



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 10:59 AM GMT

PDB ID : 4KD0  
Title : 70S Ribosome translocation intermediate GDPNP-I containing elongation factor EFG/GDPNP, MRNA, AND TRNA BOUND IN THE  $pe^*/E$  STATE. THIS ENTRY CONTAINS THE 30S RIBOSOMAL SUBUNIT B. THE 50S SUBUNIT B CAN BE FOUND IN 4KD2. MOLECULE A IN THE SAME ASYMMETRIC UNIT IS DEPOSITED AS 4KCY (30S) AND 4KCZ (50S)  
Authors : Zhou, J.; Lancaster, L.; Donohue, J.P.; Noller, H.F.  
Deposited on : 2013-04-24  
Resolution : 3.50 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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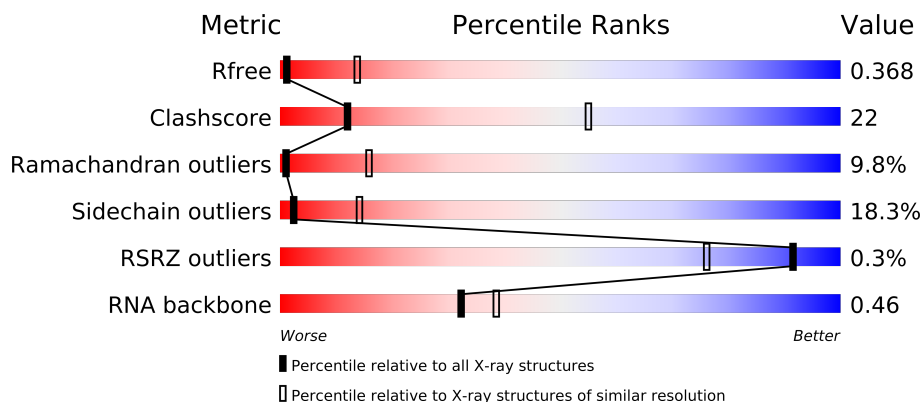
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.50 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.



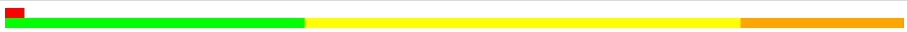
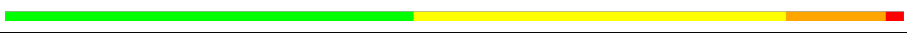
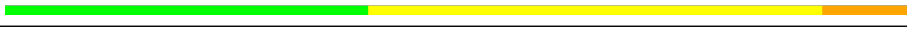

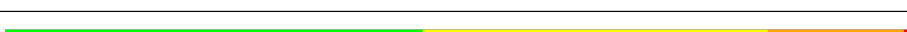

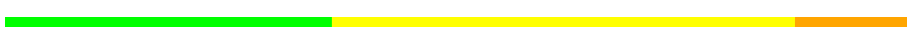
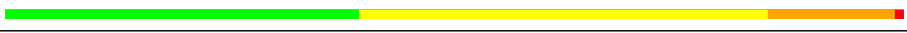
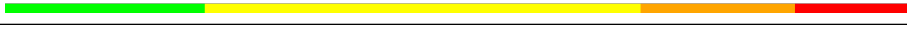

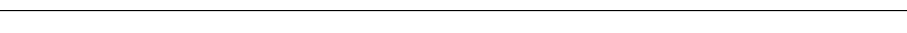

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1243 (3.70-3.30)
Clashscore	79885	1039 (3.66-3.34)
Ramachandran outliers	78287	1000 (3.66-3.34)
Sidechain outliers	78261	1000 (3.66-3.34)
RSRZ outliers	66119	1243 (3.70-3.30)
RNA backbone	1838	1007 (4.22-2.76)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	B	235	
2	C	207	
3	D	208	
4	E	151	
5	F	101	
6	G	155	
7	H	138	
8	I	127	
9	J	99	
10	K	119	
11	L	125	
12	M	125	

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Mol	Chain	Length	Quality of chain
13	N	60	
14	O	88	
15	P	84	
16	Q	100	
17	R	70	
18	S	79	
19	T	99	
20	A	1511	
21	W	77	
22	V	23	
23	Y	687	
24	U	6	

## 2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 59087 atoms, of which 0 are hydrogen and 0 are deuterium.

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 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	235	Total	C	N	O	S	0	0	0
			1910	1218	342	345	5			

- Molecule 2 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	207	Total	C	N	O	S	0	0	0
			1621	1022	315	283	1			

- Molecule 3 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	151	Total	C	N	O	S	0	0	0
			1156	729	218	205	4			

- Molecule 5 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 6 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 7 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 8 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	127	Total	C	N	O	S	0	0	0
			1011	639	198	174				

- Molecule 9 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	99	Total	C	N	O	S	0	0	0
			802	504	157	140	1			

- Molecule 10 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	K	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 11 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	125	Total	C	N	O	S	0	0	0
			976	614	196	165	1			

- Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	125	Total	C	N	O	S	0	0	0
			997	617	207	171	2			

- Molecule 13 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 14 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	O	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 15 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	P	84	Total	C	N	O	S	0	0	0
			706	446	140	119	1			

- Molecule 16 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	Q	100	Total	C	N	O	S	0	0	0
			835	534	156	143	2			

- Molecule 17 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	R	70	Total	C	N	O	S	0	0	0
			574	367	112	95				

- Molecule 18 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	S	79	Total	C	N	O	S	0	0	0
			634	405	115	112	2			

- Molecule 19 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	T	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

- Molecule 20 is a RNA chain called ribosomal RNA 16S.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	A	1511	Total	C	N	O	P	0	0	0
			32474	14455	6015	10494	1510			

- Molecule 21 is a RNA chain called transfer RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	W	77	Total	C	N	O	P	0	0	0
			1635	732	291	536	76			

- Molecule 22 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	23	Total	C	N	O	P	0	0	0
			503	227	106	148	22			

- Molecule 23 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	Y	687	Total	C	N	O	S	0	0	0
			5380	3414	922	1024	20			

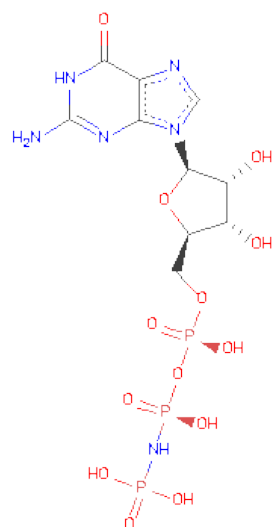
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	129	LYS	HIS	CONFLICT	UNP Q72I01
Y	226	ASN	HIS	CONFLICT	UNP Q72I01

- Molecule 24 is a protein called VIOMYCIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	U	6	Total	C	N	O	0	0	0
			48	25	13	10			

- Molecule 25 is PHOSPHOAMINOPHOSPHONICACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>13</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	Y	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

- Molecule 26 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

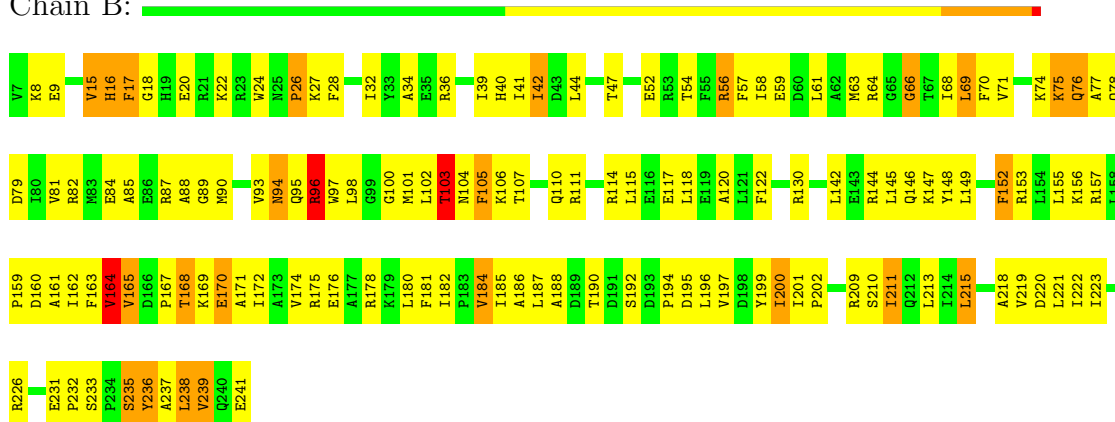
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	Y	1	Total	Mg	0	0
			1	1		

### 3 Residue-property plots

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

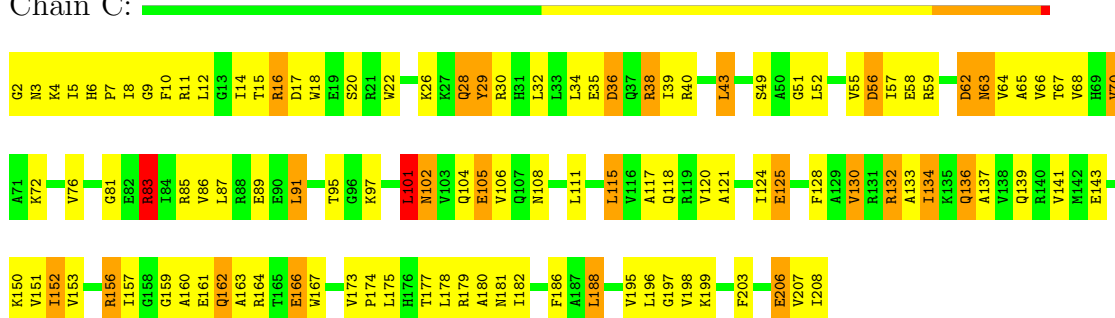
#### • Molecule 1: 30S ribosomal protein S2

Chain B:



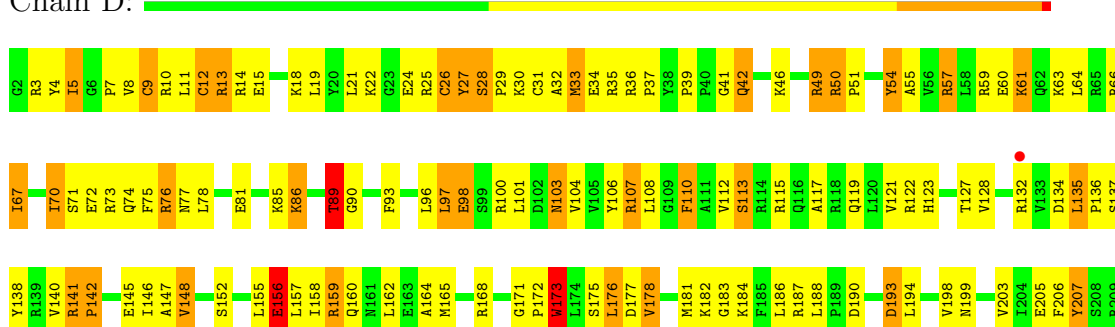
#### • Molecule 2: 30S ribosomal protein S3

Chain C:



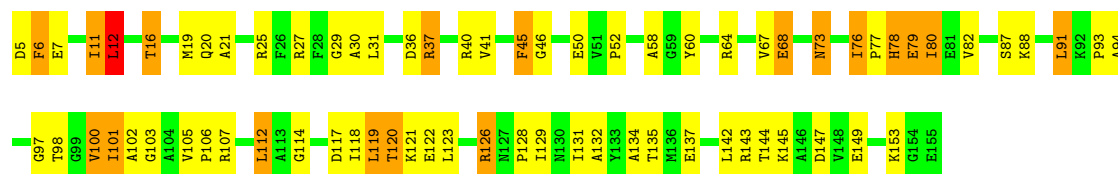
#### • Molecule 3: 30S ribosomal protein S4

Chain D:



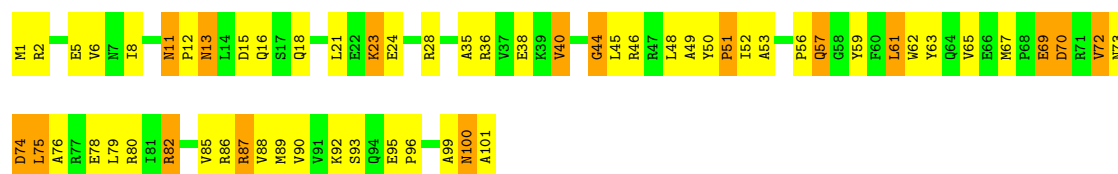
- Molecule 4: 30S ribosomal protein S5

Chain E: 



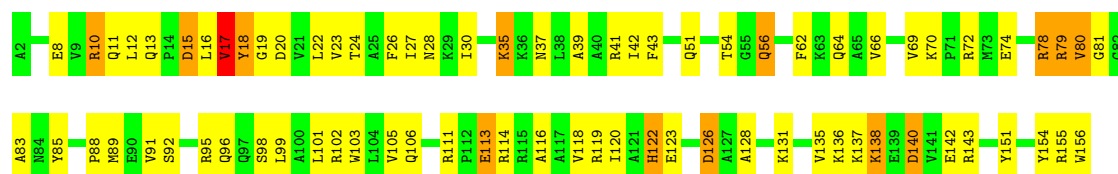
- Molecule 5: 30S ribosomal protein S6

Chain F: 



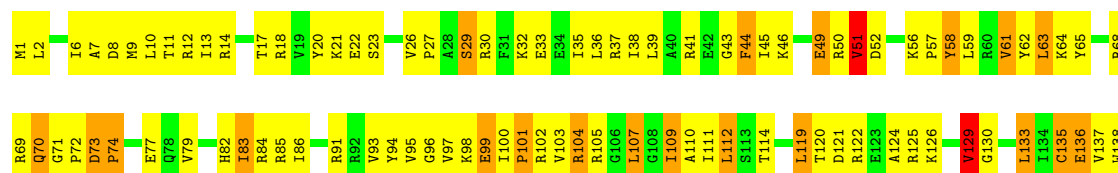
- Molecule 6: 30S ribosomal protein S7

Chain G: 



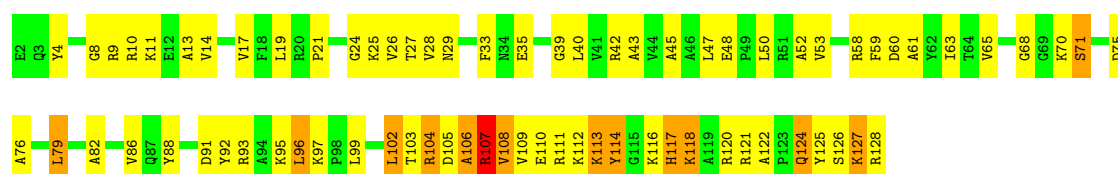
- Molecule 7: 30S ribosomal protein S8

Chain H: 



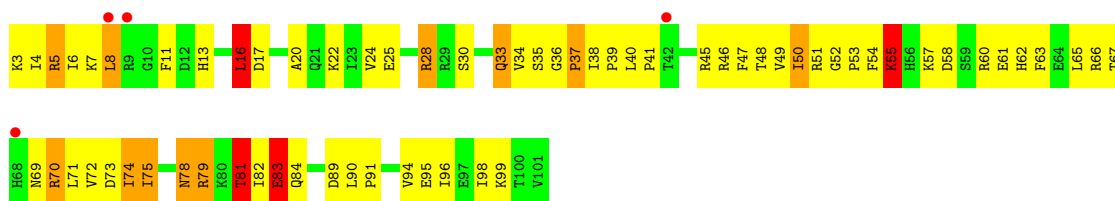
- Molecule 8: 30S ribosomal protein S9

Chain I: 



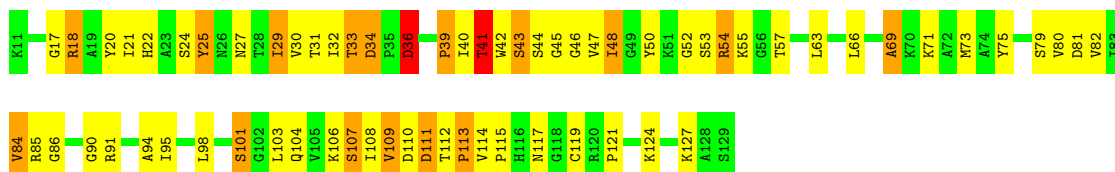
- Molecule 9: 30S ribosomal protein S10

Chain J: 



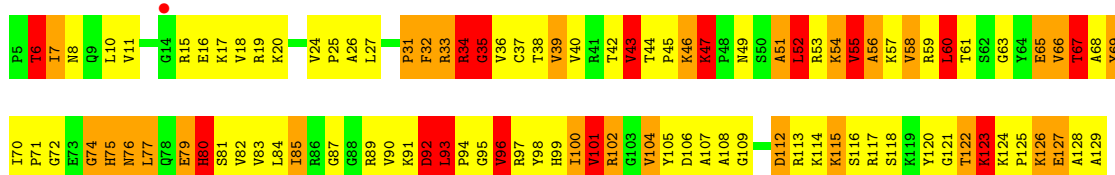
• Molecule 10: 30S ribosomal protein S11

Chain K:



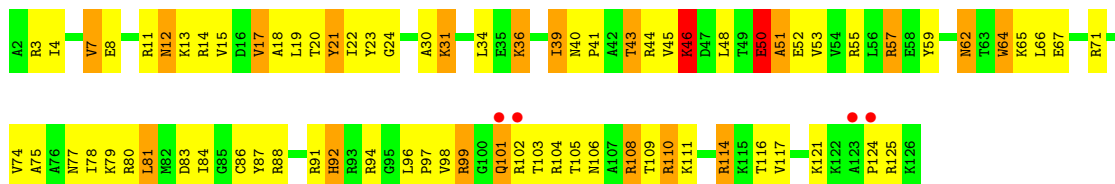
• Molecule 11: 30S ribosomal protein S12

Chain L:



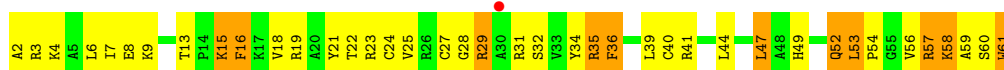
• Molecule 12: 30S ribosomal protein S13

Chain M:



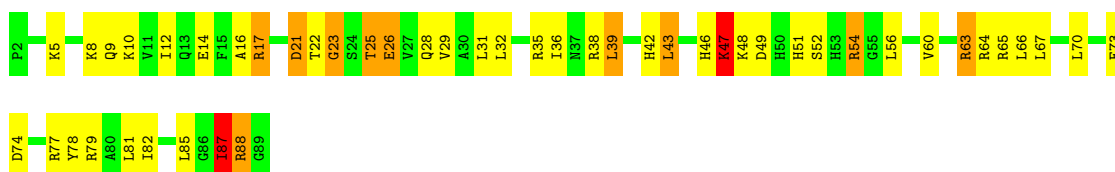
• Molecule 13: 30S ribosomal protein S14 type Z

Chain N:



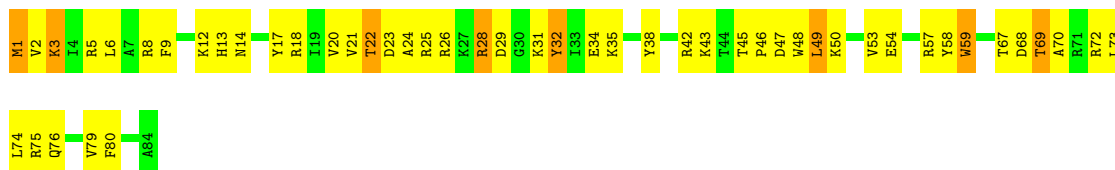
• Molecule 14: 30S ribosomal protein S15

Chain O:



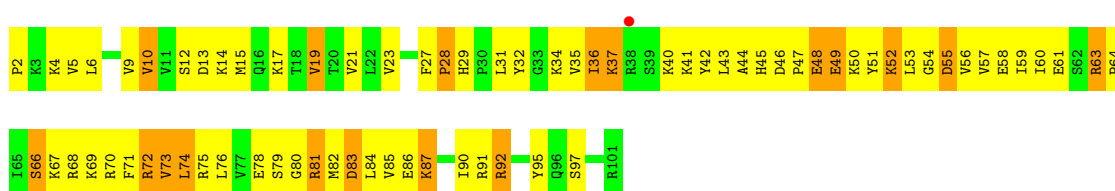
- Molecule 15: 30S ribosomal protein S16

Chain P:



- Molecule 16: 30S ribosomal protein S17

Chain Q:



- Molecule 17: 30S ribosomal protein S18

Chain R:



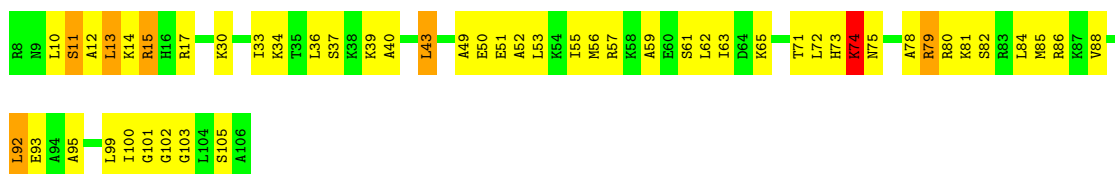
- Molecule 18: 30S ribosomal protein S19

Chain S:



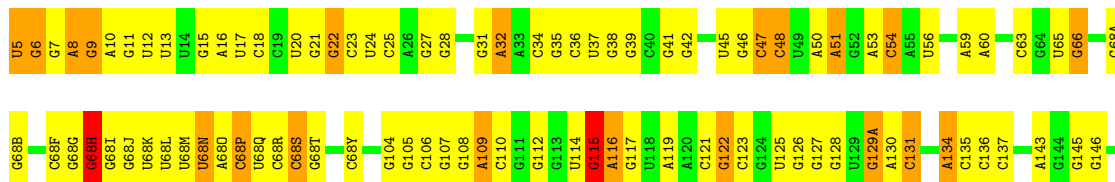
- Molecule 19: 30S ribosomal protein S20

Chain T:

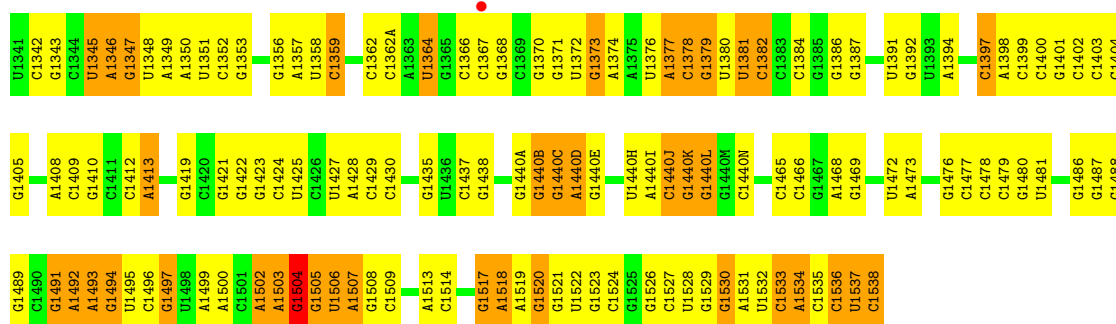


- Molecule 20: ribosomal RNA 16S

Chain A:

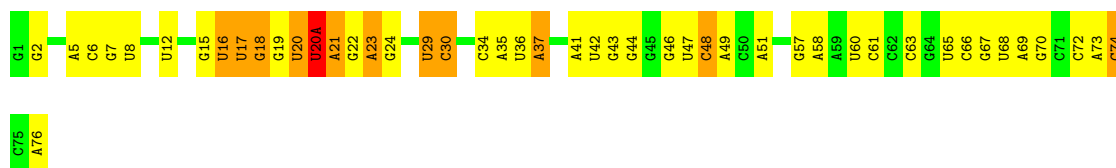


U1278	A1279	U1280	U1281	C1282	U1283	C1284	U1285	A1286	U1287	A1288	U1289	C1290	U1291	U1292	C1293	A1294	U1295	U1298	C1299	U1300	U1301	C1302	U1303	C1304	U1305	A1306	U1309	C1310	U1313	C1314	U1315	U1316	C1317	U1318	A1319	C1320	U1321	C1322	U1323	C1324	U1325	C1326	U1327	U1328	A1329	U1330	C1331	U1332	A1333	U1334	C1335	U1338	A1339																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
U1212	U1213	C1214	U1215	U1216	C1217	U1218	C1219	U1220	C1221	U1222	C1223	U1224	C1225	U1226	C1227	U1228	C1229	U1230	C1231	U1232	C1233	U1234	C1235	U1236	C1237	U1238	C1239	U1240	C1241	U1245	C1246	U1247	A1248	C1249	U1250	C1251	U1252	C1253	U1254	C1255	U1256	C1257	U1258	C1259	U1260	C1261	U1262	C1263	U1264	C1265	U1268	C1269	U1270	C1271	U1272	C1273	U1274																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
A1130	G1131	U1132	U1133	U1135	C1136	C1137	U1138	C1139	U1140	C1141	U1142	C1143	U1144	C1145	U1146	C1147	U1148	C1149	U1150	A1151	U1152	U1157	C1158	U1159	C1160	U1161	C1162	U1171	C1172	U1173	C1174	U1178	A1179	U1180	C1181	U1182	C1183	U1184	C1185	U1186	C1187	U1188	C1189	U1190	C1191	U1192	C1193	U1194	C1195	U1196	C1197	U1198	C1199	U1204	U1205	C1206	U1207	C1208	U1209	C1212	U1213	C1214	U1215	C1216	U1217	C1218	U1219	C1220	U1221	C1222	U1223	C1224	U1225	C1226	U1227	C1228	U1229	C1230	U1231	C1232	U1233	C1234	U1235	C1236	U1237	C1238	U1239	C1240	U1241	C1242	U1243	C1244	U1245	C1246	U1247	C1248	U1249	C1250	U1251	C1252	U1253	C1254	U1255	C1256	U1257	C1258	U1259	C1260	U1261	C1262	U1263	C1264	U1265	U1268	C1269	U1270	C1271	U1272	C1273	U1274	C1275	U1276	C1277	U1278	C1279	U1280	C1281	U1282	C1283	U1284	C1285	U1286	C1287	U1288	C1289	U1290	C1291	U1292	C1293	U1294	C1295	U1296	C1297	U1298	C1299	U1300	C1301	U1302	C1303	U1304	C1305	U1306	C1307	U1308	C1309	U1310	C1311	U1312	C1313	U1314	C1315	U1316	C1317	U1318	C1319	U1320	C1321	U1322	C1323	U1324	C1325	U1326	C1327	U1328	C1329	U1330	C1331	U1332	C1333	U1334	C1335	U1336	C1337	U1338	C1339	U1340	C1341	U1342	C1343	U1344	C1345	U1346	C1347	U1348	C1349	U1350	C1351	U1352	C1353	U1354	C1355	U1356	C1357	U1358	C1359	U1360	C1361	U1362	C1363	U1364	C1365	U1366	C1367	U1368	C1369	U1370	C1371	U1372	C1373	U1374	C1375	U1376	C1377	U1378	C1379	U1380	C1381	U1382	C1383	U1384	C1385	U1386	C1387	U1388	C1389	U1390	C1391	U1392	C1393	U1394	C1395	U1396	C1397	U1398	C1399	U1400	C1401	U1402	C1403	U1404	C1405	U1406	C1407	U1408	C1409	U1410	C1411	U1412	C1413	U1414	C1415	U1416	C1417	U1418	C1419	U1420	C1421	U1422	C1423	U1424	C1425	U1426	C1427	U1428	C1429	U1430	C1431	U1432	C1433	U1434	C1435	U1436	C1437	U1438	C1439	U1440	C1441	U1442	C1443	U1444	C1445	U1446	C1447	U1448	C1449	U1450	C1451	U1452	C1453	U1454	C1455	U1456	C1457	U1458	C1459	U1460	C1461	U1462	C1463	U1464	C1465	U1466	C1467	U1468	C1469	U1470	C1471	U1472	C1473	U1474	C1475	U1476	C1477	U1478	C1479	U1480	C1481	U1482	C1483	U1484	C1485	U1486	C1487	U1488	C1489	U1490	C1491	U1492	C1493	U1494	C1495	U1496	C1497	U1498	C1499	U1500	C1501	U1502	C1503	U1504	C1505	U1506	C1507	U1508	C1509	U1510	C1511	U1512	C1513	U1514	C1515	U1516	C1517	U1518	C1519	U1520	C1521	U1522	C1523	U1524	C1525	U1526	C1527	U1528	C1529	U1530	C1531	U1532	C1533	U1534	C1535	U1536	C1537	U1538	C1539	U1540	C1541	U1542	C1543	U1544	C1545	U1546	C1547	U1548	C1549	U1550	C1551	U1552	C1553	U1554	C1555	U1556	C1557	U1558	C1559	U1560	C1561	U1562	C1563	U1564	C1565	U1566	C1567	U1568	C1569	U1570	C1571	U1572	C1573	U1574	C1575	U1576	C1577	U1578	C1579	U1580	C1581	U1582	C1583	U1584	C1585	U1586	C1587	U1588	C1589	U1590	C1591	U1592	C1593	U1594	C1595	U1596	C1597	U1598	C1599	U1600	C1601	U1602	C1603	U1604	C1605	U1606	C1607	U1608	C1609	U1610	C1611	U1612	C1613	U1614	C1615	U1616	C1617	U1618	C1619	U1620	C1621	U1622	C1623	U1624	C1625	U1626	C1627	U1628	C1629	U1630	C1631	U1632	C1633	U1634	C1635	U1636	C1637	U1638	C1639	U1640	C1641	U1642	C1643	U1644	C1645	U1646	C1647	U1648	C1649	U1650	C1651	U1652	C1653	U1654	C1655	U1656	C1657	U1658	C1659	U1660	C1661	U1662	C1663	U1664	C1665	U1666	C1667	U1668	C1669	U1670	C1671	U1672	C1673	U1674	C1675	U1676	C1677	U1678	C1679	U1680	C1681	U1682	C1683	U1684	C1685	U1686	C1687	U1688	C1689	U1690	C1691	U1692	C1693	U1694	C1695	U1696	C1697	U1698	C1699	U1700	C1701	U1702	C1703	U1704	C1705	U1706	C1707	U1708	C1709	U1710	C1711	U1712	C1713	U1714	C1715	U1716	C1717	U1718	C1719	U1720	C1721	U1722	C1723	U1724	C1725	U1726	C1727	U1728	C1729	U1730	C1731	U1732	C1733	U1734	C1735	U1736	C1737	U1738	C1739	U1740	C1741	U1742	C1743	U1744	C1745	U1746	C1747	U1748	C1749	U1750	C1751	U1752	C1753	U1754	C1755	U1756	C1757	U1758	C1759	U1760	C1761	U1762	C1763	U1764	C1765	U1766	C1767	U1768	C1769	U1770	C1771	U1772	C1773	U1774	C1775	U1776	C1777	U1778	C1779	U1780	C1781	U1782	C1783	U1784	C1785	U1786	C1787	U1788	C1789	U1790	C1791	U1792	C1793	U1794	C1795	U1796	C1797	U1798	C1799	U1800	C1801	U1802	C1803	U1804	C1805	U1806	C1807	U1808	C1809	U1810	C1811	U1812	C1813	U1814	C1815	U1816	C1817	U1818	C1819	U1820	C1821	U1822	C1823	U1824	C1825	U1826	C1827	U1828	C1829	U1830	C1831	U1832	C1833	U1834	C1835	U1836	C1837	U1838	C1839	U1840	C1841	U1842	C1843	U1844	C1845	U1846	C1847	U1848	C1849	U1850	C1851	U1852	C1853	U1854	C1855	U1856	C1857	U1858	C1859	U1860	C1861	U1862	C1863	U1864	C1865	U1866	C1867	U1868	C1869	U1870	C1871	U1872	C1873	U1874	C1875	U1876	C1877	U1878	C1879	U1880	C1881	U1882	C1883	U1884	C1885	U1886	C1887	U1888	C1889	U1890	C1891	U1892	C1893	U1894	C1895	U1896	C1897	U1898	C1899	U1900	C1901	U1902	C1903	U1904	C1905	U1906	C1907	U1908	C1909	U1910	C1911	U1912	C1913	U1914	C1915	U1916	C1917	U1918	C1919	U1920	C1921	U1922	C1923	U1924	C1925	U1926	C1927	U1928	C1929	U1930	C1931	U1932	C1933	U1934	C1935	U1936	C1937	U1938	C1939	U1940	C1941	U1942	C1943	U1944	C1945	U1946	C1947	U1948	C1949	U1950	C1951	U1952	C1953	U1954	C1955	U1956	C1957	U1958	C1959	U1960	C1961	U1962	C1963	U1964	C1965	U1966	C1967	U1968	C1969	U1970	C1971	U1972	C1973	U1974	C1975	U1976	C1977	U1978	C1979	U1980	C1981	U1982	C1983	U1984	C1985	U1986	C1987	U1988	C1989	U1990	C1991	U1992	C1993	U1994	C1995	U1996	C1997	U1998	C1999	U2000	C2001	U2002	C2003	U2004	C2005	U2006	C2007	U2008	C2009	U2010	C2011	U2012	C2013	U2014	C2015	U2016	C2017	U2018	C2019	U2020	C2021	U2022	C2023	U2024	C2025	U2026	C2027	U2028	C2029	U2030	C2031	U2032	C2033	U2034	C2035	U2036	C2037	U2038	C2039	U2040	C2041	U2042	C2043	U2044	C2045	U2046	C2047	U2048	C2049	U2050	C2051	U2052	C2053	U2054	C2055	U2056	C2057	U2058	C2059	U2060	C2061	U2062	C2063	U2064	C2065	U2066	C2067	U2068	C2069	U2070	C2071	U2072	C2073	U2074	C2075	U2076	C2077	U2078	C2079	U2080	C2081	U2082	C2083	U2084	C2085	U2086	C2087	U2088	C2089	U2090	C2091	U2092	C2093	U2094	C2095	U2096	C2097	U2098	C2099	U2100	C2101	U2102	C2103	U2104	C2105	U2106	C2107	U2108	C2109	U2110	C2111	U2112	C2113	U2114	C2115	U2116	C2117	U2118	C2119	U2120	C2121	U2122	C2123	U2124	C2125	U2126	C2127	U2128	C2129	U2130	C2131	U2132	C2133	U2134	C2135	U2136	C2137	U2138	C2139	U2140	C2141	U2142	C2143	U2144	C2145	U2146	C2147	U2148	C2149	U2150	C2151	U2152	C2153	U2154	C2155	U2156	C2157	U2158	C2159	U2160	C2161	U2162	C2163	U2164	C2165	U2166	C2167	U2168	C2169	U2170	C2171	U2172	C2173	U2174	C2175	U2176	C2177	U2178	C2179	U2180	C2181	U2182	C2183	U2184	C2185	U2186	C2187	U2188	C2189	U2190	C2191	U2192	C2193	U2194	C2195	U2196	C2197	U2198	C2199	U2200	C2201	U2202	C2203	U2204	C2205	U2206	C2207	U2208	C2209	U2210	C2211	U2212	C2213	U2214	C2215	U2216	C2217	U2218	C2219	U2220	C2221	U2222	C2223	U2224	C2225	U2226	C2227	U2228	C2229	U2230	C2231	U2232	C2233	U2234	C2235	U2236	C2237	U2238	C2239	U2240	C2241	U2242	C2243	U2244	C2245	U2246	C2247	U2248	C2249	U2250	C2251	U2252	C2253	U2254	C2255	U2256	C2257	U2258	C2259	U2260	C2261	U2262	C2263	U2264	C2265	U2266	C2267	U2268	C2269	U2270	C2271	U2272	C2273	U2274	C2275	U2276	C2277	U2278	C2279	U2280	C2281	U2282	C2283	U2284	C2285	U2286	C2287	U2288	C2289	U2290	C2291	U2292	C2293	U2294	C2295	U2296	C2297	U2298	C2299	U2300	C2301	U2302	C2303	U2304	C2305	U2306	C2307	U2308	C2309	U2310	C2311	U2312	C2313	U2314	C2315	U2316	C2317	U2318	C2319	U2320	C2321	U2322	C2323	U2324	C2325	U2326	C2327	U2328	C2329	U2330	C2331	U2332	C2333	U2334	C2335	U2336	C2337	U2338	C2339	U2340	C2341	U2342	C2343



• Molecule 21: transfer RNA

Chain W:



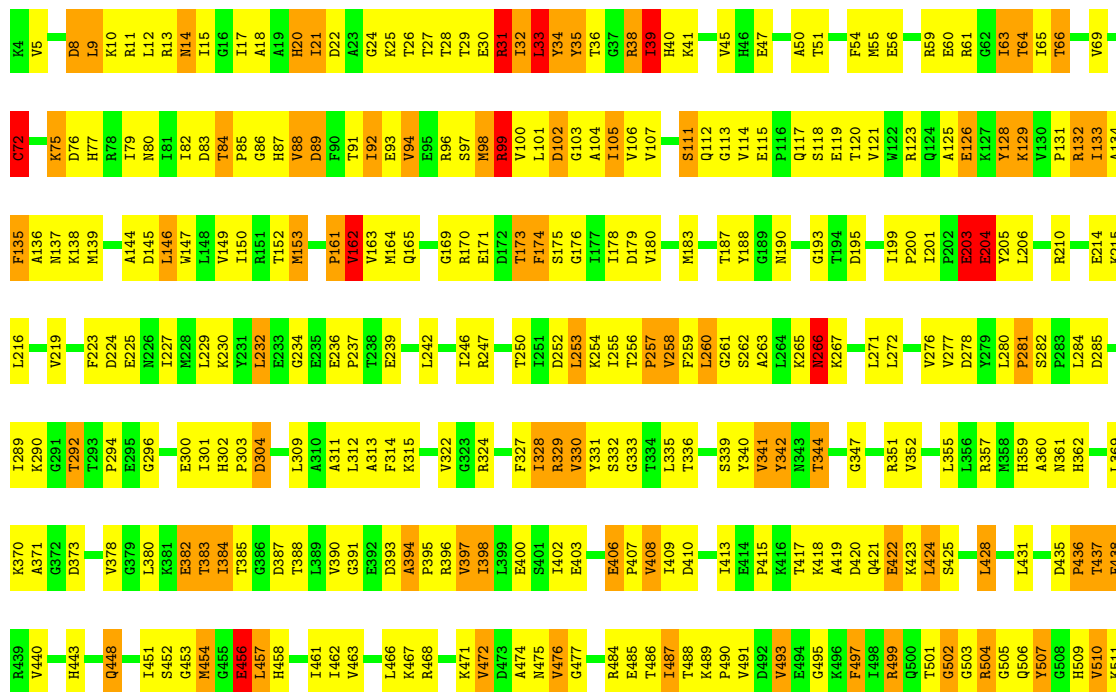
• Molecule 22: messenger RNA

Chain V:



• Molecule 23: Elongation factor G

Chain Y:





● Molecule 24: VIOMYCIN

Chain U:



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	306.01Å 673.49Å 351.98Å 90.00° 92.69° 90.00°	Depositor
Resolution (Å)	40.00 – 3.50 131.34 – 3.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.50) 74.9 (131.34-3.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.30 (at 3.49Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.262 , 0.309 0.366 , 0.368	Depositor DCC
$R_{free}$ test set	38207 reflections (4.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	80.5	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 271.9	EDS
Estimated twinning fraction	0.247 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.26$ , $\langle L^2 \rangle = 0.11$	Xtriage
Outliers	0 of 765681 reflections	Xtriage
$F_o, F_c$ correlation	0.59	EDS
Total number of atoms	59087	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GNP, DPP, MG, KBE, UAL, 5OH

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	B	0.40	0/1945	0.69	1/2621 (0.0%)
2	C	0.33	0/1645	0.58	1/2216 (0.0%)
3	D	0.34	0/1733	0.61	0/2318
4	E	0.34	0/1172	0.63	1/1576 (0.1%)
5	F	0.35	0/856	0.64	1/1154 (0.1%)
6	G	0.35	0/1276	0.58	0/1709
7	H	0.33	0/1136	0.57	0/1527
8	I	0.36	0/1029	0.61	1/1378 (0.1%)
9	J	0.33	0/815	0.65	1/1095 (0.1%)
10	K	0.37	0/900	0.63	0/1213
11	L	0.47	0/992	0.88	4/1327 (0.3%)
12	M	0.32	0/1008	0.58	0/1347
13	N	0.35	0/501	0.57	0/664
14	O	0.35	0/745	0.59	0/992
15	P	0.33	0/722	0.56	0/970
16	Q	0.42	0/848	0.71	0/1131
17	R	0.31	0/579	0.57	0/768
18	S	0.31	0/647	0.56	0/870
19	T	0.37	0/764	0.62	0/1006
20	A	0.38	0/36351	0.95	35/56736 (0.1%)
21	W	0.41	1/1827 (0.1%)	1.06	9/2845 (0.3%)
22	V	0.95	3/568 (0.5%)	1.74	19/886 (2.1%)
23	Y	0.52	7/5481 (0.1%)	0.76	12/7418 (0.2%)
24	U	1.06	0/11	1.28	0/13
All	All	0.40	11/63551 (0.0%)	0.87	85/93780 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
11	L	0	1
23	Y	0	8
All	All	0	10

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	Y	502	GLY	C-O	18.54	1.53	1.23
22	V	16	A	O3'-P	-10.50	1.48	1.61
23	Y	504	ARG	C-N	8.54	1.48	1.33
21	W	37	A	O3'-P	-8.36	1.51	1.61
22	V	15	A	N9-C4	-7.84	1.33	1.37
23	Y	499	ARG	C-N	6.39	1.48	1.34
22	V	16	A	N9-C4	6.18	1.41	1.37
23	Y	31	ARG	C-O	6.18	1.35	1.23
23	Y	72	CYS	CA-CB	-5.62	1.41	1.53
23	Y	33	LEU	CA-C	-5.30	1.39	1.52
23	Y	33	LEU	N-CA	5.27	1.56	1.46

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	W	37	A	P-O3'-C3'	19.49	143.09	119.70
22	V	16	A	P-O3'-C3'	18.93	142.41	119.70
23	Y	502	GLY	O-C-N	-12.85	101.35	123.20
23	Y	502	GLY	CA-C-N	12.59	141.38	116.20
23	Y	502	GLY	C-N-CA	11.35	146.14	122.30
22	V	15	A	N1-C6-N6	-10.80	112.12	118.60
22	V	16	A	O3'-P-O5'	-10.76	83.56	104.00
22	V	18	G	C8-N9-C4	-9.98	102.41	106.40
22	V	15	A	C8-N9-C4	9.20	109.48	105.80
21	W	74	C	C2-N1-C1'	9.09	128.80	118.80
20	A	1137	C	C2-N1-C1'	8.93	128.62	118.80
23	Y	503	GLY	O-C-N	-8.59	108.95	122.70
22	V	18	G	C2'-C3'-O3'	8.53	128.28	109.50
22	V	15	A	C4-C5-C6	-8.47	112.76	117.00
22	V	16	A	OP1-P-O3'	8.38	123.64	105.20
23	Y	33	LEU	CA-CB-CG	8.38	134.57	115.30
20	A	723	U	C2-N1-C1'	8.20	127.54	117.70
22	V	15	A	C5-C6-N1	8.16	121.78	117.70
23	Y	72	CYS	CB-CA-C	-8.07	94.26	110.40
20	A	1158	C	C2-N1-C1'	7.97	127.57	118.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1137	C	N1-C2-O2	7.94	123.67	118.90
20	A	201(C)	U	C2-N1-C1'	7.71	126.95	117.70
21	W	74	C	N1-C2-O2	7.38	123.33	118.90
22	V	15	A	C6-C5-N7	7.32	137.42	132.30
21	W	37	A	OP1-P-O3'	7.18	121.01	105.20
23	Y	72	CYS	CA-CB-SG	-7.05	101.30	114.00
20	A	1158	C	N1-C2-O2	7.05	123.13	118.90
20	A	1137	C	C6-N1-C1'	-6.85	112.58	120.80
23	Y	72	CYS	N-CA-CB	-6.80	98.36	110.60
22	V	15	A	N7-C8-N9	-6.73	110.43	113.80
8	I	58	ARG	NE-CZ-NH1	6.69	123.65	120.30
23	Y	503	GLY	C-N-CA	6.66	138.36	121.70
22	V	18	G	N7-C8-N9	6.54	116.37	113.10
20	A	748	C	P-O3'-C3'	6.52	127.53	119.70
20	A	924	C	C6-N1-C2	-6.46	117.72	120.30
21	W	74	C	C6-N1-C1'	-6.40	113.12	120.80
11	L	55	VAL	CB-CA-C	-6.38	99.28	111.40
23	Y	72	CYS	N-CA-C	6.38	128.22	111.00
20	A	1128	C	C2-N1-C1'	6.29	125.72	118.80
20	A	1158	C	C6-N1-C1'	-6.29	113.26	120.80
4	E	12	LEU	CA-CB-CG	6.19	129.54	115.30
22	V	18	G	N3-C4-C5	-6.18	125.51	128.60
20	A	881	G	C8-N9-C4	-6.17	103.93	106.40
11	L	60	LEU	CA-CB-CG	6.17	129.50	115.30
23	Y	503	GLY	CA-C-N	6.16	130.76	117.20
21	W	20(A)	U	P-O3'-C3'	6.11	127.03	119.70
21	W	74	C	N3-C2-O2	-6.01	117.69	121.90
22	V	19	G	C4-N9-C1'	5.96	134.25	126.50
20	A	872	A	O4'-C1'-N9	5.95	112.96	108.20
23	Y	33	LEU	CA-C-N	-5.75	104.55	117.20
20	A	723	U	C6-N1-C1'	-5.74	113.17	121.20
22	V	16	A	C5'-C4'-C3'	5.72	125.16	116.00
20	A	1504	G	P-O3'-C3'	5.72	126.56	119.70
20	A	201(C)	U	C5-C6-N1	5.70	125.55	122.70
22	V	18	G	C4'-C3'-O3'	5.67	124.34	113.00
20	A	1128	C	N1-C2-O2	5.66	122.30	118.90
20	A	1137	C	N3-C2-O2	-5.64	117.95	121.90
20	A	723	U	N1-C2-O2	5.62	126.74	122.80
20	A	201(C)	U	N1-C2-O2	5.62	126.73	122.80
20	A	992	U	P-O3'-C3'	5.59	126.41	119.70
21	W	74	C	C6-N1-C2	-5.58	118.07	120.30
22	V	16	A	N9-C4-C5	-5.52	103.59	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	V	17	U	C6-N1-C2	-5.50	117.70	121.00
20	A	421	U	C2-N1-C1'	5.47	124.26	117.70
2	C	188	LEU	CA-CB-CG	5.37	127.65	115.30
22	V	19	G	C8-N9-C1'	-5.37	120.02	127.00
20	A	68(H)	G	N1-C6-O6	-5.34	116.70	119.90
11	L	35	GLY	N-CA-C	5.33	126.43	113.10
21	W	30	C	C6-N1-C2	-5.31	118.18	120.30
20	A	1064	G	P-O3'-C3'	5.30	126.06	119.70
20	A	201(C)	U	N3-C2-O2	-5.30	118.49	122.20
9	J	16	LEU	CA-CB-CG	5.29	127.47	115.30
20	A	748	C	OP2-P-O3'	5.29	116.83	105.20
20	A	838(A)	U	C2-N1-C1'	5.27	124.02	117.70
20	A	421	U	N3-C2-O2	-5.26	118.52	122.20
20	A	421	U	N1-C2-O2	5.22	126.45	122.80
20	A	351	G	N3-C4-C5	-5.20	126.00	128.60
20	A	351	G	C8-N9-C4	-5.20	104.32	106.40
1	B	66	GLY	N-CA-C	5.17	126.03	113.10
5	F	75	LEU	CA-CB-CG	5.15	127.15	115.30
11	L	34	ARG	N-CA-C	5.10	124.76	111.00
20	A	1009	G	O4'-C1'-N9	5.08	112.26	108.20
20	A	687	A	P-O3'-C3'	5.03	125.73	119.70
20	A	717	C	C2-N1-C1'	5.01	124.31	118.80
20	A	115	G	P-O3'-C3'	5.01	125.71	119.70

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	163	PHE	Peptide
11	L	32	PHE	Peptide
23	Y	162	VAL	Peptide
23	Y	31	ARG	Peptide
23	Y	32	ILE	Peptide
23	Y	329	ARG	Peptide
23	Y	34	TYR	Peptide
23	Y	502	GLY	Mainchain,Peptide
23	Y	630	GLN	Peptide

## 5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1910	0	1957	98	0
2	C	1621	0	1688	67	0
3	D	1703	0	1763	120	0
4	E	1156	0	1213	54	0
5	F	843	0	857	38	0
6	G	1257	0	1296	61	0
7	H	1116	0	1177	73	0
8	I	1011	0	1043	54	0
9	J	802	0	849	61	0
10	K	885	0	904	61	0
11	L	976	0	1062	113	0
12	M	997	0	1072	72	0
13	N	492	0	529	35	0
14	O	734	0	771	42	0
15	P	706	0	725	39	0
16	Q	835	0	906	63	0
17	R	574	0	644	36	0
18	S	634	0	655	32	0
19	T	762	0	859	32	0
20	A	32474	0	16393	843	0
21	W	1635	0	831	52	0
22	V	503	0	252	34	0
23	Y	5380	0	5435	341	0
24	U	48	0	39	8	0
25	Y	32	0	13	32	0
26	Y	1	0	0	0	0
All	All	59087	0	42933	2172	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 22.

All (2172) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
21:W:37:A:C2	22:V:16:A:C2	1.85	1.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:Y:138:LYS:HE2	25:Y:701:GNP:C4	1.55	1.33
23:Y:138:LYS:HG2	25:Y:701:GNP:C6	1.57	1.31
23:Y:30:GLU:O	23:Y:33:LEU:N	1.69	1.24
23:Y:137:ASN:ND2	23:Y:263:ALA:H	1.45	1.15
20:A:1028(B):C:N4	20:A:1028(G):G:H1	1.49	1.11
21:W:37:A:C2	22:V:16:A:N3	2.19	1.10
23:Y:138:LYS:HG2	25:Y:701:GNP:N1	1.66	1.09
23:Y:25:LYS:HG3	25:Y:701:GNP:O1B	1.56	1.06
21:W:37:A:H2	22:V:16:A:N3	1.54	1.04
23:Y:138:LYS:HE2	25:Y:701:GNP:N9	1.74	1.03
20:A:1124:G:H1	20:A:1149:C:N4	1.59	1.01
1:B:87:ARG:HH22	1:B:233:SER:H	1.11	0.99
20:A:1127:G:N2	20:A:1145:C:N3	2.09	0.99
20:A:1127:G:H1	20:A:1145:C:H42	1.00	0.98
20:A:1536:C:H42	22:V:9:G:H1	1.12	0.95
20:A:1405:G:H1	20:A:1496:C:H42	1.13	0.94
21:W:37:A:N1	22:V:16:A:C2	2.34	0.94
23:Y:64:THR:HG21	25:Y:701:GNP:O3G	1.65	0.94
20:A:68(A):G:H1	20:A:68(Y):C:H42	1.14	0.94
20:A:1124:G:H1	20:A:1149:C:H42	0.97	0.94
20:A:1003:G:N1	20:A:1037:C:O2	2.00	0.94
21:W:37:A:N1	22:V:16:A:N1	2.16	0.93
23:Y:137:ASN:HD21	23:Y:263:ALA:H	1.14	0.93
20:A:376:G:H1	20:A:387:U:H3	1.17	0.93
11:L:54:LYS:HD3	11:L:70:ILE:HG12	1.50	0.92
20:A:151:A:H62	20:A:170:U:H3	0.99	0.91
20:A:1127:G:H1	20:A:1145:C:N4	1.68	0.91
3:D:157:LEU:HA	3:D:160:GLN:HB2	1.50	0.91
20:A:1028(C):G:N2	20:A:1028(F):A:C8	2.38	0.91
20:A:68(F):C:N3	20:A:68(T):G:N2	2.18	0.91
23:Y:32:ILE:O	23:Y:34:TYR:N	2.05	0.90
20:A:815:A:C2	20:A:1527:C:O2	2.25	0.90
3:D:175:SER:HB3	3:D:184:LYS:HB2	1.53	0.89
20:A:68(F):C:H42	20:A:68(T):G:H1	0.91	0.89
6:G:88:PRO:HD2	6:G:151:TYR:HB2	1.54	0.88
21:W:15:G:N2	21:W:48:C:H42	1.71	0.88
8:I:107:ARG:HA	20:A:1347:G:H5'	1.56	0.88
23:Y:137:ASN:ND2	23:Y:263:ALA:N	2.22	0.88
14:O:8:LYS:HE3	14:O:31:LEU:HD21	1.54	0.88
20:A:1028(B):C:N4	20:A:1028(G):G:N1	2.21	0.87
14:O:82:ILE:HG13	14:O:87:ILE:HG13	1.56	0.87
23:Y:138:LYS:CE	25:Y:701:GNP:C4	2.48	0.87

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:68(F):C:N4	20:A:68(T):G:H1	1.72	0.87
20:A:590:C:H42	20:A:649:G:H1	1.20	0.86
20:A:443:C:H42	20:A:491:G:H1	1.23	0.86
16:Q:27:PHE:HB3	16:Q:36:ILE:HG13	1.56	0.86
23:Y:138:LYS:CG	25:Y:701:GNP:C6	2.51	0.85
20:A:152:A:N6	20:A:169:C:O2	2.09	0.84
23:Y:56:GLU:HB2	23:Y:59:ARG:HE	1.41	0.84
11:L:33:ARG:HB3	11:L:60:LEU:HD12	1.60	0.83
11:L:54:LYS:HG2	11:L:70:ILE:HG23	1.61	0.83
9:J:40:LEU:HD22	9:J:41:PRO:HD2	1.60	0.83
21:W:37:A:C2	22:V:16:A:N1	2.46	0.83
23:Y:137:ASN:HD21	23:Y:263:ALA:N	1.75	0.82
21:W:15:G:H22	21:W:48:C:H42	1.22	0.82
23:Y:163:VAL:HG13	23:Y:258:VAL:HG23	1.59	0.82
20:A:1343:G:N2	20:A:1349:A:O2'	2.11	0.82
23:Y:524:GLU:HB2	23:Y:564:LYS:HG3	1.61	0.82
1:B:236:TYR:HA	1:B:239:VAL:HB	1.60	0.81
12:M:91:ARG:NH2	20:A:1226:C:OP2	2.14	0.81
6:G:113:GLU:HB2	6:G:119:ARG:HG2	1.63	0.81
23:Y:137:ASN:HD22	23:Y:262:SER:HA	1.46	0.80
20:A:936:C:H42	20:A:1379:G:H1	1.27	0.80
21:W:37:A:N3	22:V:16:A:C2	2.49	0.80
11:L:70:ILE:HG13	11:L:72:GLY:H	1.46	0.80
10:K:18:ARG:HB3	10:K:81:ASP:HB2	1.63	0.80
23:Y:72:CYS:SG	23:Y:79:ILE:N	2.55	0.80
21:W:15:G:H22	21:W:48:C:N4	1.79	0.79
20:A:666:G:OP2	20:A:725:G:N2	2.16	0.79
1:B:71:VAL:HB	1:B:164:VAL:HG22	1.65	0.79
23:Y:25:LYS:NZ	25:Y:701:GNP:PB	2.55	0.79
23:Y:413:ILE:HG13	23:Y:415:PRO:HD3	1.64	0.78
20:A:1028(B):C:C4	20:A:1028(G):G:N1	2.49	0.78
9:J:50:ILE:HG12	9:J:52:GLY:H	1.47	0.77
20:A:1261:A:H62	20:A:1274:G:H21	1.31	0.77
3:D:26:CYS:HA	3:D:31:CYS:HA	1.66	0.77
20:A:813:U:H2'	20:A:814:A:H8	1.48	0.77
14:O:54:ARG:HH21	20:A:579:G:H4'	1.47	0.77
23:Y:72:CYS:CB	23:Y:79:ILE:H	1.98	0.77
9:J:13:HIS:HA	9:J:16:LEU:HD12	1.66	0.77
20:A:1006:C:H42	20:A:1023:G:H1	1.32	0.77
20:A:933:G:H1	20:A:1384:C:H42	1.33	0.77
9:J:49:VAL:HG21	13:N:41:ARG:HB2	1.67	0.76
23:Y:511:LYS:HB2	23:Y:569:ASP:HB3	1.67	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:H:96:GLY:HA2	7:H:130:GLY:HA3	1.67	0.76
20:A:992:U:H3	20:A:1044:A:H62	1.31	0.76
23:Y:117:GLN:NE2	23:Y:665:GLY:O	2.19	0.76
18:S:36:ARG:NH1	18:S:52:TYR:O	2.19	0.76
1:B:235:SER:O	1:B:237:ALA:N	2.18	0.76
23:Y:25:LYS:HZ2	25:Y:701:GNP:PB	2.09	0.76
20:A:1536:C:N4	22:V:9:G:H1	1.81	0.76
23:Y:138:LYS:HG2	25:Y:701:GNP:C5	2.15	0.76
20:A:1503:A:N6	22:V:14:A:H3'	2.00	0.76
23:Y:608:VAL:HG12	23:Y:645:ALA:HB3	1.65	0.76
3:D:57:ARG:HB3	3:D:206:PHE:HB2	1.67	0.76
20:A:1405:G:H1	20:A:1496:C:N4	1.84	0.75
20:A:68(A):G:H1	20:A:68(Y):C:N4	1.84	0.75
20:A:962:C:H42	20:A:973:G:H1	1.31	0.75
1:B:88:ALA:HB1	1:B:222:ILE:HD11	1.66	0.75
3:D:24:GLU:HG2	3:D:112:VAL:HG11	1.67	0.75
1:B:171:ALA:HA	1:B:174:VAL:HB	1.69	0.75
23:Y:35:TYR:HD1	23:Y:36:THR:N	1.83	0.75
11:L:7:ILE:HA	11:L:10:LEU:HD12	1.69	0.74
23:Y:138:LYS:HE2	25:Y:701:GNP:C5	2.18	0.74
3:D:57:ARG:NH1	3:D:205:GLU:OE2	2.20	0.74
4:E:76:ILE:HG13	4:E:93:PRO:HG3	1.70	0.74
11:L:35:GLY:HA2	11:L:58:VAL:HG13	1.70	0.74
11:L:47:LYS:NZ	20:A:1492:A:OP2	2.12	0.74
19:T:65:LYS:NZ	20:A:195:A:OP1	2.21	0.74
23:Y:30:GLU:HG3	23:Y:31:ARG:HH11	1.51	0.74
11:L:85:ILE:HG23	11:L:98:TYR:HB3	1.70	0.74
23:Y:633:GLY:HA3	23:Y:644:ARG:HB2	1.69	0.73
23:Y:659:LEU:O	23:Y:663:THR:OG1	2.06	0.73
23:Y:614:GLU:HA	23:Y:617:MET:HB3	1.70	0.73
11:L:82:VAL:HB	11:L:105:TYR:HB2	1.70	0.73
23:Y:54:PHE:HB2	23:Y:60:GLU:HA	1.71	0.73
20:A:670:G:H1	20:A:736:C:H42	1.36	0.73
20:A:107:G:H3'	20:A:108:G:H21	1.54	0.73
21:W:37:A:C2	22:V:16:A:H2	1.99	0.73
20:A:922:G:H2'	20:A:923:A:C8	2.23	0.73
6:G:78:ARG:HB2	6:G:156:TRP:HB3	1.69	0.73
11:L:39:VAL:HG12	11:L:40:VAL:H	1.54	0.73
10:K:85:ARG:HG2	10:K:111:ASP:HB3	1.69	0.73
4:E:50:GLU:HG3	4:E:52:PRO:HD2	1.70	0.73
20:A:231:G:H2'	20:A:232:G:H8	1.54	0.73
20:A:151:A:N7	20:A:170:U:O4	2.22	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:Y:256:THR:O	23:Y:258:VAL:N	2.22	0.72
23:Y:30:GLU:O	23:Y:33:LEU:CA	2.37	0.72
2:C:6:HIS:HB3	2:C:9:GLY:H	1.54	0.72
20:A:68(H):G:H21	20:A:68(S):C:N4	1.88	0.72
23:Y:515:GLU:HG2	23:Y:516:PRO:HD2	1.70	0.72
11:L:31:PRO:HG3	20:A:553:A:H1'	1.70	0.72
23:Y:428:LEU:HD13	23:Y:440:VAL:HG21	1.71	0.72
20:A:1065:U:OP2	20:A:1190:G:N2	2.22	0.72
23:Y:133:ILE:HG22	23:Y:257:PRO:HG2	1.70	0.72
10:K:112:THR:O	17:R:84:LYS:NZ	2.21	0.72
3:D:147:ALA:HB2	3:D:182:LYS:HG3	1.72	0.72
14:O:74:ASP:HB3	14:O:77:ARG:HG2	1.72	0.72
20:A:1124:G:N2	20:A:1149:C:N3	2.31	0.72
23:Y:93:GLU:O	23:Y:97:SER:OG	2.07	0.72
11:L:90:VAL:HG22	11:L:96:VAL:HG11	1.70	0.71
9:J:55:LYS:HG2	20:A:963:G:H21	1.55	0.71
14:O:39:LEU:HD12	14:O:56:LEU:HB2	1.71	0.71
3:D:18:LYS:HB3	3:D:33:MET:HG2	1.71	0.71
2:C:130:VAL:HG21	2:C:157:ILE:HG23	1.72	0.71
11:L:56:ALA:HB3	11:L:68:ALA:HB3	1.72	0.71
23:Y:10:LYS:HG2	23:Y:284:LEU:HD22	1.70	0.71
20:A:112:G:H1	20:A:315:A:H61	1.38	0.71
23:Y:35:TYR:HE2	23:Y:72:CYS:HA	1.54	0.71
10:K:31:THR:HA	10:K:42:TRP:HA	1.71	0.71
10:K:33:THR:HA	10:K:39:PRO:HA	1.73	0.71
11:L:6:THR:O	11:L:8:ASN:N	2.22	0.71
19:T:74:LYS:HG2	19:T:75:ASN:H	1.55	0.71
14:O:39:LEU:HB3	14:O:56:LEU:HD13	1.72	0.71
20:A:201:C:H42	20:A:216:G:H1	1.39	0.71
23:Y:467:LYS:HA	23:Y:472:VAL:H	1.56	0.70
17:R:61:LYS:NZ	20:A:836:G:OP1	2.23	0.70
23:Y:342:TYR:HB3	23:Y:390:VAL:HG23	1.73	0.70
3:D:33:MET:N	3:D:33:MET:SD	2.63	0.70
7:H:46:LYS:HB3	7:H:62:TYR:HB2	1.71	0.70
11:L:93:LEU:O	11:L:95:GLY:N	2.24	0.70
23:Y:201:ILE:HG21	23:Y:206:LEU:HB2	1.72	0.70
12:M:3:ARG:HH12	12:M:7:VAL:HG22	1.57	0.70
20:A:293:G:O6	20:A:304:U:O2	2.09	0.70
12:M:78:ILE:HD11	20:A:1309:G:H5'	1.72	0.70
10:K:50:TYR:HB3	10:K:55:LYS:HA	1.71	0.70
1:B:167:PRO:O	1:B:171:ALA:HB2	1.91	0.70
23:Y:493:VAL:HB	23:Y:512:ILE:HD11	1.73	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
15:P:20:VAL:HG23	15:P:35:LYS:HA	1.73	0.70
13:N:24:CYS:HA	13:N:39:LEU:HA	1.73	0.70
14:O:48:LYS:HB2	20:A:668:G:H4'	1.74	0.70
20:A:7:G:H5'	20:A:298:A:H5'	1.73	0.70
20:A:664:G:N2	20:A:741:G:O6	2.24	0.70
3:D:108:LEU:HD21	3:D:183:GLY:HA3	1.73	0.70
23:Y:247:ARG:NH1	23:Y:278:ASP:O	2.24	0.69
20:A:815:A:H2	20:A:1527:C:O2	1.72	0.69
6:G:111:ARG:HB3	6:G:113:GLU:HG2	1.74	0.69
2:C:56:ASP:HB2	2:C:67:THR:HB	1.74	0.69
20:A:680:C:H42	20:A:710:G:H1	1.40	0.69
20:A:1127:G:H21	20:A:1147:C:H42	1.40	0.69
11:L:93:LEU:HB2	11:L:96:VAL:HG22	1.74	0.69
15:P:38:TYR:CZ	15:P:50:LYS:HG3	2.27	0.69
23:Y:34:TYR:OH	23:Y:47:GLU:O	2.09	0.69
23:Y:138:LYS:CG	25:Y:701:GNP:N1	2.53	0.69
8:I:110:GLU:OE2	8:I:113:LYS:NZ	2.24	0.69
23:Y:227:ILE:HA	23:Y:230:LYS:HB3	1.73	0.69
23:Y:87:HIS:NE2	23:Y:120:THR:OG1	2.25	0.69
23:Y:35:TYR:CE2	23:Y:72:CYS:HA	2.27	0.69
23:Y:72:CYS:HB3	23:Y:79:ILE:O	1.92	0.69
7:H:30:ARG:HD3	20:A:590:C:H5'	1.74	0.69
8:I:127:LYS:O	20:A:966:G:O2'	2.10	0.69
23:Y:294:PRO:HD3	23:Y:397:VAL:HA	1.74	0.69
20:A:47:C:H42	20:A:361:G:H1	1.40	0.69
1:B:88:ALA:HB2	1:B:219:VAL:HG13	1.74	0.69
20:A:231:G:H2'	20:A:232:G:C8	2.27	0.69
20:A:41:G:H2'	20:A:42:G:H8	1.58	0.69
20:A:137:C:H42	20:A:226:G:H1	1.41	0.69
11:L:25:PRO:HA	11:L:27:LEU:HG	1.74	0.69
4:E:98:THR:OG1	20:A:6:G:N2	2.24	0.69
20:A:936:C:N4	20:A:1379:G:H1	1.90	0.68
23:Y:9:LEU:HD11	23:Y:303:PRO:HB2	1.76	0.68
21:W:23:A:H2'	21:W:24:G:C8	2.28	0.68
23:Y:29:THR:O	23:Y:32:ILE:HB	1.94	0.68
3:D:115:ARG:HB3	20:A:407:G:H5''	1.76	0.68
11:L:49:ASN:ND2	20:A:529:G:O6	2.26	0.68
9:J:6:ILE:HG23	9:J:72:VAL:HB	1.76	0.68
16:Q:63:ARG:NH2	20:A:130:A:H5'	2.09	0.68
14:O:70:LEU:HD11	14:O:77:ARG:HD2	1.74	0.68
20:A:131:C:HO2'	20:A:262:A:HO2'	1.37	0.68
11:L:71:PRO:HG2	11:L:102:ARG:HG2	1.75	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:H:21:LYS:O	7:H:23:SER:N	2.27	0.68
4:E:144:THR:H	4:E:147:ASP:HB2	1.58	0.68
20:A:713:G:H21	20:A:777:A:H1'	1.58	0.68
20:A:946:A:H2'	20:A:947:G:C8	2.28	0.68
1:B:115:LEU:HA	1:B:118:LEU:HD12	1.75	0.68
11:L:89:ARG:HA	11:L:96:VAL:HB	1.76	0.67
7:H:14:ARG:NH1	20:A:876:G:O5'	2.27	0.67
23:Y:357:ARG:NH1	23:Y:373:ASP:OD1	2.27	0.67
10:K:41:THR:HB	10:K:71:LYS:HB2	1.76	0.67
11:L:58:VAL:HG12	11:L:60:LEU:H	1.58	0.67
20:A:68(F):C:H2'	20:A:68(G):G:H8	1.58	0.67
3:D:190:ASP:H	3:D:193:ASP:HB2	1.59	0.67
20:A:401:C:O2'	20:A:621:A:N3	2.27	0.67
7:H:68:ARG:HG3	7:H:74:PRO:HB3	1.75	0.67
6:G:137:LYS:HA	6:G:140:ASP:HB2	1.76	0.67
20:A:1057:G:H2'	20:A:1058:G:O4'	1.95	0.67
13:N:47:LEU:HB3	13:N:53:LEU:HD12	1.77	0.67
23:Y:509:HIS:HB3	23:Y:571:SER:HB3	1.76	0.67
20:A:590:C:N3	20:A:649:G:N2	2.36	0.67
20:A:789:U:N3	20:A:792:A:OP2	2.23	0.67
8:I:10:ARG:NH2	8:I:105:ASP:OD1	2.28	0.67
20:A:153:C:H42	20:A:168:G:H1	1.42	0.67
23:Y:91:THR:O	23:Y:93:GLU:N	2.28	0.66
8:I:61:ALA:HB1	8:I:63:ILE:HD11	1.76	0.66
21:W:18:G:O2'	21:W:57:G:N2	2.28	0.66
2:C:59:ARG:HD3	2:C:64:VAL:HG22	1.76	0.66
2:C:29:TYR:OH	13:N:54:PRO:O	2.12	0.66
1:B:42:ILE:HD11	1:B:202:PRO:HB2	1.77	0.66
23:Y:216:LEU:HD21	23:Y:246:ILE:HD11	1.77	0.66
11:L:100:ILE:HG22	11:L:101:VAL:H	1.60	0.66
5:F:6:VAL:HG22	5:F:90:VAL:HG13	1.76	0.66
11:L:87:GLY:HA2	11:L:98:TYR:H	1.60	0.66
20:A:677:U:H3	20:A:713:G:H22	1.43	0.66
21:W:72:C:H2'	21:W:73:A:O4'	1.96	0.66
12:M:109:THR:OG1	20:A:947:G:O3'	2.14	0.66
20:A:634:C:H2'	20:A:635:G:H8	1.59	0.66
20:A:590:C:N4	20:A:649:G:H1	1.91	0.66
20:A:429:U:H1'	20:A:430:A:H5''	1.78	0.66
20:A:1085:U:H3'	20:A:1086:U:H5	1.60	0.66
9:J:3:LYS:HG3	9:J:4:ILE:HD12	1.78	0.66
3:D:171:GLY:O	3:D:173:TRP:N	2.23	0.66
12:M:94:ARG:HE	18:S:81:ARG:HB3	1.61	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:328:C:H4'	20:A:329:A:H5'	1.78	0.66
23:Y:352:VAL:HG12	23:Y:380:LEU:HD11	1.77	0.66
20:A:1503:A:H61	22:V:14:A:H3'	1.60	0.65
20:A:38:G:N2	20:A:397:A:OP1	2.28	0.65
1:B:167:PRO:HG2	1:B:192:SER:HB3	1.77	0.65
23:Y:14:ASN:HD21	23:Y:80:ASN:HD22	1.43	0.65
7:H:96:GLY:H	7:H:99:GLU:HB2	1.62	0.65
10:K:32:ILE:N	10:K:41:THR:O	2.28	0.65
18:S:6:LYS:H	18:S:6:LYS:HD3	1.61	0.65
12:M:99:ARG:HB3	12:M:101:GLN:HG3	1.79	0.65
20:A:973:G:H3'	20:A:974:A:H5''	1.77	0.65
23:Y:485:GLU:HB3	23:Y:601:ILE:HG23	1.78	0.65
10:K:82:VAL:HB	10:K:108:ILE:HA	1.79	0.65
14:O:21:ASP:OD2	20:A:750:G:O2'	2.14	0.65
20:A:131:C:O2'	20:A:262:A:O2'	2.12	0.65
22:V:4:A:N6	22:V:6:G:N7	2.44	0.65
23:Y:560:VAL:HG12	23:Y:563:ILE:HD11	1.79	0.65
23:Y:27:THR:O	23:Y:30:GLU:HG2	1.97	0.65
20:A:1500:A:H5''	20:A:1508:G:H5''	1.79	0.65
23:Y:313:ALA:HA	23:Y:328:ILE:HA	1.79	0.65
1:B:100:GLY:O	1:B:104:ASN:N	2.24	0.65
10:K:33:THR:HG22	10:K:39:PRO:HB3	1.79	0.64
20:A:1040:U:H2'	20:A:1041:A:C8	2.33	0.64
20:A:384:G:H2'	20:A:385:C:C6	2.31	0.64
11:L:84:LEU:HB2	11:L:104:VAL:HG12	1.78	0.64
2:C:58:GLU:HB2	2:C:65:ALA:HB3	1.79	0.64
15:P:75:ARG:HE	15:P:80:PHE:HD1	1.43	0.64
19:T:51:GLU:O	19:T:55:ILE:HG12	1.97	0.64
20:A:673:G:H2'	20:A:674:G:C8	2.32	0.64
24:U:4:SER:HB3	24:U:6:5OH:NQ	2.11	0.64
20:A:813:U:H2'	20:A:814:A:C8	2.32	0.64
16:Q:73:VAL:O	16:Q:74:LEU:HB2	1.96	0.64
20:A:1251:A:H2'	20:A:1252:A:C8	2.32	0.64
19:T:49:ALA:O	19:T:52:ALA:N	2.29	0.64
1:B:9:GLU:N	1:B:9:GLU:OE1	2.30	0.64
6:G:126:ASP:HB3	6:G:131:LYS:O	1.98	0.64
6:G:91:VAL:O	6:G:96:GLN:NE2	2.30	0.64
20:A:354:G:H21	20:A:388:G:H2'	1.63	0.64
20:A:582:U:OP2	20:A:758:G:N1	2.26	0.64
23:Y:276:VAL:HA	23:Y:280:LEU:HD23	1.79	0.64
11:L:102:ARG:HB3	11:L:109:GLY:H	1.61	0.64
20:A:105:G:H2'	20:A:106:C:C6	2.32	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:41:G:H2'	20:A:42:G:C8	2.32	0.64
10:K:22:HIS:HB3	10:K:29:ILE:HG23	1.80	0.64
23:Y:72:CYS:HB2	23:Y:79:ILE:H	1.61	0.64
12:M:81:LEU:HD11	12:M:88:ARG:HH21	1.62	0.64
20:A:858:G:N2	20:A:870:U:OP2	2.26	0.64
20:A:68(J):G:H2'	20:A:68(K):U:O4'	1.98	0.64
4:E:119:LEU:HD11	20:A:6:G:H2'	1.80	0.64
3:D:173:TRP:HB2	3:D:186:LEU:HB2	1.79	0.63
21:W:37:A:H2	22:V:16:A:C4	2.16	0.63
23:Y:34:TYR:O	23:Y:35:TYR:CG	2.51	0.63
20:A:1006:C:N3	20:A:1023:G:N2	2.39	0.63
23:Y:420:ASP:HA	23:Y:423:LYS:HE2	1.80	0.63
23:Y:311:ALA:HA	23:Y:330:VAL:O	1.97	0.63
9:J:78:ASN:N	9:J:78:ASN:OD1	2.31	0.63
20:A:1040:U:H2'	20:A:1041:A:H8	1.63	0.63
21:W:35:A:H2	22:V:18:G:H1	1.46	0.63
23:Y:150:ILE:HG23	23:Y:161:PRO:HG3	1.81	0.63
15:P:43:LYS:NZ	20:A:452:A:OP1	2.31	0.63
7:H:63:LEU:H	7:H:63:LEU:HD22	1.63	0.63
11:L:80:HIS:NE2	23:Y:425:SER:HB3	2.13	0.63
23:Y:87:HIS:HD2	23:Y:121:VAL:HG22	1.63	0.63
1:B:84:GLU:HB3	1:B:219:VAL:HG21	1.80	0.63
1:B:168:THR:HG23	1:B:192:SER:HB2	1.80	0.63
10:K:84:VAL:HG23	10:K:110:ASP:HA	1.81	0.63
3:D:19:LEU:HD22	3:D:67:ILE:HB	1.79	0.63
4:E:11:ILE:HG22	4:E:12:LEU:HD13	1.81	0.63
20:A:1264:C:H2'	20:A:1265:G:C8	2.33	0.63
5:F:48:LEU:H	5:F:57:GLN:HA	1.63	0.63
10:K:98:LEU:O	10:K:101:SER:OG	2.17	0.63
23:Y:30:GLU:HB2	23:Y:51:THR:HG22	1.80	0.63
13:N:31:ARG:NH2	20:A:977:A:OP1	2.31	0.63
23:Y:357:ARG:HH12	23:Y:370:LYS:HD3	1.63	0.63
6:G:15:ASP:HB3	6:G:20:ASP:H	1.64	0.63
20:A:1281:U:H5'	20:A:1282:C:H5	1.64	0.63
11:L:70:ILE:HG22	11:L:100:ILE:HG13	1.80	0.63
12:M:125:ARG:NH1	20:A:969:A:N1	2.46	0.63
3:D:59:ARG:HA	3:D:59:ARG:HH11	1.64	0.63
15:P:67:THR:H	15:P:70:ALA:HB3	1.64	0.63
23:Y:458:HIS:O	23:Y:461:ILE:HG13	1.99	0.63
3:D:141:ARG:HE	3:D:142:PRO:HD2	1.64	0.63
20:A:1127:G:H21	20:A:1147:C:N4	1.96	0.62
6:G:78:ARG:HG3	6:G:79:ARG:N	2.14	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:59:ARG:HA	2:C:63:ASN:O	1.99	0.62
21:W:51:A:H61	21:W:63:C:H42	1.45	0.62
20:A:573:A:N3	20:A:883:C:O2'	2.25	0.62
11:L:58:VAL:HG11	11:L:60:LEU:HD13	1.81	0.62
14:O:8:LYS:NZ	20:A:658:G:OP1	2.24	0.62
11:L:66:VAL:HG12	11:L:67:THR:N	2.14	0.62
20:A:32:A:O2'	20:A:48:C:N4	2.32	0.62
20:A:1507:A:O5'	22:V:15:A:N6	2.32	0.62
23:Y:292:THR:HG23	23:Y:398:ILE:HB	1.80	0.62
9:J:35:SER:HB3	9:J:73:ASP:HB2	1.81	0.62
2:C:35:GLU:HA	2:C:38:ARG:HG3	1.80	0.62
22:V:8:A:H2'	22:V:9:G:H8	1.65	0.62
22:V:8:A:O2'	22:V:9:G:OP1	2.17	0.62
10:K:81:ASP:HA	10:K:106:LYS:O	1.99	0.62
20:A:1358:U:O2'	20:A:1359:C:O4'	2.17	0.62
14:O:82:ILE:HD11	14:O:88:ARG:HB2	1.81	0.62
3:D:28:SER:HB2	3:D:29:PRO:HD2	1.81	0.62
16:Q:13:ASP:HA	16:Q:19:VAL:HG12	1.82	0.62
1:B:78:GLN:HG3	1:B:94:ASN:HB2	1.82	0.62
20:A:481:G:O2'	20:A:483:C:N4	2.33	0.62
10:K:53:SER:HB2	20:A:694:A:H5''	1.82	0.62
20:A:713:G:H2'	20:A:714:G:C8	2.35	0.62
4:E:40:ARG:HG2	4:E:68:GLU:HB3	1.81	0.62
20:A:977:A:HO2'	20:A:981:U:H3	1.48	0.62
12:M:88:ARG:HA	12:M:98:VAL:HG13	1.81	0.62
2:C:133:ALA:HA	2:C:136:GLN:HB2	1.81	0.62
1:B:159:PRO:O	1:B:161:ALA:N	2.32	0.62
20:A:448:A:OP2	20:A:485:G:N1	2.22	0.62
6:G:151:TYR:HA	6:G:154:TYR:HB2	1.81	0.62
23:Y:117:GLN:O	23:Y:120:THR:OG1	2.18	0.62
11:L:70:ILE:HG13	11:L:72:GLY:N	2.15	0.61
20:A:157:G:H1	20:A:164:U:H3	1.47	0.61
3:D:128:VAL:HG13	3:D:146:ILE:HG13	1.81	0.61
2:C:6:HIS:CG	13:N:49:HIS:HB3	2.35	0.61
2:C:134:ILE:HD11	2:C:151:VAL:HG11	1.82	0.61
16:Q:63:ARG:HH21	20:A:130:A:H5'	1.66	0.61
4:E:101:ILE:HD11	4:E:119:LEU:HD22	1.83	0.61
7:H:21:LYS:NZ	20:A:828:A:OP1	2.34	0.61
16:Q:28:PRO:HA	16:Q:35:VAL:HA	1.80	0.61
1:B:103:THR:OG1	1:B:176:GLU:OE1	2.18	0.61
5:F:100:ASN:ND2	17:R:23:LYS:O	2.31	0.61
23:Y:505:GLY:HA3	23:Y:576:ASP:HA	1.80	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:G:26:PHE:O	6:G:30:ILE:HG13	2.00	0.61
17:R:73:ALA:HB3	17:R:79:LEU:HD12	1.81	0.61
23:Y:107:VAL:HG13	23:Y:135:PHE:HB3	1.81	0.61
20:A:443:C:N4	20:A:491:G:H1	1.95	0.61
10:K:21:ILE:HG12	10:K:30:VAL:HG12	1.83	0.61
20:A:563:A:O2'	20:A:567:G:OP2	2.18	0.61
20:A:816:A:OP2	20:A:1526:G:O2'	2.17	0.61
23:Y:265:LYS:O	23:Y:267:LYS:N	2.33	0.61
2:C:52:LEU:HD13	2:C:68:VAL:HG13	1.81	0.61
5:F:12:PRO:O	5:F:13:ASN:ND2	2.32	0.61
20:A:1026:G:O6	20:A:1035:A:N1	2.32	0.61
23:Y:64:THR:CG2	25:Y:701:GNP:O3G	2.41	0.61
3:D:50:ARG:NH1	3:D:51:PRO:O	2.33	0.61
20:A:933:G:H1	20:A:1384:C:N4	1.98	0.61
11:L:71:PRO:HD2	11:L:102:ARG:HD3	1.83	0.61
21:W:17:U:H5'	21:W:18:G:O5'	2.01	0.61
20:A:34:C:H2'	20:A:35:G:C8	2.36	0.61
4:E:149:GLU:O	4:E:153:LYS:HB2	2.01	0.61
23:Y:137:ASN:ND2	23:Y:138:LYS:H	1.99	0.61
20:A:259:G:H1	20:A:267:C:H42	1.48	0.61
20:A:778:G:H2'	20:A:779:C:O4'	2.00	0.61
23:Y:552:SER:O	23:Y:591:LYS:NZ	2.34	0.61
17:R:66:LEU:O	17:R:70:ILE:HG13	2.00	0.61
23:Y:25:LYS:NZ	25:Y:701:GNP:O1B	2.33	0.60
11:L:53:ARG:HG3	11:L:69:TYR:CE1	2.36	0.60
6:G:74:GLU:O	6:G:88:PRO:HA	2.01	0.60
15:P:1:MET:O	15:P:3:LYS:NZ	2.34	0.60
20:A:1347:G:N1	20:A:1374:A:OP2	2.19	0.60
1:B:211:ILE:O	1:B:215:LEU:HB2	2.00	0.60
4:E:29:GLY:HA2	4:E:46:GLY:O	2.01	0.60
20:A:156:G:H1	20:A:165:C:H42	1.49	0.60
20:A:390:C:H2'	20:A:391:G:H8	1.65	0.60
2:C:39:ILE:O	2:C:43:LEU:HB2	2.00	0.60
23:Y:679:VAL:HB	23:Y:683:VAL:HB	1.83	0.60
19:T:79:ARG:O	19:T:82:SER:OG	2.15	0.60
22:V:17:U:H2'	22:V:18:G:C8	2.36	0.60
20:A:1229:A:O2'	21:W:30:C:OP1	2.19	0.60
20:A:774:G:H1	20:A:805:C:H42	1.49	0.60
20:A:660:G:H1	20:A:745:C:H42	1.49	0.60
6:G:22:LEU:HG	6:G:62:PHE:HE2	1.66	0.60
4:E:102:ALA:HB1	4:E:106:PRO:HB2	1.83	0.60
20:A:1006:C:N4	20:A:1023:G:H1	1.98	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:1268:A:N3	20:A:1326:C:O2'	2.34	0.60
11:L:34:ARG:HD3	11:L:82:VAL:HG13	1.82	0.60
20:A:946:A:H2'	20:A:947:G:H8	1.66	0.60
1:B:161:ALA:HB1	1:B:185:ILE:HG12	1.82	0.60
23:Y:604:PRO:HB2	23:Y:649:LEU:HD12	1.84	0.60
12:M:50:GLU:O	12:M:53:VAL:N	2.35	0.60
20:A:748:C:O2'	20:A:749:C:OP2	2.13	0.60
5:F:2:ARG:HG2	5:F:92:LYS:HE2	1.82	0.60
20:A:1408:A:H61	24:U:1:KBE:HAA	1.67	0.60
8:I:120:ARG:HG3	20:A:1348:U:H4'	1.83	0.60
23:Y:18:ALA:HB1	23:Y:121:VAL:HG11	1.83	0.60
1:B:24:TRP:HZ3	1:B:26:PRO:HA	1.65	0.60
20:A:114:U:H2'	20:A:115:G:C8	2.37	0.60
20:A:1491:G:H5''	20:A:1492:A:OP2	2.02	0.60
23:Y:118:SER:HA	23:Y:121:VAL:HG23	1.83	0.60
4:E:11:ILE:O	4:E:31:LEU:HB3	2.01	0.60
8:I:71:SER:HB3	20:A:1372:U:H5''	1.84	0.60
20:A:1513:A:H2'	20:A:1514:C:C6	2.37	0.60
9:J:79:ARG:HH22	9:J:82:ILE:HD12	1.66	0.60
3:D:155:LEU:HB3	3:D:158:ILE:HD13	1.83	0.60
21:W:37:A:N1	22:V:16:A:C6	2.70	0.60
23:Y:255:ILE:HG23	23:Y:257:PRO:HD3	1.84	0.60
14:O:43:LEU:HD22	14:O:47:LYS:HA	1.83	0.60
4:E:98:THR:HB	4:E:117:ASP:HB3	1.84	0.60
20:A:566:G:H4'	20:A:567:G:H5'	1.84	0.60
20:A:1316:G:N1	20:A:1319:A:OP2	2.35	0.60
23:Y:9:LEU:H	23:Y:12:LEU:HD23	1.67	0.59
20:A:390:C:H2'	20:A:391:G:C8	2.37	0.59
23:Y:34:TYR:HB3	23:Y:36:THR:HG23	1.83	0.59
3:D:8:VAL:HG22	20:A:430:A:OP2	2.02	0.59
7:H:95:VAL:HG21	7:H:133:LEU:HD12	1.82	0.59
20:A:1022:G:H2'	20:A:1023:G:O4'	2.03	0.59
19:T:14:LYS:NZ	20:A:104:G:O6	2.23	0.59
11:L:77:LEU:HB3	11:L:81:SER:OG	2.03	0.59
3:D:89:THR:OG1	4:E:97:GLY:O	2.20	0.59
11:L:124:LYS:O	11:L:126:LYS:N	2.32	0.59
23:Y:8:ASP:HB3	23:Y:10:LYS:H	1.68	0.59
23:Y:682:GLN:HA	23:Y:685:GLU:HB2	1.83	0.59
20:A:1327:C:H2'	20:A:1328:C:C6	2.38	0.59
20:A:421:U:O2'	20:A:423:G:O6	2.16	0.59
12:M:31:LYS:HA	12:M:34:LEU:HB2	1.84	0.59
23:Y:675:HIS:NE2	23:Y:677:GLN:OE1	2.35	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
18:S:71:LEU:O	18:S:73:GLU:N	2.35	0.59
20:A:1507:A:P	22:V:15:A:H61	2.25	0.59
20:A:1427:U:H2'	20:A:1428:A:H8	1.68	0.59
15:P:59:TRP:CE3	15:P:59:TRP:HA	2.38	0.59
3:D:22:LYS:H	3:D:26:CYS:HB2	1.67	0.59
6:G:22:LEU:HG	6:G:62:PHE:CE2	2.38	0.59
18:S:62:ILE:HA	18:S:66:MET:HG3	1.85	0.59
12:M:86:CYS:HB3	18:S:74:PHE:HE1	1.68	0.59
1:B:215:LEU:O	1:B:218:ALA:N	2.35	0.59
23:Y:11:ARG:HD3	23:Y:40:HIS:CE1	2.37	0.59
13:N:24:CYS:HB3	13:N:28:GLY:H	1.68	0.59
9:J:89:ASP:OD1	9:J:90:LEU:N	2.35	0.59
4:E:121:LYS:HG3	4:E:122:GLU:H	1.67	0.59
20:A:1309:G:H2'	20:A:1310:G:C8	2.37	0.58
2:C:156:ARG:NE	2:C:159:GLY:O	2.36	0.58
6:G:80:VAL:HB	6:G:83:ALA:HB3	1.85	0.58
12:M:91:ARG:HH21	12:M:96:LEU:HD13	1.68	0.58
11:L:39:VAL:C	11:L:55:VAL:HG21	2.24	0.58
13:N:25:VAL:H	13:N:39:LEU:HD23	1.68	0.58
1:B:152:PHE:CE1	1:B:155:LEU:HB3	2.38	0.58
20:A:438:G:O2'	20:A:494:U:O4	2.16	0.58
15:P:23:ASP:O	15:P:25:ARG:N	2.35	0.58
20:A:409:G:H1	20:A:433:C:H42	1.49	0.58
2:C:68:VAL:HG12	2:C:70:VAL:HG22	1.85	0.58
20:A:197:A:C6	20:A:221:C:H4'	2.39	0.58
23:Y:409:ILE:HD11	23:Y:657:THR:H	1.68	0.58
13:N:60:SER:HB3	20:A:1187:G:H21	1.68	0.58
21:W:35:A:H2	22:V:18:G:N1	2.02	0.58
11:L:16:GLU:O	20:A:562:C:O2'	2.10	0.58
19:T:10:LEU:HG	19:T:11:SER:H	1.68	0.58
20:A:743:U:H2'	20:A:744:C:C6	2.38	0.58
20:A:1144:G:H21	20:A:1146:A:H62	1.52	0.58
20:A:1404:C:H2'	20:A:1405:G:C8	2.38	0.58
11:L:45:PRO:O	11:L:47:LYS:N	2.37	0.58
9:J:50:ILE:HA	9:J:60:ARG:HA	1.84	0.58
3:D:72:GLU:HG3	20:A:546:G:OP2	2.04	0.58
20:A:545:C:O2'	20:A:549:C:OP1	2.21	0.58
8:I:24:GLY:N	8:I:60:ASP:OD2	2.33	0.58
15:P:5:ARG:NH2	15:P:26:ARG:O	2.35	0.58
3:D:64:LEU:HB2	3:D:198:VAL:HG11	1.86	0.58
4:E:78:HIS:H	4:E:78:HIS:CD2	2.22	0.58
19:T:61:SER:O	19:T:65:LYS:HG2	2.04	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:1228:C:H2'	20:A:1229:A:H8	1.68	0.58
1:B:178:ARG:HG3	7:H:72:PRO:HA	1.86	0.58
21:W:69:A:H2'	21:W:70:G:C8	2.39	0.58
1:B:118:LEU:HD13	1:B:142:LEU:HA	1.85	0.58
20:A:1255:G:H2'	20:A:1258:G:H21	1.69	0.58
20:A:287:U:H2'	20:A:288:A:C8	2.38	0.58
10:K:17:GLY:O	10:K:80:VAL:HA	2.04	0.58
20:A:1401:G:H5''	22:V:22:A:H62	1.68	0.58
23:Y:35:TYR:CD1	23:Y:36:THR:N	2.70	0.58
20:A:1148:U:H2'	20:A:1149:C:O4'	2.04	0.58
17:R:38:GLU:O	17:R:42:ARG:HG3	2.03	0.58
20:A:811:C:O2'	20:A:901:A:N1	2.37	0.58
12:M:91:ARG:HH22	12:M:103:THR:HG21	1.68	0.58
18:S:6:LYS:HG2	18:S:7:LYS:H	1.69	0.58
1:B:24:TRP:CZ3	1:B:26:PRO:HA	2.38	0.58
20:A:894:G:H2'	20:A:895:G:H8	1.69	0.58
6:G:54:THR:OG1	6:G:56:GLN:OE1	2.21	0.58
20:A:737:A:H2'	20:A:738:C:C6	2.39	0.57
20:A:112:G:H1	20:A:315:A:N6	2.02	0.57
23:Y:359:HIS:O	23:Y:361:ASN:N	2.37	0.57
10:K:63:LEU:O	10:K:66:LEU:HB3	2.04	0.57
20:A:1376:U:H2'	20:A:1377:A:C8	2.39	0.57
20:A:1118:C:H2'	20:A:1119:C:C6	2.39	0.57
1:B:96:ARG:NE	1:B:96:ARG:H	2.01	0.57
20:A:199:G:O6	20:A:218:C:N3	2.37	0.57
12:M:45:VAL:HG23	12:M:48:LEU:HD12	1.86	0.57
15:P:53:VAL:HG12	15:P:79:VAL:HG22	1.84	0.57
11:L:104:VAL:HG23	11:L:106:ASP:H	1.68	0.57
20:A:921:U:H2'	20:A:922:G:O4'	2.04	0.57
13:N:27:CYS:SG	13:N:28:GLY:N	2.78	0.57
4:E:78:HIS:O	4:E:79:GLU:HB3	2.03	0.57
20:A:859:A:OP2	20:A:869:G:N1	2.36	0.57
16:Q:60:ILE:O	16:Q:71:PHE:HA	2.05	0.57
7:H:38:ILE:HD13	7:H:41:ARG:HH12	1.69	0.57
24:U:6:5OH:HS	24:U:6:5OH:N	2.19	0.57
20:A:232:G:H21	20:A:263:A:H2	1.52	0.57
11:L:118:SER:OG	20:A:35:G:N2	2.38	0.57
23:Y:302:HIS:O	23:Y:332:SER:OG	2.21	0.57
4:E:78:HIS:HB2	7:H:104:ARG:HG3	1.86	0.57
8:I:126:SER:O	8:I:128:ARG:N	2.37	0.57
23:Y:543:GLN:O	23:Y:546:ILE:N	2.28	0.57
23:Y:56:GLU:HB2	23:Y:59:ARG:NE	2.15	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:I:112:LYS:NZ	8:I:116:LYS:O	2.37	0.57
13:N:34:TYR:HE2	20:A:1357:A:HO2'	1.53	0.57
7:H:33:GLU:OE1	7:H:50:ARG:NE	2.36	0.57
9:J:40:LEU:HB3	9:J:69:ASN:HB2	1.86	0.57
9:J:6:ILE:HB	9:J:98:ILE:HG23	1.86	0.57
16:Q:19:VAL:HG23	16:Q:44:ALA:HB3	1.87	0.57
16:Q:6:LEU:HD13	16:Q:23:VAL:HG11	1.87	0.57
20:A:1088:G:H2'	20:A:1089:G:H8	1.70	0.57
3:D:127:THR:HA	3:D:132:ARG:HA	1.86	0.57
15:P:69:THR:HA	15:P:72:ARG:HB2	1.87	0.57
23:Y:55:MET:SD	23:Y:59:ARG:NH1	2.78	0.57
1:B:68:ILE:HG12	1:B:161:ALA:HB3	1.87	0.57
19:T:63:ILE:HG21	19:T:81:LYS:HG3	1.86	0.57
5:F:8:ILE:HD11	5:F:79:LEU:HD13	1.86	0.57
23:Y:59:ARG:HD3	23:Y:65:ILE:H	1.70	0.56
20:A:692:U:H2'	20:A:694:A:OP2	2.05	0.56
9:J:79:ARG:O	9:J:83:GLU:HB2	2.04	0.56
23:Y:486:THR:OG1	23:Y:487:ILE:N	2.34	0.56
11:L:33:ARG:HG3	11:L:34:ARG:H	1.70	0.56
3:D:5:ILE:HG21	20:A:406:G:H5''	1.87	0.56
8:I:118:LYS:HB3	20:A:1349:A:OP1	2.05	0.56
20:A:68(N):U:H3'	20:A:68(O):A:C8	2.39	0.56
20:A:299:G:H2'	20:A:300:A:C8	2.40	0.56
1:B:15:VAL:HG21	1:B:209:ARG:HE	1.70	0.56
3:D:135:LEU:HG	20:A:620:C:C2	2.40	0.56
3:D:164:ALA:O	3:D:168:ARG:NH1	2.39	0.56
14:O:64:ARG:HH21	20:A:581:G:H4'	1.70	0.56
6:G:102:ARG:HD2	20:A:940:C:OP1	2.06	0.56
9:J:5:ARG:HB3	9:J:99:LYS:O	2.05	0.56
9:J:62:HIS:NE2	20:A:1368:G:OP1	2.32	0.56
23:Y:32:ILE:O	23:Y:34:TYR:C	2.43	0.56
6:G:79:ARG:NH2	6:G:156:TRP:HB2	2.21	0.56
20:A:714:G:H2'	20:A:715:A:C8	2.41	0.56
16:Q:51:TYR:CE2	16:Q:73:VAL:HG11	2.41	0.56
20:A:510:A:N3	20:A:543:C:H1'	2.20	0.56
23:Y:229:LEU:HA	23:Y:232:LEU:HB2	1.88	0.56
12:M:4:ILE:HG23	12:M:57:ARG:HB2	1.88	0.56
8:I:9:ARG:HG2	8:I:13:ALA:O	2.05	0.56
20:A:143:A:H5'	20:A:196:A:N1	2.21	0.56
20:A:339:C:H2'	20:A:340:U:C6	2.40	0.56
8:I:4:TYR:CE1	8:I:21:PRO:HD3	2.41	0.56
21:W:15:G:P	21:W:16:U:H3	2.29	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:741:G:H3'	20:A:742:G:H8	1.71	0.56
19:T:84:LEU:O	19:T:88:VAL:HG23	2.06	0.56
20:A:701:C:O2	20:A:703:G:N2	2.37	0.56
20:A:292:G:C5	20:A:293:G:H1'	2.40	0.56
23:Y:555:LEU:HD21	23:Y:599:PRO:HB3	1.88	0.56
4:E:45:PHE:HZ	20:A:1079:G:H5''	1.71	0.56
9:J:5:ARG:NH2	9:J:73:ASP:OD2	2.39	0.56
20:A:1412:C:H2'	20:A:1413:A:C8	2.41	0.56
21:W:7:G:O6	21:W:49:A:N6	2.39	0.56
7:H:94:TYR:OH	20:A:597:G:N2	2.39	0.56
20:A:1486:G:H2'	20:A:1487:G:O4'	2.06	0.56
12:M:23:TYR:OH	12:M:71:ARG:HG3	2.06	0.56
11:L:60:LEU:HD23	11:L:63:GLY:O	2.05	0.56
9:J:54:PHE:CG	9:J:55:LYS:N	2.74	0.56
8:I:10:ARG:HD3	8:I:75:ASP:HB3	1.86	0.56
20:A:765:G:N1	20:A:812:C:O2'	2.36	0.56
7:H:12:ARG:NH2	20:A:825:G:O2'	2.31	0.56
19:T:103:GLY:HA2	20:A:192:U:H1'	1.88	0.56
20:A:1028(B):C:N3	20:A:1028(G):G:N2	2.50	0.55
12:M:40:ASN:O	12:M:43:THR:HB	2.07	0.55
20:A:892:A:H2'	20:A:893:C:C6	2.40	0.55
16:Q:9:VAL:HA	16:Q:56:VAL:HG22	1.87	0.55
20:A:891:U:H3	20:A:907:A:H62	1.55	0.55
20:A:217:C:O2'	20:A:458(C):G:O6	2.16	0.55
12:M:15:VAL:HG23	12:M:34:LEU:HD13	1.88	0.55
20:A:1109:C:H2'	20:A:1110:A:O4'	2.06	0.55
7:H:30:ARG:NH1	20:A:590:C:OP2	2.40	0.55
20:A:993:G:H1	20:A:1045:C:H42	1.52	0.55
12:M:98:VAL:HB	12:M:99:ARG:CZ	2.36	0.55
22:V:6:G:H2'	22:V:7:G:C8	2.41	0.55
20:A:255:G:H2'	20:A:256:U:C6	2.42	0.55
23:Y:25:LYS:NZ	25:Y:701:GNP:O3G	2.39	0.55
20:A:1437:C:H2'	20:A:1438:G:C8	2.41	0.55
20:A:372:C:H42	20:A:389:A:H62	1.54	0.55
20:A:1422:G:H2'	20:A:1423:G:H8	1.72	0.55
23:Y:417:THR:O	23:Y:419:ALA:N	2.35	0.55
23:Y:15:ILE:HD12	23:Y:105:ILE:HD11	1.88	0.55
1:B:164:VAL:HG12	1:B:186:ALA:HB1	1.89	0.55
23:Y:660:ARG:O	23:Y:665:GLY:N	2.40	0.55
2:C:66:VAL:HG12	2:C:68:VAL:HG23	1.88	0.55
22:V:8:A:H2'	22:V:9:G:C8	2.42	0.55
23:Y:163:VAL:HG13	23:Y:258:VAL:CG2	2.32	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:Y:20:HIS:CD2	23:Y:21:ILE:HG23	2.42	0.55
1:B:118:LEU:O	1:B:122:PHE:HB2	2.06	0.55
16:Q:66:SER:O	16:Q:70:ARG:NH1	2.39	0.55
1:B:223:ILE:HA	1:B:226:ARG:HB2	1.88	0.55
20:A:1440(J):C:H1'	20:A:1440(K):G:N2	2.22	0.55
23:Y:438:PHE:HE1	23:Y:462:ILE:HG13	1.72	0.55
3:D:8:VAL:HG23	3:D:9:CYS:H	1.71	0.55
16:Q:67:LYS:HD2	20:A:266:G:C8	2.40	0.55
20:A:1328:C:H2'	20:A:1329:A:H8	1.70	0.55
20:A:1321:C:H3'	20:A:1322:C:H5''	1.89	0.55
20:A:1237:C:H4'	20:A:1334:G:H21	1.71	0.55
3:D:70:ILE:HG12	3:D:71:SER:N	2.21	0.55
13:N:15:LYS:HD3	13:N:16:PHE:CZ	2.42	0.55
12:M:104:ARG:NH2	20:A:954:G:O6	2.37	0.55
20:A:1256:A:N6	20:A:1278:U:O4'	2.39	0.55
5:F:50:TYR:OH	17:R:77:GLY:N	2.38	0.55
7:H:7:ALA:HA	7:H:10:LEU:HD12	1.88	0.55
20:A:112:G:N2	20:A:315:A:N1	2.54	0.55
3:D:103:ASN:HA	3:D:106:TYR:HB3	1.88	0.55
1:B:111:ARG:HE	1:B:145:LEU:HD21	1.71	0.55
1:B:145:LEU:HD12	1:B:149:LEU:HD12	1.87	0.55
23:Y:616:TYR:HB3	23:Y:663:THR:HA	1.89	0.55
3:D:61:LYS:HD3	3:D:75:PHE:HE2	1.72	0.55
13:N:19:ARG:HG2	20:A:980:C:H1'	1.87	0.55
20:A:1350:A:H2'	20:A:1351:U:C6	2.42	0.55
20:A:56:U:O4	20:A:356:A:N1	2.40	0.55
3:D:33:MET:O	3:D:35:ARG:N	2.37	0.55
18:S:36:ARG:HH22	18:S:75:ALA:HB3	1.72	0.55
20:A:1422:G:H1	20:A:1478:C:H42	1.55	0.55
12:M:105:THR:O	12:M:114:ARG:NH1	2.40	0.55
20:A:835:U:H2'	20:A:836:G:H8	1.72	0.54
6:G:72:ARG:O	6:G:91:VAL:N	2.40	0.54
23:Y:438:PHE:HB2	23:Y:452:SER:O	2.06	0.54
21:W:43:G:H2'	21:W:44:G:H8	1.72	0.54
20:A:781:A:N6	20:A:802:A:H1'	2.22	0.54
10:K:117:ASN:OD1	20:A:716:A:O2'	2.25	0.54
23:Y:134:ALA:HB2	23:Y:258:VAL:HG12	1.90	0.54
23:Y:617:MET:HA	23:Y:620:VAL:HG22	1.89	0.54
10:K:108:ILE:HD13	17:R:87:ARG:HG2	1.89	0.54
20:A:509:A:N3	20:A:543:C:O2'	2.34	0.54
17:R:74:ARG:NH2	17:R:81:PHE:O	2.40	0.54
23:Y:538:TYR:OH	23:Y:577:SER:O	2.19	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:523:A:H1'	20:A:527:G:H22	1.71	0.54
23:Y:164:MET:HE2	23:Y:259:PHE:CZ	2.41	0.54
20:A:953:G:H2'	20:A:954:G:O4'	2.08	0.54
10:K:117:ASN:O	20:A:716:A:O2'	2.25	0.54
13:N:32:SER:OG	20:A:975:A:O2'	2.25	0.54
23:Y:165:GLN:HE21	23:Y:260:LEU:H	1.55	0.54
20:A:27:G:H2'	20:A:28:G:H8	1.71	0.54
6:G:156:TRP:HH2	20:A:1378:C:N3	2.05	0.54
9:J:5:ARG:HH21	9:J:71:LEU:HD21	1.73	0.54
3:D:135:LEU:HG	20:A:620:C:N3	2.22	0.54
20:A:1493:A:OP1	24:U:2:DPP:HA	2.07	0.54
1:B:84:GLU:HG3	1:B:215:LEU:HB3	1.90	0.54
1:B:196:LEU:HD12	1:B:197:VAL:HG23	1.89	0.54
5:F:1:MET:HB2	5:F:67:MET:O	2.07	0.54
23:Y:163:VAL:HG12	23:Y:164:MET:H	1.73	0.54
3:D:98:GLU:O	3:D:103:ASN:ND2	2.30	0.54
20:A:1245:A:H61	20:A:1292:U:H3	1.55	0.54
20:A:636:U:H2'	20:A:637:G:H8	1.72	0.54
9:J:69:ASN:O	9:J:70:ARG:HD2	2.08	0.54
5:F:90:VAL:O	20:A:736:C:O2'	2.21	0.54
23:Y:8:ASP:HB3	23:Y:11:ARG:H	1.73	0.54
9:J:4:ILE:HD13	9:J:74:ILE:HG12	1.89	0.54
20:A:501:C:H1'	20:A:549:C:H1'	1.89	0.54
20:A:382:A:H2'	20:A:383:A:C8	2.42	0.54
23:Y:475:ASN:O	23:Y:477:GLY:N	2.40	0.54
18:S:13:ASP:N	18:S:13:ASP:OD2	2.34	0.54
11:L:45:PRO:HA	11:L:92:ASP:HB3	1.89	0.54
20:A:68(P):C:H2'	20:A:68(Q):U:C6	2.43	0.54
1:B:167:PRO:HD3	1:B:188:ALA:HA	1.90	0.54
10:K:84:VAL:HG11	10:K:95:ILE:HD11	1.90	0.54
20:A:263:A:H2'	20:A:264:U:H6	1.71	0.54
23:Y:604:PRO:HA	23:Y:676:TYR:HB3	1.89	0.54
8:I:13:ALA:HB2	8:I:68:GLY:HA3	1.90	0.54
20:A:977:A:O2'	20:A:981:U:N3	2.37	0.54
16:Q:57:VAL:HG12	16:Q:76:LEU:HA	1.89	0.54
12:M:8:GLU:OE1	12:M:22:ILE:HG23	2.07	0.54
20:A:1496:C:H2'	20:A:1497:G:O4'	2.08	0.54
9:J:24:VAL:HG21	9:J:37:PRO:HG3	1.89	0.54
20:A:672:U:H2'	20:A:673:G:H8	1.73	0.54
20:A:533:A:O2'	20:A:536:C:N4	2.40	0.54
20:A:1218:C:H2'	20:A:1219:U:C6	2.43	0.54
20:A:979:C:OP1	20:A:1223:C:N4	2.41	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:Y:139:MET:SD	23:Y:144:ALA:HB1	2.48	0.53
20:A:68(H):G:H21	20:A:68(S):C:H41	1.52	0.53
10:K:108:ILE:HG21	17:R:88:LYS:H	1.71	0.53
20:A:166:G:H2'	20:A:167:G:C8	2.44	0.53
7:H:1:MET:HB2	20:A:824:C:H4'	1.90	0.53
7:H:121:ASP:OD2	7:H:122:ARG:N	2.35	0.53
21:W:37:A:C2	22:V:16:A:C4	2.94	0.53
23:Y:138:LYS:HE2	25:Y:701:GNP:N3	2.19	0.53
23:Y:24:GLY:CA	25:Y:701:GNP:H8	2.39	0.53
20:A:329:A:C5	20:A:332:G:C6	2.96	0.53
7:H:91:ARG:NH2	20:A:564:C:O2'	2.41	0.53
20:A:1440(E):G:H1	20:A:1440(N):C:H42	1.55	0.53
12:M:80:ARG:HA	12:M:83:ASP:OD1	2.08	0.53
20:A:729:A:H2'	20:A:730:G:H8	1.71	0.53
14:O:12:ILE:HG21	14:O:22:THR:HG22	1.90	0.53
20:A:1016:A:O5'	20:A:1016:A:H8	1.91	0.53
20:A:762:C:H2'	20:A:763:G:C8	2.43	0.53
20:A:828:A:H2'	20:A:829:G:O4'	2.08	0.53
19:T:105:SER:HB3	20:A:186(P):U:O2	2.09	0.53
20:A:1008:C:H42	20:A:1021:G:H1	1.55	0.53
23:Y:31:ARG:HA	23:Y:33:LEU:HB2	1.90	0.53
20:A:406:G:H2'	20:A:407:G:H8	1.74	0.53
20:A:1309:G:H2'	20:A:1310:G:H8	1.73	0.53
20:A:1306:A:H1'	20:A:1332:A:N1	2.24	0.53
12:M:39:ILE:HG13	12:M:52:GLU:HB3	1.91	0.53
19:T:86:ARG:HG3	20:A:186(A):C:H5''	1.89	0.53
20:A:1127:G:N2	20:A:1145:C:C2	2.74	0.53
15:P:6:LEU:HD23	15:P:17:TYR:CG	2.43	0.53
11:L:90:VAL:HG23	11:L:92:ASP:OD1	2.08	0.53
11:L:39:VAL:HB	11:L:55:VAL:HG11	1.88	0.53
20:A:263:A:H2'	20:A:264:U:C6	2.44	0.53
8:I:112:LYS:HG3	8:I:117:HIS:O	2.08	0.53
20:A:1328:C:H2'	20:A:1329:A:C8	2.44	0.53
20:A:17:U:H2'	20:A:18:C:C6	2.44	0.53
20:A:612:C:H42	20:A:628:G:H1	1.57	0.53
23:Y:24:GLY:HA3	25:Y:701:GNP:C8	2.38	0.53
7:H:49:GLU:OE2	7:H:62:TYR:OH	2.16	0.53
2:C:199:LYS:NZ	20:A:1059:C:OP2	2.41	0.53
1:B:57:PHE:CE2	1:B:185:ILE:HD11	2.44	0.53
17:R:74:ARG:HE	17:R:81:PHE:HA	1.73	0.53
23:Y:438:PHE:CE1	23:Y:462:ILE:HG13	2.44	0.53
2:C:150:LYS:HD2	2:C:167:TRP:HE1	1.74	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:Y:394:ALA:O	23:Y:396:ARG:N	2.41	0.53
16:Q:27:PHE:HD2	16:Q:36:ILE:HD11	1.74	0.53
23:Y:276:VAL:O	23:Y:280:LEU:HB2	2.09	0.53
10:K:18:ARG:HA	10:K:81:ASP:H	1.73	0.53
10:K:108:ILE:HB	17:R:87:ARG:H	1.71	0.53
23:Y:206:LEU:O	23:Y:210:ARG:NH1	2.42	0.53
12:M:125:ARG:O	20:A:966:G:H5'	2.09	0.53
9:J:45:ARG:NH1	20:A:1255:G:OP1	2.41	0.53
20:A:1493:A:OP2	20:A:1493:A:H8	1.92	0.53
4:E:19:MET:O	20:A:921:U:O2'	2.23	0.53
1:B:78:GLN:O	1:B:81:VAL:HG22	2.09	0.53
20:A:1427:U:H2'	20:A:1428:A:C8	2.44	0.53
20:A:728:A:H2'	20:A:729:A:C8	2.44	0.53
4:E:80:ILE:HG13	4:E:82:VAL:HG23	1.91	0.53
19:T:72:LEU:HD11	19:T:80:ARG:HH11	1.74	0.53
3:D:115:ARG:NH1	20:A:407:G:OP1	2.42	0.53
20:A:1062:U:H2'	20:A:1063:C:C6	2.44	0.53
20:A:186(E):C:H42	20:A:186(L):G:H1	1.57	0.53
20:A:605:U:H2'	20:A:606:G:C8	2.44	0.53
2:C:40:ARG:NH1	13:N:52:GLN:HB3	2.23	0.53
23:Y:25:LYS:NZ	25:Y:701:GNP:PG	2.81	0.53
11:L:46:LYS:O	11:L:47:LYS:HE2	2.09	0.53
10:K:18:ARG:HD2	10:K:20:TYR:HE1	1.74	0.53
20:A:266:G:O2'	20:A:268:C:OP2	2.24	0.53
1:B:155:LEU:HD11	1:B:159:PRO:HG3	1.90	0.53
14:O:60:VAL:O	14:O:63:ARG:HG3	2.08	0.53
20:A:1068:G:H1	20:A:1107:C:H42	1.56	0.53
20:A:24:U:H2'	20:A:25:C:C6	2.44	0.53
20:A:1492:A:H5'	24:U:6:5OH:HNP	1.75	0.52
10:K:53:SER:N	20:A:695:A:OP2	2.38	0.52
20:A:695:A:H2'	20:A:696:A:C8	2.44	0.52
16:Q:17:LYS:NZ	20:A:256:U:H5'	2.25	0.52
3:D:63:LYS:O	3:D:67:ILE:HG22	2.09	0.52
12:M:86:CYS:HB3	18:S:74:PHE:CE1	2.43	0.52
20:A:1211:U:H1'	20:A:1213:A:C2	2.44	0.52
3:D:117:ALA:O	3:D:121:VAL:HG23	2.09	0.52
12:M:59:TYR:HA	12:M:62:ASN:HB2	1.90	0.52
11:L:69:TYR:OH	20:A:522:C:OP2	2.27	0.52
20:A:815:A:N3	20:A:1527:C:H1'	2.25	0.52
20:A:1234:C:H4'	20:A:1364:U:H1'	1.91	0.52
8:I:47:LEU:HG	8:I:50:LEU:HD12	1.92	0.52
23:Y:533:VAL:O	23:Y:535:PRO:HD3	2.09	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:1392:G:O2'	20:A:1502:A:OP1	2.27	0.52
9:J:38:ILE:HG23	9:J:71:LEU:HB3	1.90	0.52
18:S:46:GLY:HA2	18:S:62:ILE:HG23	1.90	0.52
20:A:63:C:H5''	20:A:383:A:H61	1.74	0.52
3:D:42:GLN:N	20:A:541:G:O2'	2.31	0.52
20:A:1157:A:H4'	20:A:1158:C:O5'	2.09	0.52
4:E:6:PHE:CD2	4:E:36:ASP:HB3	2.44	0.52
20:A:1239:A:H2'	20:A:1298:C:H42	1.73	0.52
14:O:51:HIS:CE1	20:A:667:G:H4'	2.44	0.52
15:P:5:ARG:NH1	20:A:376:G:O3'	2.40	0.52
6:G:74:GLU:CD	6:G:95:ARG:HH21	2.10	0.52
23:Y:272:LEU:O	23:Y:276:VAL:HG23	2.09	0.52
2:C:40:ARG:CZ	13:N:52:GLN:HB3	2.38	0.52
2:C:180:ALA:HB1	2:C:203:PHE:CE1	2.45	0.52
1:B:238:LEU:HA	1:B:241:GLU:HG2	1.89	0.52
2:C:137:ALA:O	2:C:141:VAL:HG23	2.09	0.52
13:N:6:LEU:HB3	13:N:23:ARG:NH2	2.24	0.52
4:E:16:THR:HG21	20:A:1080:A:H5''	1.91	0.52
8:I:107:ARG:HD3	20:A:1347:G:C8	2.44	0.52
12:M:96:LEU:O	12:M:110:ARG:HD2	2.09	0.52
1:B:71:VAL:O	1:B:165:VAL:N	2.41	0.52
20:A:314:C:H2'	20:A:315:A:H8	1.74	0.52
1:B:79:ASP:O	1:B:82:ARG:HG2	2.10	0.52
20:A:145:G:H1	20:A:177:C:H42	1.58	0.52
20:A:271:C:H2'	20:A:272:C:C6	2.44	0.52
12:M:66:LEU:HB3	12:M:67:GLU:HG2	1.91	0.52
3:D:30:LYS:HD3	3:D:35:ARG:HH11	1.74	0.52
3:D:25:ARG:HB2	20:A:409:G:H5''	1.92	0.52
13:N:18:VAL:HG11	20:A:1316:G:H4'	1.90	0.52
20:A:881:G:H2'	20:A:882:C:O4'	2.10	0.52
20:A:68(A):G:H2'	20:A:68(B):G:C8	2.44	0.52
3:D:15:GLU:OE2	3:D:63:LYS:HG3	2.10	0.52
20:A:116:A:H8	20:A:116:A:O5'	1.93	0.52
7:H:69:ARG:HG2	7:H:70:GLN:H	1.75	0.52
10:K:27:ASN:HD21	10:K:44:SER:HB2	1.74	0.52
12:M:14:ARG:HG3	12:M:44:ARG:HH11	1.75	0.52
20:A:1004:A:O2'	20:A:1037:C:O2	2.26	0.52
20:A:993:G:H2'	20:A:995:C:H41	1.74	0.52
17:R:74:ARG:HG3	17:R:79:LEU:HB3	1.91	0.52
17:R:79:LEU:HD23	17:R:80:PRO:HD2	1.91	0.52
23:Y:139:MET:H	23:Y:262:SER:HB2	1.75	0.52
15:P:59:TRP:HA	15:P:59:TRP:HE3	1.73	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:861:G:O2'	20:A:874:G:O2'	2.26	0.52
20:A:45:U:H2'	20:A:46:G:H8	1.74	0.52
14:O:49:ASP:OD2	14:O:52:SER:OG	2.27	0.52
20:A:923:A:H2'	20:A:924:C:O4'	2.10	0.52
4:E:31:LEU:HA	4:E:45:PHE:HB2	1.91	0.52
18:S:29:ARG:O	18:S:48:THR:OG1	2.28	0.52
11:L:113:ARG:CZ	11:L:115:LYS:HB3	2.40	0.52
17:R:72:ARG:O	17:R:76:LEU:HG	2.10	0.52
6:G:98:SER:HA	6:G:101:LEU:HD12	1.92	0.52
2:C:12:LEU:HB2	13:N:57:ARG:NH2	2.25	0.52
20:A:68(F):C:H2'	20:A:68(G):G:C8	2.44	0.51
23:Y:133:ILE:HD12	23:Y:280:LEU:HD21	1.93	0.51
12:M:96:LEU:HD11	18:S:82:GLY:O	2.10	0.51
14:O:25:THR:O	14:O:29:VAL:HG23	2.09	0.51
20:A:116:A:H2'	20:A:117:G:O4'	2.10	0.51
4:E:78:HIS:CD2	4:E:79:GLU:H	2.28	0.51
20:A:892:A:H2'	20:A:893:C:H6	1.74	0.51
20:A:860:A:H2'	20:A:861:G:O4'	2.10	0.51
1:B:54:THR:O	1:B:58:ILE:HG12	2.10	0.51
23:Y:137:ASN:ND2	23:Y:262:SER:HA	2.22	0.51
12:M:91:ARG:HA	12:M:94:ARG:HB2	1.93	0.51
1:B:69:LEU:HB3	1:B:71:VAL:HG23	1.92	0.51
21:W:23:A:H2'	21:W:24:G:H8	1.74	0.51
21:W:35:A:C2	22:V:18:G:N1	2.78	0.51
3:D:155:LEU:O	3:D:159:ARG:NE	2.43	0.51
12:M:15:VAL:HG13	12:M:43:THR:O	2.10	0.51
23:Y:443:HIS:HB2	23:Y:448:GLN:HG2	1.92	0.51
20:A:123:C:OP1	20:A:311:C:O2'	2.25	0.51
7:H:64:LYS:HG2	7:H:79:VAL:HG21	1.91	0.51
22:V:14:A:H5'	22:V:15:A:OP2	2.10	0.51
10:K:85:ARG:NH1	20:A:707:C:OP1	2.43	0.51
20:A:745:C:H1'	20:A:836:G:O2'	2.09	0.51
16:Q:21:VAL:HG23	16:Q:44:ALA:HB2	1.92	0.51
12:M:116:THR:HA	20:A:1228:C:H4'	1.92	0.51
16:Q:92:ARG:O	16:Q:95:TYR:HB2	2.10	0.51
3:D:145:GLU:HG2	3:D:182:LYS:HG2	1.92	0.51
12:M:78:ILE:HD12	12:M:92:HIS:CE1	2.46	0.51
16:Q:67:LYS:HG2	20:A:267:C:OP2	2.10	0.51
1:B:162:ILE:HG22	1:B:184:VAL:HA	1.93	0.51
5:F:61:LEU:HB2	5:F:63:TYR:HE2	1.76	0.51
20:A:591:U:H2'	20:A:592:G:C8	2.45	0.51
20:A:373:A:H4'	20:A:480:U:O2'	2.11	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:18:GLY:HA3	1:B:41:ILE:HA	1.93	0.51
20:A:1145:C:O2'	20:A:1146:A:OP2	2.29	0.51
20:A:992:U:O2'	20:A:993:G:OP2	2.17	0.51
23:Y:14:ASN:ND2	23:Y:80:ASN:HD22	2.08	0.51
7:H:7:ALA:HB2	7:H:85:ARG:HE	1.75	0.51
20:A:1534:A:H8	20:A:1534:A:O5'	1.93	0.51
3:D:74:GLN:O	3:D:78:LEU:HG	2.11	0.51
11:L:42:THR:HA	11:L:52:LEU:HA	1.93	0.51
20:A:1507:A:H2'	20:A:1508:G:H8	1.76	0.51
9:J:8:LEU:HB3	9:J:16:LEU:HD23	1.93	0.51
20:A:966:G:C2	20:A:967:C:C2	2.99	0.51
23:Y:246:ILE:O	23:Y:250:THR:OG1	2.19	0.51
20:A:743:U:H2'	20:A:744:C:H6	1.74	0.51
20:A:1137:C:H2'	20:A:1137:C:O2	2.09	0.51
20:A:672:U:H2'	20:A:673:G:C8	2.45	0.51
16:Q:13:ASP:O	16:Q:15:MET:N	2.37	0.51
20:A:1429:C:H2'	20:A:1430:C:C6	2.46	0.51
2:C:195:VAL:HG11	20:A:1205:U:H4'	1.91	0.51
20:A:490:G:H2'	20:A:491:G:C8	2.46	0.51
6:G:111:ARG:HE	6:G:123:GLU:HB2	1.75	0.51
7:H:100:ILE:HG22	7:H:101:PRO:O	2.11	0.51
20:A:129(A):G:N2	20:A:186(J):G:OP2	2.32	0.51
6:G:26:PHE:HB2	6:G:62:PHE:HZ	1.76	0.51
23:Y:136:ALA:HB3	23:Y:260:LEU:HB2	1.93	0.51
23:Y:215:LYS:O	23:Y:219:VAL:N	2.37	0.51
20:A:1018:C:H2'	20:A:1019:C:C6	2.45	0.51
20:A:68(P):C:H2'	20:A:68(Q):U:H6	1.75	0.51
3:D:3:ARG:O	3:D:5:ILE:N	2.44	0.51
20:A:16:A:N1	20:A:919:A:H2	2.09	0.51
23:Y:8:ASP:HB2	23:Y:11:ARG:NE	2.25	0.51
6:G:16:LEU:HD22	8:I:42:ARG:HA	1.93	0.51
20:A:1151:A:HO2'	20:A:1152:A:H8	1.59	0.51
3:D:14:ARG:HG3	3:D:66:ARG:HH12	1.76	0.51
2:C:28:GLN:HB2	2:C:32:LEU:HD11	1.92	0.51
14:O:85:LEU:HD22	14:O:87:ILE:HG12	1.91	0.51
23:Y:163:VAL:HA	23:Y:258:VAL:HG22	1.92	0.51
13:N:29:ARG:NH1	20:A:974:A:OP2	2.44	0.51
9:J:61:GLU:OE2	13:N:49:HIS:NE2	2.45	0.51
20:A:1255:G:N2	20:A:1259:C:O2	2.44	0.51
3:D:42:GLN:H	20:A:541:G:HO2'	1.58	0.51
20:A:11:G:H1	20:A:23:C:H42	1.58	0.51
5:F:5:GLU:HG2	5:F:62:TRP:HZ2	1.76	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:E:131:ILE:O	4:E:135:THR:OG1	2.24	0.51
11:L:127:GLU:O	11:L:129:ALA:N	2.42	0.51
20:A:1028(B):C:N4	20:A:1028(G):G:C6	2.79	0.50
9:J:8:LEU:HB3	9:J:16:LEU:CD2	2.42	0.50
20:A:737:A:H2'	20:A:738:C:H6	1.76	0.50
10:K:108:ILE:HG21	17:R:88:LYS:N	2.26	0.50
3:D:122:ARG:HA	3:D:134:ASP:O	2.11	0.50
20:A:1134:G:H1	20:A:1140:C:H42	1.59	0.50
3:D:203:VAL:O	3:D:207:TYR:HB2	2.11	0.50
20:A:911:U:H2'	20:A:912:C:C6	2.47	0.50
20:A:551:U:H2'	20:A:552:U:C6	2.46	0.50
8:I:107:ARG:NE	20:A:1347:G:H5''	2.27	0.50
23:Y:210:ARG:O	23:Y:214:GLU:HG2	2.10	0.50
4:E:94:ALA:HB2	4:E:119:LEU:HD23	1.93	0.50
2:C:86:VAL:O	2:C:89:GLU:HB2	2.11	0.50
20:A:770:C:O2'	20:A:899:C:N3	2.42	0.50
19:T:30:LYS:O	19:T:34:LYS:HG3	2.11	0.50
11:L:123:LYS:HD3	20:A:37:U:OP1	2.12	0.50
6:G:119:ARG:HH22	20:A:1240:U:H5	1.58	0.50
20:A:1261:A:H62	20:A:1274:G:N2	2.03	0.50
3:D:35:ARG:HD3	20:A:412:A:H2	1.75	0.50
1:B:167:PRO:HD3	1:B:187:LEU:O	2.11	0.50
2:C:152:ILE:HG12	2:C:199:LYS:HB2	1.94	0.50
8:I:17:VAL:HG22	8:I:63:ILE:HD12	1.93	0.50
18:S:71:LEU:C	18:S:73:GLU:H	2.14	0.50
11:L:43:VAL:HG12	11:L:44:THR:H	1.75	0.50
20:A:1472:U:H2'	20:A:1473:A:C8	2.47	0.50
12:M:102:ARG:HG2	12:M:106:ASN:H	1.76	0.50
7:H:100:ILE:HB	7:H:125:ARG:HH21	1.76	0.50
23:Y:608:VAL:HG13	23:Y:609:GLU:O	2.12	0.50
20:A:1251:A:H2'	20:A:1252:A:H8	1.77	0.50
6:G:30:ILE:HG22	6:G:39:ALA:HB1	1.93	0.50
20:A:773:G:H1	20:A:806:C:H42	1.59	0.50
23:Y:138:LYS:CE	25:Y:701:GNP:N9	2.62	0.50
20:A:836:G:C6	20:A:851:G:C6	2.99	0.50
15:P:45:THR:O	15:P:47:ASP:N	2.45	0.50
19:T:85:MET:SD	20:A:186:C:O2'	2.63	0.50
20:A:1440(A):G:H5''	20:A:1440(B):G:O4'	2.11	0.50
19:T:37:SER:O	19:T:40:ALA:HB3	2.11	0.50
13:N:3:ARG:NH1	20:A:1204:A:OP2	2.45	0.50
3:D:162:LEU:HD11	3:D:181:MET:CG	2.41	0.50
15:P:5:ARG:HB2	20:A:376:G:H5''	1.94	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:L:84:LEU:H	11:L:104:VAL:HG11	1.77	0.50
14:O:67:LEU:HD11	14:O:87:ILE:HD12	1.92	0.50
3:D:30:LYS:HB3	3:D:35:ARG:HG2	1.93	0.50
3:D:33:MET:HG3	3:D:37:PRO:HB3	1.92	0.50
20:A:328:C:H4'	20:A:329:A:C5'	2.41	0.50
20:A:1196:U:H5'	20:A:1197:G:H5''	1.93	0.50
6:G:118:VAL:O	6:G:122:HIS:HB2	2.12	0.50
3:D:96:LEU:HD11	3:D:188:LEU:HD23	1.94	0.50
8:I:26:VAL:HG13	8:I:61:ALA:HB3	1.94	0.50
9:J:33:GLN:N	9:J:75:ILE:HD11	2.25	0.50
3:D:173:TRP:HA	3:D:186:LEU:HD12	1.92	0.50
23:Y:649:LEU:HA	23:Y:652:MET:HB3	1.93	0.50
23:Y:336:THR:HB	23:Y:339:SER:HB2	1.93	0.50
23:Y:541:ALA:HB1	23:Y:583:LYS:HD3	1.94	0.50
7:H:36:LEU:HD13	7:H:61:VAL:HG11	1.93	0.50
20:A:999:U:H2'	20:A:1000:A:H8	1.77	0.50
21:W:20(A):U:H1'	21:W:21:A:OP1	2.12	0.50
20:A:1492:A:H5'	24:U:6:5OH:NP	2.27	0.50
9:J:17:ASP:HB2	9:J:70:ARG:NH1	2.27	0.50
12:M:83:ASP:OD2	12:M:84:ILE:HG13	2.12	0.50
20:A:123:C:H5''	20:A:311:C:O2'	2.12	0.50
20:A:301:G:H2'	20:A:302:G:H8	1.76	0.50
20:A:1126:U:H1'	20:A:1280:A:C6	2.47	0.50
20:A:925:G:H1	20:A:1391:U:H3	1.59	0.50
20:A:1028(C):G:N2	20:A:1028(F):A:H8	2.02	0.50
4:E:20:GLN:HA	20:A:922:G:H4'	1.94	0.50
9:J:20:ALA:HB1	9:J:37:PRO:HB3	1.94	0.50
20:A:757:U:H2'	20:A:758:G:O4'	2.12	0.50
20:A:954:G:H2'	20:A:955:U:O4'	2.12	0.50
20:A:636:U:H2'	20:A:637:G:C8	2.47	0.50
3:D:93:PHE:O	3:D:97:LEU:HB2	2.12	0.50
4:E:126:ARG:HE	20:A:9:G:H5''	1.76	0.50
20:A:1206:G:H2'	20:A:1207:G:O4'	2.12	0.50
23:Y:25:LYS:HZ3	25:Y:701:GNP:PB	2.32	0.49
23:Y:72:CYS:HB2	23:Y:79:ILE:HD12	1.94	0.49
20:A:810:C:H2'	20:A:811:C:H6	1.77	0.49
20:A:340:U:H2'	20:A:341:C:O4'	2.11	0.49
20:A:1070:U:H3	20:A:1105:A:H61	1.60	0.49
23:Y:542:VAL:HG23	23:Y:582:PHE:HB3	1.94	0.49
20:A:1172:C:H2'	20:A:1173:G:H8	1.77	0.49
11:L:32:PHE:O	11:L:84:LEU:HG	2.11	0.49
20:A:634:C:H2'	20:A:635:G:C8	2.45	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:1085:U:H3'	20:A:1086:U:C5	2.42	0.49
6:G:99:LEU:HD13	6:G:103:TRP:CZ2	2.47	0.49
23:Y:610:VAL:O	23:Y:642:VAL:HA	2.12	0.49
23:Y:28:THR:O	23:Y:32:ILE:HG12	2.13	0.49
23:Y:428:LEU:HD22	23:Y:440:VAL:HG11	1.94	0.49
20:A:694:A:H2'	20:A:695:A:O4'	2.12	0.49
8:I:108:VAL:O	8:I:110:GLU:N	2.45	0.49
11:L:118:SER:CB	20:A:35:G:H21	2.25	0.49
20:A:302:G:N3	20:A:556:C:H4'	2.27	0.49
5:F:35:ALA:HB1	5:F:65:VAL:HG21	1.93	0.49
23:Y:103:GLY:HA2	23:Y:131:PRO:HD2	1.93	0.49
6:G:35:LYS:NZ	20:A:1289:A:O2'	2.42	0.49
23:Y:536:LYS:H	23:Y:536:LYS:HD2	1.77	0.49
9:J:54:PHE:CD1	9:J:55:LYS:HD2	2.47	0.49
23:Y:512:ILE:HG22	23:Y:567:LEU:HD12	1.93	0.49
23:Y:573:HIS:HB3	23:Y:576:ASP:HB2	1.93	0.49
20:A:287:U:H2'	20:A:288:A:H8	1.78	0.49
20:A:894:G:H2'	20:A:895:G:C8	2.47	0.49
21:W:43:G:H2'	21:W:44:G:C8	2.47	0.49
1:B:85:ALA:O	1:B:89:GLY:N	2.45	0.49
16:Q:10:VAL:HG12	16:Q:54:GLY:H	1.78	0.49
20:A:803:G:C6	20:A:804:U:C4	3.01	0.49
23:Y:85:PRO:HB3	23:Y:94:VAL:HG22	1.94	0.49
20:A:1381:U:H2'	20:A:1382:C:C6	2.46	0.49
15:P:20:VAL:HG11	15:P:32:TYR:HD1	1.78	0.49
16:Q:51:TYR:HE1	16:Q:76:LEU:HB2	1.77	0.49
20:A:1357:A:N6	20:A:1358:U:O4	2.45	0.49
21:W:65:U:H2'	21:W:66:C:H6	1.77	0.49
20:A:763:G:H2'	20:A:764:C:H6	1.78	0.49
20:A:1409:C:H2'	20:A:1410:G:C8	2.47	0.49
23:Y:45:VAL:HB	23:Y:362:HIS:ND1	2.28	0.49
23:Y:138:LYS:HG2	25:Y:701:GNP:C2	2.37	0.49
7:H:11:THR:HG21	20:A:876:G:H1'	1.93	0.49
11:L:66:VAL:HG12	11:L:67:THR:H	1.77	0.49
20:A:1402:C:H2'	20:A:1403:C:O4'	2.13	0.49
20:A:1352:C:H2'	20:A:1353:G:C8	2.46	0.49
23:Y:203:GLU:O	23:Y:205:TYR:N	2.46	0.49
11:L:83:VAL:HB	11:L:100:ILE:HG23	1.93	0.49
20:A:1343:G:N2	20:A:1349:A:HO2'	2.09	0.49
20:A:813:U:H3'	20:A:816:A:H62	1.78	0.49
20:A:1493:A:H5'	20:A:1494:G:O5'	2.13	0.49
20:A:763:G:H2'	20:A:764:C:C6	2.47	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:272:C:H2'	20:A:273:A:H8	1.78	0.49
18:S:50:ALA:HA	18:S:59:PRO:HA	1.93	0.49
20:A:1508:G:H2'	20:A:1509:C:C6	2.48	0.49
23:Y:161:PRO:O	23:Y:256:THR:N	2.45	0.49
9:J:54:PHE:HB2	20:A:1198:G:H21	1.78	0.49
20:A:691:G:H2'	20:A:692:U:C6	2.48	0.49
16:Q:21:VAL:HG21	16:Q:59:ILE:HG12	1.95	0.49
10:K:69:ALA:O	10:K:73:MET:HG2	2.13	0.49
20:A:27:G:H2'	20:A:28:G:C8	2.48	0.49
2:C:108:ASN:HB3	2:C:111:LEU:HD23	1.94	0.49
5:F:15:ASP:HB3	5:F:18:GLN:HG3	1.93	0.49
19:T:57:ARG:NH1	19:T:102:GLY:HA3	2.28	0.49
20:A:201(B):U:H5''	20:A:201(C):U:OP1	2.12	0.49
9:J:13:HIS:HB2	9:J:70:ARG:HH12	1.78	0.49
23:Y:133:ILE:HD13	23:Y:133:ILE:H	1.78	0.49
23:Y:257:PRO:O	23:Y:259:PHE:N	2.43	0.49
23:Y:512:ILE:H	23:Y:512:ILE:HD13	1.77	0.49
20:A:137:C:N4	20:A:226:G:H1	2.08	0.49
7:H:14:ARG:O	7:H:17:THR:OG1	2.26	0.49
13:N:57:ARG:O	13:N:59:ALA:N	2.46	0.49
7:H:64:LYS:HD2	7:H:79:VAL:HG11	1.94	0.49
20:A:1010:G:H1	20:A:1019:C:H42	1.61	0.49
23:Y:237:PRO:HB2	23:Y:242:LEU:HD21	1.94	0.49
20:A:1338:G:H2'	20:A:1339:A:C8	2.48	0.49
1:B:95:GLN:HG3	1:B:147:LYS:O	2.13	0.49
1:B:27:LYS:H	1:B:27:LYS:HD2	1.77	0.49
20:A:1003:G:N1	20:A:1037:C:C2	2.64	0.49
9:J:54:PHE:CE1	9:J:55:LYS:HD2	2.48	0.49
10:K:111:ASP:HA	17:R:84:LYS:HE3	1.95	0.49
23:Y:428:LEU:HA	23:Y:431:LEU:HB2	1.95	0.49
2:C:130:VAL:O	2:C:134:ILE:HB	2.13	0.49
4:E:31:LEU:HA	4:E:45:PHE:CB	2.43	0.49
3:D:86:LYS:NZ	3:D:89:THR:HG23	2.28	0.49
23:Y:489:LYS:HD3	23:Y:597:GLY:HA2	1.94	0.49
7:H:10:LEU:HB3	7:H:83:ILE:HD12	1.94	0.49
3:D:11:LEU:HA	3:D:14:ARG:HB3	1.95	0.49
20:A:1520:G:H2'	20:A:1521:G:H8	1.77	0.49
21:W:5:A:H2'	21:W:6:C:C6	2.47	0.49
20:A:1304:G:C6	20:A:1305:G:N1	2.81	0.49
6:G:24:THR:HA	6:G:27:ILE:HD12	1.94	0.49
11:L:91:LYS:NZ	20:A:526:C:OP2	2.45	0.49
11:L:39:VAL:HG12	11:L:40:VAL:N	2.24	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:402:G:H5'	20:A:621:A:H1'	1.95	0.48
12:M:116:THR:HG23	20:A:1229:A:H5'	1.94	0.48
20:A:1221:G:OP1	20:A:1320:C:N4	2.46	0.48
19:T:88:VAL:HG12	19:T:92:LEU:HG	1.95	0.48
5:F:72:VAL:HG13	5:F:73:ASN:H	1.78	0.48
20:A:762:C:H2'	20:A:763:G:H8	1.76	0.48
5:F:40:VAL:HA	5:F:62:TRP:O	2.13	0.48
23:Y:139:MET:HB3	23:Y:174:PHE:HE1	1.78	0.48
23:Y:72:CYS:CB	23:Y:79:ILE:O	2.59	0.48
18:S:36:ARG:HB2	18:S:72:GLY:HA3	1.95	0.48
20:A:1306:A:N6	20:A:1331:G:O2'	2.46	0.48
8:I:105:ASP:CG	8:I:106:ALA:H	2.15	0.48
18:S:6:LYS:HD2	20:A:1314:C:C6	2.47	0.48
6:G:92:SER:O	6:G:96:GLN:HG3	2.12	0.48
10:K:24:SER:OG	10:K:25:TYR:N	2.46	0.48
5:F:96:PRO:HA	17:R:32:ARG:HB2	1.95	0.48
23:Y:39:ILE:HG21	23:Y:76:ASP:OD2	2.12	0.48
16:Q:2:PRO:O	20:A:127:G:O2'	2.30	0.48
20:A:867:G:H2'	20:A:868:C:H6	1.78	0.48
20:A:1295:G:H21	20:A:1302:U:H3	1.60	0.48
23:Y:497:PHE:HB3	23:Y:507:TYR:HB2	1.95	0.48
23:Y:684:GLN:O	23:Y:688:ILE:N	2.47	0.48
11:L:54:LYS:HD3	11:L:70:ILE:CG1	2.32	0.48
11:L:79:GLU:O	11:L:80:HIS:ND1	2.47	0.48
11:L:92:ASP:OD1	11:L:92:ASP:N	2.45	0.48
12:M:96:LEU:HB3	12:M:97:PRO:HD2	1.93	0.48
20:A:1421:G:H2'	20:A:1422:G:O4'	2.13	0.48
20:A:1016:A:H2'	20:A:1017:G:O4'	2.14	0.48
23:Y:83:ASP:N	23:Y:83:ASP:OD1	2.46	0.48
20:A:316:G:OP2	20:A:351:G:O2'	2.30	0.48
20:A:642:A:H2'	20:A:643:C:C6	2.48	0.48
20:A:1003:G:O6	20:A:1037:C:N3	2.46	0.48
14:O:46:HIS:O	14:O:48:LYS:N	2.46	0.48
5:F:48:LEU:N	5:F:56:PRO:O	2.46	0.48
19:T:36:LEU:HB3	19:T:59:ALA:HB2	1.95	0.48
4:E:91:LEU:HD13	4:E:120:THR:HB	1.94	0.48
23:Y:138:LYS:HE2	25:Y:701:GNP:C8	2.41	0.48
20:A:670:G:H1	20:A:736:C:N4	2.09	0.48
11:L:117:ARG:NH2	20:A:501:C:OP2	2.38	0.48
23:Y:681:LYS:O	23:Y:685:GLU:N	2.44	0.48
3:D:135:LEU:HD13	3:D:135:LEU:HA	1.66	0.48
20:A:1440(J):C:O2'	20:A:1440(K):G:N2	2.47	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:1161:C:H2'	20:A:1162:C:C6	2.48	0.48
3:D:177:ASP:HB2	3:D:182:LYS:H	1.79	0.48
20:A:258:G:H2'	20:A:259:G:H8	1.78	0.48
20:A:59:A:N6	20:A:331:G:O2'	2.47	0.48
20:A:501:C:O2'	20:A:549:C:O2	2.27	0.48
21:W:69:A:H2'	21:W:70:G:H8	1.77	0.48
20:A:701:C:OP1	20:A:703:G:H5'	2.14	0.48
23:Y:17:ILE:H	23:Y:83:ASP:CB	2.27	0.48
2:C:11:ARG:HE	2:C:182:ILE:H	1.61	0.48
20:A:1290:G:H2'	20:A:1291:G:H8	1.79	0.48
20:A:1440(C):G:H3'	20:A:1440(D):A:H5'	1.96	0.48
20:A:1537:U:O2'	20:A:1538:C:OP1	2.30	0.48
23:Y:176:GLY:HA3	23:Y:187:THR:HA	1.95	0.48
4:E:88:LYS:HB3	4:E:123:LEU:HB2	1.94	0.48
15:P:9:PHE:HE2	15:P:18:ARG:HB2	1.78	0.48
6:G:140:ASP:HA	6:G:143:ARG:HD2	1.96	0.48
20:A:105:G:H2'	20:A:106:C:H6	1.75	0.48
3:D:55:ALA:HB2	20:A:509:A:H5''	1.96	0.48
20:A:1103:C:H2'	20:A:1104:G:O4'	2.14	0.48
20:A:186(L):G:H2'	20:A:186(M):G:C8	2.49	0.48
23:Y:17:ILE:H	23:Y:83:ASP:HB3	1.79	0.48
7:H:86:ILE:HD11	7:H:136:GLU:HG3	1.96	0.48
20:A:1313:U:H2'	20:A:1314:C:O4'	2.14	0.48
1:B:197:VAL:HG12	1:B:200:ILE:HG13	1.96	0.48
12:M:51:ALA:O	12:M:55:ARG:HG2	2.14	0.48
6:G:51:GLN:NE2	6:G:56:GLN:O	2.33	0.48
20:A:201(A):U:O2'	20:A:201(B):U:H5'	2.14	0.48
16:Q:64:PRO:O	20:A:265:G:H5'	2.14	0.48
20:A:128:G:H1	20:A:233:C:H42	1.62	0.48
14:O:29:VAL:HG22	14:O:66:LEU:HB3	1.94	0.48
20:A:458(A):G:O6	20:A:458(C):G:H5''	2.13	0.48
3:D:67:ILE:HG12	3:D:67:ILE:O	2.14	0.48
4:E:145:LYS:O	4:E:149:GLU:HG2	2.13	0.48
20:A:1102:A:H2'	20:A:1103:C:C6	2.49	0.48
23:Y:630:GLN:O	23:Y:646:PHE:HB2	2.13	0.48
20:A:671:G:H1	20:A:735:C:H42	1.60	0.48
6:G:66:VAL:O	6:G:70:LYS:HG3	2.14	0.48
3:D:156:GLU:HB2	3:D:157:LEU:HD12	1.96	0.48
12:M:75:ALA:O	12:M:79:LYS:HG3	2.14	0.48
1:B:111:ARG:NH1	20:A:1104:G:H4'	2.28	0.48
20:A:975:A:H4'	20:A:976:G:H5''	1.96	0.48
20:A:1197:G:H5'	20:A:1197:G:H8	1.79	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
21:W:19:G:H4'	21:W:20:U:C5	2.49	0.48
14:O:23:GLY:O	14:O:28:GLN:NE2	2.38	0.48
20:A:942:G:H2'	20:A:943:U:C6	2.49	0.48
6:G:78:ARG:HG2	6:G:85:TYR:HB2	1.96	0.47
12:M:74:VAL:O	12:M:78:ILE:HG12	2.14	0.47
12:M:31:LYS:HA	12:M:34:LEU:HD12	1.96	0.47
15:P:2:VAL:HA	15:P:23:ASP:HA	1.96	0.47
15:P:53:VAL:O	15:P:57:ARG:HB2	2.14	0.47
7:H:10:LEU:O	7:H:13:ILE:HB	2.14	0.47
20:A:122:G:H2'	20:A:123:C:H6	1.78	0.47
10:K:79:SER:HA	10:K:104:GLN:HB3	1.96	0.47
4:E:73:ASN:O	4:E:73:ASN:ND2	2.40	0.47
23:Y:25:LYS:CG	25:Y:701:GNP:O1B	2.45	0.47
11:L:35:GLY:HA3	11:L:83:VAL:O	2.14	0.47
11:L:45:PRO:CA	11:L:92:ASP:HB3	2.44	0.47
23:Y:598:ASP:HA	23:Y:599:PRO:HD2	1.76	0.47
7:H:63:LEU:HD23	7:H:65:TYR:CZ	2.49	0.47
3:D:15:GLU:HB3	3:D:63:LYS:HE2	1.95	0.47
18:S:78:ARG:HH12	20:A:1223:C:P	2.37	0.47
20:A:1015:A:H2'	20:A:1016:A:C8	2.49	0.47
1:B:61:LEU:HD12	1:B:64:ARG:HH21	1.79	0.47
7:H:98:LYS:HG2	7:H:98:LYS:H	1.44	0.47
5:F:82:ARG:HA	5:F:82:ARG:CZ	2.44	0.47
1:B:107:THR:O	1:B:110:GLN:HB2	2.14	0.47
23:Y:138:LYS:CE	25:Y:701:GNP:C5	2.85	0.47
9:J:24:VAL:HG13	9:J:34:VAL:HB	1.94	0.47
23:Y:14:ASN:HB3	23:Y:102:ASP:H	1.78	0.47
17:R:44:LEU:HD22	17:R:79:LEU:HD22	1.97	0.47
21:W:66:C:H2'	21:W:67:G:H8	1.78	0.47
20:A:939:G:H2'	20:A:940:C:C6	2.49	0.47
20:A:339:C:H2'	20:A:340:U:H6	1.79	0.47
12:M:108:ARG:HH12	12:M:111:LYS:HZ1	1.61	0.47
20:A:1178:G:N2	20:A:1181:G:OP2	2.47	0.47
20:A:184:G:H1	20:A:193:C:H42	1.62	0.47
13:N:35:ARG:HD3	13:N:36:PHE:H	1.80	0.47
23:Y:256:THR:O	23:Y:258:VAL:HG13	2.15	0.47
3:D:30:LYS:C	3:D:32:ALA:H	2.17	0.47
20:A:745:C:H5''	20:A:851:G:O2'	2.14	0.47
8:I:112:LYS:NZ	8:I:113:LYS:O	2.47	0.47
23:Y:344:THR:HB	23:Y:388:THR:HB	1.96	0.47
1:B:102:LEU:HD11	1:B:159:PRO:HG2	1.96	0.47
13:N:6:LEU:HB3	13:N:23:ARG:HH22	1.79	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:1247:U:H3	20:A:1290:G:H1	1.62	0.47
21:W:36:U:C5	21:W:37:A:N7	2.82	0.47
9:J:16:LEU:HD11	9:J:70:ARG:HD3	1.97	0.47
7:H:129:VAL:HB	7:H:130:GLY:H	1.60	0.47
3:D:122:ARG:HE	20:A:403:C:H4'	1.78	0.47
23:Y:239:GLU:HA	23:Y:242:LEU:HD12	1.97	0.47
23:Y:406:GLU:HG3	23:Y:407:PRO:HD2	1.96	0.47
20:A:950:U:H2'	20:A:951:G:H8	1.79	0.47
20:A:1194:U:H2'	20:A:1195:C:O4'	2.15	0.47
20:A:60:A:H62	20:A:110:C:N4	2.12	0.47
3:D:73:ARG:HB2	20:A:546:G:OP1	2.14	0.47
20:A:316:G:O3'	20:A:353:A:N6	2.48	0.47
8:I:92:TYR:O	8:I:96:LEU:HB2	2.15	0.47
17:R:52:PRO:HG2	17:R:55:ARG:HG2	1.95	0.47
23:Y:98:MET:C	23:Y:100:VAL:H	2.18	0.47
15:P:28:ARG:NE	15:P:29:ASP:OD1	2.36	0.47
20:A:1003:G:C2	20:A:1037:C:O2	2.65	0.47
20:A:375:U:H2'	20:A:376:G:C8	2.50	0.47
20:A:1506:U:H3'	22:V:15:A:N6	2.30	0.47
6:G:74:GLU:OE2	6:G:95:ARG:NH2	2.35	0.47
9:J:16:LEU:HD21	9:J:70:ARG:HB2	1.97	0.47
23:Y:415:PRO:HD2	23:Y:421:GLN:OE1	2.14	0.47
14:O:26:GLU:OE1	14:O:77:ARG:HD3	2.15	0.47
14:O:39:LEU:HD22	14:O:42:HIS:HB3	1.97	0.47
8:I:111:ARG:CZ	20:A:1187:G:H4'	2.44	0.47
16:Q:67:LYS:C	16:Q:69:LYS:H	2.17	0.47
9:J:79:ARG:HA	9:J:79:ARG:CZ	2.45	0.47
18:S:51:VAL:HG21	18:S:71:LEU:HD22	1.97	0.47
7:H:83:ILE:HG12	7:H:84:ARG:N	2.29	0.47
20:A:768:A:H5'	20:A:1524:C:O2'	2.15	0.47
2:C:174:PRO:HA	20:A:1107:C:H5''	1.96	0.47
20:A:146:G:H1	20:A:176:C:H42	1.62	0.47
3:D:100:ARG:HD2	3:D:137:SER:HA	1.96	0.47
18:S:14:HIS:NE2	20:A:1014:A:H4'	2.29	0.47
20:A:1011:G:H2'	20:A:1012:U:O4'	2.14	0.47
20:A:1228:C:H2'	20:A:1229:A:C8	2.48	0.47
20:A:978:A:O2'	20:A:1322:C:N3	2.41	0.47
20:A:1063:C:H42	20:A:1193:G:H1	1.62	0.47
23:Y:611:THR:HA	23:Y:642:VAL:HG22	1.96	0.47
1:B:22:LYS:HG2	1:B:40:HIS:HE2	1.80	0.47
5:F:76:ALA:O	5:F:80:ARG:HG3	2.14	0.47
20:A:1208:C:H2'	20:A:1209:C:O4'	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:I:14:VAL:HG11	20:A:1148:U:O2'	2.15	0.47
11:L:33:ARG:HG2	11:L:60:LEU:HB3	1.96	0.47
6:G:116:ALA:O	6:G:120:ILE:HG12	2.15	0.47
1:B:69:LEU:HA	1:B:69:LEU:HD22	1.76	0.47
8:I:113:LYS:HD2	20:A:1187:G:H5''	1.97	0.47
19:T:49:ALA:HB1	19:T:53:LEU:HD23	1.96	0.47
20:A:34:C:H42	20:A:550:G:H1	1.61	0.47
14:O:65:ARG:NH2	20:A:581:G:OP1	2.48	0.47
2:C:105:GLU:HG2	2:C:106:VAL:N	2.29	0.47
20:A:295:C:H2'	20:A:296:U:O4'	2.15	0.47
23:Y:289:ILE:HD12	23:Y:289:ILE:H	1.78	0.47
5:F:74:ASP:N	5:F:74:ASP:OD1	2.47	0.47
11:L:7:ILE:O	11:L:10:LEU:HB2	2.14	0.47
8:I:127:LYS:NZ	21:W:34:C:OP2	2.26	0.47
23:Y:180:VAL:HG23	23:Y:216:LEU:HD12	1.97	0.47
20:A:1281:U:H4'	20:A:1282:C:OP2	2.14	0.47
20:A:688:G:H2'	20:A:689:C:C6	2.49	0.47
11:L:114:LYS:N	20:A:538:G:OP1	2.48	0.47
3:D:54:TYR:CE2	20:A:508:C:H4'	2.50	0.47
16:Q:86:GLU:O	16:Q:90:ILE:HG13	2.15	0.47
20:A:285:G:H2'	20:A:286:G:H8	1.80	0.47
23:Y:309:LEU:O	23:Y:391:GLY:N	2.44	0.47
16:Q:68:ARG:NH2	20:A:277:C:OP1	2.34	0.46
20:A:565:U:OP2	20:A:566:G:O2'	2.19	0.46
7:H:94:TYR:CD2	20:A:598:U:H4'	2.50	0.46
1:B:231:GLU:HA	1:B:232:PRO:HD3	1.84	0.46
16:Q:87:LYS:HB3	16:Q:87:LYS:HE2	1.65	0.46
23:Y:24:GLY:HA2	25:Y:701:GNP:H8	1.97	0.46
20:A:1504:G:OP1	20:A:1507:A:H4'	2.15	0.46
23:Y:5:VAL:HG13	23:Y:11:ARG:HH12	1.79	0.46
20:A:292:G:N7	20:A:293:G:H1'	2.30	0.46
20:A:1187:G:H2'	20:A:1188:A:C8	2.50	0.46
20:A:323:U:H2'	20:A:324:G:O4'	2.14	0.46
20:A:1468:A:H2'	20:A:1469:G:O4'	2.15	0.46
11:L:92:ASP:HB2	11:L:93:LEU:H	1.30	0.46
23:Y:415:PRO:HB2	23:Y:472:VAL:HG12	1.96	0.46
20:A:277:C:H2'	20:A:278:G:H8	1.80	0.46
20:A:68(K):U:H3'	20:A:68(M):U:OP2	2.16	0.46
3:D:21:LEU:O	3:D:113:SER:OG	2.22	0.46
7:H:97:VAL:HG12	20:A:600:C:OP1	2.16	0.46
20:A:1270:C:H2'	20:A:1271:G:C8	2.50	0.46
14:O:8:LYS:HZ1	20:A:658:G:P	2.35	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:108:G:OP2	20:A:108:G:N2	2.49	0.46
8:I:127:LYS:HE3	21:W:34:C:H5"	1.97	0.46
20:A:864:A:C6	20:A:865:A:C6	3.03	0.46
20:A:38:G:H1'	20:A:397:A:N6	2.30	0.46
12:M:108:ARG:HH12	12:M:111:LYS:NZ	2.14	0.46
18:S:10:PHE:CE1	20:A:1318:A:H4'	2.50	0.46
20:A:979:C:N4	20:A:1318:A:H61	2.12	0.46
16:Q:95:TYR:C	16:Q:97:SER:H	2.18	0.46
1:B:52:GLU:O	1:B:56:ARG:HB2	2.15	0.46
10:K:109:VAL:HG13	17:R:84:LYS:HB2	1.97	0.46
20:A:1440(A):G:H4'	20:A:1440(B):G:C5	2.51	0.46
23:Y:72:CYS:SG	23:Y:79:ILE:O	2.74	0.46
11:L:36:VAL:O	11:L:80:HIS:HA	2.15	0.46
11:L:80:HIS:HB3	11:L:81:SER:H	1.46	0.46
11:L:7:ILE:O	11:L:11:VAL:HG23	2.15	0.46
10:K:53:SER:C	10:K:55:LYS:H	2.18	0.46
20:A:47:C:N4	20:A:361:G:H1	2.08	0.46
2:C:20:SER:HB2	2:C:22:TRP:HE1	1.81	0.46
9:J:24:VAL:O	9:J:28:ARG:HG2	2.16	0.46
20:A:59:A:H1'	20:A:354:G:C2	2.50	0.46
20:A:1234:C:H2'	20:A:1235:U:O4'	2.15	0.46
20:A:767:A:H2'	20:A:768:A:O4'	2.16	0.46
20:A:309:G:H2'	20:A:310:G:C8	2.51	0.46
20:A:309:G:H2'	20:A:310:G:H8	1.81	0.46
3:D:74:GLN:NE2	20:A:403:C:OP2	2.49	0.46
5:F:62:TRP:HB2	17:R:35:ARG:HH12	1.79	0.46
23:Y:38:ARG:HD2	23:Y:41:LYS:O	2.16	0.46
2:C:115:LEU:HA	2:C:118:GLN:HB2	1.98	0.46
19:T:12:ALA:HA	19:T:15:ARG:HB2	1.97	0.46
20:A:554:C:H2'	20:A:555:C:C6	2.49	0.46
18:S:82:GLY:HA3	20:A:1226:C:H4'	1.98	0.46
13:N:29:ARG:HH11	13:N:31:ARG:HB2	1.80	0.46
23:Y:617:MET:O	23:Y:621:ILE:HD12	2.15	0.46
23:Y:206:LEU:HD12	23:Y:210:ARG:HH12	1.79	0.46
1:B:74:LYS:O	1:B:76:GLN:N	2.48	0.46
10:K:119:CYS:HB3	20:A:778:G:H1'	1.97	0.46
3:D:41:GLY:HA3	20:A:542:G:H5'	1.98	0.46
20:A:1288:A:N1	20:A:1371:G:H1'	2.31	0.46
5:F:23:LYS:HE3	5:F:23:LYS:HB3	1.81	0.46
20:A:490:G:H2'	20:A:491:G:H8	1.81	0.46
3:D:9:CYS:CA	3:D:12:CYS:HB2	2.45	0.46
20:A:129(A):G:H4'	20:A:130:A:H5"	1.98	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:M:13:LYS:HE3	12:M:21:TYR:HE1	1.80	0.46
21:W:67:G:H2'	21:W:68:U:C6	2.51	0.46
20:A:1401:G:H2'	20:A:1402:C:O4'	2.16	0.46
20:A:939:G:C2	20:A:940:C:C4	3.04	0.46
20:A:689:C:H2'	20:A:690:G:O4'	2.16	0.46
3:D:148:VAL:HG23	3:D:181:MET:HB3	1.97	0.46
23:Y:96:ARG:O	23:Y:100:VAL:HG12	2.16	0.46
17:R:26:LEU:HD13	17:R:39:VAL:HG22	1.98	0.46
10:K:113:PRO:O	10:K:115:PRO:HD3	2.16	0.46
23:Y:686:LYS:HD3	23:Y:687:LEU:HD23	1.98	0.46
16:Q:91:ARG:HG2	20:A:583:A:H4'	1.98	0.46
23:Y:150:ILE:HD12	23:Y:161:PRO:HB2	1.98	0.46
23:Y:408:VAL:HG22	23:Y:454:MET:HA	1.98	0.46
6:G:79:ARG:H	6:G:79:ARG:HD2	1.81	0.46
20:A:834:C:H2'	20:A:835:U:O4'	2.16	0.46
21:W:12:U:H1'	21:W:24:G:H22	1.81	0.46
20:A:1306:A:H61	20:A:1331:G:H1'	1.81	0.46
4:E:40:ARG:HA	4:E:68:GLU:HA	1.98	0.46
12:M:48:LEU:HD13	12:M:53:VAL:HG22	1.98	0.46
20:A:869:G:H4'	20:A:872:A:C8	2.50	0.46
20:A:784:C:H2'	20:A:785:G:C8	2.51	0.46
20:A:890:G:O2'	20:A:906:G:O6	2.25	0.46
6:G:11:GLN:HG2	6:G:12:LEU:N	2.31	0.46
2:C:117:ALA:HA	2:C:120:VAL:HB	1.97	0.46
23:Y:335:LEU:HA	23:Y:335:LEU:HD12	1.74	0.46
15:P:6:LEU:HD22	20:A:375:U:H5"	1.98	0.46
11:L:45:PRO:CB	11:L:92:ASP:HB3	2.45	0.46
20:A:1343:G:H21	20:A:1349:A:HO2'	1.56	0.46
23:Y:631:ILE:O	23:Y:645:ALA:HA	2.15	0.46
8:I:28:VAL:HG13	8:I:63:ILE:HB	1.98	0.46
23:Y:485:GLU:OE2	23:Y:555:LEU:HB2	2.16	0.46
11:L:15:ARG:HB3	20:A:562:C:O2	2.16	0.46
20:A:115:G:H1'	20:A:116:A:N7	2.30	0.46
9:J:45:ARG:HA	20:A:1254:C:OP1	2.17	0.46
20:A:1523:G:H2'	20:A:1524:C:C6	2.51	0.46
2:C:87:LEU:O	2:C:91:LEU:HB2	2.16	0.46
1:B:95:GLN:HG3	1:B:148:TYR:HA	1.98	0.46
11:L:57:LYS:O	11:L:59:ARG:N	2.49	0.46
20:A:889:A:OP1	20:A:889:A:H8	1.99	0.46
9:J:58:ASP:OD2	9:J:58:ASP:N	2.48	0.46
23:Y:344:THR:HG22	23:Y:397:VAL:O	2.16	0.45
2:C:36:ASP:HA	2:C:39:ILE:HD12	1.97	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:1321:C:C3'	20:A:1322:C:H5''	2.45	0.45
2:C:7:PRO:O	2:C:11:ARG:HG2	2.16	0.45
20:A:229:U:H2'	20:A:230:G:C8	2.51	0.45
8:I:82:ALA:O	8:I:86:VAL:HG23	2.16	0.45
23:Y:25:LYS:HZ2	25:Y:701:GNP:PG	2.39	0.45
11:L:15:ARG:NH1	20:A:563:A:N3	2.64	0.45
15:P:45:THR:C	15:P:47:ASP:H	2.18	0.45
20:A:647:C:H2'	20:A:648:A:H8	1.81	0.45
10:K:18:ARG:HD2	10:K:20:TYR:CE1	2.50	0.45
3:D:12:CYS:HB3	3:D:33:MET:CE	2.47	0.45
3:D:9:CYS:HA	3:D:12:CYS:HB2	1.98	0.45
3:D:8:VAL:HG23	3:D:9:CYS:N	2.31	0.45
14:O:25:THR:OG1	14:O:26:GLU:N	2.46	0.45
9:J:24:VAL:HG22	9:J:34:VAL:HG11	1.98	0.45
20:A:1356:G:H2'	20:A:1357:A:C8	2.52	0.45
20:A:163:C:H2'	20:A:164:U:C6	2.52	0.45
18:S:40:ILE:HD11	18:S:71:LEU:HA	1.98	0.45
17:R:37:VAL:HG23	17:R:38:GLU:H	1.81	0.45
6:G:37:ASN:O	6:G:41:ARG:HG3	2.16	0.45
23:Y:45:VAL:HB	23:Y:362:HIS:CE1	2.52	0.45
4:E:25:ARG:HD3	4:E:27:ARG:NH1	2.31	0.45
2:C:139:GLN:O	2:C:143:GLU:HB2	2.16	0.45
23:Y:69:VAL:HB	23:Y:82:ILE:HG12	1.98	0.45
6:G:69:VAL:O	6:G:138:LYS:HG3	2.17	0.45
20:A:1400:C:H5'	22:V:20:U:C4	2.52	0.45
3:D:107:ARG:HA	3:D:107:ARG:HD3	1.82	0.45
20:A:522:C:H2'	20:A:523:A:O4'	2.17	0.45
20:A:1006:C:H2'	20:A:1007:C:C6	2.52	0.45
20:A:923:A:N6	20:A:1392:G:O6	2.49	0.45
20:A:947:G:O2'	20:A:1306:A:H4'	2.17	0.45
18:S:44:MET:O	18:S:46:GLY:N	2.50	0.45
20:A:186(A):C:H2'	20:A:186(B):C:C6	2.52	0.45
20:A:910:C:H2'	20:A:911:U:C6	2.51	0.45
23:Y:86:GLY:C	23:Y:88:VAL:H	2.19	0.45
3:D:101:LEU:HB2	3:D:138:TYR:HB3	1.99	0.45
5:F:24:GLU:O	5:F:28:ARG:HG3	2.17	0.45
16:Q:79:SER:OG	16:Q:80:GLY:N	2.49	0.45
23:Y:101:LEU:O	23:Y:128:TYR:OH	2.09	0.45
23:Y:387:ASP:N	23:Y:387:ASP:OD2	2.41	0.45
23:Y:569:ASP:OD2	23:Y:570:GLY:N	2.48	0.45
10:K:84:VAL:N	10:K:109:VAL:O	2.49	0.45
10:K:86:GLY:HA2	10:K:112:THR:HG23	1.98	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:313:A:H2'	20:A:314:C:C6	2.51	0.45
12:M:98:VAL:O	12:M:98:VAL:HG12	2.15	0.45
10:K:94:ALA:O	10:K:98:LEU:HG	2.16	0.45
18:S:73:GLU:HG2	20:A:1320:C:H1'	1.98	0.45
23:Y:76:ASP:O	23:Y:77:HIS:ND1	2.46	0.45
5:F:80:ARG:NH2	5:F:88:VAL:O	2.49	0.45
12:M:36:LYS:NZ	12:M:36:LYS:HA	2.31	0.45
8:I:9:ARG:HG3	8:I:14:VAL:HG23	1.98	0.45
3:D:8:VAL:HG11	3:D:115:ARG:CZ	2.46	0.45
20:A:408:A:H2'	20:A:409:G:C8	2.52	0.45
14:O:46:HIS:O	14:O:47:LYS:HG2	2.17	0.45
16:Q:46:ASP:OD1	16:Q:49:GLU:HA	2.16	0.45
17:R:40:LEU:HB3	17:R:79:LEU:HD11	1.98	0.45
20:A:872:A:C4	20:A:874:G:N7	2.85	0.45
7:H:110:ALA:HB3	7:H:121:ASP:HB3	1.99	0.45
20:A:53:A:H61	20:A:358:U:H3	1.64	0.45
16:Q:37:LYS:N	16:Q:37:LYS:HD2	2.32	0.45
16:Q:4:LYS:HD2	16:Q:4:LYS:HA	1.66	0.45
23:Y:499:ARG:HB2	23:Y:506:GLN:O	2.16	0.45
23:Y:33:LEU:HG	23:Y:34:TYR:CD2	2.52	0.45
11:L:95:GLY:C	11:L:97:ARG:H	2.19	0.45
9:J:49:VAL:HG22	9:J:50:ILE:H	1.81	0.45
9:J:78:ASN:O	9:J:81:THR:OG1	2.33	0.45
20:A:687:A:N6	20:A:701:C:O2	2.50	0.45
3:D:162:LEU:HD11	3:D:181:MET:HG2	1.99	0.45
20:A:301:G:H2'	20:A:302:G:C8	2.51	0.45
16:Q:52:LYS:HG2	16:Q:55:ASP:OD1	2.16	0.45
11:L:35:GLY:HA2	11:L:58:VAL:CG1	2.44	0.45
11:L:10:LEU:HB3	16:Q:32:TYR:CD1	2.52	0.45
20:A:1465:C:H2'	20:A:1466:C:O4'	2.16	0.45
16:Q:45:HIS:HB3	16:Q:72:ARG:HG2	1.99	0.45
7:H:20:TYR:HA	7:H:65:TYR:CZ	2.52	0.45
20:A:272:C:H2'	20:A:273:A:C8	2.52	0.45
20:A:123:C:O3'	20:A:310:G:N2	2.49	0.45
20:A:647:C:H2'	20:A:648:A:C8	2.52	0.45
20:A:346:G:H5'	20:A:347:G:OP2	2.17	0.45
20:A:1260:C:OP1	20:A:1284:C:H4'	2.17	0.45
20:A:1227:A:N3	20:A:1227:A:H2'	2.32	0.45
11:L:93:LEU:HD12	11:L:96:VAL:HG13	1.98	0.45
20:A:68(I):G:O6	20:A:68(Q):U:O4	2.35	0.45
23:Y:150:ILE:HD11	23:Y:258:VAL:HG21	1.98	0.45
20:A:663:A:H61	20:A:742:G:H1	1.65	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:201:ILE:HA	1:B:201:ILE:HD13	1.73	0.45
3:D:177:ASP:HB2	3:D:182:LYS:N	2.32	0.45
19:T:73:HIS:C	19:T:74:LYS:HZ2	2.20	0.45
11:L:74:GLY:O	11:L:102:ARG:NH2	2.48	0.45
3:D:55:ALA:O	3:D:59:ARG:HG2	2.17	0.45
2:C:2:GLY:HA2	20:A:1062:U:O4	2.17	0.45
20:A:45:U:H2'	20:A:46:G:C8	2.52	0.45
5:F:18:GLN:O	5:F:21:LEU:HB3	2.17	0.45
2:C:8:ILE:HD12	2:C:16:ARG:CZ	2.47	0.45
6:G:64:GLN:HG3	6:G:128:ALA:HA	1.99	0.45
7:H:52:ASP:HA	7:H:58:TYR:H	1.81	0.45
2:C:161:GLU:HA	20:A:1055:A:O2'	2.16	0.45
13:N:4:LYS:O	13:N:7:ILE:HG12	2.16	0.45
23:Y:119:GLU:O	23:Y:123:ARG:HB2	2.17	0.45
14:O:5:LYS:O	14:O:9:GLN:HG2	2.16	0.45
23:Y:24:GLY:HA3	25:Y:701:GNP:H8	1.98	0.45
11:L:58:VAL:HB	11:L:60:LEU:HD22	1.99	0.45
11:L:81:SER:HB2	11:L:83:VAL:HG13	1.98	0.45
11:L:90:VAL:CG2	11:L:96:VAL:HG11	2.43	0.45
9:J:55:LYS:HG3	20:A:973:G:O4'	2.16	0.45
3:D:24:GLU:HA	3:D:27:TYR:HD1	1.82	0.45
11:L:85:ILE:HD12	11:L:85:ILE:HA	1.72	0.45
14:O:43:LEU:O	14:O:47:LYS:N	2.50	0.45
1:B:142:LEU:O	1:B:146:GLN:HB2	2.17	0.45
2:C:57:ILE:HA	2:C:65:ALA:O	2.17	0.45
21:W:68:U:H2'	21:W:69:A:C8	2.52	0.45
7:H:38:ILE:HD13	7:H:41:ARG:NH1	2.32	0.45
20:A:1286:A:H2'	20:A:1287:A:H4'	1.99	0.45
18:S:18:LYS:NZ	20:A:1014:A:OP1	2.49	0.45
20:A:1262:C:H2'	20:A:1263:C:C6	2.53	0.45
1:B:172:ILE:O	1:B:175:ARG:HB3	2.17	0.45
11:L:90:VAL:HB	20:A:523:A:C2	2.52	0.44
23:Y:614:GLU:O	23:Y:617:MET:N	2.50	0.44
23:Y:11:ARG:HG2	23:Y:12:LEU:HD22	1.99	0.44
20:A:216:G:H2'	20:A:217:C:C6	2.52	0.44
20:A:251:G:C6	20:A:266:G:N1	2.86	0.44
23:Y:602:LEU:HB3	23:Y:676:TYR:HB2	1.98	0.44
5:F:50:TYR:HA	5:F:51:PRO:HD2	1.85	0.44
2:C:106:VAL:HG12	2:C:108:ASN:H	1.82	0.44
6:G:64:GLN:NE2	6:G:128:ALA:O	2.50	0.44
8:I:118:LYS:C	8:I:120:ARG:H	2.21	0.44
20:A:428:G:H4'	20:A:429:U:OP1	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:993:G:H2'	20:A:995:C:N4	2.33	0.44
12:M:94:ARG:HD3	12:M:94:ARG:HA	1.70	0.44
6:G:116:ALA:O	6:G:119:ARG:N	2.51	0.44
23:Y:616:TYR:O	23:Y:620:VAL:HG13	2.17	0.44
23:Y:183:MET:HE3	23:Y:210:ARG:HH21	1.82	0.44
10:K:32:ILE:HB	10:K:41:THR:HG23	2.00	0.44
2:C:22:TRP:CB	2:C:59:ARG:HB2	2.48	0.44
12:M:13:LYS:HE3	12:M:21:TYR:CE1	2.52	0.44
1:B:15:VAL:HB	1:B:16:HIS:ND1	2.32	0.44
19:T:15:ARG:HD3	19:T:15:ARG:HA	1.68	0.44
10:K:45:GLY:O	10:K:48:ILE:HG12	2.18	0.44
23:Y:106:VAL:HG23	23:Y:132:ARG:HG3	1.99	0.44
20:A:1144:G:N2	20:A:1146:A:H62	2.14	0.44
23:Y:150:ILE:HG23	23:Y:161:PRO:CG	2.46	0.44
20:A:1261:A:N6	20:A:1274:G:H21	2.08	0.44
20:A:1327:C:H2'	20:A:1328:C:H6	1.79	0.44
20:A:143:A:H2	20:A:220:G:H22	1.66	0.44
23:Y:165:GLN:NE2	23:Y:260:LEU:H	2.15	0.44
8:I:103:THR:HA	20:A:1179:A:O3'	2.18	0.44
9:J:7:LYS:NZ	20:A:1279:A:OP1	2.50	0.44
20:A:645:C:H2'	20:A:646:U:O4'	2.18	0.44
4:E:103:GLY:HA2	20:A:8:A:H1'	1.98	0.44
20:A:994:A:H2'	20:A:994:A:N3	2.32	0.44
20:A:68(H):G:H2'	20:A:68(I):G:N7	2.32	0.44
20:A:1240:U:H4'	20:A:1241:G:OP2	2.18	0.44
9:J:63:PHE:HZ	13:N:49:HIS:HE2	1.66	0.44
4:E:45:PHE:CZ	20:A:1079:G:H5"	2.51	0.44
11:L:117:ARG:HB3	11:L:122:THR:O	2.17	0.44
23:Y:679:VAL:O	23:Y:681:LYS:N	2.51	0.44
17:R:52:PRO:O	17:R:56:THR:HG23	2.18	0.44
16:Q:29:HIS:HB2	16:Q:34:LYS:O	2.18	0.44
20:A:615:C:H2'	20:A:616:G:O4'	2.18	0.44
2:C:164:ARG:NH1	2:C:166:GLU:OE1	2.51	0.44
23:Y:634:MET:N	23:Y:634:MET:SD	2.90	0.44
20:A:1505:G:O2'	22:V:15:A:H2'	2.17	0.44
23:Y:256:THR:HA	23:Y:257:PRO:HD2	1.80	0.44
6:G:79:ARG:H	6:G:79:ARG:CD	2.31	0.44
10:K:110:ASP:HB3	17:R:88:LYS:HG3	1.99	0.44
12:M:77:ASN:O	12:M:81:LEU:HD22	2.18	0.44
23:Y:485:GLU:HA	23:Y:601:ILE:HA	1.98	0.44
16:Q:67:LYS:HD3	20:A:254:G:OP2	2.17	0.44
23:Y:301:ILE:HG22	23:Y:332:SER:OG	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:1236:A:H2'	20:A:1237:C:C6	2.53	0.44
2:C:86:VAL:HG23	2:C:87:LEU:HD22	2.00	0.44
2:C:8:ILE:HA	2:C:11:ARG:HB2	1.99	0.44
7:H:119:LEU:HD22	7:H:124:ALA:HA	1.99	0.44
12:M:24:GLY:N	20:A:1330:U:OP1	2.51	0.44
20:A:1127:G:H1'	20:A:1148:U:C4	2.53	0.44
20:A:68(H):G:N2	20:A:68(S):C:H41	2.14	0.44
21:W:15:G:N1	21:W:48:C:N3	2.60	0.44
20:A:1342:C:H2'	20:A:1343:G:H8	1.83	0.44
12:M:87:TYR:CZ	12:M:91:ARG:HD2	2.53	0.44
23:Y:424:LEU:HD22	23:Y:472:VAL:HG11	1.99	0.44
23:Y:614:GLU:C	23:Y:617:MET:H	2.21	0.44
20:A:736:C:O2'	20:A:737:A:H5'	2.18	0.44
20:A:692:U:O2'	20:A:694:A:N7	2.39	0.44
23:Y:388:THR:HG21	23:Y:398:ILE:HA	2.00	0.44
20:A:5:U:O2'	20:A:6:G:O5'	2.35	0.44
11:L:102:ARG:HB3	11:L:109:GLY:N	2.28	0.44
11:L:102:ARG:HD2	11:L:107:ALA:HB1	2.00	0.44
7:H:14:ARG:CZ	7:H:82:HIS:HE1	2.30	0.44
7:H:110:ALA:N	7:H:121:ASP:OD1	2.36	0.44
5:F:52:ILE:HA	5:F:52:ILE:HD13	1.77	0.44
23:Y:13:ARG:O	23:Y:79:ILE:HA	2.18	0.44
20:A:411:A:H2	20:A:430:A:H62	1.60	0.44
23:Y:616:TYR:CB	23:Y:663:THR:HA	2.47	0.44
10:K:85:ARG:HA	10:K:110:ASP:O	2.18	0.44
20:A:314:C:H2'	20:A:315:A:C8	2.53	0.44
20:A:745:C:OP1	20:A:851:G:O2'	2.35	0.44
20:A:258:G:H2'	20:A:259:G:C8	2.53	0.44
20:A:266:G:H5'	20:A:268:C:H41	1.82	0.44
16:Q:17:LYS:HA	16:Q:46:ASP:O	2.17	0.44
16:Q:66:SER:OG	16:Q:67:LYS:N	2.49	0.44
1:B:68:ILE:HG23	1:B:161:ALA:C	2.38	0.44
7:H:94:TYR:CE2	20:A:598:U:H4'	2.53	0.44
20:A:781:A:H4'	20:A:1522:U:O2'	2.18	0.44
7:H:36:LEU:HA	7:H:39:LEU:HB2	1.99	0.44
2:C:30:ARG:HB2	13:N:36:PHE:O	2.17	0.44
1:B:32:ILE:HG21	1:B:40:HIS:ND1	2.32	0.44
7:H:27:PRO:HA	7:H:58:TYR:CE2	2.53	0.44
7:H:114:THR:HG23	7:H:119:LEU:HD13	2.00	0.44
23:Y:484:ARG:HD3	23:Y:559:PRO:HB2	1.98	0.44
23:Y:627:ARG:HA	23:Y:651:GLU:HG2	1.99	0.44
15:P:6:LEU:HD11	15:P:69:THR:HG23	2.00	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:L:52:LEU:HG	11:L:53:ARG:H	1.82	0.44
9:J:55:LYS:HG3	20:A:973:G:C1'	2.48	0.44
20:A:833:U:H2'	20:A:834:C:H6	1.83	0.44
23:Y:183:MET:CE	23:Y:210:ARG:HH21	2.30	0.44
15:P:38:TYR:O	15:P:50:LYS:HB2	2.17	0.44
20:A:774:G:H2'	20:A:775:G:H8	1.83	0.44
23:Y:463:VAL:HA	23:Y:466:LEU:HB2	1.99	0.44
20:A:1235:U:H2'	20:A:1236:A:O4'	2.18	0.44
20:A:1061:G:H2'	20:A:1062:U:O4'	2.18	0.44
2:C:83:ARG:HA	2:C:86:VAL:HG22	2.00	0.44
2:C:101:LEU:HD12	2:C:102:ASN:H	1.83	0.44
23:Y:266:ASN:N	23:Y:266:ASN:OD1	2.46	0.44
20:A:962:C:N4	20:A:973:G:H1	2.08	0.43
4:E:19:MET:CG	20:A:15:G:H1'	2.47	0.43
6:G:78:ARG:HD2	6:G:156:TRP:HA	2.00	0.43
20:A:68(N):U:H5''	20:A:68(O):A:OP2	2.19	0.43
23:Y:89:ASP:OD1	23:Y:457:LEU:HB3	2.18	0.43
15:P:25:ARG:NH1	20:A:134:A:H61	2.16	0.43
7:H:9:MET:HG3	7:H:26:VAL:HG21	2.00	0.43
20:A:784:C:H2'	20:A:785:G:H8	1.83	0.43
1:B:169:LYS:O	1:B:172:ILE:N	2.49	0.43
5:F:99:ALA:C	5:F:101:ALA:H	2.21	0.43
23:Y:322:VAL:HB	23:Y:378:VAL:HG13	1.99	0.43
18:S:47:HIS:HA	18:S:61:TYR:HE2	1.83	0.43
11:L:33:ARG:HB3	11:L:60:LEU:CD1	2.41	0.43
20:A:411:A:C2	20:A:430:A:N6	2.80	0.43
4:E:21:ALA:HB2	20:A:923:A:H4'	2.01	0.43
4:E:102:ALA:O	4:E:107:ARG:NH2	2.51	0.43
12:M:13:LYS:H	12:M:45:VAL:HG12	1.82	0.43
7:H:83:ILE:HB	7:H:137:VAL:HG22	1.99	0.43
20:A:122:G:H2'	20:A:123:C:C6	2.52	0.43
3:D:148:VAL:CG2	3:D:181:MET:HB3	2.49	0.43
20:A:1178:G:N2	20:A:1180:A:H3'	2.33	0.43
20:A:125:U:H3	20:A:236:G:H1	1.66	0.43
17:R:60:ALA:O	17:R:64:ARG:HG3	2.17	0.43
20:A:945:G:H2'	20:A:945:G:N3	2.33	0.43
21:W:37:A:N3	22:V:16:A:H2	2.10	0.43
20:A:1028(G):G:H2'	20:A:1028(H):G:C8	2.54	0.43
20:A:664:G:H2'	20:A:666:G:OP1	2.17	0.43
23:Y:616:TYR:CG	23:Y:663:THR:HA	2.53	0.43
20:A:232:G:H1'	20:A:262:A:N1	2.33	0.43
20:A:262:A:H2'	20:A:263:A:C8	2.53	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:Y:491:VAL:HG12	23:Y:493:VAL:HG22	2.00	0.43
19:T:53:LEU:HD13	19:T:56:MET:HG3	2.00	0.43
3:D:49:ARG:HB3	3:D:50:ARG:H	1.56	0.43
19:T:14:LYS:HA	19:T:17:ARG:HH21	1.83	0.43
12:M:40:ASN:HA	12:M:41:PRO:HD3	1.89	0.43
5:F:75:LEU:O	5:F:79:LEU:HG	2.17	0.43
7:H:12:ARG:CZ	20:A:826:C:H5'	2.48	0.43
23:Y:435:ASP:HA	23:Y:436:PRO:HD2	1.88	0.43
6:G:37:ASN:HB2	8:I:40:LEU:HG	2.00	0.43
23:Y:203:GLU:HB3	23:Y:204:GLU:H	1.52	0.43
3:D:100:ARG:O	3:D:104:VAL:HG23	2.17	0.43
23:Y:146:LEU:HB3	23:Y:147:TRP:H	1.61	0.43
20:A:445:G:H2'	20:A:446:G:C8	2.53	0.43
20:A:902:G:H2'	20:A:903:G:H8	1.83	0.43
20:A:937:A:H2'	20:A:938:A:H8	1.82	0.43
8:I:14:VAL:HG21	20:A:1148:U:H4'	2.01	0.43
3:D:31:CYS:HB3	3:D:33:MET:SD	2.59	0.43
20:A:919:A:H2'	20:A:920:U:C6	2.53	0.43
10:K:46:GLY:HA2	10:K:50:TYR:O	2.19	0.43
16:Q:46:ASP:OD2	16:Q:50:LYS:HG2	2.18	0.43
1:B:76:GLN:H	1:B:76:GLN:CD	2.21	0.43
20:A:35:G:C6	20:A:36:C:C4	3.07	0.43
20:A:1440(K):G:N2	20:A:1440(L):G:C8	2.86	0.43
20:A:1237:C:H4'	20:A:1334:G:N2	2.34	0.43
20:A:1440(E):G:H1	20:A:1440(N):C:N4	2.16	0.43
4:E:82:VAL:HG11	4:E:134:ALA:O	2.18	0.43
3:D:90:GLY:O	3:D:93:PHE:HB3	2.18	0.43
13:N:35:ARG:HD3	13:N:36:PHE:N	2.33	0.43
20:A:1324:A:O4'	20:A:1362:C:H4'	2.18	0.43
23:Y:137:ASN:ND2	25:Y:701:GNP:O6	2.51	0.43
23:Y:467:LYS:NZ	23:Y:474:ALA:HB3	2.33	0.43
16:Q:67:LYS:O	16:Q:68:ARG:HB3	2.18	0.43
3:D:135:LEU:HA	3:D:136:PRO:HD3	1.92	0.43
20:A:1423:G:H2'	20:A:1424:C:C6	2.53	0.43
23:Y:462:ILE:HD13	23:Y:462:ILE:HA	1.85	0.43
21:W:20:U:H1'	21:W:20(A):U:H2'	1.99	0.43
23:Y:98:MET:O	23:Y:100:VAL:N	2.52	0.43
8:I:33:PHE:CE2	8:I:43:ALA:HB1	2.53	0.43
4:E:7:GLU:HB3	4:E:112:LEU:HD13	2.01	0.43
23:Y:111:SER:O	23:Y:113:GLY:N	2.43	0.43
11:L:69:TYR:C	11:L:100:ILE:HG12	2.38	0.43
23:Y:247:ARG:NH2	23:Y:280:LEU:O	2.52	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:71:VAL:HG22	1:B:93:VAL:HB	2.00	0.43
3:D:25:ARG:C	3:D:27:TYR:H	2.22	0.43
20:A:696:A:H2'	20:A:697:U:C6	2.54	0.43
20:A:34:C:H2'	20:A:35:G:H8	1.82	0.43
20:A:862:C:O4'	20:A:874:G:H4'	2.18	0.43
2:C:28:GLN:HG2	2:C:28:GLN:H	1.41	0.43
5:F:62:TRP:CB	17:R:35:ARG:HH12	2.32	0.43
20:A:1000:A:H2'	20:A:1001:G:O4'	2.19	0.43
1:B:85:ALA:HB1	1:B:90:MET:O	2.18	0.43
3:D:101:LEU:HB2	3:D:138:TYR:O	2.18	0.43
4:E:37:ARG:O	4:E:114:GLY:HA2	2.18	0.43
8:I:48:GLU:O	8:I:52:ALA:N	2.51	0.43
20:A:609:A:H2'	20:A:610:G:O4'	2.19	0.43
2:C:81:GLY:O	2:C:85:ARG:HB2	2.18	0.43
12:M:46:LYS:HB2	12:M:46:LYS:HE3	1.82	0.43
20:A:1479:C:H2'	20:A:1480:G:H8	1.83	0.43
12:M:19:LEU:HD13	12:M:19:LEU:HA	1.89	0.43
23:Y:422:GLU:O	23:Y:425:SER:HB2	2.19	0.43
14:O:81:LEU:O	14:O:85:LEU:N	2.35	0.43
20:A:1380:U:H4'	20:A:1381:U:H5'	2.00	0.43
8:I:114:TYR:HD1	9:J:60:ARG:HB2	1.83	0.43
20:A:408:A:H2'	20:A:409:G:H8	1.83	0.43
6:G:140:ASP:O	6:G:143:ARG:HB2	2.19	0.43
3:D:64:LEU:O	3:D:67:ILE:HG23	2.18	0.43
12:M:108:ARG:HD3	12:M:114:ARG:HD2	2.00	0.43
3:D:199:ASN:O	3:D:203:VAL:HG23	2.18	0.43
3:D:54:TYR:HE2	20:A:508:C:H4'	1.83	0.43
1:B:117:GLU:HA	1:B:120:ALA:HB3	1.99	0.43
8:I:79:LEU:HD21	8:I:104:ARG:HA	2.01	0.43
16:Q:40:LYS:HD3	16:Q:42:TYR:OH	2.18	0.43
5:F:53:ALA:HB3	5:F:86:ARG:NH1	2.34	0.43
20:A:971:G:OP1	20:A:971:G:H3'	2.19	0.43
23:Y:579:GLU:H	23:Y:579:GLU:HG3	1.57	0.43
11:L:83:VAL:HB	11:L:100:ILE:HD12	2.00	0.43
1:B:77:ALA:O	1:B:81:VAL:HG13	2.19	0.43
20:A:548:G:C6	20:A:549:C:C4	3.07	0.43
20:A:872:A:C8	20:A:874:G:C8	3.07	0.43
20:A:1413:A:H8	20:A:1413:A:OP2	2.02	0.43
20:A:716:A:C6	20:A:717:C:C4	3.06	0.43
23:Y:583:LYS:HE2	23:Y:583:LYS:HB2	1.71	0.43
20:A:1338:G:H21	21:W:41:A:H1'	1.84	0.43
20:A:1160:G:H2'	20:A:1161:C:H5'	2.00	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:159:G:H1'	20:A:162:A:N6	2.33	0.43
20:A:528:C:H4'	20:A:535:A:C6	2.54	0.43
17:R:58:LEU:HB3	17:R:62:GLU:HB2	1.99	0.43
23:Y:615:GLU:CD	23:Y:615:GLU:H	2.22	0.43
22:V:8:A:HO2'	22:V:9:G:P	2.38	0.43
4:E:76:ILE:HD13	4:E:142:LEU:HD22	2.00	0.43
23:Y:11:ARG:HB3	23:Y:11:ARG:HE	1.54	0.43
20:A:680:C:N4	20:A:710:G:H1	2.10	0.43
21:W:57:G:H2'	21:W:57:G:N3	2.34	0.43
16:Q:72:ARG:HB3	16:Q:73:VAL:H	1.72	0.43
3:D:59:ARG:HD2	3:D:59:ARG:HA	1.80	0.43
23:Y:457:LEU:O	23:Y:461:ILE:HG23	2.18	0.43
3:D:49:ARG:HA	3:D:49:ARG:NE	2.34	0.43
20:A:546:G:H4'	20:A:548:G:H4'	2.00	0.43
11:L:120:TYR:O	11:L:122:THR:N	2.51	0.43
23:Y:546:ILE:HA	23:Y:590:ILE:HG13	2.01	0.43
11:L:114:LYS:HB2	20:A:538:G:H5''	2.00	0.43
3:D:110:PHE:CZ	3:D:148:VAL:HG22	2.54	0.43
14:O:28:GLN:O	14:O:32:LEU:HG	2.19	0.43
20:A:890:G:H22	20:A:906:G:H2'	1.83	0.43
8:I:45:ALA:O	8:I:48:GLU:HB2	2.19	0.43
23:Y:169:GLY:HA3	23:Y:173:THR:HB	2.00	0.43
14:O:10:LYS:O	14:O:14:GLU:HB2	2.18	0.43
11:L:75:HIS:CG	11:L:76:ASN:N	2.86	0.43
20:A:68(G):G:H1	20:A:68(S):C:H42	1.66	0.43
23:Y:105:ILE:HG23	23:Y:133:ILE:HD11	2.00	0.43
20:A:409:G:H1	20:A:433:C:N4	2.13	0.43
2:C:134:ILE:HD13	2:C:134:ILE:HA	1.67	0.43
3:D:193:ASP:C	3:D:194:LEU:HD22	2.39	0.43
16:Q:13:ASP:CG	16:Q:14:LYS:H	2.22	0.43
12:M:116:THR:HG21	21:W:29:U:H4'	2.01	0.43
20:A:773:G:H2'	20:A:774:G:H8	1.84	0.43
3:D:152:SER:HA	3:D:155:LEU:HB2	2.00	0.43
10:K:27:ASN:ND2	10:K:44:SER:HB2	2.34	0.43
2:C:195:VAL:CG1	20:A:1205:U:H4'	2.48	0.43
20:A:1151:A:O2'	20:A:1152:A:H8	2.01	0.43
20:A:584:G:H2'	20:A:585:G:C8	2.54	0.43
20:A:837:G:H1	20:A:849:C:H42	1.67	0.43
11:L:84:LEU:HB2	11:L:104:VAL:CG1	2.46	0.42
20:A:658:G:H2'	20:A:659:U:C6	2.54	0.42
9:J:33:GLN:OE1	9:J:34:VAL:N	2.52	0.42
20:A:1356:G:H2'	20:A:1357:A:H8	1.84	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:Y:487:ILE:HB	23:Y:597:GLY:O	2.19	0.42
3:D:42:GLN:O	3:D:46:LYS:NZ	2.41	0.42
10:K:44:SER:OG	10:K:47:VAL:HG23	2.19	0.42
4:E:91:LEU:HD13	4:E:91:LEU:HA	1.82	0.42
16:Q:83:ASP:O	16:Q:86:GLU:HB3	2.19	0.42
20:A:1480:G:H2'	20:A:1481:U:O4'	2.19	0.42
23:Y:25:LYS:HE2	23:Y:84:THR:HA	2.01	0.42
20:A:966:G:H2'	20:A:967:C:O4'	2.19	0.42
20:A:509:A:C6	20:A:510:A:N1	2.87	0.42
1:B:16:HIS:CE1	1:B:210:SER:HA	2.54	0.42
20:A:1424:C:H2'	20:A:1425:U:C6	2.55	0.42
2:C:174:PRO:CA	20:A:1107:C:H5''	2.49	0.42
3:D:207:TYR:HD2	3:D:207:TYR:HA	1.70	0.42
8:I:29:ASN:ND2	8:I:65:VAL:O	2.51	0.42
1:B:98:LEU:N	1:B:101:MET:SD	2.93	0.42
9:J:51:ARG:O	20:A:1060:C:H5'	2.19	0.42
20:A:54:C:H42	20:A:357:G:H1	1.67	0.42
19:T:39:LYS:HE3	19:T:43:LEU:HD12	2.01	0.42
1:B:180:LEU:HB3	1:B:182:ILE:HG12	2.01	0.42
20:A:568:G:N2	20:A:569:C:C2	2.86	0.42
20:A:1492:A:C5'	24:U:6:5OH:HP	2.49	0.42
11:L:75:HIS:HB2	11:L:77:LEU:HD12	2.01	0.42
20:A:741:G:H5'	20:A:742:G:OP2	2.19	0.42
9:J:49:VAL:CG2	13:N:41:ARG:HB2	2.43	0.42
16:Q:59:ILE:HA	16:Q:73:VAL:HA	2.02	0.42
20:A:1358:U:O2'	20:A:1359:C:O5'	2.38	0.42
20:A:773:G:H2'	20:A:774:G:C8	2.54	0.42
6:G:56:GLN:H	6:G:56:GLN:CD	2.22	0.42
20:A:1440(J):C:O2'	20:A:1440(K):G:H5''	2.18	0.42
23:Y:436:PRO:O	23:Y:438:PHE:N	2.52	0.42
20:A:729:A:C5	20:A:730:G:N7	2.86	0.42
3:D:76:ARG:HD3	3:D:207:TYR:CE1	2.54	0.42
20:A:867:G:H2'	20:A:868:C:C6	2.55	0.42
23:Y:149:VAL:HG12	23:Y:153:MET:SD	2.58	0.42
2:C:206:GLU:C	2:C:208:ILE:H	2.22	0.42
1:B:105:PHE:HZ	1:B:156:LYS:HA	1.84	0.42
16:Q:58:GLU:CD	16:Q:75:ARG:HE	2.23	0.42
7:H:56:LYS:HA	7:H:57:PRO:HD2	1.91	0.42
23:Y:495:GLY:HA3	23:Y:510:VAL:HG23	2.00	0.42
23:Y:32:ILE:C	23:Y:34:TYR:H	2.10	0.42
11:L:93:LEU:HD23	11:L:93:LEU:H	1.84	0.42
20:A:1347:G:O2'	20:A:1373:G:O6	2.24	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:936:C:N3	20:A:1379:G:N2	2.61	0.42
23:Y:617:MET:HG2	23:Y:618:GLY:N	2.29	0.42
10:K:53:SER:CB	20:A:694:A:H5'	2.47	0.42
4:E:101:ILE:HG13	4:E:118:ILE:O	2.18	0.42
6:G:15:ASP:HB2	6:G:20:ASP:O	2.19	0.42
5:F:11:ASN:ND2	5:F:13:ASN:O	2.52	0.42
3:D:72:GLU:HA	3:D:75:PHE:HB3	2.01	0.42
8:I:24:GLY:HA2	8:I:59:PHE:C	2.40	0.42
20:A:893:C:H2'	20:A:894:G:C8	2.54	0.42
10:K:66:LEU:O	10:K:69:ALA:HB3	2.18	0.42
7:H:9:MET:HE3	7:H:10:LEU:HG	2.01	0.42
7:H:122:ARG:O	7:H:126:LYS:HB2	2.20	0.42
8:I:40:LEU:HD22	8:I:42:ARG:HG3	2.02	0.42
7:H:35:ILE:O	7:H:39:LEU:HD23	2.19	0.42
20:A:1345:U:H4'	20:A:1346:A:H5'	2.01	0.42
20:A:436:C:H2'	20:A:437:U:O4'	2.19	0.42
20:A:1366:C:H2'	20:A:1367:C:C6	2.54	0.42
23:Y:586:GLY:O	23:Y:589:ALA:HB3	2.20	0.42
2:C:179:ARG:HG3	2:C:179:ARG:H	1.68	0.42
23:Y:135:PHE:CD2	23:Y:137:ASN:HB2	2.53	0.42
20:A:218:C:H4'	20:A:458(C):G:N1	2.35	0.42
7:H:21:LYS:HB2	7:H:21:LYS:HE3	1.85	0.42
20:A:549:C:H2'	20:A:550:G:O4'	2.19	0.42
12:M:50:GLU:O	12:M:52:GLU:N	2.52	0.42
12:M:20:THR:C	12:M:22:ILE:H	2.21	0.42
20:A:427:U:O2'	20:A:541:G:OP1	2.29	0.42
7:H:27:PRO:HA	7:H:58:TYR:CD2	2.54	0.42
2:C:161:GLU:O	2:C:163:ALA:N	2.52	0.42
23:Y:333:GLY:O	23:Y:371:ALA:HB2	2.18	0.42
19:T:33:ILE:HG13	19:T:62:LEU:HB3	2.00	0.42
15:P:21:VAL:HG13	15:P:34:GLU:H	1.84	0.42
15:P:14:ASN:HA	15:P:42:ARG:HH21	1.84	0.42
11:L:81:SER:HB3	11:L:106:ASP:HB3	2.00	0.42
23:Y:257:PRO:HB2	23:Y:259:PHE:CE1	2.55	0.42
1:B:69:LEU:HD12	1:B:71:VAL:HG22	2.02	0.42
20:A:201:C:N4	20:A:216:G:H1	2.13	0.42
8:I:125:TYR:CZ	8:I:127:LYS:HB2	2.54	0.42
20:A:360:A:H2'	20:A:361:G:C8	2.54	0.42
9:J:34:VAL:HG13	9:J:74:ILE:HG22	2.01	0.42
20:A:705:U:HO2'	20:A:706:A:P	2.42	0.42
4:E:100:VAL:O	4:E:102:ALA:N	2.52	0.42
14:O:64:ARG:NH2	20:A:581:G:H4'	2.34	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:1217:C:H2'	20:A:1218:C:C6	2.55	0.42
20:A:22:G:H2'	20:A:23:C:C6	2.55	0.42
20:A:1096:C:H2'	20:A:1097:C:C6	2.55	0.42
20:A:1495:U:O2'	20:A:1496:C:H5'	2.20	0.42
11:L:54:LYS:CD	11:L:70:ILE:HG12	2.36	0.42
1:B:69:LEU:HD12	1:B:71:VAL:CG2	2.50	0.42
20:A:918:A:H2'	20:A:919:A:O4'	2.20	0.42
21:W:12:U:H1'	21:W:24:G:N2	2.35	0.42
18:S:60:VAL:HG21	18:S:74:PHE:HB3	2.02	0.42
21:W:65:U:H2'	21:W:66:C:C6	2.55	0.42
20:A:1440(J):C:HO2'	20:A:1440(K):G:N2	2.17	0.42
20:A:1256:A:O3'	20:A:1257:U:H4'	2.20	0.42
20:A:45:U:H4'	20:A:306:G:N2	2.35	0.42
5:F:61:LEU:HB2	5:F:63:TYR:CE2	2.54	0.42
18:S:14:HIS:CD2	20:A:1014:A:H4'	2.55	0.42
23:Y:314:PHE:HE2	23:Y:329:ARG:HB3	1.84	0.42
5:F:44:GLY:HA2	5:F:59:TYR:CG	2.55	0.42
11:L:61:THR:HG21	20:A:362:G:H5''	2.02	0.42
9:J:16:LEU:CD1	9:J:70:ARG:HH11	2.33	0.42
23:Y:87:HIS:CD2	23:Y:121:VAL:HG22	2.48	0.42
16:Q:41:LYS:HE3	20:A:277:C:OP1	2.20	0.42
20:A:1230:C:H5'	21:W:30:C:H5''	2.02	0.42
20:A:11:G:C5	20:A:12:U:C4	3.07	0.42
20:A:642:A:H2'	20:A:643:C:H6	1.83	0.42
16:Q:91:ARG:NH1	20:A:584:G:OP1	2.53	0.42
7:H:56:LYS:NZ	20:A:653:A:OP1	2.51	0.42
23:Y:252:ASP:O	23:Y:253:LEU:HB2	2.20	0.42
20:A:243:A:C2	20:A:245:C:H2'	2.54	0.42
6:G:23:VAL:HG13	6:G:43:PHE:HE2	1.85	0.42
7:H:44:PHE:HE2	7:H:109:ILE:HG21	1.84	0.42
3:D:13:ARG:HH22	3:D:36:ARG:NE	2.17	0.42
11:L:104:VAL:HG23	11:L:105:TYR:N	2.35	0.42
11:L:51:ALA:HB1	11:L:52:LEU:HD23	2.01	0.42
11:L:34:ARG:O	11:L:82:VAL:HG13	2.19	0.42
1:B:164:VAL:HG13	1:B:170:GLU:HB2	2.02	0.42
7:H:18:ARG:HH12	7:H:82:HIS:HD2	1.67	0.42
17:R:74:ARG:CG	17:R:79:LEU:HB3	2.49	0.42
3:D:119:GLN:HG3	3:D:123:HIS:ND1	2.35	0.42
20:A:159:G:H1'	20:A:162:A:H62	1.85	0.42
6:G:89:MET:HB2	6:G:155:ARG:NH1	2.35	0.42
20:A:20:U:H2'	20:A:21:G:O4'	2.19	0.42
2:C:177:THR:HG23	20:A:1111:A:N1	2.34	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:177:THR:HG22	2:C:178:LEU:H	1.84	0.42
12:M:91:ARG:HH12	12:M:103:THR:HG21	1.84	0.42
23:Y:20:HIS:ND1	23:Y:118:SER:HB3	2.35	0.42
20:A:433:C:H2'	20:A:434:U:H6	1.85	0.42
19:T:73:HIS:CG	19:T:74:LYS:HD3	2.55	0.42
10:K:53:SER:H	20:A:695:A:P	2.42	0.42
16:Q:44:ALA:HA	16:Q:71:PHE:O	2.20	0.42
4:E:11:ILE:O	4:E:12:LEU:HD13	2.20	0.42
1:B:185:ILE:HD12	1:B:199:TYR:HB2	2.02	0.42
4:E:46:GLY:N	4:E:58:ALA:HB2	2.35	0.42
3:D:123:HIS:CD2	20:A:438:G:H4'	2.54	0.42
15:P:45:THR:OG1	20:A:617:G:H5'	2.20	0.42
6:G:24:THR:O	6:G:28:ASN:HB2	2.19	0.42
13:N:2:ALA:N	20:A:1049:U:HO2'	2.18	0.42
8:I:8:GLY:HA3	8:I:76:ALA:O	2.20	0.42
20:A:290:C:H2'	20:A:291:C:O4'	2.20	0.42
20:A:1488:G:C2	20:A:1489:G:C4	3.08	0.42
20:A:119:A:C5	20:A:240:C:C4	3.08	0.42
23:Y:247:ARG:HH21	23:Y:281:PRO:HA	1.85	0.41
23:Y:614:GLU:HB2	23:Y:617:MET:SD	2.60	0.41
12:M:75:ALA:O	12:M:78:ILE:HB	2.19	0.41
10:K:30:VAL:HG23	10:K:43:SER:HB3	2.01	0.41
20:A:778:G:C6	20:A:779:C:N3	2.89	0.41
7:H:29:SER:HB3	7:H:32:LYS:HE2	2.02	0.41
9:J:46:ARG:HG3	20:A:1253:G:H5''	2.02	0.41
7:H:51:VAL:HG12	7:H:52:ASP:H	1.84	0.41
3:D:176:LEU:HD11	3:D:178:VAL:HG22	2.01	0.41
23:Y:126:GLU:C	23:Y:129:LYS:H	2.23	0.41
1:B:87:ARG:NH2	1:B:233:SER:H	1.95	0.41
24:U:6:5OH:CS	24:U:6:5OH:N	2.83	0.41
20:A:724:G:C2	20:A:725:G:C8	3.08	0.41
20:A:413:G:O2'	20:A:428:G:N2	2.53	0.41
20:A:696:A:H8	20:A:696:A:O5'	2.03	0.41
15:P:31:LYS:HD3	20:A:607:A:C2	2.55	0.41
20:A:105:G:C6	20:A:106:C:N4	2.88	0.41
9:J:38:ILE:HA	9:J:39:PRO:HD2	1.94	0.41
1:B:220:ASP:HA	1:B:223:ILE:HB	2.02	0.41
5:F:95:GLU:HA	5:F:96:PRO:HD3	1.92	0.41
17:R:22:VAL:HG23	17:R:56:THR:HA	2.01	0.41
20:A:613:C:H2'	20:A:614:A:C8	2.55	0.41
20:A:1440(H):U:H4'	20:A:1440(I):A:C5	2.55	0.41
23:Y:75:LYS:HB3	23:Y:75:LYS:HE3	1.65	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:Y:137:ASN:HA	23:Y:261:GLY:O	2.20	0.41
23:Y:25:LYS:HG3	23:Y:25:LYS:H	1.51	0.41
23:Y:281:PRO:HB2	23:Y:285:ASP:HB2	2.02	0.41
23:Y:616:TYR:HB2	23:Y:663:THR:HG22	2.02	0.41
20:A:304:U:H2'	20:A:305:G:C8	2.55	0.41
8:I:113:LYS:HZ2	20:A:1187:G:P	2.43	0.41
2:C:199:LYS:HE3	20:A:1058:G:H5''	2.01	0.41
16:Q:50:LYS:HE3	16:Q:51:TYR:CZ	2.55	0.41
4:E:30:ALA:HB3	4:E:46:GLY:HA3	2.02	0.41
23:Y:409:ILE:HG13	23:Y:456:GLU:HB2	2.02	0.41
20:A:687:A:N3	20:A:688:G:H1'	2.35	0.41
7:H:9:MET:SD	7:H:32:LYS:HD2	2.61	0.41
2:C:117:ALA:HB1	2:C:198:VAL:HG12	2.02	0.41
8:I:97:LYS:C	8:I:99:LEU:H	2.23	0.41
16:Q:81:ARG:HE	16:Q:81:ARG:HA	1.84	0.41
20:A:928:G:H2'	20:A:929:G:C8	2.56	0.41
12:M:64:TRP:HB2	12:M:65:LYS:H	1.47	0.41
20:A:442:C:H42	20:A:492:G:H1	1.68	0.41
7:H:130:GLY:N	20:A:599:C:O2'	2.54	0.41
16:Q:43:LEU:HD12	16:Q:69:LYS:HA	2.02	0.41
9:J:5:ARG:HH11	9:J:5:ARG:HB2	1.85	0.41
15:P:74:LEU:HD22	15:P:79:VAL:HG21	2.02	0.41
20:A:1422:G:H2'	20:A:1423:G:C8	2.52	0.41
20:A:1068:G:H1	20:A:1107:C:N4	2.16	0.41
13:N:21:TYR:HE2	13:N:23:ARG:NH2	2.18	0.41
20:A:177:C:H2'	20:A:178:C:C6	2.54	0.41
3:D:32:ALA:HB2	20:A:429:U:H5'	2.02	0.41
15:P:31:LYS:HG3	15:P:32:TYR:N	2.35	0.41
4:E:101:ILE:HD11	4:E:119:LEU:HA	2.01	0.41
20:A:1306:A:N6	20:A:1331:G:H1'	2.35	0.41
20:A:38:G:H22	20:A:397:A:P	2.41	0.41
16:Q:5:VAL:HG12	16:Q:60:ILE:HG13	2.02	0.41
16:Q:71:PHE:O	16:Q:72:ARG:O	2.38	0.41
23:Y:462:ILE:O	23:Y:466:LEU:HB2	2.20	0.41
5:F:96:PRO:HB3	17:R:30:ASP:OD2	2.20	0.41
6:G:138:LYS:O	6:G:142:GLU:HG2	2.21	0.41
23:Y:517:LEU:HG	23:Y:518:PRO:HD2	2.01	0.41
20:A:985:C:H2'	20:A:986:A:C8	2.55	0.41
3:D:85:LYS:HA	3:D:85:LYS:HD3	1.90	0.41
23:Y:315:LYS:HB3	23:Y:327:PHE:CD2	2.55	0.41
23:Y:30:GLU:OE2	23:Y:31:ARG:NH1	2.54	0.41
23:Y:34:TYR:HB3	23:Y:36:THR:CG2	2.51	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:Y:27:THR:HG23	25:Y:701:GNP:O2A	2.20	0.41
11:L:54:LYS:HD3	11:L:70:ILE:H	1.85	0.41
1:B:69:LEU:HD13	1:B:70:PHE:H	1.85	0.41
1:B:187:LEU:HD23	1:B:201:ILE:O	2.19	0.41
20:A:232:G:C6	20:A:233:C:C4	3.08	0.41
15:P:22:THR:OG1	15:P:32:TYR:HA	2.21	0.41
21:W:66:C:H2'	21:W:67:G:C8	2.54	0.41
20:A:1472:U:H2'	20:A:1473:A:H8	1.86	0.41
23:Y:236:GLU:HA	23:Y:237:PRO:HD3	1.88	0.41
20:A:396:G:O2'	20:A:398:C:OP1	2.15	0.41
20:A:1178:G:O2'	20:A:1180:A:N7	2.50	0.41
15:P:8:ARG:HB3	15:P:28:ARG:NH2	2.36	0.41
16:Q:52:LYS:HE3	16:Q:52:LYS:HB3	1.79	0.41
16:Q:78:GLU:OE1	16:Q:81:ARG:NH1	2.54	0.41
23:Y:544:LYS:O	23:Y:548:GLU:N	2.53	0.41
23:Y:355:LEU:HD12	23:Y:369:LEU:HD22	2.03	0.41
20:A:50:A:H4'	20:A:51:A:H5'	2.02	0.41
14:O:17:ARG:HE	14:O:17:ARG:HA	1.85	0.41
3:D:156:GLU:HG2	3:D:156:GLU:H	1.36	0.41
20:A:1506:U:O2'	20:A:1507:A:H5''	2.20	0.41
3:D:25:ARG:HA	3:D:28:SER:HB3	2.03	0.41
11:L:26:ALA:HB2	11:L:98:TYR:CD2	2.56	0.41
23:Y:620:VAL:O	23:Y:624:LEU:HB2	2.21	0.41
12:M:78:ILE:HD13	12:M:78:ILE:HA	1.84	0.41
7:H:68:ARG:HG3	7:H:74:PRO:CB	2.48	0.41
3:D:15:GLU:OE1	3:D:63:LYS:HA	2.21	0.41
1:B:75:LYS:HB3	1:B:76:GLN:NE2	2.36	0.41
1:B:74:LYS:HG3	1:B:77:ALA:HB3	2.01	0.41
1:B:184:VAL:O	1:B:197:VAL:HG13	2.21	0.41
12:M:13:LYS:HE2	12:M:13:LYS:HB2	1.88	0.41
20:A:1493:A:H4'	20:A:1494:G:OP2	2.20	0.41
20:A:1287:A:H2	20:A:1353:G:N3	2.19	0.41
6:G:135:VAL:O	6:G:138:LYS:HB3	2.20	0.41
20:A:1141:C:H2'	20:A:1142:G:H8	1.85	0.41
2:C:121:ALA:O	2:C:125:GLU:HB2	2.20	0.41
20:A:431:A:H2'	20:A:432:A:C8	2.56	0.41
10:K:114:VAL:O	20:A:675:A:O2'	2.38	0.41
10:K:84:VAL:O	10:K:109:VAL:O	2.39	0.41
23:Y:328:ILE:HG13	23:Y:328:ILE:H	1.50	0.41
19:T:53:LEU:O	19:T:56:MET:HB2	2.21	0.41
23:Y:648:PRO:O	23:Y:649:LEU:HB2	2.21	0.41
12:M:50:GLU:O	12:M:51:ALA:C	2.59	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
19:T:13:LEU:HD12	19:T:14:LYS:H	1.85	0.41
2:C:28:GLN:O	2:C:32:LEU:HG	2.21	0.41
23:Y:113:GLY:C	23:Y:115:GLU:HG2	2.40	0.41
19:T:33:ILE:CD1	19:T:62:LEU:HB3	2.51	0.41
23:Y:384:ILE:HB	23:Y:385:THR:H	1.73	0.41
4:E:105:VAL:HG11	4:E:132:ALA:HB2	2.03	0.41
23:Y:524:GLU:O	23:Y:565:VAL:HG23	2.21	0.41
20:A:993:G:H1	20:A:1045:C:N4	2.18	0.41
20:A:962:C:C2	20:A:963:G:C8	3.08	0.41
1:B:28:PHE:HE2	1:B:188:ALA:HB1	1.86	0.41
14:O:39:LEU:HA	14:O:39:LEU:HD22	1.82	0.41
23:Y:341:VAL:HB	23:Y:342:TYR:H	1.68	0.41
15:P:31:LYS:HD3	20:A:607:A:N3	2.36	0.41
8:I:116:LYS:HE2	8:I:122:ALA:HB2	2.02	0.41
16:Q:21:VAL:O	16:Q:41:LYS:HA	2.21	0.41
20:A:756:C:H2'	20:A:757:U:O4'	2.21	0.41
7:H:112:LEU:HB3	7:H:133:LEU:HD23	2.03	0.41
20:A:859:A:H2'	20:A:860:A:O4'	2.21	0.41
20:A:186(M):G:H2'	20:A:186(N):U:O4'	2.21	0.41
17:R:76:LEU:O	17:R:78:LEU:N	2.51	0.41
23:Y:162:VAL:HG21	23:Y:219:VAL:HG21	2.03	0.41
20:A:1134:G:H2'	20:A:1135:U:O4'	2.21	0.41
20:A:1440(A):G:H4'	20:A:1440(B):G:C4	2.55	0.41
23:Y:610:VAL:O	23:Y:612:THR:HG22	2.21	0.41
23:Y:38:ARG:O	23:Y:39:ILE:HB	2.20	0.41
14:O:28:GLN:HG2	20:A:657:G:O2'	2.21	0.41
14:O:32:LEU:O	14:O:36:ILE:HG13	2.19	0.41
23:Y:98:MET:HE1	23:Y:104:ALA:HB2	2.03	0.41
23:Y:98:MET:HG2	23:Y:125:ALA:O	2.21	0.41
1:B:22:LYS:HG2	1:B:40:HIS:NE2	2.35	0.41
20:A:1253:G:H1	20:A:1284:C:H42	1.67	0.41
20:A:1260:C:H4'	20:A:1283:G:O2'	2.20	0.41
20:A:362:G:N2	20:A:365:U:OP2	2.53	0.41
20:A:492:G:H2'	20:A:493:G:H8	1.86	0.41
23:Y:369:LEU:HA	23:Y:369:LEU:HD12	1.79	0.41
20:A:1530:G:C2	20:A:1531:A:C4	3.09	0.41
1:B:44:LEU:O	1:B:47:THR:HB	2.21	0.41
20:A:66:G:H4'	20:A:173:U:C5	2.55	0.41
8:I:11:LYS:HB3	8:I:11:LYS:HE2	1.89	0.41
20:A:321:A:C2	20:A:333:G:C2	3.09	0.41
20:A:513:C:H2'	20:A:514:C:C6	2.56	0.41
20:A:1248:A:H2'	20:A:1249:C:C6	2.56	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:Y:64:THR:HG21	23:Y:84:THR:HG22	2.02	0.41
20:A:658:G:H2'	20:A:659:U:H6	1.86	0.41
14:O:78:TYR:O	14:O:82:ILE:HG22	2.20	0.41
3:D:31:CYS:O	3:D:33:MET:SD	2.80	0.41
20:A:920:U:HO2'	20:A:921:U:H5'	1.86	0.41
20:A:833:U:H2'	20:A:834:C:C6	2.56	0.41
10:K:52:GLY:HA2	20:A:691:G:C6	2.56	0.41
10:K:52:GLY:HA2	20:A:691:G:O6	2.21	0.41
1:B:114:ARG:O	1:B:118:LEU:HG	2.21	0.41
14:O:32:LEU:O	14:O:35:ARG:HG2	2.21	0.41
20:A:1528:U:N3	20:A:1530:G:C8	2.89	0.41
23:Y:340:TYR:CZ	23:Y:351:ARG:HD3	2.56	0.41
15:P:49:LEU:HD23	15:P:76:GLN:OE1	2.21	0.41
23:Y:223:PHE:HZ	23:Y:254:LYS:HG3	1.86	0.41
23:Y:193:GLY:C	23:Y:195:ASP:H	2.25	0.41
23:Y:382:GLU:HB3	23:Y:383:THR:H	1.63	0.41
20:A:1476:G:H2'	20:A:1477:C:C6	2.56	0.41
20:A:1386:G:H2'	20:A:1387:G:C8	2.56	0.41
23:Y:63:ILE:HG21	25:Y:701:GNP:O1A	2.21	0.40
23:Y:609:GLU:O	23:Y:669:PHE:HB2	2.21	0.40
20:A:923:A:H1'	20:A:1398:A:C2	2.57	0.40
23:Y:428:LEU:HA	23:Y:431:LEU:HD22	2.02	0.40
20:A:293:G:O6	20:A:304:U:C2	2.74	0.40
10:K:29:ILE:HG12	20:A:706:A:O2'	2.21	0.40
20:A:1523:G:H2'	20:A:1524:C:H6	1.86	0.40
5:F:67:MET:HE1	5:F:72:VAL:HA	2.02	0.40
23:Y:497:PHE:CD2	23:Y:507:TYR:HA	2.56	0.40
20:A:928:G:H2'	20:A:929:G:H8	1.86	0.40
20:A:109:A:C8	20:A:326:G:H2'	2.56	0.40
20:A:511:C:C2	20:A:512:U:C6	3.09	0.40
20:A:1114:C:H2'	20:A:1115:C:C6	2.56	0.40
7:H:6:ILE:H	7:H:6:ILE:HD12	1.85	0.40
20:A:375:U:H2'	20:A:376:G:H8	1.85	0.40
10:K:18:ARG:HH21	10:K:36:ASP:HA	1.86	0.40
7:H:96:GLY:O	7:H:100:ILE:HG13	2.21	0.40
18:S:75:ALA:HA	18:S:76:PRO:HD2	1.74	0.40
23:Y:668:SER:OG	23:Y:669:PHE:N	2.53	0.40
20:A:232:G:C5	20:A:233:C:C5	3.10	0.40
23:Y:9:LEU:O	23:Y:284:LEU:HB2	2.21	0.40
14:O:46:HIS:C	14:O:48:LYS:H	2.23	0.40
3:D:63:LYS:HG2	3:D:198:VAL:HG22	2.03	0.40
12:M:13:LYS:HB3	12:M:18:ALA:HB2	2.02	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:J:45:ARG:HB3	9:J:65:LEU:HB2	2.04	0.40
23:Y:543:GLN:HG2	23:Y:547:GLU:HG3	2.02	0.40
13:N:61:TRP:HH2	20:A:1368:G:H4'	1.86	0.40
11:L:115:LYS:HG3	11:L:116:SER:N	2.36	0.40
20:A:909:A:C8	20:A:910:C:C5	3.09	0.40
20:A:943:U:O4	20:A:1340:A:N1	2.54	0.40
11:L:57:LYS:HE3	11:L:65:GLU:HB3	2.03	0.40
20:A:586:C:O2'	20:A:878:G:H4'	2.22	0.40
6:G:17:VAL:HB	6:G:18:TYR:H	1.62	0.40
20:A:1397:C:N4	22:V:24:A:H2'	2.36	0.40
1:B:106:LYS:HD2	1:B:106:LYS:H	1.87	0.40
11:L:26:ALA:HB2	11:L:98:TYR:CE2	2.56	0.40
15:P:20:VAL:HG11	15:P:32:TYR:CD1	2.57	0.40
15:P:20:VAL:HG21	15:P:32:TYR:CD1	2.56	0.40
11:L:27:LEU:HA	11:L:27:LEU:HD23	1.87	0.40
2:C:197:GLY:N	20:A:1057:G:H4'	2.37	0.40
16:Q:60:ILE:HG12	16:Q:61:GLU:N	2.36	0.40
20:A:68(M):U:H2'	20:A:68(N):U:O4'	2.21	0.40
11:L:120:TYR:CD2	11:L:120:TYR:N	2.89	0.40
18:S:60:VAL:HG21	18:S:74:PHE:CB	2.51	0.40
6:G:102:ARG:O	6:G:105:VAL:HB	2.21	0.40
23:Y:438:PHE:HB3	23:Y:453:GLY:HA3	2.04	0.40
20:A:1522:U:H2'	20:A:1523:G:H8	1.86	0.40
8:I:50:LEU:HD23	8:I:50:LEU:HA	1.90	0.40
20:A:1533:C:H3'	20:A:1534:A:O4'	2.21	0.40
12:M:17:VAL:HG11	20:A:1302:U:H6	1.86	0.40
17:R:26:LEU:HD13	17:R:39:VAL:HG13	2.04	0.40
8:I:124:GLN:HB3	20:A:1232:U:H5"	2.02	0.40
4:E:101:ILE:HD11	4:E:119:LEU:HD13	2.02	0.40
21:W:2:G:O6	21:W:72:C:N4	2.55	0.40
9:J:5:ARG:NH1	9:J:5:ARG:HB2	2.36	0.40
1:B:162:ILE:C	1:B:185:ILE:O	2.60	0.40
20:A:1493:A:N6	23:Y:580:MET:HB2	2.36	0.40
20:A:126:G:OP1	20:A:605:U:O2'	2.33	0.40
20:A:604:G:H2'	20:A:605:U:O4'	2.21	0.40
20:A:306:G:H2'	20:A:307:C:C6	2.57	0.40
11:L:113:ARG:HD2	20:A:538:G:OP1	2.21	0.40
3:D:78:LEU:O	3:D:81:GLU:HB3	2.21	0.40
6:G:37:ASN:ND2	6:G:41:ARG:HD2	2.36	0.40
7:H:86:ILE:HG12	7:H:135:CYS:HA	2.02	0.40
20:A:878:G:C6	20:A:879:C:C4	3.09	0.40
6:G:8:GLU:HG3	6:G:10:ARG:HG3	2.03	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:160:A:HO2'	20:A:344:A:N6	2.20	0.40
2:C:95:THR:O	2:C:97:LYS:N	2.46	0.40
18:S:27:GLU:HG3	18:S:27:GLU:H	1.34	0.40
23:Y:471:LYS:HE2	23:Y:471:LYS:HB2	1.93	0.40
16:Q:84:LEU:HG	16:Q:84:LEU:H	1.63	0.40
23:Y:31:ARG:O	23:Y:32:ILE:C	2.59	0.40
20:A:1507:A:H2'	20:A:1508:G:C8	2.54	0.40
10:K:34:ASP:O	10:K:36:ASP:N	2.47	0.40
23:Y:408:VAL:HG12	23:Y:669:PHE:HE1	1.87	0.40
9:J:57:LYS:HE2	20:A:973:G:OP1	2.21	0.40
10:K:111:ASP:HA	17:R:84:LYS:HG3	2.04	0.40
23:Y:12:LEU:O	23:Y:282:SER:HA	2.22	0.40
20:A:864:A:C2	20:A:865:A:C4	3.09	0.40
5:F:50:TYR:HE2	5:F:87:ARG:NH2	2.20	0.40
1:B:111:ARG:HE	1:B:145:LEU:HD11	1.86	0.40
1:B:238:LEU:HG	1:B:241:GLU:OE1	2.21	0.40
20:A:270:A:H2'	20:A:271:C:O4'	2.22	0.40
20:A:1053:G:H4'	20:A:1055:A:OP1	2.21	0.40
13:N:4:LYS:O	13:N:8:GLU:HG2	2.22	0.40
12:M:12:ASN:HB2	12:M:46:LYS:HE2	2.04	0.40
3:D:165:MET:HE1	3:D:176:LEU:HD11	2.03	0.40
15:P:48:TRP:CE3	15:P:49:LEU:HG	2.56	0.40
20:A:1232:U:C4	20:A:1233:G:C8	3.10	0.40
1:B:181:PHE:CD1	7:H:71:GLY:HA2	2.57	0.40
20:A:786:G:H2'	20:A:787:A:O4'	2.21	0.40
20:A:1517:G:C5	20:A:1518:A:C5	3.10	0.40
23:Y:99:ARG:CZ	23:Y:403:GLU:HG2	2.51	0.40
23:Y:490:PRO:HA	23:Y:514:VAL:O	2.22	0.40
6:G:42:ILE:HA	6:G:42:ILE:HD13	1.83	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	B	233/235 (99%)	174 (75%)	36 (16%)	23 (10%)	1	15
2	C	205/207 (99%)	152 (74%)	34 (17%)	19 (9%)	1	18
3	D	206/208 (99%)	149 (72%)	46 (22%)	11 (5%)	3	35
4	E	149/151 (99%)	116 (78%)	24 (16%)	9 (6%)	2	31
5	F	99/101 (98%)	81 (82%)	7 (7%)	11 (11%)	1	13
6	G	153/155 (99%)	119 (78%)	27 (18%)	7 (5%)	4	39
7	H	136/138 (99%)	102 (75%)	21 (15%)	13 (10%)	1	17
8	I	125/127 (98%)	92 (74%)	25 (20%)	8 (6%)	2	29
9	J	97/99 (98%)	71 (73%)	16 (16%)	10 (10%)	1	14
10	K	117/119 (98%)	78 (67%)	26 (22%)	13 (11%)	1	13
11	L	123/125 (98%)	39 (32%)	44 (36%)	40 (32%)	0	0
12	M	123/125 (98%)	91 (74%)	18 (15%)	14 (11%)	1	12
13	N	58/60 (97%)	40 (69%)	14 (24%)	4 (7%)	2	27
14	O	86/88 (98%)	66 (77%)	15 (17%)	5 (6%)	3	32
15	P	82/84 (98%)	59 (72%)	18 (22%)	5 (6%)	2	30
16	Q	98/100 (98%)	68 (69%)	20 (20%)	10 (10%)	1	14
17	R	68/70 (97%)	52 (76%)	10 (15%)	6 (9%)	1	19
18	S	77/79 (98%)	56 (73%)	12 (16%)	9 (12%)	1	12
19	T	97/99 (98%)	75 (77%)	14 (14%)	8 (8%)	1	21
23	Y	685/687 (100%)	457 (67%)	156 (23%)	72 (10%)	1	14
24	U	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
All	All	3019/3063 (99%)	2138 (71%)	584 (19%)	297 (10%)	1	16

All (297) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	17	PHE
1	B	66	GLY
1	B	75	LYS
1	B	76	GLN
1	B	96	ARG
1	B	160	ASP
1	B	235	SER
1	B	236	TYR
2	C	3	ASN
2	C	4	LYS

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Mol	Chain	Res	Type
2	C	5	ILE
2	C	14	ILE
2	C	62	ASP
2	C	63	ASN
2	C	207	VAL
3	D	4	TYR
3	D	7	PRO
4	E	6	PHE
4	E	79	GLU
5	F	44	GLY
5	F	69	GLU
5	F	70	ASP
6	G	15	ASP
6	G	17	VAL
6	G	35	LYS
7	H	22	GLU
9	J	75	ILE
10	K	41	THR
10	K	43	SER
10	K	109	VAL
10	K	111	ASP
11	L	6	THR
11	L	7	ILE
11	L	34	ARG
11	L	39	VAL
11	L	43	VAL
11	L	46	LYS
11	L	51	ALA
11	L	66	VAL
11	L	67	THR
11	L	80	HIS
11	L	94	PRO
11	L	100	ILE
11	L	108	ALA
12	M	7	VAL
12	M	12	ASN
12	M	50	GLU
12	M	51	ALA
14	O	47	LYS
15	P	46	PRO
16	Q	12	SER
16	Q	72	ARG

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Mol	Chain	Res	Type
16	Q	74	LEU
17	R	28	GLU
17	R	37	VAL
18	S	28	LYS
18	S	67	VAL
19	T	50	GLU
19	T	95	ALA
19	T	100	ILE
23	Y	39	ILE
23	Y	88	VAL
23	Y	92	ILE
23	Y	111	SER
23	Y	146	LEU
23	Y	161	PRO
23	Y	204	GLU
23	Y	257	PRO
23	Y	266	ASN
23	Y	330	VAL
23	Y	331	TYR
23	Y	400	GLU
23	Y	418	LYS
23	Y	476	VAL
23	Y	544	LYS
23	Y	566	THR
23	Y	567	LEU
23	Y	631	ILE
23	Y	680	PRO
1	B	34	ALA
1	B	97	TRP
1	B	103	THR
1	B	164	VAL
1	B	165	VAL
2	C	10	PHE
2	C	162	GLN
3	D	5	ILE
3	D	172	PRO
4	E	11	ILE
4	E	67	VAL
4	E	77	PRO
5	F	38	GLU
6	G	10	ARG
6	G	19	GLY

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Mol	Chain	Res	Type
7	H	43	GLY
7	H	74	PRO
7	H	93	VAL
7	H	103	VAL
8	I	109	VAL
9	J	81	THR
10	K	69	ALA
10	K	90	GLY
11	L	58	VAL
11	L	92	ASP
11	L	96	VAL
11	L	101	VAL
11	L	104	VAL
11	L	112	ASP
11	L	121	GLY
11	L	122	THR
11	L	123	LYS
11	L	126	LYS
12	M	46	LYS
13	N	15	LYS
13	N	58	LYS
16	Q	28	PRO
16	Q	49	GLU
16	Q	82	MET
18	S	45	VAL
18	S	46	GLY
18	S	72	GLY
19	T	74	LYS
19	T	79	ARG
23	Y	21	ILE
23	Y	64	THR
23	Y	102	ASP
23	Y	162	VAL
23	Y	281	PRO
23	Y	360	ALA
23	Y	384	ILE
23	Y	437	THR
23	Y	501	THR
23	Y	528	ALA
23	Y	565	VAL
23	Y	681	LYS
1	B	8	LYS

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Mol	Chain	Res	Type
1	B	105	PHE
1	B	190	THR
2	C	49	SER
2	C	160	ALA
2	C	181	ASN
3	D	28	SER
3	D	34	GLU
3	D	156	GLU
4	E	129	ILE
5	F	49	ALA
5	F	93	SER
7	H	105	ARG
7	H	129	VAL
8	I	35	GLU
8	I	102	LEU
8	I	104	ARG
8	I	106	ALA
9	J	33	GLN
10	K	36	ASP
10	K	91	ARG
11	L	17	LYS
11	L	19	ARG
11	L	47	LYS
11	L	56	ALA
11	L	102	ARG
11	L	128	ALA
12	M	21	TYR
12	M	39	ILE
12	M	62	ASN
12	M	101	GLN
13	N	52	GLN
14	O	16	ALA
15	P	28	ARG
15	P	54	GLU
16	Q	48	GLU
17	R	43	PHE
17	R	87	ARG
19	T	78	ALA
19	T	99	LEU
23	Y	22	ASP
23	Y	33	LEU
23	Y	66	THR

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Mol	Chain	Res	Type
23	Y	72	CYS
23	Y	89	ASP
23	Y	99	ARG
23	Y	112	GLN
23	Y	129	LYS
23	Y	175	SER
23	Y	188	TYR
23	Y	200	PRO
23	Y	253	LEU
23	Y	324	ARG
23	Y	347	GLY
23	Y	383	THR
23	Y	395	PRO
23	Y	521	SER
23	Y	539	ILE
23	Y	622	GLY
23	Y	652	MET
1	B	20	GLU
1	B	157	ARG
1	B	194	PRO
1	B	215	LEU
2	C	51	GLY
2	C	102	ASN
2	C	132	ARG
2	C	156	ARG
3	D	89	THR
3	D	173	TRP
4	E	128	PRO
5	F	51	PRO
7	H	45	ILE
7	H	51	VAL
7	H	107	LEU
8	I	39	GLY
8	I	127	LYS
9	J	55	LYS
9	J	83	GLU
10	K	54	ARG
10	K	107	SER
11	L	55	VAL
11	L	74	GLY
11	L	79	GLU
11	L	93	LEU

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Mol	Chain	Res	Type
12	M	11	ARG
12	M	30	ALA
12	M	114	ARG
14	O	23	GLY
14	O	73	GLU
15	P	68	ASP
16	Q	31	LEU
17	R	60	ALA
18	S	63	THR
18	S	80	TYR
23	Y	38	ARG
23	Y	50	ALA
23	Y	63	ILE
23	Y	203	GLU
23	Y	234	GLY
23	Y	397	VAL
23	Y	456	GLU
23	Y	614	GLU
23	Y	628	ARG
1	B	26	PRO
1	B	153	ARG
2	C	83	ARG
2	C	101	LEU
4	E	100	VAL
5	F	40	VAL
5	F	85	VAL
5	F	100	ASN
8	I	107	ARG
9	J	37	PRO
9	J	91	PRO
11	L	115	LYS
12	M	124	PRO
13	N	13	THR
15	P	24	ALA
16	Q	73	VAL
18	S	29	ARG
23	Y	75	LYS
23	Y	145	ASP
23	Y	296	GLY
23	Y	304	ASP
23	Y	393	ASP
23	Y	394	ALA

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Mol	Chain	Res	Type
23	Y	535	PRO
3	D	39	PRO
6	G	81	GLY
6	G	138	LYS
7	H	2	LEU
10	K	121	PRO
11	L	31	PRO
11	L	52	LEU
11	L	65	GLU
11	L	99	HIS
14	O	87	ILE
16	Q	47	PRO
18	S	77	THR
23	Y	258	VAL
23	Y	436	PRO
1	B	130	ARG
2	C	130	VAL
7	H	73	ASP
9	J	94	VAL
10	K	113	PRO
11	L	35	GLY
11	L	125	PRO
12	M	117	VAL
9	J	36	GLY
23	Y	341	VAL
23	Y	402	ILE
3	D	142	PRO
4	E	101	ILE
9	J	53	PRO
10	K	39	PRO
23	Y	598	ASP
5	F	72	VAL
19	T	101	GLY
7	H	101	PRO
17	R	77	GLY

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	203/203 (100%)	177 (87%)	26 (13%)	6	33
2	C	161/161 (100%)	122 (76%)	39 (24%)	1	6
3	D	180/180 (100%)	142 (79%)	38 (21%)	1	9
4	E	116/116 (100%)	95 (82%)	21 (18%)	2	15
5	F	90/90 (100%)	74 (82%)	16 (18%)	2	16
6	G	126/126 (100%)	112 (89%)	14 (11%)	9	42
7	H	119/119 (100%)	91 (76%)	28 (24%)	1	7
8	I	98/98 (100%)	77 (79%)	21 (21%)	1	9
9	J	89/89 (100%)	66 (74%)	23 (26%)	1	5
10	K	90/90 (100%)	72 (80%)	18 (20%)	2	11
11	L	104/104 (100%)	77 (74%)	27 (26%)	1	5
12	M	100/100 (100%)	86 (86%)	14 (14%)	5	28
13	N	49/49 (100%)	35 (71%)	14 (29%)	0	4
14	O	79/79 (100%)	66 (84%)	13 (16%)	3	20
15	P	72/72 (100%)	61 (85%)	11 (15%)	4	25
16	Q	95/95 (100%)	80 (84%)	15 (16%)	4	23
17	R	61/61 (100%)	53 (87%)	8 (13%)	6	32
18	S	69/69 (100%)	52 (75%)	17 (25%)	1	6
19	T	76/76 (100%)	68 (90%)	8 (10%)	10	46
23	Y	579/579 (100%)	483 (83%)	96 (17%)	3	19
24	U	2/2 (100%)	2 (100%)	0	100	100
All	All	2558/2558 (100%)	2091 (82%)	467 (18%)	2	14

All (467) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	15	VAL
1	B	16	HIS
1	B	17	PHE
1	B	36	ARG
1	B	39	ILE
1	B	42	ILE
1	B	56	ARG
1	B	59	GLU
1	B	63	MET
1	B	69	LEU

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Mol	Chain	Res	Type
1	B	94	ASN
1	B	96	ARG
1	B	103	THR
1	B	144	ARG
1	B	152	PHE
1	B	164	VAL
1	B	168	THR
1	B	170	GLU
1	B	184	VAL
1	B	195	ASP
1	B	200	ILE
1	B	211	ILE
1	B	213	LEU
1	B	221	LEU
1	B	238	LEU
1	B	239	VAL
2	C	15	THR
2	C	16	ARG
2	C	17	ASP
2	C	18	TRP
2	C	26	LYS
2	C	28	GLN
2	C	29	TYR
2	C	34	LEU
2	C	36	ASP
2	C	38	ARG
2	C	43	LEU
2	C	55	VAL
2	C	56	ASP
2	C	62	ASP
2	C	70	VAL
2	C	72	LYS
2	C	76	VAL
2	C	83	ARG
2	C	91	LEU
2	C	101	LEU
2	C	104	GLN
2	C	105	GLU
2	C	115	LEU
2	C	124	ILE
2	C	125	GLU
2	C	128	PHE

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Mol	Chain	Res	Type
2	C	132	ARG
2	C	134	ILE
2	C	136	GLN
2	C	152	ILE
2	C	153	VAL
2	C	162	GLN
2	C	166	GLU
2	C	173	VAL
2	C	175	LEU
2	C	186	PHE
2	C	188	LEU
2	C	196	LEU
2	C	206	GLU
3	D	9	CYS
3	D	10	ARG
3	D	12	CYS
3	D	13	ARG
3	D	26	CYS
3	D	27	TYR
3	D	33	MET
3	D	42	GLN
3	D	49	ARG
3	D	50	ARG
3	D	54	TYR
3	D	57	ARG
3	D	60	GLU
3	D	61	LYS
3	D	67	ILE
3	D	70	ILE
3	D	76	ARG
3	D	77	ASN
3	D	86	LYS
3	D	89	THR
3	D	97	LEU
3	D	98	GLU
3	D	103	ASN
3	D	107	ARG
3	D	110	PHE
3	D	113	SER
3	D	135	LEU
3	D	140	VAL
3	D	141	ARG

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Mol	Chain	Res	Type
3	D	148	VAL
3	D	156	GLU
3	D	159	ARG
3	D	173	TRP
3	D	176	LEU
3	D	178	VAL
3	D	187	ARG
3	D	193	ASP
3	D	207	TYR
4	E	5	ASP
4	E	12	LEU
4	E	16	THR
4	E	37	ARG
4	E	41	VAL
4	E	45	PHE
4	E	60	TYR
4	E	64	ARG
4	E	68	GLU
4	E	73	ASN
4	E	76	ILE
4	E	78	HIS
4	E	80	ILE
4	E	87	SER
4	E	91	LEU
4	E	112	LEU
4	E	119	LEU
4	E	120	THR
4	E	126	ARG
4	E	137	GLU
4	E	143	ARG
5	F	11	ASN
5	F	13	ASN
5	F	16	GLN
5	F	23	LYS
5	F	36	ARG
5	F	45	LEU
5	F	46	ARG
5	F	57	GLN
5	F	61	LEU
5	F	69	GLU
5	F	70	ASP
5	F	74	ASP

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Mol	Chain	Res	Type
5	F	78	GLU
5	F	82	ARG
5	F	87	ARG
5	F	89	MET
6	G	13	GLN
6	G	17	VAL
6	G	18	TYR
6	G	56	GLN
6	G	78	ARG
6	G	79	ARG
6	G	80	VAL
6	G	106	GLN
6	G	113	GLU
6	G	114	ARG
6	G	122	HIS
6	G	126	ASP
6	G	136	LYS
6	G	140	ASP
7	H	8	ASP
7	H	29	SER
7	H	37	ARG
7	H	44	PHE
7	H	49	GLU
7	H	51	VAL
7	H	58	TYR
7	H	59	LEU
7	H	61	VAL
7	H	63	LEU
7	H	70	GLN
7	H	73	ASP
7	H	77	GLU
7	H	83	ILE
7	H	99	GLU
7	H	102	ARG
7	H	104	ARG
7	H	107	LEU
7	H	109	ILE
7	H	111	ILE
7	H	112	LEU
7	H	119	LEU
7	H	120	THR
7	H	129	VAL

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Mol	Chain	Res	Type
7	H	133	LEU
7	H	135	CYS
7	H	136	GLU
7	H	138	TRP
8	I	19	LEU
8	I	25	LYS
8	I	27	THR
8	I	53	VAL
8	I	70	LYS
8	I	71	SER
8	I	79	LEU
8	I	88	TYR
8	I	91	ASP
8	I	93	ARG
8	I	95	LYS
8	I	96	LEU
8	I	102	LEU
8	I	107	ARG
8	I	108	VAL
8	I	113	LYS
8	I	114	TYR
8	I	117	HIS
8	I	118	LYS
8	I	121	ARG
8	I	124	GLN
9	J	5	ARG
9	J	8	LEU
9	J	11	PHE
9	J	16	LEU
9	J	22	LYS
9	J	25	GLU
9	J	28	ARG
9	J	30	SER
9	J	47	PHE
9	J	48	THR
9	J	50	ILE
9	J	55	LYS
9	J	66	ARG
9	J	67	THR
9	J	70	ARG
9	J	74	ILE
9	J	78	ASN

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Mol	Chain	Res	Type
9	J	79	ARG
9	J	81	THR
9	J	83	GLU
9	J	84	GLN
9	J	95	GLU
9	J	96	ILE
10	K	18	ARG
10	K	25	TYR
10	K	29	ILE
10	K	33	THR
10	K	34	ASP
10	K	36	ASP
10	K	40	ILE
10	K	41	THR
10	K	48	ILE
10	K	54	ARG
10	K	57	THR
10	K	75	TYR
10	K	84	VAL
10	K	101	SER
10	K	103	LEU
10	K	107	SER
10	K	124	LYS
10	K	127	LYS
11	L	6	THR
11	L	18	VAL
11	L	20	LYS
11	L	24	VAL
11	L	33	ARG
11	L	37	CYS
11	L	38	THR
11	L	43	VAL
11	L	47	LYS
11	L	52	LEU
11	L	54	LYS
11	L	55	VAL
11	L	60	LEU
11	L	67	THR
11	L	69	TYR
11	L	75	HIS
11	L	76	ASN
11	L	77	LEU

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Mol	Chain	Res	Type
11	L	80	HIS
11	L	85	ILE
11	L	92	ASP
11	L	93	LEU
11	L	96	VAL
11	L	101	VAL
11	L	112	ASP
11	L	123	LYS
11	L	127	GLU
12	M	17	VAL
12	M	31	LYS
12	M	36	LYS
12	M	43	THR
12	M	46	LYS
12	M	50	GLU
12	M	57	ARG
12	M	64	TRP
12	M	81	LEU
12	M	92	HIS
12	M	99	ARG
12	M	108	ARG
12	M	110	ARG
12	M	121	LYS
13	N	9	LYS
13	N	16	PHE
13	N	22	THR
13	N	29	ARG
13	N	35	ARG
13	N	36	PHE
13	N	40	CYS
13	N	44	LEU
13	N	47	LEU
13	N	53	LEU
13	N	56	VAL
13	N	57	ARG
13	N	58	LYS
13	N	61	TRP
14	O	17	ARG
14	O	21	ASP
14	O	25	THR
14	O	26	GLU
14	O	38	ARG

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Mol	Chain	Res	Type
14	O	39	LEU
14	O	43	LEU
14	O	47	LYS
14	O	54	ARG
14	O	63	ARG
14	O	79	ARG
14	O	87	ILE
14	O	88	ARG
15	P	1	MET
15	P	3	LYS
15	P	12	LYS
15	P	13	HIS
15	P	22	THR
15	P	32	TYR
15	P	49	LEU
15	P	58	TYR
15	P	59	TRP
15	P	69	THR
15	P	73	LEU
16	Q	10	VAL
16	Q	19	VAL
16	Q	36	ILE
16	Q	37	LYS
16	Q	48	GLU
16	Q	52	LYS
16	Q	53	LEU
16	Q	55	ASP
16	Q	63	ARG
16	Q	66	SER
16	Q	81	ARG
16	Q	83	ASP
16	Q	85	VAL
16	Q	87	LYS
16	Q	92	ARG
17	R	19	LYS
17	R	23	LYS
17	R	34	TYR
17	R	38	GLU
17	R	47	THR
17	R	53	ARG
17	R	62	GLU
17	R	81	PHE

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Mol	Chain	Res	Type
18	S	5	LEU
18	S	6	LYS
18	S	9	VAL
18	S	13	ASP
18	S	25	LYS
18	S	27	GLU
18	S	29	ARG
18	S	33	THR
18	S	34	TRP
18	S	37	ARG
18	S	47	HIS
18	S	61	TYR
18	S	62	ILE
18	S	63	THR
18	S	66	MET
18	S	67	VAL
18	S	71	LEU
19	T	11	SER
19	T	13	LEU
19	T	15	ARG
19	T	43	LEU
19	T	71	THR
19	T	74	LYS
19	T	92	LEU
19	T	93	GLU
23	Y	8	ASP
23	Y	9	LEU
23	Y	14	ASN
23	Y	20	HIS
23	Y	26	THR
23	Y	33	LEU
23	Y	35	TYR
23	Y	39	ILE
23	Y	61	ARG
23	Y	66	THR
23	Y	84	THR
23	Y	92	ILE
23	Y	94	VAL
23	Y	98	MET
23	Y	99	ARG
23	Y	105	ILE
23	Y	114	VAL

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Mol	Chain	Res	Type
23	Y	126	GLU
23	Y	128	TYR
23	Y	132	ARG
23	Y	133	ILE
23	Y	135	PHE
23	Y	152	THR
23	Y	153	MET
23	Y	170	ARG
23	Y	171	GLU
23	Y	173	THR
23	Y	174	PHE
23	Y	178	ILE
23	Y	179	ASP
23	Y	190	ASN
23	Y	199	ILE
23	Y	203	GLU
23	Y	204	GLU
23	Y	224	ASP
23	Y	225	GLU
23	Y	232	LEU
23	Y	260	LEU
23	Y	266	ASN
23	Y	271	LEU
23	Y	277	VAL
23	Y	290	LYS
23	Y	292	THR
23	Y	300	GLU
23	Y	304	ASP
23	Y	312	LEU
23	Y	328	ILE
23	Y	342	TYR
23	Y	344	THR
23	Y	382	GLU
23	Y	398	ILE
23	Y	406	GLU
23	Y	408	VAL
23	Y	410	ASP
23	Y	422	GLU
23	Y	424	LEU
23	Y	428	LEU
23	Y	437	THR
23	Y	438	PHE

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Mol	Chain	Res	Type
23	Y	448	GLN
23	Y	451	ILE
23	Y	454	MET
23	Y	456	GLU
23	Y	457	LEU
23	Y	468	ARG
23	Y	472	VAL
23	Y	476	VAL
23	Y	487	ILE
23	Y	488	THR
23	Y	493	VAL
23	Y	497	PHE
23	Y	504	ARG
23	Y	507	TYR
23	Y	510	VAL
23	Y	512	ILE
23	Y	525	PHE
23	Y	526	VAL
23	Y	542	VAL
23	Y	556	ILE
23	Y	568	TYR
23	Y	572	TYR
23	Y	574	GLU
23	Y	579	GLU
23	Y	601	ILE
23	Y	606	MET
23	Y	608	VAL
23	Y	614	GLU
23	Y	617	MET
23	Y	623	ASP
23	Y	630	GLN
23	Y	663	THR
23	Y	669	PHE
23	Y	671	MET
23	Y	676	TYR
23	Y	677	GLN
23	Y	679	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	161	ASN

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Mol	Chain	Res	Type
4	E	78	HIS
5	F	32	ASN
6	G	148	ASN
10	K	27	ASN
10	K	116	HIS
12	M	92	HIS
14	O	53	HIS
16	Q	96	GLN
19	T	18	GLN
23	Y	40	HIS
23	Y	80	ASN
23	Y	137	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
20	A	1511/1511 (100%)	310 (20%)	16 (1%)
21	W	76/77 (98%)	19 (25%)	1 (1%)
22	V	22/23 (95%)	9 (40%)	3 (13%)
All	All	1609/1611 (99%)	338 (21%)	20 (1%)

All (338) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
20	A	6	G
20	A	8	A
20	A	9	G
20	A	10	A
20	A	13	U
20	A	22	G
20	A	31	G
20	A	32	A
20	A	39	G
20	A	47	C
20	A	48	C
20	A	51	A
20	A	54	C
20	A	65	U
20	A	66	G
20	A	68(H)	G
20	A	68(L)	U

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Mol	Chain	Res	Type
20	A	68(N)	U
20	A	68(P)	C
20	A	68(R)	C
20	A	68(S)	C
20	A	109	A
20	A	116	A
20	A	121	C
20	A	122	G
20	A	129(A)	G
20	A	131	C
20	A	134	A
20	A	135	C
20	A	136	C
20	A	153	C
20	A	163	C
20	A	169	C
20	A	172	A
20	A	174	C
20	A	186(I)	U
20	A	186(K)	G
20	A	192	U
20	A	195	A
20	A	197	A
20	A	201	C
20	A	201(C)	U
20	A	216	G
20	A	221	C
20	A	243	A
20	A	247	G
20	A	251	G
20	A	267	C
20	A	279	A
20	A	281	G
20	A	285	G
20	A	289	G
20	A	296	U
20	A	301	G
20	A	315	A
20	A	316	G
20	A	321	A
20	A	328	C
20	A	329	A

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Mol	Chain	Res	Type
20	A	332	G
20	A	345	C
20	A	346	G
20	A	347	G
20	A	348	G
20	A	352	C
20	A	353	A
20	A	354	G
20	A	366	C
20	A	367	U
20	A	368	U
20	A	372	C
20	A	373	A
20	A	388	G
20	A	389	A
20	A	390	C
20	A	392	G
20	A	397	A
20	A	398	C
20	A	406	G
20	A	410	G
20	A	412	A
20	A	414	A
20	A	421	U
20	A	422	C
20	A	423	G
20	A	424	G
20	A	429	U
20	A	430	A
20	A	440	A
20	A	452	A
20	A	453	A
20	A	457	C
20	A	458(B)	A
20	A	475	G
20	A	481	G
20	A	484	G
20	A	485	G
20	A	497	A
20	A	498	U
20	A	501	C
20	A	505	G

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Mol	Chain	Res	Type
20	A	509	A
20	A	511	C
20	A	512	U
20	A	518	C
20	A	521	G
20	A	524	G
20	A	525	C
20	A	527	G
20	A	531	U
20	A	532	A
20	A	533	A
20	A	535	A
20	A	547	A
20	A	552	U
20	A	559	A
20	A	562	C
20	A	567	G
20	A	568	G
20	A	572	A
20	A	573	A
20	A	574	A
20	A	575	G
20	A	576	G
20	A	577	G
20	A	603	U
20	A	653	A
20	A	659	U
20	A	665	A
20	A	666	G
20	A	688	G
20	A	693	G
20	A	695	A
20	A	702	A
20	A	703	G
20	A	706	A
20	A	711	G
20	A	717	C
20	A	721	G
20	A	737	A
20	A	741	G
20	A	749	C
20	A	753	A

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Mol	Chain	Res	Type
20	A	755	G
20	A	777	A
20	A	781	A
20	A	793	U
20	A	794	A
20	A	809	G
20	A	815	A
20	A	816	A
20	A	817	C
20	A	818	G
20	A	819	A
20	A	821	G
20	A	828	A
20	A	838(A)	U
20	A	838(B)	C
20	A	838(C)	U
20	A	848	C
20	A	849	C
20	A	859	A
20	A	867	G
20	A	872	A
20	A	885	G
20	A	889	A
20	A	890	G
20	A	916	G
20	A	926	G
20	A	927	G
20	A	934	C
20	A	935	A
20	A	946	A
20	A	960	U
20	A	961	U
20	A	966	G
20	A	969	A
20	A	971	G
20	A	972	C
20	A	974	A
20	A	976	G
20	A	977	A
20	A	978	A
20	A	979	C
20	A	980	C

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Mol	Chain	Res	Type
20	A	992	U
20	A	993	G
20	A	1004	A
20	A	1005	A
20	A	1025	U
20	A	1028	C
20	A	1028(B)	C
20	A	1028(C)	G
20	A	1037	C
20	A	1045	C
20	A	1054	C
20	A	1055	A
20	A	1060	C
20	A	1065	U
20	A	1094	G
20	A	1095	U
20	A	1101	A
20	A	1102	A
20	A	1104	G
20	A	1108	G
20	A	1125	U
20	A	1126	U
20	A	1128	C
20	A	1129	C
20	A	1130	A
20	A	1131	G
20	A	1137	C
20	A	1138	G
20	A	1139	G
20	A	1149	C
20	A	1152	A
20	A	1159	U
20	A	1171	G
20	A	1178	G
20	A	1181	G
20	A	1190	G
20	A	1191	A
20	A	1196	U
20	A	1197	G
20	A	1198	G
20	A	1204	A
20	A	1212	U

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Mol	Chain	Res	Type
20	A	1213	A
20	A	1215	G
20	A	1220	G
20	A	1225	A
20	A	1227	A
20	A	1228	C
20	A	1236	A
20	A	1238	A
20	A	1239	A
20	A	1256	A
20	A	1257	U
20	A	1260	C
20	A	1270	C
20	A	1272	G
20	A	1280	A
20	A	1281	U
20	A	1282	C
20	A	1287	A
20	A	1290	G
20	A	1293	G
20	A	1300	G
20	A	1301	U
20	A	1302	U
20	A	1305	G
20	A	1309	G
20	A	1314	C
20	A	1317	C
20	A	1320	C
20	A	1322	C
20	A	1323	G
20	A	1325	C
20	A	1331	G
20	A	1335	C
20	A	1345	U
20	A	1346	A
20	A	1347	G
20	A	1359	C
20	A	1362(A)	C
20	A	1364	U
20	A	1370	G
20	A	1373	G
20	A	1377	A

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Mol	Chain	Res	Type
20	A	1378	C
20	A	1379	G
20	A	1381	U
20	A	1382	C
20	A	1394	A
20	A	1397	C
20	A	1399	C
20	A	1413	A
20	A	1419	G
20	A	1435	G
20	A	1440(B)	G
20	A	1440(C)	G
20	A	1440(D)	A
20	A	1440(J)	C
20	A	1440(K)	G
20	A	1440(L)	G
20	A	1491	G
20	A	1492	A
20	A	1493	A
20	A	1494	G
20	A	1497	G
20	A	1499	A
20	A	1502	A
20	A	1503	A
20	A	1504	G
20	A	1505	G
20	A	1506	U
20	A	1507	A
20	A	1517	G
20	A	1518	A
20	A	1519	A
20	A	1520	G
20	A	1529	G
20	A	1530	G
20	A	1532	U
20	A	1533	C
20	A	1534	A
20	A	1535	C
20	A	1536	C
20	A	1537	U
20	A	1538	C
21	W	8	U

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Mol	Chain	Res	Type
21	W	16	U
21	W	17	U
21	W	18	G
21	W	20	U
21	W	20(A)	U
21	W	21	A
21	W	22	G
21	W	23	A
21	W	29	U
21	W	42	U
21	W	46	G
21	W	47	U
21	W	48	C
21	W	58	A
21	W	60	U
21	W	61	C
21	W	74	C
21	W	76	A
22	V	5	A
22	V	9	G
22	V	11	U
22	V	12	A
22	V	15	A
22	V	16	A
22	V	18	G
22	V	19	G
22	V	23	A

All (20) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
20	A	5	U
20	A	115	G
20	A	266	G
20	A	328	C
20	A	409	G
20	A	429	U
20	A	687	A
20	A	705	U
20	A	748	C
20	A	992	U
20	A	1064	G

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Mol	Chain	Res	Type
20	A	1101	A
20	A	1324	A
20	A	1493	A
20	A	1504	G
20	A	1537	U
21	W	20(A)	U
22	V	8	A
22	V	16	A
22	V	18	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
24	KBE	U	1	24	8,8,9	8.13	1 (12%)	6,8,10	0.58	0
24	DPP	U	2	24	5,5,6	6.82	1 (20%)	3,5,7	2.64	2 (66%)
24	UAL	U	5	24	7,8,9	1.30	1 (14%)	6,9,11	1.36	1 (16%)
24	5OH	U	6	24	12,12,13	6.61	3 (25%)	13,16,18	0.84	0

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
24	KBE	U	1	24	-	0/6/7/8	0/0/0/0
24	DPP	U	2	24	-	0/2/4/6	0/0/0/0
24	UAL	U	5	24	-	0/3/7/9	0/0/0/0
24	5OH	U	6	24	-	0/2/18/20	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	U	1	KBE	O-C	22.95	1.27	1.11
24	U	6	5OH	O-C	22.13	1.26	1.11
24	U	2	DPP	O-C	15.12	1.21	1.11
24	U	6	5OH	CQ-NP	5.15	1.40	1.34
24	U	6	5OH	CQ-NR	2.37	1.40	1.32
24	U	5	UAL	CA-N	-2.11	1.31	1.35

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	U	2	DPP	C-CA-N	-3.74	110.10	113.83
24	U	2	DPP	CB-CA-N	-2.18	104.19	111.50
24	U	5	UAL	CB-CA-N	2.06	127.80	123.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates i

There are no carbohydrates in this entry.

## 5.6 Ligand geometry i

Of 2 ligands modelled in this entry, 1 is 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	$\# Z  > 2$
25	GNP	Y	701	26	34,34,34	1.72	6 (17%)	50,54,54	5.62	14 (28%)

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
25	GNP	Y	701	26	-	0/18/38/38	0/1/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Y	701	GNP	PG-O1G	6.08	1.53	1.46
25	Y	701	GNP	PB-N3B	-4.55	1.60	1.64
25	Y	701	GNP	PA-O3A	-2.77	1.54	1.59
25	Y	701	GNP	PA-O2A	-2.18	1.45	1.55
25	Y	701	GNP	PB-O3A	-2.17	1.56	1.59
25	Y	701	GNP	PG-N3B	-2.09	1.62	1.64

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	701	GNP	C6-C5-N7	-37.53	129.09	134.14
25	Y	701	GNP	PA-O3A-PB	-4.63	115.98	131.81
25	Y	701	GNP	C2-N3-C4	-3.71	109.89	115.09
25	Y	701	GNP	C4-C5-N7	3.63	112.63	109.52
25	Y	701	GNP	C4'-O4'-C1'	-3.59	105.85	109.75
25	Y	701	GNP	C5-C4-N3	3.35	130.80	125.94
25	Y	701	GNP	C6-N1-C2	3.20	125.10	119.51
25	Y	701	GNP	O2B-PB-O1B	3.18	117.23	109.89
25	Y	701	GNP	O3G-PG-O2G	3.06	116.43	107.66
25	Y	701	GNP	O3G-PG-O1G	-2.96	106.00	113.60
25	Y	701	GNP	PB-N3B-PG	-2.89	125.22	130.07
25	Y	701	GNP	O1B-PB-N3B	2.70	115.91	111.83
25	Y	701	GNP	O1G-PG-N3B	-2.18	108.54	111.83
25	Y	701	GNP	C5'-C4'-C3'	-2.09	106.84	115.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	B	235/235 (100%)	-0.38	0 100 100	34, 86, 153, 201	0
2	C	207/207 (100%)	-0.25	0 100 100	23, 75, 130, 190	0
3	D	208/208 (100%)	-0.23	1 (0%) 88 64	23, 85, 142, 184	0
4	E	151/151 (100%)	-0.04	0 100 100	14, 58, 106, 151	0
5	F	101/101 (100%)	-0.25	0 100 100	29, 61, 123, 148	0
6	G	155/155 (100%)	-0.33	0 100 100	38, 82, 137, 180	0
7	H	138/138 (100%)	-0.24	0 100 100	25, 75, 121, 155	0
8	I	127/127 (100%)	-0.09	0 100 100	0, 84, 149, 220	0
9	J	99/99 (100%)	0.19	4 (4%) 36 16	31, 75, 127, 166	0
10	K	119/119 (100%)	-0.19	0 100 100	38, 72, 133, 151	0
11	L	125/125 (100%)	-0.11	1 (0%) 83 53	29, 69, 136, 170	0
12	M	125/125 (100%)	-0.09	4 (3%) 45 21	53, 100, 158, 223	0
13	N	60/60 (100%)	0.23	1 (1%) 67 34	39, 69, 117, 135	0
14	O	88/88 (100%)	-0.30	0 100 100	25, 68, 119, 170	0
15	P	84/84 (100%)	-0.10	0 100 100	52, 81, 127, 153	0
16	Q	100/100 (100%)	-0.01	1 (1%) 79 47	0, 68, 126, 150	0
17	R	70/70 (100%)	-0.23	0 100 100	39, 63, 113, 155	0
18	S	79/79 (100%)	-0.15	0 100 100	44, 99, 145, 189	0
19	T	99/99 (100%)	-0.13	0 100 100	0, 79, 131, 166	0
20	A	1511/1511 (100%)	-0.11	3 (0%) 93 80	18, 70, 157, 272	0
21	W	77/77 (100%)	-0.49	0 100 100	39, 101, 193, 240	0
22	V	23/23 (100%)	-0.21	0 100 100	41, 118, 186, 216	0
23	Y	687/687 (100%)	-0.27	0 100 100	40, 92, 149, 204	0
24	U	2/6 (33%)	-0.22	0 100 100	119, 119, 119, 119	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
All	All	4670/4674 (99%)	-0.17	15 (0%)	91 76	0, 77, 148, 272	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	A	1257	U	5.9
12	M	102	ARG	4.6
16	Q	38	ARG	3.9
9	J	8	LEU	2.9
12	M	101	GLN	2.7
3	D	132	ARG	2.6
13	N	30	ALA	2.6
9	J	68	HIS	2.5
12	M	124	PRO	2.5
20	A	1086	U	2.5
11	L	14	GLY	2.4
12	M	123	ALA	2.2
9	J	42	THR	2.1
9	J	9	ARG	2.1
20	A	1367	C	2.0

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

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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
24	DPP	U	2	6/7	0.16	-	118,118,118,118	0
24	UAL	U	5	9/10	0.15	-	118,118,118,118	0
24	KBE	U	1	9/10	0.19	-	118,118,118,118	0
24	5OH	U	6	12/13	0.13	-	99,101,102,102	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
25	GNP	Y	701	32/32	0.14	-	58,71,81,83	0
26	MG	Y	702	1/1	0.10	-	135,135,135,135	0

## 6.5 Other polymers

There are no such residues in this entry.