



# Full wwPDB X-ray Structure Validation Report

Sep 15, 2014 – 12:01 PM EDT

PDB ID : 1VXJ  
Title : Crystal Structure of tRNA Proline (CGG) Bound to Codon CCC-U on the Ribosome  
Authors : Maehigashi, T.; Dunkle, J.A.; Dunham, C.M.  
Deposited on : 2013-07-12  
Resolution : 2.94 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>

---

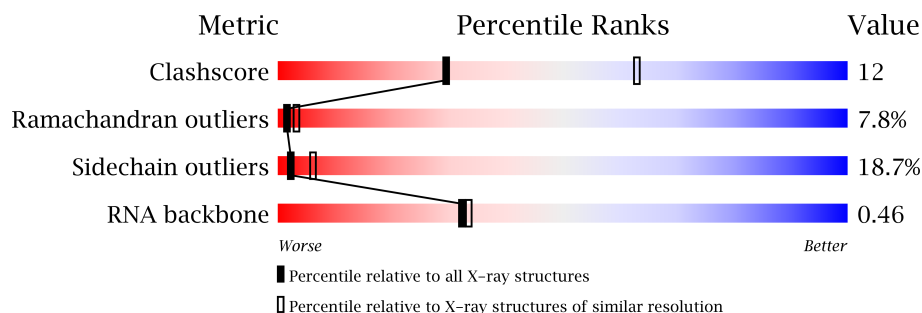
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23489

# 1 Overall quality at a glance

The reported resolution of this entry is 2.94 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1761 (2.98-2.90)
Ramachandran outliers	78287	1708 (2.98-2.90)
Sidechain outliers	78261	1710 (2.98-2.90)
RNA backbone	1838	1002 (3.44-2.44)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	2916	
2	B	122	
3	D	276	
4	E	206	
5	F	210	
6	G	182	
7	H	180	
8	I	148	
9	N	140	
10	O	122	
11	P	150	
12	Q	141	
13	R	118	
14	S	112	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
15	T	146	
16	U	118	
17	V	101	
18	W	113	
19	X	96	
20	Y	110	
21	Z	206	
22	0	85	
23	1	98	
24	2	72	
25	3	60	
26	4	71	
27	5	60	
28	6	54	
29	7	49	
30	8	65	
31	9	37	
32	a	3	

## 2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 92288 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 RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2883	Total	C	N	O	P	0	0	0
			62091	27636	11613	19960	2882			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	N	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	O	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	P	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	Q	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	R	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	S	111	Total	C	N	O	0	0	0
			882	556	176	150			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	T	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	U	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	V	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	W	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	X	92	Total	C	N	O	0	0	0
			725	471	131	123			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	Y	102	Total	C	N	O	S	0	0	0
			785	505	150	125	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	Z	183	Total	C	N	O	S	0	0	0
			1461	933	260	265	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	0	82	Total	C	N	O	S	0	0	0
			648	401	138	108	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	1	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	2	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	3	59	Total	C	N	O	0	0	0
			469	298	90	81			

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	4	71	Total	C	N	O	S	0	0	0
			581	364	108	104	5			

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	6	49	Total	C	N	O	S	0	0	0
			424	264	87	69	4			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 32 is a RNA chain called tRNA acceptor end mimic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	a	3	Total	C	N	O	P	0	0	0
			74	40	13	19	2			

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	P	2	Total	Mg	0	0
			2	2		
33	Q	1	Total	Mg	0	0
			1	1		
33	E	1	Total	Mg	0	0
			1	1		
33	B	3	Total	Mg	0	0
			3	3		
33	A	268	Total	Mg	0	0
			268	268		
33	5	1	Total	Mg	0	0
			1	1		

*Continued on next page...*



*Continued from previous page...*

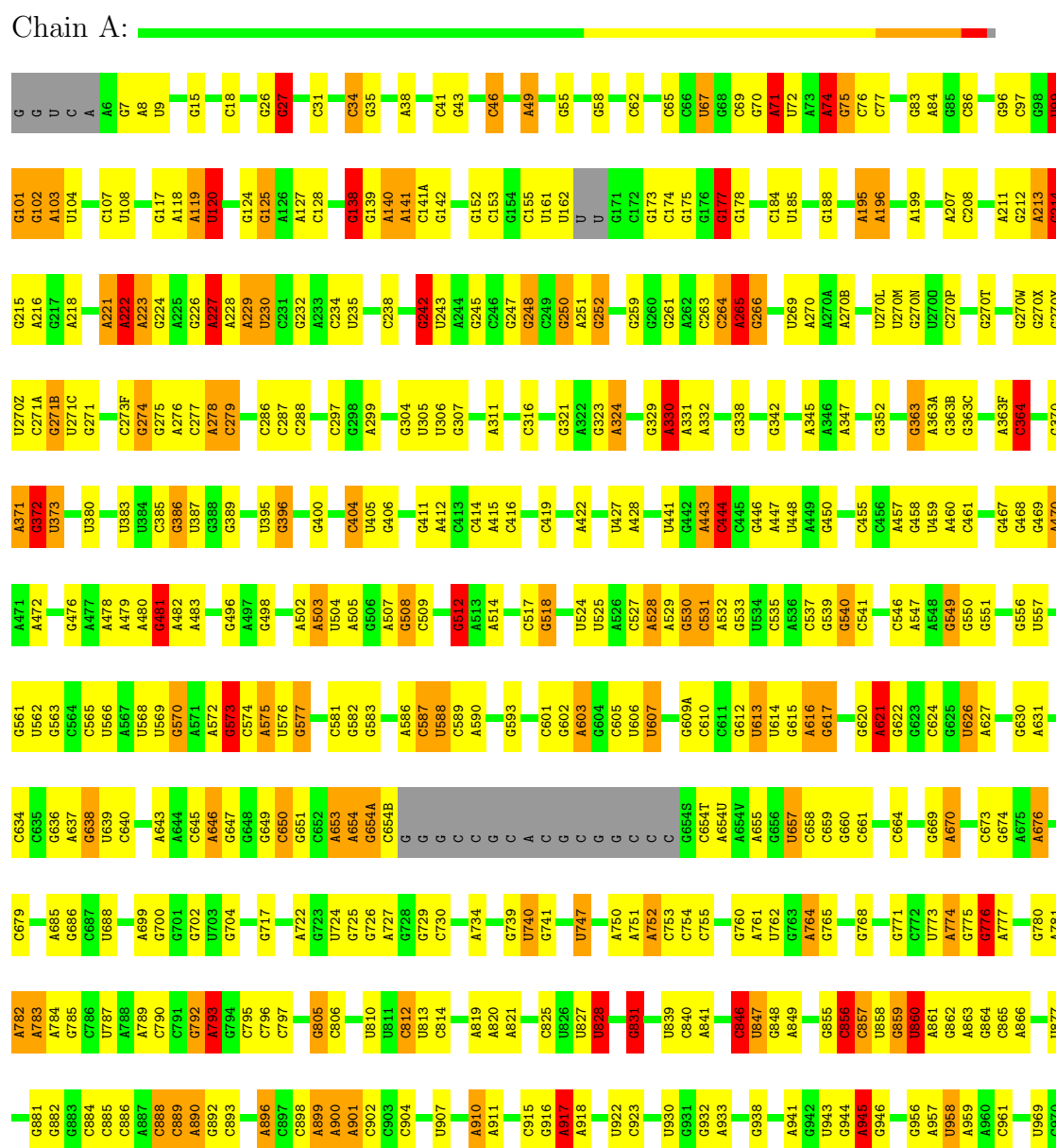
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	X	1	Total	Mg	0	0
			1	1		

### 3 Residue-property plots

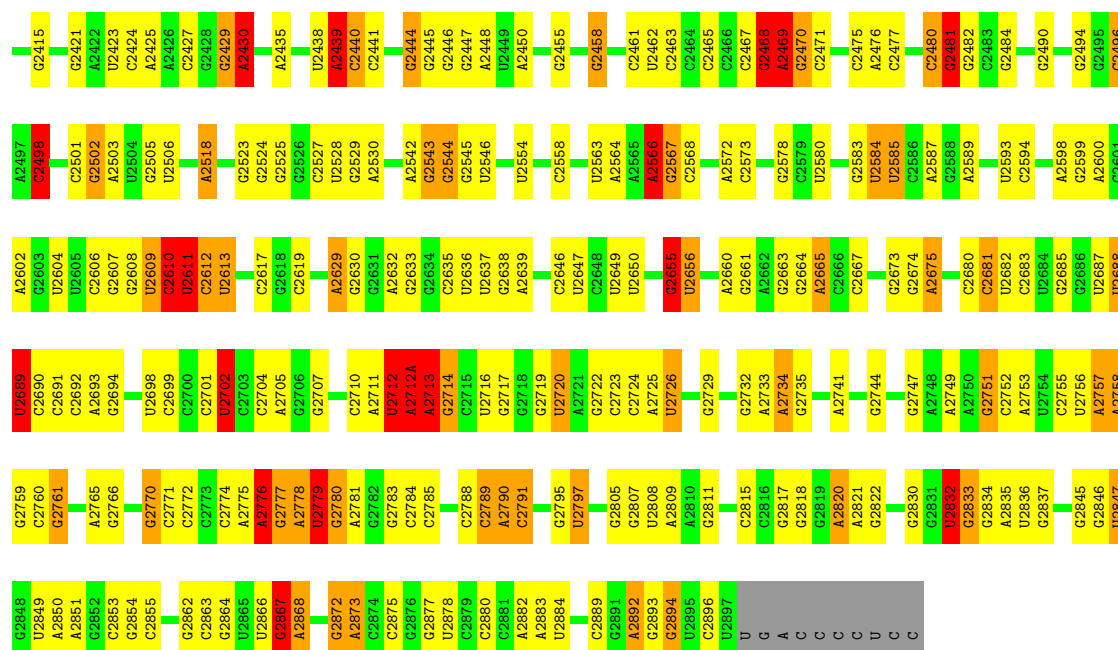
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

#### • Molecule 1: 23S rRNA

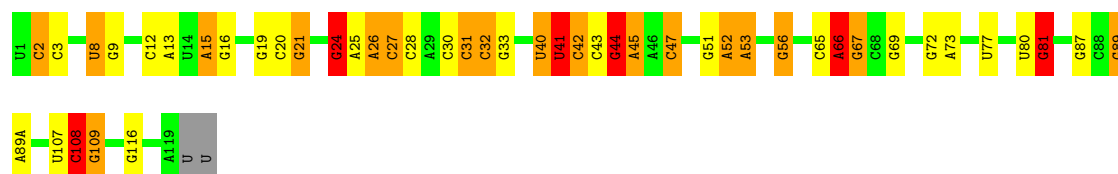


A2328	C2043	G1941	G1835	G1750	C1638	A1545A	G1461	C1386	U1300	U1205	A1126	G1055	C971
G2329	C2044	C1947	G1836	G1753	U1639	C1546	C1467	C1387	A1301	G1206	A1127	G1056	G972
G2330	C2045	C1947	G1836	G1753	C1640	C1547	C1467	C1388	C1307	G1207	A1128	A1057	A973
G2331	C2136	C2136	G1839	G1754	C1548	C1549	C1468	G1389	G1309	G1208	A1129	G1058	G974
G2334	C2050	G1950	G1839	A1755	G1647	C1549	A1469	U1390	U1310	G1209	U1130	G1059	G974A
	A2051	U1951	G1847	G1756	C1648	C1550	G1470	U1391	G1131	A1210	U1060	U1061	G975
G2335	A2051	U1951	G1847	G1756	C1648	C1550	G1470	U1391	U1313	U1211	C1135	G1061	A980
A2336	C2055	U1955	A1848	A1769	A1652	A1554	G1479	A1393	C1314	G1212	C1136	G1062	A981
A2336	C2056	U1955	G1849	A1762	G1653	C1557	G1480	A1395	G1136	A1213	G1137	G1063	A982
U2344	A2057	U1956	G1858	G1763	A1654	C1558	U1482	U1396	G1138	G1216	G1138	U1066	A983
G2345	G2151	A1960	G1859	G1764	A1655	A1558	G1483	U1397	G1139	A1220	G1139	A1067	G987
	G2152	A1960	G1859	G1764	A1655	A1558	G1483	U1397	G1139		A1069	A1070	
G2347	A2060	G1862	G1862	G1771	C1656	G1559	G1484	C1398	A1321	C1222	C1140	G1068	C991
G2350	G2061	U1963	G1863	G1772	C1657	C1565	G1485	C1399	A1322	G1228	A1142	G1071	C992
	A2062	G1965	U1864	G1773	U1659	C1566	G1486	G1400	A1400	G1238	A1148	C1076	G993
A2352	C2063	C1966	U1864	G1774	A1660	A1567	G1487	C1402	G1328	G1239	A1149	U1077	C994
G2355	C2064	G1967	G1870	U1775	G1665	G1568	A1490	C1403	G1330	G1240	C1150	U1078	C995
A2356	C2065	C1967	G1870	U1775	G1666	A1569	U1570	C1404	A1331	G1241	C1151	G1079	A996
U2357	G2067	A1969	A1871	U1776	G1667	A1571	A1495	U1571	G1332	A1241	C1153	C1080	C997
G2357	U2167	G1878	A1872	U1778	A1668	C1577	A1496	C1405	G1333	G1242	G1154	U1081	A1000
	G2276	A1971	C1879	U1779	A1668	C1577	U1497	C1406	G1334	G1243	A1155	U1082	U1083
A2360	G2069	A1972	G1882	A1780	G1674	C1577	U1497	C1408	U1335	G1244	A1156	U1083	G1004
A2361	A2071	A1972	G1882	C1761	G1674	C1577	U1497	C1408	U1335	G1245	A1156	U1083	G1004
G2364	U2074	C1979	G1883	A1784	G1678	A1579	C1498	C1411	G1338	G1256	G1169	G1089	G1011
G2365	U2075	G1980	A1884	A1784	G1681	A1579	C1499	G1418	U1339	C1257	G1170	U1090	U1012
A2366	C2174	C1982	A1889	A1786	G1682	G1581	G1500	G1413	U1340	G1257	G1171	C1013	C1013
G2366	C2175	C1982	A1889	A1786	G1682	G1581	G1500	G1413	U1341	G1258	G1172	G1093	G1093
	U2089	C1987	G1896	C1684	C1684	C1585	C1505	G1416	A1342	U1263	G1173	U1094	U1019
A2369	G2093	C1987	G1896	C1684	C1684	C1586	C1506	C1417	C1345	G1264	A1174	U1094	U1019
G2370	C2177	C1988	G1899	A1791	U1790	A1586	C1507	G1418	G1348	G1265	A1175	A1095	A1020
A2377	C2178	C1989	G1899	G1792	G1792	A1587	C1508	G1419	U1349	G1266	G1176	A1096	A1021
A2378	C2179	C1990	G1899	G1792	U1688	C1588	C1509	U1420	G1348	G1267	A1177	U1097	G1022
G2379	C2180	U1991	U2098	U1794	G1931	G1591	A1510	A1510	A1349	U1268	A1178	A1098	G1022
C2293	C2183	G1993	G1905	U1796	G1694	G1592	G1512	G1424	U1352	G1269	C1179	G1099	U1023
C2294			G1906	U1796	G1695	G1593	G1513	G1425	A1353	G1270	C1180	G1100	G1024
G2302	C2190	C1996	C1914	C1914	G1696	G1594	G1514	G1426	A1354	U1271	G1184	U1101	G1025
	G2191	U2109	U2011	C1800	G1697	G1595	U1519	G1428	A1359	G1272		U1102	U1026
A2298	G2192	G2110	A1915	C1801	G1698	C1800	G1520	C1430	A1360	G1273		C1102	U1027
G2385	G2193	C2111	A1916	G1801	G1699	G1802	U1520	U1431	G1364	A1272	G1187	A1028	A1028
G2386	G2194	A2014	U1917	A1802	A1700	A1603	G1522	U1431	A1365	U1273	G1188	A1029	A1029
G2302	C2195	A2015	A1918	C1804	A1701	A1603	G1522	U1431	G1366	A1278	A1189	G1106	
	U2113	A2015	A1919	C1804	A1701	A1603	G1522	U1431	G1366				
C2306	U2197	G2389	C2215	U1805	U1709	C1607	A1528	A1434					
G2307	A2198	C2021	C2216	U1805	A1608	A1608	A1529	A1434					
G2308					A1609	A1609	G1530	A1444A					
A2309	G2210	U2117	U2022	G1811	G1725	A1610	C1531	C1445	G1371	A1278	G1191	G1107	A1032
A2310	G2211	C2093	C2093	G1925					U1372	G1283	G1191	U1108	U1033
A2311	A2212	U2118	G2024	G1925					G1372	G1284	G1192	G1109	G1036
									U1372	G1285	G1193	G1110	
C2314	G2213	G2213	G2213	G1930	A1729	C1615	G1533	G1448	A1373	A1286	A1194	A1111	
G2315				U1931	U1730	A1616	U1535	G1449A	C1375	G1287	G1195	G1112	A1045
				G1933	A1932	C1617	A1536			U1287			A1046
				G1933	A1732	A1618	C1537		A1379	U1288	U1113	U1113	A1046
					G1823				G1380	U1289	U1198	G1114	G1047
					G1824				G1381	C1290	U1199	G1114	A1048
G2318				A1936	C1734	G1622	G1538		G1382	C1291	U1199	G1122	C1049
G2319				A1937	C1734	G1622	G1538		G1383	U1292	C1201	G1122	A1050
A2320				G1825	G1742	A1634	A1543	C1458	C1384	G1293		G1124	
U2406				G1826	G1743	A1634	A1543	C1458	C1384			G1124	
G2325				U1939	G1743	A1634	A1543	C1458	C1384			G1124	
G2326				U1939	G1743	A1634	A1543	C1458	C1384			G1124	
A2327				U1939	G1743	A1634	A1543	C1458	C1384			G1124	
G2410				U1939	G1743	A1634	A1543	C1458	C1384			G1124	
G2411				U1939	G1743	A1634	A1543	C1458	C1384			G1124	



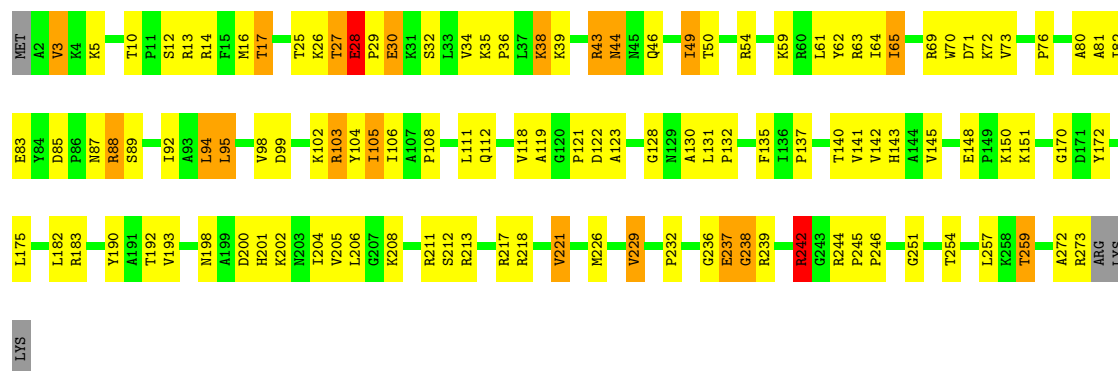
- Molecule 2: 5S rRNA

Chain B:



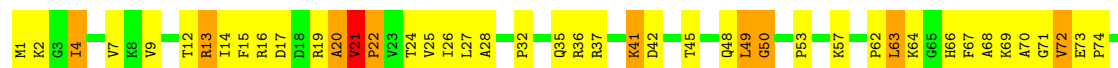
- Molecule 3: 50S ribosomal protein L2

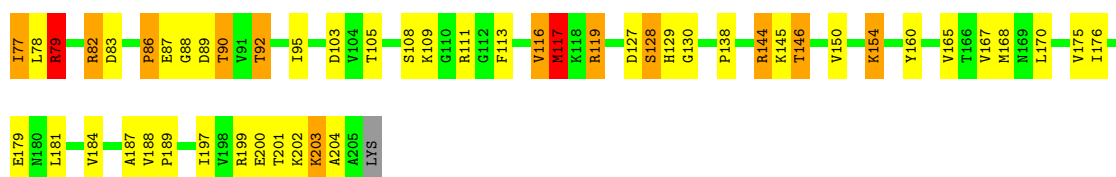
Chain D:



- Molecule 4: 50S ribosomal protein L3

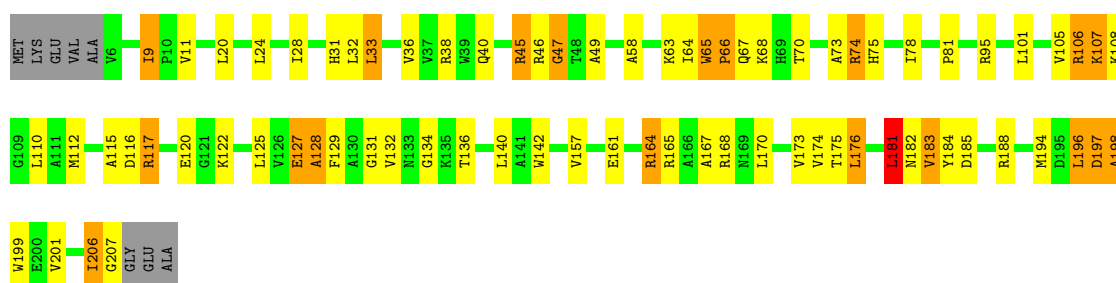
Chain E:





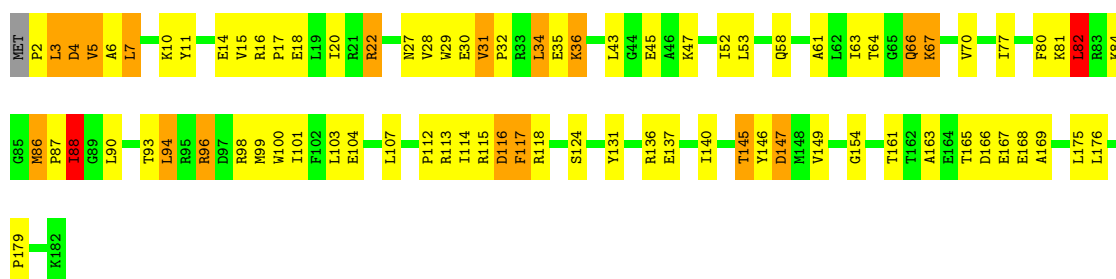
• Molecule 5: 50S ribosomal protein L4

Chain F:



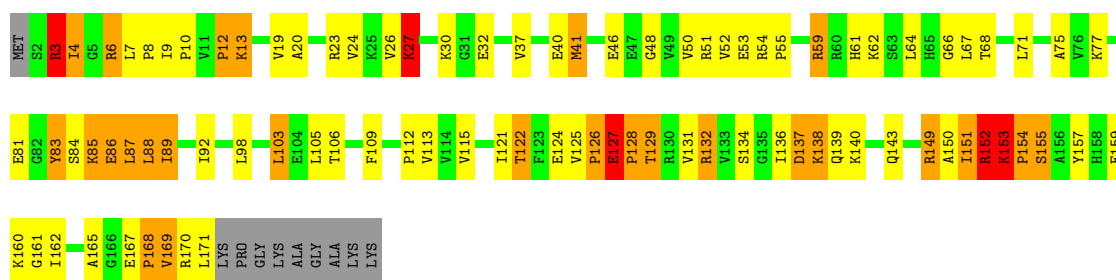
• Molecule 6: 50S ribosomal protein L5

Chain G:



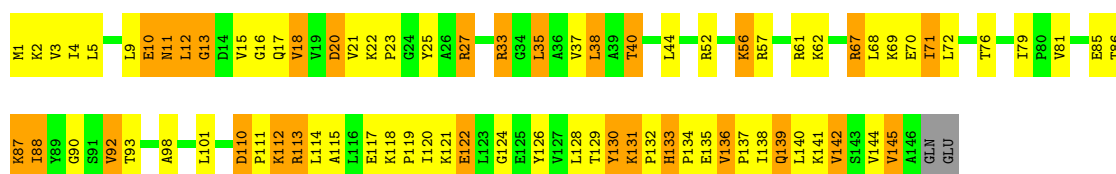
• Molecule 7: 50S ribosomal protein L6

Chain H:



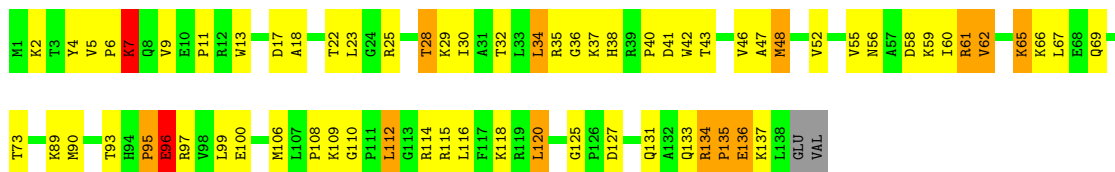
• Molecule 8: 50S ribosomal protein L9

Chain I:



- Molecule 9: 50S ribosomal protein L13

Chain N:



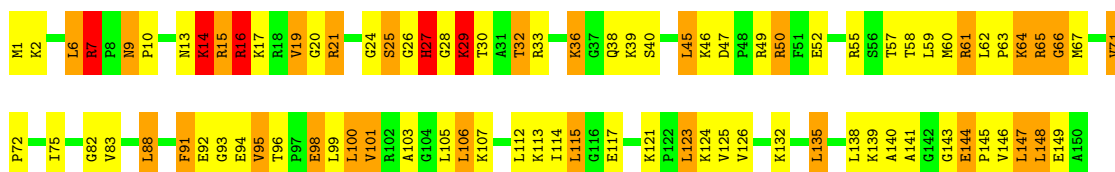
- Molecule 10: 50S ribosomal protein L14

Chain O:



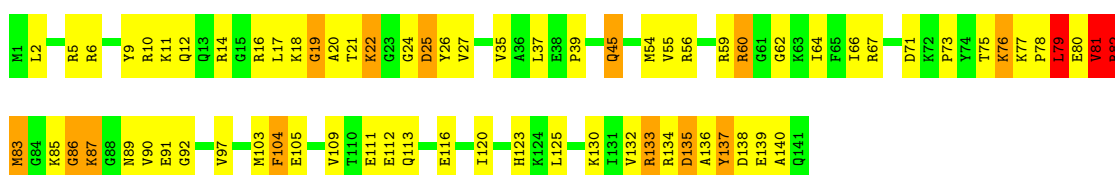
- Molecule 11: 50S ribosomal protein L15

Chain P:



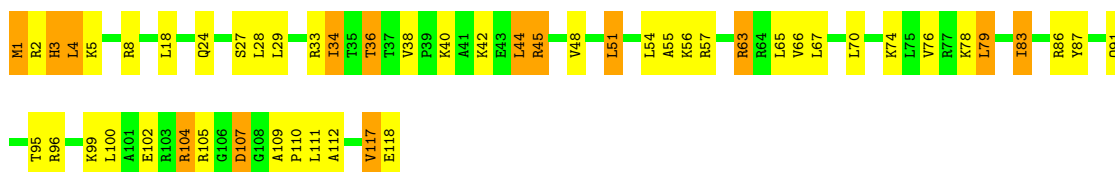
- Molecule 12: 50S ribosomal protein L16

Chain Q:



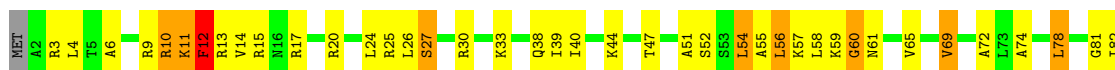
- Molecule 13: 50S ribosomal protein L17

Chain R:



- Molecule 14: 50S ribosomal protein L18

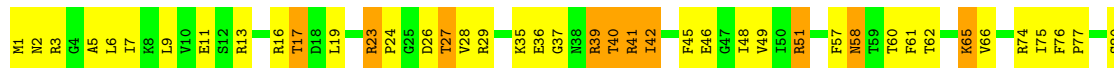
Chain S:





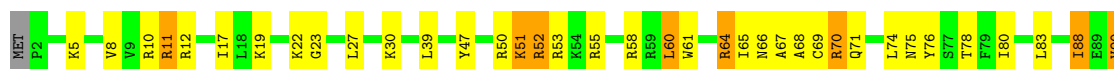
- Molecule 15: 50S ribosomal protein L19

Chain T:



- Molecule 16: 50S ribosomal protein L20

Chain U:



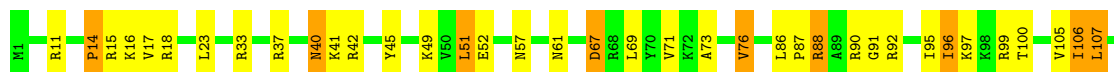
- Molecule 17: 50S ribosomal protein L21

Chain V:



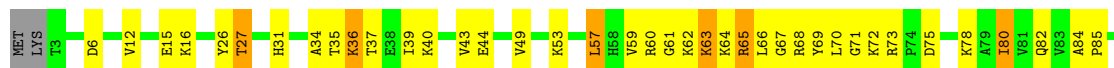
- Molecule 18: 50S ribosomal protein L22

Chain W:



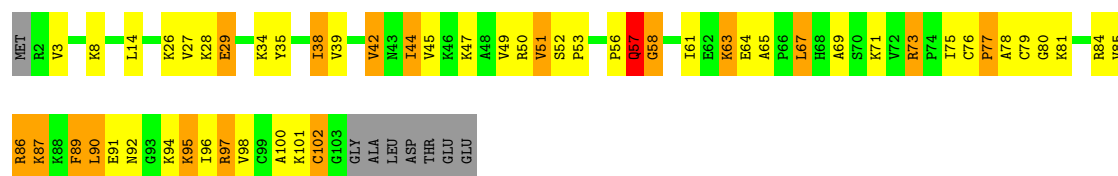
- Molecule 19: 50S ribosomal protein L23

Chain X:



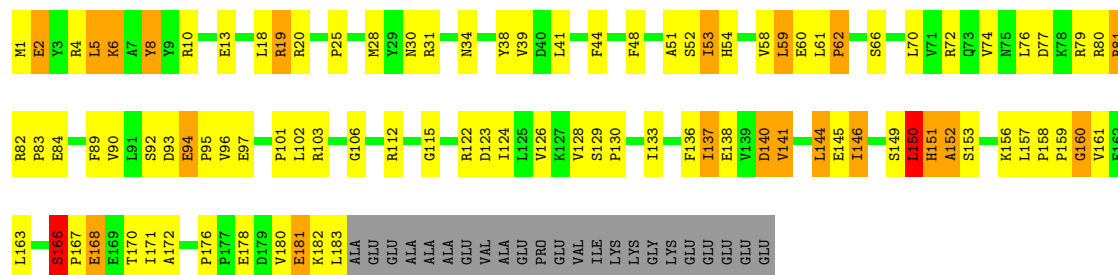
- Molecule 20: 50S ribosomal protein L24

Chain Y: 



- Molecule 21: 50S ribosomal protein L25

Chain Z: 



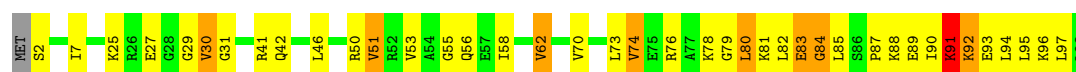
- Molecule 22: 50S ribosomal protein L27

Chain 0: 



- Molecule 23: 50S ribosomal protein L28

Chain 1: 



- Molecule 24: 50S ribosomal protein L29

Chain 2: 



- Molecule 25: 50S ribosomal protein L30

Chain 3: 



- Molecule 26: 50S ribosomal protein L31

Chain 4: 







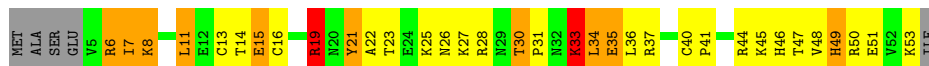
- Molecule 27: 50S ribosomal protein L32

Chain 5:



- Molecule 28: 50S ribosomal protein L33

Chain 6:



- Molecule 29: 50S ribosomal protein L34

Chain 7:



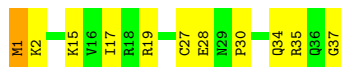
- Molecule 30: 50S ribosomal protein L35

Chain 8:



- Molecule 31: 50S ribosomal protein L36

Chain 9:



- Molecule 32: tRNA acceptor end mimic

Chain a:



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.81Å 449.41Å 620.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	155.22 – 2.94	Depositor
% Data completeness (in resolution range)	98.6 (155.22-2.94)	Depositor
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.219 , 0.265	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	92288	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.72	19/69543 (0.0%)	1.26	504/108563 (0.5%)
2	B	0.56	0/2878	1.15	18/4490 (0.4%)
3	D	0.58	0/2165	0.78	1/2919 (0.0%)
4	E	0.46	0/1601	0.75	2/2160 (0.1%)
5	F	0.48	0/1620	0.71	1/2194 (0.0%)
6	G	0.39	0/1499	0.60	0/2016
7	H	0.45	0/1332	0.73	0/1802
8	I	0.35	0/1151	0.66	0/1558
9	N	0.43	0/1131	0.64	0/1525
10	O	0.49	0/943	0.65	0/1269
11	P	0.49	0/1162	0.90	2/1544 (0.1%)
12	Q	0.57	0/1143	0.80	1/1527 (0.1%)
13	R	0.44	0/982	0.73	0/1312
14	S	0.40	0/892	0.75	1/1187 (0.1%)
15	T	0.44	0/1155	0.67	0/1542
16	U	0.50	0/982	0.68	0/1306
17	V	0.45	0/790	0.73	1/1057 (0.1%)
18	W	0.45	0/911	0.68	0/1220
19	X	0.50	0/739	0.66	0/993
20	Y	0.46	0/798	0.69	0/1064
21	Z	0.37	0/1493	0.64	2/2026 (0.1%)
22	0	0.48	0/657	0.69	0/874
23	1	0.46	0/770	0.69	0/1022
24	2	0.52	0/583	0.73	0/771
25	3	0.41	0/474	0.59	0/635
26	4	0.37	0/594	0.68	0/795
27	5	0.43	0/473	0.77	1/639 (0.2%)
28	6	0.37	0/431	0.67	0/575
29	7	0.57	0/438	0.71	0/575
30	8	0.58	0/525	0.82	0/691
31	9	0.32	0/310	0.48	0/407
32	a	0.78	0/40	1.81	1/60 (1.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.65	19/100205 (0.0%)	1.14	535/150318 (0.4%)

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
4	E	0	1
5	F	0	1
7	H	0	2
14	S	0	1
21	Z	0	1
24	2	0	1
30	8	0	2
All	All	0	9

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	528	A	N9-C4	-9.10	1.32	1.37
1	A	783	A	N9-C4	-7.66	1.33	1.37
1	A	783	A	N3-C4	-7.55	1.30	1.34
1	A	676	A	N9-C4	-7.13	1.33	1.37
1	A	1786	A	N3-C4	-6.80	1.30	1.34
1	A	1142(A)	A	N9-C4	-6.74	1.33	1.37
1	A	71	A	N9-C4	-6.52	1.33	1.37
1	A	2287	A	N9-C4	-6.37	1.34	1.37
1	A	783	A	C5-C6	-6.22	1.35	1.41
1	A	1021	A	N9-C4	-5.71	1.34	1.37
1	A	1786	A	N9-C4	-5.66	1.34	1.37
1	A	783	A	N9-C8	5.56	1.42	1.37
1	A	74	A	N9-C4	-5.53	1.34	1.37
1	A	776	G	N7-C5	5.51	1.42	1.39
1	A	1950	G	C2-N3	5.31	1.36	1.32
1	A	49	A	N7-C5	-5.29	1.36	1.39
1	A	1991	U	C2-N3	-5.27	1.34	1.37
1	A	974	G	C8-N7	5.21	1.34	1.30
1	A	774	A	C5-C6	-5.07	1.36	1.41

All (535) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1786	A	N7-C8-N9	13.21	120.41	113.80
1	A	528	A	C2-N3-C4	-13.10	104.05	110.60
1	A	783	A	C2-N3-C4	-12.39	104.41	110.60
1	A	1786	A	C5-N7-C8	-12.26	97.77	103.90
1	A	1786	A	C2-N3-C4	-11.73	104.73	110.60
1	A	783	A	C5-N7-C8	-11.48	98.16	103.90
1	A	1899	G	N3-C2-N2	11.37	127.86	119.90
1	A	774	A	N1-C6-N6	11.19	125.32	118.60
1	A	1991	U	N3-C4-O4	-10.91	111.76	119.40
1	A	265	A	O4'-C1'-N9	10.83	116.86	108.20
1	A	774	A	C2-N3-C4	-10.47	105.36	110.60
1	A	1899	G	N1-C2-N2	-10.44	106.80	116.20
1	A	1678	G	C4-C5-N7	10.44	114.97	110.80
1	A	2430	A	C2-N3-C4	-10.26	105.47	110.60
1	A	74	A	C2-N3-C4	-9.86	105.67	110.60
1	A	71	A	C2-N3-C4	-9.80	105.70	110.60
1	A	1678	G	C5-N7-C8	-9.77	99.42	104.30
1	A	530	G	N3-C2-N2	9.56	126.59	119.90
1	A	945	A	N1-C6-N6	9.44	124.27	118.60
1	A	1786	A	N1-C2-N3	9.42	134.01	129.30
1	A	1786	A	C8-N9-C4	-9.39	102.04	105.80
1	A	676	A	C5-N7-C8	-9.30	99.25	103.90
1	A	1021	A	C2-N3-C4	-9.21	105.99	110.60
1	A	528	A	N3-C4-N9	-9.17	120.06	127.40
1	A	676	A	C2-N3-C4	-9.02	106.09	110.60
1	A	1332	G	C6-C5-N7	-8.90	125.06	130.40
1	A	528	A	N3-C4-C5	8.90	133.03	126.80
1	A	783	A	C4-C5-N7	8.79	115.09	110.70
1	A	1824	G	O5'-P-OP2	-8.79	97.79	105.70
1	A	1979	C	C6-N1-C2	-8.66	116.84	120.30
1	A	2287	A	C2-N3-C4	-8.64	106.28	110.60
1	A	530	G	N1-C6-O6	-8.60	114.74	119.90
1	A	372	G	O4'-C1'-N9	8.59	115.08	108.20
1	A	776	G	C5-N7-C8	-8.56	100.02	104.30
1	A	945	A	C5-N7-C8	-8.52	99.64	103.90
1	A	776	G	N1-C6-O6	-8.51	114.79	119.90
1	A	1950	G	N7-C8-N9	8.49	117.35	113.10
1	A	1678	G	C6-C5-N7	-8.46	125.32	130.40
1	A	530	G	N1-C2-N2	-8.44	108.60	116.20
1	A	1204	A	O4'-C1'-N9	8.41	114.92	108.20
1	A	945	A	C4-C5-N7	8.39	114.90	110.70
1	A	774	A	N1-C2-N3	8.38	133.49	129.30
1	A	776	G	N7-C8-N9	8.36	117.28	113.10

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	974(A)	C	N3-C2-O2	-8.34	116.06	121.90
1	A	2490	G	C4-C5-N7	8.31	114.12	110.80
1	A	1332	G	C4-C5-N7	8.31	114.12	110.80
1	A	120	U	C5-C6-N1	-8.28	118.56	122.70
1	A	2490	G	C5-N7-C8	-8.28	100.16	104.30
1	A	1991	U	N3-C4-C5	8.26	119.56	114.60
1	A	1210	A	C8-N9-C4	-8.21	102.52	105.80
1	A	2702	U	C2-N1-C1'	8.21	127.55	117.70
1	A	330	A	C2-N3-C4	-8.17	106.52	110.60
1	A	1899	G	C6-C5-N7	-8.16	125.50	130.40
1	A	74	A	N1-C2-N3	8.13	133.37	129.30
1	A	783	A	N7-C8-N9	8.08	117.84	113.80
1	A	774	A	C6-C5-N7	-8.08	126.65	132.30
1	A	141	A	N7-C8-N9	8.03	117.82	113.80
1	A	1496	A	N7-C8-N9	8.03	117.81	113.80
1	A	1616	A	C5-N7-C8	-8.01	99.90	103.90
1	A	1950	G	C4-N9-C1'	7.98	136.88	126.50
1	A	1678	G	N7-C8-N9	7.95	117.07	113.10
1	A	2490	G	C6-C5-N7	-7.94	125.63	130.40
1	A	1786	A	C6-C5-N7	-7.87	126.79	132.30
1	A	2712(A)	A	N7-C8-N9	7.87	117.73	113.80
1	A	2447	G	C8-N9-C4	-7.85	103.26	106.40
1	A	2544	G	N1-C6-O6	7.84	124.61	119.90
1	A	945	A	C6-C5-N7	-7.84	126.81	132.30
1	A	1396	U	N3-C2-O2	-7.83	116.72	122.20
1	A	2584	U	N3-C2-O2	-7.82	116.73	122.20
1	A	1210	A	N7-C8-N9	7.77	117.69	113.80
1	A	1819	A	P-O3'-C3'	7.75	129.00	119.70
1	A	1142(A)	A	C2-N3-C4	-7.74	106.73	110.60
1	A	1899	G	N3-C4-N9	7.74	130.64	126.00
1	A	1190	G	C5-N7-C8	-7.68	100.46	104.30
1	A	470	A	O5'-P-OP1	-7.64	98.82	105.70
1	A	1678	G	N1-C6-O6	7.59	124.45	119.90
1	A	1678	G	C2-N3-C4	-7.59	108.11	111.90
1	A	1698	A	C2-N3-C4	-7.55	106.83	110.60
1	A	1130	U	P-O3'-C3'	7.54	128.75	119.70
1	A	676	A	N3-C4-C5	7.52	132.06	126.80
1	A	1404	C	O5'-P-OP1	-7.52	98.93	105.70
1	A	1396	U	N1-C2-O2	7.50	128.05	122.80
1	A	1204	A	N1-C2-N3	7.49	133.05	129.30
1	A	2713	A	C5-N7-C8	-7.46	100.17	103.90
1	A	2688	U	C4-C5-C6	7.46	124.17	119.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	450	G	C5-C6-N1	-7.44	107.78	111.50
1	A	2346	A	C2-N3-C4	-7.43	106.88	110.60
1	A	1931	U	C5-C4-O4	7.42	130.35	125.90
1	A	774	A	C5-N7-C8	-7.42	100.19	103.90
1	A	1950	G	N3-C2-N2	7.40	125.08	119.90
1	A	2490	G	N7-C8-N9	7.38	116.79	113.10
1	A	1332	G	C4-N9-C1'	7.38	136.09	126.50
1	A	774	A	C4-C5-N7	7.37	114.39	110.70
1	A	1332	G	C5-N7-C8	-7.37	100.62	104.30
1	A	2429	G	OP2-P-O3'	7.36	121.38	105.20
1	A	2688	U	N3-C2-O2	-7.33	117.07	122.20
1	A	1382	G	N1-C6-O6	7.32	124.29	119.90
1	A	1332	G	N7-C8-N9	7.30	116.75	113.10
1	A	140	A	N7-C8-N9	7.30	117.45	113.80
1	A	371	A	O5'-P-OP1	-7.29	99.14	105.70
1	A	1950	G	O4'-C1'-N9	7.28	114.02	108.20
1	A	1204	A	C2-N3-C4	-7.28	106.96	110.60
1	A	856	C	C6-N1-C2	-7.26	117.39	120.30
1	A	512	G	O4'-C1'-N9	7.26	114.01	108.20
1	A	1021	A	C5-N7-C8	-7.26	100.27	103.90
1	A	120	U	C4-C5-C6	7.25	124.05	119.70
1	A	1950	G	C8-N9-C4	-7.24	103.50	106.40
1	A	676	A	O4'-C1'-N9	7.24	113.99	108.20
1	A	141	A	C8-N9-C4	-7.22	102.91	105.80
1	A	1799	G	P-O3'-C3'	7.22	128.36	119.70
1	A	1936	A	N9-C4-C5	-7.22	102.91	105.80
1	A	1929	G	OP1-P-O3'	7.20	121.04	105.20
4	E	21	VAL	C-N-CD	-7.18	104.80	120.60
1	A	1313	U	C2-N1-C1'	7.17	126.31	117.70
1	A	621	A	C2-N3-C4	-7.16	107.02	110.60
1	A	1616	A	N7-C8-N9	7.16	117.38	113.80
1	A	141	A	C5-N7-C8	-7.13	100.33	103.90
1	A	140	A	C5-N7-C8	-7.09	100.36	103.90
1	A	446	G	N1-C6-O6	7.07	124.14	119.90
1	A	1931	U	N3-C2-O2	-7.06	117.26	122.20
2	B	31	C	C6-N1-C2	-7.03	117.49	120.30
1	A	1496	A	C8-N9-C4	-7.02	102.99	105.80
1	A	2688	U	C5-C4-O4	7.00	130.10	125.90
1	A	974(A)	C	N1-C2-O2	6.99	123.09	118.90
1	A	1614	A	C5-N7-C8	-6.96	100.42	103.90
1	A	1427	A	P-O3'-C3'	6.96	128.05	119.70
1	A	1653	G	P-O3'-C3'	6.93	128.01	119.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1929	G	C4-C5-N7	6.89	113.56	110.80
1	A	621	A	N7-C8-N9	6.89	117.24	113.80
1	A	2587	A	N1-C6-N6	-6.88	114.47	118.60
1	A	974(A)	C	N3-C4-N4	-6.88	113.18	118.00
1	A	1889	A	O5'-P-OP1	-6.85	99.54	105.70
1	A	2311	A	C2-N3-C4	-6.84	107.18	110.60
1	A	2689	U	N3-C4-O4	-6.83	114.62	119.40
1	A	2481	G	P-O3'-C3'	6.83	127.89	119.70
32	a	74	C	N1-C2-O2	6.82	122.99	118.90
1	A	783	A	N3-C4-C5	6.80	131.56	126.80
1	A	1428	C	O5'-P-OP2	6.80	118.86	110.70
1	A	1528	A	N7-C8-N9	6.79	117.19	113.80
1	A	676	A	N3-C4-N9	-6.76	121.99	127.40
1	A	1929	G	N1-C6-O6	6.75	123.95	119.90
1	A	1955	U	P-O3'-C3'	6.75	127.80	119.70
1	A	676	A	N7-C8-N9	6.74	117.17	113.80
1	A	828	U	N3-C2-O2	-6.74	117.48	122.20
1	A	242	G	P-O3'-C3'	6.71	127.76	119.70
1	A	245	G	O5'-P-OP1	-6.71	99.66	105.70
2	B	44	G	C4-N9-C1'	-6.71	117.78	126.50
1	A	71	A	N3-C4-C5	6.70	131.49	126.80
1	A	2430	A	N1-C2-N3	6.70	132.65	129.30
1	A	860	U	N3-C2-O2	-6.69	117.52	122.20
1	A	1616	A	O4'-C1'-N9	6.67	113.54	108.20
1	A	776	G	C4-C5-C6	-6.66	114.81	118.80
1	A	528	A	N1-C2-N3	6.64	132.62	129.30
1	A	828	U	C5-C4-O4	6.63	129.88	125.90
1	A	99	U	P-O3'-C3'	6.62	127.65	119.70
1	A	2439	A	N7-C8-N9	6.62	117.11	113.80
1	A	2609	U	C5-C6-N1	-6.62	119.39	122.70
1	A	588	U	O5'-P-OP1	-6.61	99.75	105.70
1	A	238	C	C5-C6-N1	-6.61	117.69	121.00
1	A	27	G	N3-C4-N9	-6.59	122.05	126.00
1	A	1929	G	C5-C6-O6	-6.58	124.65	128.60
1	A	1786	A	C4-C5-N7	6.57	113.99	110.70
1	A	1213	A	N1-C6-N6	6.55	122.53	118.60
1	A	2713	A	N1-C6-N6	6.55	122.53	118.60
1	A	1496	A	C5-N7-C8	-6.54	100.63	103.90
1	A	503	A	P-O3'-C3'	6.53	127.54	119.70
1	A	2070	G	N1-C6-O6	-6.53	115.98	119.90
1	A	372	G	C4-N9-C1'	-6.53	118.02	126.50
1	A	1694	C	P-O3'-C3'	6.53	127.53	119.70

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1428	C	O5'-P-OP1	-6.52	99.83	105.70
14	S	56	LEU	CA-CB-CG	6.52	130.30	115.30
1	A	860	U	C4-C5-C6	6.51	123.61	119.70
1	A	783	A	C6-C5-N7	-6.51	127.75	132.30
1	A	1786	A	C5-C6-N1	-6.50	114.45	117.70
1	A	1021	A	N7-C8-N9	6.50	117.05	113.80
1	A	528	A	C5-C6-N1	-6.48	114.46	117.70
1	A	2713	A	C4-C5-N7	6.48	113.94	110.70
1	A	570	G	C5-C6-N1	-6.47	108.26	111.50
1	A	1899	G	N3-C4-C5	-6.46	125.37	128.60
1	A	195	A	C5-N7-C8	-6.44	100.68	103.90
1	A	621	A	C5-N7-C8	-6.44	100.68	103.90
1	A	783	A	N1-C6-N6	6.44	122.46	118.60
1	A	1969	A	C8-N9-C4	6.43	108.37	105.80
1	A	679	C	C6-N1-C2	6.43	122.87	120.30
1	A	2458	G	N3-C4-C5	-6.42	125.39	128.60
1	A	1925	C	N1-C2-O2	-6.42	115.05	118.90
1	A	2032	G	C5-N7-C8	-6.42	101.09	104.30
1	A	1153	C	N1-C2-O2	-6.41	115.06	118.90
1	A	1799	G	N3-C4-C5	-6.40	125.40	128.60
1	A	761	A	N1-C6-N6	6.40	122.44	118.60
1	A	2587	A	C8-N9-C4	-6.39	103.24	105.80
1	A	1021	A	N1-C2-N3	6.39	132.50	129.30
1	A	1950	G	C6-C5-N7	-6.38	126.57	130.40
1	A	1528	A	C8-N9-C4	-6.37	103.25	105.80
1	A	1955	U	C5-C4-O4	6.36	129.72	125.90
1	A	2779	U	N3-C2-O2	-6.36	117.75	122.20
1	A	2502	G	O5'-P-OP1	-6.36	99.98	105.70
2	B	108	C	O4'-C1'-N1	6.35	113.28	108.20
1	A	1992	G	P-O3'-C3'	6.35	127.32	119.70
1	A	783	A	C8-N9-C4	-6.35	103.26	105.80
1	A	27	G	N9-C4-C5	6.34	107.93	105.40
1	A	1210	A	C5-N7-C8	-6.33	100.73	103.90
1	A	2584	U	C5-C4-O4	6.33	129.70	125.90
1	A	2832	U	P-O3'-C3'	6.33	127.30	119.70
1	A	577	G	N1-C6-O6	6.32	123.69	119.90
1	A	2598	A	OP2-P-O3'	6.32	119.09	105.20
1	A	372	G	OP2-P-O3'	6.31	119.09	105.20
1	A	2638	G	N3-C4-N9	6.31	129.79	126.00
1	A	2712	U	O4'-C1'-N1	6.31	113.25	108.20
1	A	2318	G	C6-C5-N7	-6.30	126.62	130.40
1	A	2430	A	C5-N7-C8	-6.30	100.75	103.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	860	U	C5-C6-N1	-6.29	119.56	122.70
1	A	1142(A)	A	N3-C4-C5	6.28	131.19	126.80
1	A	774	A	C5-C6-N6	-6.25	118.70	123.70
1	A	1614	A	C4-C5-N7	6.24	113.82	110.70
1	A	2712	U	C2-N1-C1'	6.19	125.12	117.70
2	B	66	A	P-O3'-C3'	6.17	127.11	119.70
1	A	140	A	C8-N9-C4	-6.17	103.33	105.80
1	A	1899	G	C4-N9-C1'	6.16	134.51	126.50
1	A	2447	G	C8-N9-C1'	6.15	135.00	127.00
1	A	2702	U	C5-C6-N1	6.15	125.78	122.70
1	A	1544	C	O5'-P-OP1	-6.15	100.17	105.70
1	A	1314	C	C2-N1-C1'	6.14	125.55	118.80
1	A	1614	A	N1-C6-N6	6.13	122.28	118.60
1	A	945	A	C5-C6-N6	-6.11	118.81	123.70
2	B	24	G	P-O3'-C3'	6.10	127.02	119.70
1	A	227	A	C8-N9-C4	-6.09	103.36	105.80
1	A	2681	C	P-O3'-C3'	6.09	127.01	119.70
1	A	446	G	C5-C6-O6	-6.09	124.94	128.60
1	A	859	G	P-O3'-C3'	6.09	127.00	119.70
1	A	2307	G	O4'-C1'-N9	6.08	113.06	108.20
5	F	74	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	A	570	G	C4-C5-N7	-6.08	108.37	110.80
1	A	140	A	C2-N3-C4	-6.07	107.57	110.60
1	A	1698	A	C5-N7-C8	-6.07	100.87	103.90
1	A	1991	U	C4-C5-C6	-6.05	116.07	119.70
1	A	1647	G	O5'-P-OP1	-6.05	100.25	105.70
1	A	2496	C	N3-C4-C5	6.05	124.32	121.90
1	A	2610	C	P-O3'-C3'	6.04	126.95	119.70
2	B	108	C	C2-N1-C1'	-6.04	112.16	118.80
1	A	621	A	O4'-C1'-N9	6.01	113.01	108.20
1	A	140	A	C6-C5-N7	-6.00	128.10	132.30
1	A	1332	G	C8-N9-C1'	-6.00	119.20	127.00
1	A	2518	A	C2-N3-C4	-5.98	107.61	110.60
1	A	1007	C	O5'-P-OP1	-5.97	100.32	105.70
1	A	271(B)	G	P-O3'-C3'	5.97	126.87	119.70
1	A	1559	G	N1-C6-O6	5.97	123.48	119.90
1	A	177	G	O4'-C1'-N9	5.97	112.98	108.20
1	A	1332	G	O4'-C1'-N9	-5.97	103.42	108.20
1	A	1970	A	O5'-P-OP2	-5.96	100.34	105.70
1	A	140	A	O4'-C1'-N9	5.96	112.96	108.20
1	A	1328	G	N3-C4-N9	5.95	129.57	126.00
17	V	35	LEU	CA-CB-CG	5.95	128.99	115.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2702	U	C6-N1-C1'	-5.93	112.89	121.20
1	A	74	A	P-O3'-C3'	5.93	126.81	119.70
1	A	930	U	C5-C4-O4	5.92	129.46	125.90
1	A	2287	A	N3-C4-C5	5.92	130.95	126.80
1	A	1696	G	C8-N9-C4	-5.91	104.04	106.40
1	A	2589	A	C8-N9-C4	5.90	108.16	105.80
2	B	31	C	N3-C2-O2	-5.89	117.78	121.90
1	A	97	C	N1-C2-O2	5.88	122.43	118.90
1	A	1558	A	P-O3'-C3'	5.88	126.76	119.70
1	A	575	A	O5'-P-OP1	-5.88	100.41	105.70
1	A	446	G	N9-C4-C5	-5.87	103.05	105.40
1	A	930	U	N3-C4-O4	-5.86	115.30	119.40
1	A	228	A	C8-N9-C4	-5.86	103.45	105.80
1	A	2050	C	N1-C2-O2	-5.85	115.39	118.90
1	A	1698	A	N1-C2-N3	5.85	132.22	129.30
1	A	330	A	C4-C5-N7	5.84	113.62	110.70
1	A	1313	U	C6-N1-C2	-5.84	117.49	121.00
1	A	1698	A	O4'-C1'-N9	5.83	112.86	108.20
1	A	2440	C	O5'-P-OP2	5.83	117.70	110.70
1	A	2447	G	N9-C4-C5	5.83	107.73	105.40
1	A	2481	G	OP2-P-O3'	5.83	118.03	105.20
1	A	2031	A	O4'-C1'-N9	5.82	112.85	108.20
1	A	372	G	C8-N9-C1'	5.81	134.56	127.00
1	A	27	G	P-O3'-C3'	5.80	126.66	119.70
1	A	974	G	N9-C4-C5	5.80	107.72	105.40
1	A	1559	G	C4-C5-N7	5.80	113.12	110.80
1	A	2439	A	P-O3'-C3'	5.79	126.65	119.70
1	A	1950	G	N1-C2-N2	-5.79	110.99	116.20
1	A	195	A	C8-N9-C4	-5.79	103.49	105.80
1	A	450	G	N1-C6-O6	5.78	123.37	119.90
1	A	2490	G	C4-N9-C1'	5.78	134.01	126.50
1	A	2067	G	C8-N9-C4	-5.78	104.09	106.40
1	A	1698	A	N7-C8-N9	5.77	116.69	113.80
1	A	1899	G	N7-C8-N9	5.77	115.98	113.10
1	A	1022	G	P-O3'-C3'	5.76	126.61	119.70
1	A	982	C	C6-N1-C2	-5.76	118.00	120.30
1	A	2439	A	C8-N9-C4	-5.75	103.50	105.80
1	A	1528	A	O4'-C1'-N9	5.75	112.80	108.20
1	A	2583	G	C4-C5-N7	-5.74	108.50	110.80
1	A	783	A	N3-C4-N9	-5.74	122.81	127.40
1	A	1698	A	C8-N9-C4	-5.74	103.50	105.80
1	A	2503	A	C2-N3-C4	5.74	113.47	110.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1528	A	C5-N7-C8	-5.73	101.03	103.90
1	A	2307	G	C4-N9-C1'	5.72	133.94	126.50
1	A	2867	G	P-O3'-C3'	5.72	126.56	119.70
12	Q	82	ARG	N-CA-C	5.72	126.44	111.00
1	A	444	C	C6-N1-C2	-5.71	118.01	120.30
1	A	2430	A	N1-C6-N6	5.71	122.03	118.60
1	A	1313	U	C5-C6-N1	5.71	125.55	122.70
1	A	2712	U	C6-N1-C1'	-5.70	113.22	121.20
1	A	238	C	C2-N3-C4	-5.70	117.05	119.90
1	A	752	A	P-O3'-C3'	5.70	126.54	119.70
1	A	330	A	C5-N7-C8	-5.70	101.05	103.90
11	P	59	LEU	CA-CB-CG	5.69	128.38	115.30
1	A	1950	G	C8-N9-C1'	-5.68	119.62	127.00
1	A	195	A	N7-C8-N9	5.67	116.64	113.80
1	A	2335	A	O4'-C1'-N9	5.66	112.73	108.20
1	A	573	G	O5'-P-OP2	-5.66	100.61	105.70
2	B	44	G	C6-C5-N7	5.66	133.80	130.40
1	A	195	A	P-O3'-C3'	5.66	126.49	119.70
1	A	2028	U	C5-C4-O4	-5.65	122.51	125.90
1	A	512	G	C8-N9-C1'	5.65	134.35	127.00
1	A	789	A	N1-C6-N6	-5.65	115.21	118.60
1	A	1398	C	N3-C4-C5	5.65	124.16	121.90
1	A	124	G	C5-C6-O6	-5.65	125.21	128.60
1	A	2468	G	C8-N9-C4	-5.64	104.14	106.40
1	A	1616	A	C8-N9-C4	-5.64	103.55	105.80
1	A	46	C	O5'-P-OP1	-5.63	100.64	105.70
1	A	2318	G	O4'-C1'-N9	5.63	112.70	108.20
1	A	860	U	C2-N1-C1'	5.62	124.45	117.70
1	A	2307	G	C6-C5-N7	-5.62	127.03	130.40
1	A	2447	G	N7-C8-N9	5.62	115.91	113.10
1	A	676	A	C4-C5-N7	5.61	113.51	110.70
1	A	783	A	N1-C2-N3	5.61	132.10	129.30
1	A	1678	G	C5-C6-O6	-5.59	125.24	128.60
1	A	102	G	P-O3'-C3'	5.59	126.41	119.70
11	P	25	SER	N-CA-C	-5.59	95.92	111.00
1	A	930	U	N3-C2-O2	-5.58	118.29	122.20
3	D	229	VAL	CB-CA-C	-5.58	100.79	111.40
1	A	330	A	N1-C6-N6	5.57	121.94	118.60
1	A	974	G	C8-N9-C1'	5.57	134.24	127.00
1	A	2071	A	O5'-P-OP2	5.57	117.38	110.70
1	A	2496	C	C6-N1-C2	5.55	122.52	120.30
1	A	1786	A	N9-C1'-C2'	5.54	121.21	114.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1799	G	C5-C6-O6	5.54	131.93	128.60
1	A	2566	A	P-O3'-C3'	5.54	126.35	119.70
1	A	1941	C	C6-N1-C2	-5.54	118.08	120.30
1	A	1667	G	C8-N9-C4	-5.54	104.19	106.40
1	A	1616	A	C4-C5-N7	5.54	113.47	110.70
1	A	1835	G	N3-C4-N9	5.54	129.32	126.00
1	A	2713	A	N7-C8-N9	5.54	116.57	113.80
1	A	945	A	N7-C8-N9	5.53	116.57	113.80
1	A	1930	G	C4-N9-C1'	-5.53	119.31	126.50
1	A	1647	G	O4'-C1'-N9	-5.53	103.78	108.20
1	A	2712(A)	A	C5-N7-C8	-5.53	101.14	103.90
1	A	1142(A)	A	C5-N7-C8	-5.52	101.14	103.90
1	A	2318	G	C4-N9-C1'	5.52	133.68	126.50
1	A	1929	G	C6-C5-N7	-5.51	127.10	130.40
1	A	2056	G	C5-N7-C8	-5.51	101.55	104.30
1	A	1698	A	C6-C5-N7	-5.50	128.45	132.30
1	A	2688	U	N1-C2-N3	5.50	118.20	114.90
1	A	38	A	N1-C6-N6	-5.50	115.30	118.60
1	A	621	A	N1-C2-N3	5.50	132.05	129.30
1	A	1191	G	N7-C8-N9	-5.49	110.35	113.10
1	A	1790	C	C6-N1-C2	5.49	122.50	120.30
1	A	1565	C	C6-N1-C2	5.49	122.50	120.30
1	A	1905	C	N1-C2-O2	5.49	122.19	118.90
1	A	1947	C	N3-C4-C5	5.48	124.09	121.90
1	A	1969	A	N7-C8-N9	-5.48	111.06	113.80
1	A	214	G	O4'-C1'-N9	5.48	112.58	108.20
1	A	1419	A	O4'-C1'-N9	5.47	112.58	108.20
1	A	2506	U	C2-N1-C1'	5.47	124.26	117.70
2	B	44	G	C8-N9-C1'	5.46	134.10	127.00
1	A	2655	G	P-O3'-C3'	5.46	126.25	119.70
1	A	222	A	P-O3'-C3'	5.46	126.25	119.70
1	A	1395	A	O4'-C1'-N9	5.45	112.56	108.20
1	A	1786	A	N1-C6-N6	5.45	121.87	118.60
1	A	831	G	N1-C6-O6	5.45	123.17	119.90
1	A	1674	G	C5-C6-O6	-5.45	125.33	128.60
1	A	2254	C	N1-C2-O2	-5.45	115.63	118.90
1	A	2463	C	N3-C4-C5	5.45	124.08	121.90
1	A	1774	C	N3-C4-C5	5.45	124.08	121.90
1	A	2720	U	O5'-P-OP1	-5.45	100.80	105.70
1	A	196	A	O4'-C1'-N9	5.45	112.56	108.20
1	A	2468	G	N7-C8-N9	5.45	115.82	113.10
1	A	958	U	C6-N1-C2	-5.44	117.73	121.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	865	C	O5'-P-OP1	-5.44	100.80	105.70
1	A	238	C	C6-N1-C2	5.44	122.48	120.30
1	A	383	U	O4'-C1'-N1	5.44	112.55	108.20
1	A	2031	A	C4-N9-C1'	5.43	136.08	126.30
1	A	97	C	N3-C2-O2	-5.43	118.10	121.90
1	A	250	G	C4-C5-N7	5.43	112.97	110.80
1	A	2031	A	C8-N9-C1'	-5.42	117.94	127.70
1	A	2692	C	N3-C2-O2	-5.42	118.10	121.90
1	A	841	A	N1-C6-N6	5.42	121.85	118.60
1	A	1309	G	N1-C6-O6	5.42	123.15	119.90
1	A	2468	G	C4-N9-C1'	5.42	133.55	126.50
1	A	1570	A	C8-N9-C4	5.41	107.97	105.80
1	A	762	U	C2-N1-C1'	5.41	124.19	117.70
1	A	1930	G	C6-C5-N7	5.41	133.65	130.40
2	B	30	C	N3-C2-O2	-5.41	118.11	121.90
1	A	58	G	C8-N9-C4	-5.40	104.24	106.40
1	A	1359	A	N9-C4-C5	-5.40	103.64	105.80
1	A	2318	G	N7-C8-N9	5.40	115.80	113.10
1	A	27	G	N3-C2-N2	-5.39	116.12	119.90
1	A	2713	A	C6-C5-N7	-5.39	128.53	132.30
1	A	512	G	C4-N9-C1'	-5.39	119.50	126.50
1	A	974(A)	C	P-O3'-C3'	5.39	126.17	119.70
1	A	1929	G	N9-C4-C5	-5.38	103.25	105.40
1	A	2070	G	C5-C6-O6	5.38	131.83	128.60
1	A	1950	G	C5-N7-C8	-5.38	101.61	104.30
1	A	242	G	OP2-P-O3'	5.38	117.03	105.20
1	A	2609	U	C2-N1-C1'	-5.38	111.25	117.70
21	Z	115	GLY	N-CA-C	-5.37	99.67	113.10
1	A	974(A)	C	C5-C4-N4	5.37	123.96	120.20
1	A	1396	U	C2-N1-C1'	5.37	124.15	117.70
1	A	1603	A	C8-N9-C4	-5.37	103.65	105.80
1	A	2346	A	N1-C2-N3	5.36	131.98	129.30
1	A	2446	G	OP2-P-O3'	5.35	116.97	105.20
1	A	626	U	C6-N1-C2	-5.35	117.79	121.00
1	A	773	U	C5-C6-N1	-5.35	120.03	122.70
1	A	2045	C	C6-N1-C2	5.35	122.44	120.30
1	A	2587	A	N9-C4-C5	5.34	107.94	105.80
1	A	364	C	C6-N1-C2	-5.33	118.17	120.30
1	A	2445	G	C5-C6-O6	5.33	131.80	128.60
1	A	1309	G	C8-N9-C4	5.32	108.53	106.40
1	A	846	C	C2-N1-C1'	5.32	124.65	118.80
1	A	1559	G	C5-C6-O6	-5.32	125.41	128.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1191	G	C8-N9-C4	5.32	108.53	106.40
1	A	270(Z)	U	O4'-C1'-N1	5.31	112.45	108.20
1	A	1970	A	O4'-C1'-N9	-5.31	103.95	108.20
1	A	458	G	O4'-C1'-N9	5.30	112.44	108.20
1	A	514	A	C8-N9-C4	5.30	107.92	105.80
1	A	2501	C	C2-N1-C1'	-5.30	112.97	118.80
2	B	41	U	C5-C6-N1	-5.30	120.05	122.70
1	A	213	A	OP2-P-O3'	5.30	116.86	105.20
1	A	795	C	C2-N3-C4	-5.29	117.26	119.90
1	A	1781	C	C6-N1-C1'	-5.28	114.46	120.80
1	A	670	A	OP1-P-O3'	5.28	116.82	105.20
1	A	1396	U	C5-C4-O4	5.28	129.07	125.90
1	A	141	A	O4'-C1'-N9	5.28	112.42	108.20
1	A	776	G	C6-C5-N7	5.28	133.56	130.40
1	A	793	A	C8-N9-C4	-5.28	103.69	105.80
1	A	621	A	C8-N9-C4	-5.27	103.69	105.80
1	A	2406	U	O4'-C1'-N1	-5.27	103.98	108.20
1	A	2610	C	OP2-P-O3'	5.27	116.79	105.20
1	A	99	U	OP2-P-O3'	5.26	116.78	105.20
1	A	812	C	N1-C2-O2	-5.26	115.74	118.90
27	5	4	HIS	C-N-CD	5.26	139.44	128.40
1	A	2822	G	C5-C6-O6	-5.26	125.44	128.60
1	A	1359	A	C4-C5-N7	5.25	113.33	110.70
1	A	2265	U	C5-C4-O4	-5.25	122.75	125.90
1	A	739	G	C8-N9-C4	5.25	108.50	106.40
1	A	1786	A	C4-N9-C1'	5.25	135.74	126.30
1	A	67	U	C2-N3-C4	5.25	130.15	127.00
1	A	917	A	C2-N3-C4	-5.25	107.98	110.60
1	A	2600	A	O5'-P-OP2	-5.25	100.98	105.70
1	A	2544	G	C5-C6-N1	-5.24	108.88	111.50
1	A	140	A	C4-C5-N7	5.24	113.32	110.70
1	A	2655	G	C4-N9-C1'	-5.23	119.70	126.50
1	A	2330	G	C5-C6-O6	-5.22	125.47	128.60
2	B	108	C	C6-N1-C1'	5.22	127.07	120.80
1	A	1647	G	O5'-P-OP2	5.21	116.95	110.70
1	A	46	C	C6-N1-C2	-5.20	118.22	120.30
2	B	31	C	N3-C4-C5	-5.20	119.82	121.90
1	A	1190	G	C4-C5-N7	5.20	112.88	110.80
1	A	2392	A	C5-N7-C8	-5.20	101.30	103.90
1	A	1799	G	N1-C6-O6	-5.19	116.78	119.90
1	A	481	G	O5'-P-OP2	-5.19	101.03	105.70
1	A	1142(A)	A	N3-C4-N9	-5.18	123.25	127.40

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2427	C	O5'-P-OP1	-5.18	101.03	105.70
1	A	1914	C	C2-N1-C1'	5.18	124.50	118.80
1	A	2498	C	N3-C4-C5	5.18	123.97	121.90
1	A	2307	G	C4-C5-N7	5.17	112.87	110.80
1	A	805	G	C5-C6-O6	-5.17	125.50	128.60
1	A	1882	C	C2-N1-C1'	5.17	124.49	118.80
1	A	1012	U	P-O3'-C3'	5.16	125.89	119.70
1	A	2469	A	C2-N3-C4	-5.16	108.02	110.60
1	A	1023	U	O5'-P-OP1	-5.16	101.06	105.70
1	A	1256	G	N9-C4-C5	-5.16	103.34	105.40
1	A	2584	U	N1-C2-N3	5.16	118.00	114.90
1	A	138	G	O4'-C1'-N9	5.15	112.32	108.20
1	A	395	U	O4'-C1'-N1	5.15	112.32	108.20
1	A	2126	A	P-O3'-C3'	5.15	125.88	119.70
1	A	364	C	C5-C6-N1	5.15	123.58	121.00
1	A	1899	G	C4-C5-C6	5.14	121.89	118.80
1	A	2330	G	C4-C5-N7	5.14	112.86	110.80
1	A	74	A	C5-C6-N1	-5.14	115.13	117.70
1	A	1800	C	O5'-P-OP2	5.14	116.86	110.70
1	A	2023	G	O5'-P-OP1	-5.13	101.08	105.70
1	A	2584	U	C6-N1-C2	-5.13	117.92	121.00
1	A	1328	G	N9-C4-C5	-5.13	103.35	105.40
1	A	676	A	C5-C6-N1	-5.13	115.14	117.70
1	A	2430	A	C6-C5-N7	-5.12	128.71	132.30
1	A	1300	U	N1-C2-N3	5.11	117.97	114.90
2	B	81	G	N7-C8-N9	5.11	115.66	113.10
1	A	1683	C	C6-N1-C2	-5.11	118.25	120.30
1	A	1835	G	C4-N9-C1'	5.11	133.14	126.50
2	B	31	C	N1-C2-O2	5.11	121.96	118.90
1	A	577	G	C6-C5-N7	-5.10	127.34	130.40
1	A	1930	G	OP2-P-O3'	5.10	116.43	105.20
1	A	783	A	N9-C1'-C2'	-5.10	106.39	112.00
1	A	1929	G	O4'-C1'-N9	-5.10	104.12	108.20
1	A	2402	C	O4'-C1'-N1	5.10	112.28	108.20
1	A	810	U	O5'-P-OP2	-5.10	101.11	105.70
1	A	1905	C	N3-C2-O2	-5.10	118.33	121.90
1	A	404	C	P-O3'-C3'	5.09	125.81	119.70
1	A	2681	C	C6-N1-C2	-5.09	118.27	120.30
1	A	528	A	C5-N7-C8	-5.08	101.36	103.90
1	A	503	A	C8-N9-C4	-5.08	103.77	105.80
1	A	2619	C	O5'-P-OP2	-5.07	101.13	105.70
2	B	56	G	C8-N9-C4	-5.07	104.37	106.40

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2318	G	C4-C5-N7	5.07	112.83	110.80
1	A	2688	U	N3-C4-C5	-5.07	111.56	114.60
1	A	27	G	C8-N9-C1'	5.07	133.59	127.00
1	A	2250	G	N3-C4-C5	-5.07	126.07	128.60
1	A	795	C	C5-C6-N1	-5.06	118.47	121.00
2	B	43	C	C2-N1-C1'	5.06	124.36	118.80
1	A	62	C	C6-N1-C2	5.05	122.32	120.30
1	A	71	A	N3-C4-N9	-5.05	123.36	127.40
1	A	2246	G	C8-N9-C4	5.05	108.42	106.40
1	A	2611	U	O5'-P-OP2	-5.05	101.15	105.70
1	A	2751	G	C5-N7-C8	-5.05	101.77	104.30
1	A	812	C	N3-C4-C5	-5.05	119.88	121.90
1	A	1698	A	C4-C5-N7	5.05	113.23	110.70
4	E	117	MET	CA-CB-CG	5.05	121.89	113.30
1	A	2655	G	OP2-P-O3'	5.05	116.31	105.20
1	A	1839	G	C8-N9-C1'	-5.05	120.44	127.00
1	A	2523	G	C8-N9-C4	-5.04	104.38	106.40
1	A	740	U	N3-C4-C5	5.04	117.62	114.60
1	A	1781	C	O4'-C1'-N1	5.04	112.23	108.20
1	A	1253	A	C5-N7-C8	-5.04	101.38	103.90
1	A	2776	A	P-O3'-C3'	5.03	125.74	119.70
1	A	1535	U	C2-N1-C1'	5.03	123.73	117.70
1	A	530	G	C5-C6-N1	5.03	114.01	111.50
1	A	472	A	C5-C6-N1	-5.02	115.19	117.70
1	A	1799	G	C8-N9-C4	-5.02	104.39	106.40
1	A	781	A	C8-N9-C4	5.01	107.81	105.80
21	Z	150	LEU	CA-CB-CG	5.01	126.83	115.30
1	A	1382	G	C5-C6-O6	-5.01	125.59	128.60
1	A	2444	G	O5'-P-OP2	-5.00	101.20	105.70
2	B	81	G	C5-N7-C8	-5.00	101.80	104.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
24	2	17	SER	Peptide
30	8	30	ARG	Peptide
30	8	51	ALA	Peptide
4	E	21	VAL	Peptide
5	F	47	GLY	Peptide
7	H	127	GLU	Peptide
7	H	153	LYS	Peptide

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
14	S	109	GLY	Peptide
21	Z	181	GLU	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	A	62091	0	31295	865	0
2	B	2573	0	1306	32	0
3	D	2115	0	2195	97	0
4	E	1568	0	1634	64	0
5	F	1585	0	1632	64	0
6	G	1474	0	1535	57	0
7	H	1307	0	1382	66	0
8	I	1136	0	1223	46	0
9	N	1104	0	1180	50	0
10	O	933	0	996	23	0
11	P	1145	0	1227	94	0
12	Q	1122	0	1178	48	0
13	R	968	0	1033	36	0
14	S	882	0	943	40	0
15	T	1141	0	1202	47	0
16	U	964	0	1022	58	0
17	V	779	0	852	42	0
18	W	900	0	964	28	0
19	X	725	0	778	25	0
20	Y	785	0	878	39	0
21	Z	1461	0	1493	56	0
22	0	648	0	672	27	0
23	1	763	0	848	28	0
24	2	581	0	629	26	0
25	3	469	0	518	17	0
26	4	581	0	574	41	0
27	5	459	0	480	33	0
28	6	424	0	450	30	0
29	7	430	0	480	17	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	8	517	0	582	40	0
31	9	307	0	338	7	0
32	a	74	0	51	0	0
33	5	1	0	0	0	0
33	A	268	0	0	0	0
33	B	3	0	0	0	0
33	E	1	0	0	0	0
33	P	2	0	0	0	0
33	Q	1	0	0	0	0
33	X	1	0	0	0	0
All	All	92288	0	61570	1851	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 12.

All (1851) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2701:C:H3'	1:A:2702:U:H5''	1.32	1.07
3:D:43:ARG:NH1	3:D:44:ASN:OD1	1.86	1.06
1:A:1359:A:N6	1:A:1372:U:O4	1.92	1.02
1:A:1771:C:HO2'	1:A:1786:A:H8	1.01	0.98
1:A:1496:A:H8	1:A:1577:C:HO2'	1.10	0.97
1:A:1138:G:H21	9:N:106:MET:HE3	1.30	0.95
1:A:483:A:H4'	20:Y:49:VAL:HA	1.51	0.92
1:A:774:A:H2	1:A:787:U:HO2'	1.00	0.92
1:A:620:G:H4'	1:A:621:A:H5''	1.50	0.92
1:A:1728:G:H8	1:A:1732:A:H62	1.15	0.91
1:A:67:U:H3	1:A:74:A:H2	1.11	0.91
4:E:24:THR:HG21	4:E:188:VAL:HG11	1.52	0.91
21:Z:151:HIS:HB3	21:Z:170:THR:HA	1.54	0.89
4:E:50:GLY:HA2	4:E:77:ILE:HA	1.53	0.89
20:Y:79:CYS:SG	20:Y:80:GLY:N	2.45	0.88
1:A:1021:A:OP2	9:N:65:LYS:NZ	2.06	0.88
11:P:58:THR:O	11:P:61:ARG:NE	2.08	0.87
20:Y:76:CYS:HB3	20:Y:96:ILE:HD13	1.57	0.87
27:5:40:LYS:HG2	27:5:47:PRO:HD2	1.56	0.86
1:A:993:G:OP1	16:U:50:ARG:NH2	2.09	0.86
1:A:528:A:O2'	1:A:529:A:H5'	1.75	0.86
1:A:498:G:N3	20:Y:47:LYS:NZ	2.24	0.86
21:Z:94:GLU:HB2	21:Z:130:PRO:HD2	1.58	0.85
1:A:1689:A:H62	1:A:1698:A:H2	1.21	0.85
18:W:18:ARG:HG3	18:W:76:VAL:HG13	1.58	0.84

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1479:G:N7	1:A:1510:A:N6	2.25	0.84
1:A:780:G:H21	1:A:783:A:H62	1.19	0.84
21:Z:145:GLU:HG3	21:Z:146:ILE:HG12	1.59	0.84
15:T:26:ASP:HB3	15:T:92:GLY:H	1.42	0.84
9:N:4:TYR:O	16:U:64:ARG:NH1	2.10	0.83
1:A:1728:G:N1	1:A:1730:U:OP2	2.11	0.83
6:G:27:ASN:HB3	6:G:30:GLU:HG3	1.60	0.83
1:A:2580:U:H4'	4:E:130:GLY:HA3	1.58	0.83
1:A:265:A:N6	1:A:427:U:O2'	2.12	0.83
11:P:19:VAL:HG13	11:P:21:ARG:H	1.41	0.83
1:A:674:G:H1'	5:F:74:ARG:HD3	1.61	0.83
16:U:90:VAL:O	16:U:92:ARG:N	2.11	0.82
1:A:1310:G:OP2	29:7:9:ARG:NH1	2.11	0.82
23:1:7:ILE:HD12	23:1:62:VAL:HG11	1.62	0.82
27:5:16:ARG:NH1	27:5:17:ASP:OD1	2.13	0.81
24:2:47:ASN:O	24:2:49:LYS:N	2.12	0.81
1:A:630:G:OP1	30:8:46:ARG:NH1	2.13	0.81
1:A:631:A:OP2	30:8:46:ARG:NH2	2.13	0.81
9:N:4:TYR:OH	9:N:7:LYS:NZ	2.14	0.81
1:A:1403:C:H5''	1:A:1471:A:H1'	1.61	0.80
8:I:92:VAL:HG13	8:I:120:ILE:HG23	1.64	0.80
20:Y:76:CYS:SG	20:Y:77:PRO:HD2	2.22	0.80
1:A:138:G:N2	19:X:44:GLU:OE2	2.11	0.80
1:A:2015:A:H1'	27:5:2:ALA:HA	1.64	0.80
21:Z:182:LYS:HG3	21:Z:183:LEU:HD23	1.62	0.79
19:X:67:GLY:O	19:X:69:TYR:N	2.15	0.79
1:A:2701:C:H3'	1:A:2702:U:C5'	2.13	0.79
8:I:130:TYR:HB3	8:I:136:VAL:HG13	1.62	0.78
21:Z:144:LEU:HD11	21:Z:149:SER:HA	1.63	0.78
1:A:2849:U:OP2	15:T:95:ARG:NH1	2.17	0.78
26:4:1:MET:SD	26:4:6:HIS:NE2	2.56	0.78
10:O:88:ASN:HD21	10:O:92:GLU:HB2	1.47	0.78
1:A:607:U:H3	1:A:621:A:H2	1.33	0.77
1:A:900:A:H3'	1:A:901:A:H8	1.49	0.77
3:D:69:ARG:NH2	3:D:128:GLY:O	2.18	0.77
9:N:95:PRO:O	9:N:97:ARG:N	2.18	0.77
11:P:47:ASP:OD1	11:P:50:ARG:NH2	2.17	0.77
1:A:2306:C:H3'	1:A:2307:G:H5''	1.67	0.76
5:F:197:ASP:O	5:F:199:TRP:N	2.19	0.76
1:A:1996:C:OP1	10:O:31:LYS:NZ	2.19	0.76
13:R:74:LYS:O	13:R:76:VAL:N	2.18	0.76
1:A:128:C:H4'	29:7:49:ARG:HH12	1.51	0.76

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:H:153:LYS:HG2	7:H:162:ILE:HG13	1.67	0.75
1:A:1434:A:H61	1:A:1558:A:N6	1.85	0.75
1:A:2392:A:H2	1:A:2424:C:H42	1.35	0.75
15:T:57:PHE:O	15:T:58:ASN:ND2	2.20	0.75
15:T:27:THR:HG23	15:T:90:GLN:HB3	1.67	0.75
16:U:92:ARG:O	16:U:94:ASN:N	2.20	0.75
9:N:13:TRP:HB2	9:N:133:GLN:HG3	1.69	0.75
17:V:24:LYS:HA	17:V:92:THR:HG23	1.68	0.74
1:A:2849:U:O4	15:T:23:ARG:NH2	2.21	0.74
14:S:78:LEU:HD21	14:S:108:GLY:HA3	1.68	0.74
21:Z:30:ASN:HD22	21:Z:90:VAL:HB	1.51	0.74
1:A:482:A:H4'	20:Y:47:LYS:HD2	1.70	0.74
2:B:15:A:H5'	2:B:16:G:C8	2.22	0.74
15:T:51:ARG:HG2	15:T:98:LYS:HG3	1.70	0.74
6:G:161:THR:HG22	6:G:163:ALA:H	1.53	0.74
26:4:9:LEU:H	26:4:27:THR:HG23	1.53	0.73
1:A:483:A:H5'	20:Y:49:VAL:HG22	1.69	0.73
11:P:14:LYS:O	11:P:16:ARG:N	2.22	0.73
19:X:27:THR:HB	19:X:80:ILE:HB	1.69	0.73
1:A:1667:G:O2'	1:A:1991:U:O4	2.04	0.73
1:A:2287:A:H62	1:A:2344:U:H3	1.34	0.73
1:A:49:A:N7	1:A:120:U:H5	1.86	0.73
7:H:86:GLU:HG3	7:H:165:ALA:H	1.53	0.73
12:Q:111:GLU:OE1	12:Q:133:ARG:NH2	2.22	0.73
1:A:2849:U:O2'	1:A:2866:U:O2	2.07	0.73
12:Q:104:PHE:HE1	12:Q:125:LEU:HD11	1.54	0.73
12:Q:24:GLY:O	12:Q:26:TYR:N	2.19	0.73
1:A:1210:A:H5'	1:A:1210:A:H8	1.52	0.72
26:4:48:ARG:HH12	26:4:52:THR:HG22	1.54	0.72
6:G:64:THR:HG23	6:G:66:GLN:H	1.55	0.72
6:G:6:ALA:H	26:4:23:GLU:HG2	1.54	0.72
3:D:35:LYS:HD2	3:D:104:TYR:CE1	2.25	0.72
24:2:42:GLY:O	24:2:44:LEU:N	2.20	0.72
1:A:2753:A:O2'	31:9:15:LYS:NZ	2.22	0.72
1:A:2789:C:H1'	1:A:2892:A:H2	1.55	0.72
7:H:129:THR:OG1	7:H:129:THR:O	2.08	0.72
20:Y:51:VAL:HG13	20:Y:52:SER:H	1.54	0.72
10:O:47:ILE:HG13	10:O:48:PRO:HD2	1.72	0.71
21:Z:102:LEU:HG	21:Z:123:ASP:HA	1.72	0.71
1:A:2469:A:H2	1:A:2481:G:H21	1.36	0.71
1:A:910:A:H62	12:Q:12:GLN:HA	1.56	0.71
4:E:170:LEU:HD21	4:E:187:ALA:HB3	1.72	0.71

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2415:G:H4'	11:P:67:MET:N	2.06	0.71
2:B:52:A:O2'	2:B:53:A:N7	2.24	0.71
9:N:89:LYS:O	9:N:93:THR:HG22	1.90	0.71
1:A:2760:C:H2'	1:A:2761:G:H5''	1.71	0.71
1:A:1019:U:H3	1:A:1142(A):A:H62	1.37	0.71
1:A:259:G:H21	1:A:621:A:H8	1.39	0.71
20:Y:29:GLU:HB3	20:Y:38:ILE:HG23	1.70	0.71
1:A:918:A:N3	2:B:80:U:O2'	2.23	0.71
1:A:372:G:O2'	1:A:373:U:OP2	2.08	0.71
8:I:144:VAL:HG13	8:I:145:VAL:HG13	1.70	0.71
14:S:106:ARG:HA	14:S:110:LEU:HD21	1.73	0.71
14:S:24:LEU:HB2	14:S:85:VAL:HG12	1.70	0.71
15:T:77:PRO:HB2	15:T:80:SER:HB2	1.72	0.71
10:O:2:ILE:HD12	10:O:6:THR:HG21	1.72	0.71
20:Y:42:VAL:HG12	20:Y:65:ALA:HB3	1.71	0.71
30:8:58:ILE:HD13	30:8:61:LEU:HD21	1.73	0.70
1:A:2334:G:H5'	14:S:9:ARG:HG2	1.72	0.70
6:G:47:LYS:HD3	6:G:81:LYS:HB2	1.73	0.70
1:A:860:U:H5	1:A:917:A:C2	2.10	0.70
21:Z:141:VAL:HG23	21:Z:144:LEU:HB2	1.74	0.70
18:W:17:VAL:HG12	18:W:76:VAL:HG11	1.72	0.70
1:A:2633:G:H1'	4:E:62:PRO:HG2	1.73	0.70
5:F:185:ASP:HA	5:F:188:ARG:HD3	1.72	0.70
21:Z:103:ARG:HB2	21:Z:138:GLU:HG2	1.72	0.70
1:A:226:G:O2'	1:A:227:A:O5'	2.09	0.70
3:D:43:ARG:HB3	3:D:54:ARG:HB2	1.74	0.70
1:A:2292:C:P	14:S:17:ARG:HH22	2.14	0.70
21:Z:80:ARG:HH21	21:Z:82:ARG:HH22	1.39	0.69
1:A:221:A:H4'	1:A:222:A:O5'	1.91	0.69
5:F:182:ASN:ND2	5:F:185:ASP:OD2	2.19	0.69
1:A:1754:C:OP1	15:T:96:ARG:NH1	2.26	0.69
3:D:182:LEU:H	3:D:272:ALA:HB3	1.56	0.69
1:A:252:G:OP2	11:P:50:ARG:NH1	2.26	0.69
1:A:1338:G:N7	19:X:62:LYS:NZ	2.40	0.69
28:6:11:LEU:HD11	28:6:51:GLU:HG3	1.75	0.69
1:A:1019:U:HO2'	1:A:1021:A:H2	1.39	0.69
1:A:676:A:H8	1:A:2069:G:H21	1.38	0.69
3:D:71:ASP:HB2	3:D:103:ARG:HH22	1.58	0.69
5:F:110:LEU:HD11	5:F:181:LEU:HD13	1.74	0.69
5:F:184:TYR:O	5:F:188:ARG:HG3	1.93	0.69
1:A:2401:U:H2'	1:A:2402:C:H5''	1.75	0.69
4:E:128:SER:OG	4:E:129:HIS:N	2.24	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:704:G:O2'	1:A:726:G:N2	2.25	0.69
23:1:73:LEU:HD13	23:1:90:ILE:HG22	1.76	0.68
1:A:141:A:H8	1:A:1595:G:H21	1.39	0.68
5:F:157:VAL:HB	5:F:194:MET:HB3	1.75	0.68
11:P:64:LYS:C	11:P:66:GLY:H	1.96	0.68
1:A:1509:C:H3'	1:A:1510:A:H5''	1.75	0.68
1:A:2712:U:HO2'	1:A:2712(A):A:H8	1.40	0.68
15:T:123:GLN:O	15:T:125:ARG:N	2.26	0.68
3:D:25:THR:O	3:D:27:THR:N	2.26	0.68
1:A:2527:C:H5''	31:9:30:PRO:HB2	1.73	0.68
1:A:1049:C:H2'	1:A:1050:A:H5''	1.76	0.68
1:A:1094:U:O2'	1:A:1096:A:OP1	2.09	0.68
4:E:95:ILE:HD12	4:E:95:ILE:H	1.59	0.68
3:D:142:VAL:HG23	3:D:193:VAL:HA	1.75	0.68
11:P:64:LYS:C	11:P:66:GLY:N	2.48	0.68
9:N:133:GLN:HB2	9:N:135:PRO:HD3	1.76	0.68
12:Q:37:LEU:HD21	12:Q:130:LYS:HE3	1.74	0.68
11:P:39:LYS:HG3	11:P:45:LEU:HD22	1.75	0.68
30:8:29:LYS:O	30:8:31:HIS:N	2.27	0.67
1:A:2636:U:OP1	4:E:79:ARG:HA	1.93	0.67
8:I:5:LEU:HD21	8:I:12:LEU:HB3	1.77	0.67
2:B:52:A:H62	14:S:33:LYS:HG3	1.60	0.67
4:E:1:MET:N	4:E:83:ASP:O	2.28	0.67
7:H:137:ASP:OD1	7:H:138:LYS:N	2.27	0.67
12:Q:89:ASN:O	12:Q:92:GLY:N	2.18	0.67
1:A:270(T):G:H5''	23:1:97:LEU:HD22	1.76	0.67
1:A:888:C:H3'	1:A:889:C:H4'	1.76	0.67
1:A:2393:A:H5'	11:P:62:LEU:HB3	1.77	0.67
1:A:2114:A:N6	1:A:2119:A:N7	2.43	0.67
15:T:16:ARG:NH2	15:T:83:ILE:O	2.27	0.67
17:V:52:VAL:HG21	17:V:55:ALA:HB3	1.76	0.67
1:A:1021:A:H8	1:A:1022:G:H5''	1.60	0.67
1:A:2123:G:H2'	1:A:2124:G:H8	1.58	0.67
3:D:35:LYS:HG2	3:D:64:ILE:H	1.59	0.67
13:R:78:LYS:HE2	13:R:83:ILE:HD11	1.77	0.66
27:5:4:HIS:HB3	27:5:5:PRO:HD3	1.77	0.66
1:A:1796:U:H2'	1:A:1797:C:C6	2.31	0.66
1:A:587:C:OP2	11:P:21:ARG:NH2	2.28	0.66
1:A:142:G:H1'	19:X:37:THR:HG21	1.75	0.66
8:I:4:ILE:HG12	8:I:18:VAL:HG22	1.76	0.66
1:A:2685:G:N2	1:A:2724:C:O2	2.19	0.66
18:W:45:TYR:CZ	18:W:49:LYS:HD2	2.30	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2636:U:OP2	4:E:79:ARG:NH1	2.29	0.66
7:H:86:GLU:HG3	7:H:165:ALA:N	2.10	0.66
20:Y:49:VAL:O	20:Y:51:VAL:N	2.29	0.66
21:Z:128:VAL:HB	21:Z:161:VAL:HG13	1.78	0.66
1:A:1899:G:H21	1:A:1902:C:N4	1.94	0.66
1:A:74:A:H4'	1:A:75:G:O5'	1.95	0.66
20:Y:97:ARG:HE	20:Y:98:VAL:HB	1.61	0.66
1:A:2308:G:H22	1:A:2311:A:H2	1.43	0.66
9:N:35:ARG:O	9:N:37:LYS:N	2.29	0.66
11:P:105:LEU:O	11:P:106:LEU:HB2	1.95	0.66
21:Z:60:GLU:HA	21:Z:66:SER:HA	1.76	0.66
1:A:1863:G:HO2'	1:A:2411:A:HO2'	1.44	0.66
1:A:2444:G:OP2	5:F:68:LYS:HE3	1.96	0.65
1:A:363(B):G:H2'	1:A:363(C):G:H8	1.61	0.65
17:V:21:ARG:HD2	17:V:91:TYR:CD1	2.31	0.65
23:1:29:GLY:O	23:1:31:GLY:N	2.30	0.65
15:T:16:ARG:HD3	15:T:19:LEU:HD11	1.77	0.65
1:A:2306:C:H2'	1:A:2307:G:H21	1.62	0.65
1:A:1771:C:H1'	1:A:1786:A:C8	2.32	0.65
1:A:780:G:N2	1:A:783:A:H62	1.94	0.65
16:U:8:VAL:HG23	16:U:11:ARG:HH21	1.62	0.65
1:A:1287:A:N7	13:R:107:ASP:HB2	2.11	0.65
24:2:50:ILE:HD12	24:2:51:ARG:H	1.62	0.65
27:5:40:LYS:HZ1	27:5:48:GLU:HB2	1.61	0.65
1:A:443:A:H3'	5:F:45:ARG:NH1	2.11	0.65
1:A:768:G:N2	1:A:1379:A:O2'	2.30	0.65
7:H:20:ALA:HB3	7:H:23:ARG:HG2	1.77	0.65
22:0:10:THR:HG22	22:0:12:ASN:H	1.62	0.65
1:A:31:C:O3'	1:A:1238:G:H5''	1.97	0.65
27:5:56:LYS:HD2	27:5:56:LYS:H	1.60	0.65
3:D:44:ASN:HB3	3:D:49:ILE:HA	1.78	0.65
7:H:153:LYS:HG3	7:H:161:GLY:HA2	1.78	0.65
1:A:2853:C:H2'	1:A:2854:G:H8	1.61	0.64
3:D:80:ALA:HB3	3:D:94:LEU:HD13	1.79	0.64
5:F:107:LYS:HD2	5:F:207:GLY:H	1.62	0.64
1:A:1190:G:OP1	11:P:30:THR:OG1	2.15	0.64
1:A:1639:U:H2'	1:A:1640:C:H5''	1.79	0.64
21:Z:182:LYS:HG3	21:Z:183:LEU:HA	1.78	0.64
3:D:30:GLU:HG3	3:D:63:ARG:NH2	2.12	0.64
7:H:153:LYS:HB3	7:H:162:ILE:H	1.63	0.64
12:Q:78:PRO:O	12:Q:79:LEU:HB2	1.97	0.64
1:A:2543:G:H2'	1:A:2544:G:C8	2.33	0.64

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
16:U:88:ILE:HG22	16:U:90:VAL:HG23	1.79	0.64
4:E:9:VAL:HB	4:E:25:VAL:HG23	1.80	0.64
1:A:2646:C:OP2	1:A:2732:G:O2'	2.15	0.64
13:R:51:LEU:HD13	13:R:66:VAL:HG13	1.79	0.64
1:A:1063:G:H22	1:A:1076:C:H1'	1.62	0.64
6:G:112:PRO:HB3	26:4:37:SER:HB2	1.80	0.64
1:A:127:A:H5''	1:A:128:C:C6	2.33	0.64
3:D:35:LYS:NZ	3:D:64:ILE:O	2.31	0.64
15:T:36:GLU:HG3	15:T:41:ARG:HE	1.62	0.64
1:A:1568:G:H4'	3:D:59:LYS:HB3	1.80	0.63
24:2:41:ILE:HD11	24:2:44:LEU:HG	1.80	0.63
30:8:16:ILE:HD13	30:8:57:ARG:HG2	1.80	0.63
1:A:468:G:N7	29:7:39:ARG:NH2	2.44	0.63
1:A:72:U:N3	24:2:62:THR:HG22	2.14	0.63
11:P:58:THR:HG22	11:P:61:ARG:HG3	1.80	0.63
3:D:25:THR:HG23	3:D:27:THR:HB	1.80	0.63
26:4:48:ARG:O	26:4:50:VAL:N	2.31	0.63
1:A:1405:U:H2'	1:A:1406:U:H6	1.63	0.63
3:D:35:LYS:HG2	3:D:64:ILE:N	2.13	0.63
14:S:59:LYS:HD3	14:S:60:GLY:H	1.62	0.63
20:Y:91:GLU:HG3	20:Y:92:ASN:H	1.63	0.63
26:4:23:GLU:O	26:4:25:TYR:N	2.31	0.63
29:7:9:ARG:HH21	29:7:48:LYS:HD2	1.63	0.63
1:A:1652:A:OP1	13:R:8:ARG:NH1	2.30	0.63
7:H:83:TYR:CZ	7:H:138:LYS:HD2	2.34	0.63
11:P:13:ASN:O	11:P:15:ARG:N	2.32	0.63
1:A:2470:G:H5'	12:Q:56:ARG:HH22	1.62	0.63
1:A:1786:A:H2	1:A:2606:C:H1'	1.63	0.63
1:A:2315:G:OP1	6:G:36:LYS:NZ	2.31	0.63
16:U:83:LEU:HD12	16:U:113:ALA:HB2	1.79	0.63
18:W:41:LYS:HE3	27:5:25:LEU:HD21	1.80	0.63
7:H:152:ARG:HG3	7:H:153:LYS:HD2	1.81	0.63
10:O:13:ASN:ND2	10:O:96:THR:O	2.30	0.63
28:6:41:PRO:HG2	28:6:45:LYS:H	1.63	0.63
1:A:2068:U:H3	1:A:2430:A:H2	1.46	0.63
1:A:84:A:O5'	20:Y:8:LYS:HD3	1.99	0.63
1:A:1068:G:O2'	1:A:1096:A:N3	2.32	0.62
1:A:1348:G:H2'	1:A:1349:A:H5''	1.81	0.62
1:A:2394:C:OP1	11:P:63:PRO:HD2	1.99	0.62
1:A:2817:G:OP1	13:R:99:LYS:NZ	2.27	0.62
7:H:26:VAL:HG11	7:H:75:ALA:HB1	1.81	0.62
1:A:996:A:H4'	16:U:92:ARG:HE	1.65	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2864:G:OP1	15:T:119:LYS:HD2	1.99	0.62
6:G:115:ARG:NH2	6:G:137:GLU:OE1	2.33	0.62
8:I:124:GLY:H	8:I:142:VAL:HG23	1.63	0.62
1:A:2032:G:H21	4:E:146:THR:HG23	1.64	0.62
5:F:46:ARG:HG2	5:F:46:ARG:HH11	1.65	0.62
6:G:3:LEU:HD12	6:G:4:ASP:H	1.64	0.62
8:I:81:VAL:HG21	8:I:88:ILE:HD12	1.80	0.62
15:T:1:MET:O	15:T:3:ARG:N	2.29	0.62
1:A:265:A:O2'	1:A:266:G:H4'	2.00	0.62
26:4:37:SER:HB3	26:4:42:PHE:CD1	2.35	0.62
30:8:23:VAL:HG11	30:8:46:ARG:HD3	1.81	0.62
22:0:27:GLU:HG3	22:0:68:GLU:HA	1.82	0.61
1:A:1364:G:N7	23:1:2:SER:N	2.48	0.61
1:A:2776:A:H3'	1:A:2776:A:OP1	2.00	0.61
1:A:1062:G:H2'	1:A:1063:G:C8	2.35	0.61
14:S:83:LYS:C	14:S:109:GLY:HA3	2.21	0.61
16:U:92:ARG:HD2	17:V:11:GLN:HB2	1.82	0.61
1:A:1216:G:OP2	16:U:12:ARG:NH2	2.31	0.61
5:F:197:ASP:OD2	5:F:197:ASP:N	2.33	0.61
1:A:2610:C:H4'	1:A:2611:U:OP2	1.98	0.61
1:A:1020:A:N1	1:A:1141:U:H2'	2.15	0.61
1:A:1728:G:H3'	1:A:1729:A:H5''	1.83	0.61
1:A:751:A:H5'	18:W:90:ARG:HA	1.82	0.61
23:1:83:GLU:O	23:1:85:LEU:N	2.34	0.61
1:A:99:U:H4'	1:A:101:G:H5''	1.81	0.61
1:A:1055:G:H1	1:A:1104:C:H42	1.49	0.61
1:A:71:A:H2	19:X:31:HIS:HE2	1.49	0.61
16:U:52:ARG:HA	16:U:55:ARG:HG3	1.83	0.61
1:A:1093:G:H4'	7:H:170:ARG:NH2	2.16	0.60
27:5:16:ARG:HG2	27:5:16:ARG:HH11	1.66	0.60
3:D:72:LYS:NZ	3:D:99:ASP:OD1	2.33	0.60
7:H:113:VAL:HG11	7:H:151:ILE:HD12	1.83	0.60
12:Q:35:VAL:HG13	12:Q:130:LYS:HB3	1.83	0.60
26:4:56:VAL:HA	26:4:60:GLN:HB2	1.84	0.60
1:A:1165:U:H2'	1:A:1166:C:C6	2.36	0.60
3:D:108:PRO:HB3	3:D:143:HIS:CE1	2.35	0.60
1:A:443:A:H3'	5:F:45:ARG:HH12	1.65	0.60
11:P:95:VAL:HG13	11:P:100:LEU:HD21	1.83	0.60
28:6:25:LYS:HZ2	30:8:34:TRP:HZ2	1.48	0.60
1:A:528:A:C2	1:A:2042:A:H2'	2.36	0.60
3:D:35:LYS:HD2	3:D:104:TYR:CD1	2.35	0.60
1:A:229:A:OP1	1:A:229:A:H4'	2.00	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
15:T:84:GLN:OE1	15:T:85:LYS:NZ	2.34	0.60
1:A:443:A:N7	5:F:45:ARG:HD2	2.17	0.60
10:O:96:THR:O	10:O:97:ARG:HB3	2.01	0.60
31:9:35:ARG:HH21	31:9:37:GLY:HA3	1.67	0.60
1:A:1057:A:H62	1:A:1086:A:H2'	1.66	0.60
6:G:28:VAL:HG23	6:G:29:TRP:CD1	2.36	0.60
7:H:4:ILE:HB	7:H:6:ARG:HG2	1.82	0.60
21:Z:58:VAL:O	21:Z:60:GLU:N	2.34	0.60
1:A:528:A:N1	1:A:2042:A:H2'	2.17	0.60
11:P:147:LEU:O	11:P:148:LEU:HB2	2.02	0.60
30:8:50:LEU:HD12	30:8:51:ALA:H	1.67	0.60
1:A:1430:C:H2'	1:A:1431:U:C6	2.37	0.60
1:A:1434:A:H61	1:A:1558:A:H62	1.48	0.60
1:A:2698:U:H2'	1:A:2699:C:C6	2.37	0.60
13:R:42:LYS:HA	13:R:45:ARG:HD2	1.84	0.60
1:A:831:G:O2'	11:P:38:GLN:NE2	2.35	0.59
8:I:21:VAL:HG21	8:I:25:TYR:HD1	1.66	0.59
1:A:1980:G:O2'	1:A:1982:C:OP2	2.19	0.59
1:A:593:G:O4'	30:8:4:MET:HE1	2.02	0.59
18:W:86:LEU:HD12	18:W:87:PRO:HD2	1.83	0.59
1:A:775:G:O5'	1:A:777:A:H1'	2.02	0.59
1:A:1932:A:H2'	1:A:1933:G:O4'	2.03	0.59
1:A:2314:C:H2'	1:A:2315:G:H8	1.67	0.59
1:A:2031:A:C6	1:A:2498:C:H1'	2.37	0.59
7:H:98:LEU:HD22	7:H:125:VAL:HB	1.83	0.59
8:I:129:THR:HG22	8:I:137:PRO:HB3	1.84	0.59
13:R:33:ARG:NH2	27:5:55:ARG:HG2	2.17	0.59
29:7:35:ARG:HG3	29:7:42:LEU:HD11	1.85	0.59
1:A:1081:U:H3'	1:A:1082:U:H4'	1.84	0.59
1:A:1048:A:OP2	1:A:1110:G:N2	2.35	0.59
18:W:111:HIS:CD2	18:W:112:GLY:H	2.20	0.59
25:3:6:VAL:HG13	25:3:56:VAL:HG13	1.84	0.59
4:E:36:ARG:HH21	4:E:88:GLY:HA2	1.68	0.59
7:H:6:ARG:NH2	7:H:54:ARG:HH22	2.01	0.59
11:P:26:GLY:O	11:P:28:GLY:N	2.35	0.59
1:A:2291:U:H2'	1:A:2292:C:C6	2.38	0.59
1:A:2795:G:H3'	1:A:2797:U:C5'	2.33	0.59
1:A:372:G:O2'	1:A:373:U:P	2.61	0.59
1:A:943:U:OP2	11:P:36:LYS:NZ	2.36	0.59
14:S:26:LEU:HB3	14:S:87:PHE:HA	1.85	0.59
1:A:1364:G:C8	23:1:2:SER:N	2.70	0.58
1:A:1012:U:O2'	1:A:1013:C:OP2	2.16	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:G:136:ARG:O	6:G:154:GLY:HA2	2.02	0.58
14:S:106:ARG:HA	14:S:110:LEU:HD11	1.85	0.58
9:N:40:PRO:HB3	16:U:68:ALA:HB2	1.85	0.58
27:5:4:HIS:HB3	27:5:5:PRO:CD	2.32	0.58
1:A:250:G:OP2	30:8:13:ARG:NH2	2.35	0.58
1:A:1103:A:H5'	1:A:1104:C:H5	1.66	0.58
3:D:28:GLU:OE1	3:D:29:PRO:HD2	2.03	0.58
8:I:67:ARG:HH21	8:I:68:LEU:HB2	1.68	0.58
13:R:67:LEU:HD13	13:R:76:VAL:HG21	1.84	0.58
21:Z:146:ILE:HG22	21:Z:176:PRO:HD3	1.85	0.58
23:1:51:VAL:HG11	23:1:74:VAL:HG21	1.84	0.58
1:A:1665:A:H1'	10:O:1:MET:HG3	1.83	0.58
19:X:61:GLY:N	19:X:75:ASP:OD2	2.36	0.58
1:A:2115:G:N2	1:A:2165:G:N7	2.45	0.58
1:A:612:G:N2	1:A:616:A:O2'	2.37	0.58
17:V:44:LYS:O	17:V:46:VAL:N	2.36	0.58
7:H:153:LYS:HB3	7:H:154:PRO:HD3	1.85	0.58
26:4:42:PHE:O	26:4:44:THR:N	2.36	0.58
1:A:2294:C:OP2	14:S:13:ARG:NH1	2.37	0.58
1:A:1278:A:H4'	13:R:34:ILE:HD12	1.85	0.58
1:A:1048:A:P	1:A:1110:G:H22	2.25	0.58
1:A:780:G:H21	1:A:783:A:N6	1.98	0.58
13:R:27:SER:HB3	13:R:34:ILE:HD11	1.84	0.58
1:A:1191:G:OP1	11:P:32:THR:HB	2.04	0.58
1:A:2655:G:O2'	1:A:2656:U:OP2	2.21	0.58
1:A:49:A:N7	1:A:120:U:C5	2.70	0.58
1:A:813:U:H2'	1:A:814:C:C6	2.39	0.58
2:B:41:U:C4	6:G:70:VAL:HG23	2.38	0.58
5:F:127:GLU:O	5:F:129:PHE:N	2.32	0.58
10:O:64:ARG:HG2	10:O:79:PHE:CG	2.38	0.58
21:Z:5:LEU:HD11	21:Z:39:VAL:HB	1.85	0.58
5:F:28:ILE:HG22	5:F:112:MET:HB3	1.85	0.58
13:R:24:GLN:OE1	13:R:36:THR:HG21	2.04	0.58
15:T:24:PRO:HA	15:T:49:VAL:HG13	1.85	0.58
16:U:92:ARG:HD3	16:U:94:ASN:HB3	1.85	0.58
13:R:117:VAL:HG22	13:R:118:GLU:H	1.68	0.57
14:S:59:LYS:HD3	14:S:60:GLY:N	2.19	0.57
1:A:72:U:H3	24:2:62:THR:HG22	1.68	0.57
6:G:67:LYS:HE2	26:4:6:HIS:CE1	2.38	0.57
8:I:33:ARG:HB3	8:I:35:LEU:HG	1.86	0.57
12:Q:66:ILE:HA	12:Q:104:PHE:HA	1.85	0.57
18:W:73:ALA:HB3	18:W:106:ILE:HD13	1.84	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:G:98:ARG:NH1	26:4:1:MET:SD	2.77	0.57
3:D:65:ILE:H	3:D:65:ILE:HD13	1.68	0.57
4:E:35:GLN:HB3	4:E:48:GLN:HB2	1.87	0.57
22:0:50:ASN:HB3	22:0:63:VAL:HG22	1.86	0.57
1:A:83:G:N2	1:A:103:A:OP2	2.22	0.57
1:A:1103:A:H5'	1:A:1104:C:C5	2.39	0.57
1:A:242:G:H5''	30:8:62:LEU:HD13	1.86	0.57
12:Q:116:GLU:O	12:Q:120:ILE:HG12	2.05	0.57
14:S:10:ARG:NH2	14:S:91:PRO:O	2.36	0.57
1:A:2405:G:O2'	1:A:2411:A:N6	2.36	0.57
1:A:259:G:N2	1:A:621:A:H8	2.02	0.57
8:I:40:THR:O	8:I:44:LEU:HB2	2.04	0.57
21:Z:158:PRO:O	21:Z:160:GLY:N	2.37	0.57
1:A:2233:U:H2'	1:A:2234:G:C8	2.39	0.57
6:G:98:ARG:HH12	26:4:1:MET:HB3	1.69	0.57
1:A:1309:G:H4'	29:7:7:PRO:HB2	1.85	0.57
1:A:443:A:H1'	1:A:1201:C:O4'	2.03	0.57
2:B:12:C:O2'	22:0:74:ARG:HG3	2.04	0.57
7:H:149:ARG:HG3	7:H:162:ILE:O	2.05	0.57
21:Z:19:ARG:NH1	21:Z:84:GLU:O	2.35	0.57
1:A:1405:U:H2'	1:A:1406:U:C6	2.40	0.57
3:D:71:ASP:CB	3:D:103:ARG:HH22	2.18	0.57
1:A:1142(A):A:H4'	9:N:25:ARG:HH22	1.70	0.57
11:P:135:LEU:O	11:P:139:LYS:HB2	2.04	0.57
1:A:1204:A:H2	1:A:1241:A:N1	2.01	0.57
1:A:2298:A:H62	1:A:2318:G:H8	1.51	0.57
1:A:1412:A:H2'	1:A:1413:G:C8	2.40	0.57
1:A:1590:U:H2'	1:A:1591:G:C8	2.39	0.57
8:I:56:LYS:HE3	8:I:57:ARG:HA	1.87	0.57
21:Z:77:ASP:OD2	21:Z:80:ARG:HD3	2.05	0.57
26:4:71:ARG:HB2	26:4:71:ARG:HH11	1.68	0.56
1:A:1266:G:O5'	18:W:15:ARG:NH2	2.38	0.56
1:A:1359:A:N6	1:A:1372:U:C4	2.72	0.56
1:A:2011:U:OP1	18:W:42:ARG:NH1	2.37	0.56
1:A:2111:C:N3	1:A:2118:U:O2'	2.38	0.56
1:A:2815:C:H5'	27:5:29:THR:HG21	1.87	0.56
1:A:654(A):G:H8	1:A:654(A):G:OP2	1.88	0.56
12:Q:85:LYS:O	12:Q:87:LYS:N	2.38	0.56
1:A:1359:A:H2'	1:A:1360:A:H5'	1.88	0.56
1:A:372:G:HO2'	1:A:400:G:H1	1.53	0.56
1:A:551:G:H5'	1:A:1220:A:H1'	1.87	0.56
5:F:107:LYS:HD2	5:F:206:ILE:HA	1.86	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:G:81:LYS:O	6:G:82:LEU:HB2	2.04	0.56
10:O:85:VAL:HG11	10:O:114:ILE:HD11	1.87	0.56
1:A:1204:A:H1'	1:A:1206:G:C8	2.40	0.56
1:A:2849:U:P	15:T:95:ARG:HH12	2.28	0.56
1:A:27:G:N2	1:A:512:G:O2'	2.38	0.56
11:P:101:VAL:HG23	11:P:106:LEU:HB3	1.88	0.56
15:T:60:THR:HG22	15:T:77:PRO:HA	1.86	0.56
17:V:59:ALA:HB2	17:V:96:ILE:HD13	1.87	0.56
1:A:518:G:H5'	18:W:18:ARG:HH12	1.70	0.56
1:A:1061:U:H4'	1:A:1070:A:H1'	1.87	0.56
1:A:1188:U:H4'	17:V:79:VAL:HG22	1.86	0.56
28:6:25:LYS:HE2	28:6:27:LYS:HE3	1.87	0.56
17:V:66:ARG:HH11	17:V:88:ARG:HD3	1.71	0.56
21:Z:152:ALA:HB2	21:Z:168:GLU:HA	1.87	0.56
12:Q:137:TYR:CE2	21:Z:83:PRO:HG3	2.41	0.56
1:A:2882:A:OP1	13:R:96:ARG:NH1	2.38	0.56
18:W:71:VAL:HA	18:W:107:LEU:HD12	1.87	0.56
1:A:1819:A:H4'	1:A:1820:U:O5'	2.06	0.56
1:A:860:U:C5	1:A:917:A:C2	2.94	0.56
7:H:92:ILE:H	7:H:92:ILE:HD12	1.71	0.56
8:I:79:ILE:HB	8:I:142:VAL:HA	1.88	0.56
10:O:97:ARG:HA	10:O:117:LEU:HD22	1.88	0.56
1:A:1693:U:O2'	3:D:14:ARG:NH2	2.39	0.56
1:A:2168:G:N2	1:A:2170:A:N7	2.52	0.56
1:A:2123:G:H1	1:A:2175:C:H42	1.53	0.56
1:A:573:G:OP2	17:V:78:LYS:NZ	2.38	0.56
12:Q:81:VAL:C	12:Q:82:ARG:HG2	2.25	0.56
20:Y:95:LYS:HB3	20:Y:100:ALA:HA	1.87	0.56
7:H:41:MET:HE1	7:H:64:LEU:HB3	1.86	0.56
1:A:1952:A:C6	10:O:22:ILE:HD12	2.41	0.56
9:N:40:PRO:O	16:U:64:ARG:HD2	2.06	0.56
1:A:1077:A:H5'	1:A:1078:U:H5''	1.88	0.55
1:A:1427:A:H4'	1:A:1428:C:O5'	2.05	0.55
1:A:1678:G:O5'	1:A:1678:G:H8	1.90	0.55
9:N:56:ASN:N	9:N:125:GLY:O	2.22	0.55
15:T:29:ARG:HB2	15:T:46:GLU:HG3	1.88	0.55
3:D:232:PRO:HB3	3:D:244:ARG:NH1	2.21	0.55
15:T:39:ARG:HG2	15:T:40:THR:H	1.72	0.55
1:A:1285:G:N2	1:A:1329:U:OP1	2.35	0.55
1:A:1798:U:H5'	3:D:259:THR:HG22	1.88	0.55
30:8:50:LEU:HD12	30:8:51:ALA:N	2.21	0.55
1:A:264:C:C2'	1:A:265:A:H5''	2.37	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2788:C:O2'	1:A:2809:A:N3	2.39	0.55
1:A:287:C:H2'	1:A:288:C:H6	1.71	0.55
5:F:101:LEU:O	5:F:106:ARG:NH1	2.40	0.55
6:G:67:LYS:HZ1	26:4:6:HIS:CD2	2.24	0.55
17:V:38:LEU:H	17:V:51:VAL:HG13	1.70	0.55
1:A:1026:U:H1'	1:A:1027:A:O5'	2.05	0.55
1:A:1637:A:H4'	1:A:2711:A:O2'	2.06	0.55
1:A:2680:C:H5'	4:E:189:PRO:HA	1.88	0.55
7:H:121:ILE:HG12	7:H:140:LYS:HD2	1.89	0.55
28:6:28:ARG:HB3	28:6:30:THR:H	1.71	0.55
4:E:63:LEU:HD12	4:E:64:LYS:N	2.22	0.55
11:P:52:GLU:HG3	11:P:57:THR:HG22	1.88	0.55
15:T:3:ARG:HG3	15:T:7:ILE:HG12	1.88	0.55
22:0:27:GLU:HB2	22:0:69:PHE:HD1	1.72	0.55
30:8:60:LEU:HB3	30:8:63:PRO:HG2	1.89	0.55
1:A:2126:A:H4'	1:A:2127:G:O5'	2.07	0.55
1:A:527:C:OP2	1:A:2779:U:H5	1.90	0.55
1:A:459:U:H5''	29:7:40:TRP:CD2	2.42	0.55
7:H:157:TYR:HA	7:H:171:LEU:O	2.06	0.55
11:P:62:LEU:HD12	30:8:30:ARG:NH1	2.22	0.55
17:V:34:GLU:O	17:V:36:PRO:HD3	2.06	0.55
1:A:1939:U:OP1	1:A:2604:U:O2'	2.20	0.55
1:A:2286:A:H4'	1:A:2287:A:O4'	2.07	0.55
1:A:2790:A:H2'	1:A:2791:C:H5''	1.89	0.55
1:A:863:A:H2'	1:A:864:G:C8	2.41	0.55
1:A:863:A:H2'	1:A:864:G:H8	1.72	0.55
3:D:43:ARG:HD2	3:D:44:ASN:OD1	2.07	0.55
1:A:1093:G:H5'	7:H:170:ARG:NH1	2.22	0.55
8:I:129:THR:HA	8:I:137:PRO:HA	1.88	0.55
8:I:3:VAL:HG12	8:I:38:LEU:HA	1.87	0.55
1:A:958:U:OP2	12:Q:14:ARG:NH1	2.40	0.55
15:T:26:ASP:O	15:T:49:VAL:HG12	2.07	0.55
11:P:71:VAL:HG13	11:P:72:PRO:HD3	1.89	0.55
18:W:14:PRO:O	18:W:17:VAL:N	2.40	0.55
21:Z:48:PHE:CE2	21:Z:52:SER:HA	2.42	0.55
1:A:141:A:C8	1:A:1408:C:H1'	2.41	0.55
1:A:1688:U:H1'	1:A:1701:A:C6	2.42	0.55
1:A:860:U:OP2	1:A:916:G:N1	2.37	0.55
1:A:2820:A:C8	4:E:109:LYS:HE2	2.42	0.55
17:V:61:VAL:HG23	17:V:63:GLY:H	1.71	0.55
1:A:1292:U:H2'	1:A:1293:C:C6	2.41	0.54
1:A:2777:G:OP2	1:A:2781:A:O2'	2.20	0.54

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:330:A:HO2'	1:A:331:A:H8	1.52	0.54
1:A:996:A:OP2	16:U:92:ARG:NH2	2.40	0.54
5:F:116:ASP:OD2	11:P:1:MET:N	2.26	0.54
1:A:1649:G:O2'	13:R:107:ASP:OD1	2.14	0.54
15:T:62:THR:HG22	15:T:75:ILE:HG12	1.89	0.54
1:A:2656:U:H3	1:A:2665:A:H2	1.54	0.54
1:A:740:U:H2'	1:A:741:G:C8	2.42	0.54
1:A:898:C:H2'	1:A:899:A:H5'	1.88	0.54
3:D:12:SER:O	3:D:16:MET:HB2	2.08	0.54
12:Q:109:VAL:HG13	12:Q:113:GLN:HB3	1.89	0.54
13:R:55:ALA:HB2	13:R:79:LEU:HD13	1.89	0.54
13:R:56:LYS:NZ	13:R:87:TYR:O	2.40	0.54
9:N:42:TRP:O	16:U:64:ARG:NH2	2.41	0.54
27:5:55:ARG:HG3	27:5:57:VAL:H	1.73	0.54
1:A:1113:U:H2'	1:A:1114:G:C8	2.42	0.54
1:A:2131:G:H4'	1:A:2132:U:H4'	1.88	0.54
22:0:20:ARG:O	22:0:24:LYS:NZ	2.39	0.54
1:A:987:G:O2'	1:A:1000:A:N3	2.38	0.54
2:B:40:U:H1'	2:B:45:A:H61	1.72	0.54
21:Z:149:SER:HB2	21:Z:172:ALA:O	2.07	0.54
26:4:54:GLY:O	26:4:59:PHE:HB2	2.07	0.54
1:A:1085:A:O2'	1:A:1086:A:OP1	2.23	0.54
1:A:530:G:H1'	1:A:2021:C:O2'	2.07	0.54
1:A:540:G:H5'	1:A:541:C:OP2	2.07	0.54
9:N:35:ARG:HB2	9:N:42:TRP:CH2	2.42	0.54
11:P:64:LYS:O	11:P:66:GLY:N	2.41	0.54
16:U:76:TYR:CZ	16:U:80:ILE:HG13	2.43	0.54
21:Z:5:LEU:HD21	21:Z:44:PHE:HA	1.89	0.54
24:2:35:LEU:HD12	24:2:53:LEU:HD12	1.89	0.54
1:A:141(A):C:H2'	1:A:142:G:O4'	2.08	0.54
1:A:287:C:H2'	1:A:288:C:C6	2.42	0.54
1:A:518:G:H5'	18:W:18:ARG:NH1	2.23	0.54
21:Z:82:ARG:HG3	21:Z:83:PRO:HD2	1.90	0.54
1:A:2022:U:O2'	1:A:2617:C:H5'	2.08	0.54
1:A:2089:U:H5''	1:A:2089:U:H6	1.73	0.54
1:A:460:A:H2'	1:A:461:C:O4'	2.07	0.54
1:A:125:G:H5''	29:7:19:ARG:HD3	1.90	0.54
6:G:15:VAL:HG21	6:G:176:LEU:HD23	1.90	0.54
9:N:6:PRO:HG3	9:N:41:ASP:HB2	1.89	0.54
1:A:1341:U:OP2	1:A:1394:U:O2'	2.22	0.54
1:A:1678:G:N2	1:A:1989:G:H22	2.05	0.54
1:A:1929:G:H4'	1:A:1930:G:OP1	2.08	0.54

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2126:A:N6	1:A:2163:C:O2'	2.41	0.54
1:A:649:G:H2'	1:A:650:C:C6	2.42	0.54
1:A:2212:A:H1'	1:A:2215:G:C5	2.43	0.53
1:A:2712:U:O2'	1:A:2712(A):A:OP1	2.26	0.53
1:A:528:A:HO2'	1:A:529:A:H5'	1.73	0.53
3:D:70:TRP:CH2	3:D:150:LYS:HA	2.43	0.53
4:E:111:ARG:HD2	4:E:160:TYR:CD1	2.42	0.53
4:E:78:LEU:HG	4:E:79:ARG:NE	2.23	0.53
11:P:62:LEU:HD12	30:8:30:ARG:HH11	1.72	0.53
11:P:88:LEU:HD12	11:P:95:VAL:HG11	1.90	0.53
1:A:996:A:H4'	16:U:92:ARG:NE	2.22	0.53
1:A:2114:A:N6	1:A:2119:A:H62	2.07	0.53
1:A:2712:U:O2'	1:A:2712(A):A:H8	1.90	0.53
1:A:2832:U:H4'	1:A:2833:G:H5''	1.90	0.53
3:D:43:ARG:CB	3:D:54:ARG:HB2	2.38	0.53
17:V:66:ARG:NH1	17:V:88:ARG:HD3	2.23	0.53
1:A:2564:A:C2	1:A:2647:U:H4'	2.43	0.53
1:A:443:A:H5''	1:A:444:C:OP1	2.09	0.53
9:N:30:ILE:HG23	9:N:52:VAL:HG11	1.91	0.53
24:2:15:LYS:H	24:2:67:LYS:HE2	1.73	0.53
1:A:1019:U:O2'	1:A:1021:A:H2	1.91	0.53
1:A:1614:A:N6	18:W:88:ARG:H	2.05	0.53
1:A:2853:C:H2'	1:A:2854:G:C8	2.40	0.53
1:A:796:C:H2'	1:A:797:C:C6	2.43	0.53
3:D:244:ARG:HB2	3:D:245:PRO:HD2	1.90	0.53
3:D:30:GLU:HG3	3:D:63:ARG:HH21	1.72	0.53
8:I:62:LYS:HE3	8:I:134:PRO:HG2	1.90	0.53
11:P:92:GLU:HA	11:P:123:LEU:HD23	1.89	0.53
1:A:2467:C:H4'	12:Q:123:HIS:CD2	2.42	0.53
12:Q:12:GLN:HG2	12:Q:73:PRO:HD2	1.90	0.53
31:9:27:CYS:SG	31:9:28:GLU:N	2.82	0.53
1:A:1570:A:H2'	1:A:1571:A:C8	2.42	0.53
1:A:2150:U:H2'	1:A:2151:G:C8	2.44	0.53
1:A:2438:U:O3'	1:A:2439:A:H3'	2.08	0.53
1:A:2469:A:O2'	12:Q:56:ARG:HG2	2.08	0.53
15:T:105:LEU:O	15:T:107:ASP:N	2.42	0.53
15:T:112:ARG:O	15:T:112:ARG:NE	2.39	0.53
15:T:51:ARG:CG	15:T:98:LYS:HG3	2.38	0.53
1:A:2277:G:OP2	22:0:10:THR:HG21	2.08	0.53
1:A:226:G:O2'	1:A:227:A:C8	2.61	0.53
1:A:2567:G:H2'	1:A:2568:C:C6	2.43	0.53
1:A:528:A:C2	1:A:2043:C:H4'	2.44	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:782:A:H5'	1:A:783:A:C2	2.44	0.53
1:A:888:C:H3'	1:A:889:C:C4'	2.38	0.53
1:A:1178:C:H2'	1:A:1179:C:C6	2.44	0.53
1:A:2757:A:OP1	31:9:19:ARG:HA	2.09	0.53
8:I:79:ILE:N	8:I:141:LYS:O	2.40	0.53
1:A:1061:U:H3'	1:A:1062:G:H5''	1.89	0.53
1:A:2877:G:H2'	1:A:2878:U:O4'	2.09	0.53
3:D:206:LEU:O	3:D:211:ARG:HD3	2.09	0.53
6:G:179:PRO:HG3	26:4:38:LYS:NZ	2.24	0.53
8:I:93:THR:HG22	8:I:119:PRO:HB3	1.91	0.53
9:N:96:GLU:HG2	9:N:97:ARG:N	2.24	0.53
15:T:16:ARG:HE	15:T:19:LEU:HD21	1.73	0.53
16:U:102:GLU:OE1	17:V:13:ARG:NH2	2.42	0.53
28:6:26:ASN:ND2	28:6:35:GLU:OE2	2.42	0.53
1:A:1093:G:OP1	7:H:170:ARG:NH1	2.42	0.53
1:A:1697:G:OP2	1:A:1698:A:O2'	2.12	0.53
1:A:2629:A:O2'	1:A:2630:G:H5''	2.09	0.53
1:A:2667:C:H1'	7:H:109:PHE:CD2	2.43	0.53
7:H:149:ARG:NH1	7:H:167:GLU:OE1	2.42	0.53
24:2:47:ASN:H	24:2:47:ASN:ND2	2.05	0.53
1:A:1184:G:OP1	25:3:29:ARG:NH1	2.42	0.53
28:6:40:CYS:HB2	28:6:45:LYS:HD3	1.90	0.53
1:A:2469:A:H2	1:A:2481:G:N2	2.05	0.53
1:A:286:C:H2'	1:A:287:C:C6	2.44	0.53
1:A:363(F):A:H4'	1:A:364:C:H5''	1.91	0.53
9:N:13:TRP:O	9:N:135:PRO:HD2	2.08	0.53
14:S:10:ARG:O	14:S:12:PHE:N	2.42	0.53
1:A:2496:C:P	12:Q:81:VAL:HG12	2.49	0.52
1:A:414:C:H2'	1:A:415:A:C8	2.43	0.52
3:D:85:ASP:OD2	3:D:88:ARG:HD2	2.08	0.52
8:I:20:ASP:N	8:I:20:ASP:OD2	2.39	0.52
1:A:1354:A:OP1	3:D:38:LYS:HE2	2.09	0.52
6:G:96:ARG:O	6:G:98:ARG:N	2.42	0.52
9:N:110:GLY:O	9:N:114:ARG:HG3	2.09	0.52
20:Y:35:TYR:CE1	20:Y:69:ALA:HB3	2.44	0.52
1:A:1059:G:H3'	1:A:1060:U:H5''	1.90	0.52
1:A:1332:G:H5'	1:A:1332:G:C8	2.44	0.52
1:A:2667:C:H1'	7:H:109:PHE:HD2	1.74	0.52
2:B:42:C:O2	6:G:93:THR:N	2.27	0.52
3:D:132:PRO:HD3	3:D:190:TYR:CZ	2.44	0.52
1:A:184:C:H2'	1:A:185:U:C6	2.45	0.52
1:A:2867:G:OP2	15:T:119:LYS:NZ	2.25	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:729:G:C6	3:D:208:LYS:HB2	2.44	0.52
1:A:848:G:H2'	1:A:849:A:C8	2.43	0.52
1:A:2599:G:OP2	3:D:236:GLY:HA2	2.09	0.52
14:S:6:ALA:O	14:S:10:ARG:HD3	2.09	0.52
28:6:13:CYS:O	28:6:21:TYR:HA	2.09	0.52
1:A:1149:G:H2'	1:A:1150:C:C6	2.44	0.52
1:A:1448:G:O2'	1:A:1528:A:N6	2.43	0.52
1:A:1569:A:O5'	3:D:61:LEU:HD21	2.10	0.52
1:A:1728:G:H2'	1:A:1731:G:O6	2.10	0.52
1:A:1906:G:OP2	1:A:1929:G:O2'	2.27	0.52
1:A:2262:U:OP1	1:A:2387:U:O2'	2.27	0.52
1:A:2389:G:H5''	1:A:2390:U:O4'	2.09	0.52
1:A:507:A:C5'	1:A:508:G:H5'	2.40	0.52
25:3:40:THR:HB	25:3:43:ILE:HG12	1.92	0.52
1:A:444:C:H4'	5:F:49:ALA:HB2	1.92	0.52
5:F:63:LYS:HE2	5:F:67:GLN:HB2	1.91	0.52
6:G:88:ILE:HD13	6:G:88:ILE:O	2.09	0.52
11:P:20:GLY:HA2	11:P:27:HIS:O	2.10	0.52
1:A:223:A:O4'	1:A:422:A:H5'	2.10	0.52
1:A:2327:A:H2'	1:A:2328:A:C8	2.44	0.52
1:A:363:G:H2'	1:A:363(A):A:H8	1.74	0.52
1:A:581:C:H2'	1:A:582:G:C8	2.45	0.52
1:A:581:C:H2'	1:A:582:G:H8	1.74	0.52
1:A:764:A:N3	3:D:213:ARG:NH1	2.57	0.52
5:F:24:LEU:HD23	5:F:115:ALA:HA	1.91	0.52
1:A:857:C:OP2	22:0:77:ARG:NH2	2.43	0.52
1:A:1184:G:OP1	25:3:30:ARG:HD2	2.10	0.52
30:8:11:LYS:NZ	30:8:63:PRO:HG3	2.24	0.52
1:A:1210:A:C8	1:A:1210:A:H5'	2.40	0.52
1:A:1771:C:H1'	1:A:1786:A:H8	1.75	0.52
1:A:2774:C:H2'	1:A:2775:A:O4'	2.10	0.52
1:A:286:C:H2'	1:A:287:C:H6	1.74	0.52
24:2:58:ALA:O	24:2:62:THR:HG23	2.10	0.52
28:6:7:ILE:HG13	28:6:8:LYS:H	1.75	0.52
1:A:1339:G:H5''	19:X:16:LYS:HD3	1.92	0.52
1:A:2015:A:H1'	27:5:2:ALA:CA	2.38	0.52
1:A:2123:G:H2'	1:A:2124:G:C8	2.43	0.52
2:B:77:U:P	21:Z:19:ARG:HH22	2.33	0.52
8:I:110:ASP:N	8:I:130:TYR:OH	2.43	0.52
21:Z:124:ILE:HG22	21:Z:126:VAL:HG13	1.92	0.52
23:1:83:GLU:HG2	23:1:84:GLY:N	2.24	0.52
18:W:40:ASN:O	18:W:41:LYS:HG2	2.10	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1952:A:C5	10:O:22:ILE:HD12	2.44	0.51
1:A:2239:G:H5'	3:D:251:GLY:HA3	1.92	0.51
2:B:44:G:H1'	2:B:47:C:N4	2.25	0.51
15:T:88:ILE:HD12	15:T:90:GLN:N	2.25	0.51
24:2:24:LEU:HD13	24:2:60:LEU:HD11	1.92	0.51
30:8:51:ALA:N	30:8:53:PRO:HD2	2.25	0.51
1:A:1786:A:C2	1:A:2606:C:H1'	2.45	0.51
7:H:26:VAL:HG13	7:H:27:LYS:H	1.75	0.51
16:U:107:ALA:O	16:U:110:VAL:HB	2.10	0.51
17:V:25:LEU:H	17:V:92:THR:HG21	1.74	0.51
1:A:1533:C:H42	1:A:1538:G:H1	1.57	0.51
1:A:2151:G:H2'	1:A:2152:G:C8	2.45	0.51
3:D:148:GLU:HB2	3:D:151:LYS:HD2	1.92	0.51
5:F:127:GLU:OE1	5:F:196:LEU:HB2	2.11	0.51
6:G:77:ILE:HD13	6:G:82:LEU:HD12	1.93	0.51
7:H:88:LEU:H	7:H:88:LEU:HD22	1.75	0.51
11:P:96:THR:HG22	11:P:126:VAL:HB	1.93	0.51
13:R:83:ILE:HG22	13:R:87:TYR:HE2	1.76	0.51
27:5:42:PRO:HB2	27:5:43:HIS:ND1	2.25	0.51
1:A:1245:G:OP1	11:P:13:ASN:ND2	2.40	0.51
1:A:26:G:C6	1:A:27:G:N1	2.77	0.51
1:A:324:A:N6	1:A:338:G:O2'	2.41	0.51
9:N:38:HIS:O	16:U:67:ALA:HB1	2.10	0.51
17:V:65:GLY:HA3	17:V:91:TYR:CZ	2.46	0.51
23:1:70:VAL:O	23:1:74:VAL:HG23	2.10	0.51
27:5:38:ALA:HB3	27:5:40:LYS:HE3	1.92	0.51
27:5:56:LYS:HD3	27:5:58:LEU:HD23	1.90	0.51
1:A:2734:A:H5'	1:A:2735:G:OP2	2.11	0.51
1:A:569:U:C4	1:A:570:G:C6	2.97	0.51
6:G:16:ARG:O	6:G:20:ILE:HG12	2.10	0.51
16:U:47:TYR:HA	16:U:50:ARG:NH2	2.26	0.51
21:Z:89:PHE:HE1	21:Z:96:VAL:HG21	1.75	0.51
24:2:65:ASN:HB3	24:2:69:ARG:NH2	2.26	0.51
1:A:2151:G:H2'	1:A:2152:G:H8	1.74	0.51
1:A:2572:A:N7	4:E:145:LYS:HB2	2.24	0.51
4:E:62:PRO:O	4:E:64:LYS:N	2.43	0.51
12:Q:2:LEU:H	12:Q:2:LEU:HD23	1.76	0.51
14:S:11:LYS:HB2	14:S:91:PRO:HB3	1.93	0.51
15:T:109:GLU:O	15:T:113:LYS:HB2	2.11	0.51
16:U:92:ARG:NH1	17:V:11:GLN:O	2.44	0.51
1:A:2331:G:H4'	22:0:43:THR:H	1.75	0.51
25:3:43:ILE:O	25:3:47:VAL:HG23	2.10	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1069:A:H4'	1:A:1070:A:H5''	1.93	0.51
1:A:2182:G:H2'	1:A:2183:C:C6	2.46	0.51
1:A:2328:A:H2'	1:A:2329:G:C8	2.46	0.51
1:A:2795:G:H3'	1:A:2797:U:H5'	1.93	0.51
7:H:6:ARG:NE	7:H:54:ARG:HH12	2.09	0.51
12:Q:60:ARG:HA	21:Z:178:GLU:O	2.11	0.51
27:5:45:VAL:HG11	27:5:57:VAL:HG12	1.93	0.51
1:A:1154:G:OP2	16:U:58:ARG:NH1	2.41	0.51
1:A:1548:C:H2'	1:A:1549:C:H6	1.76	0.51
1:A:1654:A:OP2	13:R:2:ARG:HD2	2.11	0.51
1:A:524:U:H2'	1:A:525:U:C6	2.45	0.51
3:D:35:LYS:NZ	3:D:104:TYR:HB2	2.26	0.51
13:R:104:ARG:HD3	13:R:111:LEU:HD21	1.92	0.51
18:W:106:ILE:O	18:W:106:ILE:HG12	2.07	0.51
20:Y:81:LYS:HG2	20:Y:97:ARG:HD3	1.93	0.51
1:A:467:G:OP2	29:7:34:ARG:NH1	2.42	0.51
30:8:23:VAL:CG1	30:8:46:ARG:HD3	2.40	0.51
1:A:2789:C:H1'	1:A:2892:A:C2	2.42	0.51
1:A:673:C:H5''	5:F:81:PRO:HD2	1.92	0.51
1:A:107:C:H2'	1:A:108:U:H6	1.75	0.51
1:A:1359:A:H61	1:A:1372:U:H3	1.59	0.51
7:H:89:ILE:HG12	7:H:89:ILE:O	2.10	0.51
2:B:8:U:O2'	14:S:40:ILE:HD13	2.10	0.51
1:A:1412:A:H2'	1:A:1413:G:H8	1.76	0.50
1:A:1614:A:N1	18:W:91:GLY:HA2	2.25	0.50
1:A:2335:A:HO2'	1:A:2336:A:P	2.34	0.50
1:A:2524:G:H5'	1:A:2525:G:OP2	2.11	0.50
2:B:15:A:H1'	2:B:109:G:C8	2.46	0.50
12:Q:66:ILE:O	12:Q:104:PHE:N	2.39	0.50
1:A:2064:C:H2'	1:A:2065:C:C6	2.45	0.50
1:A:2758:A:C2	1:A:2759:G:H1'	2.46	0.50
18:W:57:ASN:O	18:W:61:ASN:HB2	2.10	0.50
30:8:58:ILE:HA	30:8:61:LEU:HD21	1.92	0.50
1:A:265:A:C8	1:A:266:G:H1'	2.47	0.50
8:I:11:ASN:O	8:I:12:LEU:HB2	2.11	0.50
11:P:62:LEU:HD23	11:P:62:LEU:N	2.26	0.50
12:Q:89:ASN:O	12:Q:91:GLU:N	2.44	0.50
14:S:30:ARG:HG3	14:S:97:ARG:NH2	2.26	0.50
17:V:52:VAL:HG23	17:V:55:ALA:H	1.76	0.50
26:4:10:VAL:HG22	26:4:11:PRO:HD2	1.94	0.50
6:G:67:LYS:HZ1	26:4:1:MET:HB2	1.77	0.50
1:A:2057:A:H2'	1:A:2058:A:O4'	2.12	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:530:G:C5	1:A:2022:U:H5''	2.47	0.50
8:I:13:GLY:HA3	8:I:17:GLN:OE1	2.12	0.50
4:E:111:ARG:HA	13:R:1:MET:CG	2.40	0.50
21:Z:72:ARG:NH2	21:Z:97:GLU:O	2.27	0.50
1:A:1771:C:C1'	1:A:1786:A:H8	2.25	0.50
1:A:1858:G:O2'	1:A:1884:A:N6	2.44	0.50
1:A:229:A:OP1	1:A:230:U:H5'	2.12	0.50
1:A:704:G:H1'	1:A:727:A:N6	2.27	0.50
1:A:877:U:H3	1:A:899:A:H2	1.60	0.50
1:A:900:A:H3'	1:A:901:A:C8	2.39	0.50
1:A:958:U:O2	2:B:89(A):A:O2'	2.26	0.50
5:F:167:ALA:HB1	5:F:173:VAL:HG11	1.93	0.50
6:G:5:VAL:HG11	6:G:100:TRP:HB3	1.93	0.50
10:O:120:GLU:HG2	10:O:122:LEU:HG	1.94	0.50
11:P:58:THR:O	11:P:61:ARG:CZ	2.59	0.50
1:A:1639:U:C2'	1:A:1640:C:H5''	2.40	0.50
17:V:61:VAL:HA	17:V:94:LEU:HD23	1.93	0.50
29:7:5:TRP:NE1	29:7:7:PRO:HG3	2.26	0.50
5:F:108:LYS:O	5:F:112:MET:HG3	2.11	0.50
5:F:65:TRP:O	5:F:67:GLN:N	2.43	0.50
7:H:4:ILE:HG13	7:H:6:ARG:NE	2.26	0.50
7:H:84:SER:O	7:H:85:LYS:HB2	2.11	0.50
11:P:36:LYS:HB3	11:P:40:SER:HB3	1.94	0.50
28:6:47:THR:HG22	28:6:48:VAL:HG12	1.94	0.50
1:A:1424:G:H2'	1:A:1425:G:O4'	2.12	0.50
1:A:1590:U:H2'	1:A:1591:G:H8	1.75	0.50
1:A:1798:U:C5'	3:D:259:THR:HG22	2.41	0.50
1:A:2875:C:H4'	15:T:5:ALA:HB2	1.93	0.50
9:N:58:ASP:N	9:N:58:ASP:OD1	2.45	0.50
30:8:25:MET:O	30:8:47:LYS:NZ	2.44	0.50
1:A:1778:U:H2'	1:A:1784:A:N6	2.27	0.50
1:A:1805:U:O2	3:D:50:THR:HB	2.12	0.50
1:A:2336:A:H61	22:0:43:THR:CG2	2.24	0.50
1:A:278:A:H2'	1:A:279:C:C6	2.47	0.50
11:P:126:VAL:HG13	11:P:145:PRO:HB2	1.94	0.50
12:Q:66:ILE:HG13	12:Q:67:ARG:N	2.27	0.50
19:X:60:ARG:HH22	29:7:47:ARG:HH12	1.60	0.50
20:Y:97:ARG:HH21	20:Y:98:VAL:HB	1.76	0.50
1:A:1872:A:H5'	1:A:1878:G:OP2	2.12	0.49
1:A:1878:G:H2'	1:A:1879:C:C6	2.47	0.49
4:E:103:ASP:OD1	4:E:201:THR:HG23	2.12	0.49
1:A:1138:G:N2	9:N:106:MET:HE3	2.13	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2820:A:O5'	13:R:4:LEU:HD23	2.12	0.49
22:0:70:GLN:OE1	22:0:72:ARG:HD3	2.12	0.49
1:A:1520:U:H2'	1:A:1521:G:O4'	2.12	0.49
1:A:1535:U:H5''	1:A:1537:C:C4	2.47	0.49
1:A:2299:G:N2	1:A:2318:G:H1'	2.27	0.49
1:A:363(B):G:H2'	1:A:363(C):G:C8	2.45	0.49
4:E:73:GLU:HG3	4:E:74:PRO:HD2	1.92	0.49
16:U:83:LEU:HG	16:U:88:ILE:HG13	1.93	0.49
1:A:1093:G:H4'	7:H:170:ARG:HH22	1.76	0.49
1:A:140:A:C8	1:A:1408:C:O2'	2.62	0.49
1:A:2023:G:H5'	1:A:2617:C:H4'	1.93	0.49
1:A:2687:U:C4	1:A:2688:U:C5	2.99	0.49
1:A:247:G:H4'	1:A:386:G:C5	2.47	0.49
4:E:35:GLN:HG2	4:E:37:ARG:HE	1.77	0.49
9:N:7:LYS:HD2	9:N:7:LYS:N	2.28	0.49
19:X:53:LYS:HB3	19:X:82:GLN:HB3	1.93	0.49
26:4:15:ILE:HD13	26:4:15:ILE:H	1.76	0.49
1:A:1021:A:H3'	1:A:1021:A:C8	2.46	0.49
1:A:2308:G:N2	1:A:2311:A:H2	2.09	0.49
1:A:2704:C:H2'	1:A:2705:A:O4'	2.12	0.49
1:A:2770:G:H5''	1:A:2771:C:OP2	2.13	0.49
1:A:754:C:H2'	1:A:755:C:C6	2.47	0.49
3:D:121:PRO:HB3	3:D:135:PHE:CE1	2.47	0.49
1:A:153:C:OP1	23:1:88:LYS:HE2	2.12	0.49
1:A:1007:C:H4'	9:N:108:PRO:HD3	1.94	0.49
1:A:177:G:H3'	1:A:178:G:H8	1.77	0.49
1:A:2257:U:O2'	1:A:2258:C:H5'	2.13	0.49
1:A:2854:G:H2'	1:A:2855:C:C6	2.47	0.49
1:A:34:C:H41	1:A:447:A:H61	1.58	0.49
1:A:860:U:H5	1:A:917:A:N1	2.09	0.49
5:F:31:HIS:HB2	11:P:9:ASN:OD1	2.12	0.49
9:N:17:ASP:O	9:N:56:ASN:HB2	2.12	0.49
9:N:34:LEU:HD21	9:N:120:LEU:HB2	1.94	0.49
16:U:61:TRP:CD2	16:U:94:ASN:HA	2.47	0.49
16:U:95:LEU:HD22	17:V:4:ILE:HD12	1.93	0.49
1:A:77:C:OP1	24:2:59:ARG:HD3	2.13	0.49
28:6:41:PRO:HD2	28:6:46:HIS:N	2.28	0.49
3:D:27:THR:HG21	3:D:83:GLU:HG2	1.94	0.49
3:D:76:PRO:HG2	3:D:98:VAL:HG21	1.94	0.49
4:E:179:GLU:HB3	4:E:181:LEU:HD23	1.94	0.49
1:A:617:G:OP1	5:F:40:GLN:NE2	2.46	0.49
6:G:94:LEU:HD12	6:G:99:MET:HA	1.95	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:Y:86:ARG:HB2	20:Y:95:LYS:HD2	1.93	0.49
28:6:21:TYR:HE1	28:6:53:LYS:HE3	1.77	0.49
11:P:63:PRO:HD3	30:8:13:ARG:HD3	1.95	0.49
1:A:1021:A:H3'	1:A:1021:A:H8	1.78	0.49
1:A:1291:C:H5'	1:A:1536:A:H5'	1.95	0.49
1:A:589:C:H2'	1:A:590:A:C8	2.48	0.49
28:6:41:PRO:O	28:6:45:LYS:HE3	2.12	0.49
1:A:1113:U:H2'	1:A:1114:G:H8	1.78	0.49
1:A:1509:C:N3	1:A:1511:A:N6	2.61	0.49
1:A:152:G:H2'	1:A:153:C:C6	2.48	0.49
1:A:760:G:H4'	1:A:1776:G:OP1	2.13	0.49
1:A:185:U:H4'	1:A:218:A:H4'	1.95	0.49
1:A:2031:A:N3	1:A:2455:G:O2'	2.42	0.49
19:X:57:LEU:HD11	19:X:78:LYS:HD2	1.94	0.49
22:0:53:MET:HA	22:0:58:THR:O	2.13	0.49
1:A:1257:C:OP1	5:F:75:HIS:HE1	1.95	0.49
1:A:1667:G:OP2	1:A:1667:G:H8	1.95	0.49
1:A:2805:G:N2	1:A:2893:G:O6	2.40	0.49
3:D:170:GLY:C	3:D:172:TYR:H	2.16	0.49
7:H:12:PRO:HG3	7:H:48:GLY:HA2	1.95	0.49
11:P:61:ARG:HD3	30:8:13:ARG:HD2	1.94	0.49
1:A:1607:C:N4	1:A:1622:G:OP2	2.39	0.49
1:A:1803:A:O2'	3:D:259:THR:HG21	2.13	0.49
1:A:1870:C:H2'	1:A:1871:A:O4'	2.13	0.49
1:A:211:A:H2'	1:A:212:G:O4'	2.13	0.49
1:A:70:G:H21	1:A:71:A:H62	1.59	0.49
3:D:61:LEU:O	3:D:63:ARG:NH1	2.45	0.49
5:F:176:LEU:HD21	5:F:181:LEU:HA	1.94	0.49
1:A:207:A:H2'	1:A:208:C:O4'	2.13	0.48
1:A:2470:G:H5'	12:Q:56:ARG:NH2	2.28	0.48
1:A:2712:U:O2'	1:A:2712(A):A:P	2.71	0.48
1:A:278:A:O2'	1:A:279:C:O4'	2.30	0.48
1:A:639:U:H2'	1:A:640:C:C6	2.47	0.48
2:B:15:A:H5'	2:B:16:G:H8	1.73	0.48
6:G:166:ASP:HA	6:G:169:ALA:HB3	1.95	0.48
7:H:98:LEU:HD13	7:H:125:VAL:HB	1.94	0.48
10:O:4:PRO:O	10:O:5:GLN:HB2	2.11	0.48
12:Q:104:PHE:CE1	12:Q:125:LEU:HD11	2.41	0.48
15:T:107:ASP:H	15:T:110:ILE:HG22	1.78	0.48
18:W:51:LEU:HD23	18:W:105:VAL:HG11	1.94	0.48
1:A:107:C:H2'	1:A:108:U:C6	2.48	0.48
1:A:1506:C:H3'	1:A:1507:A:H5''	1.94	0.48

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2725:A:O2'	1:A:2726:U:OP2	2.29	0.48
3:D:35:LYS:HD3	3:D:63:ARG:CB	2.43	0.48
4:E:21:VAL:HG23	4:E:22:PRO:HD3	1.95	0.48
5:F:185:ASP:OD1	5:F:188:ARG:NH1	2.35	0.48
7:H:55:PRO:HG2	7:H:61:HIS:CE1	2.48	0.48
11:P:135:LEU:HD13	11:P:139:LYS:HE2	1.94	0.48
16:U:98:LEU:O	16:U:102:GLU:N	2.37	0.48
1:A:1109:C:HO2'	1:A:1110:G:P	2.35	0.48
1:A:1329:U:H5''	1:A:1330:C:H5	1.77	0.48
1:A:1510:A:H2'	1:A:1510:A:N3	2.29	0.48
1:A:1733:G:H5'	1:A:1734:C:OP2	2.13	0.48
1:A:754:C:H2'	1:A:755:C:H6	1.77	0.48
10:O:76:ALA:HB3	15:T:75:ILE:HD12	1.95	0.48
11:P:82:GLY:HA2	11:P:113:LYS:O	2.12	0.48
23:1:41:ARG:HG3	23:1:41:ARG:HH11	1.79	0.48
1:A:1026:U:H4'	1:A:1027:A:OP1	2.14	0.48
1:A:2593:U:H2'	1:A:2594:C:H6	1.79	0.48
1:A:2862:G:H2'	1:A:2863:C:H6	1.79	0.48
1:A:507:A:H5''	1:A:508:G:H5'	1.95	0.48
7:H:137:ASP:HB3	7:H:140:LYS:HB3	1.94	0.48
17:V:15:GLU:O	17:V:18:LEU:HB2	2.14	0.48
21:Z:182:LYS:CG	21:Z:183:LEU:HA	2.44	0.48
27:5:41:PRO:O	27:5:44:THR:OG1	2.32	0.48
4:E:111:ARG:HG2	13:R:1:MET:SD	2.54	0.48
15:T:102:ILE:HB	15:T:110:ILE:HD13	1.95	0.48
19:X:63:LYS:O	19:X:64:LYS:HD2	2.14	0.48
1:A:218:A:C2	1:A:235:U:H4'	2.48	0.48
1:A:2496:C:OP2	12:Q:81:VAL:HG12	2.12	0.48
1:A:2544:G:O5'	1:A:2544:G:H8	1.95	0.48
4:E:20:ALA:HB3	4:E:21:VAL:HG13	1.95	0.48
11:P:14:LYS:O	11:P:16:ARG:HG2	2.13	0.48
11:P:52:GLU:O	11:P:55:ARG:HG2	2.14	0.48
14:S:74:ALA:HB1	14:S:107:GLU:HB3	1.95	0.48
16:U:60:LEU:HD22	16:U:60:LEU:O	2.14	0.48
17:V:76:LYS:HB2	17:V:81:TYR:HB3	1.95	0.48
1:A:1533:C:H2'	1:A:1534:G:N7	2.29	0.48
1:A:2287:A:N6	1:A:2344:U:H3	2.05	0.48
1:A:1050:A:C8	1:A:2751:G:C4	3.02	0.48
1:A:27:G:H22	1:A:512:G:C2'	2.27	0.48
1:A:459:U:H2'	1:A:460:A:H8	1.78	0.48
1:A:576:U:H2'	1:A:577:G:C8	2.48	0.48
2:B:89:G:C6	2:B:89(A):A:C6	3.01	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:254:THR:O	3:D:254:THR:OG1	2.30	0.48
16:U:97:ASP:OD1	16:U:101:ARG:NH1	2.46	0.48
18:W:67:ASP:OD2	18:W:67:ASP:N	2.46	0.48
28:6:27:LYS:NZ	28:6:27:LYS:HB2	2.28	0.48
1:A:1385:G:H1'	1:A:1386:C:C6	2.49	0.48
1:A:1557:C:OP2	1:A:1558:A:O2'	2.26	0.48
1:A:776:G:H4'	1:A:777:A:O5'	2.13	0.48
8:I:69:LYS:HG3	8:I:136:VAL:HB	1.96	0.48
16:U:90:VAL:HG22	17:V:39:LEU:HB3	1.96	0.48
20:Y:35:TYR:CD1	20:Y:69:ALA:HB3	2.49	0.48
27:5:58:LEU:HD22	27:5:60:VAL:HB	1.96	0.48
1:A:1156:A:C8	16:U:51:LYS:HG3	2.49	0.48
1:A:128:C:H4'	29:7:49:ARG:NH1	2.26	0.48
1:A:1545(A):A:H2'	1:A:1546:C:O4'	2.14	0.48
1:A:1882:C:H5'	1:A:1883:G:OP2	2.13	0.48
1:A:2352:A:C4	1:A:2366:A:C2	3.01	0.48
1:A:861:A:C2	1:A:917:A:C5	3.02	0.48
7:H:6:ARG:HA	7:H:66:GLY:HA2	1.95	0.48
8:I:76:THR:OG1	8:I:139:GLN:OE1	2.31	0.48
11:P:98:GLU:HA	11:P:101:VAL:HB	1.96	0.48
11:P:46:LYS:HE3	11:P:46:LYS:HB3	1.54	0.48
16:U:92:ARG:CZ	17:V:11:GLN:H	2.26	0.48
1:A:1404:C:C2'	1:A:1405:U:H5'	2.44	0.48
1:A:603:A:O4'	1:A:655:A:N6	2.46	0.48
9:N:134:ARG:N	9:N:135:PRO:HD3	2.29	0.48
14:S:65:VAL:O	14:S:69:VAL:HG12	2.14	0.48
20:Y:44:ILE:HG13	20:Y:45:VAL:N	2.28	0.48
27:5:46:CYS:O	27:5:48:GLU:N	2.38	0.47
1:A:264:C:H2'	1:A:265:A:H5''	1.95	0.47
1:A:2655:G:N2	1:A:2665:A:OP2	2.47	0.47
2:B:44:G:H1'	2:B:47:C:H42	1.78	0.47
3:D:35:LYS:HZ1	3:D:104:TYR:HB2	1.79	0.47
1:A:1036:G:OP1	7:H:59:ARG:HB2	2.14	0.47
1:A:1535:U:N3	1:A:1537:C:H1'	2.29	0.47
2:B:27:C:H5'	2:B:28:C:OP2	2.14	0.47
11:P:144:GLU:OE1	11:P:144:GLU:N	2.40	0.47
17:V:44:LYS:O	17:V:46:VAL:HG12	2.13	0.47
23:1:91:LYS:HB3	23:1:92:LYS:H	1.44	0.47
24:2:59:ARG:O	24:2:63:VAL:HG23	2.15	0.47
1:A:2245:U:H5'	1:A:2246:G:H5'	1.96	0.47
1:A:2688:U:H5	1:A:2720:U:OP2	1.97	0.47
1:A:2849:U:H4'	1:A:2868:A:C2	2.49	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:71:ASP:HB2	3:D:103:ARG:NH2	2.27	0.47
5:F:36:VAL:HG11	5:F:183:VAL:HG11	1.95	0.47
12:Q:21:THR:HB	12:Q:22:LYS:H	1.40	0.47
15:T:11:GLU:OE1	15:T:11:GLU:N	2.43	0.47
23:1:53:VAL:HG22	23:1:74:VAL:HG13	1.96	0.47
1:A:2056:G:H1	27:5:4:HIS:HD2	1.62	0.47
11:P:50:ARG:HE	30:8:7:HIS:HE2	1.63	0.47
1:A:1379:A:H4'	1:A:1380:G:OP2	2.14	0.47
1:A:226:G:HO2'	1:A:227:A:H8	1.55	0.47
1:A:846:C:O2'	1:A:847:U:OP2	2.26	0.47
1:A:2467:C:H4'	12:Q:123:HIS:CG	2.49	0.47
30:8:36:LYS:HB3	30:8:40:GLU:HG2	1.95	0.47
1:A:7:G:H1	1:A:2896:C:H42	1.62	0.47
2:B:24:G:H1'	2:B:26:A:H62	1.79	0.47
3:D:28:GLU:HB2	3:D:29:PRO:CD	2.45	0.47
1:A:1454:U:H5'	13:R:63:ARG:NE	2.30	0.47
18:W:110:LYS:HG3	18:W:111:HIS:H	1.80	0.47
1:A:1062:G:O5'	1:A:1062:G:H8	1.97	0.47
1:A:1239:G:H2'	1:A:1240:U:O4'	2.14	0.47
1:A:1529:A:N6	1:A:1542:G:O2'	2.41	0.47
1:A:2392:A:C8	11:P:60:MET:HG2	2.50	0.47
1:A:2469:A:H5'	1:A:2470:G:OP2	2.15	0.47
5:F:164:ARG:HG3	5:F:175:THR:OG1	2.15	0.47
9:N:30:ILE:HG22	9:N:34:LEU:HD22	1.96	0.47
1:A:1453:A:O2'	1:A:1454:U:H2'	2.14	0.47
1:A:1916:A:H2'	1:A:1917:U:O4'	2.15	0.47
1:A:2319:G:N7	14:S:3:ARG:HB3	2.29	0.47
1:A:593:G:O3'	30:8:61:LEU:HD22	2.14	0.47
3:D:206:LEU:HD23	3:D:206:LEU:HA	1.51	0.47
5:F:182:ASN:HD21	5:F:185:ASP:CG	2.14	0.47
6:G:28:VAL:O	6:G:31:VAL:HG13	2.14	0.47
8:I:144:VAL:HG22	8:I:145:VAL:H	1.80	0.47
1:A:896:A:C8	21:Z:146:ILE:HD12	2.50	0.47
22:0:19:LYS:HD3	22:0:19:LYS:HA	1.66	0.47
1:A:1221:C:H2'	1:A:1222:C:H6	1.79	0.47
1:A:1665:A:C2'	1:A:1666:G:H5'	2.43	0.47
1:A:922:U:H2'	1:A:923:C:C6	2.50	0.47
3:D:237:GLU:O	3:D:239:ARG:N	2.47	0.47
6:G:113:ARG:HG2	26:4:34:GLU:OE2	2.14	0.47
6:G:34:LEU:HD22	6:G:35:GLU:N	2.30	0.47
25:3:23:LEU:HD13	25:3:50:VAL:HG11	1.96	0.47
1:A:99:U:O2'	1:A:101:G:OP2	2.28	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1728:G:H5'	1:A:1729:A:OP2	2.14	0.47
1:A:2636:U:H2'	1:A:2637:U:H6	1.79	0.47
1:A:307:G:H21	1:A:330:A:N6	2.13	0.47
4:E:116:VAL:HG11	4:E:138:PRO:HB3	1.97	0.47
5:F:140:LEU:HD12	5:F:140:LEU:HA	1.77	0.47
5:F:9:ILE:HG23	5:F:20:LEU:O	2.15	0.47
6:G:114:ILE:HD13	6:G:140:ILE:HG21	1.96	0.47
7:H:122:THR:HG22	7:H:134:SER:HB2	1.96	0.47
1:A:1614:A:H61	18:W:88:ARG:H	1.61	0.47
1:A:1586:A:H3'	1:A:1587:A:H8	1.80	0.47
1:A:1658:C:H2'	1:A:1659:U:C6	2.50	0.47
1:A:957:A:N1	1:A:2458:G:H4'	2.29	0.47
1:A:2461:C:H2'	1:A:2462:U:C6	2.49	0.47
1:A:478:A:C6	1:A:480:A:C6	3.03	0.47
5:F:129:PHE:HA	5:F:142:TRP:NE1	2.29	0.47
7:H:4:ILE:HB	7:H:6:ARG:CG	2.43	0.47
7:H:4:ILE:HG13	7:H:6:ARG:CZ	2.45	0.47
1:A:1204:A:O2'	1:A:1205:U:O5'	2.33	0.47
1:A:1289:C:H2'	1:A:1290:C:H6	1.79	0.47
1:A:2439:A:H5'	1:A:2439:A:C8	2.50	0.47
11:P:64:LYS:HB2	30:8:25:MET:HG3	1.96	0.47
20:Y:73:ARG:HB3	20:Y:73:ARG:HE	1.47	0.47
26:4:38:LYS:HD3	26:4:42:PHE:HE1	1.80	0.46
27:5:33:CYS:SG	27:5:34:PRO:HD2	2.55	0.46
1:A:1029:A:N1	1:A:2465:C:O2'	2.46	0.46
1:A:2593:U:H2'	1:A:2594:C:C6	2.50	0.46
1:A:602:G:O2'	1:A:655:A:N6	2.48	0.46
1:A:890:A:O2'	1:A:892:G:H8	1.98	0.46
3:D:17:THR:CG2	3:D:205:VAL:H	2.28	0.46
5:F:108:LYS:NZ	5:F:108:LYS:HB3	2.31	0.46
7:H:154:PRO:HD3	7:H:162:ILE:H	1.79	0.46
8:I:68:LEU:HA	8:I:71:ILE:HG22	1.97	0.46
9:N:114:ARG:O	9:N:115:ARG:HB3	2.14	0.46
11:P:88:LEU:HB2	11:P:91:PHE:HE2	1.80	0.46
11:P:96:THR:O	11:P:99:LEU:HB3	2.15	0.46
26:4:2:LYS:HA	26:4:2:LYS:HD2	1.67	0.46
1:A:234:C:H2'	1:A:235:U:C6	2.51	0.46
1:A:415:A:H2'	1:A:416:C:H6	1.81	0.46
2:B:16:G:N2	2:B:69:G:H1'	2.29	0.46
4:E:150:VAL:HG13	4:E:154:LYS:HG3	1.96	0.46
4:E:176:ILE:HB	4:E:181:LEU:HB2	1.97	0.46
6:G:11:TYR:HA	6:G:15:VAL:HB	1.95	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:P:19:VAL:HG13	11:P:21:ARG:N	2.20	0.46
14:S:52:SER:HB2	14:S:55:ALA:H	1.79	0.46
20:Y:87:LYS:HD3	20:Y:92:ASN:HB3	1.98	0.46
1:A:1102:C:H2'	1:A:1103:A:H5''	1.97	0.46
1:A:1550:C:H2'	1:A:1551:C:H6	1.80	0.46
1:A:1771:C:C1'	1:A:1786:A:C8	2.97	0.46
1:A:2059:A:H5'	1:A:2060:A:OP2	2.16	0.46
3:D:94:LEU:HD22	3:D:95:LEU:N	2.31	0.46
5:F:127:GLU:OE2	5:F:128:ALA:N	2.47	0.46
8:I:131:LYS:HB3	8:I:132:PRO:HA	1.98	0.46
11:P:121:LYS:HE2	11:P:121:LYS:HB2	1.75	0.46
11:P:29:LYS:HD2	11:P:30:THR:HG23	1.97	0.46
22:O:17:GLN:O	22:O:19:LYS:HE3	2.14	0.46
1:A:1265:A:H3'	27:5:19:ARG:NH1	2.31	0.46
1:A:1396:U:O2	1:A:1396:U:H2'	2.15	0.46
1:A:1794:U:H2'	1:A:1795:C:H6	1.80	0.46
1:A:2356:C:H2'	1:A:2357:U:O4'	2.16	0.46
1:A:2655:G:O2'	1:A:2656:U:P	2.73	0.46
3:D:25:THR:CG2	3:D:82:ILE:H	2.27	0.46
14:S:27:SER:HA	14:S:88:ASP:HB2	1.96	0.46
23:1:96:LYS:H	23:1:97:LEU:HD12	1.81	0.46
25:3:8:LEU:HD22	25:3:31:LEU:HD22	1.96	0.46
1:A:1153:C:H5'	16:U:76:TYR:HE2	1.81	0.46
1:A:224:G:O6	1:A:419:C:O2'	2.33	0.46
1:A:2545:G:H2'	1:A:2546:U:O4'	2.16	0.46
1:A:27:G:H22	1:A:512:G:H2'	1.79	0.46
20:Y:94:LYS:HD2	20:Y:101:LYS:HZ3	1.81	0.46
1:A:2392:A:H2'	1:A:2393:A:O4'	2.16	0.46
1:A:2469:A:O2'	12:Q:56:ARG:NE	2.48	0.46
3:D:118:VAL:HG22	3:D:119:ALA:N	2.31	0.46
3:D:35:LYS:HB3	3:D:63:ARG:HA	1.98	0.46
16:U:75:ASN:HB3	16:U:78:THR:H	1.81	0.46
23:1:80:LEU:HB2	23:1:81:LYS:H	1.61	0.46
1:A:2364:C:H2'	1:A:2365:G:O4'	2.16	0.46
1:A:658:C:H2'	1:A:659:C:C6	2.50	0.46
3:D:35:LYS:HE3	3:D:63:ARG:C	2.36	0.46
6:G:34:LEU:HD12	6:G:100:TRP:CH2	2.50	0.46
7:H:167:GLU:HA	7:H:168:PRO:HD3	1.79	0.46
8:I:88:ILE:HG12	8:I:122:GLU:N	2.31	0.46
12:Q:136:ALA:O	12:Q:138:ASP:N	2.40	0.46
1:A:1482:U:H5'	1:A:1483:G:OP2	2.15	0.46
1:A:2346:A:H5''	1:A:2383:G:H1'	1.98	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:270(W):G:H2'	1:A:270(X):G:O4'	2.16	0.46
1:A:528:A:C2'	1:A:529:A:H5'	2.46	0.46
1:A:969:U:O3'	25:3:14:GLY:HA2	2.16	0.46
4:E:116:VAL:O	4:E:117:MET:HB3	2.16	0.46
4:E:36:ARG:NH2	4:E:88:GLY:HA2	2.29	0.46
7:H:103:LEU:HD23	7:H:115:VAL:HB	1.97	0.46
8:I:3:VAL:O	8:I:18:VAL:HA	2.15	0.46
1:A:1049:C:C2'	1:A:1050:A:H5''	2.45	0.46
1:A:7:G:H2'	1:A:8:A:O4'	2.16	0.46
4:E:70:ALA:O	4:E:72:VAL:N	2.49	0.46
5:F:129:PHE:O	5:F:142:TRP:CD1	2.69	0.46
7:H:106:THR:HG22	7:H:112:PRO:HB3	1.97	0.46
18:W:110:LYS:HG3	18:W:111:HIS:ND1	2.31	0.46
1:A:1417:C:H2'	1:A:1418:G:O4'	2.16	0.46
1:A:2712:U:O2'	1:A:2712(A):A:C8	2.61	0.46
1:A:2689:U:H5'	1:A:2713:A:C2	2.51	0.46
1:A:612:G:H2'	1:A:613:U:O2	2.16	0.46
4:E:108:SER:HB3	4:E:165:VAL:HG21	1.98	0.46
11:P:135:LEU:HD23	11:P:135:LEU:HA	1.74	0.46
12:Q:135:ASP:N	12:Q:135:ASP:OD1	2.48	0.46
13:R:51:LEU:HD12	13:R:70:LEU:HG	1.97	0.46
1:A:997:G:OP1	16:U:93:LYS:HD2	2.16	0.46
23:1:58:ILE:N	23:1:58:ILE:HD12	2.30	0.45
1:A:771:G:OP1	29:7:14:LYS:HE3	2.15	0.45
1:A:1454:U:H5'	13:R:63:ARG:HE	1.80	0.45
1:A:1688:U:O2	1:A:1700:A:H5''	2.16	0.45
1:A:1754:C:P	15:T:96:ARG:HH12	2.39	0.45
1:A:1930:G:H2'	1:A:1968:G:C6	2.50	0.45
3:D:10:THR:OG1	3:D:13:ARG:HB2	2.16	0.45
3:D:137:PRO:O	3:D:140:THR:HG23	2.16	0.45
5:F:129:PHE:C	5:F:131:GLY:H	2.18	0.45
7:H:86:GLU:O	7:H:87:LEU:HB2	2.16	0.45
11:P:138:LEU:C	11:P:140:ALA:H	2.18	0.45
17:V:19:LYS:HA	17:V:94:LEU:O	2.15	0.45
1:A:751:A:C5'	18:W:90:ARG:HA	2.46	0.45
20:Y:84:ARG:HB3	20:Y:95:LYS:HD3	1.97	0.45
1:A:1532:C:H2'	1:A:1533:C:O4'	2.17	0.45
1:A:858:U:O2	1:A:2268:A:H2'	2.15	0.45
1:A:2584:U:H2'	1:A:2585:U:C6	2.51	0.45
1:A:2612:C:H2'	1:A:2613:U:H5'	1.99	0.45
1:A:2867:G:O2'	1:A:2868:A:H8	1.98	0.45
1:A:601:C:O2'	1:A:605:C:OP1	2.26	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:33:G:H5'	6:G:2:PRO:HG3	1.98	0.45
1:A:1006:C:O2	9:N:106:MET:HG2	2.15	0.45
13:R:78:LYS:O	13:R:83:ILE:HG12	2.16	0.45
20:Y:51:VAL:HG13	20:Y:52:SER:N	2.28	0.45
28:6:33:LYS:HB2	28:6:33:LYS:HE2	1.76	0.45
1:A:1404:C:O2'	1:A:1405:U:H5'	2.16	0.45
1:A:1530:G:O6	1:A:1542:G:N2	2.49	0.45
1:A:1794:U:H2'	1:A:1795:C:C6	2.51	0.45
1:A:1820:U:H4'	1:A:1821:A:OP2	2.16	0.45
1:A:2275:C:H5'	1:A:2275:C:H6	1.81	0.45
1:A:2314:C:H2'	1:A:2315:G:C8	2.48	0.45
1:A:2563:U:H4'	10:O:28:SER:HA	1.98	0.45
1:A:2636:U:H2'	1:A:2637:U:C6	2.52	0.45
5:F:11:VAL:HA	5:F:125:LEU:O	2.16	0.45
11:P:27:HIS:N	11:P:27:HIS:ND1	2.64	0.45
13:R:109:ALA:HA	13:R:110:PRO:HD2	1.77	0.45
16:U:68:ALA:O	16:U:71:GLN:HB2	2.16	0.45
20:Y:87:LYS:HA	20:Y:92:ASN:HB3	1.98	0.45
23:1:91:LYS:HE3	23:1:91:LYS:HA	1.98	0.45
24:2:4:SER:OG	24:2:5:GLU:OE1	2.23	0.45
6:G:6:ALA:N	26:4:23:GLU:HG2	2.28	0.45
1:A:1026:U:O2	1:A:1027:A:H3'	2.16	0.45
1:A:1055:G:H1	1:A:1104:C:N4	2.13	0.45
1:A:1826:G:H4'	3:D:242:ARG:CZ	2.46	0.45
1:A:2365:G:H4'	22:0:60:PHE:CZ	2.51	0.45
1:A:242:G:C5'	30:8:62:LEU:HD13	2.46	0.45
1:A:34:C:N4	1:A:447:A:H61	2.14	0.45
1:A:653:A:H4'	1:A:654:A:OP2	2.16	0.45
1:A:86:C:H4'	1:A:104:U:H1'	1.98	0.45
1:A:1490:A:O2'	3:D:99:ASP:OD2	2.35	0.45
11:P:106:LEU:HD23	11:P:106:LEU:HA	1.84	0.45
13:R:24:GLN:HE21	13:R:44:LEU:HG	1.81	0.45
16:U:66:ASN:O	16:U:70:ARG:HB2	2.17	0.45
20:Y:56:PRO:O	20:Y:58:GLY:N	2.49	0.45
22:0:23:VAL:HA	22:0:38:VAL:HA	1.99	0.45
24:2:21:LEU:O	24:2:25:VAL:HG23	2.17	0.45
25:3:31:LEU:O	25:3:32:GLN:HB2	2.17	0.45
28:6:15:GLU:CD	28:6:41:PRO:HB3	2.37	0.45
1:A:1012:U:O4	9:N:25:ARG:HA	2.16	0.45
1:A:609(A):G:H2'	1:A:610:C:C6	2.51	0.45
2:B:87:G:N2	2:B:89(A):A:OP2	2.29	0.45
6:G:146:TYR:O	6:G:149:VAL:HG22	2.16	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:P:124:LYS:HA	11:P:143:GLY:O	2.16	0.45
16:U:58:ARG:HA	16:U:61:TRP:CE3	2.52	0.45
17:V:19:LYS:HG3	17:V:95:LEU:HD23	1.98	0.45
17:V:36:PRO:HA	17:V:56:SER:OG	2.17	0.45
20:Y:101:LYS:HG2	20:Y:102:CYS:H	1.81	0.45
1:A:1899:G:H21	1:A:1902:C:H42	1.64	0.45
1:A:2630:G:O4'	1:A:2894:G:H1'	2.16	0.45
1:A:2836:U:H2'	1:A:2837:G:C8	2.52	0.45
1:A:304:G:H2'	1:A:305:U:C6	2.51	0.45
1:A:860:U:C5	1:A:917:A:H2	2.34	0.45
1:A:956:G:H5'	12:Q:77:LYS:HE2	1.99	0.45
2:B:15:A:H1'	2:B:109:G:N9	2.32	0.45
1:A:321:G:H5''	5:F:136:THR:HG23	1.97	0.45
7:H:150:ALA:O	7:H:152:ARG:N	2.49	0.45
15:T:6:LEU:HA	15:T:9:LEU:HB2	1.99	0.45
24:2:24:LEU:HA	24:2:24:LEU:HD23	1.67	0.45
1:A:1338:G:O2'	1:A:1393:A:N1	2.43	0.45
1:A:1655:A:H3'	1:A:1656:C:C6	2.52	0.45
1:A:2760:C:C2'	1:A:2761:G:H5''	2.43	0.45
1:A:2846:G:H2'	1:A:2847:U:C6	2.51	0.45
1:A:414:C:O2	1:A:1864:U:O2'	2.30	0.45
1:A:646:A:H2'	1:A:647:G:O4'	2.17	0.45
3:D:44:ASN:N	3:D:44:ASN:ND2	2.64	0.45
4:E:67:PHE:O	4:E:69:LYS:N	2.49	0.45
1:A:2468:G:H5''	12:Q:120:ILE:HD12	1.99	0.45
23:1:79:GLY:N	23:1:80:LEU:HD23	2.32	0.45
1:A:2074:U:H2'	1:A:2075:U:C6	2.52	0.45
1:A:2133:G:H1'	1:A:2158:A:H61	1.82	0.45
1:A:277:C:H3'	1:A:278:A:C5'	2.47	0.45
15:T:102:ILE:HA	15:T:105:LEU:CD2	2.47	0.45
18:W:97:LYS:HE2	18:W:99:ARG:NH2	2.31	0.45
21:Z:19:ARG:NH1	21:Z:84:GLU:HB2	2.32	0.45
26:4:16:CYS:HB3	26:4:33:VAL:HB	1.98	0.45
26:4:22:ILE:HG22	26:4:23:GLU:H	1.82	0.45
1:A:1349:A:N6	1:A:1598:C:N4	2.65	0.45
1:A:2283:C:H2'	1:A:2284:C:O4'	2.16	0.45
1:A:396:G:H1'	23:1:42:GLN:HB3	1.99	0.45
1:A:606:U:H4'	1:A:658:C:H4'	1.99	0.45
1:A:971:C:H2'	1:A:972:G:O4'	2.17	0.45
3:D:39:LYS:HB2	3:D:62:TYR:HB2	1.98	0.45
11:P:126:VAL:HG12	11:P:147:LEU:HD22	1.99	0.45
1:A:994:C:OP1	16:U:53:ARG:NH2	2.50	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
19:X:60:ARG:HH22	29:7:47:ARG:NH1	2.14	0.45
21:Z:80:ARG:NH2	21:Z:82:ARG:HH22	2.12	0.45
1:A:2355:C:O3'	22:0:24:LYS:HD2	2.17	0.45
1:A:1021:A:H62	1:A:1141:U:H3	1.65	0.45
1:A:1204:A:H2	1:A:1241:A:C2	2.35	0.45
1:A:1862:G:O2'	1:A:1863:G:H5'	2.17	0.45
1:A:2067:G:O2'	1:A:2069:G:H5''	2.17	0.45
1:A:2674:G:H2'	1:A:2675:A:C8	2.52	0.45
1:A:459:U:H2'	1:A:460:A:C8	2.52	0.45
4:E:167:VAL:HG21	4:E:187:ALA:CB	2.47	0.45
7:H:12:PRO:O	7:H:13:LYS:HB2	2.17	0.45
7:H:52:VAL:HG21	7:H:68:THR:HG22	1.99	0.45
1:A:1006:C:H5'	9:N:28:THR:HG23	1.98	0.45
14:S:88:ASP:HB3	14:S:89:ARG:H	1.47	0.45
24:2:41:ILE:HD11	24:2:44:LEU:CG	2.47	0.44
1:A:1187:G:H5''	17:V:81:TYR:CE2	2.52	0.44
7:H:3:ARG:NE	7:H:3:ARG:HA	2.33	0.44
1:A:2309:A:C6	1:A:2310:A:C2	3.05	0.44
1:A:643:A:N1	1:A:2369:A:O2'	2.44	0.44
1:A:862:G:H2'	1:A:863:A:O4'	2.17	0.44
8:I:120:ILE:HD11	8:I:126:TYR:CZ	2.52	0.44
10:O:17:ARG:NH2	10:O:47:ILE:HD13	2.33	0.44
10:O:86:ILE:HG22	10:O:94:ARG:HD3	2.00	0.44
18:W:33:ARG:NH2	18:W:52:GLU:OE1	2.50	0.44
19:X:35:THR:O	19:X:39:ILE:HG13	2.16	0.44
21:Z:82:ARG:HG3	21:Z:83:PRO:CD	2.47	0.44
23:1:53:VAL:HB	23:1:58:ILE:HD13	1.98	0.44
1:A:1109:C:O2'	1:A:1110:G:OP1	2.26	0.44
1:A:1164:G:H2'	1:A:1165:U:C6	2.52	0.44
1:A:1289:C:H2'	1:A:1290:C:C6	2.53	0.44
1:A:2282:G:H4'	1:A:2389:G:O2'	2.18	0.44
1:A:1638:C:H5''	1:A:2710:C:O2'	2.17	0.44
1:A:41:C:H2'	1:A:43:G:O4'	2.17	0.44
1:A:531:C:OP1	1:A:561:G:N1	2.50	0.44
1:A:99:U:H4'	1:A:101:G:C5'	2.48	0.44
9:N:62:VAL:HG12	9:N:66:LYS:HD2	1.98	0.44
1:A:587:C:O2	11:P:33:ARG:NH1	2.50	0.44
11:P:64:LYS:CB	30:8:25:MET:HG3	2.48	0.44
16:U:66:ASN:HB2	16:U:76:TYR:HB2	1.99	0.44
1:A:1204:A:C2	1:A:1241:A:C2	3.05	0.44
1:A:1371:G:HO2'	1:A:1372:U:H5	1.63	0.44
1:A:1930:G:O2'	1:A:1931:U:P	2.75	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2175:C:H2'	1:A:2176:A:O4'	2.17	0.44
1:A:2563:U:H1'	1:A:2566:A:N6	2.33	0.44
1:A:2867:G:O2'	1:A:2868:A:P	2.76	0.44
7:H:124:GLU:HB3	7:H:132:ARG:HG3	1.99	0.44
15:T:61:PHE:CE2	15:T:76:PHE:HB2	2.53	0.44
16:U:104:GLN:OE1	16:U:105:VAL:HG23	2.18	0.44
17:V:99:ILE:H	17:V:99:ILE:HD13	1.82	0.44
24:2:17:SER:CB	24:2:67:LYS:HE3	2.47	0.44
28:6:34:LEU:H	28:6:34:LEU:HD13	1.82	0.44
28:6:7:ILE:HA	28:6:7:ILE:HD12	1.85	0.44
1:A:1085:A:HO2'	1:A:1086:A:P	2.37	0.44
1:A:1469:A:H2'	1:A:1470:G:C8	2.53	0.44
1:A:1535:U:OP2	1:A:1537:C:N4	2.51	0.44
1:A:479:A:N3	1:A:481:G:H5"	2.32	0.44
5:F:63:LYS:HE3	5:F:65:TRP:O	2.18	0.44
6:G:114:ILE:HB	6:G:117:PHE:HB2	1.99	0.44
8:I:110:ASP:HB3	8:I:112:LYS:N	2.33	0.44
9:N:134:ARG:O	9:N:136:GLU:N	2.50	0.44
1:A:911:A:H2'	12:Q:9:TYR:OH	2.18	0.44
15:T:42:ILE:HG21	15:T:84:GLN:NE2	2.32	0.44
17:V:15:GLU:HG3	17:V:16:PRO:HD2	1.99	0.44
20:Y:51:VAL:O	20:Y:56:PRO:HA	2.18	0.44
22:0:43:THR:O	22:0:43:THR:HG23	2.17	0.44
1:A:77:C:O3'	24:2:14:ARG:NH2	2.51	0.44
1:A:1283:G:N2	1:A:1285:G:H3'	2.32	0.44
1:A:1537:C:H2'	1:A:1538:G:C8	2.53	0.44
1:A:2335:A:O2'	1:A:2336:A:H2'	2.17	0.44
1:A:2360:A:H2'	1:A:2361:A:O4'	2.18	0.44
1:A:71:A:H2	19:X:31:HIS:NE2	2.13	0.44
3:D:85:ASP:HB2	3:D:92:ILE:HD13	1.99	0.44
5:F:184:TYR:CE2	5:F:188:ARG:HD2	2.52	0.44
5:F:47:GLY:HA3	5:F:95:ARG:O	2.18	0.44
11:P:62:LEU:HB2	30:8:30:ARG:HH11	1.83	0.44
1:A:2336:A:H61	22:0:43:THR:HG21	1.82	0.44
26:4:48:ARG:CZ	26:4:51:ASP:HA	2.47	0.44
1:A:2056:G:H1	27:5:4:HIS:CD2	2.36	0.44
1:A:1509:C:H2'	1:A:1511:A:C8	2.53	0.44
1:A:2119:A:C2	1:A:2171:A:H1'	2.52	0.44
1:A:535:C:O3'	16:U:53:ARG:NH1	2.51	0.44
1:A:839:U:H2'	1:A:840:C:C6	2.53	0.44
3:D:61:LEU:HA	3:D:61:LEU:HD13	1.91	0.44
6:G:98:ARG:O	6:G:101:ILE:HG13	2.17	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2392:A:H8	11:P:60:MET:HG2	1.83	0.44
15:T:48:ILE:H	15:T:48:ILE:HD12	1.83	0.44
19:X:70:LEU:H	19:X:70:LEU:HD23	1.83	0.44
21:Z:52:SER:O	21:Z:54:HIS:N	2.50	0.44
24:2:31:GLU:HB2	24:2:53:LEU:HD11	2.00	0.44
26:4:35:VAL:C	26:4:37:SER:H	2.20	0.44
30:8:49:VAL:HG23	30:8:53:PRO:HB3	2.00	0.44
1:A:2051:A:H5'	1:A:2578:G:O4'	2.17	0.44
1:A:2097:C:H2'	1:A:2098:U:O4'	2.18	0.44
1:A:2872:G:O2'	1:A:2873:A:H5'	2.17	0.44
1:A:828:U:H4'	1:A:831:G:N1	2.33	0.44
4:E:37:ARG:O	4:E:45:THR:HA	2.18	0.44
1:A:674:G:C1'	5:F:74:ARG:HD3	2.41	0.44
6:G:10:LYS:HE2	6:G:175:LEU:O	2.18	0.44
6:G:47:LYS:HB2	6:G:47:LYS:HE3	1.73	0.44
21:Z:166:SER:HB2	21:Z:167:PRO:C	2.38	0.44
23:1:70:VAL:O	23:1:73:LEU:HB2	2.18	0.44
28:6:41:PRO:HD2	28:6:46:HIS:H	1.81	0.44
1:A:138:G:H2'	1:A:139:G:C8	2.52	0.44
1:A:1790:C:H2'	1:A:1791:A:C4	2.52	0.44
1:A:855:G:C6	1:A:856:C:C4	3.06	0.44
4:E:105:THR:OG1	4:E:199:ARG:NH1	2.50	0.44
8:I:130:TYR:N	8:I:136:VAL:O	2.51	0.44
1:A:636:G:OP1	11:P:132:LYS:HB2	2.18	0.44
1:A:1754:C:H5'	15:T:101:PHE:CE2	2.52	0.44
21:Z:19:ARG:HD3	21:Z:25:PRO:HD2	1.99	0.44
21:Z:52:SER:OG	21:Z:52:SER:O	2.30	0.44
1:A:1449:A:H5'	1:A:1449(A):G:OP2	2.18	0.43
1:A:1803:A:H4'	3:D:259:THR:HG23	2.00	0.43
6:G:67:LYS:HD2	6:G:67:LYS:O	2.17	0.43
11:P:126:VAL:HG12	11:P:147:LEU:CD2	2.48	0.43
23:1:94:LEU:HD23	23:1:94:LEU:HA	1.81	0.43
11:P:61:ARG:NH1	30:8:56:GLU:OE2	2.49	0.43
31:9:1:MET:O	31:9:34:GLN:HG2	2.18	0.43
1:A:1263:U:H1'	27:5:10:LYS:HG3	1.98	0.43
1:A:330:A:O2'	1:A:331:A:H8	2.01	0.43
1:A:729:G:OP2	3:D:13:ARG:NH1	2.50	0.43
1:A:892:G:N2	1:A:893:C:C2	2.86	0.43
5:F:66:PRO:O	5:F:68:LYS:N	2.51	0.43
7:H:4:ILE:HG12	7:H:4:ILE:H	1.59	0.43
7:H:67:LEU:O	7:H:71:LEU:HB2	2.17	0.43
1:A:389:G:H22	11:P:72:PRO:CG	2.30	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:1:25:LYS:C	23:1:27:GLU:H	2.22	0.43
1:A:1543:A:C2	1:A:1545:A:C4	3.06	0.43
1:A:2271:G:OP1	22:0:18:ALA:HB1	2.19	0.43
1:A:270(B):A:H61	1:A:270(Y):G:H1'	1.83	0.43
1:A:2845:G:O2'	1:A:2846:G:H5'	2.18	0.43
1:A:898:C:C2'	1:A:899:A:H5'	2.48	0.43
4:E:188:VAL:O	4:E:188:VAL:HG13	2.19	0.43
8:I:88:ILE:HG12	8:I:122:GLU:H	1.83	0.43
9:N:112:LEU:HG	9:N:112:LEU:O	2.17	0.43
13:R:38:VAL:HG22	13:R:112:ALA:HB2	2.00	0.43
13:R:34:ILE:HA	13:R:34:ILE:HD13	1.71	0.43
15:T:35:LYS:H	15:T:35:LYS:HD2	1.83	0.43
17:V:52:VAL:O	17:V:54:GLY:N	2.51	0.43
19:X:72:LYS:HG2	19:X:73:ARG:O	2.18	0.43
1:A:1268:A:H2'	1:A:1269:A:O4'	2.19	0.43
1:A:1796:U:H2'	1:A:1797:C:H6	1.79	0.43
1:A:2467:C:C2'	1:A:2468:G:H5'	2.48	0.43
1:A:2480:C:H2'	1:A:2481:G:H5'	1.99	0.43
1:A:654(A):G:N2	1:A:654(U):A:H1'	2.32	0.43
1:A:847:U:C5	1:A:933:A:N1	2.87	0.43
3:D:92:ILE:HD12	3:D:104:TYR:CD2	2.54	0.43
4:E:87:GLU:O	4:E:89:ASP:N	2.50	0.43
24:2:15:LYS:H	24:2:67:LYS:CE	2.32	0.43
25:3:51:ALA:HA	25:3:54:VAL:HG12	2.00	0.43
26:4:43:TYR:CD2	26:4:43:TYR:C	2.92	0.43
29:7:47:ARG:HB2	29:7:48:LYS:H	1.59	0.43
1:A:1021:A:C8	1:A:1022:G:H5''	2.46	0.43
1:A:1430:C:H2'	1:A:1431:U:H6	1.82	0.43
1:A:1512:G:H2'	1:A:1513:C:C6	2.54	0.43
1:A:1534:G:N3	1:A:1534:G:H2'	2.34	0.43
1:A:1742:C:H5'	1:A:1743:G:OP2	2.19	0.43
5:F:33:LEU:HD12	5:F:33:LEU:HA	1.86	0.43
5:F:64:ILE:HG23	5:F:65:TRP:CD1	2.53	0.43
10:O:64:ARG:HG2	10:O:79:PHE:CD1	2.53	0.43
10:O:88:ASN:OD1	10:O:90:GLN:HB2	2.19	0.43
10:O:88:ASN:ND2	10:O:92:GLU:HB2	2.23	0.43
1:A:956:G:C5'	12:Q:77:LYS:HE2	2.49	0.43
21:Z:5:LEU:HB3	21:Z:59:LEU:HA	2.00	0.43
13:R:33:ARG:HH21	27:5:55:ARG:HG2	1.82	0.43
1:A:1207:C:H2'	1:A:1208:C:H6	1.83	0.43
1:A:2238:G:H2'	1:A:2238:G:N3	2.31	0.43
1:A:71:A:H5''	1:A:72:U:H3'	2.01	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:825:C:O2	11:P:55:ARG:NH2	2.51	0.43
11:P:126:VAL:HG22	11:P:145:PRO:HG2	2.00	0.43
11:P:83:VAL:O	11:P:114:ILE:HA	2.19	0.43
14:S:39:ILE:HD12	14:S:85:VAL:HG11	2.00	0.43
17:V:55:ALA:HB2	17:V:101:GLY:HA2	2.00	0.43
19:X:53:LYS:H	19:X:82:GLN:HB3	1.83	0.43
20:Y:87:LYS:NZ	20:Y:87:LYS:HB2	2.33	0.43
24:2:47:ASN:HB2	24:2:48:HIS:H	1.50	0.43
1:A:2780:G:OP2	9:N:118:LYS:HE2	2.19	0.43
1:A:345:A:N3	1:A:347:A:N6	2.66	0.43
1:A:657:U:H2'	1:A:658:C:C6	2.54	0.43
3:D:132:PRO:HG3	3:D:190:TYR:CE1	2.54	0.43
4:E:119:ARG:HG2	4:E:160:TYR:HB2	2.00	0.43
11:P:113:LYS:HG2	11:P:115:LEU:HD23	2.01	0.43
11:P:30:THR:O	11:P:33:ARG:HB2	2.18	0.43
13:R:70:LEU:HA	13:R:70:LEU:HD23	1.84	0.43
1:A:1216:G:P	16:U:12:ARG:HH21	2.39	0.43
20:Y:67:LEU:HD12	20:Y:67:LEU:HA	1.78	0.43
20:Y:80:GLY:O	20:Y:81:LYS:HG3	2.18	0.43
21:Z:52:SER:C	21:Z:54:HIS:H	2.22	0.43
12:Q:20:ALA:HB3	21:Z:79:ARG:CZ	2.49	0.43
24:2:17:SER:HB3	24:2:67:LYS:HE3	2.00	0.43
1:A:1105:U:H2'	1:A:1106:G:H8	1.83	0.43
1:A:1198:U:H2'	1:A:1199:U:C6	2.54	0.43
1:A:1930:G:O2'	1:A:1931:U:O2	2.35	0.43
2:B:66:A:H61	2:B:107:U:H2'	1.84	0.43
4:E:4:ILE:HD12	4:E:28:ALA:HB1	2.01	0.43
6:G:145:THR:O	6:G:147:ASP:N	2.44	0.43
11:P:15:ARG:O	11:P:17:LYS:HG3	2.19	0.43
11:P:62:LEU:HB2	30:8:30:ARG:NH1	2.34	0.43
21:Z:70:LEU:HA	21:Z:70:LEU:HD23	1.91	0.43
25:3:7:LYS:HE2	25:3:32:GLN:O	2.19	0.43
26:4:6:HIS:HA	26:4:7:PRO:HD2	1.82	0.43
27:5:58:LEU:HB2	27:5:60:VAL:H	1.83	0.43
27:5:58:LEU:HD13	27:5:60:VAL:HB	2.01	0.43
28:6:28:ARG:HH21	28:6:30:THR:HG23	1.84	0.43
1:A:944:G:H5''	1:A:945:A:O5'	2.19	0.43
2:B:32:C:C2	2:B:51:G:N2	2.87	0.43
4:E:14:ILE:HG23	4:E:15:PHE:N	2.34	0.43
21:Z:141:VAL:CG2	21:Z:144:LEU:HB2	2.46	0.43
28:6:41:PRO:HG2	28:6:45:LYS:N	2.29	0.43
1:A:1243:G:O2'	11:P:7:ARG:NH2	2.42	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2056:G:C2	1:A:2057:A:C8	3.07	0.43
1:A:2250:G:C4	12:Q:82:ARG:HG3	2.53	0.43
1:A:2747:G:O6	1:A:2755:C:H5''	2.18	0.43
1:A:900:A:H5'	1:A:901:A:OP2	2.19	0.43
2:B:65:C:H41	2:B:108:C:H2'	1.84	0.43
4:E:201:THR:HG22	4:E:203:LYS:H	1.83	0.43
4:E:36:ARG:HH21	4:E:88:GLY:CA	2.32	0.43
12:Q:45:GLN:CD	12:Q:45:GLN:H	2.22	0.43
14:S:83:LYS:HZ1	14:S:109:GLY:HA2	1.83	0.43
17:V:64:HIS:ND1	17:V:92:THR:HG22	2.34	0.43
26:4:14:ILE:HG13	26:4:31:ILE:HB	1.99	0.42
1:A:1335:U:OP2	19:X:65:ARG:NH2	2.51	0.42
1:A:2068:U:N3	1:A:2430:A:H2	2.15	0.42
1:A:2716:U:O2'	1:A:2717:G:H5'	2.18	0.42
1:A:2850:A:C2	1:A:2851:A:C4	3.06	0.42
1:A:476:G:H4'	1:A:502:A:N1	2.34	0.42
4:E:111:ARG:HD2	4:E:160:TYR:CE1	2.54	0.42
11:P:125:VAL:CG1	11:P:138:LEU:HD21	2.49	0.42
21:Z:6:LYS:HB2	21:Z:6:LYS:HE3	1.88	0.42
1:A:1385:G:H4'	1:A:1386:C:OP1	2.19	0.42
1:A:2683:C:H4'	4:E:13:ARG:NH2	2.34	0.42
1:A:2749:A:H4'	7:H:62:LYS:HB3	2.00	0.42
2:B:80:U:H2'	2:B:81:G:H21	1.83	0.42
4:E:201:THR:HG22	4:E:203:LYS:N	2.34	0.42
6:G:31:VAL:HA	6:G:32:PRO:HD3	1.83	0.42
7:H:126:PRO:HB2	7:H:127:GLU:H	1.58	0.42
9:N:134:ARG:H	9:N:135:PRO:HD3	1.83	0.42
15:T:80:SER:HA	15:T:81:PRO:HD3	1.89	0.42
21:Z:157:LEU:HD22	21:Z:161:VAL:HB	2.01	0.42
21:Z:8:TYR:HA	21:Z:62:PRO:HD3	2.00	0.42
23:1:58:ILE:HG23	23:1:87:PRO:HG3	2.02	0.42
25:3:4:LEU:HD22	25:3:56:VAL:HG12	2.01	0.42
26:4:60:GLN:O	26:4:63:TYR:HB3	2.20	0.42
29:7:25:PRO:HA	29:7:28:ARG:CZ	2.49	0.42
1:A:1301:A:H2'	1:A:1301:A:N3	2.35	0.42
1:A:1416:G:H2'	1:A:1417:C:C6	2.54	0.42
7:H:159:GLU:O	7:H:160:LYS:HG2	2.19	0.42
15:T:45:PHE:CE1	15:T:65:LYS:HE3	2.55	0.42
18:W:86:LEU:HD22	18:W:96:ILE:HD12	2.01	0.42
22:0:53:MET:CB	22:0:59:LEU:HD23	2.50	0.42
28:6:15:GLU:HG2	28:6:49:HIS:NE2	2.34	0.42
30:8:52:LYS:N	30:8:53:PRO:HD2	2.33	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1025:G:C4	1:A:1135:C:H1'	2.53	0.42
1:A:1914:C:H2'	1:A:1915:U:O4'	2.19	0.42
1:A:2275:C:H5'	1:A:2275:C:C6	2.55	0.42
1:A:2524:G:H2'	1:A:2741:A:H2	1.84	0.42
1:A:2729:G:H1'	4:E:187:ALA:HB2	2.00	0.42
3:D:35:LYS:HE3	3:D:64:ILE:N	2.35	0.42
3:D:36:PRO:CB	3:D:61:LEU:HB3	2.50	0.42
4:E:57:LYS:HA	4:E:57:LYS:HD2	1.87	0.42
6:G:103:LEU:HA	6:G:103:LEU:HD23	1.83	0.42
6:G:16:ARG:N	6:G:17:PRO:HD2	2.34	0.42
7:H:126:PRO:HG2	7:H:128:PRO:HA	2.00	0.42
7:H:153:LYS:HB3	7:H:154:PRO:CD	2.49	0.42
9:N:96:GLU:HG2	9:N:97:ARG:H	1.84	0.42
11:P:39:LYS:HG3	11:P:45:LEU:CD2	2.45	0.42
12:Q:39:PRO:HA	12:Q:97:VAL:O	2.20	0.42
12:Q:76:LYS:HG3	12:Q:77:LYS:N	2.35	0.42
14:S:60:GLY:O	14:S:61:ASN:HB3	2.17	0.42
15:T:58:ASN:HD22	15:T:58:ASN:C	2.23	0.42
25:3:8:LEU:HB3	25:3:31:LEU:HA	2.01	0.42
1:A:2281:C:O2'	1:A:2282:G:H5'	2.20	0.42
1:A:263:C:H2'	1:A:264:C:O4'	2.18	0.42
1:A:2649:U:H2'	1:A:2650:U:C6	2.55	0.42
3:D:25:THR:HG22	3:D:82:ILE:H	1.84	0.42
1:A:1823:G:P	3:D:54:ARG:HH21	2.39	0.42
5:F:45:ARG:HH11	5:F:45:ARG:CG	2.33	0.42
6:G:64:THR:CG2	6:G:66:GLN:H	2.28	0.42
11:P:1:MET:HB3	11:P:2:LYS:H	1.61	0.42
14:S:81:GLY:O	14:S:83:LYS:N	2.53	0.42
22:0:27:GLU:HB2	22:0:69:PHE:CD1	2.53	0.42
24:2:8:LYS:HE3	24:2:8:LYS:HB2	1.83	0.42
1:A:1221:C:H2'	1:A:1222:C:C6	2.55	0.42
3:D:25:THR:HG21	3:D:81:ALA:HA	2.02	0.42
8:I:67:ARG:NH2	8:I:68:LEU:HB2	2.33	0.42
9:N:46:VAL:HG13	9:N:48:MET:HG3	2.02	0.42
10:O:21:CYS:O	10:O:22:ILE:HD13	2.20	0.42
14:S:106:ARG:HA	14:S:110:LEU:CD2	2.47	0.42
22:0:41:ARG:NE	22:0:41:ARG:HA	2.33	0.42
28:6:14:THR:HG21	28:6:19:ARG:HH21	1.85	0.42
1:A:2370:G:H21	28:6:45:LYS:CE	2.33	0.42
30:8:60:LEU:C	30:8:63:PRO:HD2	2.40	0.42
1:A:1188:U:O2'	1:A:1189:A:H5'	2.20	0.42
1:A:1792:G:P	3:D:206:LEU:HB2	2.60	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:582:G:H2'	1:A:583:G:C8	2.55	0.42
9:N:137:LYS:HD2	9:N:137:LYS:HA	1.77	0.42
1:A:1250:G:OP2	11:P:21:ARG:HD3	2.20	0.42
11:P:36:LYS:HB3	11:P:40:SER:CB	2.49	0.42
14:S:83:LYS:NZ	14:S:109:GLY:HA2	2.33	0.42
15:T:26:ASP:HB2	15:T:91:ARG:HA	2.00	0.42
16:U:109:LEU:HA	16:U:109:LEU:HD23	1.89	0.42
17:V:65:GLY:O	17:V:90:PRO:HA	2.20	0.42
26:4:68:ARG:HB2	26:4:69:LYS:H	1.51	0.42
1:A:1190:G:H5'	11:P:32:THR:HA	2.01	0.42
1:A:1859:A:N6	1:A:1883:G:O2'	2.52	0.42
1:A:2688:U:C5	1:A:2720:U:OP2	2.72	0.42
1:A:565:C:H2'	1:A:566:U:O4'	2.19	0.42
1:A:76:C:H1'	24:2:62:THR:HG21	2.00	0.42
3:D:89:SER:O	3:D:198:ASN:ND2	2.52	0.42
1:A:2784:C:O2'	4:E:37:ARG:NH1	2.52	0.42
14:S:38:GLN:HG3	14:S:47:THR:HG21	2.02	0.42
19:X:84:ALA:HB1	19:X:85:PRO:HD2	2.02	0.42
26:4:16:CYS:SG	26:4:36:CYS:HB3	2.59	0.42
26:4:39:CYS:O	26:4:40:HIS:HB2	2.20	0.42
30:8:44:LYS:N	30:8:44:LYS:HD2	2.34	0.42
1:A:1374:G:H2'	1:A:1375:C:O4'	2.20	0.42
1:A:141:A:H8	1:A:1408:C:H1'	1.85	0.42
1:A:1499:C:H2'	1:A:1500:G:H8	1.84	0.42
1:A:1510:A:O2'	1:A:1511:A:N7	2.47	0.42
1:A:70:G:H21	1:A:71:A:N6	2.17	0.42
3:D:34:VAL:HG22	3:D:35:LYS:HG3	2.00	0.42
7:H:30:LYS:HE2	7:H:81:GLU:H	1.85	0.42
8:I:133:HIS:HB2	8:I:134:PRO:CD	2.50	0.42
8:I:37:VAL:HG12	8:I:38:LEU:H	1.84	0.42
11:P:29:LYS:HD2	11:P:30:THR:CG2	2.50	0.42
19:X:26:TYR:HB3	19:X:92:LEU:HD12	2.02	0.42
21:Z:150:LEU:HD22	21:Z:171:ILE:HB	2.02	0.42
22:0:53:MET:HB3	22:0:59:LEU:HD23	2.01	0.42
26:4:37:SER:HB3	26:4:42:PHE:HB3	2.00	0.42
27:5:31:VAL:HG13	27:5:42:PRO:HG3	2.01	0.42
27:5:56:LYS:CD	27:5:56:LYS:H	2.29	0.42
30:8:26:LYS:HB3	30:8:44:LYS:HG3	2.01	0.42
1:A:142:G:H1'	19:X:37:THR:CG2	2.45	0.42
1:A:2712:U:OP1	1:A:2714:G:H4'	2.20	0.42
1:A:2845:G:H2'	1:A:2846:G:C8	2.55	0.42
1:A:415:A:H2'	1:A:416:C:C6	2.55	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:67:U:N3	1:A:74:A:H2	1.95	0.42
3:D:221:VAL:HG22	3:D:226:MET:CE	2.49	0.42
4:E:167:VAL:HG21	4:E:187:ALA:HB1	2.01	0.42
6:G:86:MET:HA	6:G:87:PRO:HD2	1.95	0.42
11:P:82:GLY:HA3	11:P:115:LEU:HD21	2.01	0.42
14:S:30:ARG:NH2	14:S:92:TYR:CD1	2.87	0.42
20:Y:51:VAL:HG23	20:Y:57:GLN:N	2.35	0.42
20:Y:96:ILE:HG13	20:Y:98:VAL:H	1.85	0.42
21:Z:1:MET:HG2	21:Z:2:GLU:H	1.85	0.42
1:A:1169:G:H1	1:A:1180:C:H42	1.68	0.41
1:A:1192:G:C2'	1:A:1193:G:H5'	2.50	0.41
1:A:565:C:H4'	1:A:1253:A:C6	2.55	0.41
1:A:1400:G:H2'	1:A:1401:G:C8	2.55	0.41
1:A:1469:A:H2'	1:A:1470:G:H8	1.84	0.41
1:A:1709:U:H2'	1:A:1710:C:C6	2.55	0.41
1:A:234:C:H2'	1:A:235:U:H6	1.84	0.41
1:A:556:G:H2'	1:A:557:U:C6	2.55	0.41
3:D:105:ILE:HA	3:D:105:ILE:HD12	1.55	0.41
3:D:232:PRO:HB3	3:D:244:ARG:CZ	2.50	0.41
8:I:98:ALA:HB2	8:I:111:PRO:HB3	2.01	0.41
9:N:35:ARG:HB2	9:N:42:TRP:CZ3	2.55	0.41
9:N:59:LYS:HE3	9:N:61:ARG:HH22	1.85	0.41
1:A:661:C:H5''	11:P:15:ARG:HH21	1.85	0.41
12:Q:85:LYS:O	12:Q:86:GLY:C	2.58	0.41
14:S:51:ALA:HB1	14:S:69:VAL:HG23	2.02	0.41
22:O:36:ILE:HD11	22:O:39:ARG:HG2	2.02	0.41
25:3:35:ARG:HB3	25:3:37:LEU:HD21	2.01	0.41
26:4:24:THR:OG1	26:4:25:TYR:N	2.53	0.41
1:A:1089:G:H21	1:A:1102:C:H42	1.68	0.41
1:A:1124:C:H2'	1:A:1125:G:O4'	2.20	0.41
1:A:729:G:H2'	1:A:1775:U:H1'	2.02	0.41
1:A:2293:C:OP1	14:S:89:ARG:NH1	2.53	0.41
1:A:251:A:H8	1:A:251:A:O5'	2.03	0.41
1:A:2693:A:H2'	1:A:2694:G:H8	1.85	0.41
1:A:2867:G:O2'	1:A:2868:A:C8	2.72	0.41
2:B:116:G:H4'	14:S:54:LEU:HD13	2.03	0.41
3:D:245:PRO:HA	3:D:246:PRO:HD3	1.87	0.41
4:E:144:ARG:HB3	4:E:145:LYS:H	1.45	0.41
4:E:181:LEU:HA	4:E:181:LEU:HD13	1.85	0.41
13:R:2:ARG:HG2	13:R:5:LYS:NZ	2.35	0.41
13:R:3:HIS:O	13:R:5:LYS:N	2.53	0.41
16:U:30:LYS:HA	16:U:30:LYS:HD3	1.90	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:1:76:ARG:HD2	23:1:76:ARG:H	1.84	0.41
23:1:89:GLU:HA	23:1:93:GLU:HB2	2.02	0.41
1:A:1107:G:H2'	1:A:1108:U:H6	1.85	0.41
1:A:2639:A:H1'	1:A:2778:A:C2	2.56	0.41
1:A:385:C:O2	11:P:71:VAL:HG21	2.20	0.41
1:A:630:G:OP2	30:8:15:LYS:NZ	2.53	0.41
1:A:685:A:H1'	1:A:688:U:O4	2.20	0.41
2:B:2:C:H2'	2:B:3:C:C6	2.55	0.41
5:F:117:ARG:HD2	5:F:120:GLU:OE2	2.20	0.41
6:G:165:THR:OG1	6:G:168:GLU:HG3	2.21	0.41
9:N:18:ALA:HB3	9:N:55:VAL:O	2.19	0.41
9:N:65:LYS:O	9:N:69:GLN:HG2	2.19	0.41
9:N:7:LYS:HD2	9:N:7:LYS:H	1.84	0.41
12:Q:54:MET:HB3	12:Q:64:ILE:HD13	2.01	0.41
16:U:69:CYS:HB3	16:U:106:PHE:CZ	2.56	0.41
17:V:22:VAL:HG12	17:V:23:GLU:H	1.85	0.41
20:Y:84:ARG:O	20:Y:95:LYS:HD3	2.20	0.41
29:7:47:ARG:HE	29:7:47:ARG:HB2	1.58	0.41
1:A:1101:U:H2'	1:A:1102:C:C6	2.56	0.41
1:A:174:C:H2'	1:A:175:G:O4'	2.21	0.41
1:A:2197:U:H1'	1:A:2198:A:C8	2.56	0.41
1:A:2210:G:H2'	1:A:2210:G:N3	2.35	0.41
1:A:2392:A:H2	1:A:2424:C:N4	2.10	0.41
1:A:2836:U:C4	1:A:2883:A:N6	2.89	0.41
1:A:572:A:H5''	1:A:573:G:OP2	2.20	0.41
1:A:593:G:O2'	30:8:61:LEU:HD13	2.20	0.41
2:B:41:U:O4	6:G:70:VAL:HG23	2.20	0.41
7:H:19:VAL:HG22	7:H:24:VAL:HG12	2.03	0.41
8:I:21:VAL:HG22	8:I:22:LYS:H	1.85	0.41
12:Q:19:GLY:O	12:Q:21:THR:OG1	2.23	0.41
1:A:2275:C:O2	12:Q:83:MET:HG3	2.19	0.41
14:S:107:GLU:N	14:S:110:LEU:HD11	2.35	0.41
17:V:38:LEU:O	17:V:51:VAL:HA	2.20	0.41
17:V:72:VAL:HG13	17:V:85:LYS:HG2	2.01	0.41
1:A:517:C:OP1	27:5:16:ARG:NH2	2.53	0.41
1:A:117:G:C6	1:A:119:A:C6	3.08	0.41
1:A:1209:G:H21	1:A:1210:A:H62	1.68	0.41
1:A:2286:A:H2'	28:6:31:PRO:HG2	2.02	0.41
1:A:2306:C:H2'	1:A:2307:G:N2	2.33	0.41
1:A:2528:U:H2'	1:A:2530:A:O5'	2.21	0.41
1:A:2811:G:H1	1:A:2889:C:H42	1.69	0.41
1:A:2862:G:H2'	1:A:2863:C:C6	2.56	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:783:A:H3'	1:A:783:A:C8	2.55	0.41
4:E:86:PRO:HB2	4:E:87:GLU:H	1.66	0.41
5:F:125:LEU:HA	5:F:194:MET:O	2.20	0.41
5:F:107:LYS:CD	5:F:207:GLY:H	2.30	0.41
6:G:166:ASP:OD1	6:G:166:ASP:N	2.54	0.41
1:A:2334:G:C2	14:S:12:PHE:CE2	3.08	0.41
20:Y:63:LYS:HD2	20:Y:63:LYS:HA	1.86	0.41
22:0:72:ARG:HB2	22:0:75:LEU:HB2	2.03	0.41
26:4:48:ARG:NH1	26:4:52:THR:H	2.19	0.41
1:A:1087:G:C5	1:A:1089:G:H1'	2.56	0.41
1:A:1411:C:H5'	1:A:1412:A:OP2	2.20	0.41
1:A:248:G:H5'	1:A:250:G:N7	2.36	0.41
1:A:792:G:H5''	1:A:793:A:H5'	2.01	0.41
1:A:2061:G:OP1	5:F:68:LYS:NZ	2.54	0.41
9:N:29:LYS:H	9:N:29:LYS:HG2	1.53	0.41
11:P:101:VAL:C	11:P:103:ALA:H	2.23	0.41
14:S:88:ASP:O	14:S:89:ARG:HB3	2.21	0.41
1:A:583:G:OP2	16:U:10:ARG:HD2	2.21	0.41
1:A:2421:G:OP1	28:6:6:ARG:NH2	2.54	0.41
1:A:1021:A:C8	1:A:1021:A:C3'	3.04	0.41
1:A:1085:A:O2'	1:A:1086:A:P	2.78	0.41
1:A:1317:A:H2'	1:A:1318:C:C6	2.55	0.41
1:A:1878:G:H2'	1:A:1879:C:H6	1.84	0.41
1:A:1919:A:H5''	1:A:1920:C:OP2	2.21	0.41
1:A:2134:A:OP2	1:A:2157:G:N2	2.53	0.41
1:A:2663:G:C6	1:A:2664:G:C4	3.09	0.41
1:A:2713:A:H3'	1:A:2714:G:H5''	2.02	0.41
1:A:273(F):C:H2'	1:A:274:G:H5''	2.03	0.41
1:A:820:A:H2'	1:A:821:A:O4'	2.20	0.41
8:I:115:ALA:HB3	8:I:128:LEU:HD12	2.02	0.41
8:I:23:PRO:O	8:I:27:ARG:HG2	2.21	0.41
12:Q:16:ARG:HB3	12:Q:17:LEU:H	1.76	0.41
16:U:98:LEU:HD23	16:U:99:ALA:N	2.36	0.41
17:V:72:VAL:CG1	17:V:85:LYS:HG2	2.50	0.41
1:A:1342:A:OP1	19:X:36:LYS:NZ	2.54	0.41
30:8:37:SER:O	30:8:40:GLU:HB3	2.21	0.41
31:9:2:LYS:HA	31:9:2:LYS:HD2	1.86	0.41
1:A:1107:G:H2'	1:A:1108:U:C6	2.56	0.41
1:A:1126:A:OP1	1:A:1126:A:H8	2.03	0.41
1:A:1265:A:OP1	1:A:1265:A:H8	2.04	0.41
1:A:2292:C:OP2	14:S:17:ARG:NH2	2.47	0.41
1:A:414:C:H1'	1:A:1864:U:O2'	2.21	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:102:LYS:C	3:D:103:ARG:HG2	2.40	0.41
3:D:3:VAL:HG13	3:D:17:THR:HG23	2.03	0.41
3:D:36:PRO:HB3	3:D:61:LEU:HB3	2.03	0.41
4:E:64:LYS:C	4:E:66:HIS:H	2.24	0.41
5:F:9:ILE:HD11	5:F:125:LEU:HG	2.03	0.41
6:G:103:LEU:O	6:G:107:LEU:HG	2.21	0.41
6:G:124:SER:HB2	6:G:131:TYR:CE1	2.56	0.41
8:I:57:ARG:O	8:I:61:ARG:HG2	2.20	0.41
9:N:7:LYS:H	9:N:7:LYS:NZ	2.18	0.41
16:U:8:VAL:O	16:U:12:ARG:HG3	2.20	0.41
21:Z:136:PHE:C	21:Z:137:ILE:HG12	2.41	0.41
1:A:1032:A:H2	1:A:1122:G:H22	1.68	0.41
1:A:1048:A:C5	1:A:1111:A:H2	2.39	0.41
1:A:1094:U:O2	1:A:1096:A:H5'	2.21	0.41
1:A:1682:G:H2'	1:A:1683:C:C6	2.55	0.41
1:A:2688:U:O2	1:A:2719:G:C6	2.74	0.41
1:A:2783:G:H2'	1:A:2784:C:C6	2.56	0.41
1:A:620:G:H4'	1:A:621:A:C5'	2.36	0.41
1:A:724:U:H2'	1:A:725:G:O4'	2.21	0.41
2:B:20:C:H2'	2:B:21:G:O4'	2.21	0.41
3:D:130:ALA:C	3:D:131:LEU:HD12	2.42	0.41
4:E:41:LYS:HA	4:E:41:LYS:HE2	2.02	0.41
9:N:96:GLU:O	9:N:100:GLU:HG3	2.20	0.41
21:Z:182:LYS:CB	21:Z:183:LEU:HA	2.51	0.41
23:1:83:GLU:C	23:1:85:LEU:H	2.24	0.41
28:6:36:LEU:HD13	28:6:50:ARG:CZ	2.51	0.41
1:A:1683:C:H2'	1:A:1684:C:C6	2.56	0.41
1:A:213:A:H2'	1:A:214:G:O4'	2.21	0.41
1:A:2772:C:H5'	4:E:168:MET:SD	2.60	0.41
1:A:2845:G:H2'	1:A:2846:G:H8	1.85	0.41
1:A:568:U:H5'	1:A:945:A:N1	2.36	0.41
1:A:649:G:C5	1:A:650:C:C4	3.08	0.41
3:D:145:VAL:HG11	3:D:175:LEU:HD11	2.02	0.41
4:E:32:PRO:HA	4:E:90:THR:HA	2.03	0.41
5:F:28:ILE:H	5:F:28:ILE:HG13	1.68	0.41
5:F:64:ILE:HD12	5:F:64:ILE:HA	1.80	0.41
5:F:67:GLN:HG3	5:F:67:GLN:O	2.21	0.41
11:P:106:LEU:O	11:P:107:LYS:HB2	2.20	0.41
12:Q:80:GLU:HB2	12:Q:81:VAL:H	1.69	0.41
13:R:44:LEU:HD22	13:R:48:VAL:HG23	2.02	0.41
16:U:17:ILE:HG23	16:U:39:LEU:HD12	2.02	0.41
16:U:92:ARG:NH2	17:V:11:GLN:H	2.18	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
16:U:92:ARG:HD2	16:U:95:LEU:HD12	2.02	0.41
19:X:31:HIS:HB3	19:X:34:ALA:HB2	2.03	0.41
21:Z:8:TYR:HD1	21:Z:38:TYR:CZ	2.39	0.41
1:A:1588:C:H2'	1:A:1589:C:H6	1.86	0.41
1:A:173:G:H2'	1:A:174:C:C6	2.56	0.41
1:A:1931:U:C5	1:A:1969:A:N7	2.89	0.41
1:A:297:C:H5''	20:Y:85:VAL:CG2	2.51	0.41
1:A:566:U:OP1	11:P:29:LYS:NZ	2.50	0.41
1:A:69:C:H2'	1:A:70:G:C8	2.55	0.41
1:A:747:U:OP2	27:5:3:LYS:HD2	2.21	0.41
3:D:201:HIS:O	3:D:204:ILE:HG12	2.21	0.41
3:D:35:LYS:HZ1	3:D:65:ILE:HA	1.86	0.41
4:E:95:ILE:CD1	4:E:95:ILE:H	2.31	0.41
10:O:4:PRO:O	10:O:5:GLN:CB	2.69	0.41
26:4:43:TYR:O	26:4:46:GLN:HA	2.20	0.40
26:4:48:ARG:HH12	26:4:52:THR:H	1.69	0.40
1:A:1331:A:C6	1:A:1333:C:C2	3.09	0.40
1:A:18:C:O3'	16:U:23:GLY:HA2	2.21	0.40
1:A:2108:C:H2'	1:A:2109:U:C6	2.56	0.40
1:A:270:A:H1'	1:A:370:G:C2	2.56	0.40
1:A:270(X):G:C6	1:A:270(Y):G:N1	2.89	0.40
1:A:654:A:O2'	1:A:654(A):G:OP2	2.36	0.40
1:A:654:A:HO2'	1:A:654(A):G:P	2.44	0.40
1:A:659:C:H2'	1:A:660:G:H8	1.85	0.40
6:G:18:GLU:OE1	6:G:22:ARG:NH1	2.49	0.40
6:G:61:ALA:HA	6:G:64:THR:HG22	2.02	0.40
7:H:125:VAL:HG22	7:H:131:VAL:HG13	2.02	0.40
11:P:29:LYS:HB3	11:P:30:THR:H	1.59	0.40
16:U:96:ALA:HA	16:U:98:LEU:HD23	2.03	0.40
28:6:13:CYS:HB2	28:6:22:ALA:HB3	2.03	0.40
1:A:1076:C:H2'	1:A:1077:A:H5''	2.03	0.40
1:A:1087:G:C4	1:A:1089:G:H1'	2.56	0.40
1:A:1209:G:N2	1:A:1210:A:H62	2.19	0.40
1:A:1550:C:H2'	1:A:1551:C:C6	2.55	0.40
1:A:2884:U:C2	27:5:51:TYR:HE1	2.39	0.40
1:A:549:G:H2'	1:A:550:G:O4'	2.21	0.40
1:A:593:G:C4'	30:8:4:MET:HE1	2.51	0.40
1:A:857:C:H1'	22:0:26:TYR:CE2	2.56	0.40
2:B:41:U:H5	6:G:70:VAL:O	2.04	0.40
3:D:62:TYR:HA	3:D:87:ASN:OD1	2.21	0.40
4:E:49:LEU:HA	4:E:49:LEU:HD12	1.71	0.40
6:G:7:LEU:HD12	6:G:104:GLU:HA	2.04	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:H:109:PHE:HZ	7:H:152:ARG:HG2	1.86	0.40
8:I:52:ARG:O	8:I:56:LYS:HB3	2.21	0.40
9:N:65:LYS:H	9:N:65:LYS:HG2	1.60	0.40
14:S:69:VAL:HA	14:S:72:ALA:HB3	2.03	0.40
28:6:11:LEU:HD13	28:6:11:LEU:HA	1.86	0.40
1:A:1071:G:O5'	1:A:1071:G:H8	2.03	0.40
1:A:1093:G:H5'	7:H:170:ARG:HH12	1.86	0.40
1:A:1790:C:H2'	1:A:1791:A:C5	2.56	0.40
1:A:1906:G:OP2	1:A:1930:G:H5''	2.21	0.40
1:A:1991:U:H2'	1:A:1992:G:H5''	2.03	0.40
1:A:2168:G:H2'	1:A:2168:G:N3	2.36	0.40
1:A:2477:C:O5'	1:A:2477:C:H6	2.04	0.40
1:A:2607:G:H2'	1:A:2608:G:O4'	2.20	0.40
1:A:2660:A:C2	1:A:2661:G:H1'	2.56	0.40
1:A:2722:G:H2'	1:A:2723:C:C6	2.56	0.40
1:A:468:G:C6	1:A:469:G:C4	3.09	0.40
1:A:849:A:N1	25:3:25:ALA:HB2	2.36	0.40
1:A:2635:C:H5'	4:E:77:ILE:HD13	2.04	0.40
5:F:168:ARG:HG3	5:F:175:THR:HG21	2.02	0.40
5:F:198:ALA:HA	5:F:201:VAL:HG12	2.03	0.40
8:I:56:LYS:HG3	8:I:57:ARG:N	2.34	0.40
21:Z:106:GLY:O	21:Z:141:VAL:HG13	2.20	0.40
25:3:12:PRO:O	25:3:14:GLY:N	2.55	0.40
25:3:52:HIS:CD2	25:3:53:LEU:HG	2.57	0.40
26:4:14:ILE:O	26:4:14:ILE:HG23	2.21	0.40
28:6:28:ARG:HB3	28:6:30:THR:C	2.41	0.40
1:A:1429:G:H2'	1:A:1430:C:C6	2.57	0.40
1:A:1698:A:H4'	1:A:1699:G:OP1	2.22	0.40
1:A:1759:A:H1'	1:A:2711:A:C2	2.57	0.40
1:A:661:C:H5''	11:P:15:ARG:NH2	2.37	0.40
1:A:699:A:H2'	1:A:700:G:O4'	2.22	0.40
2:B:66:A:O2'	2:B:67:G:P	2.80	0.40
1:A:1800:C:OP2	3:D:183:ARG:NH1	2.54	0.40
3:D:237:GLU:O	3:D:238:GLY:C	2.59	0.40
7:H:46:GLU:OE1	7:H:51:ARG:NH1	2.54	0.40
16:U:17:ILE:HD13	16:U:17:ILE:HA	1.92	0.40
16:U:19:LYS:O	16:U:22:LYS:HB2	2.22	0.40
1:A:65:C:H5'	19:X:71:GLY:HA3	2.03	0.40
20:Y:89:PHE:C	20:Y:90:LEU:HD13	2.42	0.40
21:Z:136:PHE:CD1	21:Z:138:GLU:HG3	2.56	0.40
21:Z:140:ASP:OD2	21:Z:140:ASP:N	2.51	0.40
1:A:1321:A:H2'	1:A:1322:A:O4'	2.21	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1406:U:H2'	1:A:1407:C:C6	2.57	0.40
1:A:141:A:H1'	1:A:1408:C:O4'	2.21	0.40
1:A:1547:C:O2'	1:A:1548:C:H5'	2.21	0.40
1:A:1931:U:H5	1:A:1969:A:N7	2.20	0.40
1:A:2025:C:H2'	1:A:2026:C:C6	2.55	0.40
1:A:226:G:O2'	1:A:227:A:P	2.79	0.40
1:A:305:U:H2'	1:A:306:U:C6	2.56	0.40
1:A:607:U:N3	1:A:621:A:C2	2.82	0.40
1:A:638:G:H2'	1:A:639:U:C6	2.56	0.40
1:A:69:C:H2'	1:A:70:G:H8	1.86	0.40
1:A:747:U:O2	1:A:2014:A:H1'	2.21	0.40
1:A:888:C:C3'	1:A:889:C:H4'	2.48	0.40
5:F:122:LYS:HA	5:F:122:LYS:HD3	1.86	0.40
5:F:125:LEU:HD21	5:F:199:TRP:CE3	2.57	0.40
8:I:110:ASP:HB2	8:I:130:TYR:HE1	1.87	0.40
8:I:90:GLY:O	8:I:121:LYS:HE2	2.21	0.40
16:U:61:TRP:O	16:U:65:ILE:HG13	2.22	0.40
17:V:21:ARG:HD2	17:V:91:TYR:CE1	2.56	0.40
17:V:3:ALA:HA	17:V:40:LEU:O	2.21	0.40
21:Z:28:MET:O	21:Z:34:ASN:HA	2.22	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	
3	D	270/276 (98%)	227 (84%)	34 (13%)	9 (3%)	6	23
4	E	203/206 (98%)	142 (70%)	41 (20%)	20 (10%)	1	2
5	F	200/210 (95%)	167 (84%)	25 (12%)	8 (4%)	5	16
6	G	179/182 (98%)	142 (79%)	25 (14%)	12 (7%)	2	4
7	H	168/180 (93%)	121 (72%)	23 (14%)	24 (14%)	0	1

Continued on next page...



Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	I	144/148 (97%)	104 (72%)	23 (16%)	17 (12%)	1	1
9	N	136/140 (97%)	106 (78%)	16 (12%)	14 (10%)	1	2
10	O	120/122 (98%)	108 (90%)	10 (8%)	2 (2%)	14	45
11	P	148/150 (99%)	108 (73%)	23 (16%)	17 (12%)	1	1
12	Q	139/141 (99%)	98 (70%)	22 (16%)	19 (14%)	0	1
13	R	116/118 (98%)	99 (85%)	11 (10%)	6 (5%)	3	9
14	S	109/112 (97%)	78 (72%)	18 (16%)	13 (12%)	1	1
15	T	135/146 (92%)	108 (80%)	17 (13%)	10 (7%)	2	4
16	U	115/118 (98%)	101 (88%)	10 (9%)	4 (4%)	6	21
17	V	99/101 (98%)	79 (80%)	12 (12%)	8 (8%)	1	3
18	W	111/113 (98%)	100 (90%)	9 (8%)	2 (2%)	13	43
19	X	90/96 (94%)	82 (91%)	6 (7%)	2 (2%)	10	37
20	Y	100/110 (91%)	70 (70%)	18 (18%)	12 (12%)	1	1
21	Z	181/206 (88%)	124 (68%)	40 (22%)	17 (9%)	1	2
22	0	80/85 (94%)	73 (91%)	7 (9%)	0	100	100
23	1	95/98 (97%)	72 (76%)	17 (18%)	6 (6%)	2	5
24	2	67/72 (93%)	55 (82%)	6 (9%)	6 (9%)	1	2
25	3	57/60 (95%)	52 (91%)	4 (7%)	1 (2%)	13	43
26	4	69/71 (97%)	35 (51%)	15 (22%)	19 (28%)	0	0
27	5	57/60 (95%)	46 (81%)	9 (16%)	2 (4%)	6	21
28	6	47/54 (87%)	22 (47%)	17 (36%)	8 (17%)	0	0
29	7	47/49 (96%)	43 (92%)	3 (6%)	1 (2%)	11	39
30	8	62/65 (95%)	48 (77%)	10 (16%)	4 (6%)	2	5
31	9	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
All	All	3379/3526 (96%)	2641 (78%)	475 (14%)	263 (8%)	1	3

All (263) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	26	LYS
3	D	28	GLU
3	D	122	ASP
3	D	123	ALA
4	E	2	LYS

Continued on next page...



*Continued from previous page...*

Mol	Chain	Res	Type
4	E	19	ARG
4	E	22	PRO
4	E	53	PRO
4	E	63	LEU
4	E	71	GLY
5	F	73	ALA
5	F	134	GLY
6	G	96	ARG
7	H	3	ARG
7	H	12	PRO
7	H	13	LYS
7	H	86	GLU
7	H	126	PRO
7	H	127	GLU
7	H	128	PRO
7	H	168	PRO
7	H	169	VAL
8	I	133	HIS
8	I	145	VAL
9	N	9	VAL
9	N	22	THR
9	N	36	GLY
11	P	6	LEU
11	P	10	PRO
11	P	14	LYS
11	P	15	ARG
11	P	25	SER
11	P	27	HIS
11	P	95	VAL
11	P	106	LEU
11	P	148	LEU
12	Q	18	LYS
12	Q	22	LYS
12	Q	25	ASP
12	Q	79	LEU
12	Q	86	GLY
12	Q	90	VAL
12	Q	134	ARG
13	R	3	HIS
14	S	82	ILE
14	S	88	ASP
14	S	107	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
15	T	2	ASN
15	T	123	GLN
15	T	124	ASP
16	U	90	VAL
16	U	91	ASP
16	U	93	LYS
17	V	45	THR
19	X	68	ARG
20	Y	50	ARG
20	Y	57	GLN
20	Y	77	PRO
20	Y	78	ALA
21	Z	6	LYS
21	Z	53	ILE
21	Z	146	ILE
21	Z	152	ALA
21	Z	159	PRO
23	1	30	VAL
23	1	84	GLY
23	1	91	LYS
23	1	95	LEU
24	2	16	LEU
24	2	43	GLN
24	2	47	ASN
24	2	48	HIS
26	4	24	THR
26	4	40	HIS
26	4	49	PHE
27	5	4	HIS
28	6	15	GLU
29	7	48	LYS
30	8	52	LYS
30	8	62	LEU
3	D	238	GLY
3	D	242	ARG
4	E	7	VAL
4	E	204	ALA
5	F	128	ALA
5	F	132	VAL
5	F	181	LEU
6	G	4	ASP
6	G	36	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
7	H	27	LYS
7	H	50	VAL
7	H	85	LYS
7	H	152	ARG
7	H	155	SER
9	N	23	LEU
9	N	96	GLU
10	O	5	GLN
11	P	66	GLY
11	P	93	GLY
11	P	141	ALA
12	Q	6	ARG
12	Q	60	ARG
12	Q	137	TYR
13	R	4	LEU
13	R	45	ARG
13	R	107	ASP
14	S	12	PHE
14	S	57	LYS
14	S	109	GLY
15	T	13	ARG
15	T	39	ARG
15	T	106	SER
17	V	31	ALA
17	V	48	GLY
17	V	79	VAL
18	W	111	HIS
20	Y	58	GLY
20	Y	102	CYS
21	Z	13	GLU
21	Z	81	ARG
24	2	70	GLN
24	2	71	ASN
26	4	5	ILE
26	4	18	CYS
26	4	22	ILE
26	4	37	SER
26	4	43	TYR
26	4	50	VAL
28	6	7	ILE
28	6	16	CYS
28	6	33	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	D	32	SER
4	E	20	ALA
4	E	50	GLY
4	E	79	ARG
4	E	90	THR
4	E	92	THR
4	E	117	MET
4	E	184	VAL
5	F	198	ALA
7	H	8	PRO
7	H	10	PRO
7	H	87	LEU
7	H	137	ASP
7	H	138	LYS
7	H	153	LYS
7	H	154	PRO
8	I	11	ASN
8	I	12	LEU
8	I	72	LEU
8	I	113	ARG
8	I	122	GLU
9	N	7	LYS
9	N	131	GLN
11	P	16	ARG
11	P	29	LYS
11	P	65	ARG
12	Q	19	GLY
12	Q	105	GLU
12	Q	133	ARG
13	R	86	ARG
14	S	4	LEU
14	S	11	LYS
15	T	97	ALA
17	V	49	THR
17	V	53	GLU
17	V	100	ARG
20	Y	42	VAL
20	Y	63	LYS
21	Z	59	LEU
21	Z	92	SER
21	Z	166	SER
25	3	3	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
26	4	9	LEU
26	4	23	GLU
26	4	30	GLU
26	4	34	GLU
26	4	66	SER
27	5	47	PRO
28	6	19	ARG
28	6	49	HIS
30	8	30	ARG
30	8	34	TRP
6	G	14	GLU
6	G	82	LEU
6	G	86	MET
6	G	116	ASP
7	H	83	TYR
8	I	10	GLU
8	I	87	LYS
8	I	114	LEU
9	N	11	PRO
9	N	28	THR
9	N	47	ALA
12	Q	104	PHE
12	Q	140	ALA
14	S	89	ARG
14	S	96	GLY
15	T	17	THR
19	X	40	LYS
20	Y	51	VAL
20	Y	53	PRO
21	Z	160	GLY
26	4	16	CYS
26	4	25	TYR
26	4	54	GLY
26	4	60	GLN
28	6	35	GLU
3	D	3	VAL
3	D	46	GLN
4	E	68	ALA
4	E	82	ARG
4	E	86	PRO
6	G	5	VAL
6	G	53	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
6	G	117	PHE
7	H	151	ILE
8	I	18	VAL
8	I	71	ILE
8	I	117	GLU
8	I	118	LYS
9	N	95	PRO
9	N	127	ASP
9	N	134	ARG
9	N	135	PRO
12	Q	11	LYS
12	Q	27	VAL
14	S	94	TYR
14	S	110	LEU
15	T	86	ILE
16	U	117	GLN
17	V	50	PRO
20	Y	39	VAL
21	Z	51	ALA
21	Z	61	LEU
21	Z	62	PRO
21	Z	168	GLU
21	Z	181	GLU
23	1	74	VAL
26	4	14	ILE
28	6	21	TYR
4	E	72	VAL
5	F	58	ALA
10	O	97	ARG
11	P	7	ARG
12	Q	62	GLY
12	Q	81	VAL
20	Y	3	VAL
23	1	55	GLY
8	I	15	VAL
5	F	66	PRO
8	I	16	GLY
15	T	37	GLY
21	Z	101	PRO
4	E	21	VAL
8	I	13	GLY
18	W	14	PRO

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
6	G	52	ILE
6	G	88	ILE
7	H	7	LEU
11	P	24	GLY
13	R	117	VAL
14	S	60	GLY

### 5.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	214/218 (98%)	181 (85%)	33 (15%)	4	11
4	E	165/166 (99%)	137 (83%)	28 (17%)	3	8
5	F	161/166 (97%)	137 (85%)	24 (15%)	4	12
6	G	155/156 (99%)	133 (86%)	22 (14%)	5	13
7	H	142/148 (96%)	115 (81%)	27 (19%)	2	6
8	I	122/124 (98%)	92 (75%)	30 (25%)	1	2
9	N	117/119 (98%)	96 (82%)	21 (18%)	2	7
10	O	100/100 (100%)	89 (89%)	11 (11%)	9	26
11	P	116/116 (100%)	82 (71%)	34 (29%)	0	1
12	Q	111/111 (100%)	92 (83%)	19 (17%)	3	8
13	R	101/101 (100%)	80 (79%)	21 (21%)	2	4
14	S	87/88 (99%)	68 (78%)	19 (22%)	1	4
15	T	120/127 (94%)	98 (82%)	22 (18%)	2	6
16	U	93/94 (99%)	77 (83%)	16 (17%)	3	8
17	V	82/82 (100%)	67 (82%)	15 (18%)	2	6
18	W	92/92 (100%)	76 (83%)	16 (17%)	3	8
19	X	74/78 (95%)	60 (81%)	14 (19%)	2	6
20	Y	85/91 (93%)	64 (75%)	21 (25%)	1	2
21	Z	162/179 (90%)	130 (80%)	32 (20%)	2	5
22	0	65/67 (97%)	59 (91%)	6 (9%)	13	37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	1	82/83 (99%)	70 (85%)	12 (15%)	5	12
24	2	64/67 (96%)	47 (73%)	17 (27%)	1	2
25	3	51/52 (98%)	43 (84%)	8 (16%)	4	10
26	4	63/63 (100%)	43 (68%)	20 (32%)	0	1
27	5	51/52 (98%)	37 (72%)	14 (28%)	0	1
28	6	48/52 (92%)	38 (79%)	10 (21%)	2	4
29	7	42/42 (100%)	35 (83%)	7 (17%)	3	8
30	8	54/55 (98%)	41 (76%)	13 (24%)	1	2
31	9	34/34 (100%)	32 (94%)	2 (6%)	28	63
All	All	2853/2923 (98%)	2319 (81%)	534 (19%)	2	6

All (534) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	5	LYS
3	D	17	THR
3	D	27	THR
3	D	28	GLU
3	D	30	GLU
3	D	38	LYS
3	D	43	ARG
3	D	44	ASN
3	D	49	ILE
3	D	65	ILE
3	D	73	VAL
3	D	88	ARG
3	D	94	LEU
3	D	95	LEU
3	D	103	ARG
3	D	105	ILE
3	D	106	ILE
3	D	111	LEU
3	D	112	GLN
3	D	141	VAL
3	D	192	THR
3	D	200	ASP
3	D	202	LYS
3	D	212	SER
3	D	217	ARG

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
3	D	218	ARG
3	D	221	VAL
3	D	229	VAL
3	D	237	GLU
3	D	242	ARG
3	D	257	LEU
3	D	259	THR
3	D	273	ARG
4	E	4	ILE
4	E	12	THR
4	E	13	ARG
4	E	16	ARG
4	E	17	ASP
4	E	26	ILE
4	E	27	LEU
4	E	41	LYS
4	E	42	ASP
4	E	49	LEU
4	E	77	ILE
4	E	79	ARG
4	E	82	ARG
4	E	92	THR
4	E	113	PHE
4	E	116	VAL
4	E	117	MET
4	E	119	ARG
4	E	127	ASP
4	E	128	SER
4	E	144	ARG
4	E	146	THR
4	E	154	LYS
4	E	175	VAL
4	E	197	ILE
4	E	200	GLU
4	E	202	LYS
4	E	203	LYS
5	F	9	ILE
5	F	32	LEU
5	F	33	LEU
5	F	38	ARG
5	F	45	ARG
5	F	65	TRP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	F	70	THR
5	F	78	ILE
5	F	105	VAL
5	F	106	ARG
5	F	107	LYS
5	F	117	ARG
5	F	127	GLU
5	F	161	GLU
5	F	164	ARG
5	F	165	ARG
5	F	170	LEU
5	F	174	VAL
5	F	176	LEU
5	F	181	LEU
5	F	183	VAL
5	F	196	LEU
5	F	197	ASP
5	F	206	ILE
6	G	3	LEU
6	G	7	LEU
6	G	22	ARG
6	G	31	VAL
6	G	34	LEU
6	G	43	LEU
6	G	45	GLU
6	G	58	GLN
6	G	63	ILE
6	G	66	GLN
6	G	67	LYS
6	G	80	PHE
6	G	82	LEU
6	G	84	LYS
6	G	88	ILE
6	G	90	LEU
6	G	94	LEU
6	G	116	ASP
6	G	118	ARG
6	G	145	THR
6	G	147	ASP
6	G	167	GLU
7	H	3	ARG
7	H	4	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
7	H	6	ARG
7	H	9	ILE
7	H	27	LYS
7	H	32	GLU
7	H	37	VAL
7	H	40	GLU
7	H	41	MET
7	H	53	GLU
7	H	59	ARG
7	H	77	LYS
7	H	88	LEU
7	H	89	ILE
7	H	103	LEU
7	H	105	LEU
7	H	122	THR
7	H	129	THR
7	H	132	ARG
7	H	136	ILE
7	H	139	GLN
7	H	143	GLN
7	H	149	ARG
7	H	152	ARG
7	H	153	LYS
7	H	155	SER
7	H	169	VAL
8	I	1	MET
8	I	2	LYS
8	I	9	LEU
8	I	10	GLU
8	I	20	ASP
8	I	27	ARG
8	I	33	ARG
8	I	35	LEU
8	I	38	LEU
8	I	40	THR
8	I	56	LYS
8	I	67	ARG
8	I	70	GLU
8	I	85	GLU
8	I	86	THR
8	I	87	LYS
8	I	88	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
8	I	92	VAL
8	I	101	LEU
8	I	110	ASP
8	I	112	LYS
8	I	113	ARG
8	I	130	TYR
8	I	131	LYS
8	I	135	GLU
8	I	136	VAL
8	I	138	ILE
8	I	139	GLN
8	I	140	LEU
8	I	142	VAL
9	N	2	LYS
9	N	5	VAL
9	N	7	LYS
9	N	32	THR
9	N	34	LEU
9	N	43	THR
9	N	48	MET
9	N	60	ILE
9	N	61	ARG
9	N	62	VAL
9	N	65	LYS
9	N	67	LEU
9	N	73	THR
9	N	90	MET
9	N	96	GLU
9	N	99	LEU
9	N	109	LYS
9	N	112	LEU
9	N	116	LEU
9	N	120	LEU
9	N	136	GLU
10	O	9	GLU
10	O	19	ILE
10	O	20	MET
10	O	23	ARG
10	O	24	VAL
10	O	31	LYS
10	O	47	ILE
10	O	49	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
10	O	53	LYS
10	O	66	LYS
10	O	91	LEU
11	P	6	LEU
11	P	7	ARG
11	P	9	ASN
11	P	14	LYS
11	P	16	ARG
11	P	19	VAL
11	P	21	ARG
11	P	27	HIS
11	P	29	LYS
11	P	32	THR
11	P	36	LYS
11	P	45	LEU
11	P	49	ARG
11	P	50	ARG
11	P	61	ARG
11	P	64	LYS
11	P	65	ARG
11	P	71	VAL
11	P	75	ILE
11	P	88	LEU
11	P	91	PHE
11	P	94	GLU
11	P	98	GLU
11	P	100	LEU
11	P	101	VAL
11	P	112	LEU
11	P	115	LEU
11	P	117	GLU
11	P	123	LEU
11	P	135	LEU
11	P	144	GLU
11	P	146	VAL
11	P	147	LEU
11	P	149	GLU
12	Q	5	ARG
12	Q	10	ARG
12	Q	25	ASP
12	Q	45	GLN
12	Q	55	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
12	Q	59	ARG
12	Q	71	ASP
12	Q	75	THR
12	Q	76	LYS
12	Q	79	LEU
12	Q	81	VAL
12	Q	82	ARG
12	Q	83	MET
12	Q	87	LYS
12	Q	103	MET
12	Q	112	GLU
12	Q	132	VAL
12	Q	135	ASP
12	Q	139	GLU
13	R	1	MET
13	R	18	LEU
13	R	28	LEU
13	R	29	LEU
13	R	34	ILE
13	R	36	THR
13	R	40	LYS
13	R	44	LEU
13	R	51	LEU
13	R	54	LEU
13	R	57	ARG
13	R	63	ARG
13	R	65	LEU
13	R	79	LEU
13	R	83	ILE
13	R	91	GLN
13	R	95	THR
13	R	100	LEU
13	R	102	GLU
13	R	104	ARG
13	R	105	ARG
14	S	10	ARG
14	S	12	PHE
14	S	14	VAL
14	S	15	ARG
14	S	20	ARG
14	S	25	ARG
14	S	27	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
14	S	44	LYS
14	S	54	LEU
14	S	56	LEU
14	S	58	LEU
14	S	69	VAL
14	S	78	LEU
14	S	83	LYS
14	S	85	VAL
14	S	89	ARG
14	S	103	GLU
14	S	106	ARG
14	S	111	GLU
15	T	17	THR
15	T	23	ARG
15	T	27	THR
15	T	28	VAL
15	T	40	THR
15	T	41	ARG
15	T	42	ILE
15	T	51	ARG
15	T	58	ASN
15	T	65	LYS
15	T	66	VAL
15	T	74	ARG
15	T	86	ILE
15	T	87	ASP
15	T	88	ILE
15	T	89	VAL
15	T	110	ILE
15	T	112	ARG
15	T	115	ARG
15	T	125	ARG
15	T	128	GLU
15	T	134	GLU
16	U	5	LYS
16	U	11	ARG
16	U	27	LEU
16	U	51	LYS
16	U	52	ARG
16	U	60	LEU
16	U	64	ARG
16	U	70	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
16	U	74	LEU
16	U	88	ILE
16	U	91	ASP
16	U	98	LEU
16	U	104	GLN
16	U	111	GLU
16	U	112	ARG
16	U	114	LYS
17	V	7	THR
17	V	10	LYS
17	V	13	ARG
17	V	19	LYS
17	V	35	LEU
17	V	39	LEU
17	V	40	LEU
17	V	45	THR
17	V	61	VAL
17	V	66	ARG
17	V	72	VAL
17	V	73	SER
17	V	78	LYS
17	V	79	VAL
17	V	99	ILE
18	W	11	ARG
18	W	16	LYS
18	W	23	LEU
18	W	37	ARG
18	W	40	ASN
18	W	51	LEU
18	W	67	ASP
18	W	69	LEU
18	W	76	VAL
18	W	88	ARG
18	W	92	ARG
18	W	95	ILE
18	W	96	ILE
18	W	100	THR
18	W	106	ILE
18	W	107	LEU
19	X	6	ASP
19	X	12	VAL
19	X	15	GLU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
19	X	27	THR
19	X	36	LYS
19	X	43	VAL
19	X	49	VAL
19	X	57	LEU
19	X	59	VAL
19	X	63	LYS
19	X	65	ARG
19	X	66	LEU
19	X	80	ILE
19	X	88	LYS
20	Y	14	LEU
20	Y	26	LYS
20	Y	27	VAL
20	Y	28	LYS
20	Y	29	GLU
20	Y	34	LYS
20	Y	38	ILE
20	Y	44	ILE
20	Y	57	GLN
20	Y	61	ILE
20	Y	64	GLU
20	Y	67	LEU
20	Y	71	LYS
20	Y	73	ARG
20	Y	75	ILE
20	Y	86	ARG
20	Y	87	LYS
20	Y	89	PHE
20	Y	90	LEU
20	Y	95	LYS
20	Y	97	ARG
21	Z	2	GLU
21	Z	4	ARG
21	Z	5	LEU
21	Z	8	TYR
21	Z	10	ARG
21	Z	18	LEU
21	Z	19	ARG
21	Z	20	ARG
21	Z	31	ARG
21	Z	41	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
21	Z	53	ILE
21	Z	74	VAL
21	Z	76	LEU
21	Z	81	ARG
21	Z	93	ASP
21	Z	94	GLU
21	Z	95	PRO
21	Z	112	ARG
21	Z	122	ARG
21	Z	129	SER
21	Z	133	ILE
21	Z	137	ILE
21	Z	140	ASP
21	Z	141	VAL
21	Z	144	LEU
21	Z	150	LEU
21	Z	151	HIS
21	Z	153	SER
21	Z	156	LYS
21	Z	163	LEU
21	Z	166	SER
21	Z	180	VAL
22	0	9	SER
22	0	11	ARG
22	0	36	ILE
22	0	55	ARG
22	0	64	ASP
22	0	74	ARG
23	1	30	VAL
23	1	46	LEU
23	1	50	ARG
23	1	51	VAL
23	1	56	GLN
23	1	62	VAL
23	1	78	LYS
23	1	80	LEU
23	1	82	LEU
23	1	83	GLU
23	1	91	LYS
23	1	92	LYS
24	2	4	SER
24	2	7	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
24	2	9	GLN
24	2	16	LEU
24	2	23	LYS
24	2	24	LEU
24	2	27	GLU
24	2	32	LEU
24	2	34	GLU
24	2	41	ILE
24	2	47	ASN
24	2	50	ILE
24	2	51	ARG
24	2	52	ASP
24	2	53	LEU
24	2	64	LEU
24	2	65	ASN
25	3	6	VAL
25	3	8	LEU
25	3	23	LEU
25	3	30	ARG
25	3	31	LEU
25	3	36	VAL
25	3	37	LEU
25	3	56	VAL
26	4	6	HIS
26	4	10	VAL
26	4	15	ILE
26	4	16	CYS
26	4	22	ILE
26	4	27	THR
26	4	34	GLU
26	4	39	CYS
26	4	42	PHE
26	4	43	TYR
26	4	48	ARG
26	4	49	PHE
26	4	53	GLU
26	4	57	GLU
26	4	58	ARG
26	4	61	ARG
26	4	63	TYR
26	4	67	TYR
26	4	68	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
26	4	71	ARG
27	5	3	LYS
27	5	4	HIS
27	5	6	VAL
27	5	11	THR
27	5	29	THR
27	5	36	CYS
27	5	37	LYS
27	5	40	LYS
27	5	48	GLU
27	5	49	CYS
27	5	51	TYR
27	5	52	TYR
27	5	56	LYS
27	5	58	LEU
28	6	6	ARG
28	6	8	LYS
28	6	11	LEU
28	6	19	ARG
28	6	23	THR
28	6	30	THR
28	6	33	LYS
28	6	34	LEU
28	6	37	ARG
28	6	44	ARG
29	7	1	MET
29	7	4	THR
29	7	8	ASN
29	7	9	ARG
29	7	10	ARG
29	7	14	LYS
29	7	47	ARG
30	8	13	ARG
30	8	14	VAL
30	8	15	LYS
30	8	29	LYS
30	8	30	ARG
30	8	34	TRP
30	8	43	GLN
30	8	44	LYS
30	8	47	LYS
30	8	56	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
30	8	58	ILE
30	8	64	TYR
30	8	65	GLU
31	9	1	MET
31	9	17	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
15	T	58	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2880/2916 (98%)	623 (21%)	75 (2%)
2	B	119/122 (97%)	29 (24%)	3 (2%)
32	a	1/3 (33%)	0	0
All	All	3000/3041 (98%)	652 (21%)	78 (2%)

All (652) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	U
1	A	15	G
1	A	27	G
1	A	34	C
1	A	35	G
1	A	46	C
1	A	55	G
1	A	71	A
1	A	74	A
1	A	75	G
1	A	96	G
1	A	99	U
1	A	101	G
1	A	102	G
1	A	103	A
1	A	118	A
1	A	119	A
1	A	120	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	125	G
1	A	138	G
1	A	155	C
1	A	161	U
1	A	162	U
1	A	177	G
1	A	188	G
1	A	196	A
1	A	214	G
1	A	215	G
1	A	216	A
1	A	221	A
1	A	222	A
1	A	223	A
1	A	227	A
1	A	229	A
1	A	230	U
1	A	232	G
1	A	242	G
1	A	243	U
1	A	248	G
1	A	252	G
1	A	261	G
1	A	264	C
1	A	265	A
1	A	266	G
1	A	269	U
1	A	270(L)	U
1	A	270(M)	U
1	A	270(N)	G
1	A	270(P)	C
1	A	271(A)	C
1	A	271(B)	G
1	A	271(C)	U
1	A	271	G
1	A	274	G
1	A	275	G
1	A	276	A
1	A	278	A
1	A	279	C
1	A	299	A
1	A	311	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	316	C
1	A	323	G
1	A	324	A
1	A	329	G
1	A	330	A
1	A	332	A
1	A	342	G
1	A	352	G
1	A	363	G
1	A	364	C
1	A	371	A
1	A	372	G
1	A	373	U
1	A	380	U
1	A	386	G
1	A	387	U
1	A	396	G
1	A	405	U
1	A	406	G
1	A	411	G
1	A	412	A
1	A	428	A
1	A	441	U
1	A	443	A
1	A	444	C
1	A	448	U
1	A	455	C
1	A	457	A
1	A	470	A
1	A	481	G
1	A	496	G
1	A	503	A
1	A	504	U
1	A	505	A
1	A	509	C
1	A	512	G
1	A	518	G
1	A	531	C
1	A	532	A
1	A	533	G
1	A	537	C
1	A	539	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	540	G
1	A	546	C
1	A	547	A
1	A	549	G
1	A	562	U
1	A	563	G
1	A	573	G
1	A	574	C
1	A	575	A
1	A	586	A
1	A	588	U
1	A	603	A
1	A	607	U
1	A	613	U
1	A	614	U
1	A	615	G
1	A	616	A
1	A	617	G
1	A	621	A
1	A	622	G
1	A	624	C
1	A	626	U
1	A	627	A
1	A	634	C
1	A	637	A
1	A	638	G
1	A	645	C
1	A	646	A
1	A	650	C
1	A	651	G
1	A	654	A
1	A	654(A)	G
1	A	654(B)	C
1	A	654(T)	C
1	A	657	U
1	A	664	C
1	A	670	A
1	A	686	G
1	A	702	G
1	A	717	G
1	A	722	A
1	A	730	C

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	734	A
1	A	747	U
1	A	750	A
1	A	752	A
1	A	753	C
1	A	764	A
1	A	765	G
1	A	776	G
1	A	782	A
1	A	784	A
1	A	785	G
1	A	790	C
1	A	792	G
1	A	793	A
1	A	805	G
1	A	806	C
1	A	812	C
1	A	819	A
1	A	827	U
1	A	828	U
1	A	831	G
1	A	846	C
1	A	847	U
1	A	856	C
1	A	857	C
1	A	859	G
1	A	860	U
1	A	866	A
1	A	881	G
1	A	882	G
1	A	884	C
1	A	885	C
1	A	886	C
1	A	888	C
1	A	889	C
1	A	890	A
1	A	896	A
1	A	899	A
1	A	900	A
1	A	901	A
1	A	902	C
1	A	904	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	907	U
1	A	910	A
1	A	915	C
1	A	917	A
1	A	932	G
1	A	938	G
1	A	941	A
1	A	945	A
1	A	946	G
1	A	959	A
1	A	961	C
1	A	974	G
1	A	974(A)	C
1	A	975	G
1	A	980	A
1	A	983	A
1	A	990	A
1	A	991	C
1	A	996	A
1	A	1003	G
1	A	1005	C
1	A	1011	G
1	A	1012	U
1	A	1013	C
1	A	1022	G
1	A	1023	U
1	A	1025	G
1	A	1026	U
1	A	1027	A
1	A	1033	U
1	A	1045	A
1	A	1046	A
1	A	1050	A
1	A	1054	A
1	A	1055	G
1	A	1059	G
1	A	1060	U
1	A	1061	U
1	A	1066	U
1	A	1067	A
1	A	1068	G
1	A	1071	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	1076	C
1	A	1077	A
1	A	1078	U
1	A	1079	C
1	A	1082	U
1	A	1083	U
1	A	1084	A
1	A	1085	A
1	A	1086	A
1	A	1088	A
1	A	1089	G
1	A	1090	U
1	A	1095	A
1	A	1096	A
1	A	1097	U
1	A	1099	G
1	A	1103	A
1	A	1104	C
1	A	1105	U
1	A	1110	G
1	A	1111	A
1	A	1122	G
1	A	1128	A
1	A	1130	U
1	A	1131	G
1	A	1135	C
1	A	1136	G
1	A	1139	G
1	A	1142	U
1	A	1142(A)	A
1	A	1148	A
1	A	1169	G
1	A	1170	G
1	A	1173	G
1	A	1174	A
1	A	1175	U
1	A	1176	G
1	A	1178	C
1	A	1179	C
1	A	1180	C
1	A	1195	G
1	A	1204	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	1205	U
1	A	1211	U
1	A	1220	A
1	A	1221	C
1	A	1228	G
1	A	1238	G
1	A	1241	A
1	A	1250	G
1	A	1253	A
1	A	1256	G
1	A	1265	A
1	A	1271	G
1	A	1272	A
1	A	1273	U
1	A	1284	A
1	A	1300	U
1	A	1301	A
1	A	1321	A
1	A	1329	U
1	A	1345	C
1	A	1349	A
1	A	1352	U
1	A	1365	A
1	A	1368	G
1	A	1379	A
1	A	1384	A
1	A	1385	G
1	A	1386	C
1	A	1388	G
1	A	1389	G
1	A	1390	U
1	A	1391	U
1	A	1395	A
1	A	1407	C
1	A	1411	C
1	A	1416	G
1	A	1417	C
1	A	1419	A
1	A	1420	U
1	A	1421	G
1	A	1428	C
1	A	1444(A)	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	1445	C
1	A	1449	A
1	A	1449(A)	G
1	A	1453	A
1	A	1455	G
1	A	1458	C
1	A	1460	A
1	A	1461	G
1	A	1467	C
1	A	1471	A
1	A	1482	U
1	A	1483	G
1	A	1485	G
1	A	1486	A
1	A	1487	G
1	A	1493	C
1	A	1495	A
1	A	1497	U
1	A	1505	C
1	A	1506	C
1	A	1507	A
1	A	1508	A
1	A	1510	A
1	A	1511	A
1	A	1514	U
1	A	1519	G
1	A	1520	U
1	A	1522	G
1	A	1534	G
1	A	1535	U
1	A	1536	A
1	A	1537	C
1	A	1543	A
1	A	1544	C
1	A	1545	A
1	A	1547	C
1	A	1554	A
1	A	1558	A
1	A	1559	G
1	A	1566	A
1	A	1569	A
1	A	1578	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	1579	A
1	A	1581	G
1	A	1585	C
1	A	1586	A
1	A	1591	G
1	A	1593	G
1	A	1598	C
1	A	1608	A
1	A	1609	A
1	A	1610	A
1	A	1616	A
1	A	1617	C
1	A	1618	A
1	A	1634	A
1	A	1640	C
1	A	1648	C
1	A	1654	A
1	A	1668	A
1	A	1674	G
1	A	1678	G
1	A	1681	G
1	A	1688	U
1	A	1695	G
1	A	1697	G
1	A	1699	G
1	A	1700	A
1	A	1701	A
1	A	1725	G
1	A	1729	A
1	A	1730	U
1	A	1731	G
1	A	1732	A
1	A	1733	G
1	A	1742	C
1	A	1743	G
1	A	1750	G
1	A	1753	G
1	A	1754	C
1	A	1756	G
1	A	1762	A
1	A	1763	G
1	A	1764	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	1773	A
1	A	1780	A
1	A	1786	A
1	A	1791	A
1	A	1799	G
1	A	1800	C
1	A	1801	G
1	A	1811	G
1	A	1816	G
1	A	1820	U
1	A	1829	A
1	A	1835	G
1	A	1836	C
1	A	1847	A
1	A	1848	A
1	A	1849	G
1	A	1858	G
1	A	1869	G
1	A	1870	C
1	A	1872	A
1	A	1878	G
1	A	1882	C
1	A	1889	A
1	A	1896	G
1	A	1899	G
1	A	1906	G
1	A	1919	A
1	A	1924	C
1	A	1930	G
1	A	1931	U
1	A	1937	A
1	A	1938	A
1	A	1939	U
1	A	1955	U
1	A	1956	U
1	A	1960	A
1	A	1963	U
1	A	1965	C
1	A	1967	C
1	A	1969	A
1	A	1970	A
1	A	1971	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	1972	A
1	A	1982	C
1	A	1987	G
1	A	1991	U
1	A	1992	G
1	A	1993	U
1	A	2020	A
1	A	2021	C
1	A	2023	G
1	A	2031	A
1	A	2032	G
1	A	2033	A
1	A	2034	U
1	A	2043	C
1	A	2055	C
1	A	2056	G
1	A	2059	A
1	A	2060	A
1	A	2061	G
1	A	2062	A
1	A	2069	G
1	A	2089	U
1	A	2093	G
1	A	2099	U
1	A	2100	G
1	A	2111	C
1	A	2112	G
1	A	2113	U
1	A	2114	A
1	A	2115	G
1	A	2116	G
1	A	2117	A
1	A	2119	A
1	A	2120	G
1	A	2126	A
1	A	2127	G
1	A	2128	C
1	A	2131	G
1	A	2132	U
1	A	2133	G
1	A	2136	C
1	A	2146	C

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	2148	G
1	A	2158	A
1	A	2166	G
1	A	2167	U
1	A	2168	G
1	A	2169	A
1	A	2173	A
1	A	2176	A
1	A	2178	C
1	A	2181	G
1	A	2190	G
1	A	2192	G
1	A	2194	G
1	A	2198	A
1	A	2210	G
1	A	2211	G
1	A	2212	A
1	A	2215	G
1	A	2225	A
1	A	2238	G
1	A	2239	G
1	A	2246	G
1	A	2268	A
1	A	2273	A
1	A	2275	C
1	A	2283	C
1	A	2287	A
1	A	2288	A
1	A	2302	G
1	A	2307	G
1	A	2308	G
1	A	2311	A
1	A	2319	G
1	A	2320	A
1	A	2325	G
1	A	2334	G
1	A	2346	A
1	A	2347	C
1	A	2350	C
1	A	2377	A
1	A	2379	G
1	A	2382	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	2383	G
1	A	2385	C
1	A	2395	C
1	A	2402	C
1	A	2403	C
1	A	2405	G
1	A	2406	U
1	A	2410	G
1	A	2423	U
1	A	2425	A
1	A	2429	G
1	A	2430	A
1	A	2435	A
1	A	2439	A
1	A	2440	C
1	A	2441	C
1	A	2448	A
1	A	2450	A
1	A	2468	G
1	A	2469	A
1	A	2470	G
1	A	2471	C
1	A	2475	C
1	A	2476	A
1	A	2480	C
1	A	2482	G
1	A	2484	G
1	A	2494	G
1	A	2498	C
1	A	2502	G
1	A	2505	G
1	A	2518	A
1	A	2529	G
1	A	2542	A
1	A	2543	G
1	A	2554	U
1	A	2558	C
1	A	2566	A
1	A	2567	G
1	A	2573	C
1	A	2585	U
1	A	2602	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	2609	U
1	A	2610	C
1	A	2611	U
1	A	2612	C
1	A	2613	U
1	A	2629	A
1	A	2632	A
1	A	2655	G
1	A	2656	U
1	A	2665	A
1	A	2673	G
1	A	2675	A
1	A	2682	U
1	A	2689	U
1	A	2690	C
1	A	2691	C
1	A	2702	U
1	A	2707	G
1	A	2712	U
1	A	2712(A)	A
1	A	2713	A
1	A	2714	G
1	A	2726	U
1	A	2733	A
1	A	2734	A
1	A	2744	G
1	A	2752	C
1	A	2757	A
1	A	2758	A
1	A	2761	G
1	A	2765	A
1	A	2766	G
1	A	2770	G
1	A	2777	G
1	A	2778	A
1	A	2779	U
1	A	2780	G
1	A	2785	C
1	A	2789	C
1	A	2790	A
1	A	2791	C
1	A	2797	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	2807	G
1	A	2808	U
1	A	2818	G
1	A	2820	A
1	A	2821	A
1	A	2830	G
1	A	2833	G
1	A	2834	G
1	A	2835	A
1	A	2847	U
1	A	2867	G
1	A	2868	A
1	A	2872	G
1	A	2873	A
1	A	2880	C
1	A	2892	A
1	A	2894	G
2	B	2	C
2	B	8	U
2	B	9	G
2	B	13	A
2	B	15	A
2	B	19	G
2	B	21	G
2	B	24	G
2	B	25	A
2	B	26	A
2	B	27	C
2	B	31	C
2	B	32	C
2	B	40	U
2	B	41	U
2	B	42	C
2	B	44	G
2	B	45	A
2	B	47	C
2	B	52	A
2	B	53	A
2	B	56	G
2	B	67	G
2	B	72	G
2	B	73	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	81	G
2	B	89	G
2	B	108	C
2	B	109	G

All (78) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	71	A
1	A	74	A
1	A	99	U
1	A	102	G
1	A	195	A
1	A	196	A
1	A	199	A
1	A	221	A
1	A	222	A
1	A	229	A
1	A	242	G
1	A	271(B)	G
1	A	278	A
1	A	372	G
1	A	404	C
1	A	503	A
1	A	508	G
1	A	562	U
1	A	587	C
1	A	637	A
1	A	653	A
1	A	654	A
1	A	669	G
1	A	752	A
1	A	764	A
1	A	846	C
1	A	856	C
1	A	859	G
1	A	974	G
1	A	974(A)	C
1	A	1022	G
1	A	1026	U
1	A	1045	A
1	A	1078	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	1085	A
1	A	1109	C
1	A	1130	U
1	A	1141	U
1	A	1178	C
1	A	1204	A
1	A	1210	A
1	A	1379	A
1	A	1427	A
1	A	1558	A
1	A	1608	A
1	A	1609	A
1	A	1617	C
1	A	1653	G
1	A	1694	C
1	A	1698	A
1	A	1799	G
1	A	1819	A
1	A	1847	A
1	A	1929	G
1	A	1930	G
1	A	1939	U
1	A	1955	U
1	A	1992	G
1	A	2126	A
1	A	2238	G
1	A	2288	A
1	A	2382	G
1	A	2405	G
1	A	2439	A
1	A	2481	G
1	A	2566	A
1	A	2610	C
1	A	2655	G
1	A	2681	C
1	A	2689	U
1	A	2712	U
1	A	2756	U
1	A	2776	A
1	A	2832	U
1	A	2867	G
2	B	24	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	66	A
2	B	108	C

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
32	PPU	a	76	1,32	38,40,41	2.42	9 (23%)	54,57,60	2.61	14 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	PPU	a	76	1,32	-	0/26/43/44	0/4/4/4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	a	76	PPU	O-C	9.19	1.41	1.23
32	a	76	PPU	C9-N6	-5.44	1.32	1.45
32	a	76	PPU	C-N3'	5.37	1.46	1.34
32	a	76	PPU	C10-N6	-5.11	1.32	1.45
32	a	76	PPU	C4-N9	-3.15	1.33	1.37
32	a	76	PPU	C8-N9	-3.04	1.32	1.36
32	a	76	PPU	O4'-C1'	2.91	1.44	1.41
32	a	76	PPU	C6-C5	-2.56	1.40	1.44
32	a	76	PPU	C5-N7	-2.01	1.32	1.39

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	a	76	PPU	N3-C2-N1	-8.55	121.37	128.89
32	a	76	PPU	C3'-N3'-C	-8.15	110.22	123.19
32	a	76	PPU	C5-C4-N3	-6.29	119.85	125.98
32	a	76	PPU	C2'-C1'-N9	-5.46	98.49	113.35
32	a	76	PPU	C2'-C3'-N3'	5.17	125.08	113.08
32	a	76	PPU	C2-N1-C6	4.71	121.72	111.52
32	a	76	PPU	C4'-O4'-C1'	-3.94	105.39	109.72
32	a	76	PPU	N3-C4-N9	3.87	132.03	125.39
32	a	76	PPU	C4-C5-N7	-3.56	105.97	109.41
32	a	76	PPU	CM-OC-CZ	-3.14	110.23	117.54
32	a	76	PPU	O4'-C1'-N9	-2.65	102.34	108.10
32	a	76	PPU	C4'-C3'-N3'	-2.64	108.01	113.56
32	a	76	PPU	C2-N3-C4	2.63	120.83	113.27
32	a	76	PPU	CA-C-N3'	2.04	121.69	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 277 ligands modelled in this entry, 277 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.