



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:42 PM GMT

PDB ID : 4IOC
Title : Crystal structure of compound 4f bound to large ribosomal subunit (50S) from *Deinococcus radiodurans*
Authors : Han, S.; Marr, E.S.
Deposited on : 2013-01-07
Resolution : 3.60 Å(reported)

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

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

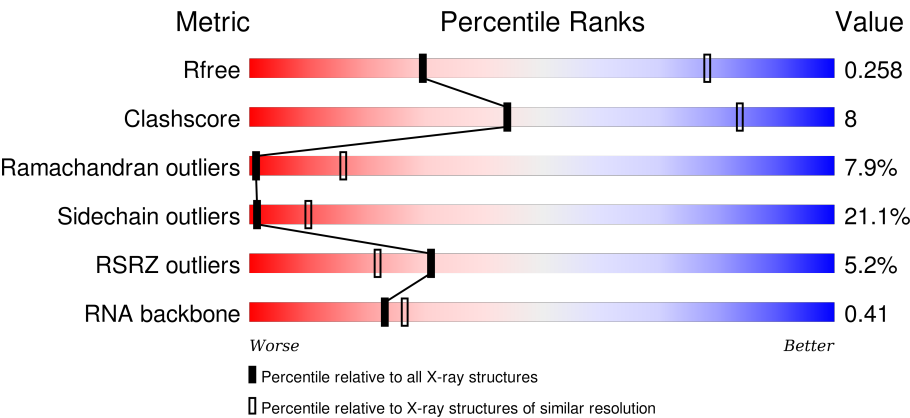
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	91344	1408 (3.80-3.40)
Clashscore	102246	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)
RSRZ outliers	91569	1003 (3.78-3.42)
RNA backbone	2183	1058 (4.40-2.80)

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

Mol	Chain	Length	Quality of chain
1	X	2880	<div><div>2%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>30%38%21%7%</div></div>
2	Y	123	<div><div>2%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>27%41%26%6%</div></div>
3	A	274	<div><div>2%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>50%26%11%12%</div></div>
4	B	211	<div><div></div><div><div></div><div></div><div></div><div></div><div></div></div><div>62%26%9%</div></div>

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
30	4	37	<div> <div>68%</div> <div>70%</div> <div>27%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	MG	X	2901	-	-	-	X
31	MG	X	2907	-	-	-	X
31	MG	X	2914	-	-	-	X
31	MG	X	2915	-	-	-	X
31	MG	X	2917	-	-	-	X
31	MG	X	2922	-	-	-	X
31	MG	X	2924	-	-	-	X
31	MG	X	2926	-	-	-	X
31	MG	Y	202	-	-	-	X

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 83877 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	2686	Total	C	N	O	P	0	0	0
			57651	25718	10642	18606	2685			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

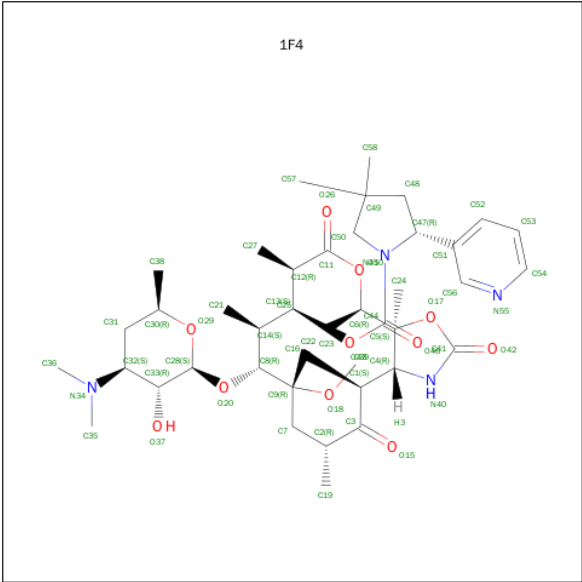
- Molecule 30 is a protein called 50S ribosomal protein L36.

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	X	28	Total Mg 28 28	0	0
31	Y	6	Total Mg 6 6	0	0
31	M	1	Total Mg 1 1	0	0

- Molecule 32 is (3AS,4R,7R,8S,9S,10R,11R,13R,15S,15AR)-4-ETHYL-11-METHOXY-3A,7,9,11,13,15-HEXAMETHYL-2,6,14-TRIOXO-10-{[3,4,6-TRIDEOXY-3-(DIMETHYLAMINO)-BETA-D-XYLO-HEXOPYRANOSYL]OXY}TETRADECAHYDRO-2H-OXACYCLO TETRADECINO[4,3-D][1,3]OXAZOL-8-YL (2R)-4,4-DIMETHYL-2-(PYRIDIN-3-YL)PYRROLIDINE-1-CARBOXYLATE (three-letter code: 1F4) (formula: C₄₃H₆₈N₄O₁₁).

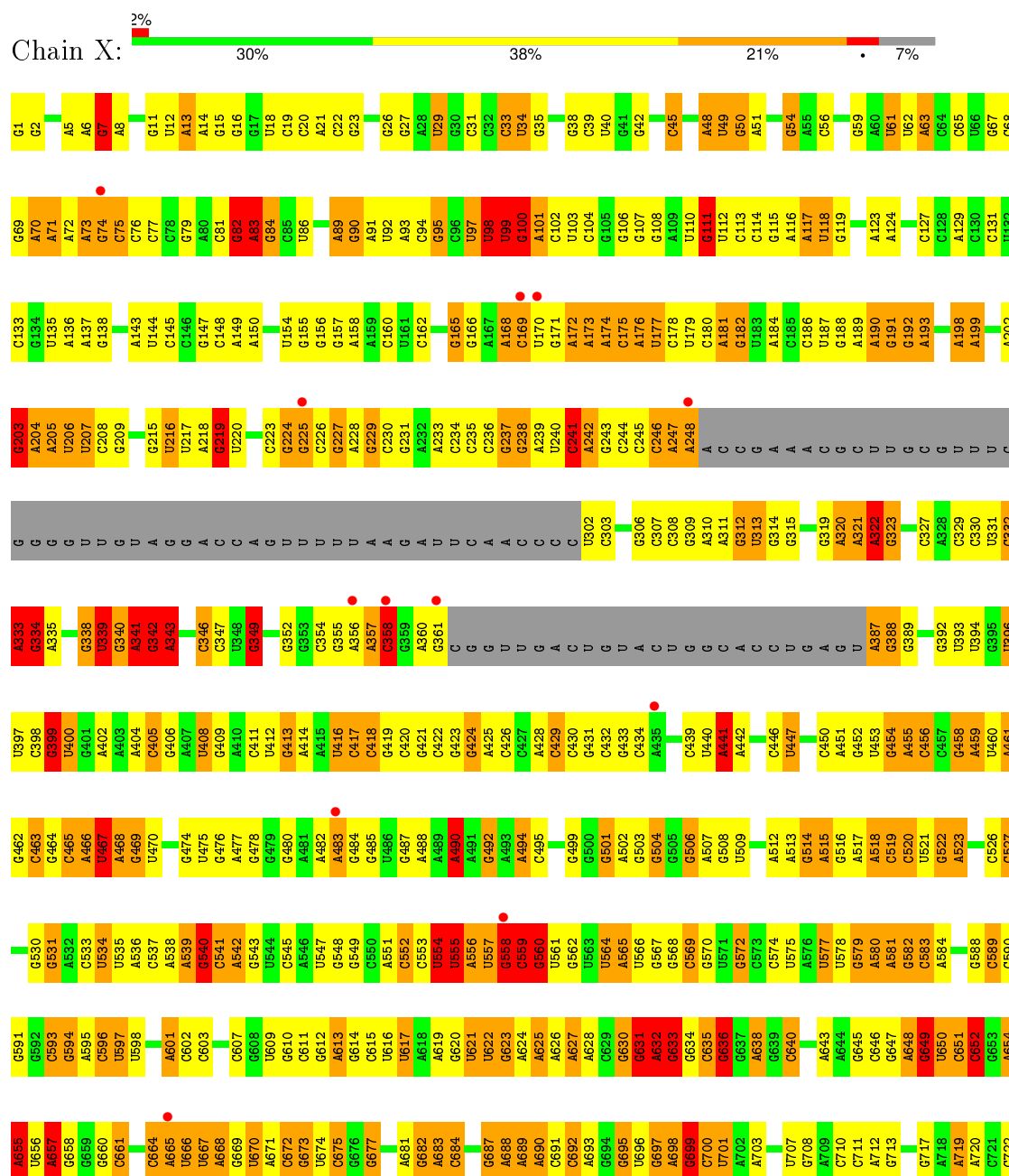


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	X	1	Total	C	N	O	0	0
			58	43	4	11		

3 Residue-property plots

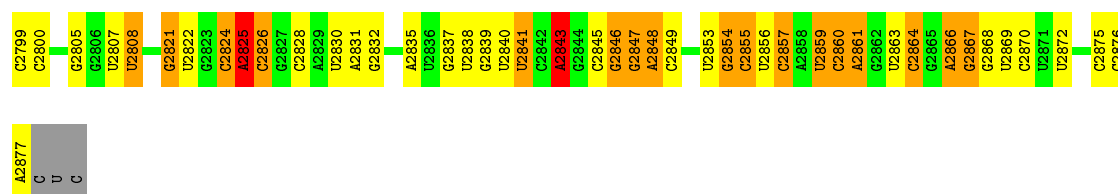
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

• Molecule 1: 23S ribosomal RNA

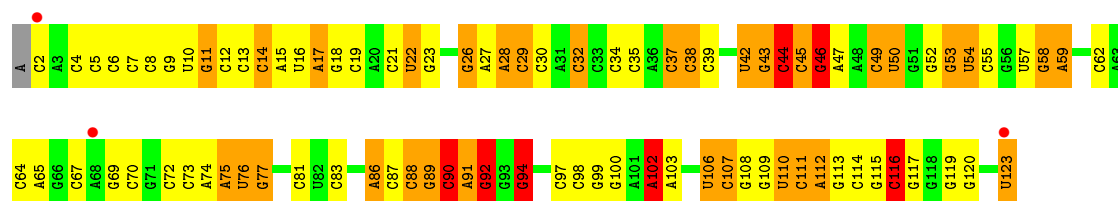


U1710	A1561	G1488	C1343	A1275	G1200	A1126	G1064	A994	U919	G854	U789	C723
C1711	G1562	C1489	C1344	A1276	G1201	C1127	G1067	A995	A922	G858	A790	C724
G1712	U1563	G1490	C1346	G1277	U1202	A1128	A1068	C996	A923	U859	G793	C725
A1643	G1491	G1495	G1347	A1278	A1203	A1129	G1069	C997	G924	U860	A794	A7726
U1647	A1567	G1496	A1348	G1279	A1208	G1130	G1070	C998	U925	C863	A795	G728
C1648	C1570	G1497	A1349	A1280	G1209	C1132	U1071	A999	U926	C864	A796	G729
U1651	G1498	C1497	A1353	A1281	G1210	G1133	U1072	G1000	C927	A965	A797	G730
C1723	C1572	G1498	A1354	A1282	G1211	C1134	G1073	A1001	G931	U866	G798	A731
G1724	A1573	G1499	A1355	A1283	C1212	C1135	G1074	C1002	G932	G867	G799	G732
C1725	G1574	U1500	A1356	A1284	G1213	G1136	G1075	C1003	U800	U868	U800	G733
U1654	C1575	G1505	G1357	A1285	U1217	A1137	U1076	C1006	G933	U869	A801	G738
C1655	G1576	C1506	U1357	A1286	C1218	G1138	U1077	A1007	G934	C870	A802	G739
U1656	G1577	C1507	C1358	A1287	G1219	A1139	U1078	G1008	C935	U871	C803	A740
A1657	U1578	A1507	G1359	A1288	G1220	A1140	G1079	A936	C937	G872	C804	G741
G1660	A1582	G1508	C1360	A1289	G1221	U1141	A1080	C1009	U941	U873	A806	G742
U1732	C1583	A1509	G1361	A1290	G1222	G1142	A1081	U1010	G938	U874	A807	A743
G1661	A1584	A1510	U1362	G1291	G1223	A1143	G1082	A1020	C939	A874	C808	G744
C1662	G1585	A1511	A1363	G1292	G1224	U1144	C1083	G1014	G940	G875	C809	G745
G1663	C1586	U1512	A1364	G1293	G1225	C1145	A1084	U1015	U942	A876	U810	G746
C1664	A1587	G1513	A1365	G1294	C1229	G1146	G1085	C1016	U943	C877	C811	G749
G1665	U1514	C1514	G1366	C1302	C1230	A1147	A1086	C1017	U944	C878	C812	C749
C1666	A1515	U1515	G1367	U1303	A1231	G1148	A1087	C1018	U945	A879	G813	C750
A1667	A1516	A1516	G1371	A1304	U1232	G1149	A1088	U1019	U946	U880	A814	C751
U1594	C1517	G1517	A1372	G1305	U1233	A1150	A1089	A1021	U947	C881	A815	G752
A1595	G1518	C1518	G1373	U1306	A1234	U1151	C1090	A1022	G951	A883	U816	U753
A1596	G1519	G1520	G1374	U1307	G1235	U1152	C1091	U1023	A952	C884	A818	C755
C1597	U1521	U1521	G1375	U1308	G1236	A1153	U1092	G1024	G953	A885	C819	C756
U1598	G1522	C1522	U1446	C1309	A1237	C1154	U1093	U1025	U954	A886	U757	U757
A1601	C1523	A1523	U1447	C1310	G1238	U1159	C1094	C1028	G955	C889	G822	C758
C1674	C1524	C1524	U1448	G1311	A1239	C1160	A1095	U1030	G956	U890	U823	C759
G1675	U1525	U1525	U1449	G1312	G1241	U1161	A1096	C1031	G957	A891	U824	U760
U1676	A1526	G1527	C1455	U1313	U1244	A1162	A1097	G1032	G958	G	C825	G761
C1677	C1528	C1528	C1456	A1314	G1245	C1163	A1098	A1033	G959	G	U826	A762
U1678	A1607	U1529	A1457	G1315	U1246	C1164	A1099	G1034	U960	G	C827	A763
G1680	U1608	G1530	A1458	G1316	U1247	A1167	U1101	G1035	G961	G	C828	A764
A1681	G1609	U1531	U1459	G1317	G1248	G1168	G1102	G1036	G967	G	C829	C765
A1682	A1610	C1531	G1460	G1318	G1249	C1169	C1103	U1037	C968	C	C830	U768
G1683	G1613	A1532	C1461	A1320	A1250	U1172	G1104	U1038	U969	U	C831	C769
G1684	C1614	G1533	U1465	A1321	C1251	G1173	A1105	A1039	A970	A	A833	U770
A1685	C1615	A1534	C1466	G1324	G1252	U1174	A1106	A1040	C971	C	A834	C771
A1686	C1616	U1539	U1467	U1325	C1253	C1181	A1107	U1044	C972	A	U837	A774
U1687	U1540	C1540	A1468	U1326	G1254	U1182	A1108	G1045	U973	G	A838	U775
U1688	A1619	G1541	U1469	C1327	A1255	C1183	C1111	C1049	U974	C	U839	G776
U1689	C1623	G1542	G1470	C1328	U1257	G1184	C1112	C1050	C975	U	U840	A777
G1690	A1624	G1543	C1471	G1329	G1261	C1185	C1113	U1051	C976	U	C841	G778
U1770	C1625	G1544	U1472	U1330	U1262	G1186	A1114	G1052	U977	A	A842	U779
A1771	A1626	G1545	C1473	G1331	G1263	A1187	C1115	C1053	U978	C	G843	U780
C1772	U1627	U1546	A1474	G1332	G1264	A1188	U1116	G1054	A979	C	U844	G781
G1773	C1628	C1548	U1475	G1333	C1265	C1189	U1117	C1055	G980	C	U845	U782
A1694	A1629	G1549	C1476	A1334	G1266	G1190	C1118	A1056	G981	C	A846	G783
U1695	G1627	U1550	U1477	U1335	G1267	C1191	G1119	U1057	C982	C	G784	U784
C1775	C1628	C1550	C1478	A1336	G1268	G1192	U1121	C914	G983	C	U850	U785
A1699	G1629	U1551	U1479	U1337	G1269	C1193	A1122	C915	A984	C	C851	U786
U1776	A1630	G1552	U1480	G1338	C1270	U1194	G1123	U1059	G985	C	U852	A787
C1777	C1631	G1553	U1481	U1339	C1271	C1198	G1125	C1060	A990	C	C853	G788
U1778	A1632	G1554	U1482	C1340	C1272	U1199						
A1779	C1633	G1559	C1487	U1342								
C1780	A1634	G1635										
U1781	G1636											
A1782												
C1783												
U1784												
A1785												

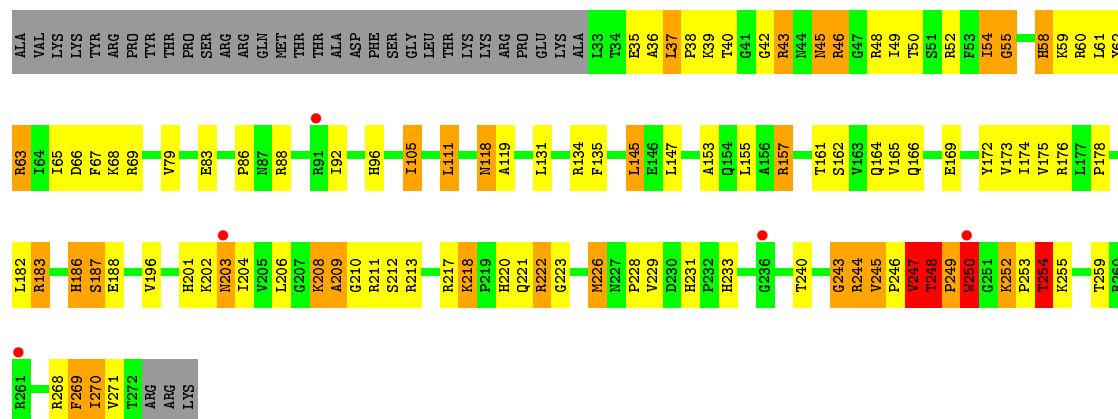
G2724	G2656	G2460	G2389	C2321	A2253	U2185	A	G2053	C1991	U1922	U1956	C1786
G2725	G2657	G2461	G2392	U2322	G2264	A2188	C	A2054	G1992	U1923	G1957	U1787
U2726	G2658	G2462	G2393	G2323	G2255	A2189	U	G2055	G1993	C1924	C1858	C1788
G2727	G2659	G2463	G2394	G2324	G2256	A2190	G	C2056	U1994	C1925	A1859	U1789
A2728	G2660	G2464	G2395	G2325	A2257	A2191	C	G2057	G1995	U1926	A1860	G1790
A2729	G2661	G2465	G2396	G2326	G2258	A2192	G	A2058	A1996	U1927	G1861	C1791
G2730	G2662	G2466	A2397	G2327	G2259	U2193	U	U2059	A1997	G1828	C1862	G1792
A2731	G2663	G2467	A2398	G2328	G2260	C2194	U	U2060	A1998	U1929	U1863	A1793
G2732	G2664	G2468	A2399	G2329	G2261	A2195	U	U2061	U1999	C1930	G1864	A1794
A2733	G2665	G2469	A2401	A2333	G2262	G2196	U	U2062	G2000	G1931	C1865	G1795
G2734	G2666	G2470	G2403	G2334	G2263	U2197	G	A2063	A2002	G1932	G1866	A1796
G2735	G2667	G2471	A2404	U2335	A2266	U2198	G	U2064	G2003	U1934	A1867	A1799
U2736	G2668	U2472	A2405	G2336	A2267	G2199	G	U2065	U2004	A1935	U1870	A1800
A2737	G2669	G2473	G2406	A2337	G2268	G2200	G	U2066	U2005	A1936	G1874	C1801
G2740	G2670	G2474	G2407	G2338	G2269	G2201	U	G2070	G2006	G1937	C1875	U1804
A2745	G2671	G2475	G2408	A2339	U2270	C2202	C	G2071	U2009	U1938	C1876	G1805
G2748	G2672	G2476	G2409	C2340	C2271	A2204	G	C2072	G2010	C1940	C1877	G1806
G2754	G2673	G2477	U2410	G2343	G2274	C2205	U	U2075	G2011	A1943	U1881	A1807
A2758	G2674	G2478	A2414	G2344	U2275	G2206	G	G2076	A2012	G	G1882	C1808
U2759	G2675	G2479	G2415	C2347	C2276	U2208	G	G2077	A2013	U1946	G1883	G1809
G2760	G2676	G2480	U2416	A2348	A2277	G2209	A	G2078	A2014	G1947	A1884	U1810
G2763	G2677	G2481	U2417	G2349	A2278	G2210	G	G2079	G2015	G1948	C1885	A1811
G2764	G2678	G2482	U2418	G2350	U2211	U2212	G	U2080	A2016	A1949	G1886	U1812
G2767	G2679	G2483	G2419	G2351	G2281	U2213	C	U2081	U2017	G1950	G1887	A1813
G2768	G2680	G2484	C2420	G2352	G2282	G2214	A	G2082	G2018	G1951	C1888	G1816
G2769	G2681	G2485	C2421	G2353	G2283	G2215	C	G2083	G2019	A1952	G	U1817
A2770	G2682	G2486	A2422	A2357	U2284	U2216	G	U2088	C2022	A1953	C	G1818
G2771	G2683	G2487	G2423	C2358	G2285	G2217	U	G2089	G2023	A1954	C	U1819
G2772	G2684	G2488	G2424	C2359	G2286	G2218	G	U2090	U2024	G1955	C	G1820
G2773	G2685	G2489	G2425	G2362	G2287	U2219	G	C	A2025	G	G	A1821
G2774	G2686	G2490	A2431	G2363	A2288	G2220	A	U	C2026	G1958	U	C1824
U2775	G2687	G2491	A2432	G2364	A2289	G2221	A	G	G2027	A	A	C1825
U2776	G2688	G2492	A2433	U2365	U2291	U2222	U	C	G2028	G1963	C	C1826
U2777	G2689	G2493	C2435	U2366	U2294	U2223	A	U	G2029	A1964	C	C1827
U2778	G2690	G2494	C2436	U2367	C2295	G2224	A	G	U2030	U1965	U	C1828
U2779	G2691	G2495	U2437	A2368	C2296	A2225	C	A	A2031	C1966	A	C1829
G2780	G2692	G2496	G2438	G2369	G2297	C2227	A	G	C2032	G1971	U	C1830
G2781	G2693	G2497	U2439	U2370	G2298	U2228	C	A	C2033	G1972	A	G1831
G2782	G2694	G2498	C2440	G2371	A2299	G2229	C	U	G2034	A1973	A	G1832
G2783	G2695	G2499	U2441	G2372	G2300	G2230	C	U	G2035	C1974	C	U1833
A2784	G2696	G2500	C2442	A2373	A2301	G2231	U	G	G2036	U1975	G	G1834
G2788	G2697	G2501	G2443	C2374	G2302	G2232	G	U	A2037	G1976	U	C1835
G2789	G2698	G2502	G2444	G2375	G2303	G2233	G	U	G2038	C1977	C	C1836
G2790	G2699	G2503	G2445	G2376	G2304	G2234	G	U	A2039	U1978	C	A1839
G2791	G2700	G2504	U2446	U2377	U2305	G2235	A	G	G2040	C1979	U	A1840
G2792	G2701	G2505	U2447	U2378	G2306	G2236	G	G	A2041	U1979	A	G1841
G2793	G2702	G2506	U2448	U2379	U2307	G2237	G	G	A2042	A1980	G	G1842
G2794	G2703	G2507	G2449	U2380	U2308	C2240	A	A	A2043	A1981	A	G1843
G2795	G2704	G2508	U2450	A2381	A2312	U2241	G	G	G2044	C1982	G	U1844
A2796	G2705	G2509	U2451	C2382	G2313	C2242	C	C	A2045	G1983	A	C1845
G2797	G2706	G2510	C2452	C2383	G2314	G2243	U	U	C2046	A1984	A	G1846
G2798	G2707	G2511	U2453	G2384	A2315	C2244	G	G	C2047	G1985	G	A1847
G2799	G2708	G2512	U2454	U2385	U2316	A2245	C	C	G2048	G1986	G	G1848
G2800	G2709	G2513	U2455	G2386	U2317	A2246	G	G	C2049	G1987	G	G1849
G2801	G2710	G2514	U2456	U2387	A2247	A2247	A	A	G2050	A1988	A	A1850
G2802	G2711	G2515	C2457	G2388	G2320	A2252	C	A	G2051	U1989	A	G1851
G2803	G2712	G2516	C2458	G2389	G2321	A2253	C	A	G2052	U1990	A	G1852



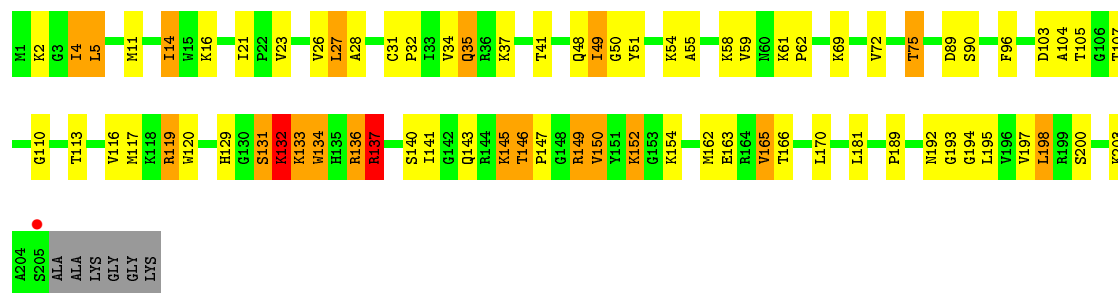
- Molecule 2: 5S ribosomal RNA



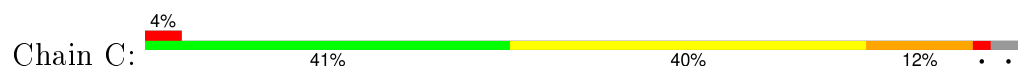
- Molecule 3: 50S ribosomal protein L2

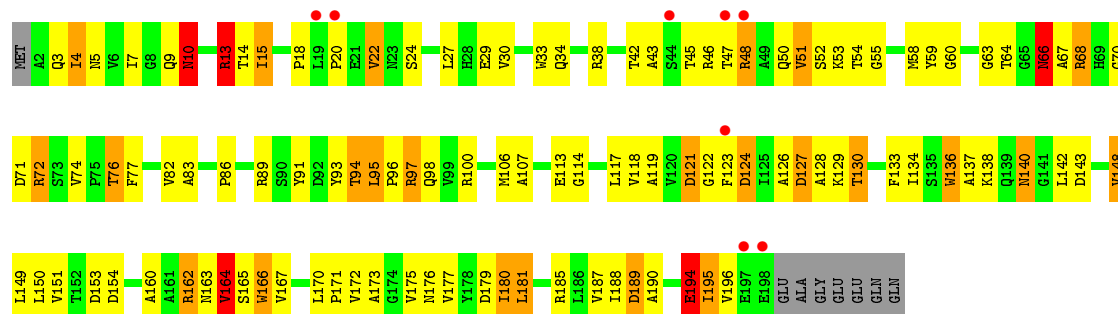


- Molecule 4: 50S ribosomal protein L3

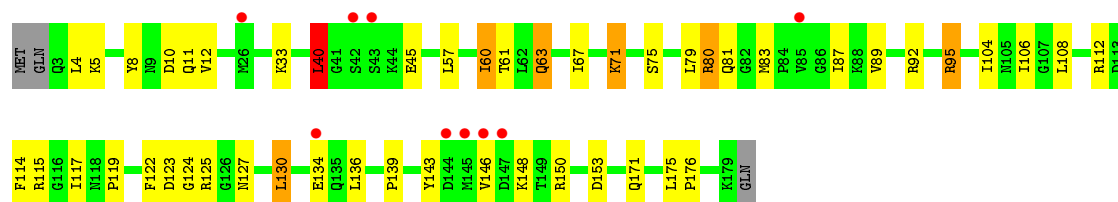


- Molecule 5: 50S ribosomal protein L4

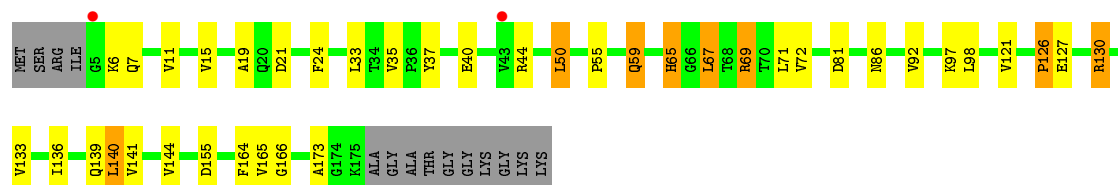




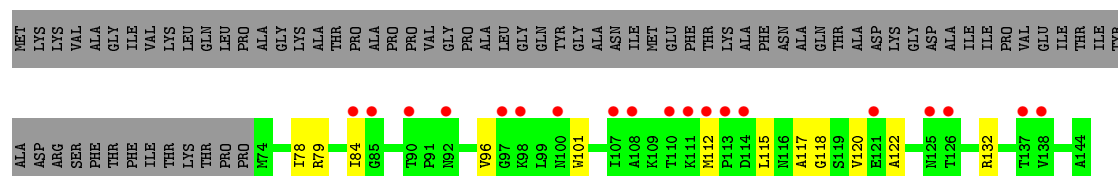
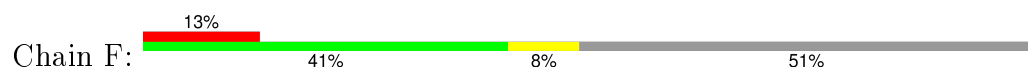
• Molecule 6: 50S ribosomal protein L5



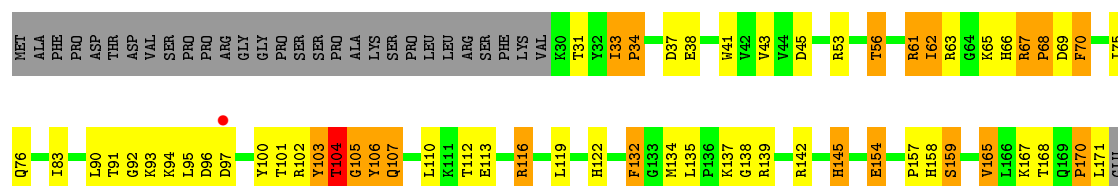
• Molecule 7: 50S ribosomal protein L6



• Molecule 8: 50S ribosomal protein L11

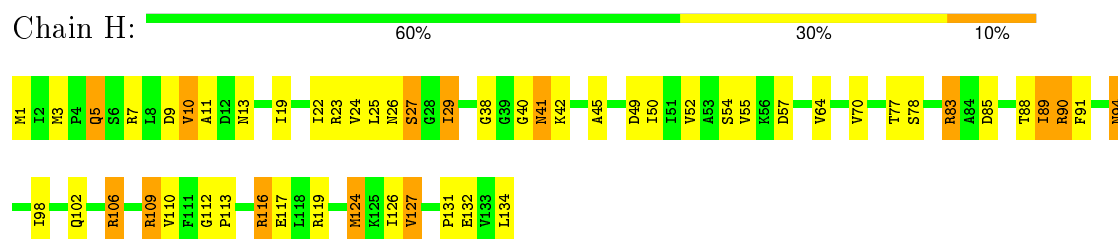


• Molecule 9: 50S ribosomal protein L13

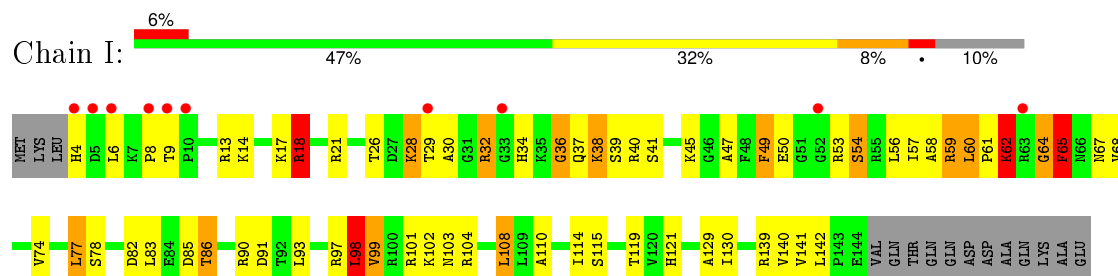


VAL
LYS

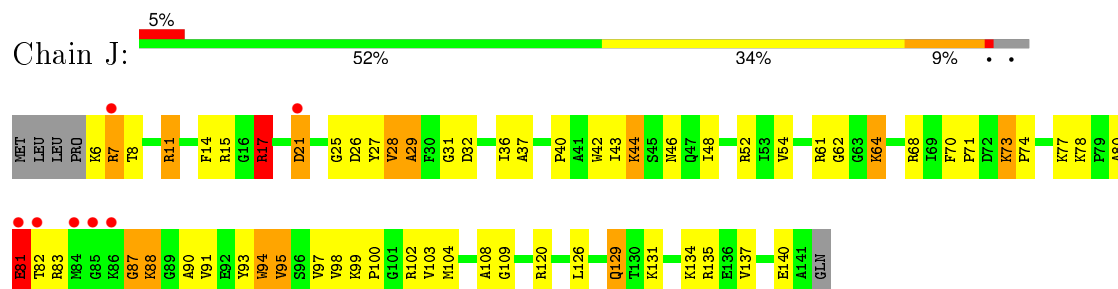
- Molecule 10: 50S ribosomal protein L14



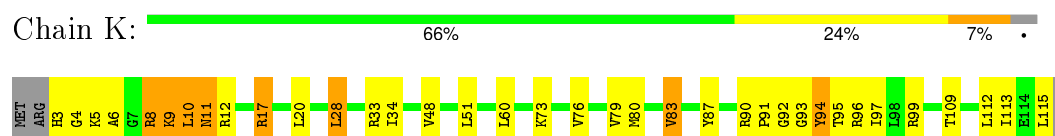
- Molecule 11: 50S ribosomal protein L15



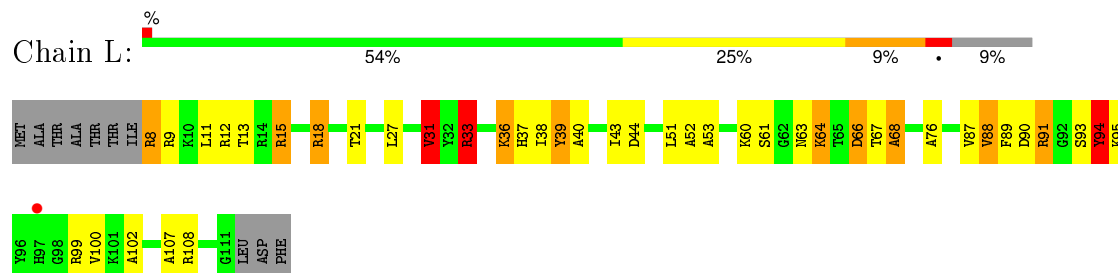
- Molecule 12: 50S ribosomal protein L16



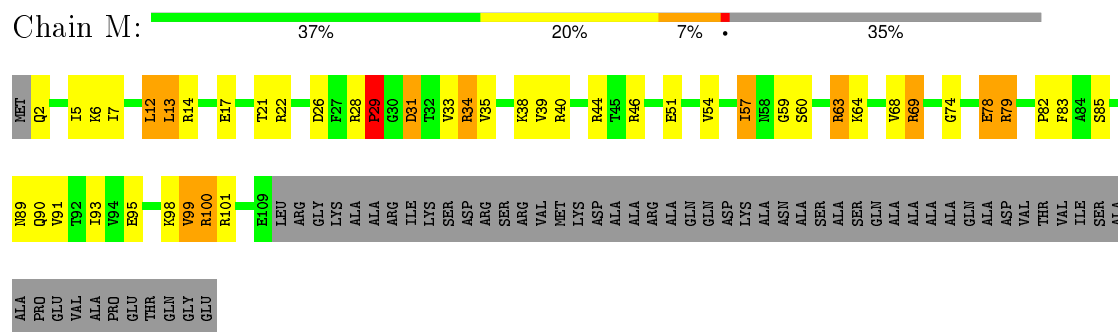
- Molecule 13: 50S ribosomal protein L17



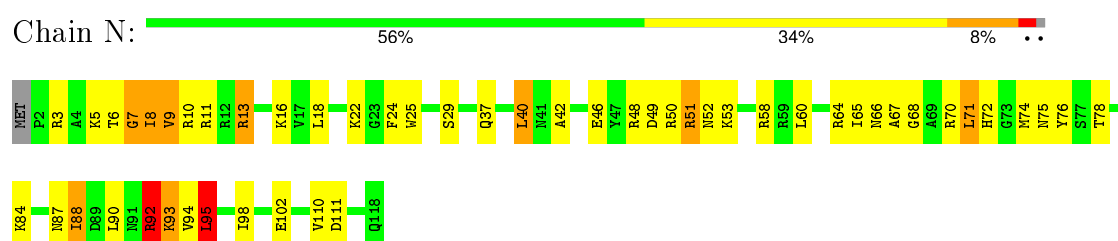
- Molecule 14: 50S ribosomal protein L18



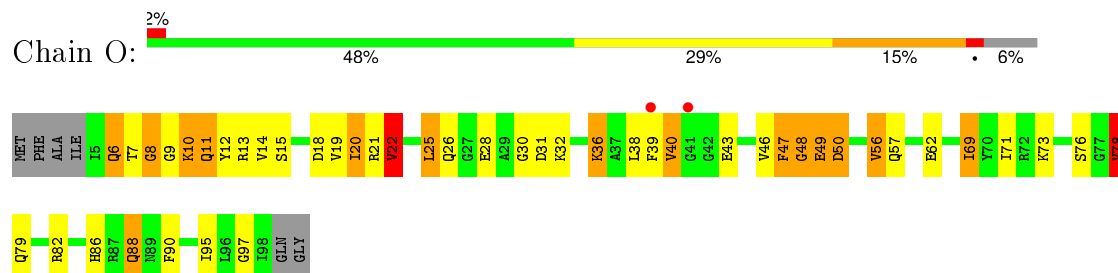
- Molecule 15: 50S ribosomal protein L19



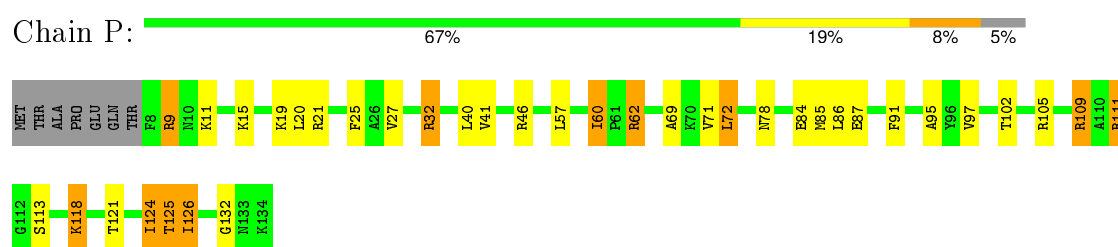
- Molecule 16: 50S ribosomal protein L20



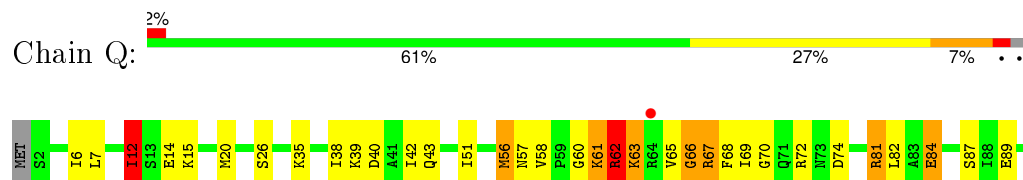
- Molecule 17: 50S ribosomal protein L21



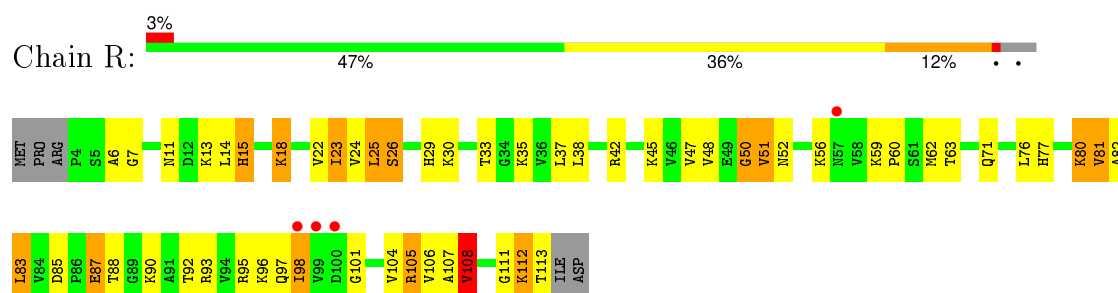
- Molecule 18: 50S ribosomal protein L22



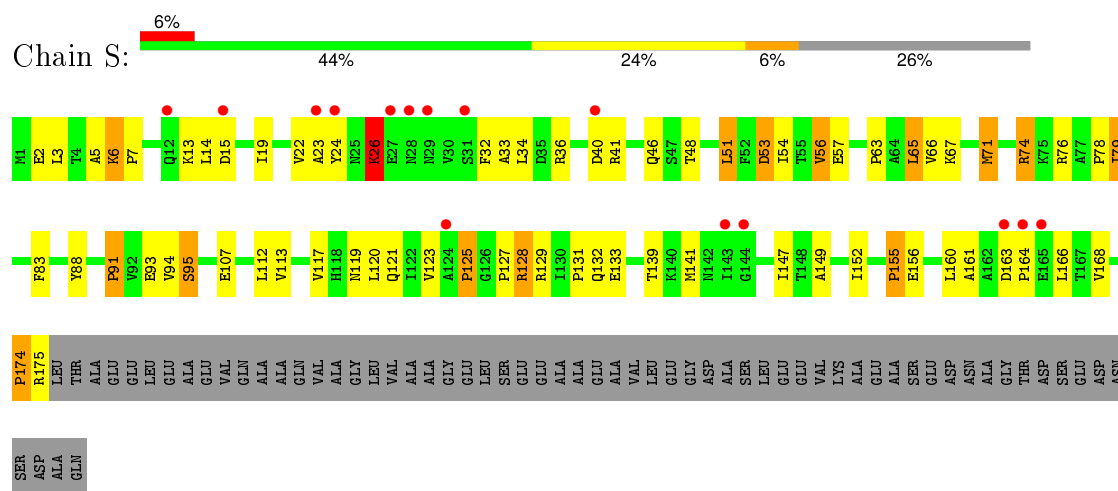
- Molecule 19: 50S ribosomal protein L23



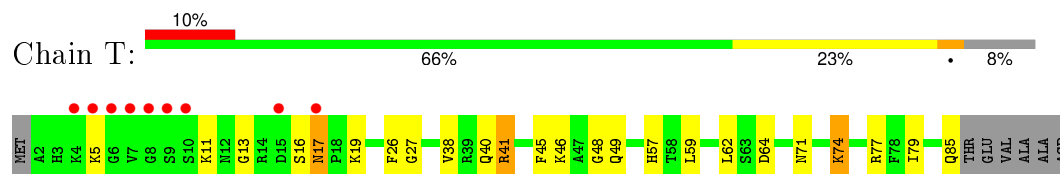
- Molecule 20: 50S ribosomal protein L24



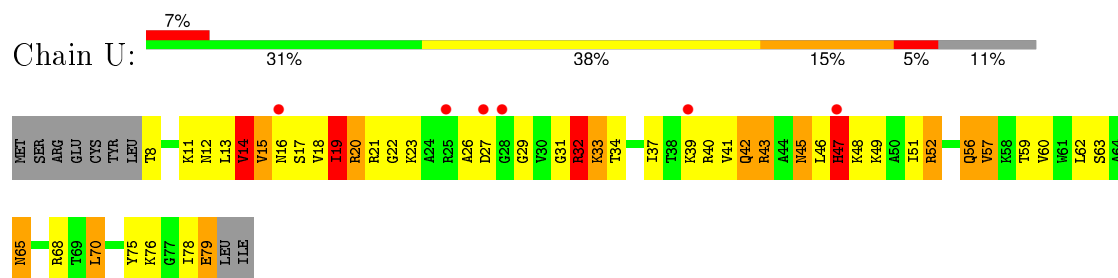
- Molecule 21: 50S ribosomal protein L25



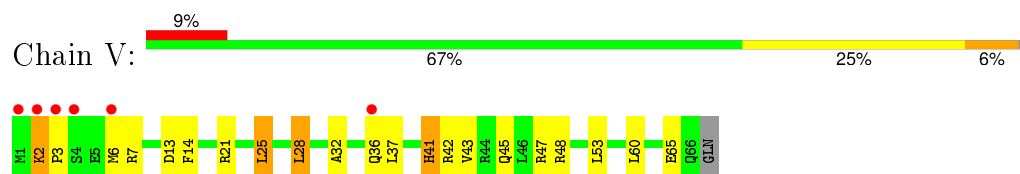
- Molecule 22: 50S ribosomal protein L27



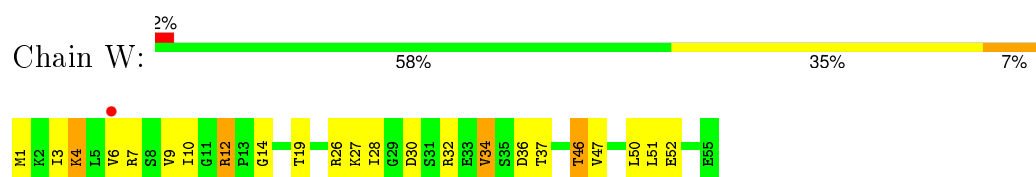
- Molecule 23: 50S ribosomal protein L28



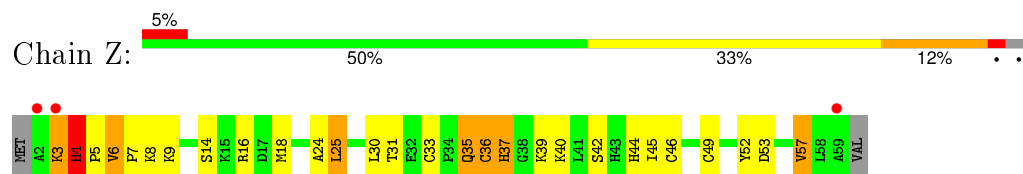
- Molecule 24: 50S ribosomal protein L29



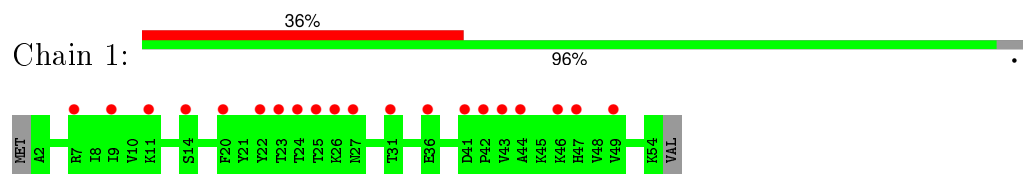
- Molecule 25: 50S ribosomal protein L30



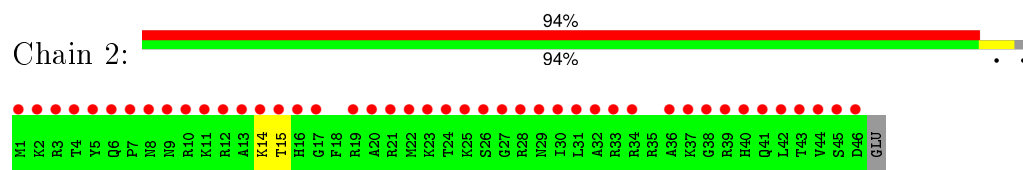
- Molecule 26: 50S ribosomal protein L32



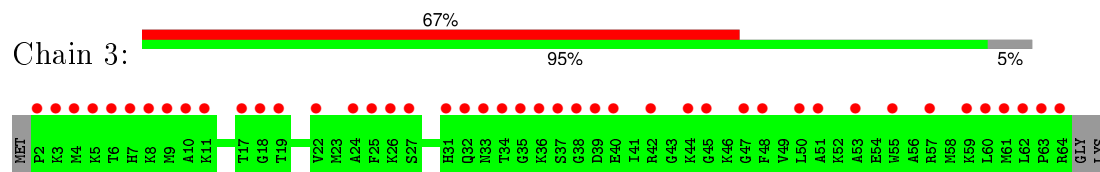
- Molecule 27: 50S ribosomal protein L33



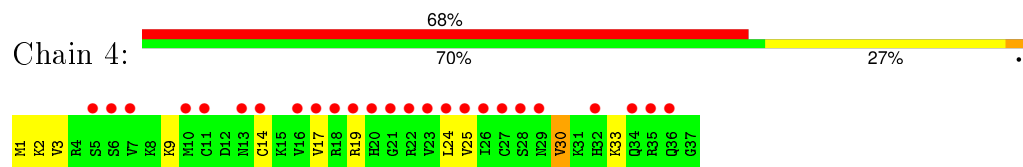
- Molecule 28: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L36



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	169.64Å 408.49Å 692.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.60 30.11 – 3.61	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-3.60) 88.4 (30.11-3.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.33 (at 3.65Å)	Xtriage
Refinement program	autobuster	Depositor
R, R_{free}	0.198 , 0.239 0.215 , 0.258	Depositor DCC
R_{free} test set	12232 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	129.2	Xtriage
Anisotropy	0.611	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 93.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 242941 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	83877	wwPDB-VP
Average B, all atoms (Å ²)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 1F4, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	X	1.02	36/64561 (0.1%)	1.86	1991/100708 (2.0%)
2	Y	1.22	2/2904 (0.1%)	1.83	99/4525 (2.2%)
3	A	0.58	0/1862	0.93	4/2510 (0.2%)
4	B	0.55	0/1567	0.88	1/2105 (0.0%)
5	C	0.62	0/1529	0.96	0/2070
6	D	0.46	0/1419	0.68	0/1903
7	E	0.47	0/1308	0.71	0/1771
8	F	0.50	0/508	0.67	0/683
9	G	0.58	0/1138	0.92	2/1539 (0.1%)
10	H	0.53	0/1007	0.84	0/1352
11	I	0.67	0/1081	1.06	2/1448 (0.1%)
12	J	0.86	0/1113	0.96	1/1486 (0.1%)
13	K	0.66	0/886	0.92	0/1188
14	L	0.52	0/785	0.93	0/1048
15	M	0.59	0/884	1.00	2/1186 (0.2%)
16	N	0.53	0/994	0.79	0/1323
17	O	0.52	0/750	0.96	1/1000 (0.1%)
18	P	0.57	0/1027	0.88	0/1373
19	Q	0.56	0/737	0.99	2/988 (0.2%)
20	R	0.59	0/835	1.02	0/1121
21	S	0.61	0/1370	0.76	0/1862
22	T	0.54	0/633	0.88	0/838
23	U	0.71	0/556	1.08	2/741 (0.3%)
24	V	0.52	0/537	0.73	0/714
25	W	0.51	0/426	0.81	0/568
26	Z	0.62	0/469	0.98	0/629
30	4	0.49	0/298	0.73	0/390
All	All	0.94	38/91184 (0.0%)	1.68	2107/137069 (1.5%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	X	0	3

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	559	C	C3'-O3'	8.19	1.53	1.42
1	X	655	A	C3'-O3'	7.84	1.53	1.42
1	X	774	A	C5-C4	7.25	1.43	1.38
1	X	699	G	N9-C4	-6.97	1.32	1.38
1	X	1688	U	C2-N3	6.58	1.42	1.37
1	X	1674	C	C3'-O3'	-6.46	1.33	1.42
1	X	393	U	C1'-N1	6.43	1.58	1.48
1	X	1468	A	N7-C5	-6.24	1.35	1.39
1	X	2189	A	C3'-O3'	6.22	1.50	1.42
1	X	343	A	N9-C4	6.22	1.41	1.37
1	X	759	C	N3-C4	6.21	1.38	1.33
1	X	236	C	C1'-N1	6.10	1.57	1.48
1	X	540	G	C2-N3	5.99	1.37	1.32
1	X	346	C	C1'-N1	5.97	1.57	1.48
1	X	774	A	C6-N1	5.88	1.39	1.35
1	X	646	C	C1'-N1	5.79	1.57	1.48
1	X	2018	G	C3'-O3'	5.78	1.50	1.42
1	X	927	C	C1'-N1	5.72	1.57	1.48
1	X	868	U	C1'-N1	5.65	1.57	1.48
1	X	917	U	C1'-N1	5.60	1.57	1.48
1	X	1522	C	C1'-N1	5.52	1.57	1.48
1	X	1946	U	C1'-N1	5.45	1.56	1.48
2	Y	87	C	C3'-O3'	5.44	1.49	1.42
1	X	774	A	N3-C4	5.37	1.38	1.34
1	X	434	C	C1'-N1	5.35	1.56	1.48
1	X	31	C	C1'-N1	5.30	1.56	1.48
2	Y	32	C	C1'-N1	5.27	1.56	1.48
1	X	1688	U	N3-C4	5.25	1.43	1.38
1	X	422	C	C1'-N1	5.18	1.56	1.48
1	X	327	C	C1'-N1	5.15	1.56	1.48
1	X	2072	C	C1'-N1	5.14	1.56	1.48
1	X	1182	U	C1'-N1	5.14	1.56	1.48
1	X	2321	C	C1'-N1	5.14	1.56	1.48
1	X	1825	C	C1'-N1	5.11	1.56	1.48
1	X	358	C	C1'-N1	5.08	1.56	1.48
1	X	558	G	C3'-O3'	5.08	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	430	C	C1'-N1	5.06	1.56	1.48
1	X	774	A	N1-C2	5.03	1.38	1.34

All (2107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1288	A	C1'-O4'-C4'	-30.77	85.29	109.90
1	X	1019	U	P-O3'-C3'	19.01	142.51	119.70
1	X	1288	A	C5'-C4'-O4'	18.79	131.64	109.10
1	X	774	A	N1-C6-N6	17.73	129.24	118.60
1	X	559	C	O4'-C1'-N1	17.43	122.14	108.20
1	X	2808	U	O4'-C1'-N1	16.51	121.41	108.20
1	X	1288	A	O4'-C1'-N9	16.46	121.37	108.20
1	X	2564	U	P-O3'-C3'	16.04	138.95	119.70
1	X	176	A	P-O3'-C3'	15.97	138.86	119.70
1	X	655	A	P-O3'-C3'	15.78	138.64	119.70
1	X	558	G	P-O3'-C3'	15.40	138.18	119.70
1	X	1775	A	P-O3'-C3'	15.14	137.87	119.70
1	X	1278	A	O4'-C1'-N9	14.65	119.92	108.20
1	X	1473	U	P-O3'-C3'	14.53	137.13	119.70
1	X	204	A	P-O3'-C3'	14.46	137.05	119.70
1	X	33	C	P-O3'-C3'	14.32	136.88	119.70
1	X	1634	A	P-O3'-C3'	14.15	136.69	119.70
1	X	100	G	P-O3'-C3'	14.14	136.66	119.70
1	X	559	C	C4'-C3'-C2'	-14.06	88.54	102.60
1	X	2497	A	P-O3'-C3'	13.90	136.38	119.70
1	X	2736	U	P-O3'-C3'	13.74	136.19	119.70
1	X	2018	G	P-O3'-C3'	13.71	136.16	119.70
1	X	814	G	P-O3'-C3'	13.68	136.11	119.70
1	X	1790	G	P-O3'-C3'	13.67	136.11	119.70
1	X	342	G	P-O3'-C3'	13.52	135.92	119.70
1	X	2312	A	P-O3'-C3'	13.31	135.68	119.70
1	X	994	A	P-O3'-C3'	13.30	135.66	119.70
1	X	774	A	N7-C8-N9	13.21	120.41	113.80
1	X	334	G	P-O3'-C3'	13.15	135.48	119.70
1	X	788	G	P-O3'-C3'	13.06	135.38	119.70
1	X	1475	U	P-O3'-C3'	12.98	135.28	119.70
1	X	181	A	P-O3'-C3'	12.91	135.19	119.70
1	X	1574	A	O4'-C1'-N9	12.86	118.49	108.20
1	X	343	A	O4'-C1'-N9	12.82	118.46	108.20
1	X	664	C	P-O3'-C3'	12.82	135.08	119.70
1	X	1468	A	C8-N9-C4	-12.70	100.72	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	48	A	P-O3'-C3'	12.66	134.89	119.70
1	X	683	A	P-O3'-C3'	12.61	134.82	119.70
1	X	1036	G	P-O3'-C3'	12.58	134.79	119.70
1	X	1938	U	P-O3'-C3'	12.51	134.71	119.70
1	X	469	G	P-O3'-C3'	12.51	134.71	119.70
1	X	2323	U	P-O3'-C3'	12.48	134.68	119.70
1	X	774	A	C5-N7-C8	-12.45	97.68	103.90
1	X	559	C	P-O3'-C3'	12.37	134.54	119.70
1	X	2854	G	C1'-O4'-C4'	-12.31	100.05	109.90
1	X	774	A	C6-C5-N7	-12.29	123.70	132.30
1	X	2691	C	P-O3'-C3'	12.27	134.42	119.70
1	X	399	G	P-O3'-C3'	12.25	134.40	119.70
1	X	1249	G	P-O3'-C3'	12.20	134.34	119.70
1	X	822	G	P-O3'-C3'	12.20	134.34	119.70
1	X	2261	G	P-O3'-C3'	12.06	134.17	119.70
1	X	537	C	N1-C2-O2	11.88	126.03	118.90
1	X	218	A	P-O3'-C3'	11.84	133.91	119.70
1	X	73	A	P-O3'-C3'	11.83	133.90	119.70
1	X	1442	C	P-O3'-C3'	11.82	133.88	119.70
1	X	33	C	O4'-C1'-N1	11.81	117.65	108.20
1	X	454	G	P-O3'-C3'	11.81	133.87	119.70
1	X	514	G	P-O3'-C3'	11.70	133.74	119.70
1	X	1441	A	P-O3'-C3'	11.69	133.72	119.70
2	Y	58	G	P-O3'-C3'	11.69	133.72	119.70
1	X	2854	G	N9-C1'-C2'	11.57	129.04	114.00
1	X	540	G	N1-C6-O6	-11.44	113.04	119.90
1	X	2298	U	P-O3'-C3'	11.43	133.41	119.70
1	X	774	A	C4-C5-N7	11.39	116.39	110.70
1	X	2189	A	P-O3'-C3'	11.34	133.30	119.70
1	X	98	U	P-O3'-C3'	11.30	133.26	119.70
1	X	1096	A	P-O3'-C3'	11.30	133.26	119.70
1	X	490	A	P-O3'-C3'	11.30	133.26	119.70
1	X	1391	A	P-O3'-C3'	11.28	133.24	119.70
1	X	2426	G	P-O3'-C3'	11.26	133.21	119.70
1	X	1122	A	P-O3'-C3'	11.22	133.16	119.70
1	X	1288	A	C4'-C3'-C2'	-11.03	91.57	102.60
2	Y	16	U	P-O3'-C3'	11.01	132.91	119.70
1	X	841	G	O4'-C4'-C3'	-11.00	93.00	104.00
1	X	1746	A	O4'-C1'-N9	10.89	116.91	108.20
1	X	1923	U	P-O3'-C3'	10.88	132.76	119.70
1	X	554	U	P-O3'-C3'	10.87	132.74	119.70
1	X	522	G	O4'-C1'-N9	10.80	116.84	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	691	C	O4'-C1'-N1	10.80	116.84	108.20
1	X	1468	A	O4'-C1'-C2'	-10.79	95.00	105.80
1	X	1261	G	P-O3'-C3'	10.78	132.64	119.70
1	X	699	G	N3-C4-N9	-10.76	119.54	126.00
1	X	2491	C	O4'-C1'-N1	10.75	116.80	108.20
1	X	71	A	P-O3'-C3'	10.72	132.57	119.70
1	X	2770	A	P-O3'-C3'	10.71	132.55	119.70
1	X	1186	G	P-O3'-C3'	10.64	132.47	119.70
1	X	2371	A	O4'-C1'-N9	10.63	116.71	108.20
1	X	242	A	C1'-O4'-C4'	-10.63	101.40	109.90
1	X	1632	A	O4'-C1'-N9	-10.53	99.78	108.20
1	X	333	A	P-O3'-C3'	10.48	132.27	119.70
1	X	2634	G	O4'-C1'-N9	10.44	116.55	108.20
1	X	1820	G	P-O3'-C3'	10.44	132.22	119.70
1	X	1732	U	P-O3'-C3'	10.42	132.21	119.70
1	X	1053	G	P-O3'-C3'	10.38	132.16	119.70
1	X	1333	G	N3-C4-N9	-10.31	119.81	126.00
1	X	1280	U	P-O3'-C3'	10.29	132.04	119.70
1	X	699	G	N3-C4-C5	10.28	133.74	128.60
1	X	1055	A	P-O3'-C3'	10.26	132.01	119.70
1	X	805	G	O4'-C1'-N9	-10.22	100.02	108.20
1	X	809	C	O4'-C1'-N1	10.21	116.37	108.20
1	X	1684	G	P-O3'-C3'	10.16	131.90	119.70
1	X	2731	G	P-O3'-C3'	10.16	131.89	119.70
1	X	1403	U	P-O3'-C3'	10.15	131.88	119.70
1	X	1409	U	P-O3'-C3'	10.14	131.87	119.70
1	X	341	A	P-O3'-C3'	10.14	131.87	119.70
1	X	2593	A	P-O3'-C3'	10.11	131.83	119.70
1	X	321	A	P-O3'-C3'	10.11	131.83	119.70
1	X	1474	A	P-O3'-C3'	10.10	131.82	119.70
1	X	2018	G	C1'-O4'-C4'	-10.01	101.89	109.90
1	X	434	C	P-O3'-C3'	9.91	131.60	119.70
1	X	666	U	O4'-C1'-N1	9.91	116.13	108.20
1	X	89	A	P-O3'-C3'	9.91	131.59	119.70
1	X	813	A	P-O3'-C3'	9.89	131.57	119.70
1	X	651	C	P-O3'-C3'	9.83	131.50	119.70
1	X	2228	U	P-O3'-C3'	9.83	131.50	119.70
1	X	1278	A	C1'-O4'-C4'	-9.83	102.03	109.90
1	X	655	A	O4'-C1'-N9	9.83	116.06	108.20
1	X	1799	A	C1'-O4'-C4'	-9.77	102.09	109.90
1	X	2229	G	P-O3'-C3'	9.77	131.42	119.70
1	X	540	G	P-O3'-C3'	9.76	131.41	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	467	U	P-O3'-C3'	9.73	131.38	119.70
1	X	2730	A	P-O3'-C3'	9.73	131.37	119.70
1	X	1601	U	P-O3'-C3'	9.68	131.32	119.70
1	X	1770	U	C1'-O4'-C4'	-9.68	102.16	109.90
1	X	1086	C	P-O3'-C3'	9.66	131.29	119.70
1	X	1976	U	O4'-C1'-N1	9.66	115.92	108.20
1	X	1353	A	P-O3'-C3'	9.65	131.28	119.70
1	X	2689	C	P-O3'-C3'	9.58	131.20	119.70
1	X	638	A	P-O3'-C3'	9.57	131.19	119.70
1	X	1975	G	P-O3'-C3'	9.56	131.17	119.70
1	X	632	A	O4'-C1'-N9	9.53	115.83	108.20
1	X	343	A	C8-N9-C4	-9.53	101.99	105.80
1	X	2330	G	N9-C1'-C2'	9.53	126.38	114.00
1	X	731	A	P-O3'-C3'	9.52	131.12	119.70
1	X	483	A	P-O3'-C3'	-9.50	108.30	119.70
1	X	1278	A	C3'-C2'-C1'	-9.50	93.90	101.50
1	X	1811	A	P-O3'-C3'	9.49	131.09	119.70
1	X	172	A	P-O3'-C3'	9.48	131.08	119.70
1	X	242	A	O4'-C1'-N9	9.46	115.77	108.20
1	X	557	U	C1'-O4'-C4'	-9.45	102.34	109.90
1	X	803	C	P-O3'-C3'	9.45	131.04	119.70
1	X	939	C	P-O3'-C3'	9.43	131.01	119.70
1	X	1575	C	P-O3'-C3'	9.43	131.01	119.70
1	X	1489	C	O4'-C1'-N1	9.39	115.71	108.20
1	X	646	C	O4'-C1'-N1	9.36	115.69	108.20
1	X	2190	A	O4'-C1'-N9	9.36	115.69	108.20
1	X	2591	C	N1-C2-O2	9.34	124.50	118.90
1	X	1574	A	C1'-O4'-C4'	-9.32	102.44	109.90
2	Y	90	C	P-O3'-C3'	-9.30	108.53	119.70
1	X	1313	U	O4'-C1'-N1	9.29	115.64	108.20
1	X	1459	U	P-O3'-C3'	9.29	130.85	119.70
1	X	1338	G	P-O3'-C3'	9.28	130.84	119.70
1	X	34	U	O4'-C1'-N1	9.27	115.62	108.20
1	X	841	G	O4'-C1'-N9	9.25	115.60	108.20
1	X	1439	G	P-O3'-C3'	9.23	130.78	119.70
1	X	941	U	O4'-C1'-N1	9.21	115.57	108.20
1	X	2222	U	O4'-C1'-N1	9.21	115.57	108.20
1	X	2324	G	P-O3'-C3'	9.17	130.71	119.70
1	X	2566	A	P-O3'-C3'	9.13	130.65	119.70
1	X	1663	C	N1-C2-O2	9.12	124.37	118.90
1	X	2634	G	C3'-C2'-C1'	-9.12	94.21	101.50
1	X	2039	G	C8-N9-C4	-9.11	102.75	106.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	247	A	C1'-O4'-C4'	-9.11	102.61	109.90
2	Y	81	C	O4'-C1'-N1	9.11	115.48	108.20
1	X	2472	U	P-O3'-C3'	-9.09	108.79	119.70
1	X	494	A	P-O3'-C3'	9.08	130.60	119.70
1	X	883	A	C5'-C4'-O4'	9.07	119.99	109.10
1	X	1790	G	O4'-C1'-N9	9.05	115.44	108.20
1	X	416	U	O4'-C1'-N1	9.01	115.41	108.20
1	X	2270	U	O4'-C1'-N1	9.01	115.41	108.20
1	X	312	G	C1'-O4'-C4'	-8.99	102.71	109.90
1	X	841	G	N9-C1'-C2'	8.97	125.66	114.00
1	X	656	U	P-O3'-C3'	8.95	130.44	119.70
1	X	1333	G	C8-N9-C4	-8.95	102.82	106.40
1	X	1984	A	C3'-C2'-C1'	-8.95	94.34	101.50
1	X	2018	G	C5-N7-C8	-8.95	99.83	104.30
1	X	2626	U	O4'-C1'-N1	8.95	115.36	108.20
1	X	1688	U	N3-C4-O4	8.93	125.65	119.40
1	X	817	A	C1'-O4'-C4'	-8.91	102.77	109.90
1	X	774	A	C5-C6-N1	-8.91	113.25	117.70
1	X	2018	G	C4-C5-N7	8.91	114.36	110.80
1	X	332	C	O4'-C1'-N1	8.84	115.27	108.20
1	X	755	C	P-O3'-C3'	-8.82	109.11	119.70
1	X	1268	U	P-O3'-C3'	8.77	130.22	119.70
1	X	825	C	P-O3'-C3'	-8.73	109.22	119.70
1	X	938	G	P-O3'-C3'	8.73	130.18	119.70
1	X	774	A	N9-C4-C5	-8.73	102.31	105.80
1	X	2228	U	N3-C4-C5	-8.73	109.36	114.60
1	X	976	C	O4'-C1'-N1	8.73	115.18	108.20
1	X	666	U	C1'-O4'-C4'	-8.71	102.94	109.90
1	X	845	U	O4'-C1'-N1	8.70	115.16	108.20
1	X	320	A	O4'-C1'-N9	8.68	115.15	108.20
1	X	2034	A	P-O3'-C3'	8.68	130.12	119.70
1	X	1496	G	P-O3'-C3'	8.67	130.11	119.70
1	X	173	A	C1'-O4'-C4'	-8.67	102.97	109.90
1	X	1574	A	C4'-C3'-C2'	-8.67	93.93	102.60
1	X	1790	G	C1'-O4'-C4'	-8.64	102.99	109.90
1	X	2204	A	P-O3'-C3'	8.60	130.02	119.70
1	X	1288	A	C3'-C2'-C1'	-8.60	94.62	101.50
1	X	99	U	P-O3'-C3'	8.58	130.00	119.70
1	X	1161	U	O4'-C1'-N1	8.58	115.06	108.20
1	X	817	A	O4'-C4'-C3'	-8.57	95.43	104.00
1	X	2824	C	P-O3'-C3'	8.57	129.98	119.70
1	X	2039	G	N9-C4-C5	8.56	108.83	105.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1710	U	P-O3'-C3'	8.56	129.97	119.70
1	X	236	C	O4'-C1'-N1	8.56	115.05	108.20
1	X	1468	A	O4'-C1'-N9	8.55	115.04	108.20
1	X	841	G	C8-N9-C4	-8.54	102.99	106.40
1	X	358	C	O4'-C1'-N1	8.53	115.02	108.20
2	Y	86	A	O4'-C1'-N9	8.49	115.00	108.20
1	X	2414	A	P-O3'-C3'	8.49	129.89	119.70
1	X	2051	U	O4'-C1'-N1	8.47	114.98	108.20
1	X	1072	U	P-O3'-C3'	8.46	129.85	119.70
1	X	761	G	C1'-O4'-C4'	-8.45	103.14	109.90
1	X	216	U	O4'-C1'-N1	8.45	114.96	108.20
1	X	432	C	O4'-C1'-N1	8.44	114.95	108.20
1	X	2452	U	P-O3'-C3'	8.44	129.83	119.70
1	X	2481	G	P-O3'-C3'	8.44	129.82	119.70
1	X	2497	A	C1'-O4'-C4'	-8.43	103.15	109.90
1	X	1468	A	P-O3'-C3'	8.43	129.82	119.70
1	X	346	C	N1-C1'-C2'	8.43	124.96	114.00
1	X	2018	G	N9-C1'-C2'	8.43	124.96	114.00
1	X	774	A	C5-C6-N6	-8.42	116.96	123.70
1	X	577	U	O4'-C1'-N1	8.41	114.93	108.20
1	X	2703	C	O4'-C1'-N1	8.41	114.93	108.20
1	X	515	A	P-O3'-C3'	8.41	129.79	119.70
1	X	117	A	P-O3'-C3'	8.40	129.78	119.70
1	X	577	U	C4'-C3'-C2'	-8.39	94.21	102.60
1	X	1333	G	O4'-C1'-N9	8.39	114.91	108.20
1	X	1705	U	O4'-C1'-N1	8.39	114.91	108.20
1	X	2025	A	O4'-C1'-N9	8.39	114.91	108.20
1	X	1466	C	C6-N1-C2	-8.36	116.96	120.30
1	X	1966	C	O4'-C1'-N1	8.34	114.88	108.20
1	X	518	A	P-O3'-C3'	8.34	129.70	119.70
1	X	1731	C	O4'-C1'-N1	8.33	114.86	108.20
2	Y	88	C	O4'-C1'-N1	8.32	114.85	108.20
1	X	2853	U	O4'-C1'-N1	8.31	114.85	108.20
1	X	1467	U	N1-C2-O2	8.30	128.61	122.80
1	X	940	G	P-O5'-C5'	8.29	134.17	120.90
1	X	1524	C	P-O3'-C3'	8.29	129.65	119.70
1	X	2196	U	P-O3'-C3'	8.29	129.64	119.70
1	X	579	G	C4-C5-N7	-8.28	107.49	110.80
1	X	2439	U	O4'-C1'-N1	8.28	114.82	108.20
1	X	387	A	C5'-C4'-O4'	8.27	119.03	109.10
1	X	2370	G	O4'-C1'-N9	8.26	114.81	108.20
1	X	2228	U	N3-C4-O4	8.26	125.18	119.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2778	U	P-O3'-C3'	8.26	129.61	119.70
1	X	2237	C	P-O3'-C3'	8.24	129.59	119.70
1	X	2198	U	P-O3'-C3'	8.23	129.58	119.70
1	X	582	G	P-O3'-C3'	8.22	129.57	119.70
1	X	2669	C	N1-C2-O2	8.21	123.83	118.90
1	X	184	A	O4'-C1'-N9	8.21	114.77	108.20
1	X	192	G	P-O3'-C3'	8.19	129.53	119.70
1	X	190	A	O4'-C1'-N9	8.19	114.75	108.20
1	X	650	U	O4'-C1'-N1	8.19	114.75	108.20
1	X	1223	G	C3'-C2'-C1'	8.19	108.05	101.50
1	X	2859	U	O4'-C1'-N1	8.19	114.75	108.20
1	X	1975	G	C2'-C3'-O3'	8.18	127.50	109.50
1	X	1917	C	O4'-C1'-N1	8.17	114.73	108.20
1	X	2409	A	C1'-O4'-C4'	-8.16	103.38	109.90
1	X	394	U	O4'-C1'-N1	8.15	114.72	108.20
1	X	1468	A	C3'-C2'-C1'	-8.14	94.99	101.50
1	X	1468	A	N7-C8-N9	8.13	117.87	113.80
1	X	1991	C	P-O3'-C3'	-8.13	109.94	119.70
1	X	969	U	P-O3'-C3'	8.13	129.45	119.70
1	X	2291	U	O4'-C1'-N1	8.13	114.70	108.20
1	X	1467	U	N1-C1'-C2'	8.12	124.56	114.00
1	X	1285	A	P-O3'-C3'	8.11	129.43	119.70
1	X	1315	A	P-O3'-C3'	8.10	129.42	119.70
1	X	2795	A	P-O3'-C3'	8.10	129.42	119.70
1	X	338	G	C8-N9-C4	-8.09	103.16	106.40
1	X	2758	A	C1'-O4'-C4'	-8.08	103.43	109.90
1	X	1749	G	C1'-O4'-C4'	-8.08	103.43	109.90
1	X	2726	U	O4'-C1'-N1	8.05	114.64	108.20
2	Y	90	C	O4'-C1'-N1	8.05	114.64	108.20
1	X	1313	U	C1'-O4'-C4'	-8.05	103.46	109.90
1	X	841	G	C1'-O4'-C4'	-8.02	103.48	109.90
1	X	1412	C	P-O3'-C3'	8.02	129.32	119.70
1	X	843	G	P-O3'-C3'	8.02	129.32	119.70
1	X	2531	U	N3-C2-O2	-7.99	116.61	122.20
1	X	2693	U	C1'-O4'-C4'	-7.99	103.51	109.90
1	X	2258	G	C4'-C3'-C2'	-7.98	94.62	102.60
1	X	2432	A	O4'-C1'-N9	7.97	114.58	108.20
1	X	1345	G	C5'-C4'-O4'	7.97	118.66	109.10
1	X	242	A	C4'-C3'-C2'	-7.96	94.64	102.60
1	X	1656	U	P-O3'-C3'	7.95	129.24	119.70
1	X	1288	A	O4'-C4'-C3'	-7.95	96.05	104.00
1	X	499	G	O4'-C1'-N9	7.94	114.55	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1523	A	P-O3'-C3'	7.93	129.22	119.70
1	X	1217	U	O4'-C1'-N1	7.92	114.54	108.20
2	Y	54	U	O4'-C1'-N1	7.92	114.53	108.20
1	X	1850	G	P-O3'-C3'	7.90	129.18	119.70
1	X	938	G	O4'-C1'-N9	7.89	114.51	108.20
1	X	458	G	P-O3'-C3'	7.87	129.14	119.70
1	X	346	C	C6-N1-C2	-7.87	117.15	120.30
1	X	882	C	O4'-C1'-N1	7.87	114.49	108.20
1	X	1188	A	P-O3'-C3'	7.85	129.12	119.70
1	X	509	U	O4'-C1'-N1	7.85	114.48	108.20
1	X	1339	U	P-O3'-C3'	7.84	129.11	119.70
1	X	2507	U	P-O3'-C3'	7.84	129.11	119.70
1	X	1830	C	P-O3'-C3'	7.84	129.10	119.70
1	X	1467	U	P-O3'-C3'	-7.83	110.30	119.70
1	X	1469	U	N3-C2-O2	-7.82	116.72	122.20
1	X	1152	C	P-O3'-C3'	7.82	129.08	119.70
1	X	593	C	O4'-C1'-N1	7.80	114.44	108.20
1	X	2702	G	C5-C6-O6	-7.78	123.93	128.60
1	X	2049	C	O4'-C1'-N1	7.76	114.41	108.20
1	X	696	U	O4'-C1'-N1	7.76	114.41	108.20
1	X	2485	U	O4'-C1'-N1	-7.75	102.00	108.20
1	X	1791	C	O4'-C1'-N1	7.74	114.39	108.20
1	X	816	U	O4'-C1'-N1	7.74	114.39	108.20
1	X	2872	U	O4'-C1'-N1	7.73	114.38	108.20
1	X	2860	C	O4'-C1'-N1	7.73	114.38	108.20
1	X	1496	G	C3'-C2'-C1'	-7.71	95.33	101.50
1	X	223	C	O4'-C1'-N1	7.71	114.36	108.20
1	X	1777	A	C1'-O4'-C4'	-7.71	103.73	109.90
1	X	2664	G	N1-C6-O6	7.70	124.52	119.90
1	X	357	A	P-O3'-C3'	7.69	128.93	119.70
1	X	1172	U	O4'-C1'-N1	7.69	114.36	108.20
1	X	2651	U	O4'-C1'-N1	7.68	114.35	108.20
1	X	2788	C	O4'-C1'-N1	7.68	114.34	108.20
1	X	2288	A	P-O3'-C3'	7.68	128.91	119.70
1	X	2039	G	O4'-C1'-N9	7.68	114.34	108.20
1	X	868	U	O4'-C1'-N1	7.67	114.34	108.20
1	X	1268	U	O4'-C1'-N1	7.67	114.34	108.20
1	X	2481	G	C5-C6-O6	-7.67	124.00	128.60
1	X	2018	G	C3'-C2'-C1'	-7.66	95.37	101.50
1	X	2530	C	P-O3'-C3'	7.66	128.90	119.70
1	X	2664	G	C6-C5-N7	-7.66	125.80	130.40
1	X	198	A	P-O3'-C3'	7.66	128.89	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	742	G	P-O3'-C3'	7.66	128.89	119.70
1	X	1071	U	P-O3'-C3'	7.66	128.89	119.70
1	X	1618	U	P-O3'-C3'	7.65	128.88	119.70
1	X	2274	C	O4'-C1'-N1	7.65	114.32	108.20
1	X	18	U	O4'-C1'-N1	7.65	114.32	108.20
1	X	308	C	O4'-C1'-N1	7.63	114.30	108.20
1	X	690	A	C4'-C3'-C2'	-7.63	94.97	102.60
1	X	788	G	C1'-O4'-C4'	-7.61	103.81	109.90
1	X	636	G	C8-N9-C4	-7.61	103.36	106.40
1	X	1302	C	O4'-C1'-N1	7.59	114.28	108.20
1	X	1935	A	N9-C1'-C2'	7.59	123.87	114.00
1	X	2005	U	O4'-C1'-N1	7.58	114.27	108.20
1	X	926	C	O4'-C1'-N1	7.58	114.27	108.20
1	X	1654	A	C3'-C2'-C1'	-7.58	95.44	101.50
1	X	774	A	P-O5'-C5'	7.56	133.00	120.90
1	X	937	C	O4'-C1'-N1	7.55	114.24	108.20
1	X	2841	U	O4'-C1'-N1	7.55	114.24	108.20
1	X	1327	C	C5-C6-N1	7.54	124.77	121.00
1	X	1001	A	P-O3'-C3'	7.54	128.75	119.70
1	X	2671	C	O4'-C1'-N1	7.54	114.23	108.20
1	X	2460	G	P-O5'-C5'	7.54	132.97	120.90
1	X	2460	G	O4'-C1'-N9	7.53	114.23	108.20
1	X	2190	A	C1'-O4'-C4'	-7.53	103.88	109.90
1	X	247	A	O4'-C1'-N9	7.52	114.22	108.20
1	X	1211	G	P-O3'-C3'	-7.52	110.68	119.70
1	X	242	A	P-O3'-C3'	7.51	128.71	119.70
2	Y	29	C	O4'-C1'-N1	7.51	114.21	108.20
1	X	1357	U	P-O3'-C3'	7.51	128.71	119.70
1	X	1433	A	O4'-C1'-N9	7.51	114.20	108.20
1	X	307	C	O4'-C1'-N1	7.50	114.20	108.20
1	X	2015	G	P-O3'-C3'	7.49	128.69	119.70
1	X	925	U	P-O3'-C3'	7.49	128.69	119.70
1	X	2431	C	O4'-C1'-N1	7.49	114.19	108.20
1	X	626	A	P-O3'-C3'	7.48	128.68	119.70
1	X	2694	G	P-O3'-C3'	7.48	128.68	119.70
2	Y	30	C	O4'-C1'-N1	7.48	114.18	108.20
1	X	1283	C	P-O3'-C3'	7.47	128.67	119.70
1	X	2710	C	O4'-C1'-N1	7.47	114.17	108.20
1	X	1221	C	O4'-C1'-N1	7.47	114.17	108.20
1	X	1223	G	P-O3'-C3'	7.47	128.66	119.70
1	X	2056	C	P-O3'-C3'	7.46	128.66	119.70
1	X	2477	C	P-O5'-C5'	7.46	132.84	120.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1985	G	O4'-C1'-N9	7.46	114.17	108.20
1	X	2384	G	P-O3'-C3'	7.46	128.65	119.70
1	X	94	C	O4'-C1'-N1	7.46	114.17	108.20
2	Y	26	G	P-O3'-C3'	7.45	128.64	119.70
1	X	2830	U	O4'-C1'-N1	7.45	114.16	108.20
1	X	2660	C	O4'-C1'-N1	7.44	114.15	108.20
1	X	2088	U	P-O3'-C3'	7.44	128.63	119.70
1	X	837	U	O4'-C1'-N1	7.44	114.15	108.20
1	X	177	U	O4'-C1'-N1	7.43	114.14	108.20
1	X	1664	G	O5'-P-OP2	7.43	119.61	110.70
1	X	2580	C	P-O3'-C3'	7.43	128.61	119.70
1	X	841	G	N7-C8-N9	7.42	116.81	113.10
1	X	117	A	O4'-C1'-N9	7.41	114.13	108.20
1	X	1607	A	P-O3'-C3'	7.41	128.59	119.70
1	X	2033	C	P-O3'-C3'	7.40	128.58	119.70
1	X	2799	C	O4'-C1'-N1	7.40	114.12	108.20
1	X	1681	A	P-O3'-C3'	7.40	128.58	119.70
1	X	2633	A	P-O3'-C3'	7.40	128.58	119.70
1	X	2564	U	C1'-O4'-C4'	-7.40	103.98	109.90
1	X	1412	C	O4'-C1'-N1	7.39	114.12	108.20
1	X	1142	G	P-O3'-C3'	7.39	128.57	119.70
1	X	2258	G	O4'-C1'-N9	7.39	114.11	108.20
1	X	1469	U	P-O5'-C5'	7.38	132.70	120.90
1	X	1412	C	C3'-C2'-C1'	-7.36	95.61	101.50
1	X	2662	C	C4'-C3'-C2'	-7.36	95.24	102.60
1	X	1559	G	P-O3'-C3'	7.35	128.52	119.70
1	X	31	C	O4'-C1'-N1	7.34	114.07	108.20
1	X	788	G	N9-C1'-C2'	7.34	123.54	114.00
1	X	796	A	C4'-C3'-C2'	-7.33	95.27	102.60
1	X	1909	U	O4'-C1'-N1	7.33	114.06	108.20
1	X	815	A	P-O3'-C3'	7.33	128.49	119.70
1	X	1688	U	N3-C4-C5	-7.32	110.21	114.60
1	X	92	U	O4'-C1'-N1	7.32	114.06	108.20
1	X	2298	U	O4'-C1'-N1	7.31	114.05	108.20
1	X	1143	A	C5'-C4'-O4'	7.30	117.86	109.10
1	X	1051	U	O4'-C1'-N1	7.30	114.04	108.20
1	X	2006	G	O4'-C1'-N9	7.30	114.04	108.20
1	X	1000	G	O4'-C1'-N9	7.29	114.03	108.20
1	X	2239	C	O4'-C1'-N1	7.29	114.03	108.20
1	X	2290	A	P-O3'-C3'	7.28	128.44	119.70
1	X	567	G	O4'-C1'-N9	7.28	114.02	108.20
1	X	742	G	C1'-O4'-C4'	-7.28	104.08	109.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	539	A	C1'-O4'-C4'	-7.27	104.09	109.90
1	X	1439	G	C3'-C2'-C1'	-7.27	95.69	101.50
1	X	180	C	O4'-C1'-N1	7.26	114.01	108.20
1	X	2702	G	N1-C6-O6	7.24	124.25	119.90
1	X	972	C	C1'-O4'-C4'	-7.24	104.11	109.90
1	X	2561	G	C5-C6-O6	-7.24	124.26	128.60
1	X	1333	G	N9-C4-C5	7.24	108.30	105.40
1	X	2870	C	O4'-C1'-N1	7.23	113.99	108.20
1	X	875	G	O4'-C1'-N9	7.23	113.99	108.20
1	X	2267	A	P-O3'-C3'	7.23	128.38	119.70
1	X	2560	G	C8-N9-C4	-7.23	103.51	106.40
1	X	2634	G	C1'-O4'-C4'	-7.23	104.12	109.90
1	X	564	U	O4'-C1'-N1	7.23	113.98	108.20
1	X	1776	A	P-O3'-C3'	7.23	128.37	119.70
1	X	1865	C	O4'-C1'-N1	7.23	113.98	108.20
1	X	1080	A	C1'-O4'-C4'	-7.22	104.12	109.90
1	X	1920	A	P-O3'-C3'	7.22	128.37	119.70
1	X	520	C	P-O3'-C3'	7.22	128.36	119.70
1	X	1513	U	O4'-C1'-N1	7.22	113.97	108.20
1	X	61	U	C1'-O4'-C4'	-7.21	104.13	109.90
1	X	631	G	O4'-C1'-N9	7.21	113.97	108.20
1	X	2608	A	C1'-O4'-C4'	-7.21	104.13	109.90
2	Y	19	C	N1-C2-O2	7.21	123.22	118.90
1	X	174	A	P-O3'-C3'	7.20	128.34	119.70
1	X	430	C	O4'-C1'-N1	7.20	113.96	108.20
1	X	802	A	O4'-C1'-N9	-7.19	102.45	108.20
1	X	1467	U	C4-C5-C6	-7.19	115.39	119.70
2	Y	106	U	O4'-C1'-N1	7.19	113.95	108.20
1	X	465	C	P-O5'-C5'	-7.19	109.40	120.90
1	X	810	U	P-O3'-C3'	-7.19	111.08	119.70
1	X	1289	A	O4'-C1'-N9	-7.18	102.45	108.20
1	X	1461	C	O4'-C1'-N1	7.18	113.95	108.20
1	X	1218	C	O4'-C1'-N1	7.18	113.94	108.20
1	X	1310	C	O4'-C1'-N1	7.18	113.94	108.20
1	X	331	U	O4'-C1'-N1	7.17	113.94	108.20
1	X	2284	U	O4'-C1'-N1	7.17	113.93	108.20
1	X	81	C	O4'-C1'-N1	7.16	113.93	108.20
1	X	531	G	P-O3'-C3'	-7.16	111.11	119.70
1	X	518	A	N9-C1'-C2'	7.15	123.29	114.00
1	X	2509	A	P-O3'-C3'	7.13	128.26	119.70
1	X	2026	C	N3-C2-O2	-7.13	116.91	121.90
1	X	117	A	C1'-O4'-C4'	-7.13	104.20	109.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2039	G	N3-C2-N2	-7.12	114.91	119.90
1	X	2449	G	O4'-C1'-N9	7.12	113.90	108.20
1	X	758	G	O4'-C1'-N9	7.12	113.90	108.20
1	X	514	G	N9-C1'-C2'	7.12	123.25	114.00
1	X	526	C	C3'-C2'-C1'	-7.11	95.81	101.50
1	X	1788	C	O4'-C1'-N1	7.11	113.89	108.20
1	X	943	U	O4'-C1'-N1	7.11	113.88	108.20
1	X	1938	U	N1-C1'-C2'	7.11	123.24	114.00
1	X	2338	C	P-O3'-C3'	7.11	128.23	119.70
1	X	455	A	P-O3'-C3'	7.10	128.22	119.70
1	X	2705	A	P-O3'-C3'	7.10	128.22	119.70
1	X	59	G	P-O3'-C3'	7.10	128.22	119.70
1	X	1652	G	P-O3'-C3'	7.09	128.21	119.70
2	Y	92	G	P-O3'-C3'	-7.09	111.19	119.70
1	X	1364	C	O4'-C1'-N1	7.09	113.87	108.20
1	X	2620	G	C4'-C3'-C2'	-7.09	95.51	102.60
2	Y	6	C	O4'-C1'-N1	7.08	113.87	108.20
1	X	2691	C	O4'-C1'-N1	7.07	113.86	108.20
1	X	2699	G	P-O3'-C3'	7.07	128.18	119.70
1	X	2243	C	O4'-C1'-N1	7.07	113.85	108.20
1	X	1950	C	O4'-C1'-N1	7.06	113.85	108.20
1	X	2498	U	P-O3'-C3'	7.06	128.17	119.70
1	X	558	G	N9-C1'-C2'	7.05	123.17	114.00
1	X	343	A	N7-C8-N9	7.04	117.32	113.80
1	X	1772	C	O4'-C1'-N1	7.04	113.84	108.20
1	X	1966	C	P-O3'-C3'	-7.04	111.25	119.70
1	X	2403	C	N1-C2-O2	7.04	123.13	118.90
1	X	2567	G	C8-N9-C4	-7.04	103.58	106.40
1	X	822	G	C4'-C3'-C2'	-7.04	95.56	102.60
1	X	1975	G	O4'-C1'-N9	-7.04	102.57	108.20
1	X	2782	G	O4'-C1'-N9	7.04	113.83	108.20
1	X	1723	U	O4'-C1'-N1	7.03	113.82	108.20
1	X	1470	G	P-O5'-C5'	-7.03	109.66	120.90
1	X	2845	C	O4'-C1'-N1	7.03	113.82	108.20
1	X	1201	G	P-O3'-C3'	7.02	128.13	119.70
1	X	2238	G	O4'-C1'-N9	7.02	113.82	108.20
1	X	190	A	C1'-O4'-C4'	-7.02	104.28	109.90
1	X	756	C	N1-C2-O2	7.02	123.11	118.90
1	X	2795	A	C3'-C2'-C1'	7.02	107.11	101.50
1	X	2593	A	O3'-P-O5'	-7.00	90.69	104.00
1	X	2080	U	O4'-C1'-N1	7.00	113.80	108.20
1	X	1403	U	O4'-C1'-N1	7.00	113.80	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	801	A	P-O3'-C3'	6.99	128.09	119.70
1	X	1754	G	P-O3'-C3'	6.99	128.08	119.70
1	X	113	C	O4'-C1'-N1	6.98	113.79	108.20
1	X	2550	C	O4'-C1'-N1	6.97	113.78	108.20
1	X	1711	C	C1'-O4'-C4'	-6.97	104.32	109.90
1	X	2406	C	P-O3'-C3'	6.96	128.06	119.70
1	X	399	G	C4'-C3'-C2'	6.96	109.56	102.60
1	X	946	U	O4'-C1'-N1	6.95	113.76	108.20
1	X	2662	C	N1-C2-O2	6.95	123.07	118.90
1	X	1458	A	P-O3'-C3'	6.94	128.03	119.70
1	X	796	A	N1-C6-N6	6.94	122.76	118.60
1	X	74	G	O4'-C4'-C3'	-6.93	97.07	104.00
1	X	2072	C	O4'-C1'-N1	6.93	113.74	108.20
1	X	814	G	N9-C1'-C2'	6.93	123.01	114.00
1	X	1308	C	C3'-C2'-C1'	-6.92	95.96	101.50
1	X	2551	A	P-O3'-C3'	6.92	128.01	119.70
1	X	1801	C	P-O3'-C3'	6.92	128.01	119.70
1	X	2782	G	C1'-O4'-C4'	-6.92	104.36	109.90
1	X	1139	A	N9-C1'-C2'	6.92	122.99	114.00
1	X	2794	G	P-O3'-C3'	6.91	127.99	119.70
2	Y	107	C	P-O3'-C3'	6.91	127.99	119.70
1	X	2488	G	P-O3'-C3'	-6.90	111.42	119.70
1	X	83	A	C1'-O4'-C4'	-6.90	104.38	109.90
1	X	95	G	P-O3'-C3'	6.90	127.98	119.70
1	X	1409	U	C1'-O4'-C4'	-6.90	104.38	109.90
1	X	2667	C	N1-C2-O2	6.90	123.04	118.90
1	X	1108	U	O4'-C1'-N1	6.89	113.71	108.20
1	X	2030	U	P-O3'-C3'	-6.89	111.43	119.70
1	X	560	G	P-O3'-C3'	-6.89	111.44	119.70
1	X	2533	U	O4'-C1'-N1	6.88	113.71	108.20
1	X	1313	U	C3'-C2'-C1'	-6.88	96.00	101.50
1	X	483	A	N9-C1'-C2'	6.88	122.94	114.00
1	X	826	U	O4'-C1'-N1	6.88	113.70	108.20
1	X	636	G	N7-C8-N9	6.87	116.54	113.10
2	Y	32	C	C6-N1-C2	-6.87	117.55	120.30
1	X	247	A	P-O3'-C3'	6.87	127.94	119.70
2	Y	74	A	P-O3'-C3'	6.87	127.94	119.70
1	X	2217	G	C1'-O4'-C4'	-6.87	104.41	109.90
1	X	796	A	C5-N7-C8	-6.87	100.47	103.90
1	X	1487	C	O4'-C1'-N1	6.87	113.69	108.20
1	X	2691	C	C1'-O4'-C4'	-6.86	104.41	109.90
1	X	1422	C	O4'-C1'-N1	6.86	113.69	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2018	G	O4'-C1'-C2'	-6.85	98.95	105.80
1	X	774	A	C8-N9-C4	-6.85	103.06	105.80
1	X	1086	C	O4'-C1'-N1	6.85	113.68	108.20
1	X	1522	C	C3'-C2'-C1'	-6.85	96.02	101.50
1	X	1602	G	P-O3'-C3'	6.84	127.91	119.70
1	X	2418	A	P-O3'-C3'	6.84	127.91	119.70
1	X	1200	G	O4'-C1'-N9	6.83	113.67	108.20
1	X	1465	G	P-O3'-C3'	-6.83	111.50	119.70
1	X	927	C	C6-N1-C2	-6.83	117.57	120.30
1	X	2245	A	P-O3'-C3'	6.82	127.89	119.70
1	X	617	U	N3-C2-O2	-6.82	117.42	122.20
2	Y	90	C	C3'-C2'-C1'	-6.82	96.05	101.50
1	X	1433	A	C1'-O4'-C4'	-6.82	104.45	109.90
2	Y	37	C	O4'-C1'-N1	6.81	113.65	108.20
1	X	1469	U	P-O3'-C3'	6.81	127.88	119.70
1	X	1963	G	P-O3'-C3'	6.81	127.87	119.70
1	X	527	C	C5-C6-N1	6.81	124.41	121.00
1	X	170	U	N3-C2-O2	-6.81	117.43	122.20
1	X	567	G	P-O3'-C3'	-6.81	111.53	119.70
1	X	1410	U	O4'-C1'-N1	6.80	113.64	108.20
1	X	580	A	N9-C1'-C2'	6.80	122.83	114.00
1	X	1686	A	C1'-O4'-C4'	-6.80	104.46	109.90
1	X	1466	C	N3-C2-O2	-6.79	117.14	121.90
1	X	1656	U	O4'-C1'-N1	6.79	113.64	108.20
1	X	1745	C	O4'-C1'-N1	6.79	113.63	108.20
1	X	2339	A	O4'-C1'-N9	6.79	113.63	108.20
2	Y	123	U	C2-N1-C1'	6.79	125.85	117.70
1	X	2554	C	O4'-C1'-N1	6.78	113.63	108.20
1	X	699	G	O4'-C1'-N9	6.78	113.62	108.20
1	X	1164	C	O4'-C1'-N1	6.78	113.62	108.20
1	X	39	C	O4'-C1'-N1	6.78	113.62	108.20
2	Y	44	C	O4'-C1'-N1	6.77	113.62	108.20
1	X	542	A	C5-N7-C8	-6.77	100.52	103.90
1	X	514	G	O4'-C1'-N9	-6.76	102.79	108.20
1	X	559	C	C5'-C4'-O4'	6.76	117.22	109.10
1	X	582	G	N3-C4-C5	-6.76	125.22	128.60
2	Y	17	A	P-O3'-C3'	6.75	127.80	119.70
1	X	1526	U	O4'-C1'-N1	6.75	113.60	108.20
1	X	2672	U	N1-C2-O2	6.75	127.52	122.80
1	X	477	A	O5'-P-OP2	-6.74	99.63	105.70
1	X	1652	G	C6-C5-N7	-6.74	126.36	130.40
1	X	886	A	C3'-C2'-C1'	-6.74	96.11	101.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2347	C	O4'-C1'-N1	6.74	113.59	108.20
1	X	2590	U	P-O5'-C5'	6.73	131.67	120.90
1	X	1608	U	O4'-C1'-N1	6.73	113.58	108.20
1	X	2479	U	C5-C6-N1	6.73	126.06	122.70
1	X	2579	A	C3'-C2'-C1'	6.72	106.88	101.50
1	X	870	C	O4'-C1'-N1	6.72	113.58	108.20
1	X	2855	C	P-O3'-C3'	-6.72	111.64	119.70
1	X	2022	C	O4'-C1'-N1	6.72	113.57	108.20
1	X	501	G	O4'-C1'-N9	6.71	113.57	108.20
1	X	697	G	O4'-C1'-N9	6.71	113.57	108.20
1	X	1958	G	O4'-C4'-C3'	-6.71	97.29	104.00
1	X	575	U	P-O3'-C3'	6.71	127.75	119.70
2	Y	53	G	N3-C4-C5	-6.71	125.25	128.60
1	X	739	G	O4'-C1'-N9	6.70	113.56	108.20
1	X	1632	A	P-O3'-C3'	6.70	127.75	119.70
1	X	1792	C	P-O3'-C3'	6.70	127.75	119.70
1	X	1833	U	O4'-C1'-N1	6.70	113.56	108.20
1	X	1184	G	P-O3'-C3'	6.70	127.74	119.70
1	X	208	C	O4'-C1'-N1	6.70	113.56	108.20
1	X	1308	C	P-O5'-C5'	-6.69	110.19	120.90
1	X	133	C	O4'-C1'-N1	6.69	113.55	108.20
1	X	699	G	P-O3'-C3'	6.69	127.73	119.70
1	X	1163	C	O4'-C1'-N1	6.69	113.55	108.20
1	X	2838	U	O4'-C1'-N1	6.69	113.55	108.20
2	Y	8	C	O4'-C1'-N1	6.69	113.55	108.20
1	X	1468	A	N9-C1'-C2'	6.69	122.70	114.00
1	X	2392	G	O4'-C1'-N9	6.69	113.55	108.20
1	X	864	C	O4'-C1'-N1	6.69	113.55	108.20
1	X	1663	C	P-O3'-C3'	6.69	127.73	119.70
1	X	1743	C	P-O3'-C3'	-6.69	111.67	119.70
1	X	1979	C	P-O3'-C3'	6.69	127.73	119.70
1	X	624	A	O4'-C1'-N9	6.69	113.55	108.20
1	X	823	U	O4'-C1'-N1	6.69	113.55	108.20
2	Y	87	C	O4'-C1'-N1	6.68	113.55	108.20
1	X	2538	C	N1-C2-O2	6.68	122.91	118.90
1	X	1744	G	C4'-C3'-C2'	-6.68	95.92	102.60
1	X	234	C	N1-C2-O2	6.68	122.91	118.90
1	X	2483	U	O4'-C1'-N1	6.67	113.54	108.20
1	X	2574	G	O4'-C1'-N9	6.67	113.54	108.20
1	X	2256	G	C8-N9-C4	-6.67	103.73	106.40
1	X	2190	A	P-O3'-C3'	6.66	127.70	119.70
1	X	83	A	P-O3'-C3'	6.66	127.69	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1068	A	P-O3'-C3'	6.66	127.69	119.70
1	X	2459	C	N1-C2-O2	6.66	122.90	118.90
1	X	649	G	O4'-C1'-N9	6.66	113.53	108.20
1	X	1404	C	O4'-C1'-N1	6.66	113.53	108.20
1	X	2854	G	P-O3'-C3'	6.66	127.69	119.70
1	X	1343	C	O4'-C1'-N1	6.65	113.52	108.20
1	X	559	C	C1'-O4'-C4'	-6.64	104.58	109.90
1	X	1232	U	O4'-C1'-N1	6.64	113.52	108.20
1	X	1927	U	P-O3'-C3'	6.64	127.67	119.70
1	X	346	C	C2-N1-C1'	6.64	126.11	118.80
1	X	1716	G	O3'-P-O5'	-6.64	91.38	104.00
1	X	559	C	C3'-C2'-C1'	6.64	106.81	101.50
1	X	996	C	N1-C2-O2	6.64	122.88	118.90
1	X	2487	G	O4'-C1'-N9	6.64	113.51	108.20
1	X	689	A	C1'-O4'-C4'	-6.63	104.59	109.90
1	X	343	A	O4'-C1'-C2'	-6.63	99.17	105.80
1	X	578	U	O4'-C1'-N1	6.63	113.51	108.20
1	X	2622	G	C5-C6-O6	-6.62	124.63	128.60
1	X	2481	G	N1-C6-O6	6.62	123.87	119.90
2	Y	62	C	O4'-C1'-N1	6.61	113.49	108.20
1	X	1749	G	C3'-C2'-C1'	-6.61	96.21	101.50
1	X	2585	C	C3'-C2'-C1'	-6.61	96.21	101.50
1	X	2208	U	O4'-C1'-N1	6.61	113.49	108.20
1	X	2276	C	O4'-C1'-N1	6.60	113.48	108.20
1	X	2199	C	P-O5'-C5'	6.60	131.45	120.90
1	X	1115	C	O4'-C1'-N1	6.59	113.47	108.20
1	X	537	C	N1-C2-N3	-6.59	114.58	119.20
1	X	2782	G	N9-C1'-C2'	-6.59	104.75	112.00
1	X	355	G	O4'-C1'-N9	6.59	113.47	108.20
1	X	2875	C	O4'-C1'-N1	6.59	113.47	108.20
1	X	1092	U	O4'-C1'-N1	6.58	113.47	108.20
1	X	1247	U	O4'-C1'-N1	6.58	113.46	108.20
1	X	42	G	C8-N9-C4	-6.58	103.77	106.40
1	X	131	C	O4'-C1'-N1	6.58	113.46	108.20
2	Y	75	A	P-O5'-C5'	6.57	131.42	120.90
1	X	2857	C	O4'-C1'-N1	6.57	113.46	108.20
1	X	1223	G	C4-C5-N7	6.57	113.43	110.80
1	X	1664	G	O5'-P-OP1	-6.57	99.79	105.70
1	X	1685	A	P-O3'-C3'	6.56	127.57	119.70
1	X	2475	C	O4'-C1'-N1	6.56	113.44	108.20
1	X	2492	G	O4'-C1'-N9	6.55	113.44	108.20
1	X	2596	C	O4'-C1'-N1	6.55	113.44	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	824	U	C1'-O4'-C4'	-6.54	104.67	109.90
1	X	1812	U	P-O3'-C3'	6.54	127.55	119.70
1	X	1333	G	N3-C4-C5	6.54	131.87	128.60
2	Y	123	U	N1-C1'-C2'	6.54	122.50	114.00
1	X	1090	C	O4'-C1'-N1	6.54	113.43	108.20
1	X	2056	C	O4'-C1'-N1	6.54	113.43	108.20
1	X	2037	A	O4'-C1'-N9	6.53	113.43	108.20
1	X	2206	C	O4'-C1'-N1	6.53	113.43	108.20
1	X	1319	C	O4'-C1'-N1	6.53	113.43	108.20
1	X	2864	C	O4'-C1'-N1	6.53	113.42	108.20
1	X	866	U	O4'-C1'-N1	6.53	113.42	108.20
1	X	1415	C	O4'-C1'-N1	6.53	113.42	108.20
1	X	1468	A	P-O5'-C5'	6.53	131.34	120.90
1	X	1939	U	N3-C2-O2	-6.53	117.63	122.20
1	X	332	C	P-O3'-C3'	6.52	127.53	119.70
1	X	2808	U	C1'-O4'-C4'	-6.52	104.68	109.90
1	X	1770	U	C5-C6-N1	-6.52	119.44	122.70
1	X	12	U	C2-N1-C1'	6.51	125.52	117.70
1	X	562	G	C3'-C2'-C1'	-6.51	96.29	101.50
1	X	1745	C	P-O3'-C3'	-6.51	111.89	119.70
1	X	2731	G	O4'-C1'-N9	6.51	113.41	108.20
1	X	1567	A	O4'-C1'-N9	6.51	113.41	108.20
1	X	1706	A	P-O5'-C5'	-6.51	110.48	120.90
1	X	2228	U	C3'-C2'-C1'	6.51	106.71	101.50
1	X	1830	C	C1'-O4'-C4'	-6.51	104.69	109.90
1	X	193	A	O4'-C1'-N9	6.50	113.40	108.20
1	X	1467	U	C5-C6-N1	6.50	125.95	122.70
2	Y	55	C	O4'-C1'-N1	6.50	113.40	108.20
1	X	1067	G	P-O3'-C3'	6.50	127.49	119.70
1	X	1009	C	N1-C2-O2	6.48	122.79	118.90
1	X	2625	U	C5-C4-O4	-6.48	122.01	125.90
1	X	2700	U	P-O3'-C3'	-6.48	111.92	119.70
1	X	182	G	P-O3'-C3'	6.48	127.47	119.70
1	X	418	C	C1'-O4'-C4'	-6.48	104.72	109.90
1	X	1764	A	C3'-C2'-C1'	-6.48	96.32	101.50
1	X	393	U	O4'-C1'-N1	6.47	113.38	108.20
1	X	1598	C	O4'-C1'-N1	6.47	113.38	108.20
2	Y	110	U	O4'-C1'-N1	6.47	113.38	108.20
1	X	689	A	C5-N7-C8	-6.47	100.67	103.90
1	X	2009	U	O4'-C1'-N1	6.47	113.37	108.20
1	X	2663	U	P-O3'-C3'	-6.47	111.94	119.70
1	X	460	U	P-O3'-C3'	6.46	127.46	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2306	A	O4'-C1'-N9	6.46	113.37	108.20
1	X	408	U	P-O3'-C3'	6.46	127.45	119.70
1	X	2671	C	N1-C2-O2	6.46	122.78	118.90
1	X	1318	A	P-O3'-C3'	6.46	127.45	119.70
1	X	1862	C	O4'-C1'-N1	6.46	113.37	108.20
1	X	1947	G	O4'-C1'-N9	-6.46	103.03	108.20
1	X	2281	C	O4'-C1'-N1	6.46	113.36	108.20
1	X	22	C	O4'-C1'-N1	6.45	113.36	108.20
1	X	2038	C	O4'-C1'-N1	6.45	113.36	108.20
2	Y	50	U	O4'-C1'-N1	6.45	113.36	108.20
1	X	873	U	O4'-C1'-N1	6.45	113.36	108.20
1	X	1223	G	C6-C5-N7	-6.45	126.53	130.40
1	X	349	G	N3-C4-C5	-6.43	125.39	128.60
1	X	1574	A	C5'-C4'-O4'	6.43	116.82	109.10
1	X	422	C	O4'-C1'-N1	6.43	113.34	108.20
1	X	1291	G	O4'-C1'-N9	6.43	113.34	108.20
1	X	1317	G	O4'-C1'-N9	6.42	113.34	108.20
1	X	1496	G	C2'-C3'-O3'	6.42	123.98	113.70
1	X	431	G	O4'-C1'-N9	6.42	113.34	108.20
1	X	446	C	N1-C2-O2	6.42	122.75	118.90
1	X	1692	C	C3'-C2'-C1'	6.42	106.64	101.50
1	X	1940	C	P-O3'-C3'	-6.42	111.99	119.70
1	X	424	G	P-O3'-C3'	6.42	127.40	119.70
1	X	2488	G	C5-C6-N1	6.42	114.71	111.50
1	X	619	A	O4'-C1'-N9	6.41	113.33	108.20
1	X	1208	A	O4'-C1'-N9	6.41	113.33	108.20
1	X	1552	C	P-O3'-C3'	6.41	127.39	119.70
1	X	559	C	C5'-C4'-C3'	6.41	126.25	116.00
1	X	1152	C	C1'-O4'-C4'	-6.41	104.78	109.90
1	X	1222	G	P-O3'-C3'	6.41	127.39	119.70
1	X	1333	G	C8-N9-C1'	6.41	135.33	127.00
1	X	244	C	O4'-C1'-N1	6.40	113.32	108.20
1	X	527	C	P-O3'-C3'	6.40	127.38	119.70
1	X	630	G	O4'-C1'-N9	6.40	113.32	108.20
2	Y	57	U	O4'-C1'-N1	6.40	113.32	108.20
1	X	956	A	P-O5'-C5'	6.39	131.13	120.90
1	X	1999	U	P-O3'-C3'	-6.39	112.03	119.70
1	X	2185	U	O4'-C1'-N1	6.39	113.32	108.20
1	X	1241	G	P-O3'-C3'	-6.39	112.03	119.70
1	X	322	A	P-O3'-C3'	6.38	127.36	119.70
1	X	429	C	O4'-C1'-N1	6.38	113.31	108.20
1	X	40	U	O4'-C1'-N1	6.38	113.31	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1229	C	N1-C2-O2	6.38	122.73	118.90
1	X	2082	C	O4'-C1'-N1	6.38	113.30	108.20
1	X	1446	U	O4'-C1'-N1	6.38	113.30	108.20
1	X	1796	A	C2-N3-C4	6.38	113.79	110.60
2	Y	17	A	O4'-C1'-N9	6.38	113.30	108.20
1	X	2032	G	C5-C6-O6	-6.38	124.78	128.60
1	X	2719	U	O4'-C1'-N1	6.38	113.30	108.20
1	X	169	C	O4'-C1'-N1	6.37	113.30	108.20
1	X	338	G	N7-C8-N9	6.37	116.29	113.10
1	X	2582	G	P-O5'-C5'	6.37	131.09	120.90
23	U	18	VAL	C-N-CA	6.37	137.63	121.70
1	X	1291	G	O4'-C4'-C3'	-6.37	97.63	104.00
1	X	1454	U	O4'-C1'-N1	6.37	113.29	108.20
1	X	1647	U	N3-C4-C5	-6.37	110.78	114.60
1	X	2032	G	O4'-C4'-C3'	-6.36	97.64	104.00
1	X	2494	C	O4'-C1'-N1	6.36	113.29	108.20
1	X	1829	C	O4'-C1'-N1	6.36	113.29	108.20
1	X	1338	G	O4'-C1'-N9	6.36	113.29	108.20
1	X	2661	G	C5-C6-O6	-6.36	124.79	128.60
1	X	2578	G	P-O5'-C5'	6.35	131.07	120.90
1	X	2653	A	O4'-C1'-N9	6.35	113.28	108.20
2	Y	86	A	C1'-O4'-C4'	-6.35	104.82	109.90
1	X	757	U	N3-C2-O2	-6.35	117.76	122.20
1	X	1670	G	O4'-C1'-N9	-6.35	103.12	108.20
1	X	1036	G	C4'-C3'-C2'	6.35	108.95	102.60
1	X	981	C	O4'-C1'-N1	6.34	113.28	108.20
1	X	1732	U	O4'-C1'-N1	6.34	113.27	108.20
1	X	309	G	C8-N9-C4	-6.34	103.86	106.40
1	X	1988	A	P-O3'-C3'	6.34	127.31	119.70
1	X	520	C	C4'-C3'-C2'	-6.34	96.26	102.60
1	X	975	C	O4'-C1'-N1	6.33	113.27	108.20
1	X	1306	U	O4'-C1'-N1	6.33	113.27	108.20
1	X	1914	U	O4'-C1'-N1	6.33	113.27	108.20
1	X	838	A	OP1-P-O3'	6.33	119.13	105.20
1	X	2772	U	O4'-C1'-N1	6.33	113.27	108.20
1	X	633	G	O4'-C1'-N9	6.33	113.26	108.20
1	X	650	U	P-O5'-C5'	6.33	131.02	120.90
1	X	967	G	P-O3'-C3'	6.32	127.29	119.70
1	X	2408	G	N3-C4-C5	-6.32	125.44	128.60
2	Y	70	C	O4'-C1'-N1	6.32	113.25	108.20
1	X	1509	A	P-O3'-C3'	6.32	127.28	119.70
1	X	1986	G	O4'-C1'-N9	6.32	113.25	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2544	A	O3'-P-O5'	-6.32	92.00	104.00
1	X	1044	U	P-O3'-C3'	6.31	127.28	119.70
1	X	774	A	C6-N1-C2	6.31	122.39	118.60
1	X	1392	U	P-O3'-C3'	6.31	127.27	119.70
1	X	2670	C	O4'-C1'-N1	6.31	113.25	108.20
1	X	2409	A	N9-C1'-C2'	6.31	122.20	114.00
1	X	1749	G	O4'-C1'-C2'	-6.30	99.50	105.80
1	X	2482	A	C2-N3-C4	6.30	113.75	110.60
2	Y	88	C	C1'-O4'-C4'	-6.30	104.86	109.90
1	X	1333	G	N7-C8-N9	6.30	116.25	113.10
1	X	90	G	P-O3'-C3'	6.30	127.26	119.70
1	X	98	U	O4'-C1'-N1	6.29	113.23	108.20
1	X	1017	C	O4'-C1'-N1	6.29	113.23	108.20
1	X	730	C	P-O3'-C3'	6.29	127.25	119.70
1	X	1407	G	N9-C1'-C2'	6.29	122.17	114.00
1	X	789	G	P-O3'-C3'	6.29	127.24	119.70
1	X	1236	G	C8-N9-C4	-6.29	103.89	106.40
1	X	779	U	O4'-C1'-N1	6.28	113.23	108.20
1	X	2808	U	P-O5'-C5'	6.28	130.95	120.90
2	Y	4	C	O4'-C1'-N1	6.28	113.23	108.20
1	X	343	A	N9-C1'-C2'	6.28	122.16	114.00
1	X	430	C	C6-N1-C2	-6.28	117.79	120.30
1	X	607	C	C3'-C2'-C1'	-6.28	96.48	101.50
1	X	805	G	N9-C1'-C2'	6.28	122.16	114.00
1	X	1792	C	N1-C1'-C2'	6.28	122.16	114.00
1	X	2375	G	O4'-C4'-C3'	-6.28	97.72	104.00
1	X	1982	C	O4'-C4'-C3'	-6.28	97.72	104.00
1	X	2043	A	P-O3'-C3'	6.28	127.23	119.70
19	Q	62	ARG	C-N-CA	6.27	137.38	121.70
1	X	1112	U	O4'-C1'-N1	6.27	113.22	108.20
1	X	1261	G	O4'-C1'-N9	-6.27	103.18	108.20
1	X	1689	U	P-O3'-C3'	6.27	127.23	119.70
1	X	1669	A	O4'-C4'-C3'	-6.27	97.73	104.00
1	X	1783	G	N9-C1'-C2'	-6.27	105.10	112.00
1	X	1882	G	C3'-C2'-C1'	6.27	106.52	101.50
1	X	968	C	C5'-C4'-O4'	6.26	116.61	109.10
1	X	1359	G	C5'-C4'-C3'	-6.26	105.98	116.00
1	X	1825	C	O4'-C1'-N1	6.26	113.21	108.20
1	X	2572	U	N3-C4-O4	6.26	123.78	119.40
1	X	672	C	O4'-C4'-C3'	-6.25	97.75	104.00
1	X	1522	C	N1-C2-O2	6.25	122.65	118.90
1	X	1938	U	C4'-C3'-C2'	6.25	108.85	102.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	456	C	O4'-C1'-N1	6.25	113.20	108.20
1	X	540	G	C5-C6-N1	6.25	114.62	111.50
1	X	655	A	C1'-O4'-C4'	-6.25	104.90	109.90
2	Y	42	U	O4'-C1'-N1	6.25	113.20	108.20
1	X	2081	U	O4'-C1'-N1	6.25	113.20	108.20
1	X	2666	U	P-O3'-C3'	6.25	127.19	119.70
1	X	1288	A	C5'-C4'-C3'	6.24	125.99	116.00
1	X	49	U	P-O3'-C3'	6.24	127.19	119.70
1	X	2258	G	O4'-C4'-C3'	-6.24	97.76	104.00
1	X	485	G	P-O3'-C3'	6.24	127.18	119.70
1	X	480	G	C5-C6-O6	-6.24	124.86	128.60
1	X	968	C	C5-C6-N1	6.24	124.12	121.00
1	X	2867	G	N7-C8-N9	6.23	116.22	113.10
1	X	517	A	P-O3'-C3'	6.23	127.17	119.70
1	X	1983	G	C3'-C2'-C1'	-6.23	96.52	101.50
1	X	2012	A	O4'-C1'-N9	6.23	113.18	108.20
1	X	2366	U	O4'-C1'-N1	6.23	113.18	108.20
1	X	2698	G	C5'-C4'-O4'	6.23	116.57	109.10
1	X	750	C	O4'-C1'-N1	6.23	113.18	108.20
1	X	79	G	C8-N9-C4	-6.22	103.91	106.40
1	X	1473	U	C4'-C3'-C2'	6.22	108.82	102.60
1	X	2667	C	C4'-C3'-C2'	-6.22	96.38	102.60
1	X	2680	U	O4'-C1'-N1	6.22	113.18	108.20
1	X	684	C	N3-C4-C5	-6.22	119.41	121.90
2	Y	90	C	C4'-C3'-C2'	6.22	108.82	102.60
1	X	1744	G	C5-C6-N1	6.21	114.61	111.50
1	X	2847	G	C8-N9-C4	-6.21	103.92	106.40
1	X	2677	U	O4'-C1'-N1	6.21	113.17	108.20
1	X	160	C	O4'-C1'-N1	6.21	113.17	108.20
1	X	699	G	C4-N9-C1'	-6.21	118.43	126.50
1	X	1190	C	O4'-C1'-N1	6.20	113.16	108.20
1	X	1230	C	O4'-C1'-N1	6.20	113.16	108.20
1	X	2717	G	O4'-C1'-N9	6.20	113.16	108.20
1	X	82	G	P-O3'-C3'	6.20	127.14	119.70
1	X	559	C	N1-C2-O2	6.20	122.62	118.90
1	X	1544	A	P-O3'-C3'	6.19	127.13	119.70
1	X	302	U	O4'-C1'-N1	6.19	113.15	108.20
1	X	2695	C	O4'-C1'-N1	6.19	113.15	108.20
1	X	725	C	O4'-C1'-N1	6.18	113.15	108.20
1	X	1819	U	O4'-C1'-N1	6.18	113.15	108.20
1	X	1412	C	C2'-C3'-O3'	6.18	123.59	113.70
1	X	699	G	C8-N9-C1'	6.18	135.03	127.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1947	G	P-O3'-C3'	6.18	127.12	119.70
1	X	2553	G	O4'-C1'-N9	6.18	113.14	108.20
1	X	2653	A	C3'-C2'-C1'	-6.18	96.56	101.50
1	X	1599	G	P-O3'-C3'	6.17	127.11	119.70
1	X	2500	C	O4'-C1'-N1	6.17	113.14	108.20
1	X	2507	U	O4'-C1'-N1	6.17	113.14	108.20
1	X	579	G	C5-C6-O6	6.17	132.30	128.60
1	X	942	U	N3-C2-O2	-6.17	117.88	122.20
1	X	1270	C	N3-C4-C5	-6.17	119.43	121.90
1	X	2344	G	P-O3'-C3'	6.17	127.11	119.70
2	Y	22	U	O4'-C1'-N1	6.17	113.14	108.20
2	Y	53	G	C8-N9-C4	-6.16	103.94	106.40
1	X	1056	U	P-O3'-C3'	6.16	127.09	119.70
1	X	2764	U	O4'-C1'-N1	6.16	113.13	108.20
1	X	607	C	N1-C2-O2	6.16	122.59	118.90
1	X	1570	C	P-O3'-C3'	6.16	127.09	119.70
1	X	2393	G	P-O3'-C3'	-6.15	112.32	119.70
1	X	1472	C	N1-C2-O2	6.15	122.59	118.90
2	Y	87	C	N1-C2-O2	6.15	122.59	118.90
1	X	729	A	P-O3'-C3'	6.15	127.08	119.70
1	X	940	G	C5'-C4'-O4'	6.15	116.48	109.10
1	X	2416	U	O4'-C1'-N1	6.14	113.11	108.20
1	X	631	G	P-O3'-C3'	6.14	127.07	119.70
1	X	1169	C	N1-C2-O2	6.14	122.58	118.90
1	X	1001	A	C8-N9-C4	-6.14	103.34	105.80
1	X	1128	G	P-O3'-C3'	6.13	127.06	119.70
1	X	2735	C	O4'-C1'-N1	6.13	113.11	108.20
1	X	2790	C	N1-C2-O2	6.13	122.58	118.90
2	Y	46	G	C3'-C2'-C1'	6.13	106.40	101.50
2	Y	54	U	P-O3'-C3'	6.13	127.05	119.70
1	X	539	A	N9-C1'-C2'	6.13	121.97	114.00
1	X	594	G	P-O3'-C3'	6.13	127.05	119.70
1	X	859	U	N1-C1'-C2'	6.12	121.96	114.00
1	X	933	G	P-O3'-C3'	-6.12	112.35	119.70
1	X	199	A	P-O3'-C3'	6.12	127.05	119.70
1	X	917	U	O4'-C1'-N1	6.12	113.10	108.20
1	X	2791	C	N1-C2-O2	6.12	122.57	118.90
1	X	35	G	O4'-C1'-N9	6.12	113.10	108.20
1	X	540	G	C8-N9-C4	-6.12	103.95	106.40
1	X	1824	C	N1-C2-O2	6.12	122.57	118.90
1	X	536	A	O4'-C1'-N9	6.11	113.09	108.20
1	X	1375	C	N1-C2-O2	6.11	122.57	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	19	C	O4'-C1'-N1	6.11	113.08	108.20
2	Y	45	C	N1-C2-O2	6.11	122.56	118.90
1	X	566	U	O4'-C1'-N1	6.10	113.08	108.20
1	X	1185	C	P-O5'-C5'	6.10	130.66	120.90
1	X	1325	U	O4'-C1'-N1	6.10	113.08	108.20
1	X	1647	U	N3-C4-O4	6.10	123.67	119.40
1	X	2465	G	O4'-C1'-N9	6.10	113.08	108.20
2	Y	13	C	O4'-C1'-N1	6.10	113.08	108.20
1	X	1469	U	N1-C1'-C2'	6.10	121.93	114.00
1	X	2223	U	P-O3'-C3'	-6.10	112.38	119.70
1	X	2275	U	P-O3'-C3'	6.10	127.02	119.70
1	X	2808	U	C5'-C4'-O4'	6.10	116.42	109.10
1	X	2240	C	N1-C2-O2	6.09	122.56	118.90
1	X	2415	G	P-O3'-C3'	6.09	127.01	119.70
1	X	476	G	N3-C4-C5	-6.09	125.56	128.60
1	X	875	G	C8-N9-C4	-6.09	103.97	106.40
2	Y	34	C	O4'-C1'-N1	6.08	113.07	108.20
1	X	1953	A	P-O5'-C5'	-6.08	111.17	120.90
1	X	2014	A	P-O3'-C3'	6.08	127.00	119.70
1	X	2609	G	O4'-C1'-N9	6.08	113.06	108.20
1	X	757	U	P-O3'-C3'	6.08	126.99	119.70
1	X	2315	A	O4'-C1'-N9	-6.08	103.34	108.20
1	X	1692	C	O4'-C1'-N1	6.08	113.06	108.20
1	X	1409	U	N1-C1'-C2'	6.07	121.89	114.00
1	X	2224	U	O4'-C1'-N1	6.07	113.06	108.20
1	X	2337	A	O4'-C1'-N9	6.07	113.06	108.20
2	Y	114	C	O4'-C1'-N1	6.07	113.06	108.20
1	X	955	G	P-O3'-C3'	6.07	126.98	119.70
1	X	246	C	N1-C2-O2	6.07	122.54	118.90
1	X	784	U	O4'-C1'-N1	6.07	113.05	108.20
1	X	2758	A	O4'-C1'-N9	6.07	113.05	108.20
1	X	56	C	O4'-C1'-N1	6.07	113.05	108.20
1	X	1249	G	N9-C1'-C2'	6.07	121.89	114.00
1	X	1183	C	O4'-C1'-N1	6.06	113.05	108.20
1	X	2329	C	O4'-C1'-N1	6.06	113.05	108.20
1	X	2869	U	O4'-C1'-N1	6.06	113.05	108.20
1	X	236	C	C6-N1-C2	-6.06	117.88	120.30
1	X	242	A	C5'-C4'-O4'	6.06	116.37	109.10
1	X	632	A	P-O3'-C3'	6.06	126.97	119.70
1	X	1986	G	P-O3'-C3'	-6.06	112.43	119.70
1	X	1773	C	N1-C2-O2	6.06	122.53	118.90
1	X	2782	G	N1-C6-O6	6.05	123.53	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	483	A	C4'-C3'-C2'	6.05	108.65	102.60
1	X	610	G	O3'-P-O5'	-6.05	92.51	104.00
1	X	2554	C	N1-C2-O2	6.04	122.53	118.90
1	X	423	G	C8-N9-C4	-6.04	103.98	106.40
1	X	794	A	N9-C1'-C2'	6.04	121.86	114.00
1	X	2795	A	C2-N3-C4	6.04	113.62	110.60
2	Y	97	C	N1-C2-O2	6.04	122.53	118.90
1	X	103	U	O4'-C1'-N1	6.04	113.03	108.20
1	X	1306	U	N3-C2-O2	-6.04	117.97	122.20
1	X	1989	C	O4'-C4'-C3'	-6.03	97.97	104.00
1	X	1388	C	O4'-C1'-N1	6.03	113.02	108.20
1	X	408	U	O4'-C1'-N1	6.03	113.02	108.20
1	X	1543	G	P-O3'-C3'	6.03	126.93	119.70
1	X	2459	C	N3-C2-O2	-6.03	117.68	121.90
1	X	1482	U	N1-C1'-C2'	6.03	121.83	114.00
1	X	2303	C	P-O3'-C3'	6.02	126.92	119.70
1	X	804	C	O4'-C1'-N1	6.02	113.01	108.20
1	X	1629	G	N9-C1'-C2'	-6.02	105.38	112.00
1	X	330	C	O4'-C1'-N1	6.01	113.01	108.20
1	X	796	A	N7-C8-N9	6.01	116.81	113.80
1	X	1594	U	O4'-C1'-N1	6.01	113.01	108.20
1	X	2178	U	O4'-C1'-N1	6.01	113.01	108.20
1	X	2840	U	P-O3'-C3'	6.01	126.92	119.70
1	X	1985	G	C3'-C2'-C1'	-6.01	96.69	101.50
1	X	2482	A	O4'-C1'-N9	6.01	113.01	108.20
1	X	2659	C	P-O3'-C3'	-6.01	112.49	119.70
1	X	343	A	P-O5'-C5'	6.00	130.51	120.90
1	X	2782	G	C5-C6-O6	-6.00	125.00	128.60
1	X	2590	U	O4'-C1'-N1	6.00	113.00	108.20
1	X	699	G	C5-N7-C8	-6.00	101.30	104.30
1	X	1217	U	C3'-C2'-C1'	-6.00	96.70	101.50
1	X	1016	C	C6-N1-C2	-5.99	117.90	120.30
2	Y	98	C	N1-C2-O2	5.99	122.50	118.90
1	X	248	A	P-O5'-C5'	5.99	130.49	120.90
1	X	1034	U	O4'-C1'-N1	5.99	112.99	108.20
1	X	2467	A	N1-C6-N6	-5.99	115.01	118.60
1	X	1407	G	C5-C6-O6	-5.99	125.01	128.60
1	X	1933	G	O4'-C1'-N9	5.99	112.99	108.20
1	X	2228	U	C6-N1-C2	-5.99	117.41	121.00
1	X	2229	G	P-O5'-C5'	-5.98	111.33	120.90
1	X	2680	U	C3'-C2'-C1'	-5.98	96.72	101.50
1	X	2688	G	O4'-C1'-N9	-5.98	103.42	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	32	C	C5-C6-N1	5.98	123.99	121.00
1	X	1030	U	O4'-C1'-N1	5.98	112.98	108.20
1	X	1284	G	N7-C8-N9	5.98	116.09	113.10
1	X	1335	A	P-O3'-C3'	-5.98	112.53	119.70
1	X	2586	G	C4'-C3'-C2'	-5.98	96.62	102.60
1	X	2808	U	C3'-C2'-C1'	-5.98	96.72	101.50
1	X	786	U	O4'-C1'-N1	5.97	112.98	108.20
1	X	1306	U	N1-C2-O2	5.97	126.98	122.80
1	X	1333	G	C5-N7-C8	-5.97	101.31	104.30
1	X	2380	U	O4'-C1'-N1	5.97	112.98	108.20
1	X	111	G	P-O5'-C5'	5.97	130.45	120.90
1	X	2724	G	O5'-C5'-C4'	-5.97	100.36	111.70
1	X	1753	A	O4'-C1'-N9	5.97	112.97	108.20
1	X	1057	A	P-O3'-C3'	5.97	126.86	119.70
1	X	1181	C	O4'-C1'-N1	5.97	112.97	108.20
1	X	1816	G	O4'-C1'-N9	5.97	112.97	108.20
1	X	675	C	C3'-C2'-C1'	-5.96	96.73	101.50
1	X	1526	U	P-O5'-C5'	5.96	130.44	120.90
1	X	1076	U	O4'-C1'-N1	5.96	112.97	108.20
1	X	1339	U	OP2-P-O3'	5.96	118.31	105.20
1	X	1249	G	C2'-C3'-O3'	5.96	123.23	113.70
1	X	1338	G	N3-C4-N9	5.96	129.57	126.00
1	X	2598	C	N1-C2-O2	5.96	122.47	118.90
1	X	1978	U	C5-C4-O4	-5.96	122.33	125.90
1	X	2672	U	N3-C2-O2	-5.96	118.03	122.20
1	X	1744	G	N3-C4-N9	5.96	129.57	126.00
1	X	2867	G	C5-N7-C8	-5.96	101.32	104.30
1	X	560	G	N9-C1'-C2'	5.95	121.74	114.00
1	X	1111	C	O4'-C1'-N1	5.95	112.96	108.20
1	X	2561	G	C6-C5-N7	-5.95	126.83	130.40
1	X	2708	U	O4'-C1'-N1	5.95	112.96	108.20
1	X	2649	A	C5'-C4'-C3'	-5.94	106.49	116.00
1	X	1142	G	O4'-C1'-C2'	-5.94	99.86	105.80
2	Y	35	C	O4'-C1'-N1	5.94	112.95	108.20
1	X	1582	A	C5'-C4'-O4'	5.94	116.23	109.10
1	X	1647	U	O4'-C1'-N1	5.94	112.95	108.20
1	X	2837	G	P-O3'-C3'	-5.94	112.57	119.70
1	X	852	U	P-O5'-C5'	-5.93	111.41	120.90
1	X	2616	U	O4'-C1'-N1	5.93	112.95	108.20
1	X	1439	G	C2'-C3'-O3'	5.93	123.19	113.70
1	X	2835	A	N1-C6-N6	5.93	122.16	118.60
1	X	580	A	C1'-O4'-C4'	-5.93	105.16	109.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1708	C	O4'-C1'-N1	5.93	112.94	108.20
1	X	2769	C	P-O3'-C3'	5.93	126.81	119.70
1	X	957	G	C5-C6-N1	5.93	114.46	111.50
1	X	2523	G	O4'-C1'-N9	5.93	112.94	108.20
1	X	1939	U	N1-C2-O2	5.93	126.95	122.80
1	X	2839	G	C5-C6-N1	5.93	114.46	111.50
1	X	1099	A	P-O3'-C3'	5.92	126.81	119.70
1	X	2201	G	C5'-C4'-O4'	5.92	116.21	109.10
1	X	1245	G	O4'-C1'-N9	5.92	112.94	108.20
1	X	2338	C	O4'-C1'-N1	5.92	112.93	108.20
2	Y	7	C	O4'-C1'-N1	5.92	112.93	108.20
1	X	938	G	C3'-C2'-C1'	5.91	106.23	101.50
1	X	2013	A	C5'-C4'-O4'	5.91	116.20	109.10
1	X	827	C	O4'-C1'-N1	5.91	112.93	108.20
1	X	26	G	C8-N9-C4	-5.91	104.03	106.40
1	X	334	G	O4'-C1'-N9	5.91	112.93	108.20
1	X	468	A	P-O3'-C3'	5.91	126.79	119.70
1	X	2493	U	O4'-C1'-N1	5.91	112.93	108.20
2	Y	49	C	C5'-C4'-O4'	5.90	116.18	109.10
1	X	2359	U	O4'-C1'-N1	5.90	112.92	108.20
1	X	540	G	C5-C6-O6	5.90	132.14	128.60
1	X	1744	G	N3-C4-C5	-5.90	125.65	128.60
1	X	2599	U	P-O5'-C5'	-5.90	111.47	120.90
1	X	1678	G	C5-C6-O6	-5.90	125.06	128.60
1	X	2015	G	N9-C1'-C2'	5.90	121.67	114.00
1	X	2444	C	O4'-C1'-N1	5.89	112.91	108.20
1	X	2636	A	O4'-C1'-N9	5.89	112.92	108.20
1	X	884	C	O4'-C1'-N1	5.89	112.91	108.20
1	X	1529	C	O4'-C1'-N1	5.89	112.91	108.20
1	X	657	A	C3'-C2'-C1'	-5.89	96.79	101.50
1	X	2017	U	O4'-C1'-N1	5.89	112.91	108.20
15	M	29	PRO	N-CA-C	5.89	127.41	112.10
1	X	1454	U	N3-C4-O4	5.88	123.52	119.40
1	X	2441	U	O4'-C1'-N1	5.88	112.90	108.20
1	X	1089	C	P-O3'-C3'	5.88	126.75	119.70
1	X	1244	U	C5-C6-N1	5.87	125.64	122.70
1	X	2572	U	O4'-C1'-N1	5.87	112.90	108.20
1	X	882	C	N1-C2-O2	5.87	122.42	118.90
1	X	1736	C	O4'-C1'-N1	5.87	112.90	108.20
1	X	155	G	O4'-C1'-N9	5.87	112.90	108.20
1	X	1429	A	P-O3'-C3'	5.87	126.74	119.70
1	X	237	G	O4'-C1'-N9	5.87	112.89	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	559	C	N3-C2-O2	-5.87	117.79	121.90
1	X	999	A	O4'-C1'-N9	5.87	112.89	108.20
1	X	2619	G	C5-C6-O6	-5.87	125.08	128.60
1	X	1678	G	O4'-C4'-C3'	-5.86	98.14	104.00
1	X	1023	U	P-O3'-C3'	5.86	126.73	119.70
1	X	2225	G	O4'-C1'-N9	5.86	112.89	108.20
1	X	2560	G	C3'-C2'-C1'	5.86	106.19	101.50
1	X	2745	A	P-O3'-C3'	5.86	126.73	119.70
1	X	2370	G	C1'-O4'-C4'	-5.86	105.21	109.90
1	X	1627	C	O4'-C1'-N1	5.86	112.89	108.20
1	X	939	C	C3'-C2'-C1'	5.85	106.18	101.50
1	X	998	C	O4'-C1'-N1	5.85	112.88	108.20
2	Y	2	C	O4'-C1'-N1	5.85	112.88	108.20
1	X	234	C	O4'-C1'-N1	5.85	112.88	108.20
1	X	771	C	C4'-C3'-C2'	-5.85	96.75	102.60
1	X	1353	A	O4'-C1'-N9	5.85	112.88	108.20
1	X	1667	A	N1-C6-N6	5.85	122.11	118.60
1	X	2797	G	P-O3'-C3'	5.85	126.72	119.70
2	Y	76	U	O4'-C1'-N1	5.85	112.88	108.20
1	X	577	U	C1'-O4'-C4'	-5.85	105.22	109.90
1	X	2797	G	N3-C4-N9	5.85	129.51	126.00
1	X	1389	C	O4'-C1'-N1	5.85	112.88	108.20
1	X	1975	G	N1-C6-O6	-5.84	116.39	119.90
1	X	2635	U	O4'-C1'-N1	5.84	112.88	108.20
1	X	2303	C	N1-C2-O2	5.84	122.41	118.90
1	X	2376	G	P-O5'-C5'	5.84	130.24	120.90
1	X	2009	U	P-O3'-C3'	-5.84	112.69	119.70
9	G	106	TYR	N-CA-CB	5.84	121.11	110.60
2	Y	116	C	O4'-C1'-N1	5.84	112.87	108.20
1	X	68	C	N1-C2-O2	5.83	122.40	118.90
1	X	422	C	C6-N1-C2	-5.83	117.97	120.30
1	X	741	G	P-O3'-C3'	5.83	126.70	119.70
1	X	1888	C	C3'-C2'-C1'	5.83	106.16	101.50
1	X	770	U	C3'-C2'-C1'	-5.83	96.84	101.50
1	X	1223	G	C5-C6-O6	-5.83	125.11	128.60
1	X	2645	C	O4'-C1'-N1	5.83	112.86	108.20
1	X	434	C	O4'-C1'-N1	5.82	112.86	108.20
1	X	522	G	N9-C1'-C2'	5.82	121.57	114.00
1	X	1993	G	C8-N9-C4	-5.82	104.07	106.40
1	X	2627	G	C5-C6-O6	-5.82	125.11	128.60
1	X	1032	A	C3'-C2'-C1'	-5.82	96.84	101.50
1	X	575	U	O4'-C1'-N1	5.82	112.86	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1682	A	C5-C6-N6	-5.82	119.05	123.70
1	X	2567	G	N7-C8-N9	5.82	116.01	113.10
1	X	533	C	O4'-C1'-N1	5.81	112.85	108.20
1	X	1778	U	O4'-C1'-N1	5.81	112.85	108.20
1	X	2797	G	C6-C5-N7	-5.81	126.92	130.40
1	X	797	A	P-O3'-C3'	5.80	126.67	119.70
1	X	220	U	O4'-C1'-N1	5.80	112.84	108.20
1	X	689	A	N7-C8-N9	5.80	116.70	113.80
1	X	582	G	C8-N9-C4	-5.80	104.08	106.40
1	X	339	U	C3'-C2'-C1'	5.80	106.14	101.50
1	X	1831	G	C8-N9-C4	-5.80	104.08	106.40
1	X	661	C	N1-C2-O2	5.79	122.38	118.90
1	X	2460	G	C8-N9-C4	-5.79	104.08	106.40
1	X	1407	G	C8-N9-C4	-5.79	104.08	106.40
1	X	1276	U	O4'-C1'-N1	5.79	112.83	108.20
1	X	466	A	P-O3'-C3'	5.79	126.64	119.70
1	X	1058	G	O4'-C1'-N9	5.79	112.83	108.20
1	X	1466	C	C4'-C3'-C2'	-5.79	96.81	102.60
1	X	1920	A	C1'-O4'-C4'	-5.79	105.27	109.90
1	X	2230	G	C5'-C4'-O4'	-5.79	102.16	109.10
1	X	2778	U	C3'-C2'-C1'	5.79	106.13	101.50
1	X	541	C	P-O3'-C3'	5.78	126.64	119.70
1	X	1987	G	C5-C6-O6	-5.78	125.13	128.60
1	X	556	A	P-O3'-C3'	5.78	126.64	119.70
1	X	461	A	C2-N3-C4	5.78	113.49	110.60
1	X	774	A	C4-C5-C6	5.78	119.89	117.00
1	X	1286	U	P-O3'-C3'	5.78	126.63	119.70
1	X	2527	G	C8-N9-C4	-5.78	104.09	106.40
1	X	467	U	N3-C2-O2	-5.78	118.16	122.20
1	X	1122	A	N9-C1'-C2'	5.78	121.51	114.00
1	X	1288	A	P-O3'-C3'	-5.77	112.77	119.70
1	X	1958	G	C5-C6-N1	5.77	114.39	111.50
1	X	1753	A	P-O5'-C5'	5.77	130.13	120.90
1	X	2487	G	C5-C6-N1	5.77	114.39	111.50
1	X	2604	G	C5-C6-N1	5.77	114.39	111.50
2	Y	64	C	O4'-C1'-N1	5.77	112.82	108.20
1	X	2571	G	C3'-C2'-C1'	-5.77	96.89	101.50
1	X	1224	A	P-O3'-C3'	5.76	126.62	119.70
1	X	202	A	O4'-C1'-N9	5.76	112.81	108.20
1	X	1058	G	C1'-O4'-C4'	-5.76	105.29	109.90
1	X	1841	G	O4'-C1'-N9	5.76	112.81	108.20
1	X	673	G	C2'-C3'-O3'	5.76	122.92	113.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1811	A	C2'-C3'-O3'	5.76	122.92	113.70
2	Y	76	U	N3-C2-O2	-5.76	118.17	122.20
1	X	29	U	O4'-C1'-N1	5.76	112.81	108.20
1	X	396	U	C1'-O4'-C4'	-5.76	105.30	109.90
1	X	764	A	O5'-P-OP2	-5.76	100.52	105.70
1	X	2840	U	O4'-C1'-N1	5.75	112.80	108.20
1	X	1311	C	N1-C2-O2	5.75	122.35	118.90
1	X	1251	G	N9-C1'-C2'	-5.75	105.68	112.00
2	Y	5	C	O4'-C1'-N1	5.75	112.80	108.20
1	X	352	G	P-O5'-C5'	5.74	130.09	120.90
1	X	603	C	N1-C2-O2	5.74	122.34	118.90
1	X	2458	U	O4'-C1'-N1	5.74	112.79	108.20
1	X	223	C	P-O3'-C3'	-5.74	112.81	119.70
1	X	1843	U	O4'-C1'-N1	5.74	112.79	108.20
1	X	2427	A	P-O3'-C3'	5.74	126.58	119.70
1	X	1081	A	P-O3'-C3'	5.74	126.58	119.70
1	X	420	C	O4'-C1'-N1	5.74	112.79	108.20
1	X	447	U	P-O3'-C3'	5.74	126.58	119.70
1	X	1729	C	O4'-C1'-N1	5.74	112.79	108.20
1	X	2572	U	C3'-C2'-C1'	-5.73	96.91	101.50
1	X	2735	C	C6-N1-C2	-5.73	118.01	120.30
1	X	67	G	O4'-C1'-N9	5.73	112.78	108.20
1	X	1442	C	N1-C2-O2	5.73	122.34	118.90
1	X	2364	C	O4'-C1'-N1	5.73	112.78	108.20
1	X	799	C	P-O5'-C5'	-5.72	111.74	120.90
1	X	860	U	C5'-C4'-O4'	5.72	115.97	109.10
1	X	2048	C	P-O5'-C5'	-5.72	111.75	120.90
1	X	2559	U	N1-C2-O2	5.72	126.80	122.80
1	X	2573	C	O4'-C1'-N1	5.72	112.78	108.20
1	X	574	C	P-O3'-C3'	-5.71	112.84	119.70
1	X	1394	G	O4'-C1'-N9	5.71	112.77	108.20
1	X	12	U	N3-C2-O2	-5.71	118.20	122.20
1	X	1093	U	O4'-C1'-N1	5.71	112.77	108.20
1	X	2018	G	C5'-C4'-C3'	-5.71	106.86	116.00
1	X	2724	G	P-O5'-C5'	5.71	130.04	120.90
2	Y	109	G	O4'-C1'-N9	5.71	112.77	108.20
1	X	421	G	P-O5'-C5'	5.71	130.03	120.90
1	X	474	G	O4'-C1'-N9	5.71	112.77	108.20
1	X	536	A	P-O3'-C3'	5.71	126.55	119.70
1	X	724	C	O4'-C1'-N1	5.71	112.77	108.20
1	X	2876	C	O4'-C1'-N1	5.71	112.77	108.20
1	X	1635	G	P-O3'-C3'	-5.70	112.86	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	924	C	N1-C2-O2	5.70	122.32	118.90
1	X	2277	A	O4'-C1'-N9	5.70	112.76	108.20
1	X	2075	U	P-O3'-C3'	5.70	126.54	119.70
1	X	464	G	C3'-C2'-C1'	5.70	106.06	101.50
1	X	1490	U	O4'-C1'-N1	5.70	112.76	108.20
1	X	2258	G	C1'-O4'-C4'	-5.70	105.34	109.90
1	X	2235	G	C3'-C2'-C1'	-5.69	96.94	101.50
2	Y	83	C	N1-C2-O2	5.69	122.32	118.90
1	X	1570	C	N1-C2-O2	5.69	122.31	118.90
1	X	2552	C	O3'-P-O5'	-5.69	93.19	104.00
1	X	516	G	C5-C6-O6	-5.69	125.19	128.60
1	X	656	U	P-O5'-C5'	5.69	130.00	120.90
1	X	2015	G	N7-C8-N9	5.69	115.94	113.10
1	X	1518	C	O4'-C1'-N1	5.68	112.75	108.20
2	Y	120	G	O4'-C1'-N9	5.68	112.75	108.20
1	X	1668	G	P-O5'-C5'	5.68	129.99	120.90
1	X	2702	G	C6-C5-N7	-5.68	126.99	130.40
1	X	156	G	C3'-C2'-C1'	-5.68	96.96	101.50
1	X	889	C	O4'-C1'-N1	5.68	112.74	108.20
1	X	689	A	N1-C6-N6	5.67	122.00	118.60
1	X	2715	C	O4'-C1'-N1	5.67	112.74	108.20
1	X	34	U	C2-N1-C1'	5.67	124.51	117.70
1	X	1341	G	C4'-C3'-C2'	5.67	108.27	102.60
1	X	2846	G	O4'-C1'-N9	5.67	112.74	108.20
15	M	28	ARG	N-CA-C	-5.67	95.69	111.00
1	X	490	A	C5'-C4'-O4'	5.67	115.90	109.10
1	X	2245	A	C5'-C4'-O4'	5.67	115.90	109.10
1	X	467	U	N1-C2-O2	5.67	126.77	122.80
1	X	1075	C	O4'-C1'-N1	5.67	112.73	108.20
1	X	225	G	O4'-C1'-N9	5.67	112.73	108.20
1	X	1222	G	N3-C4-C5	-5.67	125.77	128.60
1	X	1500	U	O4'-C1'-N1	5.66	112.73	108.20
1	X	2285	U	O4'-C1'-N1	5.66	112.73	108.20
1	X	1237	G	O4'-C1'-N9	5.66	112.73	108.20
1	X	1415	C	N1-C2-O2	5.66	122.30	118.90
1	X	1570	C	N3-C2-O2	-5.66	117.94	121.90
1	X	2013	A	C1'-O4'-C4'	-5.66	105.37	109.90
1	X	1324	G	O4'-C1'-C2'	-5.66	100.14	105.80
1	X	2671	C	C4'-C3'-C2'	-5.66	96.94	102.60
1	X	454	G	C4'-C3'-C2'	5.66	108.26	102.60
1	X	478	G	P-O3'-C3'	-5.65	112.92	119.70
1	X	1252	C	C5-C6-N1	5.65	123.83	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2300	G	O4'-C1'-N9	5.65	112.72	108.20
1	X	413	G	O4'-C1'-N9	5.65	112.72	108.20
1	X	459	A	P-O3'-C3'	5.65	126.48	119.70
1	X	1159	U	O4'-C1'-N1	5.65	112.72	108.20
1	X	1281	A	OP2-P-O3'	5.65	117.63	105.20
1	X	516	G	P-O3'-C3'	5.65	126.48	119.70
1	X	1277	G	N3-C4-C5	-5.65	125.78	128.60
1	X	915	C	O4'-C1'-N1	5.64	112.72	108.20
1	X	1421	U	O4'-C1'-N1	5.64	112.72	108.20
1	X	1700	C	P-O3'-C3'	-5.64	112.93	119.70
1	X	175	C	C5-C6-N1	5.64	123.82	121.00
1	X	2018	G	N3-C4-C5	5.64	131.42	128.60
1	X	2552	C	O4'-C1'-N1	5.64	112.71	108.20
1	X	21	A	P-O3'-C3'	-5.64	112.93	119.70
1	X	1337	G	C3'-C2'-C1'	-5.64	96.99	101.50
1	X	2791	C	N3-C2-O2	-5.64	117.95	121.90
1	X	2545	A	P-O3'-C3'	5.64	126.46	119.70
1	X	219	G	O4'-C1'-N9	-5.63	103.69	108.20
1	X	2296	U	O4'-C1'-N1	5.63	112.71	108.20
1	X	42	G	N7-C8-N9	5.63	115.92	113.10
1	X	742	G	C5'-C4'-O4'	5.63	115.86	109.10
1	X	2075	U	O4'-C1'-N1	5.63	112.71	108.20
1	X	2353	G	N3-C4-C5	-5.63	125.78	128.60
1	X	1683	G	O4'-C1'-N9	5.63	112.70	108.20
1	X	1753	A	N7-C8-N9	5.63	116.61	113.80
1	X	806	A	P-O3'-C3'	5.62	126.45	119.70
1	X	426	C	O4'-C1'-N1	5.62	112.70	108.20
1	X	2559	U	P-O3'-C3'	5.62	126.44	119.70
1	X	12	U	N1-C2-O2	5.62	126.73	122.80
1	X	1229	C	O4'-C1'-N1	5.62	112.69	108.20
1	X	75	C	O4'-C1'-N1	5.62	112.69	108.20
1	X	168	A	O4'-C1'-N9	5.62	112.69	108.20
1	X	746	G	N3-C4-C5	-5.62	125.79	128.60
1	X	749	C	C5-C6-N1	5.62	123.81	121.00
1	X	190	A	O4'-C4'-C3'	-5.61	98.39	104.00
1	X	540	G	N9-C1'-C2'	5.61	121.30	114.00
1	X	2294	U	P-O3'-C3'	5.61	126.43	119.70
1	X	2782	G	C6-C5-N7	-5.61	127.03	130.40
1	X	1201	G	C8-N9-C4	-5.61	104.16	106.40
1	X	1249	G	N1-C6-O6	-5.61	116.54	119.90
1	X	2652	G	N3-C4-C5	-5.61	125.80	128.60
1	X	2541	U	N3-C2-O2	-5.60	118.28	122.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	690	A	P-O3'-C3'	5.60	126.42	119.70
1	X	1037	U	O4'-C1'-N1	5.60	112.68	108.20
1	X	2033	C	N1-C2-O2	5.60	122.26	118.90
1	X	1086	C	C3'-C2'-C1'	5.60	105.98	101.50
1	X	1314	A	O4'-C1'-C2'	-5.60	100.20	105.80
1	X	746	G	N3-C4-N9	5.60	129.36	126.00
1	X	982	C	O4'-C1'-N1	5.60	112.68	108.20
1	X	1399	C	O4'-C1'-N1	5.60	112.68	108.20
1	X	1341	G	C5-C6-N1	5.60	114.30	111.50
1	X	1411	C	O4'-C1'-N1	5.60	112.68	108.20
1	X	1660	G	O4'-C1'-N9	5.60	112.68	108.20
1	X	441	A	P-O3'-C3'	5.60	126.42	119.70
1	X	1607	A	C2'-C3'-O3'	5.59	122.65	113.70
1	X	169	C	N1-C2-O2	5.59	122.25	118.90
1	X	392	G	P-O3'-C3'	-5.59	112.99	119.70
1	X	1257	U	O4'-C1'-N1	5.59	112.67	108.20
1	X	534	U	O4'-C1'-N1	5.59	112.67	108.20
1	X	555	U	C1'-O4'-C4'	-5.59	105.43	109.90
1	X	927	C	N3-C2-O2	-5.59	117.99	121.90
1	X	13	A	P-O3'-C3'	5.59	126.41	119.70
1	X	1986	G	O5'-P-OP2	-5.59	100.67	105.70
12	J	87	GLY	C-N-CA	5.59	135.67	121.70
1	X	327	C	N1-C2-O2	5.59	122.25	118.90
1	X	1528	C	O4'-C1'-N1	5.59	112.67	108.20
1	X	1439	G	C8-N9-C4	-5.58	104.17	106.40
1	X	1922	U	P-O3'-C3'	5.58	126.40	119.70
2	Y	14	C	N1-C2-O2	5.58	122.25	118.90
1	X	165	G	O4'-C1'-N9	5.58	112.67	108.20
1	X	719	A	P-O3'-C3'	5.58	126.40	119.70
1	X	1304	U	O4'-C1'-N1	5.58	112.66	108.20
1	X	204	A	C2'-C3'-O3'	5.58	122.63	113.70
1	X	1636	G	O4'-C1'-N9	5.58	112.66	108.20
1	X	1087	C	O4'-C1'-N1	5.58	112.66	108.20
1	X	2338	C	N1-C2-O2	5.58	122.25	118.90
1	X	2403	C	N3-C2-O2	-5.58	118.00	121.90
1	X	327	C	P-O3'-C3'	-5.58	113.01	119.70
1	X	2421	C	O4'-C1'-N1	5.57	112.66	108.20
1	X	2527	G	C2-N3-C4	5.57	114.69	111.90
1	X	1010	U	C5'-C4'-O4'	5.57	115.79	109.10
1	X	2228	U	C4-C5-C6	5.57	123.04	119.70
1	X	878	C	O4'-C1'-N1	5.57	112.66	108.20
2	Y	54	U	C3'-C2'-C1'	5.57	105.96	101.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2015	G	C8-N9-C4	-5.57	104.17	106.40
1	X	2321	C	O4'-C1'-N1	5.57	112.66	108.20
1	X	2435	C	P-O3'-C3'	-5.57	113.02	119.70
1	X	2470	U	P-O3'-C3'	5.57	126.38	119.70
2	Y	32	C	O4'-C1'-N1	5.57	112.65	108.20
1	X	687	G	C3'-C2'-C1'	-5.57	97.05	101.50
1	X	541	C	N1-C1'-C2'	5.56	121.23	114.00
1	X	842	A	C1'-O4'-C4'	-5.56	105.45	109.90
1	X	70	A	P-O3'-C3'	5.56	126.38	119.70
1	X	162	C	O4'-C1'-N1	5.56	112.65	108.20
1	X	617	U	C2-N1-C1'	5.56	124.38	117.70
1	X	2047	C	O4'-C1'-N1	5.56	112.65	108.20
1	X	2791	C	O4'-C1'-N1	5.56	112.65	108.20
1	X	2748	C	O4'-C1'-N1	5.56	112.65	108.20
1	X	2821	G	O4'-C1'-N9	5.56	112.65	108.20
1	X	1630	A	C8-N9-C4	-5.56	103.58	105.80
1	X	1771	A	N1-C6-N6	5.56	121.94	118.60
1	X	2444	C	N1-C2-O2	5.56	122.23	118.90
1	X	2702	G	N7-C8-N9	5.56	115.88	113.10
1	X	2459	C	O4'-C1'-N1	5.56	112.64	108.20
1	X	2668	U	C5-C4-O4	5.56	129.23	125.90
1	X	1593	C	O4'-C1'-N1	5.55	112.64	108.20
1	X	2016	A	N1-C2-N3	-5.55	126.52	129.30
1	X	2422	C	N3-C2-O2	-5.55	118.01	121.90
1	X	1858	C	N1-C2-O2	5.55	122.23	118.90
1	X	86	U	C3'-C2'-C1'	-5.55	97.06	101.50
1	X	1182	U	O4'-C1'-N1	5.55	112.64	108.20
1	X	1251	G	O4'-C1'-N9	5.55	112.64	108.20
1	X	1506	C	O4'-C1'-N1	5.55	112.64	108.20
1	X	467	U	O4'-C1'-N1	5.54	112.64	108.20
1	X	957	G	N3-C4-C5	-5.54	125.83	128.60
1	X	398	C	P-O5'-C5'	5.54	129.76	120.90
1	X	1850	G	O4'-C1'-N9	5.54	112.63	108.20
1	X	2367	A	O4'-C1'-N9	5.54	112.63	108.20
1	X	562	G	O4'-C4'-C3'	-5.54	98.46	104.00
1	X	956	A	C5'-C4'-O4'	5.54	115.74	109.10
1	X	537	C	C6-N1-C1'	-5.54	114.16	120.80
1	X	1275	A	P-O5'-C5'	5.54	129.76	120.90
1	X	1533	G	C5-C6-O6	-5.54	125.28	128.60
1	X	2321	C	C6-N1-C2	-5.54	118.09	120.30
1	X	2775	U	P-O3'-C3'	5.54	126.34	119.70
1	X	224	G	C3'-C2'-C1'	5.53	105.92	101.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	236	C	N1-C2-O2	5.53	122.22	118.90
1	X	2204	A	C5'-C4'-O4'	5.53	115.74	109.10
1	X	156	G	P-O3'-C3'	-5.53	113.07	119.70
1	X	640	C	O4'-C1'-N1	5.53	112.62	108.20
1	X	1142	G	N3-C4-N9	5.53	129.31	126.00
1	X	1630	A	P-O3'-C3'	-5.53	113.07	119.70
1	X	1829	C	P-O3'-C3'	-5.53	113.07	119.70
1	X	2315	A	P-O3'-C3'	5.53	126.33	119.70
1	X	612	G	O4'-C1'-N9	5.52	112.62	108.20
1	X	632	A	C4'-C3'-C2'	-5.52	97.08	102.60
1	X	1233	A	P-O3'-C3'	5.52	126.32	119.70
1	X	1539	U	O4'-C1'-N1	5.52	112.61	108.20
1	X	2496	C	O4'-C1'-N1	5.52	112.61	108.20
1	X	919	U	N1-C2-O2	5.52	126.66	122.80
1	X	1280	U	N3-C2-O2	-5.52	118.34	122.20
1	X	1707	A	P-O3'-C3'	5.52	126.32	119.70
1	X	682	G	C5-C6-N1	5.51	114.26	111.50
1	X	1626	A	N1-C2-N3	-5.51	126.54	129.30
1	X	1840	A	O4'-C1'-N9	5.51	112.61	108.20
1	X	1912	G	P-O3'-C3'	5.51	126.32	119.70
1	X	2222	U	P-O5'-C5'	5.51	129.72	120.90
1	X	440	U	O4'-C1'-N1	5.51	112.61	108.20
1	X	1447	U	O4'-C1'-N1	5.51	112.61	108.20
1	X	455	A	O4'-C1'-N9	5.51	112.61	108.20
1	X	2591	C	N1-C2-N3	-5.51	115.34	119.20
2	Y	10	U	O4'-C1'-N1	5.51	112.61	108.20
1	X	632	A	C1'-O4'-C4'	-5.51	105.49	109.90
1	X	689	A	O4'-C1'-N9	5.51	112.61	108.20
1	X	565	A	P-O3'-C3'	-5.51	113.09	119.70
1	X	2863	U	O4'-C1'-N1	5.50	112.60	108.20
1	X	1167	A	O4'-C1'-N9	-5.50	103.80	108.20
1	X	2620	G	C5-C6-O6	-5.50	125.30	128.60
1	X	2782	G	O4'-C4'-C3'	-5.50	98.50	104.00
1	X	770	U	P-O3'-C3'	-5.50	113.10	119.70
1	X	1225	G	N3-C4-C5	-5.50	125.85	128.60
1	X	1289	A	O4'-C4'-C3'	-5.50	98.50	104.00
1	X	1936	A	N1-C2-N3	-5.50	126.55	129.30
2	Y	55	C	P-O3'-C3'	5.50	126.30	119.70
1	X	1337	G	O4'-C1'-N9	5.50	112.60	108.20
1	X	1743	C	O4'-C1'-N1	5.50	112.60	108.20
1	X	1976	U	C3'-C2'-C1'	5.50	105.90	101.50
1	X	738	G	C8-N9-C4	-5.50	104.20	106.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2088	U	O4'-C1'-N1	5.50	112.60	108.20
1	X	2589	C	N1-C1'-C2'	5.50	121.14	114.00
1	X	476	G	O4'-C1'-N9	5.49	112.59	108.20
1	X	859	U	C5'-C4'-O4'	5.49	115.69	109.10
1	X	1294	G	C4'-C3'-C2'	-5.49	97.11	102.60
1	X	2628	C	C3'-C2'-C1'	-5.49	97.11	101.50
1	X	1162	A	O4'-C1'-N9	5.49	112.59	108.20
1	X	521	U	C2-N1-C1'	5.49	124.29	117.70
1	X	2382	C	O4'-C1'-N1	5.49	112.59	108.20
1	X	1782	A	P-O5'-C5'	5.49	129.68	120.90
1	X	2528	G	OP1-P-O3'	5.49	117.27	105.20
1	X	1831	G	O4'-C1'-N9	5.48	112.59	108.20
1	X	2184	C	O4'-C1'-N1	5.48	112.58	108.20
1	X	2496	C	O3'-P-O5'	-5.48	93.58	104.00
1	X	2528	G	N3-C4-C5	-5.48	125.86	128.60
1	X	796	A	C4-C5-N7	5.48	113.44	110.70
2	Y	112	A	O4'-C1'-N9	5.48	112.58	108.20
23	U	33	LYS	C-N-CA	5.48	135.40	121.70
1	X	322	A	O4'-C1'-N9	5.48	112.58	108.20
1	X	540	G	N9-C4-C5	5.48	107.59	105.40
1	X	698	A	C1'-O4'-C4'	-5.48	105.52	109.90
1	X	940	G	C4'-C3'-C2'	-5.48	97.12	102.60
1	X	1456	C	O4'-C1'-N1	5.48	112.58	108.20
2	Y	76	U	N1-C2-O2	5.48	126.63	122.80
1	X	973	U	O3'-P-O5'	-5.48	93.59	104.00
1	X	2196	U	O4'-C1'-N1	5.48	112.58	108.20
1	X	707	U	O4'-C1'-N1	5.47	112.58	108.20
1	X	1469	U	C5'-C4'-O4'	5.47	115.67	109.10
1	X	1672	A	C3'-C2'-C1'	-5.47	97.12	101.50
1	X	2552	C	OP1-P-O3'	5.47	117.24	105.20
1	X	613	A	P-O3'-C3'	5.47	126.27	119.70
1	X	1308	C	C4'-C3'-C2'	-5.47	97.13	102.60
1	X	1808	C	N1-C2-O2	5.47	122.18	118.90
1	X	2330	G	C8-N9-C4	-5.47	104.21	106.40
1	X	2494	C	N3-C2-O2	-5.47	118.07	121.90
1	X	1965	U	N1-C2-O2	5.47	126.63	122.80
1	X	467	U	C2-N1-C1'	5.47	124.26	117.70
1	X	557	U	N1-C1'-C2'	5.47	121.11	114.00
1	X	1550	C	O4'-C1'-N1	5.47	112.58	108.20
1	X	1688	U	C5-C6-N1	5.47	125.43	122.70
1	X	165	G	C8-N9-C4	-5.46	104.21	106.40
1	X	1473	U	O4'-C1'-C2'	5.46	112.52	107.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2876	C	P-O3'-C3'	5.46	126.26	119.70
1	X	1142	G	N3-C4-C5	-5.46	125.87	128.60
1	X	535	U	O4'-C1'-N1	5.46	112.57	108.20
1	X	1664	G	P-O5'-C5'	5.46	129.64	120.90
1	X	1767	G	O4'-C1'-N9	5.46	112.57	108.20
1	X	2443	C	O4'-C1'-N1	5.46	112.57	108.20
1	X	241	C	N1-C2-O2	5.46	122.17	118.90
1	X	1381	G	C8-N9-C4	-5.46	104.22	106.40
1	X	1663	C	OP1-P-O3'	5.46	117.21	105.20
1	X	2587	G	O4'-C1'-N9	5.46	112.57	108.20
1	X	358	C	C6-N1-C2	-5.46	118.12	120.30
1	X	979	A	O4'-C1'-N9	5.46	112.56	108.20
1	X	1235	C	C5-C6-N1	5.46	123.73	121.00
1	X	1439	G	N7-C8-N9	5.46	115.83	113.10
1	X	1715	A	P-O3'-C3'	5.46	126.25	119.70
1	X	2540	A	N9-C1'-C2'	-5.46	106.00	112.00
1	X	520	C	O4'-C1'-N1	5.45	112.56	108.20
1	X	1882	G	P-O5'-C5'	5.45	129.62	120.90
1	X	2539	C	O4'-C1'-N1	5.45	112.56	108.20
1	X	2330	G	P-O3'-C3'	5.45	126.24	119.70
2	Y	30	C	P-O5'-C5'	5.45	129.62	120.90
1	X	429	C	N1-C2-O2	5.45	122.17	118.90
1	X	1146	G	P-O3'-C3'	-5.44	113.17	119.70
1	X	11	G	C8-N9-C4	-5.44	104.22	106.40
1	X	144	U	O4'-C1'-N1	5.44	112.55	108.20
1	X	1766	U	P-O5'-C5'	-5.44	112.19	120.90
1	X	2268	G	O4'-C1'-N9	5.44	112.55	108.20
1	X	1924	C	N1-C2-O2	5.44	122.17	118.90
1	X	2734	U	O4'-C1'-N1	5.44	112.55	108.20
1	X	1254	G	C8-N9-C4	-5.44	104.22	106.40
1	X	227	G	P-O3'-C3'	5.44	126.22	119.70
1	X	2668	U	C5-C6-N1	-5.44	119.98	122.70
1	X	1219	C	C5-C6-N1	5.44	123.72	121.00
1	X	1466	C	N1-C2-O2	5.43	122.16	118.90
1	X	2608	A	N9-C1'-C2'	5.43	121.06	114.00
1	X	2854	G	O4'-C1'-C2'	-5.43	100.36	105.80
1	X	191	G	C8-N9-C4	-5.43	104.23	106.40
1	X	458	G	C3'-C2'-C1'	5.43	105.85	101.50
1	X	579	G	N9-C4-C5	5.43	107.57	105.40
1	X	1680	U	P-O3'-C3'	5.43	126.22	119.70
1	X	1003	C	O4'-C1'-N1	5.43	112.54	108.20
1	X	1626	A	P-O3'-C3'	5.43	126.21	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	413	G	C8-N9-C4	-5.43	104.23	106.40
1	X	692	C	C6-N1-C2	-5.43	118.13	120.30
1	X	1690	U	O4'-C1'-N1	5.42	112.54	108.20
2	Y	123	U	N1-C2-O2	5.42	126.60	122.80
1	X	417	C	O4'-C1'-N1	5.42	112.54	108.20
1	X	1627	C	N1-C2-O2	5.42	122.15	118.90
1	X	2039	G	N1-C2-N2	5.42	121.08	116.20
1	X	731	A	C3'-C2'-C1'	5.42	105.84	101.50
1	X	924	C	P-O3'-C3'	5.42	126.21	119.70
1	X	1753	A	C8-N9-C4	-5.42	103.63	105.80
1	X	1850	G	C8-N9-C4	-5.42	104.23	106.40
1	X	1514	C	O4'-C1'-N1	5.42	112.54	108.20
1	X	2039	G	O4'-C1'-C2'	-5.42	100.38	105.80
1	X	2405	A	N9-C1'-C2'	5.42	121.04	114.00
1	X	342	G	N7-C8-N9	5.42	115.81	113.10
19	Q	60	GLY	C-N-CA	5.42	135.24	121.70
1	X	2295	C	O4'-C1'-N1	5.41	112.53	108.20
4	B	132	LYS	C-N-CA	5.41	135.23	121.70
1	X	1380	C	O4'-C1'-N1	5.41	112.53	108.20
2	Y	88	C	P-O5'-C5'	5.41	129.56	120.90
1	X	1877	C	N1-C2-O2	5.41	122.15	118.90
1	X	2694	G	C4'-C3'-C2'	-5.41	97.19	102.60
1	X	926	C	N1-C1'-C2'	-5.41	106.05	112.00
1	X	2845	C	C6-N1-C2	-5.41	118.14	120.30
1	X	1141	U	C3'-C2'-C1'	-5.41	97.17	101.50
1	X	329	C	O4'-C1'-N1	5.41	112.53	108.20
1	X	731	A	O4'-C1'-N9	5.41	112.52	108.20
1	X	1454	U	N3-C4-C5	-5.41	111.36	114.60
1	X	2256	G	N7-C8-N9	5.41	115.80	113.10
1	X	2539	C	C6-N1-C2	-5.40	118.14	120.30
1	X	2656	G	P-O5'-C5'	-5.40	112.26	120.90
1	X	1225	G	N1-C6-O6	-5.40	116.66	119.90
1	X	1995	G	N3-C4-N9	5.40	129.24	126.00
1	X	549	G	O4'-C1'-N9	5.40	112.52	108.20
1	X	851	C	O4'-C1'-N1	5.40	112.52	108.20
1	X	1828	C	N1-C2-O2	5.40	122.14	118.90
1	X	2627	G	N1-C6-O6	5.40	123.14	119.90
2	Y	90	C	P-O5'-C5'	5.40	129.54	120.90
1	X	65	C	O4'-C1'-N1	5.39	112.52	108.20
1	X	583	C	O4'-C1'-N1	5.39	112.52	108.20
1	X	2043	A	C3'-C2'-C1'	-5.39	97.19	101.50
1	X	560	G	C4'-C3'-C2'	5.39	107.99	102.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	113	G	O4'-C1'-N9	5.39	112.51	108.20
1	X	1001	A	O4'-C1'-N9	5.39	112.51	108.20
1	X	1099	A	C3'-C2'-C1'	5.39	105.81	101.50
1	X	508	G	C8-N9-C4	-5.39	104.25	106.40
1	X	2335	U	O4'-C1'-N1	5.39	112.51	108.20
1	X	235	C	N1-C2-O2	5.39	122.13	118.90
1	X	647	G	O4'-C1'-N9	5.39	112.51	108.20
1	X	1255	A	O4'-C1'-N9	5.39	112.51	108.20
2	Y	45	C	O4'-C1'-N1	5.39	112.51	108.20
1	X	863	C	O4'-C1'-N1	5.38	112.51	108.20
1	X	985	G	N9-C1'-C2'	5.38	121.00	114.00
1	X	990	A	N1-C6-N6	-5.38	115.37	118.60
1	X	1632	A	N7-C8-N9	5.38	116.49	113.80
1	X	2043	A	O4'-C1'-N9	5.38	112.51	108.20
1	X	2347	C	C3'-C2'-C1'	-5.38	97.19	101.50
1	X	2659	C	O4'-C1'-N1	5.38	112.51	108.20
2	Y	44	C	N1-C2-O2	5.38	122.13	118.90
1	X	135	U	O4'-C1'-N1	5.38	112.51	108.20
1	X	2047	C	C5-C6-N1	5.38	123.69	121.00
1	X	2199	C	C5'-C4'-O4'	5.38	115.56	109.10
1	X	558	G	C8-N9-C4	-5.38	104.25	106.40
1	X	683	A	C2'-C3'-O3'	5.38	122.31	113.70
1	X	1669	A	P-O3'-C3'	5.38	126.16	119.70
1	X	1946	U	O4'-C1'-N1	5.38	112.50	108.20
1	X	2010	G	C4'-C3'-C2'	-5.38	97.22	102.60
1	X	651	C	C3'-C2'-C1'	5.38	105.80	101.50
1	X	1648	C	C5'-C4'-O4'	-5.38	102.64	109.10
1	X	306	G	P-O3'-C3'	5.38	126.16	119.70
1	X	1563	U	C5'-C4'-O4'	5.38	115.56	109.10
1	X	1979	C	O4'-C1'-N1	-5.38	103.90	108.20
1	X	2393	G	C8-N9-C4	-5.38	104.25	106.40
1	X	1825	C	C3'-C2'-C1'	-5.38	97.20	101.50
1	X	2032	G	N3-C4-N9	5.38	129.23	126.00
1	X	1694	A	O4'-C1'-N9	5.37	112.50	108.20
1	X	1811	A	C4'-C3'-C2'	5.37	107.97	102.60
1	X	2463	G	C5'-C4'-O4'	5.37	115.54	109.10
1	X	82	G	O3'-P-O5'	-5.37	93.80	104.00
1	X	1385	C	N1-C2-O2	5.37	122.12	118.90
1	X	2367	A	C5'-C4'-C3'	-5.37	107.41	116.00
1	X	2754	C	O4'-C1'-N1	5.37	112.50	108.20
1	X	1407	G	N7-C8-N9	5.37	115.78	113.10
1	X	206	U	O4'-C1'-N1	5.37	112.49	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	758	G	C5-C6-N1	5.37	114.18	111.50
3	A	203	ASN	CA-CB-CG	5.37	125.20	113.40
1	X	1761	G	O4'-C1'-N9	5.36	112.49	108.20
1	X	1975	G	C5-C6-N1	5.36	114.18	111.50
1	X	2703	C	C5'-C4'-O4'	5.36	115.54	109.10
1	X	655	A	C3'-C2'-C1'	5.36	105.79	101.50
1	X	934	G	O4'-C1'-N9	5.36	112.49	108.20
1	X	1018	C	O4'-C1'-N1	5.36	112.49	108.20
1	X	2004	U	P-O5'-C5'	-5.36	112.32	120.90
1	X	2299	A	P-O3'-C3'	5.36	126.13	119.70
1	X	90	G	N3-C4-C5	-5.36	125.92	128.60
1	X	560	G	C1'-O4'-C4'	5.36	114.19	109.90
1	X	1009	C	N3-C2-O2	-5.36	118.15	121.90
1	X	1069	G	C3'-C2'-C1'	5.36	105.79	101.50
1	X	405	C	N1-C2-O2	5.36	122.11	118.90
1	X	1311	C	O4'-C1'-N1	5.36	112.48	108.20
1	X	2172	U	O4'-C1'-N1	5.36	112.48	108.20
1	X	2841	U	N1-C1'-C2'	5.36	120.96	114.00
1	X	601	A	P-O5'-C5'	5.35	129.46	120.90
1	X	2067	U	O4'-C1'-N1	5.35	112.48	108.20
1	X	45	C	O4'-C1'-N1	5.35	112.48	108.20
1	X	803	C	N1-C2-O2	5.35	122.11	118.90
1	X	1637	U	O3'-P-O5'	-5.35	93.84	104.00
1	X	2069	U	O4'-C1'-N1	5.35	112.48	108.20
1	X	822	G	C8-N9-C4	-5.34	104.26	106.40
1	X	1652	G	N9-C4-C5	-5.34	103.26	105.40
1	X	2796	A	O4'-C1'-N9	5.34	112.48	108.20
1	X	2856	U	P-O3'-C3'	-5.34	113.29	119.70
1	X	2574	G	C8-N9-C4	-5.34	104.26	106.40
1	X	2631	C	N1-C2-O2	5.34	122.11	118.90
1	X	589	C	N1-C2-O2	5.34	122.11	118.90
1	X	701	U	O4'-C1'-N1	5.34	112.47	108.20
1	X	1231	A	P-O3'-C3'	-5.34	113.29	119.70
1	X	2060	A	N1-C6-N6	-5.34	115.39	118.60
1	X	2489	C	P-O5'-C5'	-5.34	112.36	120.90
1	X	1668	G	C6-C5-N7	-5.34	127.20	130.40
1	X	1673	C	O5'-P-OP1	5.34	117.10	110.70
1	X	233	A	O4'-C1'-N9	5.33	112.47	108.20
1	X	1392	U	N1-C1'-C2'	5.33	120.93	114.00
1	X	2776	U	P-O3'-C3'	5.33	126.10	119.70
1	X	2195	C	C6-N1-C2	-5.33	118.17	120.30
1	X	665	A	O4'-C1'-N9	5.33	112.46	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	11	G	O4'-C4'-C3'	-5.33	98.67	104.00
1	X	575	U	C3'-C2'-C1'	5.33	105.76	101.50
1	X	841	G	C5-N7-C8	-5.33	101.64	104.30
1	X	1341	G	N3-C4-C5	-5.33	125.94	128.60
1	X	598	U	O4'-C1'-N1	5.32	112.46	108.20
1	X	2188	A	O4'-C1'-N9	5.32	112.46	108.20
1	X	2856	U	N3-C2-O2	-5.32	118.47	122.20
1	X	1946	U	N3-C2-O2	-5.32	118.48	122.20
1	X	1060	C	O4'-C1'-N1	5.32	112.45	108.20
1	X	227	G	O4'-C1'-N9	5.32	112.45	108.20
1	X	621	U	O4'-C1'-N1	5.32	112.45	108.20
1	X	2417	U	O4'-C1'-N1	5.32	112.45	108.20
1	X	2621	G	C5'-C4'-C3'	5.32	124.51	116.00
1	X	613	A	N9-C1'-C2'	5.32	120.91	114.00
1	X	1428	G	O4'-C1'-N9	5.32	112.45	108.20
3	A	248	THR	CB-CA-C	5.32	125.95	111.60
1	X	2349	G	C3'-C2'-C1'	-5.31	97.25	101.50
1	X	1825	C	C5-C6-N1	5.31	123.66	121.00
1	X	998	C	N1-C2-O2	5.31	122.09	118.90
1	X	527	C	C4-C5-C6	-5.31	114.75	117.40
1	X	668	A	P-O3'-C3'	5.31	126.07	119.70
1	X	2419	C	N1-C2-O2	5.31	122.08	118.90
1	X	404	A	O4'-C1'-N9	5.30	112.44	108.20
1	X	63	A	C5'-C4'-C3'	-5.30	107.52	116.00
1	X	738	G	N3-C4-C5	-5.30	125.95	128.60
1	X	561	U	C5-C4-O4	-5.30	122.72	125.90
1	X	860	U	C1'-O4'-C4'	-5.30	105.66	109.90
1	X	1632	A	C8-N9-C4	-5.30	103.68	105.80
1	X	1730	G	C3'-C2'-C1'	-5.30	97.26	101.50
1	X	238	G	O4'-C1'-N9	5.30	112.44	108.20
2	Y	74	A	N7-C8-N9	5.30	116.45	113.80
1	X	1513	U	P-O3'-C3'	5.30	126.06	119.70
1	X	2377	U	O4'-C1'-N1	5.29	112.44	108.20
1	X	1358	C	P-O3'-C3'	5.29	126.05	119.70
1	X	469	G	N3-C4-C5	-5.29	125.95	128.60
1	X	1885	C	C4'-C3'-C2'	-5.29	97.31	102.60
1	X	2652	G	N3-C4-N9	5.29	129.18	126.00
1	X	327	C	O4'-C1'-N1	5.29	112.43	108.20
1	X	646	C	C6-N1-C2	-5.29	118.19	120.30
1	X	1497	C	C5-C6-N1	5.29	123.64	121.00
1	X	723	C	O4'-C1'-N1	5.29	112.43	108.20
1	X	2252	A	C2-N3-C4	5.29	113.24	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	145	C	O4'-C1'-N1	5.28	112.43	108.20
1	X	2867	G	C4-C5-N7	5.28	112.91	110.80
1	X	635	C	C6-N1-C2	-5.28	118.19	120.30
1	X	914	C	O4'-C1'-N1	5.28	112.42	108.20
1	X	1008	G	C5-C6-N1	5.28	114.14	111.50
1	X	1563	U	N1-C2-O2	5.28	126.50	122.80
1	X	230	C	O4'-C1'-N1	5.28	112.42	108.20
1	X	1398	G	P-O3'-C3'	5.28	126.03	119.70
1	X	309	G	N7-C8-N9	5.28	115.74	113.10
1	X	661	C	C6-N1-C2	-5.28	118.19	120.30
1	X	2729	A	O4'-C1'-N9	5.28	112.42	108.20
1	X	661	C	O4'-C1'-N1	5.28	112.42	108.20
1	X	1681	A	N7-C8-N9	5.28	116.44	113.80
1	X	2426	G	P-O5'-C5'	5.28	129.34	120.90
1	X	1033	G	P-O3'-C3'	5.27	126.03	119.70
1	X	2567	G	N3-C4-C5	-5.27	125.96	128.60
2	Y	38	C	O4'-C1'-N1	5.27	112.42	108.20
1	X	1168	G	P-O5'-C5'	5.27	129.33	120.90
1	X	1742	G	P-O3'-C3'	-5.27	113.38	119.70
1	X	2004	U	O3'-P-O5'	-5.27	93.99	104.00
1	X	2026	C	O4'-C1'-N1	5.27	112.42	108.20
1	X	2525	U	O4'-C1'-N1	5.27	112.42	108.20
1	X	1238	A	P-O5'-C5'	5.27	129.33	120.90
1	X	2607	C	O4'-C1'-N1	5.27	112.42	108.20
1	X	418	C	P-O3'-C3'	5.27	126.02	119.70
1	X	1767	G	C5-C6-N1	5.27	114.13	111.50
1	X	2556	A	P-O3'-C3'	5.27	126.02	119.70
1	X	2598	C	N3-C2-O2	-5.27	118.21	121.90
1	X	327	C	C6-N1-C2	-5.27	118.19	120.30
1	X	664	C	C3'-C2'-C1'	5.26	105.71	101.50
1	X	1312	G	N7-C8-N9	5.26	115.73	113.10
1	X	1467	U	N1-C2-N3	-5.26	111.74	114.90
1	X	2628	C	O4'-C4'-C3'	-5.26	98.74	104.00
1	X	582	G	O3'-P-O5'	-5.26	94.00	104.00
1	X	1160	C	C6-N1-C2	-5.26	118.20	120.30
1	X	2463	G	P-O3'-C3'	-5.26	113.39	119.70
1	X	1142	G	C5-C6-O6	-5.26	125.44	128.60
1	X	2038	C	OP2-P-O3'	5.26	116.76	105.20
1	X	749	C	O4'-C1'-N1	5.25	112.40	108.20
1	X	850	C	O4'-C1'-N1	5.25	112.40	108.20
1	X	1252	C	O4'-C1'-N1	5.25	112.40	108.20
1	X	1235	C	C6-N1-C2	-5.25	118.20	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1829	C	C3'-C2'-C1'	-5.25	97.30	101.50
1	X	102	C	N1-C2-O2	5.25	122.05	118.90
1	X	203	G	O4'-C1'-N9	5.25	112.40	108.20
1	X	1150	C	P-O3'-C3'	5.25	126.00	119.70
1	X	1668	G	N1-C6-O6	5.25	123.05	119.90
1	X	2698	G	O4'-C1'-N9	5.25	112.40	108.20
2	Y	111	C	P-O3'-C3'	5.25	126.00	119.70
1	X	303	C	C5-C6-N1	5.25	123.62	121.00
1	X	429	C	C6-N1-C2	-5.25	118.20	120.30
1	X	1820	G	C4'-C3'-C2'	5.25	107.85	102.60
1	X	2225	G	C3'-C2'-C1'	-5.25	97.30	101.50
1	X	2854	G	N7-C8-N9	5.25	115.72	113.10
1	X	1288	A	N9-C1'-C2'	5.25	120.82	114.00
1	X	2667	C	C5-C6-N1	5.25	123.62	121.00
1	X	2845	C	C5-C6-N1	5.25	123.62	121.00
1	X	86	U	O4'-C1'-N1	5.24	112.39	108.20
1	X	1049	C	O4'-C1'-N1	5.24	112.39	108.20
1	X	1470	G	C8-N9-C4	-5.24	104.30	106.40
1	X	1551	U	O4'-C1'-N1	5.24	112.39	108.20
1	X	1016	C	C5-C6-N1	5.24	123.62	121.00
9	G	103	TYR	C-N-CA	5.24	134.80	121.70
1	X	186	C	N1-C2-O2	5.24	122.04	118.90
1	X	488	A	O4'-C1'-N9	5.24	112.39	108.20
1	X	846	A	O4'-C1'-N9	5.24	112.39	108.20
1	X	1977	C	O4'-C1'-N1	5.24	112.39	108.20
2	Y	29	C	C6-N1-C2	-5.24	118.20	120.30
1	X	1083	C	O4'-C1'-N1	5.24	112.39	108.20
1	X	1683	G	N9-C1'-C2'	-5.24	106.24	112.00
1	X	1355	A	O4'-C1'-N9	5.24	112.39	108.20
1	X	2035	G	C8-N9-C4	-5.24	104.31	106.40
1	X	2165	A	P-O3'-C3'	5.24	125.98	119.70
1	X	2321	C	N1-C2-O2	5.24	122.04	118.90
1	X	2330	G	N3-C4-C5	-5.24	125.98	128.60
1	X	2340	C	C6-N1-C2	-5.24	118.21	120.30
1	X	683	A	O4'-C1'-N9	-5.23	104.01	108.20
1	X	1312	G	C8-N9-C4	-5.23	104.31	106.40
1	X	2602	G	N3-C4-C5	-5.23	125.98	128.60
1	X	70	A	C3'-C2'-C1'	5.23	105.69	101.50
1	X	104	C	O4'-C1'-N1	5.23	112.38	108.20
1	X	572	G	C5-C6-N1	5.23	114.11	111.50
1	X	582	G	C3'-C2'-C1'	5.23	105.68	101.50
1	X	2535	C	N1-C2-O2	5.23	122.04	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	227	G	N9-C1'-C2'	5.23	120.80	114.00
1	X	1573	G	P-O3'-C3'	5.23	125.97	119.70
1	X	2246	A	C2-N3-C4	5.23	113.21	110.60
1	X	2626	U	N3-C2-O2	-5.23	118.54	122.20
1	X	148	C	O4'-C1'-N1	5.23	112.38	108.20
1	X	1563	U	N3-C2-O2	-5.23	118.54	122.20
1	X	788	G	O4'-C1'-N9	5.22	112.38	108.20
1	X	1150	C	N1-C2-O2	5.22	122.03	118.90
1	X	2326	C	C6-N1-C2	-5.22	118.21	120.30
1	X	2432	A	C8-N9-C4	-5.22	103.71	105.80
1	X	2805	G	C8-N9-C4	-5.22	104.31	106.40
1	X	312	G	O4'-C1'-N9	5.22	112.38	108.20
1	X	1663	C	O4'-C1'-N1	5.22	112.38	108.20
1	X	2075	U	C1'-O4'-C4'	-5.22	105.72	109.90
1	X	2602	G	C5-C6-N1	5.22	114.11	111.50
1	X	689	A	C2-N3-C4	-5.22	107.99	110.60
1	X	782	U	O4'-C1'-N1	5.22	112.38	108.20
1	X	878	C	P-O3'-C3'	5.22	125.96	119.70
1	X	1284	G	C6-C5-N7	-5.22	127.27	130.40
1	X	2632	U	O4'-C1'-N1	5.22	112.38	108.20
1	X	2696	A	C4'-C3'-C2'	-5.22	97.38	102.60
1	X	349	G	P-O5'-C5'	5.21	129.24	120.90
1	X	1624	A	P-O3'-C3'	5.21	125.95	119.70
1	X	1663	C	O3'-P-O5'	-5.21	94.09	104.00
1	X	352	G	O4'-C1'-N9	5.21	112.37	108.20
1	X	413	G	N7-C8-N9	5.21	115.71	113.10
1	X	2550	C	P-O3'-C3'	5.21	125.95	119.70
1	X	2794	G	O5'-P-OP2	-5.21	101.01	105.70
1	X	1312	G	C6-C5-N7	-5.21	127.27	130.40
1	X	313	U	O4'-C1'-N1	5.21	112.37	108.20
1	X	2715	C	P-O5'-C5'	5.21	129.24	120.90
1	X	2843	A	C5'-C4'-C3'	-5.21	107.67	116.00
17	O	6	GLN	C-N-CA	5.21	134.72	121.70
1	X	475	U	N3-C2-O2	-5.21	118.56	122.20
1	X	967	G	O4'-C1'-N9	5.21	112.37	108.20
1	X	1064	C	O4'-C1'-N1	5.21	112.36	108.20
1	X	1271	C	O4'-C1'-N1	5.21	112.36	108.20
1	X	1549	C	O4'-C1'-N1	5.21	112.36	108.20
1	X	1824	C	O4'-C1'-N1	5.21	112.36	108.20
1	X	1284	G	C8-N9-C4	-5.21	104.32	106.40
1	X	1344	C	N1-C2-O2	5.21	122.02	118.90
1	X	2511	G	P-O5'-C5'	5.21	129.23	120.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2033	C	N3-C2-O2	-5.20	118.26	121.90
1	X	2326	C	P-O3'-C3'	-5.20	113.46	119.70
1	X	2671	C	P-O5'-C5'	-5.20	112.58	120.90
1	X	76	C	N1-C2-O2	5.20	122.02	118.90
1	X	1435	G	C8-N9-C4	-5.20	104.32	106.40
1	X	20	C	O4'-C1'-N1	5.20	112.36	108.20
1	X	507	A	P-O3'-C3'	-5.20	113.46	119.70
1	X	1327	C	C6-N1-C2	-5.20	118.22	120.30
1	X	1764	A	C2'-C3'-O3'	5.20	122.02	113.70
1	X	2318	U	O4'-C1'-N1	5.20	112.36	108.20
1	X	2560	G	N9-C4-C5	5.20	107.48	105.40
1	X	540	G	C4-C5-N7	-5.20	108.72	110.80
1	X	722	C	N1-C2-O2	5.20	122.02	118.90
1	X	2406	C	O4'-C1'-N1	5.19	112.36	108.20
1	X	168	A	OP1-P-O3'	5.19	116.62	105.20
1	X	1276	U	P-O3'-C3'	5.19	125.93	119.70
3	A	243	GLY	C-N-CA	5.19	134.68	121.70
1	X	682	G	C1'-O4'-C4'	-5.19	105.75	109.90
1	X	1105	U	O4'-C1'-N1	5.19	112.35	108.20
1	X	1466	C	C2-N1-C1'	5.19	124.51	118.80
1	X	2463	G	N3-C4-C5	-5.19	126.00	128.60
1	X	831	G	C8-N9-C4	-5.19	104.33	106.40
1	X	1312	G	P-O3'-C3'	5.19	125.92	119.70
1	X	2825	A	N1-C6-N6	5.19	121.71	118.60
11	I	38	LYS	C-N-CA	5.19	134.66	121.70
1	X	2537	C	O4'-C1'-N1	5.18	112.35	108.20
1	X	34	U	P-O5'-C5'	5.18	129.19	120.90
1	X	1652	G	N1-C6-O6	5.18	123.01	119.90
1	X	430	C	C5-C6-N1	5.18	123.59	121.00
1	X	883	A	O4'-C1'-N9	5.18	112.34	108.20
2	Y	23	G	O4'-C1'-N9	5.18	112.34	108.20
1	X	1223	G	N7-C8-N9	5.18	115.69	113.10
1	X	1935	A	C2-N3-C4	5.18	113.19	110.60
1	X	7	G	C8-N9-C4	-5.18	104.33	106.40
1	X	795	A	P-O3'-C3'	5.18	125.91	119.70
1	X	2018	G	N7-C8-N9	5.18	115.69	113.10
1	X	465	C	C1'-O4'-C4'	-5.17	105.76	109.90
1	X	624	A	C2-N3-C4	5.17	113.19	110.60
1	X	951	G	C3'-C2'-C1'	-5.17	97.36	101.50
1	X	1466	C	O4'-C1'-N1	5.17	112.34	108.20
1	X	174	A	P-O5'-C5'	5.17	129.17	120.90
1	X	597	U	C5-C4-O4	-5.17	122.80	125.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	765	C	N1-C2-O2	5.17	122.00	118.90
1	X	1530	U	O4'-C1'-N1	5.17	112.34	108.20
1	X	1824	C	N3-C2-O2	-5.17	118.28	121.90
1	X	2420	C	P-O5'-C5'	5.17	129.17	120.90
1	X	516	G	C4-C5-N7	5.17	112.87	110.80
1	X	652	C	C5'-C4'-C3'	-5.17	107.73	116.00
1	X	1488	G	O4'-C1'-N9	5.17	112.33	108.20
1	X	2326	C	C5-C6-N1	5.17	123.58	121.00
2	Y	92	G	C5'-C4'-O4'	5.17	115.30	109.10
1	X	7	G	C5'-C4'-C3'	-5.17	107.73	116.00
1	X	2503	G	C5-C6-O6	-5.17	125.50	128.60
1	X	956	A	O3'-P-O5'	-5.17	94.19	104.00
1	X	2854	G	C8-N9-C4	-5.17	104.33	106.40
1	X	462	G	C5-C6-N1	-5.16	108.92	111.50
1	X	540	G	N3-C4-C5	-5.16	126.02	128.60
1	X	582	G	C2-N3-C4	5.16	114.48	111.90
1	X	1000	G	O4'-C1'-C2'	-5.16	100.64	105.80
1	X	1623	C	N1-C2-O2	5.16	122.00	118.90
2	Y	14	C	C3'-C2'-C1'	5.16	105.63	101.50
1	X	545	C	O4'-C1'-N1	5.16	112.33	108.20
1	X	1426	U	O4'-C1'-N1	5.16	112.33	108.20
1	X	2626	U	N1-C2-O2	5.16	126.41	122.80
1	X	207	U	O4'-C1'-N1	5.16	112.33	108.20
1	X	648	A	P-O3'-C3'	5.16	125.89	119.70
1	X	1790	G	N9-C1'-C2'	5.16	120.71	114.00
1	X	2793	G	O4'-C1'-N9	5.16	112.33	108.20
1	X	780	U	O4'-C1'-N1	5.16	112.32	108.20
1	X	1010	U	O4'-C1'-N1	5.16	112.33	108.20
1	X	811	G	P-O3'-C3'	-5.15	113.52	119.70
2	Y	45	C	N3-C2-O2	-5.15	118.29	121.90
2	Y	102	A	O4'-C1'-N9	5.15	112.32	108.20
1	X	2170	C	O4'-C1'-N1	5.15	112.32	108.20
1	X	2825	A	P-O3'-C3'	5.15	125.88	119.70
11	I	28	LYS	C-N-CA	5.15	134.57	121.70
1	X	2776	U	O4'-C1'-N1	5.15	112.32	108.20
1	X	439	C	O4'-C1'-N1	5.15	112.32	108.20
1	X	1138	A	P-O5'-C5'	5.15	129.13	120.90
1	X	1668	G	P-O3'-C3'	-5.15	113.53	119.70
1	X	818	G	N7-C8-N9	5.14	115.67	113.10
1	X	998	C	C5'-C4'-C3'	5.14	124.23	116.00
1	X	2264	C	P-O3'-C3'	-5.14	113.53	119.70
1	X	2478	C	C5-C6-N1	5.14	123.57	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	178	C	O4'-C1'-N1	5.14	112.31	108.20
1	X	2034	A	C5-C6-N6	-5.14	119.58	123.70
1	X	1236	G	O4'-C1'-N9	5.14	112.31	108.20
1	X	2654	A	C2-N3-C4	5.14	113.17	110.60
1	X	1714	A	O4'-C1'-N9	5.14	112.31	108.20
1	X	607	C	N3-C2-O2	-5.14	118.31	121.90
1	X	1097	A	P-O3'-C3'	5.14	125.86	119.70
1	X	2028	C	O4'-C4'-C3'	-5.14	98.86	104.00
1	X	2537	C	P-O3'-C3'	-5.14	113.54	119.70
1	X	2658	A	O4'-C1'-N9	5.14	112.31	108.20
1	X	2824	C	C2'-C3'-O3'	5.14	121.92	113.70
1	X	1930	C	N1-C2-O2	5.13	121.98	118.90
1	X	1396	C	C5-C6-N1	5.13	123.57	121.00
1	X	1219	C	O4'-C1'-N1	5.13	112.31	108.20
1	X	1268	U	P-O5'-C5'	5.13	129.11	120.90
1	X	1744	G	C6-N1-C2	-5.13	122.02	125.10
1	X	2555	G	C5-C6-N1	5.13	114.07	111.50
1	X	2828	C	O4'-C1'-N1	5.13	112.30	108.20
1	X	519	C	O4'-C1'-N1	5.13	112.30	108.20
1	X	1142	G	C5-C6-N1	5.13	114.06	111.50
1	X	1345	G	P-O3'-C3'	5.13	125.86	119.70
1	X	1876	C	N1-C2-O2	5.13	121.98	118.90
1	X	2381	A	O4'-C1'-N9	5.13	112.30	108.20
1	X	540	G	C3'-C2'-C1'	5.13	105.60	101.50
1	X	1946	U	N1-C2-O2	5.13	126.39	122.80
1	X	1681	A	C8-N9-C4	-5.12	103.75	105.80
1	X	170	U	N1-C2-O2	5.12	126.39	122.80
1	X	27	G	O4'-C1'-N9	5.12	112.30	108.20
1	X	1403	U	C3'-C2'-C1'	5.12	105.60	101.50
1	X	2229	G	C2-N3-C4	5.12	114.46	111.90
1	X	1106	A	P-O3'-C3'	5.12	125.84	119.70
1	X	2688	G	C5-C6-O6	-5.12	125.53	128.60
2	Y	67	C	P-O3'-C3'	5.12	125.84	119.70
1	X	1123	G	P-O3'-C3'	5.12	125.84	119.70
1	X	1142	G	C6-N1-C2	-5.12	122.03	125.10
1	X	2016	A	P-O3'-C3'	5.12	125.84	119.70
1	X	1407	G	C6-C5-N7	-5.12	127.33	130.40
1	X	1607	A	C3'-C2'-C1'	-5.12	97.41	101.50
1	X	1725	C	P-O5'-C5'	-5.12	112.71	120.90
1	X	2615	U	O4'-C1'-N1	5.12	112.29	108.20
2	Y	90	C	C4'-C3'-O3'	5.12	123.23	113.00
1	X	2660	C	P-O5'-C5'	5.11	129.08	120.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2748	C	N1-C1'-C2'	-5.11	106.37	112.00
1	X	596	C	P-O5'-C5'	-5.11	112.72	120.90
1	X	2660	C	P-O3'-C3'	5.11	125.83	119.70
1	X	499	G	C5-C6-N1	5.11	114.06	111.50
1	X	552	C	N1-C2-O2	5.11	121.97	118.90
1	X	934	G	N7-C8-N9	5.11	115.66	113.10
1	X	1666	G	C5-C6-N1	5.11	114.06	111.50
1	X	2369	U	O4'-C1'-N1	5.11	112.29	108.20
1	X	2606	G	C5'-C4'-O4'	5.11	115.23	109.10
1	X	236	C	C5-C6-N1	5.11	123.55	121.00
1	X	247	A	C5'-C4'-O4'	5.11	115.23	109.10
1	X	1337	G	P-O5'-C5'	5.11	129.07	120.90
1	X	1540	C	O4'-C1'-N1	5.11	112.28	108.20
1	X	1663	C	C2-N1-C1'	5.10	124.41	118.80
1	X	2667	C	P-O3'-C3'	5.10	125.82	119.70
1	X	1010	U	P-O5'-C5'	5.10	129.06	120.90
1	X	1097	A	O4'-C1'-N9	5.10	112.28	108.20
1	X	2032	G	C5-C6-N1	5.10	114.05	111.50
1	X	480	G	C3'-C2'-C1'	-5.10	97.42	101.50
1	X	688	A	P-O3'-C3'	5.10	125.82	119.70
1	X	333	A	O4'-C1'-N9	5.10	112.28	108.20
1	X	854	G	C3'-C2'-C1'	-5.10	97.42	101.50
1	X	2526	U	O4'-C1'-N1	5.10	112.28	108.20
1	X	2826	C	N1-C2-O2	5.10	121.96	118.90
2	Y	19	C	N3-C2-O2	-5.10	118.33	121.90
1	X	402	A	P-O3'-C3'	-5.09	113.59	119.70
1	X	459	A	C2-N3-C4	5.09	113.15	110.60
1	X	616	U	O4'-C1'-N1	5.09	112.28	108.20
1	X	996	C	N3-C2-O2	-5.09	118.33	121.90
1	X	1254	G	N3-C4-C5	-5.09	126.05	128.60
1	X	1337	G	O5'-P-OP2	-5.09	101.11	105.70
1	X	98	U	N3-C2-O2	-5.09	118.64	122.20
1	X	542	A	N7-C8-N9	5.09	116.35	113.80
1	X	1198	C	O4'-C1'-N1	5.09	112.27	108.20
1	X	1648	C	N1-C2-O2	5.09	121.95	118.90
1	X	1870	U	O4'-C1'-N1	5.09	112.27	108.20
1	X	2774	U	P-O3'-C3'	5.09	125.81	119.70
1	X	2195	C	O4'-C1'-N1	5.08	112.27	108.20
1	X	2702	G	O4'-C1'-N9	-5.08	104.13	108.20
1	X	179	U	O4'-C1'-N1	5.08	112.27	108.20
1	X	540	G	C2-N3-C4	5.08	114.44	111.90
1	X	757	U	OP2-P-O3'	5.08	116.39	105.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2015	G	C5-N7-C8	-5.08	101.76	104.30
2	Y	100	G	O4'-C1'-N9	5.08	112.27	108.20
1	X	1015	U	O4'-C1'-N1	5.08	112.27	108.20
1	X	1321	A	C3'-C2'-C1'	-5.08	97.43	101.50
1	X	1801	C	N1-C2-O2	5.08	121.95	118.90
2	Y	53	G	O4'-C1'-N9	5.08	112.26	108.20
1	X	1497	C	O4'-C1'-N1	5.08	112.26	108.20
1	X	516	G	O4'-C1'-N9	5.08	112.26	108.20
1	X	625	A	P-O3'-C3'	5.08	125.79	119.70
1	X	1248	G	O4'-C1'-N9	-5.08	104.14	108.20
1	X	1266	G	P-O3'-C3'	5.07	125.79	119.70
1	X	1882	G	C8-N9-C4	-5.07	104.37	106.40
1	X	2727	G	O4'-C1'-N9	5.07	112.26	108.20
2	Y	94	G	C5'-C4'-O4'	5.07	115.19	109.10
1	X	227	G	C8-N9-C4	-5.07	104.37	106.40
1	X	1863	U	O4'-C1'-N1	5.07	112.26	108.20
1	X	985	G	C5-C6-N1	5.07	114.03	111.50
1	X	1384	G	P-O3'-C3'	5.07	125.78	119.70
1	X	2848	A	O4'-C1'-N9	5.07	112.26	108.20
1	X	2588	U	C5'-C4'-O4'	5.07	115.18	109.10
1	X	358	C	P-O5'-C5'	5.07	129.01	120.90
1	X	807	A	O4'-C1'-N9	5.07	112.25	108.20
1	X	934	G	C8-N9-C4	-5.07	104.37	106.40
1	X	1766	U	P-O3'-C3'	5.07	125.78	119.70
1	X	1922	U	N3-C2-O2	-5.07	118.65	122.20
1	X	2261	G	C4'-C3'-C2'	5.07	107.67	102.60
1	X	2452	U	N3-C2-O2	-5.07	118.65	122.20
1	X	16	G	N3-C4-N9	5.06	129.04	126.00
2	Y	123	U	C6-N1-C1'	-5.06	114.11	121.20
1	X	22	C	P-O3'-C3'	5.06	125.78	119.70
1	X	1037	U	C1'-O4'-C4'	-5.06	105.85	109.90
1	X	1625	A	P-O3'-C3'	5.06	125.78	119.70
1	X	1690	U	P-O5'-C5'	-5.06	112.80	120.90
1	X	2000	U	N3-C4-O4	5.06	122.94	119.40
1	X	2264	C	C3'-C2'-C1'	-5.06	97.45	101.50
1	X	2442	C	N1-C2-O2	5.06	121.94	118.90
1	X	2213	G	C8-N9-C4	-5.06	104.38	106.40
1	X	2718	A	C5'-C4'-O4'	5.06	115.17	109.10
1	X	93	A	O4'-C1'-N9	5.06	112.25	108.20
1	X	569	C	O4'-C1'-N1	5.06	112.25	108.20
1	X	2568	A	O4'-C4'-C3'	-5.06	98.94	104.00
1	X	672	C	C3'-C2'-C1'	-5.06	97.45	101.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2210	C	O4'-C1'-N1	5.06	112.25	108.20
1	X	1152	C	P-O5'-C5'	5.06	128.99	120.90
1	X	940	G	C8-N9-C4	-5.05	104.38	106.40
1	X	1608	U	P-O3'-C3'	5.05	125.77	119.70
1	X	1971	C	P-O5'-C5'	-5.05	112.81	120.90
1	X	2314	A	O4'-C1'-N9	5.05	112.24	108.20
2	Y	86	A	C5'-C4'-O4'	5.05	115.17	109.10
1	X	1965	U	C5'-C4'-C3'	-5.05	107.92	116.00
1	X	2592	U	C5'-C4'-O4'	5.05	115.16	109.10
1	X	2824	C	N1-C1'-C2'	5.05	120.57	114.00
1	X	354	C	O4'-C1'-N1	5.05	112.24	108.20
1	X	1383	C	O4'-C1'-N1	5.05	112.24	108.20
1	X	1481	U	O4'-C1'-N1	5.05	112.24	108.20
1	X	1975	G	C3'-C2'-C1'	5.05	105.54	101.50
1	X	184	A	N1-C6-N6	-5.05	115.57	118.60
1	X	998	C	C4'-C3'-C2'	-5.05	97.55	102.60
1	X	860	U	C2-N1-C1'	5.05	123.75	117.70
1	X	2468	G	C2-N3-C4	5.05	114.42	111.90
1	X	869	C	C6-N1-C2	-5.04	118.28	120.30
1	X	916	U	O4'-C1'-N1	5.04	112.23	108.20
1	X	940	G	P-O3'-C3'	5.04	125.75	119.70
1	X	1132	C	C5-C6-N1	5.04	123.52	121.00
1	X	1619	A	P-O3'-C3'	5.04	125.75	119.70
1	X	2527	G	P-O5'-C5'	-5.04	112.83	120.90
1	X	42	G	O4'-C1'-N9	5.04	112.23	108.20
1	X	332	C	C1'-O4'-C4'	-5.04	105.87	109.90
1	X	570	G	P-O3'-C3'	5.04	125.75	119.70
1	X	598	U	O4'-C4'-C3'	-5.04	98.96	104.00
1	X	1219	C	C6-N1-C2	-5.04	118.28	120.30
1	X	1337	G	C4'-C3'-C2'	5.04	107.64	102.60
1	X	1909	U	P-O3'-C3'	5.04	125.75	119.70
1	X	1496	G	C4'-C3'-O3'	5.04	123.08	113.00
1	X	670	U	N1-C2-O2	5.04	126.33	122.80
1	X	1162	A	C4'-C3'-C2'	-5.04	97.56	102.60
1	X	2620	G	P-O3'-C3'	5.04	125.75	119.70
1	X	1825	C	C6-N1-C2	-5.04	118.28	120.30
1	X	1881	U	O4'-C1'-N1	5.04	112.23	108.20
1	X	1973	C	O4'-C1'-N1	5.04	112.23	108.20
1	X	1470	G	C5-C6-O6	-5.04	125.58	128.60
1	X	1689	U	N3-C2-O2	-5.04	118.68	122.20
1	X	2311	U	O4'-C1'-N1	5.04	112.23	108.20
1	X	2702	G	C5-N7-C8	-5.04	101.78	104.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2831	A	C2-N3-C4	5.04	113.12	110.60
3	A	203	ASN	CB-CA-C	5.04	120.47	110.40
1	X	615	C	O4'-C1'-N1	5.03	112.23	108.20
1	X	689	A	C4-C5-N7	5.03	113.22	110.70
1	X	2527	G	N3-C4-C5	-5.03	126.08	128.60
2	Y	119	G	O4'-C1'-N9	5.03	112.23	108.20
1	X	684	C	C4-C5-C6	5.03	119.92	117.40
1	X	2340	C	O4'-C1'-N1	5.03	112.23	108.20
1	X	303	C	O4'-C1'-N1	5.03	112.22	108.20
1	X	636	G	C5'-C4'-C3'	-5.03	107.95	116.00
1	X	2038	C	P-O3'-C3'	5.03	125.74	119.70
1	X	2340	C	C5-C6-N1	5.03	123.52	121.00
1	X	1663	C	C3'-C2'-C1'	5.03	105.52	101.50
1	X	11	G	N7-C8-N9	5.03	115.61	113.10
1	X	311	A	O4'-C1'-N9	5.03	112.22	108.20
1	X	1010	U	N3-C2-O2	-5.03	118.68	122.20
1	X	1122	A	O4'-C1'-N9	5.03	112.22	108.20
1	X	1570	C	O4'-C1'-N1	5.03	112.22	108.20
1	X	2015	G	C5-C6-N1	5.03	114.01	111.50
1	X	2635	U	N3-C2-O2	-5.03	118.68	122.20
1	X	2780	A	P-O5'-C5'	5.03	128.94	120.90
1	X	518	A	P-O5'-C5'	5.02	128.94	120.90
1	X	1731	C	C3'-C2'-C1'	-5.02	97.48	101.50
1	X	2062	U	O4'-C1'-N1	5.02	112.22	108.20
2	Y	77	G	P-O5'-C5'	5.02	128.94	120.90
1	X	2254	C	N1-C2-O2	5.02	121.91	118.90
1	X	2740	C	N1-C2-O2	5.02	121.91	118.90
1	X	677	G	O4'-C1'-N9	5.02	112.22	108.20
1	X	2582	G	C6-C5-N7	-5.02	127.39	130.40
1	X	622	U	O4'-C1'-N1	5.02	112.22	108.20
1	X	661	C	N3-C2-O2	-5.02	118.39	121.90
1	X	978	U	O4'-C1'-N1	5.02	112.22	108.20
1	X	834	A	P-O3'-C3'	-5.02	113.68	119.70
1	X	1128	G	P-O5'-C5'	5.02	128.93	120.90
1	X	1679	U	N3-C2-O2	-5.02	118.69	122.20
1	X	2619	G	N1-C6-O6	5.02	122.91	119.90
1	X	416	U	C1'-O4'-C4'	-5.02	105.89	109.90
1	X	863	C	C6-N1-C2	-5.02	118.29	120.30
1	X	1785	A	P-O5'-C5'	-5.02	112.87	120.90
1	X	1429	A	O4'-C1'-N9	5.01	112.21	108.20
1	X	1603	A	P-O3'-C3'	5.01	125.72	119.70
1	X	534	U	P-O5'-C5'	5.01	128.92	120.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	941	U	C4'-C3'-C2'	-5.01	97.59	102.60
1	X	1661	C	N1-C2-O2	5.01	121.91	118.90
1	X	1932	G	O4'-C1'-N9	5.01	112.21	108.20
1	X	216	U	N3-C2-O2	-5.01	118.69	122.20
1	X	1533	G	N7-C8-N9	5.01	115.60	113.10
1	X	1886	G	C8-N9-C4	-5.01	104.40	106.40
2	Y	12	C	O4'-C1'-N1	5.01	112.21	108.20
1	X	19	C	P-O3'-C3'	-5.01	113.69	119.70
1	X	581	A	O3'-P-O5'	-5.01	94.49	104.00
1	X	1652	G	N3-C4-N9	5.01	129.00	126.00
1	X	349	G	O4'-C1'-N9	5.00	112.20	108.20
1	X	631	G	C1'-O4'-C4'	-5.00	105.90	109.90
1	X	2487	G	C8-N9-C4	-5.00	104.40	106.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	1251	G	Sidechain
1	X	699	G	Sidechain
1	X	967	G	Sidechain

5.2 Too-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 hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	57651	0	29049	535	0
2	Y	2598	0	1328	22	0
3	A	1826	0	1885	83	0
4	B	1539	0	1600	57	0
5	C	1506	0	1525	57	0
6	D	1400	0	1481	17	0
7	E	1286	0	1336	10	0
8	F	503	0	520	5	0
9	G	1114	0	1144	46	0
10	H	997	0	1046	30	0
11	I	1067	0	1103	39	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	J	1090	0	1125	31	0
13	K	878	0	930	24	0
14	L	779	0	820	19	0
15	M	871	0	894	25	0
16	N	978	0	1020	33	0
17	O	741	0	756	24	0
18	P	1014	0	1096	23	0
19	Q	726	0	753	11	0
20	R	825	0	881	26	0
21	S	1345	0	1372	30	0
22	T	625	0	655	11	0
23	U	552	0	604	31	0
24	V	533	0	558	7	0
25	W	424	0	470	15	0
26	Z	457	0	462	20	0
27	1	53	0	0	0	0
28	2	46	0	0	1	0
29	3	63	0	0	0	0
30	4	297	0	330	4	0
31	M	1	0	0	0	0
31	X	28	0	0	0	0
31	Y	6	0	0	0	0
32	X	58	0	67	19	0
All	All	83877	0	54810	1080	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (1080) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:117:MET:SD	4:B:117:MET:CE	2.02	1.47
9:G:100:TYR:HB2	9:G:116:ARG:NH1	1.69	1.08
9:G:33:ILE:HB	9:G:34:PRO:HD3	1.38	1.03
1:X:558:G:H4'	1:X:559:C:H5'	1.40	1.02
1:X:1448:A:H61	1:X:1574:A:H61	1.09	1.00
5:C:43:ALA:HB1	5:C:86:PRO:HB2	1.46	0.96
4:B:152:LYS:HB2	9:G:106:TYR:HB3	1.49	0.95
1:X:1542:G:H22	1:X:1562:G:H1	1.13	0.94
1:X:1007:A:H4'	16:N:93:LYS:HB3	1.46	0.94
1:X:1919:A:H2	1:X:1926:U:H3	1.09	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:116:VAL:HG22	4:B:136:ARG:HE	1.31	0.93
11:I:62:LYS:HE2	11:I:64:GLY:HA3	1.53	0.91
32:X:2929:1F4:H59	32:X:2929:1F4:H60	1.51	0.90
11:I:30:ALA:HB3	11:I:34:HIS:CE1	2.07	0.89
1:X:77:C:H42	1:X:106:G:H1	1.21	0.88
15:M:79:ARG:HH11	15:M:79:ARG:HG3	1.36	0.88
1:X:1770:U:H5	1:X:1775:A:N7	1.70	0.88
14:L:38:ILE:HG13	14:L:39:TYR:H	1.39	0.88
4:B:116:VAL:HG22	4:B:136:ARG:NE	1.88	0.87
21:S:71:MET:HA	21:S:78:PRO:HA	1.58	0.85
4:B:131:SER:HB3	4:B:134:TRP:CD1	2.11	0.85
3:A:252:LYS:HD2	3:A:253:PRO:HD3	1.59	0.84
1:X:1817:U:H4'	3:A:252:LYS:HE2	1.59	0.83
1:X:1266:G:N7	11:I:32:ARG:NH1	2.25	0.83
13:K:10:LEU:HD21	13:K:17:ARG:HB2	1.61	0.82
3:A:248:THR:HB	3:A:249:PRO:HD3	1.60	0.82
1:X:2371:A:H2	1:X:2403:C:H42	1.28	0.82
3:A:218:LYS:HE3	3:A:221:GLN:HB2	1.62	0.82
1:X:38:G:H1	1:X:453:U:H3	1.25	0.81
1:X:1278:A:H2	1:X:1997:A:H62	1.26	0.80
9:G:33:ILE:HB	9:G:34:PRO:CD	2.11	0.80
1:X:2387:U:H2'	1:X:2388:G:H8	1.45	0.80
9:G:100:TYR:HB2	9:G:116:ARG:HH11	1.47	0.79
1:X:1342:U:H5''	1:X:1343:C:H5	1.48	0.78
1:X:559:C:H2'	1:X:560:G:O4'	1.84	0.78
3:A:43:ARG:HD2	3:A:43:ARG:N	1.99	0.78
32:X:2929:1F4:H3	32:X:2929:1F4:C39	2.13	0.78
1:X:823:U:OP1	11:I:32:ARG:NH1	2.17	0.78
9:G:68:PRO:HD2	9:G:76:GLN:HB3	1.66	0.78
16:N:66:ASN:HB3	16:N:76:TYR:H	1.50	0.77
1:X:640:C:H4'	1:X:660:G:H21	1.49	0.77
15:M:59:GLY:HA3	15:M:64:LYS:HA	1.65	0.77
3:A:172:TYR:HA	3:A:186:HIS:HA	1.66	0.76
1:X:224:G:OP2	1:X:226:C:N4	2.17	0.76
5:C:29:GLU:HB2	11:I:18:ARG:HH12	1.50	0.76
1:X:673:G:H5'	5:C:93:TYR:CE1	2.20	0.76
14:L:33:ARG:HD2	14:L:38:ILE:HD13	1.66	0.76
1:X:689:A:H8	1:X:2052:G:H21	1.33	0.76
26:Z:35:GLN:O	26:Z:37:HIS:N	2.19	0.76
21:S:6:LYS:H	21:S:7:PRO:HD3	1.48	0.75
1:X:1007:A:H1'	17:O:6:GLN:HG2	1.67	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:4:HIS:HB3	26:Z:5:PRO:HD3	1.69	0.75
13:K:10:LEU:CD2	13:K:17:ARG:HB2	2.15	0.75
4:B:134:TRP:H	4:B:134:TRP:HD1	1.32	0.75
15:M:79:ARG:HH11	15:M:79:ARG:CG	2.00	0.75
2:Y:45:C:H2'	6:D:92:ARG:HH11	1.52	0.75
10:H:25:LEU:HD11	10:H:52:VAL:HG23	1.70	0.73
25:W:12:ARG:HH11	25:W:12:ARG:HG2	1.52	0.73
1:X:1919:A:H2	1:X:1926:U:N3	1.84	0.73
1:X:1329:U:H2'	1:X:1330:G:H8	1.52	0.73
17:O:73:LYS:HB2	17:O:82:ARG:HB2	1.70	0.73
1:X:652:C:H42	1:X:657:A:H61	1.35	0.73
15:M:79:ARG:HG3	15:M:79:ARG:NH1	2.02	0.73
9:G:100:TYR:HB2	9:G:116:ARG:HH12	1.51	0.72
17:O:57:GLN:H	17:O:97:GLY:HA3	1.53	0.72
1:X:2387:U:H2'	1:X:2388:G:C8	2.23	0.72
11:I:62:LYS:CE	11:I:64:GLY:HA3	2.19	0.72
1:X:1329:U:H2'	1:X:1330:G:C8	2.25	0.72
4:B:152:LYS:CB	9:G:106:TYR:HB3	2.20	0.71
5:C:48:ARG:HB2	5:C:51:VAL:HG22	1.70	0.71
11:I:62:LYS:HE2	11:I:64:GLY:CA	2.20	0.71
1:X:2241:U:H5	22:T:17:ASN:OD1	1.72	0.71
1:X:617:U:H5	1:X:632:A:H2	1.38	0.70
3:A:231:HIS:HD2	3:A:233:HIS:H	1.38	0.70
5:C:137:ALA:HB1	5:C:142:LEU:HB2	1.73	0.70
1:X:617:U:C5	1:X:632:A:C2	2.80	0.70
1:X:1673:C:H2'	1:X:1674:C:H6	1.55	0.70
3:A:243:GLY:C	3:A:244:ARG:HD3	2.11	0.70
4:B:110:GLY:O	13:K:3:HIS:CD2	2.45	0.70
1:X:2039:G:N2	26:Z:4:HIS:O	2.22	0.69
4:B:14:ILE:HG22	4:B:21:ILE:HB	1.74	0.69
1:X:1561:A:H3'	1:X:1562:G:C8	2.27	0.69
13:K:79:VAL:HA	13:K:83:VAL:HG13	1.73	0.69
23:U:48:LYS:CG	23:U:49:LYS:H	2.04	0.69
1:X:1832:G:H1	1:X:1885:C:H42	1.37	0.69
1:X:2063:A:H4'	23:U:39:LYS:HG2	1.73	0.69
3:A:231:HIS:CD2	3:A:233:HIS:H	2.11	0.69
14:L:33:ARG:NH1	14:L:38:ILE:HB	2.08	0.68
1:X:1466:C:H2'	1:X:1467:U:O4'	1.93	0.68
1:X:1278:A:N6	1:X:1996:A:H5''	2.08	0.68
1:X:501:G:H2'	1:X:502:A:C8	2.28	0.68
1:X:577:U:H2'	1:X:579:G:OP2	1.94	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2770:A:H4'	1:X:2771:C:H5'	1.74	0.67
9:G:61:ARG:NH1	9:G:66:HIS:H	1.90	0.67
1:X:1882:G:N2	1:X:1885:C:H41	1.92	0.67
1:X:1278:A:H61	1:X:1996:A:H5''	1.60	0.67
25:W:12:ARG:CG	25:W:12:ARG:HH11	2.06	0.67
1:X:2767:C:H1'	4:B:62:PRO:HG3	1.77	0.67
9:G:132:PHE:CZ	9:G:145:HIS:HB2	2.30	0.67
3:A:210:GLY:HA2	3:A:213:ARG:HB2	1.76	0.67
13:K:11:ASN:OD1	13:K:17:ARG:NH2	2.27	0.67
9:G:67:ARG:HG2	9:G:70:PHE:HA	1.76	0.67
9:G:104:THR:OG1	9:G:110:LEU:HB3	1.95	0.67
3:A:43:ARG:HE	3:A:55:GLY:HA2	1.60	0.67
20:R:7:GLY:HA3	20:R:42:ARG:O	1.94	0.67
1:X:1885:C:C4'	3:A:244:ARG:HD2	2.24	0.66
1:X:168:A:H2'	1:X:169:C:C6	2.30	0.66
1:X:341:A:HO2'	1:X:342:G:H8	1.41	0.66
32:X:2929:1F4:H3	32:X:2929:1F4:H51	1.76	0.66
1:X:1342:U:H5''	1:X:1343:C:C5	2.31	0.66
32:X:2929:1F4:C50	32:X:2929:1F4:H60	2.23	0.66
1:X:617:U:H5	1:X:632:A:C2	2.14	0.66
12:J:15:ARG:HD2	12:J:74:PRO:HD2	1.77	0.66
25:W:4:LYS:HG2	25:W:52:GLU:HB3	1.78	0.65
1:X:1673:C:C5'	4:B:136:ARG:HD3	2.26	0.65
2:Y:45:C:H2'	6:D:92:ARG:NH1	2.10	0.65
4:B:194:GLY:HA2	15:M:2:GLN:HB3	1.77	0.65
1:X:1810:U:H2'	3:A:157:ARG:HD3	1.78	0.65
1:X:2266:A:H62	1:X:2323:U:H3	1.43	0.65
1:X:2551:A:N7	4:B:145:LYS:HB2	2.10	0.65
1:X:320:A:N3	1:X:340:G:O2'	2.29	0.65
1:X:1811:A:H5''	3:A:161:THR:HG21	1.78	0.65
1:X:1673:C:H2'	1:X:1674:C:C6	2.31	0.64
1:X:797:A:C5	3:A:229:VAL:HG21	2.31	0.64
11:I:17:LYS:O	11:I:18:ARG:HB2	1.97	0.64
20:R:25:LEU:H	20:R:80:LYS:HA	1.62	0.64
24:V:25:LEU:HD21	24:V:47:ARG:HG2	1.78	0.64
12:J:48:ILE:HD12	12:J:71:PRO:HG3	1.80	0.64
5:C:48:ARG:C	5:C:50:GLN:H	2.00	0.64
1:X:1744:G:OP1	15:M:100:ARG:HD2	1.97	0.64
16:N:66:ASN:HB2	16:N:70:ARG:NH1	2.13	0.64
1:X:1609:G:H2'	1:X:1610:A:C8	2.32	0.64
12:J:28:VAL:HG23	12:J:137:VAL:HB	1.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:482:A:H2'	1:X:483:A:O4'	1.96	0.64
1:X:742:G:C6	3:A:208:LYS:HB3	2.33	0.64
12:J:28:VAL:HG12	12:J:29:ALA:H	1.63	0.63
1:X:1582:A:OP1	3:A:211:ARG:NH2	2.31	0.63
1:X:1745:C:P	15:M:101:ARG:HH22	2.20	0.63
1:X:841:G:H2'	1:X:842:A:C8	2.33	0.63
1:X:764:A:H5'	18:P:111:ARG:HA	1.79	0.63
1:X:2653:A:O2'	10:H:41:ASN:ND2	2.32	0.63
1:X:800:U:H5''	1:X:801:A:H5'	1.81	0.63
1:X:1674:C:H2'	1:X:1675:C:C6	2.34	0.63
1:X:451:A:H2'	1:X:452:G:C8	2.34	0.62
15:M:60:SER:HB3	15:M:63:ARG:HH22	1.64	0.62
3:A:67:PHE:HB3	3:A:153:ALA:H	1.64	0.62
18:P:32:ARG:HA	18:P:121:THR:HG22	1.81	0.62
4:B:152:LYS:H	9:G:106:TYR:HB3	1.64	0.62
11:I:108:LEU:HD23	11:I:129:ALA:HB1	1.82	0.62
5:C:176:ASN:HB3	5:C:179:ASP:HB2	1.81	0.62
4:B:152:LYS:HB2	9:G:106:TYR:CB	2.27	0.62
23:U:32:ARG:HG2	23:U:33:LYS:N	2.13	0.62
21:S:3:LEU:HD11	21:S:56:VAL:HG13	1.80	0.62
1:X:797:A:N7	3:A:229:VAL:HG21	2.15	0.62
6:D:143:TYR:HA	6:D:146:VAL:HG22	1.82	0.62
24:V:28:LEU:HD12	24:V:43:VAL:HG22	1.81	0.62
1:X:1753:A:O5'	1:X:1753:A:H8	1.82	0.61
13:K:3:HIS:HB3	13:K:5:LYS:HD2	1.81	0.61
11:I:28:LYS:NZ	11:I:36:GLY:HA2	2.16	0.61
10:H:124:MET:O	10:H:127:VAL:HG12	2.00	0.61
2:Y:28:A:H8	2:Y:29:C:C5	2.17	0.61
1:X:670:U:H2'	1:X:671:A:C8	2.35	0.61
23:U:51:ILE:HA	23:U:59:THR:O	2.01	0.61
1:X:2083:G:H1	1:X:2172:U:H3	1.48	0.61
1:X:746:G:N7	1:X:774:A:C6	2.69	0.61
25:W:7:ARG:HB2	25:W:50:LEU:HA	1.82	0.61
1:X:341:A:O2'	1:X:342:G:H8	1.83	0.61
1:X:564:U:H2'	1:X:565:A:C8	2.36	0.61
1:X:1574:A:O2'	1:X:1575:C:H3'	2.00	0.61
1:X:226:C:OP2	1:X:2373:C:O2'	2.19	0.60
1:X:450:C:H2'	1:X:451:A:C8	2.35	0.60
23:U:52:ARG:NE	23:U:79:GLU:HA	2.16	0.60
1:X:1745:C:OP1	15:M:101:ARG:NH2	2.33	0.60
15:M:17:GLU:O	15:M:21:THR:OG1	2.17	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1437:A:H2'	1:X:1438:G:H8	1.64	0.60
16:N:66:ASN:HB3	16:N:76:TYR:HB2	1.83	0.60
3:A:223:GLY:HA2	3:A:226:MET:SD	2.40	0.60
1:X:512:A:H4'	18:P:15:LYS:HB3	1.83	0.60
5:C:47:THR:HA	5:C:82:VAL:HB	1.83	0.60
12:J:62:GLY:HA3	12:J:64:LYS:HE3	1.84	0.60
1:X:2543:A:H5'	1:X:2627:G:H4'	1.82	0.60
1:X:960:U:H2'	1:X:961:G:C8	2.37	0.60
5:C:176:ASN:HD22	5:C:179:ASP:H	1.48	0.60
1:X:504:G:H4'	18:P:27:VAL:HG12	1.84	0.60
1:X:412:U:H5''	23:U:68:ARG:HH22	1.67	0.60
1:X:168:A:H2'	1:X:169:C:H6	1.67	0.59
1:X:2484:G:H22	32:X:2929:1F4:H56	1.67	0.59
5:C:34:GLN:HB3	5:C:38:ARG:HH11	1.66	0.59
5:C:54:THR:HG21	5:C:72:ARG:HB3	1.84	0.59
1:X:954:U:OP2	11:I:38:LYS:HG2	2.01	0.59
1:X:2528:G:H2'	1:X:2529:G:H8	1.66	0.59
1:X:38:G:H21	5:C:42:THR:HG21	1.66	0.59
4:B:50:GLY:HA3	4:B:75:THR:HG21	1.85	0.59
1:X:530:G:H2'	1:X:531:G:C8	2.37	0.59
1:X:1782:A:N6	1:X:1820:G:O2'	2.35	0.59
16:N:66:ASN:HB2	16:N:70:ARG:HH11	1.67	0.59
18:P:27:VAL:HG23	18:P:125:THR:HG22	1.85	0.59
20:R:45:LYS:HA	20:R:76:LEU:O	2.02	0.59
18:P:40:LEU:HB3	26:Z:25:LEU:HD13	1.84	0.59
21:S:93:GLU:HB3	21:S:121:GLN:HG3	1.83	0.59
1:X:187:U:H2'	1:X:188:G:C8	2.37	0.59
10:H:78:SER:HA	10:H:91:PHE:O	2.03	0.59
1:X:1885:C:H4'	3:A:244:ARG:HD2	1.83	0.58
22:T:45:PHE:HD2	22:T:77:ARG:HB3	1.67	0.58
17:O:36:LYS:HE2	17:O:56:VAL:HG22	1.85	0.58
3:A:252:LYS:CD	3:A:253:PRO:HD3	2.32	0.58
16:N:66:ASN:CB	16:N:76:TYR:H	2.17	0.58
1:X:689:A:H2	1:X:815:A:H61	1.51	0.58
1:X:165:G:H2'	1:X:166:G:O4'	2.04	0.58
1:X:501:G:H2'	1:X:502:A:H8	1.65	0.58
5:C:38:ARG:HH12	5:C:176:ASN:HD21	1.51	0.58
12:J:40:PRO:HB3	12:J:99:LYS:HD2	1.86	0.58
1:X:2504:G:H21	30:4:1:MET:HE2	1.67	0.58
4:B:4:ILE:HG22	4:B:96:PHE:HE1	1.67	0.58
15:M:82:PRO:HG2	15:M:85:SER:HB2	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1030:U:HO2'	1:X:1032:A:H2	1.50	0.58
1:X:1999:U:O2'	26:Z:7:PRO:O	2.21	0.58
1:X:553:C:H42	1:X:559:C:H42	1.49	0.58
1:X:1656:U:H4'	1:X:2678:C:H4'	1.84	0.58
1:X:742:G:H2'	1:X:1766:U:H1'	1.85	0.58
1:X:1584:G:N3	3:A:58:HIS:CE1	2.72	0.58
1:X:405:C:H2'	1:X:406:G:H8	1.69	0.58
4:B:26:VAL:HG11	4:B:198:LEU:HD11	1.85	0.58
6:D:123:ASP:HB3	6:D:127:ASN:HB2	1.83	0.58
1:X:1505:U:HO2'	1:X:1506:C:H6	1.51	0.58
1:X:1468:A:H5'	1:X:1472:C:N4	2.19	0.57
1:X:114:C:O2'	1:X:124:A:N3	2.37	0.57
23:U:48:LYS:HG2	23:U:49:LYS:H	1.68	0.57
20:R:48:VAL:HG12	20:R:50:GLY:H	1.69	0.57
1:X:1071:U:H4'	1:X:1072:U:H3'	1.85	0.57
5:C:58:MET:HB2	5:C:70:GLY:O	2.04	0.57
5:C:119:ALA:H	5:C:189:ASP:HA	1.69	0.57
1:X:482:A:O5'	1:X:482:A:H8	1.88	0.57
1:X:1040:A:H5''	12:J:129:GLN:HE22	1.69	0.57
23:U:56:GLN:HE21	23:U:57:VAL:HG23	1.70	0.57
25:W:12:ARG:HG3	25:W:50:LEU:HD21	1.85	0.57
23:U:48:LYS:CG	23:U:49:LYS:N	2.68	0.57
1:X:1437:A:H2'	1:X:1438:G:C8	2.40	0.57
12:J:25:GLY:HA3	12:J:102:ARG:HA	1.87	0.57
7:E:127:GLU:HG3	7:E:130:ARG:HB2	1.87	0.57
1:X:712:A:H2'	1:X:713:G:O4'	2.05	0.57
5:C:43:ALA:CB	5:C:86:PRO:HB2	2.29	0.57
10:H:13:ASN:HD21	10:H:109:ARG:HG2	1.70	0.57
1:X:2081:U:H3	1:X:2174:G:H1	1.53	0.57
1:X:1845:A:H2'	1:X:1846:A:C8	2.40	0.56
19:Q:68:PHE:O	19:Q:70:GLY:N	2.38	0.56
1:X:1699:A:H61	1:X:1723:U:H3	1.51	0.56
1:X:1787:U:H2'	1:X:1788:C:C6	2.41	0.56
1:X:829:C:H2'	1:X:830:C:C6	2.40	0.56
3:A:36:ALA:HB1	3:A:62:TYR:O	2.04	0.56
1:X:1982:C:H5''	1:X:2703:C:O2'	2.05	0.56
1:X:1033:G:H22	1:X:1153:A:H2	1.53	0.56
1:X:559:C:H2'	1:X:560:G:C1'	2.35	0.56
14:L:27:LEU:HD23	14:L:44:ASP:HA	1.87	0.56
23:U:14:VAL:O	23:U:15:VAL:HG22	2.06	0.56
1:X:1173:G:H4'	17:O:22:VAL:HG23	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:530:G:H2'	1:X:531:G:H8	1.69	0.56
5:C:149:LEU:HD11	5:C:170:LEU:HD13	1.87	0.56
1:X:1268:U:C2	5:C:66:ASN:HA	2.41	0.56
1:X:215:G:H21	1:X:632:A:H8	1.52	0.56
13:K:3:HIS:CE1	13:K:5:LYS:HZ2	2.23	0.56
20:R:22:VAL:HG11	20:R:80:LYS:HD2	1.88	0.56
1:X:2653:A:H2'	10:H:41:ASN:ND2	2.21	0.56
1:X:2266:A:N6	1:X:2323:U:H3	2.04	0.56
1:X:1348:C:H2'	1:X:1349:A:C8	2.40	0.56
32:X:2929:1F4:O18	32:X:2929:1F4:H9	2.06	0.55
11:I:97:ARG:O	11:I:98:LEU:HB2	2.06	0.55
1:X:2516:U:H2'	1:X:2517:C:C6	2.40	0.55
16:N:66:ASN:HB3	16:N:76:TYR:CB	2.35	0.55
1:X:187:U:H2'	1:X:188:G:H8	1.70	0.55
1:X:1468:A:H5'	1:X:1472:C:H41	1.71	0.55
1:X:1454:U:H2'	1:X:1455:C:C6	2.41	0.55
3:A:38:PRO:HA	3:A:61:LEU:HD23	1.88	0.55
1:X:1770:U:C5	1:X:1775:A:N7	2.62	0.55
1:X:1882:G:H21	1:X:1885:C:H41	1.53	0.55
1:X:1348:C:H2'	1:X:1349:A:H8	1.71	0.55
1:X:1948:C:H5''	1:X:1949:A:H2'	1.89	0.55
20:R:52:ASN:HD21	20:R:71:GLN:HE21	1.55	0.55
1:X:2212:U:H2'	1:X:2213:G:C8	2.41	0.55
1:X:1595:A:H2'	1:X:1596:A:O4'	2.07	0.55
16:N:84:LYS:HG3	16:N:92:ARG:HH22	1.70	0.55
22:T:41:ARG:HA	22:T:41:ARG:HE	1.72	0.55
6:D:104:ILE:HA	6:D:108:LEU:HD12	1.88	0.55
1:X:559:C:C2'	1:X:560:G:O4'	2.54	0.54
9:G:106:TYR:O	9:G:110:LEU:HG	2.06	0.54
1:X:774:A:H8	1:X:774:A:O5'	1.90	0.54
5:C:136:TRP:O	5:C:140:ASN:ND2	2.40	0.54
18:P:97:VAL:HG22	18:P:124:ILE:HG23	1.87	0.54
1:X:2484:G:N2	32:X:2929:1F4:H56	2.22	0.54
1:X:1032:A:H3'	1:X:1032:A:C8	2.42	0.54
16:N:37:GLN:HA	16:N:40:LEU:HD12	1.90	0.54
1:X:75:C:H5''	24:V:48:ARG:HG3	1.89	0.54
1:X:1135:C:H2'	1:X:1136:G:O4'	2.06	0.54
1:X:333:A:H2'	5:C:162:ARG:HH12	1.72	0.54
1:X:1264:C:OP1	16:N:10:ARG:HG3	2.08	0.54
1:X:2659:C:H5'	4:B:189:PRO:HA	1.90	0.54
32:X:2929:1F4:C54	32:X:2929:1F4:H18	2.38	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:95:LEU:HD23	5:C:96:PRO:HD2	1.90	0.54
8:F:79:ARG:HG2	8:F:84:ILE:HB	1.90	0.54
3:A:60:ARG:HD3	3:A:86:PRO:O	2.06	0.54
1:X:219:G:N2	1:X:231:G:H2'	2.22	0.54
21:S:91:PRO:HG2	21:S:125:PRO:HD2	1.90	0.54
1:X:2196:U:H5'	1:X:2197:U:OP2	2.08	0.54
9:G:67:ARG:CG	9:G:70:PHE:HA	2.37	0.54
1:X:356:A:H2'	1:X:357:A:C8	2.43	0.54
1:X:29:U:H5''	16:N:7:GLY:HA2	1.90	0.54
5:C:148:VAL:HG13	5:C:185:ARG:HB2	1.90	0.54
1:X:2627:G:H2'	1:X:2628:C:O4'	2.08	0.54
6:D:80:ARG:HD3	6:D:83:MET:HB2	1.91	0.53
32:X:2929:1F4:C39	32:X:2929:1F4:H9	2.38	0.53
1:X:760:U:O2	1:X:1997:A:H1'	2.08	0.53
10:H:77:THR:HA	10:H:94:ASN:HB3	1.89	0.53
21:S:123:VAL:HG23	21:S:161:ALA:HB2	1.90	0.53
16:N:6:THR:O	16:N:9:VAL:HG23	2.08	0.53
1:X:171:G:H2'	1:X:172:A:O4'	2.08	0.53
1:X:2482:A:H4'	1:X:2483:U:OP1	2.08	0.53
1:X:1134:C:H2'	1:X:1135:C:H6	1.74	0.53
15:M:29:PRO:HB2	15:M:99:VAL:HG21	1.90	0.53
3:A:182:LEU:HD12	3:A:269:PHE:HB2	1.90	0.53
13:K:87:TYR:CE1	13:K:94:TYR:HD2	2.27	0.53
1:X:2459:C:H2'	1:X:2459:C:O2	2.08	0.53
21:S:95:SER:HB3	21:S:119:ASN:HD22	1.74	0.53
1:X:1673:C:H5'	4:B:136:ARG:HD3	1.91	0.53
9:G:132:PHE:HB2	9:G:145:HIS:CE1	2.44	0.53
1:X:1223:G:H5'	1:X:1225:G:O4'	2.08	0.53
14:L:38:ILE:HG13	14:L:39:TYR:N	2.17	0.53
21:S:6:LYS:N	21:S:7:PRO:HD3	2.20	0.53
5:C:48:ARG:C	5:C:50:GLN:N	2.61	0.53
10:H:83:ARG:CZ	10:H:89:ILE:HD11	2.38	0.53
1:X:1076:U:H3	1:X:1080:A:H2'	1.74	0.53
20:R:26:SER:H	20:R:30:LYS:HG3	1.73	0.53
1:X:732:G:H2'	1:X:733:G:C8	2.43	0.53
2:Y:9:G:H1	2:Y:116:C:H42	1.56	0.53
4:B:5:LEU:HG	4:B:195:LEU:HD11	1.91	0.53
18:P:62:ARG:HE	26:Z:25:LEU:HD11	1.74	0.53
1:X:761:G:OP2	18:P:109:ARG:HG3	2.08	0.53
1:X:555:U:H5'	1:X:556:A:C8	2.43	0.53
11:I:102:LYS:O	11:I:104:ARG:N	2.35	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2041:A:H61	32:X:2929:1F4:H46	1.73	0.53
23:U:32:ARG:HG2	23:U:33:LYS:H	1.72	0.53
1:X:633:G:H2'	1:X:634:G:H8	1.73	0.53
9:G:105:GLY:O	9:G:106:TYR:C	2.46	0.52
1:X:577:U:H5''	1:X:956:A:N6	2.23	0.52
1:X:1468:A:O5'	1:X:1468:A:C8	2.62	0.52
25:W:3:ILE:HG23	25:W:51:LEU:HD22	1.92	0.52
1:X:2270:U:H2'	1:X:2271:C:C6	2.43	0.52
1:X:2225:G:H2'	1:X:2226:A:C8	2.43	0.52
1:X:1287:A:H2'	1:X:1288:A:H5''	1.91	0.52
3:A:45:ASN:CG	3:A:46:ARG:H	2.12	0.52
1:X:796:A:H8	1:X:797:A:H4'	1.74	0.52
10:H:70:VAL:CG2	10:H:98:ILE:HG23	2.38	0.52
4:B:131:SER:O	4:B:132:LYS:HG2	2.10	0.52
1:X:1998:A:O5'	1:X:1998:A:H8	1.92	0.52
1:X:1378:A:H1'	23:U:16:ASN:HD21	1.74	0.52
3:A:79:VAL:HG21	3:A:111:LEU:HD22	1.91	0.52
3:A:245:VAL:HG12	3:A:250:TRP:O	2.09	0.52
1:X:1039:A:N6	1:X:1136:G:H2'	2.24	0.52
1:X:2505:G:H1	1:X:2516:U:H3	1.58	0.52
1:X:760:U:C5	26:Z:3:LYS:HG3	2.44	0.52
1:X:1609:G:H2'	1:X:1610:A:H8	1.73	0.52
4:B:31:CYS:HB3	4:B:49:ILE:HG23	1.90	0.52
12:J:37:ALA:O	12:J:100:PRO:HA	2.09	0.52
1:X:110:U:H3'	1:X:111:G:C8	2.44	0.52
1:X:768:U:H2'	1:X:769:C:O4'	2.09	0.52
1:X:2860:C:H2'	1:X:2861:A:O4'	2.09	0.52
13:K:17:ARG:HH11	13:K:20:LEU:CD2	2.23	0.52
2:Y:46:G:H5'	6:D:92:ARG:HH12	1.73	0.52
23:U:51:ILE:HG23	23:U:59:THR:HA	1.92	0.52
23:U:51:ILE:HG12	23:U:59:THR:HB	1.92	0.52
1:X:2372:A:H5''	11:I:61:PRO:HB3	1.92	0.52
1:X:568:G:H2'	1:X:569:C:O4'	2.09	0.52
14:L:8:ARG:HG3	14:L:9:ARG:H	1.74	0.52
8:F:117:ALA:HB1	8:F:122:ALA:HB1	1.92	0.52
1:X:1859:A:H2'	1:X:1860:A:C8	2.45	0.52
1:X:83:A:H2	1:X:97:U:O2	1.92	0.52
4:B:152:LYS:H	9:G:106:TYR:CB	2.22	0.52
1:X:465:C:O2'	1:X:483:A:N6	2.42	0.52
1:X:1856:U:OP1	1:X:2389:G:O2'	2.26	0.52
13:K:28:LEU:HD12	13:K:48:VAL:HG21	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1465:G:N2	1:X:1477:C:O2	2.41	0.52
10:H:27:SER:HA	10:H:50:ILE:HD12	1.90	0.52
17:O:40:VAL:HG12	17:O:43:GLU:HA	1.91	0.52
1:X:1673:C:H5''	4:B:136:ARG:HD3	1.91	0.52
1:X:504:G:H21	18:P:78:ASN:HD21	1.57	0.52
1:X:2528:G:H5''	1:X:2528:G:C8	2.45	0.52
1:X:2594:U:C2	26:Z:7:PRO:HA	2.45	0.52
14:L:36:LYS:HB3	14:L:64:LYS:HB2	1.92	0.52
4:B:16:LYS:HB2	4:B:21:ILE:HD11	1.92	0.52
1:X:450:C:H2'	1:X:451:A:H8	1.73	0.52
1:X:1623:C:H4'	1:X:1624:A:O5'	2.10	0.52
1:X:216:U:H2'	1:X:217:U:O4'	2.10	0.52
4:B:116:VAL:CG2	4:B:136:ARG:HE	2.15	0.51
3:A:43:ARG:HB3	3:A:54:ILE:HG12	1.91	0.51
1:X:2797:G:OP2	13:K:3:HIS:NE2	2.42	0.51
2:Y:43:G:H5'	2:Y:44:C:H5''	1.91	0.51
1:X:400:U:H5	23:U:21:ARG:HH12	1.57	0.51
1:X:1804:U:H2'	1:X:1805:G:H8	1.73	0.51
1:X:627:A:H2'	1:X:628:A:C8	2.46	0.51
1:X:611:C:H5''	1:X:611:C:H6	1.75	0.51
1:X:413:G:H8	1:X:413:G:O5'	1.93	0.51
1:X:1586:A:H5'	3:A:38:PRO:HG3	1.93	0.51
9:G:93:LYS:HB3	9:G:96:ASP:HB3	1.92	0.51
21:S:117:VAL:HG22	21:S:168:VAL:HA	1.91	0.51
20:R:59:LYS:HG2	20:R:62:MET:HB3	1.93	0.51
15:M:69:ARG:HG3	15:M:78:GLU:HG3	1.93	0.51
32:X:2929:1F4:C23	32:X:2929:1F4:C41	2.88	0.51
1:X:451:A:H2'	1:X:452:G:H8	1.74	0.51
1:X:388:G:H2'	1:X:389:G:H8	1.75	0.51
1:X:1016:C:O2'	9:G:56:THR:HG21	2.11	0.51
5:C:24:SER:HA	5:C:27:LEU:HD12	1.93	0.51
1:X:2042:A:OP1	5:C:66:ASN:ND2	2.44	0.51
6:D:4:LEU:HG	6:D:5:LYS:H	1.74	0.51
6:D:114:PHE:HZ	6:D:176:PRO:HG2	1.74	0.51
1:X:2545:A:H61	10:H:40:GLY:HA3	1.74	0.51
7:E:6:LYS:HB3	7:E:69:ARG:HD3	1.93	0.51
1:X:699:G:C8	1:X:699:G:H5'	2.46	0.51
1:X:840:U:O2	1:X:2225:G:H4'	2.11	0.51
4:B:146:THR:OG1	4:B:147:PRO:HD3	2.11	0.51
17:O:8:GLY:H	17:O:20:ILE:HD13	1.75	0.51
1:X:2289:A:H3'	1:X:2290:A:H8	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1542:G:N2	1:X:1562:G:H1	1.94	0.51
1:X:334:G:OP1	1:X:349:G:N2	2.44	0.51
15:M:44:ARG:HE	15:M:46:ARG:HH21	1.58	0.51
3:A:58:HIS:O	3:A:58:HIS:ND1	2.44	0.50
1:X:1736:C:H2'	1:X:1737:G:C8	2.46	0.50
20:R:105:ARG:HH22	20:R:112:LYS:HA	1.76	0.50
1:X:1584:G:H4'	3:A:59:LYS:HG2	1.94	0.50
1:X:935:C:H2'	1:X:936:A:C8	2.45	0.50
5:C:22:VAL:HG22	5:C:106:MET:HG3	1.92	0.50
21:S:3:LEU:HD13	21:S:32:PHE:HB3	1.93	0.50
1:X:1454:U:H2'	1:X:1455:C:H6	1.76	0.50
17:O:15:SER:HA	17:O:95:ILE:O	2.11	0.50
32:X:2929:1F4:C50	32:X:2929:1F4:C52	2.90	0.50
1:X:1834:G:H1	1:X:1881:U:H3	1.59	0.50
4:B:61:LYS:HB3	4:B:62:PRO:HD3	1.93	0.50
23:U:52:ARG:HD3	23:U:70:LEU:HD22	1.92	0.50
4:B:4:ILE:HG12	4:B:28:ALA:HB1	1.94	0.50
1:X:2271:C:P	14:L:18:ARG:HH21	2.35	0.50
12:J:26:ASP:HB3	12:J:68:ARG:HH22	1.76	0.50
13:K:17:ARG:HH11	13:K:20:LEU:HD22	1.76	0.50
1:X:1656:U:H2'	1:X:1657:A:H5''	1.94	0.50
1:X:620:G:N2	1:X:630:G:H1'	2.26	0.50
1:X:2002:A:N7	26:Z:9:LYS:HD2	2.26	0.50
16:N:24:PHE:O	16:N:29:SER:HB3	2.11	0.50
4:B:35:GLN:HB2	4:B:48:GLN:HB3	1.93	0.50
1:X:1142:G:C1'	9:G:103:TYR:HD2	2.25	0.50
3:A:246:PRO:HD2	3:A:249:PRO:O	2.12	0.50
9:G:132:PHE:CE2	9:G:145:HIS:HB2	2.47	0.50
5:C:148:VAL:HB	5:C:167:VAL:HG12	1.93	0.50
3:A:182:LEU:HB2	3:A:268:ARG:O	2.11	0.50
1:X:1685:A:H5''	10:H:5:GLN:HG2	1.93	0.50
1:X:969:U:H5''	12:J:17:ARG:HH11	1.77	0.50
15:M:33:VAL:HG22	15:M:51:GLU:HB2	1.93	0.50
21:S:51:LEU:HB3	21:S:65:LEU:HD12	1.94	0.50
20:R:92:THR:HB	20:R:95:ARG:HH22	1.75	0.50
1:X:884:C:H2'	1:X:885:A:H8	1.77	0.50
1:X:2056:C:H4'	3:A:228:PRO:HB2	1.93	0.49
26:Z:30:LEU:HD22	26:Z:39:LYS:HB3	1.94	0.49
5:C:164:VAL:C	5:C:166:TRP:H	2.15	0.49
23:U:48:LYS:HG2	23:U:49:LYS:N	2.27	0.49
1:X:2861:A:O2'	26:Z:31:THR:HG23	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:504:G:H4'	18:P:27:VAL:CG1	2.42	0.49
21:S:127:PRO:C	21:S:129:ARG:H	2.16	0.49
1:X:1448:A:H61	1:X:1574:A:N6	1.93	0.49
14:L:15:ARG:HD2	14:L:91:ARG:HD2	1.95	0.49
1:X:2597:G:H21	4:B:150:VAL:HG11	1.77	0.49
5:C:4:ILE:HG22	5:C:13:ARG:HH21	1.77	0.49
8:F:112:MET:HA	8:F:115:LEU:HD12	1.94	0.49
26:Z:45:ILE:HG21	26:Z:57:VAL:HG23	1.94	0.49
1:X:1326:U:H2'	1:X:1626:A:C2	2.48	0.49
1:X:1979:C:H4'	1:X:1980:A:OP1	2.13	0.49
1:X:1632:A:H5'	1:X:1632:A:H8	1.77	0.49
13:K:11:ASN:HD21	13:K:17:ARG:NH1	2.09	0.49
1:X:2653:A:C2'	10:H:41:ASN:ND2	2.75	0.49
1:X:1089:C:H5'	8:F:132:ARG:HH12	1.77	0.49
10:H:113:PRO:HB3	10:H:134:LEU:HD12	1.94	0.49
1:X:2546:G:H2'	1:X:2547:C:C6	2.48	0.49
3:A:66:ASP:HB3	3:A:105:ILE:HD12	1.93	0.49
21:S:5:ALA:HB1	21:S:7:PRO:HD3	1.94	0.49
1:X:2039:G:H2'	1:X:2039:G:N3	2.28	0.49
21:S:56:VAL:HG12	21:S:57:GLU:H	1.78	0.49
9:G:90:LEU:HD23	9:G:94:LYS:HA	1.94	0.49
1:X:1750:A:H1'	1:X:2690:A:C2	2.47	0.49
2:Y:50:U:OP1	14:L:94:TYR:HA	2.13	0.49
1:X:347:C:H4'	20:R:15:HIS:CD2	2.48	0.49
3:A:58:HIS:O	3:A:59:LYS:HB3	2.11	0.49
2:Y:92:G:H8	2:Y:92:G:OP2	1.95	0.49
16:N:74:MET:HG2	16:N:78:THR:HG22	1.94	0.49
16:N:66:ASN:HD22	16:N:70:ARG:HH12	1.60	0.49
1:X:1030:U:H3	1:X:1153:A:H62	1.61	0.49
1:X:2035:G:H4'	4:B:143:GLN:O	2.13	0.49
3:A:164:GLN:HB3	3:A:176:ARG:HB3	1.94	0.49
1:X:1478:U:H2'	1:X:1479:G:H8	1.78	0.49
10:H:112:GLY:O	10:H:131:PRO:HD2	2.13	0.49
13:K:87:TYR:HE1	13:K:94:TYR:HD2	1.59	0.49
16:N:75:ASN:ND2	16:N:78:THR:H	2.10	0.49
1:X:229:G:OP1	11:I:49:PHE:HE1	1.96	0.49
1:X:1509:A:H8	1:X:1510:A:C8	2.30	0.49
17:O:71:ILE:HD11	17:O:86:HIS:HB2	1.94	0.48
1:X:1469:U:P	1:X:1471:G:OP2	2.71	0.48
1:X:2779:C:H2'	1:X:2780:A:C8	2.48	0.48
4:B:27:LEU:HD23	4:B:51:TYR:OH	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:X:2929:1F4:H3	32:X:2929:1F4:O18	2.12	0.48
1:X:1333:G:N2	1:X:1344:C:N4	2.61	0.48
1:X:793:G:H21	1:X:796:A:H62	1.61	0.48
1:X:643:A:H4'	11:I:67:ASN:HB3	1.95	0.48
6:D:60:ILE:HD12	6:D:61:THR:HG23	1.95	0.48
1:X:463:C:H42	1:X:467:U:H5	1.60	0.48
18:P:102:THR:HG21	18:P:118:LYS:HB3	1.95	0.48
3:A:37:LEU:HD13	3:A:38:PRO:HD2	1.95	0.48
1:X:611:C:H4'	5:C:98:GLN:HE22	1.79	0.48
1:X:1608:U:H2'	1:X:1609:G:C8	2.48	0.48
1:X:2857:C:H5'	13:K:96:ARG:HG3	1.94	0.48
11:I:30:ALA:HB3	11:I:34:HIS:HE1	1.70	0.48
25:W:4:LYS:CG	25:W:52:GLU:HB3	2.43	0.48
1:X:1478:U:H2'	1:X:1479:G:C8	2.48	0.48
1:X:1515:U:H2'	1:X:1516:A:H8	1.79	0.48
3:A:165:VAL:HA	3:A:175:VAL:HG12	1.94	0.48
16:N:50:ARG:O	16:N:53:LYS:HG2	2.13	0.48
11:I:32:ARG:HD2	17:O:79:GLN:NE2	2.29	0.48
1:X:794:A:H5'	3:A:218:LYS:NZ	2.29	0.48
23:U:48:LYS:HG3	23:U:49:LYS:H	1.79	0.48
1:X:654:A:H2	1:X:655:A:H3'	1.78	0.48
1:X:1202:U:H2'	1:X:1203:A:H8	1.78	0.48
1:X:958:G:H2'	1:X:959:C:C6	2.49	0.48
1:X:2821:G:H2'	1:X:2822:U:C6	2.49	0.48
1:X:503:G:H2'	1:X:504:G:O4'	2.14	0.48
1:X:1093:U:H5'	8:F:117:ALA:HA	1.96	0.48
20:R:38:LEU:HB3	20:R:47:VAL:HB	1.95	0.48
17:O:10:LYS:HG3	17:O:11:GLN:HG2	1.96	0.48
1:X:82:G:N1	1:X:100:G:H2'	2.29	0.48
14:L:31:VAL:HG21	14:L:100:VAL:HG23	1.96	0.48
20:R:23:ILE:HG22	20:R:33:THR:HB	1.95	0.48
1:X:527:C:OP1	26:Z:16:ARG:NH2	2.46	0.48
1:X:1167:A:H61	16:N:48:ARG:HG2	1.79	0.48
3:A:118:ASN:HD22	3:A:119:ALA:N	2.12	0.48
1:X:621:U:H2'	1:X:622:U:C6	2.49	0.48
1:X:1918:G:H1'	1:X:1947:G:N2	2.28	0.48
11:I:130:ILE:HG22	11:I:140:VAL:HG21	1.96	0.48
10:H:26:ASN:CB	10:H:38:GLY:H	2.26	0.48
1:X:2045:A:O5'	1:X:2045:A:H8	1.96	0.48
23:U:65:ASN:HA	23:U:68:ARG:HD3	1.96	0.48
1:X:1687:C:OP2	1:X:2529:G:OP1	2.32	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1736:C:H2'	1:X:1737:G:H8	1.79	0.47
6:D:8:TYR:O	6:D:12:VAL:HB	2.14	0.47
1:X:881:U:H2'	1:X:882:C:C6	2.49	0.47
1:X:1497:C:C6	1:X:1497:C:H5''	2.50	0.47
23:U:52:ARG:HE	23:U:79:GLU:HA	1.77	0.47
1:X:1515:U:H2'	1:X:1516:A:C8	2.49	0.47
2:Y:21:C:H2'	2:Y:22:U:O4'	2.13	0.47
24:V:42:ARG:NH1	24:V:45:GLN:OE1	2.47	0.47
1:X:1674:C:H2'	1:X:1675:C:H6	1.76	0.47
32:X:2929:1F4:H11	32:X:2929:1F4:C41	2.44	0.47
10:H:116:ARG:HH11	15:M:38:LYS:HD3	1.79	0.47
18:P:57:LEU:HD13	18:P:69:ALA:HA	1.96	0.47
1:X:1406:A:N6	19:Q:15:LYS:HG2	2.29	0.47
11:I:62:LYS:NZ	11:I:64:GLY:HA3	2.28	0.47
9:G:67:ARG:HE	9:G:70:PHE:HA	1.78	0.47
20:R:22:VAL:HG13	20:R:81:VAL:O	2.14	0.47
3:A:118:ASN:HD22	3:A:119:ALA:H	1.61	0.47
25:W:1:MET:HB3	25:W:34:VAL:HG12	1.96	0.47
7:E:67:LEU:O	7:E:71:LEU:HG	2.15	0.47
1:X:1673:C:H5'	4:B:136:ARG:HH11	1.78	0.47
4:B:133:LYS:HG2	4:B:137:ARG:HB3	1.96	0.47
1:X:2362:G:H2'	1:X:2363:G:C8	2.49	0.47
11:I:32:ARG:HD2	17:O:79:GLN:HE22	1.80	0.47
3:A:186:HIS:HB2	3:A:188:GLU:CG	2.44	0.47
10:H:90:ARG:HG2	15:M:78:GLU:HB2	1.96	0.47
1:X:2394:G:H4'	11:I:65:PHE:HB3	1.96	0.47
1:X:588:G:H2'	1:X:589:C:H6	1.78	0.47
1:X:1507:A:H2'	1:X:1508:G:H8	1.79	0.47
1:X:1168:G:O2'	25:W:28:ILE:HG12	2.15	0.47
4:B:149:ARG:CZ	9:G:106:TYR:HD1	2.28	0.47
4:B:149:ARG:NH1	9:G:106:TYR:HB2	2.29	0.47
11:I:58:ALA:O	11:I:59:ARG:CB	2.62	0.47
9:G:61:ARG:HH11	9:G:66:HIS:H	1.61	0.47
3:A:208:LYS:C	3:A:209:ALA:O	2.53	0.47
3:A:208:LYS:O	3:A:209:ALA:O	2.32	0.47
1:X:388:G:H2'	1:X:389:G:C8	2.50	0.47
1:X:2014:A:C6	1:X:2477:C:H1'	2.49	0.47
21:S:131:PRO:HG3	21:S:155:PRO:HG2	1.97	0.47
21:S:23:ALA:HA	21:S:83:PHE:O	2.14	0.47
1:X:2048:C:H1'	1:X:2428:U:O2	2.14	0.47
4:B:5:LEU:HD12	4:B:197:VAL:HG22	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:588:G:H2'	1:X:589:C:C6	2.49	0.47
1:X:2493:U:H2'	1:X:2494:C:C6	2.50	0.47
1:X:7:G:H2'	1:X:8:A:C8	2.50	0.47
1:X:203:G:H21	1:X:205:A:H62	1.63	0.47
13:K:97:ILE:HA	13:K:112:LEU:O	2.14	0.47
17:O:38:LEU:HD23	17:O:47:PHE:HB3	1.96	0.47
1:X:1584:G:N3	3:A:58:HIS:HE1	2.10	0.47
19:Q:61:LYS:H	19:Q:72:ARG:HA	1.79	0.47
6:D:40:LEU:HD21	6:D:87:ILE:HD12	1.96	0.47
1:X:1255:A:H2'	1:X:1256:C:C6	2.50	0.47
1:X:745:C:H2'	1:X:746:G:O4'	2.14	0.47
6:D:63:GLN:HG3	6:D:95:ARG:HH21	1.79	0.47
16:N:49:ASP:HA	16:N:52:ASN:HB2	1.97	0.47
1:X:609:U:H4'	11:I:18:ARG:HE	1.80	0.46
1:X:2653:A:H4'	10:H:42:LYS:HB2	1.97	0.46
19:Q:12:ILE:H	19:Q:12:ILE:HD13	1.80	0.46
9:G:61:ARG:HG2	9:G:65:LYS:HE3	1.96	0.46
12:J:28:VAL:HG13	12:J:135:ARG:HG2	1.98	0.46
2:Y:94:G:H5'	21:S:74:ARG:HH12	1.79	0.46
16:N:88:ILE:CG1	17:O:49:GLU:HB2	2.45	0.46
9:G:116:ARG:HA	9:G:119:LEU:HD12	1.98	0.46
1:X:2604:G:H2'	1:X:2605:C:O4'	2.15	0.46
1:X:1329:U:H5'	1:X:1405:A:H1'	1.97	0.46
3:A:244:ARG:N	3:A:244:ARG:HD3	2.30	0.46
22:T:45:PHE:CD2	22:T:77:ARG:HB3	2.47	0.46
1:X:2286:G:C2	1:X:2287:G:H1'	2.50	0.46
25:W:47:VAL:HB	25:W:50:LEU:HD12	1.98	0.46
9:G:66:HIS:HA	16:N:67:ALA:HB1	1.98	0.46
20:R:35:LYS:HE3	20:R:37:LEU:HB3	1.98	0.46
1:X:118:U:H4'	1:X:119:G:H5''	1.97	0.46
22:T:48:GLY:HA3	22:T:79:ILE:O	2.15	0.46
1:X:876:A:H2'	1:X:877:G:C8	2.50	0.46
21:S:19:ILE:HD12	21:S:79:ILE:HA	1.97	0.46
1:X:1148:G:H2'	1:X:1149:G:O4'	2.14	0.46
15:M:13:LEU:HA	15:M:13:LEU:HD12	1.70	0.46
4:B:117:MET:HG3	4:B:136:ARG:HG3	1.98	0.46
11:I:32:ARG:HB3	17:O:79:GLN:NE2	2.31	0.46
12:J:109:GLY:HA3	21:S:112:LEU:HD21	1.97	0.46
1:X:2574:G:N2	1:X:2577:A:C8	2.82	0.46
16:N:72:HIS:HB2	16:N:110:VAL:HG11	1.96	0.46
1:X:1675:C:OP1	4:B:134:TRP:CE2	2.69	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1333:G:N2	1:X:1344:C:H41	2.14	0.46
1:X:649:G:H22	1:X:661:C:H1'	1.80	0.46
1:X:1978:U:H1'	10:H:3:MET:HE1	1.97	0.46
1:X:1169:C:H4'	25:W:28:ILE:O	2.16	0.46
1:X:547:U:H2'	1:X:548:G:C8	2.50	0.46
14:L:63:ASN:HB3	14:L:66:ASP:HB2	1.96	0.46
19:Q:20:MET:HG2	19:Q:92:ALA:O	2.16	0.46
1:X:2522:G:H2'	1:X:2523:G:C8	2.50	0.46
1:X:1505:U:O2'	1:X:1506:C:H6	1.98	0.46
11:I:77:LEU:HD13	11:I:110:ALA:HA	1.98	0.46
1:X:2784:A:C6	1:X:2866:A:C8	3.04	0.46
11:I:121:HIS:HA	11:I:141:VAL:HB	1.98	0.46
1:X:2691:C:O2'	1:X:2693:U:H5'	2.16	0.46
26:Z:33:CYS:HB2	26:Z:46:CYS:SG	2.56	0.46
1:X:609:U:H5'	11:I:18:ARG:HD3	1.97	0.46
1:X:333:A:H2'	5:C:162:ARG:NH1	2.30	0.46
1:X:540:G:H1'	1:X:2004:U:O2'	2.16	0.46
19:Q:66:GLY:O	19:Q:68:PHE:N	2.34	0.46
1:X:636:G:H5''	1:X:636:G:C8	2.51	0.46
22:T:71:ASN:HD21	22:T:74:LYS:HG2	1.81	0.46
1:X:2062:U:H2'	1:X:2063:A:C8	2.52	0.45
1:X:1032:A:H3'	1:X:1032:A:H8	1.78	0.45
17:O:25:LEU:HB2	17:O:32:LYS:HE2	1.98	0.45
1:X:784:U:H2'	1:X:785:U:C6	2.51	0.45
1:X:2352:A:H2'	1:X:2353:G:H8	1.81	0.45
1:X:172:A:H61	1:X:175:C:H3'	1.81	0.45
20:R:90:LYS:HB2	20:R:108:VAL:HG21	1.98	0.45
1:X:240:U:H2'	1:X:241:C:O4'	2.16	0.45
4:B:32:PRO:HA	4:B:89:ASP:HB3	1.98	0.45
12:J:21:ASP:HA	12:J:99:LYS:HE2	1.97	0.45
14:L:66:ASP:C	14:L:68:ALA:H	2.19	0.45
12:J:42:TRP:CD1	12:J:97:VAL:HG12	2.51	0.45
6:D:106:ILE:HG21	6:D:139:PRO:HB3	1.98	0.45
1:X:2371:A:H1'	11:I:59:ARG:HG3	1.97	0.45
1:X:673:G:H5'	5:C:93:TYR:CD1	2.52	0.45
1:X:1805:G:N3	3:A:50:THR:CG2	2.80	0.45
25:W:19:THR:HG21	25:W:46:THR:HG22	1.98	0.45
5:C:5:ASN:HB3	5:C:10:ASN:HA	1.99	0.45
1:X:313:U:H2'	1:X:314:G:H8	1.81	0.45
1:X:2210:C:OP1	23:U:45:ASN:HA	2.17	0.45
1:X:2843:A:H5''	1:X:2843:A:C8	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:523:A:O2'	16:N:11:ARG:HD2	2.16	0.45
1:X:1673:C:H5'	4:B:136:ARG:NH1	2.31	0.45
1:X:631:G:H1	5:C:97:ARG:NH1	2.14	0.45
1:X:322:A:N6	1:X:339:U:H2'	2.31	0.45
1:X:1845:A:N1	1:X:2070:G:H1'	2.31	0.45
1:X:428:A:H2'	1:X:429:C:O4'	2.17	0.45
1:X:674:U:H2'	1:X:675:C:O4'	2.17	0.45
2:Y:28:A:C8	2:Y:29:C:C5	3.02	0.45
1:X:635:C:O2'	1:X:670:U:H5''	2.17	0.45
1:X:1805:G:N3	3:A:50:THR:HG22	2.31	0.45
1:X:710:C:H2'	1:X:711:C:C6	2.52	0.45
17:O:48:GLY:C	17:O:50:ASP:H	2.20	0.45
1:X:1234:C:H2'	1:X:1235:C:H6	1.82	0.45
1:X:1997:A:H2'	1:X:1998:A:C8	2.51	0.45
2:Y:46:G:H4'	6:D:92:ARG:HH12	1.82	0.45
1:X:1832:G:H1	1:X:1885:C:N4	2.09	0.45
1:X:1981:A:H2'	1:X:1982:C:O4'	2.16	0.45
20:R:105:ARG:NH2	20:R:112:LYS:HA	2.32	0.45
3:A:83:GLU:N	3:A:92:ILE:O	2.46	0.45
7:E:11:VAL:HG11	7:E:50:LEU:HD13	1.98	0.45
18:P:105:ARG:HB3	18:P:105:ARG:HE	1.64	0.45
23:U:19:ILE:HA	23:U:42:GLN:HA	1.98	0.45
12:J:31:GLY:HA2	12:J:108:ALA:HB2	1.99	0.45
1:X:1573:G:H3'	1:X:1574:A:O4'	2.17	0.45
12:J:42:TRP:CG	12:J:95:VAL:HG11	2.52	0.45
9:G:154:GLU:C	9:G:157:PRO:HD2	2.36	0.45
5:C:74:VAL:HG23	5:C:76:THR:H	1.81	0.45
10:H:11:ALA:O	10:H:110:VAL:HA	2.17	0.45
3:A:134:ARG:HG3	3:A:135:PHE:HD2	1.81	0.45
9:G:34:PRO:HA	9:G:69:ASP:CG	2.37	0.45
1:X:1164:C:H5'	16:N:76:TYR:CE2	2.52	0.45
1:X:2579:A:H2'	1:X:2580:C:C6	2.52	0.45
1:X:2222:U:H2'	1:X:2223:U:C6	2.52	0.45
1:X:2661:G:O6	1:X:2708:U:H1'	2.17	0.45
15:M:79:ARG:CG	15:M:79:ARG:NH1	2.68	0.45
1:X:640:C:C4'	1:X:660:G:H21	2.23	0.45
23:U:22:GLY:HA3	23:U:39:LYS:HD2	1.98	0.45
1:X:593:C:N4	1:X:594:G:C6	2.85	0.45
9:G:70:PHE:HB2	16:N:64:ARG:HE	1.83	0.44
1:X:636:G:O2'	1:X:669:G:H4'	2.17	0.44
1:X:1367:A:H2'	1:X:1368:G:O4'	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:97:GLN:HB2	20:R:101:GLY:HA2	1.99	0.44
1:X:1045:G:N2	1:X:1133:G:H1'	2.31	0.44
4:B:119:ARG:HG2	4:B:120:TRP:CE2	2.52	0.44
1:X:1494:G:H2'	1:X:1495:G:O4'	2.17	0.44
1:X:1769:U:H2'	1:X:1775:A:N6	2.31	0.44
3:A:79:VAL:HG21	3:A:111:LEU:CD2	2.47	0.44
1:X:2252:A:H2'	1:X:2253:A:C8	2.52	0.44
20:R:25:LEU:N	20:R:80:LYS:HA	2.30	0.44
3:A:208:LYS:HE3	3:A:208:LYS:HA	2.00	0.44
1:X:1202:U:H5'	17:O:78:VAL:HG22	1.98	0.44
1:X:2195:C:H5''	1:X:2195:C:H6	1.82	0.44
1:X:1373:G:N2	1:X:2192:U:H3	2.15	0.44
3:A:147:LEU:HD22	3:A:183:ARG:HH22	1.82	0.44
12:J:73:LYS:H	12:J:94:TRP:HD1	1.65	0.44
1:X:1117:G:H2'	1:X:1118:G:H8	1.80	0.44
2:Y:72:C:H2'	2:Y:73:C:H6	1.82	0.44
1:X:224:G:H4'	1:X:399:G:C5	2.52	0.44
1:X:1834:G:H1'	3:A:244:ARG:HH22	1.82	0.44
1:X:956:A:C4	1:X:2427:A:C2	3.06	0.44
9:G:70:PHE:HB2	16:N:64:ARG:HG2	1.98	0.44
1:X:339:U:O4	1:X:343:A:C8	2.70	0.44
1:X:796:A:H4'	1:X:2567:G:H4'	1.99	0.44
10:H:70:VAL:HG21	10:H:98:ILE:HG23	1.98	0.44
18:P:41:VAL:HG22	18:P:60:ILE:HG21	1.99	0.44
3:A:231:HIS:ND1	3:A:247:VAL:HA	2.31	0.44
3:A:42:GLY:H	3:A:43:ARG:NH1	2.15	0.44
5:C:46:ARG:HD2	5:C:51:VAL:HB	1.99	0.44
1:X:1833:U:H2'	1:X:1834:G:C8	2.53	0.44
2:Y:89:G:N2	2:Y:92:G:C8	2.86	0.44
12:J:98:VAL:HG11	12:J:104:MET:HG2	2.00	0.44
1:X:358:C:H6	1:X:358:C:O5'	2.01	0.44
1:X:2056:C:H5'	3:A:229:VAL:HG22	2.00	0.44
4:B:5:LEU:HD22	4:B:49:ILE:HG22	1.99	0.44
4:B:54:LYS:HD3	4:B:59:VAL:HG22	1.99	0.44
1:X:1819:U:OP2	3:A:222:ARG:NH2	2.50	0.44
1:X:819:C:OP2	11:I:41:SER:HA	2.17	0.44
12:J:77:LYS:O	12:J:88:LYS:HD2	2.18	0.44
1:X:2609:G:H2'	1:X:2610:G:C8	2.52	0.44
22:T:40:GLN:HE21	22:T:57:HIS:HB3	1.83	0.44
1:X:1524:C:H3'	1:X:1525:A:H8	1.82	0.44
13:K:76:VAL:HA	13:K:79:VAL:HG12	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:67:PHE:HB3	3:A:153:ALA:N	2.31	0.44
1:X:1223:G:H5''	1:X:1224:A:H3'	2.00	0.44
1:X:2002:A:N1	1:X:2018:G:O6	2.51	0.44
12:J:44:LYS:HB3	12:J:46:ASN:ND2	2.33	0.44
1:X:1725:C:H42	1:X:1741:G:H1	1.64	0.44
1:X:490:A:N3	1:X:492:G:H5''	2.33	0.44
7:E:164:PHE:O	7:E:166:GLY:N	2.51	0.44
3:A:43:ARG:HG3	3:A:54:ILE:O	2.18	0.44
3:A:209:ALA:C	3:A:211:ARG:H	2.21	0.44
18:P:72:LEU:HD12	18:P:126:ILE:HD13	2.00	0.44
12:J:78:LYS:HE2	12:J:81:GLU:HA	2.00	0.44
10:H:24:VAL:HG13	10:H:45:ALA:HB2	1.99	0.44
21:S:3:LEU:HB3	21:S:34:LEU:HB3	1.99	0.44
14:L:8:ARG:CG	14:L:9:ARG:H	2.31	0.44
19:Q:51:ILE:HD11	19:Q:81:ARG:HD3	2.00	0.44
11:I:8:PRO:HB2	11:I:14:LYS:NZ	2.32	0.44
19:Q:39:LYS:HG2	19:Q:43:GLN:HE21	1.83	0.43
1:X:2506:C:H5'	30:4:33:LYS:HD2	2.00	0.43
1:X:2506:C:H5''	30:4:30:VAL:HB	2.00	0.43
1:X:1101:U:H2'	1:X:1102:G:C8	2.53	0.43
5:C:107:ALA:HB1	5:C:180:ILE:HD11	2.00	0.43
3:A:247:VAL:CG2	3:A:248:THR:N	2.81	0.43
1:X:760:U:C6	26:Z:3:LYS:HG3	2.53	0.43
1:X:1333:G:N7	1:X:1342:U:H5'	2.32	0.43
5:C:95:LEU:CD2	5:C:96:PRO:HD2	2.48	0.43
21:S:117:VAL:HG23	21:S:168:VAL:HG13	2.00	0.43
13:K:34:ILE:HG13	13:K:113:ILE:HG23	2.01	0.43
5:C:150:LEU:HA	5:C:187:VAL:HB	2.00	0.43
1:X:2324:G:H5''	1:X:2326:C:O4'	2.18	0.43
9:G:43:VAL:HB	9:G:167:LYS:HG2	1.99	0.43
1:X:1230:C:H2'	1:X:1231:A:H8	1.83	0.43
4:B:134:TRP:CD1	4:B:134:TRP:N	2.76	0.43
11:I:54:SER:HA	11:I:58:ALA:HB3	2.00	0.43
1:X:2551:A:O5'	1:X:2553:G:H4'	2.18	0.43
1:X:114:C:H2'	1:X:115:G:C8	2.53	0.43
3:A:145:LEU:HB3	3:A:155:LEU:HD12	2.00	0.43
6:D:117:ILE:HD13	6:D:130:LEU:HD11	2.00	0.43
3:A:202:LYS:C	3:A:204:ILE:H	2.22	0.43
26:Z:4:HIS:HB3	26:Z:5:PRO:CD	2.45	0.43
1:X:342:G:O3'	1:X:343:A:C8	2.71	0.43
1:X:695:G:N2	1:X:808:C:O2	2.44	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:127:ASP:HB2	5:C:128:ALA:H	1.64	0.43
32:X:2929:1F4:C41	32:X:2929:1F4:C16	2.97	0.43
1:X:1996:A:H5'	18:P:118:LYS:NZ	2.33	0.43
12:J:62:GLY:H	21:S:175:ARG:N	2.16	0.43
1:X:2594:U:H2'	1:X:2595:C:H6	1.83	0.43
5:C:30:VAL:HG11	5:C:177:VAL:HG21	2.00	0.43
2:Y:91:A:H2'	2:Y:92:G:C8	2.54	0.43
1:X:84:G:N3	1:X:101:A:C2	2.86	0.43
1:X:314:G:H2'	1:X:315:G:C8	2.53	0.43
1:X:538:A:H5''	9:G:139:ARG:HE	1.83	0.43
1:X:1577:G:H2'	1:X:1578:U:O4'	2.19	0.43
5:C:133:PHE:HB2	5:C:160:ALA:HB1	2.00	0.43
3:A:245:VAL:N	3:A:252:LYS:HE3	2.34	0.43
1:X:339:U:H4'	20:R:77:HIS:ND1	2.34	0.43
1:X:1782:A:O3'	3:A:206:LEU:HB2	2.18	0.43
5:C:170:LEU:HA	5:C:171:PRO:HD3	1.95	0.43
17:O:69:ILE:HG22	17:O:86:HIS:HB3	2.00	0.43
5:C:74:VAL:O	5:C:77:PHE:HB2	2.18	0.43
1:X:1539:U:H2'	1:X:1540:C:C6	2.54	0.43
30:4:19:ARG:HD2	30:4:24:LEU:HD22	2.01	0.43
1:X:2006:G:H4'	1:X:2596:C:O3'	2.19	0.43
1:X:2277:A:H2'	1:X:2278:A:O4'	2.18	0.43
10:H:22:ILE:HD11	10:H:54:SER:HB2	1.99	0.43
1:X:2066:G:N2	1:X:2216:G:H1'	2.34	0.43
1:X:2170:C:H2'	1:X:2171:U:H4'	2.01	0.43
1:X:1919:A:C2	1:X:1926:U:N3	2.74	0.43
12:J:61:ARG:HD3	21:S:174:PRO:HB2	1.99	0.43
3:A:63:ARG:O	3:A:65:ILE:HD12	2.18	0.43
1:X:2825:A:H2'	1:X:2826:C:C6	2.54	0.43
18:P:25:PHE:C	18:P:25:PHE:CD2	2.90	0.43
1:X:742:G:N1	3:A:208:LYS:HD3	2.33	0.43
3:A:45:ASN:CG	3:A:46:ARG:N	2.72	0.43
10:H:27:SER:OG	10:H:49:ASP:HA	2.19	0.43
1:X:1283:C:H5''	1:X:1284:G:O5'	2.19	0.43
1:X:1148:G:O2'	9:G:134:MET:HG3	2.18	0.43
15:M:22:ARG:HD2	15:M:83:PHE:O	2.19	0.43
10:H:19:ILE:HG22	10:H:55:VAL:HA	2.01	0.43
32:X:2929:1F4:H53	32:X:2929:1F4:H9	2.00	0.43
16:N:66:ASN:HB3	16:N:76:TYR:N	2.27	0.43
1:X:1643:A:H61	1:X:1656:U:H3	1.67	0.43
5:C:148:VAL:O	5:C:167:VAL:HA	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:10:VAL:HG11	10:H:98:ILE:HD12	2.00	0.43
1:X:1469:U:OP1	1:X:1471:G:OP2	2.36	0.43
1:X:205:A:C8	1:X:205:A:H3'	2.54	0.43
13:K:33:ARG:HD3	13:K:112:LEU:HD22	2.01	0.43
1:X:551:A:H2'	1:X:552:C:O4'	2.19	0.43
20:R:24:VAL:HB	20:R:29:HIS:O	2.19	0.43
1:X:2320:G:H2'	1:X:2321:C:O4'	2.19	0.43
4:B:11:MET:HA	4:B:23:VAL:O	2.19	0.43
1:X:504:G:N2	18:P:78:ASN:HD21	2.17	0.43
1:X:1268:U:H5	5:C:68:ARG:HB2	1.84	0.43
1:X:882:C:H2'	1:X:883:A:O4'	2.19	0.43
1:X:1497:C:H5''	1:X:1497:C:H6	1.84	0.43
25:W:27:LYS:O	25:W:30:ASP:HB2	2.19	0.43
2:Y:32:C:H1'	2:Y:59:A:H61	1.84	0.43
2:Y:107:C:H2'	2:Y:108:G:O4'	2.19	0.43
20:R:18:LYS:HD3	20:R:18:LYS:H	1.84	0.43
1:X:487:G:H4'	1:X:512:A:N1	2.34	0.42
1:X:1978:U:H3'	1:X:1979:C:H2'	2.01	0.42
1:X:1373:G:H22	1:X:2192:U:H3	1.67	0.42
3:A:201:HIS:CD2	3:A:204:ILE:HD12	2.54	0.42
5:C:130:THR:HG23	5:C:160:ALA:HA	2.00	0.42
21:S:149:ALA:HB3	21:S:164:PRO:HA	1.99	0.42
7:E:33:LEU:HD13	7:E:136:ILE:HG22	2.01	0.42
9:G:45:ASP:HA	9:G:83:ILE:HG13	2.01	0.42
13:K:90:ARG:HA	13:K:91:PRO:HD3	1.89	0.42
1:X:2235:G:N2	1:X:2254:C:C4	2.87	0.42
25:W:12:ARG:CG	25:W:12:ARG:NH1	2.76	0.42
1:X:322:A:H3'	1:X:323:G:H8	1.83	0.42
26:Z:6:VAL:HG22	26:Z:7:PRO:HD2	2.00	0.42
7:E:6:LYS:H	7:E:65:HIS:HE1	1.66	0.42
1:X:636:G:H8	1:X:636:G:H5''	1.84	0.42
1:X:1337:G:OP2	18:P:105:ARG:NH1	2.52	0.42
1:X:719:A:H2'	1:X:720:A:O4'	2.19	0.42
7:E:126:PRO:HG2	7:E:130:ARG:HH22	1.85	0.42
20:R:93:ARG:HG2	20:R:108:VAL:HA	2.01	0.42
1:X:2011:U:H2'	1:X:2012:A:O4'	2.19	0.42
1:X:812:G:H3'	1:X:813:A:H2'	2.01	0.42
1:X:2024:U:H2'	1:X:2025:A:O4'	2.20	0.42
1:X:2489:C:C4	1:X:2490:U:C5	3.08	0.42
1:X:5:A:H2'	1:X:6:A:C8	2.54	0.42
1:X:2220:A:H2'	1:X:2221:G:C8	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1371:G:H8	1:X:1371:G:O5'	2.02	0.42
18:P:46:ARG:HG3	18:P:95:ALA:HB3	2.01	0.42
1:X:2427:A:HO2'	1:X:2428:U:H5	1.64	0.42
1:X:346:C:O2	1:X:347:C:C5	2.72	0.42
2:Y:108:G:H4'	21:S:26:LYS:HB3	2.02	0.42
1:X:441:A:H3'	1:X:442:A:H8	1.84	0.42
1:X:638:A:C8	11:I:74:VAL:HG11	2.55	0.42
10:H:64:VAL:HG22	10:H:106:ARG:NH1	2.35	0.42
15:M:34:ARG:HH22	15:M:90:GLN:N	2.17	0.42
1:X:1656:U:C2'	1:X:1657:A:H5''	2.50	0.42
14:L:44:ASP:HB2	14:L:51:LEU:HD13	2.01	0.42
2:Y:91:A:H8	2:Y:91:A:OP2	2.03	0.42
1:X:958:G:H2'	1:X:959:C:H6	1.84	0.42
1:X:877:G:H2'	1:X:878:C:C6	2.55	0.42
5:C:117:LEU:HD23	5:C:187:VAL:HG22	2.01	0.42
5:C:122:GLY:C	5:C:124:ASP:H	2.22	0.42
1:X:2200:G:H2'	1:X:2201:G:C8	2.55	0.42
1:X:1332:G:C6	1:X:1333:G:N1	2.88	0.42
3:A:43:ARG:H	3:A:43:ARG:HD2	1.78	0.42
4:B:16:LYS:HB2	4:B:21:ILE:CD1	2.49	0.42
11:I:119:THR:HG23	11:I:139:ARG:HB3	2.02	0.42
1:X:2683:C:H2'	1:X:2684:A:O4'	2.19	0.42
1:X:50:G:H4'	1:X:51:A:H5'	2.02	0.42
1:X:700:C:H2'	1:X:701:U:O4'	2.20	0.42
4:B:131:SER:HB3	4:B:134:TRP:HD1	1.79	0.42
4:B:152:LYS:N	9:G:106:TYR:HB3	2.33	0.42
17:O:12:TYR:HB2	17:O:40:VAL:H	1.84	0.42
1:X:2545:A:H61	10:H:40:GLY:CA	2.32	0.42
1:X:1737:G:H2'	1:X:1738:U:C6	2.55	0.42
2:Y:89:G:H5''	2:Y:90:C:OP2	2.19	0.42
1:X:205:A:H8	1:X:205:A:H3'	1.84	0.42
1:X:810:U:H2'	1:X:811:G:O4'	2.20	0.42
16:N:13:ARG:HA	16:N:16:LYS:HE2	2.02	0.42
1:X:2658:A:H4'	4:B:165:VAL:HG11	2.02	0.42
2:Y:102:A:H2'	2:Y:103:A:C8	2.54	0.42
17:O:88:GLN:HE21	17:O:88:GLN:HA	1.85	0.42
1:X:2241:U:C5	22:T:17:ASN:OD1	2.63	0.42
23:U:22:GLY:HA3	23:U:39:LYS:CD	2.49	0.42
1:X:2528:G:H2'	1:X:2529:G:C8	2.49	0.42
19:Q:62:ARG:O	19:Q:70:GLY:HA3	2.19	0.42
14:L:68:ALA:HB1	14:L:102:ALA:HB3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2352:A:H2'	1:X:2353:G:C8	2.54	0.42
1:X:1381:G:H8	1:X:1381:G:O5'	2.03	0.42
11:I:82:ASP:H	11:I:114:ILE:HG21	1.84	0.42
1:X:2687:G:H2'	1:X:2688:G:H8	1.85	0.42
3:A:173:VAL:HG23	3:A:187:SER:HB3	2.02	0.42
1:X:590:C:H2'	1:X:591:G:C8	2.55	0.42
1:X:1279:G:O2'	1:X:1995:G:O6	2.26	0.42
1:X:631:G:H4'	1:X:632:A:H5'	2.02	0.42
4:B:193:GLY:O	15:M:2:GLN:N	2.53	0.42
23:U:31:GLY:HA2	23:U:32:ARG:HH11	1.85	0.42
5:C:33:TRP:CE3	5:C:95:LEU:HD12	2.54	0.42
1:X:1804:U:H2'	1:X:1805:G:C8	2.54	0.42
9:G:157:PRO:C	9:G:159:SER:H	2.23	0.42
5:C:194:GLU:O	5:C:195:ILE:HG12	2.20	0.42
1:X:1314:A:H2	1:X:1642:G:N3	2.17	0.42
1:X:1100:G:H21	1:X:1113:C:H42	1.67	0.42
1:X:666:U:O2'	1:X:667:U:H5''	2.20	0.42
1:X:1035:G:C8	1:X:1036:G:H2'	2.55	0.42
1:X:1774:A:C6	1:X:2566:A:C2	3.08	0.42
1:X:688:A:N3	1:X:2422:C:O2'	2.46	0.42
1:X:1765:C:O5'	1:X:1765:C:H6	2.03	0.42
1:X:708:G:OP1	1:X:1393:G:O2'	2.37	0.42
1:X:1447:U:HO2'	1:X:1448:A:H8	1.65	0.42
15:M:38:LYS:HB3	15:M:46:ARG:HB3	2.01	0.42
5:C:180:ILE:HG13	5:C:181:LEU:N	2.35	0.42
1:X:1929:U:H2'	1:X:1930:C:C6	2.54	0.42
9:G:170:PRO:HB2	9:G:171:LEU:H	1.75	0.42
13:K:76:VAL:O	13:K:80:MET:HB2	2.20	0.41
9:G:132:PHE:HZ	9:G:142:ARG:HA	1.85	0.41
11:I:28:LYS:HZ1	11:I:36:GLY:HA2	1.83	0.41
1:X:554:U:H4'	1:X:555:U:OP2	2.20	0.41
10:H:132:GLU:HG2	10:H:134:LEU:HG	2.02	0.41
1:X:1167:A:C5	16:N:51:ARG:HD3	2.55	0.41
20:R:29:HIS:CD2	20:R:51:VAL:HG22	2.55	0.41
5:C:94:THR:HG22	5:C:100:ARG:HH12	1.84	0.41
13:K:8:ARG:O	13:K:9:LYS:HB3	2.20	0.41
1:X:1302:C:H2'	1:X:1303:U:H6	1.85	0.41
1:X:149:A:H2'	1:X:150:A:H8	1.84	0.41
32:X:2929:1F4:H18	32:X:2929:1F4:C53	2.50	0.41
1:X:224:G:H4'	1:X:399:G:C4	2.55	0.41
1:X:2796:A:H2'	1:X:2797:G:C8	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:54:G:C2	1:X:114:C:C2	3.08	0.41
1:X:1975:G:N2	1:X:1979:C:O2'	2.52	0.41
1:X:622:U:H2'	1:X:623:G:O4'	2.21	0.41
24:V:32:ALA:HB2	24:V:37:LEU:HG	2.02	0.41
1:X:2053:G:H2'	1:X:2054:A:C8	2.54	0.41
23:U:47:HIS:HB2	23:U:48:LYS:H	1.71	0.41
12:J:6:LYS:O	12:J:71:PRO:HD2	2.20	0.41
1:X:1032:A:C3'	1:X:1032:A:C8	3.03	0.41
1:X:1287:A:H2	1:X:1661:C:O2	2.03	0.41
1:X:1385:C:H2'	1:X:1386:A:O4'	2.20	0.41
1:X:2859:U:N3	26:Z:52:TYR:CE1	2.88	0.41
1:X:692:C:H2'	1:X:693:A:C8	2.55	0.41
1:X:1973:C:H2'	1:X:1974:U:O4'	2.21	0.41
1:X:1249:G:O2'	1:X:1250:A:H8	2.03	0.41
1:X:1266:G:C8	11:I:32:ARG:NH1	2.85	0.41
1:X:649:G:H2'	1:X:650:U:C6	2.55	0.41
1:X:237:G:H1'	1:X:632:A:H1'	2.02	0.41
25:W:4:LYS:HE3	25:W:52:GLU:O	2.20	0.41
1:X:1811:A:H3'	3:A:178:PRO:HB2	2.02	0.41
12:J:64:LYS:HG2	21:S:112:LEU:HD22	2.02	0.41
1:X:960:U:H2'	1:X:961:G:H8	1.82	0.41
1:X:934:G:H1'	22:T:26:PHE:CD1	2.55	0.41
1:X:2209:G:H4'	23:U:46:LEU:HB2	2.02	0.41
11:I:60:LEU:HA	11:I:60:LEU:HD12	1.89	0.41
12:J:6:LYS:HE3	12:J:7:ARG:HE	1.86	0.41
1:X:1687:C:H6	1:X:1687:C:O5'	2.02	0.41
1:X:1224:A:H4'	1:X:1225:G:OP2	2.20	0.41
1:X:1381:G:H2'	1:X:1799:A:H61	1.86	0.41
6:D:75:SER:HB2	6:D:79:LEU:HB2	2.03	0.41
12:J:36:ILE:HG13	12:J:103:VAL:HA	2.03	0.41
1:X:2590:U:O4'	32:X:2929:1F4:H32	2.21	0.41
11:I:28:LYS:HZ3	11:I:36:GLY:HA2	1.86	0.41
23:U:65:ASN:N	23:U:65:ASN:OD1	2.54	0.41
1:X:2556:A:H5''	1:X:2557:G:H5'	2.02	0.41
1:X:2225:G:H2'	1:X:2226:A:H8	1.85	0.41
13:K:96:ARG:O	13:K:113:ILE:HA	2.20	0.41
4:B:104:ALA:HB3	4:B:170:LEU:HD12	2.02	0.41
1:X:1792:C:N4	1:X:2185:U:H5'	2.36	0.41
3:A:213:ARG:HD2	3:A:213:ARG:HA	1.97	0.41
5:C:171:PRO:O	5:C:173:ALA:N	2.54	0.41
1:X:1117:G:H2'	1:X:1118:G:C8	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:34:ARG:NH1	15:M:91:VAL:HB	2.36	0.41
1:X:2519:C:O2'	1:X:2720:A:N3	2.44	0.41
1:X:2633:A:N1	1:X:2644:A:H5''	2.35	0.41
1:X:946:U:H2'	1:X:947:C:C6	2.56	0.41
9:G:62:ILE:HG23	9:G:135:LEU:HD21	2.02	0.41
1:X:1:G:H2'	1:X:1:G:N3	2.36	0.41
21:S:141:MET:SD	21:S:147:ILE:HG12	2.61	0.41
1:X:654:A:C2	1:X:655:A:H3'	2.56	0.41
9:G:53:ARG:HH22	9:G:171:LEU:HD12	1.85	0.41
1:X:2395:C:H2'	1:X:2396:C:H5''	2.02	0.41
12:J:14:PHE:CE1	12:J:90:ALA:HB2	2.56	0.41
1:X:1132:C:H6	1:X:1132:C:O5'	2.03	0.41
14:L:31:VAL:HG23	14:L:38:ILE:HD11	2.01	0.41
1:X:322:A:H3'	1:X:323:G:C8	2.55	0.41
20:R:22:VAL:HG22	20:R:83:LEU:H	1.85	0.41
12:J:27:TYR:HB2	12:J:137:VAL:HG21	2.02	0.41
21:S:107:GLU:HG3	21:S:112:LEU:HA	2.02	0.41
23:U:14:VAL:HB	23:U:15:VAL:H	1.75	0.41
1:X:762:A:H4'	1:X:1284:G:N3	2.36	0.41
16:N:68:GLY:HA2	16:N:71:LEU:HD23	2.02	0.41
4:B:105:THR:HB	4:B:166:THR:HG23	2.03	0.41
7:E:24:PHE:HB2	7:E:37:TYR:HD1	1.85	0.41
1:X:1009:C:H2'	1:X:1010:U:O4'	2.21	0.41
1:X:494:A:C8	20:R:56:LYS:HD2	2.56	0.41
1:X:1106:A:H2'	1:X:1107:A:H8	1.86	0.41
4:B:55:ALA:HB3	4:B:58:LYS:HD2	2.01	0.41
1:X:95:G:H4'	24:V:41:HIS:ND1	2.35	0.41
1:X:1494:G:HO2'	1:X:1574:A:H2	1.66	0.41
1:X:657:A:H3'	1:X:657:A:C8	2.56	0.41
1:X:1467:U:H3'	1:X:1467:U:H6	1.85	0.41
5:C:176:ASN:ND2	5:C:179:ASP:H	2.16	0.41
1:X:188:G:H2'	1:X:189:A:C8	2.56	0.41
1:X:1469:U:H5'	1:X:1470:G:N7	2.36	0.41
1:X:98:U:H1'	1:X:100:G:C4	2.56	0.41
1:X:1533:G:H2'	1:X:1534:A:H8	1.86	0.41
17:O:19:VAL:HG13	17:O:90:PHE:CD1	2.56	0.41
14:L:76:ALA:HB2	14:L:107:ALA:HA	2.02	0.41
1:X:874:A:H2'	1:X:875:G:O4'	2.21	0.41
1:X:2357:A:H1'	14:L:88:VAL:HG11	2.02	0.41
22:T:38:VAL:CG1	22:T:59:LEU:HD12	2.50	0.41
1:X:1615:C:OP2	19:Q:35:LYS:HD2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:956:A:C5	1:X:2427:A:C2	3.09	0.40
5:C:30:VAL:HA	5:C:95:LEU:HD11	2.02	0.40
1:X:99:U:H5''	1:X:100:G:C8	2.57	0.40
16:N:88:ILE:HG13	17:O:49:GLU:HB2	2.03	0.40
24:V:2:LYS:H	24:V:3:PRO:CD	2.33	0.40
1:X:1835:C:H2'	1:X:1836:C:C6	2.56	0.40
1:X:2526:U:H2'	1:X:2527:G:C8	2.57	0.40
28:2:14:LYS:CA	28:2:15:THR:CA	2.98	0.40
18:P:19:LYS:HB3	18:P:19:LYS:HE2	1.76	0.40
1:X:2796:A:OP2	13:K:5:LYS:NZ	2.55	0.40
22:T:41:ARG:HA	22:T:41:ARG:NE	2.34	0.40
1:X:957:G:H2'	1:X:958:G:H8	1.86	0.40
3:A:147:LEU:HD22	3:A:183:ARG:NH2	2.35	0.40
1:X:1835:C:O2'	3:A:254:THR:HB	2.21	0.40
19:Q:56:MET:SD	19:Q:57:ASN:N	2.91	0.40
21:S:53:ASP:HA	21:S:63:PRO:HA	2.03	0.40
23:U:43:ARG:HH21	23:U:43:ARG:HB2	1.85	0.40
1:X:1248:G:O5'	1:X:1248:G:H8	2.04	0.40
32:X:2929:1F4:O46	32:X:2929:1F4:H7	2.22	0.40
1:X:649:G:N2	1:X:660:G:N2	2.69	0.40
1:X:651:C:H2'	1:X:652:C:H6	1.86	0.40
12:J:70:PHE:HA	12:J:71:PRO:HD3	1.95	0.40
2:Y:22:U:H3	2:Y:65:A:H61	1.68	0.40
3:A:202:LYS:C	3:A:204:ILE:N	2.75	0.40
23:U:20:ARG:HB2	23:U:43:ARG:HD2	2.02	0.40
3:A:166:GLN:HB2	3:A:174:ILE:HG22	2.03	0.40
26:Z:36:CYS:HB3	26:Z:49:CYS:HB3	1.94	0.40
1:X:2419:C:N3	1:X:2420:C:H1'	2.37	0.40
1:X:2064:U:H2'	1:X:2065:A:C8	2.56	0.40
26:Z:42:SER:O	26:Z:44:HIS:HD2	2.03	0.40
16:N:42:ALA:O	16:N:46:GLU:N	2.51	0.40
1:X:1796:A:N3	3:A:50:THR:HG23	2.36	0.40
1:X:877:G:H2'	1:X:878:C:H6	1.86	0.40
1:X:1519:G:H2'	1:X:1520:G:H8	1.86	0.40
21:S:36:ARG:O	21:S:40:ASP:HB2	2.22	0.40
1:X:506:G:H4'	18:P:21:ARG:HH21	1.85	0.40
1:X:1467:U:H5''	1:X:1467:U:C6	2.57	0.40
1:X:2042:A:O3'	5:C:63:GLY:HA2	2.21	0.40
9:G:103:TYR:HB3	9:G:107:GLN:HE21	1.85	0.40
17:O:10:LYS:HE3	17:O:11:GLN:HG2	2.03	0.40
1:X:1255:A:H2'	1:X:1256:C:H6	1.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2422:C:H2'	1:X:2423:G:C8	2.56	0.40
16:N:95:LEU:HA	16:N:98:ILE:HD12	2.04	0.40
4:B:181:LEU:HD21	15:M:12:LEU:CD2	2.51	0.40
7:E:140:LEU:O	7:E:144:VAL:HG23	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	238/274 (87%)	173 (73%)	47 (20%)	18 (8%)	1	17
4	B	203/211 (96%)	173 (85%)	25 (12%)	5 (2%)	7	48
5	C	195/205 (95%)	127 (65%)	40 (20%)	28 (14%)	0	5
6	D	175/180 (97%)	142 (81%)	26 (15%)	7 (4%)	4	35
7	E	169/185 (91%)	134 (79%)	26 (15%)	9 (5%)	2	27
8	F	69/144 (48%)	57 (83%)	9 (13%)	3 (4%)	3	33
9	G	140/174 (80%)	99 (71%)	26 (19%)	15 (11%)	0	10
10	H	132/134 (98%)	117 (89%)	12 (9%)	3 (2%)	8	50
11	I	139/156 (89%)	81 (58%)	39 (28%)	19 (14%)	0	6
12	J	134/141 (95%)	98 (73%)	24 (18%)	12 (9%)	1	13
13	K	111/116 (96%)	92 (83%)	13 (12%)	6 (5%)	2	27
14	L	102/114 (90%)	75 (74%)	15 (15%)	12 (12%)	0	8
15	M	106/166 (64%)	90 (85%)	10 (9%)	6 (6%)	2	25
16	N	115/118 (98%)	91 (79%)	17 (15%)	7 (6%)	2	24
17	O	92/100 (92%)	66 (72%)	13 (14%)	13 (14%)	0	5
18	P	125/134 (93%)	104 (83%)	17 (14%)	4 (3%)	5	42

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	Q	91/95 (96%)	63 (69%)	16 (18%)	12 (13%)	0	6
20	R	108/115 (94%)	65 (60%)	26 (24%)	17 (16%)	0	4
21	S	173/237 (73%)	135 (78%)	27 (16%)	11 (6%)	2	23
22	T	82/91 (90%)	65 (79%)	12 (15%)	5 (6%)	2	24
23	U	70/81 (86%)	41 (59%)	15 (21%)	14 (20%)	0	2
24	V	64/67 (96%)	57 (89%)	5 (8%)	2 (3%)	5	43
25	W	53/55 (96%)	47 (89%)	5 (9%)	1 (2%)	10	53
26	Z	56/60 (93%)	45 (80%)	6 (11%)	5 (9%)	1	13
30	4	35/37 (95%)	23 (66%)	11 (31%)	1 (3%)	6	44
All	All	2977/3390 (88%)	2260 (76%)	482 (16%)	235 (8%)	1	16

All (235) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	45	ASN
3	A	209	ALA
3	A	217	ARG
3	A	248	THR
3	A	249	PRO
3	A	250	TRP
3	A	271	VAL
5	C	4	ILE
5	C	20	PRO
5	C	60	GLY
5	C	66	ASN
5	C	129	LYS
5	C	164	VAL
5	C	165	SER
5	C	172	VAL
5	C	195	ILE
6	D	10	ASP
6	D	81	GLN
6	D	122	PHE
7	E	165	VAL
9	G	33	ILE
9	G	67	ARG
9	G	92	GLY
9	G	97	ASP
9	G	104	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	G	170	PRO
10	H	27	SER
11	I	18	ARG
11	I	47	ALA
11	I	49	PHE
11	I	64	GLY
11	I	98	LEU
11	I	99	VAL
11	I	103	ASN
12	J	80	ALA
12	J	82	THR
12	J	88	LYS
13	K	6	ALA
13	K	92	GLY
14	L	21	THR
14	L	61	SER
14	L	68	ALA
14	L	95	LYS
15	M	29	PRO
16	N	8	ILE
16	N	95	LEU
17	O	7	THR
17	O	10	LYS
17	O	22	VAL
17	O	48	GLY
19	Q	6	ILE
19	Q	61	LYS
19	Q	63	LYS
19	Q	67	ARG
19	Q	69	ILE
20	R	11	ASN
20	R	15	HIS
20	R	60	PRO
20	R	82	ALA
20	R	107	ALA
21	S	6	LYS
21	S	26	LYS
21	S	56	VAL
21	S	91	PRO
21	S	156	GLU
22	T	19	LYS
23	U	15	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	U	19	ILE
23	U	32	ARG
23	U	34	THR
23	U	56	GLN
23	U	60	VAL
26	Z	4	HIS
26	Z	36	CYS
26	Z	53	ASP
3	A	35	GLU
3	A	58	HIS
3	A	220	HIS
4	B	132	LYS
5	C	22	VAL
5	C	83	ALA
5	C	121	ASP
5	C	190	ALA
5	C	196	VAL
6	D	124	GLY
7	E	59	GLN
7	E	173	ALA
9	G	37	ASP
9	G	105	GLY
9	G	107	GLN
9	G	158	HIS
10	H	5	GLN
10	H	29	ILE
11	I	36	GLY
11	I	54	SER
11	I	62	LYS
11	I	68	VAL
12	J	11	ARG
12	J	83	ARG
12	J	87	GLY
12	J	91	VAL
13	K	4	GLY
13	K	9	LYS
14	L	31	VAL
14	L	40	ALA
14	L	94	TYR
15	M	26	ASP
15	M	31	ASP
15	M	39	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	M	57	ILE
16	N	7	GLY
16	N	87	ASN
17	O	8	GLY
17	O	9	GLY
17	O	14	VAL
18	P	9	ARG
18	P	85	MET
19	Q	12	ILE
19	Q	84	GLU
20	R	85	ASP
20	R	98	ILE
22	T	11	LYS
23	U	29	GLY
23	U	41	VAL
23	U	76	LYS
24	V	2	LYS
24	V	36	GLN
30	4	3	VAL
3	A	254	THR
3	A	269	PHE
4	B	129	HIS
4	B	146	THR
5	C	9	GLN
5	C	10	ASN
5	C	15	ILE
5	C	67	ALA
5	C	113	GLU
5	C	114	GLY
5	C	163	ASN
5	C	189	ASP
6	D	71	LYS
6	D	119	PRO
9	G	34	PRO
11	I	91	ASP
12	J	81	GLU
14	L	33	ARG
14	L	52	ALA
15	M	74	GLY
16	N	92	ARG
16	N	94	VAL
17	O	11	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	O	49	GLU
18	P	132	GLY
19	Q	62	ARG
19	Q	74	ASP
19	Q	89	GLU
20	R	14	LEU
20	R	83	LEU
20	R	87	GLU
20	R	96	LYS
21	S	88	TYR
21	S	128	ARG
22	T	74	LYS
23	U	27	ASP
26	Z	24	ALA
26	Z	37	HIS
3	A	54	ILE
3	A	55	GLY
5	C	13	ARG
5	C	18	PRO
5	C	194	GLU
6	D	40	LEU
7	E	19	ALA
7	E	65	HIS
8	F	118	GLY
9	G	159	SER
11	I	59	ARG
11	I	65	PHE
11	I	90	ARG
12	J	17	ARG
12	J	29	ALA
13	K	95	THR
14	L	60	LYS
17	O	31	ASP
17	O	36	LYS
17	O	78	VAL
19	Q	87	SER
20	R	63	THR
21	S	33	ALA
21	S	74	ARG
22	T	13	GLY
22	T	27	GLY
3	A	247	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	255	LYS
4	B	90	SER
5	C	55	GLY
5	C	68	ARG
7	E	7	GLN
7	E	55	PRO
7	E	92	VAL
11	I	37	GLN
11	I	115	SER
12	J	21	ASP
14	L	53	ALA
17	O	30	GLY
20	R	6	ALA
20	R	108	VAL
23	U	26	ALA
23	U	47	HIS
25	W	14	GLY
3	A	187	SER
4	B	137	ARG
5	C	126	ALA
9	G	165	VAL
11	I	86	THR
13	K	93	GLY
14	L	39	TYR
16	N	65	ILE
18	P	20	LEU
20	R	50	GLY
21	S	125	PRO
23	U	12	ASN
9	G	68	PRO
12	J	28	VAL
20	R	51	VAL
7	E	126	PRO
8	F	96	VAL
11	I	9	THR
21	S	174	PRO
8	F	120	VAL
20	R	111	GLY
3	A	270	ILE
9	G	138	GLY
19	Q	66	GLY
23	U	14	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	185/215 (86%)	145 (78%)	40 (22%)	1	9
4	B	155/157 (99%)	119 (77%)	36 (23%)	1	7
5	C	157/163 (96%)	112 (71%)	45 (29%)	0	4
6	D	153/156 (98%)	130 (85%)	23 (15%)	3	25
7	E	136/144 (94%)	115 (85%)	21 (15%)	3	23
8	F	51/107 (48%)	49 (96%)	2 (4%)	39	77
9	G	118/146 (81%)	94 (80%)	24 (20%)	1	11
10	H	103/103 (100%)	80 (78%)	23 (22%)	1	8
11	I	108/121 (89%)	79 (73%)	29 (27%)	0	4
12	J	110/115 (96%)	89 (81%)	21 (19%)	2	12
13	K	90/93 (97%)	76 (84%)	14 (16%)	3	23
14	L	74/82 (90%)	51 (69%)	23 (31%)	0	3
15	M	94/134 (70%)	71 (76%)	23 (24%)	1	6
16	N	96/97 (99%)	76 (79%)	20 (21%)	1	10
17	O	75/79 (95%)	56 (75%)	19 (25%)	1	6
18	P	109/115 (95%)	91 (84%)	18 (16%)	3	19
19	Q	75/76 (99%)	60 (80%)	15 (20%)	1	11
20	R	91/96 (95%)	75 (82%)	16 (18%)	2	16
21	S	149/192 (78%)	117 (78%)	32 (22%)	1	9
22	T	62/67 (92%)	53 (86%)	9 (14%)	4	26
23	U	57/66 (86%)	33 (58%)	24 (42%)	0	1
24	V	54/55 (98%)	43 (80%)	11 (20%)	1	11
25	W	48/48 (100%)	37 (77%)	11 (23%)	1	8
26	Z	51/53 (96%)	41 (80%)	10 (20%)	1	12
30	4	35/35 (100%)	29 (83%)	6 (17%)	2	18
All	All	2436/2715 (90%)	1921 (79%)	515 (21%)	1	10

All (515) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	37	LEU
3	A	39	LYS
3	A	40	THR
3	A	43	ARG
3	A	46	ARG
3	A	48	ARG
3	A	49	ILE
3	A	52	ARG
3	A	63	ARG
3	A	68	LYS
3	A	69	ARG
3	A	88	ARG
3	A	96	HIS
3	A	105	ILE
3	A	111	LEU
3	A	118	ASN
3	A	131	LEU
3	A	145	LEU
3	A	157	ARG
3	A	162	SER
3	A	169	GLU
3	A	183	ARG
3	A	186	HIS
3	A	196	VAL
3	A	203	ASN
3	A	208	LYS
3	A	212	SER
3	A	218	LYS
3	A	222	ARG
3	A	226	MET
3	A	240	THR
3	A	244	ARG
3	A	245	VAL
3	A	247	VAL
3	A	248	THR
3	A	250	TRP
3	A	252	LYS
3	A	254	THR
3	A	259	THR
3	A	270	ILE
4	B	2	LYS
4	B	4	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	B	5	LEU
4	B	14	ILE
4	B	27	LEU
4	B	34	VAL
4	B	35	GLN
4	B	37	LYS
4	B	41	THR
4	B	49	ILE
4	B	69	LYS
4	B	72	VAL
4	B	75	THR
4	B	103	ASP
4	B	107	THR
4	B	113	THR
4	B	119	ARG
4	B	131	SER
4	B	133	LYS
4	B	134	TRP
4	B	136	ARG
4	B	137	ARG
4	B	140	SER
4	B	141	ILE
4	B	145	LYS
4	B	149	ARG
4	B	150	VAL
4	B	152	LYS
4	B	154	LYS
4	B	162	MET
4	B	163	GLU
4	B	165	VAL
4	B	192	ASN
4	B	198	LEU
4	B	200	SER
4	B	203	LYS
5	C	3	GLN
5	C	7	ILE
5	C	10	ASN
5	C	13	ARG
5	C	14	THR
5	C	15	ILE
5	C	45	THR
5	C	48	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	C	51	VAL
5	C	52	SER
5	C	53	LYS
5	C	59	TYR
5	C	64	THR
5	C	66	ASN
5	C	71	ASP
5	C	72	ARG
5	C	76	THR
5	C	89	ARG
5	C	91	TYR
5	C	94	THR
5	C	95	LEU
5	C	97	ARG
5	C	118	VAL
5	C	121	ASP
5	C	123	PHE
5	C	124	ASP
5	C	127	ASP
5	C	130	THR
5	C	134	ILE
5	C	136	TRP
5	C	138	LYS
5	C	140	ASN
5	C	143	ASP
5	C	148	VAL
5	C	151	VAL
5	C	153	ASP
5	C	154	ASP
5	C	162	ARG
5	C	164	VAL
5	C	166	TRP
5	C	175	VAL
5	C	180	ILE
5	C	181	LEU
5	C	188	ILE
5	C	194	GLU
6	D	11	GLN
6	D	33	LYS
6	D	40	LEU
6	D	45	GLU
6	D	57	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	D	60	ILE
6	D	63	GLN
6	D	67	ILE
6	D	71	LYS
6	D	80	ARG
6	D	89	VAL
6	D	95	ARG
6	D	112	ARG
6	D	115	ARG
6	D	125	ARG
6	D	130	LEU
6	D	134	GLU
6	D	136	LEU
6	D	148	LYS
6	D	150	ARG
6	D	153	ASP
6	D	171	GLN
6	D	175	LEU
7	E	15	VAL
7	E	21	ASP
7	E	35	VAL
7	E	40	GLU
7	E	44	ARG
7	E	50	LEU
7	E	59	GLN
7	E	67	LEU
7	E	69	ARG
7	E	72	VAL
7	E	81	ASP
7	E	86	ASN
7	E	97	LYS
7	E	98	LEU
7	E	121	VAL
7	E	130	ARG
7	E	133	VAL
7	E	139	GLN
7	E	140	LEU
7	E	141	VAL
7	E	155	ASP
8	F	78	ILE
8	F	101	TRP
9	G	31	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	G	38	GLU
9	G	41	TRP
9	G	56	THR
9	G	61	ARG
9	G	62	ILE
9	G	63	ARG
9	G	70	PHE
9	G	75	ILE
9	G	91	THR
9	G	95	LEU
9	G	101	THR
9	G	102	ARG
9	G	104	THR
9	G	112	THR
9	G	113	GLU
9	G	116	ARG
9	G	122	HIS
9	G	132	PHE
9	G	137	LYS
9	G	145	HIS
9	G	154	GLU
9	G	165	VAL
9	G	168	THR
10	H	1	MET
10	H	7	ARG
10	H	9	ASP
10	H	10	VAL
10	H	23	ARG
10	H	29	ILE
10	H	41	ASN
10	H	57	ASP
10	H	83	ARG
10	H	85	ASP
10	H	88	THR
10	H	89	ILE
10	H	90	ARG
10	H	94	ASN
10	H	102	GLN
10	H	106	ARG
10	H	109	ARG
10	H	116	ARG
10	H	117	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	H	119	ARG
10	H	124	MET
10	H	126	ILE
10	H	127	VAL
11	I	4	HIS
11	I	6	LEU
11	I	13	ARG
11	I	18	ARG
11	I	21	ARG
11	I	26	THR
11	I	29	THR
11	I	32	ARG
11	I	39	SER
11	I	40	ARG
11	I	45	LYS
11	I	50	GLU
11	I	53	ARG
11	I	56	LEU
11	I	57	ILE
11	I	60	LEU
11	I	62	LYS
11	I	65	PHE
11	I	77	LEU
11	I	78	SER
11	I	83	LEU
11	I	85	ASP
11	I	86	THR
11	I	93	LEU
11	I	98	LEU
11	I	99	VAL
11	I	101	ARG
11	I	108	LEU
11	I	142	LEU
12	J	7	ARG
12	J	8	THR
12	J	11	ARG
12	J	17	ARG
12	J	32	ASP
12	J	43	ILE
12	J	44	LYS
12	J	52	ARG
12	J	54	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	J	64	LYS
12	J	73	LYS
12	J	81	GLU
12	J	93	TYR
12	J	94	TRP
12	J	95	VAL
12	J	120	ARG
12	J	126	LEU
12	J	129	GLN
12	J	131	LYS
12	J	134	LYS
12	J	140	GLU
13	K	8	ARG
13	K	10	LEU
13	K	11	ASN
13	K	12	ARG
13	K	17	ARG
13	K	28	LEU
13	K	51	LEU
13	K	60	LEU
13	K	73	LYS
13	K	83	VAL
13	K	94	TYR
13	K	99	ARG
13	K	109	THR
13	K	115	LEU
14	L	8	ARG
14	L	11	LEU
14	L	12	ARG
14	L	13	THR
14	L	15	ARG
14	L	18	ARG
14	L	31	VAL
14	L	33	ARG
14	L	36	LYS
14	L	37	HIS
14	L	43	ILE
14	L	64	LYS
14	L	66	ASP
14	L	67	THR
14	L	87	VAL
14	L	88	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	L	89	PHE
14	L	90	ASP
14	L	91	ARG
14	L	93	SER
14	L	94	TYR
14	L	99	ARG
14	L	108	ARG
15	M	5	ILE
15	M	6	LYS
15	M	7	ILE
15	M	12	LEU
15	M	13	LEU
15	M	14	ARG
15	M	31	ASP
15	M	34	ARG
15	M	35	VAL
15	M	40	ARG
15	M	54	VAL
15	M	57	ILE
15	M	63	ARG
15	M	68	VAL
15	M	69	ARG
15	M	78	GLU
15	M	79	ARG
15	M	89	ASN
15	M	93	ILE
15	M	95	GLU
15	M	98	LYS
15	M	99	VAL
15	M	100	ARG
16	N	3	ARG
16	N	5	LYS
16	N	8	ILE
16	N	9	VAL
16	N	13	ARG
16	N	18	LEU
16	N	22	LYS
16	N	25	TRP
16	N	40	LEU
16	N	51	ARG
16	N	58	ARG
16	N	60	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	N	71	LEU
16	N	88	ILE
16	N	90	LEU
16	N	92	ARG
16	N	93	LYS
16	N	95	LEU
16	N	102	GLU
16	N	111	ASP
17	O	13	ARG
17	O	18	ASP
17	O	20	ILE
17	O	21	ARG
17	O	22	VAL
17	O	25	LEU
17	O	26	GLN
17	O	28	GLU
17	O	39	PHE
17	O	40	VAL
17	O	46	VAL
17	O	47	PHE
17	O	50	ASP
17	O	56	VAL
17	O	62	GLU
17	O	69	ILE
17	O	76	SER
17	O	78	VAL
17	O	88	GLN
18	P	9	ARG
18	P	11	LYS
18	P	32	ARG
18	P	60	ILE
18	P	62	ARG
18	P	71	VAL
18	P	72	LEU
18	P	84	GLU
18	P	86	LEU
18	P	87	GLU
18	P	91	PHE
18	P	109	ARG
18	P	111	ARG
18	P	113	SER
18	P	118	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	P	124	ILE
18	P	125	THR
18	P	126	ILE
19	Q	7	LEU
19	Q	12	ILE
19	Q	14	GLU
19	Q	26	SER
19	Q	38	ILE
19	Q	40	ASP
19	Q	42	ILE
19	Q	56	MET
19	Q	58	VAL
19	Q	63	LYS
19	Q	65	VAL
19	Q	67	ARG
19	Q	81	ARG
19	Q	82	LEU
19	Q	84	GLU
20	R	13	LYS
20	R	18	LYS
20	R	23	ILE
20	R	25	LEU
20	R	26	SER
20	R	80	LYS
20	R	81	VAL
20	R	87	GLU
20	R	88	THR
20	R	98	ILE
20	R	104	VAL
20	R	105	ARG
20	R	106	VAL
20	R	108	VAL
20	R	112	LYS
20	R	113	THR
21	S	2	GLU
21	S	13	LYS
21	S	14	LEU
21	S	15	ASP
21	S	22	VAL
21	S	24	TYR
21	S	26	LYS
21	S	41	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	S	46	GLN
21	S	48	THR
21	S	51	LEU
21	S	53	ASP
21	S	54	ILE
21	S	65	LEU
21	S	66	VAL
21	S	67	LYS
21	S	71	MET
21	S	76	ARG
21	S	79	ILE
21	S	94	VAL
21	S	95	SER
21	S	113	VAL
21	S	120	LEU
21	S	128	ARG
21	S	132	GLN
21	S	133	GLU
21	S	139	THR
21	S	152	ILE
21	S	155	PRO
21	S	160	LEU
21	S	163	ASP
21	S	166	LEU
22	T	5	LYS
22	T	16	SER
22	T	17	ASN
22	T	41	ARG
22	T	46	LYS
22	T	49	GLN
22	T	62	LEU
22	T	64	ASP
22	T	85	GLN
23	U	8	THR
23	U	11	LYS
23	U	13	LEU
23	U	14	VAL
23	U	17	SER
23	U	19	ILE
23	U	20	ARG
23	U	23	LYS
23	U	32	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	U	37	ILE
23	U	40	ARG
23	U	42	GLN
23	U	43	ARG
23	U	45	ASN
23	U	47	HIS
23	U	52	ARG
23	U	57	VAL
23	U	62	LEU
23	U	63	SER
23	U	65	ASN
23	U	70	LEU
23	U	75	TYR
23	U	78	ILE
23	U	79	GLU
24	V	6	MET
24	V	7	ARG
24	V	13	ASP
24	V	14	PHE
24	V	21	ARG
24	V	25	LEU
24	V	28	LEU
24	V	41	HIS
24	V	53	LEU
24	V	60	LEU
24	V	65	GLU
25	W	4	LYS
25	W	6	VAL
25	W	9	VAL
25	W	10	ILE
25	W	12	ARG
25	W	26	ARG
25	W	32	ARG
25	W	34	VAL
25	W	36	ASP
25	W	37	THR
25	W	46	THR
26	Z	3	LYS
26	Z	4	HIS
26	Z	6	VAL
26	Z	8	LYS
26	Z	14	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	Z	18	MET
26	Z	25	LEU
26	Z	35	GLN
26	Z	40	LYS
26	Z	57	VAL
30	4	2	LYS
30	4	9	LYS
30	4	14	CYS
30	4	17	VAL
30	4	25	VAL
30	4	30	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	76	ASN
3	A	118	ASN
3	A	201	HIS
3	A	231	HIS
4	B	129	HIS
4	B	180	ASN
5	C	61	GLN
5	C	66	ASN
5	C	98	GLN
5	C	140	ASN
5	C	176	ASN
6	D	63	GLN
6	D	129	ASN
7	E	18	ASN
7	E	59	GLN
7	E	65	HIS
7	E	86	ASN
9	G	73	ASN
9	G	76	GLN
10	H	41	ASN
11	I	34	HIS
11	I	37	GLN
12	J	46	ASN
12	J	129	GLN
13	K	13	ASN
14	L	41	GLN
14	L	49	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	M	58	ASN
15	M	90	GLN
16	N	31	GLN
16	N	66	ASN
16	N	75	ASN
17	O	6	GLN
17	O	11	GLN
17	O	79	GLN
17	O	88	GLN
18	P	78	ASN
18	P	81	HIS
18	P	115	ASN
19	Q	43	GLN
19	Q	44	GLN
19	Q	57	ASN
20	R	10	HIS
20	R	15	HIS
20	R	29	HIS
20	R	44	GLN
20	R	64	ASN
20	R	71	GLN
21	S	80	HIS
21	S	119	ASN
22	T	3	HIS
22	T	17	ASN
22	T	35	ASN
22	T	49	GLN
22	T	71	ASN
23	U	56	GLN
25	W	54	GLN
26	Z	23	HIS
26	Z	43	HIS
26	Z	44	HIS
26	Z	48	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2683/2880 (93%)	701 (26%)	250 (9%)
2	Y	121/123 (98%)	41 (33%)	12 (9%)
All	All	2804/3003 (93%)	742 (26%)	262 (9%)

All (742) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	2	G
1	X	7	G
1	X	13	A
1	X	14	A
1	X	15	G
1	X	23	G
1	X	34	U
1	X	45	C
1	X	48	A
1	X	49	U
1	X	50	G
1	X	54	G
1	X	62	U
1	X	63	A
1	X	69	G
1	X	70	A
1	X	71	A
1	X	72	A
1	X	73	A
1	X	74	G
1	X	82	G
1	X	83	A
1	X	84	G
1	X	89	A
1	X	90	G
1	X	91	A
1	X	97	U
1	X	99	U
1	X	100	G
1	X	101	A
1	X	107	G
1	X	108	G
1	X	111	G
1	X	112	U
1	X	116	A
1	X	117	A
1	X	118	U
1	X	123	A
1	X	127	C
1	X	129	A
1	X	136	A
1	X	137	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	138	G
1	X	143	A
1	X	147	G
1	X	154	U
1	X	157	G
1	X	158	A
1	X	173	A
1	X	174	A
1	X	176	A
1	X	177	U
1	X	181	A
1	X	182	G
1	X	191	G
1	X	192	G
1	X	193	A
1	X	199	A
1	X	203	G
1	X	205	A
1	X	206	U
1	X	207	U
1	X	209	G
1	X	219	G
1	X	225	G
1	X	227	G
1	X	228	A
1	X	229	G
1	X	238	G
1	X	239	A
1	X	241	C
1	X	242	A
1	X	243	G
1	X	245	C
1	X	246	C
1	X	248	A
1	X	310	A
1	X	312	G
1	X	319	G
1	X	321	A
1	X	322	A
1	X	323	G
1	X	332	C
1	X	333	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	334	G
1	X	335	A
1	X	338	G
1	X	340	G
1	X	342	G
1	X	343	A
1	X	349	G
1	X	358	C
1	X	360	A
1	X	361	G
1	X	388	G
1	X	396	U
1	X	397	U
1	X	399	G
1	X	400	U
1	X	409	G
1	X	411	C
1	X	414	A
1	X	416	U
1	X	417	C
1	X	418	C
1	X	419	G
1	X	424	G
1	X	425	A
1	X	433	G
1	X	441	A
1	X	455	A
1	X	456	C
1	X	458	G
1	X	459	A
1	X	461	A
1	X	463	C
1	X	467	U
1	X	468	A
1	X	469	G
1	X	470	U
1	X	484	G
1	X	490	A
1	X	492	G
1	X	495	C
1	X	504	G
1	X	506	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	513	A
1	X	514	G
1	X	515	A
1	X	518	A
1	X	519	C
1	X	520	C
1	X	522	G
1	X	523	A
1	X	534	U
1	X	539	A
1	X	540	G
1	X	541	C
1	X	542	A
1	X	543	G
1	X	554	U
1	X	555	U
1	X	557	U
1	X	558	G
1	X	559	C
1	X	560	G
1	X	572	G
1	X	580	A
1	X	581	A
1	X	582	G
1	X	583	C
1	X	584	A
1	X	595	A
1	X	596	C
1	X	597	U
1	X	601	A
1	X	602	C
1	X	613	A
1	X	614	G
1	X	623	G
1	X	625	A
1	X	627	A
1	X	631	G
1	X	632	A
1	X	633	G
1	X	636	G
1	X	645	G
1	X	648	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	649	G
1	X	652	C
1	X	654	A
1	X	655	A
1	X	657	A
1	X	658	G
1	X	664	C
1	X	665	A
1	X	667	U
1	X	668	A
1	X	677	G
1	X	681	A
1	X	683	A
1	X	684	C
1	X	690	A
1	X	695	G
1	X	697	G
1	X	699	G
1	X	700	C
1	X	703	A
1	X	717	G
1	X	723	C
1	X	725	C
1	X	727	U
1	X	728	G
1	X	729	A
1	X	730	C
1	X	731	A
1	X	732	G
1	X	739	G
1	X	742	G
1	X	743	A
1	X	751	G
1	X	753	U
1	X	754	G
1	X	760	U
1	X	777	A
1	X	778	G
1	X	788	G
1	X	789	G
1	X	790	A
1	X	795	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	797	A
1	X	798	G
1	X	801	A
1	X	802	A
1	X	803	C
1	X	804	C
1	X	805	G
1	X	806	A
1	X	807	A
1	X	814	G
1	X	815	A
1	X	816	U
1	X	818	G
1	X	824	U
1	X	825	C
1	X	832	A
1	X	840	U
1	X	841	G
1	X	842	A
1	X	843	G
1	X	859	U
1	X	860	U
1	X	872	G
1	X	879	A
1	X	883	A
1	X	886	A
1	X	891	A
1	X	919	U
1	X	922	A
1	X	926	C
1	X	931	G
1	X	938	G
1	X	939	C
1	X	940	G
1	X	941	U
1	X	943	U
1	X	944	A
1	X	952	A
1	X	956	A
1	X	957	G
1	X	967	G
1	X	968	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	969	U
1	X	970	A
1	X	972	C
1	X	979	A
1	X	984	A
1	X	985	G
1	X	994	A
1	X	995	A
1	X	996	C
1	X	998	C
1	X	1001	A
1	X	1002	C
1	X	1006	C
1	X	1007	A
1	X	1010	U
1	X	1014	G
1	X	1016	C
1	X	1019	U
1	X	1020	A
1	X	1022	A
1	X	1023	U
1	X	1024	G
1	X	1028	G
1	X	1033	G
1	X	1034	U
1	X	1036	G
1	X	1037	U
1	X	1044	U
1	X	1053	G
1	X	1054	C
1	X	1055	A
1	X	1056	U
1	X	1057	A
1	X	1058	G
1	X	1068	A
1	X	1069	G
1	X	1072	U
1	X	1073	G
1	X	1077	U
1	X	1081	A
1	X	1082	G
1	X	1086	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	1087	C
1	X	1090	C
1	X	1094	C
1	X	1097	A
1	X	1098	G
1	X	1099	A
1	X	1100	G
1	X	1101	U
1	X	1108	U
1	X	1121	G
1	X	1122	A
1	X	1123	G
1	X	1125	G
1	X	1127	C
1	X	1128	G
1	X	1129	A
1	X	1130	U
1	X	1141	U
1	X	1143	A
1	X	1145	C
1	X	1146	G
1	X	1152	C
1	X	1153	A
1	X	1161	U
1	X	1168	G
1	X	1182	U
1	X	1184	G
1	X	1185	C
1	X	1186	G
1	X	1187	A
1	X	1189	G
1	X	1192	A
1	X	1194	U
1	X	1209	G
1	X	1223	G
1	X	1224	A
1	X	1233	A
1	X	1250	A
1	X	1251	G
1	X	1261	G
1	X	1262	U
1	X	1263	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	1264	C
1	X	1266	G
1	X	1269	G
1	X	1282	A
1	X	1284	G
1	X	1285	A
1	X	1288	A
1	X	1289	A
1	X	1302	C
1	X	1313	U
1	X	1314	A
1	X	1315	A
1	X	1319	C
1	X	1326	U
1	X	1334	A
1	X	1342	U
1	X	1345	G
1	X	1346	C
1	X	1353	A
1	X	1354	A
1	X	1357	U
1	X	1358	C
1	X	1359	G
1	X	1365	U
1	X	1372	A
1	X	1378	A
1	X	1379	A
1	X	1381	G
1	X	1392	U
1	X	1399	C
1	X	1404	C
1	X	1409	U
1	X	1410	U
1	X	1412	C
1	X	1413	U
1	X	1428	G
1	X	1429	A
1	X	1430	G
1	X	1432	G
1	X	1433	A
1	X	1434	U
1	X	1439	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	1440	G
1	X	1441	A
1	X	1442	C
1	X	1443	G
1	X	1460	G
1	X	1465	G
1	X	1467	U
1	X	1468	A
1	X	1469	U
1	X	1470	G
1	X	1474	A
1	X	1475	U
1	X	1476	G
1	X	1489	C
1	X	1490	U
1	X	1497	C
1	X	1498	G
1	X	1505	U
1	X	1506	C
1	X	1508	G
1	X	1513	U
1	X	1514	C
1	X	1523	A
1	X	1524	C
1	X	1525	A
1	X	1528	C
1	X	1529	C
1	X	1531	C
1	X	1533	G
1	X	1545	G
1	X	1548	U
1	X	1551	U
1	X	1552	C
1	X	1553	G
1	X	1554	G
1	X	1562	G
1	X	1563	U
1	X	1571	G
1	X	1574	A
1	X	1575	C
1	X	1576	G
1	X	1582	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	1585	A
1	X	1594	U
1	X	1600	U
1	X	1601	U
1	X	1602	G
1	X	1603	A
1	X	1608	U
1	X	1609	G
1	X	1613	G
1	X	1614	C
1	X	1624	A
1	X	1625	A
1	X	1626	A
1	X	1631	C
1	X	1632	A
1	X	1634	A
1	X	1635	G
1	X	1648	C
1	X	1651	U
1	X	1656	U
1	X	1657	A
1	X	1665	C
1	X	1668	G
1	X	1685	A
1	X	1686	A
1	X	1691	G
1	X	1695	U
1	X	1699	A
1	X	1710	U
1	X	1711	C
1	X	1713	G
1	X	1714	A
1	X	1717	A
1	X	1732	U
1	X	1733	U
1	X	1734	C
1	X	1746	A
1	X	1749	G
1	X	1754	G
1	X	1755	G
1	X	1764	A
1	X	1773	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	1776	A
1	X	1777	A
1	X	1782	A
1	X	1790	G
1	X	1791	C
1	X	1792	C
1	X	1793	A
1	X	1799	A
1	X	1800	A
1	X	1801	C
1	X	1807	A
1	X	1808	C
1	X	1810	U
1	X	1811	A
1	X	1812	U
1	X	1813	A
1	X	1821	A
1	X	1825	C
1	X	1830	C
1	X	1831	G
1	X	1839	A
1	X	1840	A
1	X	1852	G
1	X	1861	G
1	X	1867	A
1	X	1874	G
1	X	1883	A
1	X	1886	G
1	X	1910	A
1	X	1912	G
1	X	1913	G
1	X	1919	A
1	X	1921	A
1	X	1923	U
1	X	1924	C
1	X	1927	U
1	X	1937	G
1	X	1938	U
1	X	1939	U
1	X	1943	A
1	X	1946	U
1	X	1947	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	1950	C
1	X	1953	A
1	X	1954	A
1	X	1955	G
1	X	1964	A
1	X	1965	U
1	X	1976	U
1	X	1980	A
1	X	2003	A
1	X	2006	G
1	X	2014	A
1	X	2015	G
1	X	2018	G
1	X	2019	C
1	X	2026	C
1	X	2033	C
1	X	2035	G
1	X	2038	C
1	X	2039	G
1	X	2043	A
1	X	2044	G
1	X	2045	A
1	X	2046	C
1	X	2052	G
1	X	2063	A
1	X	2076	G
1	X	2078	G
1	X	2079	A
1	X	2089	C
1	X	2166	G
1	X	2171	U
1	X	2181	A
1	X	2189	A
1	X	2190	A
1	X	2191	A
1	X	2193	C
1	X	2195	C
1	X	2196	U
1	X	2197	U
1	X	2199	C
1	X	2204	A
1	X	2205	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	2214	G
1	X	2217	G
1	X	2218	G
1	X	2228	U
1	X	2229	G
1	X	2246	A
1	X	2247	A
1	X	2257	A
1	X	2262	C
1	X	2265	A
1	X	2266	A
1	X	2268	G
1	X	2283	G
1	X	2284	U
1	X	2285	U
1	X	2286	G
1	X	2287	G
1	X	2288	A
1	X	2289	A
1	X	2291	U
1	X	2295	C
1	X	2298	U
1	X	2299	A
1	X	2300	G
1	X	2301	A
1	X	2305	C
1	X	2306	A
1	X	2313	G
1	X	2315	A
1	X	2323	U
1	X	2324	G
1	X	2326	C
1	X	2329	C
1	X	2330	G
1	X	2333	A
1	X	2340	C
1	X	2351	G
1	X	2358	C
1	X	2362	G
1	X	2363	G
1	X	2364	C
1	X	2374	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	2381	A
1	X	2385	U
1	X	2389	G
1	X	2396	C
1	X	2397	A
1	X	2402	U
1	X	2404	A
1	X	2405	A
1	X	2406	C
1	X	2407	G
1	X	2408	G
1	X	2409	A
1	X	2410	U
1	X	2415	G
1	X	2420	C
1	X	2426	G
1	X	2427	A
1	X	2438	A
1	X	2447	G
1	X	2448	A
1	X	2453	C
1	X	2455	A
1	X	2457	A
1	X	2459	C
1	X	2461	G
1	X	2463	G
1	X	2466	G
1	X	2470	U
1	X	2477	C
1	X	2480	C
1	X	2481	G
1	X	2483	U
1	X	2484	G
1	X	2485	U
1	X	2498	U
1	X	2499	C
1	X	2508	G
1	X	2514	G
1	X	2545	A
1	X	2546	G
1	X	2548	G
1	X	2552	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	2557	G
1	X	2561	G
1	X	2564	U
1	X	2565	C
1	X	2580	C
1	X	2581	A
1	X	2582	G
1	X	2588	U
1	X	2590	U
1	X	2591	C
1	X	2593	A
1	X	2594	U
1	X	2608	A
1	X	2609	G
1	X	2611	A
1	X	2613	A
1	X	2615	U
1	X	2616	U
1	X	2618	A
1	X	2621	G
1	X	2633	A
1	X	2634	G
1	X	2640	G
1	X	2642	G
1	X	2650	G
1	X	2668	U
1	X	2692	A
1	X	2693	U
1	X	2694	G
1	X	2706	U
1	X	2713	A
1	X	2718	A
1	X	2719	U
1	X	2728	A
1	X	2731	G
1	X	2732	C
1	X	2735	C
1	X	2737	A
1	X	2745	A
1	X	2758	A
1	X	2759	U
1	X	2760	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	2769	C
1	X	2770	A
1	X	2771	C
1	X	2774	U
1	X	2776	U
1	X	2778	U
1	X	2779	C
1	X	2780	A
1	X	2793	G
1	X	2795	A
1	X	2796	A
1	X	2798	A
1	X	2800	C
1	X	2808	U
1	X	2824	C
1	X	2825	A
1	X	2841	U
1	X	2843	A
1	X	2846	G
1	X	2847	G
1	X	2848	A
1	X	2849	C
1	X	2854	G
1	X	2855	C
1	X	2861	A
1	X	2864	C
1	X	2866	A
1	X	2868	G
1	X	2877	A
2	Y	11	G
2	Y	14	C
2	Y	15	A
2	Y	17	A
2	Y	18	G
2	Y	26	G
2	Y	27	A
2	Y	28	A
2	Y	37	C
2	Y	38	C
2	Y	39	C
2	Y	42	U
2	Y	43	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	Y	44	C
2	Y	46	G
2	Y	47	A
2	Y	49	C
2	Y	52	G
2	Y	53	G
2	Y	54	U
2	Y	58	G
2	Y	59	A
2	Y	69	G
2	Y	75	A
2	Y	76	U
2	Y	77	G
2	Y	86	A
2	Y	88	C
2	Y	89	G
2	Y	90	C
2	Y	91	A
2	Y	92	G
2	Y	99	G
2	Y	102	A
2	Y	106	U
2	Y	110	U
2	Y	111	C
2	Y	112	A
2	Y	115	G
2	Y	116	C
2	Y	123	U

All (262) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	13	A
1	X	33	C
1	X	34	U
1	X	48	A
1	X	61	U
1	X	62	U
1	X	70	A
1	X	71	A
1	X	73	A
1	X	74	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	82	G
1	X	83	A
1	X	89	A
1	X	98	U
1	X	99	U
1	X	100	G
1	X	117	A
1	X	173	A
1	X	176	A
1	X	181	A
1	X	190	A
1	X	198	A
1	X	204	A
1	X	242	A
1	X	247	A
1	X	312	G
1	X	321	A
1	X	322	A
1	X	332	C
1	X	333	A
1	X	334	G
1	X	339	U
1	X	341	A
1	X	342	G
1	X	343	A
1	X	387	A
1	X	396	U
1	X	399	G
1	X	400	U
1	X	408	U
1	X	416	U
1	X	417	C
1	X	425	A
1	X	447	U
1	X	454	G
1	X	458	G
1	X	466	A
1	X	467	U
1	X	469	G
1	X	513	A
1	X	522	G
1	X	539	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	540	G
1	X	557	U
1	X	558	G
1	X	559	C
1	X	580	A
1	X	582	G
1	X	583	C
1	X	596	C
1	X	631	G
1	X	648	A
1	X	657	A
1	X	664	C
1	X	672	C
1	X	682	G
1	X	683	A
1	X	687	G
1	X	698	A
1	X	717	G
1	X	731	A
1	X	765	C
1	X	775	U
1	X	777	A
1	X	788	G
1	X	802	A
1	X	803	C
1	X	806	A
1	X	813	A
1	X	824	U
1	X	840	U
1	X	841	G
1	X	842	A
1	X	858	G
1	X	859	U
1	X	878	C
1	X	883	A
1	X	886	A
1	X	925	U
1	X	938	G
1	X	939	C
1	X	943	U
1	X	956	A
1	X	969	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	970	A
1	X	972	C
1	X	995	A
1	X	1000	G
1	X	1019	U
1	X	1036	G
1	X	1037	U
1	X	1053	G
1	X	1055	A
1	X	1056	U
1	X	1057	A
1	X	1072	U
1	X	1080	A
1	X	1081	A
1	X	1086	C
1	X	1096	A
1	X	1099	A
1	X	1122	A
1	X	1129	A
1	X	1139	A
1	X	1142	G
1	X	1143	A
1	X	1152	C
1	X	1185	C
1	X	1186	G
1	X	1191	G
1	X	1223	G
1	X	1249	G
1	X	1250	A
1	X	1266	G
1	X	1278	A
1	X	1288	A
1	X	1313	U
1	X	1314	A
1	X	1325	U
1	X	1333	G
1	X	1337	G
1	X	1345	G
1	X	1353	A
1	X	1357	U
1	X	1404	C
1	X	1409	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	1412	C
1	X	1433	A
1	X	1434	U
1	X	1439	G
1	X	1441	A
1	X	1442	C
1	X	1459	U
1	X	1467	U
1	X	1473	U
1	X	1474	A
1	X	1475	U
1	X	1489	C
1	X	1496	G
1	X	1508	G
1	X	1513	U
1	X	1562	G
1	X	1570	C
1	X	1574	A
1	X	1575	C
1	X	1583	A
1	X	1600	U
1	X	1601	U
1	X	1602	G
1	X	1607	A
1	X	1613	G
1	X	1618	U
1	X	1624	A
1	X	1631	C
1	X	1632	A
1	X	1634	A
1	X	1685	A
1	X	1686	A
1	X	1710	U
1	X	1711	C
1	X	1732	U
1	X	1749	G
1	X	1775	A
1	X	1777	A
1	X	1790	G
1	X	1791	C
1	X	1795	C
1	X	1799	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	1800	A
1	X	1810	U
1	X	1811	A
1	X	1820	G
1	X	1830	C
1	X	1839	A
1	X	1883	A
1	X	1909	U
1	X	1920	A
1	X	1921	A
1	X	1923	U
1	X	1937	G
1	X	1938	U
1	X	1953	A
1	X	1975	G
1	X	2018	G
1	X	2032	G
1	X	2075	U
1	X	2165	A
1	X	2189	A
1	X	2204	A
1	X	2217	G
1	X	2228	U
1	X	2254	C
1	X	2258	G
1	X	2261	G
1	X	2295	C
1	X	2298	U
1	X	2299	A
1	X	2305	C
1	X	2312	A
1	X	2314	A
1	X	2323	U
1	X	2343	C
1	X	2363	G
1	X	2370	G
1	X	2381	A
1	X	2396	C
1	X	2401	A
1	X	2409	A
1	X	2447	G
1	X	2482	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	2497	A
1	X	2508	G
1	X	2528	G
1	X	2545	A
1	X	2560	G
1	X	2561	G
1	X	2564	U
1	X	2580	C
1	X	2593	A
1	X	2608	A
1	X	2615	U
1	X	2660	C
1	X	2669	C
1	X	2691	C
1	X	2693	U
1	X	2731	G
1	X	2736	U
1	X	2758	A
1	X	2759	U
1	X	2770	A
1	X	2778	U
1	X	2795	A
1	X	2807	U
1	X	2808	U
1	X	2824	C
1	X	2832	G
1	X	2846	G
1	X	2848	A
1	X	2854	G
1	X	2867	G
2	Y	14	C
2	Y	46	G
2	Y	47	A
2	Y	49	C
2	Y	58	G
2	Y	86	A
2	Y	90	C
2	Y	92	G
2	Y	94	G
2	Y	111	C
2	Y	116	C
2	Y	117	G

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
32	1F4	X	2929	-	60,62,62	1.24	4 (6%)	82,95,95	2.85	37 (45%)

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	1F4	X	2929	-	-	0/74/119/119	1/5/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	X	2929	1F4	O46-C44	2.10	1.24	1.21
32	X	2929	1F4	C22-C9	2.57	1.58	1.52
32	X	2929	1F4	C52-C51	3.33	1.44	1.39
32	X	2929	1F4	C41-N40	4.13	1.39	1.33

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	X	2929	1F4	C5-O17-C41	-11.29	99.90	109.28
32	X	2929	1F4	C58-C49-C50	-5.36	104.57	110.59
32	X	2929	1F4	C4-N40-C41	-5.32	106.10	112.55
32	X	2929	1F4	C22-C9-C7	-4.56	103.00	111.05
32	X	2929	1F4	C9-C7-C2	-4.43	108.70	116.09
32	X	2929	1F4	O42-C41-N40	-4.05	124.25	129.16
32	X	2929	1F4	C57-C49-C48	-4.05	105.87	111.22
32	X	2929	1F4	C51-C56-N55	-3.60	118.45	124.27
32	X	2929	1F4	O46-C44-N45	-3.39	120.22	124.28
32	X	2929	1F4	C22-C9-C8	-3.35	104.32	109.97
32	X	2929	1F4	O20-C28-O29	-3.26	102.43	110.68
32	X	2929	1F4	C28-O20-C8	-2.83	111.22	116.30
32	X	2929	1F4	C19-C2-C7	-2.72	104.01	109.69
32	X	2929	1F4	C5-C4-N40	-2.69	95.86	101.59
32	X	2929	1F4	C48-C47-C51	-2.66	108.23	113.73
32	X	2929	1F4	C28-O29-C30	-2.54	108.70	112.97
32	X	2929	1F4	C7-C2-C3	-2.12	109.54	113.47
32	X	2929	1F4	O15-C3-C2	-2.07	116.59	120.95
32	X	2929	1F4	C23-C6-C5	-2.03	112.26	115.25
32	X	2929	1F4	C48-C47-N45	2.10	107.03	103.25
32	X	2929	1F4	C16-C1-C3	2.30	112.41	108.21
32	X	2929	1F4	C24-C5-C6	2.40	116.81	112.40
32	X	2929	1F4	C31-C32-C33	2.46	113.61	110.03
32	X	2929	1F4	C58-C49-C48	2.56	114.61	111.22
32	X	2929	1F4	C13-O43-C44	2.62	120.33	116.84
32	X	2929	1F4	C7-C9-C8	2.83	113.41	110.03
32	X	2929	1F4	C5-C4-C1	2.87	122.97	117.50
32	X	2929	1F4	C2-C3-C1	3.29	125.24	119.16
32	X	2929	1F4	O10-C6-C23	3.31	113.37	107.36
32	X	2929	1F4	C54-N55-C56	3.52	123.32	116.84
32	X	2929	1F4	C21-C14-C8	3.62	120.06	112.85
32	X	2929	1F4	C9-C8-C14	4.05	120.20	113.74
32	X	2929	1F4	O43-C13-C14	4.21	119.16	107.56
32	X	2929	1F4	O18-C9-C8	4.26	115.63	108.14
32	X	2929	1F4	C21-C14-C13	4.80	120.37	111.38
32	X	2929	1F4	C57-C49-C58	5.10	115.94	109.53
32	X	2929	1F4	C6-O10-C11	7.03	129.97	118.12

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	X	2929	1F4	C1-C11-C12-C13-C14-C2-C3-C4-C5-C6-C7-C8-C9-O10

1 monomer is involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	X	2929	1F4	19	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	X	2686/2880 (93%)	-0.09	66 (2%) 61 46	43, 92, 197, 276	0
2	Y	122/123 (99%)	-0.08	3 (2%) 61 46	83, 135, 170, 191	0
3	A	240/274 (87%)	-0.18	5 (2%) 67 52	68, 115, 146, 172	0
4	B	205/211 (97%)	-0.32	1 (0%) 91 86	45, 73, 105, 154	0
5	C	197/205 (96%)	-0.12	8 (4%) 41 29	57, 114, 154, 187	0
6	D	177/180 (98%)	-0.15	9 (5%) 32 22	146, 183, 216, 227	0
7	E	171/185 (92%)	-0.49	2 (1%) 81 69	92, 143, 192, 206	0
8	F	71/144 (49%)	1.56	19 (26%) 1 1	211, 236, 252, 257	0
9	G	142/174 (81%)	-0.29	1 (0%) 89 81	72, 97, 144, 161	0
10	H	134/134 (100%)	-0.38	0 100 100	50, 70, 97, 121	0
11	I	141/156 (90%)	0.33	10 (7%) 19 12	67, 129, 174, 204	0
12	J	136/141 (96%)	0.27	7 (5%) 32 22	74, 103, 149, 184	0
13	K	113/116 (97%)	-0.35	0 100 100	35, 60, 79, 91	0
14	L	104/114 (91%)	-0.12	1 (0%) 84 73	98, 134, 156, 168	0
15	M	108/166 (65%)	-0.58	0 100 100	50, 73, 111, 145	0
16	N	117/118 (99%)	-0.40	0 100 100	59, 90, 128, 159	0
17	O	94/100 (94%)	-0.27	2 (2%) 67 52	66, 115, 157, 173	0
18	P	127/134 (94%)	-0.47	0 100 100	50, 68, 107, 158	0
19	Q	93/95 (97%)	-0.22	2 (2%) 65 50	73, 106, 162, 195	0
20	R	110/115 (95%)	-0.14	4 (3%) 46 33	88, 117, 170, 178	0
21	S	175/237 (73%)	0.38	15 (8%) 13 10	121, 155, 175, 190	0
22	T	84/91 (92%)	0.49	9 (10%) 8 6	79, 107, 186, 200	0
23	U	72/81 (88%)	0.08	6 (8%) 14 10	92, 128, 153, 161	0
24	V	66/67 (98%)	0.05	6 (9%) 11 8	100, 132, 211, 216	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	55/55 (100%)	-0.45	1 (1%) 71 58	80, 98, 126, 152	0
26	Z	58/60 (96%)	-0.14	3 (5%) 31 22	49, 70, 105, 114	0
27	1	53/55 (96%)	2.48	20 (37%) 0 0	8, 32, 62, 93	0
28	2	46/47 (97%)	5.87	44 (95%) 0 0	3, 15, 38, 59	0
29	3	63/66 (95%)	3.42	44 (69%) 0 0	3, 25, 40, 61	0
30	4	37/37 (100%)	4.00	25 (67%) 0 0	228, 254, 266, 269	0
All	All	5997/6561 (91%)	0.03	313 (5%) 31 22	3, 100, 196, 276	0

All (313) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
27	1	7	ARG	18.6
28	2	27	GLY	13.6
22	T	9	SER	13.0
30	4	25	VAL	12.8
28	2	8	ASN	12.5
29	3	35	GLY	12.1
28	2	4	THR	11.9
28	2	37	LYS	11.4
27	1	25	THR	10.8
1	X	731	A	10.3
24	V	1	MET	10.3
30	4	24	LEU	10.2
28	2	32	ALA	10.1
28	2	24	THR	10.0
28	2	33	ARG	9.9
27	1	24	THR	9.7
29	3	42	ARG	9.6
28	2	9	ASN	9.4
27	1	43	VAL	9.4
28	2	26	SER	9.1
30	4	17	VAL	9.1
27	1	44	ALA	9.0
30	4	29	ASN	8.7
28	2	25	LYS	8.6
28	2	29	ASN	8.5
11	I	9	THR	8.5
28	2	22	MET	8.4
27	1	26	LYS	8.3
28	2	7	PRO	8.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	X	1089	C	8.0
28	2	2	LYS	7.9
28	2	36	ALA	7.8
27	1	23	THR	7.8
29	3	8	LYS	7.7
29	3	32	GLN	7.7
28	2	23	LYS	7.5
30	4	28	SER	7.5
29	3	31	HIS	7.4
29	3	2	PRO	7.3
29	3	22	VAL	7.3
29	3	6	THR	7.3
22	T	10	SER	7.1
28	2	11	LYS	7.0
1	X	1091	C	6.9
8	F	114	ASP	6.9
28	2	6	GLN	6.7
1	X	1090	C	6.6
30	4	34	GLN	6.6
28	2	13	ALA	6.5
12	J	84	MET	6.5
28	2	38	GLY	6.4
3	A	203	ASN	6.4
29	3	10	ALA	6.4
11	I	8	PRO	6.3
2	Y	123	U	6.2
28	2	15	THR	6.1
30	4	6	SER	6.1
1	X	1067	G	6.0
26	Z	2	ALA	5.9
1	X	1079	G	5.8
30	4	16	VAL	5.6
8	F	137	THR	5.6
28	2	16	HIS	5.6
12	J	82	THR	5.6
28	2	28	ARG	5.5
29	3	7	HIS	5.5
30	4	35	ARG	5.5
1	X	1106	A	5.5
28	2	20	ALA	5.4
29	3	27	SER	5.4
30	4	23	VAL	5.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
22	T	8	GLY	5.3
1	X	1086	C	5.3
30	4	22	ARG	5.3
29	3	51	ALA	5.2
1	X	248	A	5.2
29	3	40	GLU	5.1
29	3	63	PRO	5.1
30	4	19	ARG	5.1
4	B	205	SER	5.0
1	X	1078	A	5.0
30	4	32	HIS	4.9
8	F	125	ASN	4.8
11	I	10	PRO	4.8
30	4	21	GLY	4.8
29	3	36	LYS	4.8
28	2	5	TYR	4.8
11	I	4	HIS	4.8
1	X	1068	A	4.8
11	I	5	ASP	4.8
27	1	41	ASP	4.7
11	I	52	GLY	4.7
30	4	20	HIS	4.6
28	2	41	GLN	4.6
30	4	27	CYS	4.6
11	I	29	THR	4.5
24	V	4	SER	4.5
1	X	1107	A	4.5
21	S	29	ASN	4.5
1	X	2776	U	4.4
1	X	1084	A	4.4
29	3	34	THR	4.4
30	4	36	GLN	4.4
19	Q	64	ARG	4.4
24	V	3	PRO	4.4
5	C	47	THR	4.3
8	F	98	LYS	4.3
3	A	250	TRP	4.3
29	3	9	MET	4.3
5	C	44	SER	4.3
12	J	85	GLY	4.2
20	R	100	ASP	4.2
8	F	108	ALA	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	X	1077	U	4.2
29	3	39	ASP	4.1
29	3	33	ASN	4.1
6	D	42	SER	4.1
6	D	43	SER	4.1
1	X	730	C	4.1
1	X	2289	A	4.1
28	2	40	HIS	4.0
29	3	3	LYS	4.0
29	3	60	LEU	3.9
28	2	43	THR	3.9
29	3	59	LYS	3.9
29	3	18	GLY	3.9
21	S	28	ASN	3.9
1	X	1099	A	3.8
22	T	6	GLY	3.8
8	F	111	LYS	3.8
29	3	5	LYS	3.8
5	C	123	PHE	3.8
1	X	1186	G	3.8
8	F	113	PRO	3.8
1	X	1073	G	3.7
1	X	1085	G	3.7
8	F	92	ASN	3.6
11	I	6	LEU	3.6
28	2	3	ARG	3.6
29	3	64	ARG	3.6
22	T	15	ASP	3.6
8	F	84	ILE	3.5
28	2	1	MET	3.5
28	2	34	ARG	3.5
27	1	47	HIS	3.5
21	S	23	ALA	3.5
29	3	4	MET	3.5
27	1	11	LYS	3.5
1	X	1094	C	3.5
1	X	1104	G	3.5
29	3	19	THR	3.4
20	R	99	VAL	3.4
28	2	10	ARG	3.4
5	C	197	GLU	3.4
22	T	17	ASN	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
12	J	81	GLU	3.4
23	U	27	ASP	3.4
24	V	2	LYS	3.4
1	X	74	G	3.4
1	X	1081	A	3.3
29	3	55	TRP	3.3
20	R	57	ASN	3.3
28	2	19	ARG	3.3
1	X	1080	A	3.3
29	3	47	GLY	3.2
30	4	26	ILE	3.2
21	S	24	TYR	3.2
27	1	20	PHE	3.2
5	C	198	GLU	3.2
8	F	107	ILE	3.2
1	X	2777	A	3.2
23	U	16	ASN	3.2
21	S	143	ILE	3.2
23	U	47	HIS	3.2
2	Y	68	A	3.2
8	F	121	GLU	3.1
30	4	18	ARG	3.1
28	2	45	SER	3.1
27	1	22	TYR	3.1
30	4	7	VAL	3.1
1	X	891	A	3.1
1	X	1114	A	3.1
22	T	4	LYS	3.1
28	2	12	ARG	3.1
5	C	20	PRO	3.1
21	S	165	GLU	3.1
30	4	10	MET	3.0
8	F	100	ASN	3.0
27	1	31	THR	3.0
8	F	97	GLY	3.0
28	2	17	GLY	3.0
29	3	53	ALA	3.0
28	2	30	ILE	3.0
27	1	14	SER	3.0
1	X	1072	U	2.9
8	F	112	MET	2.9
1	X	1098	G	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	4	5	SER	2.9
6	D	146	VAL	2.9
28	2	46	ASP	2.9
1	X	728	G	2.9
1	X	2329	C	2.9
11	I	33	GLY	2.9
29	3	17	THR	2.8
7	E	5	GLY	2.8
29	3	57	ARG	2.8
2	Y	2	C	2.8
1	X	358	C	2.8
27	1	27	ASN	2.8
1	X	1109	A	2.8
27	1	9	ILE	2.7
19	Q	94	GLN	2.7
6	D	145	MET	2.7
21	S	15	ASP	2.7
1	X	1087	C	2.7
21	S	144	GLY	2.7
9	G	97	ASP	2.7
29	3	26	LYS	2.7
1	X	225	G	2.7
11	I	63	ARG	2.7
29	3	37	SER	2.7
29	3	11	LYS	2.6
7	E	43	VAL	2.6
1	X	1088	A	2.6
1	X	1951	G	2.6
17	O	41	GLY	2.6
29	3	25	PHE	2.6
6	D	85	VAL	2.6
27	1	46	LYS	2.6
12	J	21	ASP	2.6
22	T	7	VAL	2.6
6	D	147	ASP	2.6
21	S	124	ALA	2.6
22	T	5	LYS	2.5
21	S	12	GLN	2.5
26	Z	59	ALA	2.5
8	F	110	THR	2.5
1	X	435	A	2.5
1	X	170	U	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	X	1187	A	2.5
1	X	2174	G	2.5
6	D	26	MET	2.5
21	S	31	SER	2.5
1	X	2287	G	2.4
1	X	169	C	2.4
3	A	261	ARG	2.4
1	X	1093	U	2.4
8	F	85	GLY	2.4
21	S	163	ASP	2.4
1	X	361	G	2.4
29	3	38	GLY	2.4
28	2	31	LEU	2.3
1	X	727	U	2.3
29	3	61	MET	2.3
30	4	14	CYS	2.3
1	X	2775	U	2.3
28	2	44	VAL	2.3
12	J	7	ARG	2.3
29	3	50	LEU	2.3
1	X	2088	U	2.3
17	O	39	PHE	2.3
1	X	2778	U	2.3
1	X	1524	C	2.3
28	2	42	LEU	2.3
1	X	2089	C	2.2
1	X	1115	C	2.2
20	R	98	ILE	2.2
28	2	21	ARG	2.2
1	X	558	G	2.2
1	X	1103	C	2.2
23	U	25	ARG	2.2
21	S	27	GLU	2.2
21	S	164	PRO	2.2
6	D	134	GLU	2.2
5	C	48	ARG	2.2
1	X	729	A	2.2
29	3	24	ALA	2.2
29	3	45	GLY	2.2
1	X	356	A	2.2
1	X	1913	G	2.2
30	4	11	CYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
29	3	62	LEU	2.1
23	U	39	LYS	2.1
24	V	6	MET	2.1
28	2	14	LYS	2.1
8	F	138	VAL	2.1
27	1	42	PRO	2.1
5	C	19	LEU	2.1
25	W	6	VAL	2.1
27	1	49	VAL	2.1
29	3	48	PHE	2.1
3	A	91	ARG	2.1
8	F	90	THR	2.1
6	D	144	ASP	2.1
1	X	665	A	2.1
1	X	2323	U	2.1
28	2	39	ARG	2.1
26	Z	3	LYS	2.1
1	X	1110	G	2.1
1	X	1121	G	2.1
1	X	2270	U	2.1
3	A	236	GLY	2.0
14	L	97	HIS	2.0
21	S	40	ASP	2.0
12	J	86	LYS	2.0
23	U	28	GLY	2.0
1	X	483	A	2.0
8	F	126	THR	2.0
29	3	44	LYS	2.0
30	4	13	ASN	2.0
24	V	36	GLN	2.0
27	1	36	GLU	2.0
1	X	1076	U	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
31	MG	X	2926	1/1	0.79	1.78	49.42	45,45,45,45	0
31	MG	X	2917	1/1	0.94	1.09	36.65	55,55,55,55	0
31	MG	X	2924	1/1	0.79	1.09	25.25	70,70,70,70	0
31	MG	X	2907	1/1	0.97	0.81	22.51	51,51,51,51	0
31	MG	Y	202	1/1	0.88	1.43	21.89	88,88,88,88	0
31	MG	X	2901	1/1	0.53	0.69	19.73	50,50,50,50	0
31	MG	X	2915	1/1	0.85	0.73	16.42	57,57,57,57	0
31	MG	X	2922	1/1	0.95	0.86	12.18	44,44,44,44	0
31	MG	X	2914	1/1	0.96	0.64	4.42	27,27,27,27	0
32	1F4	X	2929	58/58	0.96	0.21	-0.27	20,20,20,20	0
31	MG	X	2925	1/1	0.97	0.27	-	122,122,122,122	0
31	MG	X	2927	1/1	0.68	0.53	-	64,64,64,64	0
31	MG	M	201	1/1	0.98	1.39	-	23,23,23,23	0
31	MG	X	2902	1/1	0.93	0.31	-	94,94,94,94	0
31	MG	X	2910	1/1	0.99	0.69	-	41,41,41,41	0
31	MG	Y	201	1/1	0.93	0.46	-	98,98,98,98	0
31	MG	X	2921	1/1	0.91	0.70	-	80,80,80,80	0
31	MG	X	2913	1/1	0.37	1.00	-	60,60,60,60	0
31	MG	Y	204	1/1	0.34	0.97	-	86,86,86,86	0
31	MG	X	2920	1/1	0.54	0.46	-	113,113,113,113	0
31	MG	X	2928	1/1	0.56	0.81	-	61,61,61,61	0
31	MG	X	2916	1/1	0.86	1.18	-	37,37,37,37	0
31	MG	Y	203	1/1	0.81	0.89	-	59,59,59,59	0
31	MG	X	2903	1/1	0.45	0.63	-	89,89,89,89	0
31	MG	X	2906	1/1	0.94	0.95	-	58,58,58,58	0
31	MG	X	2919	1/1	0.92	0.92	-	30,30,30,30	0
31	MG	X	2905	1/1	0.89	0.49	-	65,65,65,65	0
31	MG	Y	205	1/1	0.92	0.40	-	82,82,82,82	0
31	MG	X	2923	1/1	0.96	0.34	-	34,34,34,34	0
31	MG	X	2909	1/1	0.33	0.62	-	97,97,97,97	0
31	MG	X	2908	1/1	0.82	2.34	-	37,37,37,37	0
31	MG	Y	206	1/1	0.84	0.29	-	78,78,78,78	0
31	MG	X	2911	1/1	0.77	0.39	-	68,68,68,68	0
31	MG	X	2904	1/1	0.92	0.30	-	110,110,110,110	0
31	MG	X	2918	1/1	0.84	1.24	-	42,42,42,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
31	MG	X	2912	1/1	0.70	0.58	-	71,71,71,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.