23S RIBOSOMAL RNA

Chain 0:



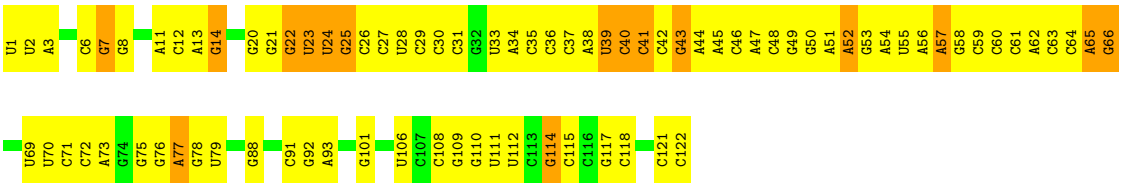



A1236 U1237 C1238 G1239 A1242 C1243 U1244 C1245 A1246 U1249 C1250 C1251 A1255 G1260 U1266 C1267 C1268 G1269 C1273 A1278 U1279 G1284 U1285 A1286 A1287 U1288 C1289 G1290 A1294 G1295 A1296 U1297 U1298 G1299 G1300 C1305 U1306 A1307 A1308 U1309 U1310 G1311 G1312 A1313 U1314 G1315 G1316 C1320 A1321
G1322 G1323 G1324 G1325 A1328 U1333 C1334 G1340 A1341 C1342 C1343 G1344 A1345 U1346 U1347 U1350 G1351 A1352 C1353 G1354 A1355 C1360 G1364 C1365 C1366 A1367 U1368 A1372 A1375 G1376 C1377 G1378 A1381 G1382 U1383 C1384 G1385 G1386 G1387 G1391 A1392 A1393 C1394 C1395 C1396 C1397 G1398 A1399 C1400 G1401
A1406 A1407 U1408 G1409 G1410 A1413 A1414 G1415 G1416 G1417 U1418 U1419 C1420 C1421 U1422 C1423 C1426 G1441 A1442 G1445 U1446 C1451 G1452 G1453 U1454 C1455 U1461 C1462 U1463 C1464 A1471 C1472 U1473 C1474 C1477 A1482 C1483 G1484 C1495 A1496 G1497 A1501 A1502 U1503 A1504 U1505 U1506
U1511 G1512 C1513 C1514 A1515 U1516 C1517 G1520 C1521 A1522 G1523 U1524 G1525 A1526 A1527 A1528 G1529 G1535 C1536 G1543 U1544 C1545 G1546 G1555 G1556 G1557 C1558 A1559 U U1561 C1562 G1568 U1569 A1573 C1574 U1577 C1578 U1583 C1584 C1585 G1586 U1587 G1588 G1589 G1592 G1593 C1594 G1595 U1596 A1597 A1598
U1599 A1603 G1604 G1605 A1606 A1607 G1608 C1613 G1614 A1615 A1616 C1617 U1625 A1626 G1627 A1630 A1631 A1632 C1633 G1634 U1635 G1636 A1637 A1641 A1642 C1643 A1653 U1654 G1655 A1656 G1663 A1664 G1665 C1666 A1667 U1668 G1669 A1670 C1675 C1676 U1677 A1678 C1679 A1682 G1683 A1684 A1685 C1686 C1687 G1688
C1692 G1695 U1696 C1700 A1701 U1702 C1705 G1706 G1707 A1710 A1711 A1712 A1717 G1718 G1719 C1720 C1721 U1722 G1723 U1724 C1725 G1730 C1731 A1732 A1733 C1734 C1735 A1736 U1741 A1742 G1752 C1753 A1754 A1755 G1756 C1762 U1766 A1767 C1768 C1769 U1770 U1771 C1772 G1773 U1774 G1777 A1778 A1779
A1783 U1784 G1785 C1786 C1787 U1788 G1789 C1790 U1791 G1795 A1796 A1797 C1798 G1799 G1800 C1803 A1804 G1805 C1810 A1815 C1816 U1817 C1818 G1819 G1820 U1825 C1826 A1829 C1830 C1834 U1835 A1836 G1837 U1838 A1839 A1840 C1841 A1845 U1846 U1850 G1851 A1852 C1853 C1854 G1855 C1856 A1857 A1858 G1868
U1871 C1872 G1873 U1874 A1875 C1876 G1877 G1878 U1879 C1880 A1881 C1882 U1883 G1884 A1885 A1886 U1887 C1888 C1889 U1890 C1894 G1902 U1903 A1904 U1905 A1909 A1910 U1915 C1916 A1919 C1920 A1921 A1922 G1925 G1926 A1927 C1928 G1929 A1930 A1931 G1932 G1933 A1934 C1935 C1936 U1939 A1942 C1946 G1947 G1948 G1949
G1950 G1951 U A A C U A U G A C C C U1964 C1965 U1966 U1967 A1968 A1969 G1970 G1971 U1972 A1973 G1974 C1975 G1976 U1977 A1978 G1979 U1980 U1992 C1993 A1994 G1995 U1996 A1997 C2002 U2003 U2004 G2005 C2006 A2007 U2008 G2009 A2010 A2011 U2012 G2013 G2014 A2015 U2016 A2022 U2032 G2033 U2034
A2039 C2040 G2044 G2050 A2054 U2059 A2060 C2061 A2062 U2063 U2064 C2065 C2066 C2071 G2072 G2073 A2074 G2075 U2076 A2081 C2087 C2088 A2089 G2090 G2091 G2092 G2093 A2096 A2100 A2101 G2102 A2103 C2104 C2105 C2106 U2107 A2108 U2109 G2110 G2111 A2112 G2113 A2118 C2119 U2120 G2121 C2122 G2128
C2132 U2133 G2134 A2135 G2136 A C G U G G U C G C C G A U G U G C A G C A U A G G U A G G A G U C G U U A C A G A G G U A C C C G C G C U
A G C G G G C C A C C C A G A C A A C A G U G A A A U A C U A C C C G U C G G U G A C U G C G2237 A2238 C2241 U2242 C2243 A2244 C2247 C2248 G2249 G2250 G2251 A2252
G2253 G2254 A2255 G2256 G2257 A2258 U2265 A2266 C2269 G2270 G2271 G2272 C2273 C2281 U2282 G2283 G2284 A2291 C2292 G2293 U2297 C2298 G2299 A2300 A2301 A2302 A2303 G2304 A2305 U2308 C2309 G2310 A2311 G2314 C2315 G2316 C2317 U2320 A2321 G2324 U2325 C2326 A2327 U2328 C2329 U2330 C2331 A2332 G2333 C2334 C2335
G2336 G2337 G2338 A C A G A G2344 A2345 C2346 C2347 C2348 G2349 G2350 C2351 G2352 A2353 A2354 G2355 A2361 A2362 G2363 A2364 C2365 A2368 A2369 A2372 U2373 G2374 A2375 C2376 U2377 U2378 G2379 G2385 U2386 U2387 C2388 U2389 A2401 A2402 C2411 G2412 A2413 A2414 A2415 G2416 U2419 G2420 G2421 U2422 C2423
U2424 A2425 G2426 A2430 A2433 A2434 U2435 U2436 A2437 G2438 C2443 U2444 U2445 G2446 G2453 A2456 U2457 A2460 U2461 G2462 A2465 G2466 U2467 A2468 A2469 A2470 G2471 C2472 C2476 C2477 U2478 A2479 G2480 G2481 G2482 A2483 U2484 A2485 G2489 A2490 G2491 U2492 C2493 A2497 C2498 U2499 C2500 G2501 C2502 A2503



• Molecule 31: 5S RIBOSOMAL RNA

Chain 9:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	212.83Å 299.90Å 576.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.33 – 2.75 85.81 – 2.41	Depositor EDS
% Data completeness (in resolution range)	81.3 (49.33-2.75) 81.1 (85.81-2.41)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.183 , 0.232 0.311 , 0.324	Depositor DCC
R_{free} test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å^2)	45.6	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 78.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	99124	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.24% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 1MA, CD, SR, OMU, PSU, OMG, NA, UR3, MG, CL, K

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.34	0/1786	0.65	0/2408
2	B	0.33	0/2690	0.64	0/3652
3	C	0.36	0/1885	0.65	0/2552
4	D	0.33	0/1111	0.55	0/1498
5	E	0.33	0/1382	0.56	0/1880
6	F	0.34	0/901	0.57	0/1224
7	G	0.30	0/241	0.50	0/324
8	H	0.35	0/1302	0.61	0/1743
9	I	0.30	0/526	0.50	0/716
10	J	0.34	0/1136	0.59	0/1530
11	K	0.35	0/1004	0.66	0/1351
12	L	0.31	0/1130	0.64	0/1509
13	M	0.34	0/1582	0.63	0/2116
14	N	0.30	0/1474	0.62	0/1999
15	O	0.34	0/874	0.60	0/1181
16	P	0.32	0/1147	0.53	0/1528
17	Q	0.34	0/749	0.65	0/1005
18	R	0.35	0/1172	0.64	0/1578
19	S	0.35	0/648	0.59	0/875
20	T	0.33	0/958	0.62	0/1289
21	U	0.34	0/417	0.57	0/562
22	V	0.31	0/502	0.49	0/675
23	W	0.34	0/1219	0.61	0/1655
24	X	0.34	0/664	0.60	0/895
25	Y	0.36	0/1146	0.62	0/1536
26	Z	0.36	0/584	0.58	0/781
27	1	0.40	0/438	0.63	0/578
28	2	0.34	0/401	0.60	0/529
29	3	0.36	0/771	0.59	0/1024
30	0	0.37	0/65960	0.68	6/102872 (0.0%)
31	9	0.32	0/2904	0.67	1/4526 (0.0%)
All	All	0.36	0/98704	0.66	7/147591 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
23	W	0	1
30	0	0	26
All	All	0	27

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	0	1819	G	C5'-C4'-C3'	6.12	125.79	116.00
30	0	871	G	C5'-C4'-O4'	-6.04	101.86	109.10
30	0	1504	A	C1'-O4'-C4'	-5.84	105.22	109.90
30	0	1504	A	N9-C1'-C2'	5.53	121.18	114.00
30	0	841	A	C1'-O4'-C4'	-5.34	105.63	109.90
30	0	2726	U	N1-C1'-C2'	5.27	120.85	114.00
31	9	39	U	N1-C1'-C2'	5.25	120.82	114.00

There are no chirality outliers.

All (27) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	1039	G	Sidechain
30	0	1078	A	Sidechain
30	0	1340	G	Sidechain
30	0	1417	G	Sidechain
30	0	1445	G	Sidechain
30	0	1653	A	Sidechain
30	0	1777	G	Sidechain
30	0	1829	A	Sidechain
30	0	1877	G	Sidechain
30	0	1878	G	Sidechain
30	0	1972	U	Sidechain
30	0	2076	U	Sidechain
30	0	22	U	Sidechain
30	0	2412	G	Sidechain
30	0	2465	A	Sidechain
30	0	2493	C	Sidechain
30	0	2503	A	Sidechain

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Mol	Chain	Res	Type	Group
30	0	2552	C	Sidechain
30	0	26	U	Sidechain
30	0	2607	U	Sidechain
30	0	2842	G	Sidechain
30	0	396	U	Sidechain
30	0	458	G	Sidechain
30	0	470	U	Sidechain
30	0	471	G	Sidechain
30	0	518	G	Sidechain
23	W	90	TYR	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	A	1753	0	1766	80	0
2	B	2625	0	2533	110	0
3	C	1860	0	1813	73	0
4	D	1094	0	1085	56	0
5	E	1357	0	1266	42	0
6	F	890	0	843	23	0
7	G	240	0	231	7	0
8	H	1282	0	1292	33	0
9	I	519	0	500	24	0
10	J	1120	0	1098	36	0
11	K	994	0	1027	37	0
12	L	1118	0	1076	30	0
13	M	1558	0	1573	48	0
14	N	1445	0	1401	61	0
15	O	865	0	873	22	0
16	P	1136	0	1123	36	0
17	Q	735	0	729	20	0
18	R	1149	0	1122	33	0
19	S	641	0	605	13	0
20	T	950	0	924	21	0
21	U	410	0	364	16	0
22	V	499	0	511	16	0
23	W	1196	0	1137	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	X	654	0	653	21	0
25	Y	1130	0	1133	41	0
26	Z	573	0	531	18	0
27	1	431	0	426	25	0
28	2	396	0	413	21	0
29	3	755	0	729	15	0
30	0	59022	0	29809	1550	0
31	9	2599	0	1325	114	0
32	0	86	0	0	0	0
32	9	1	0	0	0	0
32	A	2	0	0	0	0
32	B	1	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0
32	Y	1	0	0	0	0
33	0	10	0	0	1	0
33	3	1	0	0	0	0
33	A	1	0	0	0	0
33	B	1	0	0	0	0
33	J	3	0	0	5	0
33	L	1	0	0	0	0
33	M	1	0	0	0	0
33	N	1	0	0	1	0
33	O	1	0	0	0	0
33	Q	1	0	0	0	0
33	R	1	0	0	0	0
34	0	92	0	0	0	0
34	1	2	0	0	0	0
34	3	2	0	0	0	0
34	9	4	0	0	0	0
34	A	3	0	0	0	0
34	B	2	0	0	0	0
34	F	1	0	0	0	0
34	R	1	0	0	0	0
34	S	1	0	0	0	0
35	0	67	0	0	0	0
35	9	2	0	0	0	0
35	C	1	0	0	0	0
35	J	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	S	1	0	0	0	0
36	1	1	0	0	0	0
36	3	1	0	0	0	0
36	O	1	0	0	0	0
36	U	1	0	0	0	0
36	Z	1	0	0	0	0
37	0	2	0	0	0	0
38	0	5927	0	0	235	0
38	1	55	0	0	3	0
38	2	42	0	0	3	0
38	3	63	0	0	3	0
38	9	144	0	0	10	0
38	A	118	0	0	7	0
38	B	144	0	0	11	0
38	C	179	0	0	19	0
38	D	46	0	0	4	0
38	E	40	0	0	2	0
38	F	27	0	0	1	0
38	G	19	0	0	0	0
38	H	68	0	0	5	0
38	I	5	0	0	1	0
38	J	55	0	0	2	0
38	K	52	0	0	2	0
38	L	84	0	0	10	0
38	M	127	0	0	5	0
38	N	63	0	0	4	0
38	O	40	0	0	2	0
38	P	61	0	0	1	0
38	Q	43	0	0	1	0
38	R	84	0	0	5	0
38	S	33	0	0	2	0
38	T	33	0	0	2	0
38	U	28	0	0	2	0
38	V	14	0	0	1	0
38	W	67	0	0	5	0
38	X	30	0	0	0	0
38	Y	100	0	0	10	0
38	Z	32	0	0	0	0
All	All	99124	0	59911	2446	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 16.

All (2446) 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)
14:N:37:ARG:NH1	31:9:6:C:H5"	1.60	1.15
13:M:171:ARG:HD3	30:0:156:C:H5"	1.32	1.11
30:0:1160:G:C5'	30:0:1161:A:H5'	1.78	1.11
30:0:871:G:H5'	30:0:871:G:H8	1.12	1.11
30:0:871:G:H5'	30:0:871:G:C8	1.84	1.11
30:0:2717:C:H2'	30:0:2718:C:H5"	1.33	1.10
30:0:2291:A:C8	30:0:2309:C:H5'	1.87	1.09
30:0:1160:G:H5'	30:0:1161:A:C5'	1.82	1.08
30:0:381:G:H5"	38:0:4322:HOH:O	1.54	1.07
31:9:56:A:H2'	31:9:57:A:H5"	1.38	1.05
30:0:2502:C:H2'	30:0:2503:A:H5'	1.33	1.05
30:0:2502:C:C2'	30:0:2503:A:H5'	1.89	1.01
10:J:82:THR:HG23	30:0:1242:A:H5'	1.39	1.01
30:0:1209:C:H2'	30:0:1210:G:H8	1.19	1.01
31:9:76:G:H3'	31:9:77:A:H5"	1.39	1.01
30:0:282:C:H1'	30:0:368:C:N4	1.77	1.00
30:0:2717:C:C2'	30:0:2718:C:H5"	1.91	0.99
22:V:1:THR:HB	30:0:93:C:H5"	1.42	0.99
16:P:115:SER:H	16:P:118:GLN:HE21	1.08	0.99
30:0:2812:A:H2	30:0:2814:A:H62	1.07	0.98
30:0:1118:A:H8	30:0:1118:A:H3'	1.28	0.98
30:0:1372:A:H3'	38:0:7202:HOH:O	1.64	0.98
15:O:3:THR:HG22	30:0:656:G:H5'	1.45	0.97
30:0:1116:U:H3	30:0:1246:A:H62	1.11	0.96
8:H:59:GLN:HE21	8:H:129:ARG:HE	1.12	0.95
30:0:545:G:H5'	30:0:545:G:H8	1.30	0.95
30:0:2908:A:H2'	30:0:2909:G:O4'	1.66	0.95
30:0:542:A:H5'	30:0:542:A:H8	1.32	0.95
30:0:1160:G:H5'	30:0:1161:A:H5'	0.96	0.94
30:0:1666:C:O2'	30:0:1667:A:H5"	1.67	0.94
11:K:10:GLN:HE21	11:K:10:GLN:H	1.15	0.93
30:0:2769:C:C2'	30:0:2770:G:H5'	1.98	0.93
30:0:2497:A:H1'	30:0:2526:C:N4	1.84	0.93
30:0:1603:A:H5'	30:0:1605:G:O4'	1.68	0.92
30:0:1118:A:H3'	30:0:1118:A:C8	2.04	0.92
30:0:1701:A:H4'	30:0:1702:U:H5"	1.49	0.92
31:9:14:G:H5'	31:9:14:G:H8	1.36	0.91
30:0:1205:U:H2'	30:0:1206:U:H5"	1.52	0.91
30:0:960:G:H3'	30:0:960:G:N3	1.85	0.91
30:0:2812:A:H1'	38:0:5804:HOH:O	1.71	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:143:GLN:HE21	30:0:2780:C:H1'	1.34	0.91
30:0:871:G:H8	30:0:871:G:C5'	1.85	0.90
31:9:3:A:N6	31:9:22:G:H1'	1.86	0.90
30:0:282:C:O2'	30:0:283:U:H5'	1.71	0.90
30:0:870:G:H2'	30:0:871:G:H5"	1.53	0.90
2:B:212:GLN:HB2	2:B:257:THR:HG21	1.54	0.89
30:0:1679:C:H5'	38:0:9328:HOH:O	1.72	0.89
24:X:37:LEU:HD13	24:X:85:VAL:HG21	1.55	0.89
30:0:182:G:H5'	38:0:5169:HOH:O	1.72	0.88
30:0:1474:C:H6	30:0:1474:C:H5'	1.36	0.88
30:0:2524:G:N2	30:0:2526:C:H41	1.71	0.88
30:0:1119:G:N2	30:0:1246:A:C2	2.42	0.88
30:0:1666:C:H2'	30:0:1667:A:H5'	1.55	0.87
30:0:2769:C:H2'	30:0:2770:G:H5'	1.55	0.87
30:0:2508:C:H2'	38:0:6774:HOH:O	1.72	0.87
8:H:59:GLN:NE2	8:H:129:ARG:HE	1.71	0.87
30:0:1118:A:H62	30:0:1244:U:H3	1.23	0.87
31:9:56:A:C2'	31:9:57:A:H5"	2.05	0.87
30:0:2506:A:HO2'	30:0:2507:G:H8	1.16	0.87
30:0:1278:A:H4'	30:0:1279:U:C4	2.10	0.86
30:0:2637:A:H5'	38:0:9279:HOH:O	1.74	0.86
15:O:3:THR:CG2	30:0:656:G:H5'	2.05	0.86
30:0:1130:U:H5'	38:0:7684:HOH:O	1.75	0.86
30:0:541:C:C2'	30:0:542:A:H5"	2.05	0.86
2:B:238:ASN:HD22	2:B:240:GLY:H	1.22	0.85
23:W:88:THR:HB	38:W:6679:HOH:O	1.75	0.85
30:0:558:C:C2'	30:0:559:U:H5"	2.06	0.85
31:9:49:G:H5"	38:9:9088:HOH:O	1.75	0.85
30:0:1116:U:HO2'	30:0:1118:A:H2	0.86	0.85
30:0:1119:G:H22	30:0:1246:A:H2	1.19	0.85
30:0:2884:G:H5'	38:0:4133:HOH:O	1.76	0.84
30:0:506:G:H22	30:0:509:A:C5'	1.89	0.84
31:9:54:A:O2'	31:9:55:U:H5'	1.77	0.84
30:0:1451:C:H5'	30:0:1505:U:C5	2.12	0.84
23:W:137:GLN:HE21	23:W:141:HIS:HE1	1.21	0.84
23:W:88:THR:HG22	23:W:89:ASP:H	1.41	0.83
30:0:2586:U:H3	30:0:2592:G:H22	1.23	0.83
30:0:558:C:O2'	30:0:559:U:H5"	1.79	0.83
30:0:1183:C:H2'	38:0:6259:HOH:O	1.77	0.83
30:0:877:G:H5'	30:0:878:G:OP1	1.79	0.82
30:0:282:C:H1'	30:0:368:C:H41	1.41	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:32:ARG:HE	15:O:35:LYS:HD2	1.43	0.82
30:0:1209:C:H2'	30:0:1210:G:C8	2.10	0.82
31:9:92:G:H2'	31:9:93:A:C8	2.14	0.82
11:K:39:GLY:HA2	38:0:5233:HOH:O	1.79	0.82
30:0:2524:G:H21	30:0:2526:C:H41	1.23	0.82
4:D:154:LYS:H	4:D:154:LYS:HD2	1.42	0.82
30:0:1835:U:H5	30:0:1840:A:N7	1.76	0.82
30:0:2896:A:H5"	38:0:6114:HOH:O	1.78	0.82
1:A:223:ARG:HH12	30:0:2270:G:H4'	1.44	0.82
30:0:855:U:H5"	38:0:3639:HOH:O	1.80	0.82
30:0:559:U:H6	30:0:559:U:H5'	1.45	0.81
30:0:1741:U:H5'	30:0:1742:A:OP1	1.80	0.81
10:J:75:PRO:HG2	10:J:105:LEU:HD21	1.61	0.81
30:0:2748:G:H2'	38:0:7557:HOH:O	1.78	0.81
23:W:88:THR:HG23	23:W:110:GLN:HB3	1.62	0.81
30:0:1527:A:H1'	30:0:1528:A:C8	2.16	0.81
30:0:2529:G:H3'	38:0:7196:HOH:O	1.80	0.81
30:0:506:G:H22	30:0:509:A:H5"	1.45	0.81
22:V:12:THR:HG22	22:V:15:GLU:HG3	1.61	0.81
17:Q:15:LYS:HD3	30:0:2364:A:H5"	1.62	0.80
30:0:2497:A:H1'	30:0:2526:C:H42	1.46	0.80
30:0:541:C:H2'	30:0:542:A:C5'	2.11	0.80
11:K:29:LEU:HB3	11:K:55:VAL:HG11	1.63	0.80
22:V:1:THR:HG23	22:V:2:VAL:H	1.47	0.80
27:1:25:LYS:HD2	28:2:49:GLU:H	1.47	0.80
30:0:545:G:H5'	30:0:545:G:C8	2.15	0.80
16:P:117:SER:HB3	30:0:1593:C:OP1	1.82	0.80
30:0:2505:G:O2'	30:0:2506:A:H5'	1.82	0.80
30:0:541:C:H2'	30:0:542:A:H5"	1.64	0.79
30:0:2506:A:O2'	30:0:2507:G:H8	1.65	0.79
30:0:2570:G:H5"	38:0:4925:HOH:O	1.82	0.79
3:C:115:LEU:HD13	3:C:223:LEU:HD21	1.63	0.79
23:W:4:LEU:HD23	23:W:54:PHE:HB3	1.64	0.79
14:N:37:ARG:HH11	31:9:6:C:H5"	1.44	0.79
31:9:20:G:H3'	38:9:9054:HOH:O	1.82	0.79
30:0:1878:G:H1'	38:0:6135:HOH:O	1.81	0.79
14:N:83:LEU:HD13	14:N:175:LEU:HD23	1.65	0.79
30:0:1165:G:H21	30:0:1173:A:H5"	1.48	0.78
30:0:2604:A:H5'	38:0:5805:HOH:O	1.83	0.78
2:B:206:THR:HG21	30:0:2716:G:H5"	1.65	0.78
30:0:567:U:H5"	38:0:6420:HOH:O	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1856:C:H5'	30:0:1858:A:O4'	1.83	0.78
13:M:99:ARG:HD2	13:M:167:GLY:HA2	1.66	0.78
30:0:1206:U:H5'	30:0:1206:U:H6	1.47	0.78
30:0:2635:A:O2'	30:0:2636:C:H5'	1.83	0.78
30:0:2769:C:H2'	30:0:2770:G:C5'	2.14	0.78
10:J:52:GLN:NE2	30:0:1119:G:H2'	1.99	0.78
14:N:37:ARG:HH12	31:9:6:C:H5"	1.49	0.78
13:M:164:THR:HG22	13:M:167:GLY:H	1.46	0.77
30:0:69:A:H5'	30:0:69:A:H8	1.49	0.77
30:0:254:C:O2	30:0:254:C:H2'	1.84	0.77
30:0:2565:C:H4'	38:0:4847:HOH:O	1.84	0.77
1:A:199:HIS:HD2	1:A:201:PHE:H	1.31	0.77
30:0:2563:U:H2'	30:0:2565:C:O5'	1.85	0.77
16:P:115:SER:H	16:P:118:GLN:NE2	1.83	0.77
30:0:711:G:H1'	38:0:7109:HOH:O	1.84	0.77
30:0:1205:U:H2'	30:0:1206:U:C5'	2.13	0.77
30:0:1300:G:H1'	38:0:4697:HOH:O	1.84	0.77
16:P:88:GLN:NE2	30:0:1800:G:H1'	1.98	0.77
3:C:127:ARG:NH2	3:C:225:PRO:HG2	1.99	0.77
30:0:1205:U:C2'	30:0:1206:U:H5"	2.15	0.76
30:0:2812:A:H2	30:0:2814:A:N6	1.83	0.76
29:3:25:VAL:HG22	29:3:68:LYS:HG3	1.67	0.76
30:0:1973:A:H5'	30:0:1973:A:H8	1.49	0.76
30:0:1184:C:H1'	38:0:7483:HOH:O	1.85	0.76
30:0:536:A:H3'	38:0:5057:HOH:O	1.86	0.76
30:0:1342:C:C2'	30:0:1343:C:H5'	2.14	0.76
30:0:2587:OMU:H5	38:0:7502:HOH:O	1.85	0.76
31:9:14:G:H5'	31:9:14:G:C8	2.18	0.76
30:0:1641:A:H2'	30:0:1642:A:H5'	1.67	0.76
30:0:1979:G:H2'	38:0:3302:HOH:O	1.85	0.76
30:0:69:A:H5'	30:0:69:A:C8	2.21	0.76
30:0:1185:U:H2'	30:0:1186:C:H6	1.50	0.76
30:0:396:U:H1'	38:0:7643:HOH:O	1.86	0.75
30:0:1474:C:H5'	30:0:1474:C:C6	2.20	0.75
30:0:1701:A:H5"	30:0:1702:U:H3'	1.68	0.75
18:R:8:ALA:HB1	18:R:13:THR:HG21	1.69	0.75
26:Z:44:ARG:HH21	30:0:1771:U:H5'	1.52	0.75
22:V:39:ALA:H	22:V:40:PRO:HD2	1.51	0.75
23:W:6:GLN:HB2	23:W:26:ILE:HD12	1.69	0.75
1:A:223:ARG:NH1	30:0:2270:G:H4'	2.02	0.75
30:0:1182:C:H1'	30:0:1192:A:H8	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:31:C:H2'	38:0:7701:HOH:O	1.86	0.75
30:0:282:C:O2	30:0:282:C:H2'	1.85	0.75
30:0:2498:C:O2'	30:0:2499:U:H5'	1.87	0.75
30:0:1455:C:H3'	38:0:7887:HOH:O	1.86	0.74
20:T:24:ARG:HH21	20:T:39:ASN:HD22	1.34	0.74
30:0:1919:A:H4'	38:0:4863:HOH:O	1.86	0.74
30:0:2426:G:H1'	38:0:6107:HOH:O	1.87	0.74
14:N:144:GLY:O	14:N:147:ILE:HG22	1.88	0.74
30:0:1118:A:C8	30:0:1118:A:C3'	2.69	0.74
13:M:134:ILE:HG23	13:M:141:ILE:HD13	1.69	0.74
30:0:2456:A:H1'	38:0:6611:HOH:O	1.87	0.74
10:J:131:THR:HB	10:J:134:GLU:HG3	1.70	0.74
14:N:113:SER:HB2	38:N:8854:HOH:O	1.88	0.74
30:0:582:U:H2'	30:0:583:C:H6	1.53	0.74
31:9:54:A:H2	38:9:9061:HOH:O	1.70	0.74
10:J:82:THR:CG2	30:0:1242:A:H5'	2.16	0.73
30:0:564:G:H1'	38:0:6328:HOH:O	1.86	0.73
30:0:1634:G:H3'	38:0:3900:HOH:O	1.87	0.73
30:0:2073:G:H5"	38:0:3832:HOH:O	1.88	0.73
17:Q:95:GLU:HA	30:0:949:U:H4'	1.71	0.73
18:R:39:THR:HG22	18:R:42:GLU:H	1.53	0.73
23:W:80:ASP:O	23:W:84:VAL:HG23	1.88	0.73
30:0:2004:U:H4'	38:0:5318:HOH:O	1.87	0.73
30:0:2851:G:O2'	30:0:2852:A:H5'	1.89	0.73
28:2:43:ARG:HH22	30:0:1684:A:H1'	1.53	0.73
30:0:542:A:H5'	30:0:542:A:C8	2.21	0.73
30:0:1615:A:H4'	38:0:5899:HOH:O	1.88	0.73
10:J:127:ILE:HG22	33:J:8801:CL:CL	2.24	0.73
21:U:47:ARG:HG3	38:U:4381:HOH:O	1.89	0.73
2:B:18:ARG:HE	2:B:256:GLN:HE21	1.35	0.73
30:0:603:A:H5"	30:0:604:G:OP1	1.88	0.73
30:0:854:G:H5"	38:0:3639:HOH:O	1.88	0.73
30:0:2524:G:H21	30:0:2526:C:N4	1.85	0.73
30:0:1060:C:H6	30:0:1060:C:H5'	1.53	0.73
9:I:73:LEU:HD12	9:I:107:LYS:NZ	2.04	0.73
30:0:318:U:H5'	30:0:339:A:C2	2.24	0.73
30:0:558:C:H2'	30:0:559:U:C5'	2.19	0.73
3:C:78:ARG:HH11	3:C:78:ARG:HG3	1.54	0.73
10:J:18:ILE:HD13	30:0:1244:U:OP1	1.89	0.73
30:0:1157:C:H2'	30:0:1158:G:H8	1.53	0.73
30:0:2420:G:O2'	30:0:2421:G:H5'	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2769:C:O2'	30:0:2770:G:H5'	1.89	0.73
3:C:139:VAL:HG13	38:C:8654:HOH:O	1.87	0.73
30:0:1213:C:O2'	30:0:1214:G:H5'	1.89	0.73
30:0:1119:G:N2	30:0:1246:A:H2	1.84	0.73
31:9:55:U:H4'	31:9:56:A:C8	2.24	0.73
30:0:871:G:C8	30:0:871:G:C5'	2.63	0.72
30:0:214:U:H5'	38:0:6153:HOH:O	1.88	0.72
30:0:1666:C:H2'	30:0:1667:A:C5'	2.19	0.72
31:9:75:G:H1	31:9:106:U:H3	1.37	0.72
30:0:848:C:H5'	38:0:7287:HOH:O	1.89	0.72
30:0:1942:A:H3'	38:0:7363:HOH:O	1.88	0.72
30:0:1942:A:H5'	38:0:7363:HOH:O	1.88	0.72
3:C:1:MET:HG2	3:C:2:GLN:H	1.52	0.72
30:0:2010:A:H2'	38:0:5975:HOH:O	1.90	0.72
23:W:84:VAL:HG12	38:W:6679:HOH:O	1.89	0.72
23:W:21:LEU:HD21	23:W:48:VAL:HG11	1.72	0.72
30:0:1528:A:H2'	30:0:1529:G:O4'	1.88	0.72
30:0:1595:G:O2'	30:0:1596:U:H5'	1.89	0.72
30:0:1964:U:H2'	30:0:1964:U:O2	1.88	0.72
30:0:2787:C:H5	38:0:4647:HOH:O	1.72	0.72
2:B:258:GLY:H	2:B:260:HIS:CE1	2.08	0.72
25:Y:216:ARG:HD3	38:Y:8139:HOH:O	1.90	0.72
30:0:1603:A:H5"	30:0:1605:G:H5'	1.72	0.72
30:0:1834:C:H2'	30:0:1840:A:N6	2.04	0.72
30:0:12:U:H2'	30:0:13:G:H5'	1.72	0.71
30:0:2481:G:H5"	38:0:4556:HOH:O	1.89	0.71
30:0:272:A:H5'	30:0:273:G:OP2	1.89	0.71
30:0:363:C:H1'	38:0:5292:HOH:O	1.90	0.71
30:0:969:G:H1	30:0:999:C:H42	1.38	0.71
13:M:102:GLU:OE1	13:M:164:THR:HG21	1.88	0.71
30:0:603:A:H1'	30:0:605:C:C2	2.25	0.71
19:S:51:GLN:HE21	19:S:53:ASN:HD21	1.38	0.71
22:V:1:THR:CB	30:0:93:C:H5"	2.17	0.71
30:0:2748:G:H1'	38:0:7912:HOH:O	1.91	0.71
30:0:2768:A:H2'	30:0:2769:C:O4'	1.90	0.71
1:A:47:HIS:HD2	30:0:1654:U:H2'	1.56	0.71
30:0:2533:C:H5'	30:0:2533:C:H6	1.54	0.71
14:N:141:ARG:HH12	31:9:35:C:H2'	1.56	0.71
3:C:162:VAL:HG22	3:C:232:LEU:HD21	1.73	0.71
30:0:1701:A:H5'	38:0:6302:HOH:O	1.89	0.71
4:D:172:VAL:HG12	4:D:173:GLU:H	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:870:G:C2'	30:0:871:G:H5"	2.20	0.71
1:A:72:GLU:HG3	26:Z:90:GLY:HA2	1.72	0.70
2:B:195:ARG:HG2	2:B:323:LEU:HD22	1.72	0.70
31:9:7:G:H5'	38:9:9098:HOH:O	1.91	0.70
1:A:192:VAL:CG1	1:A:207:GLN:HB3	2.21	0.70
5:E:81:GLU:HG2	5:E:134:SER:HB3	1.73	0.70
30:0:2243:C:H5"	38:0:3756:HOH:O	1.91	0.70
3:C:140:VAL:HB	38:C:8657:HOH:O	1.91	0.70
30:0:560:U:H2'	30:0:561:G:H8	1.56	0.70
30:0:960:G:N3	30:0:960:G:C3'	2.54	0.70
30:0:2502:C:H2'	30:0:2503:A:C5'	2.17	0.70
10:J:70:PHE:CE1	30:0:2676:C:H4'	2.26	0.70
23:W:72:PRO:HG2	23:W:77:ALA:HB3	1.73	0.70
30:0:2453:G:H3'	38:0:5935:HOH:O	1.91	0.70
23:W:6:GLN:HB2	23:W:26:ILE:CD1	2.21	0.70
30:0:1116:U:O2'	30:0:1118:A:H2	1.69	0.70
30:0:1666:C:C2'	30:0:1667:A:C5'	2.70	0.70
31:9:3:A:H61	31:9:22:G:H1'	1.56	0.70
14:N:40:ASN:ND2	31:9:28:U:H5"	2.06	0.70
30:0:2005:G:H3'	30:0:2005:G:OP2	1.91	0.70
30:0:1377:C:H5'	30:0:1377:C:H6	1.57	0.69
30:0:2578:G:H5'	30:0:2578:G:H8	1.56	0.69
30:0:2372:A:H2'	30:0:2373:U:C6	2.27	0.69
2:B:201:ASP:HB2	2:B:312:ARG:HD2	1.75	0.69
30:0:401:C:H2'	30:0:402:U:C6	2.27	0.69
30:0:441:A:H1'	30:0:442:A:N7	2.08	0.69
30:0:613:C:H2'	30:0:614:U:H6	1.57	0.69
30:0:1701:A:H4'	30:0:1702:U:C5'	2.19	0.69
30:0:2073:G:OP2	30:0:2490:A:H5'	1.93	0.69
30:0:2717:C:H2'	30:0:2718:C:C5'	2.18	0.69
31:9:13:A:O2'	31:9:14:G:H5"	1.92	0.69
9:I:110:ASP:O	30:0:1163:G:H5'	1.91	0.69
31:9:36:C:C5	31:9:37:C:C5	2.80	0.69
29:3:70:ARG:HD3	38:3:9059:HOH:O	1.90	0.69
30:0:1441:G:O2'	30:0:1442:A:H5'	1.92	0.69
4:D:135:VAL:HG21	4:D:139:TYR:CD1	2.27	0.69
14:N:49:THR:HG22	14:N:56:ASP:HB2	1.75	0.69
30:0:625:U:H5"	30:0:1044:C:N4	2.08	0.69
30:0:1477:C:H5'	30:0:1868:G:C5'	2.22	0.69
30:0:1667:A:H5'	30:0:1667:A:H8	1.57	0.69
28:2:41:HIS:H	28:2:45:ASN:HD22	1.39	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:74:VAL:HG11	11:K:113:ILE:HG12	1.74	0.69
11:K:98:VAL:HG13	11:K:102:GLU:HA	1.74	0.69
30:0:249:G:O2'	30:0:250:C:H5'	1.93	0.69
30:0:271:C:H41	30:0:378:A:H2	1.36	0.69
26:Z:70:ARG:HD3	26:Z:83:TYR:HB2	1.74	0.68
30:0:544:G:H2'	30:0:545:G:H5"	1.75	0.68
30:0:2535:A:H2	38:0:4805:HOH:O	1.75	0.68
30:0:2616:G:H1'	38:0:9426:HOH:O	1.93	0.68
31:9:29:C:H2'	31:9:30:C:H5'	1.75	0.68
30:0:816:G:C6	30:0:817:G:N1	2.61	0.68
30:0:1204:C:H2'	30:0:1205:U:O4'	1.92	0.68
30:0:1730:G:H5'	30:0:1731:C:C5	2.28	0.68
30:0:1819:G:H2'	30:0:1820:G:H4'	1.73	0.68
1:A:100:PRO:HG2	1:A:103:VAL:HG21	1.73	0.68
26:Z:66:CYS:SG	26:Z:68:GLU:HB2	2.33	0.68
6:F:63:ILE:HB	6:F:64:PRO:HD3	1.74	0.68
13:M:178:LYS:HB2	38:0:6895:HOH:O	1.92	0.68
30:0:2768:A:O2'	30:0:2769:C:H5'	1.94	0.68
15:O:47:ARG:HH11	15:O:47:ARG:HG3	1.58	0.68
30:0:1201:C:H2'	30:0:1202:A:H5'	1.75	0.68
30:0:1342:C:H2'	30:0:1343:C:H5'	1.76	0.68
30:0:2812:A:C2	30:0:2814:A:N6	2.58	0.68
11:K:87:ARG:HG3	30:0:2721:U:H4'	1.76	0.67
14:N:48:VAL:CG1	14:N:55:ASP:HB3	2.24	0.67
30:0:1183:C:N4	30:0:1184:C:H41	1.92	0.67
30:0:1191:A:H2'	30:0:1193:A:H5'	1.76	0.67
30:0:2534:C:H1'	38:0:3501:HOH:O	1.95	0.67
30:0:2659:U:H5"	38:0:4130:HOH:O	1.95	0.67
8:H:6:ALA:HA	8:H:61:ARG:HH12	1.59	0.67
30:0:1422:U:H2'	30:0:1423:C:C6	2.29	0.67
31:9:24:U:H3'	31:9:25:G:H5'	1.77	0.67
2:B:207:LYS:HG3	30:0:2717:C:OP1	1.95	0.67
1:A:199:HIS:CD2	1:A:201:PHE:H	2.12	0.67
30:0:308:U:H5'	30:0:309:C:OP1	1.93	0.67
30:0:2703:A:H2'	30:0:2704:C:H6	1.60	0.66
30:0:1165:G:H21	30:0:1173:A:C5'	2.08	0.66
2:B:41:PHE:CD1	2:B:79:MET:HE2	2.31	0.66
11:K:74:VAL:CG1	11:K:113:ILE:HG12	2.25	0.66
30:0:2485:A:H3'	38:0:4900:HOH:O	1.95	0.66
18:R:99:ALA:HB1	18:R:109:MET:HE1	1.77	0.66
30:0:559:U:H5'	30:0:559:U:C6	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1185:U:H2'	30:0:1186:C:C6	2.28	0.66
30:0:1603:A:C5'	30:0:1605:G:H5'	2.25	0.66
27:1:1:THR:HA	38:1:8959:HOH:O	1.94	0.66
30:0:1857:A:H5"	38:0:6720:HOH:O	1.94	0.66
23:W:21:LEU:HD21	23:W:48:VAL:CG1	2.26	0.66
30:0:1477:C:H5'	30:0:1868:G:H5'	1.77	0.66
31:9:49:G:O2'	31:9:50:G:H5'	1.96	0.66
30:0:280:C:H2'	30:0:281:U:O4'	1.96	0.66
30:0:281:U:H2'	30:0:282:C:O4'	1.94	0.66
30:0:582:U:H2'	30:0:583:C:C6	2.31	0.66
1:A:192:VAL:HG12	38:A:9055:HOH:O	1.96	0.65
30:0:506:G:H22	30:0:509:A:H5'	1.61	0.65
30:0:2509:A:H2'	30:0:2510:C:O4'	1.96	0.65
1:A:94:LEU:HG	1:A:99:ILE:HD11	1.77	0.65
30:0:969:G:H1	30:0:999:C:N4	1.94	0.65
30:0:1855:G:H4'	30:0:1856:C:O5'	1.96	0.65
3:C:118:THR:O	3:C:136:VAL:HG13	1.96	0.65
30:0:625:U:H5'	38:0:3191:HOH:O	1.96	0.65
1:A:36:ASP:HB2	1:A:85:SER:H	1.60	0.65
30:0:1157:C:H2'	30:0:1158:G:C8	2.31	0.65
30:0:1189:A:H3'	38:0:7692:HOH:O	1.95	0.65
30:0:1211:G:H2'	30:0:1212:C:H6	1.61	0.65
30:0:1687:C:H3'	38:0:9459:HOH:O	1.94	0.65
8:H:168:VAL:HG13	38:H:212:HOH:O	1.95	0.65
18:R:117:HIS:HD2	30:0:20:G:H21	1.45	0.65
30:0:1186:C:H42	30:0:1190:G:H22	1.44	0.65
6:F:30:LYS:HE2	6:F:99:THR:HG21	1.79	0.65
22:V:55:ARG:O	22:V:59:ILE:HG12	1.97	0.65
30:0:714:U:H4'	38:0:5753:HOH:O	1.95	0.65
30:0:2672:C:H1'	38:0:6699:HOH:O	1.96	0.65
6:F:77:VAL:HG21	6:F:83:LEU:HD13	1.77	0.65
11:K:63:GLU:HB2	38:K:6344:HOH:O	1.97	0.65
30:0:1834:C:H2'	30:0:1840:A:H62	1.61	0.65
30:0:2004:U:O5'	30:0:2004:U:H6	1.80	0.65
31:9:20:G:O2'	31:9:21:G:H5'	1.97	0.65
8:H:29:SER:HA	8:H:62:HIS:HD2	1.61	0.65
1:A:51:ARG:HB2	38:A:9068:HOH:O	1.97	0.65
30:0:2781:U:H2'	30:0:2782:G:H5'	1.77	0.65
30:0:558:C:C2'	30:0:559:U:C5'	2.75	0.64
30:0:1632:A:H2'	30:0:1633:C:H5'	1.79	0.64
4:D:25:MET:SD	4:D:40:ILE:HD11	2.36	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:380:A:H2'	38:0:7242:HOH:O	1.96	0.64
30:0:558:C:H2'	30:0:559:U:H5"	1.76	0.64
30:0:1058:A:H2'	30:0:1060:C:H5"	1.79	0.64
30:0:1342:C:O2'	30:0:1343:C:H5'	1.98	0.64
30:0:1666:C:C2'	30:0:1667:A:H5"	2.27	0.64
11:K:14:LYS:HB2	11:K:45:PRO:HG2	1.80	0.64
30:0:272:A:H3'	38:0:7547:HOH:O	1.96	0.64
30:0:595:U:H2'	30:0:596:C:H6	1.63	0.64
31:9:1:U:H4'	31:9:3:A:OP1	1.97	0.64
25:Y:169:ARG:HD2	30:0:1328:A:OP1	1.97	0.64
30:0:2894:C:O2'	30:0:2895:C:H5'	1.97	0.64
12:L:41:HIS:HD2	30:0:926:A:O2'	1.79	0.64
18:R:128:ARG:NH2	30:0:2054:A:N3	2.45	0.64
30:0:2361:A:H5"	38:0:9009:HOH:O	1.97	0.64
31:9:64:C:C2'	31:9:65:A:H5'	2.27	0.64
30:0:1175:G:H1'	30:0:1193:A:C8	2.32	0.64
30:0:2824:C:H5"	30:0:2825:C:H5'	1.79	0.64
18:R:18:LEU:HB2	18:R:143:VAL:HG13	1.79	0.64
30:0:1116:U:H3	30:0:1246:A:N6	1.89	0.64
30:0:1398:G:O2'	30:0:1399:A:H5'	1.98	0.64
30:0:2781:U:C2'	30:0:2782:G:H5'	2.28	0.64
5:E:100:ASP:HB2	38:E:2789:HOH:O	1.97	0.64
15:O:42:GLU:HB2	38:O:2176:HOH:O	1.97	0.64
20:T:61:GLU:HG2	38:T:3851:HOH:O	1.97	0.63
28:2:41:HIS:HD2	28:2:44:ARG:H	1.44	0.63
30:0:541:C:C2'	30:0:542:A:C5'	2.74	0.63
30:0:544:G:C2'	30:0:545:G:H5"	2.28	0.63
30:0:1180:U:O2'	30:0:1181:A:H5'	1.98	0.63
8:H:72:ALA:HB2	8:H:156:ALA:HB2	1.80	0.63
30:0:1307:A:H2'	30:0:1308:A:C8	2.33	0.63
30:0:2510:C:H42	30:0:2564:G:H22	1.47	0.63
24:X:74:ALA:HB2	24:X:85:VAL:HG13	1.80	0.63
30:0:1165:G:H4'	30:0:1174:A:O2'	1.98	0.63
30:0:1634:G:H2'	30:0:1635:U:H6	1.63	0.63
30:0:2335:C:H2'	30:0:2336:G:H8	1.64	0.63
2:B:320:GLN:HE21	2:B:321:PRO:HD2	1.62	0.63
5:E:93:MET:HE1	5:E:165:GLY:H	1.61	0.63
25:Y:187:VAL:HG23	25:Y:192:ASP:CB	2.28	0.63
3:C:214:THR:HG23	38:C:8640:HOH:O	1.96	0.63
23:W:13:MET:HE1	23:W:18:GLN:HA	1.80	0.63
30:0:236:A:H4'	30:0:237:G:H5'	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:281:U:O2'	30:0:282:C:H5'	1.99	0.63
30:0:316:A:N3	30:0:336:G:O2'	2.30	0.63
31:9:56:A:C3'	31:9:57:A:H5"	2.29	0.63
27:1:25:LYS:HD2	28:2:49:GLU:N	2.13	0.63
30:0:74:G:H2'	30:0:75:U:C6	2.34	0.63
30:0:1878:G:C1'	38:0:6135:HOH:O	2.43	0.63
3:C:27:ARG:NH2	30:0:657:G:OP1	2.31	0.63
14:N:37:ARG:NH1	31:9:6:C:C5'	2.52	0.63
30:0:541:C:H2'	30:0:542:A:H5'	1.80	0.63
30:0:2717:C:O2'	30:0:2718:C:H5"	1.97	0.63
3:C:218:VAL:HG12	38:C:8628:HOH:O	1.99	0.63
6:F:91:VAL:HG12	6:F:92:GLY:N	2.13	0.63
30:0:1278:A:H4'	30:0:1279:U:N3	2.13	0.63
30:0:1377:C:H5'	30:0:1377:C:C6	2.34	0.63
31:9:33:U:H2'	38:9:9065:HOH:O	1.98	0.63
18:R:99:ALA:HB1	18:R:109:MET:CE	2.29	0.62
30:0:285:A:H2'	30:0:286:U:O4'	1.98	0.62
30:0:694:A:H2'	30:0:695:C:H5'	1.80	0.62
14:N:7:LYS:HE3	17:Q:21:ARG:O	1.99	0.62
25:Y:115:ARG:HH21	30:0:1266:U:H4'	1.64	0.62
30:0:533:U:H3'	38:0:3754:HOH:O	1.98	0.62
30:0:2071:C:H5'	38:0:9532:HOH:O	1.99	0.62
30:0:2670:G:O2'	30:0:2671:U:H5'	1.99	0.62
31:9:64:C:H2'	31:9:65:A:H5'	1.81	0.62
3:C:236:THR:HG22	3:C:239:ALA:HB2	1.80	0.62
30:0:2320:U:H4'	30:0:2321:A:O4'	1.99	0.62
30:0:2414:A:H2'	30:0:2415:A:C8	2.34	0.62
3:C:236:THR:HG22	3:C:239:ALA:CB	2.30	0.62
30:0:200:C:H2'	38:0:3449:HOH:O	2.00	0.62
1:A:191:GLY:HA2	1:A:194:MET:HE3	1.81	0.62
2:B:179:LEU:O	2:B:183:GLU:HG2	2.00	0.62
3:C:2:GLN:HB3	38:C:8587:HOH:O	1.98	0.62
5:E:49:ILE:HD11	5:E:69:ILE:HD12	1.82	0.62
30:0:920:C:H4'	30:0:921:G:C2	2.34	0.62
30:0:1398:G:H2'	30:0:1399:A:C8	2.34	0.62
2:B:262:ARG:HG3	30:0:2716:G:H5'	1.82	0.62
27:1:10:LYS:HG3	38:1:8981:HOH:O	2.00	0.62
30:0:2512:U:H4'	30:0:2514:U:O4	1.99	0.62
30:0:162:C:H2'	30:0:163:U:H5'	1.80	0.62
2:B:162:MET:HG3	2:B:310:ARG:HD3	1.82	0.61
25:Y:187:VAL:HG23	25:Y:192:ASP:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:585:C:H5”	38:0:4883:HOH:O	1.99	0.61
30:0:1132:A:N6	30:0:1229:C:H2’	2.16	0.61
30:0:1524:U:H6	30:0:1524:U:H5”	1.63	0.61
30:0:2900:G:H2’	30:0:2901:C:O4’	1.99	0.61
31:9:55:U:H4’	31:9:56:A:H8	1.62	0.61
38:C:8669:HOH:O	30:0:2100:A:H5’	1.99	0.61
5:E:20:ILE:HD11	5:E:40:VAL:HG11	1.83	0.61
30:0:137:U:H2’	30:0:139:C:C5	2.35	0.61
30:0:1654:U:H5”	38:0:7439:HOH:O	1.99	0.61
30:0:1838:U:H3’	38:0:5538:HOH:O	1.98	0.61
2:B:307:ARG:HH11	2:B:307:ARG:HG3	1.66	0.61
9:I:108:HIS:H	9:I:109:PRO:HD2	1.66	0.61
30:0:1350:U:H4’	38:0:5132:HOH:O	2.00	0.61
30:0:2507:G:H2’	30:0:2510:C:N4	2.15	0.61
1:A:211:LYS:HB2	38:A:9083:HOH:O	2.00	0.61
30:0:1603:A:H5’	30:0:1605:G:C4’	2.30	0.61
30:0:1972:U:H2’	30:0:1973:A:H5”	1.83	0.61
30:0:2064:U:H5’	30:0:2652:U:H4’	1.82	0.61
12:L:18:HIS:HD2	30:0:902:G:N7	1.99	0.61
30:0:2908:A:O5’	30:0:2908:A:H8	1.83	0.61
2:B:212:GLN:HB2	2:B:257:THR:CG2	2.28	0.61
12:L:133:VAL:HA	38:L:8873:HOH:O	2.00	0.61
29:3:48:ASN:HD21	30:0:2468:A:H61	1.48	0.61
30:0:1835:U:C5	30:0:1840:A:N7	2.65	0.61
3:C:37:ALA:HA	3:C:100:LEU:HD12	1.82	0.61
3:C:127:ARG:HD3	3:C:129:HIS:HE1	1.65	0.61
30:0:1226:G:H5’	38:0:4541:HOH:O	1.99	0.61
2:B:145:HIS:HD2	2:B:146:THR:O	1.83	0.61
12:L:6:ARG:HD3	30:0:1299:G:O6	2.00	0.61
21:U:17:THR:HG22	21:U:18:GLY:N	2.16	0.61
23:W:4:LEU:HD22	23:W:52:VAL:HG21	1.83	0.61
25:Y:132:ASP:OD2	30:0:621:C:H5’	2.00	0.61
2:B:74:ILE:HD13	2:B:309:VAL:HG21	1.82	0.60
25:Y:235:GLU:CD	25:Y:235:GLU:H	2.04	0.60
2:B:304:PRO:HD2	2:B:307:ARG:NE	2.16	0.60
3:C:95:GLU:HG3	38:C:8682:HOH:O	2.00	0.60
26:Z:60:ASP:HB3	26:Z:69:ASP:HB3	1.83	0.60
28:2:40:ARG:HD2	28:2:47:THR:HG22	1.83	0.60
30:0:401:C:H2’	30:0:402:U:H6	1.64	0.60
30:0:1181:A:C2’	30:0:1182:C:H5’	2.32	0.60
30:0:1741:U:O2’	30:0:2723:G:H4’	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1819:G:H5'	38:0:4725:HOH:O	2.00	0.60
3:C:76:ARG:HG2	3:C:78:ARG:NH1	2.15	0.60
21:U:52:THR:HG22	21:U:54:THR:H	1.66	0.60
30:0:10:U:C4	30:0:532:A:N7	2.70	0.60
30:0:1819:G:H2'	30:0:1820:G:C5'	2.31	0.60
18:R:128:ARG:NH2	30:0:2054:A:C2	2.70	0.60
20:T:24:ARG:HH21	20:T:39:ASN:ND2	1.98	0.60
30:0:447:A:O2'	30:0:448:G:H5'	2.01	0.60
30:0:595:U:H2'	30:0:596:C:C6	2.37	0.60
30:0:1587:U:H2'	30:0:1588:G:O4'	2.02	0.60
8:H:155:ARG:NH1	30:0:2503:A:H5"	2.17	0.60
10:J:19:MET:HE1	10:J:132:LEU:HD21	1.83	0.60
10:J:26:VAL:HG13	10:J:36:VAL:HG11	1.82	0.60
29:3:73:GLU:HB3	38:3:9049:HOH:O	2.01	0.60
30:0:558:C:H2'	30:0:559:U:H5'	1.83	0.60
30:0:847:C:H4'	38:0:3759:HOH:O	1.99	0.60
30:0:2372:A:H2'	30:0:2373:U:H6	1.66	0.60
8:H:6:ALA:HA	8:H:61:ARG:NH1	2.17	0.60
29:3:67:LEU:HD11	29:3:88:LEU:HD21	1.82	0.60
30:0:396:U:O2'	30:0:418:C:H4'	2.02	0.60
30:0:407:A:H2'	30:0:408:A:C8	2.37	0.60
30:0:541:C:O2'	30:0:542:A:H5"	2.02	0.60
30:0:1202:A:C2'	30:0:1203:G:H5'	2.32	0.60
30:0:282:C:O2'	30:0:283:U:C5'	2.49	0.60
30:0:1583:U:H1'	38:0:9989:HOH:O	2.02	0.60
30:0:2281:C:C2'	30:0:2282:U:H5'	2.32	0.60
3:C:238:SER:HB2	38:C:8577:HOH:O	2.01	0.60
13:M:163:LEU:HD21	30:0:188:C:H5"	1.84	0.60
13:M:179:GLY:O	30:0:399:C:H5'	2.02	0.60
21:U:46:ALA:HB1	21:U:52:THR:HG21	1.83	0.60
23:W:21:LEU:HD22	23:W:26:ILE:CD1	2.32	0.60
30:0:130:C:H2'	38:0:3166:HOH:O	2.02	0.60
30:0:807:A:O2'	30:0:808:A:H5'	2.01	0.60
7:G:12:ILE:HG23	38:0:5471:HOH:O	2.02	0.59
9:I:86:GLU:HG2	30:0:1180:U:H4'	1.83	0.59
11:K:98:VAL:CG1	11:K:102:GLU:HA	2.32	0.59
13:M:164:THR:HG23	13:M:165:GLY:N	2.17	0.59
19:S:55:GLN:NE2	30:0:1446:U:H2'	2.18	0.59
30:0:1172:G:H5"	38:0:7275:HOH:O	2.01	0.59
30:0:1676:G:O2'	30:0:1677:U:H5'	2.03	0.59
31:9:47:A:C2	31:9:48:C:C2	2.89	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:18:ARG:HG3	2:B:256:GLN:HG3	1.82	0.59
2:B:51:VAL:HG23	2:B:330:VAL:HG22	1.83	0.59
30:0:1206:U:H2'	30:0:1207:A:O4'	2.01	0.59
30:0:2135:A:O2'	30:0:2136:G:H5'	2.03	0.59
4:D:65:GLU:HA	38:D:6752:HOH:O	2.02	0.59
4:D:105:SER:OG	30:0:2338:G:H1'	2.03	0.59
5:E:68:HIS:O	5:E:72:MET:HG3	2.01	0.59
10:J:45:VAL:HG23	10:J:130:VAL:O	2.00	0.59
11:K:32:ILE:HD11	11:K:56:SER:HB3	1.84	0.59
30:0:1165:G:N2	30:0:1173:A:H5"	2.15	0.59
30:0:2826:G:C6	30:0:2913:A:N6	2.70	0.59
1:A:186:TRP:CG	1:A:187:PRO:HA	2.38	0.59
13:M:164:THR:HG22	13:M:167:GLY:N	2.16	0.59
25:Y:126:PRO:HG2	25:Y:128:PHE:CE1	2.37	0.59
30:0:1524:U:H6	30:0:1524:U:C5'	2.16	0.59
30:0:1766:U:O2	30:0:1778:A:H5'	2.01	0.59
30:0:2505:G:C2'	30:0:2506:A:H5'	2.32	0.59
31:9:92:G:H2'	31:9:93:A:H8	1.67	0.59
3:C:16:VAL:HG21	38:C:8634:HOH:O	2.02	0.59
13:M:125:ARG:HD2	38:M:8893:HOH:O	2.02	0.59
14:N:34:LEU:HD22	14:N:129:ILE:HD13	1.83	0.59
30:0:424:C:H2'	30:0:425:U:C6	2.38	0.59
30:0:1042:U:O2'	30:0:1043:C:H5'	2.02	0.59
30:0:1165:G:N2	30:0:1173:A:C5'	2.66	0.59
30:0:2748:G:H5'	38:0:7557:HOH:O	2.02	0.59
10:J:63:ILE:HD11	30:0:1236:A:C8	2.38	0.59
30:0:482:G:H4'	30:0:508:A:N1	2.18	0.59
30:0:522:U:O2'	30:0:1366:C:H5'	2.02	0.59
30:0:853:C:H3'	38:0:4563:HOH:O	2.03	0.59
30:0:1511:U:O2'	30:0:1512:G:H5'	2.03	0.59
30:0:1641:A:C2'	30:0:1642:A:H5'	2.32	0.59
30:0:2374:G:H2'	30:0:2375:A:C8	2.37	0.59
16:P:10:ALA:HA	16:P:13:VAL:HG12	1.85	0.59
28:2:39:ARG:HG2	38:2:3143:HOH:O	2.03	0.59
30:0:255:A:H2'	30:0:256:C:C6	2.38	0.59
30:0:1790:C:H2'	30:0:1791:U:H6	1.67	0.59
30:0:1973:A:H5'	30:0:1973:A:C8	2.36	0.59
30:0:2324:G:N2	30:0:2377:U:H1'	2.17	0.59
1:A:36:ASP:O	1:A:38:ILE:N	2.36	0.58
10:J:52:GLN:HE22	30:0:1119:G:H2'	1.67	0.58
27:1:9:GLY:HA2	30:0:1687:C:O2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:368:C:H2'	30:0:369:G:H5'	1.84	0.58
30:0:1321:A:H2'	30:0:1322:G:C8	2.38	0.58
8:H:15:PRO:HG3	30:0:1053:G:OP1	2.02	0.58
30:0:123:U:H5'	38:0:6671:HOH:O	2.03	0.58
30:0:1196:C:N4	30:0:1204:C:H42	2.01	0.58
30:0:1904:A:H2'	30:0:1905:U:O4'	2.03	0.58
30:0:2467:A:O2'	30:0:2468:A:H2'	2.02	0.58
1:A:94:LEU:HG	1:A:99:ILE:CD1	2.33	0.58
3:C:79:ARG:O	3:C:87:ARG:HG2	2.03	0.58
17:Q:21:ARG:HH12	30:0:2353:A:H1'	1.67	0.58
30:0:10:U:C4	30:0:532:A:C8	2.91	0.58
30:0:2335:C:H2'	30:0:2336:G:C8	2.38	0.58
11:K:4:LEU:HD22	11:K:116:GLU:HB3	1.85	0.58
28:2:41:HIS:HB3	28:2:44:ARG:HB2	1.84	0.58
30:0:1170:U:H2'	30:0:1172:G:OP2	2.02	0.58
30:0:1182:C:C1'	30:0:1192:A:H8	2.16	0.58
30:0:1948:G:H2'	30:0:1949:G:C8	2.39	0.58
30:0:2878:U:H2'	30:0:2879:A:O4'	2.02	0.58
3:C:78:ARG:HG3	3:C:78:ARG:NH1	2.15	0.58
30:0:2281:C:H2'	30:0:2282:U:H5'	1.85	0.58
1:A:121:ALA:O	1:A:124:VAL:HG22	2.03	0.58
8:H:174:LEU:HD21	30:0:1220:U:H4'	1.85	0.58
30:0:960:G:H8	38:0:5987:HOH:O	1.85	0.58
30:0:2852:A:H5"	38:0:5246:HOH:O	2.03	0.58
3:C:76:ARG:HG2	3:C:78:ARG:HH12	1.69	0.58
3:C:237:GLU:HG3	38:C:8634:HOH:O	2.04	0.58
9:I:112:LEU:CD1	30:0:1162:G:H1'	2.34	0.58
12:L:14:GLY:O	30:0:1295:G:H5"	2.03	0.58
30:0:2768:A:H5"	38:0:4434:HOH:O	2.03	0.58
22:V:64:GLY:O	22:V:65:ASP:HB2	2.04	0.58
24:X:23:HIS:HE1	30:0:2044:G:OP1	1.86	0.58
25:Y:141:THR:HG23	38:Y:8158:HOH:O	2.03	0.58
30:0:440:C:H2'	30:0:441:A:C8	2.39	0.58
30:0:1819:G:H2'	30:0:1820:G:C4'	2.34	0.58
31:9:37:C:H2'	31:9:38:A:H8	1.68	0.58
13:M:134:ILE:CG2	13:M:141:ILE:HD13	2.34	0.58
14:N:71:TRP:CE3	14:N:175:LEU:HD22	2.38	0.58
30:0:681:G:N3	30:0:681:G:H5'	2.19	0.58
30:0:2643:G:H5"	38:0:3933:HOH:O	2.03	0.58
30:0:2820:A:H2'	30:0:2821:C:C6	2.38	0.58
14:N:141:ARG:NH1	31:9:35:C:H2'	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:68:THR:HG23	23:W:69:ARG:HG2	1.86	0.58
11:K:20:CYS:HB2	11:K:29:LEU:HG	1.86	0.57
19:S:76:GLU:HB3	38:S:8992:HOH:O	2.04	0.57
30:0:1947:G:H2'	30:0:1948:G:H8	1.69	0.57
30:0:2760:C:H5"	38:0:5337:HOH:O	2.03	0.57
2:B:27:ASN:HD22	2:B:27:ASN:H	1.51	0.57
3:C:174:ILE:HD11	30:0:338:C:H4'	1.85	0.57
24:X:47:ALA:HB1	24:X:82:GLU:HB3	1.86	0.57
27:1:16:HIS:HD2	30:0:470:U:O2'	1.86	0.57
28:2:38:LYS:HE3	38:0:4231:HOH:O	2.04	0.57
30:0:249:G:N2	30:0:250:C:C2	2.72	0.57
30:0:1730:G:C5'	30:0:1731:C:C6	2.86	0.57
2:B:238:ASN:HD22	2:B:240:GLY:N	1.97	0.57
6:F:91:VAL:HG12	6:F:92:GLY:H	1.68	0.57
3:C:129:HIS:CE1	3:C:231:ARG:HA	2.38	0.57
30:0:185:G:H4'	30:0:186:A:OP1	2.04	0.57
30:0:360:A:H2'	30:0:361:C:O4'	2.04	0.57
30:0:395:A:H5"	38:0:3928:HOH:O	2.05	0.57
30:0:1191:A:C2	30:0:1207:A:C2	2.93	0.57
30:0:1965:C:O2'	30:0:1966:U:H5'	2.04	0.57
30:0:2003:U:HO2'	30:0:2004:U:H5	1.52	0.57
30:0:2254:G:O2'	30:0:2255:A:H5'	2.04	0.57
30:0:2532:A:H2	38:0:7579:HOH:O	1.87	0.57
31:9:76:G:C3'	31:9:77:A:H5"	2.25	0.57
13:M:188:ARG:HD3	30:0:155:C:OP2	2.03	0.57
38:O:7674:HOH:O	30:0:653:U:H5"	2.05	0.57
31:9:3:A:C8	31:9:26:C:C2	2.93	0.57
31:9:23:U:O2'	31:9:24:U:H4'	2.05	0.57
2:B:244:PRO:HB3	30:0:1234:U:N3	2.19	0.57
21:U:14:GLU:O	21:U:17:THR:HB	2.05	0.57
28:2:35:ARG:HB2	38:2:2691:HOH:O	2.05	0.57
30:0:65:C:O2'	30:0:66:G:H5'	2.03	0.57
30:0:119:A:H2'	30:0:120:A:H5"	1.86	0.57
30:0:602:A:O2'	30:0:605:C:H4'	2.04	0.57
30:0:1524:U:OP1	30:0:1524:U:H4'	2.05	0.57
30:0:2314:G:C2'	30:0:2315:C:H5'	2.34	0.57
30:0:1116:U:O2'	30:0:1118:A:C2	2.50	0.57
9:I:73:LEU:HD12	9:I:107:LYS:HZ2	1.67	0.57
30:0:1333:U:H2'	30:0:1334:C:C6	2.40	0.57
1:A:192:VAL:HG13	1:A:207:GLN:HB3	1.87	0.57
5:E:93:MET:HE1	5:E:165:GLY:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:30:GLU:O	13:M:34:GLU:HG3	2.04	0.57
14:N:13:ARG:NH1	30:0:2368:A:C6	2.72	0.57
18:R:39:THR:HG23	18:R:107:GLU:O	2.05	0.57
30:0:1515:A:H2'	30:0:1516:U:C6	2.40	0.57
30:0:2282:U:H4'	30:0:2309:C:C5	2.39	0.57
30:0:2507:G:H2'	30:0:2510:C:H42	1.70	0.57
8:H:98:LEU:HD11	8:H:127:ALA:HB2	1.86	0.57
30:0:291:C:H2'	30:0:292:G:O4'	2.05	0.57
30:0:711:G:C2	30:0:718:C:C2	2.92	0.57
30:0:1351:G:H1'	38:0:4693:HOH:O	2.04	0.57
3:C:174:ILE:CD1	30:0:338:C:H4'	2.35	0.56
16:P:59:ARG:O	16:P:63:ARG:HG3	2.05	0.56
23:W:13:MET:CE	23:W:18:GLN:HA	2.35	0.56
30:0:538:C:H5"	30:0:539:G:C8	2.40	0.56
30:0:1189:A:O2'	30:0:1208:C:H2'	2.05	0.56
30:0:2533:C:H5'	30:0:2533:C:C6	2.38	0.56
30:0:2831:C:O2'	30:0:2832:C:H5'	2.05	0.56
30:0:2897:C:O2'	30:0:2898:G:H5'	2.05	0.56
5:E:116:THR:HG22	5:E:151:LEU:HD22	1.87	0.56
11:K:118:ALA:HA	11:K:125:ALA:HB2	1.85	0.56
30:0:432:G:O2'	30:0:433:C:H5'	2.05	0.56
30:0:1504:A:H4'	30:0:1506:U:C5	2.40	0.56
1:A:105:VAL:CG1	1:A:154:ALA:HB1	2.35	0.56
2:B:294:TYR:HE2	38:B:9116:HOH:O	1.88	0.56
15:O:14:LEU:HD23	15:O:102:ILE:HD11	1.88	0.56
19:S:11:THR:H	19:S:14:ALA:HB3	1.69	0.56
19:S:57:THR:HG23	38:S:8980:HOH:O	2.05	0.56
23:W:5:VAL:HG11	23:W:153:MET:CE	2.35	0.56
26:Z:81:CYS:SG	26:Z:83:TYR:HB3	2.45	0.56
30:0:812:A:H2'	30:0:813:C:C6	2.40	0.56
14:N:139:TRP:HA	14:N:139:TRP:CE3	2.40	0.56
30:0:851:C:O2	30:0:2022:A:H2	1.87	0.56
30:0:1634:G:H2'	30:0:1635:U:C6	2.41	0.56
30:0:2297:U:H1'	38:0:5188:HOH:O	2.04	0.56
30:0:2781:U:H2'	30:0:2782:G:C5'	2.35	0.56
25:Y:130:ARG:HB2	25:Y:142:SER:O	2.05	0.56
30:0:483:C:C4	30:0:484:A:C6	2.94	0.56
30:0:484:A:N1	30:0:506:G:H4'	2.21	0.56
30:0:2282:U:H4'	30:0:2309:C:H5	1.71	0.56
30:0:2300:A:H4'	30:0:2301:A:O5'	2.05	0.56
30:0:2472:C:O2'	30:0:2634:G:H4'	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:7:ARG:HG2	2:B:7:ARG:HH11	1.70	0.56
4:D:56:ARG:NH2	30:0:2332:A:H5'	2.21	0.56
4:D:159:PRO:O	4:D:163:VAL:HG23	2.06	0.56
8:H:22:TYR:CZ	30:0:1007:A:H2'	2.41	0.56
8:H:59:GLN:HE21	8:H:129:ARG:NE	1.94	0.56
13:M:24:GLN:NE2	13:M:27:ARG:HH11	2.04	0.56
24:X:72:VAL:HG22	24:X:85:VAL:HG12	1.86	0.56
30:0:1189:A:H1'	30:0:1209:C:O4'	2.05	0.56
31:9:35:C:H5"	38:9:9075:HOH:O	2.06	0.56
1:A:47:HIS:CD2	30:0:1654:U:H2'	2.37	0.56
30:0:559:U:C5	30:0:560:U:C5	2.94	0.56
30:0:1130:U:H2'	30:0:1131:G:O4'	2.06	0.56
30:0:2482:G:H5'	38:0:5036:HOH:O	2.05	0.56
2:B:162:MET:HE2	2:B:310:ARG:HD3	1.87	0.56
18:R:29:LYS:HB3	38:R:8936:HOH:O	2.06	0.56
22:V:42:ASN:HB3	38:V:7247:HOH:O	2.06	0.56
30:0:151:A:C2	30:0:152:A:C2	2.94	0.56
30:0:282:C:O2	30:0:282:C:C2'	2.54	0.56
30:0:1772:C:H5'	30:0:1773:G:C5	2.41	0.56
30:0:2831:C:C2'	30:0:2832:C:H5'	2.36	0.56
4:D:103:ASN:ND2	4:D:134:LEU:H	2.04	0.56
10:J:74:ARG:HB3	10:J:74:ARG:HH11	1.70	0.56
2:B:156:LYS:HD3	38:0:3870:HOH:O	2.05	0.55
38:M:8868:HOH:O	30:0:2244:A:H1'	2.06	0.55
15:O:32:ARG:HH21	15:O:35:LYS:NZ	2.04	0.55
3:C:47:GLY:HA2	3:C:92:PRO:HB2	1.87	0.55
14:N:61:ALA:HB3	14:N:88:ALA:HB2	1.88	0.55
30:0:553:G:O4'	30:0:1325:G:H5'	2.06	0.55
30:0:1426:C:H2'	38:0:9598:HOH:O	2.06	0.55
30:0:1545:C:H2'	30:0:1546:G:O4'	2.06	0.55
30:0:1787:C:H4'	30:0:2883:A:O4'	2.06	0.55
31:9:49:G:H2'	31:9:50:G:O4'	2.05	0.55
2:B:211:THR:HG23	30:0:2840:A:OP1	2.06	0.55
2:B:265:LEU:HD21	2:B:316:ARG:HD3	1.88	0.55
11:K:45:PRO:HB2	38:0:7387:HOH:O	2.06	0.55
12:L:136:ALA:HB3	38:L:8873:HOH:O	2.05	0.55
14:N:37:ARG:HH11	31:9:6:C:C5'	2.15	0.55
14:N:80:SER:HB2	38:N:8833:HOH:O	2.05	0.55
30:0:1972:U:C2'	30:0:1973:A:H5"	2.36	0.55
30:0:2886:C:O2'	30:0:2887:G:H5'	2.07	0.55
21:U:39:ASN:ND2	21:U:44:ARG:HH11	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:3:3:MET:O	29:3:90:PHE:HA	2.06	0.55
30:0:960:G:N3	30:0:960:G:C2'	2.69	0.55
30:0:1191:A:C2'	30:0:1193:A:H5'	2.37	0.55
2:B:98:THR:HG22	30:0:2820:A:OP1	2.07	0.55
20:T:9:LYS:HD3	38:0:3761:HOH:O	2.06	0.55
23:W:35:VAL:HG23	23:W:41:TYR:CD2	2.42	0.55
30:0:1202:A:H2'	30:0:1203:G:C5'	2.37	0.55
30:0:2599:A:H5"	38:0:3384:HOH:O	2.05	0.55
6:F:58:GLU:CD	13:M:27:ARG:HH22	2.08	0.55
9:I:87:PRO:HG2	30:0:1181:A:H4'	1.87	0.55
14:N:12:ARG:HD3	14:N:18:THR:OG1	2.06	0.55
14:N:37:ARG:HD3	33:N:8807:CL:CL	2.44	0.55
18:R:111:ILE:HG23	18:R:145:LEU:HD11	1.89	0.55
18:R:132:ARG:HG2	18:R:133:ALA:N	2.21	0.55
30:0:669:G:O2'	30:0:670:G:H5'	2.07	0.55
30:0:1120:U:H5'	30:0:1121:G:OP2	2.07	0.55
4:D:173:GLU:HG3	4:D:174:VAL:H	1.71	0.55
15:O:25:VAL:CG1	30:0:710:G:H5'	2.36	0.55
18:R:98:ASN:HD21	30:0:500:G:H21	1.54	0.55
27:1:21:ARG:HD2	27:1:37:CYS:SG	2.47	0.55
30:0:1790:C:H2'	30:0:1791:U:C6	2.41	0.55
2:B:86:ALA:HA	38:B:9045:HOH:O	2.05	0.55
2:B:267:LYS:HE2	38:B:8994:HOH:O	2.06	0.55
3:C:236:THR:HA	38:C:8657:HOH:O	2.07	0.55
10:J:69:TYR:CE1	30:0:2081:A:H4'	2.42	0.55
18:R:59:PHE:O	18:R:63:ASN:HB3	2.06	0.55
25:Y:117:LEU:HA	25:Y:174:VAL:HG11	1.88	0.55
30:0:1972:U:H2'	30:0:1973:A:C5'	2.37	0.55
4:D:103:ASN:HD22	4:D:134:LEU:H	1.54	0.55
13:M:46:LEU:HG	38:M:8921:HOH:O	2.06	0.55
13:M:65:VAL:HG21	13:M:105:ALA:HB2	1.89	0.55
15:O:96:VAL:HG13	15:O:100:GLN:HB2	1.89	0.55
23:W:154:ARG:NH1	30:0:588:G:O6	2.40	0.55
30:0:512:G:O3'	30:0:513:A:H8	1.89	0.55
30:0:794:U:H3	30:0:819:A:H61	1.54	0.55
30:0:1544:U:O2'	30:0:1545:C:H5'	2.05	0.55
30:0:1706:G:C6	30:0:1707:G:C6	2.95	0.55
30:0:2297:U:H2'	30:0:2298:C:H6	1.71	0.55
30:0:2514:U:OP1	30:0:2572:G:H1'	2.06	0.55
31:9:24:U:H3'	31:9:25:G:C5'	2.35	0.55
6:F:96:ALA:HA	38:F:3111:HOH:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:88:G:H8	30:0:88:G:H5'	1.72	0.54
30:0:713:U:O5'	30:0:713:U:H6	1.90	0.54
30:0:1504:A:H5'	38:0:4423:HOH:O	2.06	0.54
30:0:1915:U:O2'	30:0:1916:C:H5'	2.06	0.54
30:0:2851:G:C2'	30:0:2852:A:H5'	2.37	0.54
4:D:131:THR:HG21	30:0:2348:C:H1'	1.89	0.54
30:0:515:C:H5"	38:0:5660:HOH:O	2.06	0.54
30:0:1202:A:H2'	30:0:1203:G:O4'	2.08	0.54
30:0:2790:C:HO2'	30:0:2791:U:H6	1.54	0.54
1:A:190:ARG:NH2	1:A:207:GLN:OE1	2.40	0.54
23:W:137:GLN:HE21	23:W:141:HIS:CE1	2.13	0.54
30:0:644:G:H5'	30:0:644:G:N3	2.22	0.54
30:0:1160:G:H2'	38:0:5647:HOH:O	2.07	0.54
30:0:1202:A:O2'	30:0:1203:G:H5'	2.07	0.54
30:0:1903:U:O2'	30:0:1904:A:N7	2.40	0.54
23:W:88:THR:HG23	23:W:110:GLN:HE21	1.72	0.54
30:0:1730:G:H5"	30:0:1731:C:H6	1.71	0.54
2:B:119:HIS:O	2:B:121:PRO:HD3	2.07	0.54
10:J:127:ILE:CG2	33:J:8801:CL:CL	2.91	0.54
20:T:38:ARG:NH1	38:T:6217:HOH:O	2.41	0.54
14:N:4:PRO:HG3	31:9:69:U:OP1	2.07	0.54
21:U:9:CYS:HA	21:U:52:THR:HG23	1.90	0.54
27:1:20:ARG:HG2	30:0:111:C:O2'	2.08	0.54
30:0:1521:C:H2'	30:0:1522:A:H8	1.72	0.54
30:0:2326:C:H4'	30:0:2412:G:H4'	1.89	0.54
2:B:51:VAL:HG13	2:B:53:LEU:HD13	1.90	0.54
2:B:162:MET:HE1	2:B:308:LEU:HD21	1.89	0.54
19:S:17:ASP:HB3	19:S:23:LYS:HB2	1.90	0.54
27:1:25:LYS:CD	28:2:49:GLU:H	2.18	0.54
30:0:553:G:H5'	38:0:3505:HOH:O	2.08	0.54
30:0:1406:A:H5'	30:0:1407:A:C8	2.42	0.54
30:0:2314:G:H2'	30:0:2315:C:H5'	1.90	0.54
12:L:46:LEU:O	30:0:2430:A:H4'	2.07	0.54
15:O:37:ARG:HD2	30:0:656:G:OP2	2.08	0.54
30:0:1041:U:H2'	30:0:1042:U:H5'	1.89	0.54
30:0:1559:A:H4'	38:0:5879:HOH:O	2.08	0.54
4:D:64:ARG:HD3	4:D:67:ASP:HB3	1.90	0.54
9:I:118:ASN:HB3	30:0:1185:U:H5"	1.88	0.54
19:S:33:SER:O	19:S:37:VAL:HG23	2.08	0.54
30:0:920:C:H5"	30:0:921:G:O5'	2.08	0.54
30:0:1573:A:H2'	30:0:1574:C:O4'	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2329:C:O2'	30:0:2330:U:H5'	2.08	0.54
30:0:2421:G:H2'	38:0:4085:HOH:O	2.07	0.54
1:A:101:GLU:OE2	1:A:131:HIS:HB2	2.08	0.54
2:B:212:GLN:HA	30:0:1733:A:H4'	1.89	0.54
17:Q:25:PRO:HB2	38:9:9079:HOH:O	2.07	0.54
23:W:21:LEU:HD22	23:W:26:ILE:HD13	1.89	0.54
30:0:812:A:H1'	38:0:3964:HOH:O	2.08	0.54
30:0:1165:G:O3'	30:0:1174:A:H4'	2.08	0.54
30:0:1193:A:C2	30:0:1194:A:N6	2.76	0.54
30:0:2460:A:C2	30:0:2461:U:C2	2.95	0.54
25:Y:151:SER:HB3	25:Y:154:ARG:CB	2.38	0.53
30:0:1495:C:H1'	30:0:1573:A:H1'	1.90	0.53
30:0:1544:U:H2'	30:0:1545:C:H6	1.72	0.53
2:B:84:LEU:HD23	2:B:142:LEU:HD23	1.91	0.53
16:P:76:GLY:HA3	30:0:1785:G:OP1	2.08	0.53
30:0:822:C:H2'	30:0:823:U:H6	1.73	0.53
22:V:57:LYS:HA	22:V:60:GLN:HE21	1.72	0.53
24:X:76:ARG:HH11	24:X:76:ARG:HG3	1.71	0.53
30:0:1803:C:H2'	30:0:1804:A:C8	2.43	0.53
30:0:2134:G:N2	30:0:2242:U:C2	2.76	0.53
4:D:27:ILE:HB	4:D:69:ILE:O	2.08	0.53
8:H:35:LYS:HE3	30:0:968:G:H1'	1.88	0.53
26:Z:61:HIS:HB2	26:Z:71:VAL:HB	1.90	0.53
30:0:963:C:H2'	30:0:964:G:C8	2.43	0.53
30:0:1289:C:O2'	30:0:1290:G:H5'	2.09	0.53
30:0:2510:C:H5'	30:0:2511:A:OP2	2.08	0.53
30:0:2667:G:H1'	30:0:2914:A:N3	2.24	0.53
31:9:54:A:C2'	31:9:55:U:H5'	2.38	0.53
9:I:69:PRO:HA	30:0:1164:U:OP1	2.09	0.53
25:Y:187:VAL:HB	38:Y:8140:HOH:O	2.08	0.53
30:0:2241:C:O2'	30:0:2242:U:H5'	2.09	0.53
16:P:13:VAL:HG21	16:P:41:ARG:HG2	1.89	0.53
30:0:349:U:H2'	30:0:350:G:O4'	2.09	0.53
30:0:821:U:O2'	30:0:822:C:H5'	2.08	0.53
30:0:1118:A:N6	30:0:1244:U:H3	1.99	0.53
30:0:2251:G:H2'	30:0:2252:A:C8	2.43	0.53
31:9:29:C:C2'	31:9:30:C:H5'	2.38	0.53
1:A:51:ARG:NH1	1:A:120:ARG:O	2.39	0.53
2:B:53:LEU:HD11	2:B:327:VAL:HG22	1.89	0.53
2:B:141:ARG:HD2	2:B:163:GLU:OE2	2.09	0.53
3:C:184:ARG:NH2	30:0:450:C:OP1	2.29	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:91:VAL:HG11	30:0:262:A:OP2	2.09	0.53
10:J:76:ASP:HA	38:J:8865:HOH:O	2.09	0.53
30:0:635:A:H2'	30:0:636:G:H5"	1.90	0.53
30:0:1632:A:C2'	30:0:1633:C:H5'	2.39	0.53
30:0:1909:A:N1	30:0:2128:G:H1'	2.24	0.53
2:B:312:ARG:HD3	2:B:315:VAL:HG13	1.90	0.53
5:E:107:PHE:CE1	5:E:152:THR:HB	2.43	0.53
8:H:26:ILE:HA	8:H:123:ILE:HG21	1.89	0.53
12:L:67:ARG:HB2	12:L:112:GLY:HA3	1.90	0.53
14:N:35:VAL:HG12	14:N:37:ARG:HG2	1.91	0.53
25:Y:151:SER:HB3	25:Y:154:ARG:HB2	1.90	0.53
27:1:12:ASN:O	30:0:1415:G:H5'	2.08	0.53
30:0:222:A:H2'	30:0:223:G:O4'	2.08	0.53
30:0:574:G:O2'	30:0:575:A:H5'	2.09	0.53
30:0:1166:A:C6	30:0:1167:G:C6	2.97	0.53
10:J:107:ASN:HD22	10:J:109:TYR:H	1.57	0.53
14:N:25:ARG:HG2	30:0:2416:G:O2'	2.09	0.53
14:N:132:ASN:O	14:N:135:VAL:HG12	2.09	0.53
30:0:128:A:O2'	30:0:129:A:H5'	2.09	0.53
30:0:559:U:H6	30:0:559:U:C5'	2.19	0.53
30:0:2065:C:O2'	30:0:2066:C:H5'	2.09	0.53
30:0:2073:G:C6	30:0:2489:G:H4'	2.44	0.53
30:0:2111:G:H1'	38:0:9051:HOH:O	2.08	0.53
5:E:139:GLU:OE2	30:0:2781:U:H1'	2.09	0.53
6:F:34:ASN:HA	13:M:4:ALA:HB2	1.91	0.53
14:N:139:TRP:HA	14:N:139:TRP:HE3	1.74	0.53
30:0:290:C:O2'	30:0:291:C:H5'	2.09	0.53
30:0:441:A:H8	30:0:441:A:O5'	1.92	0.53
30:0:2769:C:H2'	30:0:2770:G:O4'	2.09	0.53
30:0:24:G:N2	30:0:518:G:H1'	2.24	0.52
30:0:1181:A:H2'	30:0:1182:C:H5'	1.90	0.52
30:0:1594:C:O2'	30:0:1595:G:H5'	2.09	0.52
30:0:1625:U:H5"	38:0:6037:HOH:O	2.09	0.52
31:9:3:A:H1'	38:9:9037:HOH:O	2.09	0.52
5:E:143:GLN:NE2	30:0:2780:C:H1'	2.13	0.52
30:0:615:G:H2'	30:0:616:U:C6	2.44	0.52
4:D:57:THR:HG23	4:D:63:ILE:HA	1.91	0.52
4:D:58:VAL:HB	4:D:62:ASP:HB3	1.89	0.52
14:N:48:VAL:HG11	14:N:55:ASP:HB3	1.90	0.52
30:0:90:A:H2'	30:0:91:G:O4'	2.08	0.52
30:0:204:A:H2'	30:0:205:U:H5'	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1419:U:H2'	30:0:1685:A:C2	2.44	0.52
30:0:1733:A:C6	30:0:1734:C:C2	2.98	0.52
30:0:2500:C:O2'	30:0:2501:G:H5'	2.08	0.52
31:9:59:C:H2'	31:9:60:C:C6	2.43	0.52
1:A:223:ARG:HB2	30:0:2272:G:H5'	1.90	0.52
4:D:28:GLY:HA2	4:D:69:ILE:HG23	1.91	0.52
5:E:91:PHE:CE1	30:0:2694:A:H4'	2.43	0.52
38:L:8841:HOH:O	30:0:2453:G:H5"	2.09	0.52
15:O:47:ARG:HG3	15:O:47:ARG:NH1	2.25	0.52
23:W:48:VAL:HG12	23:W:52:VAL:HB	1.90	0.52
28:2:49:GLU:HB2	38:2:719:HOH:O	2.10	0.52
30:0:1181:A:H1'	38:0:7132:HOH:O	2.09	0.52
30:0:1216:G:O2'	30:0:1217:G:H5'	2.10	0.52
30:0:1461:U:H2'	30:0:1462:C:C6	2.44	0.52
30:0:2598:U:O2	30:0:2600:A:H8	1.92	0.52
33:0:8813:CL:CL	38:0:4697:HOH:O	2.56	0.52
1:A:206:ARG:HD3	38:0:4620:HOH:O	2.08	0.52
2:B:305:ASP:O	2:B:306:LYS:HB2	2.10	0.52
8:H:6:ALA:HB3	30:0:2521:A:OP2	2.09	0.52
16:P:134:VAL:O	16:P:137:LEU:HB3	2.10	0.52
25:Y:99:ALA:HB2	25:Y:233:TYR:CE2	2.44	0.52
26:Z:74:GLN:HB2	26:Z:78:ILE:HG22	1.90	0.52
30:0:899:C:H5'	38:0:3209:HOH:O	2.09	0.52
30:0:1161:A:C6	30:0:1162:G:N7	2.77	0.52
30:0:1189:A:H1'	30:0:1209:C:C1'	2.40	0.52
30:0:1482:A:O2'	30:0:1483:C:H5'	2.10	0.52
30:0:1588:G:C6	30:0:1589:G:N1	2.77	0.52
2:B:17:LYS:O	2:B:260:HIS:HD2	1.91	0.52
17:Q:19:ARG:HH21	31:9:11:A:P	2.33	0.52
30:0:1196:C:H42	30:0:1204:C:H42	1.58	0.52
30:0:1202:A:H2'	30:0:1203:G:H5'	1.90	0.52
30:0:1309:U:O2'	30:0:1310:U:H5'	2.09	0.52
30:0:1871:U:O4'	30:0:1873:G:C8	2.63	0.52
31:9:91:C:H2'	31:9:92:G:O4'	2.10	0.52
3:C:63:SER:OG	30:0:2101:A:H2'	2.09	0.52
16:P:91:LYS:O	16:P:95:GLU:HG3	2.08	0.52
21:U:6:CYS:HB2	21:U:32:CYS:HB3	1.90	0.52
25:Y:169:ARG:HD3	30:0:1328:A:C8	2.44	0.52
11:K:113:ILE:HD12	11:K:128:ALA:HB2	1.92	0.52
14:N:67:ALA:HA	14:N:71:TRP:HB3	1.92	0.52
20:T:38:ARG:HH21	30:0:306:A:P	2.33	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:136:C:H2'	30:0:137:U:O4'	2.09	0.52
30:0:2866:U:C2	30:0:2891:A:C8	2.98	0.52
23:W:117:ARG:HD3	30:0:1287:A:O4'	2.10	0.52
30:0:1029:U:O2'	30:0:1273:C:OP1	2.25	0.52
30:0:2273:C:H5"	38:0:4515:HOH:O	2.10	0.52
31:9:108:C:H2'	31:9:109:G:C8	2.45	0.52
3:C:217:GLU:HG3	30:0:672:G:O6	2.10	0.52
9:I:73:LEU:HD12	9:I:107:LYS:HZ1	1.73	0.52
11:K:10:GLN:H	11:K:10:GLN:NE2	1.96	0.52
11:K:18:ILE:HG22	11:K:93:ASN:HB2	1.92	0.52
18:R:33:ARG:NH1	38:R:8947:HOH:O	2.42	0.52
30:0:1964:U:O2	30:0:1964:U:C2'	2.58	0.52
30:0:2032:U:O2'	30:0:2033:G:H5"	2.09	0.52
30:0:2112:A:H2'	30:0:2113:G:C8	2.45	0.52
8:H:70:LEU:O	8:H:74:ARG:HB2	2.09	0.51
9:I:112:LEU:HD12	30:0:1162:G:H1'	1.92	0.51
22:V:56:ILE:O	22:V:60:GLN:HG3	2.09	0.51
30:0:152:A:H2'	30:0:153:C:C6	2.45	0.51
30:0:407:A:H8	38:0:4468:HOH:O	1.93	0.51
30:0:951:A:C2'	30:0:952:G:H5'	2.39	0.51
30:0:1333:U:H2'	30:0:1334:C:H6	1.75	0.51
30:0:2827:A:H2'	30:0:2828:G:O4'	2.10	0.51
31:9:59:C:O5'	31:9:59:C:H6	1.92	0.51
10:J:54:VAL:HG11	10:J:138:THR:HG21	1.92	0.51
30:0:638:C:H2'	30:0:639:A:C8	2.46	0.51
30:0:792:G:O2'	30:0:793:A:H5'	2.11	0.51
30:0:876:A:H2'	30:0:876:A:N3	2.23	0.51
30:0:2636:C:H3'	38:0:9279:HOH:O	2.09	0.51
31:9:42:C:H5'	31:9:43:G:OP2	2.10	0.51
31:9:58:G:H1'	38:9:9067:HOH:O	2.09	0.51
24:X:21:PRO:HG2	24:X:24:LYS:HD3	1.91	0.51
30:0:154:C:H2'	30:0:155:C:H6	1.76	0.51
30:0:821:U:H2'	30:0:822:C:H6	1.75	0.51
30:0:1163:G:H2'	30:0:1164:U:C5	2.44	0.51
30:0:2896:A:N3	30:0:2896:A:H2'	2.25	0.51
2:B:125:GLU:O	2:B:129:ARG:HG3	2.10	0.51
2:B:254:GLN:HG2	2:B:255:GLY:N	2.25	0.51
5:E:84:MET:HG2	5:E:168:ILE:HA	1.93	0.51
22:V:12:THR:HG23	22:V:14:ALA:H	1.74	0.51
30:0:255:A:H2'	30:0:256:C:H6	1.74	0.51
30:0:603:A:H4'	30:0:605:C:C6	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1081:A:H5”	38:0:3158:HOH:O	2.10	0.51
30:0:1137:G:H1’	38:0:3884:HOH:O	2.09	0.51
30:0:1279:U:O2	30:0:1279:U:H2’	2.09	0.51
30:0:1525:G:H5’	30:0:1526:A:OP2	2.11	0.51
30:0:1755:A:H2’	30:0:1756:G:O4’	2.11	0.51
30:0:2478:U:O2’	30:0:2479:A:H5’	2.10	0.51
30:0:2566:A:C2	30:0:2696:G:O4’	2.63	0.51
30:0:2724:U:H2’	30:0:2725:G:O4’	2.10	0.51
2:B:248:ARG:O	2:B:251:VAL:HG22	2.11	0.51
23:W:43:GLY:HA3	30:0:945:U:O2’	2.11	0.51
30:0:684:G:H2’	30:0:685:C:C6	2.46	0.51
30:0:877:G:C2	30:0:885:G:O4’	2.63	0.51
30:0:1524:U:H5”	30:0:1524:U:C6	2.46	0.51
30:0:2758:G:H2’	30:0:2759:C:C6	2.46	0.51
1:A:33:GLU:H	1:A:33:GLU:CD	2.14	0.51
1:A:69:LEU:HB3	38:A:9039:HOH:O	2.11	0.51
3:C:43:LYS:HG2	30:0:449:A:N7	2.26	0.51
3:C:111:VAL:HB	38:C:8519:HOH:O	2.11	0.51
6:F:39:SER:HB3	6:F:45:ALA:HB2	1.91	0.51
23:W:88:THR:HG22	23:W:89:ASP:N	2.18	0.51
24:X:43:VAL:HG12	24:X:44:ASP:N	2.26	0.51
30:0:2823:G:H4’	30:0:2827:A:O4’	2.11	0.51
31:9:31:C:C2	31:9:50:G:C2	2.99	0.51
31:9:54:A:HO2’	31:9:55:U:H5’	1.75	0.51
4:D:99:ASP:HB3	4:D:103:ASN:HB2	1.90	0.51
12:L:148:GLU:HA	38:L:8872:HOH:O	2.10	0.51
25:Y:189:ASN:HA	25:Y:217:ILE:HD11	1.93	0.51
30:0:10:U:C6	30:0:10:U:H3’	2.46	0.51
30:0:821:U:H2’	30:0:822:C:C6	2.46	0.51
30:0:955:A:C2	30:0:1013:A:C4	2.99	0.51
30:0:958:G:O2’	30:0:959:C:H5’	2.10	0.51
30:0:1185:U:H5’	38:0:7483:HOH:O	2.09	0.51
30:0:2344:G:H2’	30:0:2344:G:N3	2.26	0.51
30:0:2830:U:O2’	30:0:2831:C:H5’	2.11	0.51
2:B:5:ARG:NH1	30:0:2547:C:OP2	2.44	0.51
10:J:45:VAL:HG21	10:J:129:PHE:CD1	2.45	0.51
11:K:10:GLN:HE21	11:K:10:GLN:N	1.97	0.51
16:P:40:VAL:O	16:P:44:VAL:HG23	2.11	0.51
30:0:1245:C:O5’	30:0:1245:C:H6	1.93	0.51
30:0:2638:G:H1’	38:0:4596:HOH:O	2.11	0.51
30:0:2768:A:H3’	30:0:2768:A:N3	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:MET:HG2	1:A:186:TRP:CB	2.41	0.51
19:S:57:THR:HG22	19:S:58:MET:N	2.26	0.51
25:Y:204:ARG:HH22	30:0:553:G:P	2.33	0.51
30:0:407:A:H5'	38:0:6041:HOH:O	2.11	0.51
30:0:1614:G:H2'	38:0:4642:HOH:O	2.10	0.51
30:0:2102:G:H5'	30:0:2538:A:C2	2.45	0.51
2:B:36:PRO:HA	2:B:168:GLY:HA3	1.93	0.51
2:B:190:MET:HE2	2:B:194:PHE:CD1	2.46	0.51
26:Z:57:MET:SD	26:Z:73:ARG:HD2	2.51	0.51
30:0:18:C:H2'	30:0:19:U:C6	2.46	0.51
30:0:1118:A:C8	30:0:1119:G:H5"	2.46	0.51
30:0:1667:A:H5'	30:0:1667:A:C8	2.44	0.51
2:B:140:LEU:HD12	2:B:174:ARG:HG3	1.91	0.50
2:B:221:GLN:HE22	11:K:42:ASN:HD22	1.59	0.50
6:F:38:LYS:HE3	30:0:244:C:OP2	2.11	0.50
14:N:169:PRO:O	14:N:172:PHE:HB3	2.11	0.50
30:0:877:G:C5'	30:0:878:G:OP1	2.55	0.50
30:0:1857:A:N6	30:0:2247:C:H1'	2.26	0.50
30:0:2858:U:H2'	30:0:2859:C:C6	2.46	0.50
2:B:36:PRO:HG3	2:B:169:GLY:H	1.75	0.50
30:0:1284:G:O2'	30:0:1285:U:H5'	2.11	0.50
30:0:1829:A:C2'	30:0:1830:C:H5'	2.40	0.50
30:0:1829:A:H2'	30:0:1830:C:H5'	1.94	0.50
30:0:2347:C:H2'	30:0:2348:C:H6	1.76	0.50
30:0:2681:A:H8	38:0:5592:HOH:O	1.92	0.50
31:9:52:A:H2'	31:9:53:G:O4'	2.10	0.50
2:B:280:VAL:HG13	2:B:334:SER:HA	1.93	0.50
38:I:5331:HOH:O	30:0:1164:U:H5	1.94	0.50
30:0:694:A:C2'	30:0:695:C:H5'	2.41	0.50
30:0:1194:A:N1	30:0:1195:G:C6	2.79	0.50
30:0:2505:G:H8	38:0:5653:HOH:O	1.94	0.50
1:A:109:GLU:HG2	1:A:116:GLY:H	1.75	0.50
2:B:62:ARG:HA	2:B:65:MET:CE	2.41	0.50
4:D:69:ILE:HD12	30:0:2346:C:H5'	1.93	0.50
14:N:143:ARG:HH21	14:N:169:PRO:HB2	1.75	0.50
24:X:78:GLU:HG2	24:X:79:GLU:H	1.75	0.50
30:0:1163:G:H2'	30:0:1164:U:C6	2.45	0.50
30:0:1166:A:C6	30:0:1181:A:C2	2.99	0.50
30:0:1921:A:O2'	30:0:1922:A:H5'	2.12	0.50
30:0:2102:G:C2	30:0:2104:C:C4	3.00	0.50
17:Q:66:LYS:HB2	17:Q:70:ALA:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:255:A:O2'	30:0:256:C:H5'	2.12	0.50
30:0:920:C:H5'	30:0:921:G:C4	2.46	0.50
30:0:1118:A:H8	30:0:1119:G:H5"	1.77	0.50
30:0:1190:G:H3'	30:0:1190:G:N3	2.26	0.50
30:0:1762:C:H4'	38:0:4668:HOH:O	2.11	0.50
30:0:2256:G:C2'	30:0:2257:G:H5'	2.42	0.50
30:0:2718:C:H6	30:0:2718:C:H5'	1.77	0.50
1:A:191:GLY:HA2	1:A:194:MET:CE	2.41	0.50
1:A:212:PRO:HB2	38:0:4369:HOH:O	2.12	0.50
8:H:59:GLN:HG2	8:H:129:ARG:HG2	1.92	0.50
10:J:74:ARG:O	10:J:78:ILE:HG12	2.11	0.50
10:J:107:ASN:ND2	10:J:109:TYR:H	2.09	0.50
10:J:107:ASN:HD21	10:J:109:TYR:HB2	1.76	0.50
30:0:12:U:C2'	30:0:13:G:H5'	2.41	0.50
30:0:368:C:C2'	30:0:369:G:H5'	2.42	0.50
30:0:1521:C:C2	30:0:1522:A:C8	3.00	0.50
30:0:1819:G:C2'	30:0:1820:G:H5'	2.41	0.50
30:0:2553:A:H2'	30:0:2553:A:N3	2.26	0.50
30:0:2730:G:O2'	30:0:2731:G:H5'	2.11	0.50
9:I:82:THR:CG2	30:0:1168:C:H5"	2.42	0.50
30:0:559:U:C6	30:0:559:U:C3'	2.95	0.50
30:0:1131:G:C6	30:0:1230:A:C4	3.00	0.50
30:0:1522:A:C2	30:0:1665:G:C6	2.99	0.50
30:0:2729:C:O2'	30:0:2730:G:H5'	2.10	0.50
5:E:143:GLN:NE2	30:0:2779:G:H21	2.10	0.50
9:I:95:LEU:HD23	9:I:99:GLN:OE1	2.11	0.50
30:0:1205:U:C2'	30:0:1206:U:C5'	2.84	0.50
30:0:1406:A:H4'	30:0:1407:A:H5"	1.93	0.50
30:0:2445:U:H2'	30:0:2446:G:C8	2.47	0.50
30:0:2597:U:H2'	30:0:2598:U:H5'	1.94	0.50
4:D:88:LEU:HB2	4:D:89:PRO:HD3	1.94	0.50
6:F:58:GLU:HA	6:F:61:MET:HE2	1.94	0.50
9:I:87:PRO:HD3	38:0:3242:HOH:O	2.12	0.50
13:M:28:GLN:O	13:M:32:ARG:HG3	2.12	0.50
30:0:204:A:C2'	30:0:205:U:H5'	2.41	0.50
30:0:2291:A:N9	30:0:2309:C:H5'	2.26	0.50
30:0:2756:U:H3	30:0:2896:A:H2	1.57	0.50
30:0:2909:G:H2'	30:0:2910:A:H8	1.76	0.50
1:A:199:HIS:HE1	30:0:1881:A:OP1	1.95	0.49
2:B:320:GLN:HE21	2:B:321:PRO:CD	2.24	0.49
13:M:171:ARG:NH2	30:0:189:A:OP1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:77:ASN:OD1	14:N:79:PRO:HD2	2.12	0.49
23:W:64:THR:O	23:W:68:THR:HG22	2.11	0.49
26:Z:34:SER:HA	30:0:797:A:H5'	1.94	0.49
30:0:67:A:H5"	30:0:69:A:C8	2.47	0.49
30:0:73:U:O2'	30:0:74:G:H5'	2.12	0.49
30:0:941:G:C5	30:0:942:U:C4	3.00	0.49
30:0:1209:C:C2	30:0:1210:G:C8	3.00	0.49
30:0:1707:G:H1'	30:0:1711:A:N6	2.26	0.49
31:9:3:A:H2'	38:9:9040:HOH:O	2.11	0.49
2:B:62:ARG:HA	2:B:65:MET:HE2	1.93	0.49
10:J:75:PRO:HG2	10:J:105:LEU:CD2	2.38	0.49
30:0:256:C:H2'	30:0:257:G:O4'	2.12	0.49
30:0:2712:G:H5'	38:0:5233:HOH:O	2.11	0.49
1:A:33:GLU:O	1:A:34:ASP:HB2	2.12	0.49
2:B:144:THR:HG22	2:B:145:HIS:N	2.27	0.49
3:C:107:ARG:O	3:C:111:VAL:HG23	2.13	0.49
6:F:58:GLU:HB3	13:M:8:ILE:HG23	1.93	0.49
10:J:88:PRO:HA	33:J:8802:CL:CL	2.49	0.49
27:1:28:HIS:HE1	30:0:776:A:OP1	1.94	0.49
30:0:333:G:O2'	30:0:334:G:H5'	2.13	0.49
30:0:652:G:H8	38:0:3021:HOH:O	1.95	0.49
30:0:702:G:C2	30:0:703:G:C8	3.00	0.49
30:0:946:C:O2'	30:0:947:U:H5'	2.12	0.49
30:0:1878:G:O2'	30:0:1879:U:OP2	2.30	0.49
30:0:2831:C:C2	30:0:2910:A:C2	3.00	0.49
4:D:50:VAL:HG13	31:9:41:C:O4'	2.12	0.49
11:K:34:VAL:HG21	11:K:46:LYS:O	2.12	0.49
16:P:81:LYS:HG2	38:0:9543:HOH:O	2.12	0.49
30:0:185:G:H4'	30:0:186:A:H4'	1.93	0.49
30:0:1909:A:H2'	30:0:1910:A:C8	2.48	0.49
4:D:51:ARG:HH11	4:D:68:PRO:HB3	1.76	0.49
16:P:7:LYS:HD3	16:P:21:VAL:CG2	2.41	0.49
27:1:16:HIS:HE1	30:0:775:G:OP1	1.95	0.49
30:0:95:A:H5"	30:0:97:G:O4'	2.13	0.49
30:0:711:G:N2	30:0:718:C:C2	2.80	0.49
30:0:947:U:H2'	30:0:948:G:H8	1.77	0.49
30:0:1187:U:O2'	30:0:1189:A:H2	1.95	0.49
30:0:1377:C:H1'	38:0:9041:HOH:O	2.12	0.49
30:0:1607:A:C4	30:0:1608:G:C8	3.00	0.49
30:0:1768:C:H2'	30:0:1769:C:O4'	2.13	0.49
30:0:2004:U:H5"	30:0:2005:G:C8	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2781:U:O2'	30:0:2782:G:H5'	2.12	0.49
2:B:162:MET:CE	2:B:308:LEU:HD21	2.42	0.49
5:E:47:VAL:HG11	5:E:69:ILE:HD13	1.94	0.49
11:K:130:MET:SD	21:U:25:ASP:O	2.70	0.49
15:O:25:VAL:HG12	30:0:709:G:O3'	2.13	0.49
18:R:29:LYS:HE2	30:0:524:A:C5'	2.42	0.49
20:T:18:GLU:O	20:T:21:LYS:HG2	2.11	0.49
23:W:5:VAL:HG11	23:W:153:MET:HE3	1.94	0.49
30:0:363:C:H2'	30:0:364:U:H6	1.77	0.49
30:0:734:U:O2'	30:0:736:A:N7	2.44	0.49
30:0:951:A:O2'	30:0:952:G:H5'	2.13	0.49
30:0:1588:G:C6	30:0:1589:G:C6	3.01	0.49
30:0:1854:C:H2'	30:0:1875:A:H61	1.78	0.49
30:0:2112:A:H2'	30:0:2113:G:H8	1.77	0.49
10:J:70:PHE:CD1	30:0:2676:C:H4'	2.46	0.49
29:3:11:CYS:SG	29:3:14:CYS:HB2	2.52	0.49
29:3:30:GLN:NE2	38:3:9043:HOH:O	2.43	0.49
30:0:952:G:N3	30:0:2302:A:H2'	2.28	0.49
30:0:1189:A:N7	30:0:1190:G:C8	2.81	0.49
30:0:1568:G:C5	30:0:1569:U:C5	3.01	0.49
30:0:1730:G:C5'	30:0:1731:C:H6	2.25	0.49
30:0:1778:A:H2'	30:0:1779:A:H5'	1.94	0.49
1:A:53:ALA:HB3	38:A:9068:HOH:O	2.12	0.49
2:B:142:LEU:HD21	2:B:178:ALA:HB1	1.94	0.49
25:Y:149:GLN:O	25:Y:154:ARG:NH1	2.46	0.49
30:0:1066:U:H2'	30:0:1067:A:C8	2.47	0.49
30:0:1682:A:H5"	38:0:9457:HOH:O	2.13	0.49
30:0:1730:G:H5'	30:0:1731:C:H5	1.78	0.49
30:0:2481:G:C3'	30:0:2482:G:H5"	2.42	0.49
30:0:2498:C:C2'	30:0:2499:U:H5'	2.43	0.49
31:9:31:C:C2	31:9:50:G:N2	2.81	0.49
31:9:73:A:N1	31:9:108:C:O2	2.45	0.49
1:A:81:GLN:HB2	1:A:92:ASN:ND2	2.28	0.49
8:H:150:LYS:HA	38:H:230:HOH:O	2.13	0.49
10:J:131:THR:HG22	10:J:133:GLY:H	1.78	0.49
20:T:97:ARG:NH2	30:0:309:C:OP1	2.46	0.49
25:Y:189:ASN:HD22	25:Y:192:ASP:H	1.61	0.49
26:Z:55:SER:O	26:Z:59:GLU:HG3	2.12	0.49
30:0:503:G:H2'	30:0:504:G:H8	1.77	0.49
30:0:1783:A:O2'	30:0:1784:U:H5'	2.12	0.49
30:0:2829:G:O2'	30:0:2830:U:H5'	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2890:A:H5”	30:0:2890:A:H8	1.77	0.49
1:A:48:ASP:HB3	38:A:9068:HOH:O	2.13	0.49
1:A:211:LYS:HD2	38:A:9083:HOH:O	2.13	0.49
11:K:82:ARG:NH2	11:K:115:ARG:HG2	2.28	0.49
25:Y:170:SER:OG	25:Y:175:ARG:HG3	2.12	0.49
30:0:1007:A:H1’	38:0:3138:HOH:O	2.12	0.49
30:0:1398:G:H2’	30:0:1399:A:H8	1.75	0.49
30:0:1816:C:H2’	30:0:1817:U:O4’	2.13	0.49
30:0:2064:U:H5’	30:0:2652:U:O3’	2.13	0.49
30:0:2578:G:H5’	30:0:2578:G:C8	2.43	0.49
30:0:2756:U:N3	30:0:2896:A:C2	2.75	0.49
30:0:2847:G:O2’	30:0:2848:G:H5’	2.12	0.49
3:C:76:ARG:HD3	38:C:8570:HOH:O	2.13	0.48
20:T:2:LYS:HG2	30:0:447:A:OP1	2.13	0.48
23:W:125:HIS:CE1	30:0:1097:A:H5”	2.47	0.48
24:X:23:HIS:HD2	38:0:9959:HOH:O	1.96	0.48
30:0:703:G:O2’	30:0:704:C:H5’	2.13	0.48
30:0:1016:U:O2’	30:0:2303:A:N7	2.38	0.48
30:0:1180:U:H2’	30:0:1181:A:O4’	2.13	0.48
30:0:1497:G:H4’	30:0:1627:G:O2’	2.13	0.48
2:B:140:LEU:CD1	2:B:174:ARG:HG3	2.44	0.48
12:L:18:HIS:HB2	30:0:903:U:O4	2.13	0.48
15:O:32:ARG:O	15:O:32:ARG:HD3	2.13	0.48
22:V:39:ALA:N	22:V:40:PRO:HD2	2.25	0.48
30:0:69:A:H2’	30:0:70:A:OP2	2.12	0.48
30:0:499:G:O2’	30:0:500:G:H5’	2.13	0.48
30:0:613:C:H2’	30:0:614:U:C6	2.44	0.48
30:0:626:U:C4	30:0:627:G:C6	3.01	0.48
30:0:814:G:H2’	30:0:815:U:C6	2.48	0.48
30:0:1323:G:H5’	38:0:4709:HOH:O	2.13	0.48
30:0:1676:G:H1’	38:0:9434:HOH:O	2.13	0.48
31:9:61:C:H2’	31:9:62:A:H8	1.77	0.48
31:9:92:G:C6	31:9:93:A:C6	3.01	0.48
4:D:76:ARG:NE	31:9:44:A:O4’	2.46	0.48
16:P:88:GLN:HE21	30:0:1800:G:H1’	1.76	0.48
24:X:30:MET:HG2	30:0:1384:C:H5’	1.94	0.48
25:Y:154:ARG:HH22	30:0:1071:G:H4’	1.78	0.48
25:Y:187:VAL:HG23	25:Y:192:ASP:HB3	1.93	0.48
30:0:308:U:C4	30:0:342:C:H1’	2.48	0.48
30:0:371:U:O2’	30:0:372:A:H5’	2.13	0.48
30:0:961:A:H4’	38:0:6790:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2353:A:H4'	30:0:2354:A:O5'	2.13	0.48
30:0:2433:A:H2'	30:0:2434:A:C8	2.48	0.48
30:0:2510:C:H42	30:0:2564:G:N2	2.11	0.48
5:E:69:ILE:HA	5:E:72:MET:CE	2.44	0.48
14:N:110:THR:HB	14:N:113:SER:OG	2.13	0.48
17:Q:7:LEU:HD12	30:0:2424:U:H1'	1.96	0.48
30:0:466:A:H2'	30:0:467:G:O4'	2.13	0.48
30:0:581:G:O2'	30:0:582:U:H5'	2.12	0.48
30:0:1087:G:H4'	30:0:1088:A:OP1	2.12	0.48
30:0:1377:C:H6	30:0:1377:C:C5'	2.25	0.48
30:0:2831:C:H6	38:0:7228:HOH:O	1.96	0.48
31:9:39:U:H1'	31:9:44:A:H61	1.78	0.48
1:A:140:LEU:HB3	1:A:141:PRO:HD2	1.94	0.48
2:B:223:ARG:HG3	2:B:232:TRP:O	2.13	0.48
11:K:12:LEU:HB2	11:K:47:ALA:HB3	1.96	0.48
13:M:99:ARG:HD2	13:M:167:GLY:CA	2.41	0.48
15:O:14:LEU:CD2	15:O:102:ILE:HD11	2.43	0.48
24:X:61:ARG:O	30:0:2744:G:H5"	2.14	0.48
27:1:1:THR:HB	38:0:7157:HOH:O	2.13	0.48
30:0:513:A:N3	38:0:3665:HOH:O	2.35	0.48
30:0:790:A:H1'	30:0:1710:A:H2'	1.95	0.48
30:0:802:G:O2'	30:0:803:C:H5'	2.13	0.48
30:0:1190:G:H2'	38:0:4064:HOH:O	2.13	0.48
30:0:2256:G:O2'	30:0:2257:G:H5'	2.14	0.48
30:0:2754:G:C2'	30:0:2755:G:H5'	2.43	0.48
30:0:2768:A:C2'	30:0:2769:C:O4'	2.61	0.48
30:0:2908:A:O2'	30:0:2909:G:H5'	2.13	0.48
31:9:71:C:H2'	31:9:72:C:H6	1.79	0.48
4:D:23:VAL:HG12	4:D:130:VAL:HG22	1.96	0.48
8:H:165:ARG:HB3	38:H:235:HOH:O	2.13	0.48
11:K:41:LYS:HA	30:0:2582:G:O3'	2.14	0.48
14:N:65:ASP:HB3	38:N:8821:HOH:O	2.13	0.48
16:P:7:LYS:HD3	16:P:21:VAL:HG22	1.95	0.48
30:0:305:A:C5	30:0:329:A:C2	3.02	0.48
30:0:1311:G:C2	30:0:1312:G:C8	3.01	0.48
30:0:1343:C:H2'	30:0:1344:G:O5'	2.14	0.48
30:0:1520:G:H2'	30:0:1521:C:C6	2.48	0.48
1:A:135:VAL:HG21	1:A:147:ARG:HB3	1.96	0.48
3:C:246:ARG:NE	38:C:8628:HOH:O	2.43	0.48
8:H:61:ARG:HH11	8:H:61:ARG:HG3	1.78	0.48
8:H:170:ARG:HD2	38:H:194:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:55:VAL:HG12	11:K:56:SER:N	2.28	0.48
12:L:117:GLU:HA	38:L:8852:HOH:O	2.13	0.48
21:U:17:THR:CG2	21:U:18:GLY:N	2.77	0.48
23:W:21:LEU:HD13	23:W:26:ILE:HD11	1.95	0.48
27:1:28:HIS:HD2	27:1:30:LYS:H	1.59	0.48
30:0:661:G:C5	30:0:686:A:C2	3.02	0.48
30:0:735:C:O5'	30:0:735:C:H6	1.97	0.48
30:0:1422:U:H2'	30:0:1423:C:H6	1.76	0.48
5:E:72:MET:O	5:E:76:VAL:HG22	2.14	0.48
11:K:9:THR:HA	38:0:3293:HOH:O	2.14	0.48
12:L:143:THR:HG22	12:L:144:ASP:N	2.28	0.48
30:0:285:A:N6	30:0:367:G:H1'	2.28	0.48
30:0:1188:A:C5	30:0:1189:A:C2	3.01	0.48
30:0:1201:C:C2'	30:0:1202:A:H5'	2.42	0.48
30:0:1789:G:H2'	30:0:1790:C:O5'	2.13	0.48
30:0:1976:G:O2'	30:0:1977:U:H5'	2.14	0.48
30:0:2090:G:H2'	30:0:2091:G:C8	2.49	0.48
6:F:53:ASP:OD1	6:F:80:GLN:HB2	2.14	0.48
9:I:97:VAL:HG12	9:I:101:LYS:HE3	1.94	0.48
30:0:675:U:H6	30:0:675:U:O5'	1.97	0.48
30:0:732:C:O2'	30:0:733:U:H5'	2.13	0.48
30:0:1159:G:H1	30:0:1208:C:H42	1.61	0.48
30:0:1543:G:N1	30:0:1641:A:OP2	2.34	0.48
30:0:2419:U:H5"	30:0:2420:G:H5'	1.95	0.48
30:0:2635:A:C2'	30:0:2636:C:H5'	2.44	0.48
30:0:2656:G:C2'	30:0:2657:G:H5'	2.44	0.48
1:A:88:ILE:HD13	1:A:100:PRO:HD3	1.95	0.48
10:J:39:VAL:HG13	10:J:106:GLY:O	2.13	0.48
13:M:171:ARG:CD	30:0:156:C:H5"	2.23	0.48
20:T:77:VAL:HG11	20:T:91:LEU:HD11	1.95	0.48
23:W:41:TYR:OH	30:0:1024:G:H4'	2.14	0.48
30:0:363:C:H2'	30:0:364:U:C6	2.49	0.48
30:0:506:G:N2	30:0:509:A:H5"	2.20	0.48
30:0:1506:U:H6	30:0:1506:U:H5'	1.79	0.48
30:0:1613:C:H2'	30:0:1614:G:O4'	2.14	0.48
30:0:1902:G:N2	30:0:1936:C:C2	2.82	0.48
30:0:2837:U:H2'	38:0:6856:HOH:O	2.14	0.48
30:0:2858:U:H2'	30:0:2859:C:H6	1.78	0.48
38:C:8666:HOH:O	30:0:656:G:H1'	2.14	0.47
13:M:64:ARG:HD2	38:M:8880:HOH:O	2.14	0.47
14:N:4:PRO:HB2	30:0:1010:C:H4'	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:250:C:H2'	30:0:251:C:H6	1.79	0.47
30:0:947:U:O2'	30:0:948:G:H5'	2.14	0.47
30:0:1512:G:O2'	30:0:1513:C:H5'	2.14	0.47
30:0:2074:A:H1'	38:0:9890:HOH:O	2.14	0.47
30:0:2769:C:C2'	30:0:2770:G:C5'	2.78	0.47
31:9:1:U:C4'	31:9:3:A:OP1	2.62	0.47
13:M:34:GLU:HB3	13:M:38:GLU:HG3	1.96	0.47
29:3:65:THR:HB	29:3:83:TRP:H	1.79	0.47
30:0:101:C:H2'	30:0:102:A:C8	2.49	0.47
30:0:128:A:O2'	30:0:129:A:C5'	2.62	0.47
30:0:800:G:H2'	30:0:801:U:C6	2.49	0.47
30:0:814:G:H4'	38:0:3141:HOH:O	2.14	0.47
30:0:843:A:C2	30:0:846:A:C8	3.02	0.47
30:0:1562:C:O2	30:0:1562:C:H2'	2.12	0.47
30:0:2493:C:O2	30:0:2493:C:H2'	2.14	0.47
30:0:2672:C:H2'	30:0:2673:U:H6	1.78	0.47
30:0:2869:G:H5'	38:0:5510:HOH:O	2.14	0.47
31:9:108:C:H2'	31:9:109:G:H8	1.78	0.47
1:A:65:ARG:O	1:A:66:ARG:HG3	2.15	0.47
1:A:171:LYS:HB2	30:0:820:G:C6	2.49	0.47
1:A:217:ARG:HG2	1:A:229:ALA:HB2	1.96	0.47
9:I:108:HIS:N	9:I:109:PRO:HD2	2.29	0.47
9:I:120:ALA:O	9:I:124:VAL:HG23	2.14	0.47
12:L:41:HIS:CD2	30:0:926:A:O2'	2.65	0.47
26:Z:45:VAL:HG23	30:0:1887:U:OP1	2.14	0.47
29:3:11:CYS:HB2	29:3:20:HIS:CE1	2.49	0.47
30:0:814:G:H2'	30:0:815:U:H6	1.79	0.47
30:0:1268:C:H2'	30:0:1269:G:H8	1.79	0.47
30:0:1321:A:H2'	30:0:1322:G:H8	1.80	0.47
30:0:2134:G:H2'	30:0:2135:A:H8	1.79	0.47
30:0:2253:G:H2'	30:0:2254:G:H8	1.79	0.47
30:0:2795:C:O2'	30:0:2796:U:H5'	2.15	0.47
31:9:114:G:H2'	31:9:115:C:C6	2.49	0.47
1:A:171:LYS:HB2	30:0:820:G:C5	2.50	0.47
2:B:41:PHE:HB3	2:B:190:MET:HE1	1.96	0.47
3:C:58:ALA:HA	3:C:73:GLN:HE21	1.79	0.47
3:C:197:SER:HB3	38:C:8577:HOH:O	2.15	0.47
4:D:41:LEU:HA	4:D:44:ILE:HG22	1.96	0.47
5:E:143:GLN:HE21	30:0:2780:C:C1'	2.15	0.47
26:Z:43:GLY:O	26:Z:47:ARG:HG2	2.14	0.47
30:0:660:A:H4'	30:0:661:G:O5'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:671:A:O2'	30:0:672:G:H2'	2.14	0.47
30:0:834:G:H3'	30:0:835:U:H4'	1.95	0.47
30:0:1165:G:C4'	30:0:1174:A:O2'	2.60	0.47
30:0:1568:G:O2'	30:0:1569:U:H5'	2.14	0.47
30:0:1667:A:H2'	30:0:1668:U:C6	2.49	0.47
30:0:2256:G:H2'	30:0:2257:G:C5'	2.45	0.47
2:B:229:ARG:NH2	30:0:1753:C:O2	2.45	0.47
5:E:108:LEU:HD11	5:E:164:ASP:HB2	1.96	0.47
8:H:5:PRO:HD2	8:H:8:MET:SD	2.55	0.47
12:L:92:ASP:HA	12:L:121:ILE:HB	1.96	0.47
30:0:69:A:H8	30:0:69:A:C5'	2.21	0.47
30:0:1126:C:O5'	30:0:1126:C:H6	1.97	0.47
30:0:1187:U:H2'	38:0:6916:HOH:O	2.15	0.47
30:0:2105:C:O2'	30:0:2284:G:N2	2.48	0.47
30:0:2826:G:C6	30:0:2913:A:C6	3.02	0.47
1:A:186:TRP:CD1	1:A:187:PRO:HA	2.49	0.47
3:C:34:ALA:HB3	3:C:220:THR:HG21	1.97	0.47
3:C:114:ALA:HB1	3:C:223:LEU:HB3	1.96	0.47
5:E:91:PHE:HE1	30:0:2694:A:H4'	1.78	0.47
8:H:64:SER:OG	30:0:2520:G:H5'	2.13	0.47
12:L:35:ARG:O	12:L:40:PHE:HA	2.15	0.47
12:L:134:GLU:HG3	38:L:8856:HOH:O	2.15	0.47
14:N:61:ALA:CB	14:N:88:ALA:HB2	2.44	0.47
30:0:423:A:C5	30:0:424:C:C5	3.02	0.47
30:0:559:U:C6	30:0:559:U:H3'	2.50	0.47
30:0:1014:A:H5"	31:9:101:G:O2'	2.14	0.47
30:0:1126:C:HO2'	30:0:1128:U:H6	1.60	0.47
30:0:1166:A:H1'	30:0:1192:A:C2	2.50	0.47
30:0:1883:U:H5"	30:0:2013:G:OP2	2.14	0.47
30:0:2265:U:H2'	30:0:2266:A:C8	2.49	0.47
30:0:2411:C:H4'	38:0:4964:HOH:O	2.13	0.47
31:9:39:U:C2'	31:9:40:C:OP1	2.63	0.47
1:A:36:ASP:HA	1:A:83:GLY:HA3	1.97	0.47
3:C:154:VAL:O	3:C:158:GLU:HG3	2.15	0.47
4:D:37:ALA:O	4:D:40:ILE:HG12	2.14	0.47
6:F:50:VAL:HG13	6:F:60:VAL:HG11	1.96	0.47
12:L:71:GLU:HG2	30:0:700:A:C2	2.49	0.47
13:M:99:ARG:CD	13:M:167:GLY:HA2	2.41	0.47
13:M:124:GLY:HA3	30:0:2132:C:H1'	1.96	0.47
18:R:82:GLU:O	18:R:86:LYS:HG3	2.13	0.47
24:X:43:VAL:HG11	24:X:82:GLU:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:155:ARG:NH1	38:Y:8128:HOH:O	2.48	0.47
30:0:36:C:C2	30:0:447:A:C2	3.03	0.47
30:0:304:G:H1'	30:0:347:A:N6	2.29	0.47
30:0:1391:G:H2'	30:0:1392:A:H5'	1.97	0.47
30:0:1471:A:H5'	38:0:3197:HOH:O	2.15	0.47
30:0:1477:C:C5'	30:0:1868:G:H5"	2.44	0.47
30:0:1730:G:H5'	30:0:1731:C:C6	2.48	0.47
30:0:1948:G:H2'	30:0:1949:G:H8	1.79	0.47
30:0:2531:U:O2'	30:0:2532:A:H5'	2.14	0.47
30:0:2831:C:H2'	30:0:2832:C:C5'	2.45	0.47
1:A:27:LEU:HD12	1:A:69:LEU:HD22	1.95	0.47
12:L:133:VAL:HB	38:L:8856:HOH:O	2.15	0.47
14:N:11:ARG:HG3	14:N:14:ARG:NH1	2.30	0.47
16:P:54:LYS:HB2	30:0:1717:A:H5"	1.95	0.47
30:0:151:A:H2'	30:0:152:A:O4'	2.14	0.47
30:0:1182:C:C1'	30:0:1192:A:C8	2.97	0.47
30:0:2829:G:C2	30:0:2912:C:C2	3.03	0.47
30:0:2871:G:H2'	30:0:2872:U:C6	2.50	0.47
30:0:2891:A:H2'	30:0:2891:A:N3	2.29	0.47
2:B:199:TYR:HE2	2:B:268:ARG:HB2	1.79	0.47
12:L:50:GLY:C	30:0:2453:G:H4'	2.35	0.47
27:1:28:HIS:CD2	27:1:31:LYS:HG3	2.50	0.47
27:1:46:ARG:HA	38:0:3028:HOH:O	2.15	0.47
30:0:485:A:N3	30:0:487:G:H5"	2.29	0.47
30:0:560:U:H2'	30:0:561:G:C8	2.44	0.47
30:0:960:G:H3'	30:0:960:G:C4	2.47	0.47
30:0:2087:C:O2'	30:0:2088:C:H5'	2.15	0.47
30:0:1205:U:H2'	30:0:1206:U:H5'	1.96	0.47
30:0:1788:U:C2	30:0:1805:G:N2	2.83	0.47
30:0:1789:G:C2'	30:0:1790:C:O5'	2.63	0.47
30:0:2326:C:H4'	30:0:2412:G:C4'	2.44	0.47
30:0:2831:C:H2'	30:0:2832:C:H5'	1.97	0.47
2:B:314:ALA:HB3	2:B:317:PRO:HG3	1.97	0.46
14:N:11:ARG:NH1	31:9:8:G:O6	2.48	0.46
14:N:86:LEU:O	14:N:90:LEU:HG	2.14	0.46
23:W:61:THR:HG23	23:W:151:GLU:HG3	1.97	0.46
24:X:43:VAL:HG22	24:X:76:ARG:NH1	2.29	0.46
30:0:254:C:O2	30:0:254:C:C2'	2.54	0.46
30:0:820:G:O2'	30:0:856:G:H4'	2.14	0.46
30:0:825:U:H5"	30:0:826:U:OP1	2.15	0.46
30:0:1947:G:N2	30:0:1966:U:O2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2072:G:C6	30:0:2533:C:H1'	2.50	0.46
30:0:2256:G:H2'	30:0:2257:G:H5'	1.97	0.46
30:0:2833:C:H1'	30:0:2848:G:N2	2.30	0.46
1:A:233:THR:HB	30:0:1942:A:H5"	1.98	0.46
3:C:35:VAL:HG21	3:C:227:GLY:HA2	1.96	0.46
3:C:200:PRO:HB3	3:C:212:VAL:HG23	1.97	0.46
13:M:43:PRO:HG3	13:M:62:VAL:HG21	1.98	0.46
14:N:86:LEU:HD12	14:N:125:ALA:HB2	1.97	0.46
14:N:141:ARG:HH21	31:9:48:C:H4'	1.79	0.46
24:X:30:MET:HE1	24:X:58:ALA:HB3	1.97	0.46
28:2:22:PRO:HG2	28:2:25:VAL:HG23	1.97	0.46
28:2:28:LYS:O	30:0:87:C:H2'	2.15	0.46
30:0:10:U:C6	30:0:10:U:C3'	2.98	0.46
30:0:789:C:H5'	38:0:6228:HOH:O	2.15	0.46
30:0:920:C:H4'	30:0:921:G:N2	2.30	0.46
30:0:1174:A:C5	30:0:1201:C:H4'	2.50	0.46
30:0:1706:G:C5	30:0:1707:G:C6	3.03	0.46
30:0:1771:U:O2'	30:0:1773:G:N7	2.46	0.46
30:0:2092:G:H2'	30:0:2613:G:OP1	2.15	0.46
30:0:2106:C:H1'	30:0:2484:U:C2	2.49	0.46
30:0:2577:A:H8	38:0:9606:HOH:O	1.98	0.46
30:0:2825:C:H4'	30:0:2826:G:O5'	2.15	0.46
30:0:2911:C:O2'	30:0:2912:C:H5'	2.15	0.46
1:A:211:LYS:HD3	38:0:6884:HOH:O	2.15	0.46
25:Y:99:ALA:HB2	25:Y:233:TYR:CZ	2.50	0.46
30:0:277:U:O2'	30:0:278:A:H5'	2.15	0.46
30:0:544:G:C3'	30:0:545:G:H5"	2.45	0.46
30:0:1400:C:O2'	30:0:1401:G:H5'	2.15	0.46
30:0:1557:G:O2'	30:0:1558:C:H5'	2.15	0.46
30:0:1596:U:H2'	30:0:1598:A:OP2	2.14	0.46
30:0:1634:G:C4	30:0:1635:U:C5	3.03	0.46
30:0:2598:U:O2	30:0:2600:A:C8	2.68	0.46
30:0:2871:G:H2'	30:0:2872:U:H6	1.79	0.46
31:9:3:A:H2	31:9:21:G:N3	2.14	0.46
1:A:123:GLY:HA3	1:A:162:GLY:HA2	1.96	0.46
2:B:41:PHE:CZ	2:B:79:MET:HG3	2.50	0.46
13:M:80:GLY:O	13:M:81:ARG:HD2	2.14	0.46
15:O:25:VAL:HG12	30:0:709:G:O2'	2.16	0.46
30:0:354:A:H2'	30:0:355:C:H6	1.80	0.46
30:0:876:A:N3	30:0:876:A:C2'	2.79	0.46
30:0:1102:C:H5	38:0:3497:HOH:O	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1200:A:H3'	38:0:5769:HOH:O	2.15	0.46
30:0:1878:G:C4'	38:0:6135:HOH:O	2.64	0.46
30:0:2105:C:H2'	30:0:2106:C:C6	2.50	0.46
30:0:2284:G:H1'	38:0:9576:HOH:O	2.15	0.46
30:0:2482:G:H4'	30:0:2483:A:C5'	2.45	0.46
30:0:2802:C:H2'	30:0:2803:C:C6	2.50	0.46
31:9:27:C:H2'	31:9:28:U:O4'	2.16	0.46
2:B:243:ASN:HA	2:B:244:PRO:C	2.35	0.46
3:C:127:ARG:HD3	3:C:129:HIS:CE1	2.48	0.46
14:N:11:ARG:HD3	31:9:114:G:O6	2.15	0.46
16:P:101:GLN:HG3	38:0:3511:HOH:O	2.15	0.46
21:U:49:LEU:HG	38:U:3805:HOH:O	2.15	0.46
29:3:61:PRO:HG3	30:0:2462:G:O6	2.16	0.46
30:0:228:C:H2'	30:0:229:G:H5'	1.96	0.46
30:0:343:C:O2'	30:0:344:C:H5'	2.15	0.46
30:0:445:U:H2'	30:0:446:G:H8	1.81	0.46
30:0:590:A:H2'	30:0:591:A:H5'	1.97	0.46
30:0:716:G:C6	30:0:717:C:N4	2.83	0.46
30:0:1125:U:H3'	30:0:1126:C:C6	2.51	0.46
30:0:1515:A:H2'	30:0:1516:U:H6	1.80	0.46
2:B:214:PRO:HD2	38:0:9081:HOH:O	2.15	0.46
5:E:11:VAL:HG12	5:E:12:ASP:N	2.31	0.46
14:N:112:GLY:HA2	14:N:137:ALA:HB2	1.96	0.46
16:P:59:ARG:HH22	16:P:66:GLN:NE2	2.12	0.46
17:Q:53:HIS:CD2	30:0:2389:U:H4'	2.50	0.46
30:0:241:A:C2	30:0:378:A:H4'	2.51	0.46
30:0:1067:A:H5'	38:0:4351:HOH:O	2.15	0.46
30:0:1175:G:N7	30:0:1176:C:N3	2.63	0.46
30:0:1346:U:H2'	30:0:1347:U:C6	2.51	0.46
30:0:1420:C:H2'	30:0:1420:C:O2	2.15	0.46
30:0:1616:A:H5"	30:0:1617:C:OP1	2.16	0.46
30:0:2613:G:O2'	30:0:2614:C:H5'	2.15	0.46
30:0:2703:A:H2'	30:0:2704:C:C6	2.46	0.46
31:9:12:C:H5'	31:9:70:U:O4'	2.15	0.46
1:A:71:PRO:HD2	1:A:74:VAL:HG21	1.98	0.46
1:A:127:GLN:HB3	1:A:139:LYS:HB3	1.98	0.46
2:B:202:VAL:HG11	2:B:301:VAL:HG13	1.98	0.46
2:B:307:ARG:HG3	2:B:307:ARG:NH1	2.30	0.46
3:C:1:MET:CG	3:C:2:GLN:H	2.26	0.46
4:D:64:ARG:HB3	4:D:67:ASP:OD2	2.15	0.46
9:I:130:LEU:HA	38:0:7420:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:175:LEU:O	14:N:179:LEU:HG	2.15	0.46
16:P:64:GLU:HG3	38:P:166:HOH:O	2.15	0.46
30:0:138:U:OP2	30:0:139:C:C5	2.69	0.46
30:0:889:C:H2'	30:0:890:C:C6	2.51	0.46
30:0:1617:C:C4	30:0:1643:C:H4'	2.50	0.46
30:0:2061:C:C2'	30:0:2062:A:H5'	2.46	0.46
30:0:2093:G:H5"	38:0:9483:HOH:O	2.15	0.46
30:0:2346:C:H6	30:0:2346:C:O5'	1.98	0.46
30:0:2401:A:H2'	30:0:2402:A:C8	2.51	0.46
30:0:2840:A:H3'	38:0:7661:HOH:O	2.15	0.46
1:A:110:SER:HB2	1:A:117:LYS:HG3	1.98	0.46
3:C:103:ASN:HB3	38:0:9117:HOH:O	2.16	0.46
4:D:20:LYS:HA	4:D:75:LEU:O	2.15	0.46
5:E:3:VAL:HG22	5:E:49:ILE:HB	1.97	0.46
30:0:370:G:O2'	30:0:371:U:H5'	2.15	0.46
30:0:510:U:O5'	30:0:510:U:H6	1.99	0.46
30:0:729:C:C2	30:0:743:G:C2	3.04	0.46
30:0:1202:A:C8	30:0:1203:G:C8	3.04	0.46
30:0:1463:U:H2'	30:0:1464:C:C6	2.51	0.46
30:0:1741:U:C4	30:0:2033:G:C8	3.04	0.46
30:0:2908:A:C2'	30:0:2909:G:H5'	2.46	0.46
31:9:34:A:H2'	31:9:35:C:O4'	2.16	0.46
1:A:206:ARG:O	1:A:208:HIS:HD2	1.98	0.46
4:D:56:ARG:HH22	30:0:2332:A:H5'	1.79	0.46
5:E:137:ASP:O	5:E:141:VAL:HG23	2.16	0.46
6:F:13:GLU:OE2	6:F:78:GLU:HG2	2.15	0.46
16:P:80:ARG:HG2	16:P:87:ARG:CZ	2.46	0.46
17:Q:25:PRO:HA	17:Q:26:PRO:HD3	1.81	0.46
30:0:39:G:N2	30:0:444:C:C2	2.84	0.46
30:0:162:C:C2'	30:0:163:U:H5'	2.45	0.46
30:0:417:G:P	38:0:7436:HOH:O	2.73	0.46
30:0:932:U:H2'	30:0:933:C:C6	2.51	0.46
30:0:1008:C:O2'	30:0:1009:U:H5'	2.16	0.46
30:0:1309:U:C2'	30:0:1310:U:H5'	2.46	0.46
30:0:1453:G:C2	30:0:1675:C:C2	3.04	0.46
30:0:1845:A:O2'	30:0:1846:U:H5'	2.15	0.46
30:0:1873:G:H2'	30:0:1874:U:H5'	1.98	0.46
30:0:2764:C:O2'	30:0:2765:C:H5'	2.16	0.46
2:B:102:THR:HG23	2:B:182:VAL:HG12	1.98	0.46
3:C:156:LEU:O	3:C:160:LEU:HG	2.16	0.46
4:D:91:ALA:HB1	38:D:5198:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:118:LEU:HD12	23:W:153:MET:HE3	1.97	0.46
24:X:56:GLU:HG2	30:0:1400:C:H4'	1.98	0.46
25:Y:165:GLU:HB3	38:Y:8163:HOH:O	2.16	0.46
27:1:42:SER:HB2	38:1:8957:HOH:O	2.16	0.46
30:0:238:C:H4'	30:0:287:C:OP1	2.16	0.46
30:0:560:U:C2	30:0:561:G:C8	3.04	0.46
30:0:567:U:C5'	38:0:5300:HOH:O	2.63	0.46
30:0:1156:C:O5'	30:0:1156:C:H6	1.99	0.46
30:0:1535:G:H2'	30:0:1536:C:C6	2.50	0.46
30:0:1700:C:H5"	30:0:1701:A:OP2	2.15	0.46
30:0:1838:U:C4	30:0:2644:C:N4	2.84	0.46
30:0:2103:A:N3	30:0:2103:A:H2'	2.30	0.46
31:9:3:A:OP2	31:9:25:G:N2	2.48	0.46
1:A:190:ARG:NH1	30:0:1845:A:OP2	2.47	0.45
21:U:42:LEU:HD22	30:0:1810:C:H1'	1.98	0.45
28:2:22:PRO:HG2	28:2:25:VAL:CG2	2.46	0.45
30:0:369:G:C2	30:0:370:G:C8	3.04	0.45
30:0:630:A:H5'	38:0:9367:HOH:O	2.16	0.45
30:0:1393:A:H2'	30:0:1394:C:C6	2.51	0.45
30:0:1675:C:O2'	30:0:1676:G:H5'	2.16	0.45
30:0:1735:C:H2'	30:0:1736:A:C8	2.50	0.45
30:0:2526:C:H2'	30:0:2527:U:H5'	1.98	0.45
31:9:52:A:O2'	31:9:53:G:H5'	2.16	0.45
4:D:15:GLU:HA	4:D:16:PRO:HD3	1.78	0.45
11:K:34:VAL:HB	38:0:7387:HOH:O	2.15	0.45
30:0:80:A:C2	30:0:94:G:N3	2.85	0.45
30:0:137:U:OP1	30:0:259:G:O2'	2.34	0.45
30:0:340:A:C8	30:0:340:A:O5'	2.69	0.45
30:0:536:A:N1	30:0:2075:G:O2'	2.44	0.45
30:0:735:C:H2'	30:0:736:A:H5'	1.99	0.45
30:0:797:A:H2'	30:0:798:G:O4'	2.16	0.45
30:0:1501:A:H4'	38:0:5614:HOH:O	2.15	0.45
30:0:1636:G:O2'	30:0:1637:A:H5'	2.16	0.45
30:0:1741:U:H3'	38:0:9774:HOH:O	2.16	0.45
30:0:1973:A:H2'	30:0:1974:G:O4'	2.15	0.45
30:0:2499:U:H2'	30:0:2500:C:C6	2.51	0.45
31:9:37:C:H2'	31:9:38:A:C8	2.48	0.45
2:B:14:GLY:HA2	2:B:15:PRO:C	2.37	0.45
17:Q:45:PRO:O	30:0:2365:G:H4'	2.16	0.45
38:Y:8136:HOH:O	30:0:1316:G:H5"	2.15	0.45
30:0:497:A:H2'	30:0:498:A:C5'	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:806:A:H2'	30:0:807:A:O4'	2.17	0.45
30:0:2121:G:O2'	30:0:2122:C:H5'	2.16	0.45
30:0:2435:U:H1'	38:0:5442:HOH:O	2.16	0.45
30:0:2883:A:H2'	30:0:2884:G:O4'	2.17	0.45
3:C:127:ARG:CZ	3:C:225:PRO:HG2	2.45	0.45
5:E:119:HIS:O	5:E:140:ALA:HB1	2.17	0.45
10:J:46:ILE:HD11	10:J:53:ILE:HG23	1.97	0.45
16:P:105:LEU:HD21	16:P:137:LEU:HD11	1.99	0.45
20:T:41:ARG:HG2	20:T:41:ARG:HH11	1.82	0.45
30:0:364:U:H2'	30:0:365:G:C8	2.51	0.45
30:0:883:U:O2	30:0:883:U:C2'	2.64	0.45
30:0:1041:U:C2'	30:0:1042:U:H5'	2.47	0.45
30:0:1160:G:O2'	30:0:1190:G:H1'	2.17	0.45
30:0:1477:C:C5'	30:0:1868:G:C5'	2.93	0.45
30:0:1730:G:H5"	30:0:1731:C:C6	2.51	0.45
30:0:2909:G:H2'	30:0:2910:A:C8	2.51	0.45
1:A:231:LYS:HG3	30:0:1853:C:OP1	2.17	0.45
2:B:141:ARG:HG2	2:B:165:ARG:HA	1.98	0.45
4:D:22:VAL:HG22	4:D:74:THR:HG22	1.97	0.45
4:D:104:PHE:CE2	4:D:132:VAL:HB	2.52	0.45
5:E:69:ILE:HA	5:E:72:MET:HE2	1.99	0.45
5:E:143:GLN:NE2	30:0:2780:C:C1'	2.79	0.45
12:L:33:ALA:HB3	38:L:8892:HOH:O	2.17	0.45
19:S:57:THR:HG22	19:S:59:ASP:H	1.80	0.45
22:V:39:ALA:C	22:V:41:GLU:H	2.20	0.45
30:0:281:U:H5	38:0:7610:HOH:O	2.00	0.45
30:0:282:C:C2'	30:0:283:U:H5'	2.46	0.45
30:0:1163:G:N2	38:0:4740:HOH:O	2.49	0.45
30:0:2064:U:H2'	30:0:2065:C:H6	1.81	0.45
30:0:2308:U:C5	30:0:2310:G:C8	3.05	0.45
30:0:2499:U:H2'	30:0:2500:C:H6	1.81	0.45
31:9:3:A:C8	31:9:26:C:O2	2.69	0.45
31:9:3:A:H8	31:9:26:C:O2	1.99	0.45
2:B:262:ARG:HD2	30:0:2715:G:O2'	2.17	0.45
3:C:236:THR:HG21	38:C:8577:HOH:O	2.17	0.45
12:L:12:THR:HG21	12:L:16:GLY:O	2.17	0.45
14:N:4:PRO:HD2	38:0:6790:HOH:O	2.17	0.45
30:0:134:U:C2	30:0:145:A:C2	3.05	0.45
30:0:517:U:H1'	38:0:7592:HOH:O	2.16	0.45
30:0:1098:A:H2'	30:0:1099:G:O4'	2.17	0.45
30:0:1120:U:H5"	30:0:1120:U:C6	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1149:U:C5	30:0:1215:A:C5	3.04	0.45
30:0:1521:C:H2'	30:0:1522:A:C8	2.50	0.45
30:0:1815:A:H4'	30:0:2751:C:O4'	2.17	0.45
30:0:1903:U:O2'	30:0:1904:A:C8	2.69	0.45
30:0:1992:U:H2'	30:0:1994:A:OP2	2.17	0.45
30:0:2421:G:H3'	30:0:2422:U:C5'	2.47	0.45
30:0:2515:C:H2'	30:0:2516:G:O4'	2.16	0.45
30:0:2908:A:H2'	30:0:2909:G:C4'	2.45	0.45
31:9:39:U:H3'	31:9:40:C:H5"	1.99	0.45
2:B:69:VAL:HA	2:B:70:PRO:HD3	1.82	0.45
2:B:234:ARG:NH2	30:0:2039:A:OP2	2.50	0.45
3:C:54:LEU:HD23	3:C:79:ARG:HG3	1.99	0.45
4:D:10:PHE:HA	38:D:7345:HOH:O	2.15	0.45
19:S:57:THR:CG2	19:S:58:MET:N	2.79	0.45
22:V:49:LEU:O	22:V:53:ILE:HG13	2.17	0.45
30:0:61:G:C6	30:0:62:C:C4	3.05	0.45
30:0:283:U:H5	30:0:284:C:N3	2.13	0.45
30:0:581:G:H5'	38:0:7694:HOH:O	2.16	0.45
30:0:1165:G:N2	30:0:1173:A:H5'	2.32	0.45
30:0:1175:G:C1'	30:0:1193:A:C8	2.98	0.45
30:0:1196:C:H42	30:0:1204:C:N4	2.14	0.45
30:0:1249:U:H2'	30:0:1250:C:C6	2.51	0.45
30:0:1773:G:N2	30:0:1774:G:C8	2.84	0.45
30:0:1996:U:O2'	30:0:1997:A:H5'	2.16	0.45
30:0:2004:U:H6	30:0:2004:U:P	2.40	0.45
31:9:63:C:O2'	31:9:64:C:H5'	2.17	0.45
1:A:206:ARG:HH11	1:A:206:ARG:HG3	1.82	0.45
2:B:81:ALA:HB1	2:B:142:LEU:HD13	1.99	0.45
4:D:75:LEU:HD22	4:D:79:MET:HB3	1.98	0.45
14:N:171:HIS:CE1	38:N:8861:HOH:O	2.69	0.45
25:Y:144:ARG:NE	38:Y:8181:HOH:O	2.49	0.45
26:Z:34:SER:HB3	30:0:797:A:H4'	1.99	0.45
30:0:31:C:H4'	38:0:7442:HOH:O	2.17	0.45
30:0:168:C:O2'	30:0:169:A:H5'	2.16	0.45
30:0:844:A:C6	30:0:882:A:C5	3.05	0.45
30:0:2583:A:H5'	38:0:9803:HOH:O	2.17	0.45
1:A:35:GLY:O	1:A:36:ASP:HB3	2.16	0.45
1:A:54:PRO:HG2	1:A:160:ALA:HB3	1.99	0.45
2:B:5:ARG:NH2	30:0:2548:C:OP2	2.50	0.45
2:B:211:THR:HG21	38:0:7472:HOH:O	2.17	0.45
3:C:72:LYS:HE3	38:C:8505:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:2:VAL:HG22	6:F:57:GLU:OE1	2.17	0.45
11:K:64:MET:HA	11:K:67:GLN:HE21	1.81	0.45
13:M:24:GLN:HE22	13:M:27:ARG:HH11	1.64	0.45
14:N:109:PRO:HB3	30:0:2413:A:N7	2.32	0.45
18:R:15:LYS:HE3	38:R:8982:HOH:O	2.16	0.45
23:W:52:VAL:HG22	23:W:53:ALA:H	1.82	0.45
23:W:130:HIS:O	23:W:136:GLY:HA3	2.17	0.45
30:0:240:C:O2	30:0:240:C:H2'	2.17	0.45
30:0:553:G:H3'	38:0:4084:HOH:O	2.15	0.45
30:0:559:U:H2'	30:0:560:U:O4'	2.17	0.45
30:0:968:G:H2'	30:0:969:G:H8	1.82	0.45
30:0:1577:U:O2'	30:0:1578:C:H5'	2.17	0.45
30:0:1711:A:O2'	30:0:1712:A:H5'	2.16	0.45
30:0:1825:U:O2'	30:0:1826:C:H5'	2.16	0.45
30:0:2072:G:H3'	30:0:2073:G:C5'	2.47	0.45
2:B:217:ARG:HG3	2:B:257:THR:HB	1.99	0.45
8:H:31:ILE:HG23	38:H:233:HOH:O	2.16	0.45
13:M:81:ARG:HG3	13:M:85:ARG:HB2	1.99	0.45
16:P:20:ARG:NH1	16:P:54:LYS:HD3	2.32	0.45
18:R:40:ALA:O	18:R:44:VAL:HG23	2.16	0.45
27:1:16:HIS:CD2	30:0:470:U:O2'	2.68	0.45
30:0:68:U:O2'	30:0:69:A:H5"	2.17	0.45
30:0:407:A:H3'	38:0:4468:HOH:O	2.16	0.45
30:0:884:C:H3'	38:0:9406:HOH:O	2.17	0.45
30:0:960:G:C3'	30:0:960:G:C4	3.00	0.45
30:0:1626:A:H2'	30:0:1627:G:C5'	2.47	0.45
30:0:2361:A:C5'	38:0:9009:HOH:O	2.60	0.45
30:0:2624:A:O2'	30:0:2625:C:H5'	2.17	0.45
30:0:2828:G:C6	30:0:2913:A:C2	3.05	0.45
1:A:179:MET:HA	1:A:179:MET:CE	2.47	0.44
2:B:214:PRO:C	2:B:220:VAL:HG22	2.37	0.44
3:C:39:GLN:O	3:C:43:LYS:HD3	2.18	0.44
3:C:46:TYR:CE1	3:C:92:PRO:HB3	2.51	0.44
4:D:12:GLU:O	4:D:15:GLU:HG2	2.17	0.44
5:E:75:GLY:HA3	5:E:136:PRO:O	2.18	0.44
14:N:37:ARG:NH1	31:9:6:C:OP1	2.50	0.44
16:P:1:THR:O	30:0:1396:C:H1'	2.17	0.44
17:Q:26:PRO:O	17:Q:30:VAL:HG23	2.16	0.44
23:W:122:ARG:HH12	23:W:154:ARG:N	2.14	0.44
30:0:45:A:H5"	30:0:47:G:O4'	2.17	0.44
30:0:1718:G:O2'	30:0:1719:G:H5'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1735:C:H2'	30:0:1736:A:H8	1.82	0.44
30:0:2269:C:H2'	30:0:2270:G:C5'	2.47	0.44
30:0:2653:A:H2'	30:0:2654:C:C6	2.52	0.44
2:B:10:SER:O	2:B:16:ARG:NH1	2.49	0.44
2:B:27:ASN:HD21	30:0:2807:U:P	2.40	0.44
3:C:1:MET:HG2	3:C:2:GLN:N	2.27	0.44
4:D:52:THR:HG21	30:0:2346:C:O2'	2.17	0.44
5:E:15:GLN:HG3	5:E:20:ILE:HG12	1.99	0.44
9:I:121:LYS:HB3	30:0:1184:C:H4'	1.98	0.44
11:K:8:VAL:HG13	11:K:80:ILE:HG22	1.98	0.44
13:M:159:VAL:HG13	13:M:160:PHE:N	2.32	0.44
14:N:22:GLN:HA	14:N:25:ARG:CZ	2.47	0.44
18:R:29:LYS:HE2	30:0:524:A:H5'	1.99	0.44
23:W:13:MET:HE2	23:W:17:ILE:HG22	1.98	0.44
25:Y:235:GLU:CD	25:Y:235:GLU:N	2.70	0.44
28:2:8:LYS:NZ	30:0:1677:U:OP2	2.48	0.44
29:3:60:LYS:HG3	29:3:61:PRO:HD2	1.98	0.44
30:0:255:A:H2'	30:0:256:C:O4'	2.17	0.44
30:0:1676:G:C2'	30:0:1677:U:H5'	2.47	0.44
30:0:1894:C:N4	30:0:1939:U:H2'	2.31	0.44
30:0:2510:C:N4	30:0:2564:G:H22	2.12	0.44
31:9:14:G:H8	31:9:14:G:C5'	2.20	0.44
3:C:95:GLU:CD	3:C:95:GLU:H	2.20	0.44
4:D:137:PRO:O	31:9:30:C:OP1	2.35	0.44
8:H:77:ILE:HG23	8:H:82:GLU:HG2	2.00	0.44
12:L:6:ARG:NH1	30:0:1299:G:N7	2.65	0.44
13:M:59:GLY:HA3	13:M:141:ILE:CD1	2.47	0.44
13:M:184:ARG:HG3	13:M:185:PRO:HA	2.00	0.44
16:P:137:LEU:O	16:P:141:ILE:HG13	2.17	0.44
23:W:21:LEU:HB3	23:W:26:ILE:HG12	1.99	0.44
25:Y:126:PRO:HG2	25:Y:128:PHE:CZ	2.52	0.44
25:Y:154:ARG:NH2	30:0:1071:G:H4'	2.31	0.44
30:0:74:G:H2'	30:0:75:U:H6	1.82	0.44
30:0:271:C:C2	30:0:273:G:O4'	2.70	0.44
30:0:542:A:H1'	38:0:4691:HOH:O	2.16	0.44
30:0:649:U:O2'	30:0:650:C:H5'	2.16	0.44
30:0:2505:G:H2'	30:0:2506:A:H5'	2.00	0.44
30:0:2526:C:C2'	30:0:2527:U:H5'	2.47	0.44
30:0:2587:OMU:H2'	30:0:2589:U:H5"	1.99	0.44
31:9:3:A:C8	31:9:26:C:N3	2.86	0.44
31:9:65:A:N6	31:9:112:U:C6	2.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:162:MET:CE	2:B:310:ARG:HD3	2.46	0.44
3:C:233:THR:HG22	3:C:234:VAL:N	2.32	0.44
4:D:54:ALA:HB2	4:D:69:ILE:CD1	2.48	0.44
5:E:95:VAL:HG11	5:E:131:LEU:HD21	1.98	0.44
11:K:55:VAL:CG1	11:K:56:SER:N	2.80	0.44
16:P:19:ASN:OD1	30:0:1720:C:H5	2.00	0.44
27:1:8:GLN:HG3	30:0:1688:G:H4'	1.99	0.44
30:0:195:C:H2'	30:0:196:G:H5'	1.99	0.44
30:0:796:A:C2	30:0:797:A:C4	3.05	0.44
30:0:957:A:H8	30:0:957:A:O5'	2.01	0.44
30:0:1116:U:N3	30:0:1246:A:N6	2.59	0.44
30:0:1268:C:O2'	30:0:1269:G:H5'	2.16	0.44
30:0:1503:U:H2'	30:0:1504:A:O4'	2.17	0.44
30:0:1850:U:H2'	30:0:1851:G:H8	1.82	0.44
30:0:1925:G:O2'	30:0:1926:G:H5'	2.18	0.44
30:0:2064:U:H4'	30:0:2653:A:OP1	2.17	0.44
30:0:2502:C:O2'	30:0:2503:A:H5'	2.17	0.44
31:9:45:A:C5	31:9:46:C:C5	3.05	0.44
1:A:70:ALA:HA	1:A:71:PRO:HD3	1.77	0.44
1:A:164:ARG:HB2	26:Z:92:SER:OG	2.17	0.44
10:J:70:PHE:HE1	30:0:2676:C:H4'	1.79	0.44
30:0:299:U:H5'	38:0:7352:HOH:O	2.16	0.44
30:0:348:C:H5	38:0:6349:HOH:O	1.99	0.44
30:0:397:A:O2'	30:0:417:G:N3	2.36	0.44
30:0:731:U:O2'	30:0:732:C:H5'	2.18	0.44
30:0:970:U:H2'	38:0:6346:HOH:O	2.18	0.44
30:0:1268:C:H2'	30:0:1269:G:C8	2.53	0.44
30:0:1416:G:C2'	30:0:1417:G:H5'	2.47	0.44
30:0:2734:G:O2'	30:0:2735:U:H5'	2.18	0.44
2:B:198:GLU:HA	38:B:9123:HOH:O	2.17	0.44
12:L:79:ASP:HB2	38:L:8858:HOH:O	2.17	0.44
13:M:92:THR:HB	30:0:401:C:O2'	2.17	0.44
18:R:61:GLN:NE2	38:0:4737:HOH:O	2.50	0.44
25:Y:122:ARG:NH2	38:Y:8101:HOH:O	2.51	0.44
27:1:1:THR:O	30:0:1836:A:H1'	2.18	0.44
27:1:28:HIS:CE1	27:1:31:LYS:HE2	2.53	0.44
30:0:99:A:C8	30:0:100:C:C5	3.06	0.44
30:0:283:U:H5	30:0:284:C:C4	2.36	0.44
30:0:312:U:C2	30:0:320:G:N2	2.86	0.44
30:0:354:A:H2'	30:0:355:C:C6	2.53	0.44
30:0:535:G:C6	30:0:2064:U:C5	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:816:G:H5'	30:0:1598:A:H4'	2.00	0.44
30:0:1020:A:H2'	30:0:1021:G:C8	2.52	0.44
30:0:1058:A:H2'	30:0:1060:C:C5'	2.47	0.44
30:0:1421:C:H2'	30:0:1422:U:H6	1.82	0.44
30:0:2324:G:H21	30:0:2377:U:H1'	1.83	0.44
30:0:2612:A:H4'	38:0:3687:HOH:O	2.16	0.44
2:B:256:GLN:HG2	38:B:9122:HOH:O	2.17	0.44
5:E:35:TYR:CD2	5:E:36:PRO:HD2	2.53	0.44
6:F:107:ASP:O	6:F:111:ILE:HG13	2.18	0.44
7:G:19:GLU:O	7:G:23:ILE:HG13	2.18	0.44
11:K:118:ALA:CA	11:K:125:ALA:HB2	2.48	0.44
14:N:160:SER:HB3	31:9:51:A:H5'	1.99	0.44
20:T:19:ARG:HD3	20:T:67:LEU:O	2.18	0.44
24:X:34:ARG:NH1	24:X:48:VAL:O	2.49	0.44
27:1:21:ARG:HD2	27:1:39:PHE:HB2	1.98	0.44
30:0:545:G:H8	30:0:545:G:C5'	2.14	0.44
30:0:565:A:C6	30:0:566:A:C6	3.05	0.44
30:0:1224:G:H2'	30:0:1225:C:C6	2.52	0.44
30:0:1666:C:C2'	30:0:1667:A:H5'	2.31	0.44
30:0:2672:C:H2'	30:0:2673:U:C6	2.52	0.44
31:9:56:A:H2'	31:9:57:A:C5'	2.28	0.44
1:A:48:ASP:HA	1:A:49:PRO:HD3	1.86	0.44
3:C:40:ALA:O	3:C:43:LYS:HB2	2.18	0.44
3:C:153:VAL:O	3:C:157:LEU:HG	2.16	0.44
4:D:84:LEU:HA	4:D:87:ALA:HB3	1.99	0.44
5:E:81:GLU:HG2	5:E:134:SER:CB	2.45	0.44
13:M:169:ARG:HD2	38:M:8886:HOH:O	2.16	0.44
14:N:154:LEU:C	14:N:156:GLU:H	2.20	0.44
18:R:113:HIS:HE1	18:R:144:GLU:CD	2.21	0.44
23:W:75:GLY:HA3	38:W:5763:HOH:O	2.17	0.44
30:0:363:C:O2'	30:0:364:U:H5'	2.18	0.44
30:0:777:U:OP2	30:0:777:U:H4'	2.17	0.44
30:0:1947:G:N2	30:0:1966:U:C2	2.86	0.44
3:C:51:TYR:CE2	27:1:53:LYS:HB3	2.53	0.44
30:0:537:G:O4'	30:0:538:C:C5	2.70	0.44
30:0:970:U:O5'	30:0:970:U:H6	2.01	0.44
30:0:1079:A:OP2	30:0:1080:C:N4	2.46	0.44
30:0:1186:C:N4	30:0:1187:U:C4	2.86	0.44
30:0:1206:U:H6	30:0:1206:U:C5'	2.24	0.44
30:0:1236:A:H2'	30:0:1237:U:O4'	2.17	0.44
30:0:1520:G:C2	30:0:1521:C:C2	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2310:G:C2	30:0:2311:A:C5	3.05	0.44
30:0:2456:A:H5'	38:0:5708:HOH:O	2.18	0.44
3:C:195:VAL:HA	3:C:213:ALA:O	2.17	0.43
12:L:27:ARG:HH21	12:L:30:ARG:HG2	1.82	0.43
13:M:115:LEU:HD13	13:M:116:ASN:HB2	2.00	0.43
15:O:65:LEU:HD13	30:0:746:A:C6	2.53	0.43
30:0:192:A:H5'	38:0:7657:HOH:O	2.17	0.43
30:0:758:A:H2'	30:0:759:C:O4'	2.17	0.43
30:0:1593:C:O2'	30:0:1594:C:H5'	2.18	0.43
30:0:1695:G:C6	30:0:1696:U:C4	3.06	0.43
30:0:2015:A:H2'	30:0:2016:U:O4'	2.18	0.43
30:0:2387:U:H2'	30:0:2388:C:C6	2.53	0.43
30:0:2717:C:C2'	30:0:2718:C:C5'	2.81	0.43
30:0:2842:G:H2'	30:0:2843:A:H5'	2.00	0.43
5:E:53:GLU:HB3	5:E:55:ASN:ND2	2.33	0.43
5:E:84:MET:HG2	5:E:168:ILE:HD13	2.00	0.43
10:J:88:PRO:CA	33:J:8802:CL:CL	3.03	0.43
17:Q:94:GLN:O	17:Q:95:GLU:HB2	2.18	0.43
18:R:80:TYR:O	30:0:2050:G:H5"	2.18	0.43
22:V:4:HIS:O	22:V:8:ILE:HG13	2.18	0.43
30:0:327:A:H4'	30:0:329:A:C8	2.52	0.43
30:0:682:A:H2'	30:0:683:G:O4'	2.18	0.43
30:0:705:C:O2	30:0:705:C:H2'	2.17	0.43
30:0:958:G:H2'	30:0:959:C:C6	2.53	0.43
30:0:1069:C:H2'	30:0:1070:A:O4'	2.18	0.43
30:0:1164:U:H3	30:0:1192:A:H2	1.65	0.43
30:0:1626:A:C2'	30:0:1627:G:H5'	2.48	0.43
30:0:2107:U:O2'	30:0:2108:A:H5'	2.19	0.43
30:0:2269:C:H2'	30:0:2270:G:H5'	2.00	0.43
30:0:2595:U:O2'	30:0:2596:A:H5'	2.18	0.43
30:0:2642:G:H2'	30:0:2643:G:O4'	2.18	0.43
30:0:2649:A:H5'	30:0:2649:A:C8	2.53	0.43
30:0:2906:A:H5'	30:0:2907:C:O4'	2.17	0.43
4:D:146:LYS:HE2	14:N:107:ASN:ND2	2.34	0.43
7:G:23:ILE:O	7:G:27:ILE:HG13	2.18	0.43
9:I:87:PRO:HG3	38:0:7132:HOH:O	2.18	0.43
16:P:73:HIS:HE1	30:0:1789:G:O6	2.01	0.43
27:1:9:GLY:HA3	30:0:1695:G:H1'	2.00	0.43
30:0:100:C:H2'	30:0:101:C:H6	1.84	0.43
30:0:130:C:H4'	38:0:5803:HOH:O	2.17	0.43
30:0:622:G:O2'	30:0:623:U:H5'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:711:G:C2	30:0:718:C:N3	2.87	0.43
30:0:745:G:H5"	30:0:746:A:OP1	2.18	0.43
30:0:1205:U:H5	38:0:4448:HOH:O	2.00	0.43
30:0:1298:U:H2'	30:0:1299:G:C8	2.53	0.43
30:0:1631:A:C6	30:0:1632:A:N1	2.86	0.43
30:0:1889:C:O2	30:0:2010:A:H2	2.02	0.43
30:0:2349:G:O2'	30:0:2350:G:H5'	2.17	0.43
30:0:2801:A:H2'	30:0:2801:A:N3	2.33	0.43
31:9:23:U:C2'	31:9:24:U:H4'	2.48	0.43
6:F:91:VAL:CG1	6:F:92:GLY:N	2.81	0.43
8:H:12:ILE:HG23	8:H:129:ARG:CZ	2.48	0.43
10:J:80:LYS:HE3	10:J:101:VAL:O	2.19	0.43
13:M:67:VAL:HB	13:M:97:ILE:HG23	2.01	0.43
16:P:98:ILE:HD12	16:P:102:ARG:CZ	2.48	0.43
30:0:367:G:H8	30:0:367:G:OP2	2.01	0.43
30:0:483:C:N4	30:0:484:A:C6	2.86	0.43
30:0:871:G:H4'	38:0:4418:HOH:O	2.18	0.43
30:0:1074:G:H4'	30:0:1260:G:C6	2.54	0.43
30:0:1368:U:O5'	30:0:1368:U:H6	2.01	0.43
30:0:1503:U:H6	30:0:1503:U:H3'	1.82	0.43
30:0:2040:C:H5"	30:0:2759:C:O2'	2.18	0.43
30:0:2315:C:H4'	30:0:2425:A:C6	2.53	0.43
30:0:2649:A:H5'	30:0:2649:A:H8	1.83	0.43
31:9:110:G:C5	31:9:111:U:C5	3.07	0.43
1:A:64:ASP:OD1	1:A:66:ARG:HD3	2.18	0.43
14:N:37:ARG:HH21	14:N:105:GLY:N	2.16	0.43
14:N:86:LEU:HD23	14:N:179:LEU:HD12	1.98	0.43
15:O:29:VAL:HG11	15:O:98:LEU:HD21	1.99	0.43
15:O:32:ARG:HH21	15:O:35:LYS:HZ2	1.67	0.43
16:P:59:ARG:NH2	16:P:66:GLN:HE22	2.17	0.43
16:P:83:LYS:HG2	30:0:793:A:H5"	1.99	0.43
30:0:113:A:H2'	30:0:115:U:O4	2.19	0.43
30:0:666:A:H2'	30:0:667:C:O4'	2.18	0.43
30:0:725:C:H2'	30:0:726:C:O5'	2.17	0.43
30:0:1416:G:H2'	30:0:1417:G:H5'	1.99	0.43
30:0:1568:G:C6	30:0:1569:U:C4	3.06	0.43
30:0:1626:A:H2'	30:0:1627:G:H5'	1.99	0.43
30:0:2010:A:C2'	38:0:5975:HOH:O	2.59	0.43
30:0:2470:A:H5"	38:0:3249:HOH:O	2.18	0.43
30:0:2902:A:H4'	30:0:2903:C:OP1	2.19	0.43
31:9:117:G:H2'	31:9:118:C:H6	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:27:ARG:NH1	3:C:29:ASP:OD1	2.50	0.43
3:C:96:LYS:NZ	30:0:1351:G:OP1	2.39	0.43
15:O:3:THR:HG22	30:0:656:G:C5'	2.31	0.43
15:O:25:VAL:HG11	30:0:710:G:H5'	1.99	0.43
16:P:94:TRP:CH2	16:P:98:ILE:HG13	2.53	0.43
17:Q:47:VAL:HA	17:Q:48:PRO:HD3	1.81	0.43
22:V:59:ILE:O	22:V:63:GLU:HG2	2.17	0.43
23:W:139:GLY:O	23:W:141:HIS:CD2	2.71	0.43
25:Y:204:ARG:NH2	30:0:1324:G:H21	2.16	0.43
30:0:1023:C:H2'	30:0:1024:G:O4'	2.18	0.43
30:0:1163:G:H1	30:0:1184:C:N4	2.17	0.43
30:0:1314:U:H5"	30:0:1316:G:O4'	2.19	0.43
30:0:1585:C:H2'	30:0:1586:G:H8	1.84	0.43
30:0:2829:G:N2	30:0:2912:C:C2	2.86	0.43
1:A:94:LEU:HD23	1:A:94:LEU:N	2.33	0.43
1:A:94:LEU:HD12	1:A:98:GLU:HB2	2.00	0.43
2:B:51:VAL:CG2	2:B:330:VAL:HG22	2.48	0.43
3:C:118:THR:HG22	3:C:137:PRO:HB3	1.99	0.43
5:E:7:ILE:HG22	5:E:45:ASP:O	2.19	0.43
15:O:24:ALA:HB3	30:0:710:G:OP1	2.19	0.43
30:0:790:A:H2'	30:0:791:A:O4'	2.18	0.43
30:0:912:A:C4	30:0:1294:A:C2	3.06	0.43
30:0:1181:A:O2'	30:0:1182:C:H5'	2.18	0.43
30:0:1474:C:H6	30:0:1474:C:C5'	2.18	0.43
30:0:1626:A:H2'	30:0:1627:G:O4'	2.19	0.43
30:0:1950:G:O2'	30:0:1951:G:H5'	2.19	0.43
30:0:2421:G:H3'	30:0:2422:U:H5"	2.00	0.43
30:0:2716:G:O2'	30:0:2717:C:H5'	2.19	0.43
31:9:59:C:H2'	31:9:60:C:H6	1.83	0.43
31:9:64:C:O2'	31:9:65:A:H5'	2.18	0.43
2:B:242:TRP:CZ2	30:0:2607:U:C4	3.06	0.43
3:C:25:PRO:HG2	38:C:8520:HOH:O	2.17	0.43
12:L:67:ARG:O	12:L:71:GLU:HG3	2.19	0.43
13:M:49:ALA:C	13:M:54:TYR:HB3	2.39	0.43
14:N:108:SER:HA	14:N:109:PRO:HD3	1.78	0.43
30:0:512:G:O3'	30:0:513:A:C8	2.70	0.43
30:0:1132:A:H3'	38:0:4832:HOH:O	2.18	0.43
30:0:1175:G:O2'	30:0:1193:A:H2'	2.19	0.43
30:0:1453:G:N2	30:0:1675:C:C2	2.87	0.43
30:0:1705:C:H2'	30:0:1706:G:O4'	2.19	0.43
1:A:217:ARG:NH2	30:0:1853:C:O2'	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:154:LYS:H	4:D:154:LYS:CD	2.20	0.43
6:F:59:ILE:CD1	30:0:263:U:C2	3.02	0.43
6:F:61:MET:HB3	13:M:19:GLN:OE1	2.19	0.43
14:N:44:ARG:HG3	14:N:45:ALA:N	2.34	0.43
20:T:71:VAL:HG11	20:T:90:PRO:HB3	1.99	0.43
23:W:119:HIS:HE1	38:0:9560:HOH:O	2.02	0.43
30:0:64:G:H2'	30:0:65:C:O4'	2.19	0.43
30:0:590:A:C2'	30:0:591:A:H5'	2.48	0.43
30:0:1138:G:H4'	38:0:5722:HOH:O	2.18	0.43
30:0:1463:U:H2'	30:0:1464:C:H6	1.83	0.43
30:0:1971:G:H5"	38:0:7084:HOH:O	2.18	0.43
30:0:2241:C:H2'	30:0:2242:U:C6	2.54	0.43
30:0:2362:A:H2'	30:0:2363:G:C8	2.54	0.43
30:0:2589:U:H2'	30:0:2590:U:C6	2.54	0.43
30:0:2761:A:H2'	38:0:5654:HOH:O	2.19	0.43
31:9:65:A:C2'	31:9:66:G:OP2	2.66	0.43
31:9:117:G:H2'	31:9:118:C:C6	2.53	0.43
1:A:173:GLY:O	1:A:176:HIS:HB3	2.19	0.43
1:A:217:ARG:HH11	1:A:217:ARG:CG	2.32	0.43
3:C:27:ARG:HH11	3:C:27:ARG:HG3	1.83	0.43
4:D:96:SER:O	30:0:2337:G:H5"	2.19	0.43
5:E:108:LEU:CD1	5:E:164:ASP:HB2	2.49	0.43
7:G:63:ARG:O	7:G:67:LEU:HG	2.18	0.43
10:J:75:PRO:HD3	10:J:136:SER:OG	2.18	0.43
18:R:29:LYS:HE2	30:0:524:A:H5"	2.01	0.43
23:W:26:ILE:HB	38:W:5420:HOH:O	2.18	0.43
30:0:764:C:H2'	30:0:765:G:O4'	2.19	0.43
30:0:779:U:H5'	30:0:1836:A:C2	2.54	0.43
30:0:1015:C:H2'	30:0:1016:U:C6	2.54	0.43
30:0:1158:G:O2'	30:0:1159:G:H5'	2.19	0.43
30:0:1409:G:C2	30:0:1410:G:C8	3.07	0.43
30:0:1483:C:O2'	30:0:1484:G:H5'	2.18	0.43
30:0:1528:A:H61	30:0:1663:G:H1'	1.84	0.43
30:0:1559:A:OP2	30:0:1559:A:H8	2.02	0.43
30:0:1829:A:C8	30:0:1885:A:C8	3.07	0.43
30:0:2249:G:C2	30:0:2253:G:C6	3.07	0.43
30:0:2314:G:O2'	30:0:2315:C:H5'	2.19	0.43
31:9:121:C:O5'	31:9:121:C:H6	2.02	0.43
2:B:82:VAL:O	2:B:82:VAL:HG12	2.19	0.42
14:N:29:SER:HB3	30:0:2415:A:O2'	2.19	0.42
24:X:61:ARG:HD2	24:X:65:ASN:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:2:20:ARG:HG2	28:2:21:VAL:N	2.33	0.42
30:0:69:A:C8	30:0:69:A:C5'	2.98	0.42
30:0:1213:C:C2'	30:0:1214:G:H5'	2.48	0.42
30:0:1413:A:H2'	30:0:1414:A:O4'	2.19	0.42
30:0:1482:A:H1'	38:0:9422:HOH:O	2.19	0.42
30:0:1555:G:H4'	30:0:1630:A:H2	1.84	0.42
30:0:2293:G:C2	30:0:2316:G:C6	3.07	0.42
30:0:2374:G:H2'	30:0:2375:A:H8	1.83	0.42
5:E:91:PHE:HA	5:E:92:PRO:HD3	1.80	0.42
14:N:73:ALA:HB1	14:N:74:PRO:CD	2.49	0.42
17:Q:55:ARG:HD2	38:Q:2875:HOH:O	2.18	0.42
18:R:128:ARG:HH22	30:0:2054:A:H2	1.65	0.42
20:T:9:LYS:HE3	20:T:13:ARG:NH1	2.33	0.42
23:W:6:GLN:HB2	23:W:26:ILE:HD11	1.98	0.42
30:0:56:G:N3	30:0:70:A:C2	2.87	0.42
30:0:137:U:H3'	30:0:139:C:H41	1.83	0.42
30:0:216:A:O2'	30:0:217:C:H5'	2.19	0.42
30:0:319:A:H4'	30:0:338:C:C4	2.53	0.42
30:0:808:A:C5	30:0:809:G:H1'	2.54	0.42
30:0:917:U:O5'	30:0:917:U:H6	2.02	0.42
30:0:941:G:C6	30:0:942:U:C4	3.08	0.42
30:0:1116:U:C2	30:0:1246:A:N6	2.87	0.42
30:0:1406:A:H4'	30:0:1407:A:C5'	2.50	0.42
30:0:1769:C:C4	30:0:1770:U:C4	3.08	0.42
30:0:2347:C:H2'	30:0:2348:C:C6	2.54	0.42
30:0:2519:C:H2'	30:0:2520:G:O4'	2.19	0.42
30:0:2726:U:O2	30:0:2749:U:O5'	2.36	0.42
1:A:211:LYS:HG2	38:0:7044:HOH:O	2.19	0.42
2:B:70:PRO:HG3	30:0:2719:A:C2	2.54	0.42
4:D:22:VAL:HA	4:D:73:VAL:O	2.19	0.42
5:E:77:THR:OG1	5:E:78:GLU:N	2.53	0.42
5:E:107:PHE:CZ	5:E:152:THR:HB	2.55	0.42
21:U:52:THR:HG22	21:U:54:THR:N	2.32	0.42
30:0:78:G:C6	30:0:79:G:C6	3.07	0.42
30:0:699:C:C6	30:0:744:G:C4	3.07	0.42
30:0:1185:U:C5'	38:0:7483:HOH:O	2.66	0.42
30:0:2755:G:H1'	38:0:4696:HOH:O	2.19	0.42
30:0:2822:C:O2'	30:0:2827:A:H4'	2.19	0.42
4:D:23:VAL:HG21	4:D:45:THR:CG2	2.49	0.42
16:P:16:VAL:HG22	16:P:20:ARG:CZ	2.50	0.42
26:Z:40:ALA:HA	30:0:1773:G:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:69:A:C2'	30:0:70:A:OP2	2.67	0.42
30:0:305:A:C6	30:0:329:A:N3	2.87	0.42
30:0:536:A:H8	38:0:5057:HOH:O	2.01	0.42
30:0:1057:A:H1'	30:0:2492:U:O2'	2.19	0.42
30:0:1163:G:N2	30:0:1184:C:N3	2.67	0.42
30:0:1167:G:H3'	38:0:7514:HOH:O	2.19	0.42
30:0:1189:A:N7	30:0:1190:G:N7	2.67	0.42
30:0:1211:G:H2'	30:0:1212:C:C6	2.48	0.42
30:0:1400:C:C2'	30:0:1401:G:H5'	2.49	0.42
30:0:1603:A:H5'	30:0:1605:G:C5'	2.48	0.42
30:0:1850:U:H2'	30:0:1851:G:C8	2.53	0.42
30:0:2061:C:H2'	30:0:2062:A:H5'	2.00	0.42
30:0:2119:C:O2'	30:0:2120:U:H5'	2.19	0.42
30:0:2456:A:H2'	30:0:2457:U:C6	2.55	0.42
30:0:2512:U:O5'	30:0:2512:U:H6	2.02	0.42
2:B:275:GLY:O	2:B:291:ASP:HA	2.19	0.42
2:B:304:PRO:HD2	2:B:307:ARG:HE	1.84	0.42
4:D:76:ARG:NH1	31:9:42:C:O2	2.53	0.42
9:I:82:THR:HG22	30:0:1168:C:H5"	2.00	0.42
14:N:55:ASP:OD2	31:9:7:G:H4'	2.20	0.42
30:0:138:U:OP2	30:0:139:C:H5	2.02	0.42
30:0:459:A:H4'	38:0:9454:HOH:O	2.20	0.42
30:0:470:U:H2'	30:0:471:G:O4'	2.20	0.42
30:0:807:A:H2'	30:0:808:A:O4'	2.19	0.42
30:0:939:A:C2	30:0:1027:G:N3	2.88	0.42
30:0:952:G:H4'	38:0:4039:HOH:O	2.19	0.42
30:0:1015:C:H2'	30:0:1016:U:H6	1.85	0.42
30:0:1381:A:N3	30:0:1382:G:H1'	2.35	0.42
30:0:2310:G:N1	30:0:2311:A:C5	2.88	0.42
30:0:2661:U:H3	30:0:2812:A:H62	1.66	0.42
30:0:2879:A:H2'	30:0:2880:A:O4'	2.19	0.42
31:9:14:G:C8	31:9:14:G:C5'	2.99	0.42
31:9:39:U:H1'	31:9:44:A:N6	2.35	0.42
2:B:310:ARG:HD2	38:B:9114:HOH:O	2.19	0.42
3:C:206:ASN:HB2	30:0:329:A:OP2	2.19	0.42
4:D:101:THR:O	4:D:101:THR:HG22	2.19	0.42
9:I:118:ASN:HB3	30:0:1185:U:C5'	2.49	0.42
9:I:130:LEU:HD21	30:0:1167:G:H4'	2.02	0.42
18:R:72:VAL:CG1	18:R:75:TRP:HB3	2.50	0.42
28:2:10:ARG:NH2	30:0:121:U:OP2	2.39	0.42
28:2:48:ASP:O	28:2:49:GLU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:191:A:C4	30:0:237:G:N7	2.88	0.42
30:0:657:G:H2'	30:0:658:C:C6	2.55	0.42
30:0:722:G:H22	30:0:938:G:P	2.42	0.42
30:0:849:C:H1'	38:0:6632:HOH:O	2.19	0.42
30:0:1211:G:O2'	30:0:1212:C:H5'	2.19	0.42
30:0:1603:A:C5'	30:0:1605:G:C5'	2.96	0.42
30:0:1966:U:H2'	30:0:1967:U:H2'	2.00	0.42
30:0:1976:G:O2'	30:0:1977:U:C5'	2.68	0.42
30:0:2388:C:O2'	30:0:2389:U:H5'	2.19	0.42
30:0:2816:A:H5"	30:0:2817:G:H5'	2.01	0.42
2:B:140:LEU:HD13	2:B:175:LEU:HA	2.01	0.42
3:C:73:GLN:NE2	3:C:73:GLN:HA	2.35	0.42
18:R:99:ALA:O	18:R:104:PHE:HB2	2.19	0.42
38:W:7873:HOH:O	30:0:1287:A:H8	2.03	0.42
30:0:85:C:H5"	30:0:86:A:OP2	2.20	0.42
30:0:120:A:H2'	30:0:120:A:N3	2.34	0.42
30:0:137:U:O5'	30:0:137:U:H6	2.02	0.42
30:0:212:A:O4'	30:0:214:U:C6	2.72	0.42
30:0:287:C:H6	30:0:287:C:O5'	2.03	0.42
30:0:307:G:H3'	30:0:342:C:OP2	2.19	0.42
30:0:485:A:H4'	30:0:486:A:OP1	2.20	0.42
30:0:1097:A:C6	30:0:1098:A:C6	3.08	0.42
30:0:1193:A:H1'	30:0:1194:A:N7	2.35	0.42
30:0:1754:A:H2'	30:0:1755:A:O4'	2.19	0.42
30:0:2355:G:H2'	38:0:5650:HOH:O	2.18	0.42
30:0:2524:G:H5"	38:0:4744:HOH:O	2.19	0.42
1:A:30:ARG:HG2	1:A:31:LYS:N	2.35	0.42
2:B:254:GLN:NE2	38:B:9058:HOH:O	2.52	0.42
8:H:6:ALA:CA	8:H:61:ARG:HH12	2.29	0.42
20:T:41:ARG:NH1	20:T:42:VAL:O	2.53	0.42
30:0:2333:G:H2'	30:0:2334:C:H6	1.84	0.42
30:0:2575:C:H2'	30:0:2576:A:O4'	2.19	0.42
1:A:164:ARG:NH2	30:0:1876:C:O3'	2.53	0.42
2:B:53:LEU:HD21	2:B:270:ILE:HD12	2.01	0.42
2:B:137:LEU:HD21	2:B:140:LEU:HD21	2.02	0.42
2:B:215:VAL:HA	2:B:220:VAL:HG22	2.01	0.42
4:D:19:GLU:O	4:D:76:ARG:HG2	2.19	0.42
4:D:21:VAL:HA	4:D:131:THR:O	2.20	0.42
4:D:51:ARG:HD3	38:D:7636:HOH:O	2.20	0.42
11:K:78:LYS:HA	11:K:79:PRO:HD3	1.94	0.42
20:T:9:LYS:HB2	38:0:7442:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:293:A:C4	30:0:360:A:C2	3.08	0.42
30:0:295:C:H2'	30:0:296:G:O4'	2.20	0.42
30:0:834:G:H4'	30:0:835:U:OP2	2.19	0.42
30:0:2324:G:C2	30:0:2377:U:O2	2.73	0.42
30:0:2497:A:C2	30:0:2524:G:C2	3.07	0.42
2:B:75:GLU:C	2:B:77:PRO:HD3	2.39	0.42
17:Q:18:PRO:O	17:Q:21:ARG:HB2	2.20	0.42
21:U:50:GLU:HB2	30:0:2866:U:C5	2.54	0.42
23:W:48:VAL:HG12	23:W:48:VAL:O	2.20	0.42
27:1:25:LYS:HG3	28:2:49:GLU:H	1.85	0.42
30:0:130:C:H5'	38:0:5226:HOH:O	2.20	0.42
30:0:264:G:H1'	30:0:265:U:H5	1.85	0.42
30:0:844:A:C6	30:0:882:A:C6	3.08	0.42
30:0:1544:U:H2'	30:0:1545:C:C6	2.53	0.42
30:0:2134:G:C6	30:0:2258:A:C8	3.08	0.42
30:0:2727:A:C6	30:0:2756:U:C2	3.08	0.42
30:0:2911:C:H2'	30:0:2912:C:C6	2.54	0.42
2:B:84:LEU:O	2:B:99:GLU:HA	2.20	0.41
7:G:20:VAL:O	7:G:24:VAL:HG23	2.20	0.41
11:K:14:LYS:CB	11:K:45:PRO:HG2	2.50	0.41
12:L:57:VAL:HG21	30:0:2443:C:H5'	2.02	0.41
12:L:57:VAL:O	12:L:57:VAL:HG12	2.20	0.41
13:M:47:ASP:CG	13:M:48:LYS:N	2.74	0.41
17:Q:40:HIS:HE1	30:0:949:U:O2'	2.03	0.41
20:T:48:VAL:HG22	20:T:97:ARG:O	2.19	0.41
30:0:212:A:N1	30:0:226:A:H5"	2.35	0.41
30:0:583:C:C2	30:0:584:U:C5	3.08	0.41
30:0:803:C:H2'	30:0:804:C:C6	2.55	0.41
30:0:1175:G:H1'	30:0:1193:A:N9	2.33	0.41
30:0:2269:C:C2'	30:0:2270:G:H5'	2.50	0.41
30:0:2297:U:H2'	30:0:2298:C:C6	2.53	0.41
30:0:2333:G:H2'	30:0:2334:C:C6	2.55	0.41
30:0:2534:C:H2'	30:0:2535:A:C8	2.55	0.41
1:A:97:ALA:HB2	1:A:150:PRO:HB2	2.02	0.41
1:A:179:MET:HG2	1:A:186:TRP:HB2	2.02	0.41
2:B:229:ARG:HD2	38:B:8989:HOH:O	2.20	0.41
5:E:10:ASP:HA	38:E:6017:HOH:O	2.20	0.41
6:F:99:THR:HG23	6:F:99:THR:O	2.20	0.41
8:H:91:ARG:H	8:H:91:ARG:HG2	1.54	0.41
10:J:107:ASN:HD22	10:J:107:ASN:C	2.24	0.41
11:K:41:LYS:O	11:K:42:ASN:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:9:ARG:HD2	30:0:380:A:OP2	2.20	0.41
18:R:79:ARG:HB3	30:0:2050:G:OP1	2.20	0.41
18:R:96:VAL:HG13	18:R:106:GLY:HA3	2.02	0.41
20:T:28:SER:O	20:T:32:ARG:HG3	2.19	0.41
20:T:71:VAL:CG1	20:T:90:PRO:HB3	2.50	0.41
26:Z:34:SER:CB	30:0:797:A:H4'	2.50	0.41
30:0:226:A:H1'	30:0:393:G:C5	2.55	0.41
30:0:636:G:H5'	30:0:2059:U:OP2	2.20	0.41
30:0:830:G:C5	30:0:831:U:C4	3.08	0.41
30:0:1355:A:H4'	38:0:5766:HOH:O	2.19	0.41
30:0:2350:G:H2'	30:0:2351:C:C6	2.56	0.41
1:A:141:PRO:HG2	30:0:1855:G:O6	2.20	0.41
2:B:124:ALA:O	2:B:128:ILE:HG13	2.21	0.41
2:B:199:TYR:CE2	2:B:268:ARG:HB2	2.54	0.41
18:R:132:ARG:NH2	38:R:8987:HOH:O	2.53	0.41
23:W:35:VAL:HA	23:W:36:PRO:HD3	1.83	0.41
30:0:349:U:O2'	30:0:350:G:H5'	2.20	0.41
30:0:567:U:H5"	38:0:5300:HOH:O	2.19	0.41
30:0:696:C:O2'	30:0:697:G:H5'	2.19	0.41
30:0:1056:U:H2'	30:0:1057:A:O4'	2.20	0.41
30:0:1154:A:H2'	30:0:1155:G:O4'	2.20	0.41
30:0:1162:G:C6	30:0:1163:G:C6	3.09	0.41
30:0:1172:G:H1'	38:0:4984:HOH:O	2.20	0.41
30:0:1598:A:C2	30:0:1599:U:C2	3.07	0.41
30:0:1971:G:C5'	38:0:7084:HOH:O	2.67	0.41
30:0:2766:A:O2'	30:0:2767:C:H5'	2.20	0.41
31:9:3:A:C6	31:9:22:G:H1'	2.52	0.41
4:D:129:ASP:OD1	30:0:2338:G:H2'	2.20	0.41
8:H:46:TYR:HA	8:H:47:PRO:HD3	1.88	0.41
11:K:22:ASP:HB2	38:K:5264:HOH:O	2.20	0.41
17:Q:34:ASP:O	17:Q:37:GLU:HB2	2.20	0.41
23:W:74:GLU:OE1	30:0:1285:U:H4'	2.21	0.41
30:0:30:U:O2	30:0:460:A:C2	2.74	0.41
30:0:177:A:O2'	30:0:892:G:H4'	2.20	0.41
30:0:283:U:C5	30:0:284:C:N3	2.87	0.41
30:0:445:U:H2'	30:0:446:G:C8	2.55	0.41
30:0:594:C:C4	30:0:595:U:C4	3.09	0.41
30:0:1139:U:H2'	30:0:1140:C:C6	2.55	0.41
30:0:1149:U:H5"	30:0:1151:G:O4'	2.21	0.41
30:0:1421:C:H2'	30:0:1422:U:C6	2.55	0.41
30:0:1471:A:H2'	30:0:1472:C:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1795:G:H2'	30:0:1796:A:O4'	2.20	0.41
30:0:1904:A:C2	30:0:1905:U:H1'	2.54	0.41
30:0:1946:C:O4'	30:0:1969:A:C2	2.73	0.41
30:0:2310:G:C2	30:0:2311:A:C8	3.08	0.41
30:0:2600:A:H2'	30:0:2601:A:O4'	2.20	0.41
30:0:2699:A:H2'	30:0:2700:G:O4'	2.20	0.41
2:B:248:ARG:NH2	30:0:2549:C:H1'	2.35	0.41
3:C:184:ARG:HD2	30:0:1306:U:OP1	2.21	0.41
5:E:19:ASP:HA	5:E:31:ARG:O	2.21	0.41
5:E:111:LYS:CE	30:0:2690:U:H4'	2.50	0.41
13:M:72:ALA:HB2	13:M:93:ARG:HG2	2.01	0.41
24:X:43:VAL:HG12	24:X:44:ASP:H	1.85	0.41
29:3:38:ARG:HD2	30:0:396:U:OP2	2.20	0.41
30:0:113:A:OP2	30:0:114:A:H2'	2.20	0.41
30:0:154:C:O2'	30:0:155:C:H5'	2.20	0.41
30:0:625:U:H3'	38:0:3262:HOH:O	2.20	0.41
30:0:815:U:O2'	30:0:1598:A:H4'	2.20	0.41
30:0:968:G:H2'	30:0:969:G:C8	2.54	0.41
30:0:1060:C:H6	30:0:1060:C:C5'	2.29	0.41
30:0:1933:G:O2'	30:0:1934:A:H5'	2.20	0.41
30:0:2250:G:N2	30:0:2251:G:H1'	2.36	0.41
31:9:110:G:C6	31:9:111:U:C5	3.08	0.41
8:H:91:ARG:HA	30:0:1002:G:O2'	2.20	0.41
16:P:115:SER:OG	16:P:118:GLN:HG3	2.21	0.41
19:S:57:THR:HG22	19:S:59:ASP:N	2.34	0.41
30:0:168:C:O5'	30:0:168:C:H6	2.04	0.41
30:0:563:C:H2'	30:0:564:G:O4'	2.21	0.41
30:0:571:C:H6	30:0:571:C:O5'	2.03	0.41
30:0:929:A:O5'	30:0:929:A:H8	2.04	0.41
30:0:1006:A:N3	30:0:2298:C:O2'	2.50	0.41
30:0:1163:G:C2	30:0:1184:C:N3	2.89	0.41
30:0:1184:C:O2'	30:0:1185:U:OP2	2.35	0.41
30:0:1189:A:C8	30:0:1190:G:C8	3.09	0.41
30:0:1947:G:H2'	30:0:1948:G:C8	2.52	0.41
30:0:2003:U:O2'	30:0:2004:U:H5	2.02	0.41
30:0:2328:U:C4	30:0:2329:C:C5	3.08	0.41
30:0:2722:G:C2	30:0:2761:A:C2	3.09	0.41
30:0:2860:G:H2'	30:0:2861:G:O4'	2.20	0.41
30:0:2891:A:C2	30:0:2892:G:C4	3.09	0.41
31:9:28:U:O2	31:9:57:A:N6	2.53	0.41
1:A:36:ASP:CB	1:A:85:SER:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:30:ARG:NH1	38:L:8811:HOH:O	2.48	0.41
13:M:164:THR:CG2	13:M:165:GLY:N	2.82	0.41
19:S:6:LYS:HB2	19:S:27:ALA:O	2.20	0.41
21:U:56:ARG:NH1	30:0:2890:A:C2	2.89	0.41
25:Y:145:LYS:HD2	38:0:9965:HOH:O	2.20	0.41
25:Y:234:VAL:HG12	25:Y:235:GLU:N	2.36	0.41
30:0:301:C:O2'	30:0:302:A:H5'	2.21	0.41
30:0:681:G:N3	30:0:681:G:H2'	2.36	0.41
30:0:940:G:C5	30:0:1027:G:C2	3.09	0.41
30:0:1051:C:H2'	30:0:1052:G:O4'	2.21	0.41
30:0:1615:A:H5'	38:0:4187:HOH:O	2.19	0.41
30:0:1733:A:H2'	30:0:1734:C:O4'	2.20	0.41
30:0:1797:A:H2'	30:0:1799:G:O5'	2.21	0.41
31:9:78:G:O2'	31:9:79:U:OP2	2.38	0.41
2:B:140:LEU:HA	38:B:9045:HOH:O	2.20	0.41
2:B:307:ARG:HD2	38:B:9119:HOH:O	2.20	0.41
9:I:87:PRO:HD2	30:0:1180:U:O2'	2.20	0.41
16:P:55:LYS:HA	38:0:5633:HOH:O	2.21	0.41
23:W:38:THR:HG22	23:W:39:ASP:N	2.35	0.41
23:W:130:HIS:NE2	31:9:88:G:OP1	2.45	0.41
25:Y:151:SER:HB3	25:Y:154:ARG:HB3	2.03	0.41
30:0:24:G:H22	30:0:518:G:H1'	1.86	0.41
30:0:250:C:H2'	30:0:251:C:C6	2.55	0.41
30:0:506:G:N1	30:0:509:A:OP2	2.54	0.41
30:0:510:U:H5"	30:0:512:G:OP2	2.21	0.41
30:0:519:A:H4'	30:0:1320:C:O3'	2.21	0.41
30:0:1255:A:N3	38:0:7772:HOH:O	2.37	0.41
30:0:1517:C:O2	30:0:1670:A:C2	2.74	0.41
30:0:1597:A:C4	30:0:1598:A:C8	3.09	0.41
30:0:1730:G:N3	30:0:1730:G:H2'	2.36	0.41
30:0:1819:G:C2'	30:0:1820:G:C5'	2.97	0.41
30:0:2712:G:O2'	30:0:2713:G:H5'	2.21	0.41
30:0:2756:U:C2	30:0:2896:A:H2	2.39	0.41
30:0:2866:U:H4'	30:0:2867:G:H5'	2.01	0.41
31:9:23:U:H2'	31:9:24:U:H4'	2.03	0.41
1:A:105:VAL:HG11	1:A:154:ALA:HB1	2.01	0.41
2:B:80:ARG:O	2:B:82:VAL:HG23	2.21	0.41
2:B:234:ARG:HD3	30:0:1734:C:OP1	2.21	0.41
2:B:254:GLN:HG3	38:0:9708:HOH:O	2.21	0.41
4:D:18:ILE:HG12	4:D:134:LEU:HD21	2.03	0.41
4:D:49:PRO:HA	4:D:73:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:173:GLU:HG3	4:D:174:VAL:N	2.36	0.41
8:H:52:LEU:HD13	8:H:153:PHE:HB3	2.02	0.41
13:M:75:ARG:HH21	13:M:78:LYS:HE3	1.85	0.41
14:N:7:LYS:HB3	30:0:2353:A:O2'	2.20	0.41
16:P:28:GLN:HE22	30:0:1387:G:C1'	2.33	0.41
17:Q:30:VAL:HG12	17:Q:30:VAL:O	2.21	0.41
18:R:17:MET:HE3	18:R:19:ARG:NH2	2.36	0.41
23:W:4:LEU:HD22	23:W:52:VAL:CG2	2.49	0.41
23:W:5:VAL:HG22	23:W:32:CYS:HB2	2.02	0.41
23:W:88:THR:HG23	23:W:110:GLN:CB	2.43	0.41
23:W:120:PRO:HG2	30:0:1095:U:O2	2.20	0.41
23:W:125:HIS:HD2	23:W:127:GLY:H	1.68	0.41
25:Y:134:HIS:HE1	30:0:538:C:OP2	2.04	0.41
29:3:60:LYS:HG3	38:0:7573:HOH:O	2.19	0.41
30:0:106:A:H2'	30:0:107:U:O4'	2.21	0.41
30:0:271:C:H4'	30:0:272:A:OP1	2.21	0.41
30:0:278:A:H2'	30:0:279:C:O4'	2.19	0.41
30:0:652:G:H2'	30:0:653:U:O4'	2.20	0.41
30:0:694:A:H2'	30:0:695:C:C5'	2.50	0.41
30:0:822:C:H2'	30:0:823:U:C6	2.54	0.41
30:0:827:A:H2'	30:0:828:G:O4'	2.21	0.41
30:0:1222:A:H2'	30:0:1223:G:O4'	2.21	0.41
30:0:1305:C:H5'	38:0:9844:HOH:O	2.20	0.41
30:0:1364:G:H1'	38:0:4812:HOH:O	2.20	0.41
30:0:1597:A:C5	30:0:1598:A:C8	3.08	0.41
30:0:1706:G:C6	30:0:1707:G:N1	2.89	0.41
30:0:1718:G:C6	30:0:1719:G:C5	3.08	0.41
30:0:1840:A:H4'	30:0:1841:C:O5'	2.21	0.41
30:0:1873:G:C2'	30:0:1874:U:H5'	2.51	0.41
30:0:1890:U:H4'	30:0:2010:A:C6	2.56	0.41
30:0:1942:A:C1'	38:0:9044:HOH:O	2.69	0.41
30:0:2361:A:H2'	30:0:2362:A:C8	2.55	0.41
30:0:2479:A:H5"	38:0:4665:HOH:O	2.21	0.41
30:0:2689:A:H2'	30:0:2690:U:H5'	2.02	0.41
30:0:2756:U:N3	30:0:2896:A:H2	2.17	0.41
30:0:2864:U:C5	30:0:2865:G:C6	3.09	0.41
31:9:65:A:O2'	31:9:66:G:P	2.79	0.41
3:C:73:GLN:HG2	30:0:475:G:OP1	2.20	0.41
29:3:48:ASN:ND2	30:0:169:A:H1'	2.36	0.41
30:0:146:U:O2'	30:0:147:G:H5'	2.21	0.41
30:0:364:U:H2'	30:0:365:G:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:413:G:H2'	30:0:414:C:C6	2.55	0.41
30:0:424:C:C2	30:0:425:U:C5	3.09	0.41
30:0:426:G:H2'	30:0:427:C:O4'	2.19	0.41
30:0:580:A:O4'	30:0:1111:U:H4'	2.21	0.41
30:0:1175:G:H1'	30:0:1193:A:H2'	2.03	0.41
30:0:1819:G:H2'	30:0:1820:G:H5'	1.98	0.41
30:0:2722:G:N3	30:0:2761:A:C2	2.89	0.41
30:0:2780:C:H2'	30:0:2781:U:C6	2.56	0.41
2:B:24:PRO:HD3	38:B:8991:HOH:O	2.22	0.40
4:D:135:VAL:HG22	4:D:136:ARG:N	2.36	0.40
10:J:41:ALA:HB3	38:J:8865:HOH:O	2.19	0.40
19:S:38:ALA:O	19:S:42:GLU:HG3	2.21	0.40
25:Y:144:ARG:CZ	38:Y:8181:HOH:O	2.69	0.40
30:0:275:G:C2	30:0:376:C:N3	2.88	0.40
30:0:334:G:C5	30:0:335:U:C5	3.09	0.40
30:0:772:G:H2'	30:0:773:A:O4'	2.21	0.40
30:0:1217:G:C2	30:0:1218:U:C2	3.09	0.40
30:0:1250:C:O2'	30:0:1251:C:H5'	2.21	0.40
30:0:2002:C:H2'	30:0:2003:U:H5'	2.03	0.40
3:C:138:VAL:O	3:C:234:VAL:HA	2.21	0.40
3:C:236:THR:CG2	3:C:239:ALA:H	2.34	0.40
7:G:63:ARG:NH1	30:0:1151:G:OP1	2.54	0.40
8:H:27:PRO:HD3	8:H:123:ILE:HG22	2.02	0.40
13:M:167:GLY:O	13:M:171:ARG:HG3	2.21	0.40
21:U:31:PHE:CG	21:U:37:GLU:HG2	2.56	0.40
23:W:11:VAL:HG11	30:0:1086:A:C6	2.55	0.40
25:Y:152:LYS:HB3	25:Y:160:LYS:HG3	2.03	0.40
30:0:293:A:C2	30:0:294:C:C6	3.09	0.40
30:0:371:U:H2'	30:0:372:A:H8	1.86	0.40
30:0:423:A:C4	30:0:424:C:C6	3.09	0.40
30:0:725:C:C2'	30:0:726:C:O5'	2.69	0.40
30:0:921:G:H4'	30:0:924:G:N1	2.36	0.40
30:0:921:G:H4'	30:0:924:G:C6	2.56	0.40
30:0:1295:G:H2'	30:0:1296:A:C8	2.56	0.40
30:0:1587:U:C4	30:0:1588:G:C5	3.09	0.40
30:0:1669:G:H2'	30:0:1670:A:C8	2.56	0.40
30:0:1928:C:C2'	30:0:1929:G:H5'	2.51	0.40
30:0:2385:G:H2'	30:0:2386:U:C6	2.56	0.40
30:0:2846:C:H3'	38:0:7101:HOH:O	2.20	0.40
1:A:38:ILE:HD13	1:A:38:ILE:HA	1.90	0.40
2:B:209:LYS:HB2	2:B:257:THR:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:226:GLY:HA3	30:0:1308:A:O4'	2.21	0.40
10:J:90:LYS:HB2	33:J:8802:CL:CL	2.58	0.40
11:K:81:ARG:HD3	11:K:87:ARG:NH2	2.36	0.40
13:M:42:ARG:HA	13:M:43:PRO:HD3	1.93	0.40
16:P:87:ARG:HG2	38:0:5961:HOH:O	2.22	0.40
17:Q:59:GLN:NE2	30:0:1018:A:H4'	2.36	0.40
23:W:5:VAL:HG11	23:W:153:MET:HE1	2.04	0.40
23:W:139:GLY:O	23:W:141:HIS:HD2	2.04	0.40
24:X:30:MET:HE1	24:X:55:ASN:HA	2.03	0.40
25:Y:148:GLY:HA3	30:0:622:G:P	2.61	0.40
30:0:123:U:H2'	30:0:124:C:C6	2.55	0.40
30:0:303:C:N4	30:0:304:G:C6	2.89	0.40
30:0:319:A:H2'	30:0:320:G:C8	2.56	0.40
30:0:549:A:C6	30:0:550:C:C4	3.10	0.40
30:0:1182:C:H1'	30:0:1192:A:C8	2.41	0.40
30:0:1198:U:H1'	30:0:1201:C:H5	1.86	0.40
30:0:1205:U:H2'	30:0:1205:U:O2	2.21	0.40
30:0:1375:A:C2'	30:0:1376:G:H5'	2.51	0.40
30:0:1947:G:OP1	30:0:1971:G:N7	2.54	0.40
30:0:2765:C:H2'	30:0:2766:A:C8	2.56	0.40
30:0:2831:C:H2'	30:0:2832:C:O4'	2.22	0.40
1:A:109:GLU:HG2	1:A:116:GLY:N	2.36	0.40
4:D:25:MET:HE1	4:D:37:ALA:O	2.22	0.40
6:F:56:PRO:HB2	6:F:58:GLU:OE1	2.21	0.40
12:L:30:ARG:HD3	30:0:164:G:H4'	2.04	0.40
20:T:21:LYS:HA	20:T:24:ARG:HG3	2.04	0.40
23:W:108:ARG:HG3	23:W:114:PRO:HG3	2.03	0.40
24:X:79:GLU:CD	24:X:80:GLU:H	2.25	0.40
25:Y:187:VAL:HG13	25:Y:205:ILE:HA	2.02	0.40
28:2:41:HIS:CD2	28:2:44:ARG:H	2.31	0.40
30:0:27:U:H5	38:0:5902:HOH:O	2.04	0.40
30:0:272:A:N1	30:0:369:G:H5"	2.35	0.40
30:0:545:G:C8	30:0:545:G:C5'	2.95	0.40
30:0:803:C:H2'	30:0:804:C:H6	1.87	0.40
30:0:963:C:O2	30:0:1005:A:N1	2.54	0.40
30:0:1167:G:O2'	30:0:1168:C:H5'	2.22	0.40
30:0:1386:G:O2'	30:0:1387:G:H5'	2.22	0.40
30:0:1931:A:H2'	30:0:1932:G:H5'	2.04	0.40
30:0:2118:A:C5	30:0:2470:A:C5	3.09	0.40
30:0:2437:A:H2'	30:0:2438:G:C8	2.57	0.40
30:0:2505:G:HO2'	30:0:2506:A:H5'	1.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2802:C:H2'	30:0:2803:C:H6	1.85	0.40
30:0:2887:G:H2'	30:0:2888:U:O4'	2.22	0.40
31:9:24:U:H3'	31:9:24:U:H6	1.87	0.40
7:G:64:ASN:N	7:G:64:ASN:HD22	2.18	0.40
12:L:113:GLN:C	30:0:700:A:H62	2.24	0.40
14:N:143:ARG:HG2	14:N:172:PHE:CD2	2.56	0.40
15:O:44:ASN:OD1	15:O:65:LEU:HB2	2.22	0.40
16:P:104:LYS:HE2	16:P:138:GLU:OE2	2.20	0.40
18:R:46:TYR:O	18:R:50:VAL:HG23	2.22	0.40
18:R:132:ARG:CZ	38:R:8987:HOH:O	2.70	0.40
20:T:49:GLU:OE2	20:T:97:ARG:HD2	2.22	0.40
25:Y:133:HIS:HD2	38:Y:8150:HOH:O	2.04	0.40
26:Z:50:VAL:O	26:Z:54:GLU:HG3	2.21	0.40
30:0:365:G:C6	30:0:366:U:C4	3.09	0.40
30:0:461:C:N3	30:0:479:G:H5'	2.36	0.40
30:0:820:G:H5'	30:0:821:U:H5'	2.02	0.40
30:0:1102:C:H4'	38:0:9561:HOH:O	2.20	0.40
30:0:1189:A:H1'	30:0:1209:C:H1'	2.02	0.40
30:0:1191:A:H2	30:0:1206:U:H3	1.69	0.40
30:0:1207:A:H5'	30:0:1208:C:OP2	2.21	0.40
30:0:1342:C:H2'	30:0:1343:C:C5'	2.47	0.40
30:0:1589:G:H4'	38:0:6875:HOH:O	2.20	0.40
30:0:2133:U:H4'	30:0:2134:G:H5'	2.02	0.40
30:0:2237:G:O2'	30:0:2238:A:C8	2.72	0.40
30:0:2304:G:C6	30:0:2305:A:C5	3.10	0.40
30:0:2346:C:O5'	30:0:2346:C:C6	2.74	0.40
30:0:2543:G:H2'	30:0:2544:G:O4'	2.21	0.40
30:0:2712:G:P	38:0:5233:HOH:O	2.79	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
1	A	235/240 (98%)	211 (90%)	22 (9%)	2 (1%)	17 31
2	B	335/338 (99%)	309 (92%)	21 (6%)	5 (2%)	10 18
3	C	244/246 (99%)	228 (93%)	16 (7%)	0	100 100
4	D	134/177 (76%)	110 (82%)	22 (16%)	2 (2%)	10 18
5	E	170/178 (96%)	160 (94%)	9 (5%)	1 (1%)	25 42
6	F	117/120 (98%)	107 (92%)	8 (7%)	2 (2%)	9 16
7	G	25/348 (7%)	23 (92%)	2 (8%)	0	100 100
8	H	156/177 (88%)	141 (90%)	14 (9%)	1 (1%)	25 42
9	I	68/162 (42%)	53 (78%)	13 (19%)	2 (3%)	4 6
10	J	140/145 (97%)	131 (94%)	8 (6%)	1 (1%)	22 39
11	K	130/132 (98%)	122 (94%)	8 (6%)	0	100 100
12	L	141/165 (86%)	125 (89%)	13 (9%)	3 (2%)	7 12
13	M	192/196 (98%)	181 (94%)	10 (5%)	1 (0%)	29 47
14	N	184/187 (98%)	164 (89%)	16 (9%)	4 (2%)	6 11
15	O	113/116 (97%)	110 (97%)	3 (3%)	0	100 100
16	P	141/149 (95%)	137 (97%)	4 (3%)	0	100 100
17	Q	93/96 (97%)	89 (96%)	3 (3%)	1 (1%)	14 25
18	R	148/155 (96%)	141 (95%)	7 (5%)	0	100 100
19	S	79/85 (93%)	74 (94%)	5 (6%)	0	100 100
20	T	117/120 (98%)	108 (92%)	8 (7%)	1 (1%)	17 31
21	U	51/67 (76%)	48 (94%)	3 (6%)	0	100 100
22	V	63/71 (89%)	59 (94%)	3 (5%)	1 (2%)	9 16
23	W	152/154 (99%)	146 (96%)	6 (4%)	0	100 100
24	X	80/92 (87%)	73 (91%)	5 (6%)	2 (2%)	5 9
25	Y	140/241 (58%)	139 (99%)	1 (1%)	0	100 100
26	Z	71/116 (61%)	62 (87%)	9 (13%)	0	100 100
27	1	54/57 (95%)	52 (96%)	2 (4%)	0	100 100
28	2	42/50 (84%)	41 (98%)	1 (2%)	0	100 100
29	3	90/92 (98%)	88 (98%)	2 (2%)	0	100 100
All	All	3705/4472 (83%)	3432 (93%)	244 (7%)	29 (1%)	19 34

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
8	H	19	ARG
10	J	5	GLU
14	N	154	LEU
14	N	183	ASP
14	N	184	ILE
2	B	184	ASP
9	I	107	LYS
12	L	149	ARG
14	N	162	ASP
1	A	34	ASP
2	B	34	GLY
6	F	101	ALA
12	L	80	ASP
2	B	2	GLN
2	B	245	SER
4	D	56	ARG
12	L	21	ARG
20	T	53	GLY
24	X	87	ALA
4	D	137	PRO
6	F	100	ASP
24	X	70	ILE
22	V	39	ALA
2	B	185	GLY
17	Q	78	GLY
5	E	44	GLY
9	I	83	GLY
13	M	88	VAL

5.3.2 Protein sidechains (i)

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	
1	A	179/182 (98%)	166 (93%)	13 (7%)	14	25
2	B	282/283 (100%)	264 (94%)	18 (6%)	17	31
3	C	193/193 (100%)	179 (93%)	14 (7%)	14	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	D	117/148 (79%)	113 (97%)	4 (3%)	37 58
5	E	152/156 (97%)	150 (99%)	2 (1%)	69 81
6	F	93/94 (99%)	92 (99%)	1 (1%)	73 84
7	G	27/282 (10%)	25 (93%)	2 (7%)	13 24
8	H	134/145 (92%)	129 (96%)	5 (4%)	34 54
9	I	58/130 (45%)	58 (100%)	0	100 100
10	J	118/121 (98%)	112 (95%)	6 (5%)	24 41
11	K	106/106 (100%)	105 (99%)	1 (1%)	78 87
12	L	113/127 (89%)	107 (95%)	6 (5%)	22 38
13	M	158/160 (99%)	152 (96%)	6 (4%)	33 53
14	N	149/150 (99%)	142 (95%)	7 (5%)	26 45
15	O	93/94 (99%)	93 (100%)	0	100 100
16	P	113/117 (97%)	110 (97%)	3 (3%)	44 65
17	Q	79/80 (99%)	75 (95%)	4 (5%)	24 41
18	R	117/122 (96%)	111 (95%)	6 (5%)	24 41
19	S	71/74 (96%)	70 (99%)	1 (1%)	67 79
20	T	105/106 (99%)	98 (93%)	7 (7%)	16 28
21	U	44/53 (83%)	44 (100%)	0	100 100
22	V	51/57 (90%)	50 (98%)	1 (2%)	55 72
23	W	130/130 (100%)	126 (97%)	4 (3%)	40 60
24	X	66/74 (89%)	62 (94%)	4 (6%)	18 33
25	Y	120/196 (61%)	116 (97%)	4 (3%)	38 58
26	Z	60/94 (64%)	59 (98%)	1 (2%)	60 76
27	1	46/47 (98%)	45 (98%)	1 (2%)	52 70
28	2	42/46 (91%)	41 (98%)	1 (2%)	49 68
29	3	79/79 (100%)	76 (96%)	3 (4%)	33 53
All	All	3095/3646 (85%)	2970 (96%)	125 (4%)	31 51

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	26	ASP

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Mol	Chain	Res	Type
1	A	36	ASP
1	A	38	ILE
1	A	68	ILE
1	A	69	LEU
1	A	94	LEU
1	A	131	HIS
1	A	165	THR
1	A	179	MET
1	A	192	VAL
1	A	206	ARG
1	A	217	ARG
2	B	7	ARG
2	B	11	LEU
2	B	16	ARG
2	B	27	ASN
2	B	51	VAL
2	B	53	LEU
2	B	71	VAL
2	B	88	GLU
2	B	97	LEU
2	B	98	THR
2	B	132	HIS
2	B	149	ASP
2	B	162	MET
2	B	175	LEU
2	B	234	ARG
2	B	254	GLN
2	B	257	THR
2	B	265	LEU
3	C	78	ARG
3	C	91	PRO
3	C	94	THR
3	C	101	ASP
3	C	115	LEU
3	C	132	ASP
3	C	136	VAL
3	C	162	VAL
3	C	187	ARG
3	C	214	THR
3	C	222	ASP
3	C	223	LEU
3	C	234	VAL

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Mol	Chain	Res	Type
3	C	243	VAL
4	D	24	HIS
4	D	29	HIS
4	D	50	VAL
4	D	161	ASP
5	E	102	VAL
5	E	156	ASP
6	F	12	LEU
7	G	72	ASP
7	G	73	ASP
8	H	21	GLU
8	H	62	HIS
8	H	87	LYS
8	H	91	ARG
8	H	157	TYR
10	J	46	ILE
10	J	52	GLN
10	J	74	ARG
10	J	79	PHE
10	J	93	ARG
10	J	107	ASN
11	K	10	GLN
12	L	35	ARG
12	L	37	LYS
12	L	102	ASP
12	L	104	ASP
12	L	114	VAL
12	L	140	VAL
13	M	46	LEU
13	M	68	ARG
13	M	93	ARG
13	M	99	ARG
13	M	116	ASN
13	M	164	THR
14	N	23	ARG
14	N	26	LEU
14	N	49	THR
14	N	101	VAL
14	N	127	LEU
14	N	139	TRP
14	N	173	ASP
16	P	16	VAL

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Mol	Chain	Res	Type
16	P	91	LYS
16	P	98	ILE
17	Q	11	ARG
17	Q	16	ASN
17	Q	18	PRO
17	Q	57	ASP
18	R	39	THR
18	R	82	GLU
18	R	119	VAL
18	R	132	ARG
18	R	143	VAL
18	R	150	PRO
19	S	44	GLN
20	T	39	ASN
20	T	48	VAL
20	T	71	VAL
20	T	73	HIS
20	T	89	ARG
20	T	115	GLU
20	T	117	ASP
22	V	12	THR
23	W	26	ILE
23	W	52	VAL
23	W	108	ARG
23	W	146	ILE
24	X	27	ASP
24	X	52	PRO
24	X	72	VAL
24	X	82	GLU
25	Y	95	THR
25	Y	189	ASN
25	Y	191	ASP
25	Y	203	VAL
26	Z	68	GLU
27	1	14	THR
28	2	18	ASN
29	3	14	CYS
29	3	56	PRO
29	3	87	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	HIS
1	A	199	HIS
2	B	2	GLN
2	B	27	ASN
2	B	106	HIS
2	B	145	HIS
2	B	221	GLN
2	B	238	ASN
2	B	256	GLN
2	B	260	HIS
2	B	320	GLN
2	B	332	ASN
3	C	73	GLN
3	C	129	HIS
3	C	151	GLN
3	C	163	HIS
4	D	85	GLN
4	D	103	ASN
5	E	143	GLN
7	G	64	ASN
8	H	34	HIS
8	H	59	GLN
8	H	62	HIS
10	J	52	GLN
10	J	107	ASN
10	J	126	ASN
10	J	142	ASN
11	K	10	GLN
11	K	44	HIS
11	K	67	GLN
12	L	18	HIS
12	L	41	HIS
13	M	24	GLN
13	M	58	GLN
13	M	137	ASN
13	M	143	ASN
13	M	170	ASN
14	N	40	ASN
14	N	53	ASN
14	N	107	ASN
14	N	132	ASN
16	P	50	GLN
16	P	66	GLN

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Mol	Chain	Res	Type
16	P	73	HIS
16	P	88	GLN
16	P	118	GLN
17	Q	40	HIS
18	R	22	GLN
18	R	61	GLN
18	R	94	ASN
18	R	98	ASN
18	R	113	HIS
18	R	117	HIS
18	R	122	GLN
18	R	123	GLN
19	S	44	GLN
19	S	53	ASN
20	T	39	ASN
21	U	39	ASN
22	V	60	GLN
23	W	27	HIS
23	W	110	GLN
23	W	119	HIS
23	W	125	HIS
23	W	141	HIS
24	X	23	HIS
25	Y	134	HIS
25	Y	189	ASN
27	1	8	GLN
27	1	16	HIS
27	1	28	HIS
28	2	18	ASN
28	2	41	HIS
28	2	45	ASN
29	3	15	ASN
29	3	20	HIS
29	3	48	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	232 (8%)	18 (0%)
31	9	121/122 (99%)	16 (13%)	1 (0%)
All	All	2866/3045 (94%)	248 (8%)	19 (0%)

All (248) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	0	31	C
30	0	67	A
30	0	69	A
30	0	70	A
30	0	71	G
30	0	86	A
30	0	87	C
30	0	88	G
30	0	114	A
30	0	115	U
30	0	130	C
30	0	141	C
30	0	151	A
30	0	166	A
30	0	169	A
30	0	186	A
30	0	191	A
30	0	192	A
30	0	198	A
30	0	200	C
30	0	204	A
30	0	219	G
30	0	237	G
30	0	271	C
30	0	272	A
30	0	273	G
30	0	283	U
30	0	284	C
30	0	308	U
30	0	309	C
30	0	318	U
30	0	336	G
30	0	337	A
30	0	358	G
30	0	368	C
30	0	381	G
30	0	397	A
30	0	417	G
30	0	461	C
30	0	487	G
30	0	498	A
30	0	510	U

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Mol	Chain	Res	Type
30	0	511	A
30	0	514	G
30	0	537	G
30	0	538	C
30	0	539	G
30	0	542	A
30	0	545	G
30	0	553	G
30	0	559	U
30	0	588	G
30	0	604	G
30	0	620	A
30	0	632	A
30	0	644	G
30	0	660	A
30	0	688	A
30	0	701	U
30	0	746	A
30	0	759	C
30	0	777	U
30	0	809	G
30	0	821	U
30	0	835	U
30	0	840	U
30	0	857	A
30	0	858	U
30	0	868	G
30	0	869	G
30	0	871	G
30	0	872	U
30	0	875	A
30	0	877	G
30	0	878	G
30	0	884	C
30	0	885	G
30	0	905	C
30	0	920	C
30	0	921	G
30	0	923	A
30	0	953	G
30	0	960	G
30	0	961	A

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Mol	Chain	Res	Type
30	0	1006	A
30	0	1008	C
30	0	1029	U
30	0	1045	G
30	0	1059	G
30	0	1060	C
30	0	1072	G
30	0	1081	A
30	0	1088	A
30	0	1109	U
30	0	1110	G
30	0	1119	G
30	0	1124	A
30	0	1130	U
30	0	1151	G
30	0	1165	G
30	0	1174	A
30	0	1175	G
30	0	1185	U
30	0	1192	A
30	0	1193	A
30	0	1206	U
30	0	1208	C
30	0	1216	G
30	0	1237	U
30	0	1238	C
30	0	1239	G
30	0	1242	A
30	0	1279	U
30	0	1289	C
30	0	1342	C
30	0	1353	C
30	0	1360	C
30	0	1377	C
30	0	1378	G
30	0	1407	A
30	0	1409	G
30	0	1474	C
30	0	1505	U
30	0	1506	U
30	0	1524	U
30	0	1525	G

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Mol	Chain	Res	Type
30	0	1526	A
30	0	1535	G
30	0	1562	C
30	0	1592	G
30	0	1605	G
30	0	1625	U
30	0	1626	A
30	0	1634	G
30	0	1656	A
30	0	1667	A
30	0	1682	A
30	0	1684	A
30	0	1685	A
30	0	1692	C
30	0	1701	A
30	0	1710	A
30	0	1722	U
30	0	1723	G
30	0	1725	C
30	0	1731	C
30	0	1732	A
30	0	1742	A
30	0	1752	G
30	0	1778	A
30	0	1798	C
30	0	1820	G
30	0	1829	A
30	0	1856	C
30	0	1879	U
30	0	1919	A
30	0	1942	A
30	0	1968	A
30	0	1971	G
30	0	1973	A
30	0	1979	G
30	0	1980	U
30	0	1996	U
30	0	2006	C
30	0	2008	U
30	0	2011	A
30	0	2012	U
30	0	2013	G

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Mol	Chain	Res	Type
30	0	2033	G
30	0	2034	U
30	0	2064	U
30	0	2072	G
30	0	2073	G
30	0	2074	A
30	0	2096	A
30	0	2101	A
30	0	2102	G
30	0	2110	G
30	0	2238	A
30	0	2243	C
30	0	2258	A
30	0	2271	G
30	0	2272	G
30	0	2291	A
30	0	2317	C
30	0	2321	A
30	0	2354	A
30	0	2361	A
30	0	2369	A
30	0	2379	G
30	0	2422	U
30	0	2462	G
30	0	2465	A
30	0	2467	A
30	0	2476	C
30	0	2483	A
30	0	2507	G
30	0	2509	A
30	0	2511	A
30	0	2533	C
30	0	2537	G
30	0	2541	U
30	0	2553	A
30	0	2564	G
30	0	2589	U
30	0	2601	A
30	0	2602	G
30	0	2608	C
30	0	2613	G
30	0	2637	A

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Mol	Chain	Res	Type
30	0	2638	G
30	0	2649	A
30	0	2664	A
30	0	2681	A
30	0	2682	C
30	0	2726	U
30	0	2747	C
30	0	2748	G
30	0	2749	U
30	0	2750	G
30	0	2762	C
30	0	2768	A
30	0	2800	A
30	0	2811	A
30	0	2812	A
30	0	2825	C
30	0	2867	G
30	0	2876	G
30	0	2890	A
30	0	2896	A
30	0	2903	C
30	0	2914	A
31	9	2	U
31	9	7	G
31	9	14	G
31	9	22	G
31	9	23	U
31	9	24	U
31	9	25	G
31	9	40	C
31	9	41	C
31	9	43	G
31	9	52	A
31	9	57	A
31	9	66	G
31	9	77	A
31	9	114	G
31	9	122	C

All (19) RNA pucker outliers are listed below:

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Mol	Chain	Res	Type
30	0	129	A
30	0	603	A
30	0	699	C
30	0	834	G
30	0	857	A
30	0	871	G
30	0	877	G
30	0	1237	U
30	0	1352	A
30	0	1377	C
30	0	1506	U
30	0	1685	A
30	0	1979	G
30	0	2467	A
30	0	2649	A
30	0	2718	C
30	0	2726	U
30	0	2761	A
31	9	65	A

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

5 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
30	OMG	0	2588	30	18,26,27	0.99	2 (11%)	19,38,41	0.70	1 (5%)
30	UR3	0	2619	30	19,22,23	0.42	0	26,32,35	0.63	1 (3%)
30	OMU	0	2587	30	19,22,23	0.29	0	26,31,34	0.39	0
30	PSU	0	2621	30	18,21,22	1.49	2 (11%)	22,30,33	1.26	3 (13%)
30	1MA	0	628	30,35	16,25,26	1.36	3 (18%)	18,37,40	1.02	2 (11%)

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
30	OMG	0	2588	30	-	0/5/27/28	0/3/3/3
30	UR3	0	2619	30	-	0/7/25/26	0/2/2/2
30	OMU	0	2587	30	-	0/9/27/28	0/2/2/2
30	PSU	0	2621	30	-	0/7/25/26	0/2/2/2
30	1MA	0	628	30,35	-	0/3/25/26	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C2-N1	4.94	1.43	1.36
30	0	628	1MA	C2-N3	3.53	1.33	1.29
30	0	2621	PSU	C6-C5	2.69	1.38	1.35
30	0	628	1MA	C6-N6	2.56	1.34	1.27
30	0	2588	OMG	C8-N7	-2.45	1.30	1.35
30	0	2588	OMG	C5-C6	-2.41	1.42	1.47
30	0	628	1MA	C8-N7	-2.03	1.31	1.35

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	0	2621	PSU	C6-C5-C4	3.37	120.56	118.20
30	0	2621	PSU	O2-C2-N1	2.76	125.83	122.79
30	0	628	1MA	N1-C2-N3	2.76	129.24	126.02
30	0	2621	PSU	C6-N1-C2	-2.72	119.90	122.68
30	0	628	1MA	C5-C6-N1	2.49	117.62	113.90
30	0	2619	UR3	C4-N3-C2	2.38	126.81	124.56
30	0	2588	OMG	O6-C6-C5	2.15	128.57	124.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	0	2587	OMU	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 305 ligands modelled in this entry, 305 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.