Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 11:15 PM GMT

PDB ID	:	5DM7
Title	:	Crystal structure of the 50S ribosomal subunit from Deinococcus radiodurans in complex with hygromycin A
Authors	:	Kaminishi, T.; Schedlbauer, A.; Ochoa-Lizarralde, B.; Connell, S.R.; Fucini, P.
Deposited on	:	2015-09-08
Resolution	:	3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

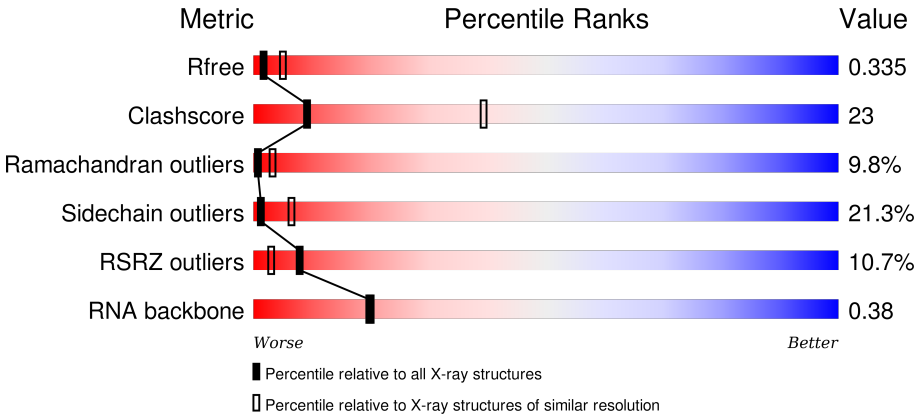
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)
RNA backbone	2183	1036 (3.40-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	224	80% 54% 39% 6%
2	A	274	14% 43% 47% 9% •
3	B	205	2% 33% 50% 17%
4	C	197	5% 30% 50% 17% •

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Mol	Chain	Length	Quality of chain
5	D	177	8% 38% 49% 13%
6	E	171	6% 46% 44% 9%
7	F	144	42% 60% 33% 6%
8	G	142	6% 47% 45% 6%
9	H	134	3% 29% 46% 23%
10	I	141	24% 43% 43% 11%
11	J	136	18% 39% 44% 15%
12	K	113	5% 29% 51% 17%
13	L	104	25% 29% 46% 24%
14	M	109	3% 32% 44% 23%
15	N	117	9% 30% 62% 8%
16	O	94	6% 38% 45% 16%
17	P	127	4% 31% 53% 15%
18	Q	93	13% 46% 39% 14%
19	R	110	7% 34% 41% 25%
20	S	175	14% 41% 43% 13%
21	T	84	21% 42% 46% 11%
22	U	72	29% 24% 51% 17% 8%
23	V	66	18% 61% 32% 8%
24	W	55	11% 38% 56% 5%
25	Z	57	5% 30% 51% 18%
26	1	54	43% 46% 39% 13%
27	2	47	4% 40% 47% 13%
28	3	65	40% 17% 60% 20%
29	X	2881	3% 22% 44% 25% 5%

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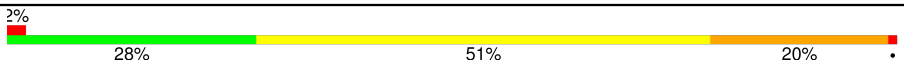
Mol	Chain	Length	Quality of chain
30	Y	122	

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
31	MG	M	201	-	-	-	X
31	MG	N	201	-	-	-	X
31	MG	X	6001	-	-	-	X
31	MG	X	6002	-	-	-	X
31	MG	X	6006	-	-	-	X
31	MG	X	6007	-	-	-	X
31	MG	X	6008	-	-	-	X
31	MG	X	6011	-	-	-	X
31	MG	X	6014	-	-	-	X
31	MG	X	6016	-	-	-	X
31	MG	X	6017	-	-	-	X
31	MG	X	6018	-	-	-	X
31	MG	X	6019	-	-	-	X
31	MG	X	6021	-	-	-	X
31	MG	X	6022	-	-	-	X
31	MG	X	6032	-	-	-	X
31	MG	X	6033	-	-	-	X
31	MG	X	6037	-	-	-	X
31	MG	X	6051	-	-	-	X
31	MG	X	6053	-	-	-	X
31	MG	X	6054	-	-	-	X
31	MG	X	6055	-	-	-	X
31	MG	X	6056	-	-	-	X
31	MG	X	6059	-	-	-	X
31	MG	X	6060	-	-	-	X
31	MG	X	6062	-	-	-	X
31	MG	X	6066	-	-	-	X
31	MG	X	6068	-	-	-	X
31	MG	X	6071	-	-	-	X
31	MG	X	6078	-	-	-	X
31	MG	X	6085	-	-	-	X
31	MG	X	6087	-	-	-	X
31	MG	X	6093	-	-	-	X
31	MG	X	6105	-	-	-	X
31	MG	X	6108	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	MG	X	6110	-	-	-	X
31	MG	X	6115	-	-	-	X
31	MG	X	6129	-	-	-	X
31	MG	X	6131	-	-	-	X
31	MG	X	6132	-	-	-	X
31	MG	X	6142	-	-	-	X
31	MG	X	6144	-	-	-	X
31	MG	X	6147	-	-	-	X
31	MG	X	6162	-	-	-	X
31	MG	X	6167	-	-	-	X
31	MG	X	6171	-	-	-	X
31	MG	Y	201	-	-	-	X

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 89361 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 L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	224	Total	C	N	O	S	0	0	0
			1651	1031	302	313	5			

- Molecule 2 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	274	Total	C	N	O	S	0	0	0
			2107	1313	423	368	3			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	LYS	ARG	conflict	UNP Q9RXJ9
A	25	ALA	THR	conflict	UNP Q9RXJ9
A	270	LEU	ILE	conflict	UNP Q9RXJ9

- Molecule 3 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	205	Total	C	N	O	S	0	0	0
			1540	965	295	272	8			

- Molecule 4 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	197	Total	C	N	O	S	0	0	0
			1507	935	287	283	2			

- Molecule 5 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	177	Total	C	N	O	S	0	0	0
			1401	892	247	255	7			

- Molecule 6 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	E	171	Total	C	N	O	S	0	0	0
			1287	812	237	237	1			

- Molecule 7 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	F	144	Total	C	N	O	S	0	0	0
			1048	663	183	197	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	2	ARG	LYS	conflict	UNP Q9RSS7
F	3	ARG	LYS	conflict	UNP Q9RSS7

- Molecule 8 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	G	142	Total	C	N	O	S	0	0	0
			1115	704	209	199	3			

- Molecule 9 is a protein called 50S ribosomal protein L14.

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

- Molecule 10 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	I	141	Total	C	N	O	0	0	0
			1068	655	216	197			

- Molecule 11 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	136	Total	C	N	O	S	0	0	0
			1091	696	202	186	7			

- Molecule 12 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	113	Total	C	N	O	S	0	0	0
			879	541	178	158	2			

- Molecule 13 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	L	104	Total	C	N	O	0	0	0
			778	476	159	143			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	26	LYS	ARG	conflict	UNP Q9RSL2

- Molecule 14 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	M	109	Total	C	N	O	0	0	0
			867	540	171	156			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	?	-	LEU	deletion	UNP Q9RWB4
M	?	-	ARG	deletion	UNP Q9RWB4
M	?	-	GLU	deletion	UNP Q9RWB4
M	?	-	LEU	deletion	UNP Q9RWB4

- Molecule 15 is a protein called 50S ribosomal protein L20.

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

- Molecule 16 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	O	94	Total	C	N	O	0	0	0
			742	465	139	138			

- Molecule 17 is a protein called 50S ribosomal protein L22.

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

- Molecule 18 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Q	93	Total	C	N	O	S	0	0	0
			727	458	136	131	2			

- Molecule 19 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	R	110	Total	C	N	O	S	0	0	0
			826	513	160	152	1			

- Molecule 20 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	S	175	Total	C	N	O	S	0	0	0
			1346	849	236	255	6			

- Molecule 21 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	T	84	Total	C	N	O	S	0	0	0
			626	393	122	110	1			

- Molecule 22 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	U	72	Total	C	N	O	0	0	0
			553	341	116	96			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	67	ILE	LEU	conflict	UNP Q9RRG8

- Molecule 23 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	V	66	Total	C	N	O	S	0	0	0
			534	327	107	97	3			

- Molecule 24 is a protein called 50S ribosomal protein L30.

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

- Molecule 25 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Z	57	Total	C	N	O	S	0	0	0
			453	278	93	77	5			

- Molecule 26 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	1	54	Total	C	N	O	S	0	0	0
			404	256	73	74	1			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	0	ALA	-	insertion	UNP Q9RSS4
1	1	ALA	-	insertion	UNP Q9RSS4
1	3	GLY	LYS	conflict	UNP Q9RSS4
1	4	ALA	ASP	conflict	UNP Q9RSS4
1	5	ALA	GLY	conflict	UNP Q9RSS4
1	45	ALA	LYS	conflict	UNP Q9RSS4
1	46	HIS	LYS	conflict	UNP Q9RSS4
1	47	VAL	HIS	conflict	UNP Q9RSS4
1	49	PHE	VAL	conflict	UNP Q9RSS4
1	50	ALA	PHE	conflict	UNP Q9RSS4
1	51	ALA	-	insertion	UNP Q9RSS4
1	52	ALA	-	insertion	UNP Q9RSS4
1	53	ALA	-	insertion	UNP Q9RSS4

- Molecule 27 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	2	47	Total	C	N	O	S	0	0	0
			393	235	92	64	2			

- Molecule 28 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	3	65	Total	C	N	O	S	0	0	0
			509	320	104	80	5			

- Molecule 29 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	X	2780	Total	C	N	O	P	0	0	0
			59673	26617	11011	19265	2780			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	1526	U	UNK	conflict	GB 11612676

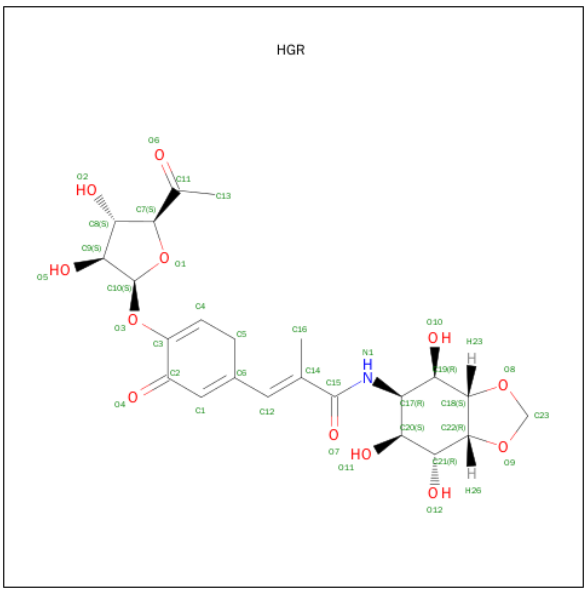
- Molecule 30 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	Y	122	Total	C	N	O	P	0	0	0
			2601	1161	476	842	122			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
31	H	1	Total	Mg	0	0
			1	1		
31	A	1	Total	Mg	0	0
			1	1		
31	N	1	Total	Mg	0	0
			1	1		
31	X	177	Total	Mg	0	0
			177	177		
31	Y	5	Total	Mg	0	0
			5	5		
31	M	1	Total	Mg	0	0
			1	1		

- Molecule 32 is Hygromycin A (three-letter code: HGR) (formula: $C_{23}H_{29}NO_{12}$).



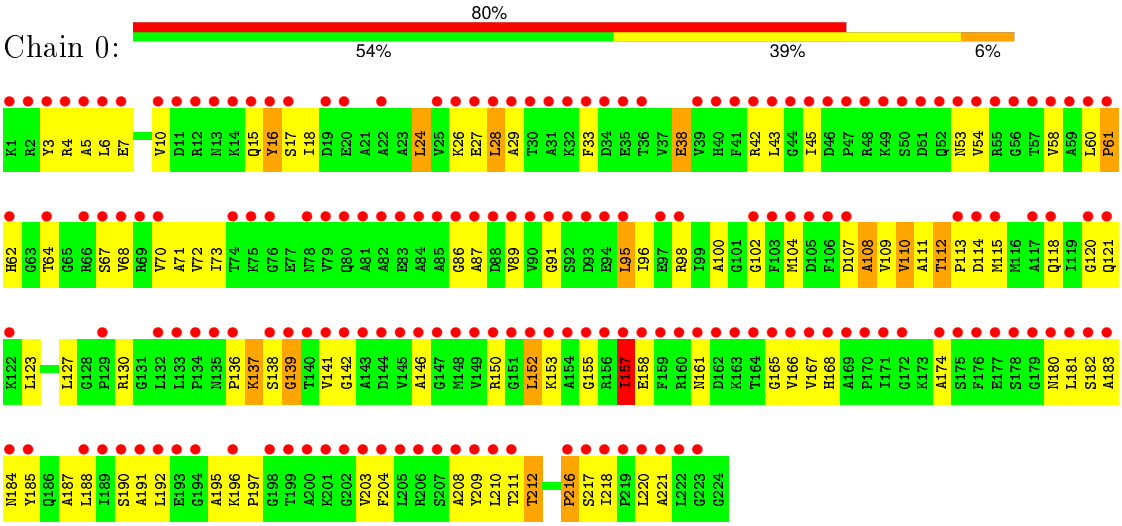
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
32	X	1	36	23	1	12	0	0

3 Residue-property plots (i)

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

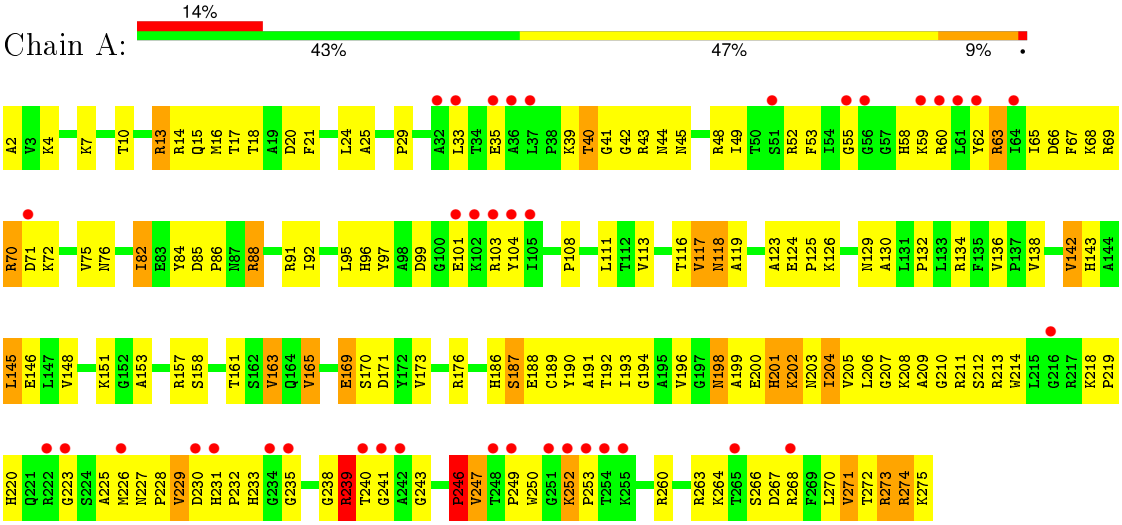
- Molecule 1: 50S ribosomal protein L1

Chain 0:



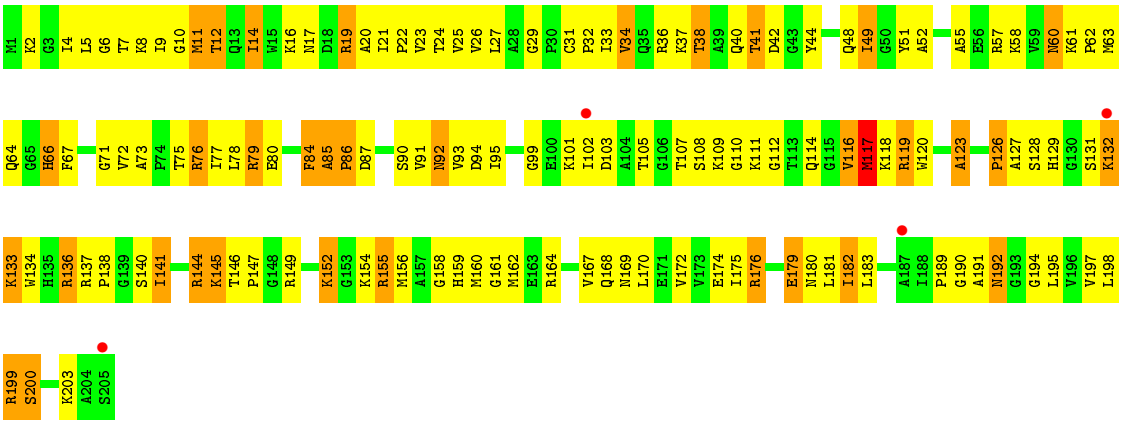
- Molecule 2: 50S ribosomal protein L2

Chain A:



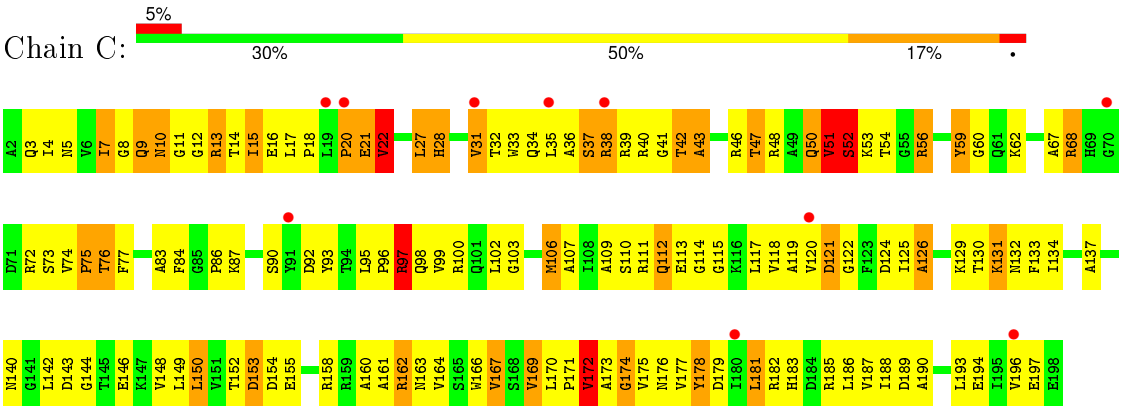
- Molecule 3: 50S ribosomal protein L3

Chain B:



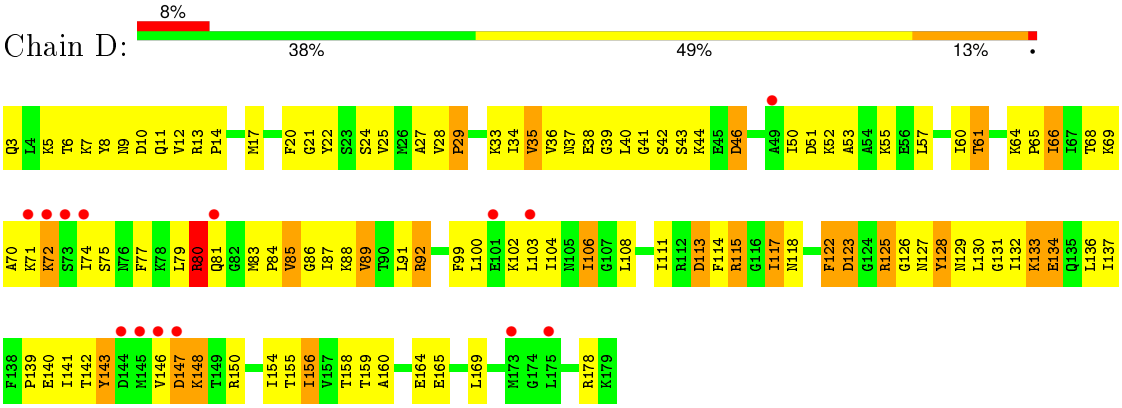
• Molecule 4: 50S ribosomal protein L4

Chain C:



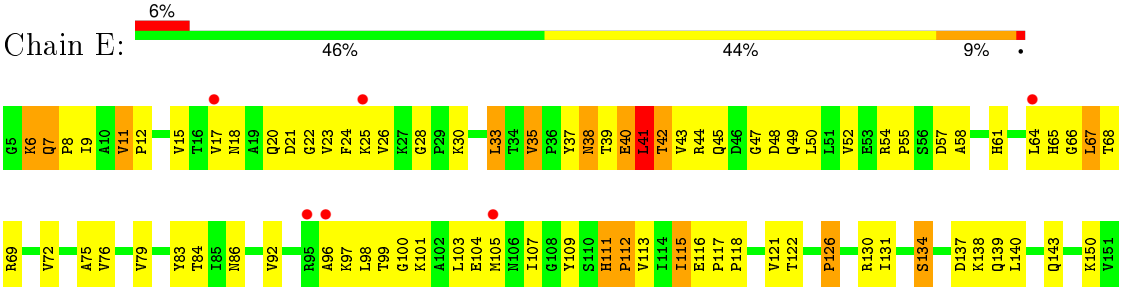
• Molecule 5: 50S ribosomal protein L5

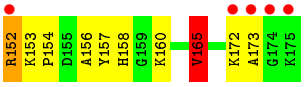
Chain D:



• Molecule 6: 50S ribosomal protein L6

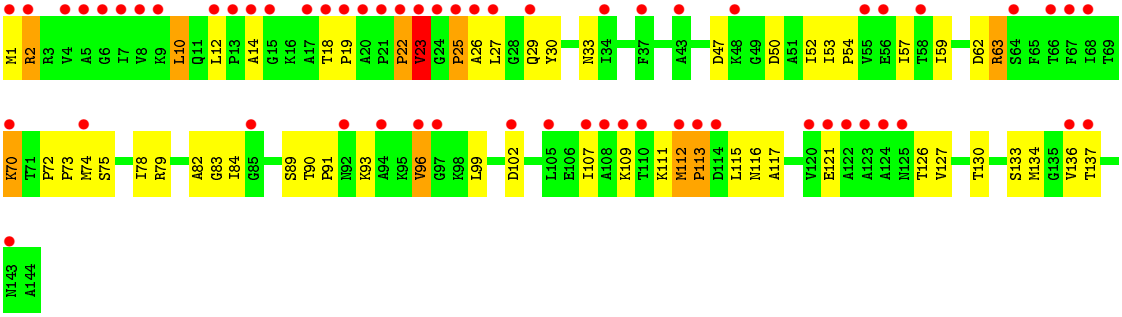
Chain E:





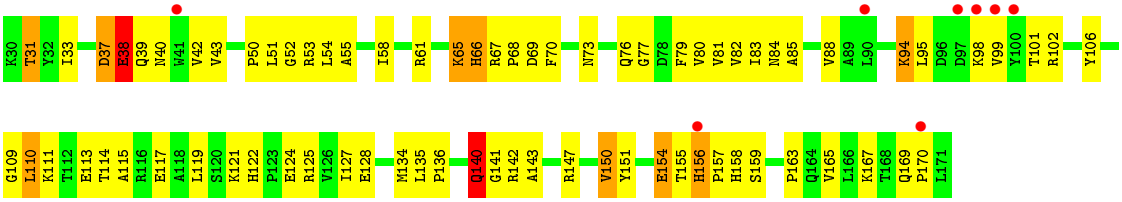
• Molecule 7: 50S ribosomal protein L11

Chain F:



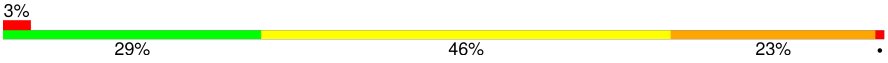
• Molecule 8: 50S ribosomal protein L13

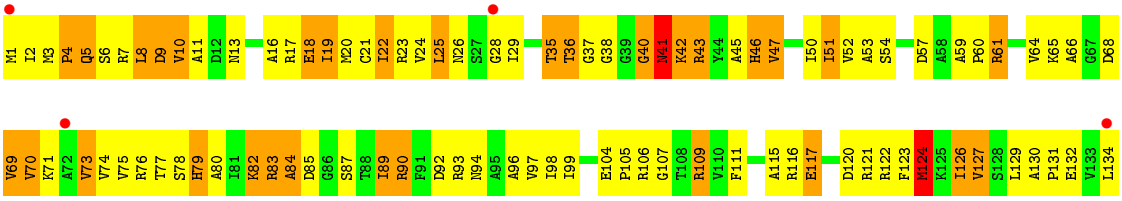
Chain G:



• Molecule 9: 50S ribosomal protein L14

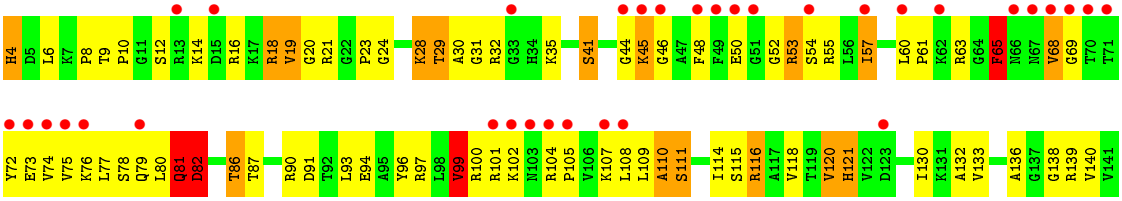
Chain H:





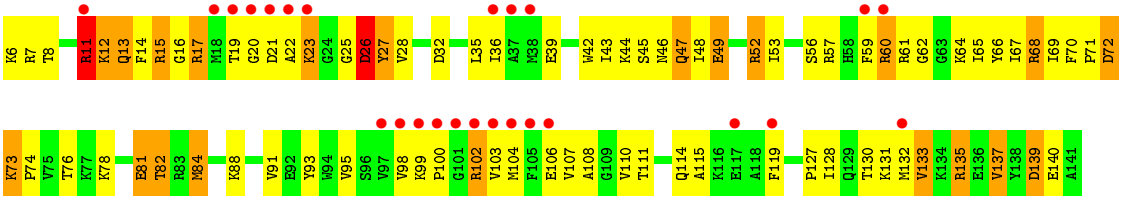
• Molecule 10: 50S ribosomal protein L15

Chain I:



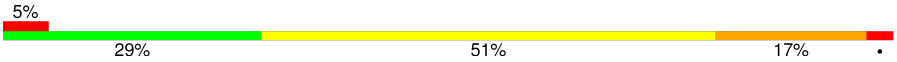
- Molecule 11: 50S ribosomal protein L16

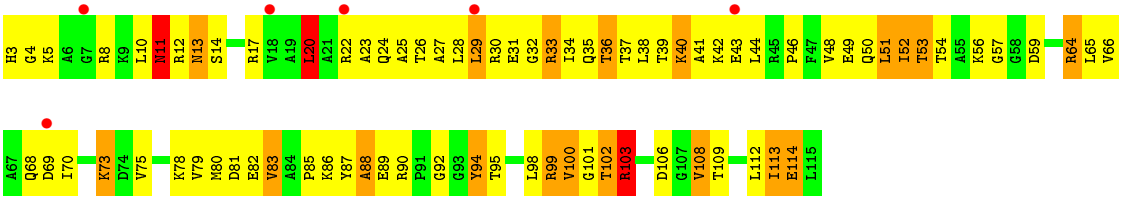
Chain J:



- Molecule 12: 50S ribosomal protein L17

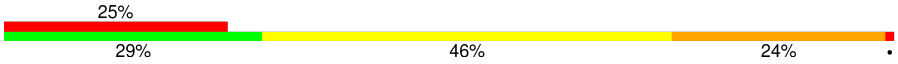
Chain K:

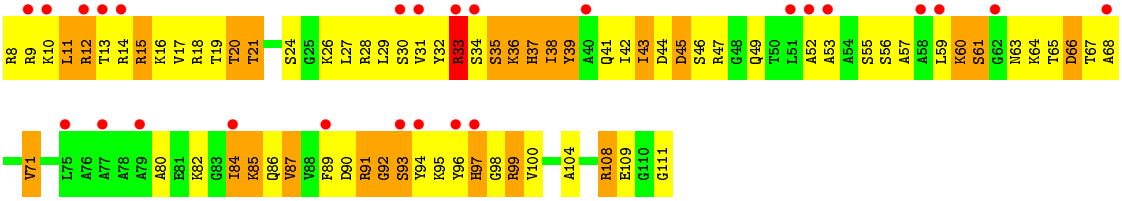




- Molecule 13: 50S ribosomal protein L18

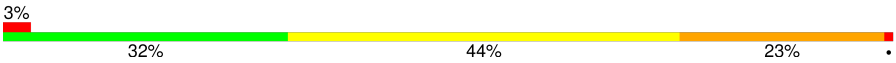
Chain L:

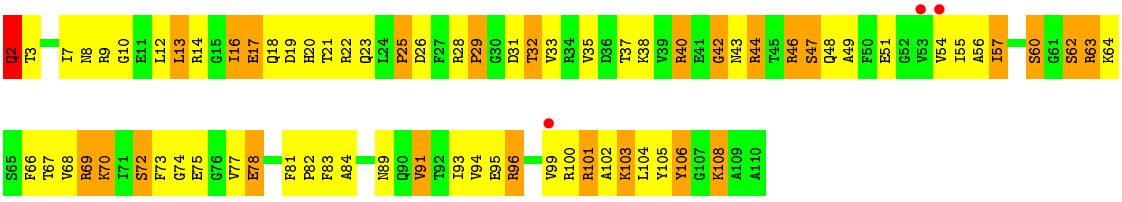




- Molecule 14: 50S ribosomal protein L19

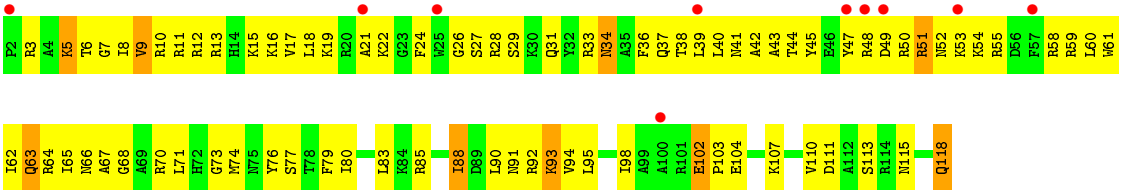
Chain M:





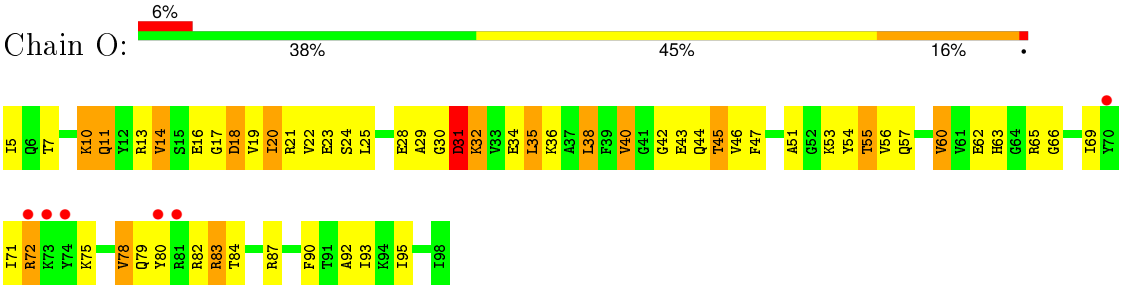
- Molecule 15: 50S ribosomal protein L20

Chain N:



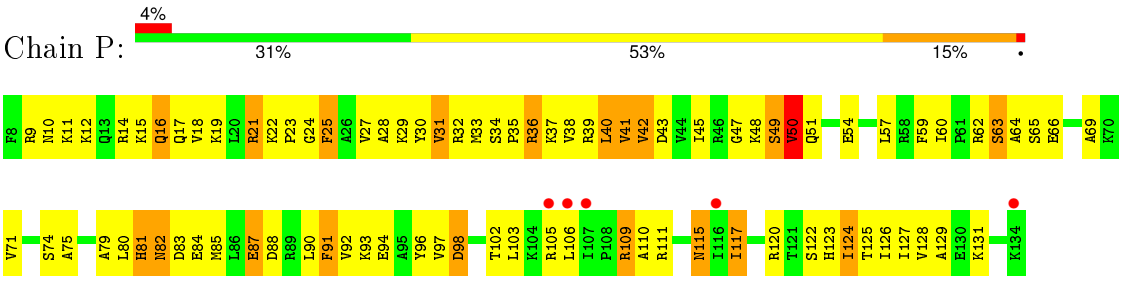
• Molecule 16: 50S ribosomal protein L21

Chain O:



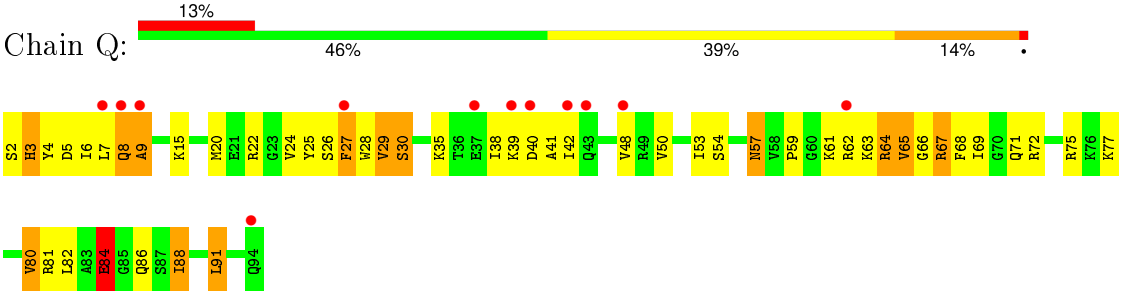
• Molecule 17: 50S ribosomal protein L22

Chain P:



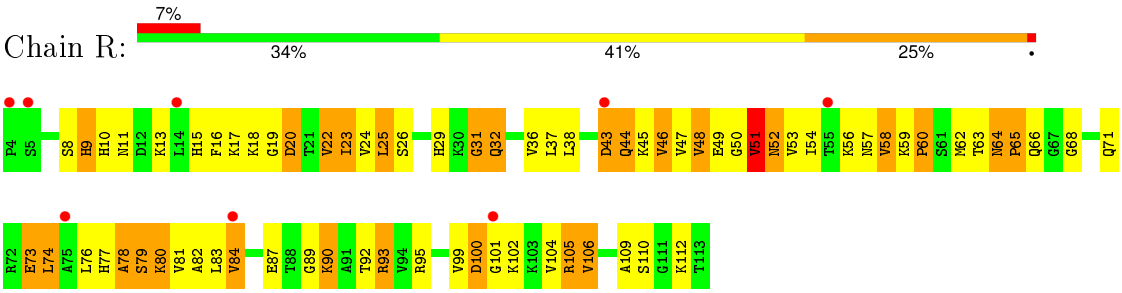
• Molecule 18: 50S ribosomal protein L23

Chain Q:



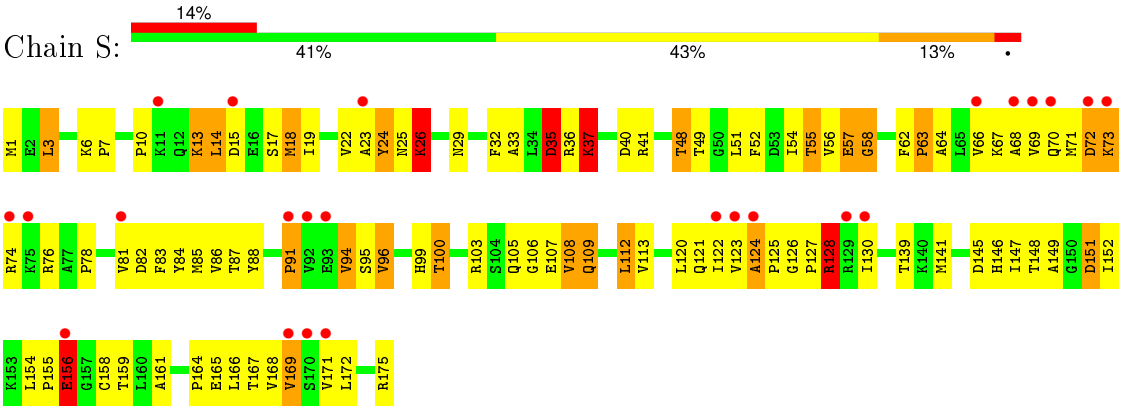
• Molecule 19: 50S ribosomal protein L24

Chain R:



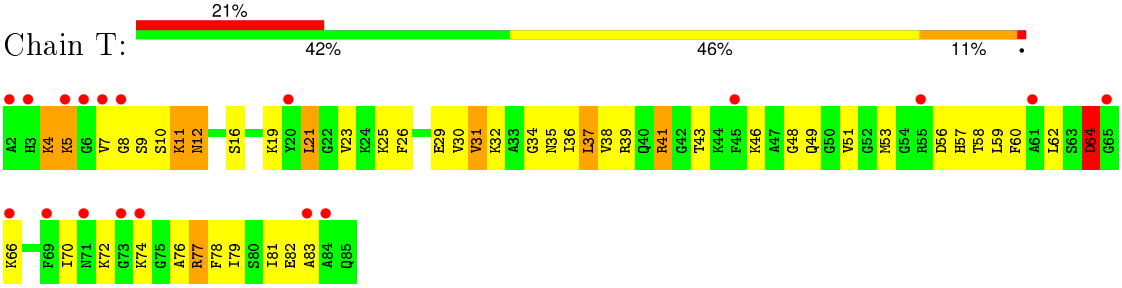
• Molecule 20: 50S ribosomal protein L25

Chain S:



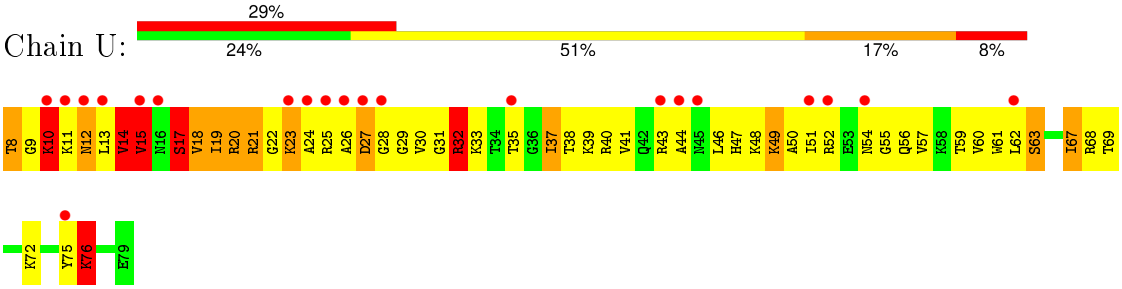
- Molecule 21: 50S ribosomal protein L27

Chain T:



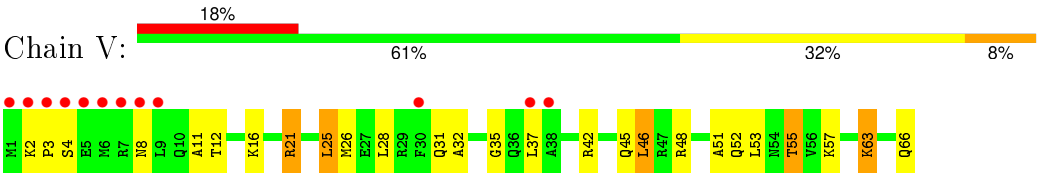
- Molecule 22: 50S ribosomal protein L28

Chain U:



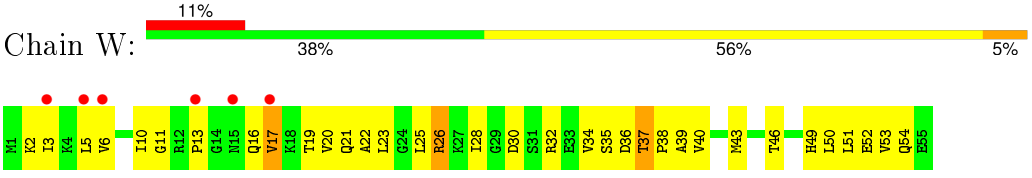
- Molecule 23: 50S ribosomal protein L29

Chain V:



- Molecule 24: 50S ribosomal protein L30

Chain W:

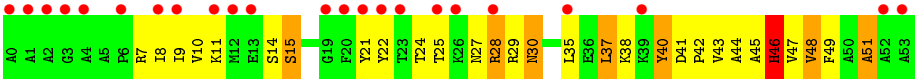


- Molecule 25: 50S ribosomal protein L32

Chain Z:

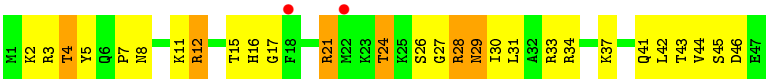
• Molecule 26: 50S ribosomal protein L33

Chain 1:



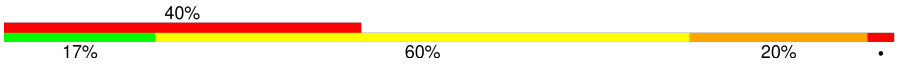
• Molecule 27: 50S ribosomal protein L34

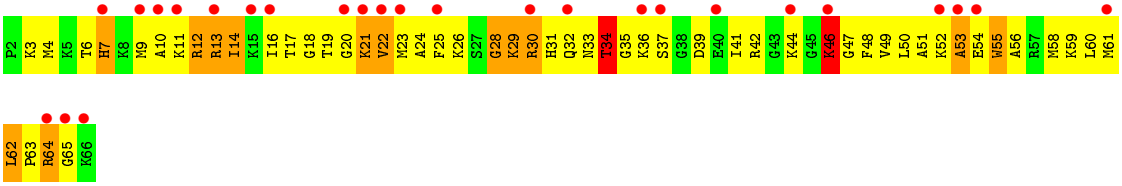
Chain 2:



• Molecule 28: 50S ribosomal protein L35

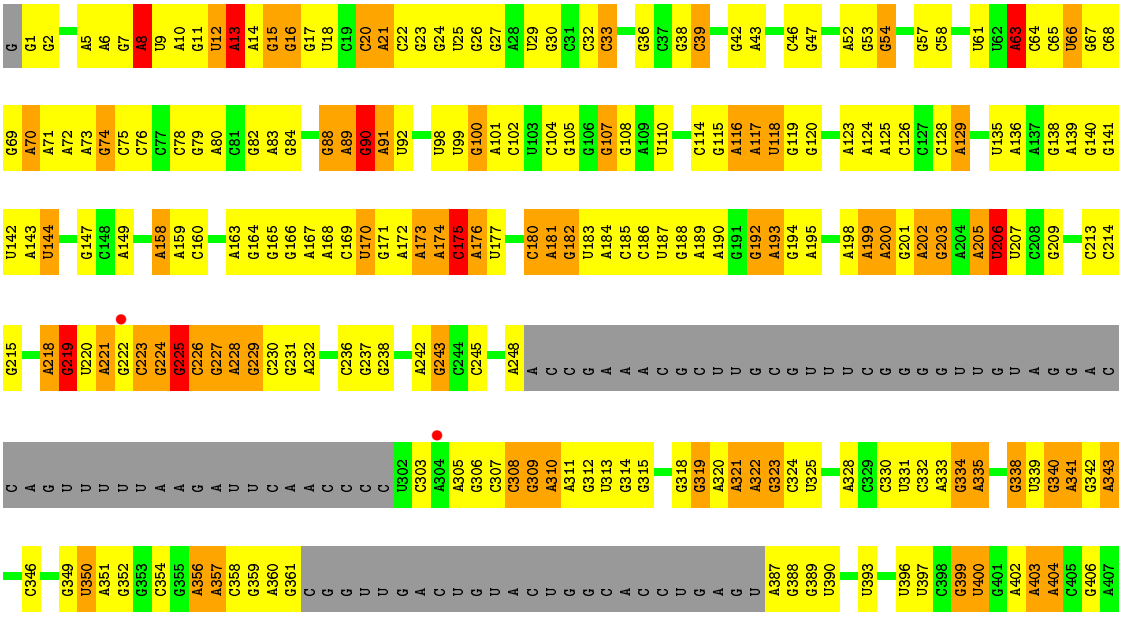
Chain 3:

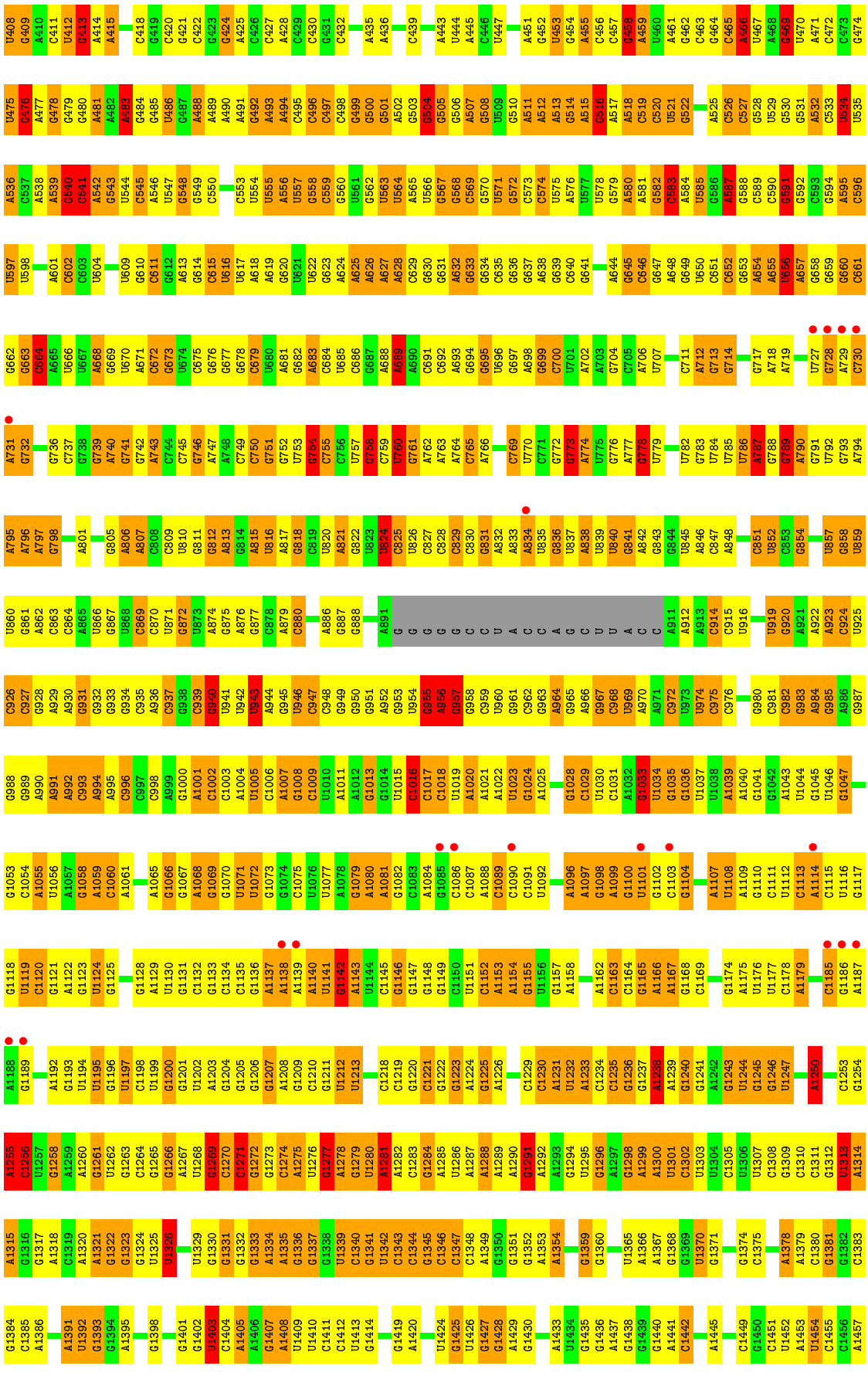


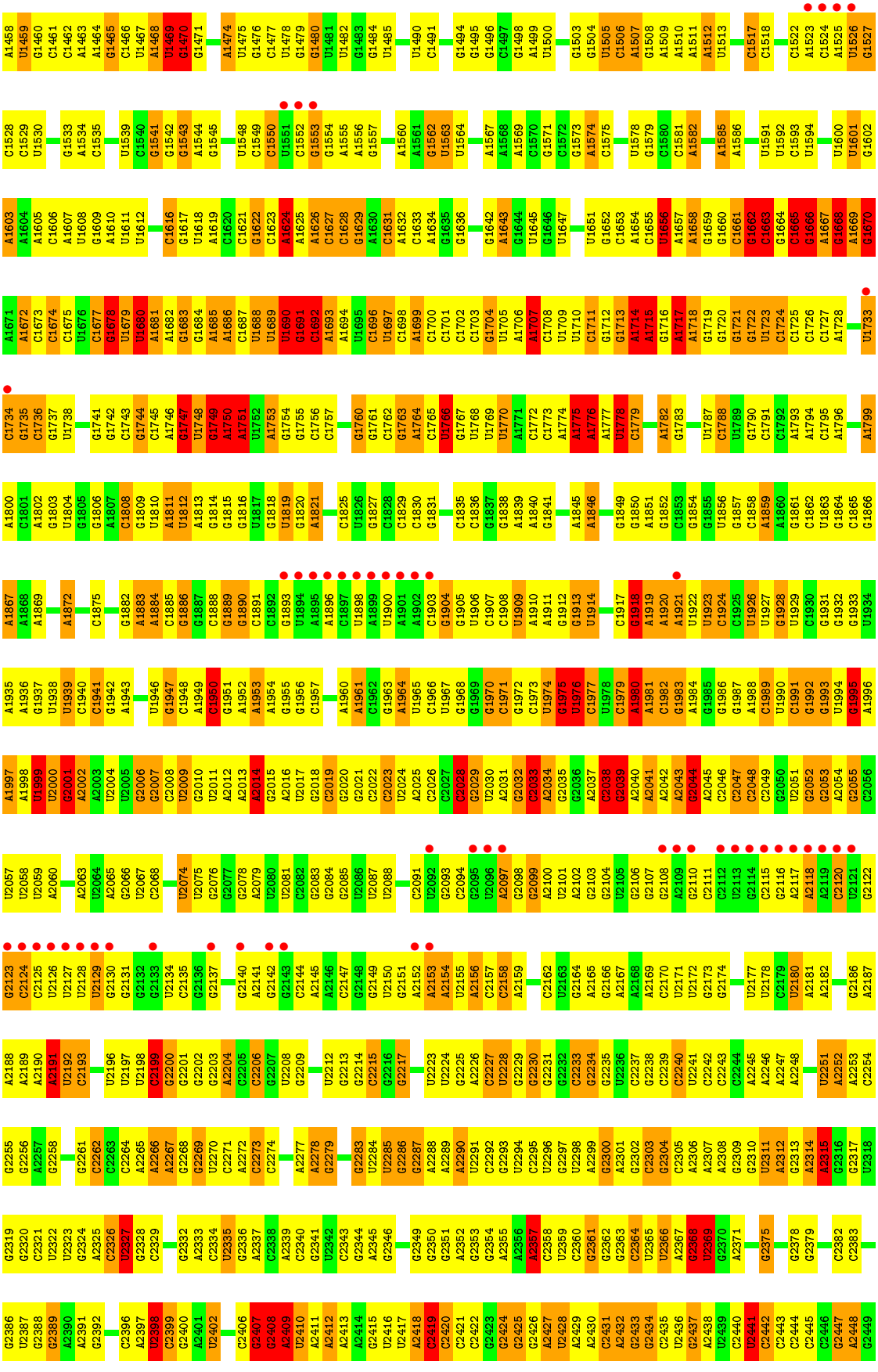


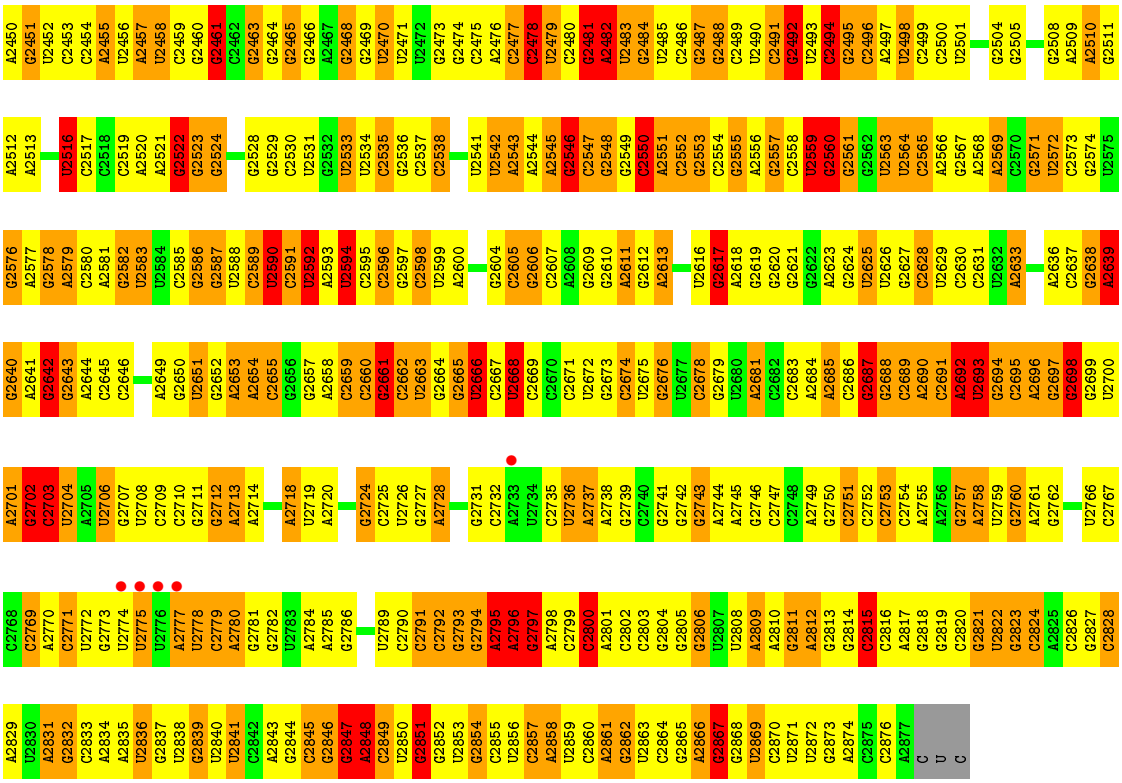
• Molecule 29: 23S ribosomal RNA

Chain X:

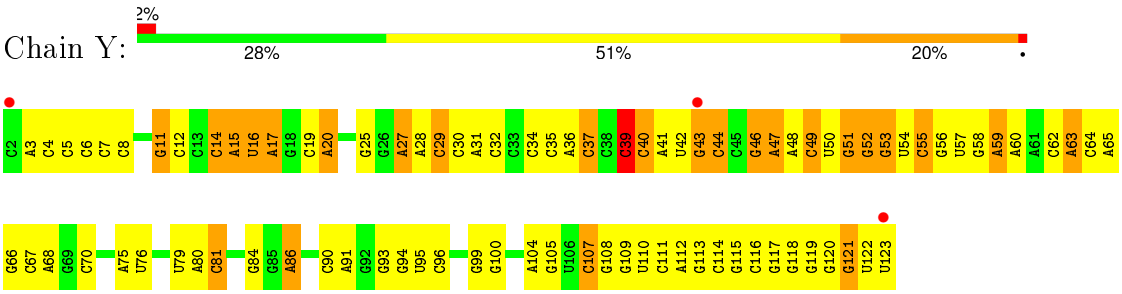





A1458 U1459 G1460 C1461 C1462 A1463 A1464 G1465 C1466 U1467 A1468 U1469 G1470 G1471 A1474 U1475 G1476 C1477 U1478 G1479 G1480 U1481 U1482 G1483 G1484 U1485 U1490 C1491 G1494 G1495 G1496 C1497 G1498 A1499 U1500 G1503 G1504 U1505 C1506 A1507 G1508 A1509 A1510 A1511 A1512 U1513 C1517 C1518 C1522 A1523 C1524 A1525 U1526 G1527
C1528 C1529 U1530 G1533 A1534 C1535 U1539 C1540 G1541 G1542 G1543 A1544 G1545 U1548 C1549 C1550 U1551 C1552 G1553 G1554 A1555 A1556 G1557 A1560 A1561 G1562 U1563 U1564 A1567 A1568 A1569 C1570 G1571 G1572 G1573 A1574 C1575 U1578 G1579 C1580 C1581 A1582 A1585 A1586 U1591 U1592 C1593 U1594 U1600 U1601 G1602
A1603 A1604 A1605 C1606 A1607 U1608 G1609 A1610 U1611 U1612 C1616 G1617 U1618 A1619 C1620 C1621 G1622 C1623 A1624 A1625 A1626 C1627 C1628 A1629 A1630 C1631 A1632 C1633 A1634 G1635 G1636 G1642 A1643 G1644 U1645 G1646 U1647 U1651 G1652 C1653 A1654 C1655 U1656 A1657 A1658 G1659 G1660 C1661 G1662 C1663 G1664 C1665 G1666 A1667 G1668 A1669 G1670
A1671 A1672 C1673 C1674 C1675 U1676 C1677 G1678 U1679 U1680 A1681 A1682 G1683 G1684 A1685 A1686 C1687 U1688 U1689 U1690 G1691 C1692 A1693 A1694 U1695 C1696 U1697 C1698 A1699 C1700 C1701 C1702 C1703 G1704 U1705 A1706 A1707 C1708 U1709 U1710 C1711 G1712 G1713 A1714 A1715 G1716 A1717 A1718 G1719 G1720 G1721 G1722 U1723 C1724 C1725 C1726 C1727 A1728 U1733
C1734 G1735 C1736 G1737 U1738 G1741 G1742 C1743 G1744 C1745 A1746 G1747 U1748 G1749 A1750 A1751 U1752 A1753 G1754 G1755 C1756 C1757 G1760 C1761 C1762 G1763 A1764 C1765 U1766 G1767 U1768 U1769 U1770 A1771 C1772 C1773 A1774 A1775 A1776 A1777 U1778 C1779 A1782 G1783 U1787 C1788 U1789 G1790 C1791 C1792 A1793 A1794 C1795 A1796 A1799
A1800 C1801 A1802 G1803 U1804 G1805 G1806 A1807 C1808 G1809 U1810 A1811 U1812 A1813 G1814 G1815 G1816 U1817 U1818 U1819 G1820 A1821 C1825 U1826 G1827 C1828 C1829 C1830 G1831 C1835 C1836 G1837 G1838 A1839 A1840 G1841 A1845 A1846 G1849 G1850 A1851 G1852 C1853 G1854 G1855 U1856 G1857 C1858 A1859 A1860 G1861 C1862 U1863 G1864 C1865 G1866
A1867 A1868 A1869 A1872 C1875 G1882 A1883 A1884 C1885 G1886 G1887 C1888 G1889 G1890 C1891 C1892 G1893 U1894 A1895 A1896 C1897 U1898 A1899 U1900 A1901 A1902 C1903 G1904 G1905 U1906 C1907 C1908 U1909 A1910 A1911 G1912 G1913 U1914 C1917 G1918 A1919 A1920 A1921 U1922 U1923 C1924 C1925 U1926 U1927 G1928 U1929 C1930 G1931 G1932 G1933 U1934
A1935 A1936 G1937 U1938 U1939 C1940 C1941 G1942 A1943 U1946 G1947 C1948 A1949 C1950 G1951 A1952 A1953 A1954 G1955 G1956 C1957 A1960 A1961 C1962 G1963 A1964 U1965 C1966 U1967 G1968 G1969 G1970 C1971 G1972 C1973 U1974 G1975 U1976 C1977 U1978 C1979 A1980 A1981 C1982 G1983 A1984 G1985 G1986 G1987 A1988 C1989 U1990 C1991 G1992 G1993 U1994 G1995 A1996
A1997 A1998 U1999 U2000 G2001 A2002 A2003 U2004 U2005 G2006 G2007 C2008 U2009 G2010 U2011 A2012 A2013 A2014 G2015 A2016 U2017 G2018 C2019 G2020 G2021 C2022 C2023 U2024 A2025 C2026 C2027 C2028 G2029 U2030 A2031 G2032 C2033 A2034 G2035 G2036 A2037 C2038 G2039 A2040 A2041 A2042 A2043 G2044 A2045 C2046 C2047 C2048 C2049 G2050 U2051 G2052 G2053 A2054 G2055 C2056
U2057 U2058 U2059 A2060 A2063 U2064 A2065 G2066 U2067 C2068 U2074 U2075 G2076 G2077 G2078 A2079 U2080 U2081 C2082 G2083 G2084 C2085 U2086 U2087 U2088 C2091 U2092 G2093 C2094 G2095 U2096 A2097 G2098 G2099 A2100 U2101 A2102 G2103 G2104 U2105 G2106 G2107 G2108 A2109 G2110 C2111 C2112 U2113 G2114 C2115 C2116 A2117 A2118 A2119 C2120 U2121 G2122
G2123 C2124 C2125 U2126 U2127 U2128 U2129 G2130 G2131 G2132 G2133 U2134 C2135 G2136 G2137 G2140 A2141 G2142 G2143 C2144 A2145 A2146 C2147 G2148 G2149 U2150 G2151 A2152 A2153 A2154 U2155 A2156 C2157 C2158 A2159 C2162 U2163 G2164 A2165 G2166 A2167 A2168 A2169 C2170 U2171 U2172 G2173 G2174 U2177 U2178 C2179 U2180 A2181 A2182 G2186 A2187
A2188 A2189 A2190 A2191 U2192 C2193 U2196 U2197 U2198 C2199 G2200 G2201 G2202 G2203 A2204 C2205 C2206 G2207 U2208 G2209 U2212 G2213 G2214 C2215 G2216 G2217 U2223 U2224 G2225 A2226 C2227 C2228 G2229 G2230 G2231 G2232 C2233 G2234 G2235 U2236 C2237 G2238 C2239 C2240 U2241 C2242 C2243 C2244 A2245 A2246 A2247 A2248 U2251 A2252 A2253 C2254
G2255 G2256 A2257 G2258 G2261 C2262 C2263 C2264 A2265 A2266 A2267 G2268 G2269 U2270 C2271 A2272 C2273 C2274 A2277 A2278 G2279 G2283 U2284 U2285 G2286 G2287 A2288 A2289 A2290 U2291 C2292 G2293 U2294 C2295 U2296 G2297 U2298 A2299 G2300 A2301 G2302 C2303 G2304 C2305 A2306 A2307 A2308 G2309 G2310 U2311 A2312 G2313 A2314 A2315 G2316 G2317 U2318
G2319 G2320 C2321 U2322 U2323 G2324 A2325 C2326 U2327 G2328 C2329 G2332 A2333 C2334 U2335 G2336 A2337 C2338 A2339 C2340 G2341 U2342 C2343 G2344 A2345 G2346 G2349 G2350 G2351 A2352 G2353 G2354 A2355 A2356 A2357 C2358 U2359 C2360 G2361 G2362 G2363 C2364 U2365 U2366 A2367 G2368 U2369 G2370 A2371 G2375 G2378 G2379 C2382 C2383
G2386 U2387 G2388 G2389 A2390 A2391 G2392 C2396 A2397 U2398 C2399 G2400 A2401 U2402 C2406 G2407 G2408 A2409 U2410 A2411 A2412 A2413 A2414 G2415 U2416 U2417 A2418 G2419 C2420 C2421 C2422 G2423 G2424 G2425 G2426 A2427 U2428 A2429 A2430 C2431 A2432 G2433 G2434 C2435 U2436 G2437 A2438 U2439 C2440 U2441 C2442 C2443 C2444 C2445 G2446 G2447 A2448 G2449



- Molecule 30: 5S ribosomal RNA



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	169.82Å 411.54Å 695.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.02 – 3.00 59.03 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.9 (57.02-3.00) 76.2 (59.03-3.00)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.32 (at 3.01Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.284 , 0.326 0.291 , 0.335	Depositor DCC
R_{free} test set	22814 reflections (6.53%)	DCC
Wilson B-factor (Å^2)	66.7	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.16 , 40.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Outliers	6 of 478148 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	89361	wwPDB-VP
Average B, all atoms (Å^2)	142.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, HGR

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	0	0.25	0/1674	0.46	0/2257
2	A	0.40	0/2149	0.62	0/2890
3	B	0.66	0/1568	0.92	2/2105 (0.1%)
4	C	0.50	0/1530	0.75	0/2070
5	D	0.36	0/1420	0.59	0/1903
6	E	0.39	0/1309	0.61	0/1771
7	F	0.30	0/1067	0.55	0/1446
8	G	0.47	0/1139	0.74	0/1539
9	H	0.72	0/1007	1.02	1/1352 (0.1%)
10	I	0.49	0/1082	0.78	0/1448
11	J	0.60	0/1114	0.83	1/1486 (0.1%)
12	K	0.81	0/887	1.11	4/1188 (0.3%)
13	L	0.54	0/784	0.79	1/1045 (0.1%)
14	M	0.76	0/880	1.02	3/1179 (0.3%)
15	N	0.65	0/994	0.77	0/1323
16	O	0.54	0/751	0.75	0/1000
17	P	0.75	0/1027	0.93	0/1373
18	Q	0.46	0/738	0.63	0/988
19	R	0.58	0/836	0.87	0/1121
20	S	0.40	0/1371	0.68	0/1862
21	T	0.52	0/634	0.70	0/838
22	U	0.52	0/557	0.88	1/741 (0.1%)
23	V	0.40	0/538	0.58	0/714
24	W	0.51	0/426	0.74	0/568
25	Z	0.67	0/465	0.99	1/622 (0.2%)
26	1	0.47	0/411	0.68	0/554
27	2	0.47	0/397	0.70	0/521
28	3	0.56	0/516	0.75	0/673
29	X	0.79	28/66826 (0.0%)	1.38	1078/104247 (1.0%)
30	Y	0.61	0/2907	1.12	10/4529 (0.2%)
All	All	0.73	28/97004 (0.0%)	1.25	1102/145353 (0.8%)

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
3	B	0	1
9	H	0	1
10	I	0	1
13	L	0	1
14	M	0	2
19	R	0	1
All	All	0	7

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	X	774	A	N3-C4	7.61	1.39	1.34
29	X	774	A	C5-C4	7.18	1.43	1.38
29	X	1682	A	N7-C5	-6.86	1.35	1.39
29	X	1975	G	N7-C5	6.29	1.43	1.39
29	X	2823	G	N9-C8	-6.08	1.33	1.37
29	X	2409	A	N9-C4	5.99	1.41	1.37
29	X	1750	A	N3-C4	-5.93	1.31	1.34
29	X	1686	A	N3-C4	-5.84	1.31	1.34
29	X	1680	U	N1-C2	5.74	1.43	1.38
29	X	2611	A	N9-C4	-5.67	1.34	1.37
29	X	1680	U	C2-N3	5.62	1.41	1.37
29	X	2618	A	N9-C4	5.59	1.41	1.37
29	X	2795	A	N9-C4	5.46	1.41	1.37
29	X	513	A	N3-C4	-5.40	1.31	1.34
29	X	2488	G	C6-N1	-5.35	1.35	1.39
29	X	1681	A	C5-C6	-5.34	1.36	1.41
29	X	1680	U	C2-O2	5.33	1.27	1.22
29	X	1278	A	N7-C5	-5.29	1.36	1.39
29	X	2398	U	C2-N3	5.25	1.41	1.37
29	X	540	G	C5-C4	5.22	1.42	1.38
29	X	2548	G	C6-O6	5.20	1.28	1.24
29	X	2489	C	C4-C5	-5.19	1.38	1.43
29	X	774	A	C6-N1	5.08	1.39	1.35
29	X	1692	C	N1-C6	-5.07	1.34	1.37
29	X	527	C	N1-C2	5.06	1.45	1.40
29	X	1678	G	N7-C5	5.05	1.42	1.39
29	X	1975	G	N9-C4	-5.03	1.33	1.38
29	X	2797	G	N1-C2	-5.02	1.33	1.37

All (1102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	X	1678	G	C8-N9-C4	14.96	112.38	106.40
29	X	1292	A	C8-N9-C4	14.80	111.72	105.80
29	X	774	A	N1-C6-N6	13.97	126.98	118.60
29	X	1679	U	C5-C6-N1	-13.00	116.20	122.70
29	X	1678	G	N7-C8-N9	-12.95	106.62	113.10
29	X	1724	C	C6-N1-C2	12.83	125.43	120.30
29	X	1681	A	N1-C6-N6	12.46	126.08	118.60
29	X	2704	U	N1-C2-O2	-12.39	114.12	122.80
29	X	497	C	N1-C2-O2	-11.87	111.78	118.90
29	X	2548	G	C5-C6-N1	-11.76	105.62	111.50
29	X	1679	U	C2-N3-C4	-11.74	119.95	127.00
29	X	1647	U	N3-C4-C5	-11.63	107.62	114.60
29	X	527	C	C6-N1-C2	-11.22	115.81	120.30
29	X	774	A	C5-N7-C8	-10.93	98.43	103.90
29	X	1992	G	C8-N9-C4	10.93	110.77	106.40
29	X	2019	C	C6-N1-C2	-10.90	115.94	120.30
29	X	522	G	N1-C6-O6	10.89	126.43	119.90
29	X	2550	C	C6-N1-C2	-10.87	115.95	120.30
29	X	1973	C	C6-N1-C2	-10.77	115.99	120.30
29	X	774	A	N7-C8-N9	10.66	119.13	113.80
29	X	2857	C	C6-N1-C2	-10.49	116.11	120.30
29	X	774	A	C4-C5-N7	10.39	115.90	110.70
29	X	1702	C	C6-N1-C2	10.38	124.45	120.30
29	X	661	C	C6-N1-C2	-9.98	116.31	120.30
29	X	1647	U	C6-N1-C2	-9.93	115.05	121.00
29	X	563	U	C6-N1-C2	9.90	126.94	121.00
29	X	1670	G	C8-N9-C4	9.90	110.36	106.40
29	X	2845	C	C6-N1-C2	-9.87	116.35	120.30
29	X	1681	A	C5-C6-N6	-9.84	115.83	123.70
29	X	2624	G	C8-N9-C4	-9.75	102.50	106.40
29	X	957	G	N1-C6-O6	-9.67	114.10	119.90
29	X	1289	A	C8-N9-C4	9.50	109.60	105.80
29	X	2815	C	C6-N1-C2	9.50	124.10	120.30
29	X	2854	G	C4-C5-N7	9.42	114.57	110.80
29	X	1336	G	C5-C6-O6	-9.36	122.98	128.60
29	X	1681	A	N9-C4-C5	-9.34	102.06	105.80
29	X	2523	G	C8-N9-C4	-9.33	102.67	106.40
29	X	1999	U	C2-N1-C1'	9.31	128.87	117.70
29	X	2523	G	C6-C5-N7	-9.28	124.83	130.40
29	X	1678	G	C5-N7-C8	9.26	108.93	104.30
29	X	2541	U	N3-C2-O2	-9.21	115.75	122.20
29	X	2867	G	N3-C4-C5	9.19	133.19	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	X	1682	A	C8-N9-C4	-9.14	102.14	105.80
29	X	2655	C	C6-N1-C2	9.13	123.95	120.30
29	X	955	G	C6-C5-N7	-9.12	124.92	130.40
29	X	2049	C	C6-N1-C2	-9.09	116.66	120.30
29	X	2369	U	C5-C6-N1	9.08	127.24	122.70
29	X	1313	U	C2-N1-C1'	-9.01	106.89	117.70
29	X	1681	A	C6-C5-N7	-9.01	126.00	132.30
29	X	1775	A	C8-N9-C4	9.00	109.40	105.80
29	X	2478	C	C6-N1-C2	-8.98	116.71	120.30
29	X	2594	U	N1-C2-N3	-8.97	109.52	114.90
29	X	2822	U	N3-C4-O4	8.97	125.68	119.40
29	X	1756	C	C6-N1-C2	8.94	123.87	120.30
29	X	2662	C	C6-N1-C2	-8.93	116.73	120.30
29	X	774	A	C6-C5-N7	-8.93	126.05	132.30
29	X	1163	C	C6-N1-C2	-8.90	116.74	120.30
29	X	2554	C	C6-N1-C2	-8.90	116.74	120.30
29	X	2038	C	C6-N1-C2	-8.86	116.76	120.30
29	X	2590	U	C2-N1-C1'	8.82	128.28	117.70
29	X	1933	G	C8-N9-C4	-8.81	102.87	106.40
29	X	1715	A	N1-C6-N6	8.78	123.87	118.60
29	X	1335	A	C8-N9-C4	8.74	109.30	105.80
29	X	497	C	N3-C2-O2	8.73	128.01	121.90
29	X	1992	G	N7-C8-N9	-8.73	108.74	113.10
29	X	579	G	C8-N9-C4	-8.71	102.92	106.40
29	X	1244	U	C5-C6-N1	8.67	127.04	122.70
29	X	2695	C	C6-N1-C2	-8.66	116.83	120.30
29	X	2522	G	N3-C4-C5	-8.65	124.27	128.60
29	X	2576	G	N1-C6-O6	8.65	125.09	119.90
29	X	1339	U	N3-C4-O4	8.64	125.45	119.40
29	X	2523	G	N7-C8-N9	8.61	117.41	113.10
29	X	1155	G	C8-N9-C4	8.57	109.83	106.40
29	X	1336	G	C4-C5-N7	8.56	114.22	110.80
29	X	1292	A	N7-C8-N9	-8.53	109.53	113.80
29	X	2433	G	N1-C6-O6	-8.53	114.78	119.90
29	X	1725	C	C6-N1-C2	-8.53	116.89	120.30
29	X	563	U	C5-C6-N1	-8.53	118.44	122.70
29	X	754	G	C4-C5-N7	8.51	114.20	110.80
29	X	1678	G	C4-C5-N7	-8.51	107.40	110.80
29	X	2596	C	C6-N1-C2	8.51	123.70	120.30
29	X	2495	G	N3-C4-C5	-8.49	124.35	128.60
29	X	1975	G	N3-C4-N9	-8.49	120.91	126.00
29	X	2523	G	N3-C4-C5	-8.49	124.36	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	X	1681	A	C4-C5-N7	8.47	114.94	110.70
29	X	1973	C	C5-C6-N1	8.45	125.22	121.00
29	X	527	C	N3-C2-O2	-8.43	116.00	121.90
29	X	1679	U	N1-C2-N3	8.43	119.96	114.90
29	X	1678	G	C6-C5-N7	8.41	135.44	130.40
29	X	1339	U	C5-C6-N1	8.40	126.90	122.70
29	X	206	U	N1-C2-O2	8.39	128.68	122.80
29	X	1634	A	N1-C6-N6	-8.39	113.56	118.60
29	X	1340	C	C6-N1-C2	-8.36	116.96	120.30
29	X	1704	G	C4-C5-N7	8.35	114.14	110.80
29	X	496	C	C6-N1-C2	8.34	123.63	120.30
29	X	2033	C	N3-C2-O2	-8.31	116.08	121.90
29	X	2240	C	C6-N1-C2	-8.28	116.99	120.30
30	Y	32	C	C6-N1-C2	-8.23	117.01	120.30
29	X	1244	U	C6-N1-C2	-8.20	116.08	121.00
30	Y	81	C	C6-N1-C2	-8.16	117.04	120.30
29	X	16	G	C8-N9-C4	8.15	109.66	106.40
29	X	1751	A	C8-N9-C4	8.11	109.05	105.80
29	X	2718	A	C8-N9-C4	8.11	109.05	105.80
29	X	540	G	C5-C6-N1	-8.11	107.45	111.50
29	X	1339	U	C5-C4-O4	-8.11	121.04	125.90
29	X	2038	C	C5-C6-N1	8.09	125.04	121.00
29	X	1679	U	N3-C4-O4	-8.07	113.75	119.40
29	X	2867	G	N3-C4-N9	-8.06	121.16	126.00
29	X	1312	G	N1-C6-O6	8.03	124.72	119.90
29	X	1683	G	N1-C6-O6	-8.01	115.09	119.90
29	X	1749	G	C8-N9-C4	-7.99	103.20	106.40
29	X	955	G	N7-C8-N9	7.99	117.09	113.10
14	M	3	THR	N-CA-C	-7.94	89.56	111.00
29	X	1636	G	N1-C6-O6	7.94	124.66	119.90
29	X	1333	G	C8-N9-C4	-7.93	103.23	106.40
29	X	1961	A	C8-N9-C4	-7.88	102.65	105.80
29	X	1975	G	N1-C6-O6	-7.84	115.19	119.90
29	X	1313	U	C5-C6-N1	-7.83	118.78	122.70
29	X	1001	A	C8-N9-C4	-7.83	102.67	105.80
29	X	1652	G	C4-C5-N7	7.83	113.93	110.80
29	X	2747	C	C6-N1-C2	7.81	123.42	120.30
29	X	1238	A	N1-C6-N6	-7.80	113.92	118.60
29	X	1696	C	N3-C4-C5	-7.79	118.78	121.90
29	X	1775	A	N9-C4-C5	-7.79	102.69	105.80
29	X	472	C	C6-N1-C2	-7.78	117.19	120.30
29	X	1305	C	C6-N1-C2	7.77	123.41	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	X	2624	G	N7-C8-N9	7.77	116.98	113.10
29	X	2862	G	N3-C4-C5	-7.77	124.72	128.60
29	X	806	A	C8-N9-C4	7.77	108.91	105.80
29	X	522	G	C6-C5-N7	-7.76	125.74	130.40
29	X	2661	G	C5-C6-O6	-7.75	123.95	128.60
29	X	2698	G	N1-C6-O6	7.74	124.54	119.90
29	X	1704	G	C5-C6-O6	-7.74	123.96	128.60
29	X	1974	U	C6-N1-C2	-7.71	116.37	121.00
9	H	25	LEU	CA-CB-CG	7.70	133.00	115.30
29	X	206	U	C2-N1-C1'	7.70	126.94	117.70
29	X	522	G	C4-C5-N7	7.70	113.88	110.80
29	X	2433	G	C5-C6-O6	7.69	133.21	128.60
29	X	175	C	C2-N1-C1'	7.68	127.25	118.80
29	X	1677	C	N3-C2-O2	-7.66	116.54	121.90
29	X	574	C	C5-C6-N1	7.66	124.83	121.00
29	X	2009	U	C5-C6-N1	7.65	126.52	122.70
12	K	103	ARG	NE-CZ-NH2	-7.62	116.49	120.30
29	X	2704	U	N1-C2-N3	7.62	119.47	114.90
29	X	2369	U	C6-N1-C2	-7.61	116.43	121.00
29	X	2693	U	N3-C2-O2	-7.61	116.87	122.20
29	X	2797	G	N3-C4-N9	7.59	130.55	126.00
29	X	990	A	N1-C6-N6	-7.59	114.05	118.60
29	X	1770	U	C5-C6-N1	-7.58	118.91	122.70
29	X	2495	G	C2-N3-C4	7.55	115.68	111.90
29	X	2854	G	C6-C5-N7	-7.55	125.87	130.40
29	X	955	G	C4-C5-N7	7.54	113.82	110.80
29	X	1480	G	N1-C6-O6	7.54	124.42	119.90
29	X	660	G	N3-C4-N9	-7.54	121.48	126.00
29	X	2839	G	N1-C6-O6	-7.53	115.38	119.90
29	X	2854	G	C5-N7-C8	-7.51	100.54	104.30
29	X	1292	A	N9-C4-C5	-7.51	102.80	105.80
29	X	2799	C	C6-N1-C2	-7.50	117.30	120.30
29	X	1269	G	N1-C6-O6	7.50	124.40	119.90
29	X	1715	A	C5-C6-N6	-7.50	117.70	123.70
29	X	1721	G	C4-N9-C1'	-7.48	116.78	126.50
30	Y	39	C	C2-N1-C1'	7.48	127.03	118.80
29	X	1269	G	C5-C6-O6	-7.47	124.12	128.60
29	X	2623	A	C8-N9-C4	7.44	108.77	105.80
29	X	2815	C	C5-C6-N1	-7.43	117.28	121.00
29	X	774	A	N9-C4-C5	-7.43	102.83	105.80
29	X	1277	G	N1-C6-O6	-7.42	115.44	119.90
29	X	1663	C	C5-C6-N1	7.42	124.71	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	X	2845	C	C5-C6-N1	7.42	124.71	121.00
29	X	527	C	N1-C2-O2	7.39	123.33	118.90
29	X	2522	G	C8-N9-C4	-7.39	103.44	106.40
29	X	501	G	C5-C6-O6	7.37	133.02	128.60
29	X	1963	G	C8-N9-C4	-7.37	103.45	106.40
29	X	1977	C	N3-C4-C5	7.35	124.84	121.90
29	X	1760	G	N7-C8-N9	7.35	116.77	113.10
29	X	2700	U	N3-C2-O2	-7.34	117.06	122.20
29	X	2668	U	C6-N1-C2	7.34	125.41	121.00
29	X	2854	G	C5-C6-O6	-7.34	124.20	128.60
29	X	1776	A	C8-N9-C4	-7.33	102.87	105.80
29	X	2659	C	N3-C4-C5	-7.33	118.97	121.90
29	X	1269	G	C4-C5-N7	7.32	113.73	110.80
29	X	955	G	N1-C6-O6	7.31	124.29	119.90
29	X	1933	G	C2-N3-C4	7.31	115.55	111.90
29	X	1345	G	C4-N9-C1'	7.30	136.00	126.50
29	X	2835	A	N1-C6-N6	7.30	122.98	118.60
29	X	1009	C	C5-C6-N1	-7.30	117.35	121.00
29	X	2523	G	N3-C4-N9	7.27	130.36	126.00
29	X	20	C	C6-N1-C2	-7.26	117.40	120.30
29	X	527	C	C2-N1-C1'	7.24	126.76	118.80
29	X	1714	A	N1-C6-N6	7.24	122.94	118.60
29	X	656	U	N3-C2-O2	-7.22	117.14	122.20
29	X	1270	C	N3-C4-C5	-7.22	119.01	121.90
29	X	2671	C	N3-C4-N4	7.22	123.06	118.00
29	X	206	U	N3-C2-O2	-7.21	117.15	122.20
29	X	661	C	C5-C6-N1	7.21	124.60	121.00
29	X	943	U	C2-N1-C1'	7.20	126.34	117.70
29	X	1336	G	N9-C4-C5	-7.20	102.52	105.40
29	X	538	A	N1-C6-N6	-7.18	114.29	118.60
29	X	1652	G	C5-C6-O6	-7.18	124.29	128.60
29	X	2019	C	C5-C6-N1	7.17	124.58	121.00
29	X	2542	U	N3-C2-O2	-7.15	117.19	122.20
29	X	672	C	C6-N1-C2	7.13	123.15	120.30
29	X	1313	U	C5-C4-O4	7.13	130.18	125.90
29	X	1336	G	N1-C6-O6	7.13	124.18	119.90
29	X	1684	G	N9-C4-C5	7.13	108.25	105.40
29	X	1219	C	N1-C2-O2	7.12	123.17	118.90
29	X	2478	C	C5-C6-N1	7.11	124.56	121.00
29	X	1665	C	C5-C6-N1	-7.09	117.45	121.00
29	X	1341	G	C5-C6-N1	7.09	115.05	111.50
29	X	2688	G	C8-N9-C4	7.07	109.23	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	X	1704	G	N1-C6-O6	7.07	124.14	119.90
29	X	2857	C	N3-C4-C5	-7.07	119.07	121.90
29	X	2523	G	C4-N9-C1'	7.07	135.68	126.50
29	X	1016	C	C2-N1-C1'	7.05	126.56	118.80
29	X	700	C	C6-N1-C2	-7.04	117.48	120.30
29	X	1167	A	C8-N9-C4	7.04	108.62	105.80
29	X	1278	A	C4-C5-C6	7.03	120.52	117.00
29	X	1989	C	C5-C6-N1	7.03	124.52	121.00
29	X	1974	U	N3-C2-O2	-7.03	117.28	122.20
29	X	2314	A	C8-N9-C4	-7.02	102.99	105.80
29	X	754	G	C6-C5-N7	-7.02	126.19	130.40
29	X	2273	C	C6-N1-C2	-7.01	117.49	120.30
29	X	1167	A	N9-C4-C5	-7.01	103.00	105.80
29	X	2749	A	N1-C6-N6	7.00	122.80	118.60
29	X	2662	C	C5-C6-N1	6.99	124.50	121.00
29	X	2535	C	C6-N1-C2	6.99	123.10	120.30
29	X	2398	U	N3-C4-C5	-6.99	110.41	114.60
29	X	1269	G	N9-C4-C5	-6.98	102.61	105.40
29	X	2433	G	C4-C5-N7	-6.98	108.01	110.80
29	X	1770	U	C4-C5-C6	6.97	123.88	119.70
29	X	1647	U	C4-C5-C6	6.96	123.88	119.70
29	X	1647	U	N1-C2-N3	6.95	119.07	114.90
29	X	2854	G	N9-C4-C5	-6.95	102.62	105.40
29	X	2500	C	C6-N1-C2	-6.94	117.52	120.30
29	X	2597	G	N3-C4-N9	6.93	130.16	126.00
29	X	1270	C	C6-N1-C2	-6.92	117.53	120.30
29	X	1636	G	C8-N9-C4	6.92	109.17	106.40
29	X	1474	A	C8-N9-C4	-6.92	103.03	105.80
29	X	466	A	N1-C6-N6	-6.92	114.45	118.60
29	X	989	G	C8-N9-C4	6.92	109.17	106.40
29	X	1704	G	C6-C5-N7	-6.90	126.26	130.40
29	X	2862	G	N3-C4-N9	6.90	130.14	126.00
29	X	2555	G	C8-N9-C4	6.90	109.16	106.40
29	X	985	G	C8-N9-C4	-6.89	103.64	106.40
29	X	2867	G	C2-N3-C4	-6.89	108.45	111.90
29	X	1033	G	N3-C4-C5	-6.89	125.16	128.60
29	X	943	U	N1-C2-O2	6.88	127.61	122.80
29	X	1941	C	C6-N1-C2	6.88	123.05	120.30
29	X	1984	A	N3-C4-C5	6.86	131.60	126.80
29	X	773	G	N3-C4-N9	6.86	130.11	126.00
29	X	22	C	C2-N1-C1'	6.85	126.33	118.80
29	X	1312	G	C5-C6-O6	-6.85	124.49	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	Y	39	C	C6-N1-C1'	-6.85	112.58	120.80
29	X	700	C	C5-C6-N1	6.83	124.41	121.00
29	X	591	G	C8-N9-C4	6.82	109.13	106.40
29	X	2422	C	C6-N1-C2	-6.81	117.58	120.30
29	X	2028	C	C5-C4-N4	-6.81	115.44	120.20
29	X	501	G	N1-C6-O6	-6.80	115.82	119.90
29	X	2702	G	N3-C4-C5	-6.79	125.21	128.60
29	X	1343	C	N3-C4-N4	6.78	122.75	118.00
29	X	1974	U	C5-C4-O4	6.78	129.97	125.90
29	X	2592	U	N1-C2-O2	-6.78	118.05	122.80
29	X	774	A	C5-C6-N6	-6.78	118.28	123.70
29	X	2023	C	C6-N1-C2	6.77	123.01	120.30
29	X	2037	A	C8-N9-C4	-6.76	103.09	105.80
29	X	615	C	N3-C2-O2	-6.76	117.17	121.90
29	X	1343	C	C5-C4-N4	-6.76	115.47	120.20
29	X	2800	C	N1-C2-O2	6.75	122.95	118.90
29	X	1016	C	C5-C6-N1	6.74	124.37	121.00
29	X	1652	G	N9-C4-C5	-6.74	102.70	105.40
29	X	522	G	N9-C4-C5	-6.74	102.70	105.40
29	X	1305	C	C5-C6-N1	-6.74	117.63	121.00
29	X	2624	G	C4-N9-C1'	6.74	135.26	126.50
29	X	2465	G	C8-N9-C4	-6.73	103.71	106.40
29	X	1975	G	C6-C5-N7	6.72	134.43	130.40
29	X	1696	C	C6-N1-C2	-6.72	117.61	120.30
29	X	2421	C	C6-N1-C2	-6.72	117.61	120.30
29	X	2552	C	C6-N1-C2	-6.72	117.61	120.30
29	X	1347	C	C6-N1-C2	-6.71	117.61	120.30
29	X	1279	G	N3-C2-N2	6.71	124.60	119.90
29	X	1950	C	C6-N1-C2	-6.71	117.62	120.30
29	X	2704	U	C5-C6-N1	-6.70	119.35	122.70
29	X	2572	U	C6-N1-C2	-6.69	116.99	121.00
29	X	2573	C	C6-N1-C2	-6.69	117.62	120.30
29	X	2662	C	N3-C4-C5	-6.68	119.23	121.90
29	X	2523	G	C4-C5-C6	6.68	122.81	118.80
29	X	2851	G	C8-N9-C4	6.68	109.07	106.40
29	X	519	C	N3-C4-C5	-6.67	119.23	121.90
29	X	522	G	C5-N7-C8	-6.66	100.97	104.30
29	X	968	C	C5-C6-N1	6.66	124.33	121.00
29	X	2586	G	C6-C5-N7	-6.66	126.40	130.40
29	X	2597	G	C8-N9-C1'	-6.66	118.34	127.00
29	X	1326	U	N3-C2-O2	-6.66	117.54	122.20
29	X	2548	G	C4-C5-C6	6.64	122.79	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	X	1634	A	C5-C6-N6	6.64	129.01	123.70
29	X	576	A	N1-C6-N6	-6.64	114.62	118.60
29	X	1039	A	C8-N9-C4	-6.64	103.14	105.80
29	X	1995	G	N3-C4-N9	6.64	129.98	126.00
25	Z	16	ARG	NE-CZ-NH2	-6.63	116.98	120.30
29	X	1474	A	N1-C6-N6	-6.63	114.62	118.60
29	X	1686	A	C8-N9-C4	-6.63	103.15	105.80
29	X	787	A	N1-C6-N6	6.63	122.58	118.60
29	X	2524	G	C5-C6-N1	6.62	114.81	111.50
29	X	2870	C	C6-N1-C2	-6.62	117.65	120.30
29	X	22	C	N3-C2-O2	-6.61	117.27	121.90
29	X	225	G	N1-C6-O6	6.61	123.87	119.90
29	X	1770	U	N3-C2-O2	-6.61	117.57	122.20
29	X	689	A	N7-C8-N9	6.61	117.10	113.80
29	X	983	G	C8-N9-C4	-6.61	103.76	106.40
29	X	2822	U	C5-C4-O4	-6.60	121.94	125.90
29	X	957	G	N3-C4-C5	-6.59	125.30	128.60
29	X	1289	A	N7-C8-N9	-6.59	110.50	113.80
29	X	1975	G	C4-C5-C6	-6.59	114.84	118.80
29	X	1683	G	C5-C6-O6	6.58	132.55	128.60
29	X	2854	G	N1-C6-O6	6.58	123.85	119.90
29	X	2398	U	C6-N1-C2	-6.58	117.05	121.00
29	X	430	C	C6-N1-C2	-6.58	117.67	120.30
29	X	2687	G	C8-N9-C4	6.57	109.03	106.40
29	X	2598	C	C6-N1-C2	-6.57	117.67	120.30
29	X	955	G	C5-N7-C8	-6.57	101.02	104.30
29	X	2479	U	C5-C6-N1	6.57	125.98	122.70
29	X	526	C	N3-C2-O2	-6.56	117.31	121.90
29	X	2554	C	N3-C4-N4	6.56	122.59	118.00
29	X	2576	G	C6-C5-N7	-6.56	126.47	130.40
29	X	1744	G	N3-C4-C5	-6.56	125.32	128.60
29	X	2821	G	C8-N9-C4	6.55	109.02	106.40
29	X	1016	C	C6-N1-C2	-6.55	117.68	120.30
29	X	1207	G	N1-C6-O6	6.55	123.83	119.90
29	X	2757	G	N9-C4-C5	-6.55	102.78	105.40
29	X	1212	U	C5-C6-N1	-6.54	119.43	122.70
29	X	124	A	C8-N9-C4	-6.54	103.19	105.80
29	X	1636	G	N9-C4-C5	-6.53	102.79	105.40
29	X	2867	G	C4-N9-C1'	-6.53	118.02	126.50
29	X	2698	G	C5-C6-O6	-6.53	124.69	128.60
14	M	42	GLY	N-CA-C	-6.52	96.79	113.10
29	X	2060	A	C8-N9-C4	-6.51	103.19	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	X	2659	C	C6-N1-C2	-6.51	117.70	120.30
29	X	2697	G	C8-N9-C4	-6.51	103.80	106.40
29	X	497	C	N3-C4-N4	6.50	122.55	118.00
29	X	1760	G	C8-N9-C4	-6.50	103.80	106.40
29	X	1652	G	N1-C6-O6	6.50	123.80	119.90
29	X	2548	G	N1-C6-O6	6.50	123.80	119.90
29	X	2039	G	C8-N9-C4	-6.50	103.80	106.40
29	X	557	U	N3-C2-O2	-6.50	117.65	122.20
29	X	2488	G	C5-C6-N1	6.50	114.75	111.50
29	X	2279	G	N1-C6-O6	6.49	123.80	119.90
29	X	1142	G	N9-C4-C5	-6.48	102.81	105.40
29	X	1721	G	N3-C4-C5	6.48	131.84	128.60
29	X	2704	U	C2-N1-C1'	-6.48	109.92	117.70
29	X	2828	C	C6-N1-C2	-6.48	117.71	120.30
29	X	576	A	N9-C4-C5	6.48	108.39	105.80
29	X	493	A	C8-N9-C4	6.47	108.39	105.80
29	X	1661	C	N3-C2-O2	-6.47	117.37	121.90
29	X	2481	G	N3-C4-C5	-6.46	125.37	128.60
29	X	2696	A	C8-N9-C4	-6.46	103.21	105.80
29	X	2712	G	N1-C2-N2	-6.46	110.38	116.20
29	X	225	G	C4-C5-N7	6.46	113.38	110.80
14	M	35	VAL	CB-CA-C	-6.46	99.13	111.40
29	X	991	A	C8-N9-C4	-6.46	103.22	105.80
29	X	2666	U	N1-C2-O2	-6.45	118.28	122.80
29	X	1656	U	C6-N1-C2	6.44	124.86	121.00
29	X	1647	U	C5-C4-O4	6.43	129.76	125.90
29	X	646	C	C6-N1-C2	-6.42	117.73	120.30
29	X	2419	C	N1-C2-O2	-6.41	115.05	118.90
29	X	2383	C	C6-N1-C2	-6.41	117.74	120.30
29	X	1667	A	C8-N9-C4	6.40	108.36	105.80
29	X	2703	C	N1-C2-O2	-6.40	115.06	118.90
29	X	2538	C	C5-C6-N1	6.39	124.20	121.00
3	B	179	GLU	N-CA-C	-6.39	93.75	111.00
29	X	522	G	C2-N3-C4	-6.38	108.71	111.90
29	X	1333	G	N1-C6-O6	-6.38	116.07	119.90
29	X	1964	A	C8-N9-C4	-6.37	103.25	105.80
29	X	2587	G	C8-N9-C4	-6.37	103.85	106.40
29	X	2240	C	C5-C6-N1	6.37	124.18	121.00
29	X	660	G	N3-C4-C5	6.37	131.78	128.60
29	X	1313	U	C6-N1-C1'	6.37	130.11	121.20
29	X	2617	G	N1-C6-O6	-6.36	116.08	119.90
29	X	968	C	N1-C2-O2	6.35	122.71	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	X	338	G	C8-N9-C4	-6.35	103.86	106.40
29	X	2044	G	N3-C4-C5	-6.33	125.44	128.60
29	X	175	C	C6-N1-C1'	-6.33	113.21	120.80
29	X	2479	U	C6-N1-C2	-6.33	117.20	121.00
29	X	2007	G	C8-N9-C4	6.32	108.93	106.40
29	X	2538	C	C6-N1-C2	-6.31	117.78	120.30
29	X	2757	G	C5-C6-O6	-6.31	124.81	128.60
29	X	2563	U	C2-N1-C1'	6.30	125.26	117.70
29	X	2841	U	N3-C2-O2	-6.30	117.79	122.20
29	X	854	G	C8-N9-C4	-6.30	103.88	106.40
29	X	540	G	C4-C5-N7	-6.30	108.28	110.80
29	X	773	G	N3-C4-C5	-6.29	125.45	128.60
29	X	1457	A	C8-N9-C4	6.29	108.32	105.80
29	X	2554	C	C5-C6-N1	6.28	124.14	121.00
29	X	2623	A	N7-C8-N9	-6.28	110.66	113.80
29	X	1002	C	C6-N1-C2	-6.27	117.79	120.30
29	X	1281	A	C8-N9-C4	6.27	108.31	105.80
29	X	1713	G	N9-C4-C5	6.26	107.91	105.40
29	X	2273	C	C5-C6-N1	6.26	124.13	121.00
29	X	2847	G	N3-C2-N2	-6.26	115.52	119.90
29	X	750	C	C6-N1-C2	-6.26	117.80	120.30
29	X	2867	G	C8-N9-C1'	6.26	135.14	127.00
12	K	103	ARG	NE-CZ-NH1	6.26	123.43	120.30
29	X	2695	C	C5-C6-N1	6.26	124.13	121.00
29	X	2606	G	N1-C6-O6	6.26	123.65	119.90
29	X	774	A	C6-N1-C2	6.25	122.35	118.60
29	X	587	A	N1-C6-N6	-6.25	114.85	118.60
29	X	2797	G	C8-N9-C1'	-6.24	118.89	127.00
29	X	2300	G	C8-N9-C4	-6.24	103.90	106.40
29	X	972	C	C6-N1-C2	-6.24	117.81	120.30
29	X	1999	U	C6-N1-C1'	-6.24	112.47	121.20
29	X	993	C	N1-C2-O2	6.23	122.64	118.90
29	X	1271	C	N3-C2-O2	-6.22	117.54	121.90
29	X	774	A	C2-N3-C4	-6.22	107.49	110.60
29	X	508	G	N1-C6-O6	6.22	123.63	119.90
29	X	2048	C	C6-N1-C2	-6.22	117.81	120.30
29	X	2693	U	N1-C2-N3	6.22	118.63	114.90
29	X	2845	C	N3-C4-N4	6.22	122.35	118.00
29	X	1289	A	N9-C4-C5	-6.21	103.31	105.80
29	X	1465	G	C8-N9-C4	-6.21	103.92	106.40
29	X	1672	A	N1-C6-N6	6.21	122.32	118.60
29	X	2639	A	C2-N3-C4	6.20	113.70	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	X	1981	A	N1-C6-N6	6.20	122.32	118.60
29	X	2637	C	C6-N1-C2	6.20	122.78	120.30
29	X	1142	G	N1-C6-O6	6.20	123.62	119.90
29	X	1339	U	C2-N1-C1'	6.19	125.13	117.70
29	X	2199	C	N1-C2-O2	6.19	122.61	118.90
29	X	219	G	C4-N9-C1'	-6.19	118.45	126.50
29	X	2597	G	C4-N9-C1'	6.19	134.55	126.50
29	X	993	C	N3-C2-O2	-6.18	117.57	121.90
29	X	2858	A	C8-N9-C4	-6.18	103.33	105.80
29	X	334	G	N1-C6-O6	6.18	123.61	119.90
29	X	540	G	C4-N9-C1'	6.18	134.53	126.50
29	X	2797	G	N9-C4-C5	-6.17	102.93	105.40
29	X	2690	A	N1-C2-N3	6.16	132.38	129.30
29	X	2822	U	C5-C6-N1	6.16	125.78	122.70
29	X	880	C	N1-C2-O2	6.15	122.59	118.90
29	X	2590	U	N3-C2-O2	-6.13	117.91	122.20
29	X	579	G	N7-C8-N9	6.13	116.16	113.10
29	X	576	A	C4-C5-N7	-6.13	107.64	110.70
29	X	1208	A	C8-N9-C4	-6.12	103.35	105.80
29	X	1308	C	C2-N1-C1'	6.12	125.53	118.80
29	X	615	C	N1-C2-O2	6.12	122.57	118.90
29	X	2671	C	C6-N1-C2	-6.11	117.86	120.30
29	X	1315	A	C4-C5-N7	-6.11	107.65	110.70
29	X	107	G	C4-N9-C1'	6.11	134.44	126.50
29	X	2383	C	C2-N1-C1'	6.10	125.51	118.80
29	X	2233	C	C6-N1-C2	6.10	122.74	120.30
29	X	528	G	N3-C2-N2	-6.10	115.63	119.90
29	X	713	G	N1-C6-O6	6.10	123.56	119.90
29	X	2628	C	N3-C2-O2	-6.10	117.63	121.90
29	X	774	A	C5-C6-N1	-6.09	114.65	117.70
29	X	2371	A	C8-N9-C4	-6.09	103.36	105.80
29	X	1256	C	C6-N1-C2	6.09	122.73	120.30
29	X	1990	U	N3-C4-C5	-6.09	110.95	114.60
29	X	2662	C	C2-N3-C4	6.09	122.94	119.90
29	X	931	G	N3-C4-N9	6.08	129.65	126.00
29	X	2841	U	N1-C2-O2	6.08	127.05	122.80
29	X	2009	U	C6-N1-C2	-6.08	117.35	121.00
29	X	1744	G	N3-C4-N9	6.08	129.65	126.00
29	X	2240	C	N1-C2-O2	6.08	122.55	118.90
29	X	931	G	N9-C4-C5	-6.07	102.97	105.40
29	X	2015	G	C5-N7-C8	-6.07	101.26	104.30
29	X	2592	U	N3-C2-O2	6.07	126.45	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	X	1984	A	C4-C5-C6	-6.07	113.97	117.00
29	X	2594	U	N3-C4-O4	6.07	123.65	119.40
29	X	1990	U	N3-C4-O4	6.06	123.64	119.40
29	X	20	C	C5-C6-N1	6.06	124.03	121.00
29	X	2561	G	N1-C6-O6	-6.06	116.27	119.90
29	X	688	A	C8-N9-C4	-6.05	103.38	105.80
29	X	1668	G	C4-C5-N7	6.05	113.22	110.80
29	X	2655	C	N3-C4-C5	6.05	124.32	121.90
29	X	319	G	C4-C5-N7	6.05	113.22	110.80
29	X	673	G	C8-N9-C4	6.04	108.82	106.40
29	X	2382	C	C6-N1-C2	-6.04	117.88	120.30
29	X	1775	A	N1-C6-N6	6.03	122.22	118.60
29	X	2828	C	C5-C6-N1	6.03	124.02	121.00
29	X	968	C	C2-N1-C1'	6.03	125.43	118.80
29	X	574	C	C6-N1-C2	-6.03	117.89	120.30
29	X	1736	C	C6-N1-C2	-6.03	117.89	120.30
29	X	2617	G	N3-C2-N2	6.02	124.12	119.90
29	X	2696	A	N1-C6-N6	-6.02	114.99	118.60
29	X	1407	G	C5-C6-O6	-6.01	124.99	128.60
29	X	1724	C	C5-C6-N1	-6.01	117.99	121.00
29	X	2690	A	C2-N3-C4	-6.01	107.59	110.60
29	X	754	G	N9-C4-C5	-6.01	103.00	105.40
29	X	2704	U	N3-C2-O2	6.01	126.41	122.20
29	X	1231	A	N7-C8-N9	6.00	116.80	113.80
29	X	1982	C	N3-C2-O2	-6.00	117.70	121.90
29	X	2524	G	N3-C4-C5	-6.00	125.60	128.60
29	X	1706	A	N1-C6-N6	6.00	122.20	118.60
29	X	2044	G	C4-C5-N7	-6.00	108.40	110.80
29	X	672	C	N3-C4-C5	5.99	124.30	121.90
29	X	2569	A	C8-N9-C4	5.99	108.20	105.80
29	X	1950	C	C5-C6-N1	5.99	123.99	121.00
29	X	1684	G	C4-C5-N7	-5.99	108.41	110.80
29	X	2546	G	N3-C4-C5	-5.98	125.61	128.60
29	X	652	C	C6-N1-C2	5.98	122.69	120.30
29	X	2704	U	C2-N3-C4	-5.97	123.42	127.00
29	X	522	G	C5-C6-O6	-5.97	125.02	128.60
29	X	2522	G	C5-C6-O6	5.97	132.18	128.60
29	X	968	C	C4-C5-C6	-5.97	114.42	117.40
29	X	1684	G	C5-C6-O6	5.97	132.18	128.60
29	X	673	G	C4-N9-C1'	-5.96	118.75	126.50
29	X	1337	G	C5-C6-N1	5.96	114.48	111.50
29	X	1679	U	N3-C4-C5	5.96	118.18	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	X	2412	A	N1-C6-N6	-5.96	115.02	118.60
29	X	1681	A	C8-N9-C1'	-5.95	116.99	127.70
29	X	2408	G	N3-C4-C5	-5.95	125.63	128.60
29	X	2561	G	C5-C6-N1	5.95	114.47	111.50
29	X	1681	A	C4-N9-C1'	5.94	136.99	126.30
29	X	1983	G	N1-C2-N3	5.94	127.46	123.90
29	X	1950	C	C2-N1-C1'	5.94	125.33	118.80
29	X	2590	U	N1-C2-O2	5.94	126.95	122.80
29	X	2666	U	C2-N1-C1'	-5.93	110.58	117.70
29	X	1995	G	C5-C6-N1	5.93	114.47	111.50
29	X	1339	U	C6-N1-C2	-5.93	117.44	121.00
29	X	2239	C	C6-N1-C2	-5.92	117.93	120.30
29	X	2492	G	N1-C6-O6	-5.92	116.35	119.90
29	X	1323	G	N1-C6-O6	5.91	123.45	119.90
29	X	931	G	N3-C2-N2	5.91	124.04	119.90
29	X	2724	G	C8-N9-C4	-5.91	104.04	106.40
29	X	1763	G	C8-N9-C4	5.90	108.76	106.40
29	X	1721	G	C8-N9-C1'	5.90	134.67	127.00
29	X	522	G	C5-C6-N1	-5.90	108.55	111.50
29	X	1747	G	N3-C4-N9	5.90	129.54	126.00
29	X	2550	C	C5-C6-N1	5.90	123.95	121.00
29	X	2696	A	C2-N3-C4	5.89	113.55	110.60
29	X	1980	A	N1-C2-N3	5.89	132.25	129.30
29	X	2191	A	N1-C6-N6	-5.89	115.07	118.60
29	X	1989	C	N3-C2-O2	5.89	126.02	121.90
29	X	689	A	C5-N7-C8	-5.89	100.96	103.90
29	X	1221	C	C6-N1-C2	-5.89	117.94	120.30
29	X	2831	A	C8-N9-C4	-5.88	103.45	105.80
29	X	2598	C	N1-C2-O2	5.88	122.43	118.90
29	X	1744	G	N3-C2-N2	5.88	124.02	119.90
29	X	1999	U	C5-C6-N1	5.88	125.64	122.70
29	X	927	C	C6-N1-C2	-5.87	117.95	120.30
29	X	1627	C	C6-N1-C2	-5.87	117.95	120.30
29	X	566	U	C5-C6-N1	5.87	125.64	122.70
29	X	1683	G	N9-C4-C5	5.87	107.75	105.40
29	X	1219	C	C5-C6-N1	5.87	123.93	121.00
29	X	1333	G	C4-N9-C1'	5.87	134.13	126.50
29	X	526	C	N1-C2-O2	5.86	122.42	118.90
29	X	919	U	C5-C6-N1	-5.86	119.77	122.70
29	X	1219	C	C6-N1-C2	-5.86	117.96	120.30
29	X	2484	G	C8-N9-C4	-5.86	104.06	106.40
29	X	1269	G	C6-C5-N7	-5.85	126.89	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	X	1474	A	C5-C6-N6	5.85	128.38	123.70
29	X	458	G	C4-C5-N7	5.84	113.14	110.80
29	X	1636	G	N3-C4-C5	5.84	131.52	128.60
29	X	863	C	C6-N1-C2	-5.84	117.96	120.30
29	X	1470	G	N1-C6-O6	-5.84	116.39	119.90
29	X	968	C	N1-C2-N3	-5.84	115.11	119.20
29	X	1008	G	N9-C4-C5	-5.84	103.06	105.40
29	X	1258	G	C8-N9-C4	-5.84	104.06	106.40
29	X	2273	C	C2-N1-C1'	5.84	125.22	118.80
29	X	2028	C	N3-C4-N4	5.83	122.08	118.00
30	Y	84	G	C8-N9-C4	5.83	108.73	106.40
29	X	2605	C	N3-C2-O2	-5.83	117.82	121.90
29	X	2797	G	C4-N9-C1'	5.83	134.08	126.50
29	X	1778	U	N3-C2-O2	-5.83	118.12	122.20
29	X	1661	C	C2-N1-C1'	5.83	125.21	118.80
29	X	2671	C	N3-C4-C5	-5.83	119.57	121.90
29	X	1132	C	C6-N1-C2	-5.82	117.97	120.30
29	X	2846	G	C8-N9-C1'	-5.82	119.43	127.00
29	X	1672	A	C5-C6-N6	-5.82	119.04	123.70
29	X	2698	G	C6-C5-N7	-5.82	126.91	130.40
29	X	1631	C	N1-C2-O2	-5.82	115.41	118.90
29	X	920	G	C8-N9-C4	5.82	108.73	106.40
29	X	2858	A	N9-C4-C5	5.81	108.12	105.80
29	X	2516	U	C6-N1-C2	5.81	124.49	121.00
29	X	1662	G	N1-C6-O6	-5.80	116.42	119.90
29	X	1940	C	C6-N1-C1'	-5.80	113.84	120.80
29	X	1315	A	C5-C6-N6	5.80	128.34	123.70
29	X	2797	G	C4-C5-N7	5.80	113.12	110.80
29	X	2757	G	C8-N9-C4	5.79	108.72	106.40
29	X	2465	G	N7-C8-N9	5.79	116.00	113.10
29	X	1678	G	C4-N9-C1'	-5.78	118.98	126.50
29	X	2823	G	C4-C5-N7	-5.78	108.49	110.80
29	X	2489	C	C5-C4-N4	-5.78	116.15	120.20
29	X	923	A	N1-C6-N6	5.78	122.07	118.60
29	X	2199	C	N3-C2-O2	-5.78	117.86	121.90
29	X	2568	A	C8-N9-C4	5.78	108.11	105.80
29	X	1134	C	C6-N1-C2	-5.77	117.99	120.30
29	X	2033	C	C6-N1-C2	-5.77	117.99	120.30
29	X	2437	G	C6-C5-N7	-5.76	126.94	130.40
29	X	749	C	C6-N1-C2	-5.76	118.00	120.30
29	X	1308	C	C6-N1-C2	-5.76	118.00	120.30
29	X	1768	U	N1-C2-O2	5.76	126.83	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	X	2420	C	C6-N1-C2	-5.76	118.00	120.30
29	X	2366	U	N1-C2-O2	-5.75	118.77	122.80
29	X	548	G	N1-C6-O6	5.75	123.35	119.90
29	X	1744	G	N1-C2-N2	-5.75	111.02	116.20
29	X	1405	A	C2-N3-C4	5.75	113.47	110.60
29	X	90	G	N3-C4-C5	-5.75	125.73	128.60
29	X	2553	G	C4-C5-N7	5.75	113.10	110.80
29	X	1294	G	C8-N9-C4	-5.75	104.10	106.40
29	X	773	G	C4-N9-C1'	5.74	133.97	126.50
29	X	2559	U	C2-N3-C4	5.74	130.45	127.00
29	X	2598	C	C5-C6-N1	5.74	123.87	121.00
29	X	1260	A	C8-N9-C4	5.74	108.10	105.80
29	X	2597	G	N3-C4-C5	-5.74	125.73	128.60
29	X	1301	U	N3-C4-C5	-5.74	111.16	114.60
29	X	2240	C	C2-N1-C1'	5.73	125.11	118.80
29	X	476	G	C4-C5-N7	-5.73	108.51	110.80
29	X	493	A	N7-C8-N9	-5.73	110.93	113.80
29	X	2594	U	N3-C2-O2	5.73	126.21	122.20
29	X	1281	A	N7-C8-N9	-5.73	110.93	113.80
29	X	1155	G	N7-C8-N9	-5.73	110.24	113.10
29	X	508	G	C5-C6-O6	-5.73	125.16	128.60
29	X	796	A	N7-C8-N9	5.73	116.66	113.80
29	X	2279	G	C6-C5-N7	-5.73	126.96	130.40
29	X	2846	G	N9-C4-C5	-5.73	103.11	105.40
29	X	1345	G	C8-N9-C1'	-5.73	119.56	127.00
29	X	1766	U	C5-C6-N1	-5.73	119.84	122.70
29	X	1692	C	C4-C5-C6	5.72	120.26	117.40
29	X	2491	C	N3-C4-C5	5.72	124.19	121.90
29	X	2492	G	C4-C5-N7	-5.72	108.51	110.80
29	X	2642	G	C8-N9-C4	5.72	108.69	106.40
29	X	1332	G	C6-C5-N7	-5.72	126.97	130.40
29	X	2654	A	C8-N9-C4	5.72	108.09	105.80
29	X	968	C	C2-N3-C4	5.71	122.76	119.90
29	X	2794	G	C6-N1-C2	-5.71	121.67	125.10
29	X	501	G	C4-C5-N7	-5.71	108.52	110.80
29	X	1292	A	C2-N3-C4	-5.71	107.74	110.60
29	X	789	G	C6-C5-N7	-5.71	126.97	130.40
29	X	2661	G	N1-C2-N2	5.71	121.34	116.20
29	X	2594	U	C2-N3-C4	5.70	130.42	127.00
29	X	545	C	C2-N1-C1'	-5.70	112.53	118.80
29	X	16	G	N7-C8-N9	-5.70	110.25	113.10
29	X	1332	G	C4-N9-C1'	5.70	133.91	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	X	2851	G	N3-C2-N2	5.69	123.89	119.90
29	X	237	G	N3-C4-C5	-5.69	125.75	128.60
29	X	596	C	C6-N1-C2	-5.69	118.02	120.30
29	X	1975	G	N3-C4-C5	5.68	131.44	128.60
29	X	2300	G	C2-N3-C4	5.68	114.74	111.90
29	X	1318	A	C8-N9-C4	5.68	108.07	105.80
29	X	2712	G	N9-C4-C5	-5.68	103.13	105.40
29	X	761	G	N3-C4-C5	5.68	131.44	128.60
29	X	1332	G	N3-C4-N9	5.67	129.40	126.00
29	X	1142	G	C8-N9-C4	5.67	108.67	106.40
29	X	1315	A	N1-C6-N6	-5.67	115.20	118.60
29	X	1326	U	C2-N1-C1'	5.67	124.50	117.70
29	X	2451	G	N3-C4-C5	-5.67	125.77	128.60
29	X	2590	U	C6-N1-C1'	-5.67	113.27	121.20
29	X	927	C	N1-C2-O2	5.67	122.30	118.90
12	K	29	LEU	CB-CG-CD1	-5.66	101.37	111.00
29	X	758	G	C8-N9-C4	5.66	108.67	106.40
29	X	1989	C	C2-N3-C4	5.66	122.73	119.90
29	X	1681	A	N3-C4-N9	5.66	131.93	127.40
29	X	1672	A	C6-C5-N7	-5.66	128.34	132.30
29	X	1550	C	C6-N1-C2	-5.66	118.04	120.30
29	X	2366	U	N3-C2-O2	5.66	126.16	122.20
29	X	516	G	C4-C5-N7	5.65	113.06	110.80
29	X	2831	A	N9-C4-C5	5.65	108.06	105.80
29	X	2368	G	N3-C4-C5	-5.65	125.78	128.60
29	X	1747	G	N3-C4-C5	-5.64	125.78	128.60
29	X	1685	A	C8-N9-C4	5.64	108.06	105.80
29	X	2857	C	C5-C4-N4	5.64	124.15	120.20
29	X	343	A	N9-C4-C5	5.64	108.06	105.80
29	X	968	C	C6-N1-C1'	-5.64	114.03	120.80
29	X	1207	G	C5-C6-O6	-5.64	125.22	128.60
29	X	2597	G	N1-C2-N2	-5.64	111.12	116.20
29	X	1465	G	N1-C2-N3	5.64	127.28	123.90
29	X	1312	G	C4-C5-N7	5.63	113.05	110.80
29	X	2002	A	C2-N3-C4	5.63	113.42	110.60
29	X	2419	C	C6-N1-C2	-5.63	118.05	120.30
29	X	2848	A	C8-N9-C4	-5.63	103.55	105.80
29	X	1403	U	C2-N1-C1'	5.63	124.46	117.70
29	X	2693	U	C4-C5-C6	5.62	123.08	119.70
29	X	319	G	C5-C6-O6	-5.62	125.23	128.60
30	Y	32	C	C5-C6-N1	5.62	123.81	121.00
29	X	700	C	N3-C4-C5	-5.61	119.66	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	X	1274	C	N1-C2-O2	5.61	122.27	118.90
29	X	1335	A	N7-C8-N9	-5.61	111.00	113.80
29	X	2618	A	C2-N3-C4	5.61	113.41	110.60
29	X	2806	G	C2-N3-C4	-5.61	109.09	111.90
29	X	2848	A	N1-C6-N6	-5.61	115.24	118.60
29	X	1197	U	N1-C2-O2	5.61	126.72	122.80
29	X	1997	A	C4-C5-C6	5.61	119.80	117.00
29	X	2666	U	C6-N1-C1'	5.60	129.04	121.20
29	X	1272	G	N1-C6-O6	-5.60	116.54	119.90
29	X	769	C	N1-C2-O2	-5.60	115.54	118.90
29	X	2812	A	C8-N9-C4	-5.60	103.56	105.80
29	X	943	U	N3-C2-O2	-5.59	118.28	122.20
29	X	2317	G	C8-N9-C4	-5.59	104.16	106.40
29	X	1645	U	N3-C2-O2	-5.59	118.29	122.20
29	X	1707	A	N1-C6-N6	5.59	121.95	118.60
29	X	1918	G	N1-C6-O6	-5.59	116.55	119.90
29	X	2495	G	N3-C4-N9	5.59	129.35	126.00
29	X	2839	G	C6-C5-N7	5.59	133.75	130.40
29	X	1775	A	C8-N9-C1'	-5.59	117.64	127.70
29	X	1966	C	C6-N1-C2	5.59	122.54	120.30
29	X	2572	U	C5-C6-N1	5.59	125.49	122.70
29	X	2668	U	C5-C6-N1	-5.58	119.91	122.70
29	X	2434	G	C8-N9-C1'	-5.58	119.74	127.00
29	X	2681	A	N1-C6-N6	5.58	121.95	118.60
29	X	1678	G	N1-C6-O6	-5.58	116.55	119.90
29	X	499	G	N3-C4-N9	5.58	129.35	126.00
29	X	1008	G	C8-N9-C4	5.58	108.63	106.40
29	X	1272	G	C5-C6-O6	5.58	131.94	128.60
29	X	2033	C	N1-C2-O2	5.58	122.25	118.90
29	X	2665	G	N3-C4-N9	-5.58	122.65	126.00
29	X	2598	C	C2-N1-C1'	5.57	124.93	118.80
29	X	1288	A	C5-C6-N6	-5.57	119.24	123.70
29	X	1298	G	C6-C5-N7	-5.57	127.06	130.40
29	X	2311	U	C2-N1-C1'	5.56	124.38	117.70
29	X	563	U	N3-C4-C5	5.56	117.94	114.60
29	X	661	C	C2-N1-C1'	5.56	124.92	118.80
29	X	1298	G	N9-C4-C5	-5.56	103.18	105.40
29	X	1345	G	N7-C8-N9	5.56	115.88	113.10
29	X	1344	C	N3-C4-C5	5.55	124.12	121.90
29	X	1656	U	N1-C2-N3	-5.55	111.57	114.90
29	X	2757	G	N1-C6-O6	5.55	123.23	119.90
29	X	2366	U	C2-N1-C1'	-5.55	111.04	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	X	1670	G	N9-C4-C5	-5.55	103.18	105.40
29	X	2233	C	C5-C6-N1	-5.55	118.23	121.00
29	X	2794	G	N3-C4-C5	-5.55	125.83	128.60
29	X	343	A	C4-C5-N7	-5.55	107.93	110.70
29	X	1232	U	C6-N1-C2	-5.54	117.67	121.00
29	X	1405	A	C8-N9-C4	-5.54	103.58	105.80
29	X	1681	A	C5-N7-C8	-5.54	101.13	103.90
29	X	1683	G	C8-N9-C1'	5.54	134.20	127.00
29	X	2610	G	N3-C4-N9	-5.54	122.68	126.00
29	X	2618	A	N3-C4-C5	-5.54	122.92	126.80
29	X	1965	U	C2-N1-C1'	5.54	124.35	117.70
29	X	1333	G	N3-C4-C5	-5.54	125.83	128.60
29	X	1947	G	N1-C6-O6	-5.54	116.58	119.90
29	X	1973	C	C2-N1-C1'	5.53	124.89	118.80
29	X	2041	A	N1-C6-N6	5.53	121.92	118.60
29	X	2546	G	N3-C4-N9	5.53	129.32	126.00
29	X	528	G	N1-C2-N2	5.53	121.17	116.20
29	X	567	G	C4-C5-N7	-5.53	108.59	110.80
29	X	1776	A	N9-C4-C5	5.53	108.01	105.80
29	X	2311	U	N3-C2-O2	-5.53	118.33	122.20
29	X	1918	G	C8-N9-C4	-5.52	104.19	106.40
29	X	1332	G	C5-C6-O6	-5.51	125.29	128.60
29	X	792	U	C5-C6-N1	-5.51	119.94	122.70
29	X	1658	A	C8-N9-C4	-5.51	103.59	105.80
29	X	12	U	C6-N1-C2	-5.51	117.69	121.00
29	X	919	U	C2-N1-C1'	-5.51	111.09	117.70
29	X	505	G	C2-N3-C4	-5.51	109.15	111.90
29	X	1461	C	C6-N1-C2	-5.51	118.10	120.30
29	X	236	C	C6-N1-C2	-5.50	118.10	120.30
29	X	789	G	C4-N9-C1'	5.50	133.65	126.50
29	X	583	C	C6-N1-C2	-5.50	118.10	120.30
29	X	1704	G	C5-N7-C8	-5.50	101.55	104.30
29	X	1296	G	C8-N9-C4	-5.49	104.20	106.40
29	X	2582	G	C8-N9-C1'	-5.49	119.86	127.00
29	X	2824	C	C5-C6-N1	-5.49	118.25	121.00
29	X	778	G	C6-C5-N7	-5.49	127.11	130.40
29	X	2712	G	N3-C2-N2	5.49	123.74	119.90
29	X	1670	G	N7-C8-N9	-5.49	110.36	113.10
29	X	2437	G	C5-C6-O6	-5.48	125.31	128.60
3	B	119	ARG	NE-CZ-NH2	-5.48	117.56	120.30
29	X	319	G	N1-C6-O6	5.48	123.19	119.90
29	X	1691	G	C5-C6-N1	5.48	114.24	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	X	2637	C	N3-C4-C5	5.48	124.09	121.90
29	X	2357	A	N1-C6-N6	5.47	121.89	118.60
29	X	107	G	C8-N9-C1'	-5.47	119.89	127.00
29	X	824	U	N1-C2-N3	5.47	118.18	114.90
29	X	1213	U	C5-C6-N1	5.47	125.43	122.70
29	X	2669	C	N1-C2-O2	5.47	122.18	118.90
29	X	1694	A	C5-N7-C8	-5.46	101.17	103.90
29	X	2699	G	C5-C6-O6	5.46	131.88	128.60
29	X	1714	A	N9-C4-C5	-5.46	103.61	105.80
29	X	2227	C	C6-N1-C1'	-5.46	114.25	120.80
29	X	1747	G	C2-N3-C4	5.46	114.63	111.90
29	X	2547	C	C5-C6-N1	5.46	123.73	121.00
29	X	585	U	N3-C4-O4	5.45	123.22	119.40
29	X	63	A	N1-C6-N6	5.45	121.87	118.60
29	X	1709	U	N3-C2-O2	-5.45	118.39	122.20
29	X	751	G	N3-C4-C5	-5.45	125.88	128.60
29	X	548	G	C6-C5-N7	-5.45	127.13	130.40
29	X	2481	G	N1-C2-N2	-5.45	111.30	116.20
29	X	9	U	N3-C2-O2	-5.44	118.39	122.20
29	X	996	C	C6-N1-C2	5.44	122.48	120.30
29	X	2696	A	N9-C4-C5	5.44	107.98	105.80
29	X	568	G	N1-C6-O6	-5.44	116.64	119.90
29	X	470	U	N3-C2-O2	-5.44	118.39	122.20
29	X	1449	C	C6-N1-C2	-5.43	118.13	120.30
29	X	1975	G	N9-C4-C5	5.43	107.57	105.40
29	X	2048	C	C5-C6-N1	5.43	123.72	121.00
30	Y	79	U	C5-C6-N1	-5.43	119.98	122.70
29	X	2412	A	C8-N9-C4	-5.43	103.63	105.80
29	X	2560	G	C8-N9-C4	-5.43	104.23	106.40
29	X	1991	C	C5-C6-N1	-5.43	118.29	121.00
29	X	793	G	C2-N3-C4	-5.42	109.19	111.90
29	X	1250	A	N1-C6-N6	5.42	121.85	118.60
29	X	1230	C	C6-N1-C2	-5.42	118.13	120.30
29	X	2470	U	C2-N1-C1'	5.42	124.21	117.70
29	X	1321	A	N1-C6-N6	-5.42	115.35	118.60
29	X	1960	A	C8-N9-C4	5.42	107.97	105.80
29	X	2704	U	C6-N1-C1'	5.42	128.78	121.20
29	X	2487	G	C5-C6-N1	5.42	114.21	111.50
29	X	528	G	N3-C4-N9	-5.41	122.75	126.00
29	X	993	C	C4-C5-C6	5.41	120.11	117.40
29	X	1933	G	N9-C4-C5	5.41	107.56	105.40
29	X	2851	G	N9-C4-C5	-5.41	103.23	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	X	1929	U	C5-C6-N1	-5.41	120.00	122.70
29	X	1946	U	C5-C6-N1	5.41	125.40	122.70
29	X	2698	G	C4-C5-C6	5.41	122.04	118.80
12	K	108	VAL	CB-CA-C	-5.41	101.13	111.40
29	X	931	G	N1-C2-N2	-5.41	111.34	116.20
29	X	1717	A	N1-C6-N6	-5.40	115.36	118.60
29	X	2638	G	N1-C6-O6	5.40	123.14	119.90
29	X	774	A	C8-N9-C4	-5.40	103.64	105.80
29	X	1689	U	C6-N1-C2	5.40	124.24	121.00
29	X	2496	C	N3-C4-C5	5.40	124.06	121.90
29	X	2796	A	N1-C6-N6	-5.40	115.36	118.60
29	X	760	U	N1-C2-N3	5.40	118.14	114.90
29	X	2543	A	C5-C6-N6	-5.40	119.38	123.70
29	X	2583	U	C5-C6-N1	-5.40	120.00	122.70
29	X	2553	G	N3-C4-C5	5.39	131.30	128.60
29	X	2753	C	C6-N1-C2	-5.39	118.14	120.30
29	X	1469	U	N1-C2-O2	-5.39	119.03	122.80
29	X	2227	C	C2-N1-C1'	5.39	124.73	118.80
29	X	507	A	N1-C6-N6	-5.39	115.37	118.60
29	X	2599	U	C5-C6-N1	5.39	125.39	122.70
29	X	504	G	C4-C5-N7	5.38	112.95	110.80
29	X	1712	G	N3-C4-N9	5.38	129.23	126.00
29	X	2437	G	N1-C6-O6	5.38	123.13	119.90
29	X	1624	A	C4-C5-C6	5.38	119.69	117.00
29	X	1480	G	C6-C5-N7	-5.38	127.17	130.40
29	X	1636	G	C2-N3-C4	-5.38	109.21	111.90
29	X	2500	C	N3-C2-O2	-5.38	118.14	121.90
29	X	2314	A	N9-C4-C5	5.37	107.95	105.80
29	X	789	G	C8-N9-C1'	-5.37	120.02	127.00
29	X	2407	G	C8-N9-C4	-5.37	104.25	106.40
29	X	2408	G	N3-C4-N9	5.37	129.22	126.00
29	X	940	G	N1-C6-O6	-5.37	116.68	119.90
29	X	1933	G	N3-C4-C5	-5.37	125.92	128.60
29	X	1995	G	N3-C4-C5	-5.37	125.92	128.60
29	X	2669	C	N3-C2-O2	-5.36	118.14	121.90
29	X	2698	G	N3-C4-C5	-5.36	125.92	128.60
29	X	1986	G	C4-C5-N7	-5.36	108.66	110.80
29	X	2483	U	C5-C6-N1	5.36	125.38	122.70
29	X	2689	C	C2-N1-C1'	-5.36	112.91	118.80
29	X	1984	A	C6-N1-C2	5.35	121.81	118.60
29	X	1243	G	C5-C6-O6	-5.35	125.39	128.60
29	X	30	G	C8-N9-C4	-5.35	104.26	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	X	1775	A	N7-C8-N9	-5.35	111.13	113.80
29	X	2014	A	C8-N9-C4	-5.35	103.66	105.80
29	X	2307	A	C2-N3-C4	-5.35	107.93	110.60
29	X	845	U	C5-C6-N1	5.34	125.37	122.70
29	X	1704	G	N9-C4-C5	-5.34	103.26	105.40
29	X	2661	G	N1-C6-O6	5.34	123.11	119.90
29	X	1976	U	N3-C2-O2	-5.34	118.46	122.20
29	X	741	G	C8-N9-C4	5.34	108.53	106.40
22	U	17	SER	C-N-CA	5.33	135.03	121.70
29	X	1704	G	N3-C4-N9	5.33	129.20	126.00
29	X	1305	C	N1-C2-O2	-5.33	115.70	118.90
29	X	2687	G	N3-C4-C5	5.33	131.26	128.60
29	X	2843	A	C8-N9-C4	5.33	107.93	105.80
29	X	33	C	N1-C2-O2	5.32	122.09	118.90
29	X	2598	C	N3-C2-O2	-5.32	118.18	121.90
29	X	567	G	N3-C4-N9	-5.32	122.81	126.00
29	X	576	A	C5-C6-N6	5.32	127.95	123.70
29	X	1346	C	C6-N1-C2	-5.32	118.17	120.30
29	X	488	A	C8-N9-C4	-5.32	103.67	105.80
29	X	786	U	N3-C2-O2	-5.31	118.48	122.20
29	X	1300	A	C8-N9-C4	-5.31	103.67	105.80
29	X	2315	A	N1-C6-N6	-5.31	115.41	118.60
29	X	12	U	N3-C2-O2	-5.31	118.48	122.20
29	X	2679	G	C8-N9-C4	5.31	108.52	106.40
29	X	749	C	C2-N1-C1'	5.31	124.64	118.80
29	X	2699	G	C6-N1-C2	5.31	128.28	125.10
29	X	557	U	C6-N1-C2	-5.30	117.82	121.00
29	X	749	C	C5-C6-N1	5.30	123.65	121.00
29	X	2692	A	C4-C5-C6	-5.30	114.35	117.00
29	X	1668	G	C5-N7-C8	-5.30	101.65	104.30
29	X	2700	U	N1-C2-O2	5.30	126.51	122.80
29	X	1333	G	C5-C6-O6	5.30	131.78	128.60
29	X	1756	C	N3-C2-O2	5.30	125.61	121.90
29	X	2697	G	N7-C8-N9	5.30	115.75	113.10
29	X	2015	G	C4-C5-N7	5.29	112.92	110.80
29	X	2594	U	C5-C6-N1	5.29	125.35	122.70
29	X	1751	A	N7-C8-N9	-5.29	111.16	113.80
29	X	957	G	C5-C6-O6	5.29	131.77	128.60
29	X	2561	G	C4-C5-C6	-5.29	115.63	118.80
29	X	829	C	N3-C4-C5	5.29	124.01	121.90
29	X	2055	G	N3-C2-N2	5.28	123.60	119.90
29	X	1308	C	N3-C4-N4	5.28	121.70	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	X	2853	U	C5-C6-N1	-5.28	120.06	122.70
29	X	536	A	C6-N1-C2	-5.27	115.44	118.60
29	X	755	C	C6-N1-C2	5.27	122.41	120.30
29	X	1295	U	C6-N1-C2	-5.27	117.84	121.00
29	X	2665	G	C4-N9-C1'	-5.27	119.65	126.50
29	X	956	A	C2-N3-C4	5.27	113.23	110.60
29	X	664	C	N1-C2-O2	5.26	122.06	118.90
29	X	2498	U	N3-C4-C5	-5.26	111.44	114.60
29	X	689	A	N1-C6-N6	5.26	121.76	118.60
29	X	2702	G	N3-C4-N9	5.26	129.16	126.00
29	X	350	U	C5-C6-N1	5.26	125.33	122.70
29	X	13	A	C4-C5-C6	5.26	119.63	117.00
29	X	2049	C	N3-C2-O2	-5.26	118.22	121.90
29	X	2554	C	C5-C4-N4	-5.26	116.52	120.20
29	X	957	G	C5-C6-N1	5.25	114.13	111.50
29	X	2239	C	N3-C2-O2	-5.25	118.22	121.90
29	X	2251	U	C6-N1-C2	5.25	124.15	121.00
29	X	778	G	N1-C6-O6	5.25	123.05	119.90
29	X	2398	U	N3-C4-O4	5.25	123.07	119.40
29	X	1686	A	N7-C8-N9	5.24	116.42	113.80
29	X	2051	U	N3-C2-O2	-5.24	118.53	122.20
29	X	2383	C	N3-C2-O2	-5.24	118.23	121.90
29	X	2441	U	N3-C2-O2	-5.24	118.53	122.20
29	X	2561	G	C2-N3-C4	5.24	114.52	111.90
29	X	579	G	N9-C4-C5	5.24	107.50	105.40
29	X	2297	G	C4-C5-N7	-5.24	108.70	110.80
29	X	21	A	C8-N9-C4	-5.24	103.70	105.80
29	X	2795	A	C8-N9-C4	-5.24	103.70	105.80
29	X	1250	A	C6-C5-N7	-5.24	128.63	132.30
29	X	2660	C	C4-C5-C6	5.24	120.02	117.40
29	X	2015	G	C8-N9-C1'	5.24	133.81	127.00
29	X	2524	G	C2-N3-C4	5.23	114.52	111.90
29	X	2845	C	N3-C4-C5	-5.23	119.81	121.90
29	X	700	C	C2-N3-C4	5.23	122.51	119.90
29	X	1715	A	C4-C5-N7	5.23	113.31	110.70
29	X	2569	A	N7-C8-N9	-5.23	111.19	113.80
29	X	2578	G	N3-C4-N9	5.23	129.14	126.00
29	X	1693	A	N9-C4-C5	-5.23	103.71	105.80
29	X	1993	G	N1-C6-O6	5.23	123.03	119.90
29	X	2482	A	N1-C2-N3	5.23	131.91	129.30
29	X	1683	G	C6-C5-N7	5.22	133.53	130.40
29	X	1766	U	C6-N1-C2	5.22	124.14	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	X	2543	A	N1-C6-N6	5.22	121.73	118.60
29	X	2620	G	N1-C6-O6	5.22	123.03	119.90
29	X	2001	G	C8-N9-C4	-5.22	104.31	106.40
29	X	2402	U	C6-N1-C2	-5.22	117.87	121.00
29	X	1981	A	C8-N9-C4	5.22	107.89	105.80
29	X	2695	C	N3-C2-O2	-5.21	118.25	121.90
29	X	2843	A	N7-C8-N9	-5.21	111.19	113.80
29	X	1663	C	N3-C4-N4	5.21	121.65	118.00
29	X	1939	U	C6-N1-C2	-5.21	117.87	121.00
29	X	1666	G	C8-N9-C4	5.21	108.48	106.40
29	X	1690	U	C5-C6-N1	5.21	125.31	122.70
29	X	955	G	C8-N9-C4	-5.21	104.32	106.40
29	X	2483	U	N1-C2-O2	5.21	126.45	122.80
30	Y	34	C	C6-N1-C2	-5.21	118.22	120.30
29	X	12	U	C2-N1-C1'	5.21	123.95	117.70
29	X	746	G	N3-C4-C5	-5.20	126.00	128.60
29	X	22	C	C6-N1-C1'	-5.20	114.56	120.80
29	X	2000	U	N1-C2-O2	-5.20	119.16	122.80
29	X	1721	G	N3-C4-N9	-5.20	122.88	126.00
29	X	679	C	N3-C2-O2	-5.20	118.26	121.90
29	X	754	G	C5-N7-C8	-5.20	101.70	104.30
29	X	989	G	C4-N9-C1'	-5.20	119.74	126.50
29	X	1245	G	N7-C8-N9	5.20	115.70	113.10
29	X	1629	G	N1-C6-O6	-5.20	116.78	119.90
29	X	2300	G	N3-C4-C5	-5.20	126.00	128.60
29	X	2712	G	C8-N9-C1'	-5.20	120.25	127.00
29	X	796	A	C8-N9-C4	-5.19	103.72	105.80
29	X	2009	U	N3-C4-O4	5.19	123.03	119.40
29	X	2053	G	C4-N9-C1'	-5.19	119.75	126.50
29	X	1465	G	N3-C4-C5	-5.19	126.01	128.60
29	X	2611	A	C2-N3-C4	-5.19	108.01	110.60
29	X	1974	U	N3-C4-C5	-5.19	111.49	114.60
29	X	469	G	N1-C6-O6	-5.18	116.79	119.90
29	X	2606	G	C6-C5-N7	-5.18	127.29	130.40
29	X	2676	G	C4-C5-C6	5.18	121.91	118.80
29	X	2792	C	C5-C6-N1	-5.18	118.41	121.00
29	X	1255	A	N1-C6-N6	-5.18	115.49	118.60
29	X	1674	C	C5-C6-N1	-5.18	118.41	121.00
29	X	219	G	C8-N9-C1'	5.17	133.73	127.00
29	X	1317	G	C8-N9-C1'	5.17	133.73	127.00
29	X	2437	G	N3-C4-N9	5.17	129.10	126.00
29	X	544	U	N1-C2-O2	5.17	126.42	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	X	1142	G	C5-C6-O6	-5.17	125.50	128.60
29	X	224	G	N3-C4-N9	5.17	129.10	126.00
29	X	1970	G	N3-C4-C5	-5.17	126.02	128.60
29	X	2215	C	C6-N1-C2	5.17	122.37	120.30
29	X	2821	G	N7-C8-N9	-5.17	110.52	113.10
29	X	1704	G	N7-C8-N9	5.16	115.68	113.10
29	X	567	G	C6-C5-N7	5.16	133.50	130.40
29	X	2542	U	C5-C4-O4	5.16	129.00	125.90
29	X	1753	A	N7-C8-N9	5.16	116.38	113.80
29	X	595	A	C4-C5-C6	-5.16	114.42	117.00
29	X	1975	G	C8-N9-C1'	5.16	133.70	127.00
29	X	2524	G	N1-C6-O6	-5.16	116.81	119.90
29	X	1035	G	N3-C4-C5	-5.15	126.02	128.60
29	X	1323	G	C6-C5-N7	-5.15	127.31	130.40
29	X	945	G	C8-N9-C4	-5.15	104.34	106.40
29	X	1291	G	C8-N9-C4	5.15	108.46	106.40
29	X	1315	A	N9-C4-C5	5.15	107.86	105.80
29	X	1476	G	C8-N9-C4	-5.15	104.34	106.40
29	X	2870	C	N3-C2-O2	-5.15	118.30	121.90
29	X	943	U	C6-N1-C1'	-5.15	113.99	121.20
29	X	968	C	C5-C4-N4	-5.15	116.60	120.20
29	X	2806	G	N1-C2-N2	-5.15	111.57	116.20
29	X	2835	A	N9-C4-C5	-5.15	103.74	105.80
29	X	1714	A	C5-C6-N6	-5.14	119.58	123.70
29	X	2854	G	N7-C8-N9	5.14	115.67	113.10
29	X	2327	U	C5-C6-N1	5.14	125.27	122.70
29	X	2461	G	C4-N9-C1'	5.14	133.19	126.50
29	X	472	C	C5-C6-N1	5.14	123.57	121.00
29	X	1279	G	N1-C2-N2	-5.14	111.57	116.20
29	X	1632	A	N1-C6-N6	5.14	121.69	118.60
29	X	1679	U	C4-C5-C6	5.14	122.78	119.70
29	X	1238	A	C6-C5-N7	5.14	135.90	132.30
29	X	1931	G	N1-C6-O6	5.14	122.98	119.90
29	X	854	G	N7-C8-N9	5.13	115.67	113.10
29	X	2869	U	C6-N1-C2	-5.13	117.92	121.00
29	X	483	A	C2-N3-C4	-5.13	108.03	110.60
29	X	1862	C	C6-N1-C2	-5.13	118.25	120.30
29	X	526	C	C6-N1-C2	-5.13	118.25	120.30
29	X	545	C	C6-N1-C1'	5.13	126.96	120.80
29	X	1690	U	C5-C4-O4	-5.13	122.82	125.90
29	X	1984	A	C2-N3-C4	-5.13	108.03	110.60
29	X	2422	C	N3-C2-O2	-5.13	118.31	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	J	42	TRP	N-CA-C	-5.13	97.15	111.00
29	X	1984	A	N3-C4-N9	-5.13	123.30	127.40
29	X	2541	U	N1-C2-O2	5.13	126.39	122.80
29	X	2559	U	C5-C6-N1	5.13	125.26	122.70
29	X	8	A	C6-N1-C2	-5.13	115.52	118.60
29	X	1940	C	C2-N1-C1'	5.13	124.44	118.80
29	X	1989	C	C4-C5-C6	-5.13	114.84	117.40
30	Y	93	G	N1-C6-O6	5.13	122.98	119.90
29	X	990	A	N7-C8-N9	-5.12	111.24	113.80
29	X	1663	C	N1-C2-O2	5.12	121.97	118.90
29	X	2442	C	C6-N1-C2	-5.12	118.25	120.30
29	X	2492	G	C5-C6-O6	5.12	131.67	128.60
29	X	1661	C	C6-N1-C2	-5.12	118.25	120.30
29	X	2227	C	N1-C2-O2	5.12	121.97	118.90
29	X	2559	U	C2-N1-C1'	5.12	123.85	117.70
29	X	2489	C	N3-C4-N4	5.12	121.58	118.00
29	X	541	C	C5-C6-N1	-5.12	118.44	121.00
29	X	934	G	C8-N9-C4	-5.12	104.35	106.40
29	X	931	G	C8-N9-C1'	-5.12	120.35	127.00
29	X	1013	G	N3-C4-N9	5.11	129.07	126.00
29	X	1308	C	C5-C6-N1	5.11	123.56	121.00
29	X	1779	C	C6-N1-C2	5.11	122.34	120.30
29	X	2660	C	C5-C6-N1	-5.11	118.44	121.00
29	X	39	C	C6-N1-C2	-5.11	118.26	120.30
29	X	1663	C	C6-N1-C2	-5.11	118.26	120.30
29	X	1971	C	N3-C4-C5	5.11	123.94	121.90
29	X	1344	C	C6-N1-C2	5.10	122.34	120.30
29	X	534	U	N1-C2-O2	-5.10	119.23	122.80
29	X	689	A	C8-N9-C4	-5.10	103.76	105.80
29	X	1298	G	N3-C4-N9	5.10	129.06	126.00
29	X	2017	U	C5-C6-N1	5.10	125.25	122.70
29	X	2800	C	C5-C6-N1	5.10	123.55	121.00
29	X	1332	G	C4-C5-N7	5.10	112.84	110.80
29	X	2494	C	C6-N1-C2	5.10	122.34	120.30
29	X	1939	U	N3-C2-O2	-5.10	118.63	122.20
29	X	2007	G	N7-C8-N9	-5.09	110.55	113.10
29	X	2559	U	N1-C2-N3	-5.09	111.85	114.90
29	X	852	U	C6-N1-C2	5.09	124.05	121.00
29	X	974	U	N3-C4-O4	5.09	122.96	119.40
29	X	1138	A	C8-N9-C4	-5.09	103.76	105.80
29	X	660	G	N3-C2-N2	-5.09	116.34	119.90
29	X	2599	U	C6-N1-C2	-5.09	117.95	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	X	540	G	N3-C2-N2	-5.08	116.34	119.90
29	X	2510	A	N1-C6-N6	5.08	121.65	118.60
29	X	597	U	C6-N1-C2	5.08	124.05	121.00
29	X	1016	C	N3-C4-N4	5.07	121.55	118.00
13	L	92	GLY	N-CA-C	-5.07	100.42	113.10
29	X	1750	A	C4-C5-C6	5.07	119.53	117.00
29	X	2398	U	C5-C6-N1	5.07	125.23	122.70
29	X	812	G	C8-N9-C4	-5.06	104.38	106.40
30	Y	107	C	C6-N1-C2	-5.06	118.28	120.30
29	X	1292	A	N3-C4-C5	5.06	130.34	126.80
29	X	1332	G	C8-N9-C1'	-5.06	120.42	127.00
29	X	2718	A	N7-C8-N9	-5.06	111.27	113.80
29	X	1301	U	C2-N3-C4	5.06	130.03	127.00
29	X	496	C	N1-C2-N3	-5.05	115.66	119.20
29	X	1238	A	C5-C6-N6	5.05	127.74	123.70
29	X	2542	U	N1-C2-N3	5.05	117.93	114.90
29	X	1663	C	C2-N3-C4	5.05	122.42	119.90
29	X	1652	G	C6-C5-N7	-5.05	127.37	130.40
29	X	2576	G	C5-C6-N1	-5.05	108.98	111.50
29	X	1723	U	N3-C2-O2	-5.04	118.67	122.20
29	X	1750	A	C8-N9-C4	-5.04	103.78	105.80
29	X	2563	U	N3-C2-O2	-5.04	118.67	122.20
29	X	2685	A	N1-C6-N6	-5.04	115.58	118.60
29	X	559	C	C5-C6-N1	5.03	123.52	121.00
29	X	174	A	C2-N3-C4	5.03	113.12	110.60
29	X	1231	A	C8-N9-C4	-5.03	103.79	105.80
29	X	1748	U	N3-C2-O2	5.03	125.72	122.20
29	X	2425	G	C4-N9-C1'	5.03	133.04	126.50
29	X	2553	G	N3-C4-N9	-5.03	122.98	126.00
29	X	632	A	N1-C6-N6	-5.03	115.58	118.60
29	X	1692	C	N1-C2-O2	-5.03	115.88	118.90
29	X	1253	C	N3-C2-O2	-5.03	118.38	121.90
29	X	1975	G	C4-N9-C1'	-5.03	119.96	126.50
29	X	413	G	N3-C4-C5	-5.02	126.09	128.60
29	X	2522	G	N1-C6-O6	-5.02	116.89	119.90
29	X	476	G	C5-C6-O6	5.02	131.61	128.60
29	X	2605	C	N1-C2-O2	5.02	121.91	118.90
29	X	2704	U	C4-C5-C6	5.02	122.71	119.70
29	X	90	G	N3-C4-N9	5.01	129.01	126.00
29	X	1250	A	C4-C5-C6	5.01	119.51	117.00
29	X	1657	A	C8-N9-C4	5.01	107.81	105.80
29	X	2483	U	C2-N1-C1'	5.01	123.72	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	X	1333	G	N1-C2-N2	-5.01	111.69	116.20
29	X	1715	A	C6-C5-N7	-5.01	128.79	132.30
29	X	1138	A	N7-C8-N9	5.01	116.30	113.80
29	X	2586	G	N3-C4-N9	5.01	129.00	126.00
29	X	2597	G	C4-C5-C6	5.01	121.81	118.80
29	X	223	C	C6-N1-C2	-5.01	118.30	120.30
29	X	540	G	C8-N9-C4	-5.01	104.40	106.40
29	X	829	C	C5-C6-N1	-5.01	118.50	121.00
29	X	334	G	C5-C6-O6	-5.00	125.60	128.60
29	X	762	A	C4-C5-N7	5.00	113.20	110.70

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	85	ALA	Peptide
9	H	36	THR	Peptide
10	I	52	GLY	Peptide
13	L	87	VAL	Peptide
14	M	108	LYS	Peptide
14	M	2	GLN	Peptide
19	R	105	ARG	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	1651	0	1693	51	0
2	A	2107	0	2190	133	0
3	B	1540	0	1600	117	0
4	C	1507	0	1525	115	0
5	D	1401	0	1481	81	0
6	E	1287	0	1336	53	0
7	F	1048	0	1088	35	0
8	G	1115	0	1144	50	0
9	H	997	0	1046	81	0
10	I	1068	0	1103	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	J	1091	0	1125	66	0
12	K	879	0	930	79	0
13	L	778	0	820	57	0
14	M	867	0	890	64	0
15	N	978	0	1020	95	0
16	O	742	0	756	37	0
17	P	1014	0	1096	80	0
18	Q	727	0	753	31	0
19	R	826	0	881	65	0
20	S	1346	0	1372	71	0
21	T	626	0	655	38	0
22	U	553	0	604	50	0
23	V	534	0	558	13	0
24	W	424	0	470	24	0
25	Z	453	0	455	49	0
26	1	404	0	416	25	0
27	2	393	0	420	24	0
28	3	509	0	565	56	0
29	X	59673	0	30060	1967	0
30	Y	2601	0	1327	91	0
31	A	1	0	0	0	0
31	H	1	0	0	0	0
31	M	1	0	0	0	0
31	N	1	0	0	0	0
31	X	177	0	0	1	0
31	Y	5	0	0	0	0
32	X	36	0	29	2	0
All	All	89361	0	59408	3326	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 23.

All (3326) 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)
3:B:14:ILE:HB	14:M:20:HIS:HD2	1.16	1.11
12:K:79:VAL:HA	12:K:83:VAL:HG13	1.35	1.06
29:X:1225:G:H1'	29:X:1250:A:H61	1.21	1.03
29:X:517:A:H5"	29:X:518:A:H5'	1.37	1.02
29:X:2690:A:OP1	29:X:2692:A:OP2	1.78	0.99
29:X:2550:C:H5"	29:X:2551:A:H5'	1.42	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:U:21:ARG:HH12	29:X:400:U:H5'	1.28	0.98
15:N:48:ARG:HD2	29:X:1167:A:H61	1.27	0.97
29:X:320:A:N3	29:X:340:G:O2'	1.96	0.97
24:W:43:MET:HE1	29:X:940:G:H21	1.30	0.97
29:X:2796:A:H2'	29:X:2797:G:H8	1.30	0.96
10:I:21:ARG:NH2	29:X:596:C:OP2	1.99	0.96
29:X:623:G:O2'	29:X:626:A:N6	1.99	0.95
29:X:1230:C:H2'	29:X:1231:A:H8	1.31	0.94
3:B:14:ILE:HB	14:M:20:HIS:CD2	2.03	0.93
28:3:29:LYS:NZ	29:X:2398:U:OP2	2.01	0.93
25:Z:19:ARG:NH2	29:X:1277:G:OP1	2.02	0.92
14:M:25:PRO:HB3	14:M:93:ILE:HD11	1.53	0.91
29:X:2796:A:H2'	29:X:2797:G:C8	2.05	0.91
29:X:646:C:O2'	29:X:650:U:OP1	1.90	0.90
14:M:82:PRO:O	14:M:84:ALA:N	2.04	0.90
11:J:19:THR:HG22	11:J:20:GLY:H	1.37	0.89
12:K:36:THR:OG1	29:X:1291:G:OP1	1.91	0.89
17:P:31:VAL:HG11	17:P:124:ILE:HD11	1.54	0.89
8:G:140:GLN:HG3	29:X:567:G:H5'	1.55	0.88
29:X:2083:G:H1	29:X:2172:U:H3	1.21	0.88
14:M:42:GLY:O	14:M:44:ARG:N	2.08	0.87
28:3:34:THR:OG1	29:X:2399:C:OP1	1.92	0.86
3:B:75:THR:HG22	3:B:77:ILE:H	1.38	0.86
10:I:21:ARG:HA	29:X:824:U:H2'	1.55	0.86
6:E:22:GLY:HA3	6:E:39:THR:HG22	1.56	0.86
14:M:29:PRO:HD3	14:M:57:ILE:HD11	1.57	0.86
29:X:320:A:N6	29:X:1223:G:O2'	2.08	0.86
29:X:578:U:O2'	29:X:994:A:N1	2.08	0.86
24:W:25:LEU:HD22	24:W:30:ASP:HB3	1.57	0.85
12:K:53:THR:OG1	29:X:2815:C:OP1	1.92	0.85
17:P:49:SER:O	17:P:51:GLN:N	2.08	0.85
29:X:834:A:H1'	29:X:955:G:H5'	1.58	0.85
29:X:1230:C:H2'	29:X:1231:A:C8	2.12	0.84
29:X:1919:A:H2	29:X:1926:U:H3	1.24	0.84
13:L:18:ARG:NH2	29:X:2271:C:OP2	2.10	0.84
29:X:469:G:N2	29:X:481:A:OP2	2.08	0.84
29:X:1989:C:O2'	29:X:2798:A:N3	2.11	0.84
29:X:2821:G:H2'	29:X:2822:U:C6	2.12	0.83
12:K:11:ASN:HD22	12:K:11:ASN:H	1.25	0.83
29:X:841:G:H2'	29:X:842:A:C8	2.13	0.83
29:X:1202:U:H2'	29:X:1203:A:H8	1.44	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:2:43:THR:HG22	27:2:45:SER:H	1.41	0.83
22:U:17:SER:HB2	22:U:18:VAL:HB	1.60	0.83
29:X:2352:A:H2'	29:X:2353:G:C8	2.14	0.82
27:2:46:ASP:OD1	29:X:125:A:N6	2.13	0.82
29:X:1983:G:N2	29:X:2668:U:O4	2.10	0.82
29:X:2522:G:H2'	29:X:2523:G:C8	2.14	0.82
20:S:141:MET:HG2	20:S:145:ASP:HB2	1.62	0.81
29:X:1060:C:H42	29:X:2731:G:H1	1.26	0.81
29:X:693:A:H2'	29:X:694:G:H8	1.45	0.81
3:B:111:LYS:NZ	29:X:2704:U:OP1	2.13	0.81
15:N:37:GLN:HA	15:N:40:LEU:HD12	1.60	0.81
29:X:1244:U:H2'	29:X:1245:G:H8	1.45	0.81
12:K:13:ASN:O	12:K:17:ARG:NH2	2.14	0.81
29:X:1909:U:OP2	29:X:1912:G:N1	2.13	0.80
29:X:2668:U:O2	29:X:2693:U:H5"	1.82	0.80
29:X:2543:A:OP1	29:X:2627:G:O2'	1.97	0.80
29:X:1681:A:N6	29:X:1975:G:O6	2.14	0.80
3:B:189:PRO:HA	29:X:2659:C:H5'	1.61	0.80
15:N:49:ASP:HA	15:N:52:ASN:HB2	1.61	0.80
28:3:64:ARG:NH2	29:X:219:G:OP1	2.15	0.80
29:X:1336:G:H2'	29:X:1337:G:H5'	1.63	0.79
29:X:652:C:H42	29:X:657:A:H61	1.28	0.79
29:X:1674:C:H2'	29:X:1675:C:C6	2.17	0.79
29:X:2309:G:N2	29:X:2365:U:O2	2.16	0.79
29:X:698:A:OP1	29:X:699:G:N2	2.15	0.79
29:X:1573:G:H3'	29:X:1574:A:H5"	1.61	0.79
29:X:79:G:H2'	29:X:80:A:H8	1.48	0.79
22:U:48:LYS:HG2	22:U:49:LYS:H	1.48	0.79
29:X:833:A:N3	29:X:954:U:O2'	2.15	0.79
29:X:2118:A:N6	29:X:2140:G:O6	2.15	0.79
17:P:109:ARG:NH1	29:X:760:U:O2'	2.15	0.79
11:J:26:ASP:N	11:J:26:ASP:OD1	2.14	0.78
2:A:60:ARG:HD3	2:A:86:PRO:HB2	1.65	0.78
29:X:312:G:HO2'	29:X:313:U:H6	1.31	0.78
12:K:103:ARG:HH21	12:K:108:VAL:HB	1.48	0.78
29:X:2303:C:H5"	29:X:2304:G:H5"	1.66	0.78
29:X:546:A:H2'	29:X:547:U:H6	1.49	0.78
2:A:16:MET:HG3	2:A:207:GLY:HA3	1.65	0.78
26:1:45:ALA:HB1	29:X:2350:G:H4'	1.66	0.78
14:M:69:ARG:HD2	14:M:78:GLU:HG2	1.64	0.78
16:O:46:VAL:HG13	16:O:51:ALA:HB2	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:32:ARG:NH1	17:P:120:ARG:O	2.16	0.78
29:X:1164:C:H2'	29:X:1165:G:C8	2.18	0.78
5:D:75:SER:H	5:D:79:LEU:HD22	1.49	0.77
17:P:15:LYS:NZ	29:X:512:A:O2'	2.12	0.77
17:P:28:ALA:HB2	17:P:71:VAL:HG21	1.66	0.77
4:C:150:LEU:HA	4:C:187:VAL:HB	1.64	0.77
9:H:64:VAL:HG22	9:H:106:ARG:HH21	1.48	0.77
10:I:28:LYS:HB3	10:I:29:THR:HG23	1.67	0.77
2:A:157:ARG:NH1	29:X:1810:U:OP2	2.18	0.77
29:X:226:C:H4'	29:X:227:G:H5"	1.66	0.77
29:X:2283:G:H22	29:X:2291:U:H3	1.32	0.77
29:X:2772:U:H2'	29:X:2773:G:H8	1.48	0.77
14:M:60:SER:HA	14:M:64:LYS:HB2	1.64	0.77
20:S:67:LYS:HD2	20:S:84:TYR:HB2	1.66	0.77
22:U:32:ARG:NE	22:U:32:ARG:H	1.81	0.77
29:X:1097:A:O2'	29:X:1098:G:N7	2.17	0.77
17:P:117:ILE:HD11	29:X:1995:G:H4'	1.66	0.77
29:X:7:G:H2'	29:X:8:A:H8	1.50	0.77
8:G:88:VAL:HG21	8:G:127:ILE:HD11	1.67	0.77
29:X:2494:C:H42	29:X:2548:G:H1	1.30	0.77
3:B:6:GLY:HA3	3:B:27:LEU:O	1.85	0.77
2:A:69:ARG:HH12	2:A:192:THR:HG22	1.50	0.77
29:X:2418:A:H4'	29:X:2419:C:C5'	2.16	0.76
30:Y:40:C:O2	30:Y:50:U:O2'	2.01	0.76
15:N:102:GLU:OE1	16:O:13:ARG:NH2	2.18	0.76
29:X:1770:U:H5	29:X:1775:A:N7	1.83	0.76
29:X:1674:C:H2'	29:X:1675:C:H6	1.49	0.76
27:2:12:ARG:NH1	29:X:476:G:OP1	2.19	0.76
17:P:81:HIS:O	17:P:83:ASP:N	2.18	0.76
25:Z:15:LYS:O	25:Z:18:MET:N	2.18	0.76
29:X:1058:G:O2'	29:X:1120:C:N4	2.19	0.76
10:I:28:LYS:O	10:I:30:ALA:N	2.19	0.76
3:B:78:LEU:O	3:B:79:ARG:NE	2.17	0.76
29:X:693:A:H2'	29:X:694:G:C8	2.20	0.76
6:E:107:ILE:O	6:E:152:ARG:NH1	2.19	0.76
29:X:857:U:H3'	29:X:858:G:C8	2.21	0.76
11:J:32:ASP:H	11:J:108:ALA:HB2	1.51	0.76
20:S:25:ASN:HA	20:S:85:MET:HB2	1.68	0.76
24:W:40:VAL:HA	24:W:43:MET:HE3	1.67	0.75
19:R:37:LEU:HD11	19:R:49:GLU:HG3	1.68	0.75
5:D:111:ILE:HG12	5:D:137:ILE:HD12	1.65	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1225:G:H1'	29:X:1250:A:N6	1.98	0.75
29:X:1104:G:H21	29:X:1109:A:H62	1.33	0.75
29:X:2629:U:H2'	29:X:2630:C:H6	1.52	0.75
21:T:25:LYS:HB2	21:T:37:LEU:HA	1.67	0.75
17:P:15:LYS:HB3	29:X:512:A:H4'	1.67	0.74
16:O:14:VAL:HG11	16:O:95:ILE:HG13	1.69	0.74
9:H:22:ILE:HD11	29:X:1935:A:C6	2.22	0.74
29:X:43:A:H61	29:X:447:U:H3	1.36	0.74
5:D:14:PRO:HA	5:D:17:MET:HB2	1.68	0.74
15:N:12:ARG:NH1	29:X:1229:C:OP2	2.21	0.74
19:R:15:HIS:CD2	19:R:16:PHE:HD2	2.06	0.74
29:X:867:G:H1	29:X:935:C:H42	1.32	0.74
14:M:93:ILE:HD12	14:M:93:ILE:H	1.52	0.74
29:X:455:A:H2	29:X:1258:G:N3	1.85	0.74
29:X:1437:A:H2'	29:X:1438:G:H8	1.52	0.74
30:Y:4:C:N4	30:Y:121:G:O6	2.18	0.74
29:X:2543:A:H5'	29:X:2627:G:H4'	1.69	0.74
29:X:2789:U:H3	29:X:2861:A:H61	1.36	0.74
29:X:2672:U:H2'	29:X:2673:G:H8	1.52	0.74
5:D:131:GLY:HA2	5:D:154:ILE:H	1.52	0.73
13:L:39:TYR:OH	30:Y:118:G:N3	2.21	0.73
29:X:205:A:H2'	29:X:206:U:H5'	1.68	0.73
29:X:2639:A:H5"	29:X:2639:A:N3	2.02	0.73
5:D:38:GLU:HB3	5:D:87:ILE:HB	1.70	0.73
29:X:517:A:C5'	29:X:518:A:H5'	2.18	0.73
17:P:109:ARG:NH2	29:X:1996:A:N3	2.37	0.73
29:X:333:A:H5'	29:X:351:A:H1'	1.70	0.73
7:F:73:PRO:O	7:F:75:SER:N	2.20	0.73
29:X:2417:U:O2'	29:X:2419:C:OP1	2.06	0.73
29:X:2811:G:H2'	29:X:2812:A:C8	2.23	0.73
8:G:151:TYR:OH	8:G:158:HIS:NE2	2.21	0.73
5:D:92:ARG:NH2	30:Y:47:A:OP1	2.21	0.73
12:K:81:ASP:O	12:K:85:PRO:HG3	1.88	0.73
29:X:2550:C:H5"	29:X:2551:A:C5'	2.18	0.73
29:X:692:C:H2'	29:X:693:A:H8	1.54	0.73
5:D:60:ILE:HG22	5:D:140:GLU:HB2	1.70	0.73
10:I:130:ILE:HG12	10:I:140:VAL:HG21	1.70	0.73
19:R:93:ARG:NH2	29:X:312:G:OP2	2.19	0.73
29:X:1279:G:O2'	29:X:1995:G:O6	2.06	0.73
19:R:16:PHE:CE2	19:R:81:VAL:HG11	2.23	0.73
17:P:62:ARG:HH11	25:Z:25:LEU:HD11	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1726:C:O2'	29:X:2834:A:N3	2.21	0.72
29:X:1479:G:H2'	29:X:1480:G:C8	2.24	0.72
29:X:2270:U:O2'	29:X:2353:G:N3	2.21	0.72
29:X:402:A:N7	29:X:2392:G:O2'	2.22	0.72
2:A:201:HIS:O	2:A:203:ASN:N	2.21	0.72
29:X:2611:A:H61	29:X:2766:U:H3	1.36	0.72
29:X:421:G:H2'	29:X:422:C:H6	1.54	0.72
23:V:51:ALA:O	23:V:55:THR:OG1	2.08	0.72
2:A:108:PRO:HB3	2:A:143:HIS:HE1	1.53	0.72
29:X:834:A:H5'	29:X:835:U:H6	1.53	0.72
9:H:21:CYS:SG	9:H:22:ILE:N	2.62	0.72
13:L:89:PHE:O	13:L:91:ARG:NH2	2.22	0.72
15:N:48:ARG:NH2	29:X:987:G:OP1	2.22	0.72
9:H:22:ILE:HG22	9:H:52:VAL:HG12	1.70	0.72
29:X:488:A:H2'	29:X:489:A:C8	2.25	0.72
29:X:2014:A:C6	29:X:2477:C:H1'	2.25	0.72
3:B:84:PHE:CD2	3:B:86:PRO:HD3	2.25	0.72
2:A:17:THR:OG1	2:A:205:VAL:N	2.22	0.72
28:3:52:LYS:O	28:3:54:GLU:N	2.23	0.72
29:X:1164:C:H2'	29:X:1165:G:H8	1.53	0.72
2:A:239:ARG:HG3	29:X:2569:A:H5"	1.72	0.72
12:K:87:TYR:CD1	12:K:90:ARG:HD2	2.25	0.72
24:W:5:LEU:HB2	24:W:25:LEU:HD13	1.71	0.72
29:X:46:C:H2'	29:X:47:G:H8	1.52	0.72
29:X:2336:G:N2	29:X:2339:A:OP2	2.22	0.72
2:A:39:LYS:NZ	2:A:58:HIS:H	1.88	0.71
29:X:2522:G:H2'	29:X:2523:G:H8	1.54	0.71
20:S:54:ILE:HB	20:S:62:PHE:HB2	1.70	0.71
29:X:1437:A:H2'	29:X:1438:G:C8	2.25	0.71
9:H:47:VAL:HG23	9:H:77:THR:HG23	1.72	0.71
10:I:63:ARG:NH1	29:X:2396:C:OP1	2.22	0.71
15:N:26:GLY:O	15:N:28:ARG:N	2.23	0.71
20:S:148:THR:HB	20:S:165:GLU:HA	1.71	0.71
29:X:1333:G:C2	29:X:1342:U:H5"	2.26	0.71
29:X:2761:A:H5"	29:X:2762:G:H5'	1.72	0.71
12:K:3:HIS:O	12:K:5:LYS:N	2.21	0.71
19:R:77:HIS:HD2	29:X:339:U:H4'	1.55	0.71
15:N:111:ASP:O	15:N:115:ASN:ND2	2.22	0.71
19:R:22:VAL:HG11	19:R:81:VAL:HG22	1.70	0.71
23:V:2:LYS:NZ	29:X:76:C:OP1	2.17	0.71
12:K:10:LEU:O	12:K:12:ARG:N	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:75:SER:O	7:F:79:ARG:NH1	2.23	0.71
29:X:789:G:N1	29:X:2055:G:OP1	2.17	0.71
30:Y:25:G:H1	30:Y:62:C:H42	1.37	0.71
22:U:31:GLY:HA2	22:U:32:ARG:HH11	1.56	0.70
29:X:1030:U:H3	29:X:1153:A:N6	1.89	0.70
29:X:1505:U:H1'	29:X:1506:C:H2'	1.73	0.70
29:X:2665:G:C2	29:X:2704:U:O2	2.44	0.70
4:C:148:VAL:HG13	4:C:185:ARG:HB3	1.73	0.70
29:X:1997:A:H2'	29:X:1998:A:C8	2.26	0.70
29:X:542:A:OP1	29:X:570:G:N2	2.24	0.70
29:X:1212:U:H2'	29:X:1213:U:C6	2.26	0.70
28:3:13:ARG:NH2	29:X:227:G:OP2	2.24	0.70
29:X:2013:A:H4'	29:X:2014:A:C8	2.26	0.70
29:X:713:G:H22	29:X:745:C:H5	1.38	0.70
29:X:870:C:N4	29:X:871:U:O4	2.25	0.70
24:W:35:SER:O	24:W:37:THR:N	2.22	0.70
15:N:37:GLN:HG3	29:X:1265:G:H1	1.55	0.70
29:X:2418:A:H4'	29:X:2419:C:H5"	1.74	0.70
12:K:90:ARG:NH1	29:X:2855:C:O2'	2.25	0.70
3:B:176:ARG:HH21	14:M:16:ILE:HA	1.54	0.70
29:X:1662:G:H5"	29:X:1663:C:H5'	1.71	0.70
25:Z:33:CYS:O	25:Z:35:GLN:N	2.23	0.70
29:X:1939:U:H1'	29:X:2531:U:OP1	1.90	0.70
20:S:74:ARG:HH22	30:Y:94:G:H5"	1.54	0.70
29:X:2387:U:H2'	29:X:2388:G:C8	2.27	0.70
29:X:1053:G:H1	29:X:1124:U:H3	1.38	0.70
8:G:169:GLN:HG2	8:G:170:PRO:HD2	1.73	0.70
29:X:2123:G:N2	29:X:2134:U:O2	2.25	0.70
13:L:44:ASP:O	13:L:46:SER:N	2.24	0.70
19:R:100:ASP:HB3	19:R:101:GLY:HA3	1.74	0.70
29:X:2378:G:H1	29:X:2396:C:H42	1.40	0.69
5:D:39:GLY:HA2	5:D:86:GLY:HA2	1.74	0.69
29:X:1267:A:H5"	29:X:1268:U:H5"	1.72	0.69
3:B:110:GLY:HA2	3:B:161:GLY:HA3	1.74	0.69
30:Y:64:C:H2'	30:Y:65:A:C8	2.27	0.69
29:X:1937:G:O2'	29:X:1939:U:O4	2.10	0.69
1:0:42:ARG:HH22	1:0:209:TYR:HB2	1.56	0.69
29:X:172:A:H5"	29:X:173:A:OP2	1.92	0.69
2:A:274:ARG:NH2	29:X:1788:C:OP2	2.24	0.69
5:D:50:ILE:HG22	5:D:87:ILE:HD11	1.74	0.69
29:X:2187:A:H2	29:X:2198:U:H3	1.38	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:2775:U:O2'	29:X:2778:U:OP2	2.08	0.69
14:M:104:LEU:HA	14:M:106:TYR:CE2	2.27	0.69
4:C:111:ARG:HH11	4:C:181:LEU:HA	1.56	0.69
29:X:2845:C:N4	29:X:2846:G:O6	2.25	0.69
30:Y:27:A:OP2	30:Y:27:A:H8	1.75	0.69
10:I:86:THR:OG1	10:I:116:ARG:NH1	2.26	0.69
29:X:57:G:N2	29:X:68:C:O2	2.24	0.69
2:A:198:ASN:O	2:A:200:GLU:N	2.26	0.69
10:I:60:LEU:O	28:3:13:ARG:NH1	2.26	0.69
11:J:22:ALA:HB2	11:J:99:LYS:HB2	1.74	0.69
6:E:143:GLN:HG3	29:X:2725:C:H1'	1.74	0.69
11:J:65:ILE:HA	11:J:107:VAL:HG12	1.74	0.69
22:U:31:GLY:HA2	22:U:32:ARG:NH1	2.08	0.69
11:J:15:ARG:HG2	11:J:74:PRO:HD2	1.75	0.69
29:X:711:C:O2'	29:X:747:A:N6	2.25	0.69
12:K:3:HIS:N	29:X:2795:A:H4'	2.08	0.69
21:T:34:GLY:HA3	29:X:2332:G:H1'	1.75	0.69
29:X:877:G:H1	29:X:924:C:H42	1.39	0.69
10:I:75:VAL:HG22	10:I:99:VAL:HG11	1.75	0.68
29:X:1185:C:H2'	29:X:1186:G:H2'	1.74	0.68
12:K:29:LEU:HD13	12:K:79:VAL:HB	1.75	0.68
30:Y:5:C:N3	30:Y:120:G:N2	2.37	0.68
13:L:33:ARG:HE	13:L:38:ILE:HG21	1.57	0.68
2:A:243:GLY:HA3	29:X:2576:G:H5'	1.74	0.68
17:P:50:VAL:HB	17:P:91:PHE:HA	1.75	0.68
29:X:796:A:H4'	29:X:2567:G:H4'	1.75	0.68
4:C:72:ARG:HE	4:C:77:PHE:HE2	1.41	0.68
8:G:109:GLY:O	8:G:111:LYS:N	2.26	0.68
15:N:54:LYS:NZ	29:X:1006:C:OP2	2.27	0.68
9:H:69:VAL:HG12	9:H:70:VAL:H	1.58	0.68
9:H:23:ARG:HG3	9:H:24:VAL:H	1.57	0.68
29:X:1043:A:H2	29:X:1133:G:H22	1.39	0.68
29:X:511:A:O2'	29:X:512:A:OP1	2.09	0.68
29:X:1255:A:H2'	29:X:1256:C:H6	1.59	0.68
1:0:208:ALA:HB3	1:0:220:LEU:HB2	1.75	0.68
29:X:2032:G:N2	29:X:2598:C:O2	2.24	0.68
9:H:134:LEU:HA	14:M:48:GLN:HE22	1.59	0.68
26:1:15:SER:OG	26:1:48:VAL:O	2.12	0.68
2:A:161:THR:H	2:A:196:VAL:HB	1.59	0.68
4:C:47:THR:H	4:C:50:GLN:HG3	1.58	0.68
3:B:132:LYS:NZ	29:X:2590:U:OP1	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1116:U:H2'	29:X:1117:G:C8	2.29	0.68
15:N:76:TYR:HE2	29:X:1163:C:HO2'	1.41	0.68
29:X:33:C:N4	29:X:458:G:O2'	2.27	0.68
29:X:2690:A:OP1	29:X:2692:A:P	2.52	0.67
15:N:92:ARG:NH2	29:X:1009:C:OP2	2.26	0.67
29:X:796:A:OP1	29:X:1778:U:O2'	2.12	0.67
29:X:1556:A:H2'	29:X:1557:G:H8	1.58	0.67
29:X:1850:G:O4'	29:X:1867:A:N6	2.26	0.67
29:X:654:A:O2'	29:X:655:A:OP1	2.12	0.67
29:X:79:G:H2'	29:X:80:A:C8	2.28	0.67
29:X:2485:U:O2	32:X:6178:HGR:H23	1.93	0.67
24:W:43:MET:HE1	29:X:940:G:N2	2.05	0.67
8:G:142:ARG:NH2	29:X:539:A:OP2	2.24	0.67
29:X:677:G:O2'	29:X:952:A:OP2	2.12	0.67
29:X:198:A:N1	29:X:242:A:O2'	2.26	0.67
29:X:580:A:H4'	29:X:581:A:OP1	1.95	0.67
29:X:2440:C:H2'	29:X:2441:U:H6	1.58	0.67
29:X:1005:U:O2'	29:X:1007:A:OP1	2.10	0.67
2:A:173:VAL:HG23	2:A:187:SER:HB3	1.76	0.67
29:X:2043:A:H1'	29:X:2481:G:C1'	2.24	0.67
4:C:62:LYS:NZ	29:X:2043:A:H3'	2.10	0.67
29:X:1407:G:O6	29:X:1408:A:N6	2.28	0.67
4:C:129:LYS:HB3	4:C:132:ASN:ND2	2.10	0.67
29:X:2225:G:H2'	29:X:2226:A:H8	1.58	0.67
29:X:1401:G:H1	29:X:1412:C:H42	1.40	0.67
29:X:2816:C:C2	29:X:2852:G:N2	2.63	0.67
29:X:219:G:N2	29:X:231:G:H2'	2.10	0.67
29:X:1507:A:H2'	29:X:1508:G:C8	2.30	0.67
4:C:112:GLN:HA	4:C:117:LEU:HG	1.76	0.67
1:0:104:MET:SD	1:0:130:ARG:NH1	2.68	0.67
20:S:1:MET:HG3	20:S:52:PHE:HD2	1.60	0.67
29:X:168:A:H2'	29:X:169:C:C6	2.30	0.67
16:O:35:LEU:HD23	16:O:36:LYS:H	1.60	0.67
28:3:58:MET:HA	28:3:61:MET:HG3	1.76	0.66
9:H:25:LEU:HD22	9:H:52:VAL:HG23	1.77	0.66
4:C:4:ILE:HG22	4:C:13:ARG:HH12	1.60	0.66
2:A:55:GLY:HA3	2:A:218:LYS:HG3	1.77	0.66
29:X:1686:A:OP2	31:X:6021:MG:MG	1.38	0.66
29:X:1679:U:O2	29:X:2666:U:H5"	1.94	0.66
29:X:1301:U:O2'	29:X:1664:G:N2	2.29	0.66
29:X:546:A:H2'	29:X:547:U:C6	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1195:U:H2'	29:X:1196:G:C8	2.30	0.66
29:X:2873:G:H2'	29:X:2874:A:C8	2.29	0.66
29:X:403:A:H4'	29:X:404:A:H5'	1.76	0.66
20:S:3:LEU:HG	20:S:32:PHE:CD1	2.30	0.66
27:2:8:ASN:HB3	27:2:11:LYS:HB3	1.77	0.66
29:X:474:G:N2	29:X:477:A:OP2	2.28	0.66
29:X:2791:C:C2	29:X:2806:G:N2	2.63	0.66
15:N:24:PHE:HB2	15:N:29:SER:HB3	1.76	0.66
30:Y:64:C:H2'	30:Y:65:A:H8	1.60	0.66
21:T:46:LYS:HE2	21:T:77:ARG:H	1.60	0.66
10:I:68:VAL:HG13	10:I:69:GLY:H	1.60	0.66
12:K:31:GLU:O	12:K:33:ARG:N	2.25	0.66
29:X:1454:U:H2'	29:X:1455:C:H6	1.61	0.66
29:X:2241:U:H2'	29:X:2242:C:H6	1.61	0.66
2:A:274:ARG:HH22	29:X:1788:C:P	2.18	0.66
29:X:2826:C:H2'	29:X:2827:G:O4'	1.95	0.66
11:J:68:ARG:O	11:J:102:ARG:NH2	2.29	0.66
29:X:1030:U:H3	29:X:1153:A:H62	1.44	0.66
29:X:2226:A:H2'	29:X:2227:C:H6	1.61	0.66
1:0:127:LEU:HD23	1:0:130:ARG:HG3	1.76	0.66
24:W:39:ALA:O	29:X:864:C:O2'	2.14	0.66
29:X:1697:U:O2'	29:X:1754:G:N7	2.25	0.66
9:H:40:GLY:HA3	29:X:2545:A:H61	1.61	0.66
7:F:96:VAL:HB	7:F:136:VAL:HG12	1.75	0.66
29:X:1223:G:H4'	29:X:1224:A:H5"	1.78	0.66
3:B:119:ARG:HG2	3:B:120:TRP:CD1	2.31	0.66
16:O:22:VAL:HG12	16:O:23:GLU:H	1.60	0.66
29:X:1624:A:H1'	29:X:1626:A:OP2	1.96	0.66
29:X:2690:A:P	29:X:2692:A:OP2	2.54	0.66
29:X:1454:U:H2'	29:X:1455:C:C6	2.30	0.66
26:1:14:SER:HB2	26:1:47:VAL:HG11	1.77	0.66
29:X:2450:A:N6	29:X:2455:A:O2'	2.29	0.66
15:N:13:ARG:NH1	29:X:1264:C:H5"	2.11	0.65
12:K:46:PRO:O	12:K:50:GLN:HG3	1.96	0.65
4:C:9:GLN:O	4:C:10:ASN:ND2	2.16	0.65
7:F:12:LEU:HD22	7:F:18:THR:HG21	1.78	0.65
1:0:212:THR:O	29:X:2106:G:N2	2.28	0.65
29:X:1753:A:O5'	29:X:1753:A:H8	1.78	0.65
29:X:1856:U:OP1	29:X:2389:G:O2'	2.12	0.65
26:1:7:ARG:NH2	29:X:2265:A:OP2	2.28	0.65
29:X:573:C:H2'	29:X:574:C:H6	1.59	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:66:ASN:HA	15:N:76:TYR:HB2	1.77	0.65
29:X:335:A:N6	29:X:349:G:O2'	2.28	0.65
29:X:1482:U:O4'	29:X:1562:G:N2	2.30	0.65
10:I:90:ARG:HB2	10:I:93:LEU:HB2	1.76	0.65
5:D:37:ASN:OD1	29:X:2291:U:O2'	2.13	0.65
14:M:40:ARG:HB3	14:M:40:ARG:HH11	1.59	0.65
17:P:90:LEU:HD11	17:P:128:VAL:HB	1.76	0.65
6:E:28:GLY:HA3	6:E:79:VAL:HB	1.78	0.65
12:K:20:LEU:O	12:K:22:ARG:N	2.29	0.65
29:X:1467:U:O2	29:X:1468:A:N6	2.30	0.65
7:F:112:MET:HG3	7:F:113:PRO:HD3	1.77	0.65
29:X:421:G:H1	29:X:432:C:H42	1.44	0.65
29:X:1359:G:O6	29:X:1616:C:N4	2.27	0.65
12:K:108:VAL:HG12	12:K:109:THR:O	1.96	0.65
5:D:36:VAL:HB	5:D:89:VAL:HG23	1.79	0.65
29:X:2191:A:H5"	29:X:2192:U:H5	1.61	0.65
29:X:992:A:N1	29:X:2010:G:O2'	2.25	0.65
2:A:238:GLY:O	2:A:240:THR:OG1	2.13	0.65
6:E:45:GLN:NE2	6:E:47:GLY:O	2.30	0.65
26:1:29:ARG:O	26:1:30:ASN:ND2	2.30	0.65
12:K:11:ASN:HD22	12:K:11:ASN:N	1.92	0.65
29:X:1255:A:H2'	29:X:1256:C:C6	2.32	0.65
2:A:206:LEU:HB2	29:X:1782:A:O3'	1.97	0.65
1:0:152:LEU:HD23	1:0:157:ILE:HD12	1.79	0.65
12:K:87:TYR:HD1	12:K:90:ARG:HD2	1.62	0.65
29:X:510:G:H22	29:X:513:A:H5'	1.61	0.65
29:X:1140:A:O2'	29:X:2494:C:O2	2.14	0.65
4:C:164:VAL:HB	4:C:167:VAL:HG22	1.79	0.65
11:J:81:GLU:HB3	21:T:4:LYS:HE2	1.80	0.65
2:A:225:ALA:HB1	29:X:795:A:O2'	1.98	0.64
7:F:115:LEU:O	7:F:117:ALA:N	2.24	0.64
29:X:2410:U:O2	29:X:2412:A:H8	1.79	0.64
13:L:16:LYS:NZ	13:L:90:ASP:OD1	2.29	0.64
18:Q:66:GLY:O	18:Q:68:PHE:N	2.29	0.64
19:R:58:VAL:HA	29:X:494:A:H5'	1.79	0.64
11:J:23:LYS:O	20:S:73:LYS:NZ	2.29	0.64
29:X:876:A:H2'	29:X:877:G:C8	2.33	0.64
2:A:223:GLY:HA2	2:A:226:MET:HG3	1.77	0.64
29:X:104:C:H2'	29:X:105:G:H8	1.62	0.64
13:L:33:ARG:HG2	13:L:99:ARG:HG3	1.79	0.64
12:K:73:LYS:H	12:K:73:LYS:CE	2.10	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:52:ARG:HG3	11:J:67:ILE:HD11	1.79	0.64
8:G:124:GLU:HB3	8:G:150:VAL:HB	1.80	0.64
29:X:1981:A:HO2'	29:X:2704:U:HO2'	1.40	0.64
23:V:2:LYS:HE2	23:V:52:GLN:NE2	2.12	0.64
30:Y:16:U:H1'	30:Y:109:G:H21	1.62	0.64
29:X:746:G:N7	29:X:774:A:C6	2.66	0.64
29:X:2691:C:O2'	29:X:2692:A:O5'	2.13	0.64
29:X:7:G:H2'	29:X:8:A:C8	2.33	0.64
29:X:540:G:N2	29:X:2006:G:OP1	2.27	0.64
29:X:10:A:H2'	29:X:11:G:H8	1.63	0.64
29:X:531:G:H2'	29:X:532:A:H8	1.61	0.64
29:X:1838:G:H2'	29:X:1839:A:C8	2.33	0.64
29:X:2099:G:OP2	29:X:2149:G:O2'	2.14	0.64
18:Q:29:VAL:HG12	18:Q:30:SER:H	1.63	0.64
29:X:2299:A:N6	29:X:2312:A:O2'	2.30	0.64
29:X:794:A:H2	29:X:1767:G:N3	1.96	0.64
29:X:14:A:C6	29:X:536:A:C2	2.86	0.64
22:U:28:GLY:O	22:U:30:VAL:N	2.30	0.64
29:X:2775:U:H4'	29:X:2777:A:H3'	1.79	0.64
26:1:38:LYS:HG2	26:1:48:VAL:HG22	1.80	0.64
15:N:6:THR:HG21	15:N:10:ARG:HB2	1.80	0.64
3:B:51:TYR:N	3:B:75:THR:HG21	2.13	0.64
13:L:90:ASP:OD2	13:L:91:ARG:N	2.31	0.64
3:B:149:ARG:O	29:X:2035:G:H1'	1.98	0.64
29:X:2617:G:O2'	29:X:2755:A:N1	2.31	0.64
29:X:1237:G:O2'	29:X:1238:A:H5'	1.97	0.64
6:E:137:ASP:OD1	6:E:138:LYS:N	2.30	0.64
29:X:88:G:H5"	29:X:89:A:H5"	1.79	0.64
29:X:1090:C:N4	29:X:1099:A:OP1	2.28	0.63
29:X:1116:U:H2'	29:X:1117:G:H8	1.60	0.63
29:X:1366:A:H2'	29:X:1367:A:C8	2.32	0.63
10:I:18:ARG:NH2	29:X:1263:G:N7	2.47	0.63
11:J:82:THR:HG23	21:T:4:LYS:HG3	1.81	0.63
29:X:2040:A:H2'	29:X:2041:A:C8	2.33	0.63
1:0:10:VAL:HG21	1:0:216:PRO:HG2	1.80	0.63
29:X:104:C:H2'	29:X:105:G:C8	2.33	0.63
2:A:134:ARG:HB3	2:A:187:SER:HB2	1.79	0.63
29:X:1393:G:O2'	29:X:1585:A:N6	2.31	0.63
29:X:2278:A:H61	29:X:2296:U:H3	1.45	0.63
4:C:173:ALA:O	4:C:175:VAL:N	2.32	0.63
29:X:942:U:H2'	29:X:943:U:H6	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:2:5:TYR:HE1	29:X:699:G:C8	2.17	0.63
10:I:90:ARG:O	10:I:121:HIS:ND1	2.32	0.63
29:X:1429:A:C6	29:X:1600:U:H4'	2.34	0.63
29:X:1329:U:H2'	29:X:1330:G:H8	1.63	0.63
28:3:22:VAL:HG13	28:3:55:TRP:CD1	2.33	0.63
29:X:2043:A:H1'	29:X:2481:G:O4'	1.97	0.63
4:C:126:ALA:HB3	4:C:132:ASN:ND2	2.14	0.63
29:X:2736:U:H4'	29:X:2737:A:OP1	1.99	0.63
29:X:5:A:H2'	29:X:6:A:C8	2.33	0.63
12:K:11:ASN:ND2	12:K:11:ASN:H	1.95	0.63
20:S:68:ALA:HB3	20:S:82:ASP:HB2	1.80	0.63
10:I:16:ARG:HH22	29:X:598:U:P	2.22	0.63
29:X:1507:A:H2'	29:X:1508:G:H8	1.62	0.63
29:X:89:A:H4'	29:X:90:G:O5'	1.97	0.63
15:N:50:ARG:HA	15:N:53:LYS:HE2	1.81	0.63
5:D:34:ILE:HG22	5:D:91:LEU:HB2	1.79	0.63
21:T:56:ASP:HB2	21:T:58:THR:OG1	1.99	0.63
17:P:93:LYS:HD3	17:P:94:GLU:HG3	1.81	0.62
29:X:1705:U:O4'	29:X:1718:A:N6	2.32	0.62
9:H:76:ARG:O	9:H:94:ASN:HA	1.98	0.62
19:R:23:ILE:HA	19:R:32:GLN:O	1.98	0.62
2:A:71:ASP:HB3	2:A:103:ARG:HH12	1.64	0.62
7:F:90:THR:HB	29:X:1087:C:H1'	1.80	0.62
29:X:652:C:N4	29:X:657:A:H61	1.95	0.62
29:X:858:G:O2'	29:X:859:U:OP2	2.17	0.62
13:L:37:HIS:HE1	13:L:39:TYR:CD1	2.18	0.62
3:B:102:ILE:N	3:B:170:LEU:O	2.31	0.62
29:X:2674:C:H2'	29:X:2675:U:C6	2.33	0.62
29:X:2191:A:OP1	29:X:2193:C:N4	2.32	0.62
15:N:3:ARG:HB3	29:X:1261:G:C5	2.34	0.62
29:X:2369:U:H3'	29:X:2369:U:H6	1.64	0.62
6:E:17:VAL:HG22	6:E:26:VAL:HG13	1.81	0.62
29:X:2102:A:O4'	29:X:2155:U:O2'	2.17	0.62
2:A:123:ALA:HB1	2:A:129:ASN:HD22	1.64	0.62
29:X:2240:C:O2	29:X:2258:G:N2	2.19	0.62
28:3:25:PHE:HA	28:3:47:GLY:HA2	1.80	0.62
10:I:94:GLU:N	10:I:97:ARG:HH11	1.97	0.62
29:X:1703:C:H2'	29:X:1704:G:O4'	1.99	0.62
3:B:27:LEU:HD23	3:B:29:GLY:H	1.64	0.62
26:1:46:HIS:HD2	29:X:2350:G:O2'	1.83	0.62
29:X:2640:G:H2'	29:X:2641:A:C8	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:334:G:OP1	29:X:349:G:N2	2.32	0.62
29:X:1654:A:H4'	29:X:2690:A:O2'	2.00	0.62
22:U:23:LYS:HD2	22:U:35:THR:HG21	1.81	0.62
29:X:421:G:H2'	29:X:422:C:C6	2.34	0.62
29:X:1454:U:H3	29:X:1567:A:H61	1.47	0.62
7:F:62:ASP:OD1	7:F:63:ARG:NH1	2.32	0.62
25:Z:14:SER:O	25:Z:18:MET:HG3	2.00	0.62
14:M:104:LEU:HA	14:M:106:TYR:HE2	1.64	0.62
3:B:132:LYS:O	3:B:134:TRP:N	2.33	0.62
29:X:494:A:H3'	29:X:495:C:H6	1.65	0.62
9:H:124:MET:O	9:H:127:VAL:HG12	1.99	0.62
29:X:2285:U:H5'	29:X:2286:G:C8	2.35	0.62
29:X:160:C:O2'	29:X:445:A:N3	2.31	0.62
29:X:427:C:H2'	29:X:428:A:C8	2.34	0.62
28:3:17:THR:OG1	28:3:18:GLY:N	2.33	0.62
29:X:2033:C:N4	29:X:2034:A:N1	2.48	0.62
29:X:1642:G:H5"	29:X:1643:A:OP1	2.00	0.62
30:Y:68:A:N6	30:Y:111:C:OP2	2.33	0.62
19:R:84:VAL:HG22	19:R:89:GLY:HA2	1.80	0.62
29:X:170:U:N3	29:X:180:C:O2	2.32	0.61
13:L:27:LEU:HD13	13:L:84:ILE:HG23	1.82	0.61
29:X:1192:A:H2'	29:X:1193:G:H8	1.63	0.61
29:X:555:U:C2	29:X:1243:G:C2	2.88	0.61
4:C:149:LEU:HD21	4:C:170:LEU:HD12	1.82	0.61
2:A:63:ARG:HH21	2:A:86:PRO:HD3	1.65	0.61
29:X:1790:G:N2	29:X:1811:A:OP2	2.31	0.61
29:X:571:U:HO2'	29:X:581:A:H8	1.47	0.61
29:X:2186:G:H2'	29:X:2187:A:C8	2.36	0.61
29:X:753:U:H2'	29:X:754:G:C8	2.34	0.61
29:X:1030:U:O2	29:X:1155:G:N2	2.33	0.61
29:X:1066:G:H1	29:X:1115:C:H42	1.48	0.61
9:H:2:ILE:N	9:H:45:ALA:O	2.27	0.61
29:X:510:G:N2	29:X:513:A:H5'	2.16	0.61
19:R:93:ARG:NH2	29:X:311:A:O5'	2.33	0.61
29:X:1077:U:O2'	29:X:1079:G:N7	2.28	0.61
19:R:51:VAL:HG13	19:R:73:GLU:HB3	1.81	0.61
11:J:43:ILE:O	11:J:95:VAL:HA	2.00	0.61
29:X:759:C:OP1	29:X:761:G:H4'	2.01	0.61
9:H:51:ILE:HD11	9:H:53:ALA:HB2	1.81	0.61
29:X:1511:A:N1	29:X:1512:A:N6	2.48	0.61
29:X:98:U:O2	29:X:100:G:N1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:67:ALA:HA	29:X:1268:U:C5	2.35	0.61
17:P:94:GLU:HB2	17:P:127:ILE:HB	1.83	0.61
29:X:1608:U:H2'	29:X:1609:G:C8	2.36	0.61
9:H:41:ASN:HB2	29:X:2654:A:H5'	1.83	0.61
29:X:220:U:H2'	29:X:221:A:H8	1.65	0.61
3:B:12:THR:OG1	14:M:17:GLU:OE1	2.18	0.61
17:P:111:ARG:HG2	29:X:764:A:O4'	2.01	0.61
29:X:1770:U:H6	29:X:1775:A:H62	1.49	0.61
17:P:98:ASP:OD1	29:X:23:G:N2	2.29	0.61
8:G:67:ARG:O	8:G:70:PHE:HB2	2.01	0.61
3:B:55:ALA:H	3:B:58:LYS:NZ	1.97	0.61
16:O:55:THR:OG1	16:O:56:VAL:N	2.33	0.61
18:Q:2:SER:OG	18:Q:3:HIS:N	2.32	0.61
2:A:142:VAL:HG23	2:A:193:ILE:HA	1.82	0.61
19:R:25:LEU:HD11	19:R:82:ALA:HB2	1.83	0.61
29:X:2672:U:H2'	29:X:2673:G:C8	2.35	0.61
19:R:68:GLY:N	29:X:494:A:O2'	2.33	0.61
29:X:90:G:H5"	29:X:91:A:OP2	2.01	0.61
29:X:926:C:H42	30:Y:104:A:H5'	1.66	0.61
16:O:40:VAL:HG12	16:O:42:GLY:H	1.66	0.61
29:X:653:G:H21	29:X:656:U:H3	1.49	0.60
29:X:761:G:C8	29:X:763:A:C8	2.89	0.60
29:X:836:G:H2'	29:X:837:U:C6	2.36	0.60
29:X:2201:G:H2'	29:X:2202:G:H8	1.66	0.60
15:N:18:LEU:HA	15:N:21:ALA:HB3	1.83	0.60
13:L:104:ALA:O	13:L:108:ARG:N	2.31	0.60
22:U:20:ARG:NE	29:X:393:U:OP1	2.34	0.60
29:X:761:G:C8	29:X:763:A:N7	2.69	0.60
29:X:588:G:O2'	29:X:2002:A:OP1	2.14	0.60
29:X:174:A:N6	29:X:2409:A:O2'	2.33	0.60
9:H:16:ALA:CB	9:H:98:ILE:HD11	2.31	0.60
2:A:210:GLY:HA2	29:X:777:A:H5'	1.82	0.60
3:B:26:VAL:HG12	3:B:182:ILE:HB	1.82	0.60
29:X:1863:U:H2'	29:X:1864:G:C8	2.34	0.60
12:K:46:PRO:HB3	29:X:2814:G:H5'	1.82	0.60
3:B:189:PRO:HA	29:X:2659:C:C5'	2.31	0.60
1:0:123:LEU:HB3	1:0:127:LEU:HB2	1.84	0.60
4:C:133:PHE:HB2	4:C:160:ALA:HB1	1.82	0.60
4:C:40:ARG:NH2	29:X:39:C:O2	2.32	0.60
29:X:1690:U:O2'	29:X:1691:G:OP1	2.18	0.60
29:X:957:G:H2'	29:X:958:G:H8	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:106:ASP:N	29:X:1300:A:N7	2.49	0.60
29:X:531:G:H2'	29:X:532:A:C8	2.35	0.60
29:X:2208:U:H2'	29:X:2209:G:H8	1.66	0.60
20:S:127:PRO:HA	20:S:130:ILE:HD11	1.82	0.60
9:H:8:LEU:H	9:H:8:LEU:HD23	1.64	0.60
19:R:83:LEU:O	19:R:92:THR:OG1	2.20	0.60
22:U:51:ILE:HG23	22:U:59:THR:HA	1.83	0.60
30:Y:6:C:H2'	30:Y:7:C:C6	2.36	0.60
29:X:2038:C:H2'	29:X:2483:U:H4'	1.82	0.60
29:X:2246:A:H61	29:X:2251:U:H3	1.48	0.60
12:K:11:ASN:OD1	29:X:1669:A:N6	2.35	0.60
29:X:1982:C:OP1	29:X:2703:C:O2'	2.19	0.60
11:J:36:ILE:HG12	11:J:103:VAL:HG13	1.83	0.60
5:D:72:LYS:HG3	5:D:81:GLN:HG3	1.83	0.60
29:X:2639:A:H3'	29:X:2640:G:C8	2.37	0.60
20:S:167:THR:OG1	29:X:888:G:H4'	2.01	0.60
29:X:490:A:N3	29:X:492:G:H5"	2.17	0.60
29:X:505:G:O5'	29:X:505:G:H8	1.84	0.60
29:X:691:C:H2'	29:X:692:C:H6	1.65	0.60
29:X:330:C:H2'	29:X:331:U:H6	1.67	0.60
30:Y:17:A:OP1	30:Y:110:U:O2'	2.13	0.60
9:H:40:GLY:CA	29:X:2545:A:H61	2.14	0.60
17:P:24:GLY:O	17:P:127:ILE:HA	2.01	0.60
5:D:34:ILE:HG13	5:D:156:ILE:HG23	1.83	0.60
13:L:19:THR:O	13:L:21:THR:N	2.34	0.60
5:D:35:VAL:HG11	29:X:2293:G:H5'	1.83	0.60
4:C:62:LYS:HZ2	29:X:2043:A:H5'	1.67	0.60
29:X:2579:A:H2'	29:X:2580:C:C6	2.37	0.60
6:E:137:ASP:OD1	6:E:139:GLN:N	2.35	0.60
4:C:142:LEU:HB3	4:C:166:TRP:HH2	1.66	0.60
9:H:38:GLY:O	29:X:2627:G:H1'	2.01	0.60
29:X:1681:A:N3	29:X:2706:U:C2	2.69	0.60
17:P:63:SER:HB2	29:X:1993:G:H5"	1.83	0.60
29:X:1992:G:O2'	29:X:1993:G:H5'	2.02	0.60
29:X:1479:G:H2'	29:X:1480:G:H8	1.66	0.60
29:X:2277:A:C2	29:X:2278:A:H1'	2.36	0.60
20:S:91:PRO:HG3	20:S:126:GLY:H	1.66	0.60
16:O:32:LYS:HZ3	16:O:57:GLN:HB3	1.66	0.60
29:X:633:G:C2	29:X:634:G:C8	2.90	0.60
20:S:154:LEU:HD22	20:S:158:CYS:HB2	1.83	0.60
29:X:1556:A:H2'	29:X:1557:G:C8	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:825:C:H2'	29:X:826:U:H6	1.67	0.59
6:E:83:TYR:CE1	6:E:138:LYS:HB2	2.37	0.59
13:L:87:VAL:HG21	13:L:108:ARG:HH12	1.67	0.59
22:U:51:ILE:O	22:U:52:ARG:NH2	2.33	0.59
29:X:389:G:H1	29:X:411:C:H42	1.50	0.59
29:X:70:A:H4'	29:X:71:A:H5"	1.84	0.59
28:3:33:ASN:O	28:3:35:GLY:N	2.35	0.59
25:Z:19:ARG:HA	29:X:2029:G:H5'	1.84	0.59
2:A:208:LYS:HB2	29:X:742:G:C5	2.37	0.59
20:S:105:GLN:O	20:S:109:GLN:NE2	2.35	0.59
6:E:17:VAL:HG13	6:E:26:VAL:HG22	1.82	0.59
11:J:39:GLU:HB2	11:J:128:ILE:HG22	1.83	0.59
29:X:1701:C:C2	29:X:1722:G:N2	2.69	0.59
29:X:2013:A:H4'	29:X:2014:A:H8	1.66	0.59
21:T:23:VAL:HB	21:T:38:VAL:HG22	1.83	0.59
29:X:1117:G:H2'	29:X:1118:G:H8	1.66	0.59
12:K:20:LEU:O	12:K:23:ALA:N	2.36	0.59
29:X:451:A:H2'	29:X:452:G:C8	2.37	0.59
5:D:113:ASP:HB3	5:D:115:ARG:HH12	1.65	0.59
29:X:663:G:H2'	29:X:664:C:H4'	1.84	0.59
7:F:89:SER:HA	29:X:1075:C:H4'	1.84	0.59
7:F:54:PRO:HG2	7:F:70:LYS:HB2	1.83	0.59
19:R:77:HIS:O	19:R:79:SER:N	2.35	0.59
29:X:1504:G:N2	29:X:1517:C:O2	2.35	0.59
29:X:388:G:OP1	29:X:406:G:OP1	2.20	0.59
12:K:37:THR:HB	12:K:40:LYS:HG3	1.85	0.59
2:A:273:ARG:HB2	2:A:275:LYS:HE2	1.85	0.59
2:A:33:LEU:HD13	2:A:104:TYR:HD2	1.66	0.59
11:J:72:ASP:N	11:J:72:ASP:OD2	2.35	0.59
29:X:1909:U:H5"	29:X:1911:A:OP2	2.02	0.59
29:X:2791:C:O2	29:X:2858:A:O2'	2.19	0.59
14:M:16:ILE:O	14:M:18:GLN:N	2.32	0.59
11:J:47:GLN:OE1	11:J:127:PRO:HD3	2.01	0.59
9:H:75:VAL:HG22	9:H:96:ALA:HA	1.84	0.59
4:C:131:LYS:HA	4:C:134:ILE:HD12	1.85	0.59
1:0:113:PRO:HG3	1:0:142:GLY:HA2	1.84	0.59
29:X:118:U:H4'	29:X:119:G:H5"	1.83	0.59
29:X:129:A:H61	29:X:142:U:H3	1.50	0.59
3:B:9:ILE:HD11	3:B:27:LEU:HB2	1.83	0.59
29:X:2821:G:H2'	29:X:2822:U:H6	1.64	0.59
5:D:37:ASN:ND2	29:X:2291:U:O2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1053:G:N2	29:X:1124:U:O2	2.29	0.59
2:A:70:ARG:NH1	2:A:146:GLU:OE2	2.35	0.59
19:R:19:GLY:H	19:R:36:VAL:HB	1.68	0.59
29:X:575:U:O2'	29:X:822:G:OP2	2.20	0.59
29:X:627:A:H2'	29:X:628:A:C8	2.38	0.59
2:A:263:ARG:NH1	29:X:2206:C:OP1	2.35	0.59
29:X:2180:U:H2'	29:X:2203:G:H1	1.67	0.59
1:0:174:ALA:HA	1:0:181:LEU:HD21	1.83	0.59
29:X:511:A:HO2'	29:X:512:A:P	2.26	0.59
15:N:33:ARG:HB3	29:X:1265:G:C2	2.38	0.59
29:X:712:A:H2'	29:X:713:G:O4'	2.03	0.59
29:X:2559:U:H5"	29:X:2560:G:OP2	2.03	0.59
29:X:847:C:HO2'	29:X:2337:A:HO2'	1.51	0.59
1:0:138:SER:OG	1:0:139:GLY:N	2.34	0.59
29:X:1827:G:H1'	29:X:1914:U:C2	2.38	0.59
29:X:2792:C:C2	29:X:2805:G:N2	2.71	0.59
29:X:2088:U:H3	29:X:2167:A:H61	1.50	0.59
13:L:38:ILE:HD12	13:L:39:TYR:H	1.67	0.59
30:Y:25:G:H1	30:Y:62:C:N4	2.01	0.59
26:1:35:LEU:HB3	26:1:51:ALA:HB2	1.83	0.59
18:Q:35:LYS:HD2	18:Q:53:ILE:HD13	1.85	0.59
25:Z:38:GLY:O	25:Z:39:LYS:HG2	2.01	0.59
19:R:77:HIS:CD2	29:X:339:U:H4'	2.37	0.58
29:X:1465:G:N2	29:X:1466:C:C2	2.71	0.58
29:X:82:G:N2	29:X:100:G:H1'	2.18	0.58
1:0:136:PRO:HA	1:0:141:VAL:HG11	1.84	0.58
29:X:641:G:N2	29:X:644:A:OP2	2.34	0.58
1:0:15:GLN:HB3	1:0:221:ALA:HB2	1.85	0.58
4:C:84:PHE:CE1	29:X:596:C:H5'	2.38	0.58
29:X:1679:U:H2'	29:X:1680:U:O4'	2.02	0.58
29:X:455:A:C2	29:X:1258:G:N3	2.68	0.58
29:X:1326:U:H4'	29:X:1345:G:H4'	1.85	0.58
3:B:4:ILE:HG12	3:B:5:LEU:H	1.67	0.58
29:X:2516:U:H2'	29:X:2517:C:C6	2.37	0.58
12:K:92:GLY:HA2	12:K:94:TYR:CE2	2.38	0.58
19:R:26:SER:HB2	29:X:321:A:H5'	1.85	0.58
8:G:140:GLN:HG3	29:X:567:G:C5'	2.30	0.58
29:X:548:G:H1	29:X:564:U:H3	1.50	0.58
29:X:1100:G:H5'	29:X:1101:U:OP2	2.04	0.58
9:H:115:ALA:O	9:H:117:GLU:N	2.36	0.58
23:V:32:ALA:HA	23:V:37:LEU:HB2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:103:ARG:HH22	20:S:107:GLU:HB3	1.67	0.58
29:X:970:A:N3	29:X:2436:U:O2'	2.33	0.58
29:X:958:G:H2'	29:X:959:C:C6	2.38	0.58
8:G:31:THR:OG1	29:X:1006:C:N3	2.37	0.58
29:X:243:G:H1	29:X:439:C:H42	1.50	0.58
4:C:125:ILE:HD12	4:C:133:PHE:HA	1.85	0.58
23:V:42:ARG:NH1	23:V:45:GLN:OE1	2.36	0.58
29:X:930:A:H4'	30:Y:100:G:N3	2.18	0.58
18:Q:88:ILE:HD11	18:Q:91:LEU:HB2	1.85	0.58
15:N:91:ASN:HD22	15:N:93:LYS:HB3	1.69	0.58
12:K:3:HIS:O	12:K:3:HIS:CD2	2.56	0.58
15:N:31:GLN:NE2	29:X:589:C:H4'	2.18	0.58
29:X:1117:G:H2'	29:X:1118:G:C8	2.38	0.58
29:X:2226:A:H2'	29:X:2227:C:C6	2.37	0.58
29:X:1655:C:H5"	29:X:2689:C:H1'	1.85	0.58
29:X:1815:G:H2'	29:X:1816:G:H8	1.68	0.58
10:I:77:LEU:O	10:I:79:GLN:N	2.37	0.58
14:M:102:ALA:O	14:M:103:LYS:NZ	2.26	0.58
15:N:19:LYS:NZ	29:X:1233:A:OP1	2.36	0.58
29:X:622:U:H2'	29:X:623:G:C8	2.38	0.58
29:X:2418:A:H4'	29:X:2419:C:H5'	1.84	0.58
26:1:42:PRO:HG3	29:X:2327:U:O2'	2.03	0.58
11:J:16:GLY:O	11:J:73:LYS:NZ	2.36	0.58
5:D:128:TYR:HB3	5:D:156:ILE:HD12	1.84	0.58
6:E:150:LYS:NZ	29:X:2741:G:H21	2.00	0.58
29:X:2633:A:N1	29:X:2644:A:H5"	2.17	0.58
13:L:32:TYR:O	13:L:34:SER:N	2.36	0.58
19:R:8:SER:OG	19:R:9:HIS:N	2.36	0.58
28:3:64:ARG:HH21	29:X:219:G:P	2.26	0.58
13:L:43:ILE:HG22	13:L:45:ASP:H	1.69	0.58
15:N:83:LEU:HD22	15:N:88:ILE:HD12	1.85	0.58
29:X:2565:C:H2'	29:X:2566:A:C8	2.39	0.58
14:M:70:LYS:NZ	14:M:72:SER:OG	2.37	0.58
29:X:1298:G:C6	29:X:1342:U:C6	2.92	0.58
29:X:1035:G:C6	29:X:1036:G:C6	2.92	0.58
29:X:1124:U:H2'	29:X:1125:G:C8	2.39	0.58
29:X:1621:C:O2	29:X:1626:A:O2'	2.20	0.58
29:X:2625:U:O5'	29:X:2625:U:H6	1.87	0.58
10:I:72:TYR:HD1	10:I:107:LYS:HZ2	1.52	0.58
17:P:41:VAL:HG11	17:P:65:SER:HA	1.84	0.58
29:X:1921:A:O2'	29:X:1922:U:H5'	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:49:GLN:HG2	30:Y:116:C:H4'	1.86	0.58
29:X:1040:A:C8	29:X:1041:G:C8	2.92	0.58
22:U:48:LYS:HE3	29:X:2074:U:H1'	1.85	0.58
29:X:1033:G:N2	29:X:1034:U:O4	2.28	0.58
10:I:75:VAL:HG12	10:I:108:LEU:HD13	1.85	0.58
14:M:31:ASP:OD1	14:M:96:ARG:HA	2.04	0.58
29:X:834:A:H5'	29:X:835:U:C6	2.38	0.58
14:M:106:TYR:CE1	29:X:1745:C:H5'	2.39	0.58
15:N:3:ARG:HB3	29:X:1261:G:C4	2.39	0.58
1:0:182:SER:HA	1:0:185:TYR:HB3	1.86	0.58
21:T:53:MET:HG2	21:T:57:HIS:HA	1.86	0.58
15:N:58:ARG:O	15:N:62:ILE:HG13	2.04	0.57
29:X:333:A:H5'	29:X:351:A:C1'	2.33	0.57
9:H:90:ARG:NH2	14:M:78:GLU:OE1	2.37	0.57
30:Y:58:G:H4'	30:Y:59:A:H5"	1.84	0.57
29:X:2531:U:H2'	29:X:2533:U:OP2	2.04	0.57
4:C:86:PRO:HD3	29:X:1261:G:C8	2.38	0.57
19:R:13:LYS:NZ	29:X:349:G:OP1	2.30	0.57
9:H:97:VAL:HG11	9:H:126:ILE:HD13	1.86	0.57
24:W:2:LYS:HB3	24:W:54:GLN:HB2	1.87	0.57
14:M:46:ARG:HG2	14:M:47:SER:H	1.68	0.57
29:X:501:G:H2'	29:X:502:A:O4'	2.04	0.57
20:S:123:VAL:HG23	20:S:161:ALA:HB2	1.84	0.57
29:X:1281:A:H2'	29:X:1282:A:C8	2.40	0.57
29:X:622:U:H2'	29:X:623:G:H8	1.68	0.57
29:X:2198:U:H3'	29:X:2199:C:H4'	1.85	0.57
25:Z:3:LYS:HD2	29:X:2556:A:H4'	1.84	0.57
29:X:484:G:H2'	29:X:485:G:H8	1.69	0.57
6:E:66:GLY:HA3	29:X:2728:A:H4'	1.86	0.57
29:X:1608:U:H2'	29:X:1609:G:H8	1.68	0.57
29:X:836:G:N2	29:X:847:C:O2	2.37	0.57
2:A:62:TYR:HE1	29:X:1808:C:H3'	1.69	0.57
15:N:59:ARG:HH22	29:X:1019:U:H4'	1.69	0.57
29:X:2424:G:H2'	29:X:2425:G:H8	1.69	0.57
5:D:66:ILE:HD11	30:Y:43:G:H2'	1.85	0.57
16:O:71:ILE:HB	16:O:84:THR:OG1	2.04	0.57
29:X:936:A:H2'	29:X:937:C:C6	2.40	0.57
29:X:1336:G:C2'	29:X:1337:G:H5'	2.32	0.57
29:X:548:G:C2	29:X:549:G:C8	2.91	0.57
29:X:1067:G:H1'	29:X:1114:A:H61	1.69	0.57
9:H:25:LEU:CD2	9:H:52:VAL:HG23	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:35:SER:OG	13:L:36:LYS:N	2.37	0.57
29:X:1072:U:N3	29:X:1080:A:OP1	2.38	0.57
29:X:2391:A:C8	29:X:2392:G:C8	2.91	0.57
29:X:992:A:H5"	29:X:993:C:OP2	2.04	0.57
19:R:58:VAL:HG13	19:R:60:PRO:HD2	1.85	0.57
11:J:11:ARG:NH2	11:J:72:ASP:HB2	2.19	0.57
1:0:187:ALA:HA	1:0:190:SER:HB3	1.86	0.57
8:G:33:ILE:HG21	29:X:548:G:H5'	1.84	0.57
29:X:2197:U:H2'	29:X:2198:U:C6	2.38	0.57
2:A:210:GLY:HA3	29:X:777:A:OP1	2.04	0.57
11:J:27:TYR:HB3	11:J:137:VAL:HB	1.85	0.57
29:X:668:A:H4'	29:X:669:G:H5'	1.85	0.57
19:R:106:VAL:O	19:R:112:LYS:HB2	2.04	0.57
17:P:31:VAL:HG12	17:P:122:SER:O	2.05	0.57
29:X:691:C:H2'	29:X:692:C:C6	2.39	0.57
16:O:34:GLU:HG3	16:O:57:GLN:HA	1.86	0.57
17:P:59:PHE:HD1	25:Z:30:LEU:HD11	1.70	0.57
30:Y:39:C:H5"	30:Y:40:C:C5	2.39	0.57
13:L:37:HIS:CE1	13:L:39:TYR:HD1	2.23	0.57
2:A:108:PRO:HB3	2:A:143:HIS:CE1	2.36	0.57
29:X:1464:A:H61	29:X:1477:C:H42	1.50	0.57
15:N:6:THR:O	15:N:8:ILE:N	2.35	0.57
29:X:485:G:C6	29:X:520:C:N4	2.73	0.57
29:X:497:C:O2	29:X:505:G:N2	2.38	0.57
16:O:32:LYS:NZ	16:O:57:GLN:HB3	2.20	0.57
4:C:8:GLY:H	4:C:121:ASP:HB3	1.70	0.57
3:B:92:ASN:N	3:B:92:ASN:OD1	2.37	0.57
29:X:308:C:H2'	29:X:309:G:C8	2.40	0.57
20:S:63:PRO:HB2	20:S:86:VAL:HG22	1.87	0.57
29:X:1981:A:H4'	29:X:2704:U:O2'	2.03	0.57
27:2:12:ARG:HD2	27:2:44:VAL:HG11	1.87	0.57
29:X:1787:U:H2'	29:X:1788:C:H6	1.70	0.57
2:A:142:VAL:HA	2:A:194:GLY:H	1.69	0.57
8:G:84:ASN:ND2	8:G:154:GLU:OE1	2.34	0.57
5:D:5:LYS:HA	5:D:8:TYR:CD2	2.40	0.57
17:P:80:LEU:HD11	17:P:87:GLU:HB2	1.87	0.57
5:D:126:GLY:O	5:D:160:ALA:HB3	2.04	0.57
29:X:2691:C:H2'	29:X:2694:G:H5"	1.85	0.57
29:X:958:G:H2'	29:X:959:C:H6	1.70	0.57
29:X:1071:U:H4'	29:X:1072:U:H5'	1.86	0.57
15:N:24:PHE:CE1	29:X:543:G:H5'	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1192:A:H2'	29:X:1193:G:C8	2.40	0.57
29:X:2354:G:N2	29:X:2357:A:OP2	2.34	0.57
12:K:24:GLN:HB3	12:K:44:LEU:HD22	1.87	0.57
2:A:211:ARG:HD2	2:A:214:TRP:CZ3	2.40	0.57
29:X:2124:C:N4	29:X:2125:C:N3	2.53	0.57
2:A:260:ARG:NH2	2:A:267:ASP:OD1	2.24	0.57
17:P:31:VAL:HG11	17:P:124:ILE:CD1	2.33	0.57
15:N:50:ARG:O	15:N:53:LYS:HG2	2.04	0.57
29:X:533:C:H5"	29:X:550:C:O2'	2.05	0.57
1:0:53:ASN:ND2	1:0:161:ASN:OD1	2.37	0.57
29:X:654:A:H2'	29:X:655:A:C8	2.39	0.56
29:X:1982:C:H2'	29:X:1983:G:O4'	2.05	0.56
29:X:1529:C:H2'	29:X:1530:U:C6	2.40	0.56
28:3:24:ALA:O	28:3:48:PHE:N	2.33	0.56
29:X:1458:A:H5"	29:X:1459:U:OP2	2.05	0.56
29:X:602:C:H42	29:X:678:G:H1	1.52	0.56
29:X:1935:A:C6	29:X:1936:A:N1	2.73	0.56
4:C:189:ASP:OD1	4:C:190:ALA:N	2.37	0.56
29:X:874:A:H2'	29:X:875:G:O4'	2.05	0.56
24:W:13:PRO:HG2	24:W:16:GLN:HB2	1.87	0.56
28:3:28:GLY:HA3	28:3:32:GLN:OE1	2.06	0.56
29:X:1845:A:H2'	29:X:1846:A:C8	2.40	0.56
29:X:2048:C:H5"	29:X:2231:G:H1'	1.86	0.56
3:B:144:ARG:HD3	29:X:2551:A:C8	2.41	0.56
29:X:340:G:H4'	29:X:341:A:OP2	2.06	0.56
28:3:3:LYS:HA	29:X:602:C:H1'	1.88	0.56
19:R:43:ASP:N	19:R:43:ASP:OD2	2.38	0.56
3:B:141:ILE:HD12	29:X:2035:G:C8	2.40	0.56
29:X:2197:U:H2'	29:X:2198:U:C5	2.40	0.56
30:Y:16:U:O2'	30:Y:17:A:OP2	2.21	0.56
29:X:837:U:H2'	29:X:838:A:C8	2.39	0.56
22:U:20:ARG:HB3	22:U:43:ARG:NH2	2.20	0.56
29:X:2251:U:H5"	29:X:2252:A:OP1	2.05	0.56
1:0:73:ILE:HG12	1:0:95:LEU:HB3	1.86	0.56
14:M:100:ARG:NH2	29:X:1744:G:OP1	2.34	0.56
29:X:1793:A:H2'	29:X:1794:A:C8	2.40	0.56
29:X:1002:C:H5'	29:X:1200:G:OP2	2.05	0.56
3:B:152:LYS:HB3	8:G:106:TYR:CE1	2.41	0.56
17:P:36:ARG:NH1	25:Z:20:ARG:HH21	2.04	0.56
15:N:37:GLN:HG3	29:X:1265:G:N1	2.20	0.56
14:M:69:ARG:NH2	14:M:108:LYS:HA	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:12:LYS:O	11:J:13:GLN:HB2	2.05	0.56
17:P:27:VAL:HG22	17:P:125:THR:OG1	2.05	0.56
5:D:69:LYS:NZ	30:Y:43:G:H1	2.04	0.56
8:G:95:LEU:HA	8:G:115:ALA:HB3	1.88	0.56
29:X:224:G:H4'	29:X:399:G:C4	2.41	0.56
29:X:16:G:H2'	29:X:17:G:H8	1.71	0.56
29:X:2605:C:H2'	29:X:2606:G:H8	1.70	0.56
29:X:858:G:OP2	29:X:858:G:H8	1.87	0.56
29:X:1863:U:H2'	29:X:1864:G:H8	1.70	0.56
4:C:97:ARG:NH2	29:X:630:G:N7	2.53	0.56
29:X:2662:C:C2'	29:X:2663:U:H5'	2.35	0.56
29:X:52:A:H5"	29:X:53:G:OP2	2.05	0.56
29:X:1989:C:O5'	29:X:1989:C:H6	1.88	0.56
3:B:7:THR:HG23	3:B:194:GLY:O	2.06	0.56
29:X:1909:U:P	29:X:1912:G:H1	2.26	0.56
8:G:51:LEU:HD12	8:G:88:VAL:HG11	1.87	0.56
29:X:1329:U:H2'	29:X:1330:G:C8	2.40	0.56
2:A:48:ARG:HH21	29:X:791:G:H5'	1.70	0.56
3:B:109:LYS:HG2	3:B:191:ALA:HB2	1.87	0.56
28:3:56:ALA:HA	28:3:59:LYS:HG3	1.88	0.56
29:X:1956:G:H2'	29:X:1957:C:C6	2.41	0.56
29:X:840:U:H4'	29:X:841:G:C8	2.41	0.56
29:X:2308:A:H2'	29:X:2309:G:C8	2.40	0.56
3:B:2:LYS:HA	3:B:84:PHE:HE1	1.70	0.56
2:A:142:VAL:HG23	2:A:193:ILE:HD13	1.86	0.56
3:B:107:THR:O	3:B:190:GLY:HA3	2.05	0.56
29:X:2129:U:H2'	29:X:2130:G:H8	1.70	0.56
29:X:1428:G:HO2'	29:X:1429:A:H8	1.53	0.56
4:C:158:ARG:O	4:C:161:ALA:N	2.39	0.56
8:G:136:PRO:O	8:G:141:GLY:HA3	2.06	0.56
13:L:11:LEU:HD21	29:X:2273:C:OP1	2.06	0.56
29:X:1016:C:H1'	29:X:1023:U:N3	2.20	0.56
29:X:628:A:H2'	29:X:629:C:C6	2.40	0.56
29:X:692:C:H2'	29:X:693:A:C8	2.37	0.56
4:C:188:ILE:HB	4:C:189:ASP:O	2.05	0.56
20:S:3:LEU:HB2	20:S:33:ALA:O	2.06	0.56
26:1:9:ILE:HA	26:1:25:THR:HG22	1.87	0.56
12:K:73:LYS:HE2	12:K:73:LYS:H	1.71	0.56
29:X:10:A:H2'	29:X:11:G:C8	2.40	0.56
29:X:1736:C:H2'	29:X:1737:G:C8	2.41	0.56
29:X:1383:C:H3'	29:X:1384:G:H8	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:861:G:H22	29:X:943:U:H1'	1.69	0.56
29:X:861:G:N3	29:X:944:A:H1'	2.21	0.56
29:X:995:A:P	29:X:996:C:H41	2.28	0.56
15:N:94:VAL:O	15:N:98:ILE:HG12	2.06	0.56
25:Z:7:PRO:HA	29:X:2594:U:C2	2.42	0.56
29:X:2387:U:H2'	29:X:2388:G:H8	1.70	0.56
29:X:2225:G:H2'	29:X:2226:A:C8	2.40	0.56
29:X:1856:U:H3	29:X:1861:G:H1	1.52	0.56
29:X:1656:U:OP1	29:X:2688:G:N2	2.39	0.56
29:X:1707:A:H3'	29:X:1708:C:H6	1.71	0.56
29:X:415:A:H61	29:X:435:A:H61	1.54	0.56
29:X:1426:U:H3	29:X:1605:A:H61	1.54	0.56
21:T:9:SER:HB3	29:X:2235:G:O2'	2.05	0.56
29:X:806:A:OP2	29:X:2054:A:O2'	2.24	0.56
2:A:52:ARG:HG2	2:A:53:PHE:CD2	2.41	0.56
29:X:1342:U:O5'	29:X:1343:C:H5	1.87	0.55
22:U:30:VAL:O	22:U:32:ARG:NH1	2.39	0.55
13:L:37:HIS:HD2	30:Y:29:C:O3'	1.89	0.55
29:X:2434:G:H2'	29:X:2435:C:C6	2.41	0.55
29:X:1690:U:H6	29:X:1690:U:H3'	1.72	0.55
4:C:146:GLU:O	4:C:166:TRP:HE3	1.90	0.55
29:X:2516:U:H2'	29:X:2517:C:H6	1.70	0.55
17:P:60:ILE:HD11	25:Z:28:PRO:HD3	1.88	0.55
29:X:1244:U:H2'	29:X:1245:G:C8	2.36	0.55
5:D:85:VAL:HG23	29:X:2291:U:H5'	1.88	0.55
5:D:13:ARG:HB2	5:D:14:PRO:HD3	1.88	0.55
29:X:2198:U:C2	29:X:2199:C:H1'	2.41	0.55
9:H:2:ILE:HD12	9:H:6:SER:OG	2.06	0.55
16:O:66:GLY:O	16:O:87:ARG:HD2	2.06	0.55
20:S:69:VAL:HG22	20:S:81:VAL:HG22	1.88	0.55
22:U:22:GLY:C	22:U:39:LYS:HZ3	2.08	0.55
29:X:652:C:N3	29:X:658:G:N2	2.54	0.55
29:X:568:G:H2'	29:X:569:C:O4'	2.07	0.55
29:X:810:U:H2'	29:X:811:G:O4'	2.06	0.55
15:N:61:TRP:O	15:N:65:ILE:HG13	2.05	0.55
2:A:142:VAL:HG21	2:A:191:ALA:HB1	1.89	0.55
29:X:787:A:O2'	29:X:788:G:O4'	2.24	0.55
29:X:165:G:O2'	29:X:1378:A:N6	2.39	0.55
20:S:151:ASP:N	20:S:151:ASP:OD2	2.37	0.55
16:O:28:GLU:O	16:O:30:GLY:N	2.39	0.55
29:X:1975:G:N2	29:X:1979:C:O2'	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:2586:G:H2'	29:X:2587:G:O4'	2.05	0.55
29:X:2031:A:H2'	29:X:2032:G:H5"	1.89	0.55
16:O:23:GLU:O	16:O:25:LEU:N	2.38	0.55
19:R:58:VAL:HA	29:X:494:A:H4'	1.87	0.55
29:X:2234:G:H2'	29:X:2235:G:O4'	2.07	0.55
2:A:246:PRO:HG2	29:X:1884:A:O2'	2.07	0.55
22:U:54:ASN:O	22:U:56:GLN:N	2.39	0.55
15:N:13:ARG:O	15:N:16:LYS:HB2	2.06	0.55
28:3:52:LYS:O	28:3:55:TRP:N	2.39	0.55
29:X:877:G:H1	29:X:924:C:N4	2.03	0.55
21:T:46:LYS:HZ3	21:T:76:ALA:HA	1.71	0.55
29:X:1325:U:H4'	29:X:1326:U:O5'	2.05	0.55
29:X:1819:U:H2'	29:X:1820:G:O4'	2.06	0.55
2:A:208:LYS:HB2	29:X:742:G:C6	2.41	0.55
8:G:94:LYS:O	8:G:98:LYS:N	2.31	0.55
2:A:43:ARG:HA	2:A:48:ARG:O	2.06	0.55
29:X:2443:C:H42	29:X:2465:G:H1	1.52	0.55
1:0:68:VAL:HG22	1:0:153:LYS:HA	1.89	0.55
29:X:1283:C:H5"	29:X:1284:G:H5'	1.88	0.55
8:G:125:ARG:NH1	29:X:2619:G:OP1	2.36	0.55
28:3:33:ASN:HB3	29:X:2398:U:H5"	1.89	0.55
29:X:2328:G:O6	29:X:2361:G:N2	2.30	0.55
29:X:495:C:H2'	29:X:496:C:C6	2.42	0.55
29:X:1550:C:H2'	29:X:1553:G:H1	1.71	0.55
29:X:2546:G:H2'	29:X:2547:C:C6	2.42	0.55
29:X:774:A:H8	29:X:774:A:O5'	1.90	0.55
19:R:23:ILE:HG13	19:R:31:GLY:HA2	1.88	0.55
29:X:1922:U:OP1	29:X:2583:U:O2'	2.25	0.55
29:X:1710:U:H3	29:X:1821:A:H61	1.55	0.55
5:D:99:PHE:HA	5:D:102:LYS:HD2	1.88	0.55
30:Y:41:A:O2'	30:Y:48:A:N1	2.35	0.55
29:X:2604:G:H2'	29:X:2605:C:O4'	2.07	0.55
5:D:92:ARG:NH2	30:Y:46:G:H3'	2.22	0.55
1:0:123:LEU:HD13	1:0:127:LEU:HD12	1.87	0.55
29:X:2277:A:H2'	29:X:2278:A:O4'	2.07	0.55
8:G:61:ARG:HD3	8:G:66:HIS:CE1	2.42	0.55
29:X:1221:C:C2	29:X:1222:G:C8	2.95	0.55
29:X:518:A:H5"	29:X:518:A:H8	1.71	0.55
14:M:63:ARG:HD3	29:X:2661:G:H4'	1.88	0.55
27:2:12:ARG:CD	27:2:44:VAL:HG11	2.36	0.55
25:Z:17:ASP:HB3	29:X:16:G:OP1	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1108:U:H3'	29:X:1109:A:C8	2.41	0.55
11:J:78:LYS:NZ	11:J:84:MET:HG3	2.22	0.55
29:X:2053:G:H2'	29:X:2054:A:C8	2.41	0.55
29:X:974:U:H2'	29:X:975:C:C6	2.42	0.55
11:J:66:TYR:HE2	29:X:886:A:HO2'	1.55	0.55
21:T:64:ASP:N	21:T:64:ASP:OD1	2.40	0.55
10:I:65:PHE:HA	28:3:12:ARG:HD2	1.89	0.55
29:X:1484:G:H2'	29:X:1485:U:C6	2.42	0.55
21:T:21:LEU:HD11	21:T:41:ARG:NE	2.21	0.55
3:B:84:PHE:HD2	3:B:86:PRO:HD3	1.71	0.55
29:X:713:G:O5'	29:X:713:G:H8	1.90	0.55
29:X:68:C:H2'	29:X:69:G:C8	2.41	0.55
25:Z:3:LYS:HB2	29:X:2590:U:O2	2.07	0.55
29:X:2145:A:H4'	29:X:2155:U:H5"	1.89	0.55
29:X:751:G:H2'	29:X:752:G:C8	2.41	0.55
24:W:17:VAL:O	24:W:20:VAL:N	2.40	0.55
1:0:38:GLU:HB2	1:0:211:THR:HB	1.88	0.55
20:S:168:VAL:HG12	20:S:169:VAL:H	1.71	0.55
13:L:64:LYS:HZ3	30:Y:53:G:H5"	1.72	0.55
15:N:10:ARG:HG3	15:N:13:ARG:HH22	1.72	0.54
3:B:22:PRO:HB3	29:X:2661:G:C2	2.42	0.54
30:Y:7:C:H2'	30:Y:8:C:H6	1.72	0.54
3:B:134:TRP:CD1	3:B:137:ARG:HB2	2.42	0.54
29:X:825:C:HO2'	29:X:1239:A:HO2'	1.55	0.54
13:L:19:THR:HG21	13:L:28:ARG:HD3	1.88	0.54
29:X:618:A:H2'	29:X:619:A:C8	2.43	0.54
29:X:562:G:H2'	29:X:563:U:O4'	2.07	0.54
9:H:4:PRO:O	9:H:5:GLN:HB2	2.07	0.54
27:2:37:LYS:HG2	29:X:469:G:C8	2.41	0.54
29:X:313:U:H2'	29:X:314:G:H8	1.72	0.54
20:S:26:LYS:HE3	30:Y:107:C:H4'	1.89	0.54
5:D:65:PRO:HA	5:D:89:VAL:HG13	1.89	0.54
26:1:37:LEU:HG	29:X:2323:U:O2'	2.06	0.54
10:I:90:ARG:HD2	10:I:93:LEU:HG	1.88	0.54
29:X:165:G:H2'	29:X:166:G:O4'	2.08	0.54
21:T:12:ASN:OD1	21:T:12:ASN:N	2.40	0.54
3:B:116:VAL:HG11	3:B:138:PRO:HB3	1.89	0.54
18:Q:84:GLU:OE2	18:Q:86:GLN:NE2	2.40	0.54
5:D:24:SER:OG	30:Y:57:U:O3'	2.15	0.54
29:X:1773:C:O4'	29:X:2588:U:C2	2.60	0.54
14:M:82:PRO:C	14:M:84:ALA:H	2.09	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1298:G:C6	29:X:1342:U:C5	2.95	0.54
29:X:2605:C:H2'	29:X:2606:G:C8	2.43	0.54
29:X:867:G:H1	29:X:935:C:N4	2.02	0.54
29:X:2482:A:H4'	29:X:2483:U:OP1	2.06	0.54
13:L:85:LYS:HD2	13:L:86:GLN:HG2	1.89	0.54
29:X:1987:G:C5	29:X:1988:A:C8	2.96	0.54
24:W:19:THR:HG23	24:W:43:MET:HG2	1.88	0.54
29:X:2495:G:N2	29:X:2548:G:H1'	2.23	0.54
29:X:2030:U:H2'	29:X:2031:A:C8	2.42	0.54
4:C:117:LEU:HD22	4:C:188:ILE:HD11	1.88	0.54
29:X:1818:G:H2'	29:X:1819:U:H6	1.71	0.54
30:Y:86:A:C2	30:Y:96:C:N3	2.76	0.54
29:X:2574:G:N2	29:X:2577:A:OP2	2.39	0.54
29:X:2779:C:H2'	29:X:2780:A:H8	1.72	0.54
29:X:510:G:H2'	29:X:511:A:H3'	1.88	0.54
29:X:659:G:H2'	29:X:660:G:C8	2.41	0.54
29:X:573:C:H2'	29:X:574:C:C6	2.41	0.54
29:X:1974:U:H2'	29:X:1975:G:H5'	1.89	0.54
3:B:57:ARG:NH2	29:X:2809:A:H5'	2.21	0.54
14:M:106:TYR:CD2	14:M:106:TYR:N	2.75	0.54
18:Q:2:SER:O	18:Q:4:TYR:N	2.34	0.54
2:A:145:LEU:HD22	2:A:163:VAL:HG11	1.90	0.54
3:B:108:SER:OG	3:B:162:MET:N	2.41	0.54
5:D:117:ILE:HG21	5:D:130:LEU:HD21	1.89	0.54
29:X:1296:G:N2	29:X:1299:A:H5'	2.23	0.54
6:E:96:ALA:HA	6:E:104:GLU:O	2.08	0.54
29:X:2660:C:C4	29:X:2704:U:C5	2.95	0.54
8:G:31:THR:HG21	15:N:61:TRP:HE1	1.71	0.54
16:O:18:ASP:OD1	16:O:18:ASP:N	2.39	0.54
2:A:39:LYS:HZ1	2:A:58:HIS:H	1.54	0.54
29:X:1030:U:OP1	29:X:1046:U:O2'	2.21	0.54
14:M:40:ARG:NH1	14:M:40:ARG:HB3	2.21	0.54
29:X:2285:U:H5	29:X:2290:A:C6	2.26	0.54
1:0:112:THR:HB	1:0:115:MET:HB2	1.89	0.54
29:X:854:G:H1'	29:X:949:G:H22	1.71	0.54
27:2:34:ARG:HD3	29:X:478:G:OP2	2.07	0.54
16:O:78:VAL:HG23	16:O:80:TYR:H	1.73	0.54
29:X:1385:C:H2'	29:X:1386:A:O4'	2.08	0.54
29:X:932:G:H2'	29:X:933:G:C8	2.42	0.54
29:X:994:A:N7	29:X:995:A:C6	2.76	0.54
29:X:2557:G:H2'	29:X:2558:C:C6	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:588:G:H1	29:X:1274:C:H42	1.55	0.54
29:X:1353:A:H3'	29:X:1354:A:C8	2.42	0.54
3:B:175:ILE:HG12	3:B:182:ILE:HD11	1.90	0.54
29:X:706:A:H2'	29:X:707:U:O4'	2.08	0.54
3:B:164:ARG:O	29:X:2753:C:H5"	2.08	0.54
20:S:49:THR:HG21	20:S:96:VAL:HG13	1.89	0.54
13:L:80:ALA:HB2	13:L:111:GLY:O	2.08	0.54
10:I:61:PRO:HG2	28:3:25:PHE:HB2	1.89	0.54
29:X:1818:G:H2'	29:X:1819:U:C6	2.43	0.54
29:X:597:U:H2'	29:X:598:U:C6	2.42	0.54
17:P:45:ILE:HD11	17:P:57:LEU:HG	1.90	0.54
5:D:64:LYS:HD3	30:Y:44:C:H4'	1.90	0.54
29:X:2594:U:H2'	29:X:2595:C:H6	1.73	0.54
29:X:521:U:O4	29:X:522:G:N2	2.41	0.54
2:A:260:ARG:HH22	2:A:266:SER:HB2	1.72	0.54
29:X:2819:G:H2'	29:X:2820:C:H6	1.73	0.54
29:X:24:G:H2'	29:X:25:U:C6	2.43	0.54
29:X:2433:G:H2'	29:X:2434:G:H8	1.73	0.54
29:X:1542:G:H2'	29:X:1543:G:C8	2.43	0.54
8:G:106:TYR:CD2	29:X:2621:G:H5'	2.42	0.54
23:V:21:ARG:HG3	23:V:46:LEU:HD23	1.89	0.54
14:M:8:ASN:HA	29:X:2851:G:OP1	2.08	0.54
29:X:555:U:H5'	29:X:556:A:C2	2.43	0.53
5:D:74:ILE:HA	5:D:79:LEU:HB2	1.90	0.53
29:X:525:A:H2'	29:X:526:C:H5'	1.90	0.53
18:Q:65:VAL:HG23	29:X:63:A:H1'	1.88	0.53
29:X:1329:U:H5'	29:X:1405:A:H1'	1.89	0.53
11:J:78:LYS:HZ2	11:J:84:MET:HG3	1.73	0.53
29:X:1324:G:OP2	29:X:1324:G:N2	2.29	0.53
6:E:41:LEU:HG	6:E:54:ARG:HA	1.90	0.53
18:Q:64:ARG:HB2	18:Q:69:ILE:HD13	1.90	0.53
25:Z:45:ILE:HD13	25:Z:57:VAL:HG22	1.90	0.53
17:P:11:LYS:HG3	17:P:14:ARG:NH2	2.22	0.53
29:X:957:G:H2'	29:X:958:G:C8	2.43	0.53
26:1:22:TYR:OH	29:X:2326:C:O2'	2.20	0.53
20:S:52:PHE:N	20:S:64:ALA:O	2.32	0.53
29:X:1359:G:H2'	29:X:1360:G:H8	1.73	0.53
29:X:2245:A:H4'	29:X:2246:A:C2	2.43	0.53
28:3:56:ALA:O	28:3:60:LEU:HG	2.08	0.53
3:B:105:THR:HB	3:B:197:VAL:HG13	1.90	0.53
22:U:21:ARG:HH21	22:U:23:LYS:HG2	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:130:THR:HG21	29:X:331:U:H2'	1.90	0.53
29:X:175:C:O2'	29:X:176:A:H5'	2.08	0.53
20:S:55:THR:OG1	20:S:55:THR:O	2.23	0.53
29:X:163:A:H2'	29:X:164:G:C8	2.43	0.53
10:I:35:LYS:HE2	29:X:820:U:P	2.48	0.53
19:R:48:VAL:HG13	19:R:50:GLY:H	1.72	0.53
25:Z:36:CYS:SG	25:Z:49:CYS:N	2.73	0.53
28:3:36:LYS:HB3	28:3:41:ILE:HG13	1.90	0.53
29:X:651:C:H2'	29:X:652:C:C6	2.44	0.53
29:X:2310:G:C6	29:X:2311:U:C5	2.97	0.53
15:N:24:PHE:HB3	15:N:28:ARG:HB3	1.89	0.53
14:M:106:TYR:N	14:M:106:TYR:HD2	2.07	0.53
21:T:32:LYS:HB3	21:T:35:ASN:OD1	2.09	0.53
12:K:34:ILE:O	12:K:112:LEU:HA	2.08	0.53
15:N:104:GLU:O	15:N:107:LYS:HB3	2.09	0.53
29:X:2490:U:H2'	29:X:2491:C:O4'	2.09	0.53
29:X:1840:A:H2'	29:X:1841:G:O4'	2.09	0.53
9:H:132:GLU:HB2	14:M:73:PHE:CE1	2.44	0.53
29:X:2081:U:H3	29:X:2174:G:H1	1.55	0.53
29:X:645:G:H2'	29:X:646:C:C6	2.43	0.53
3:B:11:MET:HG2	3:B:24:THR:OG1	2.09	0.53
29:X:548:G:N2	29:X:564:U:O2	2.33	0.53
29:X:1770:U:C2	29:X:1774:A:N7	2.77	0.53
3:B:176:ARG:NH2	14:M:16:ILE:HA	2.20	0.53
29:X:2451:G:H2'	29:X:2454:C:H42	1.74	0.53
29:X:2200:G:H2'	29:X:2201:G:C8	2.43	0.53
20:S:103:ARG:NH2	20:S:107:GLU:HB3	2.22	0.53
29:X:2726:U:O2	29:X:2739:G:N2	2.41	0.53
4:C:74:VAL:HG12	4:C:76:THR:H	1.74	0.53
11:J:111:THR:HG22	11:J:114:GLN:HG3	1.91	0.53
29:X:839:U:OP1	29:X:2408:G:OP1	2.26	0.53
8:G:110:LEU:HD22	29:X:1142:G:H4'	1.91	0.53
12:K:83:VAL:HG23	12:K:87:TYR:CE2	2.43	0.53
29:X:493:A:OP2	29:X:517:A:N6	2.28	0.53
29:X:2820:C:C2	29:X:2821:G:C8	2.97	0.53
15:N:54:LYS:NZ	29:X:1005:U:H3'	2.24	0.53
29:X:1007:A:H2'	29:X:1008:G:H8	1.71	0.53
29:X:310:A:N3	29:X:330:C:O2'	2.40	0.53
29:X:1020:A:N7	29:X:1021:A:C6	2.76	0.53
4:C:67:ALA:HA	29:X:1268:U:C6	2.44	0.53
29:X:2198:U:H3'	29:X:2199:C:C4'	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:68:ARG:NH2	29:X:2043:A:N6	2.55	0.53
12:K:27:ALA:O	12:K:30:ARG:N	2.42	0.53
29:X:2375:G:C2	29:X:2400:G:C2	2.96	0.53
4:C:106:MET:O	4:C:110:SER:OG	2.15	0.53
29:X:1430:G:O2'	29:X:1603:A:N3	2.41	0.53
4:C:33:TRP:HD1	4:C:93:TYR:CE1	2.27	0.53
29:X:1699:A:H61	29:X:1723:U:H3	1.57	0.53
29:X:513:A:C6	29:X:516:G:C6	2.97	0.53
29:X:2084:G:H2'	29:X:2085:G:C8	2.43	0.53
29:X:218:A:N1	29:X:232:A:H5"	2.23	0.53
29:X:1340:C:H2'	29:X:1341:G:C8	2.44	0.53
3:B:147:PRO:HG2	3:B:149:ARG:HG2	1.90	0.53
29:X:1662:G:H5"	29:X:1663:C:C5'	2.38	0.53
22:U:20:ARG:HD2	22:U:43:ARG:NH1	2.23	0.53
25:Z:36:CYS:SG	25:Z:48:ASN:HB2	2.49	0.53
3:B:37:LYS:NZ	3:B:80:GLU:OE2	2.38	0.53
29:X:186:C:H2'	29:X:187:U:O4'	2.09	0.53
13:L:63:ASN:HB3	13:L:66:ASP:HB2	1.91	0.53
29:X:1991:C:H2'	29:X:1992:G:C8	2.44	0.53
29:X:571:U:O2'	29:X:581:A:H8	1.91	0.53
29:X:1436:G:O3'	29:X:1508:G:O2'	2.27	0.53
19:R:100:ASP:HB3	19:R:101:GLY:CA	2.38	0.53
29:X:2369:U:C6	29:X:2369:U:H3'	2.43	0.53
29:X:1495:G:H2'	29:X:1496:G:C8	2.44	0.53
13:L:64:LYS:NZ	30:Y:53:G:H5"	2.24	0.53
29:X:2817:A:C2	29:X:2851:G:C2	2.96	0.53
8:G:122:HIS:O	8:G:122:HIS:ND1	2.39	0.53
29:X:1069:G:H2'	29:X:1070:G:H8	1.73	0.53
29:X:2769:C:H1'	29:X:2866:A:H2	1.73	0.53
8:G:50:PRO:HG3	29:X:1152:C:C5	2.44	0.53
9:H:35:THR:HG21	29:X:2628:C:O3'	2.09	0.53
17:P:97:VAL:HG22	17:P:124:ILE:HG23	1.89	0.53
15:N:91:ASN:HB3	15:N:94:VAL:HG23	1.91	0.53
27:2:12:ARG:HD3	29:X:699:G:O6	2.09	0.53
5:D:74:ILE:HG12	5:D:80:ARG:O	2.09	0.53
22:U:32:ARG:H	22:U:32:ARG:HE	1.54	0.53
19:R:44:GLN:HG2	19:R:77:HIS:HE1	1.72	0.53
29:X:1692:C:C5	29:X:1693:A:N7	2.77	0.53
2:A:229:VAL:HG11	29:X:797:A:C4	2.43	0.53
29:X:500:G:H5"	29:X:501:G:OP2	2.09	0.53
29:X:937:C:H1'	29:X:939:C:H41	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:82:LYS:HB3	9:H:82:LYS:NZ	2.24	0.53
29:X:2750:G:O5'	29:X:2750:G:H8	1.92	0.53
12:K:39:THR:O	12:K:42:LYS:N	2.42	0.53
3:B:99:GLY:N	3:B:172:VAL:O	2.42	0.53
3:B:145:LYS:HB2	29:X:2551:A:N7	2.24	0.53
15:N:13:ARG:HH12	29:X:1264:C:P	2.30	0.53
4:C:34:GLN:HE21	29:X:627:A:P	2.31	0.53
29:X:1104:G:N3	29:X:1110:G:N2	2.56	0.53
13:L:35:SER:OG	30:Y:30:C:OP1	2.10	0.53
10:I:87:THR:OG1	10:I:97:ARG:NH2	2.41	0.53
1:0:157:ILE:HD13	1:0:157:ILE:H	1.73	0.53
7:F:115:LEU:HD22	7:F:126:THR:HG21	1.91	0.53
19:R:58:VAL:HA	29:X:494:A:C5'	2.39	0.53
10:I:23:PRO:HD2	29:X:826:U:OP1	2.08	0.53
29:X:2098:G:O2'	29:X:2154:A:N6	2.42	0.53
11:J:84:MET:HE3	29:X:970:A:H62	1.73	0.53
29:X:307:C:C2'	29:X:308:C:H5'	2.38	0.53
20:S:149:ALA:HB3	20:S:164:PRO:HA	1.91	0.53
29:X:1924:C:N4	29:X:1948:C:OP2	2.42	0.53
29:X:359:G:H2'	29:X:360:A:C8	2.43	0.53
22:U:17:SER:CB	22:U:18:VAL:HB	2.36	0.52
29:X:220:U:H2'	29:X:221:A:C8	2.43	0.52
29:X:2606:G:H21	29:X:2761:A:H2	1.56	0.52
21:T:26:PHE:CE1	29:X:870:C:H1'	2.44	0.52
29:X:2038:C:H2'	29:X:2483:U:C4'	2.40	0.52
8:G:37:ASP:HB2	8:G:38:GLU:HG3	1.91	0.52
29:X:1794:A:N6	29:X:1806:G:O2'	2.42	0.52
29:X:1728:A:H61	29:X:1738:U:H3	1.57	0.52
11:J:115:ALA:O	11:J:119:PHE:HB2	2.09	0.52
15:N:11:ARG:O	15:N:15:LYS:HG3	2.08	0.52
3:B:16:LYS:HB2	3:B:21:ILE:HD11	1.92	0.52
29:X:2262:C:C5	29:X:2368:G:H2'	2.45	0.52
15:N:6:THR:O	15:N:9:VAL:HG23	2.10	0.52
29:X:627:A:C6	29:X:628:A:C6	2.96	0.52
29:X:218:A:H61	29:X:232:A:H3'	1.74	0.52
29:X:2630:C:H2'	29:X:2631:C:C6	2.44	0.52
19:R:59:LYS:N	19:R:60:PRO:HD2	2.24	0.52
9:H:2:ILE:O	9:H:45:ALA:N	2.43	0.52
22:U:51:ILE:HA	22:U:59:THR:O	2.09	0.52
1:0:112:THR:HG22	1:0:113:PRO:HD2	1.91	0.52
10:I:77:LEU:C	10:I:79:GLN:H	2.12	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:10:LYS:HB2	29:X:2000:U:O2	2.09	0.52
6:E:103:LEU:HD21	6:E:131:ILE:HD13	1.91	0.52
29:X:670:U:H2'	29:X:671:A:C8	2.44	0.52
28:3:17:THR:HG21	28:3:21:LYS:HG3	1.90	0.52
29:X:16:G:O2'	29:X:17:G:H5'	2.10	0.52
9:H:16:ALA:HB2	9:H:98:ILE:HD11	1.91	0.52
29:X:2651:U:C2	29:X:2652:G:C8	2.98	0.52
6:E:99:THR:O	6:E:101:LYS:N	2.40	0.52
21:T:39:ARG:HH21	29:X:2334:C:H1'	1.73	0.52
22:U:22:GLY:O	22:U:39:LYS:HG3	2.09	0.52
9:H:38:GLY:HA2	29:X:2627:G:N3	2.24	0.52
29:X:2707:G:H2'	29:X:2708:U:H6	1.74	0.52
29:X:1672:A:H3'	29:X:1673:C:C6	2.44	0.52
9:H:54:SER:HA	9:H:69:VAL:HA	1.91	0.52
29:X:1030:U:N3	29:X:1031:C:H5	2.06	0.52
29:X:24:G:H2'	29:X:25:U:H6	1.73	0.52
29:X:1686:A:H5"	29:X:1687:C:OP2	2.09	0.52
29:X:529:U:C2	29:X:530:G:C8	2.98	0.52
29:X:490:A:H4'	29:X:491:A:OP1	2.09	0.52
14:M:55:ILE:O	14:M:103:LYS:O	2.28	0.52
14:M:73:PHE:O	14:M:75:GLU:N	2.42	0.52
17:P:40:LEU:HA	17:P:43:ASP:OD2	2.08	0.52
29:X:58:C:H1'	29:X:72:A:H2'	1.91	0.52
29:X:1282:A:H8	29:X:1282:A:O5'	1.92	0.52
11:J:100:PRO:HG2	20:S:74:ARG:HH11	1.74	0.52
29:X:1774:A:H5'	29:X:2587:G:H4'	1.90	0.52
13:L:89:PHE:HZ	13:L:100:VAL:HG22	1.74	0.52
29:X:2001:G:C6	29:X:2002:A:C6	2.97	0.52
18:Q:15:LYS:NZ	29:X:1353:A:OP1	2.38	0.52
30:Y:16:U:O2'	30:Y:17:A:P	2.67	0.52
10:I:114:ILE:HG21	10:I:132:ALA:O	2.09	0.52
20:S:155:PRO:O	20:S:156:GLU:HB3	2.10	0.52
11:J:49:GLU:O	11:J:53:ILE:HG13	2.10	0.52
29:X:812:G:H3'	29:X:813:A:H2'	1.91	0.52
29:X:483:A:H3'	29:X:484:G:H5'	1.91	0.52
10:I:93:LEU:HB3	10:I:97:ARG:NH1	2.24	0.52
29:X:2779:C:H2'	29:X:2780:A:C8	2.45	0.52
29:X:1903:C:H5'	29:X:1904:G:OP2	2.09	0.52
9:H:70:VAL:HG21	9:H:106:ARG:NH1	2.25	0.52
26:1:21:TYR:OH	29:X:2397:A:N3	2.43	0.52
29:X:2198:U:C3'	29:X:2199:C:H4'	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1238:A:O2'	29:X:1239:A:O4'	2.25	0.52
29:X:739:G:O2'	29:X:740:A:OP2	2.27	0.52
12:K:54:THR:HG22	12:K:66:VAL:HG23	1.90	0.52
13:L:15:ARG:HH21	29:X:2272:A:P	2.32	0.52
13:L:60:LYS:HG2	13:L:61:SER:H	1.74	0.52
11:J:19:THR:HG22	11:J:20:GLY:N	2.16	0.52
30:Y:39:C:H5"	30:Y:40:C:C6	2.45	0.52
29:X:2791:C:N3	29:X:2806:G:N2	2.57	0.52
25:Z:3:LYS:HA	29:X:2556:A:O2'	2.10	0.52
13:L:65:THR:OG1	30:Y:52:G:OP1	2.25	0.52
29:X:501:G:H2'	29:X:502:A:C8	2.44	0.52
29:X:2230:G:H5"	29:X:2231:G:OP2	2.09	0.52
29:X:1744:G:C2	29:X:1747:G:C2	2.98	0.52
23:V:31:GLN:O	23:V:35:GLY:N	2.43	0.52
10:I:20:GLY:HA3	10:I:21:ARG:NH1	2.24	0.52
4:C:84:PHE:HE1	29:X:596:C:H5'	1.75	0.52
7:F:133:SER:OG	29:X:1073:G:N3	2.43	0.52
29:X:1462:C:O2'	29:X:1560:A:N3	2.32	0.52
29:X:242:A:H1'	29:X:243:G:H1'	1.91	0.52
29:X:1234:C:H42	29:X:1241:G:H1	1.58	0.52
29:X:1889:G:O2'	29:X:1890:G:H5"	2.09	0.52
29:X:1533:G:H2'	29:X:1534:A:C8	2.44	0.52
11:J:59:PHE:CD2	11:J:110:VAL:HG11	2.44	0.52
2:A:250:TRP:CE2	29:X:1796:A:H5"	2.45	0.52
29:X:1578:U:H2'	29:X:1579:G:H8	1.75	0.52
25:Z:5:PRO:HG3	29:X:2593:A:C8	2.45	0.52
29:X:1323:G:H1'	29:X:1627:C:H5'	1.91	0.52
29:X:2676:G:C2	29:X:2690:A:C2	2.98	0.52
29:X:2551:A:H5"	29:X:2553:G:H4'	1.91	0.52
10:I:18:ARG:HH22	29:X:1262:U:H2'	1.74	0.52
29:X:1982:C:H4'	29:X:2703:C:O2	2.09	0.52
29:X:13:A:O2'	29:X:15:G:N7	2.43	0.52
22:U:27:ASP:O	22:U:32:ARG:HD3	2.10	0.52
30:Y:59:A:H5'	30:Y:60:A:OP2	2.09	0.52
29:X:1065:A:H2'	29:X:1066:G:C8	2.45	0.52
29:X:1194:U:H2'	29:X:1195:U:C6	2.45	0.52
2:A:238:GLY:O	2:A:240:THR:N	2.43	0.52
29:X:2579:A:H2'	29:X:2580:C:C5	2.44	0.52
29:X:1905:G:OP2	29:X:1905:G:H8	1.92	0.52
4:C:51:VAL:O	4:C:53:LYS:N	2.43	0.52
29:X:2308:A:N6	29:X:2365:U:O4	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:46:VAL:N	19:R:76:LEU:O	2.44	0.51
2:A:48:ARG:NH2	29:X:791:G:H5'	2.25	0.51
4:C:18:PRO:HB2	4:C:106:MET:HG3	1.92	0.51
29:X:1533:G:H2'	29:X:1534:A:H8	1.74	0.51
7:F:2:ARG:NH2	7:F:29:GLN:O	2.43	0.51
29:X:1278:A:H5'	29:X:1280:U:H1'	1.91	0.51
29:X:2120:C:N4	29:X:2137:G:O6	2.42	0.51
18:Q:28:TRP:CZ3	18:Q:77:LYS:HB2	2.45	0.51
15:N:90:LEU:HD13	15:N:95:LEU:HD21	1.92	0.51
29:X:1673:C:C2	29:X:1674:C:C5	2.98	0.51
13:L:37:HIS:CE1	13:L:39:TYR:CD1	2.96	0.51
15:N:3:ARG:HG2	29:X:457:C:H5"	1.92	0.51
29:X:826:U:H2'	29:X:827:C:C6	2.45	0.51
2:A:124:GLU:O	2:A:126:LYS:N	2.44	0.51
2:A:231:HIS:CG	2:A:232:PRO:HD2	2.45	0.51
29:X:1548:U:H3	29:X:1555:A:H61	1.57	0.51
7:F:107:ILE:HG21	7:F:127:VAL:HG11	1.92	0.51
8:G:81:VAL:HG11	8:G:156:HIS:CD2	2.45	0.51
4:C:130:THR:HG23	29:X:332:C:H5"	1.92	0.51
29:X:1354:A:H2'	29:X:1410:U:O2	2.10	0.51
29:X:1441:A:H4'	29:X:1442:C:O5'	2.09	0.51
29:X:915:C:H2'	29:X:916:U:C6	2.45	0.51
29:X:2859:U:C5	29:X:2860:C:C2	2.98	0.51
22:U:21:ARG:NH1	29:X:400:U:H5'	2.12	0.51
29:X:2340:C:H2'	29:X:2341:G:O4'	2.11	0.51
29:X:1662:G:OP1	29:X:1663:C:H5'	2.10	0.51
10:I:86:THR:HG1	10:I:116:ARG:HH11	1.57	0.51
17:P:48:LYS:O	17:P:50:VAL:N	2.37	0.51
22:U:38:THR:HG22	29:X:2412:A:H2	1.75	0.51
29:X:389:G:H1	29:X:411:C:N4	2.08	0.51
1:0:61:PRO:HG2	1:0:184:ASN:HA	1.91	0.51
17:P:12:LYS:NZ	29:X:319:G:N7	2.41	0.51
28:3:29:LYS:O	28:3:30:ARG:HD3	2.11	0.51
29:X:1681:A:O5'	29:X:1681:A:C8	2.63	0.51
28:3:64:ARG:HD2	29:X:220:U:H5'	1.92	0.51
29:X:2440:C:H2'	29:X:2441:U:C6	2.42	0.51
29:X:1685:A:N6	29:X:1693:A:H61	2.09	0.51
27:2:7:PRO:HB2	29:X:1322:G:H4'	1.93	0.51
29:X:854:G:H1'	29:X:949:G:N2	2.26	0.51
29:X:929:A:H2	30:Y:81:C:O2	1.93	0.51
2:A:85:ASP:HB2	2:A:92:ILE:HD13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:10:GLY:O	14:M:13:LEU:HB2	2.11	0.51
2:A:14:ARG:HG3	2:A:15:GLN:H	1.76	0.51
29:X:1334:A:H2'	29:X:1335:A:O4'	2.11	0.51
23:V:25:LEU:HA	23:V:28:LEU:HD12	1.92	0.51
19:R:95:ARG:HH22	19:R:109:ALA:HA	1.75	0.51
3:B:112:GLY:O	3:B:159:HIS:HA	2.10	0.51
29:X:556:A:H4'	29:X:558:G:H21	1.76	0.51
4:C:149:LEU:HD11	4:C:170:LEU:HG	1.92	0.51
4:C:174:GLY:HA3	29:X:626:A:C4	2.45	0.51
29:X:1680:U:H4'	29:X:2666:U:OP1	2.10	0.51
29:X:2665:G:N2	29:X:2704:U:O2	2.43	0.51
29:X:2607:C:H1'	29:X:2761:A:C2	2.46	0.51
29:X:2494:C:O2	29:X:2549:G:C2	2.63	0.51
29:X:67:G:H2'	29:X:68:C:H6	1.76	0.51
3:B:134:TRP:HA	3:B:137:ARG:HD3	1.93	0.51
20:S:56:VAL:O	20:S:58:GLY:N	2.39	0.51
21:T:16:SER:OG	29:X:2241:U:OP2	2.20	0.51
12:K:22:ARG:HD3	12:K:69:ASP:HA	1.93	0.51
9:H:83:ARG:CZ	9:H:89:ILE:HD11	2.40	0.51
29:X:2144:C:O2'	29:X:2156:A:H1'	2.10	0.51
29:X:2528:G:C2	29:X:2529:G:N7	2.79	0.51
3:B:144:ARG:HD3	29:X:2551:A:N7	2.25	0.51
29:X:227:G:C6	29:X:228:A:C6	2.98	0.51
29:X:942:U:H2'	29:X:943:U:C6	2.46	0.51
29:X:2542:U:O2	29:X:2544:A:H8	1.93	0.51
29:X:2477:C:O2'	29:X:2478:C:H5'	2.11	0.51
14:M:106:TYR:HE1	29:X:1745:C:H5'	1.75	0.51
29:X:2097:A:H61	29:X:2102:A:N6	2.09	0.51
22:U:46:LEU:HB2	29:X:2209:G:H4'	1.92	0.51
17:P:9:ARG:NH2	29:X:318:G:OP1	2.43	0.51
29:X:1578:U:H2'	29:X:1579:G:C8	2.46	0.51
29:X:2867:G:H8	29:X:2867:G:OP2	1.92	0.51
1:0:71:ALA:HB3	1:0:109:VAL:HG22	1.93	0.51
3:B:174:GLU:HB3	3:B:183:LEU:HD12	1.93	0.51
28:3:22:VAL:HG22	28:3:50:LEU:HD23	1.91	0.51
29:X:959:C:H2'	29:X:960:U:C6	2.45	0.51
11:J:28:VAL:HB	11:J:135:ARG:HA	1.93	0.51
30:Y:7:C:H2'	30:Y:8:C:C6	2.45	0.51
13:L:39:TYR:OH	30:Y:118:G:H1'	2.10	0.51
29:X:1764:A:H2'	29:X:1765:C:H5'	1.92	0.51
29:X:1851:A:H3'	29:X:1852:G:H8	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:74:MET:HE2	15:N:110:VAL:HG13	1.93	0.51
4:C:193:LEU:HA	4:C:196:VAL:HG22	1.93	0.51
29:X:2629:U:H2'	29:X:2630:C:C6	2.40	0.51
29:X:1478:U:H2'	29:X:1479:G:H8	1.75	0.51
14:M:2:GLN:N	29:X:2795:A:H61	2.09	0.51
19:R:44:GLN:HG2	19:R:77:HIS:CE1	2.46	0.51
15:N:31:GLN:HB3	29:X:590:C:OP1	2.11	0.51
7:F:12:LEU:HD21	7:F:23:VAL:HG22	1.93	0.51
29:X:1889:G:H1	29:X:1908:C:H5"	1.76	0.51
29:X:914:C:H2'	29:X:915:C:C6	2.46	0.51
2:A:24:LEU:HD22	2:A:82:ILE:O	2.11	0.51
5:D:129:ASN:HA	5:D:155:THR:HA	1.93	0.51
12:K:8:ARG:HB2	12:K:43:GLU:OE1	2.11	0.51
11:J:26:ASP:HA	11:J:103:VAL:HG23	1.93	0.51
5:D:27:ALA:HB2	30:Y:59:A:H1'	1.91	0.51
7:F:10:LEU:HD22	7:F:27:LEU:HD21	1.92	0.51
29:X:1683:G:H1	29:X:1977:C:N4	2.08	0.51
23:V:63:LYS:HG2	23:V:66:GLN:NE2	2.25	0.51
20:S:17:SER:HA	20:S:36:ARG:HH22	1.75	0.51
29:X:2847:G:C2	29:X:2848:A:N6	2.79	0.51
29:X:2447:G:HO2'	29:X:2448:A:H8	1.57	0.51
29:X:1281:A:OP1	29:X:1989:C:OP1	2.28	0.50
29:X:1231:A:N6	29:X:1245:G:O6	2.44	0.50
27:2:37:LYS:O	29:X:469:G:H2'	2.11	0.50
29:X:2283:G:N2	29:X:2291:U:H3	2.05	0.50
25:Z:7:PRO:HB3	29:X:2594:U:H1'	1.93	0.50
29:X:1211:G:C2	29:X:1212:U:C5	2.98	0.50
7:F:90:THR:OG1	7:F:93:LYS:HB2	2.10	0.50
5:D:115:ARG:HB2	5:D:178:ARG:HG3	1.93	0.50
10:I:101:ARG:O	10:I:102:LYS:HB2	2.11	0.50
29:X:1707:A:H3'	29:X:1708:C:C6	2.46	0.50
5:D:117:ILE:HG22	5:D:118:ASN:H	1.76	0.50
12:K:28:LEU:HD23	12:K:48:VAL:HG11	1.92	0.50
29:X:2695:C:H2'	29:X:2696:A:H8	1.76	0.50
29:X:1971:C:H2'	29:X:1972:G:O4'	2.11	0.50
29:X:640:C:H4'	29:X:660:G:H21	1.75	0.50
4:C:72:ARG:NE	4:C:77:PHE:HE2	2.07	0.50
29:X:522:G:OP1	29:X:1247:U:O2'	2.27	0.50
29:X:1468:A:N7	29:X:2681:A:N6	2.59	0.50
19:R:18:LYS:HA	19:R:36:VAL:CG1	2.40	0.50
29:X:967:G:H2'	29:X:968:C:H2'	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1039:A:N6	29:X:1137:A:OP1	2.35	0.50
15:N:48:ARG:CD	29:X:1167:A:H61	2.13	0.50
29:X:653:G:H2'	29:X:654:A:H3'	1.93	0.50
12:K:103:ARG:NH2	12:K:108:VAL:HB	2.24	0.50
30:Y:39:C:H5'	30:Y:40:C:OP2	2.11	0.50
5:D:10:ASP:HA	5:D:13:ARG:HG3	1.94	0.50
7:F:54:PRO:HD3	7:F:73:PRO:HD3	1.94	0.50
30:Y:16:U:HO2'	30:Y:17:A:P	2.34	0.50
29:X:1238:A:H2'	29:X:1239:A:C8	2.46	0.50
18:Q:2:SER:C	18:Q:4:TYR:H	2.15	0.50
12:K:52:ILE:HG21	12:K:94:TYR:CG	2.45	0.50
11:J:88:LYS:HG3	29:X:966:A:H5"	1.92	0.50
29:X:503:G:H2'	29:X:504:G:O4'	2.11	0.50
4:C:179:ASP:O	4:C:182:ARG:HB3	2.11	0.50
29:X:661:C:H2'	29:X:662:G:C8	2.46	0.50
29:X:125:A:H5"	29:X:126:C:O4'	2.11	0.50
29:X:2659:C:C2	29:X:2660:C:C5	3.00	0.50
12:K:103:ARG:CZ	12:K:106:ASP:OD2	2.59	0.50
29:X:1991:C:H2'	29:X:1992:G:H8	1.77	0.50
29:X:866:U:H2'	29:X:867:G:C8	2.45	0.50
30:Y:36:A:N6	30:Y:46:G:O2'	2.44	0.50
29:X:2595:C:H2'	29:X:2596:C:H6	1.76	0.50
29:X:1856:U:H2'	29:X:1857:G:C8	2.46	0.50
6:E:45:GLN:HG2	6:E:47:GLY:H	1.77	0.50
29:X:2425:G:H2'	29:X:2480:C:H5	1.76	0.50
21:T:41:ARG:HA	21:T:41:ARG:HE	1.77	0.50
29:X:2563:U:HO2'	29:X:2564:U:H5	1.58	0.50
20:S:37:LYS:O	20:S:41:ARG:HG2	2.12	0.50
29:X:213:C:H2'	29:X:214:C:H6	1.75	0.50
8:G:52:GLY:O	8:G:55:ALA:HB3	2.12	0.50
17:P:81:HIS:HD1	17:P:82:ASN:N	2.10	0.50
29:X:2630:C:H2'	29:X:2631:C:H6	1.76	0.50
29:X:46:C:H2'	29:X:47:G:C8	2.41	0.50
29:X:991:A:C4	29:X:1146:G:O4'	2.64	0.50
11:J:44:LYS:O	11:J:47:GLN:N	2.44	0.50
19:R:20:ASP:O	19:R:36:VAL:HG23	2.11	0.50
6:E:150:LYS:HZ1	29:X:2741:G:H21	1.60	0.50
10:I:72:TYR:HE2	10:I:105:PRO:HB2	1.76	0.50
3:B:8:LYS:HG2	3:B:192:ASN:HD22	1.76	0.50
1:0:150:ARG:HG2	1:0:153:LYS:HD2	1.92	0.50
29:X:2649:A:H2'	29:X:2650:G:O4'	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:106:LEU:HA	17:P:115:ASN:O	2.11	0.50
12:K:98:LEU:HD23	12:K:99:ARG:NH2	2.27	0.50
10:I:57:ILE:HD12	28:3:61:MET:SD	2.52	0.50
17:P:39:ARG:NH2	29:X:527:C:O2'	2.44	0.50
8:G:157:PRO:HG2	8:G:158:HIS:CE1	2.47	0.50
4:C:46:ARG:HB3	4:C:50:GLN:HB2	1.94	0.50
29:X:1353:A:H3'	29:X:1354:A:H8	1.76	0.50
29:X:98:U:H4'	29:X:100:G:C8	2.45	0.50
29:X:1142:G:H1'	29:X:1143:A:C8	2.47	0.50
6:E:6:LYS:HB3	6:E:6:LYS:HZ3	1.76	0.50
6:E:67:LEU:HD11	29:X:2738:A:C5	2.47	0.50
6:E:158:HIS:NE2	29:X:2638:G:OP1	2.45	0.50
2:A:40:THR:O	2:A:40:THR:OG1	2.26	0.50
29:X:513:A:OP1	29:X:514:G:N2	2.39	0.50
9:H:43:ARG:HH21	29:X:1979:C:P	2.34	0.50
29:X:1066:G:O2'	29:X:1096:A:N1	2.33	0.50
29:X:5:A:H2'	29:X:6:A:H8	1.73	0.50
9:H:1:MET:SD	9:H:79:HIS:NE2	2.84	0.50
2:A:208:LYS:HD2	29:X:742:G:C8	2.47	0.50
29:X:2230:G:H3'	29:X:2231:G:H8	1.76	0.50
29:X:2407:G:H4'	29:X:2408:G:C4	2.47	0.50
2:A:40:THR:O	2:A:42:GLY:N	2.44	0.50
3:B:146:THR:HG23	29:X:1141:U:C5	2.47	0.50
22:U:21:ARG:O	22:U:39:LYS:HD2	2.11	0.50
29:X:2291:U:H2'	29:X:2292:C:H6	1.77	0.50
30:Y:35:C:H2'	30:Y:36:A:C8	2.47	0.50
2:A:219:PRO:HG3	29:X:794:A:C8	2.46	0.50
29:X:61:U:H3	29:X:91:A:H2	1.58	0.50
29:X:1742:G:C2	29:X:1743:C:N3	2.80	0.50
2:A:202:LYS:HB2	29:X:1812:U:C2	2.46	0.50
15:N:33:ARG:HB3	29:X:1265:G:N2	2.27	0.50
3:B:11:MET:O	29:X:2661:G:H5'	2.12	0.50
29:X:79:G:N2	29:X:104:C:O2	2.45	0.50
29:X:525:A:C2'	29:X:526:C:H5'	2.42	0.50
2:A:227:ASN:CG	29:X:797:A:H5"	2.31	0.50
29:X:746:G:O6	29:X:774:A:C8	2.65	0.50
2:A:18:THR:HG21	29:X:1581:C:H5"	1.92	0.50
29:X:12:U:H2'	29:X:12:U:O2	2.12	0.50
13:L:67:THR:HG22	13:L:71:VAL:HG12	1.94	0.50
17:P:39:ARG:O	17:P:42:VAL:HG12	2.11	0.49
29:X:2587:G:H8	29:X:2587:G:O5'	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1354:A:H5"	29:X:1410:U:O2	2.11	0.49
29:X:2410:U:O2	29:X:2412:A:C8	2.63	0.49
10:I:16:ARG:NH2	29:X:598:U:OP2	2.44	0.49
18:Q:53:ILE:HG12	18:Q:54:SER:N	2.27	0.49
29:X:1815:G:H2'	29:X:1816:G:C8	2.46	0.49
29:X:668:A:H2'	29:X:668:A:OP2	2.12	0.49
11:J:53:ILE:O	11:J:57:ARG:HG2	2.11	0.49
12:K:99:ARG:NE	12:K:99:ARG:H	2.10	0.49
25:Z:4:HIS:ND1	25:Z:4:HIS:O	2.45	0.49
10:I:50:GLU:HA	29:X:846:A:C4'	2.42	0.49
29:X:2642:G:H2'	29:X:2643:G:O4'	2.12	0.49
22:U:9:GLY:H	22:U:14:VAL:HG22	1.77	0.49
20:S:100:THR:HG21	20:S:113:VAL:HG11	1.93	0.49
29:X:513:A:C6	29:X:515:A:C6	3.00	0.49
29:X:224:G:OP2	29:X:226:C:N4	2.44	0.49
28:3:36:LYS:HB2	28:3:37:SER:HA	1.94	0.49
12:K:102:THR:O	12:K:103:ARG:HB2	2.12	0.49
29:X:580:A:N3	29:X:582:G:C8	2.80	0.49
19:R:99:VAL:HB	19:R:105:ARG:HD2	1.93	0.49
4:C:152:THR:HA	4:C:189:ASP:OD2	2.12	0.49
29:X:991:A:N6	29:X:992:A:N6	2.60	0.49
29:X:2180:U:H2'	29:X:2203:G:N1	2.27	0.49
24:W:26:ARG:NH1	29:X:1197:U:H5"	2.28	0.49
29:X:1017:C:H2'	29:X:1018:C:H6	1.76	0.49
29:X:1830:C:H4'	29:X:1831:G:C8	2.47	0.49
12:K:83:VAL:O	12:K:86:LYS:HB2	2.11	0.49
22:U:23:LYS:HB3	22:U:37:ILE:HG22	1.95	0.49
28:3:33:ASN:O	28:3:36:LYS:HA	2.13	0.49
11:J:15:ARG:HG3	11:J:73:LYS:HG3	1.93	0.49
4:C:72:ARG:NH1	29:X:1271:C:OP1	2.32	0.49
14:M:48:GLN:HG2	14:M:49:ALA:H	1.76	0.49
29:X:1542:G:H2'	29:X:1543:G:H8	1.76	0.49
29:X:1428:G:N2	29:X:1601:U:O4'	2.45	0.49
5:D:8:TYR:O	5:D:12:VAL:HG23	2.12	0.49
29:X:2273:C:H2'	29:X:2274:C:C6	2.47	0.49
29:X:974:U:H2'	29:X:975:C:H6	1.77	0.49
20:S:149:ALA:HA	20:S:152:ILE:HD13	1.94	0.49
29:X:1451:C:O2'	29:X:1533:G:H4'	2.10	0.49
29:X:1872:A:N1	29:X:2213:G:H1'	2.27	0.49
20:S:66:VAL:HG22	20:S:83:PHE:HE1	1.77	0.49
29:X:1669:A:H2	29:X:1989:C:N3	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:9:ILE:HD11	3:B:27:LEU:CB	2.42	0.49
29:X:1681:A:C2	29:X:2706:U:C2	3.00	0.49
5:D:92:ARG:HD3	30:Y:47:A:H8	1.77	0.49
30:Y:63:A:H2'	30:Y:64:C:H6	1.77	0.49
26:1:38:LYS:HB2	29:X:2323:U:H2'	1.94	0.49
29:X:1326:U:O3'	29:X:1345:G:H5'	2.13	0.49
9:H:10:VAL:HG22	9:H:19:ILE:HG22	1.94	0.49
10:I:100:ARG:C	10:I:101:ARG:HD2	2.33	0.49
29:X:358:C:H2'	29:X:359:G:H5'	1.95	0.49
7:F:78:ILE:HD11	7:F:107:ILE:HD11	1.93	0.49
6:E:153:LYS:HG3	6:E:154:PRO:HD2	1.94	0.49
22:U:50:ALA:HB3	22:U:62:LEU:HB3	1.93	0.49
29:X:2837:G:H2'	29:X:2838:U:H6	1.77	0.49
29:X:464:G:H2'	29:X:465:C:C6	2.48	0.49
10:I:31:GLY:O	29:X:1204:G:H5"	2.12	0.49
29:X:583:C:C5	29:X:2016:A:H4'	2.47	0.49
29:X:2511:G:H2'	29:X:2512:A:O4'	2.12	0.49
1:0:58:VAL:HG13	1:0:191:ALA:HB3	1.94	0.49
3:B:159:HIS:NE2	29:X:2797:G:OP1	2.45	0.49
4:C:176:ASN:OD1	4:C:179:ASP:N	2.41	0.49
25:Z:16:ARG:HG3	29:X:1277:G:OP1	2.12	0.49
29:X:2661:G:O6	29:X:2708:U:H1'	2.13	0.49
29:X:78:C:H2'	29:X:79:G:H8	1.77	0.49
29:X:206:U:H2'	29:X:206:U:O2	2.11	0.49
7:F:73:PRO:HB3	29:X:1071:U:OP1	2.13	0.49
29:X:1313:U:O2	29:X:1642:G:N1	2.46	0.49
14:M:55:ILE:HD11	14:M:67:THR:HG21	1.93	0.49
2:A:4:LYS:NZ	29:X:1581:C:OP1	2.40	0.49
28:3:32:GLN:OE1	28:3:44:LYS:HE2	2.12	0.49
10:I:50:GLU:HA	29:X:846:A:H4'	1.94	0.49
29:X:1174:G:C2	29:X:1175:A:N7	2.80	0.49
29:X:54:G:C2	29:X:114:C:C2	2.99	0.49
9:H:42:LYS:HA	29:X:2653:A:O3'	2.13	0.49
29:X:2802:C:H2'	29:X:2803:C:H6	1.76	0.49
11:J:19:THR:CG2	11:J:20:GLY:H	2.16	0.49
29:X:1919:A:C2	29:X:1928:G:C8	3.00	0.49
29:X:356:A:H2'	29:X:357:A:N7	2.26	0.49
29:X:2140:G:H2'	29:X:2140:G:N3	2.27	0.49
29:X:564:U:H2'	29:X:565:A:C8	2.48	0.49
13:L:37:HIS:CD2	30:Y:29:C:O3'	2.65	0.49
25:Z:7:PRO:O	29:X:1999:U:O2'	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:712:A:H8	29:X:712:A:H5'	1.75	0.49
29:X:457:C:H2'	29:X:458:G:H5"	1.93	0.49
29:X:1660:G:C6	29:X:1661:C:C5	3.01	0.49
29:X:1913:G:N2	29:X:1914:U:O4	2.38	0.49
17:P:29:LYS:HB2	29:X:503:G:H4'	1.95	0.49
20:S:23:ALA:HA	20:S:83:PHE:HB2	1.94	0.49
29:X:661:C:H2'	29:X:662:G:H8	1.77	0.49
29:X:1673:C:H2'	29:X:1674:C:H6	1.78	0.49
29:X:858:G:OP2	29:X:858:G:C8	2.65	0.49
29:X:2378:G:H1	29:X:2396:C:N4	2.08	0.49
29:X:754:G:H2'	29:X:755:C:C6	2.47	0.49
29:X:1299:A:C6	29:X:1302:C:C2	3.01	0.49
25:Z:49:CYS:SG	25:Z:51:TYR:HB2	2.53	0.49
4:C:95:LEU:HD12	4:C:96:PRO:CD	2.42	0.49
29:X:2713:A:H2'	29:X:2714:A:H8	1.78	0.49
29:X:2794:G:C6	29:X:2796:A:C2	3.00	0.49
29:X:331:U:H4'	29:X:333:A:C8	2.48	0.49
30:Y:30:C:H42	30:Y:58:G:H1	1.58	0.49
29:X:1099:A:H2'	29:X:1099:A:N3	2.28	0.49
28:3:46:LYS:HB3	28:3:47:GLY:H	1.40	0.49
29:X:2097:A:H2'	29:X:2098:G:O4'	2.13	0.49
20:S:106:GLY:HA2	20:S:109:GLN:HE22	1.77	0.49
12:K:51:LEU:HD13	12:K:70:ILE:HD11	1.95	0.49
3:B:133:LYS:NZ	29:X:758:G:OP2	2.28	0.49
18:Q:7:LEU:HD11	18:Q:41:ALA:HB1	1.94	0.49
29:X:229:G:H2'	29:X:230:C:H6	1.78	0.49
29:X:1669:A:C2	29:X:1989:C:N3	2.81	0.49
29:X:219:G:O2'	29:X:231:G:O6	2.19	0.49
29:X:1505:U:O2	29:X:1506:C:O2'	2.21	0.49
3:B:141:ILE:HD11	29:X:2034:A:O4'	2.12	0.49
29:X:2034:A:H2	29:X:2035:G:O6	1.95	0.49
29:X:171:G:H2'	29:X:172:A:C8	2.48	0.49
29:X:2431:C:H1'	32:X:6178:HGR:C1	2.43	0.49
19:R:17:LYS:HG3	29:X:83:A:H3'	1.95	0.49
10:I:72:TYR:HB3	10:I:107:LYS:HB2	1.94	0.49
29:X:1129:A:H2'	29:X:1130:U:O4'	2.13	0.49
4:C:33:TRP:HD1	4:C:93:TYR:CZ	2.31	0.49
29:X:635:C:O2	29:X:670:U:H4'	2.12	0.49
29:X:1174:G:C2	29:X:1175:A:C5	3.00	0.49
29:X:2592:U:H6	29:X:2592:U:H5'	1.78	0.49
29:X:1611:U:H2'	29:X:1612:U:C6	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:8:ILE:HD12	26:1:28:ARG:NE	2.28	0.49
29:X:1379:A:H2'	29:X:1380:C:C6	2.47	0.49
29:X:1499:A:H2'	29:X:1500:U:C6	2.48	0.49
28:3:17:THR:HG21	28:3:21:LYS:CG	2.43	0.49
29:X:1982:C:H5"	29:X:2703:C:H1'	1.95	0.49
9:H:64:VAL:HG13	9:H:68:ASP:OD2	2.13	0.49
29:X:408:U:H2'	29:X:409:G:C8	2.48	0.49
29:X:820:U:H2'	29:X:821:A:H8	1.78	0.49
2:A:199:ALA:HA	29:X:1812:U:H3	1.77	0.49
22:U:14:VAL:HB	22:U:15:VAL:H	1.41	0.49
15:N:60:LEU:HD11	15:N:64:ARG:HE	1.78	0.49
8:G:58:ILE:HG12	8:G:80:VAL:HG11	1.94	0.49
15:N:22:LYS:NZ	29:X:1232:U:OP1	2.46	0.49
29:X:987:G:C2	29:X:988:G:N7	2.80	0.48
29:X:1989:C:C6	29:X:1989:C:O5'	2.65	0.48
9:H:21:CYS:SG	9:H:51:ILE:HG13	2.53	0.48
2:A:201:HIS:O	2:A:204:ILE:HG13	2.13	0.48
29:X:590:C:H2'	29:X:591:G:H8	1.78	0.48
29:X:746:G:C8	29:X:774:A:C6	3.00	0.48
2:A:124:GLU:C	2:A:126:LYS:H	2.17	0.48
3:B:175:ILE:HG12	3:B:182:ILE:CD1	2.43	0.48
29:X:742:G:H2'	29:X:1766:U:O2	2.13	0.48
9:H:10:VAL:HA	9:H:96:ALA:O	2.12	0.48
11:J:70:PHE:HA	11:J:71:PRO:HD2	1.63	0.48
29:X:1761:G:C5	29:X:1762:C:C5	3.01	0.48
29:X:2047:C:O2	29:X:2429:A:N6	2.46	0.48
25:Z:55:ARG:HH21	25:Z:58:LEU:HA	1.77	0.48
4:C:56:ARG:HB2	29:X:810:U:OP1	2.13	0.48
3:B:22:PRO:HB3	29:X:2661:G:N3	2.28	0.48
29:X:1503:G:H2'	29:X:1504:G:C8	2.48	0.48
21:T:23:VAL:HG11	29:X:870:C:H4'	1.94	0.48
29:X:2409:A:O2'	29:X:2410:U:O5'	2.25	0.48
29:X:966:A:N6	29:X:967:G:C6	2.81	0.48
29:X:1426:U:H3'	29:X:1427:G:H5"	1.95	0.48
27:2:34:ARG:NH2	27:2:41:GLN:HG3	2.28	0.48
29:X:1904:G:H2'	29:X:1905:G:O4'	2.13	0.48
29:X:1491:C:N3	29:X:1533:G:N2	2.60	0.48
29:X:625:A:H4'	29:X:625:A:OP2	2.13	0.48
2:A:132:PRO:O	2:A:136:VAL:HG23	2.12	0.48
29:X:1917:C:C2'	29:X:1918:G:H5'	2.43	0.48
29:X:202:A:C4	29:X:203:G:H1'	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:689:A:H8	29:X:2052:G:H21	1.60	0.48
29:X:1919:A:H2	29:X:1926:U:N3	2.02	0.48
29:X:1108:U:H2'	29:X:1109:A:O4'	2.13	0.48
13:L:91:ARG:HB2	13:L:94:TYR:HD1	1.78	0.48
29:X:1920:A:N7	29:X:1923:U:H5	2.11	0.48
20:S:3:LEU:HD11	20:S:56:VAL:HG22	1.95	0.48
29:X:750:C:H4'	29:X:779:U:O3'	2.14	0.48
19:R:18:LYS:HB2	29:X:84:G:OP2	2.13	0.48
6:E:54:ARG:NE	6:E:57:ASP:OD2	2.37	0.48
16:O:21:ARG:HD3	16:O:90:PHE:CE1	2.48	0.48
2:A:2:ALA:N	2:A:20:ASP:OD1	2.46	0.48
17:P:14:ARG:O	17:P:18:VAL:HG22	2.13	0.48
29:X:1337:G:N2	29:X:1344:C:C2	2.82	0.48
29:X:956:A:C4	29:X:2427:A:C2	3.01	0.48
29:X:870:C:C4	29:X:871:U:C4	3.02	0.48
29:X:2425:G:H2'	29:X:2480:C:C5	2.47	0.48
29:X:306:G:H2'	29:X:307:C:C6	2.49	0.48
29:X:2769:C:H1'	29:X:2866:A:C2	2.48	0.48
25:Z:10:LYS:HG3	29:X:1276:U:H1'	1.96	0.48
9:H:83:ARG:O	9:H:85:ASP:N	2.41	0.48
29:X:1174:G:C2	29:X:1175:A:C8	3.02	0.48
29:X:731:A:H2'	29:X:732:G:H5'	1.94	0.48
29:X:1469:U:H4'	29:X:1470:G:OP1	2.14	0.48
29:X:965:G:O2'	29:X:2253:A:N1	2.34	0.48
3:B:144:ARG:NH1	29:X:2551:A:C4	2.81	0.48
29:X:647:G:O2'	29:X:649:G:O2'	2.26	0.48
29:X:2708:U:H2'	29:X:2709:C:C6	2.48	0.48
29:X:219:G:H22	29:X:231:G:H2'	1.78	0.48
27:2:11:LYS:HE2	29:X:699:G:H5"	1.96	0.48
3:B:57:ARG:HH21	29:X:2809:A:H5'	1.78	0.48
29:X:2533:U:H2'	29:X:2534:U:C6	2.48	0.48
13:L:46:SER:OG	13:L:47:ARG:N	2.47	0.48
2:A:243:GLY:HA3	29:X:2576:G:C5'	2.42	0.48
29:X:82:G:H21	29:X:83:A:N6	2.11	0.48
29:X:1882:G:O2'	29:X:1883:A:OP2	2.27	0.48
29:X:2279:G:O5'	29:X:2279:G:H8	1.95	0.48
29:X:149:A:OP2	29:X:149:A:H8	1.97	0.48
29:X:2840:U:C4	29:X:2841:U:C4	3.01	0.48
24:W:49:HIS:CD2	24:W:50:LEU:HG	2.49	0.48
29:X:2498:U:C5	29:X:2520:A:C6	3.02	0.48
29:X:772:G:H2'	29:X:773:G:H8	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:10:ARG:HG3	15:N:13:ARG:NH2	2.28	0.48
15:N:51:ARG:HA	15:N:54:LYS:HD2	1.96	0.48
27:2:30:ILE:HD13	29:X:477:A:H4'	1.95	0.48
29:X:2495:G:C6	29:X:2496:C:N4	2.81	0.48
30:Y:65:A:H2'	30:Y:66:G:H8	1.79	0.48
17:P:93:LYS:HB2	17:P:129:ALA:HB3	1.95	0.48
29:X:1509:A:H8	29:X:1510:A:C8	2.32	0.48
19:R:25:LEU:CD1	19:R:82:ALA:HB2	2.42	0.48
2:A:211:ARG:NE	29:X:1582:A:OP1	2.40	0.48
20:S:147:ILE:HG23	20:S:151:ASP:HB2	1.95	0.48
11:J:46:ASN:OD1	11:J:46:ASN:N	2.34	0.48
29:X:1370:U:H3'	29:X:1371:G:C8	2.48	0.48
1:0:16:TYR:CZ	1:0:24:LEU:HD22	2.49	0.48
10:I:55:ARG:NH1	29:X:228:A:OP1	2.35	0.48
12:K:11:ASN:ND2	12:K:11:ASN:N	2.59	0.48
29:X:218:A:H5'	29:X:220:U:O4'	2.12	0.48
29:X:713:G:H2'	29:X:714:G:O4'	2.13	0.48
29:X:1096:A:H1'	29:X:1116:U:H1'	1.95	0.48
4:C:142:LEU:HB3	4:C:166:TRP:CH2	2.48	0.48
29:X:2784:A:C2	29:X:2866:A:C4	3.02	0.48
29:X:2047:C:H1'	29:X:2429:A:C6	2.49	0.48
29:X:1727:C:O2'	29:X:2833:C:N3	2.43	0.48
1:0:210:LEU:HB2	1:0:217:SER:HA	1.94	0.48
6:E:7:GLN:H	6:E:8:PRO:CD	2.27	0.48
29:X:639:G:O2'	29:X:661:C:O2'	2.22	0.48
20:S:24:TYR:O	20:S:26:LYS:NZ	2.42	0.48
29:X:1401:G:H1	29:X:1412:C:N4	2.08	0.48
29:X:2265:A:H4'	29:X:2266:A:O4'	2.14	0.48
6:E:83:TYR:O	6:E:134:SER:OG	2.20	0.48
1:0:10:VAL:HG22	1:0:218:ILE:HD11	1.96	0.48
4:C:137:ALA:HB1	4:C:142:LEU:HD12	1.95	0.48
2:A:52:ARG:CZ	2:A:53:PHE:HE2	2.26	0.48
5:D:122:PHE:HE2	5:D:130:LEU:N	2.12	0.48
29:X:1054:C:H2'	29:X:1055:A:C8	2.49	0.48
5:D:52:LYS:HE2	5:D:146:VAL:HB	1.96	0.48
10:I:81:GLN:HB3	10:I:82:ASP:H	1.43	0.48
29:X:341:A:H2'	29:X:341:A:N3	2.29	0.48
24:W:35:SER:O	24:W:37:THR:OG1	2.28	0.48
29:X:691:C:C2	29:X:692:C:C5	3.01	0.48
29:X:1979:C:H4'	29:X:1980:A:OP1	2.14	0.48
29:X:1672:A:C8	29:X:1673:C:C5	3.01	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:26:LYS:HD2	30:Y:107:C:O2'	2.14	0.48
29:X:2492:G:H2'	29:X:2493:U:C6	2.48	0.48
29:X:174:A:C5	29:X:175:C:C5	3.02	0.48
24:W:2:LYS:HD2	24:W:32:ARG:O	2.14	0.48
10:I:115:SER:O	10:I:136:ALA:HB1	2.14	0.48
27:2:2:LYS:HG2	27:2:3:ARG:N	2.28	0.48
3:B:44:TYR:CE1	29:X:2616:U:H5'	2.49	0.48
11:J:99:LYS:O	11:J:102:ARG:HB3	2.14	0.48
21:T:46:LYS:HB3	21:T:78:PHE:CD2	2.49	0.48
29:X:2565:C:H2'	29:X:2566:A:H8	1.78	0.48
29:X:1378:A:H2'	29:X:1378:A:N3	2.29	0.48
29:X:187:U:H2'	29:X:188:G:C8	2.48	0.48
24:W:26:ARG:HH12	29:X:1197:U:H5"	1.78	0.48
29:X:1882:G:N7	29:X:1885:C:N4	2.46	0.48
29:X:772:G:H2'	29:X:773:G:C8	2.49	0.48
26:1:40:TYR:CG	26:1:41:ASP:N	2.82	0.48
14:M:105:TYR:HD2	29:X:2698:G:H5'	1.79	0.48
29:X:2345:A:H2'	29:X:2346:G:O4'	2.14	0.48
29:X:322:A:H3'	29:X:323:G:C8	2.49	0.48
12:K:88:ALA:O	12:K:90:ARG:N	2.47	0.47
29:X:2796:A:C6	29:X:2797:G:C6	3.02	0.47
4:C:149:LEU:HB2	4:C:183:HIS:ND1	2.29	0.47
29:X:2813:G:C4	29:X:2814:G:C8	3.02	0.47
29:X:2702:G:C2'	29:X:2703:C:H5'	2.44	0.47
29:X:2707:G:C4	29:X:2708:U:C5	3.02	0.47
15:N:52:ASN:O	15:N:55:ARG:N	2.47	0.47
22:U:49:LYS:HB2	22:U:61:TRP:CZ3	2.47	0.47
29:X:2495:G:C6	29:X:2548:G:C2	3.01	0.47
16:O:14:VAL:HG13	16:O:20:ILE:HD11	1.96	0.47
26:1:11:LYS:HB2	26:1:22:TYR:O	2.14	0.47
29:X:2432:A:H2'	29:X:2433:G:H8	1.79	0.47
29:X:797:A:O2'	29:X:798:G:H8	1.97	0.47
29:X:2728:A:C6	29:X:2737:A:N7	2.83	0.47
29:X:1658:A:N6	29:X:1659:G:C2	2.83	0.47
29:X:303:C:N3	29:X:359:G:N2	2.44	0.47
9:H:109:ARG:HA	9:H:129:LEU:HD22	1.95	0.47
6:E:35:VAL:HB	6:E:37:TYR:CZ	2.49	0.47
29:X:181:A:H2	29:X:182:G:H21	1.61	0.47
29:X:2456:U:H4'	29:X:2458:U:O4	2.14	0.47
22:U:10:LYS:HD3	22:U:11:LYS:H	1.78	0.47
17:P:11:LYS:NZ	17:P:15:LYS:HE2	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:18:VAL:O	17:P:19:LYS:HB2	2.14	0.47
9:H:37:GLY:O	29:X:2627:G:O2'	2.32	0.47
29:X:699:G:H2'	29:X:801:A:N1	2.29	0.47
13:L:92:GLY:O	13:L:94:TYR:N	2.43	0.47
4:C:119:ALA:HA	4:C:188:ILE:HB	1.95	0.47
29:X:2662:C:C6	29:X:2663:U:H5	2.32	0.47
29:X:1987:G:C4	29:X:1988:A:C8	3.02	0.47
12:K:34:ILE:HG13	12:K:113:ILE:HG22	1.97	0.47
1:0:72:VAL:HG13	1:0:110:VAL:HB	1.96	0.47
10:I:110:ALA:O	10:I:111:SER:OG	2.26	0.47
29:X:1606:C:H2'	29:X:1607:A:C8	2.48	0.47
29:X:1606:C:H2'	29:X:1607:A:H8	1.79	0.47
21:T:48:GLY:H	21:T:51:VAL:CG2	2.27	0.47
29:X:2675:U:H2'	29:X:2676:G:C8	2.49	0.47
9:H:26:ASN:HB3	9:H:38:GLY:H	1.78	0.47
15:N:61:TRP:HZ2	29:X:1006:C:O2	1.96	0.47
29:X:1337:G:C4	29:X:1341:G:O6	2.67	0.47
3:B:136:ARG:NH1	29:X:1673:C:OP1	2.46	0.47
5:D:70:ALA:HB3	5:D:81:GLN:O	2.14	0.47
17:P:30:TYR:CD1	17:P:123:HIS:HE1	2.32	0.47
15:N:34:ASN:O	15:N:38:THR:OG1	2.29	0.47
25:Z:33:CYS:HB3	25:Z:40:LYS:HB3	1.95	0.47
9:H:8:LEU:N	9:H:8:LEU:HD23	2.28	0.47
29:X:617:U:H5"	29:X:630:G:O6	2.14	0.47
29:X:1724:C:H42	29:X:1742:G:H1	1.61	0.47
29:X:2367:A:N7	29:X:2368:G:C5	2.83	0.47
2:A:44:ASN:HB2	29:X:1804:U:O2'	2.13	0.47
15:N:13:ARG:CZ	29:X:1264:C:H5"	2.43	0.47
15:N:91:ASN:HB2	16:O:11:GLN:HB2	1.97	0.47
12:K:106:ASP:HB3	29:X:1666:G:O2'	2.13	0.47
29:X:536:A:N6	29:X:2605:C:H4'	2.29	0.47
7:F:133:SER:HB2	29:X:1099:A:N6	2.29	0.47
29:X:2335:U:H2'	29:X:2336:G:C8	2.50	0.47
19:R:77:HIS:O	19:R:80:LYS:HG3	2.15	0.47
12:K:30:ARG:HG2	12:K:31:GLU:OE1	2.14	0.47
29:X:1452:U:H2'	29:X:1453:A:O4'	2.13	0.47
29:X:1309:G:H1	29:X:1661:C:H42	1.62	0.47
22:U:19:ILE:HD12	22:U:20:ARG:N	2.29	0.47
6:E:97:LYS:HB3	6:E:98:LEU:H	1.49	0.47
25:Z:21:SER:OG	25:Z:21:SER:O	2.32	0.47
21:T:5:LYS:HE3	21:T:5:LYS:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:2645:C:H3'	29:X:2646:C:C6	2.49	0.47
29:X:2757:G:H4'	29:X:2758:A:H5"	1.96	0.47
13:L:30:SER:HB3	13:L:41:GLN:HB2	1.96	0.47
29:X:1391:A:O2'	29:X:1392:U:OP2	2.33	0.47
28:3:6:THR:HG23	28:3:62:LEU:HB3	1.96	0.47
3:B:169:ASN:ND2	29:X:2711:G:OP1	2.38	0.47
24:W:35:SER:HB3	29:X:941:U:OP1	2.13	0.47
29:X:553:C:H1'	29:X:556:A:H8	1.79	0.47
29:X:840:U:H4'	29:X:841:G:N7	2.29	0.47
29:X:1909:U:P	29:X:1912:G:H22	2.37	0.47
30:Y:39:C:N4	30:Y:50:U:O2'	2.47	0.47
29:X:1998:A:C8	29:X:1999:U:C5	3.02	0.47
19:R:99:VAL:O	19:R:100:ASP:HB2	2.14	0.47
29:X:2827:G:H2'	29:X:2828:C:O4'	2.15	0.47
29:X:746:G:N7	29:X:774:A:C5	2.83	0.47
5:D:104:ILE:HA	5:D:108:LEU:HD12	1.97	0.47
15:N:11:ARG:HH12	29:X:29:U:C4'	2.28	0.47
16:O:10:LYS:H	16:O:10:LYS:HD3	1.80	0.47
25:Z:44:HIS:ND1	25:Z:44:HIS:N	2.63	0.47
4:C:194:GLU:O	4:C:197:GLU:HB3	2.14	0.47
10:I:9:THR:HB	10:I:12:SER:HB2	1.97	0.47
29:X:2158:C:H2'	29:X:2159:A:C8	2.49	0.47
29:X:2659:C:N4	29:X:2660:C:H41	2.11	0.47
29:X:2658:A:H2'	29:X:2659:C:O4'	2.15	0.47
17:P:81:HIS:ND1	17:P:82:ASN:OD1	2.48	0.47
29:X:2033:C:C4	29:X:2034:A:C6	3.03	0.47
29:X:2594:U:H2'	29:X:2595:C:C6	2.49	0.47
29:X:1212:U:H2'	29:X:1213:U:H6	1.75	0.47
29:X:1463:A:H2'	29:X:1464:A:H8	1.79	0.47
2:A:227:ASN:OD1	29:X:797:A:H5"	2.14	0.47
22:U:20:ARG:HB2	22:U:43:ARG:HD2	1.96	0.47
9:H:10:VAL:HG23	9:H:17:ARG:O	2.14	0.47
11:J:14:PHE:CD1	11:J:88:LYS:HD3	2.50	0.47
5:D:5:LYS:HE2	5:D:104:ILE:HD12	1.96	0.47
20:S:94:VAL:HG12	20:S:96:VAL:HG22	1.97	0.47
29:X:717:G:N3	29:X:739:G:N1	2.63	0.47
5:D:41:GLY:O	5:D:43:SER:N	2.47	0.47
30:Y:19:C:H2'	30:Y:20:A:C8	2.49	0.47
29:X:640:C:H5"	29:X:660:G:O2'	2.14	0.47
15:N:55:ARG:O	15:N:58:ARG:HB3	2.15	0.47
8:G:33:ILE:CD1	29:X:547:U:H4'	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:85:ALA:HB1	8:G:127:ILE:HG13	1.96	0.47
21:T:37:LEU:HD12	21:T:59:LEU:O	2.14	0.47
19:R:16:PHE:CZ	19:R:46:VAL:HG21	2.50	0.47
30:Y:5:C:H42	30:Y:120:G:H1	1.63	0.47
12:K:82:GLU:O	12:K:85:PRO:HG2	2.14	0.47
29:X:2396:C:H2'	29:X:2397:A:O4'	2.14	0.47
12:K:3:HIS:CG	12:K:3:HIS:O	2.68	0.47
17:P:90:LEU:HA	17:P:129:ALA:O	2.14	0.47
29:X:176:A:N6	29:X:2413:A:C6	2.83	0.47
29:X:2145:A:H5"	29:X:2155:U:C6	2.49	0.47
29:X:2044:G:N2	29:X:2046:C:C2	2.83	0.47
30:Y:80:A:H2'	30:Y:81:C:O4'	2.13	0.47
29:X:2662:C:H2'	29:X:2663:U:H5'	1.95	0.47
29:X:1987:G:N7	29:X:1988:A:N7	2.62	0.47
2:A:233:HIS:HE2	2:A:247:VAL:HG12	1.79	0.47
29:X:2836:U:O2'	29:X:2837:G:H5'	2.14	0.47
9:H:13:ASN:ND2	9:H:109:ARG:HG2	2.30	0.47
6:E:11:VAL:HG12	6:E:15:VAL:HG11	1.95	0.47
1:0:60:LEU:HB2	1:0:155:GLY:HA2	1.97	0.47
3:B:61:LYS:N	3:B:62:PRO:HD2	2.29	0.47
11:J:61:ARG:HG2	20:S:175:ARG:H	1.79	0.47
29:X:2871:U:H2'	29:X:2872:U:C6	2.50	0.47
29:X:2612:G:H2'	29:X:2613:A:O4'	2.15	0.47
29:X:2542:U:C2	29:X:2544:A:OP2	2.67	0.47
29:X:475:U:C4	29:X:801:A:C5	3.03	0.47
25:Z:18:MET:CE	29:X:2028:C:H5'	2.45	0.47
29:X:494:A:H3'	29:X:495:C:C6	2.46	0.47
12:K:73:LYS:H	12:K:73:LYS:HE3	1.77	0.47
4:C:153:ASP:HA	4:C:158:ARG:HH22	1.78	0.47
29:X:389:G:H2'	29:X:390:U:C6	2.50	0.47
29:X:2087:U:H2'	29:X:2088:U:C6	2.49	0.47
3:B:8:LYS:HG2	3:B:192:ASN:HA	1.96	0.47
29:X:1174:G:N3	29:X:1175:A:C8	2.83	0.47
29:X:2697:G:H2'	29:X:2698:G:C8	2.49	0.47
29:X:2711:G:H2'	29:X:2712:G:C8	2.50	0.47
23:V:4:SER:O	23:V:8:ASN:ND2	2.48	0.47
29:X:459:A:H5"	29:X:461:A:C5	2.50	0.47
29:X:2474:G:C6	29:X:2475:C:N3	2.82	0.47
13:L:42:ILE:HB	13:L:52:ALA:HB3	1.97	0.47
29:X:981:C:N4	29:X:982:C:N4	2.63	0.47
12:K:8:ARG:HD2	12:K:10:LEU:HD21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:2796:A:C4	29:X:2797:G:N7	2.83	0.47
15:N:58:ARG:HH21	15:N:92:ARG:HH12	1.61	0.47
4:C:39:ARG:HD2	29:X:455:A:N7	2.30	0.47
13:L:37:HIS:HB3	30:Y:30:C:OP1	2.14	0.47
5:D:57:LEU:HD23	5:D:60:ILE:HD11	1.97	0.47
15:N:115:ASN:HA	15:N:118:GLN:OE1	2.15	0.47
17:P:98:ASP:OD2	17:P:98:ASP:N	2.47	0.47
21:T:35:ASN:OD1	29:X:2332:G:O2'	2.25	0.47
20:S:146:HIS:HB3	20:S:167:THR:HG23	1.97	0.47
29:X:2663:U:C2	29:X:2664:G:C8	3.02	0.47
1:0:150:ARG:HA	1:0:153:LYS:HB2	1.97	0.47
29:X:1141:U:O5'	29:X:1141:U:H6	1.98	0.47
29:X:202:A:C5	29:X:203:G:H1'	2.50	0.47
29:X:2519:C:O2	29:X:2720:A:H2	1.98	0.47
5:D:22:TYR:HE1	5:D:28:VAL:HG13	1.80	0.47
29:X:828:C:N4	29:X:1206:G:H1	2.13	0.47
29:X:116:A:OP2	29:X:117:A:H2'	2.15	0.47
29:X:649:G:N2	29:X:661:C:H1'	2.30	0.47
29:X:2820:C:H42	29:X:2846:G:H1	1.62	0.47
29:X:2789:U:H2'	29:X:2790:C:C6	2.50	0.47
29:X:587:A:OP1	29:X:1268:U:O2'	2.15	0.47
29:X:754:G:H2'	29:X:755:C:H6	1.80	0.47
4:C:137:ALA:CB	4:C:142:LEU:HD12	2.44	0.47
12:K:24:GLN:HB3	12:K:44:LEU:HD13	1.96	0.47
29:X:2487:G:C6	29:X:2561:G:O6	2.68	0.47
29:X:2701:A:H1'	29:X:2848:A:O2'	2.15	0.47
17:P:47:GLY:H	17:P:92:VAL:HB	1.78	0.47
29:X:218:A:H4'	29:X:219:G:OP1	2.14	0.46
2:A:171:ASP:O	2:A:187:SER:OG	2.27	0.46
29:X:2411:A:H8	29:X:2411:A:O5'	1.98	0.46
29:X:1690:U:C6	29:X:1690:U:H3'	2.50	0.46
29:X:790:A:C2	29:X:791:G:C4	3.03	0.46
9:H:130:ALA:HA	9:H:131:PRO:HD3	1.81	0.46
22:U:68:ARG:NH1	29:X:413:G:O4'	2.39	0.46
14:M:20:HIS:O	14:M:62:SER:HB2	2.15	0.46
29:X:646:C:H2'	29:X:647:G:O4'	2.16	0.46
29:X:1340:C:H2'	29:X:1341:G:O4'	2.16	0.46
27:2:15:THR:HG22	27:2:16:HIS:CG	2.50	0.46
5:D:57:LEU:O	5:D:61:THR:HG23	2.15	0.46
4:C:47:THR:N	4:C:50:GLN:HG3	2.28	0.46
29:X:1687:C:C4	29:X:1688:U:C2	3.03	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:991:A:H62	29:X:992:A:N6	2.13	0.46
29:X:2040:A:H2'	29:X:2041:A:H8	1.76	0.46
2:A:163:VAL:HA	2:A:176:ARG:O	2.15	0.46
10:I:72:TYR:CE2	10:I:105:PRO:HB2	2.50	0.46
29:X:1794:A:H5"	29:X:1795:C:OP2	2.15	0.46
8:G:115:ALA:O	8:G:119:LEU:HB2	2.15	0.46
29:X:2406:C:H5"	29:X:2407:G:OP1	2.15	0.46
9:H:59:ALA:O	9:H:61:ARG:N	2.48	0.46
3:B:103:ASP:OD1	3:B:168:GLN:HA	2.14	0.46
29:X:1301:U:C2	29:X:1340:C:O2	2.68	0.46
17:P:109:ARG:HD2	29:X:761:G:OP2	2.15	0.46
20:S:26:LYS:HE2	20:S:84:TYR:CE1	2.51	0.46
29:X:402:A:H8	29:X:2392:G:H4'	1.79	0.46
29:X:1153:A:C5	29:X:1155:G:C5	3.03	0.46
29:X:1179:A:C2	29:X:1196:G:C2	3.04	0.46
29:X:1511:A:C6	29:X:1512:A:C6	3.03	0.46
29:X:2505:G:N2	29:X:2517:C:H1'	2.31	0.46
29:X:2859:U:H5	29:X:2860:C:C4	2.33	0.46
29:X:2802:C:H2'	29:X:2803:C:C6	2.50	0.46
6:E:157:TYR:CE2	29:X:2510:A:H4'	2.50	0.46
19:R:10:HIS:NE2	29:X:338:G:H1'	2.31	0.46
29:X:1715:A:C8	29:X:1717:A:O4'	2.68	0.46
28:3:23:MET:HA	28:3:49:VAL:HA	1.97	0.46
29:X:518:A:H5"	29:X:518:A:C8	2.50	0.46
29:X:223:C:C4	29:X:224:G:N7	2.84	0.46
29:X:860:U:H5'	29:X:861:G:OP2	2.16	0.46
28:3:33:ASN:C	28:3:35:GLY:H	2.18	0.46
29:X:471:A:C2	29:X:481:A:C4	3.03	0.46
29:X:713:G:N2	29:X:745:C:H5	2.09	0.46
21:T:60:PHE:CE2	29:X:2344:G:H4'	2.51	0.46
29:X:1118:G:N1	29:X:1119:U:O2	2.47	0.46
29:X:2455:A:N3	29:X:2460:G:N1	2.54	0.46
7:F:23:VAL:HA	7:F:26:ALA:HB3	1.98	0.46
29:X:2151:G:N2	29:X:2154:A:O5'	2.46	0.46
2:A:123:ALA:HB1	2:A:129:ASN:ND2	2.29	0.46
13:L:15:ARG:HA	13:L:15:ARG:HD3	1.38	0.46
2:A:232:PRO:HB2	2:A:233:HIS:CD2	2.50	0.46
25:Z:43:HIS:HA	25:Z:52:TYR:OH	2.15	0.46
5:D:46:ASP:N	5:D:46:ASP:OD2	2.49	0.46
8:G:117:GLU:O	8:G:121:LYS:HB2	2.16	0.46
29:X:1513:U:H6	29:X:1593:C:H5"	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:48:ARG:HD2	4:C:75:PRO:HD2	1.97	0.46
15:N:44:THR:O	15:N:48:ARG:HG2	2.15	0.46
29:X:1994:U:H2'	29:X:1995:G:C5'	2.45	0.46
2:A:201:HIS:C	2:A:203:ASN:H	2.19	0.46
14:M:2:GLN:HB3	29:X:2795:A:C2	2.51	0.46
26:1:38:LYS:HD2	29:X:2323:U:OP1	2.15	0.46
29:X:1542:G:N2	29:X:1562:G:H1	2.14	0.46
29:X:1235:C:H2'	29:X:1236:G:C8	2.51	0.46
29:X:2042:A:C5	29:X:2482:A:C2	3.03	0.46
29:X:828:C:H42	29:X:1206:G:H1	1.64	0.46
29:X:143:A:H2'	29:X:144:U:C6	2.51	0.46
18:Q:63:LYS:HD2	18:Q:72:ARG:NH2	2.30	0.46
14:M:32:THR:HG22	14:M:94:VAL:HB	1.98	0.46
29:X:784:U:H2'	29:X:785:U:H6	1.81	0.46
28:3:21:LYS:HE2	29:X:661:C:OP1	2.16	0.46
19:R:76:LEU:HD23	19:R:76:LEU:HA	1.69	0.46
30:Y:119:G:C6	30:Y:120:G:C5	3.04	0.46
29:X:169:C:H5"	29:X:170:U:OP2	2.15	0.46
29:X:1655:C:O3'	29:X:2688:G:N2	2.48	0.46
29:X:1079:G:N2	29:X:1107:A:O5'	2.49	0.46
8:G:38:GLU:OE2	8:G:67:ARG:NH2	2.48	0.46
29:X:1683:G:H1	29:X:1977:C:H42	1.62	0.46
29:X:1:G:H2'	29:X:2:G:C8	2.51	0.46
17:P:74:SER:HA	29:X:498:C:H1'	1.98	0.46
29:X:1222:G:O2'	29:X:1250:A:N1	2.42	0.46
29:X:515:A:H2'	29:X:516:G:H5'	1.97	0.46
28:3:7:HIS:O	28:3:10:ALA:N	2.43	0.46
29:X:1067:G:O2'	29:X:1098:G:O6	2.34	0.46
29:X:1103:C:H2'	29:X:1104:G:O4'	2.15	0.46
3:B:2:LYS:NZ	3:B:95:ILE:HA	2.30	0.46
29:X:590:C:H2'	29:X:591:G:C8	2.50	0.46
29:X:2441:U:H2'	29:X:2442:C:C6	2.50	0.46
4:C:62:LYS:HZ1	29:X:2043:A:H3'	1.81	0.46
3:B:128:SER:OG	29:X:1693:A:H1'	2.15	0.46
29:X:1685:A:O4'	29:X:1686:A:C2	2.68	0.46
17:P:27:VAL:HB	29:X:504:G:H4'	1.98	0.46
29:X:2237:C:O2'	29:X:2406:C:OP2	2.25	0.46
9:H:42:LYS:NZ	29:X:2653:A:H5'	2.31	0.46
29:X:695:G:H2'	29:X:696:U:C6	2.51	0.46
29:X:861:G:C4	29:X:862:A:C8	3.03	0.46
29:X:824:U:O2	29:X:1263:G:H3'	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:149:LEU:HD22	4:C:179:ASP:HB3	1.98	0.46
29:X:573:C:O2'	29:X:574:C:H5'	2.16	0.46
29:X:78:C:H2'	29:X:79:G:C8	2.51	0.46
9:H:92:ASP:OD2	14:M:69:ARG:NH1	2.48	0.46
29:X:1067:G:H5"	29:X:1068:A:O4'	2.15	0.46
29:X:2585:C:H2'	29:X:2586:G:H5'	1.98	0.46
29:X:1850:G:H2'	29:X:1850:G:N3	2.30	0.46
29:X:1511:A:H8	29:X:1594:U:HO2'	1.64	0.46
13:L:28:ARG:HH22	30:Y:11:G:H5'	1.81	0.46
17:P:60:ILE:CD1	25:Z:28:PRO:HD3	2.46	0.46
12:K:25:ALA:N	12:K:44:LEU:HD11	2.31	0.46
29:X:1495:G:N2	29:X:1529:C:O2	2.29	0.46
24:W:16:GLN:O	24:W:20:VAL:HG23	2.15	0.46
17:P:34:SER:HB3	17:P:37:LYS:HG3	1.98	0.46
29:X:1733:U:H2'	29:X:1734:C:C5	2.50	0.46
5:D:3:GLN:O	5:D:6:THR:OG1	2.17	0.46
29:X:2415:G:H2'	29:X:2416:U:C6	2.51	0.46
19:R:62:MET:HA	19:R:63:THR:HA	1.70	0.46
29:X:2494:C:C2	29:X:2549:G:C2	3.04	0.46
13:L:57:ALA:HB3	30:Y:119:G:H4'	1.97	0.46
5:D:60:ILE:HG13	5:D:61:THR:HG22	1.98	0.46
29:X:2767:C:HO2'	29:X:2785:A:HO2'	1.63	0.46
29:X:1765:C:O5'	29:X:1765:C:H6	1.98	0.46
9:H:23:ARG:HG3	9:H:24:VAL:N	2.29	0.46
29:X:1698:C:O2'	29:X:1753:A:N3	2.37	0.46
29:X:1464:A:C6	29:X:1465:G:C6	3.04	0.46
20:S:126:GLY:HA3	20:S:128:ARG:NH2	2.31	0.46
29:X:2447:G:O2'	29:X:2448:A:H8	1.99	0.46
29:X:2695:C:H2'	29:X:2696:A:C8	2.51	0.46
5:D:147:ASP:HB2	5:D:148:LYS:H	1.57	0.46
29:X:1402:G:H2'	29:X:1403:U:C6	2.51	0.46
29:X:1669:A:N7	29:X:1670:G:C6	2.84	0.46
3:B:27:LEU:HD22	3:B:51:TYR:OH	2.15	0.46
29:X:1008:G:H1	29:X:1169:C:H42	1.64	0.46
5:D:70:ALA:O	5:D:72:LYS:N	2.43	0.46
2:A:69:ARG:HD2	2:A:130:ALA:HB2	1.98	0.46
29:X:1769:U:H2'	29:X:1775:A:N6	2.31	0.46
29:X:2790:C:H2'	29:X:2791:C:C6	2.51	0.46
29:X:992:A:H2	29:X:2010:G:N3	2.13	0.46
29:X:1661:C:H2'	29:X:1661:C:O2	2.16	0.46
29:X:38:G:C2	29:X:454:G:C2	3.04	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:119:G:H1	29:X:128:C:H42	1.63	0.46
29:X:1017:C:O2'	29:X:1018:C:H5'	2.16	0.46
29:X:1470:G:C2	29:X:1471:G:C8	3.04	0.46
20:S:10:PRO:O	20:S:13:LYS:HG3	2.16	0.46
29:X:194:G:H2'	29:X:195:A:O4'	2.16	0.46
29:X:998:C:O2'	29:X:1011:A:N3	2.37	0.46
8:G:79:PHE:CE2	8:G:147:ARG:HD3	2.50	0.46
6:E:117:PRO:HA	6:E:118:PRO:HD2	1.84	0.46
4:C:34:GLN:OE1	4:C:176:ASN:HB2	2.17	0.45
12:K:106:ASP:OD2	29:X:1300:A:C8	2.69	0.45
5:D:79:LEU:HD21	29:X:2289:A:H2	1.81	0.45
29:X:1813:A:H2'	29:X:1814:G:H8	1.81	0.45
26:1:21:TYR:CE2	29:X:2378:G:H1'	2.51	0.45
29:X:1033:G:H22	29:X:1153:A:H2	1.63	0.45
29:X:1685:A:H61	29:X:1693:A:H61	1.63	0.45
29:X:1194:U:H2'	29:X:1195:U:H6	1.80	0.45
20:S:6:LYS:HA	20:S:32:PHE:HA	1.98	0.45
29:X:1510:A:H2'	29:X:1511:A:O4'	2.16	0.45
3:B:91:VAL:HG12	3:B:92:ASN:H	1.81	0.45
29:X:165:G:H4'	29:X:1378:A:C5	2.51	0.45
28:3:62:LEU:HD13	28:3:65:GLY:HA2	1.97	0.45
4:C:36:ALA:O	4:C:38:ARG:N	2.49	0.45
29:X:1670:G:OP2	29:X:1670:G:H8	2.00	0.45
29:X:15:G:C5	29:X:16:G:N7	2.84	0.45
5:D:92:ARG:HD3	30:Y:47:A:C8	2.50	0.45
13:L:12:ARG:O	13:L:16:LYS:HB2	2.16	0.45
3:B:140:SER:HB2	29:X:2557:G:N7	2.31	0.45
29:X:2227:C:H5"	29:X:2228:U:OP2	2.16	0.45
19:R:58:VAL:HG13	19:R:60:PRO:CD	2.46	0.45
29:X:2754:C:N4	29:X:2755:A:C5	2.84	0.45
16:O:83:ARG:N	29:X:827:C:OP1	2.45	0.45
29:X:742:G:H2'	29:X:1766:U:H1'	1.98	0.45
4:C:53:LYS:HB2	4:C:73:SER:HB3	1.98	0.45
22:U:8:THR:HA	22:U:13:LEU:HD12	1.98	0.45
3:B:60:ASN:HB2	3:B:63:MET:HB2	1.98	0.45
30:Y:54:U:H4'	30:Y:54:U:OP1	2.16	0.45
29:X:2727:G:O6	29:X:2735:C:H5"	2.15	0.45
27:2:4:THR:O	29:X:700:C:H5'	2.16	0.45
3:B:38:THR:HG23	3:B:41:THR:OG1	2.16	0.45
29:X:628:A:H8	29:X:628:A:O5'	1.99	0.45
29:X:1336:G:H8	29:X:1336:G:O5'	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:314:G:H2'	29:X:315:G:C8	2.52	0.45
5:D:74:ILE:HG23	5:D:80:ARG:HA	1.97	0.45
29:X:571:U:C2	29:X:581:A:C8	3.05	0.45
2:A:39:LYS:NZ	2:A:58:HIS:O	2.34	0.45
14:M:2:GLN:N	29:X:2795:A:N1	2.64	0.45
29:X:2431:C:H2'	29:X:2432:A:C8	2.51	0.45
29:X:38:G:H2'	29:X:39:C:H6	1.81	0.45
9:H:115:ALA:C	9:H:117:GLU:H	2.18	0.45
18:Q:91:LEU:HD12	18:Q:91:LEU:HA	1.80	0.45
29:X:2235:G:N2	29:X:2254:C:C4	2.85	0.45
29:X:1296:G:N2	29:X:1299:A:OP2	2.49	0.45
29:X:1302:C:O2'	29:X:1303:U:H5'	2.17	0.45
29:X:615:C:H1'	29:X:670:U:H1'	1.98	0.45
7:F:25:PRO:HB2	7:F:29:GLN:NE2	2.31	0.45
18:Q:42:ILE:HD12	18:Q:80:VAL:HG21	1.99	0.45
29:X:2555:G:H3'	29:X:2555:G:OP1	2.16	0.45
9:H:9:ASP:N	9:H:9:ASP:OD2	2.48	0.45
29:X:2468:G:C6	29:X:2469:G:C6	3.04	0.45
22:U:75:TYR:O	22:U:76:LYS:HB2	2.16	0.45
29:X:2686:C:C2'	29:X:2687:G:H5'	2.46	0.45
18:Q:62:ARG:HA	18:Q:71:GLN:HA	1.98	0.45
6:E:38:ASN:OD1	6:E:64:LEU:HD22	2.16	0.45
14:M:38:LYS:HZ2	14:M:89:ASN:HB2	1.82	0.45
29:X:1202:U:H2'	29:X:1203:A:C8	2.36	0.45
29:X:573:C:H2'	29:X:574:C:O4'	2.17	0.45
29:X:602:C:N4	29:X:678:G:H1	2.14	0.45
29:X:158:A:H2	29:X:447:U:H4'	1.81	0.45
29:X:2286:G:H3'	29:X:2287:G:H8	1.81	0.45
29:X:99:U:H5"	29:X:100:G:N7	2.32	0.45
29:X:2792:C:C2	29:X:2805:G:C2	3.05	0.45
17:P:9:ARG:HG3	17:P:10:ASN:H	1.82	0.45
1:0:95:LEU:HD13	1:0:98:ARG:HB2	1.98	0.45
5:D:114:PHE:HE1	5:D:117:ILE:HG13	1.81	0.45
25:Z:36:CYS:HB3	25:Z:49:CYS:HB3	1.55	0.45
13:L:14:ARG:HG2	13:L:15:ARG:HH12	1.82	0.45
29:X:1888:C:OP1	29:X:1889:G:H5'	2.14	0.45
8:G:69:ASP:HA	15:N:64:ARG:HH22	1.82	0.45
29:X:1918:G:H1'	29:X:1947:G:N2	2.31	0.45
5:D:143:TYR:HA	5:D:146:VAL:HG22	1.98	0.45
11:J:69:ILE:HG23	11:J:104:MET:HA	1.99	0.45
16:O:92:ALA:C	16:O:93:ILE:HD12	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:872:G:O2'	29:X:928:G:O6	2.30	0.45
29:X:1932:G:N2	29:X:1941:C:C2	2.85	0.45
28:3:58:MET:CA	28:3:61:MET:HG3	2.45	0.45
29:X:650:U:H2'	29:X:651:C:C6	2.51	0.45
6:E:40:GLU:H	6:E:40:GLU:HG3	1.55	0.45
29:X:2523:G:N3	29:X:2524:G:C8	2.85	0.45
4:C:162:ARG:HG3	4:C:169:VAL:HG21	1.98	0.45
29:X:534:U:H2'	29:X:535:U:C6	2.51	0.45
29:X:42:G:H2'	29:X:43:A:H8	1.81	0.45
3:B:176:ARG:NE	14:M:16:ILE:HD13	2.31	0.45
29:X:588:G:N2	29:X:1275:A:C4	2.85	0.45
29:X:591:G:C6	29:X:592:G:C6	3.04	0.45
29:X:585:U:H4'	29:X:2481:G:N7	2.31	0.45
29:X:1310:C:C2	29:X:1311:C:C5	3.05	0.45
29:X:1069:G:H2'	29:X:1070:G:C8	2.52	0.45
18:Q:38:ILE:O	18:Q:42:ILE:HG13	2.16	0.45
12:K:64:ARG:O	12:K:68:GLN:HG3	2.17	0.45
5:D:164:GLU:HG3	5:D:165:GLU:HG2	1.98	0.45
12:K:11:ASN:ND2	29:X:1670:G:O6	2.49	0.45
17:P:97:VAL:HG22	17:P:124:ILE:HA	1.99	0.45
29:X:2523:G:C4	29:X:2524:G:C8	3.05	0.45
29:X:476:G:H2'	29:X:477:A:C8	2.52	0.45
4:C:148:VAL:HG12	4:C:187:VAL:HG23	1.99	0.45
29:X:1810:U:H4'	29:X:1813:A:H1'	1.99	0.45
20:S:26:LYS:HD3	20:S:26:LYS:N	2.31	0.45
11:J:32:ASP:OD2	11:J:135:ARG:NH2	2.40	0.45
29:X:2007:G:C2	29:X:2023:C:C2	3.05	0.45
26:1:27:ASN:C	26:1:29:ARG:H	2.20	0.45
29:X:1367:A:H2'	29:X:1368:G:O4'	2.16	0.45
1:0:7:GLU:HA	1:0:10:VAL:HB	1.98	0.45
2:A:186:HIS:O	2:A:189:CYS:N	2.47	0.45
20:S:103:ARG:NH1	20:S:108:VAL:HG22	2.32	0.45
29:X:306:G:H2'	29:X:307:C:H6	1.82	0.45
3:B:20:ALA:HB2	9:H:85:ASP:O	2.16	0.45
29:X:2529:G:C4	29:X:2530:C:C5	3.05	0.45
29:X:2837:G:H2'	29:X:2838:U:C6	2.51	0.45
29:X:2430:A:OP1	29:X:2476:A:N6	2.49	0.45
3:B:61:LYS:O	3:B:64:GLN:HB2	2.16	0.45
29:X:115:G:OP2	29:X:117:A:O2'	2.29	0.45
29:X:1269:G:N3	29:X:1269:G:H2'	2.32	0.45
29:X:311:A:H1'	29:X:330:C:O4'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:46:HIS:CE1	29:X:2351:G:HO2'	2.35	0.45
9:H:64:VAL:HG22	9:H:106:ARG:NH2	2.25	0.45
29:X:2589:C:H4'	29:X:2590:U:H5'	1.99	0.45
29:X:458:G:H5"	29:X:458:G:H8	1.82	0.45
21:T:46:LYS:NZ	21:T:76:ALA:HA	2.31	0.45
11:J:11:ARG:HB3	11:J:12:LYS:H	1.41	0.45
29:X:2792:C:N3	29:X:2805:G:C2	2.84	0.45
21:T:57:HIS:CD2	21:T:57:HIS:N	2.84	0.45
6:E:97:LYS:H	6:E:104:GLU:HB2	1.80	0.45
22:U:14:VAL:O	22:U:15:VAL:HG22	2.16	0.45
20:S:112:LEU:HD12	20:S:113:VAL:H	1.82	0.45
29:X:2683:C:H2'	29:X:2684:A:O4'	2.17	0.45
3:B:9:ILE:N	3:B:9:ILE:HD12	2.32	0.45
29:X:2819:G:H2'	29:X:2820:C:C6	2.51	0.45
29:X:1298:G:N2	29:X:1341:G:H5'	2.32	0.45
29:X:2302:G:H1	29:X:2311:U:H5	1.65	0.45
29:X:697:G:C2	29:X:807:A:C2	3.05	0.45
29:X:2611:A:C2	29:X:2767:C:O2	2.70	0.45
29:X:2264:C:H4'	29:X:2267:A:N7	2.32	0.45
21:T:36:ILE:HD11	29:X:2343:C:O2	2.16	0.45
29:X:491:A:H3'	29:X:492:G:H5"	1.97	0.45
29:X:2345:A:C6	29:X:2346:G:C4	3.05	0.45
14:M:33:VAL:HG11	14:M:91:VAL:HG12	1.98	0.45
29:X:1628:C:N3	29:X:1629:G:C8	2.85	0.45
29:X:1750:A:H2'	29:X:1751:A:H8	1.81	0.45
29:X:769:C:C4	29:X:770:U:C4	3.05	0.45
29:X:1029:C:O3'	29:X:1131:G:N2	2.49	0.45
1:0:43:LEU:HD12	1:0:167:VAL:HG11	1.99	0.45
24:W:5:LEU:HB2	24:W:25:LEU:CD1	2.43	0.45
11:J:102:ARG:NH1	11:J:103:VAL:O	2.49	0.45
11:J:22:ALA:HB2	11:J:99:LYS:CB	2.46	0.45
2:A:63:ARG:O	2:A:65:ILE:HG13	2.17	0.45
29:X:2494:C:N4	29:X:2548:G:H1	2.06	0.45
2:A:69:ARG:HH11	2:A:130:ALA:HB2	1.82	0.45
13:L:99:ARG:HG2	13:L:99:ARG:H	1.52	0.45
29:X:1478:U:C2	29:X:1479:G:C8	3.05	0.45
10:I:63:ARG:HD3	28:3:25:PHE:CE1	2.52	0.45
2:A:218:LYS:HB3	2:A:218:LYS:HE3	1.49	0.45
4:C:172:VAL:HB	4:C:173:ALA:H	1.64	0.45
29:X:1309:G:H1	29:X:1661:C:N4	2.15	0.45
2:A:186:HIS:NE2	29:X:2201:G:H5'	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:2248:A:H2'	29:X:2248:A:N3	2.30	0.45
29:X:820:U:OP1	29:X:843:G:N2	2.50	0.45
12:K:51:LEU:CD2	12:K:66:VAL:HG22	2.47	0.45
14:M:33:VAL:CG1	14:M:91:VAL:HG12	2.46	0.45
10:I:80:LEU:HA	10:I:80:LEU:HD23	1.75	0.45
29:X:2217:G:H2'	29:X:2217:G:N3	2.32	0.45
11:J:139:ASP:N	11:J:139:ASP:OD2	2.50	0.45
29:X:831:G:N7	29:X:1201:G:C6	2.85	0.45
4:C:3:GLN:O	4:C:12:GLY:HA3	2.17	0.45
4:C:14:THR:HB	4:C:15:ILE:H	1.58	0.45
2:A:76:ASN:HB2	2:A:117:VAL:O	2.17	0.45
29:X:2691:C:HO2'	29:X:2692:A:P	2.36	0.45
22:U:21:ARG:CG	22:U:22:GLY:H	2.30	0.45
29:X:567:G:H2'	29:X:568:G:C8	2.52	0.45
29:X:1775:A:H4'	29:X:1776:A:OP1	2.15	0.45
19:R:15:HIS:CD2	19:R:16:PHE:CD2	2.96	0.45
29:X:1408:A:N1	29:X:1411:C:C2	2.85	0.45
16:O:35:LEU:HD23	16:O:36:LYS:N	2.28	0.45
30:Y:15:A:H4'	30:Y:17:A:H2'	1.99	0.45
3:B:5:LEU:HD22	3:B:195:LEU:HD11	1.98	0.45
2:A:43:ARG:HH21	29:X:704:G:H4'	1.82	0.45
5:D:22:TYR:CE1	5:D:28:VAL:HG13	2.52	0.45
29:X:1:G:H1	29:X:2876:C:H42	1.65	0.45
10:I:4:HIS:CD2	10:I:4:HIS:C	2.90	0.45
29:X:1713:G:C6	29:X:1714:A:C5	3.05	0.45
6:E:9:ILE:HD11	6:E:52:VAL:HG23	1.99	0.45
10:I:14:LYS:HD3	29:X:675:C:O2'	2.17	0.45
29:X:2078:G:H2'	29:X:2079:A:C8	2.52	0.45
29:X:944:A:H8	29:X:944:A:OP2	2.00	0.44
14:M:93:ILE:N	14:M:93:ILE:HD12	2.26	0.44
28:3:17:THR:HG23	28:3:20:GLY:H	1.82	0.44
14:M:81:PHE:HA	14:M:82:PRO:HD3	1.74	0.44
8:G:140:GLN:O	8:G:143:ALA:N	2.50	0.44
29:X:2283:G:N3	29:X:2283:G:H2'	2.32	0.44
17:P:91:PHE:CZ	17:P:131:LYS:HG3	2.52	0.44
4:C:62:LYS:HZ2	29:X:2043:A:H3'	1.82	0.44
4:C:118:VAL:O	4:C:120:VAL:HG23	2.17	0.44
29:X:404:A:H1'	29:X:424:G:O4'	2.17	0.44
29:X:2020:G:H2'	29:X:2021:G:C8	2.52	0.44
29:X:1236:G:C6	29:X:1240:G:C6	3.05	0.44
4:C:133:PHE:CE1	4:C:161:ALA:HB2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:452:G:H2'	29:X:453:U:C6	2.51	0.44
29:X:2048:C:H1'	29:X:2428:U:N3	2.32	0.44
18:Q:64:ARG:HH21	18:Q:69:ILE:HD11	1.82	0.44
2:A:232:PRO:HB2	2:A:233:HIS:HD2	1.82	0.44
18:Q:7:LEU:HD21	18:Q:42:ILE:HG12	1.99	0.44
29:X:1611:U:H2'	29:X:1612:U:H6	1.82	0.44
29:X:498:C:N4	29:X:499:G:C6	2.85	0.44
16:O:5:ILE:N	16:O:38:LEU:HD12	2.33	0.44
29:X:2831:A:H2'	29:X:2832:G:O4'	2.17	0.44
18:Q:8:GLN:O	18:Q:9:ALA:HB2	2.16	0.44
10:I:118:VAL:O	10:I:138:GLY:HA3	2.17	0.44
6:E:126:PRO:HG2	6:E:130:ARG:HB2	1.99	0.44
10:I:19:VAL:O	10:I:21:ARG:NH1	2.51	0.44
29:X:1229:C:H6	29:X:1229:C:O5'	2.00	0.44
25:Z:13:LYS:HD3	29:X:527:C:OP2	2.17	0.44
29:X:654:A:HO2'	29:X:655:A:P	2.40	0.44
15:N:40:LEU:O	15:N:43:ALA:HB3	2.18	0.44
30:Y:58:G:C4'	30:Y:59:A:H5"	2.47	0.44
29:X:420:C:H2'	29:X:421:G:H8	1.83	0.44
29:X:2034:A:H2'	29:X:2557:G:OP1	2.17	0.44
29:X:1787:U:H2'	29:X:1788:C:C6	2.52	0.44
29:X:1352:G:C6	29:X:1353:A:N6	2.85	0.44
12:K:27:ALA:O	12:K:31:GLU:N	2.49	0.44
3:B:119:ARG:HG2	3:B:120:TRP:NE1	2.33	0.44
1:0:68:VAL:HG21	1:0:153:LYS:HG2	2.00	0.44
20:S:36:ARG:HG2	20:S:40:ASP:OD2	2.17	0.44
29:X:1882:G:N3	29:X:1882:G:H2'	2.32	0.44
4:C:95:LEU:O	4:C:100:ARG:NH1	2.45	0.44
24:W:49:HIS:HD2	24:W:50:LEU:HG	1.82	0.44
18:Q:62:ARG:HG2	18:Q:71:GLN:HG3	1.98	0.44
29:X:1348:C:H2'	29:X:1349:A:C8	2.52	0.44
2:A:271:VAL:HG22	2:A:272:THR:HG23	1.98	0.44
28:3:64:ARG:HH21	29:X:219:G:H5'	1.82	0.44
29:X:1067:G:H2'	29:X:1113:C:H41	1.81	0.44
29:X:1770:U:C5	29:X:1775:A:N7	2.73	0.44
29:X:587:A:H8	29:X:587:A:OP2	2.00	0.44
29:X:2241:U:H2'	29:X:2242:C:C6	2.48	0.44
30:Y:16:U:O2'	30:Y:110:U:H1'	2.18	0.44
29:X:443:A:H5"	29:X:444:U:OP2	2.18	0.44
29:X:742:G:H5'	29:X:743:A:H5"	2.00	0.44
29:X:1815:G:C4	29:X:1816:G:C8	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:2662:C:H2'	29:X:2663:U:H6	1.82	0.44
29:X:1142:G:C8	29:X:2008:C:H4'	2.52	0.44
29:X:2375:G:N3	29:X:2400:G:N2	2.65	0.44
4:C:17:LEU:HA	4:C:18:PRO:HD3	1.77	0.44
29:X:1733:U:H3	29:X:1734:C:H41	1.64	0.44
12:K:54:THR:CG2	12:K:66:VAL:HG23	2.47	0.44
2:A:233:HIS:NE2	2:A:247:VAL:HG12	2.33	0.44
29:X:1174:G:N2	29:X:1175:A:C4	2.85	0.44
29:X:828:C:H2'	29:X:829:C:H6	1.82	0.44
29:X:1858:C:H2'	29:X:1859:A:O4'	2.16	0.44
17:P:22:LYS:HA	17:P:23:PRO:HD3	1.56	0.44
28:3:21:LYS:HB3	28:3:55:TRP:CH2	2.53	0.44
16:O:14:VAL:HG12	16:O:18:ASP:OD2	2.18	0.44
9:H:20:MET:HG2	9:H:21:CYS:N	2.29	0.44
30:Y:30:C:H2'	30:Y:31:A:O4'	2.18	0.44
29:X:526:C:H1'	29:X:1274:C:O2'	2.16	0.44
14:M:106:TYR:HD1	29:X:1745:C:H4'	1.83	0.44
29:X:198:A:O2'	29:X:243:G:O6	2.35	0.44
29:X:1623:C:H4'	29:X:1624:A:O5'	2.17	0.44
29:X:1359:G:C6	29:X:1617:G:C6	3.05	0.44
29:X:2022:C:H2'	29:X:2023:C:C6	2.53	0.44
2:A:225:ALA:HB1	29:X:795:A:HO2'	1.82	0.44
29:X:619:A:N6	29:X:630:G:O2'	2.51	0.44
20:S:121:GLN:O	20:S:161:ALA:HB3	2.18	0.44
29:X:1283:C:H5"	29:X:1284:G:C5'	2.47	0.44
29:X:2229:G:HO2'	29:X:2475:C:P	2.40	0.44
18:Q:9:ALA:O	18:Q:27:PHE:HB3	2.17	0.44
3:B:19:ARG:HH11	9:H:84:ALA:HB1	1.82	0.44
29:X:2067:U:H2'	29:X:2068:C:C6	2.53	0.44
4:C:178:TYR:O	4:C:182:ARG:N	2.42	0.44
15:N:47:TYR:CE2	15:N:51:ARG:CZ	3.00	0.44
7:F:130:THR:HG1	29:X:1071:U:H5	1.65	0.44
29:X:2427:A:OP1	29:X:2478:C:OP1	2.35	0.44
4:C:68:ARG:NH2	29:X:2043:A:H62	2.16	0.44
8:G:128:GLU:HG3	8:G:150:VAL:HG21	1.99	0.44
30:Y:16:U:O2'	30:Y:110:U:O2	2.34	0.44
30:Y:67:C:N4	30:Y:111:C:O2'	2.43	0.44
9:H:1:MET:O	9:H:2:ILE:HD13	2.17	0.44
8:G:70:PHE:HA	8:G:76:GLN:OE1	2.18	0.44
20:S:91:PRO:HG2	20:S:124:ALA:HA	1.99	0.44
29:X:318:G:N1	29:X:321:A:OP2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:2741:G:C6	29:X:2742:G:N7	2.86	0.44
29:X:875:G:O2'	30:Y:80:A:N3	2.38	0.44
29:X:1724:C:N3	29:X:1747:G:C6	2.85	0.44
29:X:1283:C:H6	29:X:1283:C:O5'	1.99	0.44
29:X:2817:A:H2'	29:X:2818:G:O4'	2.16	0.44
12:K:39:THR:O	12:K:41:ALA:N	2.51	0.44
12:K:38:LEU:O	12:K:41:ALA:HB3	2.18	0.44
20:S:66:VAL:HG22	20:S:83:PHE:CE1	2.53	0.44
29:X:757:U:H2'	29:X:758:G:O4'	2.17	0.44
29:X:1629:G:C6	29:X:1633:C:C6	3.05	0.44
21:T:11:LYS:HE2	21:T:11:LYS:HB2	1.61	0.44
7:F:109:LYS:HA	7:F:109:LYS:HD2	1.60	0.44
29:X:2011:U:H2'	29:X:2012:A:O4'	2.18	0.44
29:X:1951:G:O2'	29:X:1952:A:O4'	2.26	0.44
29:X:223:C:N4	29:X:224:G:O6	2.50	0.44
14:M:60:SER:O	14:M:63:ARG:NH1	2.51	0.44
29:X:7:G:C4	29:X:8:A:C8	3.06	0.44
29:X:42:G:H2'	29:X:43:A:C8	2.52	0.44
29:X:1819:U:H5'	29:X:1954:A:O3'	2.17	0.44
29:X:2038:C:O5'	29:X:2039:G:H5"	2.17	0.44
29:X:2039:G:N2	29:X:2040:A:C4	2.86	0.44
29:X:1329:U:O2'	29:X:1330:G:H5'	2.17	0.44
29:X:2290:A:N3	29:X:2290:A:H2'	2.33	0.44
19:R:51:VAL:HG13	19:R:73:GLU:CB	2.48	0.44
2:A:142:VAL:HG12	2:A:163:VAL:O	2.17	0.44
29:X:389:G:N2	29:X:412:U:H1'	2.32	0.44
29:X:2233:C:C2'	29:X:2234:G:H5'	2.48	0.44
29:X:1835:C:H2'	29:X:1836:C:C6	2.52	0.44
5:D:106:ILE:HB	5:D:139:PRO:HB3	2.00	0.44
29:X:2800:C:H5"	29:X:2801:A:OP2	2.17	0.44
29:X:488:A:OP1	29:X:488:A:H8	2.01	0.44
28:3:42:ARG:HD3	29:X:2328:G:OP2	2.16	0.44
29:X:580:A:C8	29:X:2013:A:N6	2.86	0.44
29:X:1506:C:H4'	29:X:1507:A:OP1	2.17	0.44
29:X:349:G:H2'	29:X:350:U:C6	2.53	0.44
17:P:75:ALA:HB1	17:P:128:VAL:HG22	1.99	0.44
7:F:111:LYS:HD3	7:F:115:LEU:HG	1.99	0.44
29:X:1310:C:OP1	29:X:2689:C:H4'	2.17	0.44
29:X:1430:G:O2'	29:X:1603:A:H1'	2.18	0.44
15:N:68:GLY:HA2	15:N:71:LEU:HD12	2.00	0.44
6:E:7:GLN:H	6:E:8:PRO:HD3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:387:A:N6	29:X:413:G:O2'	2.51	0.44
16:O:53:LYS:HG3	16:O:54:TYR:CD1	2.53	0.44
29:X:1177:U:C2	29:X:1198:C:O2	2.71	0.44
17:P:33:MET:SD	17:P:64:ALA:HB2	2.58	0.44
11:J:25:GLY:HA3	29:X:919:U:OP1	2.18	0.44
20:S:18:MET:HA	20:S:35:ASP:HA	1.98	0.44
6:E:111:HIS:HA	6:E:112:PRO:HD2	1.55	0.44
16:O:31:ASP:HB2	16:O:60:VAL:HG21	2.00	0.44
29:X:2793:G:N2	29:X:2804:G:C4	2.86	0.44
3:B:7:THR:O	3:B:9:ILE:HD12	2.17	0.44
29:X:471:A:C2	29:X:481:A:C5	3.06	0.44
28:3:3:LYS:HE3	29:X:219:G:OP2	2.17	0.44
29:X:2309:G:H2'	29:X:2310:G:O4'	2.18	0.44
2:A:29:PRO:HG2	2:A:63:ARG:NH1	2.33	0.44
29:X:534:U:P	29:X:549:G:H21	2.40	0.44
29:X:2857:C:N3	29:X:2858:A:C8	2.86	0.44
13:L:91:ARG:CG	13:L:92:GLY:H	2.31	0.44
14:M:101:ARG:NH1	29:X:1745:C:OP1	2.47	0.44
29:X:1065:A:H2'	29:X:1066:G:H8	1.82	0.44
1:0:96:ILE:HG23	1:0:123:LEU:HG	2.00	0.44
1:0:96:ILE:HD11	1:0:118:GLN:HB3	2.00	0.44
29:X:2578:G:C2	29:X:2579:A:C8	3.05	0.44
3:B:55:ALA:H	3:B:58:LYS:HZ2	1.61	0.44
20:S:91:PRO:HG3	20:S:126:GLY:N	2.32	0.44
11:J:12:LYS:HG2	29:X:923:A:N6	2.33	0.44
14:M:56:ALA:HB1	14:M:103:LYS:HE3	2.00	0.44
29:X:790:A:H2'	29:X:791:G:H8	1.83	0.44
13:L:9:ARG:O	13:L:11:LEU:N	2.51	0.44
5:D:122:PHE:HB3	5:D:123:ASP:H	1.63	0.44
29:X:213:C:H2'	29:X:214:C:C6	2.53	0.44
29:X:464:G:H2'	29:X:465:C:H6	1.83	0.44
28:3:11:LYS:HB3	28:3:11:LYS:HE2	1.68	0.44
29:X:2571:G:C6	29:X:2572:U:N3	2.86	0.44
29:X:228:A:C5	29:X:229:G:H1'	2.53	0.44
29:X:2813:G:C5	29:X:2814:G:N7	2.86	0.44
15:N:91:ASN:ND2	15:N:93:LYS:HB3	2.33	0.44
29:X:65:C:H2'	29:X:66:U:O4'	2.18	0.44
29:X:1254:G:C2	29:X:1255:A:C5	3.06	0.44
29:X:1236:G:N2	29:X:1239:A:OP2	2.37	0.44
29:X:1642:G:O5'	29:X:1642:G:H8	2.01	0.44
3:B:5:LEU:HD12	3:B:49:ILE:CD1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:501:G:H2'	29:X:502:A:H8	1.82	0.44
3:B:123:ALA:HB2	29:X:2491:C:OP1	2.17	0.44
29:X:1174:G:H2'	29:X:1175:A:H8	1.82	0.44
29:X:2508:G:H5"	29:X:2509:A:H5"	2.00	0.44
4:C:5:ASN:N	4:C:5:ASN:OD1	2.51	0.44
3:B:199:ARG:H	3:B:199:ARG:HG3	1.65	0.44
29:X:199:A:O2'	29:X:200:A:O5'	2.29	0.44
29:X:1024:G:H2'	29:X:1025:A:C8	2.53	0.44
3:B:10:GLY:O	3:B:25:VAL:HG23	2.18	0.44
1:0:4:ARG:HG2	1:0:5:ALA:H	1.82	0.44
10:I:41:SER:OG	29:X:684:C:H3'	2.18	0.44
28:3:17:THR:HG22	28:3:21:LYS:O	2.18	0.43
29:X:567:G:H2'	29:X:568:G:H8	1.83	0.43
29:X:1494:G:O2'	29:X:1574:A:N7	2.51	0.43
5:D:92:ARG:CZ	30:Y:46:G:H5"	2.48	0.43
29:X:2433:G:C4	29:X:2434:G:C8	3.06	0.43
20:S:3:LEU:HD13	20:S:56:VAL:HA	2.00	0.43
29:X:1600:U:H5"	29:X:1601:U:H5'	1.99	0.43
16:O:32:LYS:HB3	16:O:32:LYS:HE3	1.80	0.43
11:J:84:MET:HE2	29:X:967:G:H4'	2.00	0.43
11:J:111:THR:H	11:J:114:GLN:HG3	1.83	0.43
29:X:1734:C:H2'	29:X:1735:G:H5'	1.99	0.43
25:Z:52:TYR:OH	29:X:2859:U:N3	2.50	0.43
29:X:758:G:N2	29:X:766:A:C6	2.86	0.43
3:B:60:ASN:HB3	3:B:62:PRO:HD2	2.00	0.43
28:3:23:MET:HG2	28:3:49:VAL:HG22	1.99	0.43
29:X:2684:A:H8	29:X:2684:A:O5'	2.01	0.43
29:X:1474:A:H2'	29:X:1474:A:N3	2.32	0.43
4:C:154:ASP:N	4:C:154:ASP:OD1	2.50	0.43
17:P:36:ARG:NH1	25:Z:20:ARG:NH2	2.65	0.43
29:X:2814:G:C2	29:X:2815:C:C2	3.06	0.43
29:X:818:G:N2	29:X:842:A:OP1	2.51	0.43
29:X:312:G:N2	29:X:328:A:H1'	2.32	0.43
5:D:88:LYS:HD3	29:X:2292:C:H5"	1.99	0.43
3:B:48:GLN:HA	3:B:79:ARG:O	2.19	0.43
13:L:33:ARG:NH2	13:L:38:ILE:HD13	2.32	0.43
19:R:24:VAL:HA	19:R:80:LYS:O	2.18	0.43
29:X:1436:G:O2'	29:X:1508:G:N3	2.51	0.43
29:X:1562:G:H3'	29:X:1563:U:H5'	2.01	0.43
29:X:1146:G:N2	29:X:1147:G:C4	2.86	0.43
29:X:825:C:H2'	29:X:826:U:C6	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:2273:C:H2'	29:X:2274:C:H6	1.82	0.43
29:X:2407:G:H5"	29:X:2408:G:O5'	2.17	0.43
29:X:616:U:H4'	29:X:671:A:H4'	1.99	0.43
20:S:19:ILE:HD11	20:S:36:ARG:HG3	2.00	0.43
1:0:110:VAL:HG12	1:0:111:ALA:H	1.83	0.43
9:H:7:ARG:HD3	9:H:18:GLU:OE2	2.17	0.43
29:X:2269:G:N2	29:X:2322:U:O2'	2.51	0.43
1:0:196:LYS:HE2	1:0:204:PHE:CZ	2.53	0.43
24:W:37:THR:CB	29:X:940:G:H5'	2.48	0.43
22:U:17:SER:OG	22:U:44:ALA:HA	2.18	0.43
15:N:51:ARG:O	15:N:54:LYS:HB2	2.18	0.43
29:X:2349:G:C6	29:X:2350:G:C5	3.07	0.43
29:X:2294:U:H2'	29:X:2295:C:C6	2.53	0.43
29:X:1089:C:H1'	29:X:1099:A:H2	1.83	0.43
29:X:851:C:C2	29:X:952:A:C6	3.07	0.43
18:Q:29:VAL:HG12	18:Q:30:SER:N	2.32	0.43
29:X:2097:A:H61	29:X:2102:A:H62	1.65	0.43
29:X:2678:C:O2	29:X:2688:G:N1	2.52	0.43
2:A:210:GLY:O	2:A:213:ARG:N	2.50	0.43
29:X:18:U:O2'	29:X:563:U:OP1	2.33	0.43
16:O:78:VAL:O	16:O:79:GLN:HB2	2.18	0.43
4:C:103:GLY:O	4:C:106:MET:N	2.51	0.43
7:F:1:MET:HE2	7:F:2:ARG:HH11	1.83	0.43
5:D:129:ASN:HB3	5:D:155:THR:HG22	2.00	0.43
29:X:2212:U:H2'	29:X:2213:G:C8	2.53	0.43
29:X:2511:G:C5	29:X:2512:A:N7	2.86	0.43
2:A:76:ASN:HB3	2:A:118:ASN:CG	2.39	0.43
29:X:1424:U:H2'	29:X:1425:G:O4'	2.18	0.43
4:C:27:LEU:O	4:C:31:VAL:HG23	2.18	0.43
29:X:1229:C:H2'	29:X:1230:C:C6	2.52	0.43
29:X:2659:C:N3	29:X:2660:C:C5	2.86	0.43
29:X:574:C:H4'	29:X:1266:G:C6	2.54	0.43
29:X:312:G:O2'	29:X:313:U:H6	1.95	0.43
2:A:69:ARG:HH22	2:A:192:THR:HG21	1.84	0.43
9:H:22:ILE:HD11	29:X:1935:A:N6	2.33	0.43
19:R:78:ALA:HA	19:R:81:VAL:HB	2.01	0.43
29:X:714:G:C2	29:X:745:C:C5	3.07	0.43
3:B:129:HIS:CE1	29:X:1692:C:N3	2.86	0.43
12:K:33:ARG:CB	12:K:114:GLU:HB2	2.49	0.43
7:F:10:LEU:HD21	7:F:57:ILE:HG13	2.00	0.43
29:X:350:U:O5'	29:X:350:U:H6	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:25:LYS:HG2	6:E:26:VAL:N	2.32	0.43
29:X:1310:C:H2'	29:X:1311:C:H6	1.84	0.43
29:X:82:G:H1	29:X:100:G:HO2'	1.66	0.43
29:X:717:G:H1'	29:X:739:G:H22	1.84	0.43
15:N:67:ALA:O	15:N:71:LEU:HG	2.18	0.43
4:C:28:HIS:CD2	10:I:8:PRO:HA	2.54	0.43
29:X:2445:C:H42	29:X:2463:G:H1	1.66	0.43
7:F:53:ILE:HG12	7:F:72:PRO:HB3	2.00	0.43
29:X:2666:U:O2'	29:X:2667:C:H5'	2.18	0.43
29:X:2499:C:C4	29:X:2546:G:C8	3.06	0.43
15:N:28:ARG:HG2	15:N:38:THR:OG1	2.19	0.43
25:Z:35:GLN:O	25:Z:37:HIS:N	2.52	0.43
7:F:10:LEU:HD12	7:F:12:LEU:HG	2.00	0.43
10:I:73:GLU:HG3	10:I:105:PRO:O	2.19	0.43
29:X:502:A:H2'	29:X:503:G:O4'	2.19	0.43
2:A:62:TYR:CE1	29:X:1808:C:H3'	2.51	0.43
20:S:49:THR:HG22	20:S:94:VAL:HG13	2.00	0.43
29:X:1749:G:H5"	29:X:1749:G:N3	2.34	0.43
19:R:54:ILE:HD12	19:R:71:GLN:NE2	2.33	0.43
4:C:43:ALA:HB2	29:X:456:C:H4'	2.01	0.43
20:S:72:ASP:O	20:S:76:ARG:N	2.49	0.43
17:P:36:ARG:CZ	25:Z:20:ARG:HH21	2.31	0.43
29:X:1678:G:C4	29:X:1983:G:N2	2.87	0.43
5:D:70:ALA:C	5:D:72:LYS:H	2.21	0.43
29:X:1071:U:O4'	29:X:1073:G:H5'	2.18	0.43
30:Y:25:G:N2	30:Y:62:C:N3	2.52	0.43
29:X:539:A:N7	29:X:2025:A:C2	2.87	0.43
29:X:676:G:C5	29:X:677:G:C8	3.07	0.43
18:Q:15:LYS:HZ3	29:X:1354:A:H62	1.67	0.43
19:R:58:VAL:HA	29:X:494:A:C4'	2.48	0.43
21:T:56:ASP:CG	29:X:2343:C:H5'	2.39	0.43
29:X:777:A:O2'	29:X:778:G:H5'	2.19	0.43
30:Y:86:A:C2	30:Y:96:C:C2	3.07	0.43
29:X:2487:G:C2	29:X:2561:G:C6	3.07	0.43
29:X:2528:G:C2	29:X:2529:G:C8	3.05	0.43
29:X:1175:A:H2'	29:X:1176:U:C6	2.54	0.43
11:J:8:THR:HG22	11:J:70:PHE:CE2	2.53	0.43
29:X:1715:A:O5'	29:X:1715:A:H8	2.01	0.43
29:X:783:G:N1	29:X:784:U:C2	2.87	0.43
5:D:147:ASP:N	5:D:147:ASP:OD1	2.52	0.43
29:X:2269:G:N2	29:X:2322:U:H1'	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:436:A:H2'	29:X:436:A:N3	2.34	0.43
29:X:1539:U:H6	29:X:1539:U:O5'	2.02	0.43
18:Q:57:ASN:N	18:Q:57:ASN:OD1	2.51	0.43
29:X:26:G:O2'	29:X:27:G:H5'	2.18	0.43
29:X:1865:C:H2'	29:X:1866:G:O4'	2.19	0.43
23:V:11:ALA:HB1	23:V:57:LYS:HD2	2.01	0.43
29:X:1419:G:H2'	29:X:1420:A:C8	2.53	0.43
29:X:1670:G:H5"	29:X:2797:G:N2	2.33	0.43
29:X:1110:G:O5'	29:X:1110:G:H8	2.01	0.43
19:R:38:LEU:O	19:R:46:VAL:HG23	2.19	0.43
7:F:22:PRO:HB2	7:F:23:VAL:H	1.61	0.43
29:X:1609:G:H2'	29:X:1610:A:O4'	2.18	0.43
10:I:73:GLU:OE2	10:I:104:ARG:HB2	2.19	0.43
29:X:717:G:N3	29:X:739:G:C2	2.87	0.43
29:X:998:C:O2	29:X:1011:A:H2	2.02	0.43
4:C:59:TYR:HD1	4:C:60:GLY:N	2.15	0.43
4:C:114:GLY:N	4:C:115:GLY:HA2	2.33	0.43
29:X:649:G:C5	29:X:650:U:C5	3.06	0.43
29:X:655:A:H8	29:X:655:A:O5'	2.01	0.43
29:X:817:A:H5"	29:X:818:G:OP1	2.19	0.43
12:K:102:THR:HG22	12:K:103:ARG:H	1.83	0.43
29:X:1339:U:C4'	29:X:1993:G:H21	2.32	0.43
29:X:330:C:C2	29:X:331:U:C6	3.06	0.43
29:X:547:U:H2'	29:X:548:G:C8	2.54	0.43
29:X:1030:U:C4	29:X:1031:C:H5	2.36	0.43
30:Y:63:A:H2'	30:Y:64:C:C6	2.53	0.43
29:X:2021:G:C2	29:X:2022:C:C2	3.07	0.43
2:A:226:MET:HB3	2:A:230:ASP:HB2	2.01	0.43
11:J:52:ARG:O	11:J:56:SER:HB3	2.18	0.43
29:X:1210:C:H1'	29:X:1239:A:C4	2.53	0.43
29:X:444:U:O2'	29:X:445:A:H5'	2.19	0.43
3:B:55:ALA:H	3:B:58:LYS:HZ1	1.64	0.43
9:H:11:ALA:O	9:H:111:PHE:N	2.46	0.43
15:N:63:GLN:HG2	15:N:63:GLN:H	1.56	0.43
29:X:2662:C:C2	29:X:2663:U:C5	3.07	0.43
29:X:1723:U:C6	29:X:1748:U:OP2	2.71	0.43
3:B:44:TYR:CZ	29:X:2616:U:H5'	2.54	0.43
29:X:2655:C:O2	29:X:2712:G:N2	2.51	0.43
29:X:1402:G:H2'	29:X:1403:U:H6	1.84	0.43
21:T:72:LYS:HD3	30:Y:14:C:H5	1.84	0.43
29:X:1527:G:H2'	29:X:1528:C:H6	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:32:GLU:O	25:Z:34:PRO:HD3	2.18	0.43
1:0:188:LEU:O	1:0:192:LEU:HB2	2.18	0.43
29:X:2238:G:C6	29:X:2261:G:O6	2.72	0.43
29:X:628:A:H2'	29:X:629:C:H6	1.80	0.43
29:X:578:U:H1'	29:X:958:G:O4'	2.19	0.43
15:N:37:GLN:CG	29:X:1265:G:H1	2.27	0.43
29:X:2707:G:H2'	29:X:2708:U:C6	2.53	0.43
29:X:78:C:O2'	29:X:357:A:N3	2.43	0.43
29:X:312:G:C4	29:X:313:U:C5	3.06	0.43
14:M:69:ARG:CZ	14:M:108:LYS:HG2	2.48	0.43
29:X:402:A:C8	29:X:2392:G:H4'	2.54	0.43
29:X:2006:G:C2	29:X:2024:U:O2	2.72	0.43
29:X:2033:C:H5"	29:X:2034:A:OP2	2.19	0.43
29:X:2043:A:H1'	29:X:2481:G:H1'	1.99	0.43
29:X:167:A:H3'	29:X:168:A:H8	1.84	0.43
22:U:38:THR:HG22	29:X:2412:A:C2	2.53	0.43
2:A:71:ASP:CG	2:A:103:ARG:HH22	2.22	0.43
17:P:9:ARG:HG3	17:P:10:ASN:N	2.33	0.43
10:I:73:GLU:OE2	10:I:101:ARG:HB2	2.19	0.43
20:S:168:VAL:HG12	20:S:169:VAL:N	2.34	0.43
29:X:1299:A:N6	29:X:1302:C:C2	2.87	0.43
2:A:247:VAL:HA	2:A:253:PRO:HA	2.01	0.43
29:X:1883:A:H5'	29:X:1953:A:H5'	2.00	0.43
8:G:68:PRO:O	15:N:64:ARG:HG2	2.19	0.43
4:C:59:TYR:CD1	4:C:60:GLY:N	2.87	0.43
29:X:1287:A:C2	29:X:1315:A:C2	3.07	0.43
29:X:225:G:H2'	29:X:226:C:OP1	2.19	0.43
29:X:987:G:C2	29:X:988:G:C5	3.07	0.43
29:X:320:A:C6	29:X:341:A:C6	3.07	0.43
12:K:8:ARG:NH1	29:X:1669:A:OP1	2.47	0.43
15:N:10:ARG:HG3	29:X:1264:C:OP1	2.18	0.43
4:C:176:ASN:OD1	4:C:178:TYR:HB3	2.19	0.43
17:P:36:ARG:HA	17:P:39:ARG:HD2	2.01	0.43
29:X:815:A:C5	29:X:816:U:C5	3.07	0.43
29:X:2604:G:C5	29:X:2605:C:C4	3.07	0.43
29:X:1021:A:N3	29:X:1164:C:H1'	2.34	0.43
29:X:2493:U:H2'	29:X:2494:C:C6	2.54	0.43
14:M:2:GLN:HB3	29:X:2795:A:N1	2.33	0.43
15:N:31:GLN:HE22	29:X:589:C:H4'	1.83	0.43
4:C:129:LYS:HB3	4:C:132:ASN:HD22	1.83	0.43
4:C:189:ASP:CG	4:C:190:ALA:H	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1322:G:H1	29:X:1621:C:H42	1.67	0.43
29:X:1321:A:H61	29:X:1624:A:H61	1.66	0.43
29:X:2369:U:C3'	29:X:2369:U:C6	3.02	0.43
2:A:126:LYS:HE2	2:A:126:LYS:HB3	1.81	0.43
29:X:854:G:H22	29:X:948:C:N4	2.17	0.43
30:Y:42:U:H3'	30:Y:43:G:H5"	2.01	0.43
15:N:107:LYS:O	15:N:110:VAL:HB	2.19	0.43
9:H:85:ASP:CG	9:H:87:SER:H	2.22	0.43
22:U:8:THR:N	22:U:14:VAL:HG23	2.34	0.43
29:X:2429:A:OP1	29:X:2476:A:C8	2.71	0.43
29:X:469:G:N2	29:X:480:G:H2'	2.34	0.42
29:X:815:A:H5"	29:X:816:U:OP2	2.19	0.42
9:H:43:ARG:NH2	29:X:1979:C:OP2	2.49	0.42
29:X:1672:A:H3'	29:X:1673:C:H6	1.84	0.42
29:X:351:A:H2'	29:X:352:G:H5'	2.01	0.42
29:X:1104:G:N2	29:X:1109:A:H62	2.09	0.42
29:X:2326:C:H2'	29:X:2327:U:C6	2.54	0.42
29:X:520:C:H2'	29:X:521:U:O4'	2.19	0.42
29:X:951:G:H2'	29:X:952:A:O4'	2.19	0.42
29:X:585:U:H4'	29:X:2481:G:C8	2.54	0.42
6:E:45:GLN:HG3	6:E:49:GLN:O	2.18	0.42
11:J:88:LYS:HG2	29:X:967:G:OP1	2.20	0.42
12:K:112:LEU:HD11	25:Z:57:VAL:HG13	2.01	0.42
25:Z:52:TYR:CZ	29:X:2859:U:N3	2.84	0.42
29:X:2512:A:H2'	29:X:2513:A:O4'	2.18	0.42
29:X:1287:A:C2	29:X:1315:A:H2	2.37	0.42
3:B:52:ALA:O	3:B:76:ARG:N	2.48	0.42
29:X:1746:A:H8	29:X:1746:A:O5'	2.02	0.42
27:2:24:THR:O	27:2:28:ARG:HD3	2.19	0.42
2:A:88:ARG:NH1	29:X:1809:G:OP1	2.51	0.42
29:X:2214:G:H2'	29:X:2215:C:C6	2.54	0.42
28:3:4:MET:HE3	28:3:4:MET:HB2	1.91	0.42
30:Y:55:C:H2'	30:Y:56:G:O4'	2.18	0.42
3:B:34:VAL:HG21	3:B:67:PHE:HE1	1.83	0.42
29:X:1028:G:C2	29:X:1157:G:C4	3.06	0.42
15:N:9:VAL:O	15:N:12:ARG:HB2	2.20	0.42
28:3:33:ASN:ND2	29:X:2398:U:O5'	2.50	0.42
6:E:21:ASP:HB3	6:E:22:GLY:H	1.41	0.42
29:X:2660:C:C2	29:X:2704:U:O4	2.72	0.42
29:X:218:A:C6	29:X:232:A:H5"	2.54	0.42
29:X:351:A:N6	29:X:352:G:C2	2.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:24:TYR:HB3	20:S:29:ASN:HB2	2.00	0.42
29:X:1088:A:N1	29:X:1099:A:O2'	2.34	0.42
29:X:2595:C:H2'	29:X:2596:C:C6	2.53	0.42
29:X:2432:A:H2'	29:X:2433:G:C8	2.54	0.42
6:E:75:ALA:O	6:E:79:VAL:HG22	2.19	0.42
19:R:51:VAL:HG22	19:R:52:ASN:N	2.34	0.42
4:C:22:VAL:HG22	4:C:106:MET:HG2	2.01	0.42
2:A:252:LYS:HA	2:A:253:PRO:HD3	1.90	0.42
23:V:25:LEU:O	23:V:28:LEU:HB2	2.19	0.42
3:B:23:VAL:HG11	3:B:183:LEU:HB3	2.00	0.42
4:C:48:ARG:NH2	29:X:686:C:OP1	2.52	0.42
29:X:1:G:H2'	29:X:2:G:H8	1.83	0.42
4:C:102:LEU:O	4:C:102:LEU:HD12	2.18	0.42
17:P:25:PHE:CD2	17:P:25:PHE:C	2.92	0.42
2:A:67:PHE:HB3	2:A:153:ALA:H	1.84	0.42
3:B:33:ILE:HG12	3:B:36:ARG:HH21	1.84	0.42
28:3:7:HIS:HD2	28:3:61:MET:CE	2.32	0.42
29:X:2543:A:C6	29:X:2544:A:N1	2.88	0.42
29:X:1674:C:C2	29:X:1675:C:C5	3.07	0.42
29:X:1080:A:H4'	29:X:1081:A:H8	1.84	0.42
30:Y:36:A:H4'	30:Y:37:C:H5	1.84	0.42
29:X:1179:A:C2	29:X:1196:G:N1	2.87	0.42
29:X:2450:A:C4	29:X:2451:G:C8	3.08	0.42
7:F:126:THR:HA	29:X:1091:C:O2'	2.19	0.42
29:X:1091:C:H2'	29:X:1092:U:C6	2.54	0.42
29:X:746:G:N7	29:X:774:A:N6	2.66	0.42
29:X:836:G:H2'	29:X:837:U:H6	1.80	0.42
17:P:38:VAL:O	17:P:41:VAL:HG23	2.18	0.42
15:N:59:ARG:O	15:N:63:GLN:HG2	2.19	0.42
16:O:71:ILE:HG13	29:X:1003:C:O2'	2.19	0.42
29:X:828:C:N3	29:X:1207:G:C2	2.87	0.42
29:X:782:U:H2'	29:X:783:G:C8	2.54	0.42
29:X:2057:U:C2	29:X:2415:G:C2	3.07	0.42
4:C:35:LEU:O	4:C:38:ARG:HG3	2.19	0.42
29:X:1950:C:N4	29:X:1951:G:C6	2.88	0.42
29:X:919:U:HO2'	29:X:920:G:H8	1.68	0.42
13:L:8:ARG:HA	13:L:8:ARG:HD2	1.80	0.42
29:X:1381:G:C2'	29:X:1799:A:H61	2.31	0.42
5:D:7:LYS:O	5:D:11:GLN:HG3	2.19	0.42
16:O:72:ARG:HA	16:O:82:ARG:O	2.19	0.42
19:R:64:ASN:HA	19:R:65:PRO:HD2	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1942:G:H2'	29:X:1943:A:O4'	2.20	0.42
13:L:98:GLY:HA3	30:Y:51:G:OP1	2.19	0.42
29:X:2691:C:O2	29:X:2692:A:H2'	2.19	0.42
25:Z:16:ARG:HD2	25:Z:20:ARG:HH12	1.85	0.42
11:J:100:PRO:C	11:J:102:ARG:H	2.22	0.42
29:X:587:A:H2'	29:X:588:G:H5"	1.99	0.42
19:R:58:VAL:C	19:R:60:PRO:HD2	2.39	0.42
29:X:2041:A:O5'	29:X:2041:A:H8	2.02	0.42
4:C:42:THR:HG21	29:X:454:G:N3	2.33	0.42
13:L:65:THR:HG21	30:Y:52:G:OP2	2.19	0.42
29:X:1977:C:O2	29:X:1977:C:H2'	2.19	0.42
16:O:75:LYS:HG3	16:O:80:TYR:HD1	1.84	0.42
29:X:887:G:H1	29:X:915:C:H42	1.67	0.42
2:A:72:LYS:O	2:A:75:VAL:HG12	2.19	0.42
29:X:718:A:H2'	29:X:719:A:C8	2.55	0.42
29:X:1720:G:C2	29:X:1721:G:C4	3.07	0.42
11:J:60:ARG:O	11:J:62:GLY:HA2	2.19	0.42
29:X:1667:A:H5"	29:X:1668:G:OP2	2.20	0.42
4:C:20:PRO:C	4:C:21:GLU:HG2	2.39	0.42
29:X:2255:G:C2	29:X:2256:G:C8	3.07	0.42
17:P:16:GLN:NE2	29:X:511:A:O2'	2.52	0.42
29:X:2169:A:H2'	29:X:2170:C:C6	2.54	0.42
29:X:2844:G:C6	29:X:2845:C:N3	2.88	0.42
29:X:816:U:O2'	29:X:817:A:H5'	2.20	0.42
29:X:953:G:O2'	29:X:1203:A:N3	2.44	0.42
29:X:2543:A:C2	29:X:2626:U:H4'	2.54	0.42
29:X:1672:A:H3'	29:X:1673:C:C5	2.54	0.42
17:P:30:TYR:H	17:P:123:HIS:CE1	2.37	0.42
29:X:1811:A:H1'	29:X:1813:A:C6	2.54	0.42
10:I:94:GLU:HA	10:I:97:ARG:HE	1.84	0.42
21:T:4:LYS:HD3	21:T:4:LYS:HA	1.42	0.42
8:G:128:GLU:CD	29:X:2760:G:H1	2.23	0.42
29:X:192:G:H4'	29:X:193:A:H4'	2.01	0.42
29:X:752:G:H4'	29:X:753:U:OP1	2.20	0.42
19:R:90:LYS:C	19:R:92:THR:HG23	2.39	0.42
8:G:61:ARG:HA	8:G:66:HIS:CE1	2.54	0.42
29:X:1699:A:H2'	29:X:1700:C:C6	2.55	0.42
29:X:303:C:H42	29:X:359:G:H1	1.66	0.42
29:X:813:A:O5'	29:X:813:A:H8	2.02	0.42
29:X:2564:U:C6	29:X:2564:U:H5'	2.54	0.42
29:X:1830:C:H41	29:X:1882:G:P	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:2720:A:C8	29:X:2743:G:N2	2.87	0.42
29:X:919:U:HO2'	29:X:920:G:C5'	2.32	0.42
29:X:2223:U:H2'	29:X:2224:U:O4'	2.20	0.42
29:X:681:A:C2	29:X:683:A:C6	3.07	0.42
29:X:2536:G:O2'	29:X:2537:C:H5'	2.20	0.42
29:X:984:A:O4'	29:X:1202:U:C6	2.72	0.42
29:X:2706:U:H3'	29:X:2707:G:H8	1.85	0.42
19:R:45:LYS:HA	19:R:76:LEU:O	2.19	0.42
17:P:62:ARG:NH1	25:Z:25:LEU:HD11	2.28	0.42
29:X:74:G:OP1	29:X:74:G:H4'	2.20	0.42
11:J:78:LYS:HE3	11:J:78:LYS:HB2	1.64	0.42
29:X:740:A:OP1	29:X:1445:A:O2'	2.30	0.42
3:B:146:THR:HG23	29:X:1141:U:H5	1.84	0.42
15:N:64:ARG:O	15:N:67:ALA:HB3	2.19	0.42
29:X:1762:C:C2	29:X:1763:G:C8	3.08	0.42
29:X:1713:G:H21	29:X:1961:A:H5'	1.85	0.42
29:X:399:G:O2'	29:X:400:U:OP1	2.29	0.42
29:X:1298:G:C5	29:X:1342:U:C5	3.08	0.42
27:2:16:HIS:HD2	29:X:699:G:O6	2.02	0.42
30:Y:7:C:O2	30:Y:119:G:N2	2.52	0.42
25:Z:6:VAL:O	29:X:2594:U:C4	2.71	0.42
29:X:2001:G:C6	29:X:2002:A:C5	3.07	0.42
14:M:101:ARG:NH1	29:X:1745:C:P	2.92	0.42
3:B:117:MET:O	3:B:119:ARG:N	2.53	0.42
29:X:1541:G:C4	29:X:1542:G:C8	3.07	0.42
2:A:229:VAL:HG11	29:X:797:A:C5	2.54	0.42
21:T:56:ASP:OD1	29:X:2343:C:H5'	2.19	0.42
9:H:73:VAL:HG12	9:H:99:ILE:HD13	2.00	0.42
29:X:389:G:H2'	29:X:390:U:H6	1.85	0.42
29:X:18:U:H6	29:X:18:U:O5'	2.03	0.42
29:X:1554:G:H2'	29:X:1555:A:C8	2.54	0.42
3:B:203:LYS:NZ	29:X:2712:G:OP1	2.43	0.42
29:X:1750:A:C2	29:X:1751:A:C5	3.08	0.42
3:B:19:ARG:HA	9:H:84:ALA:O	2.20	0.42
22:U:72:LYS:HA	22:U:72:LYS:HD3	1.89	0.42
29:X:2849:C:H2'	29:X:2850:U:H6	1.84	0.42
29:X:1374:G:O2'	29:X:1375:C:H5'	2.19	0.42
29:X:1569:A:N6	29:X:1571:G:H1'	2.35	0.42
15:N:39:LEU:HA	15:N:42:ALA:HB3	2.01	0.42
29:X:511:A:C6	29:X:512:A:C2	3.08	0.42
15:N:91:ASN:O	15:N:95:LEU:HG	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:763:A:C2	29:X:765:C:H4'	2.54	0.42
29:X:14:A:N6	29:X:15:G:C2	2.88	0.42
29:X:13:A:N3	29:X:15:G:C6	2.88	0.42
17:P:28:ALA:O	17:P:123:HIS:HA	2.20	0.42
16:O:19:VAL:HG12	16:O:20:ILE:H	1.84	0.42
16:O:95:ILE:HD13	16:O:95:ILE:HA	1.83	0.42
29:X:1693:A:C2	29:X:1976:U:H5'	2.55	0.42
29:X:1345:G:N7	29:X:1626:A:C8	2.88	0.42
26:1:14:SER:HB3	26:1:49:PHE:CE1	2.54	0.42
29:X:2019:C:O2'	29:X:2020:G:H5'	2.19	0.42
29:X:1643:A:H61	29:X:1656:U:H3	1.66	0.42
29:X:946:U:C2	29:X:947:C:C6	3.08	0.42
29:X:1040:A:H2	29:X:2444:C:O2	2.02	0.42
29:X:2425:G:N2	29:X:2480:C:N3	2.67	0.42
29:X:790:A:C2	29:X:791:G:C5	3.07	0.42
29:X:1733:U:C5	29:X:1735:G:H1'	2.54	0.42
4:C:95:LEU:HD12	4:C:96:PRO:HD2	2.00	0.42
3:B:41:THR:HB	3:B:42:ASP:OD1	2.20	0.42
27:2:28:ARG:O	27:2:31:LEU:HB2	2.19	0.42
11:J:6:LYS:HB3	11:J:7:ARG:H	1.67	0.42
29:X:728:G:H22	29:X:730:C:N4	2.18	0.42
6:E:86:ASN:HB2	6:E:165:VAL:HG22	2.02	0.42
29:X:1135:C:C2	29:X:1136:G:C8	3.08	0.42
6:E:39:THR:OG1	6:E:40:GLU:N	2.53	0.42
29:X:1681:A:O5'	29:X:1681:A:H8	2.01	0.42
29:X:2709:C:H2'	29:X:2710:C:C6	2.55	0.42
29:X:2310:G:N2	29:X:2364:C:C4	2.87	0.42
29:X:2494:C:H2'	29:X:2495:G:H8	1.85	0.42
2:A:108:PRO:HA	2:A:196:VAL:O	2.20	0.42
29:X:541:C:O2'	29:X:572:G:H5"	2.19	0.42
29:X:877:G:N2	29:X:925:U:O2	2.53	0.42
4:C:186:LEU:HG	4:C:188:ILE:HA	2.02	0.42
12:K:27:ALA:HA	12:K:30:ARG:HB3	2.02	0.42
26:1:7:ARG:NH1	26:1:25:THR:O	2.53	0.42
12:K:20:LEU:C	12:K:22:ARG:N	2.73	0.42
29:X:2038:C:H6	29:X:2483:U:H5'	1.83	0.42
5:D:34:ILE:HA	5:D:156:ILE:HG23	2.02	0.42
2:A:126:LYS:HB2	2:A:129:ASN:OD1	2.20	0.42
29:X:2201:G:C4	29:X:2202:G:C8	3.07	0.42
9:H:73:VAL:HG21	9:H:123:PHE:CE2	2.55	0.42
29:X:1689:U:C2'	29:X:1690:U:H5'	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1701:C:C2	29:X:1722:G:C2	3.08	0.42
14:M:56:ALA:CB	14:M:103:LYS:HE3	2.50	0.42
2:A:235:GLY:HA3	29:X:2577:A:H5"	2.01	0.42
4:C:106:MET:HE2	4:C:106:MET:HB3	1.86	0.42
29:X:1699:A:C2	29:X:1700:C:C2	3.08	0.42
8:G:69:ASP:HA	15:N:64:ARG:NH2	2.33	0.42
20:S:13:LYS:HB2	20:S:14:LEU:H	1.51	0.42
30:Y:90:C:H2'	30:Y:91:A:O4'	2.20	0.42
2:A:13:ARG:HD3	2:A:13:ARG:HA	1.44	0.42
20:S:48:THR:O	20:S:48:THR:OG1	2.32	0.42
29:X:2829:A:C2	29:X:2839:G:C4	3.08	0.42
12:K:100:VAL:HG12	12:K:101:GLY:N	2.34	0.42
29:X:963:G:H5'	29:X:964:A:OP2	2.20	0.42
29:X:139:A:H2'	29:X:140:G:C8	2.55	0.42
15:N:13:ARG:NH2	29:X:1264:C:OP1	2.50	0.42
14:M:82:PRO:C	14:M:84:ALA:N	2.71	0.42
29:X:1059:A:H8	29:X:1059:A:O5'	2.03	0.42
17:P:110:ALA:HB2	29:X:761:G:O5'	2.20	0.42
17:P:102:THR:HG22	17:P:120:ARG:HA	2.02	0.42
19:R:24:VAL:HB	19:R:29:HIS:O	2.19	0.42
25:Z:3:LYS:HG3	29:X:2591:C:OP2	2.20	0.42
29:X:457:C:C2'	29:X:458:G:H5"	2.50	0.42
29:X:167:A:C2	29:X:168:A:C4	3.07	0.42
29:X:2150:U:H2'	29:X:2151:G:C8	2.55	0.42
29:X:1704:G:H1'	29:X:1719:G:N2	2.34	0.42
29:X:1314:A:H2	29:X:1642:G:N3	2.18	0.42
2:A:209:ALA:O	2:A:210:GLY:C	2.57	0.42
3:B:26:VAL:HG11	3:B:198:LEU:HD11	2.01	0.42
29:X:215:G:H1'	29:X:619:A:H1'	2.01	0.42
13:L:32:TYR:O	13:L:32:TYR:CG	2.72	0.42
12:K:44:LEU:O	12:K:44:LEU:HG	2.18	0.42
29:X:1016:C:C2	29:X:1154:A:C5	3.08	0.42
30:Y:48:A:C5	30:Y:49:C:C4	3.07	0.42
29:X:2685:A:N1	29:X:2686:C:C2	2.87	0.42
21:T:66:LYS:HB3	21:T:66:LYS:HE2	1.72	0.42
29:X:2461:G:N3	29:X:2461:G:H2'	2.34	0.42
4:C:7:ILE:HA	4:C:7:ILE:HD13	1.74	0.42
4:C:107:ALA:HB2	4:C:177:VAL:HG13	2.02	0.42
29:X:961:G:C6	29:X:962:C:C4	3.08	0.42
29:X:824:U:H1'	29:X:1264:C:O4'	2.20	0.41
29:X:2665:G:C6	29:X:2666:U:N3	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:U:27:ASP:CA	22:U:32:ARG:HH21	2.33	0.41
30:Y:3:A:C6	30:Y:4:C:N4	2.88	0.41
29:X:76:C:C2	29:X:108:G:C2	3.08	0.41
2:A:151:LYS:HD3	29:X:2186:G:H4'	2.02	0.41
29:X:66:U:H2'	29:X:67:G:H8	1.85	0.41
21:T:31:VAL:HG22	21:T:35:ASN:HB2	2.01	0.41
29:X:63:A:O2'	29:X:64:C:H5'	2.19	0.41
4:C:153:ASP:HA	4:C:158:ARG:NH2	2.35	0.41
29:X:71:A:O2'	29:X:74:G:N2	2.53	0.41
29:X:830:C:O2	29:X:1205:G:N2	2.53	0.41
29:X:2437:G:C8	29:X:2469:G:C6	3.08	0.41
29:X:2269:G:H22	29:X:2322:U:H1'	1.85	0.41
4:C:28:HIS:NE2	10:I:8:PRO:HB3	2.34	0.41
11:J:131:LYS:HD2	11:J:131:LYS:HA	1.93	0.41
10:I:120:VAL:HG23	10:I:139:ARG:O	2.20	0.41
29:X:736:G:H2'	29:X:737:C:O4'	2.20	0.41
29:X:2770:A:H4'	29:X:2771:C:O5'	2.20	0.41
29:X:656:U:C5	29:X:657:A:C4	3.08	0.41
29:X:658:G:H2'	29:X:659:G:H8	1.85	0.41
15:N:33:ARG:HD3	29:X:1265:G:N3	2.35	0.41
29:X:1298:G:N1	29:X:1342:U:OP1	2.49	0.41
5:D:125:ARG:HD2	29:X:2295:C:O4'	2.20	0.41
29:X:2639:A:H3'	29:X:2640:G:H8	1.81	0.41
29:X:2326:C:C5	29:X:2361:G:H1'	2.55	0.41
29:X:1920:A:N7	29:X:1923:U:C5	2.88	0.41
29:X:1045:G:C6	29:X:1133:G:C2	3.08	0.41
29:X:198:A:C8	29:X:243:G:C5	3.08	0.41
29:X:1407:G:C6	29:X:1408:A:N6	2.89	0.41
29:X:753:U:O4'	29:X:1964:A:C4	2.73	0.41
29:X:632:A:H2'	29:X:633:G:O4'	2.20	0.41
17:P:41:VAL:HG13	17:P:60:ILE:HG21	2.03	0.41
29:X:786:U:H2'	29:X:787:A:H5'	2.02	0.41
29:X:787:A:O2'	29:X:790:A:H1'	2.21	0.41
29:X:1987:G:C6	29:X:1988:A:C4	3.08	0.41
29:X:1302:C:H2'	29:X:1303:U:H6	1.84	0.41
15:N:74:MET:CE	15:N:79:PHE:HD1	2.33	0.41
20:S:112:LEU:O	20:S:171:VAL:HA	2.20	0.41
8:G:39:GLN:HG3	8:G:79:PHE:CE1	2.55	0.41
29:X:1526:U:H4'	29:X:1527:G:OP1	2.20	0.41
6:E:68:THR:O	6:E:72:VAL:HG23	2.21	0.41
3:B:179:GLU:O	3:B:181:LEU:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1665:C:C4	29:X:1666:G:N7	2.88	0.41
5:D:36:VAL:HG22	5:D:154:ILE:HG13	2.01	0.41
30:Y:58:G:H4'	30:Y:59:A:O4'	2.21	0.41
5:D:60:ILE:HG21	5:D:141:ILE:HG12	2.02	0.41
3:B:141:ILE:HD11	29:X:2034:A:C1'	2.50	0.41
4:C:50:GLN:O	4:C:52:SER:N	2.53	0.41
29:X:1353:A:H4'	29:X:1407:G:H1'	2.02	0.41
6:E:30:LYS:HB2	6:E:79:VAL:O	2.21	0.41
29:X:1467:U:H4'	29:X:1468:A:C4	2.54	0.41
29:X:1147:G:N2	29:X:1148:G:H1'	2.35	0.41
29:X:2010:G:C2	29:X:2020:G:C5	3.09	0.41
29:X:750:C:N3	29:X:751:G:C8	2.88	0.41
29:X:854:G:H8	29:X:854:G:O5'	2.03	0.41
29:X:2044:G:N7	29:X:2480:C:H4'	2.34	0.41
29:X:1710:U:H4'	29:X:1711:C:OP2	2.20	0.41
4:C:17:LEU:HG	4:C:109:ALA:HB2	2.02	0.41
2:A:231:HIS:ND1	2:A:249:PRO:HA	2.35	0.41
29:X:202:A:N6	29:X:203:G:N3	2.68	0.41
29:X:1135:C:H2'	29:X:1136:G:H8	1.84	0.41
22:U:67:ILE:HD13	22:U:67:ILE:HA	1.89	0.41
30:Y:117:G:H8	30:Y:117:G:O5'	2.03	0.41
29:X:2781:G:H2'	29:X:2782:G:C8	2.55	0.41
29:X:1243:G:C2	29:X:1244:U:O2	2.73	0.41
4:C:179:ASP:HA	4:C:182:ARG:HB3	2.02	0.41
29:X:841:G:C2	29:X:842:A:N6	2.89	0.41
15:N:47:TYR:CZ	15:N:51:ARG:NH2	2.88	0.41
29:X:2311:U:H4'	29:X:2315:A:H62	1.85	0.41
29:X:2332:G:C6	29:X:2344:G:N2	2.88	0.41
4:C:77:PHE:CE1	29:X:1270:C:H4'	2.55	0.41
29:X:2560:G:H22	29:X:2589:C:H2'	1.85	0.41
29:X:1261:G:O5'	29:X:1261:G:H8	2.04	0.41
29:X:1194:U:C4	29:X:1195:U:C4	3.08	0.41
29:X:2022:C:H2'	29:X:2023:C:H6	1.85	0.41
29:X:88:G:H5"	29:X:89:A:C5'	2.49	0.41
3:B:101:LYS:HA	3:B:170:LEU:O	2.20	0.41
9:H:98:ILE:HG22	9:H:99:ILE:N	2.35	0.41
2:A:260:ARG:NH2	2:A:264:LYS:HD3	2.34	0.41
17:P:57:LEU:HD13	17:P:69:ALA:HA	2.03	0.41
29:X:1440:G:C6	29:X:1441:A:C6	3.08	0.41
29:X:1917:C:O2'	29:X:1918:G:H5'	2.19	0.41
29:X:1802:A:H3'	29:X:1803:G:H8	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:982:C:H2'	29:X:983:G:O4'	2.21	0.41
17:P:21:ARG:O	17:P:23:PRO:HD3	2.20	0.41
29:X:1374:G:H2'	29:X:1375:C:H6	1.85	0.41
2:A:95:LEU:HA	2:A:95:LEU:HD23	1.85	0.41
6:E:115:ILE:HA	6:E:115:ILE:HD12	1.83	0.41
18:Q:20:MET:HG3	18:Q:25:TYR:CE1	2.55	0.41
18:Q:22:ARG:HH12	18:Q:24:VAL:HG21	1.85	0.41
5:D:100:LEU:O	5:D:103:LEU:HB3	2.20	0.41
29:X:980:G:O5'	29:X:980:G:H8	2.03	0.41
29:X:2177:U:H2'	29:X:2178:U:O4'	2.21	0.41
28:3:29:LYS:HZ3	28:3:41:ILE:HG23	1.84	0.41
5:D:83:MET:HA	5:D:84:PRO:HD3	1.86	0.41
29:X:1109:A:H8	29:X:1109:A:O5'	2.02	0.41
9:H:22:ILE:HD12	9:H:22:ILE:HA	1.92	0.41
19:R:38:LEU:HB3	19:R:47:VAL:HG23	2.03	0.41
29:X:2325:A:H4'	29:X:2326:C:OP2	2.18	0.41
23:V:48:ARG:HG2	23:V:52:GLN:HE21	1.85	0.41
2:A:170:SER:HB3	2:A:171:ASP:H	1.67	0.41
20:S:3:LEU:HG	20:S:32:PHE:HD1	1.84	0.41
18:Q:68:PHE:CD1	29:X:64:C:H1'	2.54	0.41
29:X:530:G:O2'	29:X:531:G:H5'	2.21	0.41
9:H:79:HIS:CG	9:H:80:ALA:H	2.38	0.41
2:A:209:ALA:O	2:A:212:SER:N	2.52	0.41
29:X:318:G:N2	29:X:321:A:C8	2.89	0.41
29:X:1581:C:O2'	29:X:1582:A:OP2	2.33	0.41
1:0:95:LEU:HD22	1:0:98:ARG:HD2	2.02	0.41
29:X:2487:G:H2'	29:X:2488:G:O4'	2.21	0.41
29:X:1204:G:H2'	29:X:1205:G:C8	2.55	0.41
29:X:182:G:O2'	29:X:183:U:OP2	2.37	0.41
10:I:14:LYS:O	29:X:675:C:H5'	2.20	0.41
10:I:32:ARG:HH22	29:X:684:C:P	2.43	0.41
27:2:21:ARG:O	27:2:27:GLY:HA3	2.21	0.41
29:X:184:A:H2'	29:X:185:C:O4'	2.21	0.41
6:E:160:LYS:NZ	29:X:2636:A:O3'	2.52	0.41
29:X:2359:U:H2'	29:X:2360:C:C6	2.56	0.41
17:P:19:LYS:HD2	17:P:19:LYS:N	2.35	0.41
11:J:19:THR:CG2	11:J:20:GLY:N	2.81	0.41
29:X:1666:G:C6	29:X:1992:G:O6	2.74	0.41
29:X:2604:G:H2'	29:X:2605:C:C6	2.55	0.41
29:X:1994:U:H2'	29:X:1995:G:H5'	2.01	0.41
8:G:51:LEU:HD11	8:G:127:ILE:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:119:ALA:HA	2:A:130:ALA:HB3	2.02	0.41
29:X:1935:A:N6	29:X:1936:A:N1	2.68	0.41
29:X:205:A:C2'	29:X:206:U:H5'	2.44	0.41
29:X:1066:G:H1	29:X:1115:C:N4	2.15	0.41
6:E:45:GLN:HA	6:E:50:LEU:HA	2.02	0.41
26:1:27:ASN:ND2	29:X:2264:C:OP1	2.53	0.41
1:0:28:LEU:HB3	1:0:216:PRO:HD3	2.02	0.41
30:Y:104:A:C6	30:Y:105:G:C5	3.09	0.41
13:L:28:ARG:HH21	13:L:45:ASP:HB3	1.85	0.41
2:A:231:HIS:CE1	2:A:249:PRO:HA	2.55	0.41
29:X:1513:U:C6	29:X:1593:C:H5"	2.56	0.41
29:X:2415:G:H2'	29:X:2416:U:H6	1.85	0.41
29:X:2801:A:N3	29:X:2801:A:H2'	2.36	0.41
3:B:33:ILE:HG12	3:B:36:ARG:HE	1.85	0.41
4:C:7:ILE:CG2	4:C:122:GLY:HA3	2.51	0.41
16:O:62:GLU:HG2	16:O:63:HIS:N	2.35	0.41
29:X:36:G:N3	29:X:462:G:O2'	2.53	0.41
6:E:105:MET:HB2	6:E:113:VAL:O	2.20	0.41
29:X:2320:G:H2'	29:X:2321:C:O4'	2.20	0.41
29:X:399:G:HO2'	29:X:400:U:P	2.43	0.41
29:X:2352:A:C6	29:X:2353:G:C6	3.09	0.41
29:X:1340:C:C4	29:X:1341:G:C6	3.08	0.41
29:X:315:G:C2	29:X:325:U:O2	2.74	0.41
8:G:33:ILE:HG12	29:X:547:U:O2'	2.21	0.41
5:D:125:ARG:HG2	5:D:125:ARG:H	1.50	0.41
29:X:2292:C:C2	29:X:2293:G:C8	3.09	0.41
29:X:2494:C:H2'	29:X:2495:G:C8	2.55	0.41
5:D:38:GLU:HG2	5:D:53:ALA:HB1	2.03	0.41
19:R:44:GLN:HB2	19:R:44:GLN:HE21	1.70	0.41
2:A:206:LEU:HD23	29:X:1783:G:OP1	2.21	0.41
29:X:797:A:HO2'	29:X:798:G:H8	1.66	0.41
29:X:2728:A:C5	29:X:2737:A:N6	2.89	0.41
29:X:2151:G:N2	29:X:2153:A:H3'	2.35	0.41
29:X:1656:U:O2'	29:X:2678:C:H4'	2.20	0.41
9:H:1:MET:N	9:H:46:HIS:HB3	2.35	0.41
9:H:117:GLU:O	9:H:120:ASP:HB2	2.21	0.41
29:X:1495:G:H2'	29:X:1496:G:H8	1.84	0.41
29:X:790:A:N3	29:X:791:G:C8	2.89	0.41
21:T:41:ARG:NH1	29:X:2366:U:H1'	2.35	0.41
2:A:24:LEU:CD1	2:A:84:TYR:HB2	2.50	0.41
12:K:99:ARG:HE	12:K:99:ARG:H	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:55:ARG:NH2	25:Z:58:LEU:HA	2.36	0.41
29:X:1750:A:H2'	29:X:1751:A:C8	2.55	0.41
29:X:2445:C:N3	29:X:2464:G:C2	2.89	0.41
8:G:134:MET:O	8:G:135:LEU:HG	2.20	0.41
10:I:45:LYS:H	10:I:46:GLY:HA2	1.86	0.41
29:X:623:G:N1	29:X:627:A:C6	2.88	0.41
28:3:52:LYS:HB3	28:3:53:ALA:H	1.68	0.41
29:X:1098:G:O6	29:X:1100:G:N2	2.54	0.41
20:S:62:PHE:HB3	20:S:85:MET:SD	2.60	0.41
2:A:204:ILE:HG13	2:A:204:ILE:H	1.64	0.41
29:X:23:G:C2	29:X:24:G:C8	3.09	0.41
29:X:1787:U:O2'	29:X:1788:C:H5'	2.20	0.41
26:1:37:LEU:HD12	26:1:37:LEU:HA	1.80	0.41
29:X:1716:G:O6	29:X:1754:G:H1'	2.20	0.41
29:X:2459:C:N4	29:X:2460:G:O6	2.54	0.41
17:P:90:LEU:CD1	17:P:128:VAL:HB	2.47	0.41
15:N:50:ARG:NH1	29:X:1004:A:OP1	2.42	0.41
29:X:2145:A:H5"	29:X:2155:U:H6	1.84	0.41
19:R:51:VAL:HG21	19:R:74:LEU:O	2.20	0.41
15:N:74:MET:HE1	15:N:79:PHE:HD1	1.85	0.41
17:P:37:LYS:O	17:P:40:LEU:HB2	2.20	0.41
7:F:2:ARG:NH2	7:F:30:TYR:HA	2.36	0.41
29:X:1885:C:C2	29:X:1886:G:H1'	2.56	0.41
29:X:784:U:H2'	29:X:785:U:C6	2.55	0.41
6:E:116:GLU:HA	6:E:117:PRO:HD2	1.96	0.41
29:X:140:G:H2'	29:X:141:G:C8	2.56	0.41
24:W:28:ILE:HG13	24:W:28:ILE:H	1.71	0.41
20:S:172:LEU:HA	20:S:172:LEU:HD23	1.92	0.41
29:X:2751:C:H2'	29:X:2752:C:C6	2.55	0.41
1:0:27:GLU:O	1:0:29:ALA:N	2.48	0.41
29:X:2165:A:H2'	29:X:2166:G:C8	2.55	0.41
29:X:507:A:H2'	29:X:508:G:C8	2.56	0.41
10:I:55:ARG:HB3	10:I:57:ILE:HG12	2.03	0.41
4:C:176:ASN:ND2	29:X:626:A:O2'	2.54	0.41
29:X:1203:A:N3	29:X:1203:A:H2'	2.35	0.41
29:X:1300:A:C2	29:X:1301:U:C2	3.09	0.41
29:X:698:A:C2	29:X:702:A:C5	3.09	0.41
22:U:48:LYS:HB2	22:U:48:LYS:HE2	1.85	0.41
4:C:162:ARG:HH21	29:X:333:A:P	2.44	0.41
29:X:2630:C:C2	29:X:2631:C:C5	3.09	0.41
9:H:22:ILE:CG2	9:H:52:VAL:HG12	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:33:ARG:CZ	13:L:33:ARG:HB2	2.51	0.41
12:K:80:MET:O	12:K:85:PRO:HD3	2.21	0.41
29:X:2006:G:H5'	29:X:2596:C:H4'	2.03	0.41
17:P:50:VAL:O	17:P:54:GLU:HG3	2.21	0.41
29:X:1850:G:O3'	29:X:1851:A:H8	2.04	0.41
3:B:126:PRO:O	3:B:128:SER:N	2.53	0.41
21:T:46:LYS:HB2	21:T:77:ARG:O	2.20	0.41
29:X:1453:A:H3'	29:X:1454:U:C6	2.55	0.41
29:X:2265:A:H4'	29:X:2266:A:N9	2.35	0.41
29:X:1782:A:N6	29:X:1820:G:O2'	2.54	0.41
29:X:2411:A:H2'	29:X:2412:A:O4'	2.21	0.41
29:X:1238:A:O2'	29:X:1239:A:O5'	2.35	0.41
29:X:2038:C:H3'	29:X:2038:C:H6	1.85	0.41
1:0:3:TYR:O	1:0:7:GLU:HB3	2.21	0.41
9:H:2:ILE:HB	9:H:45:ALA:HB3	2.02	0.41
2:A:186:HIS:O	2:A:188:GLU:N	2.53	0.41
29:X:71:A:H62	29:X:110:U:H5'	1.85	0.41
29:X:2230:G:OP2	29:X:2230:G:H8	2.03	0.41
29:X:1724:C:C2	29:X:1747:G:C4	3.09	0.41
29:X:2662:C:C5	29:X:2663:U:H5	2.39	0.41
29:X:1549:C:H2'	29:X:1550:C:O4'	2.21	0.41
29:X:1554:G:H2'	29:X:1555:A:H8	1.86	0.41
29:X:2457:A:H3'	29:X:2458:U:H6	1.86	0.41
29:X:1047:G:C2	29:X:1131:G:C4	3.09	0.41
29:X:184:A:C6	29:X:185:C:C2	3.09	0.41
10:I:53:ARG:CG	10:I:54:SER:H	2.34	0.41
15:N:41:ASN:HB3	15:N:45:TYR:HE2	1.86	0.41
10:I:76:LYS:HB2	10:I:76:LYS:HE3	1.93	0.41
5:D:51:ASP:O	5:D:55:LYS:HG2	2.21	0.41
3:B:31:CYS:HA	3:B:32:PRO:HD3	1.75	0.41
29:X:1967:U:H2'	29:X:1968:G:H8	1.86	0.41
11:J:17:ARG:NH2	29:X:969:U:O5'	2.54	0.41
5:D:29:PRO:HB2	5:D:169:LEU:HD13	2.03	0.41
29:X:493:A:O2'	29:X:507:A:N1	2.50	0.41
10:I:18:ARG:NH2	29:X:1262:U:C2	2.89	0.41
29:X:1059:A:H2'	29:X:1060:C:OP1	2.21	0.41
11:J:36:ILE:HG23	11:J:103:VAL:HG22	2.03	0.41
29:X:2293:G:H2'	29:X:2294:U:C6	2.56	0.41
29:X:858:G:P	29:X:858:G:H8	2.44	0.41
3:B:2:LYS:HB2	3:B:200:SER:HB3	2.03	0.41
11:J:15:ARG:HB3	11:J:16:GLY:H	1.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:66:ASN:OD1	15:N:70:ARG:HD2	2.21	0.41
29:X:1354:A:P	29:X:1410:U:H3	2.43	0.41
29:X:1330:G:C4	29:X:1331:G:C8	3.09	0.41
3:B:170:LEU:HA	3:B:170:LEU:HD23	1.48	0.41
29:X:837:U:H2'	29:X:838:A:H8	1.83	0.41
4:C:144:GLY:HA2	4:C:166:TRP:CZ2	2.55	0.41
29:X:2662:C:C4	29:X:2663:U:C5	3.09	0.41
29:X:2529:G:C6	29:X:2530:C:N4	2.89	0.41
29:X:465:C:HO2'	29:X:466:A:P	2.42	0.41
29:X:459:A:H4'	29:X:461:A:N7	2.35	0.41
29:X:2229:G:O2'	29:X:2475:C:OP1	2.36	0.41
9:H:59:ALA:HA	9:H:60:PRO:HD3	1.89	0.41
6:E:156:ALA:HB3	29:X:2509:A:H61	1.85	0.41
1:0:107:ASP:HB3	1:0:108:ALA:H	1.63	0.41
24:W:21:GLN:C	24:W:23:LEU:H	2.25	0.41
18:Q:39:LYS:NZ	18:Q:50:VAL:HG12	2.36	0.41
2:A:268:ARG:NH2	29:X:2204:A:OP1	2.54	0.41
22:U:24:ALA:C	22:U:26:ALA:H	2.25	0.41
29:X:1245:G:C2	29:X:1246:G:C8	3.09	0.40
25:Z:19:ARG:HA	29:X:2029:G:C5'	2.51	0.40
3:B:27:LEU:HD23	3:B:29:GLY:N	2.32	0.40
15:N:55:ARG:HD3	29:X:1166:A:H5"	2.04	0.40
27:2:11:LYS:NZ	29:X:699:G:OP1	2.29	0.40
2:A:158:SER:O	2:A:196:VAL:HG11	2.20	0.40
2:A:99:ASP:HB2	29:X:1506:C:O2	2.21	0.40
29:X:2033:C:N4	29:X:2034:A:C6	2.89	0.40
29:X:2197:U:H2'	29:X:2198:U:H6	1.82	0.40
14:M:106:TYR:H	14:M:106:TYR:HD2	1.67	0.40
29:X:484:G:C2	29:X:485:G:N7	2.89	0.40
29:X:1659:G:C4	29:X:1660:G:C8	3.09	0.40
14:M:56:ALA:O	14:M:66:PHE:HA	2.21	0.40
11:J:27:TYR:HA	11:J:137:VAL:HG21	2.03	0.40
3:B:8:LYS:HD3	3:B:190:GLY:O	2.21	0.40
21:T:21:LEU:HD11	21:T:41:ARG:CZ	2.50	0.40
29:X:869:C:H42	29:X:933:G:H1	1.69	0.40
29:X:611:C:O2	29:X:615:C:H4'	2.20	0.40
29:X:1903:C:O3'	29:X:1904:G:H8	2.04	0.40
28:3:4:MET:CE	29:X:679:C:H1'	2.51	0.40
16:O:43:GLU:O	16:O:45:THR:N	2.46	0.40
27:2:29:ASN:O	27:2:33:ARG:HG2	2.21	0.40
3:B:114:GLN:HB2	3:B:160:MET:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:43:VAL:HG23	8:G:163:PRO:HB2	2.02	0.40
1:0:180:ASN:HA	1:0:183:ALA:HB3	2.04	0.40
20:S:71:MET:HA	20:S:78:PRO:HA	2.03	0.40
29:X:1413:U:H2'	29:X:1414:G:H8	1.86	0.40
3:B:144:ARG:NH1	29:X:2551:A:N3	2.70	0.40
15:N:6:THR:OG1	15:N:10:ARG:NH2	2.54	0.40
29:X:815:A:H3'	29:X:816:U:H6	1.87	0.40
5:D:72:LYS:O	5:D:74:ILE:HG13	2.22	0.40
9:H:50:ILE:HG22	9:H:51:ILE:N	2.36	0.40
19:R:43:ASP:HB2	19:R:45:LYS:HG3	2.03	0.40
30:Y:3:A:H2'	30:Y:4:C:C6	2.57	0.40
14:M:106:TYR:HD1	29:X:1745:C:C4'	2.33	0.40
29:X:1255:A:C4	29:X:1256:C:C5	3.10	0.40
29:X:2590:U:O2	29:X:2590:U:H2'	2.21	0.40
29:X:1477:C:O2'	29:X:2681:A:H1'	2.21	0.40
29:X:174:A:C6	29:X:2409:A:N3	2.89	0.40
29:X:2617:G:N2	29:X:2755:A:H2'	2.36	0.40
7:F:91:PRO:HD2	29:X:1087:C:O2	2.21	0.40
29:X:193:A:C8	29:X:445:A:C6	3.08	0.40
8:G:37:ASP:N	8:G:38:GLU:OE1	2.54	0.40
2:A:53:PHE:CE1	2:A:220:HIS:HA	2.56	0.40
12:K:51:LEU:HD23	12:K:66:VAL:HG22	2.03	0.40
29:X:1534:A:H2'	29:X:1535:C:C6	2.56	0.40
29:X:2528:G:N3	29:X:2529:G:C8	2.90	0.40
2:A:24:LEU:HD13	2:A:84:TYR:HB2	2.02	0.40
29:X:2697:G:H2'	29:X:2698:G:H8	1.86	0.40
29:X:2011:U:H2'	29:X:2012:A:C8	2.56	0.40
29:X:1135:C:C4	29:X:1136:G:N7	2.89	0.40
6:E:33:LEU:HD12	6:E:33:LEU:HA	1.89	0.40
29:X:614:G:C6	29:X:636:G:C2	3.10	0.40
29:X:20:C:H2'	29:X:21:A:C8	2.57	0.40
29:X:1757:C:C2	29:X:1970:G:C2	3.09	0.40
29:X:2065:A:C2	29:X:2066:G:H1'	2.57	0.40
2:A:97:TYR:HB2	2:A:101:GLU:O	2.22	0.40
29:X:486:U:O2'	29:X:515:A:H1'	2.21	0.40
12:K:8:ARG:HB3	12:K:10:LEU:HG	2.03	0.40
29:X:1673:C:H2'	29:X:1674:C:C6	2.56	0.40
29:X:356:A:H2'	29:X:357:A:C8	2.56	0.40
5:D:80:ARG:HD3	5:D:83:MET:HB2	2.02	0.40
22:U:27:ASP:C	22:U:32:ARG:HD3	2.42	0.40
30:Y:120:G:C2	30:Y:121:G:C5	3.09	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1504:G:C6	29:X:1505:U:O4	2.75	0.40
29:X:67:G:H2'	29:X:68:C:C6	2.54	0.40
4:C:120:VAL:N	4:C:189:ASP:O	2.43	0.40
29:X:404:A:C5	29:X:424:G:C2	3.09	0.40
29:X:1326:U:H2'	29:X:1626:A:C2	2.56	0.40
2:A:229:VAL:HG13	2:A:230:ASP:OD2	2.20	0.40
7:F:63:ARG:HE	7:F:63:ARG:HB2	1.73	0.40
19:R:83:LEU:HA	19:R:83:LEU:HD23	1.92	0.40
22:U:51:ILE:O	22:U:52:ARG:HD3	2.22	0.40
9:H:11:ALA:HB3	9:H:97:VAL:HG23	2.03	0.40
17:P:59:PHE:CD1	25:Z:30:LEU:HD11	2.52	0.40
2:A:48:ARG:HE	29:X:791:G:H5"	1.86	0.40
29:X:933:G:H4'	29:X:2248:A:C6	2.56	0.40
29:X:2701:A:C2	29:X:2848:A:C4	3.10	0.40
29:X:965:G:N3	29:X:2253:A:C2	2.90	0.40
29:X:2535:C:H2'	29:X:2536:G:C8	2.56	0.40
29:X:963:G:C6	29:X:964:A:N7	2.89	0.40
29:X:2165:A:H2'	29:X:2166:G:H8	1.87	0.40
29:X:189:A:H2'	29:X:190:A:H8	1.85	0.40
3:B:155:ARG:O	3:B:156:MET:HB3	2.21	0.40
17:P:79:ALA:O	17:P:85:MET:HB2	2.21	0.40
29:X:1591:U:H2'	29:X:1592:U:C6	2.57	0.40
28:3:10:ALA:HB1	28:3:14:ILE:HG13	2.02	0.40
29:X:941:U:H2'	29:X:942:U:C6	2.57	0.40
12:K:46:PRO:HA	12:K:49:GLU:HB2	2.02	0.40
29:X:2666:U:C5	29:X:2667:C:C4	3.09	0.40
30:Y:94:G:N2	30:Y:95:U:C2	2.89	0.40
29:X:2585:C:C2'	29:X:2586:G:H5'	2.50	0.40
30:Y:35:C:H2'	30:Y:36:A:H8	1.85	0.40
12:K:78:LYS:O	12:K:82:GLU:HB2	2.20	0.40
10:I:63:ARG:HB3	28:3:25:PHE:CZ	2.56	0.40
29:X:572:G:H22	29:X:587:A:H2	1.68	0.40
29:X:66:U:H2'	29:X:67:G:C8	2.55	0.40
29:X:1272:G:H2'	29:X:1273:G:C8	2.57	0.40
29:X:2559:U:C5	29:X:2560:G:C6	3.10	0.40
29:X:746:G:C8	29:X:774:A:N6	2.89	0.40
29:X:1235:C:C2	29:X:1241:G:N2	2.89	0.40
29:X:2039:G:H2'	29:X:2039:G:N3	2.37	0.40
29:X:1079:G:H8	29:X:1079:G:OP2	2.03	0.40
29:X:836:G:O2'	29:X:837:U:H5'	2.22	0.40
8:G:98:LYS:HB3	8:G:115:ALA:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:2345:A:N6	29:X:2346:G:C2	2.89	0.40
9:H:129:LEU:HA	9:H:129:LEU:HD23	1.89	0.40
6:E:12:PRO:HG2	6:E:15:VAL:HG13	2.03	0.40
29:X:695:G:N2	29:X:809:C:C2	2.89	0.40
16:O:53:LYS:H	16:O:53:LYS:HG2	1.67	0.40
4:C:28:HIS:O	4:C:32:THR:HG23	2.21	0.40
29:X:2320:G:H2'	29:X:2321:C:C6	2.56	0.40
29:X:2863:U:N3	29:X:2864:C:C5	2.90	0.40
5:D:133:LYS:HB2	5:D:134:GLU:H	1.61	0.40
11:J:76:THR:HG22	11:J:91:VAL:HA	2.03	0.40
30:Y:12:C:H42	30:Y:113:G:H1	1.69	0.40
1:0:54:VAL:HG13	1:0:195:ALA:HB2	2.03	0.40
29:X:654:A:O2'	29:X:655:A:P	2.80	0.40
29:X:955:G:H3'	29:X:955:G:C8	2.57	0.40
29:X:1265:G:O2'	29:X:1266:G:C8	2.75	0.40
15:N:91:ASN:HD21	29:X:1007:A:H4'	1.86	0.40
15:N:92:ARG:HG2	29:X:1008:G:OP1	2.21	0.40
29:X:2302:G:C6	29:X:2303:C:C4	3.10	0.40
29:X:2309:G:N2	29:X:2365:U:C2	2.88	0.40
29:X:697:G:O2'	29:X:801:A:N7	2.46	0.40
29:X:2856:U:H2'	29:X:2857:C:H6	1.86	0.40
29:X:1080:A:H4'	29:X:1081:A:C8	2.57	0.40
29:X:2785:A:C8	29:X:2786:G:C8	3.10	0.40
29:X:1033:G:N2	29:X:1035:G:N2	2.69	0.40
29:X:1503:G:C6	29:X:1504:G:C6	3.09	0.40
29:X:32:C:H2'	29:X:33:C:C6	2.56	0.40
29:X:2225:G:C4	29:X:2226:A:C8	3.09	0.40
3:B:119:ARG:NH1	3:B:158:GLY:HA3	2.36	0.40
29:X:1359:G:C5	29:X:1360:G:N7	2.90	0.40
29:X:947:C:C2	29:X:948:C:C5	3.10	0.40
14:M:96:ARG:HA	14:M:96:ARG:HD2	1.84	0.40
1:0:18:ILE:HG12	1:0:185:TYR:HE1	1.85	0.40
29:X:2424:G:H2'	29:X:2425:G:C8	2.51	0.40
29:X:874:A:C2	29:X:875:G:H1'	2.57	0.40
29:X:2262:C:C6	29:X:2368:G:H2'	2.56	0.40
29:X:2563:U:H2'	29:X:2564:U:H6	1.85	0.40
10:I:41:SER:OG	29:X:685:U:OP2	2.33	0.40
24:W:11:GLY:HA2	29:X:980:G:O2'	2.22	0.40
9:H:105:PRO:HB2	9:H:107:GLY:H	1.87	0.40
29:X:1320:A:N6	29:X:1622:G:O2'	2.55	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	0	222/224 (99%)	139 (63%)	58 (26%)	25 (11%)	0 2
2	A	272/274 (99%)	206 (76%)	50 (18%)	16 (6%)	2 11
3	B	203/205 (99%)	152 (75%)	33 (16%)	18 (9%)	1 4
4	C	195/197 (99%)	123 (63%)	50 (26%)	22 (11%)	0 2
5	D	175/177 (99%)	117 (67%)	42 (24%)	16 (9%)	1 4
6	E	169/171 (99%)	119 (70%)	33 (20%)	17 (10%)	1 3
7	F	142/144 (99%)	100 (70%)	27 (19%)	15 (11%)	0 3
8	G	140/142 (99%)	111 (79%)	19 (14%)	10 (7%)	1 7
9	H	132/134 (98%)	96 (73%)	18 (14%)	18 (14%)	0 1
10	I	139/141 (99%)	93 (67%)	30 (22%)	16 (12%)	0 2
11	J	134/136 (98%)	97 (72%)	28 (21%)	9 (7%)	1 8
12	K	111/113 (98%)	81 (73%)	18 (16%)	12 (11%)	0 2
13	L	102/104 (98%)	68 (67%)	18 (18%)	16 (16%)	0 1
14	M	107/109 (98%)	83 (78%)	14 (13%)	10 (9%)	1 4
15	N	115/117 (98%)	90 (78%)	19 (16%)	6 (5%)	2 15
16	O	92/94 (98%)	69 (75%)	13 (14%)	10 (11%)	0 2
17	P	125/127 (98%)	102 (82%)	17 (14%)	6 (5%)	3 17
18	Q	91/93 (98%)	67 (74%)	16 (18%)	8 (9%)	1 4
19	R	108/110 (98%)	63 (58%)	28 (26%)	17 (16%)	0 1
20	S	173/175 (99%)	123 (71%)	32 (18%)	18 (10%)	1 3
21	T	82/84 (98%)	68 (83%)	8 (10%)	6 (7%)	1 6
22	U	70/72 (97%)	39 (56%)	15 (21%)	16 (23%)	0 0
23	V	64/66 (97%)	54 (84%)	9 (14%)	1 (2%)	12 48
24	W	53/55 (96%)	36 (68%)	13 (24%)	4 (8%)	1 6
25	Z	55/57 (96%)	36 (66%)	13 (24%)	6 (11%)	0 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
26	1	52/54 (96%)	31 (60%)	13 (25%)	8 (15%)	0 1
27	2	45/47 (96%)	38 (84%)	6 (13%)	1 (2%)	8 38
28	3	63/65 (97%)	38 (60%)	17 (27%)	8 (13%)	0 1
All	All	3431/3487 (98%)	2439 (71%)	657 (19%)	335 (10%)	1 3

All (335) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	17	SER
1	0	61	PRO
1	0	157	ILE
1	0	216	PRO
2	A	25	ALA
2	A	111	LEU
2	A	202	LYS
3	B	34	VAL
3	B	85	ALA
3	B	86	PRO
3	B	117	MET
3	B	123	ALA
3	B	133	LYS
3	B	180	ASN
4	C	9	GLN
4	C	20	PRO
4	C	51	VAL
4	C	52	SER
4	C	54	THR
4	C	97	ARG
4	C	126	ALA
4	C	172	VAL
4	C	174	GLY
5	D	40	LEU
5	D	134	GLU
6	E	24	PHE
6	E	42	THR
6	E	55	PRO
6	E	58	ALA
6	E	65	HIS
6	E	112	PRO
6	E	126	PRO
6	E	165	VAL

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Mol	Chain	Res	Type
7	F	23	VAL
7	F	50	ASP
7	F	74	MET
7	F	116	ASN
8	G	37	ASP
8	G	66	HIS
8	G	110	LEU
9	H	5	GLN
9	H	29	ILE
9	H	41	ASN
9	H	47	VAL
9	H	61	ARG
9	H	84	ALA
9	H	116	ARG
10	I	29	THR
10	I	78	SER
10	I	82	ASP
10	I	110	ALA
10	I	111	SER
11	J	21	ASP
11	J	23	LYS
11	J	135	ARG
12	K	4	GLY
12	K	11	ASN
12	K	13	ASN
12	K	20	LEU
12	K	32	GLY
12	K	88	ALA
12	K	100	VAL
13	L	10	LYS
13	L	21	THR
13	L	33	ARG
13	L	45	ASP
13	L	53	ALA
14	M	25	PRO
14	M	43	ASN
14	M	83	PHE
15	N	5	LYS
15	N	7	GLY
15	N	27	SER
16	O	24	SER
16	O	29	ALA

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Mol	Chain	Res	Type
17	P	49	SER
17	P	50	VAL
17	P	81	HIS
17	P	82	ASN
17	P	87	GLU
19	R	11	ASN
19	R	51	VAL
19	R	58	VAL
19	R	60	PRO
19	R	78	ALA
19	R	93	ARG
19	R	110	SER
20	S	91	PRO
20	S	124	ALA
20	S	169	VAL
21	T	30	VAL
21	T	64	ASP
21	T	74	LYS
22	U	14	VAL
22	U	15	VAL
22	U	18	VAL
22	U	25	ARG
22	U	55	GLY
22	U	60	VAL
22	U	76	LYS
24	W	36	ASP
24	W	38	PRO
25	Z	34	PRO
26	1	40	TYR
26	1	44	ALA
28	3	53	ALA
1	0	62	HIS
1	0	87	ALA
1	0	100	ALA
1	0	108	ALA
1	0	137	LYS
2	A	41	GLY
2	A	125	PRO
2	A	169	GLU
2	A	239	ARG
3	B	60	ASN
3	B	71	GLY

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Mol	Chain	Res	Type
3	B	118	LYS
4	C	11	GLY
4	C	22	VAL
4	C	37	SER
4	C	43	ALA
4	C	56	ARG
4	C	75	PRO
4	C	178	TYR
5	D	33	LYS
5	D	42	SER
5	D	122	PHE
5	D	132	ILE
5	D	133	LYS
6	E	18	ASN
6	E	100	GLY
6	E	173	ALA
7	F	14	ALA
7	F	22	PRO
7	F	82	ALA
8	G	38	GLU
8	G	77	GLY
8	G	94	LYS
9	H	4	PRO
9	H	22	ILE
9	H	42	LYS
9	H	66	ALA
9	H	69	VAL
9	H	79	HIS
10	I	41	SER
10	I	44	GLY
10	I	57	ILE
10	I	86	THR
10	I	99	VAL
11	J	13	GLN
11	J	26	ASP
11	J	98	VAL
12	K	40	LYS
12	K	103	ARG
13	L	20	THR
13	L	55	SER
13	L	56	SER
13	L	59	LEU

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Mol	Chain	Res	Type
13	L	61	SER
13	L	93	SER
13	L	96	TYR
14	M	16	ILE
14	M	17	GLU
14	M	26	ASP
16	O	16	GLU
18	Q	3	HIS
18	Q	59	PRO
18	Q	61	LYS
18	Q	67	ARG
19	R	25	LEU
19	R	79	SER
20	S	26	LYS
22	U	10	LYS
22	U	29	GLY
22	U	32	ARG
22	U	63	SER
25	Z	36	CYS
26	1	30	ASN
28	3	12	ARG
28	3	34	THR
28	3	51	ALA
1	0	28	LEU
1	0	33	PHE
1	0	45	ILE
1	0	102	GLY
1	0	146	ALA
1	0	203	VAL
2	A	187	SER
2	A	198	ASN
2	A	241	GLY
2	A	246	PRO
3	B	17	ASN
3	B	127	ALA
3	B	155	ARG
4	C	83	ALA
4	C	171	PRO
5	D	71	LYS
5	D	80	ARG
6	E	7	GLN
6	E	41	LEU

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Mol	Chain	Res	Type
6	E	172	LYS
7	F	47	ASP
8	G	65	LYS
8	G	113	GLU
9	H	28	GLY
9	H	71	LYS
10	I	65	PHE
10	I	68	VAL
10	I	81	GLN
11	J	11	ARG
12	K	56	LYS
13	L	26	LYS
14	M	46	ARG
14	M	47	SER
15	N	73	GLY
15	N	103	PRO
16	O	45	THR
18	Q	8	GLN
19	R	20	ASP
19	R	87	GLU
20	S	7	PRO
20	S	14	LEU
20	S	51	LEU
20	S	58	GLY
20	S	63	PRO
20	S	94	VAL
20	S	156	GLU
21	T	83	ALA
22	U	17	SER
22	U	27	ASP
22	U	47	HIS
24	W	17	VAL
24	W	22	ALA
25	Z	21	SER
26	1	28	ARG
26	1	46	HIS
26	1	48	VAL
27	2	17	GLY
28	3	46	LYS
1	0	6	LEU
1	0	139	GLY
1	0	158	GLU

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Mol	Chain	Res	Type
1	0	197	PRO
2	A	45	ASN
3	B	66	HIS
3	B	73	ALA
3	B	144	ARG
3	B	154	LYS
4	C	90	SER
5	D	20	PHE
5	D	35	VAL
5	D	77	PHE
7	F	19	PRO
7	F	25	PRO
7	F	70	LYS
7	F	83	GLY
8	G	140	GLN
10	I	116	ARG
12	K	102	THR
13	L	68	ALA
13	L	97	HIS
14	M	74	GLY
16	O	20	ILE
16	O	40	VAL
16	O	44	GLN
18	Q	84	GLU
19	R	52	ASN
19	R	64	ASN
19	R	102	LYS
20	S	37	LYS
20	S	57	GLU
20	S	88	TYR
20	S	122	ILE
20	S	128	ARG
21	T	8	GLY
23	V	3	PRO
25	Z	24	ALA
2	A	228	PRO
3	B	131	SER
4	C	15	ILE
4	C	27	LEU
4	C	41	GLY
5	D	29	PRO
5	D	44	LYS

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Mol	Chain	Res	Type
6	E	23	VAL
7	F	113	PRO
9	H	70	VAL
9	H	124	MET
11	J	81	GLU
11	J	133	VAL
12	K	57	GLY
16	O	31	ASP
19	R	65	PRO
25	Z	4	HIS
25	Z	20	ARG
26	1	51	ALA
28	3	63	PRO
1	0	67	SER
1	0	120	GLY
2	A	201	HIS
5	D	21	GLY
5	D	113	ASP
6	E	92	VAL
8	G	165	VAL
13	L	84	ILE
16	O	60	VAL
19	R	31	GLY
19	R	100	ASP
20	S	35	ASP
22	U	12	ASN
22	U	41	VAL
1	0	89	VAL
2	A	165	VAL
7	F	52	ILE
10	I	24	GLY
14	M	7	ILE
15	N	88	ILE
20	S	125	PRO
26	1	43	VAL
16	O	17	GLY
18	Q	9	ALA
18	Q	29	VAL
21	T	31	VAL
28	3	16	ILE
1	0	86	GLY
1	0	165	GLY

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Mol	Chain	Res	Type
2	A	229	VAL
9	H	40	GLY
17	P	35	PRO
10	I	10	PRO
28	3	28	GLY
1	0	91	GLY
6	E	76	VAL
7	F	96	VAL

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	0	167/167 (100%)	150 (90%)	17 (10%)	9 33
2	A	214/214 (100%)	177 (83%)	37 (17%)	2 12
3	B	155/155 (100%)	123 (79%)	32 (21%)	1 7
4	C	157/157 (100%)	117 (74%)	40 (26%)	1 3
5	D	153/153 (100%)	126 (82%)	27 (18%)	2 12
6	E	136/136 (100%)	111 (82%)	25 (18%)	2 10
7	F	107/107 (100%)	94 (88%)	13 (12%)	6 25
8	G	118/118 (100%)	97 (82%)	21 (18%)	2 11
9	H	103/103 (100%)	73 (71%)	30 (29%)	0 2
10	I	108/108 (100%)	88 (82%)	20 (18%)	2 10
11	J	110/110 (100%)	82 (74%)	28 (26%)	1 3
12	K	90/90 (100%)	68 (76%)	22 (24%)	1 4
13	L	74/74 (100%)	46 (62%)	28 (38%)	0 1
14	M	92/92 (100%)	58 (63%)	34 (37%)	0 1
15	N	96/96 (100%)	82 (85%)	14 (15%)	4 18
16	O	75/75 (100%)	59 (79%)	16 (21%)	1 6
17	P	109/109 (100%)	85 (78%)	24 (22%)	1 6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
18	Q	75/75 (100%)	57 (76%)	18 (24%)	1 4
19	R	91/91 (100%)	71 (78%)	20 (22%)	1 6
20	S	149/149 (100%)	119 (80%)	30 (20%)	1 8
21	T	62/62 (100%)	42 (68%)	20 (32%)	0 1
22	U	57/57 (100%)	38 (67%)	19 (33%)	0 1
23	V	54/54 (100%)	45 (83%)	9 (17%)	3 13
24	W	48/48 (100%)	38 (79%)	10 (21%)	1 7
25	Z	51/51 (100%)	43 (84%)	8 (16%)	3 15
26	1	38/38 (100%)	33 (87%)	5 (13%)	5 22
27	2	40/40 (100%)	32 (80%)	8 (20%)	1 8
28	3	51/51 (100%)	34 (67%)	17 (33%)	0 1
All	All	2780/2780 (100%)	2188 (79%)	592 (21%)	1 6

All (592) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	16	TYR
1	0	24	LEU
1	0	26	LYS
1	0	38	GLU
1	0	64	THR
1	0	70	VAL
1	0	95	LEU
1	0	110	VAL
1	0	112	THR
1	0	114	ASP
1	0	121	GLN
1	0	137	LYS
1	0	152	LEU
1	0	157	ILE
1	0	166	VAL
1	0	168	HIS
1	0	212	THR
2	A	7	LYS
2	A	10	THR
2	A	13	ARG
2	A	21	PHE
2	A	35	GLU

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Mol	Chain	Res	Type
2	A	40	THR
2	A	49	ILE
2	A	59	LYS
2	A	63	ARG
2	A	66	ASP
2	A	68	LYS
2	A	70	ARG
2	A	82	ILE
2	A	88	ARG
2	A	91	ARG
2	A	96	HIS
2	A	113	VAL
2	A	116	THR
2	A	117	VAL
2	A	118	ASN
2	A	138	VAL
2	A	142	VAL
2	A	145	LEU
2	A	148	VAL
2	A	163	VAL
2	A	165	VAL
2	A	169	GLU
2	A	190	TYR
2	A	204	ILE
2	A	239	ARG
2	A	246	PRO
2	A	247	VAL
2	A	252	LYS
2	A	270	LEU
2	A	271	VAL
2	A	273	ARG
2	A	274	ARG
3	B	11	MET
3	B	12	THR
3	B	14	ILE
3	B	19	ARG
3	B	38	THR
3	B	40	GLN
3	B	41	THR
3	B	49	ILE
3	B	66	HIS
3	B	72	VAL

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Mol	Chain	Res	Type
3	B	76	ARG
3	B	79	ARG
3	B	84	PHE
3	B	87	ASP
3	B	90	SER
3	B	92	ASN
3	B	93	VAL
3	B	94	ASP
3	B	116	VAL
3	B	117	MET
3	B	126	PRO
3	B	132	LYS
3	B	136	ARG
3	B	141	ILE
3	B	145	LYS
3	B	152	LYS
3	B	167	VAL
3	B	176	ARG
3	B	182	ILE
3	B	192	ASN
3	B	199	ARG
3	B	200	SER
4	C	7	ILE
4	C	10	ASN
4	C	13	ARG
4	C	16	GLU
4	C	21	GLU
4	C	22	VAL
4	C	28	HIS
4	C	31	VAL
4	C	37	SER
4	C	38	ARG
4	C	42	THR
4	C	47	THR
4	C	50	GLN
4	C	51	VAL
4	C	52	SER
4	C	59	TYR
4	C	68	ARG
4	C	76	THR
4	C	87	LYS
4	C	92	ASP

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Mol	Chain	Res	Type
4	C	97	ARG
4	C	98	GLN
4	C	99	VAL
4	C	106	MET
4	C	112	GLN
4	C	113	GLU
4	C	121	ASP
4	C	124	ASP
4	C	131	LYS
4	C	140	ASN
4	C	143	ASP
4	C	150	LEU
4	C	153	ASP
4	C	155	GLU
4	C	162	ARG
4	C	163	ASN
4	C	167	VAL
4	C	169	VAL
4	C	172	VAL
4	C	181	LEU
5	D	9	ASN
5	D	25	VAL
5	D	46	ASP
5	D	61	THR
5	D	66	ILE
5	D	68	THR
5	D	72	LYS
5	D	80	ARG
5	D	85	VAL
5	D	89	VAL
5	D	92	ARG
5	D	106	ILE
5	D	115	ARG
5	D	117	ILE
5	D	123	ASP
5	D	125	ARG
5	D	127	ASN
5	D	128	TYR
5	D	136	LEU
5	D	142	THR
5	D	143	TYR
5	D	147	ASP

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Mol	Chain	Res	Type
5	D	148	LYS
5	D	150	ARG
5	D	156	ILE
5	D	158	THR
5	D	159	THR
6	E	6	LYS
6	E	11	VAL
6	E	20	GLN
6	E	33	LEU
6	E	35	VAL
6	E	38	ASN
6	E	40	GLU
6	E	41	LEU
6	E	42	THR
6	E	43	VAL
6	E	44	ARG
6	E	48	ASP
6	E	61	HIS
6	E	67	LEU
6	E	69	ARG
6	E	84	THR
6	E	109	TYR
6	E	111	HIS
6	E	115	ILE
6	E	121	VAL
6	E	122	THR
6	E	134	SER
6	E	140	LEU
6	E	152	ARG
6	E	165	VAL
7	F	2	ARG
7	F	10	LEU
7	F	23	VAL
7	F	33	ASN
7	F	59	ILE
7	F	63	ARG
7	F	84	ILE
7	F	99	LEU
7	F	102	ASP
7	F	112	MET
7	F	121	GLU
7	F	134	MET

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Mol	Chain	Res	Type
7	F	137	THR
8	G	31	THR
8	G	38	GLU
8	G	40	ASN
8	G	42	VAL
8	G	53	ARG
8	G	54	LEU
8	G	65	LYS
8	G	73	ASN
8	G	82	VAL
8	G	83	ILE
8	G	99	VAL
8	G	101	THR
8	G	102	ARG
8	G	114	THR
8	G	140	GLN
8	G	150	VAL
8	G	154	GLU
8	G	155	THR
8	G	156	HIS
8	G	159	SER
8	G	167	LYS
9	H	3	MET
9	H	8	LEU
9	H	9	ASP
9	H	10	VAL
9	H	18	GLU
9	H	19	ILE
9	H	35	THR
9	H	36	THR
9	H	41	ASN
9	H	43	ARG
9	H	46	HIS
9	H	51	ILE
9	H	57	ASP
9	H	65	LYS
9	H	73	VAL
9	H	74	VAL
9	H	78	SER
9	H	82	LYS
9	H	83	ARG
9	H	89	ILE

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Mol	Chain	Res	Type
9	H	90	ARG
9	H	93	ARG
9	H	104	GLU
9	H	109	ARG
9	H	117	GLU
9	H	121	ARG
9	H	122	ARG
9	H	124	MET
9	H	126	ILE
9	H	127	VAL
10	I	4	HIS
10	I	6	LEU
10	I	18	ARG
10	I	19	VAL
10	I	28	LYS
10	I	45	LYS
10	I	48	PHE
10	I	53	ARG
10	I	65	PHE
10	I	74	VAL
10	I	81	GLN
10	I	82	ASP
10	I	91	ASP
10	I	96	TYR
10	I	99	VAL
10	I	109	LEU
10	I	120	VAL
10	I	121	HIS
10	I	133	VAL
10	I	142	LEU
11	J	11	ARG
11	J	12	LYS
11	J	15	ARG
11	J	17	ARG
11	J	26	ASP
11	J	27	TYR
11	J	35	LEU
11	J	45	SER
11	J	47	GLN
11	J	48	ILE
11	J	49	GLU
11	J	52	ARG

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Mol	Chain	Res	Type
11	J	60	ARG
11	J	64	LYS
11	J	68	ARG
11	J	72	ASP
11	J	73	LYS
11	J	82	THR
11	J	84	MET
11	J	93	TYR
11	J	102	ARG
11	J	106	GLU
11	J	130	THR
11	J	132	MET
11	J	133	VAL
11	J	137	VAL
11	J	139	ASP
11	J	140	GLU
12	K	11	ASN
12	K	14	SER
12	K	20	LEU
12	K	26	THR
12	K	33	ARG
12	K	35	GLN
12	K	36	THR
12	K	51	LEU
12	K	52	ILE
12	K	53	THR
12	K	59	ASP
12	K	64	ARG
12	K	65	LEU
12	K	73	LYS
12	K	75	VAL
12	K	83	VAL
12	K	89	GLU
12	K	94	TYR
12	K	95	THR
12	K	99	ARG
12	K	113	ILE
12	K	114	GLU
13	L	11	LEU
13	L	12	ARG
13	L	13	THR
13	L	15	ARG

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Mol	Chain	Res	Type
13	L	17	VAL
13	L	20	THR
13	L	24	SER
13	L	29	LEU
13	L	31	VAL
13	L	33	ARG
13	L	35	SER
13	L	36	LYS
13	L	37	HIS
13	L	38	ILE
13	L	39	TYR
13	L	43	ILE
13	L	60	LYS
13	L	66	ASP
13	L	71	VAL
13	L	82	LYS
13	L	85	LYS
13	L	91	ARG
13	L	93	SER
13	L	95	LYS
13	L	97	HIS
13	L	99	ARG
13	L	108	ARG
13	L	109	GLU
14	M	2	GLN
14	M	9	ARG
14	M	12	LEU
14	M	13	LEU
14	M	14	ARG
14	M	19	ASP
14	M	21	THR
14	M	22	ARG
14	M	23	GLN
14	M	28	ARG
14	M	29	PRO
14	M	32	THR
14	M	37	THR
14	M	40	ARG
14	M	44	ARG
14	M	51	GLU
14	M	54	VAL
14	M	57	ILE

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Mol	Chain	Res	Type
14	M	60	SER
14	M	62	SER
14	M	63	ARG
14	M	68	VAL
14	M	69	ARG
14	M	70	LYS
14	M	72	SER
14	M	77	VAL
14	M	78	GLU
14	M	91	VAL
14	M	95	GLU
14	M	96	ARG
14	M	99	VAL
14	M	101	ARG
14	M	103	LYS
14	M	106	TYR
15	N	5	LYS
15	N	9	VAL
15	N	17	VAL
15	N	34	ASN
15	N	36	PHE
15	N	51	ARG
15	N	63	GLN
15	N	77	SER
15	N	80	ILE
15	N	85	ARG
15	N	93	LYS
15	N	102	GLU
15	N	113	SER
15	N	118	GLN
16	O	7	THR
16	O	10	LYS
16	O	11	GLN
16	O	14	VAL
16	O	18	ASP
16	O	31	ASP
16	O	32	LYS
16	O	35	LEU
16	O	38	LEU
16	O	47	PHE
16	O	55	THR
16	O	65	ARG

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Mol	Chain	Res	Type
16	O	69	ILE
16	O	72	ARG
16	O	78	VAL
16	O	83	ARG
17	P	16	GLN
17	P	17	GLN
17	P	21	ARG
17	P	25	PHE
17	P	31	VAL
17	P	36	ARG
17	P	40	LEU
17	P	41	VAL
17	P	42	VAL
17	P	50	VAL
17	P	63	SER
17	P	66	GLU
17	P	84	GLU
17	P	88	ASP
17	P	91	PHE
17	P	96	TYR
17	P	98	ASP
17	P	103	LEU
17	P	105	ARG
17	P	109	ARG
17	P	115	ASN
17	P	117	ILE
17	P	124	ILE
17	P	126	ILE
18	Q	5	ASP
18	Q	6	ILE
18	Q	26	SER
18	Q	27	PHE
18	Q	30	SER
18	Q	40	ASP
18	Q	48	VAL
18	Q	57	ASN
18	Q	64	ARG
18	Q	65	VAL
18	Q	67	ARG
18	Q	75	ARG
18	Q	80	VAL
18	Q	81	ARG

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Mol	Chain	Res	Type
18	Q	82	LEU
18	Q	84	GLU
18	Q	88	ILE
18	Q	91	LEU
19	R	9	HIS
19	R	22	VAL
19	R	23	ILE
19	R	32	GLN
19	R	43	ASP
19	R	44	GLN
19	R	46	VAL
19	R	48	VAL
19	R	51	VAL
19	R	53	VAL
19	R	56	LYS
19	R	57	ASN
19	R	66	GLN
19	R	73	GLU
19	R	74	LEU
19	R	80	LYS
19	R	84	VAL
19	R	90	LYS
19	R	104	VAL
19	R	106	VAL
20	S	3	LEU
20	S	13	LYS
20	S	15	ASP
20	S	18	MET
20	S	22	VAL
20	S	24	TYR
20	S	26	LYS
20	S	35	ASP
20	S	37	LYS
20	S	48	THR
20	S	55	THR
20	S	57	GLU
20	S	70	GLN
20	S	72	ASP
20	S	73	LYS
20	S	87	THR
20	S	95	SER
20	S	96	VAL

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Mol	Chain	Res	Type
20	S	99	HIS
20	S	100	THR
20	S	108	VAL
20	S	109	GLN
20	S	112	LEU
20	S	120	LEU
20	S	128	ARG
20	S	139	THR
20	S	151	ASP
20	S	156	GLU
20	S	159	THR
20	S	166	LEU
21	T	4	LYS
21	T	5	LYS
21	T	7	VAL
21	T	10	SER
21	T	11	LYS
21	T	12	ASN
21	T	19	LYS
21	T	21	LEU
21	T	29	GLU
21	T	37	LEU
21	T	41	ARG
21	T	43	THR
21	T	49	GLN
21	T	62	LEU
21	T	64	ASP
21	T	70	ILE
21	T	77	ARG
21	T	79	ILE
21	T	81	ILE
21	T	82	GLU
22	U	8	THR
22	U	10	LYS
22	U	12	ASN
22	U	14	VAL
22	U	15	VAL
22	U	19	ILE
22	U	20	ARG
22	U	21	ARG
22	U	23	LYS
22	U	32	ARG

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Mol	Chain	Res	Type
22	U	33	LYS
22	U	37	ILE
22	U	40	ARG
22	U	49	LYS
22	U	57	VAL
22	U	63	SER
22	U	67	ILE
22	U	69	THR
22	U	76	LYS
23	V	12	THR
23	V	16	LYS
23	V	21	ARG
23	V	25	LEU
23	V	26	MET
23	V	46	LEU
23	V	53	LEU
23	V	55	THR
23	V	63	LYS
24	W	3	ILE
24	W	6	VAL
24	W	10	ILE
24	W	26	ARG
24	W	34	VAL
24	W	37	THR
24	W	46	THR
24	W	51	LEU
24	W	52	GLU
24	W	53	VAL
25	Z	9	LYS
25	Z	25	LEU
25	Z	26	THR
25	Z	34	PRO
25	Z	44	HIS
25	Z	48	ASN
25	Z	52	TYR
25	Z	57	VAL
26	1	10	VAL
26	1	15	SER
26	1	24	THR
26	1	37	LEU
26	1	46	HIS
27	2	4	THR

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Mol	Chain	Res	Type
27	2	12	ARG
27	2	21	ARG
27	2	24	THR
27	2	26	SER
27	2	28	ARG
27	2	29	ASN
27	2	42	LEU
28	3	7	HIS
28	3	9	MET
28	3	13	ARG
28	3	14	ILE
28	3	19	THR
28	3	21	LYS
28	3	22	VAL
28	3	26	LYS
28	3	29	LYS
28	3	30	ARG
28	3	31	HIS
28	3	34	THR
28	3	39	ASP
28	3	46	LYS
28	3	55	TRP
28	3	62	LEU
28	3	64	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	186	GLN
2	A	129	ASN
2	A	227	ASN
3	B	60	ASN
3	B	192	ASN
4	C	132	ASN
6	E	139	GLN
7	F	11	GLN
13	L	37	HIS
14	M	48	GLN
15	N	37	GLN
16	O	57	GLN
20	S	109	GLN
23	V	52	GLN

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Mol	Chain	Res	Type
26	1	30	ASN
26	1	46	HIS
28	3	7	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
29	X	2776/2881 (96%)	839 (30%)	30 (1%)
30	Y	121/122 (99%)	35 (28%)	1 (0%)
All	All	2897/3003 (96%)	874 (30%)	31 (1%)

All (874) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
29	X	8	A
29	X	13	A
29	X	15	G
29	X	54	G
29	X	63	A
29	X	66	U
29	X	70	A
29	X	73	A
29	X	74	G
29	X	75	C
29	X	88	G
29	X	89	A
29	X	90	G
29	X	91	A
29	X	92	U
29	X	100	G
29	X	101	A
29	X	102	C
29	X	107	G
29	X	116	A
29	X	117	A
29	X	118	U
29	X	120	G
29	X	123	A
29	X	129	A
29	X	135	U
29	X	136	A

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Mol	Chain	Res	Type
29	X	138	G
29	X	144	U
29	X	147	G
29	X	158	A
29	X	159	A
29	X	170	U
29	X	173	A
29	X	175	C
29	X	176	A
29	X	177	U
29	X	180	C
29	X	181	A
29	X	182	G
29	X	192	G
29	X	193	A
29	X	199	A
29	X	200	A
29	X	201	G
29	X	202	A
29	X	203	G
29	X	205	A
29	X	206	U
29	X	207	U
29	X	209	G
29	X	218	A
29	X	219	G
29	X	221	A
29	X	222	G
29	X	225	G
29	X	226	C
29	X	227	G
29	X	228	A
29	X	229	G
29	X	238	G
29	X	243	G
29	X	245	C
29	X	248	A
29	X	305	A
29	X	308	C
29	X	309	G
29	X	310	A
29	X	321	A

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Mol	Chain	Res	Type
29	X	322	A
29	X	323	G
29	X	324	C
29	X	335	A
29	X	340	G
29	X	341	A
29	X	342	G
29	X	343	A
29	X	346	C
29	X	354	C
29	X	356	A
29	X	357	A
29	X	361	G
29	X	396	U
29	X	397	U
29	X	399	G
29	X	400	U
29	X	403	A
29	X	404	A
29	X	408	U
29	X	409	G
29	X	412	U
29	X	413	G
29	X	414	A
29	X	415	A
29	X	418	C
29	X	424	G
29	X	425	A
29	X	453	U
29	X	455	A
29	X	458	G
29	X	459	A
29	X	463	C
29	X	466	A
29	X	467	U
29	X	469	G
29	X	475	U
29	X	476	G
29	X	478	G
29	X	479	G
29	X	481	A
29	X	483	A

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Mol	Chain	Res	Type
29	X	486	U
29	X	492	G
29	X	494	A
29	X	500	G
29	X	504	G
29	X	506	G
29	X	511	A
29	X	512	A
29	X	514	G
29	X	515	A
29	X	516	G
29	X	518	A
29	X	519	C
29	X	520	C
29	X	521	U
29	X	532	A
29	X	534	U
29	X	539	A
29	X	540	G
29	X	541	C
29	X	542	A
29	X	543	G
29	X	545	C
29	X	554	U
29	X	555	U
29	X	556	A
29	X	557	U
29	X	558	G
29	X	559	C
29	X	560	G
29	X	564	U
29	X	569	C
29	X	571	U
29	X	572	G
29	X	580	A
29	X	582	G
29	X	583	C
29	X	584	A
29	X	587	A
29	X	591	G
29	X	594	G
29	X	595	A

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Mol	Chain	Res	Type
29	X	601	A
29	X	602	C
29	X	604	U
29	X	609	U
29	X	610	G
29	X	611	C
29	X	613	A
29	X	616	U
29	X	620	G
29	X	624	A
29	X	625	A
29	X	626	A
29	X	627	A
29	X	628	A
29	X	631	G
29	X	633	G
29	X	637	G
29	X	638	A
29	X	645	G
29	X	648	A
29	X	655	A
29	X	656	U
29	X	657	A
29	X	663	G
29	X	664	C
29	X	666	U
29	X	668	A
29	X	672	C
29	X	673	G
29	X	682	G
29	X	683	A
29	X	689	A
29	X	695	G
29	X	699	G
29	X	712	A
29	X	714	G
29	X	727	U
29	X	728	G
29	X	729	A
29	X	730	C
29	X	731	A
29	X	732	G

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Mol	Chain	Res	Type
29	X	739	G
29	X	740	A
29	X	741	G
29	X	743	A
29	X	754	G
29	X	758	G
29	X	760	U
29	X	765	C
29	X	773	G
29	X	776	G
29	X	778	G
29	X	787	A
29	X	789	G
29	X	790	A
29	X	795	A
29	X	797	A
29	X	798	G
29	X	805	G
29	X	807	A
29	X	815	A
29	X	816	U
29	X	818	G
29	X	821	A
29	X	824	U
29	X	825	C
29	X	831	G
29	X	832	A
29	X	834	A
29	X	836	G
29	X	838	A
29	X	840	U
29	X	841	G
29	X	848	A
29	X	851	C
29	X	852	U
29	X	857	U
29	X	858	G
29	X	859	U
29	X	869	C
29	X	872	G
29	X	879	A
29	X	880	C

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Mol	Chain	Res	Type
29	X	912	A
29	X	914	C
29	X	922	A
29	X	924	C
29	X	926	C
29	X	927	C
29	X	931	G
29	X	937	C
29	X	939	C
29	X	940	G
29	X	943	U
29	X	946	U
29	X	947	C
29	X	950	G
29	X	955	G
29	X	956	A
29	X	957	G
29	X	964	A
29	X	967	G
29	X	969	U
29	X	972	C
29	X	975	C
29	X	976	C
29	X	982	C
29	X	984	A
29	X	985	G
29	X	992	A
29	X	994	A
29	X	1001	A
29	X	1005	U
29	X	1007	A
29	X	1013	G
29	X	1015	U
29	X	1016	C
29	X	1017	C
29	X	1018	C
29	X	1020	A
29	X	1022	A
29	X	1023	U
29	X	1024	G
29	X	1028	G
29	X	1029	C

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Mol	Chain	Res	Type
29	X	1033	G
29	X	1034	U
29	X	1036	G
29	X	1037	U
29	X	1044	U
29	X	1047	G
29	X	1055	A
29	X	1056	U
29	X	1058	G
29	X	1059	A
29	X	1060	C
29	X	1061	A
29	X	1066	G
29	X	1068	A
29	X	1069	G
29	X	1071	U
29	X	1072	U
29	X	1079	G
29	X	1080	A
29	X	1081	A
29	X	1082	G
29	X	1084	A
29	X	1086	C
29	X	1089	C
29	X	1096	A
29	X	1097	A
29	X	1098	G
29	X	1099	A
29	X	1100	G
29	X	1101	U
29	X	1102	G
29	X	1104	G
29	X	1107	A
29	X	1108	U
29	X	1111	C
29	X	1112	U
29	X	1113	C
29	X	1114	A
29	X	1119	U
29	X	1120	C
29	X	1121	G
29	X	1122	A

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Mol	Chain	Res	Type
29	X	1123	G
29	X	1124	U
29	X	1128	G
29	X	1137	A
29	X	1138	A
29	X	1139	A
29	X	1140	A
29	X	1141	U
29	X	1142	G
29	X	1143	A
29	X	1145	C
29	X	1146	G
29	X	1149	G
29	X	1151	U
29	X	1152	C
29	X	1153	A
29	X	1154	A
29	X	1158	A
29	X	1162	A
29	X	1165	G
29	X	1166	A
29	X	1168	G
29	X	1178	C
29	X	1179	A
29	X	1185	C
29	X	1187	A
29	X	1189	G
29	X	1195	U
29	X	1199	U
29	X	1200	G
29	X	1209	G
29	X	1218	C
29	X	1220	G
29	X	1223	G
29	X	1225	G
29	X	1226	A
29	X	1233	A
29	X	1235	C
29	X	1236	G
29	X	1238	A
29	X	1240	G
29	X	1246	G

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Mol	Chain	Res	Type
29	X	1247	U
29	X	1250	A
29	X	1255	A
29	X	1256	C
29	X	1261	G
29	X	1266	G
29	X	1269	G
29	X	1271	C
29	X	1275	A
29	X	1277	G
29	X	1280	U
29	X	1281	A
29	X	1284	G
29	X	1285	A
29	X	1286	U
29	X	1288	A
29	X	1290	A
29	X	1291	G
29	X	1299	A
29	X	1302	C
29	X	1307	U
29	X	1313	U
29	X	1314	A
29	X	1322	G
29	X	1326	U
29	X	1331	G
29	X	1334	A
29	X	1342	U
29	X	1346	C
29	X	1347	C
29	X	1351	G
29	X	1354	A
29	X	1359	G
29	X	1365	U
29	X	1370	U
29	X	1378	A
29	X	1381	G
29	X	1391	A
29	X	1392	U
29	X	1393	G
29	X	1395	A
29	X	1398	G

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Mol	Chain	Res	Type
29	X	1403	U
29	X	1404	C
29	X	1408	A
29	X	1409	U
29	X	1425	G
29	X	1427	G
29	X	1428	G
29	X	1433	A
29	X	1435	G
29	X	1442	C
29	X	1454	U
29	X	1459	U
29	X	1460	G
29	X	1468	A
29	X	1469	U
29	X	1470	G
29	X	1475	U
29	X	1490	U
29	X	1498	G
29	X	1505	U
29	X	1506	C
29	X	1507	A
29	X	1512	A
29	X	1517	C
29	X	1518	C
29	X	1522	C
29	X	1523	A
29	X	1524	C
29	X	1525	A
29	X	1527	G
29	X	1541	G
29	X	1543	G
29	X	1544	A
29	X	1545	G
29	X	1552	C
29	X	1553	G
29	X	1562	G
29	X	1563	U
29	X	1564	U
29	X	1574	A
29	X	1575	C
29	X	1582	A

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Mol	Chain	Res	Type
29	X	1585	A
29	X	1586	A
29	X	1601	U
29	X	1602	G
29	X	1603	A
29	X	1616	C
29	X	1618	U
29	X	1619	A
29	X	1622	G
29	X	1624	A
29	X	1625	A
29	X	1626	A
29	X	1628	C
29	X	1631	C
29	X	1643	A
29	X	1651	U
29	X	1653	C
29	X	1656	U
29	X	1662	G
29	X	1663	C
29	X	1665	C
29	X	1666	G
29	X	1668	G
29	X	1669	A
29	X	1670	G
29	X	1677	C
29	X	1678	G
29	X	1680	U
29	X	1688	U
29	X	1690	U
29	X	1691	G
29	X	1692	C
29	X	1696	C
29	X	1697	U
29	X	1699	A
29	X	1707	A
29	X	1711	C
29	X	1714	A
29	X	1717	A
29	X	1718	A
29	X	1722	G
29	X	1733	U

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Mol	Chain	Res	Type
29	X	1734	C
29	X	1735	G
29	X	1741	G
29	X	1747	G
29	X	1749	G
29	X	1750	A
29	X	1751	A
29	X	1755	G
29	X	1760	G
29	X	1764	A
29	X	1766	U
29	X	1772	C
29	X	1775	A
29	X	1776	A
29	X	1777	A
29	X	1778	U
29	X	1779	C
29	X	1782	A
29	X	1788	C
29	X	1791	C
29	X	1799	A
29	X	1800	A
29	X	1808	C
29	X	1811	A
29	X	1812	U
29	X	1819	U
29	X	1821	A
29	X	1825	C
29	X	1829	C
29	X	1846	A
29	X	1849	G
29	X	1854	G
29	X	1859	A
29	X	1867	A
29	X	1869	A
29	X	1872	A
29	X	1875	C
29	X	1883	A
29	X	1884	A
29	X	1886	G
29	X	1889	G
29	X	1890	G

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Mol	Chain	Res	Type
29	X	1891	C
29	X	1893	G
29	X	1896	A
29	X	1898	U
29	X	1900	U
29	X	1904	G
29	X	1906	U
29	X	1907	C
29	X	1909	U
29	X	1910	A
29	X	1913	G
29	X	1914	U
29	X	1918	G
29	X	1919	A
29	X	1920	A
29	X	1921	A
29	X	1923	U
29	X	1924	C
29	X	1926	U
29	X	1927	U
29	X	1928	G
29	X	1938	U
29	X	1949	A
29	X	1950	C
29	X	1953	A
29	X	1955	G
29	X	1975	G
29	X	1976	U
29	X	1979	C
29	X	1980	A
29	X	1995	G
29	X	1999	U
29	X	2001	G
29	X	2004	U
29	X	2006	G
29	X	2009	U
29	X	2014	A
29	X	2018	G
29	X	2026	C
29	X	2028	C
29	X	2029	G
29	X	2032	G

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Mol	Chain	Res	Type
29	X	2033	C
29	X	2034	A
29	X	2038	C
29	X	2039	G
29	X	2043	A
29	X	2044	G
29	X	2045	A
29	X	2047	C
29	X	2052	G
29	X	2058	U
29	X	2059	U
29	X	2063	A
29	X	2074	U
29	X	2075	U
29	X	2076	G
29	X	2091	C
29	X	2093	G
29	X	2094	C
29	X	2097	A
29	X	2099	G
29	X	2100	A
29	X	2101	U
29	X	2103	G
29	X	2104	G
29	X	2107	G
29	X	2108	G
29	X	2110	G
29	X	2111	C
29	X	2115	C
29	X	2116	G
29	X	2117	A
29	X	2118	A
29	X	2120	C
29	X	2122	G
29	X	2123	G
29	X	2124	C
29	X	2126	U
29	X	2127	U
29	X	2128	U
29	X	2129	U
29	X	2131	G
29	X	2135	C

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Mol	Chain	Res	Type
29	X	2141	A
29	X	2142	G
29	X	2147	C
29	X	2152	A
29	X	2153	A
29	X	2154	A
29	X	2156	A
29	X	2157	C
29	X	2158	C
29	X	2162	C
29	X	2164	G
29	X	2171	U
29	X	2173	G
29	X	2180	U
29	X	2181	A
29	X	2182	A
29	X	2188	A
29	X	2189	A
29	X	2190	A
29	X	2191	A
29	X	2192	U
29	X	2193	C
29	X	2196	U
29	X	2199	C
29	X	2200	G
29	X	2204	A
29	X	2206	C
29	X	2217	G
29	X	2228	U
29	X	2230	G
29	X	2234	G
29	X	2243	C
29	X	2247	A
29	X	2252	A
29	X	2262	C
29	X	2266	A
29	X	2267	A
29	X	2268	G
29	X	2269	G
29	X	2278	A
29	X	2283	G
29	X	2284	U

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Mol	Chain	Res	Type
29	X	2285	U
29	X	2286	G
29	X	2287	G
29	X	2288	A
29	X	2290	A
29	X	2298	U
29	X	2300	G
29	X	2301	A
29	X	2303	C
29	X	2304	G
29	X	2305	C
29	X	2306	A
29	X	2312	A
29	X	2313	G
29	X	2314	A
29	X	2315	A
29	X	2319	G
29	X	2324	G
29	X	2326	C
29	X	2327	U
29	X	2329	C
29	X	2333	A
29	X	2335	U
29	X	2355	A
29	X	2357	A
29	X	2358	C
29	X	2361	G
29	X	2362	G
29	X	2363	G
29	X	2364	C
29	X	2368	G
29	X	2369	U
29	X	2375	G
29	X	2379	G
29	X	2386	G
29	X	2389	G
29	X	2398	U
29	X	2399	C
29	X	2402	U
29	X	2407	G
29	X	2408	G
29	X	2409	A

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Mol	Chain	Res	Type
29	X	2410	U
29	X	2418	A
29	X	2419	C
29	X	2420	C
29	X	2424	G
29	X	2426	G
29	X	2427	A
29	X	2428	U
29	X	2431	C
29	X	2432	A
29	X	2438	A
29	X	2441	U
29	X	2447	G
29	X	2448	A
29	X	2452	U
29	X	2453	C
29	X	2455	A
29	X	2457	A
29	X	2458	U
29	X	2461	G
29	X	2463	G
29	X	2466	G
29	X	2468	G
29	X	2470	U
29	X	2471	U
29	X	2473	G
29	X	2477	C
29	X	2478	C
29	X	2479	U
29	X	2481	G
29	X	2482	A
29	X	2484	G
29	X	2486	C
29	X	2492	G
29	X	2494	C
29	X	2497	A
29	X	2501	U
29	X	2504	G
29	X	2516	U
29	X	2521	A
29	X	2522	G
29	X	2533	U

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Mol	Chain	Res	Type
29	X	2538	C
29	X	2545	A
29	X	2546	G
29	X	2550	C
29	X	2551	A
29	X	2552	C
29	X	2557	G
29	X	2559	U
29	X	2560	G
29	X	2564	U
29	X	2565	C
29	X	2571	G
29	X	2579	A
29	X	2581	A
29	X	2582	G
29	X	2589	C
29	X	2590	U
29	X	2591	C
29	X	2594	U
29	X	2600	A
29	X	2609	G
29	X	2613	A
29	X	2617	G
29	X	2625	U
29	X	2633	A
29	X	2639	A
29	X	2640	G
29	X	2642	G
29	X	2643	G
29	X	2651	U
29	X	2653	A
29	X	2657	G
29	X	2661	G
29	X	2663	U
29	X	2666	U
29	X	2668	U
29	X	2674	C
29	X	2678	C
29	X	2687	G
29	X	2691	C
29	X	2692	A
29	X	2693	U

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Mol	Chain	Res	Type
29	X	2694	G
29	X	2698	G
29	X	2701	A
29	X	2702	G
29	X	2703	C
29	X	2706	U
29	X	2713	A
29	X	2718	A
29	X	2719	U
29	X	2724	G
29	X	2728	A
29	X	2732	C
29	X	2737	A
29	X	2743	G
29	X	2744	A
29	X	2745	A
29	X	2746	G
29	X	2751	C
29	X	2758	A
29	X	2759	U
29	X	2760	G
29	X	2769	C
29	X	2771	C
29	X	2774	U
29	X	2775	U
29	X	2777	A
29	X	2778	U
29	X	2779	C
29	X	2780	A
29	X	2791	C
29	X	2793	G
29	X	2795	A
29	X	2796	A
29	X	2797	G
29	X	2800	C
29	X	2808	U
29	X	2809	A
29	X	2810	A
29	X	2811	G
29	X	2815	C
29	X	2823	G
29	X	2824	C

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Mol	Chain	Res	Type
29	X	2832	G
29	X	2836	U
29	X	2847	G
29	X	2848	A
29	X	2849	C
29	X	2851	G
29	X	2854	G
29	X	2861	A
29	X	2862	G
29	X	2865	G
29	X	2866	A
29	X	2867	G
29	X	2868	G
29	X	2869	U
30	Y	11	G
30	Y	14	C
30	Y	15	A
30	Y	16	U
30	Y	17	A
30	Y	20	A
30	Y	27	A
30	Y	28	A
30	Y	29	C
30	Y	37	C
30	Y	39	C
30	Y	40	C
30	Y	43	G
30	Y	44	C
30	Y	46	G
30	Y	47	A
30	Y	49	C
30	Y	51	G
30	Y	52	G
30	Y	53	G
30	Y	55	C
30	Y	59	A
30	Y	63	A
30	Y	70	C
30	Y	75	A
30	Y	76	U
30	Y	86	A
30	Y	99	G

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Mol	Chain	Res	Type
30	Y	108	G
30	Y	112	A
30	Y	114	C
30	Y	115	G
30	Y	121	G
30	Y	122	U
30	Y	123	U

All (31) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
29	X	459	A
29	X	465	C
29	X	475	U
29	X	511	A
29	X	518	A
29	X	654	A
29	X	655	A
29	X	813	A
29	X	939	C
29	X	940	G
29	X	1000	G
29	X	1123	G
29	X	1138	A
29	X	1225	G
29	X	1506	C
29	X	1526	U
29	X	1601	U
29	X	1602	G
29	X	1690	U
29	X	1715	A
29	X	1777	A
29	X	2044	G
29	X	2228	U
29	X	2550	C
29	X	2551	A
29	X	2592	U
29	X	2736	U
29	X	2758	A
29	X	2823	G
29	X	2854	G
30	Y	16	U

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 187 ligands modelled in this entry, 186 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
32	HGR	X	6178	-	38,39,39	1.83	7 (18%)	44,58,58	1.94	8 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	HGR	X	6178	-	-	0/20/79/79	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	X	6178	HGR	C5-C6	-4.36	1.42	1.50
32	X	6178	HGR	C3-C2	-3.69	1.41	1.48
32	X	6178	HGR	C5-C4	-3.53	1.43	1.49
32	X	6178	HGR	C17-N1	2.07	1.49	1.45
32	X	6178	HGR	C12-C14	3.65	1.43	1.33
32	X	6178	HGR	C12-C6	3.84	1.55	1.44
32	X	6178	HGR	C1-C6	4.64	1.41	1.35

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	X	6178	HGR	C5-C6-C1	-4.70	116.95	120.38
32	X	6178	HGR	C4-C3-C2	-2.98	118.17	122.09
32	X	6178	HGR	O1-C10-C9	-2.44	101.47	104.83
32	X	6178	HGR	C1-C2-C3	2.27	120.84	115.81
32	X	6178	HGR	O10-C19-C17	2.56	114.88	109.57
32	X	6178	HGR	C5-C6-C12	3.61	124.39	120.24
32	X	6178	HGR	O3-C3-C2	4.00	118.43	112.33
32	X	6178	HGR	C10-O3-C3	7.53	126.09	115.16

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
32	X	6178	HGR	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	0	224/224 (100%)	4.90	180 (80%) 0 0	291, 311, 319, 322	0
2	A	274/274 (100%)	0.62	39 (14%) 4 1	108, 151, 172, 185	0
3	B	205/205 (100%)	0.04	4 (1%) 68 39	67, 102, 129, 146	0
4	C	197/197 (100%)	0.12	10 (5%) 32 12	93, 133, 158, 177	0
5	D	177/177 (100%)	0.30	14 (7%) 15 5	165, 183, 200, 214	0
6	E	171/171 (100%)	0.09	11 (6%) 23 8	116, 167, 191, 198	0
7	F	144/144 (100%)	2.34	60 (41%) 0 0	233, 259, 275, 281	0
8	G	142/142 (100%)	0.28	8 (5%) 28 11	87, 125, 139, 169	0
9	H	134/134 (100%)	-0.10	4 (2%) 54 25	70, 92, 108, 118	0
10	I	141/141 (100%)	1.05	34 (24%) 1 1	98, 150, 173, 182	0
11	J	136/136 (100%)	0.94	25 (18%) 2 1	107, 126, 156, 159	0
12	K	113/113 (100%)	0.23	6 (5%) 30 12	63, 82, 95, 99	0
13	L	104/104 (100%)	1.12	26 (25%) 1 1	126, 147, 162, 173	0
14	M	109/109 (100%)	-0.06	3 (2%) 56 27	72, 89, 117, 147	0
15	N	117/117 (100%)	0.36	10 (8%) 13 5	90, 118, 144, 153	0
16	O	94/94 (100%)	-0.28	6 (6%) 23 8	103, 129, 156, 173	0
17	P	127/127 (100%)	0.16	5 (3%) 43 18	81, 96, 120, 180	0
18	Q	93/93 (100%)	0.59	12 (12%) 5 2	108, 137, 160, 176	0
19	R	110/110 (100%)	0.37	8 (7%) 18 6	111, 131, 166, 180	0
20	S	175/175 (100%)	0.48	24 (13%) 4 1	134, 167, 185, 193	0
21	T	84/84 (100%)	1.16	18 (21%) 1 1	111, 130, 148, 171	0
22	U	72/72 (100%)	1.51	21 (29%) 1 0	134, 163, 177, 182	0
23	V	66/66 (100%)	0.82	12 (18%) 2 1	147, 163, 190, 201	0
24	W	55/55 (100%)	0.66	6 (10%) 7 3	112, 124, 142, 157	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	Z	57/57 (100%)	0.05	3 (5%) 30 12	82, 97, 120, 130	0
26	1	54/54 (100%)	1.72	23 (42%) 0 0	140, 153, 179, 189	0
27	2	47/47 (100%)	0.17	2 (4%) 39 16	108, 121, 132, 134	0
28	3	65/65 (100%)	1.63	26 (40%) 0 0	115, 132, 143, 153	0
29	X	2780/2881 (96%)	-0.15	79 (2%) 56 27	59, 127, 241, 397	0
30	Y	122/122 (100%)	-0.36	3 (2%) 61 30	110, 157, 182, 203	0
All	All	6389/6490 (98%)	0.37	682 (10%) 8 3	59, 134, 276, 397	0

All (682) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	0	204	PHE	18.3
1	0	200	ALA	18.1
1	0	205	LEU	17.3
1	0	85	ALA	15.6
29	X	2127	U	15.3
1	0	47	PRO	15.2
1	0	162	ASP	15.0
29	X	1899	A	14.2
29	X	1900	U	12.1
1	0	147	GLY	12.1
1	0	222	LEU	11.8
7	F	113	PRO	11.7
29	X	2114	G	11.5
29	X	1901	A	11.3
1	0	54	VAL	11.2
1	0	206	ARG	11.1
1	0	171	ILE	11.1
1	0	56	GLY	10.8
1	0	202	GLY	10.8
29	X	1897	C	10.7
1	0	159	PHE	10.6
1	0	48	ARG	10.6
10	I	69	GLY	10.5
1	0	143	ALA	10.5
1	0	146	ALA	10.3
7	F	4	VAL	10.3
1	0	14	LYS	10.2
1	0	199	THR	10.2
1	0	188	LEU	10.1

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Mol	Chain	Res	Type	RSRZ
1	0	165	GLY	9.9
23	V	3	PRO	9.9
1	0	33	PHE	9.8
1	0	55	ARG	9.8
1	0	87	ALA	9.6
1	0	86	GLY	9.5
29	X	2095	G	9.4
1	0	208	ALA	9.4
1	0	15	GLN	9.3
21	T	2	ALA	9.2
1	0	148	MET	9.1
29	X	731	A	9.1
1	0	46	ASP	9.0
7	F	23	VAL	8.8
7	F	5	ALA	8.8
1	0	192	LEU	8.8
1	0	201	LYS	8.7
29	X	2120	C	8.7
1	0	69	ARG	8.6
10	I	67	ASN	8.5
29	X	1187	A	8.5
29	X	1525	A	8.4
1	0	209	TYR	8.4
7	F	18	THR	8.3
7	F	22	PRO	8.3
29	X	2128	U	8.3
1	0	219	PRO	8.2
29	X	2109	A	8.2
1	0	42	ARG	8.1
1	0	44	GLY	7.9
1	0	207	SER	7.9
1	0	129	PRO	7.8
1	0	203	VAL	7.8
23	V	4	SER	7.8
20	S	92	VAL	7.7
29	X	730	C	7.7
23	V	6	MET	7.6
1	0	140	THR	7.6
1	0	78	ASN	7.5
29	X	2116	G	7.5
7	F	68	ILE	7.5
1	0	158	GLU	7.4

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Mol	Chain	Res	Type	RSRZ
1	0	107	ASP	7.3
13	L	40	ALA	7.3
1	0	220	LEU	7.3
29	X	2115	C	7.3
1	0	217	SER	7.3
1	0	218	ILE	7.2
29	X	1902	A	7.2
1	0	84	ALA	7.1
1	0	41	PHE	7.1
23	V	1	MET	7.1
1	0	193	GLU	7.1
7	F	21	PRO	7.1
1	0	145	VAL	7.0
13	L	31	VAL	7.0
1	0	67	SER	6.9
29	X	728	G	6.9
1	0	142	GLY	6.8
1	0	216	PRO	6.8
1	0	210	LEU	6.8
21	T	3	HIS	6.8
1	0	68	VAL	6.8
7	F	7	ILE	6.7
29	X	1524	C	6.6
11	J	37	ALA	6.6
5	D	145	MET	6.6
7	F	25	PRO	6.6
10	I	68	VAL	6.6
3	B	205	SER	6.5
29	X	2776	U	6.5
1	0	135	ASN	6.5
29	X	1523	A	6.5
22	U	27	ASP	6.5
1	0	40	HIS	6.5
1	0	185	TYR	6.5
20	S	68	ALA	6.5
1	0	50	SER	6.4
1	0	174	ALA	6.4
1	0	194	GLY	6.4
1	0	74	THR	6.4
7	F	112	MET	6.3
1	0	189	ILE	6.3
1	0	49	LYS	6.2

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Mol	Chain	Res	Type	RSRZ
10	I	70	THR	6.2
29	X	2129	U	6.2
11	J	22	ALA	6.2
1	0	172	GLY	6.1
29	X	1086	C	6.1
29	X	1898	U	6.1
1	0	149	VAL	6.0
11	J	21	ASP	6.0
1	0	57	THR	5.9
1	0	144	ASP	5.9
1	0	20	GLU	5.9
22	U	26	ALA	5.9
29	X	1189	G	5.9
7	F	6	GLY	5.9
29	X	1186	G	5.9
28	3	32	GLN	5.8
21	T	8	GLY	5.8
1	0	157	ILE	5.8
22	U	45	ASN	5.8
1	0	82	ALA	5.8
7	F	114	ASP	5.8
28	3	65	GLY	5.8
26	1	21	TYR	5.8
1	0	191	ALA	5.8
13	L	12	ARG	5.8
1	0	13	ASN	5.7
1	0	53	ASN	5.6
1	0	184	ASN	5.6
1	0	170	PRO	5.6
5	D	146	VAL	5.6
1	0	45	ILE	5.6
23	V	7	ARG	5.6
7	F	58	THR	5.6
1	0	52	GLN	5.5
1	0	61	PRO	5.5
22	U	16	ASN	5.5
29	X	729	A	5.5
1	0	133	LEU	5.5
29	X	1552	C	5.5
10	I	74	VAL	5.5
1	0	39	VAL	5.4
1	0	83	GLU	5.4

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Mol	Chain	Res	Type	RSRZ
13	L	96	TYR	5.4
1	0	58	VAL	5.4
2	A	231	HIS	5.4
1	0	150	ARG	5.4
13	L	30	SER	5.4
23	V	2	LYS	5.4
1	0	16	TYR	5.4
1	0	180	ASN	5.4
11	J	20	GLY	5.3
1	0	178	SER	5.3
7	F	26	ALA	5.3
29	X	2774	U	5.3
7	F	110	THR	5.2
29	X	2777	A	5.2
7	F	66	THR	5.2
10	I	33	GLY	5.2
30	Y	123	U	5.2
7	F	24	GLY	5.1
1	0	43	LEU	5.1
1	0	164	THR	5.1
7	F	20	ALA	5.1
22	U	25	ARG	5.1
1	0	106	PHE	5.0
11	J	36	ILE	5.0
10	I	66	ASN	5.0
7	F	12	LEU	5.0
1	0	59	ALA	5.0
1	0	163	LYS	5.0
1	0	1	LYS	5.0
1	0	11	ASP	5.0
1	0	182	SER	5.0
29	X	1188	A	4.9
19	R	5	SER	4.9
29	X	2096	U	4.9
21	T	6	GLY	4.9
2	A	242	ALA	4.9
29	X	2110	G	4.9
26	1	23	THR	4.8
7	F	56	GLU	4.8
20	S	74	ARG	4.8
7	F	97	GLY	4.8
29	X	2119	A	4.8

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Mol	Chain	Res	Type	RSRZ
29	X	2092	U	4.8
23	V	5	GLU	4.7
26	1	11	LYS	4.7
1	0	36	THR	4.7
1	0	34	ASP	4.7
29	X	2133	G	4.7
1	0	31	ALA	4.6
1	0	51	ASP	4.6
1	0	156	ARG	4.6
1	0	151	GLY	4.6
1	0	60	LEU	4.6
11	J	99	LYS	4.6
26	1	53	ALA	4.6
10	I	72	TYR	4.6
1	0	32	LYS	4.6
1	0	190	SER	4.6
1	0	155	GLY	4.6
10	I	75	VAL	4.5
2	A	55	GLY	4.5
17	P	134	LYS	4.5
1	0	105	ASP	4.5
23	V	37	LEU	4.5
4	C	20	PRO	4.5
26	1	22	TYR	4.5
1	0	62	HIS	4.5
2	A	104	TYR	4.5
21	T	7	VAL	4.5
6	E	64	LEU	4.5
7	F	1	MET	4.4
5	D	73	SER	4.4
28	3	37	SER	4.4
7	F	19	PRO	4.4
11	J	105	PHE	4.4
19	R	14	LEU	4.4
28	3	22	VAL	4.4
7	F	29	GLN	4.4
7	F	27	LEU	4.4
30	Y	43	G	4.4
1	0	161	ASN	4.3
1	0	93	ASP	4.3
1	0	30	THR	4.3
29	X	2108	G	4.3

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Mol	Chain	Res	Type	RSRZ
1	0	66	ARG	4.3
10	I	103	ASN	4.3
14	M	99	VAL	4.3
28	3	54	GLU	4.3
1	0	113	PRO	4.3
1	0	4	ARG	4.3
1	0	81	ALA	4.3
22	U	11	LYS	4.3
29	X	2113	U	4.2
12	K	7	GLY	4.2
13	L	97	HIS	4.2
21	T	45	PHE	4.2
1	0	28	LEU	4.2
11	J	98	VAL	4.2
2	A	35	GLU	4.2
7	F	125	ASN	4.2
2	A	32	ALA	4.2
11	J	59	PHE	4.2
11	J	119	PHE	4.2
2	A	265	THR	4.1
6	E	173	ALA	4.1
29	X	2152	A	4.1
11	J	106	GLU	4.1
29	X	1895	A	4.1
7	F	102	ASP	4.1
29	X	2125	C	4.1
1	0	75	LYS	4.1
29	X	1139	A	4.1
22	U	28	GLY	4.0
1	0	70	VAL	4.0
22	U	51	ILE	4.0
8	G	99	VAL	4.0
20	S	124	ALA	4.0
5	D	81	GLN	4.0
5	D	72	LYS	4.0
7	F	70	LYS	4.0
1	0	152	LEU	4.0
1	0	90	VAL	4.0
7	F	120	VAL	4.0
16	O	74	TYR	3.9
29	X	2142	G	3.9
22	U	62	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	0	160	ARG	3.9
28	3	23	MET	3.9
2	A	251	GLY	3.9
29	X	1185	C	3.9
5	D	144	ASP	3.9
1	0	91	GLY	3.9
11	J	100	PRO	3.9
13	L	13	THR	3.9
21	T	74	LYS	3.9
29	X	2124	C	3.9
13	L	33	ARG	3.9
7	F	109	LYS	3.9
1	0	177	GLU	3.9
21	T	71	ASN	3.9
7	F	34	ILE	3.8
10	I	79	GLN	3.8
20	S	73	LYS	3.8
7	F	67	PHE	3.8
26	1	8	ILE	3.8
9	H	134	LEU	3.8
18	Q	27	PHE	3.8
26	1	26	LYS	3.8
29	X	2775	U	3.8
14	M	53	VAL	3.8
1	0	98	ARG	3.8
1	0	88	ASP	3.7
26	1	12	MET	3.7
1	0	183	ALA	3.7
22	U	44	ALA	3.7
24	W	13	PRO	3.7
1	0	80	GLN	3.7
10	I	50	GLU	3.7
29	X	2126	U	3.7
20	S	69	VAL	3.7
5	D	147	ASP	3.7
28	3	10	ALA	3.7
22	U	10	LYS	3.7
29	X	727	U	3.7
1	0	95	LEU	3.7
5	D	71	LYS	3.7
13	L	94	TYR	3.7
1	0	102	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
26	1	28	ARG	3.6
7	F	55	VAL	3.6
29	X	1894	U	3.6
28	3	7	HIS	3.6
1	0	169	ALA	3.6
1	0	134	PRO	3.6
1	0	2	ARG	3.6
23	V	38	ALA	3.6
2	A	62	TYR	3.6
13	L	84	ILE	3.6
11	J	117	GLU	3.6
10	I	104	ARG	3.5
21	T	65	GLY	3.5
29	X	1085	G	3.5
1	0	132	LEU	3.5
1	0	17	SER	3.5
21	T	83	ALA	3.5
7	F	94	ALA	3.5
13	L	62	GLY	3.5
28	3	20	GLY	3.5
7	F	96	VAL	3.5
11	J	97	VAL	3.5
13	L	89	PHE	3.5
26	1	1	ALA	3.5
29	X	2121	U	3.5
8	G	97	ASP	3.4
29	X	2118	A	3.4
1	0	25	VAL	3.4
4	C	196	VAL	3.4
22	U	15	VAL	3.4
1	0	92	SER	3.4
1	0	29	ALA	3.4
29	X	1526	U	3.4
1	0	121	GLN	3.4
28	3	61	MET	3.4
2	A	255	LYS	3.4
20	S	169	VAL	3.4
10	I	71	THR	3.3
22	U	75	TYR	3.3
2	A	230	ASP	3.3
18	Q	7	LEU	3.3
13	L	93	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	0	223	GLY	3.3
26	1	13	GLU	3.3
1	0	181	LEU	3.3
8	G	170	PRO	3.3
28	3	66	LYS	3.3
1	0	114	ASP	3.3
1	0	7	GLU	3.3
1	0	27	GLU	3.3
7	F	14	ALA	3.3
20	S	171	VAL	3.3
10	I	73	GLU	3.2
11	J	101	GLY	3.2
29	X	1551	U	3.2
26	1	20	PHE	3.2
24	W	6	VAL	3.2
2	A	103	ARG	3.2
10	I	48	PHE	3.2
1	0	120	GLY	3.2
13	L	59	LEU	3.2
13	L	9	ARG	3.2
2	A	33	LEU	3.2
29	X	1893	G	3.2
12	K	22	ARG	3.2
1	0	141	VAL	3.2
26	1	2	ALA	3.2
4	C	91	TYR	3.2
7	F	105	LEU	3.2
22	U	12	ASN	3.2
7	F	137	THR	3.2
1	0	26	LYS	3.1
2	A	64	ILE	3.1
2	A	61	LEU	3.1
1	0	176	PHE	3.1
11	J	18	MET	3.1
20	S	66	VAL	3.1
2	A	71	ASP	3.1
24	W	3	ILE	3.1
26	1	6	PRO	3.1
20	S	93	GLU	3.1
1	0	167	VAL	3.1
1	0	6	LEU	3.1
15	N	48	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
11	J	23	LYS	3.1
7	F	13	PRO	3.1
29	X	834	A	3.1
10	I	54	SER	3.0
12	K	69	ASP	3.0
26	1	9	ILE	3.0
19	R	75	ALA	3.0
21	T	84	ALA	3.0
6	E	172	LYS	3.0
1	0	166	VAL	3.0
16	O	80	TYR	3.0
1	0	153	LYS	3.0
13	L	52	ALA	3.0
7	F	107	ILE	3.0
19	R	4	PRO	3.0
18	Q	43	GLN	3.0
19	R	84	VAL	3.0
13	L	75	LEU	3.0
20	S	129	ARG	3.0
1	0	179	GLY	3.0
20	S	130	ILE	3.0
28	3	9	MET	3.0
11	J	60	ARG	3.0
1	0	136	PRO	3.0
1	0	154	ALA	3.0
17	P	116	ILE	3.0
29	X	1101	U	3.0
4	C	38	ARG	3.0
18	Q	39	LYS	2.9
20	S	75	LYS	2.9
2	A	234	GLY	2.9
26	1	52	ALA	2.9
29	X	222	G	2.9
10	I	13	ARG	2.9
13	L	14	ARG	2.9
7	F	64	SER	2.9
1	0	221	ALA	2.9
20	S	81	VAL	2.9
25	Z	4	HIS	2.9
2	A	56	GLY	2.9
10	I	101	ARG	2.9
8	G	98	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
2	A	235	GLY	2.9
13	L	10	LYS	2.9
2	A	253	PRO	2.9
7	F	17	ALA	2.8
18	Q	37	GLU	2.8
22	U	13	LEU	2.8
6	E	95	ARG	2.8
20	S	122	ILE	2.8
4	C	180	ILE	2.8
11	J	103	VAL	2.8
1	0	139	GLY	2.8
10	I	60	LEU	2.8
26	1	25	THR	2.8
4	C	35	LEU	2.8
2	A	226	MET	2.8
11	J	19	THR	2.8
2	A	223	GLY	2.8
13	L	34	SER	2.8
2	A	268	ARG	2.8
10	I	45	LYS	2.8
11	J	11	ARG	2.8
19	R	43	ASP	2.8
21	T	69	PHE	2.8
23	V	8	ASN	2.8
2	A	51	SER	2.8
7	F	108	ALA	2.8
22	U	52	ARG	2.8
28	3	15	LYS	2.8
1	0	104	MET	2.7
1	0	97	GLU	2.7
28	3	16	ILE	2.7
2	A	254	THR	2.7
20	S	72	ASP	2.7
2	A	216	GLY	2.7
15	N	47	TYR	2.7
16	O	73	LYS	2.7
28	3	46	LYS	2.7
22	U	54	ASN	2.7
13	L	68	ALA	2.7
2	A	37	LEU	2.7
3	B	102	ILE	2.7
6	E	174	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
7	F	2	ARG	2.7
18	Q	9	ALA	2.7
29	X	2123	G	2.7
29	X	2137	G	2.7
1	0	117	ALA	2.7
2	A	36	ALA	2.7
21	T	66	LYS	2.7
29	X	1896	A	2.7
1	0	5	ALA	2.7
7	F	37	PHE	2.6
5	D	74	ILE	2.6
29	X	1090	C	2.6
29	X	1103	C	2.6
17	P	105	ARG	2.6
10	I	49	PHE	2.6
16	O	81	ARG	2.6
18	Q	94	GLN	2.6
29	X	2153	A	2.6
10	I	76	LYS	2.6
20	S	15	ASP	2.6
15	N	21	ALA	2.6
28	3	36	LYS	2.6
1	0	19	ASP	2.6
7	F	8	VAL	2.6
15	N	2	PRO	2.6
26	1	3	GLY	2.6
29	X	1734	C	2.6
7	F	74	MET	2.6
11	J	102	ARG	2.6
1	0	3	TYR	2.6
2	A	60	ARG	2.6
5	D	103	LEU	2.6
29	X	2130	G	2.5
12	K	29	LEU	2.5
11	J	104	MET	2.5
29	X	1114	A	2.5
1	0	12	ARG	2.5
10	I	46	GLY	2.5
17	P	107	ILE	2.5
26	1	19	GLY	2.5
12	K	18	VAL	2.5
15	N	100	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
30	Y	2	C	2.5
7	F	121	GLU	2.5
10	I	15	ASP	2.5
14	M	54	VAL	2.5
1	0	22	ALA	2.5
28	3	40	GLU	2.5
6	E	25	LYS	2.5
7	F	143	ASN	2.5
22	U	43	ARG	2.5
24	W	15	ASN	2.5
7	F	15	GLY	2.5
15	N	49	ASP	2.5
1	0	138	SER	2.5
29	X	1903	C	2.4
29	X	2112	C	2.4
1	0	198	GLY	2.4
28	3	21	LYS	2.4
21	T	73	GLY	2.4
7	F	124	ALA	2.4
1	0	168	HIS	2.4
10	I	123	ASP	2.4
10	I	51	GLY	2.4
10	I	108	LEU	2.4
19	R	55	THR	2.4
25	Z	56	GLN	2.4
23	V	9	LEU	2.4
29	X	2117	A	2.4
15	N	25	TRP	2.4
10	I	57	ILE	2.4
1	0	64	THR	2.4
4	C	120	VAL	2.4
29	X	1138	A	2.4
29	X	1921	A	2.4
29	X	2140	G	2.4
1	0	94	GLU	2.4
13	L	79	ALA	2.4
7	F	122	ALA	2.4
26	1	0	ALA	2.4
7	F	136	VAL	2.4
9	H	1	MET	2.4
27	2	18	PHE	2.4
2	A	241	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
2	A	101	GLU	2.4
1	0	10	VAL	2.3
1	0	175	SER	2.3
10	I	102	LYS	2.3
22	U	23	LYS	2.3
3	B	187	ALA	2.3
20	S	23	ALA	2.3
15	N	57	PHE	2.3
29	X	2097	A	2.3
4	C	19	LEU	2.3
4	C	31	VAL	2.3
1	0	211	THR	2.3
2	A	222	ARG	2.3
10	I	44	GLY	2.3
18	Q	48	VAL	2.3
1	0	115	MET	2.3
5	D	49	ALA	2.3
13	L	53	ALA	2.3
2	A	248	THR	2.3
1	0	103	PHE	2.3
6	E	96	ALA	2.3
22	U	35	THR	2.3
20	S	123	VAL	2.3
28	3	25	PHE	2.3
4	C	70	GLY	2.3
2	A	249	PRO	2.3
5	D	173	MET	2.3
15	N	39	LEU	2.3
2	A	102	LYS	2.3
10	I	107	LYS	2.3
1	0	89	VAL	2.3
29	X	2143	G	2.2
7	F	92	ASN	2.2
1	0	76	GLY	2.2
6	E	152	ARG	2.2
29	X	2733	A	2.2
25	Z	59	ALA	2.2
29	X	304	A	2.2
10	I	105	PRO	2.2
16	O	72	ARG	2.2
29	X	1733	U	2.2
2	A	240	THR	2.2

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Mol	Chain	Res	Type	RSRZ
18	Q	62	ARG	2.2
8	G	41	TRP	2.2
28	3	64	ARG	2.2
18	Q	40	ASP	2.2
21	T	20	TYR	2.2
11	J	38	MET	2.2
1	0	122	LYS	2.2
2	A	59	LYS	2.2
2	A	252	LYS	2.2
29	X	1553	G	2.2
1	0	35	GLU	2.2
22	U	24	ALA	2.2
5	D	101	GLU	2.2
8	G	100	TYR	2.2
13	L	51	LEU	2.2
28	3	11	LYS	2.2
6	E	17	VAL	2.2
18	Q	42	ILE	2.2
20	S	91	PRO	2.2
23	V	30	PHE	2.2
7	F	85	GLY	2.2
9	H	28	GLY	2.1
1	0	79	VAL	2.1
17	P	106	LEU	2.1
26	1	4	ALA	2.1
26	1	39	LYS	2.1
24	W	5	LEU	2.1
3	B	132	LYS	2.1
13	L	58	ALA	2.1
28	3	44	LYS	2.1
5	D	175	LEU	2.1
7	F	43	ALA	2.1
28	3	30	ARG	2.1
20	S	156	GLU	2.1
7	F	48	LYS	2.1
6	E	105	MET	2.1
18	Q	8	GLN	2.1
15	N	53	LYS	2.1
12	K	43	GLU	2.1
20	S	11	LYS	2.1
1	0	118	GLN	2.1
21	T	61	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
8	G	156	HIS	2.1
11	J	132	MET	2.1
28	3	13	ARG	2.0
2	A	105	ILE	2.0
27	2	22	MET	2.0
28	3	52	LYS	2.0
20	S	70	GLN	2.0
16	O	70	TYR	2.0
19	R	101	GLY	2.0
7	F	123	ALA	2.0
20	S	170	SER	2.0
1	0	196	LYS	2.0
13	L	77	ALA	2.0
21	T	5	LYS	2.0
24	W	17	VAL	2.0
8	G	90	LEU	2.0
26	1	35	LEU	2.0
28	3	53	ALA	2.0
7	F	9	LYS	2.0
9	H	72	ALA	2.0
21	T	55	ARG	2.0
6	E	175	LYS	2.0
10	I	62	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
31	MG	X	6033	1/1	0.83	0.69	51.06	76,76,76,76	0
31	MG	X	6001	1/1	0.88	0.73	46.93	67,67,67,67	0
31	MG	X	6162	1/1	0.75	0.78	41.49	104,104,104,104	0
31	MG	X	6147	1/1	0.93	1.08	31.86	93,93,93,93	0
31	MG	X	6018	1/1	0.95	0.78	25.76	86,86,86,86	0
31	MG	X	6167	1/1	0.90	1.05	25.76	97,97,97,97	0
31	MG	X	6129	1/1	0.90	0.46	19.40	89,89,89,89	0
31	MG	X	6132	1/1	0.92	0.56	19.08	84,84,84,84	0
31	MG	X	6087	1/1	0.82	0.62	19.04	85,85,85,85	0
31	MG	X	6085	1/1	0.82	0.41	17.62	66,66,66,66	0
31	MG	X	6105	1/1	0.90	0.41	14.70	86,86,86,86	0
31	MG	X	6014	1/1	0.80	0.47	13.98	99,99,99,99	0
31	MG	X	6142	1/1	0.91	0.56	12.84	106,106,106,106	0
31	MG	X	6011	1/1	0.90	0.39	12.12	104,104,104,104	0
31	MG	X	6016	1/1	0.96	0.35	11.13	74,74,74,74	0
31	MG	X	6019	1/1	0.92	0.48	10.85	75,75,75,75	0
31	MG	X	6054	1/1	0.96	0.39	10.58	79,79,79,79	0
31	MG	X	6066	1/1	0.93	0.40	10.56	105,105,105,105	0
31	MG	X	6053	1/1	0.94	0.36	9.82	85,85,85,85	0
31	MG	X	6006	1/1	0.77	0.57	9.63	70,70,70,70	0
31	MG	M	201	1/1	0.94	0.67	9.21	71,71,71,71	0
31	MG	Y	201	1/1	0.81	0.41	8.79	96,96,96,96	0
31	MG	X	6022	1/1	0.84	0.58	8.55	92,92,92,92	0
31	MG	X	6017	1/1	0.85	0.45	8.53	54,54,54,54	0
31	MG	X	6068	1/1	0.93	0.38	8.32	111,111,111,111	0
31	MG	X	6007	1/1	0.96	0.39	7.69	78,78,78,78	0
31	MG	X	6062	1/1	0.86	0.72	6.96	87,87,87,87	0
31	MG	X	6055	1/1	0.97	0.46	6.88	85,85,85,85	0
31	MG	X	6037	1/1	0.89	0.41	5.86	65,65,65,65	0
31	MG	X	6093	1/1	0.65	0.35	5.85	96,96,96,96	0
31	MG	X	6171	1/1	0.86	0.32	5.66	118,118,118,118	0
31	MG	N	201	1/1	0.77	0.39	5.47	74,74,74,74	0
31	MG	X	6115	1/1	0.91	0.30	5.27	133,133,133,133	0
31	MG	X	6008	1/1	0.95	0.26	4.65	58,58,58,58	0
31	MG	X	6032	1/1	0.95	0.36	4.29	86,86,86,86	0
31	MG	X	6060	1/1	0.92	0.65	4.26	80,80,80,80	0
31	MG	X	6078	1/1	0.81	0.37	3.57	89,89,89,89	0
31	MG	X	6071	1/1	0.89	0.34	3.26	99,99,99,99	0
31	MG	X	6056	1/1	0.92	0.32	3.15	81,81,81,81	0
31	MG	X	6021	1/1	0.94	0.26	3.13	91,91,91,91	0
31	MG	X	6144	1/1	0.81	0.26	3.12	132,132,132,132	0
31	MG	X	6131	1/1	0.80	0.40	3.00	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
31	MG	X	6110	1/1	0.91	0.23	2.80	84,84,84,84	0
31	MG	X	6002	1/1	0.85	0.32	2.77	91,91,91,91	0
31	MG	X	6051	1/1	0.73	0.54	2.65	83,83,83,83	0
31	MG	X	6059	1/1	0.91	0.24	2.19	88,88,88,88	0
32	HGR	X	6178	36/36	0.90	0.25	1.98	79,99,109,111	0
31	MG	X	6108	1/1	0.92	0.52	1.96	108,108,108,108	0
31	MG	X	6158	1/1	0.87	0.21	1.66	76,76,76,76	0
31	MG	X	6023	1/1	0.97	0.37	1.37	83,83,83,83	0
31	MG	X	6012	1/1	0.86	0.24	1.28	78,78,78,78	0
31	MG	X	6004	1/1	0.96	0.28	1.06	93,93,93,93	0
31	MG	A	301	1/1	0.73	0.35	-0.13	108,108,108,108	0
31	MG	X	6086	1/1	0.96	0.17	-0.21	104,104,104,104	0
31	MG	X	6038	1/1	0.94	0.09	-4.23	82,82,82,82	0
31	MG	X	6119	1/1	0.91	0.41	-	89,89,89,89	0
31	MG	X	6042	1/1	0.86	1.02	-	96,96,96,96	0
31	MG	X	6036	1/1	0.94	0.36	-	70,70,70,70	0
31	MG	X	6174	1/1	0.72	0.30	-	117,117,117,117	0
31	MG	X	6101	1/1	0.07	1.27	-	138,138,138,138	0
31	MG	X	6127	1/1	0.81	0.62	-	81,81,81,81	0
31	MG	X	6172	1/1	0.77	0.35	-	88,88,88,88	0
31	MG	X	6044	1/1	0.93	0.42	-	66,66,66,66	0
31	MG	X	6100	1/1	0.90	0.42	-	111,111,111,111	0
31	MG	X	6140	1/1	0.46	0.42	-	97,97,97,97	0
31	MG	X	6126	1/1	0.87	0.42	-	114,114,114,114	0
31	MG	X	6107	1/1	0.92	0.22	-	76,76,76,76	0
31	MG	X	6079	1/1	0.86	0.33	-	99,99,99,99	0
31	MG	X	6164	1/1	0.86	0.23	-	86,86,86,86	0
31	MG	X	6092	1/1	0.92	0.72	-	97,97,97,97	0
31	MG	X	6169	1/1	0.77	0.49	-	91,91,91,91	0
31	MG	X	6143	1/1	0.97	0.64	-	99,99,99,99	0
31	MG	X	6076	1/1	0.73	0.56	-	73,73,73,73	0
31	MG	X	6120	1/1	0.88	0.27	-	78,78,78,78	0
31	MG	X	6046	1/1	0.85	0.58	-	76,76,76,76	0
31	MG	X	6005	1/1	0.98	0.56	-	58,58,58,58	0
31	MG	X	6039	1/1	0.90	0.40	-	79,79,79,79	0
31	MG	X	6177	1/1	0.90	0.49	-	125,125,125,125	0
31	MG	X	6088	1/1	0.99	0.29	-	88,88,88,88	0
31	MG	X	6149	1/1	0.74	0.41	-	99,99,99,99	0
31	MG	X	6074	1/1	0.84	0.39	-	89,89,89,89	0
31	MG	X	6003	1/1	0.81	0.31	-	72,72,72,72	0
31	MG	X	6045	1/1	0.86	0.73	-	94,94,94,94	0
31	MG	X	6109	1/1	0.94	0.37	-	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
31	MG	X	6137	1/1	0.84	0.47	-	136,136,136,136	0
31	MG	X	6083	1/1	0.88	0.29	-	83,83,83,83	0
31	MG	X	6134	1/1	0.94	0.11	-	100,100,100,100	0
31	MG	X	6072	1/1	0.96	0.51	-	101,101,101,101	0
31	MG	X	6152	1/1	0.57	0.30	-	158,158,158,158	0
31	MG	X	6165	1/1	0.89	0.45	-	88,88,88,88	0
31	MG	X	6025	1/1	0.91	0.66	-	76,76,76,76	0
31	MG	X	6135	1/1	0.44	1.17	-	129,129,129,129	0
31	MG	X	6031	1/1	0.94	0.62	-	85,85,85,85	0
31	MG	X	6026	1/1	0.97	0.34	-	79,79,79,79	0
31	MG	X	6013	1/1	0.92	0.49	-	76,76,76,76	0
31	MG	X	6148	1/1	0.83	0.31	-	104,104,104,104	0
31	MG	X	6099	1/1	0.59	0.86	-	120,120,120,120	0
31	MG	Y	202	1/1	0.92	0.18	-	130,130,130,130	0
31	MG	X	6090	1/1	0.80	0.47	-	72,72,72,72	0
31	MG	X	6160	1/1	0.73	0.72	-	108,108,108,108	0
31	MG	X	6024	1/1	0.95	0.37	-	100,100,100,100	0
31	MG	X	6104	1/1	0.93	0.54	-	89,89,89,89	0
31	MG	X	6156	1/1	0.83	0.25	-	91,91,91,91	0
31	MG	X	6064	1/1	0.85	0.48	-	77,77,77,77	0
31	MG	X	6041	1/1	0.91	0.41	-	64,64,64,64	0
31	MG	X	6166	1/1	0.92	0.12	-	76,76,76,76	0
31	MG	X	6084	1/1	0.94	0.29	-	124,124,124,124	0
31	MG	X	6063	1/1	0.97	0.31	-	87,87,87,87	0
31	MG	X	6124	1/1	0.68	0.58	-	100,100,100,100	0
31	MG	X	6028	1/1	0.92	0.31	-	75,75,75,75	0
31	MG	X	6081	1/1	0.96	0.34	-	90,90,90,90	0
31	MG	X	6168	1/1	0.54	0.67	-	100,100,100,100	0
31	MG	X	6154	1/1	0.90	0.67	-	96,96,96,96	0
31	MG	X	6111	1/1	0.71	0.41	-	98,98,98,98	0
31	MG	X	6096	1/1	0.93	0.33	-	99,99,99,99	0
31	MG	X	6141	1/1	0.78	0.39	-	87,87,87,87	0
31	MG	X	6009	1/1	0.94	0.31	-	50,50,50,50	0
31	MG	X	6048	1/1	0.95	0.57	-	66,66,66,66	0
31	MG	X	6098	1/1	0.87	0.21	-	71,71,71,71	0
31	MG	X	6035	1/1	0.76	0.46	-	80,80,80,80	0
31	MG	X	6123	1/1	0.93	0.55	-	89,89,89,89	0
31	MG	X	6175	1/1	0.86	0.54	-	121,121,121,121	0
31	MG	X	6052	1/1	0.81	0.43	-	86,86,86,86	0
31	MG	X	6128	1/1	0.96	0.22	-	131,131,131,131	0
31	MG	X	6146	1/1	0.89	0.16	-	125,125,125,125	0
31	MG	X	6112	1/1	0.71	0.34	-	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
31	MG	X	6113	1/1	0.93	0.59	-	143,143,143,143	0
31	MG	X	6057	1/1	0.95	0.69	-	92,92,92,92	0
31	MG	X	6145	1/1	0.94	0.39	-	84,84,84,84	0
31	MG	X	6094	1/1	0.94	0.38	-	95,95,95,95	0
31	MG	X	6163	1/1	0.75	0.33	-	82,82,82,82	0
31	MG	X	6097	1/1	0.90	0.52	-	122,122,122,122	0
31	MG	X	6106	1/1	0.92	0.50	-	100,100,100,100	0
31	MG	Y	204	1/1	0.88	0.60	-	116,116,116,116	0
31	MG	X	6077	1/1	0.92	0.56	-	80,80,80,80	0
31	MG	X	6116	1/1	0.78	0.68	-	99,99,99,99	0
31	MG	X	6058	1/1	0.86	0.34	-	70,70,70,70	0
31	MG	X	6091	1/1	0.88	0.27	-	72,72,72,72	0
31	MG	Y	203	1/1	0.81	0.76	-	96,96,96,96	0
31	MG	X	6010	1/1	0.90	0.50	-	64,64,64,64	0
31	MG	X	6118	1/1	0.62	0.42	-	82,82,82,82	0
31	MG	X	6153	1/1	0.88	0.30	-	114,114,114,114	0
31	MG	X	6114	1/1	0.61	0.71	-	93,93,93,93	0
31	MG	X	6015	1/1	0.82	0.27	-	74,74,74,74	0
31	MG	X	6047	1/1	0.84	0.26	-	79,79,79,79	0
31	MG	X	6065	1/1	0.87	0.28	-	93,93,93,93	0
31	MG	X	6159	1/1	0.77	1.14	-	109,109,109,109	0
31	MG	X	6138	1/1	0.93	0.16	-	86,86,86,86	0
31	MG	X	6103	1/1	0.50	0.24	-	126,126,126,126	0
31	MG	X	6161	1/1	0.68	0.23	-	113,113,113,113	0
31	MG	Y	205	1/1	0.77	0.65	-	123,123,123,123	0
31	MG	X	6151	1/1	0.94	0.16	-	88,88,88,88	0
31	MG	X	6133	1/1	0.81	0.48	-	91,91,91,91	0
31	MG	X	6030	1/1	0.82	0.33	-	101,101,101,101	0
31	MG	X	6102	1/1	0.96	0.30	-	98,98,98,98	0
31	MG	X	6061	1/1	0.83	0.23	-	100,100,100,100	0
31	MG	X	6027	1/1	0.94	0.72	-	65,65,65,65	0
31	MG	X	6050	1/1	0.98	0.45	-	91,91,91,91	0
31	MG	X	6029	1/1	0.91	0.40	-	82,82,82,82	0
31	MG	X	6157	1/1	0.90	0.56	-	96,96,96,96	0
31	MG	X	6136	1/1	0.95	0.68	-	84,84,84,84	0
31	MG	X	6125	1/1	0.72	0.49	-	109,109,109,109	0
31	MG	X	6034	1/1	0.94	0.27	-	69,69,69,69	0
31	MG	X	6080	1/1	0.94	0.70	-	82,82,82,82	0
31	MG	X	6150	1/1	0.80	0.47	-	97,97,97,97	0
31	MG	X	6075	1/1	0.81	0.26	-	85,85,85,85	0
31	MG	X	6117	1/1	0.90	0.42	-	130,130,130,130	0
31	MG	X	6173	1/1	0.81	0.14	-	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
31	MG	X	6095	1/1	0.93	0.58	-	78,78,78,78	0
31	MG	X	6170	1/1	0.81	0.37	-	97,97,97,97	0
31	MG	X	6049	1/1	0.78	0.40	-	91,91,91,91	0
31	MG	H	201	1/1	0.90	0.14	-	104,104,104,104	0
31	MG	X	6130	1/1	0.87	0.41	-	132,132,132,132	0
31	MG	X	6122	1/1	0.91	0.36	-	84,84,84,84	0
31	MG	X	6121	1/1	0.93	0.60	-	85,85,85,85	0
31	MG	X	6176	1/1	0.69	0.56	-	73,73,73,73	0
31	MG	X	6020	1/1	0.82	0.45	-	76,76,76,76	0
31	MG	X	6082	1/1	0.94	0.69	-	105,105,105,105	0
31	MG	X	6069	1/1	0.91	0.35	-	65,65,65,65	0
31	MG	X	6067	1/1	0.98	0.18	-	72,72,72,72	0
31	MG	X	6070	1/1	0.81	0.47	-	69,69,69,69	0
31	MG	X	6043	1/1	0.92	0.39	-	106,106,106,106	0
31	MG	X	6073	1/1	0.93	0.30	-	105,105,105,105	0
31	MG	X	6139	1/1	0.72	0.43	-	113,113,113,113	0
31	MG	X	6155	1/1	0.81	0.80	-	108,108,108,108	0
31	MG	X	6040	1/1	0.94	0.55	-	63,63,63,63	0
31	MG	X	6089	1/1	0.94	0.26	-	89,89,89,89	0

6.5 Other polymers (i)

There are no such residues in this entry.