



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 04:49 pm BST

PDB ID : 4JI8  
Title : Crystal Structure of 30S ribosomal subunit from *Thermus thermophilus*  
Authors : Demirci, H.; Wang, L.; Murphy IV, F.; Murphy, E.; Carr, J.; Blanchard, S.;  
Jogl, G.; Dahlberg, A.E.; Gregory, S.T.  
Deposited on : 2013-03-05  
Resolution : 3.74 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

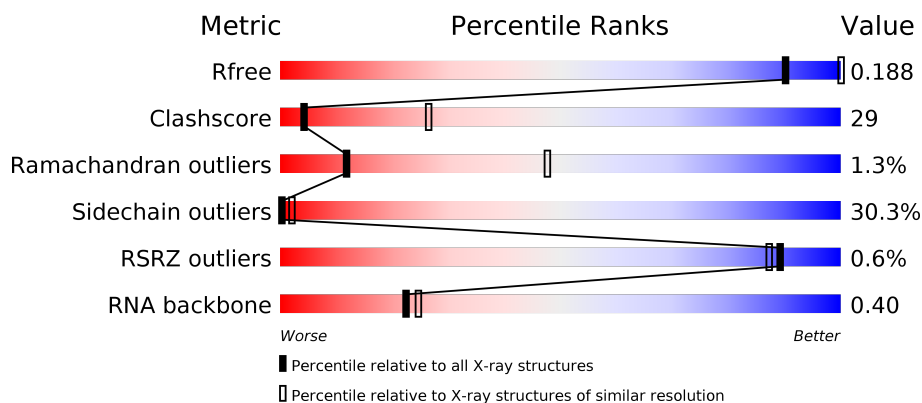
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.74 Å.

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



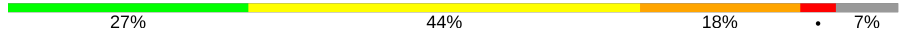

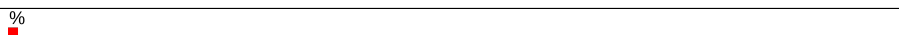
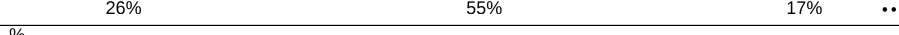
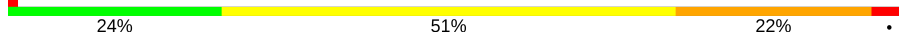

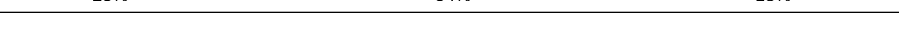
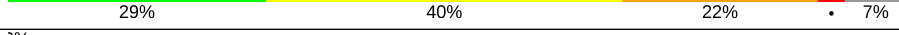
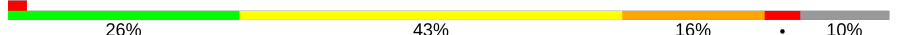

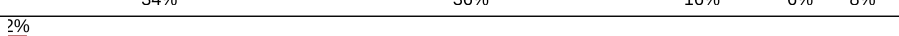
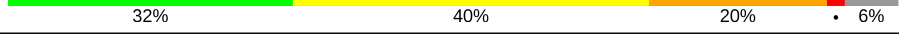
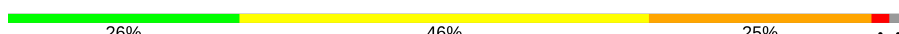
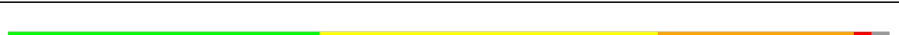
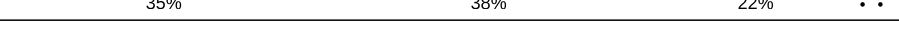
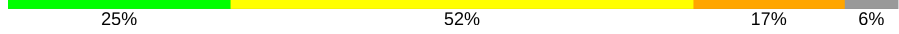
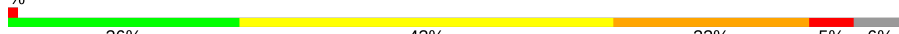
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1001 (3.90-3.58)
Clashscore	141614	1063 (3.90-3.58)
Ramachandran outliers	138981	1027 (3.90-3.58)
Sidechain outliers	138945	1023 (3.90-3.58)
RSRZ outliers	127900	1006 (3.92-3.56)
RNA backbone	3102	1028 (4.46-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	A	1522	
2	B	256	
3	C	239	
4	D	209	

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Mol	Chain	Length	Quality of chain
5	E	162	
6	F	101	
7	G	156	
8	H	138	
9	I	128	
10	J	105	
11	K	129	
12	L	135	
13	M	126	
14	N	61	
15	O	89	
16	P	88	
17	Q	105	
18	R	88	
19	S	93	
20	T	106	
21	U	27	

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
23	MG	A	1602	-	-	-	X
23	MG	A	1637	-	-	-	X
23	MG	A	1657	-	-	-	X
23	MG	A	1659	-	-	-	X
23	MG	A	1664	-	-	-	X
23	MG	A	1681	-	-	-	X
23	MG	A	1691	-	-	-	X
23	MG	A	1697	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	MG	A	1702	-	-	-	X
23	MG	A	1704	-	-	-	X
23	MG	A	1717	-	-	-	X
23	MG	A	1718	-	-	-	X
23	MG	A	1728	-	-	-	X
23	MG	A	1731	-	-	-	X
23	MG	A	1739	-	-	-	X
23	MG	A	1752	-	-	-	X
23	MG	A	1763	-	-	-	X
23	MG	A	1769	-	-	-	X
23	MG	A	1770	-	-	-	X
23	MG	A	1772	-	-	-	X
23	MG	A	1774	-	-	-	X
23	MG	A	1776	-	-	-	X
23	MG	A	1795	-	-	-	X
23	MG	A	1800	-	-	-	X
23	MG	A	1814	-	-	-	X
23	MG	A	1815	-	-	-	X
23	MG	A	1819	-	-	-	X
23	MG	A	1824	-	-	-	X
23	MG	A	1834	-	-	-	X
23	MG	A	1855	-	-	-	X
23	MG	A	1856	-	-	-	X
23	MG	A	1923	-	-	-	X
23	MG	A	1936	-	-	-	X
23	MG	A	1942	-	-	-	X
23	MG	A	1943	-	-	-	X
23	MG	A	1944	-	-	-	X
23	MG	A	1947	-	-	-	X
23	MG	A	1961	-	-	-	X
23	MG	A	1962	-	-	-	X
23	MG	A	1966	-	-	-	X
23	MG	A	1986	-	-	-	X
23	MG	A	1987	-	-	-	X
23	MG	A	1989	-	-	-	X
23	MG	E	203	-	-	-	X
23	MG	Q	201	-	-	-	X

## 2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 53563 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 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1514	Total	C	N	O	P	0	0	0
			32550	14496	6018	10522	1514			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1534	C	A	CONFLICT	GB M26923.1
A	1535	A	C	CONFLICT	GB M26923.1

- Molecule 2 is a protein called RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			

- Molecule 3 is a protein called RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 4 is a protein called RIBOSOMAL PROTEIN S4.

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

- Molecule 5 is a protein called RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	150	Total	C	N	O	S	0	0	0
			1146	724	217	201	4			

- Molecule 6 is a protein called RIBOSOMAL PROTEIN S6.

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

- Molecule 7 is a protein called RIBOSOMAL PROTEIN S7.

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

- Molecule 8 is a protein called RIBOSOMAL PROTEIN S8.

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

- Molecule 9 is a protein called RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	127	Total	C	N	O	0	0	0
			1010	639	197	174			

- Molecule 10 is a protein called RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	98	Total	C	N	O	S	0	0	0
			792	498	156	137	1			

- Molecule 11 is a protein called RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			

- Molecule 12 is a protein called RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	124	Total	C	N	O	S	0	0	0
			977	617	196	163	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	94	TRP	PRO	CONFLICT	UNP F6DEQ7

- Molecule 13 is a protein called RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	118	Total	C	N	O	S	0	0	0
			937	579	193	163	2			

- Molecule 14 is a protein called RIBOSOMAL PROTEIN S14.

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

- Molecule 15 is a protein called RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	87	Total	C	N	O	S	0	0	0
			729	457	146	124	2			

- Molecule 16 is a protein called RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

- Molecule 17 is a protein called RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 18 is a protein called RIBOSOMAL PROTEIN S18.

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

- Molecule 19 is a protein called RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	80	Total	C	N	O	S	0	0	0
			647	414	119	112	2			

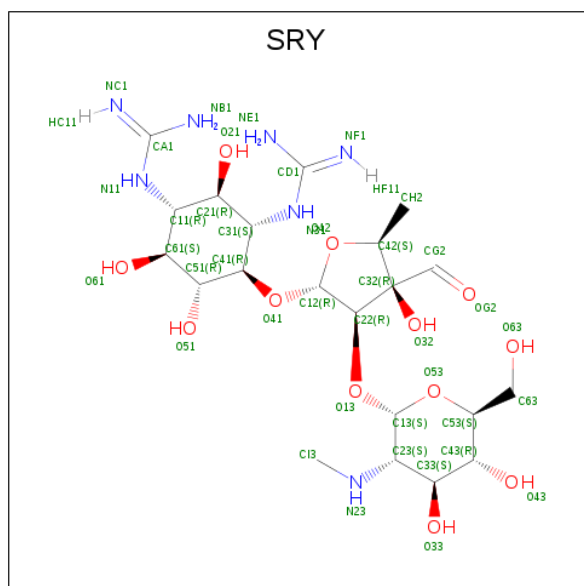
- Molecule 20 is a protein called RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 21 is a protein called RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	24	Total	C	N	O	0	0	0
			208	128	50	30			

- Molecule 22 is STREPTOMYCIN (three-letter code: SRY) (formula:  $C_{21}H_{39}N_7O_{12}$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
22	A	1	Total	C	N	O	0	0
			40	21	7	12		

- Molecule 23 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	P	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	Q	2	Total 2	Mg 2	0	0
23	D	6	Total 6	Mg 6	0	0
23	E	3	Total 3	Mg 3	0	0
23	H	1	Total 1	Mg 1	0	0
23	B	3	Total 3	Mg 3	0	0
23	C	4	Total 4	Mg 4	0	0
23	A	389	Total 389	Mg 389	0	0
23	N	1	Total 1	Mg 1	0	0
23	O	1	Total 1	Mg 1	0	0
23	L	1	Total 1	Mg 1	0	0
23	S	1	Total 1	Mg 1	0	0
23	F	1	Total 1	Mg 1	0	0

- Molecule 24 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	D	1	Total 1	Zn 1	0	0
24	N	1	Total 1	Zn 1	0	0

- Molecule 25 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	1371	Total 1371	O 1371	0	0
25	C	16	Total 16	O 16	0	0
25	D	24	Total 24	O 24	0	0

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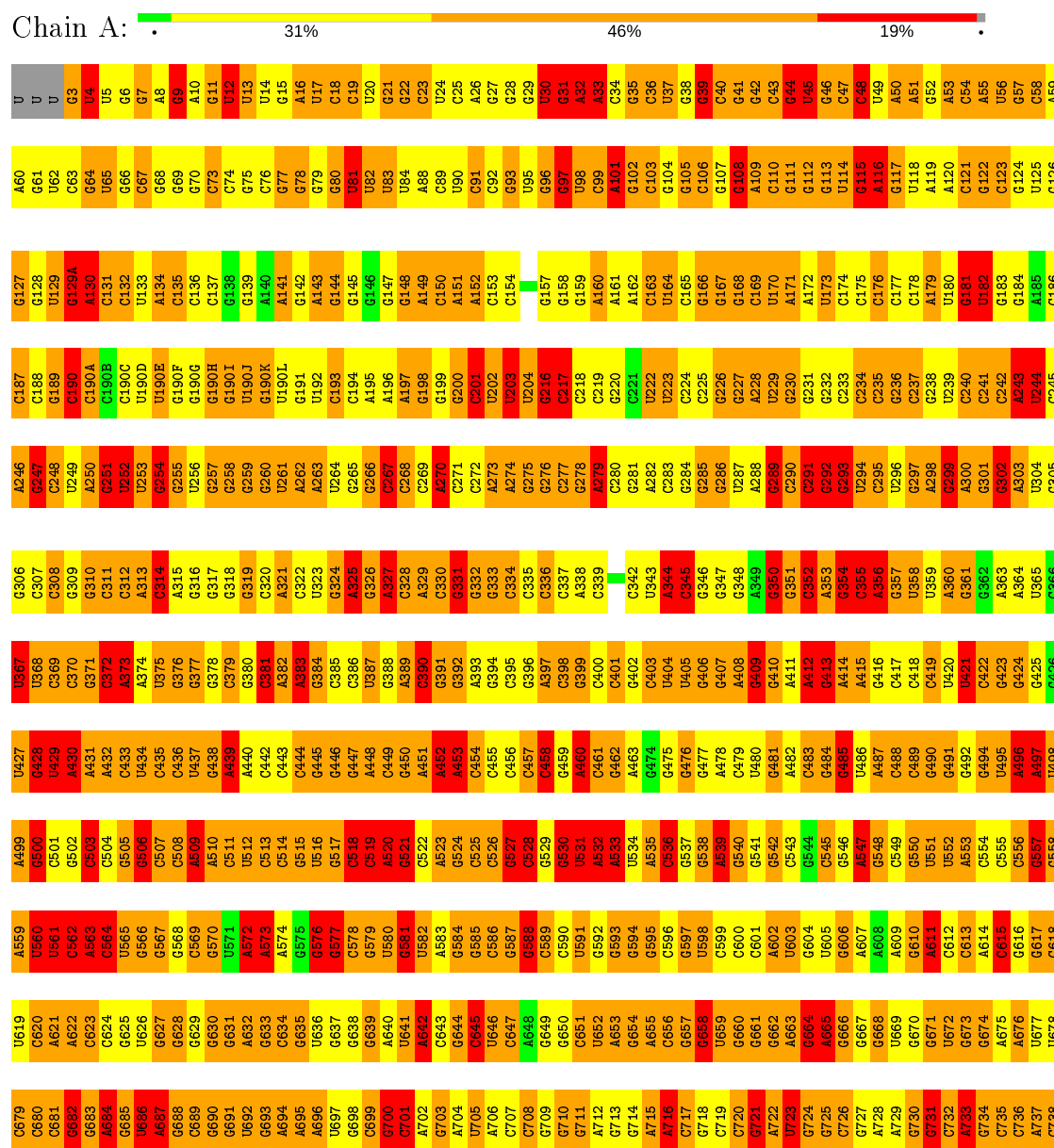
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	E	8	Total	O	0	0
			8	8		
25	F	6	Total	O	0	0
			6	6		
25	G	6	Total	O	0	0
			6	6		
25	H	5	Total	O	0	0
			5	5		
25	I	1	Total	O	0	0
			1	1		
25	L	7	Total	O	0	0
			7	7		
25	M	4	Total	O	0	0
			4	4		
25	N	4	Total	O	0	0
			4	4		
25	O	2	Total	O	0	0
			2	2		
25	P	1	Total	O	0	0
			1	1		
25	Q	8	Total	O	0	0
			8	8		
25	T	1	Total	O	0	0
			1	1		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: 16S rRNA

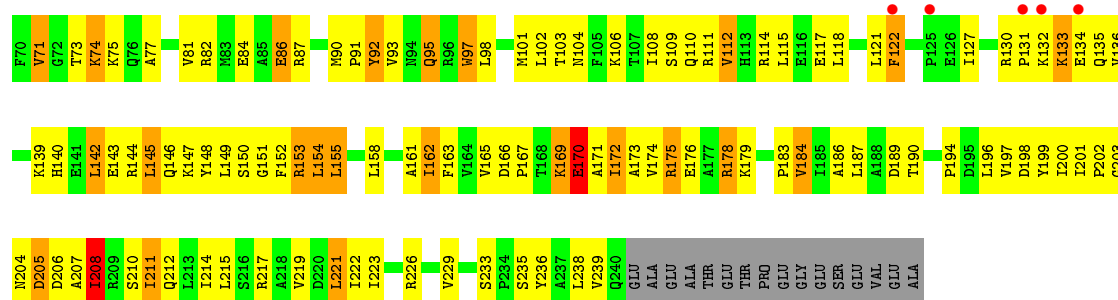


G1529	G1469	C1404	U1345	A1285	A1225	G1164	G1103	G1042	C985	G925	A865	G799	C739
G1530	G1470	G1405	A1346	A1286	C1226	C1165	G1104	C1043	A986	G926	C866	G800	U740
A1531	U1406	U1406	G1347	A1287	C1227	C1166	A1105	A1044	G987	U801	C867	U801	G741
C1533	U1472	C1407	U1348	A1288	C1228	A1167	G1106	C1045	G988	G928	C868	A802	G742
C	A1473	A1408	A1349	A1289	C1229	A1168	G1107	A1046	C989	G929	C869	U804	U743
A	G1474	C1350	A1350	A1290	C1230	A1169	G1108	G1047	C990	C930	U870	U804	C744
C	G1475	U1351	U1351	G1291	C1231	G1171	G1109	G1048	G991	C931	U871	C865	C745
C	G1476	C1352	C1352	U1292	U1232	G1172	A1110	U1049	G992	C932	A872	C806	C746
U	C1477	G1353	G1353	G1293	G1233	G1173	A1111	G1050	G993	G933	A873	A807	A747
C	C1478	C1354	C1354	G1294	C1234	G1174	G1112	C1051	A994	C934	C874	C808	C748
C1539	C1479	U1413	G1355	G1295	U1235	G1175	C1113	U1052	C995	A935	C875	C809	C749
U1540	G1480	G1415	A1356	C1296	A1236	A1176	C1114	G1053	A996	C936	C876	C810	C750
U1541	U1481	G1416	G1357	C1297	C1237	G1177	G1115	C1054	U997	A937	C877	G811	U751
U1542	G1482	G1417	U1358	C1298	A1238	G1178	C1116	A1055	G998	A938	C878	C812	G752
C1543	A1483	A1418	C1359	A1299	A1239	A1179	G1117	U1056	C	G999	C879	U813	G753
U1544	C1484	G1419	A1360	G1300	U1240	A1180	G1118	G1057	A1001	C940	C880	A814	A754
	U1485	C1420	G1361	U1301	G1241	G1181	C1119	G1058	G1002	C941	G881	A815	G755
	G1486	G1421	C1361A	U1302	C1242	G1182	G1120	C1059	G1003	G942	C882	A816	G756
	G1487	G1422	C1362	C1303	C1243	A1183	U1121	C1060	G1003A	U943	C883	C817	U757
	G1488	G1423	A1363	G1304	C1244	G1184	U1122	G1061	A1004	G944	U884	G818	G758
	G1489	C1424	U1364	G1305	A1245	G1185	A1123	U1062	A1005	G945	C885	A819	A759
	C1490	U1425	G1365	U1306	C1246	G1186	G1124	C1063	C1006	A946	G886	U820	G760
	G1491	C1426	C1366	U1307	U1247	G1187	G1125	G1064	C1007	G947	G887	G821	G761
	A1492	U1427	C1367	U1308	A1248	A1188	U1126	U1065	C1008	C948	G888	C822	C762
	A1493	A1428	G1368	G1309	C1249	C1189	G1127	C1066	A889	C949	G889	G823	G763
	G1494	C1429	C1369	G1310	A1250	G1190	C1128	A1067	G1010	U950	C890	C824	C764
	U1495	C1430	G1370	G1311	A1251	A1191	G1129	G1068	G1011	G951	U891	G825	G765
	C1496	G1431	G1371	G1312	A1252	A1192	A1130	U1012	G952	U952	A892	C826	A766
	G1497	A1432	U1372	U1313	G1253	G1193	G1131	U1070	G1013	G953	C893	U832	A767
	Y33	G1498	G1373	C1314	C1254	U1194	G1132	C1071	A1014	G954	G894	A828	A768
	A1499	A1434	A1374	U1315	G1255	G1195	G1133	G1072	A1015	U955	G895	G829	G769
	A1500	G1435	A1375	G1316	A1256	U1196	G1134	U1073	A1016	U956	C896	G830	C770
	C1501	U1436	U1376	C1317	U1257	G1197	U1135	G1074	G1017	U957	C897	G831	G771
	A1502	G1437	A1377	A1318	G1258	G1198	U1136	C1075	C1018	A958	G898	C832	U772
	A1503	G1438	G1378	A1319	C1259	U1199	G1137	C1076	C1019	A959	C899	U833	G773
	G1504	C1439	G1379	C1320	C1260	U1200	G1138	G1077	U1020	U960	A900	G774	G774
	U1505	G1440	U1380	C1321	A1261	A1201	G1139	U1078	G1021	U961	A901	U835	G775
	U1506	G1441	U1381	C1322	C1262	G1202	C1140	G1079	G1022	C962	G902	G836	G776
	A1507	G1442	C1382	G1323	G1263	C1203	C1141	A1080	G1023	G963	G903	G837	A777
	G1508	G1443	C1383	A1324	C1264	A1204	G1142	G1081	G1024	A964	C904	G838	G778
	A1509	A1446	G1384	C1325	G1265	U1205	G1143	G1082	U1025	U965	U839	U839	C779
	U1510	G1447	G1385	C1326	G1266	G1206	G1144	U1083	G1026	G966	G906	C840	A780
	G1511	C1448	G1386	C1327	C1267	G1207	G1145	G1084	C1027	C967	A907	U841	A781
	U1512	C1449	G1387	C1328	A1268	C1208	A1146	U1085	C1028	A968	A908	C843	A782
	A1513	U1450	C1388	A1329	A1269	C1209	C1147	U1086	C1029	A969	A909	C849	C783
	C1514	A1451	C1389	U1330	C1270	C1210	U1148	G1087	C1030	C970	C910	U850	C784
	E52	C1452	U1390	G1331	G1271	U1211	C1149	C1077	U911	G971	U911	G851	G785
	R53	G1453	A1391	A1332	G1272	U1212	U1150	U1095	C912	C972	G912	G852	G786
	T54	G1454	G1392	A1333	G1273	A1213	A1151	C1096	G913	G973	A913	G853	A787
	F55	G1455	U1393	G1334	G1274	C1214	A1152	G1097	A914	A974	A914	G854	U788
	A1518	A1456	A1394	C1335	A1275	G1215	G1155	A1092	A915	A975	A915	G855	U789
	A1519	A1459	C1395	C1336	G1276	G1216	G1156	A1093	G916	C976	G916	G856	A790
	G1520	G1461	C1396	G1337	C1277	C1217	G1157	U1096	G917	A977	G917	C857	A791
	U1521	G1462	C1397	A1338	U1278	C1218	A1158	C1098	A918	A978	G918	G858	A792
	C1523	C1463	A1398	A1339	A1279	U1219	G1159	G1099	A919	C979	A919	A859	U793
	G1524	G1464	A1399	A1340	A1280	G1220	U1159	C1098	U920	C980	U920	A860	A794
	G1525	C1465	C1400	U1341	U1281	G1221	G1160	G1099	U921	U981	U921	G861	C795
	G1526	G1466	G1401	C1342	C1282	G1222	C1161	C1100	U982	U982	G922	C862	C796
	G1527	G1467	C1402	G1343	C1283	G1223	G1162	A1101	A983	U983	A983	U863	C797
	U1528	A1468	C1403	C1344	C1284	G1224	C1163	A1102	A1041	C984	C924	A864	G798

## • Molecule 2: RIBOSOMAL PROTEIN S2

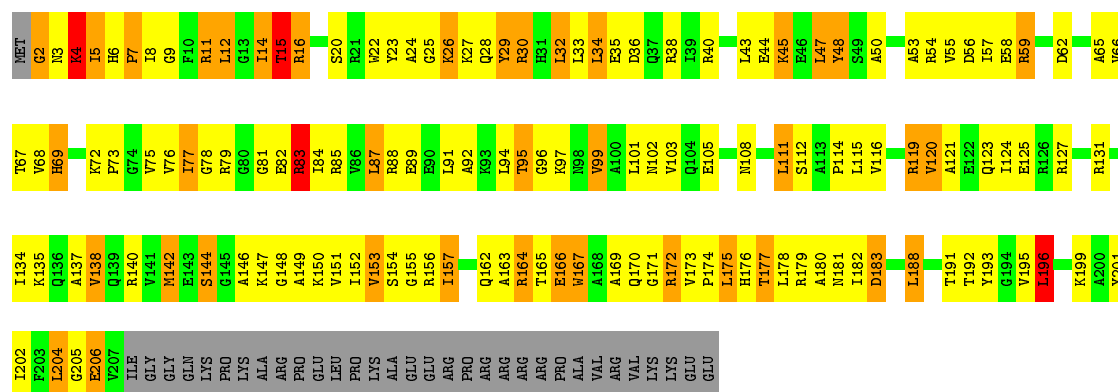


MET	PRO	VAL	GLU	ILE	THR	V7	K8	E9	L10	L11	L12	E12	H16	F17	G18	H19	E20	R21	K22	R23	W24	N25	F28	L29	R30	Y31	I32	Y33	A34	E35	I39	H40	I41	I42	D43	L44	Q45	K46	T47	M48	E49	E50	L51	E52	R53	T54	F55	R56	F57	D60	R64	T67	I68	L69
-----	-----	-----	-----	-----	-----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----



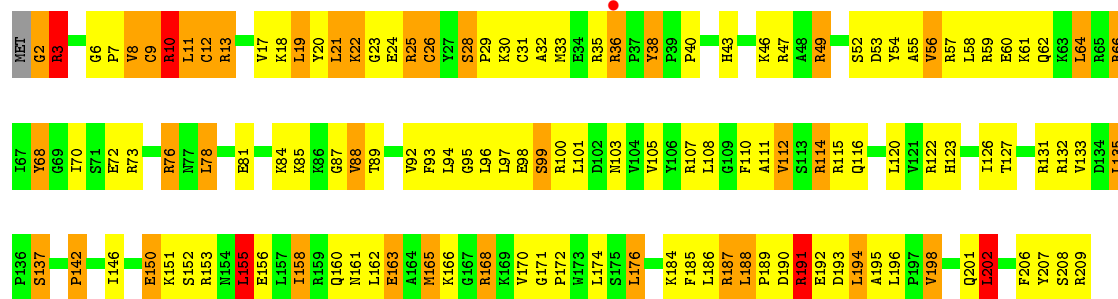
### • Molecule 3: RIBOSOMAL PROTEIN S3

Chain C: 27% 41% 16% 14%



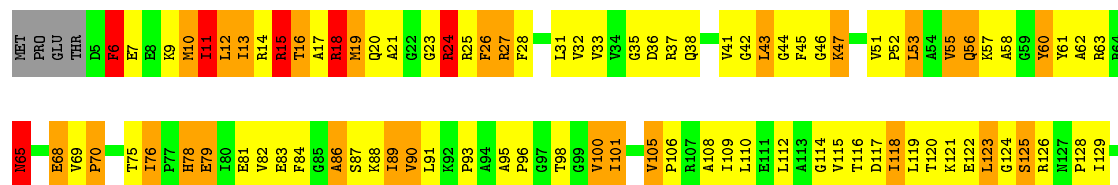
### • Molecule 4: RIBOSOMAL PROTEIN S4

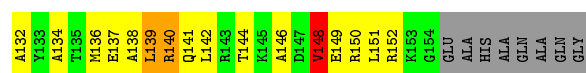
Chain D: 37% 42% 18%



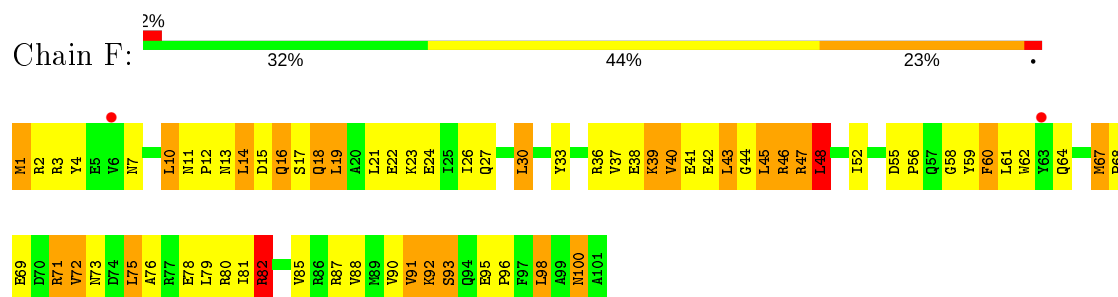
### • Molecule 5: RIBOSOMAL PROTEIN S5

Chain E: 27% 44% 18% 7%

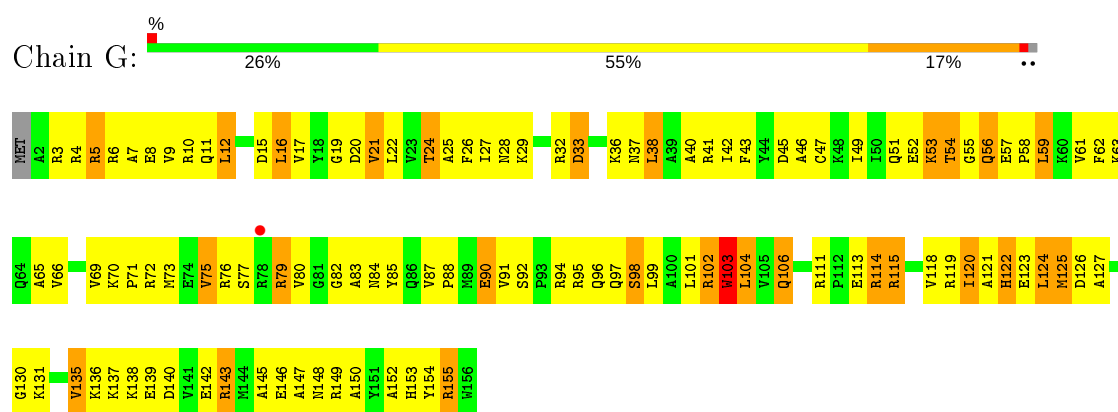




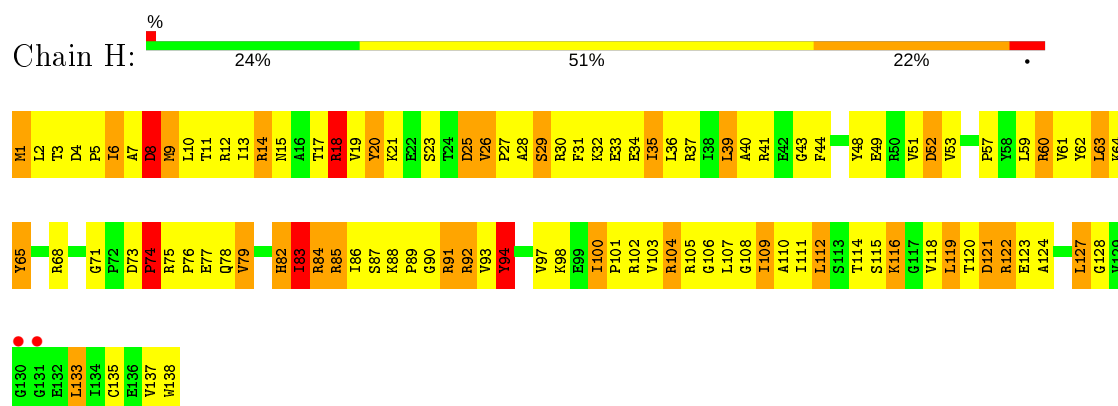
• Molecule 6: RIBOSOMAL PROTEIN S6



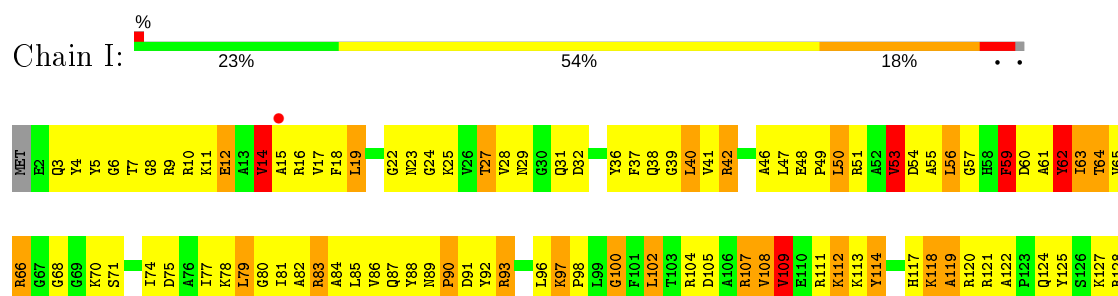
• Molecule 7: RIBOSOMAL PROTEIN S7



• Molecule 8: RIBOSOMAL PROTEIN S8

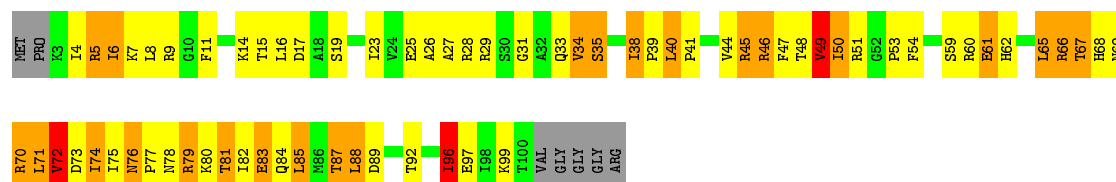


• Molecule 9: RIBOSOMAL PROTEIN S9



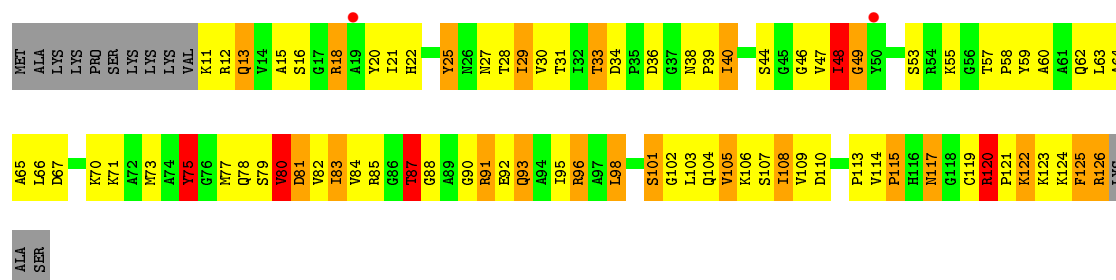
- Molecule 10: RIBOSOMAL PROTEIN S10

Chain J: 



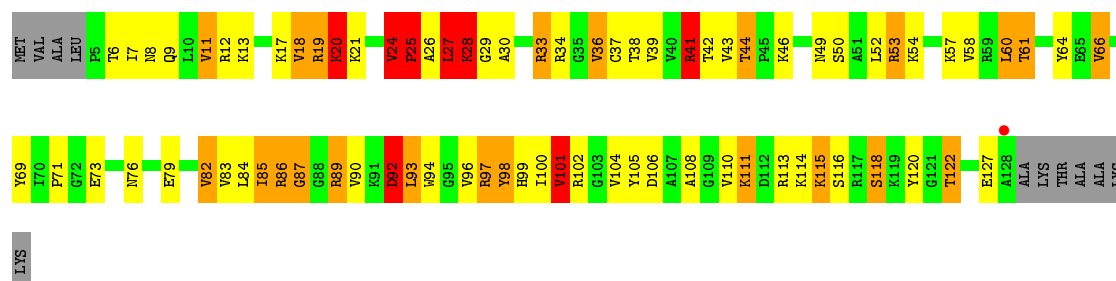
- Molecule 11: RIBOSOMAL PROTEIN S11

Chain K:  2% 26% 43% 16% 10%



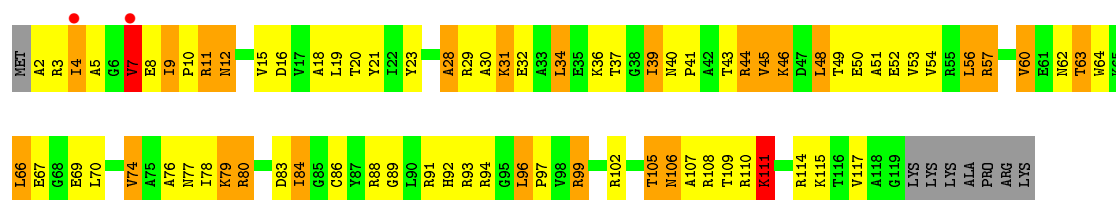
- Molecule 12: RIBOSOMAL PROTEIN S12

Chain L: 



- Molecule 13: RIBOSOMAL PROTEIN S13

Chain M:  2% 32% 40% 20% 6%



- Molecule 14: RIBOSOMAL PROTEIN S14

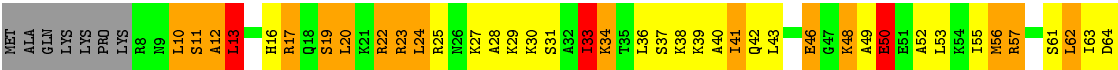
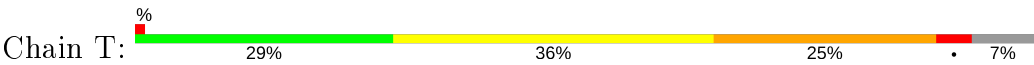
Chain N:  26% 46% 25% .



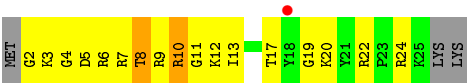




• Molecule 20: RIBOSOMAL PROTEIN S20



• Molecule 21: RIBOSOMAL PROTEIN THX



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	400.31Å 400.31Å 214.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.85 – 3.74 49.85 – 3.74	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.85-3.74) 99.7 (49.85-3.74)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.05 (at 3.77Å)	Xtriage
Refinement program	PHENIX dev_1119	Depositor
R, $R_{free}$	0.137 , 0.187 0.137 , 0.188	Depositor DCC
$R_{free}$ test set	8973 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	154.8	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 160.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	53563	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	154.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.70% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, M2G, MA6, MG, 2MG, 5MC, UR3, 4OC, SRY, 7MG, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	1.86	872/36088 (2.4%)	3.13	6102/56318 (10.8%)
2	B	1.17	6/1935 (0.3%)	1.37	17/2609 (0.7%)
3	C	1.15	3/1636 (0.2%)	1.30	10/2205 (0.5%)
4	D	1.26	4/1733 (0.2%)	1.43	16/2318 (0.7%)
5	E	1.45	9/1162 (0.8%)	1.57	14/1564 (0.9%)
6	F	1.20	0/856	1.37	5/1154 (0.4%)
7	G	1.12	3/1276 (0.2%)	1.25	3/1709 (0.2%)
8	H	1.41	5/1136 (0.4%)	1.55	13/1527 (0.9%)
9	I	1.00	0/1029	1.36	16/1379 (1.2%)
10	J	1.17	0/805	1.47	9/1082 (0.8%)
11	K	1.12	2/879 (0.2%)	1.40	9/1187 (0.8%)
12	L	1.74	21/994 (2.1%)	1.80	27/1331 (2.0%)
13	M	1.08	1/947 (0.1%)	1.22	3/1270 (0.2%)
14	N	1.24	2/501 (0.4%)	1.42	6/664 (0.9%)
15	O	1.25	5/740 (0.7%)	1.48	11/987 (1.1%)
16	P	1.23	0/716	1.45	7/963 (0.7%)
17	Q	1.54	9/836 (1.1%)	1.66	17/1117 (1.5%)
18	R	1.25	0/579	1.47	5/768 (0.7%)
19	S	1.16	2/661 (0.3%)	1.39	9/890 (1.0%)
20	T	1.23	2/765 (0.3%)	1.52	12/1007 (1.2%)
21	U	1.20	0/212	1.20	1/277 (0.4%)
All	All	1.67	946/55486 (1.7%)	2.71	6312/82326 (7.7%)

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
2	B	0	4
3	C	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	5
5	E	0	2
6	F	0	1
8	H	0	1
9	I	0	1
10	J	0	2
11	K	0	2
12	L	0	5
13	M	0	3
14	N	0	1
17	Q	0	2
18	R	0	3
19	S	0	1
20	T	0	3
All	All	0	40

All (946) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	279	A	N9-C4	-16.47	1.27	1.37
1	A	1415	G	N9-C4	15.77	1.50	1.38
1	A	1393	U	C4-O4	13.77	1.34	1.23
1	A	239	U	C4-O4	12.59	1.33	1.23
1	A	372	C	N1-C2	12.45	1.52	1.40
1	A	1397	C	N3-C4	12.26	1.42	1.33
1	A	1502	A	N9-C4	-12.25	1.30	1.37
1	A	333	G	C6-O6	12.24	1.35	1.24
1	A	1492	A	N9-C4	12.23	1.45	1.37
1	A	1509	C	N1-C6	-12.05	1.29	1.37
1	A	1502	A	C5-C6	-12.00	1.30	1.41
4	D	12	CYS	CB-SG	11.98	2.02	1.82
1	A	523	A	N3-C4	-11.85	1.27	1.34
1	A	1346	A	N9-C4	-11.56	1.30	1.37
1	A	782	A	N3-C4	-11.24	1.28	1.34
1	A	839	U	C4-C5	11.11	1.53	1.43
1	A	814	A	N9-C4	-11.08	1.31	1.37
1	A	1529	G	N7-C5	-10.95	1.32	1.39
1	A	439	A	N9-C4	-10.95	1.31	1.37
1	A	1499	A	N3-C4	-10.87	1.28	1.34
1	A	975	A	N9-C4	-10.82	1.31	1.37
1	A	279	A	N7-C5	-10.82	1.32	1.39
1	A	108	G	N9-C4	-10.64	1.29	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	266	G	N9-C4	-10.60	1.29	1.38
1	A	484	G	C6-N1	-10.50	1.32	1.39
1	A	1513	A	N9-C4	-10.49	1.31	1.37
1	A	26	A	N3-C4	-10.47	1.28	1.34
1	A	903	G	N3-C4	-10.46	1.28	1.35
1	A	580	U	C4-O4	10.35	1.31	1.23
1	A	1497	G	N7-C5	-10.28	1.33	1.39
1	A	108	G	N1-C2	10.27	1.46	1.37
1	A	47	C	N1-C6	-10.24	1.31	1.37
1	A	569	C	N3-C4	-10.17	1.26	1.33
1	A	1530	G	C6-N1	10.15	1.46	1.39
12	L	127	GLU	CG-CD	10.13	1.67	1.51
1	A	403	C	N1-C6	-10.10	1.31	1.37
1	A	1397	C	N1-C6	10.06	1.43	1.37
1	A	792	A	N3-C4	-10.02	1.28	1.34
1	A	1393	U	C2-N3	10.00	1.44	1.37
1	A	918	A	C5-C4	-9.95	1.31	1.38
12	L	127	GLU	CB-CG	9.94	1.71	1.52
1	A	325	A	N9-C4	-9.89	1.31	1.37
1	A	1492	A	N3-C4	9.89	1.40	1.34
1	A	144	G	C6-N1	9.79	1.46	1.39
1	A	1414	U	C4-O4	9.72	1.31	1.23
1	A	204	U	C2-N3	9.70	1.44	1.37
1	A	298	A	N3-C4	-9.70	1.29	1.34
1	A	1415	G	C2-N3	9.67	1.40	1.32
1	A	859	A	N9-C4	-9.62	1.32	1.37
1	A	109	A	N9-C4	-9.59	1.32	1.37
1	A	729	A	N3-C4	-9.58	1.29	1.34
1	A	889	A	N3-C4	-9.58	1.29	1.34
1	A	250	A	C5-C4	9.57	1.45	1.38
1	A	651	C	C2-N3	9.56	1.43	1.35
1	A	1523	G	N7-C5	-9.54	1.33	1.39
1	A	1499	A	N9-C4	-9.49	1.32	1.37
1	A	758	G	N7-C5	-9.47	1.33	1.39
1	A	144	G	C5-C4	9.46	1.45	1.38
1	A	144	G	N1-C2	9.41	1.45	1.37
1	A	859	A	N3-C4	-9.37	1.29	1.34
1	A	1393	U	N3-C4	9.29	1.46	1.38
1	A	903	G	C5-C4	-9.26	1.31	1.38
1	A	532	A	N9-C4	9.21	1.43	1.37
1	A	1529	G	N3-C4	-9.20	1.29	1.35
1	A	781	A	N9-C4	-9.17	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	789	U	C4-O4	9.13	1.30	1.23
1	A	1506	U	C2-O2	9.09	1.30	1.22
1	A	1415	G	C5-C4	9.08	1.44	1.38
1	A	930	C	N3-C4	-9.02	1.27	1.33
12	L	98	TYR	CZ-OH	8.97	1.53	1.37
8	H	94	TYR	CD2-CE2	8.92	1.52	1.39
1	A	144	G	C6-O6	8.89	1.32	1.24
1	A	715	A	N9-C4	-8.88	1.32	1.37
1	A	26	A	C6-N1	-8.87	1.29	1.35
1	A	289	G	N7-C5	-8.85	1.33	1.39
1	A	1514	C	N3-C4	-8.84	1.27	1.33
1	A	782	A	N9-C4	-8.83	1.32	1.37
1	A	778	G	N9-C8	-8.73	1.31	1.37
1	A	635	G	C6-O6	8.70	1.31	1.24
1	A	130	A	N3-C4	-8.67	1.29	1.34
1	A	556	C	N1-C6	-8.66	1.31	1.37
1	A	1397	C	C2-N3	8.64	1.42	1.35
1	A	792	A	N9-C4	-8.63	1.32	1.37
1	A	1529	G	N9-C8	-8.59	1.31	1.37
1	A	569	C	N1-C6	-8.57	1.32	1.37
1	A	1401	G	C5-C4	-8.57	1.32	1.38
1	A	1075	C	N1-C6	-8.55	1.32	1.37
1	A	360	A	N9-C4	-8.54	1.32	1.37
1	A	1124	G	N9-C4	8.53	1.44	1.38
1	A	920	U	C2-N3	-8.52	1.31	1.37
1	A	529	G	N7-C5	-8.51	1.34	1.39
1	A	830	G	N7-C5	8.51	1.44	1.39
1	A	524	G	C5-C4	-8.50	1.32	1.38
1	A	722	A	N9-C4	-8.49	1.32	1.37
1	A	149	A	N3-C4	-8.48	1.29	1.34
1	A	389	A	N9-C4	8.45	1.43	1.37
1	A	203	U	C2-N3	8.42	1.43	1.37
1	A	360	A	N3-C4	-8.41	1.29	1.34
1	A	900	A	N7-C5	-8.39	1.34	1.39
1	A	1442	G	N3-C4	8.37	1.41	1.35
1	A	1450	U	C4-O4	8.33	1.30	1.23
1	A	1516	G	C6-N1	8.29	1.45	1.39
1	A	1529	G	N9-C4	-8.29	1.31	1.38
1	A	964	A	N3-C4	-8.28	1.29	1.34
12	L	26	ALA	CA-CB	8.25	1.69	1.52
1	A	439	A	N3-C4	-8.24	1.29	1.34
1	A	964	A	N9-C4	-8.23	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1126	U	P-O5'	8.20	1.68	1.59
1	A	803	G	N3-C4	-8.19	1.29	1.35
1	A	1136	U	C2-N3	8.18	1.43	1.37
1	A	968	A	N3-C4	8.13	1.39	1.34
1	A	651	C	C2-O2	8.12	1.31	1.24
12	L	57	LYS	CD-CE	8.12	1.71	1.51
1	A	509	A	N7-C5	-8.10	1.34	1.39
1	A	14	U	C2-N3	-8.06	1.32	1.37
1	A	518	C	N1-C2	8.06	1.48	1.40
1	A	903	G	C6-N1	-8.02	1.33	1.39
1	A	120	A	N3-C4	-8.01	1.30	1.34
1	A	62	U	C4-O4	8.00	1.30	1.23
1	A	601	C	N1-C6	-7.98	1.32	1.37
1	A	1521	G	C5-C4	-7.96	1.32	1.38
1	A	122	G	N7-C5	-7.94	1.34	1.39
1	A	1125	U	C5-C6	-7.93	1.27	1.34
1	A	1505	G	N9-C8	-7.92	1.32	1.37
1	A	1508	G	C6-N1	-7.88	1.34	1.39
1	A	669	U	C2-O2	7.87	1.29	1.22
1	A	900	A	N9-C4	-7.86	1.33	1.37
1	A	762	C	N1-C6	-7.83	1.32	1.37
1	A	289	G	C5-C4	-7.82	1.32	1.38
1	A	563	A	N9-C4	-7.81	1.33	1.37
1	A	122	G	C5-C6	-7.79	1.34	1.42
1	A	550	G	C6-N1	-7.78	1.34	1.39
1	A	1530	G	N7-C5	7.78	1.44	1.39
1	A	801	U	C2-N3	-7.77	1.32	1.37
1	A	267	C	N3-C4	-7.73	1.28	1.33
1	A	279	A	N3-C4	-7.73	1.30	1.34
1	A	62	U	C2-N3	7.71	1.43	1.37
1	A	1502	A	N7-C5	-7.71	1.34	1.39
1	A	1003	G	N9-C4	7.67	1.44	1.38
1	A	1442	G	N9-C4	7.67	1.44	1.38
1	A	236	G	N1-C2	-7.64	1.31	1.37
1	A	70	G	N9-C4	-7.63	1.31	1.38
1	A	1095	U	C2-O2	-7.63	1.15	1.22
1	A	1102	A	N7-C5	-7.62	1.34	1.39
1	A	130	A	N9-C4	-7.60	1.33	1.37
1	A	622	A	N9-C4	-7.60	1.33	1.37
1	A	320	C	N1-C6	-7.59	1.32	1.37
1	A	818	G	C6-O6	7.59	1.30	1.24
1	A	664	G	N9-C8	-7.58	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	722	A	N3-C4	-7.58	1.30	1.34
1	A	149	A	N9-C4	-7.55	1.33	1.37
1	A	333	G	C6-N1	7.53	1.44	1.39
1	A	1394	A	N9-C4	-7.53	1.33	1.37
1	A	154	C	C2-N3	-7.52	1.29	1.35
1	A	262	A	N7-C5	7.52	1.43	1.39
1	A	1227	A	N3-C4	-7.52	1.30	1.34
1	A	817	C	N1-C6	-7.52	1.32	1.37
1	A	746	A	N3-C4	-7.51	1.30	1.34
1	A	841	U	N1-C2	7.50	1.45	1.38
1	A	720	C	N1-C2	7.50	1.47	1.40
1	A	1499	A	C6-N1	-7.48	1.30	1.35
1	A	815	A	N3-C4	-7.47	1.30	1.34
1	A	883	C	N1-C6	-7.47	1.32	1.37
1	A	1509	C	N3-C4	-7.47	1.28	1.33
12	L	98	TYR	CD2-CE2	7.46	1.50	1.39
8	H	135	CYS	CB-SG	-7.46	1.69	1.82
1	A	523	A	N9-C4	-7.45	1.33	1.37
1	A	531	U	C4-O4	7.45	1.29	1.23
1	A	1392	G	C6-N1	-7.45	1.34	1.39
1	A	452	A	N9-C4	-7.44	1.33	1.37
1	A	778	G	C8-N7	-7.44	1.26	1.30
1	A	910	C	N1-C6	-7.41	1.32	1.37
1	A	379	C	N1-C6	-7.41	1.32	1.37
1	A	715	A	N3-C4	-7.40	1.30	1.34
1	A	54	C	N1-C6	-7.40	1.32	1.37
1	A	883	C	N1-C2	-7.40	1.32	1.40
1	A	524	G	N9-C8	-7.38	1.32	1.37
1	A	1236	A	C5-C6	-7.38	1.34	1.41
1	A	768	A	N7-C5	-7.37	1.34	1.39
1	A	6	G	N9-C4	-7.37	1.32	1.38
1	A	1302	U	N1-C2	7.37	1.45	1.38
1	A	1516	G	N1-C2	7.36	1.43	1.37
1	A	60	A	N3-C4	-7.33	1.30	1.34
1	A	590	C	N1-C6	-7.32	1.32	1.37
1	A	1125	U	P-O5'	7.31	1.67	1.59
13	M	7	VAL	CA-CB	7.30	1.70	1.54
1	A	898	G	N7-C5	-7.29	1.34	1.39
1	A	1308	U	C4-O4	7.27	1.29	1.23
1	A	1127	G	N7-C5	-7.26	1.34	1.39
1	A	1397	C	C2-O2	7.26	1.30	1.24
1	A	579	G	N7-C5	-7.25	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	810	C	N3-C4	-7.25	1.28	1.33
1	A	579	G	C5-C6	-7.25	1.35	1.42
1	A	484	G	N1-C2	-7.24	1.31	1.37
1	A	81	U	C2-N3	7.22	1.42	1.37
1	A	250	A	C6-N1	7.22	1.40	1.35
1	A	532	A	C5-C4	7.22	1.43	1.38
1	A	108	G	N3-C4	-7.22	1.30	1.35
17	Q	28	PRO	CA-C	-7.21	1.38	1.52
17	Q	67	LYS	CD-CE	7.21	1.69	1.51
1	A	1110	A	N3-C4	-7.20	1.30	1.34
1	A	50	A	C6-N1	-7.19	1.30	1.35
1	A	1086	U	C2-N3	7.19	1.42	1.37
1	A	1501	C	N3-C4	-7.19	1.28	1.33
1	A	532	A	N3-C4	7.18	1.39	1.34
1	A	729	A	N9-C8	-7.18	1.32	1.37
1	A	43	C	C2-O2	7.17	1.30	1.24
1	A	1205	U	C2-N3	-7.16	1.32	1.37
1	A	300	A	N9-C4	-7.15	1.33	1.37
1	A	51	A	C5-C6	-7.14	1.34	1.41
12	L	57	LYS	CB-CG	7.14	1.71	1.52
1	A	1461	G	N9-C4	-7.13	1.32	1.38
1	A	839	U	N1-C2	7.13	1.45	1.38
1	A	276	G	C6-O6	7.13	1.30	1.24
1	A	887	G	N3-C4	-7.11	1.30	1.35
1	A	122	G	C5-C4	-7.11	1.33	1.38
1	A	1506	U	N1-C2	7.10	1.45	1.38
1	A	900	A	C5-C6	-7.09	1.34	1.41
1	A	722	A	C5-C6	-7.08	1.34	1.41
1	A	364	A	N7-C5	-7.07	1.35	1.39
1	A	1393	U	C5-C6	7.06	1.40	1.34
1	A	251	G	C5-C4	7.05	1.43	1.38
1	A	26	A	N7-C5	-7.05	1.35	1.39
1	A	729	A	C5-C4	-7.03	1.33	1.38
1	A	1125	U	O3'-P	7.02	1.69	1.61
1	A	1438	G	N3-C4	-7.01	1.30	1.35
1	A	1502	A	N3-C4	-7.00	1.30	1.34
1	A	787	A	N9-C4	-6.99	1.33	1.37
1	A	769	G	N7-C5	-6.99	1.35	1.39
1	A	949	A	N9-C4	-6.99	1.33	1.37
1	A	1230	C	C2-O2	6.98	1.30	1.24
1	A	778	G	C6-O6	6.98	1.30	1.24
1	A	898	G	C5-C6	-6.97	1.35	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1086	U	N1-C2	6.97	1.44	1.38
1	A	250	A	N1-C2	6.96	1.40	1.34
1	A	986	A	N9-C4	-6.95	1.33	1.37
1	A	787	A	N3-C4	-6.95	1.30	1.34
1	A	293	G	N3-C4	-6.94	1.30	1.35
1	A	1106	G	N7-C5	-6.93	1.35	1.39
15	O	34	LEU	CG-CD1	6.93	1.77	1.51
1	A	553	A	N3-C4	-6.93	1.30	1.34
1	A	282	A	C5-C6	-6.90	1.34	1.41
1	A	357	G	C5-C4	-6.90	1.33	1.38
1	A	1139	G	C5-C4	6.90	1.43	1.38
1	A	823	G	N9-C4	-6.89	1.32	1.38
1	A	236	G	C6-N1	-6.88	1.34	1.39
1	A	799	G	C6-N1	-6.87	1.34	1.39
1	A	722	A	N7-C5	-6.87	1.35	1.39
1	A	251	G	N7-C5	6.86	1.43	1.39
1	A	1492	A	N7-C5	6.86	1.43	1.39
1	A	32	A	C6-N1	-6.84	1.30	1.35
1	A	396	G	N7-C5	-6.84	1.35	1.39
1	A	676	A	N1-C2	-6.84	1.28	1.34
1	A	584	G	C5-C4	-6.84	1.33	1.38
1	A	701	C	N1-C6	-6.83	1.33	1.37
1	A	41	G	N3-C4	-6.82	1.30	1.35
1	A	134	A	N3-C4	-6.82	1.30	1.34
1	A	1191	A	C5-C6	-6.80	1.34	1.41
1	A	1529	G	C6-N1	-6.80	1.34	1.39
1	A	1487	G	N1-C2	-6.79	1.32	1.37
1	A	284	G	C6-O6	6.79	1.30	1.24
12	L	57	LYS	CE-NZ	6.74	1.66	1.49
1	A	364	A	N9-C4	-6.74	1.33	1.37
1	A	1127	G	N9-C4	-6.73	1.32	1.38
1	A	767	A	N9-C4	-6.73	1.33	1.37
1	A	1505	G	C6-O6	6.73	1.30	1.24
1	A	313	A	N9-C4	-6.73	1.33	1.37
1	A	325	A	N3-C4	-6.73	1.30	1.34
1	A	310	G	C5-C4	-6.72	1.33	1.38
1	A	921	U	C2-N3	6.72	1.42	1.37
1	A	760	G	N7-C5	6.72	1.43	1.39
1	A	43	C	N1-C6	-6.71	1.33	1.37
1	A	1177	G	N7-C5	-6.71	1.35	1.39
1	A	1493	A	N9-C4	6.71	1.41	1.37
1	A	1394	A	N3-C4	-6.71	1.30	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1487	G	C6-N1	-6.71	1.34	1.39
1	A	338	A	N9-C4	-6.70	1.33	1.37
1	A	735	C	C5-C6	-6.69	1.28	1.34
1	A	926	G	C5-C4	-6.69	1.33	1.38
12	L	98	TYR	CD1-CE1	6.69	1.49	1.39
1	A	230	G	C6-O6	6.69	1.30	1.24
1	A	1252	A	C5-C4	-6.69	1.34	1.38
1	A	651	C	N1-C6	6.69	1.41	1.37
1	A	1080	A	C5-C4	-6.68	1.34	1.38
1	A	284	G	C6-N1	6.68	1.44	1.39
1	A	908	A	C6-N1	-6.68	1.30	1.35
1	A	1190	G	C6-O6	6.68	1.30	1.24
1	A	59	A	N9-C4	-6.68	1.33	1.37
1	A	116	A	N9-C4	-6.67	1.33	1.37
1	A	1350	A	C5-C4	-6.67	1.34	1.38
1	A	521	G	N7-C5	6.67	1.43	1.39
1	A	329	A	C5-C6	-6.67	1.35	1.41
1	A	1530	G	N3-C4	6.64	1.40	1.35
1	A	819	A	N9-C4	-6.64	1.33	1.37
1	A	902	G	N9-C8	-6.64	1.33	1.37
1	A	47	C	N3-C4	-6.64	1.29	1.33
1	A	975	A	C5-C4	6.64	1.43	1.38
1	A	1528	U	C4-O4	-6.64	1.18	1.23
1	A	714	G	N9-C8	-6.63	1.33	1.37
1	A	767	A	N3-C4	-6.62	1.30	1.34
1	A	618	C	C2-O2	6.62	1.30	1.24
1	A	810	C	N1-C6	-6.61	1.33	1.37
1	A	6	G	N3-C4	-6.61	1.30	1.35
1	A	203	U	N3-C4	6.59	1.44	1.38
1	A	1529	G	C5-C4	-6.59	1.33	1.38
1	A	396	G	C6-N1	-6.59	1.34	1.39
1	A	1379	G	N9-C4	-6.59	1.32	1.38
1	A	734	G	C5-C6	-6.58	1.35	1.42
1	A	251	G	C6-O6	6.58	1.30	1.24
1	A	1373	G	N7-C5	-6.57	1.35	1.39
1	A	1177	G	C5-C6	-6.57	1.35	1.42
1	A	930	C	N1-C6	-6.56	1.33	1.37
1	A	198	G	C8-N7	-6.56	1.27	1.30
1	A	566	G	N7-C5	-6.56	1.35	1.39
1	A	193	C	N1-C6	-6.56	1.33	1.37
1	A	300	A	N3-C4	-6.56	1.30	1.34
1	A	55	A	N3-C4	-6.55	1.30	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	897	C	N3-C4	-6.55	1.29	1.33
1	A	908	A	N3-C4	-6.55	1.30	1.34
1	A	111	G	N9-C4	-6.54	1.32	1.38
14	N	61	TRP	CB-CG	-6.54	1.38	1.50
1	A	154	C	N1-C6	-6.53	1.33	1.37
1	A	500	G	N9-C4	-6.53	1.32	1.38
1	A	730	G	N9-C8	-6.53	1.33	1.37
1	A	653	A	N9-C4	6.53	1.41	1.37
1	A	394	G	C5-C4	-6.52	1.33	1.38
1	A	1054	C	N3-C4	6.52	1.38	1.33
1	A	1279	A	N7-C5	-6.52	1.35	1.39
1	A	1197	G	C6-N1	-6.52	1.34	1.39
1	A	319	G	N7-C5	-6.51	1.35	1.39
1	A	308	C	C2-O2	6.50	1.30	1.24
1	A	558	G	N3-C4	-6.49	1.30	1.35
1	A	1379	G	N7-C5	-6.49	1.35	1.39
1	A	1236	A	C5-C4	-6.49	1.34	1.38
1	A	109	A	N3-C4	-6.48	1.30	1.34
1	A	300	A	C6-N1	-6.47	1.31	1.35
1	A	108	G	N7-C5	-6.47	1.35	1.39
1	A	1136	U	N3-C4	6.47	1.44	1.38
1	A	184	G	C6-N1	-6.47	1.35	1.39
3	C	125	GLU	CG-CD	6.46	1.61	1.51
5	E	16	THR	CA-CB	6.46	1.70	1.53
1	A	51	A	C6-N6	-6.45	1.28	1.33
1	A	515	G	N7-C5	-6.45	1.35	1.39
1	A	769	G	N9-C8	-6.45	1.33	1.37
1	A	282	A	N3-C4	-6.44	1.30	1.34
1	A	545	C	N3-C4	-6.44	1.29	1.33
1	A	1528	U	N1-C6	-6.43	1.32	1.38
1	A	53	A	N3-C4	-6.42	1.30	1.34
1	A	728	A	N7-C5	-6.41	1.35	1.39
1	A	883	C	C2-O2	-6.41	1.18	1.24
1	A	839	U	C4-O4	6.41	1.28	1.23
1	A	862	C	N1-C6	-6.41	1.33	1.37
1	A	379	C	N3-C4	-6.41	1.29	1.33
1	A	929	G	C5-C4	-6.41	1.33	1.38
1	A	328	C	C2-O2	-6.40	1.18	1.24
1	A	666	G	C6-O6	6.40	1.29	1.24
1	A	1438	G	N9-C4	-6.39	1.32	1.38
12	L	36	VAL	CA-CB	-6.39	1.41	1.54
1	A	562	C	C2-N3	-6.39	1.30	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	57	LYS	CG-CD	6.39	1.74	1.52
1	A	44	G	C8-N7	-6.38	1.27	1.30
1	A	732	C	N1-C6	-6.37	1.33	1.37
1	A	396	G	N3-C4	-6.37	1.30	1.35
1	A	126	G	N3-C4	-6.37	1.30	1.35
1	A	276	G	C2-N2	-6.36	1.28	1.34
1	A	1194	U	N1-C6	-6.36	1.32	1.38
1	A	542	G	C2-N3	-6.35	1.27	1.32
1	A	289	G	C6-N1	-6.35	1.35	1.39
1	A	41	G	C2-N3	-6.34	1.27	1.32
1	A	721	G	N9-C4	6.33	1.43	1.38
1	A	1174	G	N7-C5	6.33	1.43	1.39
1	A	150	C	C2-O2	6.33	1.30	1.24
1	A	899	C	C2-N3	6.32	1.40	1.35
1	A	132	C	C2-O2	-6.32	1.18	1.24
1	A	723	U	C2-N3	6.32	1.42	1.37
1	A	1193	G	N9-C4	-6.30	1.32	1.38
1	A	230	G	C8-N7	-6.30	1.27	1.30
1	A	1504	G	N7-C5	-6.30	1.35	1.39
1	A	760	G	C5-C6	6.30	1.48	1.42
1	A	889	A	C6-N1	-6.30	1.31	1.35
1	A	121	C	C2-O2	6.30	1.30	1.24
12	L	66	VAL	CB-CG1	-6.30	1.39	1.52
1	A	734	G	N7-C5	-6.29	1.35	1.39
1	A	177	C	N1-C6	-6.29	1.33	1.37
1	A	234	C	C2-N3	-6.29	1.30	1.35
1	A	1514	C	N1-C6	-6.28	1.33	1.37
1	A	779	C	N1-C6	-6.27	1.33	1.37
5	E	148	VAL	CA-CB	-6.27	1.41	1.54
1	A	236	G	C5-C4	-6.27	1.33	1.38
1	A	311	C	N1-C6	-6.27	1.33	1.37
1	A	729	A	C6-N1	-6.25	1.31	1.35
1	A	574	A	C5-C6	-6.25	1.35	1.41
1	A	836	G	C6-N1	6.25	1.44	1.39
1	A	915	A	N9-C4	-6.24	1.34	1.37
1	A	1521	G	N9-C8	-6.24	1.33	1.37
1	A	510	A	N3-C4	-6.23	1.31	1.34
1	A	1405	G	C5-C6	-6.23	1.36	1.42
1	A	318	G	C2-N3	-6.23	1.27	1.32
1	A	722	A	C6-N1	-6.22	1.31	1.35
1	A	841	U	C2-N3	6.22	1.42	1.37
1	A	927	G	N9-C8	6.22	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	840	C	N3-C4	6.22	1.38	1.33
1	A	728	A	C6-N1	-6.22	1.31	1.35
1	A	1227	A	C5-C6	-6.21	1.35	1.41
12	L	98	TYR	CE2-CZ	6.21	1.46	1.38
1	A	741	G	N9-C8	-6.20	1.33	1.37
1	A	122	G	C8-N7	-6.19	1.27	1.30
1	A	190(D)	U	N1-C2	6.19	1.44	1.38
1	A	1451	A	N9-C4	-6.19	1.34	1.37
1	A	319	G	N3-C4	-6.19	1.31	1.35
1	A	874	G	N9-C8	-6.18	1.33	1.37
1	A	1139	G	C5-C6	6.18	1.48	1.42
1	A	574	A	N7-C5	-6.18	1.35	1.39
1	A	1460	A	N9-C4	-6.18	1.34	1.37
1	A	576	G	C6-N1	-6.17	1.35	1.39
1	A	676	A	N7-C5	6.17	1.43	1.39
1	A	938	A	N3-C4	-6.16	1.31	1.34
1	A	955	U	C2-N3	-6.16	1.33	1.37
1	A	1493	A	N3-C4	6.16	1.38	1.34
1	A	723	U	C4-O4	6.16	1.28	1.23
1	A	1124	G	C5-C4	6.16	1.42	1.38
1	A	786	G	N7-C5	-6.15	1.35	1.39
1	A	923	A	C6-N1	-6.15	1.31	1.35
1	A	282	A	C5-C4	-6.15	1.34	1.38
1	A	357	G	N1-C2	-6.15	1.32	1.37
1	A	1488	G	N9-C8	-6.15	1.33	1.37
1	A	553	A	C6-N1	-6.15	1.31	1.35
1	A	769	G	C5-C4	-6.15	1.34	1.38
15	O	3	ILE	CA-CB	6.15	1.69	1.54
5	E	149	GLU	CG-CD	6.14	1.61	1.51
1	A	687	A	N9-C8	-6.13	1.32	1.37
2	B	97	TRP	CG-CD1	6.13	1.45	1.36
1	A	524	G	N7-C5	-6.11	1.35	1.39
1	A	307	C	N3-C4	6.11	1.38	1.33
1	A	1236	A	N9-C4	-6.11	1.34	1.37
1	A	497	A	N3-C4	-6.11	1.31	1.34
1	A	655	A	C6-N6	-6.11	1.29	1.33
1	A	333	G	C2-N3	-6.10	1.27	1.32
1	A	1197	G	N3-C4	-6.10	1.31	1.35
1	A	1497	G	N9-C8	-6.09	1.33	1.37
1	A	494	G	N7-C5	-6.09	1.35	1.39
1	A	1075	C	N3-C4	-6.09	1.29	1.33
1	A	782	A	C6-N1	-6.08	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	712	A	N3-C4	-6.08	1.31	1.34
1	A	921	U	C4-O4	6.08	1.28	1.23
1	A	875	C	N3-C4	-6.07	1.29	1.33
1	A	293	G	N9-C4	-6.07	1.33	1.38
1	A	662	G	C5-C4	6.07	1.42	1.38
1	A	818	G	C5-C6	6.07	1.48	1.42
1	A	853	G	C2-N3	6.06	1.37	1.32
1	A	784	C	N1-C6	-6.06	1.33	1.37
8	H	49	GLU	CG-CD	6.06	1.61	1.51
1	A	569	C	C2-N3	-6.06	1.30	1.35
1	A	1485	U	C4-O4	6.06	1.28	1.23
1	A	792	A	N7-C5	-6.05	1.35	1.39
1	A	672	U	C4-O4	6.05	1.28	1.23
1	A	315	A	N9-C4	-6.04	1.34	1.37
1	A	28	G	N3-C4	-6.04	1.31	1.35
1	A	887	G	C2-N3	-6.04	1.27	1.32
1	A	1222	G	N1-C2	6.03	1.42	1.37
1	A	900	A	C5-C4	-6.02	1.34	1.38
1	A	1490	C	N3-C4	-6.02	1.29	1.33
1	A	1505	G	C8-N7	-6.02	1.27	1.30
1	A	413	G	N9-C4	-6.01	1.33	1.38
1	A	644	G	C5-C4	-6.01	1.34	1.38
1	A	803	G	N1-C2	-6.01	1.32	1.37
1	A	1443	G	N9-C4	-6.01	1.33	1.38
1	A	836	G	N1-C2	6.01	1.42	1.37
1	A	929	G	N9-C8	-6.01	1.33	1.37
1	A	578	C	N3-C4	-6.00	1.29	1.33
1	A	1147	C	N1-C2	6.00	1.46	1.40
17	Q	24	GLU	CG-CD	6.00	1.60	1.51
1	A	51	A	N9-C4	-5.99	1.34	1.37
1	A	81	U	N3-C4	5.99	1.43	1.38
1	A	918	A	C6-N1	-5.99	1.31	1.35
1	A	832	C	N1-C6	-5.99	1.33	1.37
1	A	553	A	N9-C4	-5.98	1.34	1.37
1	A	542	G	N3-C4	-5.97	1.31	1.35
1	A	1370	G	N7-C5	-5.97	1.35	1.39
19	S	80	TYR	CD2-CE2	5.97	1.48	1.39
1	A	910	C	C2-O2	-5.97	1.19	1.24
1	A	1366	C	C2-N3	-5.97	1.30	1.35
1	A	1526	G	C2-N3	-5.97	1.27	1.32
1	A	228	A	C6-N1	-5.97	1.31	1.35
1	A	289	G	N3-C4	-5.97	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	865	A	N7-C5	-5.96	1.35	1.39
1	A	220	G	N7-C5	-5.95	1.35	1.39
1	A	1014	A	N9-C4	5.95	1.41	1.37
1	A	1202	G	N9-C4	-5.95	1.33	1.38
1	A	365	U	N1-C6	-5.95	1.32	1.38
1	A	906	G	N7-C5	-5.95	1.35	1.39
5	E	60	TYR	CE1-CZ	5.95	1.46	1.38
1	A	282	A	N9-C4	-5.95	1.34	1.37
15	O	60	VAL	CA-CB	-5.94	1.42	1.54
1	A	1374	A	C6-N1	-5.94	1.31	1.35
1	A	55	A	C6-N1	-5.94	1.31	1.35
1	A	263	A	N9-C4	-5.93	1.34	1.37
1	A	663	A	N9-C4	-5.93	1.34	1.37
1	A	797	C	N1-C6	-5.93	1.33	1.37
1	A	759	A	N9-C4	-5.92	1.34	1.37
1	A	907	A	N3-C4	-5.92	1.31	1.34
1	A	573	A	N7-C5	-5.92	1.35	1.39
1	A	266	G	N7-C5	-5.91	1.35	1.39
1	A	1092	A	N9-C4	-5.91	1.34	1.37
1	A	338	A	N7-C5	-5.91	1.35	1.39
1	A	204	U	N3-C4	5.90	1.43	1.38
1	A	36	C	N1-C6	-5.90	1.33	1.37
1	A	111	G	C6-N1	5.90	1.43	1.39
1	A	760	G	N3-C4	-5.90	1.31	1.35
1	A	676	A	N9-C4	5.90	1.41	1.37
1	A	281	G	N1-C2	-5.90	1.33	1.37
14	N	27	CYS	CB-SG	-5.89	1.72	1.81
1	A	224	C	N1-C6	-5.89	1.33	1.37
1	A	481	G	N7-C5	-5.89	1.35	1.39
1	A	596	C	N3-C4	-5.88	1.29	1.33
11	K	105	VAL	CB-CG2	5.88	1.65	1.52
1	A	44	G	N3-C4	-5.88	1.31	1.35
1	A	576	G	N7-C5	-5.88	1.35	1.39
1	A	1529	G	C5-C6	-5.87	1.36	1.42
1	A	299	G	N3-C4	-5.87	1.31	1.35
1	A	515	G	N3-C4	-5.87	1.31	1.35
11	K	75	TYR	CE2-CZ	5.87	1.46	1.38
1	A	1079	G	N7-C5	-5.86	1.35	1.39
1	A	1124	G	N3-C4	5.86	1.39	1.35
1	A	1101	A	C6-N6	5.86	1.38	1.33
1	A	1514	C	C4-N4	-5.86	1.28	1.33
1	A	1252	A	N9-C8	-5.85	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	566	G	C5-C6	-5.85	1.36	1.42
1	A	331	G	N7-C5	-5.84	1.35	1.39
1	A	1193	G	N3-C4	-5.84	1.31	1.35
1	A	117	G	C6-N1	5.84	1.43	1.39
1	A	892	A	N3-C4	-5.84	1.31	1.34
1	A	61	G	N9-C4	-5.84	1.33	1.38
1	A	885	G	C2-N3	-5.83	1.28	1.32
1	A	438	G	C5-C6	5.83	1.48	1.42
1	A	1093	A	C5-C4	-5.82	1.34	1.38
1	A	1386	G	N9-C8	-5.82	1.33	1.37
1	A	133	U	C4-O4	5.82	1.28	1.23
1	A	298	A	N9-C4	-5.82	1.34	1.37
1	A	1510	U	C2-O2	5.82	1.27	1.22
1	A	908	A	N9-C4	-5.82	1.34	1.37
1	A	431	A	N9-C4	-5.81	1.34	1.37
1	A	1397	C	N1-C2	5.81	1.46	1.40
1	A	331	G	N9-C8	-5.81	1.33	1.37
1	A	533	A	C6-N1	-5.81	1.31	1.35
1	A	614	A	C5-C6	-5.80	1.35	1.41
1	A	900	A	N3-C4	-5.80	1.31	1.34
1	A	930	C	C2-N3	-5.79	1.31	1.35
1	A	675	A	N9-C4	-5.79	1.34	1.37
1	A	1374	A	N3-C4	-5.79	1.31	1.34
1	A	560	U	C2-N3	-5.79	1.33	1.37
1	A	568	G	C6-N1	-5.79	1.35	1.39
1	A	184	G	N9-C8	-5.78	1.33	1.37
8	H	20	TYR	CE2-CZ	5.78	1.46	1.38
1	A	1487	G	N9-C4	5.78	1.42	1.38
1	A	54	C	C4-C5	-5.77	1.38	1.43
1	A	1351	U	C2-N3	-5.77	1.33	1.37
1	A	814	A	N7-C5	-5.77	1.35	1.39
1	A	898	G	N3-C4	-5.77	1.31	1.35
1	A	975	A	N3-C4	-5.76	1.31	1.34
1	A	582	U	C2-N3	-5.76	1.33	1.37
1	A	896	C	N1-C6	-5.75	1.33	1.37
1	A	246	A	C5-C4	-5.75	1.34	1.38
17	Q	67	LYS	CB-CG	5.75	1.68	1.52
1	A	10	A	C6-N1	-5.75	1.31	1.35
1	A	1336	C	N1-C6	-5.75	1.33	1.37
1	A	1495	U	C4-O4	5.75	1.28	1.23
1	A	1506	U	C2-N3	5.75	1.41	1.37
1	A	1526	G	N3-C4	-5.75	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	42	G	C5-C6	-5.75	1.36	1.42
1	A	1388	C	N3-C4	-5.75	1.29	1.33
19	S	80	TYR	CE2-CZ	5.74	1.46	1.38
1	A	873	A	C5-C4	-5.74	1.34	1.38
1	A	854	G	N7-C5	-5.74	1.35	1.39
1	A	855	G	N3-C4	-5.73	1.31	1.35
1	A	149	A	C6-N1	-5.73	1.31	1.35
1	A	137	C	C2-O2	5.73	1.29	1.24
1	A	117	G	N1-C2	5.73	1.42	1.37
1	A	730	G	N3-C4	-5.72	1.31	1.35
4	D	112	VAL	CB-CG1	5.72	1.64	1.52
1	A	137	C	N1-C2	5.72	1.45	1.40
1	A	315	A	C6-N1	-5.72	1.31	1.35
1	A	802	A	N7-C5	-5.72	1.35	1.39
1	A	885	G	N3-C4	-5.72	1.31	1.35
1	A	53	A	C6-N1	-5.71	1.31	1.35
1	A	1468	A	N9-C4	-5.71	1.34	1.37
1	A	111	G	C6-O6	5.71	1.29	1.24
1	A	799	G	N9-C4	-5.71	1.33	1.38
1	A	19	C	N1-C6	-5.71	1.33	1.37
1	A	526	C	N1-C6	-5.71	1.33	1.37
1	A	623	C	N1-C6	-5.70	1.33	1.37
1	A	523	A	C6-N1	-5.70	1.31	1.35
1	A	637	G	N7-C5	5.69	1.42	1.39
7	G	103	TRP	CB-CG	-5.69	1.40	1.50
1	A	277	C	N1-C6	-5.69	1.33	1.37
1	A	235	C	N1-C6	-5.68	1.33	1.37
1	A	1020	U	N1-C2	5.68	1.43	1.38
1	A	44	G	N9-C8	-5.67	1.33	1.37
1	A	890	G	N9-C8	-5.67	1.33	1.37
1	A	331	G	C8-N7	-5.67	1.27	1.30
1	A	723	U	N1-C2	5.67	1.43	1.38
1	A	807	A	N7-C5	-5.66	1.35	1.39
1	A	903	G	N7-C5	-5.66	1.35	1.39
1	A	1414	U	C2-N3	5.66	1.41	1.37
1	A	1497	G	C6-N1	-5.65	1.35	1.39
1	A	1401	G	N9-C8	-5.65	1.33	1.37
1	A	1095	U	N1-C2	-5.64	1.33	1.38
1	A	1126	U	O3'-P	5.64	1.68	1.61
1	A	570	G	C5-C4	-5.64	1.34	1.38
1	A	1544	U	C4-O4	5.64	1.28	1.23
1	A	234	C	N3-C4	-5.63	1.30	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	60	TYR	CZ-OH	5.63	1.47	1.37
1	A	26	A	C5-C6	-5.63	1.35	1.41
1	A	338	A	N3-C4	-5.63	1.31	1.34
1	A	887	G	C5-C4	-5.62	1.34	1.38
1	A	806	C	C4-C5	-5.62	1.38	1.43
1	A	143	A	N3-C4	5.61	1.38	1.34
1	A	303	A	N3-C4	-5.61	1.31	1.34
1	A	750	G	N7-C5	5.61	1.42	1.39
1	A	691	G	N7-C5	-5.61	1.35	1.39
1	A	1508	G	N3-C4	-5.60	1.31	1.35
1	A	199	G	N9-C4	-5.60	1.33	1.38
1	A	333	G	N3-C4	-5.60	1.31	1.35
1	A	1415	G	N3-C4	5.60	1.39	1.35
17	Q	67	LYS	CE-NZ	5.60	1.63	1.49
1	A	785	G	C5-C4	-5.59	1.34	1.38
1	A	236	G	C8-N7	-5.59	1.27	1.30
1	A	635	G	C6-N1	5.59	1.43	1.39
1	A	1499	A	C5-C4	-5.59	1.34	1.38
20	T	12	ALA	CA-C	5.59	1.67	1.52
1	A	1222	G	C6-O6	5.58	1.29	1.24
1	A	903	G	N9-C8	-5.58	1.33	1.37
1	A	416	G	C6-N1	-5.57	1.35	1.39
1	A	58	C	N1-C6	-5.57	1.33	1.37
1	A	242	C	C5-C6	-5.57	1.29	1.34
1	A	368	U	N1-C6	-5.57	1.32	1.38
1	A	1251	A	N7-C5	-5.57	1.35	1.39
1	A	1442	G	C2-N3	5.57	1.37	1.32
1	A	828	A	N7-C5	-5.56	1.35	1.39
1	A	42	G	N7-C5	-5.56	1.35	1.39
1	A	117	G	N7-C5	-5.56	1.35	1.39
1	A	1495	U	C2-N3	5.56	1.41	1.37
1	A	1438	G	N9-C8	-5.55	1.33	1.37
7	G	83	ALA	CA-CB	5.54	1.64	1.52
1	A	402	G	N1-C2	-5.54	1.33	1.37
1	A	965	A	N9-C4	-5.54	1.34	1.37
1	A	281	G	C8-N7	-5.54	1.27	1.30
1	A	886	G	N7-C5	-5.54	1.35	1.39
1	A	1478	C	C2-N3	5.54	1.40	1.35
1	A	1499	A	N9-C8	-5.54	1.33	1.37
1	A	1439	C	C2-O2	5.54	1.29	1.24
1	A	566	G	C5-C4	-5.53	1.34	1.38
1	A	1080	A	N9-C8	-5.53	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	446	G	N3-C4	-5.53	1.31	1.35
1	A	62	U	C5-C6	5.52	1.39	1.34
1	A	1413	A	N3-C4	-5.52	1.31	1.34
1	A	590	C	C2-N3	-5.52	1.31	1.35
1	A	918	A	N3-C4	-5.52	1.31	1.34
1	A	111	G	N1-C2	5.51	1.42	1.37
1	A	678	U	C2-N3	-5.51	1.33	1.37
1	A	704	A	N9-C4	-5.51	1.34	1.37
1	A	117	G	C6-O6	5.51	1.29	1.24
1	A	728	A	N9-C4	-5.51	1.34	1.37
1	A	27	G	C5-C6	-5.51	1.36	1.42
7	G	76	ARG	CG-CD	5.51	1.65	1.51
1	A	239	U	C2-N3	5.50	1.41	1.37
1	A	1013	G	C5-C6	5.50	1.47	1.42
1	A	584	G	N9-C8	-5.50	1.33	1.37
1	A	955	U	N1-C6	-5.50	1.32	1.38
1	A	260	G	C5-C4	5.50	1.42	1.38
1	A	58	C	C4-C5	-5.50	1.38	1.43
1	A	506	G	C8-N7	-5.49	1.27	1.30
1	A	926	G	C2-N3	-5.49	1.28	1.32
1	A	522	C	C2-O2	5.49	1.29	1.24
1	A	43	C	N3-C4	-5.49	1.30	1.33
1	A	899	C	C2-O2	5.49	1.29	1.24
1	A	875	C	N1-C6	-5.49	1.33	1.37
1	A	543	C	N3-C4	-5.48	1.30	1.33
1	A	310	G	N9-C8	-5.48	1.34	1.37
1	A	357	G	N3-C4	-5.48	1.31	1.35
1	A	1222	G	C5-C4	5.48	1.42	1.38
1	A	1347	G	N3-C4	-5.47	1.31	1.35
12	L	120	TYR	CD2-CE2	5.47	1.47	1.39
1	A	123	C	N1-C6	-5.47	1.33	1.37
1	A	728	A	N3-C4	-5.47	1.31	1.34
1	A	921	U	N3-C4	5.47	1.43	1.38
12	L	18	VAL	CB-CG1	5.47	1.64	1.52
1	A	726	C	C4-C5	-5.46	1.38	1.43
1	A	1373	G	N9-C4	5.46	1.42	1.38
1	A	266	G	C5-C6	-5.45	1.36	1.42
1	A	1366	C	C2-O2	-5.45	1.19	1.24
1	A	308	C	C4-C5	-5.45	1.38	1.43
1	A	585	G	C5-C4	5.45	1.42	1.38
1	A	171	A	N9-C4	-5.45	1.34	1.37
1	A	300	A	N7-C5	-5.44	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1212	U	C2-N3	5.44	1.41	1.37
1	A	1521	G	N7-C5	-5.44	1.35	1.39
1	A	117	G	P-O5'	-5.44	1.54	1.59
1	A	776	G	C5-C6	5.44	1.47	1.42
4	D	191	ARG	CG-CD	5.44	1.65	1.51
1	A	770	C	C2-N3	-5.44	1.31	1.35
1	A	196	A	N9-C4	-5.43	1.34	1.37
12	L	108	ALA	CA-CB	-5.43	1.41	1.52
1	A	757	U	C4-O4	5.43	1.27	1.23
1	A	353	A	C5-C4	-5.42	1.34	1.38
1	A	1225	A	N3-C4	-5.42	1.31	1.34
1	A	360	A	C5-C6	-5.42	1.36	1.41
17	Q	11	VAL	CB-CG2	-5.42	1.41	1.52
1	A	1357	A	C6-N1	-5.42	1.31	1.35
1	A	564	C	N1-C6	-5.41	1.33	1.37
12	L	39	VAL	CA-CB	-5.41	1.43	1.54
1	A	903	G	N9-C4	-5.41	1.33	1.38
1	A	50	A	N9-C4	-5.40	1.34	1.37
1	A	480	U	N1-C6	-5.40	1.33	1.38
1	A	839	U	C2-N3	5.40	1.41	1.37
5	E	148	VAL	CB-CG2	-5.40	1.41	1.52
1	A	236	G	N9-C8	-5.39	1.34	1.37
1	A	703	G	C6-O6	5.39	1.29	1.24
1	A	355	C	C4-C5	-5.39	1.38	1.43
1	A	357	G	C2-N3	-5.39	1.28	1.32
1	A	1388	C	N1-C6	-5.39	1.33	1.37
1	A	50	A	N3-C4	-5.39	1.31	1.34
1	A	262	A	N9-C4	-5.39	1.34	1.37
1	A	1521	G	C6-N1	-5.39	1.35	1.39
1	A	733	A	N9-C4	-5.38	1.34	1.37
1	A	1265	G	C6-O6	5.38	1.28	1.24
1	A	579	G	C5-C4	-5.38	1.34	1.38
1	A	53	A	C5-C6	-5.38	1.36	1.41
1	A	1333	A	N7-C5	-5.38	1.36	1.39
1	A	139	G	N3-C4	-5.38	1.31	1.35
1	A	372	C	C3'-C2'	5.38	1.58	1.52
17	Q	95	TYR	CE2-CZ	5.38	1.45	1.38
1	A	402	G	C2-N2	-5.37	1.29	1.34
1	A	545	C	N1-C6	-5.37	1.33	1.37
1	A	32	A	N3-C4	-5.37	1.31	1.34
2	B	170	GLU	CD-OE1	5.37	1.31	1.25
12	L	7	ILE	CA-CB	-5.37	1.42	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	93	G	N9-C4	-5.37	1.33	1.38
1	A	108	G	C5-C4	5.37	1.42	1.38
1	A	431	A	N3-C4	-5.36	1.31	1.34
1	A	241	C	N3-C4	-5.36	1.30	1.33
5	E	6	PHE	CB-CG	-5.36	1.42	1.51
1	A	550	G	C6-O6	-5.36	1.19	1.24
1	A	506	G	N3-C4	-5.36	1.31	1.35
1	A	120	A	C6-N1	-5.35	1.31	1.35
1	A	1401	G	N7-C5	-5.35	1.36	1.39
1	A	1348	U	C2-N3	-5.35	1.34	1.37
8	H	44	PHE	CB-CG	-5.34	1.42	1.51
1	A	814	A	N3-C4	-5.34	1.31	1.34
1	A	1099	G	N1-C2	5.34	1.42	1.37
1	A	1496	C	N3-C4	-5.34	1.30	1.33
17	Q	67	LYS	CG-CD	5.34	1.70	1.52
1	A	387	U	N1-C6	-5.33	1.33	1.38
1	A	1278	U	N3-C4	5.33	1.43	1.38
1	A	1196	U	N1-C2	5.33	1.43	1.38
1	A	1227	A	C5-C4	5.33	1.42	1.38
1	A	533	A	N3-C4	-5.33	1.31	1.34
1	A	1502	A	P-O5'	-5.33	1.54	1.59
1	A	873	A	N3-C4	-5.32	1.31	1.34
1	A	785	G	C2-N3	-5.32	1.28	1.32
1	A	452	A	N7-C5	-5.32	1.36	1.39
1	A	1068	G	N7-C5	-5.32	1.36	1.39
1	A	1080	A	C6-N1	-5.32	1.31	1.35
1	A	818	G	P-OP2	5.32	1.57	1.49
1	A	332	G	C2-N3	-5.31	1.28	1.32
1	A	356	A	N3-C4	-5.31	1.31	1.34
1	A	574	A	C5-C4	-5.30	1.35	1.38
1	A	547	A	N7-C5	-5.30	1.36	1.39
1	A	783	C	C2-O2	5.29	1.29	1.24
1	A	851	G	N7-C5	-5.29	1.36	1.39
1	A	1179	A	N9-C4	-5.29	1.34	1.37
1	A	1469	G	N3-C4	-5.29	1.31	1.35
1	A	828	A	N3-C4	5.29	1.38	1.34
1	A	304	U	N1-C2	5.28	1.43	1.38
1	A	1415	G	C1'-N9	5.28	1.56	1.48
1	A	1061	G	C6-O6	5.28	1.28	1.24
1	A	1236	A	C6-N6	-5.28	1.29	1.33
1	A	920	U	N3-C4	-5.28	1.33	1.38
1	A	1485	U	N1-C2	5.28	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	O	48	LYS	CD-CE	5.27	1.64	1.51
1	A	885	G	N7-C5	-5.27	1.36	1.39
1	A	856	C	N1-C6	-5.26	1.33	1.37
1	A	899	C	N1-C6	5.26	1.40	1.37
1	A	83	U	C2-N3	5.26	1.41	1.37
1	A	405	U	C4-O4	5.26	1.27	1.23
1	A	1496	C	N1-C2	5.26	1.45	1.40
1	A	530	G	N3-C4	-5.25	1.31	1.35
1	A	1514	C	C2-N3	-5.25	1.31	1.35
5	E	101	ILE	CA-CB	-5.25	1.42	1.54
2	B	17	PHE	CB-CG	5.25	1.60	1.51
1	A	1250	A	N7-C5	-5.25	1.36	1.39
1	A	250	A	N3-C4	5.25	1.38	1.34
1	A	563	A	N3-C4	-5.25	1.31	1.34
1	A	248	C	C4-N4	-5.24	1.29	1.33
1	A	1348	U	C2-O2	-5.24	1.17	1.22
1	A	1483	A	N7-C5	5.24	1.42	1.39
1	A	674	G	C6-N1	-5.24	1.35	1.39
2	B	97	TRP	CG-CD2	-5.24	1.34	1.43
1	A	786	G	C5-C4	-5.24	1.34	1.38
1	A	978	A	N9-C4	5.23	1.41	1.37
1	A	975	A	C6-N1	-5.23	1.31	1.35
1	A	134	A	C6-N6	5.23	1.38	1.33
1	A	1528	U	N3-C4	-5.23	1.33	1.38
1	A	1385	G	N3-C4	-5.22	1.31	1.35
1	A	131	C	N1-C2	-5.22	1.34	1.40
1	A	1291	G	N9-C4	-5.22	1.33	1.38
1	A	729	A	N1-C2	-5.22	1.29	1.34
1	A	1139	G	N9-C4	5.22	1.42	1.38
20	T	12	ALA	CA-CB	5.22	1.63	1.52
1	A	632	A	C5-C6	-5.21	1.36	1.41
2	B	17	PHE	CD2-CE2	5.21	1.49	1.39
1	A	53	A	N7-C5	-5.21	1.36	1.39
1	A	703	G	C5-C6	5.21	1.47	1.42
1	A	1354	C	N3-C4	5.21	1.37	1.33
1	A	1405	G	N9-C4	-5.21	1.33	1.38
1	A	1322	C	N3-C4	5.21	1.37	1.33
1	A	1501	C	C4-N4	-5.21	1.29	1.33
1	A	246	A	N9-C8	-5.21	1.33	1.37
1	A	487	A	C5-C4	-5.21	1.35	1.38
1	A	125	U	C2-O2	-5.21	1.17	1.22
1	A	623	C	N3-C4	-5.20	1.30	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	759	A	C6-N1	-5.20	1.31	1.35
1	A	48	C	N1-C6	-5.20	1.34	1.37
1	A	139	G	C6-N1	-5.20	1.35	1.39
1	A	14	U	N3-C4	-5.20	1.33	1.38
1	A	14	U	N1-C2	-5.20	1.33	1.38
1	A	447	G	C8-N7	-5.19	1.27	1.30
1	A	484	G	C2-N3	5.19	1.36	1.32
1	A	828	A	N9-C8	-5.19	1.33	1.37
1	A	289	G	N9-C8	-5.19	1.34	1.37
1	A	1492	A	C5-C6	5.18	1.45	1.41
1	A	714	G	N3-C4	-5.18	1.31	1.35
1	A	26	A	C6-N6	-5.18	1.29	1.33
1	A	79	G	N7-C5	-5.18	1.36	1.39
1	A	238	G	N3-C4	-5.18	1.31	1.35
1	A	898	G	C5-C4	-5.18	1.34	1.38
1	A	1076	C	C4-C5	-5.18	1.38	1.43
1	A	535	A	C6-N1	-5.17	1.31	1.35
1	A	671	G	C5-C4	-5.17	1.34	1.38
1	A	110	C	C4-N4	5.17	1.38	1.33
1	A	52	G	N9-C4	-5.16	1.33	1.38
1	A	55	A	C5-C4	-5.16	1.35	1.38
1	A	62	U	N3-C4	5.16	1.43	1.38
1	A	302	G	C6-N1	-5.16	1.35	1.39
1	A	1191	A	N7-C5	-5.16	1.36	1.39
1	A	1485	U	C2-N3	5.16	1.41	1.37
1	A	485	G	N1-C2	-5.16	1.33	1.37
1	A	47	C	C2-N3	-5.15	1.31	1.35
1	A	684	A	N9-C4	-5.15	1.34	1.37
1	A	59	A	C5-C4	-5.14	1.35	1.38
1	A	1212	U	N3-C4	5.14	1.43	1.38
1	A	1356	G	N3-C4	-5.14	1.31	1.35
1	A	573	A	N3-C4	-5.14	1.31	1.34
12	L	58	VAL	CB-CG2	-5.14	1.42	1.52
1	A	771	G	C2-N3	-5.14	1.28	1.32
1	A	306	G	C6-N1	5.14	1.43	1.39
1	A	651	C	N3-C4	5.14	1.37	1.33
1	A	137	C	C2-N3	5.13	1.39	1.35
1	A	152	A	N9-C4	-5.13	1.34	1.37
1	A	570	G	N7-C5	-5.13	1.36	1.39
1	A	918	A	N1-C2	-5.13	1.29	1.34
1	A	1202	G	N3-C4	-5.13	1.31	1.35
1	A	576	G	N3-C4	-5.12	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	177	C	N3-C4	-5.12	1.30	1.33
1	A	394	G	C2-N3	-5.12	1.28	1.32
1	A	664	G	C5-C6	5.12	1.47	1.42
1	A	1308	U	C2-N3	5.12	1.41	1.37
3	C	173	VAL	CA-CB	5.12	1.65	1.54
1	A	1356	G	C6-O6	5.12	1.28	1.24
1	A	197	A	C6-N1	-5.12	1.31	1.35
1	A	616	G	C6-O6	5.12	1.28	1.24
1	A	981	U	C2-N3	5.12	1.41	1.37
1	A	1251	A	N9-C8	-5.12	1.33	1.37
1	A	49	U	C2-N3	5.11	1.41	1.37
1	A	204	U	N1-C6	5.11	1.42	1.38
1	A	907	A	C6-N1	-5.11	1.31	1.35
1	A	16	A	C6-N1	-5.11	1.31	1.35
1	A	794	A	N7-C5	-5.11	1.36	1.39
1	A	684	A	C5-C6	-5.10	1.36	1.41
1	A	1197	G	C5-C6	-5.10	1.37	1.42
1	A	799	G	N3-C4	-5.10	1.31	1.35
1	A	1513	A	C2'-C1'	-5.10	1.47	1.53
1	A	196	A	N7-C5	5.09	1.42	1.39
1	A	809	G	N7-C5	5.09	1.42	1.39
1	A	1286	A	N9-C4	-5.09	1.34	1.37
1	A	1406	U	C4-O4	5.09	1.27	1.23
1	A	228	A	N3-C4	-5.09	1.31	1.34
1	A	786	G	C5-C6	-5.09	1.37	1.42
1	A	255	G	C8-N7	-5.08	1.27	1.30
1	A	752	G	N9-C8	-5.08	1.34	1.37
5	E	68	GLU	CG-CD	5.08	1.59	1.51
1	A	321	A	C6-N6	-5.08	1.29	1.33
1	A	819	A	C5-C6	-5.08	1.36	1.41
1	A	132	C	C4-C5	5.08	1.47	1.43
1	A	539	A	C5-C4	-5.08	1.35	1.38
1	A	585	G	N7-C5	5.08	1.42	1.39
1	A	858	G	C2-N3	5.08	1.36	1.32
1	A	922	G	C2-N3	-5.08	1.28	1.32
1	A	1068	G	C5-C6	-5.07	1.37	1.42
1	A	147	G	N1-C2	5.07	1.41	1.37
1	A	1379	G	N1-C2	5.07	1.41	1.37
17	Q	99	SER	CA-C	5.07	1.66	1.52
1	A	1347	G	N9-C4	-5.07	1.33	1.38
2	B	35	GLU	CG-CD	5.07	1.59	1.51
15	O	76	GLU	CG-CD	5.07	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	355	C	N1-C6	-5.07	1.34	1.37
1	A	1087	G	N7-C5	-5.06	1.36	1.39
1	A	447	G	N9-C8	-5.06	1.34	1.37
1	A	66	G	C6-N1	5.05	1.43	1.39
1	A	1507	A	C5-C4	-5.05	1.35	1.38
1	A	1477	C	N1-C6	5.05	1.40	1.37
1	A	1186	G	C5-C4	5.05	1.41	1.38
1	A	1451	A	N7-C5	5.04	1.42	1.39
1	A	897	C	C2-N3	-5.04	1.31	1.35
1	A	963	G	N9-C8	-5.04	1.34	1.37
1	A	124	G	N9-C4	-5.04	1.33	1.38
1	A	926	G	N7-C5	-5.04	1.36	1.39
12	L	58	VAL	CB-CG1	-5.04	1.42	1.52
1	A	28	G	C2-N3	-5.04	1.28	1.32
1	A	1433	A	N9-C4	-5.04	1.34	1.37
1	A	497	A	C5-C6	5.03	1.45	1.41
1	A	839	U	C5-C6	5.03	1.38	1.34
1	A	865	A	C5-C6	-5.03	1.36	1.41
1	A	1201	A	N3-C4	-5.03	1.31	1.34
1	A	61	G	N3-C4	-5.03	1.31	1.35
1	A	176	C	C2-O2	5.03	1.28	1.24
1	A	249	U	N1-C6	-5.03	1.33	1.38
1	A	760	G	N9-C4	-5.03	1.33	1.38
1	A	891	U	C4-O4	-5.03	1.19	1.23
12	L	28	LYS	CB-CG	5.03	1.66	1.52
1	A	808	C	N1-C6	-5.02	1.34	1.37
1	A	582	U	C2-O2	-5.02	1.17	1.22
4	D	68	TYR	CE1-CZ	5.02	1.45	1.38
1	A	260	G	C6-O6	5.02	1.28	1.24
1	A	1416	G	N9-C8	5.02	1.41	1.37
1	A	1447	G	N9-C8	5.02	1.41	1.37
1	A	543	C	N1-C6	-5.01	1.34	1.37
1	A	684	A	N7-C5	-5.01	1.36	1.39
1	A	1125	U	N1-C6	-5.01	1.33	1.38
1	A	230	G	N9-C8	-5.01	1.34	1.37
1	A	1394	A	C6-N1	-5.01	1.32	1.35
1	A	1357	A	C5-C6	-5.00	1.36	1.41
1	A	733	A	C6-N1	-5.00	1.32	1.35
3	C	199	LYS	CE-NZ	5.00	1.61	1.49
1	A	147	G	C5-C4	5.00	1.41	1.38
1	A	813	U	P-O5'	-5.00	1.54	1.59

All (6312) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1415	G	C8-N9-C4	-28.43	95.03	106.40
1	A	1393	U	N3-C4-C5	-27.65	98.01	114.60
1	A	398	C	O5'-P-OP1	-27.14	78.14	110.70
1	A	1227	A	N1-C6-N6	26.33	134.40	118.60
1	A	1415	G	N3-C4-C5	-24.93	116.14	128.60
1	A	518	C	N1-C2-O2	24.59	133.65	118.90
1	A	239	U	N3-C4-C5	-23.49	100.50	114.60
1	A	975	A	C2-N3-C4	-23.39	98.90	110.60
1	A	284	G	N1-C6-O6	23.24	133.85	119.90
1	A	1393	U	C6-N1-C2	-23.02	107.19	121.00
1	A	1393	U	N3-C4-O4	22.73	135.31	119.40
1	A	144	G	C5-C6-N1	-22.32	100.34	111.50
1	A	1502	A	C2-N3-C4	-22.16	99.52	110.60
1	A	814	A	C2-N3-C4	-21.13	100.03	110.60
1	A	518	C	N3-C2-O2	-21.03	107.18	121.90
1	A	1415	G	N7-C8-N9	20.34	123.27	113.10
1	A	927	G	N1-C6-O6	20.32	132.09	119.90
1	A	734	G	N1-C6-O6	20.06	131.93	119.90
1	A	290	C	O5'-P-OP2	-20.05	86.64	110.70
1	A	117	G	N1-C6-O6	19.65	131.69	119.90
1	A	635	G	C5-C6-N1	-19.59	101.70	111.50
1	A	144	G	N1-C6-O6	19.53	131.62	119.90
1	A	901	A	O5'-P-OP1	-19.43	87.38	110.70
1	A	619	U	O5'-P-OP2	-19.21	87.64	110.70
1	A	266	G	C5-N7-C8	-19.14	94.73	104.30
1	A	113	G	N1-C6-O6	19.12	131.37	119.90
1	A	1528	U	O5'-P-OP2	-19.08	87.80	110.70
1	A	862	C	C6-N1-C2	19.06	127.92	120.30
1	A	1227	A	C6-C5-N7	-19.02	118.98	132.30
1	A	1502	A	N1-C6-N6	18.98	129.99	118.60
1	A	333	G	C5-C6-N1	-18.80	102.10	111.50
1	A	481	G	O5'-P-OP2	-18.56	88.42	110.70
1	A	635	G	N1-C6-O6	18.54	131.02	119.90
1	A	1515	C	C6-N1-C2	18.32	127.63	120.30
1	A	79	G	N1-C6-O6	18.22	130.83	119.90
1	A	1496	C	N1-C2-O2	18.03	129.72	118.90
1	A	1496	C	N3-C2-O2	-17.95	109.33	121.90
1	A	108	G	C2-N3-C4	-17.85	102.97	111.90
1	A	117	G	C6-C5-N7	-17.37	119.98	130.40
1	A	1539	C	C6-N1-C2	-17.34	113.37	120.30
1	A	484	G	N1-C2-N2	-17.12	100.79	116.20
1	A	266	G	C4-C5-N7	17.12	117.65	110.80
1	A	1502	A	C4-C5-N7	17.11	119.25	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1530	G	C4-N9-C1'	-17.04	104.35	126.50
1	A	1502	A	C6-C5-N7	-17.02	120.39	132.30
1	A	1502	A	C5-N7-C8	-16.99	95.41	103.90
1	A	1302	U	N3-C2-O2	-16.98	110.32	122.20
1	A	560	U	N3-C2-O2	-16.96	110.33	122.20
1	A	372	C	N3-C2-O2	-16.72	110.20	121.90
1	A	108	G	N1-C6-O6	16.59	129.85	119.90
1	A	147	G	C5-C6-N1	-16.49	103.26	111.50
1	A	120	A	N1-C2-N3	16.29	137.45	129.30
1	A	614	A	N1-C6-N6	16.26	128.35	118.60
1	A	62	U	N3-C4-C5	-16.17	104.90	114.60
1	A	624	C	C6-N1-C2	16.08	126.73	120.30
1	A	579	G	C5-C6-O6	-16.04	118.97	128.60
1	A	123	C	O5'-P-OP1	-16.02	91.28	105.70
1	A	144	G	C2-N3-C4	-15.94	103.93	111.90
1	A	108	G	C5-C6-N1	-15.87	103.57	111.50
1	A	1414	U	N3-C4-C5	-15.83	105.11	114.60
1	A	1393	U	C4-C5-C6	15.82	129.19	119.70
1	A	664	G	C5-C6-O6	15.76	138.06	128.60
1	A	664	G	N1-C6-O6	-15.74	110.45	119.90
1	A	1227	A	C5-N7-C8	-15.72	96.04	103.90
1	A	413	G	N3-C4-N9	-15.72	116.57	126.00
1	A	662	G	C2-N3-C4	-15.70	104.05	111.90
1	A	333	G	N3-C2-N2	-15.66	108.94	119.90
1	A	108	G	C6-C5-N7	-15.58	121.05	130.40
1	A	484	G	N3-C2-N2	15.55	130.79	119.90
1	A	789	U	O5'-P-OP2	-15.55	91.70	105.70
1	A	855	G	C2-N3-C4	-15.34	104.23	111.90
1	A	314	C	C6-N1-C2	15.33	126.43	120.30
1	A	372	C	N1-C2-O2	15.28	128.07	118.90
1	A	1222	G	C5-C6-N1	-15.20	103.90	111.50
1	A	122	G	N1-C6-O6	15.17	129.00	119.90
1	A	734	G	C5-C6-O6	-15.16	119.50	128.60
1	A	509	A	C8-N9-C4	-15.06	99.78	105.80
1	A	418	C	C6-N1-C2	15.06	126.32	120.30
1	A	562	C	N1-C2-O2	15.03	127.92	118.90
1	A	46	G	O5'-P-OP1	-15.02	92.19	105.70
1	A	122	G	C6-C5-N7	-14.91	121.45	130.40
1	A	975	A	C5-C6-N1	-14.88	110.26	117.70
1	A	314	C	N3-C4-C5	14.88	127.85	121.90
1	A	279	A	C2-N3-C4	-14.87	103.16	110.60
1	A	438	G	C4-C5-N7	-14.87	104.85	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1415	G	O5'-P-OP2	-14.87	92.32	105.70
1	A	1067	A	O5'-P-OP1	-14.81	92.37	105.70
1	A	1490	C	N1-C2-O2	14.79	127.77	118.90
1	A	520	A	O5'-P-OP2	-14.75	92.43	105.70
1	A	693	G	N9-C4-C5	14.75	111.30	105.40
1	A	61	G	N1-C6-O6	14.73	128.74	119.90
1	A	111	G	N3-C4-N9	-14.73	117.16	126.00
1	A	144	G	N3-C2-N2	-14.73	109.59	119.90
1	A	1196	U	N1-C2-O2	14.71	133.10	122.80
1	A	1415	G	N3-C4-N9	14.71	134.83	126.00
1	A	1003	G	C8-N9-C4	-14.68	100.53	106.40
1	A	110	C	N3-C4-C5	-14.67	116.03	121.90
1	A	108	G	C5-N7-C8	-14.66	96.97	104.30
1	A	116	A	C8-N9-C4	14.64	111.66	105.80
1	A	518	C	C2-N1-C1'	14.62	134.89	118.80
1	A	814	A	C5-C6-N1	-14.60	110.40	117.70
1	A	496	A	O5'-P-OP1	-14.59	92.57	105.70
1	A	734	G	C6-C5-N7	-14.58	121.65	130.40
1	A	22	G	N1-C6-O6	14.52	128.61	119.90
1	A	851	G	N1-C6-O6	14.52	128.61	119.90
1	A	855	G	C5-C6-N1	-14.51	104.25	111.50
1	A	236	G	N3-C2-N2	14.50	130.05	119.90
1	A	836	G	N1-C6-O6	14.49	128.59	119.90
1	A	321	A	O5'-P-OP2	-14.47	92.68	105.70
1	A	284	G	C5-C6-N1	-14.45	104.27	111.50
1	A	887	G	N3-C2-N2	-14.45	109.79	119.90
1	A	1393	U	N1-C2-N3	14.44	123.57	114.90
1	A	1125	U	C5-C6-N1	14.44	129.92	122.70
1	A	1393	U	C5-C6-N1	14.44	129.92	122.70
1	A	1397	C	C2-N3-C4	14.37	127.08	119.90
1	A	239	U	C6-N1-C2	-14.35	112.39	121.00
1	A	194	C	C6-N1-C2	14.35	126.04	120.30
1	A	789	U	N3-C4-C5	-14.34	106.00	114.60
1	A	674	G	C2-N3-C4	-14.32	104.74	111.90
1	A	47	C	C5-C6-N1	-14.29	113.85	121.00
1	A	578	C	C5-C6-N1	-14.28	113.86	121.00
1	A	333	G	N1-C6-O6	14.22	128.43	119.90
1	A	757	U	N3-C4-C5	-14.22	106.07	114.60
1	A	945	G	C5-C6-N1	14.18	118.59	111.50
1	A	204	U	C5-C6-N1	14.12	129.76	122.70
1	A	1485	U	N3-C4-C5	-14.09	106.15	114.60
1	A	1505	G	N3-C4-C5	-14.08	121.56	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1227	A	C2-N3-C4	-14.07	103.56	110.60
1	A	1342	C	C6-N1-C2	14.04	125.92	120.30
1	A	733	A	N1-C2-N3	14.03	136.32	129.30
1	A	484	G	N3-C4-N9	14.02	134.41	126.00
1	A	1370	G	C8-N9-C4	-14.02	100.79	106.40
1	A	438	G	C5-C6-O6	14.02	137.01	128.60
1	A	693	G	N3-C2-N2	-14.00	110.10	119.90
1	A	1530	G	N3-C4-C5	13.99	135.60	128.60
1	A	530	G	C5-C6-N1	-13.99	104.50	111.50
1	A	199	G	N1-C6-O6	13.96	128.28	119.90
1	A	1415	G	C4-N9-C1'	13.96	144.65	126.50
1	A	24	U	O5'-P-OP2	-13.96	93.14	105.70
1	A	1415	G	C4-C5-C6	13.93	127.16	118.80
1	A	9	G	O5'-P-OP2	-13.93	93.16	105.70
1	A	500	G	N1-C6-O6	13.90	128.24	119.90
1	A	1374	A	N1-C6-N6	-13.89	110.26	118.60
1	A	224	C	C5-C6-N1	-13.89	114.06	121.00
1	A	1125	U	C5-C4-O4	-13.88	117.57	125.90
1	A	242	C	N3-C4-C5	13.85	127.44	121.90
1	A	733	A	C2-N3-C4	-13.85	103.68	110.60
1	A	927	G	C4-C5-N7	13.85	116.34	110.80
1	A	266	G	N7-C8-N9	13.83	120.01	113.10
1	A	1269	A	N1-C6-N6	-13.80	110.32	118.60
1	A	867	G	N1-C6-O6	13.80	128.18	119.90
1	A	1454	G	O5'-P-OP2	-13.79	93.29	105.70
1	A	184	G	C4-C5-N7	-13.76	105.30	110.80
1	A	790	A	C2-N3-C4	-13.76	103.72	110.60
1	A	79	G	C6-C5-N7	-13.76	122.14	130.40
1	A	1450	U	N3-C4-C5	-13.75	106.35	114.60
1	A	1542	U	O5'-P-OP2	-13.75	93.32	105.70
1	A	1227	A	C4-C5-N7	13.70	117.55	110.70
1	A	579	G	N1-C6-O6	13.70	128.12	119.90
1	A	729	A	N9-C4-C5	13.69	111.28	105.80
1	A	752	G	C5-C6-O6	13.69	136.81	128.60
1	A	927	G	C5-N7-C8	-13.68	97.46	104.30
1	A	801	U	O5'-P-OP2	-13.67	93.40	105.70
1	A	664	G	C4-C5-N7	-13.66	105.34	110.80
1	A	1374	A	N9-C4-C5	13.66	111.26	105.80
1	A	122	G	N9-C4-C5	-13.65	99.94	105.40
1	A	1125	U	N3-C4-O4	13.65	128.96	119.40
1	A	279	A	C5-N7-C8	-13.61	97.09	103.90
1	A	230	G	C5-C6-N1	-13.61	104.69	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1302	U	N1-C2-O2	13.61	132.32	122.80
1	A	1397	C	C5-C6-N1	13.61	127.80	121.00
1	A	927	G	C2-N3-C4	-13.60	105.10	111.90
1	A	1190	G	C5-C6-N1	-13.59	104.70	111.50
1	A	1060	C	C6-N1-C2	-13.57	114.87	120.30
1	A	1100	C	N1-C2-O2	13.56	127.04	118.90
1	A	722	A	C2-N3-C4	-13.55	103.82	110.60
1	A	479	C	C6-N1-C2	-13.52	114.89	120.30
1	A	839	U	C5-C4-O4	13.52	134.01	125.90
1	A	1530	G	N1-C2-N3	-13.49	115.81	123.90
1	A	1521	G	O5'-P-OP2	-13.48	93.56	105.70
1	A	674	G	N1-C2-N2	-13.44	104.11	116.20
1	A	914	A	O5'-P-OP1	-13.41	93.63	105.70
1	A	921	U	N3-C4-O4	13.41	128.78	119.40
1	A	968	A	N1-C2-N3	-13.40	122.60	129.30
1	A	260	G	C5-C6-N1	-13.36	104.82	111.50
1	A	1145	C	C6-N1-C2	-13.33	114.97	120.30
1	A	701	C	N3-C4-C5	-13.32	116.57	121.90
1	A	281	G	N9-C4-C5	-13.31	100.07	105.40
1	A	746	A	N1-C6-N6	-13.31	110.61	118.60
1	A	572	A	N1-C6-N6	-13.29	110.63	118.60
1	A	190(E)	U	N1-C2-O2	13.28	132.10	122.80
1	A	239	U	N3-C4-O4	13.28	128.69	119.40
1	A	285	G	N1-C6-O6	13.27	127.86	119.90
1	A	1530	G	C8-N9-C4	13.27	111.71	106.40
1	A	403	C	N3-C4-C5	-13.27	116.59	121.90
1	A	833	U	C5-C4-O4	13.26	133.86	125.90
1	A	239	U	C4-C5-C6	13.22	127.63	119.70
1	A	962	C	C6-N1-C2	13.21	125.59	120.30
1	A	184	G	C5-N7-C8	13.20	110.90	104.30
1	A	1506	U	N1-C2-N3	-13.20	106.98	114.90
1	A	450	G	N1-C6-O6	13.18	127.81	119.90
1	A	794	A	O5'-P-OP1	13.17	126.51	110.70
1	A	1509	C	C4-C5-C6	13.16	123.98	117.40
1	A	1485	U	C6-N1-C2	-13.15	113.11	121.00
1	A	1057	G	N1-C2-N2	13.14	128.02	116.20
1	A	1484	C	C6-N1-C2	-13.14	115.04	120.30
1	A	1057	G	N3-C4-N9	-13.11	118.13	126.00
1	A	120	A	C6-N1-C2	-13.10	110.74	118.60
1	A	284	G	C6-C5-N7	-13.10	122.54	130.40
1	A	104	G	C2-N3-C4	-13.10	105.35	111.90
1	A	284	G	C2-N3-C4	-13.09	105.35	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	836	G	N3-C2-N2	-13.01	110.79	119.90
1	A	1397	C	N1-C2-N3	-13.00	110.10	119.20
1	A	484	G	N3-C4-C5	-12.99	122.10	128.60
1	A	187	C	N3-C4-C5	-12.98	116.71	121.90
1	A	1530	G	C8-N9-C1'	12.97	143.87	127.00
1	A	1339	A	N1-C6-N6	-12.97	110.82	118.60
1	A	766	A	O5'-P-OP2	-12.96	94.03	105.70
1	A	1487	G	N3-C4-C5	-12.96	122.12	128.60
1	A	26	A	N1-C2-N3	12.95	135.77	129.30
1	A	1227	A	C4-C5-C6	12.93	123.47	117.00
1	A	20	U	C6-N1-C2	12.93	128.76	121.00
1	A	268	C	O5'-P-OP2	12.93	126.22	110.70
1	A	135	C	N3-C4-C5	-12.91	116.73	121.90
1	A	79	G	C5-C6-N1	-12.91	105.05	111.50
1	A	108	G	N3-C4-C5	12.90	135.05	128.60
1	A	693	G	N3-C4-N9	-12.89	118.27	126.00
1	A	111	G	N3-C4-C5	12.86	135.03	128.60
1	A	1450	U	C4-C5-C6	12.86	127.41	119.70
1	A	1050	G	N1-C6-O6	12.84	127.60	119.90
1	A	657	G	N1-C6-O6	12.83	127.60	119.90
1	A	342	C	C6-N1-C2	-12.82	115.17	120.30
1	A	1230	C	C6-N1-C2	12.82	125.43	120.30
1	A	980	C	C6-N1-C2	-12.81	115.17	120.30
1	A	1530	G	C4-C5-C6	-12.79	111.12	118.80
1	A	810	C	O5'-P-OP2	-12.79	94.19	105.70
1	A	909	A	C5-C6-N1	12.78	124.09	117.70
1	A	1492	A	C2-N3-C4	12.77	116.99	110.60
1	A	884	U	C5-C6-N1	-12.77	116.32	122.70
1	A	1228	C	N1-C2-O2	12.76	126.55	118.90
1	A	117	G	C2-N3-C4	-12.75	105.52	111.90
1	A	536	C	C6-N1-C2	-12.73	115.21	120.30
1	A	279	A	N7-C8-N9	12.72	120.16	113.80
1	A	1227	A	C5-C6-N1	-12.72	111.34	117.70
1	A	254	G	N1-C6-O6	12.71	127.53	119.90
1	A	734	G	C4-C5-N7	12.70	115.88	110.80
1	A	506	G	C8-N9-C4	-12.68	101.33	106.40
1	A	954	G	O5'-P-OP2	-12.68	94.29	105.70
1	A	1082	G	N1-C6-O6	12.67	127.50	119.90
1	A	1191	A	O5'-P-OP1	-12.66	94.31	105.70
1	A	720	C	N1-C2-O2	12.65	126.49	118.90
1	A	500	G	C2-N3-C4	-12.65	105.58	111.90
1	A	1177	G	N1-C6-O6	12.65	127.49	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	730	G	C4-C5-N7	-12.65	105.74	110.80
1	A	446	G	C8-N9-C4	-12.63	101.35	106.40
1	A	884	U	C4-C5-C6	12.62	127.27	119.70
1	A	332	G	N1-C6-O6	12.61	127.46	119.90
1	A	293	G	C2-N3-C4	-12.60	105.60	111.90
1	A	918	A	C6-N1-C2	-12.59	111.04	118.60
1	A	790	A	N1-C6-N6	12.56	126.14	118.60
1	A	779	C	O5'-P-OP2	-12.56	94.40	105.70
1	A	752	G	C4-C5-N7	-12.54	105.78	110.80
1	A	413	G	N3-C4-C5	12.54	134.87	128.60
1	A	484	G	C8-N9-C1'	-12.53	110.71	127.00
1	A	1377	A	C2-N3-C4	-12.53	104.34	110.60
1	A	769	G	O5'-P-OP2	-12.52	94.43	105.70
1	A	109	A	N1-C6-N6	-12.48	111.11	118.60
1	A	108	G	N7-C8-N9	12.46	119.33	113.10
1	A	545	C	C6-N1-C2	-12.46	115.32	120.30
1	A	41	G	N3-C2-N2	-12.45	111.18	119.90
1	A	117	G	C5-C6-N1	-12.44	105.28	111.50
1	A	920	U	N3-C4-O4	-12.40	110.72	119.40
1	A	70	G	N3-C4-C5	12.40	134.80	128.60
1	A	484	G	N1-C6-O6	-12.40	112.46	119.90
1	A	909	A	C6-N1-C2	-12.34	111.19	118.60
1	A	674	G	C6-C5-N7	-12.34	123.00	130.40
1	A	203	U	C5-C6-N1	12.32	128.86	122.70
1	A	760	G	C4-C5-N7	-12.31	105.88	110.80
1	A	706	A	O5'-P-OP2	-12.31	94.62	105.70
1	A	314	C	N3-C4-N4	-12.31	109.39	118.00
1	A	275	G	N1-C6-O6	12.30	127.28	119.90
1	A	975	A	C5-N7-C8	-12.30	97.75	103.90
1	A	113	G	C5-C6-N1	-12.29	105.35	111.50
1	A	1451	A	C8-N9-C4	12.28	110.71	105.80
1	A	1057	G	N3-C2-N2	-12.26	111.32	119.90
1	A	279	A	C5-C6-N1	-12.24	111.58	117.70
1	A	1227	A	N1-C2-N3	12.24	135.42	129.30
1	A	484	G	C4-N9-C1'	12.23	142.39	126.50
1	A	497	A	N9-C4-C5	12.22	110.69	105.80
1	A	1505	G	N3-C4-N9	12.21	133.33	126.00
1	A	190(E)	U	O5'-P-OP2	-12.21	94.71	105.70
1	A	1276	G	N1-C6-O6	12.20	127.22	119.90
1	A	889	A	N9-C4-C5	12.20	110.68	105.80
1	A	945	G	N1-C6-O6	-12.20	112.58	119.90
1	A	167	G	N1-C6-O6	12.17	127.20	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	497	A	N1-C6-N6	-12.16	111.31	118.60
1	A	1490	C	N3-C2-O2	-12.16	113.39	121.90
1	A	553	A	N1-C2-N3	12.15	135.38	129.30
1	A	804	U	O5'-P-OP2	-12.15	94.76	105.70
1	A	818	G	C5-C6-O6	12.15	135.89	128.60
1	A	975	A	N3-C4-C5	12.15	135.31	126.80
1	A	1506	U	C5-C4-O4	-12.14	118.61	125.90
1	A	635	G	C6-C5-N7	-12.14	123.12	130.40
1	A	814	A	N1-C2-N3	12.14	135.37	129.30
1	A	662	G	C5-C6-N1	-12.13	105.44	111.50
1	A	693	G	N1-C2-N2	12.10	127.09	116.20
1	A	10	A	N1-C6-N6	-12.10	111.34	118.60
1	A	101	A	C8-N9-C4	-12.10	100.96	105.80
15	O	34	LEU	CB-CG-CD1	12.10	131.56	111.00
1	A	1217	C	O5'-P-OP2	-12.09	94.82	105.70
1	A	506	G	N7-C8-N9	12.08	119.14	113.10
1	A	930	C	C2-N3-C4	-12.08	113.86	119.90
1	A	906	G	N1-C6-O6	12.07	127.14	119.90
1	A	778	G	C8-N9-C1'	-12.06	111.31	127.00
1	A	899	C	N3-C2-O2	12.06	130.34	121.90
1	A	1227	A	N7-C8-N9	12.05	119.83	113.80
1	A	1276	G	C5-C6-N1	-12.03	105.49	111.50
1	A	562	C	N3-C2-O2	-12.02	113.48	121.90
1	A	729	A	C4-C5-N7	-12.02	104.69	110.70
1	A	1252	A	N7-C8-N9	-12.02	107.79	113.80
1	A	836	G	N3-C4-C5	12.01	134.61	128.60
1	A	332	G	C5-C6-O6	-12.01	121.39	128.60
1	A	956	U	C5-C6-N1	-11.99	116.70	122.70
1	A	635	G	C4-C5-C6	11.97	125.98	118.80
1	A	945	G	C8-N9-C4	-11.95	101.62	106.40
1	A	554	C	N3-C4-C5	-11.94	117.12	121.90
1	A	685	G	N3-C4-N9	-11.94	118.84	126.00
1	A	1072	G	O5'-P-OP2	-11.94	94.96	105.70
1	A	1401	G	C5-C6-N1	11.93	117.47	111.50
1	A	1374	A	C5-C6-N6	11.92	133.24	123.70
1	A	841	U	C5-C6-N1	11.92	128.66	122.70
1	A	590	C	C6-N1-C2	11.91	125.06	120.30
1	A	132	C	C5-C6-N1	-11.91	115.05	121.00
1	A	927	G	N3-C4-C5	11.91	134.56	128.60
1	A	757	U	C4-C5-C6	11.91	126.84	119.70
1	A	1063	C	N1-C2-O2	-11.90	111.76	118.90
1	A	113	G	C6-C5-N7	-11.90	123.26	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	799	G	C2-N3-C4	-11.90	105.95	111.90
1	A	1342	C	C5-C4-N4	-11.87	111.89	120.20
1	A	1485	U	N3-C2-O2	-11.85	113.90	122.20
1	A	693	G	C8-N9-C4	-11.84	101.66	106.40
1	A	580	U	N3-C4-C5	-11.84	107.50	114.60
1	A	238	G	C5-C6-N1	-11.84	105.58	111.50
1	A	971	G	N1-C6-O6	11.83	127.00	119.90
1	A	580	U	C4-C5-C6	11.83	126.80	119.70
1	A	1442	G	C2-N3-C4	11.82	117.81	111.90
1	A	1064	G	N3-C4-N9	-11.82	118.91	126.00
1	A	724	G	C8-N9-C4	-11.82	101.67	106.40
1	A	1393	U	N1-C2-O2	-11.81	114.53	122.80
1	A	908	A	N1-C6-N6	-11.81	111.52	118.60
1	A	1227	A	C5-C6-N6	-11.80	114.26	123.70
12	L	92	ASP	CB-CG-OD2	-11.78	107.69	118.30
1	A	1415	G	C6-C5-N7	-11.78	123.33	130.40
1	A	186	C	N3-C4-C5	-11.77	117.19	121.90
1	A	990	C	O5'-P-OP1	-11.77	95.11	105.70
1	A	190(E)	U	C2-N1-C1'	11.77	131.82	117.70
1	A	61	G	O5'-P-OP1	-11.76	95.11	105.70
1	A	1075	C	N3-C4-C5	-11.76	117.19	121.90
1	A	1492	A	O5'-P-OP2	-11.76	95.11	105.70
1	A	41	G	N1-C6-O6	11.76	126.95	119.90
1	A	241	C	C6-N1-C2	11.76	125.00	120.30
1	A	579	G	C6-C5-N7	-11.76	123.35	130.40
1	A	546	G	C8-N9-C4	-11.75	101.70	106.40
1	A	1403	C	C4-C5-C6	11.75	123.27	117.40
1	A	241	C	N3-C4-C5	11.74	126.60	121.90
1	A	1057	G	N9-C4-C5	11.74	110.10	105.40
1	A	529	G	N1-C6-O6	11.74	126.94	119.90
1	A	1354	C	C6-N1-C2	-11.72	115.61	120.30
1	A	405	U	N3-C4-C5	-11.71	107.57	114.60
1	A	276	G	N1-C6-O6	11.70	126.92	119.90
1	A	236	G	N3-C4-N9	11.69	133.02	126.00
1	A	927	G	C5-C6-N1	-11.69	105.65	111.50
1	A	747	C	C5-C6-N1	-11.69	115.15	121.00
1	A	1145	C	N3-C4-C5	-11.68	117.23	121.90
1	A	144	G	N3-C4-C5	11.66	134.43	128.60
1	A	927	G	C6-C5-N7	-11.66	123.40	130.40
1	A	255	G	C8-N9-C4	11.66	111.06	106.40
1	A	770	C	N3-C4-C5	11.64	126.56	121.90
1	A	920	U	C5-C4-O4	11.63	132.88	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	190(E)	U	C6-N1-C1'	-11.62	104.94	121.20
1	A	47	C	C6-N1-C2	11.60	124.94	120.30
1	A	1539	C	C5-C6-N1	11.58	126.79	121.00
1	A	729	A	N1-C6-N6	-11.57	111.66	118.60
1	A	1502	A	C5-C6-N1	-11.56	111.92	117.70
1	A	226	G	N1-C6-O6	11.56	126.83	119.90
1	A	262	A	N1-C6-N6	-11.54	111.68	118.60
1	A	859	A	N1-C2-N3	11.53	135.06	129.30
1	A	1373	G	C4-C5-C6	11.52	125.71	118.80
1	A	760	G	C5-C6-O6	11.51	135.51	128.60
1	A	387	U	O5'-P-OP2	-11.51	95.34	105.70
1	A	277	C	C6-N1-C2	11.50	124.90	120.30
1	A	1265	G	C5-C6-N1	-11.49	105.76	111.50
1	A	885	G	N1-C6-O6	11.47	126.78	119.90
1	A	1177	G	C6-C5-N7	-11.46	123.53	130.40
1	A	266	G	C6-C5-N7	-11.45	123.53	130.40
1	A	918	A	C5-C6-N1	11.45	123.42	117.70
1	A	1520	G	O5'-P-OP2	-11.45	95.40	105.70
1	A	907	A	N1-C2-N3	11.45	135.02	129.30
1	A	54	C	C6-N1-C2	11.44	124.88	120.30
1	A	281	G	C4-C5-N7	11.42	115.37	110.80
1	A	1523	G	C8-N9-C4	-11.41	101.83	106.40
1	A	1509	C	N3-C4-C5	-11.41	117.34	121.90
1	A	1516	G	N3-C4-C5	11.39	134.30	128.60
1	A	117	G	C4-C5-C6	11.39	125.63	118.80
1	A	27	G	C4-C5-N7	11.37	115.35	110.80
1	A	509	A	N7-C8-N9	11.37	119.48	113.80
1	A	111	G	C5-C6-N1	-11.36	105.82	111.50
1	A	514	C	N3-C4-C5	-11.35	117.36	121.90
1	A	1080	A	N1-C6-N6	-11.35	111.79	118.60
1	A	671	G	C5-C6-N1	11.34	117.17	111.50
1	A	1050	G	C5-C6-N1	-11.33	105.83	111.50
1	A	144	G	N3-C4-N9	-11.33	119.20	126.00
1	A	917	G	O5'-P-OP2	-11.33	95.51	105.70
1	A	276	G	C8-N9-C4	11.32	110.93	106.40
1	A	873	A	C8-N9-C4	-11.31	101.28	105.80
1	A	147	G	C2-N3-C4	-11.29	106.25	111.90
1	A	1323	G	N1-C6-O6	11.28	126.67	119.90
1	A	1363	A	N1-C6-N6	-11.28	111.83	118.60
1	A	889	A	N1-C2-N3	11.27	134.94	129.30
1	A	234	C	C6-N1-C2	11.27	124.81	120.30
1	A	1070	U	O5'-P-OP2	-11.25	95.58	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	672	U	N3-C4-C5	-11.24	107.86	114.60
1	A	419	C	C6-N1-C2	11.23	124.79	120.30
1	A	1125	U	C2-N1-C1'	11.22	131.16	117.70
1	A	524	G	O5'-P-OP2	-11.22	95.60	105.70
1	A	1469	G	N1-C2-N3	11.22	130.63	123.90
1	A	726	C	C6-N1-C2	-11.21	115.82	120.30
1	A	284	G	C5-C6-O6	-11.20	121.88	128.60
1	A	760	G	N3-C4-N9	-11.20	119.28	126.00
1	A	500	G	N3-C4-C5	11.20	134.20	128.60
1	A	1478	C	C5-C6-N1	11.20	126.60	121.00
1	A	220	G	N1-C6-O6	11.18	126.61	119.90
1	A	234	C	C5-C6-N1	-11.18	115.41	121.00
1	A	753	A	N1-C6-N6	-11.17	111.90	118.60
1	A	1429	C	N3-C4-C5	-11.17	117.43	121.90
1	A	1338	G	C8-N9-C4	-11.17	101.93	106.40
1	A	370	C	N1-C2-O2	11.16	125.60	118.90
1	A	250	A	O5'-P-OP2	-11.15	95.67	105.70
1	A	1064	G	N9-C4-C5	11.14	109.86	105.40
1	A	1405	G	C4-C5-N7	11.14	115.26	110.80
1	A	760	G	N1-C6-O6	-11.13	113.22	119.90
1	A	1490	C	N3-C4-C5	11.13	126.35	121.90
1	A	1388	C	C6-N1-C2	-11.13	115.85	120.30
1	A	1331	G	C8-N9-C4	-11.11	101.95	106.40
1	A	519	C	N3-C4-C5	-11.11	117.46	121.90
1	A	1529	G	O5'-P-OP1	-11.11	95.70	105.70
1	A	141	A	N1-C6-N6	11.11	125.26	118.60
1	A	711	G	N1-C6-O6	11.10	126.56	119.90
1	A	117	G	N9-C4-C5	-11.06	100.98	105.40
1	A	583	A	C2-N3-C4	-11.06	105.07	110.60
1	A	975	A	N3-C4-N9	-11.06	118.55	127.40
1	A	757	U	C6-N1-C2	-11.05	114.37	121.00
1	A	1442	G	N3-C4-C5	-11.04	123.08	128.60
1	A	316	G	N1-C6-O6	11.03	126.52	119.90
1	A	1003	G	N7-C8-N9	11.03	118.61	113.10
1	A	522	C	C6-N1-C2	11.02	124.71	120.30
1	A	776	G	OP1-P-O3'	11.02	129.44	105.20
1	A	1442	G	N3-C4-N9	11.02	132.61	126.00
1	A	1284	C	C6-N1-C2	11.01	124.70	120.30
1	A	275	G	C5-C6-N1	-11.01	106.00	111.50
1	A	1351	U	C5-C4-O4	11.01	132.51	125.90
1	A	39	G	C5-C6-N1	11.00	117.00	111.50
1	A	885	G	N3-C2-N2	-11.00	112.20	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1290	G	N1-C6-O6	11.00	126.50	119.90
1	A	389	A	C2-N3-C4	10.99	116.10	110.60
1	A	921	U	N3-C4-C5	-10.99	108.00	114.60
1	A	1528	U	OP1-P-OP2	10.98	136.08	119.60
1	A	1416	G	OP1-P-OP2	-10.98	103.13	119.60
1	A	1095	U	N1-C2-N3	10.97	121.48	114.90
1	A	132	C	N1-C2-N3	10.97	126.88	119.20
1	A	189	G	C8-N9-C4	10.97	110.79	106.40
1	A	747	C	C6-N1-C2	10.97	124.69	120.30
1	A	814	A	N1-C6-N6	10.96	125.18	118.60
1	A	523	A	N1-C2-N3	10.96	134.78	129.30
1	A	669	U	N1-C2-N3	-10.96	108.33	114.90
1	A	1484	C	C5-C6-N1	10.96	126.48	121.00
1	A	1082	G	C2-N3-C4	-10.95	106.42	111.90
1	A	1388	C	N3-C2-O2	-10.95	114.23	121.90
1	A	110	C	N3-C4-N4	10.95	125.67	118.00
1	A	242	C	C6-N1-C2	10.95	124.68	120.30
1	A	319	G	C6-C5-N7	-10.94	123.83	130.40
1	A	1305	G	C8-N9-C4	-10.95	102.02	106.40
1	A	266	G	N3-C4-C5	10.94	134.07	128.60
1	A	1158	C	C2-N1-C1'	10.94	130.84	118.80
1	A	284	G	N9-C4-C5	-10.94	101.02	105.40
1	A	1354	C	C5-C6-N1	10.94	126.47	121.00
1	A	620	C	C6-N1-C2	10.93	124.67	120.30
1	A	1127	G	N1-C6-O6	10.93	126.46	119.90
8	H	85	ARG	NE-CZ-NH1	-10.93	114.83	120.30
1	A	132	C	C4-C5-C6	10.92	122.86	117.40
1	A	385	C	N3-C4-C5	10.92	126.27	121.90
1	A	1087	G	N1-C6-O6	10.92	126.45	119.90
1	A	224	C	C2-N3-C4	-10.91	114.45	119.90
1	A	590	C	C5-C6-N1	-10.90	115.55	121.00
1	A	49	U	O5'-P-OP1	-10.90	95.89	105.70
1	A	1499	A	N1-C2-N3	10.89	134.75	129.30
1	A	981	U	N3-C4-O4	10.89	127.03	119.40
1	A	388	G	N1-C6-O6	10.88	126.43	119.90
1	A	728	A	C8-N9-C4	-10.87	101.45	105.80
1	A	754	C	N3-C4-C5	10.87	126.25	121.90
1	A	530	G	C6-C5-N7	-10.86	123.89	130.40
1	A	446	G	C2-N3-C4	-10.86	106.47	111.90
1	A	332	G	OP1-P-O3'	-10.86	81.32	105.20
1	A	108	G	N3-C4-N9	-10.85	119.49	126.00
1	A	1252	A	C5-N7-C8	10.85	109.33	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1139	G	C4-C5-N7	-10.85	106.46	110.80
1	A	629	G	N1-C6-O6	-10.84	113.39	119.90
1	A	518	C	C6-N1-C1'	-10.84	107.79	120.80
1	A	224	C	C4-C5-C6	10.84	122.82	117.40
1	A	1070	U	C6-N1-C2	10.83	127.50	121.00
1	A	791	G	C5-C6-N1	-10.82	106.09	111.50
1	A	204	U	C2-N1-C1'	10.82	130.68	117.70
1	A	760	G	C6-C5-N7	10.81	136.89	130.40
1	A	635	G	C2-N3-C4	-10.81	106.50	111.90
1	A	196	A	C8-N9-C4	10.80	110.12	105.80
1	A	1020	U	C5-C4-O4	10.80	132.38	125.90
1	A	555	C	O5'-P-OP2	-10.80	95.98	105.70
1	A	858	G	C4-N9-C1'	10.79	140.52	126.50
1	A	1502	A	N9-C4-C5	-10.78	101.49	105.80
1	A	823	G	N1-C6-O6	10.78	126.37	119.90
1	A	309	G	N1-C6-O6	10.76	126.36	119.90
1	A	1203	C	C6-N1-C2	10.76	124.60	120.30
1	A	1416	G	N7-C8-N9	10.76	118.48	113.10
1	A	1323	G	C4-C5-N7	10.75	115.10	110.80
1	A	662	G	N1-C2-N3	10.75	130.35	123.90
1	A	1321	C	N3-C4-C5	-10.75	117.60	121.90
1	A	1530	G	N1-C2-N2	10.75	125.88	116.20
1	A	823	G	C2-N3-C4	-10.75	106.53	111.90
1	A	1058	G	N9-C4-C5	-10.73	101.11	105.40
1	A	789	U	C6-N1-C2	-10.73	114.56	121.00
1	A	1515	C	N3-C2-O2	10.72	129.40	121.90
1	A	851	G	C6-C5-N7	-10.71	123.97	130.40
1	A	62	U	N3-C4-O4	10.71	126.90	119.40
1	A	281	G	N3-C4-N9	10.71	132.43	126.00
1	A	706	A	C8-N9-C4	10.71	110.08	105.80
1	A	1315	U	O5'-P-OP2	-10.71	96.06	105.70
1	A	762	C	C2-N3-C4	-10.71	114.55	119.90
1	A	1437	C	O5'-P-OP2	-10.70	96.07	105.70
1	A	1037	C	C5-C6-N1	10.70	126.35	121.00
1	A	1307	U	O5'-P-OP2	-10.70	96.07	105.70
1	A	1057	G	C8-N9-C1'	10.69	140.90	127.00
1	A	1196	U	C2-N1-C1'	10.69	130.52	117.70
1	A	1321	C	C6-N1-C2	-10.69	116.03	120.30
1	A	546	G	N9-C4-C5	10.68	109.67	105.40
1	A	725	G	N1-C6-O6	10.68	126.31	119.90
1	A	133	U	N3-C4-C5	-10.67	108.20	114.60
1	A	397	A	C8-N9-C4	-10.67	101.53	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	223	U	N1-C2-N3	10.67	121.30	114.90
1	A	889	A	N1-C6-N6	-10.67	112.20	118.60
1	A	818	G	C5-C6-N1	-10.66	106.17	111.50
1	A	255	G	C2-N3-C4	-10.65	106.58	111.90
1	A	293	G	N1-C6-O6	10.65	126.29	119.90
1	A	564	C	N3-C4-C5	-10.63	117.65	121.90
1	A	1446	A	N1-C6-N6	-10.64	112.22	118.60
1	A	614	A	C5-C6-N6	-10.63	115.19	123.70
1	A	281	G	N3-C2-N2	10.63	127.34	119.90
1	A	1524	C	O5'-P-OP1	-10.63	96.13	105.70
1	A	578	C	N3-C4-N4	-10.63	110.56	118.00
1	A	198	G	C8-N9-C4	10.63	110.65	106.40
1	A	760	G	N9-C4-C5	10.63	109.65	105.40
1	A	667	G	C2-N3-C4	-10.61	106.60	111.90
1	A	1350	A	O5'-P-OP2	-10.60	96.16	105.70
1	A	250	A	C2-N3-C4	-10.60	105.30	110.60
1	A	901	A	C2-N3-C4	-10.60	105.30	110.60
1	A	22	G	C6-C5-N7	-10.60	124.04	130.40
1	A	199	G	C2-N3-C4	-10.60	106.60	111.90
1	A	783	C	C6-N1-C2	10.59	124.54	120.30
1	A	720	C	N3-C2-O2	-10.59	114.49	121.90
1	A	27	G	C5-C6-O6	-10.58	122.25	128.60
1	A	1054	C	N3-C4-C5	-10.58	117.67	121.90
1	A	1203	C	C5-C6-N1	-10.58	115.71	121.00
4	D	12	CYS	CA-CB-SG	10.58	133.04	114.00
1	A	438	G	N9-C4-C5	10.58	109.63	105.40
1	A	927	G	C5-C6-O6	-10.58	122.25	128.60
1	A	572	A	N9-C4-C5	10.56	110.03	105.80
1	A	530	G	N1-C6-O6	10.56	126.24	119.90
1	A	122	G	C4-C5-N7	10.55	115.02	110.80
1	A	1417	G	C5-C6-O6	-10.55	122.27	128.60
1	A	111	G	O5'-P-OP1	-10.55	96.21	105.70
1	A	33	A	C5-C6-N6	-10.55	115.26	123.70
1	A	632	A	C8-N9-C4	-10.54	101.58	105.80
1	A	1405	G	N1-C6-O6	10.54	126.22	119.90
1	A	372	C	C2-N1-C1'	10.53	130.38	118.80
1	A	432	A	N1-C6-N6	-10.53	112.28	118.60
1	A	550	G	C2-N3-C4	-10.53	106.64	111.90
1	A	274	A	O5'-P-OP2	-10.52	96.23	105.70
1	A	109	A	C5-C6-N6	10.52	132.11	123.70
1	A	723	U	C6-N1-C2	-10.50	114.70	121.00
1	A	255	G	N1-C2-N3	10.50	130.20	123.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1373	G	N3-C4-C5	-10.50	123.35	128.60
1	A	1526	G	N3-C2-N2	-10.50	112.55	119.90
1	A	70	G	N3-C4-N9	-10.50	119.70	126.00
1	A	740	U	C5-C4-O4	10.50	132.20	125.90
1	A	1079	G	C6-C5-N7	-10.49	124.10	130.40
1	A	238	G	N1-C6-O6	10.49	126.19	119.90
1	A	858	G	N7-C8-N9	10.48	118.34	113.10
1	A	536	C	O5'-P-OP1	-10.47	96.28	105.70
1	A	830	G	N3-C4-C5	10.47	133.83	128.60
1	A	1066	C	N3-C4-N4	10.46	125.32	118.00
1	A	783	C	N3-C2-O2	10.45	129.22	121.90
1	A	1528	U	C5-C6-N1	-10.45	117.47	122.70
1	A	678	U	N1-C2-N3	10.45	121.17	114.90
1	A	897	C	N3-C4-C5	10.43	126.07	121.90
1	A	1093	A	C5-C6-N1	10.43	122.92	117.70
1	A	109	A	N9-C4-C5	10.43	109.97	105.80
1	A	239	U	C2-N3-C4	10.43	133.25	127.00
1	A	629	G	C5-C6-O6	10.42	134.85	128.60
1	A	300	A	N1-C6-N6	-10.41	112.35	118.60
1	A	1373	G	C6-C5-N7	-10.41	124.15	130.40
1	A	658	G	N3-C4-N9	10.41	132.25	126.00
1	A	590	C	C2-N3-C4	-10.41	114.70	119.90
1	A	1505	G	C4-C5-C6	10.40	125.04	118.80
1	A	1236	A	C5-C6-N6	-10.40	115.38	123.70
1	A	624	C	N3-C2-O2	10.40	129.18	121.90
1	A	278	G	N1-C6-O6	-10.39	113.67	119.90
1	A	242	C	C2-N3-C4	-10.39	114.71	119.90
1	A	482	A	C2-N3-C4	-10.38	105.41	110.60
1	A	674	G	N1-C2-N3	10.38	130.13	123.90
1	A	803	G	OP2-P-O3'	10.38	128.03	105.20
1	A	720	C	N3-C4-C5	10.38	126.05	121.90
1	A	953	G	C8-N9-C4	10.38	110.55	106.40
1	A	122	G	C8-N9-C4	10.36	110.55	106.40
1	A	380	G	O5'-P-OP2	-10.36	96.38	105.70
1	A	1196	U	C6-N1-C1'	-10.36	106.70	121.20
1	A	319	G	N1-C6-O6	10.35	126.11	119.90
1	A	373	A	N1-C2-N3	10.35	134.47	129.30
1	A	865	A	O5'-P-OP1	-10.35	96.39	105.70
1	A	540	G	C2-N3-C4	-10.34	106.73	111.90
1	A	1286	A	C5-N7-C8	-10.34	98.73	103.90
1	A	51	A	O5'-P-OP1	10.34	123.10	110.70
1	A	240	C	N3-C4-C5	10.33	126.03	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	262	A	C4-C5-C6	-10.33	111.83	117.00
1	A	1442	G	C5-C6-N1	10.33	116.67	111.50
1	A	927	G	O5'-P-OP1	-10.32	96.41	105.70
1	A	1461	G	N3-C4-C5	10.31	133.75	128.60
1	A	746	A	N1-C2-N3	10.30	134.45	129.30
1	A	659	U	N3-C2-O2	-10.30	114.99	122.20
1	A	391	G	C8-N9-C4	10.30	110.52	106.40
1	A	234	C	N3-C4-N4	-10.29	110.80	118.00
1	A	1188	A	N1-C2-N3	10.29	134.45	129.30
1	A	1058	G	C8-N9-C4	10.29	110.51	106.40
1	A	253	U	O5'-P-OP1	10.28	123.04	110.70
1	A	927	G	N7-C8-N9	10.29	118.24	113.10
1	A	120	A	C4-C5-C6	10.28	122.14	117.00
1	A	363	A	C2-N3-C4	-10.28	105.46	110.60
1	A	190(E)	U	C5-C4-O4	-10.27	119.74	125.90
1	A	532	A	O4'-C1'-N9	10.27	116.42	108.20
1	A	281	G	N1-C2-N2	-10.27	106.96	116.20
1	A	370	C	N3-C4-C5	10.26	126.00	121.90
1	A	830	G	C4-N9-C1'	-10.26	113.16	126.50
1	A	856	C	N3-C4-C5	-10.26	117.80	121.90
1	A	1528	U	O5'-P-OP1	10.26	123.01	110.70
1	A	793	U	N1-C2-N3	10.25	121.05	114.90
1	A	16	A	N1-C6-N6	-10.25	112.45	118.60
1	A	24	U	C5-C6-N1	-10.25	117.58	122.70
1	A	403	C	O5'-P-OP2	-10.24	96.49	105.70
1	A	79	G	C2-N3-C4	-10.23	106.78	111.90
1	A	930	C	C5-C6-N1	-10.23	115.89	121.00
1	A	522	C	N3-C2-O2	10.23	129.06	121.90
1	A	833	U	C4-C5-C6	10.23	125.84	119.70
1	A	372	C	O4'-C1'-N1	10.22	116.38	108.20
1	A	1075	C	N1-C2-O2	-10.22	112.77	118.90
1	A	1109	C	C5-C4-N4	10.22	127.35	120.20
1	A	664	G	O5'-P-OP2	-10.21	96.51	105.70
1	A	1177	G	C5-C6-O6	-10.21	122.47	128.60
1	A	1471	G	C2-N3-C4	-10.21	106.80	111.90
1	A	1490	C	N3-C4-N4	-10.20	110.86	118.00
1	A	1127	G	O5'-P-OP1	-10.20	96.52	105.70
1	A	1512	U	N3-C4-C5	-10.20	108.48	114.60
1	A	970	C	N1-C2-O2	10.20	125.02	118.90
1	A	252	U	N3-C4-C5	-10.19	108.48	114.60
1	A	970	C	N3-C4-C5	10.19	125.98	121.90
1	A	1502	A	N3-C4-C5	10.19	133.93	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	971	G	C5-C6-N1	-10.19	106.41	111.50
1	A	1131	G	N1-C6-O6	10.19	126.01	119.90
1	A	840	C	O5'-P-OP1	-10.18	96.54	105.70
1	A	1109	C	N3-C2-O2	-10.18	114.78	121.90
1	A	76	C	C5-C6-N1	10.17	126.09	121.00
1	A	604	G	C4-C5-N7	10.17	114.87	110.80
1	A	1020	U	C6-N1-C2	-10.16	114.91	121.00
1	A	396	G	C8-N9-C4	-10.15	102.34	106.40
1	A	553	A	C2-N3-C4	-10.15	105.53	110.60
1	A	721	G	N3-C4-N9	10.15	132.09	126.00
1	A	1478	C	C6-N1-C2	-10.15	116.24	120.30
1	A	43	C	C6-N1-C2	10.13	124.35	120.30
1	A	225	C	O5'-P-OP1	10.12	122.84	110.70
1	A	279	A	C8-N9-C4	-10.11	101.76	105.80
1	A	21	G	N3-C4-N9	10.11	132.06	126.00
1	A	593	G	C5-C6-N1	-10.10	106.45	111.50
1	A	320	C	N1-C2-O2	-10.10	112.84	118.90
1	A	66	G	N1-C6-O6	10.09	125.96	119.90
1	A	250	A	N1-C6-N6	10.09	124.66	118.60
1	A	266	G	C2-N3-C4	-10.09	106.85	111.90
1	A	289	G	N3-C4-C5	-10.09	123.56	128.60
1	A	889	A	C6-N1-C2	-10.09	112.55	118.60
1	A	1460	A	C8-N9-C4	10.08	109.83	105.80
1	A	286	G	N1-C6-O6	10.08	125.95	119.90
1	A	907	A	N1-C6-N6	-10.08	112.55	118.60
1	A	1076	C	C5-C4-N4	-10.08	113.14	120.20
1	A	851	G	C5-C6-N1	-10.07	106.47	111.50
1	A	873	A	N9-C4-C5	10.07	109.83	105.80
1	A	1374	A	C8-N9-C4	-10.07	101.77	105.80
1	A	674	G	C4-C5-C6	10.07	124.84	118.80
1	A	357	G	C8-N9-C4	10.06	110.42	106.40
1	A	723	U	C5-C4-O4	10.06	131.94	125.90
1	A	530	G	C2-N3-C4	-10.06	106.87	111.90
12	L	24	VAL	C-N-CD	-10.05	98.49	120.60
1	A	1311	G	N1-C6-O6	10.05	125.93	119.90
1	A	418	C	N3-C4-C5	10.04	125.92	121.90
1	A	816	A	N1-C6-N6	-10.05	112.57	118.60
1	A	1348	U	N3-C2-O2	-10.03	115.18	122.20
1	A	1057	G	C6-C5-N7	10.03	136.42	130.40
1	A	1111	A	O5'-P-OP2	-10.03	96.67	105.70
1	A	685	G	C8-N9-C1'	10.01	140.01	127.00
1	A	839	U	C5-C6-N1	-10.01	117.69	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1158	C	C6-N1-C2	-10.01	116.30	120.30
1	A	746	A	C6-N1-C2	-10.01	112.60	118.60
1	A	556	C	C6-N1-C2	10.00	124.30	120.30
1	A	885	G	C5-C6-N1	-9.99	106.50	111.50
1	A	224	C	O5'-P-OP2	-9.99	96.71	105.70
1	A	1279	A	N1-C6-N6	9.99	124.59	118.60
1	A	220	G	C6-C5-N7	-9.99	124.41	130.40
1	A	403	C	C4-C5-C6	9.99	122.39	117.40
1	A	182	U	C5-C6-N1	9.98	127.69	122.70
1	A	446	G	N7-C8-N9	9.98	118.09	113.10
1	A	859	A	C2-N3-C4	-9.98	105.61	110.60
1	A	836	G	N1-C2-N2	9.98	125.18	116.20
1	A	664	G	C5-N7-C8	9.98	109.29	104.30
1	A	723	U	N3-C4-C5	-9.98	108.61	114.60
1	A	1099	G	N3-C4-N9	-9.96	120.02	126.00
1	A	236	G	N1-C2-N2	-9.95	107.25	116.20
1	A	1054	C	N1-C2-O2	9.95	124.87	118.90
1	A	15	G	C4-C5-N7	9.94	114.77	110.80
1	A	614	A	C4-C5-N7	9.92	115.66	110.70
1	A	763	G	C5-C6-O6	-9.92	122.65	128.60
1	A	14	U	C5-C4-O4	9.92	131.85	125.90
1	A	757	U	N1-C2-N3	9.92	120.85	114.90
1	A	249	U	C5-C6-N1	-9.92	117.74	122.70
1	A	970	C	O5'-P-OP2	9.91	122.59	110.70
1	A	701	C	C4-C5-C6	9.91	122.35	117.40
1	A	328	C	C2-N1-C1'	9.90	129.69	118.80
1	A	1516	G	N1-C6-O6	9.90	125.84	119.90
1	A	51	A	C5-C6-N6	-9.90	115.78	123.70
1	A	658	G	C8-N9-C1'	-9.90	114.13	127.00
1	A	801	U	O5'-P-OP1	9.90	122.58	110.70
1	A	1109	C	C6-N1-C2	-9.90	116.34	120.30
1	A	651	C	N3-C2-O2	9.89	128.82	121.90
1	A	769	G	C5-C6-N1	-9.89	106.56	111.50
1	A	1303	C	N3-C2-O2	-9.88	114.98	121.90
1	A	108	G	C4-C5-N7	9.88	114.75	110.80
1	A	144	G	N7-C8-N9	9.88	118.04	113.10
1	A	254	G	C2-N3-C4	-9.87	106.96	111.90
1	A	1081	G	N1-C6-O6	-9.88	113.97	119.90
1	A	1398	A	O5'-P-OP1	-9.87	96.81	105.70
1	A	559	A	C5-C6-N1	9.87	122.64	117.70
1	A	132	C	N3-C2-O2	-9.87	114.99	121.90
1	A	184	G	C5-C6-O6	9.86	134.52	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	147	G	C4-C5-C6	9.85	124.71	118.80
1	A	333	G	C4-C5-N7	-9.85	106.86	110.80
1	A	109	A	C8-N9-C4	-9.84	101.86	105.80
1	A	309	G	C8-N9-C4	-9.84	102.46	106.40
1	A	776	G	C6-C5-N7	9.83	136.30	130.40
1	A	1461	G	C2-N3-C4	-9.83	106.99	111.90
1	A	742	G	C8-N9-C4	9.82	110.33	106.40
1	A	1250	A	N1-C6-N6	9.82	124.49	118.60
1	A	913	A	P-O3'-C3'	9.81	131.48	119.70
1	A	735	C	C5-C4-N4	-9.81	113.33	120.20
1	A	1279	A	C6-C5-N7	-9.80	125.44	132.30
1	A	873	A	N1-C6-N6	-9.79	112.72	118.60
1	A	1100	C	N3-C2-O2	-9.80	115.04	121.90
1	A	1177	G	C4-C5-N7	9.79	114.72	110.80
1	A	975	A	N7-C8-N9	9.79	118.69	113.80
1	A	674	G	C5-C6-N1	-9.79	106.61	111.50
1	A	1196	U	N3-C2-O2	-9.78	115.35	122.20
1	A	754	C	C4-C5-C6	-9.78	112.51	117.40
1	A	1405	G	N3-C4-C5	9.78	133.49	128.60
1	A	745	C	N3-C4-N4	-9.77	111.16	118.00
1	A	504	C	C6-N1-C2	-9.77	116.39	120.30
1	A	1147	C	N1-C2-O2	9.77	124.76	118.90
1	A	632	A	N7-C8-N9	9.77	118.69	113.80
1	A	693	G	C8-N9-C1'	9.77	139.70	127.00
1	A	902	G	C8-N9-C4	9.77	110.31	106.40
1	A	277	C	O5'-P-OP1	-9.77	96.91	105.70
1	A	358	U	N3-C4-O4	9.77	126.24	119.40
1	A	908	A	N1-C2-N3	9.77	134.18	129.30
1	A	540	G	N1-C2-N3	9.76	129.76	123.90
1	A	604	G	N3-C4-C5	9.76	133.48	128.60
1	A	712	A	C4-C5-C6	9.76	121.88	117.00
1	A	728	A	N9-C4-C5	9.76	109.70	105.80
1	A	578	C	C2-N3-C4	-9.76	115.02	119.90
1	A	721	G	N3-C4-C5	-9.76	123.72	128.60
1	A	1447	G	C5-N7-C8	-9.76	99.42	104.30
1	A	598	U	O5'-P-OP2	-9.75	96.92	105.70
1	A	829	G	O5'-P-OP2	-9.75	96.92	105.70
1	A	530	G	N7-C8-N9	9.75	117.97	113.10
1	A	669	U	O5'-P-OP2	-9.75	96.93	105.70
1	A	858	G	N3-C2-N2	9.75	126.72	119.90
1	A	569	C	C5-C6-N1	-9.74	116.13	121.00
1	A	637	G	C8-N9-C4	9.74	110.30	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	662	G	C6-C5-N7	-9.74	124.56	130.40
1	A	1037	C	C6-N1-C2	-9.74	116.40	120.30
1	A	1374	A	C4-C5-N7	-9.74	105.83	110.70
1	A	22	G	C5-C6-O6	-9.74	122.76	128.60
1	A	79	G	N9-C4-C5	-9.73	101.51	105.40
1	A	712	A	N1-C2-N3	9.73	134.17	129.30
1	A	408	A	C8-N9-C4	-9.73	101.91	105.80
1	A	601	C	C4-C5-C6	9.73	122.26	117.40
1	A	1512	U	N1-C2-O2	-9.73	115.99	122.80
1	A	22	G	OP1-P-O3'	-9.72	83.81	105.20
1	A	560	U	C5-C4-O4	9.72	131.73	125.90
1	A	887	G	O5'-P-OP2	-9.72	96.95	105.70
1	A	515	G	C8-N9-C4	-9.72	102.51	106.40
1	A	446	G	C5-C6-N1	-9.71	106.65	111.50
1	A	1028	C	C5-C6-N1	9.70	125.85	121.00
1	A	276	G	N1-C2-N3	9.70	129.72	123.90
1	A	322	C	C6-N1-C2	-9.70	116.42	120.30
1	A	323	U	N1-C2-N3	9.70	120.72	114.90
1	A	512	U	N3-C4-O4	9.69	126.18	119.40
1	A	147	G	N3-C2-N2	-9.68	113.12	119.90
1	A	226	G	C5-C6-N1	-9.68	106.66	111.50
1	A	1464	G	C2-N3-C4	-9.68	107.06	111.90
1	A	514	C	C6-N1-C2	-9.67	116.43	120.30
1	A	1512	U	N1-C2-N3	9.67	120.70	114.90
1	A	104	G	N1-C2-N3	9.67	129.70	123.90
1	A	167	G	C6-C5-N7	-9.66	124.60	130.40
1	A	257	G	O5'-P-OP2	-9.66	97.00	105.70
1	A	901	A	C5-C6-N1	-9.66	112.87	117.70
1	A	802	A	C6-N1-C2	-9.66	112.81	118.60
1	A	279	A	N3-C4-N9	-9.65	119.68	127.40
1	A	761	G	N1-C6-O6	9.65	125.69	119.90
1	A	1501	C	N3-C4-C5	9.65	125.76	121.90
1	A	1515	C	O5'-P-OP1	9.64	122.27	110.70
1	A	20	U	N3-C2-O2	9.64	128.95	122.20
1	A	1467	G	OP1-P-OP2	9.64	134.06	119.60
1	A	10	A	O5'-P-OP2	-9.64	97.03	105.70
1	A	552	U	N3-C4-O4	9.64	126.15	119.40
1	A	649	G	C8-N9-C4	9.64	110.26	106.40
1	A	557	G	N1-C6-O6	-9.64	114.12	119.90
1	A	691	G	C8-N9-C4	-9.64	102.55	106.40
1	A	380	G	C5-C6-O6	9.63	134.38	128.60
1	A	672	U	C4-C5-C6	9.63	125.48	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1501	C	N3-C4-N4	-9.63	111.26	118.00
1	A	1147	C	N3-C2-O2	-9.62	115.17	121.90
1	A	251	G	C5-C6-N1	-9.62	106.69	111.50
1	A	893	C	N1-C2-O2	9.62	124.67	118.90
1	A	372	C	C5-C4-N4	-9.62	113.47	120.20
1	A	721	G	OP1-P-OP2	9.62	134.02	119.60
1	A	624	C	O5'-P-OP2	-9.61	97.05	105.70
1	A	1252	A	N1-C6-N6	-9.61	112.83	118.60
1	A	295	C	C6-N1-C2	-9.61	116.46	120.30
1	A	150	C	C6-N1-C2	9.60	124.14	120.30
1	A	1414	U	C4-C5-C6	9.60	125.46	119.70
1	A	497	A	C5-C6-N6	9.60	131.38	123.70
1	A	807	A	C2-N3-C4	-9.60	105.80	110.60
1	A	804	U	C5-C6-N1	-9.60	117.90	122.70
1	A	1530	G	C6-C5-N7	9.60	136.16	130.40
1	A	184	G	N7-C8-N9	-9.59	108.30	113.10
1	A	223	U	C5-C6-N1	-9.59	117.90	122.70
1	A	767	A	N1-C2-N3	9.59	134.10	129.30
1	A	789	U	C5-C4-O4	9.59	131.66	125.90
1	A	559	A	N3-C4-C5	-9.59	120.09	126.80
1	A	561	U	N3-C4-O4	9.59	126.11	119.40
1	A	104	G	C5-C6-N1	-9.59	106.71	111.50
1	A	1050	G	C6-C5-N7	-9.59	124.65	130.40
1	A	184	G	N1-C6-O6	-9.58	114.15	119.90
1	A	1504	G	C8-N9-C4	-9.58	102.57	106.40
1	A	1485	U	C5-C4-O4	9.58	131.65	125.90
1	A	718	G	N1-C6-O6	9.58	125.65	119.90
1	A	1202	G	N3-C4-N9	-9.58	120.25	126.00
1	A	528	C	N1-C2-O2	-9.57	113.16	118.90
1	A	47	C	C4-C5-C6	9.56	122.18	117.40
1	A	482	A	N1-C2-N3	9.56	134.08	129.30
1	A	1014	A	C2-N3-C4	9.56	115.38	110.60
1	A	770	C	C6-N1-C2	9.56	124.12	120.30
1	A	1171	G	C8-N9-C4	-9.56	102.58	106.40
1	A	1516	G	C4-N9-C1'	-9.56	114.07	126.50
1	A	117	G	C8-N9-C1'	-9.55	114.58	127.00
1	A	1485	U	C4-C5-C6	9.55	125.43	119.70
1	A	821	G	C2-N3-C4	-9.55	107.13	111.90
1	A	1451	A	N7-C8-N9	-9.55	109.03	113.80
1	A	187	C	C4-C5-C6	9.55	122.17	117.40
1	A	862	C	C5-C6-N1	-9.54	116.23	121.00
1	A	116	A	N7-C8-N9	-9.54	109.03	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	147	G	N1-C6-O6	9.54	125.62	119.90
1	A	238	G	C2-N3-C4	-9.54	107.13	111.90
1	A	1341	U	C5-C6-N1	-9.54	117.93	122.70
1	A	906	G	C6-C5-N7	-9.54	124.68	130.40
1	A	916	G	C8-N9-C4	-9.53	102.59	106.40
1	A	569	C	C2-N3-C4	-9.53	115.14	119.90
1	A	685	G	C4-N9-C1'	-9.53	114.11	126.50
1	A	1397	C	N1-C2-O2	9.53	124.62	118.90
1	A	760	G	N3-C2-N2	-9.52	113.23	119.90
1	A	513	C	O5'-P-OP2	9.52	122.13	110.70
1	A	633	G	C4-C5-N7	9.52	114.61	110.80
1	A	1496	C	N3-C4-N4	-9.52	111.34	118.00
1	A	1354	C	N3-C4-C5	-9.52	118.09	121.90
1	A	1323	G	C5-C6-O6	-9.51	122.89	128.60
1	A	304	U	N1-C2-O2	9.51	129.46	122.80
1	A	886	G	C6-C5-N7	-9.51	124.69	130.40
1	A	886	G	N1-C6-O6	9.51	125.61	119.90
1	A	515	G	C6-C5-N7	-9.51	124.70	130.40
1	A	729	A	C5-C6-N6	9.51	131.30	123.70
1	A	855	G	C6-C5-N7	-9.51	124.70	130.40
1	A	675	A	C2-N3-C4	-9.50	105.85	110.60
1	A	113	G	N9-C4-C5	-9.50	101.60	105.40
1	A	256	U	C5-C4-O4	-9.50	120.20	125.90
1	A	618	C	N3-C2-O2	9.50	128.55	121.90
1	A	20	U	C5-C6-N1	-9.50	117.95	122.70
1	A	494	G	C8-N9-C4	-9.50	102.60	106.40
1	A	778	G	C4-C5-C6	9.50	124.50	118.80
1	A	6	G	N3-C2-N2	-9.49	113.25	119.90
1	A	239	U	N1-C2-O2	-9.49	116.15	122.80
1	A	275	G	C6-C5-N7	-9.49	124.70	130.40
1	A	916	G	O5'-P-OP2	-9.49	97.16	105.70
1	A	254	G	O5'-P-OP1	-9.49	97.16	105.70
1	A	639	G	N1-C6-O6	9.49	125.59	119.90
1	A	860	A	C8-N9-C4	9.49	109.59	105.80
1	A	113	G	O5'-P-OP1	9.48	122.08	110.70
1	A	1215	G	C8-N9-C4	-9.48	102.61	106.40
1	A	1502	A	N7-C8-N9	9.48	118.54	113.80
1	A	446	G	N1-C2-N3	9.47	129.59	123.90
1	A	1505	G	C4-N9-C1'	9.47	138.82	126.50
1	A	1211	U	N1-C2-O2	9.47	129.43	122.80
1	A	901	A	C6-N1-C2	9.47	124.28	118.60
1	A	122	G	C5-C6-N1	-9.47	106.77	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	284	G	C8-N9-C4	9.47	110.19	106.40
1	A	809	G	O5'-P-OP2	-9.46	97.19	105.70
1	A	256	U	N3-C2-O2	9.46	128.82	122.20
1	A	1068	G	C4-C5-N7	9.45	114.58	110.80
1	A	774	G	N1-C6-O6	9.45	125.57	119.90
1	A	33	A	O5'-P-OP2	-9.45	97.19	105.70
1	A	373	A	N1-C6-N6	-9.45	112.93	118.60
1	A	802	A	C5-C6-N6	-9.45	116.14	123.70
1	A	1344	C	C6-N1-C2	9.45	124.08	120.30
1	A	33	A	N1-C6-N6	9.45	124.27	118.60
1	A	251	G	N9-C4-C5	-9.45	101.62	105.40
1	A	1487	G	N3-C4-N9	9.44	131.66	126.00
1	A	132	C	C2-N3-C4	-9.44	115.18	119.90
1	A	26	A	C8-N9-C4	-9.43	102.03	105.80
1	A	877	C	O5'-P-OP1	-9.43	97.21	105.70
1	A	965	A	C8-N9-C4	9.43	109.57	105.80
1	A	814	A	N3-C4-C5	9.43	133.40	126.80
1	A	1487	G	C5-N7-C8	9.43	109.02	104.30
1	A	721	G	C8-N9-C1'	-9.43	114.75	127.00
1	A	854	G	C6-C5-N7	-9.42	124.75	130.40
1	A	920	U	C5-C6-N1	-9.42	117.99	122.70
1	A	318	G	N3-C2-N2	-9.42	113.31	119.90
1	A	18	C	C4-C5-C6	9.41	122.11	117.40
1	A	821	G	N1-C2-N3	9.41	129.55	123.90
1	A	776	G	N1-C6-O6	-9.40	114.26	119.90
1	A	885	G	C2-N3-C4	-9.40	107.20	111.90
1	A	629	G	N9-C4-C5	9.39	109.16	105.40
1	A	332	G	OP2-P-O3'	9.39	125.86	105.20
1	A	976	G	C8-N9-C4	9.39	110.16	106.40
1	A	265	G	N1-C2-N2	-9.39	107.75	116.20
1	A	333	G	C4-C5-C6	9.39	124.43	118.80
1	A	1471	G	C5-C6-N1	-9.39	106.81	111.50
1	A	49	U	N3-C2-O2	9.39	128.77	122.20
1	A	55	A	N1-C6-N6	-9.38	112.97	118.60
1	A	302	G	O5'-P-OP2	-9.37	97.26	105.70
1	A	944	G	N1-C2-N2	-9.37	107.76	116.20
1	A	1227	A	N9-C4-C5	-9.37	102.05	105.80
1	A	16	A	N7-C8-N9	-9.37	109.11	113.80
1	A	1510	U	C5-C4-O4	-9.37	120.28	125.90
1	A	357	G	N7-C8-N9	-9.37	108.42	113.10
1	A	364	A	C2-N3-C4	-9.37	105.92	110.60
1	A	657	G	C6-C5-N7	-9.37	124.78	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	348	G	C5-C6-O6	-9.36	122.98	128.60
1	A	1333	A	C6-N1-C2	-9.36	112.98	118.60
1	A	1237	C	C4-C5-C6	9.36	122.08	117.40
1	A	365	U	N3-C4-O4	9.35	125.95	119.40
1	A	438	G	C5-N7-C8	9.35	108.97	104.30
1	A	533	A	OP1-P-OP2	-9.35	105.58	119.60
1	A	1254	C	N1-C2-O2	-9.34	113.29	118.90
1	A	560	U	N1-C2-O2	9.34	129.34	122.80
1	A	125	U	N1-C2-N3	9.34	120.50	114.90
1	A	759	A	C8-N9-C4	-9.34	102.06	105.80
1	A	254	G	C5-C6-O6	-9.33	123.00	128.60
1	A	230	G	C5-C6-O6	9.33	134.20	128.60
1	A	811	C	O5'-P-OP2	-9.33	97.30	105.70
1	A	855	G	O5'-P-OP2	9.33	121.90	110.70
1	A	858	G	C8-N9-C4	-9.33	102.67	106.40
1	A	41	G	C5-C6-O6	-9.32	123.00	128.60
1	A	586	C	O5'-P-OP2	-9.32	97.31	105.70
1	A	611	A	O5'-P-OP2	-9.32	97.31	105.70
1	A	1116	C	C6-N1-C2	9.32	124.03	120.30
1	A	1098	C	C6-N1-C2	9.32	124.03	120.30
1	A	1454	G	O5'-P-OP1	9.32	121.88	110.70
1	A	405	U	C4-C5-C6	9.32	125.29	119.70
1	A	103	C	N3-C2-O2	-9.31	115.38	121.90
1	A	1338	G	N3-C4-C5	-9.31	123.94	128.60
1	A	3	G	O4'-C1'-N9	9.31	115.65	108.20
1	A	551	U	C6-N1-C2	9.31	126.59	121.00
1	A	1054	C	N3-C4-N4	9.31	124.52	118.00
1	A	318	G	C5-N7-C8	9.31	108.95	104.30
1	A	1488	G	N1-C6-O6	9.31	125.48	119.90
1	A	778	G	C8-N9-C4	9.31	110.12	106.40
1	A	79	G	C4-C5-N7	9.30	114.52	110.80
1	A	927	G	N3-C2-N2	-9.30	113.39	119.90
1	A	8	A	C5-C6-N6	9.30	131.14	123.70
1	A	278	G	C5-C6-O6	9.29	134.18	128.60
1	A	1474	G	C5-C6-N1	-9.29	106.85	111.50
1	A	160	A	O5'-P-OP2	-9.29	97.34	105.70
1	A	894	G	C4-C5-N7	9.29	114.52	110.80
1	A	403	C	N3-C4-N4	9.28	124.50	118.00
1	A	1082	G	C6-C5-N7	-9.29	124.83	130.40
1	A	1191	A	N1-C6-N6	9.28	124.17	118.60
1	A	1510	U	N1-C2-N3	-9.28	109.33	114.90
1	A	952	U	N3-C4-O4	9.28	125.90	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1178	G	C4-C5-N7	-9.28	107.09	110.80
1	A	117	G	C5-C6-O6	-9.28	123.03	128.60
1	A	199	G	N3-C4-C5	9.28	133.24	128.60
1	A	58	C	C6-N1-C2	-9.27	116.59	120.30
1	A	320	C	N3-C4-N4	9.27	124.49	118.00
1	A	363	A	N1-C2-N3	9.27	133.94	129.30
1	A	1020	U	O4'-C1'-N1	9.27	115.62	108.20
1	A	778	G	C4-N9-C1'	9.27	138.55	126.50
1	A	1235	U	N1-C2-N3	9.27	120.46	114.90
1	A	1416	G	C8-N9-C4	-9.27	102.69	106.40
1	A	564	C	N3-C4-N4	9.26	124.48	118.00
1	A	922	G	N3-C2-N2	-9.26	113.42	119.90
1	A	1212	U	C2-N1-C1'	9.26	128.81	117.70
1	A	318	G	N7-C8-N9	-9.26	108.47	113.10
1	A	508	C	O5'-P-OP2	-9.26	97.37	105.70
1	A	794	A	O5'-P-OP2	-9.26	97.37	105.70
1	A	1298	C	O5'-P-OP1	-9.26	97.37	105.70
1	A	228	A	N1-C6-N6	-9.25	113.05	118.60
1	A	1079	G	N3-C4-N9	9.25	131.55	126.00
1	A	304	U	N3-C2-O2	-9.25	115.73	122.20
1	A	1441	G	O5'-P-OP2	-9.25	97.38	105.70
1	A	1280	A	C4-C5-N7	-9.24	106.08	110.70
1	A	577	G	C2-N3-C4	-9.24	107.28	111.90
1	A	1202	G	O5'-P-OP1	-9.24	97.39	105.70
1	A	15	G	N1-C6-O6	9.24	125.44	119.90
1	A	782	A	N9-C4-C5	9.24	109.50	105.80
1	A	1212	U	O4'-C1'-N1	9.24	115.59	108.20
1	A	837	G	N1-C6-O6	9.23	125.44	119.90
1	A	975	A	N1-C2-N3	9.23	133.91	129.30
1	A	752	G	N1-C6-O6	-9.23	114.36	119.90
1	A	766	A	C2-N3-C4	-9.23	105.99	110.60
1	A	18	C	C5-C6-N1	-9.22	116.39	121.00
1	A	18	C	C2-N3-C4	-9.22	115.29	119.90
1	A	242	C	C5-C6-N1	-9.22	116.39	121.00
1	A	390	C	N3-C4-C5	-9.22	118.21	121.90
1	A	619	U	O5'-P-OP1	9.22	121.76	110.70
1	A	243	A	N1-C6-N6	9.21	124.13	118.60
1	A	730	G	C5-N7-C8	9.21	108.91	104.30
1	A	521	G	C5-C6-N1	9.21	116.10	111.50
1	A	1338	G	N1-C6-O6	-9.21	114.38	119.90
1	A	753	A	C4-C5-N7	-9.20	106.10	110.70
1	A	779	C	C5-C6-N1	-9.20	116.40	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	550	G	N1-C2-N3	9.20	129.42	123.90
1	A	883	C	N3-C4-C5	-9.20	118.22	121.90
1	A	1222	G	N3-C2-N2	-9.20	113.46	119.90
1	A	181	G	C4-N9-C1'	9.19	138.45	126.50
1	A	204	U	C6-N1-C2	-9.18	115.49	121.00
1	A	721	G	C4-N9-C1'	9.18	138.43	126.50
1	A	658	G	C4-N9-C1'	9.18	138.43	126.50
1	A	1483	A	C5-C6-N1	9.18	122.29	117.70
1	A	619	U	N1-C2-N3	9.17	120.40	114.90
1	A	442	C	C6-N1-C2	9.17	123.97	120.30
1	A	901	A	OP2-P-O3'	9.17	125.37	105.20
1	A	1214	C	C5-C4-N4	9.17	126.62	120.20
1	A	1003	G	N3-C4-C5	-9.16	124.02	128.60
1	A	531	U	C2-N1-C1'	-9.16	106.71	117.70
1	A	753	A	N9-C4-C5	9.16	109.46	105.80
1	A	953	G	N1-C2-N2	-9.16	107.95	116.20
1	A	778	G	C5-C6-N1	-9.16	106.92	111.50
1	A	908	A	C5-C6-N6	9.16	131.03	123.70
1	A	199	G	C5-C6-N1	-9.15	106.92	111.50
1	A	895	G	C8-N9-C4	-9.15	102.74	106.40
1	A	1252	A	C8-N9-C4	9.15	109.46	105.80
1	A	328	C	N3-C2-O2	-9.15	115.50	121.90
1	A	446	G	C6-C5-N7	-9.15	124.91	130.40
1	A	93	G	N1-C6-O6	9.14	125.39	119.90
1	A	323	U	O5'-P-OP2	-9.14	97.47	105.70
1	A	836	G	C5-C6-O6	-9.14	123.11	128.60
1	A	1210	C	N3-C4-C5	-9.14	118.24	121.90
1	A	60	A	O5'-P-OP1	-9.14	97.48	105.70
1	A	26	A	C2-N3-C4	-9.14	106.03	110.60
1	A	506	G	C4-N9-C1'	9.13	138.37	126.50
1	A	818	G	N3-C4-N9	-9.13	120.52	126.00
1	A	143	A	C8-N9-C4	9.12	109.45	105.80
1	A	413	G	C2-N3-C4	-9.12	107.34	111.90
1	A	1245	A	N1-C6-N6	-9.12	113.13	118.60
1	A	1394	A	O5'-P-OP2	-9.12	97.49	105.70
1	A	278	G	N1-C2-N2	-9.12	107.99	116.20
1	A	793	U	N3-C2-O2	-9.12	115.82	122.20
1	A	1201	A	P-O3'-C3'	9.12	130.64	119.70
1	A	625	G	N1-C6-O6	9.11	125.37	119.90
1	A	1252	A	C4-C5-N7	-9.11	106.14	110.70
1	A	1139	G	C8-N9-C4	-9.11	102.76	106.40
1	A	1229	A	C2-N3-C4	-9.11	106.05	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	152	A	O5'-P-OP2	9.11	121.63	110.70
1	A	348	G	C5-N7-C8	-9.10	99.75	104.30
1	A	559	A	C2-N3-C4	9.10	115.15	110.60
1	A	1392	G	O5'-P-OP2	-9.10	97.51	105.70
1	A	266	G	N1-C6-O6	9.10	125.36	119.90
1	A	308	C	C5-C6-N1	9.10	125.55	121.00
1	A	447	G	C8-N9-C4	9.09	110.04	106.40
1	A	557	G	C4-C5-N7	-9.09	107.16	110.80
1	A	199	G	C8-N9-C4	9.09	110.04	106.40
1	A	524	G	C2-N3-C4	9.09	116.44	111.90
1	A	17	U	C5-C6-N1	-9.09	118.16	122.70
1	A	1530	G	C5-C6-O6	-9.09	123.15	128.60
1	A	1055	A	N1-C6-N6	9.08	124.05	118.60
1	A	401	C	C5-C4-N4	-9.08	113.84	120.20
1	A	62	U	C4-C5-C6	9.08	125.15	119.70
1	A	615	C	N3-C4-N4	9.08	124.36	118.00
1	A	806	C	C5-C4-N4	-9.08	113.84	120.20
1	A	788	U	N3-C4-O4	9.08	125.75	119.40
1	A	823	G	C5-C6-O6	-9.08	123.15	128.60
1	A	1070	U	C5-C6-N1	-9.07	118.16	122.70
1	A	1341	U	O5'-P-OP2	-9.07	97.53	105.70
1	A	839	U	N3-C4-O4	-9.07	113.05	119.40
1	A	632	A	C5-N7-C8	-9.07	99.37	103.90
1	A	1354	C	N3-C4-N4	9.07	124.35	118.00
1	A	1415	G	N9-C4-C5	9.06	109.03	105.40
1	A	334	C	C6-N1-C2	-9.06	116.68	120.30
1	A	1258	G	C8-N9-C4	-9.06	102.78	106.40
1	A	511	C	O5'-P-OP2	-9.06	97.55	105.70
1	A	1212	U	N1-C2-N3	-9.06	109.46	114.90
1	A	730	G	C4-C5-C6	9.05	124.23	118.80
1	A	1188	A	O5'-P-OP1	-9.05	97.55	105.70
1	A	557	G	N9-C4-C5	9.05	109.02	105.40
1	A	560	U	N1-C2-N3	9.05	120.33	114.90
1	A	1117	G	N9-C4-C5	-9.05	101.78	105.40
1	A	1409	C	C5-C4-N4	-9.05	113.86	120.20
1	A	1486	G	O5'-P-OP2	-9.05	97.56	105.70
1	A	832	C	O5'-P-OP2	-9.05	97.56	105.70
1	A	529	G	C6-C5-N7	-9.04	124.97	130.40
1	A	724	G	N3-C4-C5	-9.05	124.08	128.60
1	A	1173	G	C8-N9-C4	9.05	110.02	106.40
1	A	1417	G	N1-C6-O6	9.04	125.33	119.90
1	A	361	G	OP2-P-O3'	9.04	125.08	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	724	G	N7-C8-N9	9.04	117.62	113.10
1	A	1323	G	C2-N3-C4	-9.04	107.38	111.90
12	L	53	ARG	NE-CZ-NH1	9.03	124.82	120.30
1	A	855	G	N1-C2-N3	9.03	129.32	123.90
1	A	181	G	C8-N9-C1'	-9.03	115.26	127.00
1	A	450	G	N3-C2-N2	-9.03	113.58	119.90
1	A	721	G	O5'-P-OP2	-9.02	97.58	105.70
1	A	1121	U	C6-N1-C2	9.02	126.41	121.00
1	A	797	C	N3-C4-N4	9.01	124.31	118.00
1	A	858	G	N3-C4-C5	-9.01	124.09	128.60
1	A	174	C	OP2-P-O3'	9.01	125.02	105.20
1	A	279	A	N3-C4-C5	9.01	133.11	126.80
1	A	912	C	C6-N1-C2	-9.01	116.70	120.30
1	A	1215	G	N1-C6-O6	9.01	125.30	119.90
1	A	793	U	C6-N1-C2	-9.00	115.60	121.00
1	A	1067	A	C8-N9-C4	-9.00	102.20	105.80
1	A	46	G	N1-C2-N2	9.00	124.30	116.20
1	A	144	G	C6-C5-N7	-9.00	125.00	130.40
1	A	1331	G	N9-C4-C5	9.00	109.00	105.40
1	A	963	G	N3-C4-C5	-9.00	124.10	128.60
1	A	1237	C	N1-C2-N3	8.99	125.50	119.20
1	A	663	A	C8-N9-C4	8.99	109.40	105.80
1	A	108	G	C4-C5-C6	8.99	124.19	118.80
1	A	890	G	O4'-C1'-N9	8.99	115.39	108.20
1	A	1335	C	N3-C4-N4	-8.99	111.71	118.00
1	A	1371	G	O5'-P-OP2	8.99	121.48	110.70
1	A	490	G	C8-N9-C4	8.98	109.99	106.40
1	A	667	G	C5-C6-N1	-8.98	107.01	111.50
1	A	721	G	O5'-P-OP1	-8.98	97.62	105.70
1	A	804	U	N3-C2-O2	-8.98	115.92	122.20
1	A	911	U	O5'-P-OP2	-8.98	97.62	105.70
1	A	1222	G	C2-N3-C4	-8.97	107.41	111.90
1	A	528	C	N3-C4-N4	8.97	124.28	118.00
1	A	117	G	C4-C5-N7	8.97	114.39	110.80
1	A	551	U	C5-C6-N1	-8.97	118.22	122.70
1	A	1447	G	N7-C8-N9	8.97	117.58	113.10
1	A	1516	G	N3-C4-N9	-8.97	120.62	126.00
1	A	582	U	C2-N3-C4	-8.96	121.62	127.00
1	A	284	G	N3-C2-N2	-8.96	113.63	119.90
1	A	604	G	N1-C6-O6	8.96	125.28	119.90
1	A	321	A	O5'-P-OP1	8.95	121.44	110.70
1	A	665	A	O5'-P-OP2	-8.96	97.64	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1488	G	C5-C6-N1	-8.95	107.02	111.50
1	A	309	G	N3-C2-N2	-8.95	113.64	119.90
1	A	1415	G	N1-C2-N2	-8.95	108.14	116.20
1	A	1197	G	O5'-P-OP2	-8.95	97.65	105.70
1	A	1499	A	N1-C6-N6	-8.95	113.23	118.60
1	A	1515	C	N3-C4-C5	8.94	125.48	121.90
1	A	153	C	O5'-P-OP2	-8.94	97.65	105.70
1	A	1148	U	N3-C2-O2	-8.94	115.94	122.20
1	A	109	A	N3-C4-N9	-8.94	120.25	127.40
1	A	752	G	C5-N7-C8	8.93	108.77	104.30
1	A	1189	C	OP2-P-O3'	8.93	124.85	105.20
1	A	667	G	N1-C6-O6	8.93	125.26	119.90
1	A	522	C	C2-N1-C1'	-8.93	108.98	118.80
1	A	1502	A	N1-C2-N3	8.93	133.76	129.30
1	A	116	A	C2-N3-C4	-8.93	106.14	110.60
1	A	61	G	C5-C6-O6	-8.92	123.25	128.60
1	A	483	C	OP1-P-OP2	8.92	132.98	119.60
1	A	396	G	C5-C6-O6	8.91	133.95	128.60
1	A	497	A	C4-C5-N7	-8.91	106.24	110.70
1	A	421	U	O5'-P-OP1	-8.91	97.68	105.70
1	A	629	G	C4-C5-N7	-8.91	107.24	110.80
1	A	1082	G	C5-C6-N1	-8.91	107.05	111.50
1	A	1397	C	C4-C5-C6	-8.91	112.95	117.40
1	A	281	G	C6-C5-N7	-8.90	125.06	130.40
1	A	802	A	N1-C6-N6	8.90	123.94	118.60
1	A	7	G	O5'-P-OP1	-8.90	97.69	105.70
1	A	1388	C	C2-N1-C1'	8.90	128.59	118.80
1	A	583	A	N1-C6-N6	8.89	123.94	118.60
1	A	779	C	C4-C5-C6	8.88	121.84	117.40
1	A	254	G	C8-N9-C4	8.88	109.95	106.40
1	A	1356	G	C5-C6-N1	-8.88	107.06	111.50
1	A	113	G	C5-C6-O6	-8.88	123.27	128.60
1	A	1308	U	N3-C4-C5	-8.88	109.27	114.60
1	A	53	A	N1-C2-N3	8.87	133.74	129.30
1	A	578	C	C6-N1-C2	8.88	123.85	120.30
1	A	761	G	C5-C6-O6	-8.87	123.28	128.60
1	A	539	A	O5'-P-OP2	-8.87	97.72	105.70
1	A	601	C	C5-C6-N1	-8.87	116.56	121.00
1	A	120	A	O5'-P-OP1	-8.87	97.72	105.70
1	A	761	G	C4-C5-N7	8.87	114.35	110.80
1	A	74	C	OP1-P-OP2	-8.86	106.31	119.60
1	A	783	C	OP2-P-O3'	8.86	124.69	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1254	C	N3-C2-O2	8.86	128.10	121.90
1	A	81	U	C5-C6-N1	8.86	127.13	122.70
1	A	583	A	N1-C2-N3	8.86	133.73	129.30
1	A	1415	G	C2-N3-C4	8.86	116.33	111.90
1	A	276	G	N9-C4-C5	-8.86	101.86	105.40
1	A	1443	G	N3-C4-C5	8.85	133.03	128.60
1	A	746	A	N9-C4-C5	8.85	109.34	105.80
1	A	1506	U	N3-C4-O4	8.85	125.59	119.40
1	A	1539	C	C2-N1-C1'	8.85	128.53	118.80
1	A	101	A	O5'-P-OP2	-8.85	97.74	105.70
1	A	300	A	C5-C6-N6	8.85	130.78	123.70
1	A	699	C	C6-N1-C2	8.84	123.84	120.30
1	A	824	C	N3-C4-C5	-8.84	118.36	121.90
1	A	1050	G	C2-N3-C4	-8.84	107.48	111.90
1	A	616	G	O5'-P-OP2	-8.84	97.74	105.70
1	A	193	C	C4-C5-C6	8.84	121.82	117.40
1	A	101	A	O5'-P-OP1	8.83	121.30	110.70
1	A	557	G	C6-N1-C2	-8.83	119.80	125.10
1	A	1190	G	P-O3'-C3'	8.83	130.30	119.70
1	A	66	G	N3-C2-N2	-8.83	113.72	119.90
1	A	633	G	C6-C5-N7	-8.83	125.10	130.40
1	A	866	C	N3-C4-C5	-8.83	118.37	121.90
1	A	113	G	C8-N9-C1'	-8.82	115.53	127.00
1	A	586	C	N1-C2-O2	-8.82	113.61	118.90
1	A	1064	G	N3-C2-N2	-8.82	113.72	119.90
1	A	576	G	O5'-P-OP1	-8.82	97.77	105.70
1	A	1222	G	C4-C5-N7	-8.82	107.27	110.80
1	A	542	G	N3-C2-N2	-8.81	113.73	119.90
1	A	32	A	N1-C2-N3	8.81	133.71	129.30
1	A	237	C	OP2-P-O3'	8.80	124.56	105.20
1	A	306	G	N3-C2-N2	-8.80	113.74	119.90
1	A	1144	G	N1-C6-O6	8.80	125.18	119.90
1	A	31	G	O5'-P-OP2	-8.80	97.78	105.70
1	A	250	A	C5-C6-N1	-8.80	113.30	117.70
1	A	542	G	N1-C6-O6	8.79	125.18	119.90
1	A	818	G	C4-C5-N7	-8.79	107.28	110.80
1	A	1191	A	C4-C5-N7	8.79	115.10	110.70
1	A	817	C	C2-N1-C1'	8.79	128.47	118.80
1	A	1212	U	C5-C6-N1	8.79	127.10	122.70
1	A	380	G	C4-C5-N7	-8.79	107.28	110.80
1	A	438	G	N1-C6-O6	-8.78	114.63	119.90
1	A	177	C	OP1-P-OP2	8.78	132.77	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1064	G	C8-N9-C1'	8.78	138.42	127.00
1	A	239	U	N1-C2-N3	8.78	120.17	114.90
1	A	313	A	C8-N9-C4	8.78	109.31	105.80
1	A	1303	C	N1-C2-O2	8.78	124.17	118.90
1	A	668	G	C6-C5-N7	-8.78	125.14	130.40
1	A	641	U	N3-C4-O4	8.77	125.54	119.40
1	A	1047	G	N1-C6-O6	8.77	125.16	119.90
1	A	113	G	C2-N3-C4	-8.76	107.52	111.90
1	A	795	C	C6-N1-C2	8.76	123.81	120.30
1	A	615	C	N3-C4-C5	-8.76	118.40	121.90
1	A	742	G	N7-C8-N9	-8.76	108.72	113.10
1	A	1411	C	C6-N1-C2	-8.76	116.80	120.30
1	A	293	G	N1-C2-N3	8.75	129.15	123.90
1	A	632	A	N1-C6-N6	8.75	123.85	118.60
1	A	14	U	N1-C2-N3	8.74	120.15	114.90
1	A	668	G	N1-C6-O6	8.74	125.15	119.90
1	A	1342	C	N3-C2-O2	8.74	128.02	121.90
1	A	840	C	C5-C6-N1	8.74	125.37	121.00
1	A	1168	A	C4-C5-C6	8.74	121.37	117.00
1	A	117	G	N1-C2-N3	8.73	129.14	123.90
1	A	260	G	C4-C5-C6	8.73	124.04	118.80
1	A	904	C	C5-C6-N1	-8.73	116.63	121.00
1	A	218	C	N1-C2-O2	-8.73	113.66	118.90
1	A	564	C	C4-C5-C6	8.73	121.77	117.40
1	A	658	G	N1-C2-N2	-8.73	108.34	116.20
1	A	1286	A	C4-C5-N7	8.73	115.06	110.70
1	A	1062	U	C5-C4-O4	8.73	131.14	125.90
1	A	1057	G	C4-N9-C1'	-8.73	115.16	126.50
1	A	1286	A	N1-C6-N6	8.73	123.84	118.60
1	A	1323	G	N9-C4-C5	-8.73	101.91	105.40
1	A	1193	G	C5-N7-C8	-8.72	99.94	104.30
1	A	910	C	N1-C2-O2	-8.72	113.67	118.90
1	A	1223	C	C6-N1-C2	-8.72	116.81	120.30
1	A	893	C	C2-N3-C4	8.72	124.26	119.90
1	A	47	C	N1-C2-O2	8.71	124.13	118.90
1	A	331	G	C5-C6-N1	-8.71	107.14	111.50
1	A	554	C	C4-C5-C6	8.71	121.76	117.40
1	A	858	G	N1-C2-N2	-8.71	108.36	116.20
1	A	372	C	C5'-C4'-O4'	8.71	119.55	109.10
1	A	490	G	N9-C4-C5	-8.71	101.92	105.40
1	A	1053	G	N3-C4-C5	8.70	132.95	128.60
1	A	1316	G	N3-C4-N9	-8.70	120.78	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	26	A	C6-N1-C2	-8.70	113.38	118.60
1	A	579	G	C6-N1-C2	-8.70	119.88	125.10
1	A	284	G	C4-C5-C6	8.70	124.02	118.80
1	A	446	G	C4-C5-C6	8.69	124.02	118.80
1	A	1100	C	C6-N1-C1'	-8.69	110.37	120.80
1	A	1283	G	N1-C6-O6	8.69	125.11	119.90
1	A	117	G	O5'-P-OP2	-8.69	97.88	105.70
1	A	227	G	N1-C6-O6	8.68	125.11	119.90
1	A	818	G	C6-N1-C2	8.68	130.31	125.10
1	A	1094	G	C8-N9-C1'	-8.68	115.72	127.00
1	A	1331	G	N3-C4-N9	-8.68	120.79	126.00
1	A	803	G	N1-C6-O6	-8.68	114.69	119.90
1	A	55	A	C6-N1-C2	-8.67	113.40	118.60
1	A	536	C	N1-C2-O2	-8.67	113.70	118.90
1	A	15	G	C6-C5-N7	-8.67	125.20	130.40
1	A	513	C	O5'-P-OP1	-8.67	97.90	105.70
1	A	685	G	N3-C4-C5	8.67	132.93	128.60
1	A	1060	C	N3-C4-C5	-8.66	118.43	121.90
1	A	289	G	C8-N9-C4	-8.66	102.94	106.40
1	A	956	U	C6-N1-C2	8.66	126.20	121.00
1	A	1309	G	C5-C6-N1	8.66	115.83	111.50
1	A	280	C	N3-C4-C5	-8.66	118.44	121.90
1	A	728	A	N1-C6-N6	-8.66	113.41	118.60
1	A	318	G	C4-C5-N7	-8.65	107.34	110.80
1	A	1071	C	C6-N1-C2	8.65	123.76	120.30
1	A	1264	C	N3-C4-C5	-8.65	118.44	121.90
1	A	1405	G	C5-C6-O6	-8.65	123.41	128.60
1	A	348	G	N1-C6-O6	8.64	125.09	119.90
1	A	352	C	C4-C5-C6	8.64	121.72	117.40
1	A	970	C	O5'-P-OP1	-8.64	97.92	105.70
1	A	1004	A	O4'-C1'-N9	8.64	115.11	108.20
1	A	1342	C	N1-C2-N3	-8.64	113.15	119.20
1	A	1514	C	N3-C4-C5	8.64	125.36	121.90
1	A	121	C	C6-N1-C2	8.64	123.76	120.30
1	A	236	G	C8-N9-C1'	-8.64	115.77	127.00
1	A	559	A	C5-C6-N6	-8.64	116.79	123.70
1	A	1286	A	O5'-P-OP1	-8.64	97.93	105.70
1	A	1416	G	C4-C5-N7	8.64	114.25	110.80
1	A	190(G)	G	N1-C6-O6	8.63	125.08	119.90
1	A	431	A	N1-C2-N3	8.63	133.62	129.30
1	A	886	G	C2-N3-C4	-8.63	107.58	111.90
1	A	1526	G	N1-C6-O6	8.63	125.08	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	251	G	C8-N9-C4	8.63	109.85	106.40
1	A	361	G	O5'-P-OP1	-8.63	97.94	105.70
1	A	1269	A	C6-C5-N7	8.63	138.34	132.30
1	A	389	A	N3-C4-C5	-8.62	120.76	126.80
1	A	497	A	C8-N9-C4	-8.62	102.35	105.80
1	A	763	G	C4-C5-N7	8.62	114.25	110.80
1	A	296	U	O5'-P-OP2	-8.62	97.94	105.70
1	A	710	G	C2-N3-C4	-8.62	107.59	111.90
1	A	1319	A	C2-N3-C4	-8.62	106.29	110.60
4	D	88	VAL	CB-CA-C	-8.61	95.03	111.40
1	A	945	G	C2-N3-C4	8.61	116.21	111.90
1	A	1371	G	O5'-P-OP1	-8.61	97.95	105.70
1	A	1432	G	C5-C6-O6	8.61	133.76	128.60
1	A	402	G	N1-C2-N3	8.60	129.06	123.90
1	A	1478	C	C2-N3-C4	8.60	124.20	119.90
1	A	423	G	N3-C4-N9	8.60	131.16	126.00
1	A	47	C	N3-C2-O2	-8.60	115.88	121.90
1	A	1508	G	N9-C4-C5	8.60	108.84	105.40
1	A	837	G	O5'-P-OP1	8.60	121.02	110.70
1	A	807	A	N7-C8-N9	8.59	118.10	113.80
1	A	855	G	O5'-P-OP1	-8.59	97.97	105.70
1	A	1403	C	C5-C6-N1	-8.59	116.70	121.00
1	A	187	C	N1-C2-O2	-8.59	113.75	118.90
1	A	515	G	C2-N3-C4	-8.58	107.61	111.90
1	A	674	G	C8-N9-C1'	-8.58	115.84	127.00
1	A	1370	G	N7-C8-N9	8.58	117.39	113.10
1	A	319	G	C8-N9-C4	-8.58	102.97	106.40
1	A	561	U	N3-C4-C5	-8.58	109.45	114.60
1	A	41	G	C8-N9-C4	-8.58	102.97	106.40
1	A	620	C	OP1-P-O3'	8.58	124.07	105.20
1	A	762	C	C6-N1-C2	8.58	123.73	120.30
1	A	1051	C	C6-N1-C2	8.58	123.73	120.30
1	A	1520	G	C5-C6-O6	-8.57	123.46	128.60
1	A	70	G	N1-C6-O6	8.57	125.04	119.90
1	A	559	A	C6-N1-C2	-8.57	113.46	118.60
1	A	761	G	O5'-P-OP2	-8.56	98.00	105.70
12	L	86	ARG	NE-CZ-NH2	-8.56	116.02	120.30
1	A	659	U	N1-C2-N3	8.56	120.03	114.90
1	A	870	U	N1-C2-O2	-8.56	116.81	122.80
1	A	902	G	O5'-P-OP2	-8.56	98.00	105.70
1	A	1373	G	C4-N9-C1'	8.56	137.62	126.50
1	A	112	G	N3-C2-N2	-8.56	113.91	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	G	C2-N3-C4	-8.55	107.62	111.90
1	A	76	C	C6-N1-C2	-8.55	116.88	120.30
1	A	703	G	C8-N9-C1'	-8.55	115.89	127.00
1	A	1066	C	N3-C2-O2	8.55	127.88	121.90
1	A	1152	A	N1-C6-N6	-8.55	113.47	118.60
1	A	1487	G	C4-N9-C1'	8.55	137.61	126.50
1	A	811	C	C2-N3-C4	-8.54	115.63	119.90
1	A	122	G	O5'-P-OP2	8.54	120.95	110.70
1	A	804	U	C5-C4-O4	8.54	131.03	125.90
1	A	790	A	C5-C6-N1	-8.54	113.43	117.70
1	A	1212	U	C6-N1-C1'	-8.54	109.25	121.20
1	A	101	A	N7-C8-N9	8.54	118.07	113.80
1	A	398	C	C4-C5-C6	-8.54	113.13	117.40
1	A	577	G	N3-C2-N2	-8.53	113.93	119.90
1	A	53	A	C6-N1-C2	-8.53	113.48	118.60
1	A	875	C	C5-C6-N1	-8.53	116.73	121.00
1	A	859	A	N1-C6-N6	8.53	123.72	118.60
1	A	1188	A	C2-N3-C4	-8.53	106.34	110.60
1	A	167	G	C5-C6-N1	-8.53	107.24	111.50
1	A	1438	G	C2-N3-C4	-8.53	107.64	111.90
1	A	1096	C	C5-C6-N1	8.53	125.26	121.00
1	A	1510	U	C6-N1-C2	8.53	126.11	121.00
1	A	855	G	N1-C2-N2	-8.52	108.53	116.20
1	A	762	C	N3-C4-C5	8.52	125.31	121.90
1	A	778	G	C4-C5-N7	-8.52	107.39	110.80
1	A	390	C	C6-N1-C2	8.51	123.70	120.30
1	A	769	G	N1-C6-O6	8.51	125.01	119.90
1	A	203	U	N3-C4-O4	8.51	125.36	119.40
1	A	410	G	C4-C5-N7	-8.51	107.40	110.80
1	A	1346	A	N3-C4-C5	8.51	132.76	126.80
1	A	1358	U	N3-C4-O4	8.51	125.36	119.40
1	A	604	G	C5-N7-C8	-8.51	100.05	104.30
1	A	478	A	N1-C6-N6	8.51	123.70	118.60
1	A	1139	G	N9-C4-C5	8.51	108.80	105.40
1	A	1393	U	C2-N3-C4	8.50	132.10	127.00
1	A	579	G	N3-C2-N2	-8.50	113.95	119.90
1	A	315	A	N1-C2-N3	8.50	133.55	129.30
1	A	329	A	C6-N1-C2	8.49	123.70	118.60
1	A	445	G	N1-C6-O6	8.49	125.00	119.90
1	A	1230	C	N1-C2-N3	-8.49	113.26	119.20
1	A	1450	U	N1-C2-N3	8.49	120.00	114.90
1	A	300	A	N9-C4-C5	8.49	109.19	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	295	C	N3-C4-N4	8.49	123.94	118.00
1	A	530	G	C5-N7-C8	-8.48	100.06	104.30
1	A	916	G	C5-C6-O6	-8.48	123.51	128.60
1	A	361	G	OP1-P-O3'	-8.48	86.54	105.20
1	A	670	G	N9-C4-C5	-8.48	102.01	105.40
1	A	1446	A	C5-N7-C8	8.47	108.14	103.90
1	A	1101	A	C5-C6-N1	-8.47	113.46	117.70
8	H	39	LEU	CB-CG-CD2	-8.47	96.59	111.00
1	A	255	G	C5-C6-N1	-8.47	107.27	111.50
1	A	10	A	C5-C6-N1	8.47	121.93	117.70
1	A	252	U	C5-C4-O4	8.47	130.98	125.90
1	A	767	A	O5'-P-OP2	-8.47	98.08	105.70
1	A	768	A	OP2-P-O3'	8.46	123.82	105.20
1	A	765	G	O5'-P-OP1	8.46	120.85	110.70
1	A	196	A	C4-C5-C6	-8.46	112.77	117.00
1	A	405	U	C6-N1-C2	-8.46	115.93	121.00
1	A	181	G	P-O3'-C3'	8.45	129.84	119.70
1	A	762	C	C5-C6-N1	-8.45	116.78	121.00
1	A	331	G	C4-C5-C6	8.45	123.87	118.80
1	A	916	G	N7-C8-N9	8.45	117.32	113.10
1	A	1313	U	N3-C4-O4	8.45	125.31	119.40
1	A	1389	C	C6-N1-C2	-8.44	116.92	120.30
1	A	783	C	N3-C4-C5	8.44	125.28	121.90
1	A	316	G	C5-C6-O6	-8.44	123.54	128.60
1	A	5	U	C5-C6-N1	-8.44	118.48	122.70
1	A	46	G	C5-C6-O6	-8.44	123.54	128.60
1	A	731	G	C8-N9-C4	-8.44	103.03	106.40
1	A	760	G	N1-C2-N3	8.44	128.96	123.90
1	A	1285	A	N1-C6-N6	-8.44	113.54	118.60
1	A	1374	A	N1-C2-N3	8.44	133.52	129.30
1	A	12	U	O5'-P-OP1	-8.43	98.11	105.70
1	A	894	G	C2-N3-C4	-8.43	107.68	111.90
1	A	1351	U	N3-C4-O4	-8.43	113.50	119.40
1	A	737	A	N1-C6-N6	8.43	123.66	118.60
1	A	948	C	C6-N1-C2	8.43	123.67	120.30
1	A	410	G	N1-C6-O6	-8.42	114.85	119.90
1	A	869	G	N3-C2-N2	8.42	125.79	119.90
1	A	1050	G	C4-C5-C6	8.42	123.85	118.80
1	A	801	U	N3-C4-C5	8.42	119.65	114.60
1	A	883	C	OP2-P-O3'	8.42	123.72	105.20
1	A	381	C	C6-N1-C2	-8.41	116.93	120.30
1	A	1468	A	C2-N3-C4	-8.41	106.39	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1237	C	C6-N1-C2	-8.41	116.94	120.30
1	A	1349	A	N1-C2-N3	8.41	133.50	129.30
1	A	1377	A	C5-C6-N1	-8.41	113.50	117.70
1	A	44	G	C6-C5-N7	-8.41	125.36	130.40
1	A	190(G)	G	O5'-P-OP1	-8.41	98.13	105.70
1	A	236	G	N1-C6-O6	-8.40	114.86	119.90
1	A	396	G	C4-C5-C6	8.40	123.84	118.80
1	A	262	A	C6-C5-N7	8.40	138.18	132.30
1	A	981	U	N3-C4-C5	-8.40	109.56	114.60
1	A	1280	A	N9-C4-C5	8.40	109.16	105.80
1	A	1290	G	C6-C5-N7	-8.40	125.36	130.40
1	A	852	G	C2-N3-C4	-8.40	107.70	111.90
1	A	6	G	N3-C4-N9	-8.39	120.96	126.00
1	A	1447	G	C4-C5-N7	8.39	114.16	110.80
1	A	805	C	C5-C6-N1	8.39	125.20	121.00
1	A	1439	C	C6-N1-C2	8.38	123.65	120.30
1	A	674	G	N3-C2-N2	8.38	125.77	119.90
1	A	122	G	O5'-P-OP1	-8.38	98.16	105.70
1	A	257	G	C5-C6-N1	-8.38	107.31	111.50
1	A	753	A	C5-C6-N6	8.38	130.40	123.70
1	A	1516	G	N1-C2-N2	8.38	123.74	116.20
1	A	227	G	C6-C5-N7	-8.37	125.38	130.40
1	A	1342	C	N3-C4-C5	8.38	125.25	121.90
1	A	397	A	N7-C8-N9	8.37	117.99	113.80
1	A	904	C	N3-C4-C5	8.37	125.25	121.90
1	A	1305	G	N9-C4-C5	8.37	108.75	105.40
1	A	1439	C	N1-C2-N3	-8.37	113.34	119.20
1	A	778	G	N3-C4-N9	8.37	131.02	126.00
1	A	767	A	OP1-P-OP2	8.36	132.14	119.60
1	A	1151	A	N7-C8-N9	-8.36	109.62	113.80
1	A	1299	A	N7-C8-N9	8.36	117.98	113.80
1	A	117	G	C4-N9-C1'	8.36	137.37	126.50
1	A	1127	G	N3-C4-C5	8.36	132.78	128.60
1	A	792	A	N1-C2-N3	8.36	133.48	129.30
1	A	1515	C	OP2-P-O3'	8.36	123.59	105.20
1	A	625	G	C6-C5-N7	-8.36	125.39	130.40
1	A	670	G	C8-N9-C4	8.36	109.74	106.40
1	A	807	A	C8-N9-C4	-8.35	102.46	105.80
1	A	858	G	N3-C4-N9	8.35	131.01	126.00
1	A	1281	U	N3-C4-C5	-8.35	109.59	114.60
1	A	51	A	N1-C6-N6	8.35	123.61	118.60
1	A	184	G	N3-C4-C5	-8.35	124.43	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	773	G	N1-C2-N3	8.35	128.91	123.90
1	A	823	G	N3-C4-C5	8.35	132.77	128.60
1	A	223	U	C2-N3-C4	-8.34	121.99	127.00
1	A	616	G	N1-C6-O6	8.34	124.91	119.90
1	A	332	G	C4-C5-N7	8.34	114.14	110.80
1	A	722	A	N1-C2-N3	8.34	133.47	129.30
1	A	1059	C	O5'-P-OP2	-8.34	98.19	105.70
1	A	975	A	C6-N1-C2	8.34	123.60	118.60
1	A	501	C	O5'-P-OP1	-8.34	98.20	105.70
1	A	729	A	C2-N3-C4	8.34	114.77	110.60
1	A	1179	A	N1-C6-N6	-8.34	113.60	118.60
1	A	1215	G	N7-C8-N9	8.34	117.27	113.10
1	A	447	G	N9-C4-C5	-8.33	102.07	105.40
1	A	190(D)	U	N1-C2-O2	8.33	128.63	122.80
1	A	193	C	N3-C4-C5	-8.33	118.57	121.90
1	A	232	G	C5-C6-N1	-8.33	107.33	111.50
1	A	1279	A	C4-C5-C6	8.33	121.16	117.00
1	A	1399	C	N3-C4-C5	-8.33	118.57	121.90
1	A	122	G	C2-N3-C4	-8.32	107.74	111.90
1	A	1516	G	C8-N9-C1'	8.32	137.82	127.00
1	A	8	A	N9-C4-C5	8.32	109.13	105.80
1	A	308	C	C2-N3-C4	8.32	124.06	119.90
1	A	759	A	OP1-P-O3'	-8.32	86.90	105.20
1	A	851	G	C4-C5-C6	8.32	123.79	118.80
1	A	1322	C	OP1-P-OP2	-8.32	107.12	119.60
1	A	1058	G	N3-C4-N9	8.31	130.99	126.00
1	A	1184	G	C4-C5-C6	8.31	123.79	118.80
1	A	832	C	N3-C4-C5	-8.31	118.58	121.90
1	A	1236	A	C5-C6-N1	8.31	121.85	117.70
1	A	1193	G	N1-C6-O6	8.31	124.88	119.90
1	A	1373	G	N3-C4-N9	8.31	130.98	126.00
1	A	108	G	C4-N9-C1'	8.30	137.29	126.50
1	A	223	U	O5'-P-OP2	-8.30	98.22	105.70
1	A	1396	A	O5'-P-OP1	-8.30	98.23	105.70
1	A	515	G	N1-C6-O6	8.30	124.88	119.90
1	A	1136	U	C5-C6-N1	8.30	126.85	122.70
1	A	1184	G	C6-C5-N7	-8.30	125.42	130.40
1	A	1447	G	C8-N9-C4	-8.30	103.08	106.40
1	A	314	C	C2-N1-C1'	-8.30	109.67	118.80
1	A	906	G	C5-C6-N1	-8.30	107.35	111.50
1	A	946	A	C5-C6-N6	-8.30	117.06	123.70
7	G	102	ARG	NE-CZ-NH2	-8.30	116.15	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	381	C	O5'-P-OP2	-8.30	98.23	105.70
1	A	741	G	C4-C5-N7	-8.30	107.48	110.80
1	A	1267	C	N1-C2-O2	8.30	123.88	118.90
1	A	662	G	N1-C2-N2	-8.30	108.73	116.20
1	A	897	C	C2-N3-C4	-8.29	115.75	119.90
1	A	1158	C	N3-C4-C5	-8.29	118.58	121.90
1	A	154	C	N3-C2-O2	-8.29	116.10	121.90
1	A	61	G	N3-C4-C5	8.29	132.74	128.60
1	A	7	G	O4'-C1'-N9	8.28	114.83	108.20
1	A	270	A	C8-N9-C4	-8.29	102.49	105.80
1	A	1303	C	N3-C4-N4	-8.28	112.20	118.00
1	A	619	U	N3-C2-O2	-8.28	116.40	122.20
1	A	1348	U	N1-C2-N3	8.28	119.87	114.90
1	A	1514	C	C2-N3-C4	-8.28	115.76	119.90
1	A	1131	G	N7-C8-N9	8.28	117.24	113.10
1	A	435	C	O5'-P-OP1	-8.28	98.25	105.70
1	A	609	A	C8-N9-C4	-8.27	102.49	105.80
1	A	624	C	O5'-P-OP1	8.27	120.63	110.70
1	A	125	U	O5'-P-OP2	-8.27	98.26	105.70
1	A	654	G	C8-N9-C4	-8.27	103.09	106.40
1	A	1226	C	O5'-P-OP1	8.27	120.63	110.70
1	A	576	G	N3-C4-C5	-8.27	124.47	128.60
1	A	1500	A	C2-N3-C4	8.27	114.73	110.60
1	A	315	A	C2-N3-C4	-8.26	106.47	110.60
1	A	1452	C	N3-C4-N4	8.26	123.78	118.00
1	A	97	G	O5'-P-OP1	8.26	120.61	110.70
1	A	199	G	N3-C2-N2	-8.26	114.12	119.90
1	A	879	C	OP1-P-OP2	-8.26	107.22	119.60
1	A	1304	G	C5-C6-N1	-8.26	107.37	111.50
1	A	635	G	N3-C2-N2	-8.25	114.12	119.90
1	A	728	A	N3-C4-N9	-8.25	120.80	127.40
1	A	566	G	O5'-P-OP1	-8.25	98.28	105.70
1	A	734	G	C5-N7-C8	-8.25	100.18	104.30
1	A	833	U	N3-C4-C5	-8.25	109.65	114.60
1	A	1416	G	C5-N7-C8	-8.25	100.18	104.30
1	A	1486	G	C6-N1-C2	-8.25	120.15	125.10
1	A	1522	U	N3-C2-O2	-8.25	116.43	122.20
8	H	94	TYR	CB-CG-CD2	8.25	125.95	121.00
1	A	830	G	C8-N9-C4	8.24	109.70	106.40
1	A	319	G	C2-N3-C4	-8.24	107.78	111.90
1	A	727	G	C2-N3-C4	-8.24	107.78	111.90
1	A	176	C	OP1-P-O3'	-8.23	87.08	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	241	C	N3-C4-N4	-8.23	112.23	118.00
1	A	633	G	C5-N7-C8	-8.23	100.18	104.30
1	A	511	C	N1-C2-O2	-8.23	113.96	118.90
1	A	769	G	OP2-P-O3'	8.23	123.30	105.20
1	A	778	G	C5-N7-C8	8.23	108.41	104.30
1	A	783	C	OP1-P-O3'	-8.23	87.10	105.20
1	A	1339	A	C4-C5-N7	-8.22	106.59	110.70
1	A	167	G	C2-N3-C4	-8.22	107.79	111.90
1	A	1497	G	C8-N9-C4	-8.22	103.11	106.40
1	A	616	G	C5-C6-N1	-8.22	107.39	111.50
1	A	907	A	C5-C6-N6	8.21	130.27	123.70
1	A	603	U	C6-N1-C2	-8.21	116.08	121.00
1	A	858	G	C6-C5-N7	-8.21	125.47	130.40
1	A	658	G	N1-C2-N3	8.21	128.82	123.90
1	A	1505	G	C6-C5-N7	-8.21	125.48	130.40
18	R	35	ARG	NE-CZ-NH1	-8.21	116.20	120.30
1	A	333	G	N1-C2-N3	8.20	128.82	123.90
1	A	614	A	C6-C5-N7	-8.20	126.56	132.30
5	E	18	ARG	NE-CZ-NH2	-8.20	116.20	120.30
1	A	645	C	N1-C2-O2	8.20	123.82	118.90
1	A	930	C	N1-C2-N3	8.20	124.94	119.20
1	A	198	G	C8-N9-C1'	-8.19	116.35	127.00
1	A	452	A	C8-N9-C4	-8.20	102.52	105.80
1	A	886	G	O5'-P-OP2	-8.20	98.33	105.70
1	A	1184	G	C4-N9-C1'	8.20	137.16	126.50
1	A	1299	A	C8-N9-C4	-8.19	102.52	105.80
1	A	1526	G	C5-C6-N1	-8.19	107.41	111.50
1	A	1383	C	N1-C2-N3	-8.18	113.47	119.20
1	A	62	U	C6-N1-C2	-8.18	116.09	121.00
1	A	224	C	N1-C2-N3	8.18	124.92	119.20
1	A	533	A	C4-C5-C6	8.18	121.09	117.00
1	A	899	C	C2-N1-C1'	-8.17	109.81	118.80
1	A	946	A	N9-C4-C5	-8.17	102.53	105.80
1	A	1061	G	C5-C6-N1	-8.17	107.42	111.50
1	A	1055	A	C5-C6-N6	-8.17	117.17	123.70
1	A	298	A	N1-C2-N3	8.16	133.38	129.30
1	A	479	C	N3-C4-C5	-8.16	118.64	121.90
17	Q	67	LYS	CD-CE-NZ	8.16	130.47	111.70
1	A	241	C	C5-C6-N1	-8.16	116.92	121.00
1	A	291	C	C6-N1-C2	-8.16	117.04	120.30
1	A	572	A	C4-C5-N7	-8.15	106.62	110.70
1	A	952	U	N1-C2-O2	-8.15	117.09	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1515	C	C5-C6-N1	-8.15	116.92	121.00
1	A	6	G	N9-C4-C5	8.15	108.66	105.40
9	I	83	ARG	NE-CZ-NH1	-8.15	116.22	120.30
1	A	880	C	C6-N1-C2	8.15	123.56	120.30
1	A	1194	U	N3-C4-O4	8.15	125.10	119.40
1	A	239	U	C5-C4-O4	8.14	130.79	125.90
1	A	1276	G	N3-C2-N2	-8.14	114.20	119.90
1	A	482	A	C4-C5-C6	8.14	121.07	117.00
1	A	890	G	C4-C5-C6	8.14	123.69	118.80
1	A	1352	C	N3-C4-C5	-8.14	118.64	121.90
1	A	173	U	O5'-P-OP2	-8.14	98.37	105.70
1	A	169	C	O5'-P-OP1	8.14	120.47	110.70
1	A	1094	G	N3-C4-N9	8.14	130.88	126.00
1	A	12	U	N1-C2-O2	8.13	128.49	122.80
1	A	181	G	C4-C5-C6	8.13	123.68	118.80
1	A	755	G	C6-C5-N7	-8.13	125.52	130.40
1	A	1067	A	C5-C6-N1	-8.13	113.64	117.70
1	A	1222	G	N1-C6-O6	8.13	124.78	119.90
1	A	265	G	N3-C2-N2	8.12	125.59	119.90
1	A	260	G	C8-N9-C4	-8.12	103.15	106.40
1	A	730	G	C5-C6-N1	-8.12	107.44	111.50
1	A	115	G	N1-C6-O6	8.12	124.77	119.90
1	A	236	G	N3-C4-C5	-8.12	124.54	128.60
1	A	726	C	N3-C4-N4	8.12	123.68	118.00
1	A	1091	U	C4-C5-C6	8.12	124.57	119.70
1	A	1187	G	C8-N9-C4	-8.11	103.15	106.40
1	A	62	U	N1-C2-O2	-8.11	117.12	122.80
1	A	110	C	OP1-P-OP2	-8.11	107.43	119.60
1	A	568	G	N1-C6-O6	-8.11	115.03	119.90
1	A	668	G	C2-N3-C4	-8.11	107.85	111.90
1	A	1079	G	N3-C4-C5	-8.11	124.55	128.60
12	L	57	LYS	CD-CE-NZ	8.11	130.35	111.70
1	A	547	A	C8-N9-C4	-8.11	102.56	105.80
1	A	945	G	C6-N1-C2	-8.11	120.24	125.10
1	A	1471	G	N1-C2-N3	8.11	128.76	123.90
1	A	115	G	C8-N9-C4	8.10	109.64	106.40
1	A	781	A	OP1-P-O3'	8.10	123.03	105.20
1	A	711	G	C6-C5-N7	-8.10	125.54	130.40
1	A	981	U	N1-C2-O2	-8.10	117.13	122.80
1	A	1231	G	N3-C4-N9	-8.10	121.14	126.00
1	A	1084	G	C5-N7-C8	8.10	108.35	104.30
1	A	182	U	C5-C4-O4	-8.09	121.05	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	437	U	C4-C5-C6	8.09	124.55	119.70
1	A	730	G	C5-C6-O6	8.09	133.45	128.60
1	A	1289	A	C5-C6-N1	-8.09	113.66	117.70
1	A	823	G	OP1-P-O3'	-8.09	87.41	105.20
1	A	46	G	N3-C2-N2	-8.09	114.24	119.90
1	A	348	G	C4-C5-N7	8.09	114.03	110.80
5	E	15	ARG	NE-CZ-NH1	8.08	124.34	120.30
1	A	39	G	N1-C6-O6	-8.07	115.06	119.90
1	A	306	G	N1-C6-O6	8.07	124.74	119.90
1	A	439	A	C2-N3-C4	-8.07	106.56	110.60
1	A	807	A	N1-C2-N3	8.07	133.34	129.30
1	A	852	G	N1-C6-O6	8.07	124.74	119.90
1	A	855	G	C4-C5-C6	8.07	123.64	118.80
1	A	1280	A	C4-C5-C6	8.07	121.03	117.00
1	A	204	U	C2-N3-C4	8.07	131.84	127.00
1	A	514	C	N3-C4-N4	8.07	123.65	118.00
1	A	503	C	O5'-P-OP2	-8.07	98.44	105.70
1	A	667	G	N3-C4-C5	8.07	132.63	128.60
1	A	742	G	C5-N7-C8	8.07	108.33	104.30
1	A	37	U	C6-N1-C2	-8.06	116.16	121.00
1	A	729	A	C5-N7-C8	8.06	107.93	103.90
1	A	755	G	N1-C2-N3	8.06	128.74	123.90
1	A	791	G	C8-N9-C1'	-8.06	116.52	127.00
1	A	144	G	C4-C5-C6	8.06	123.64	118.80
1	A	418	C	C5-C6-N1	-8.06	116.97	121.00
1	A	450	G	C5-C6-N1	-8.06	107.47	111.50
1	A	763	G	C6-C5-N7	-8.06	125.56	130.40
1	A	259	G	N1-C6-O6	8.05	124.73	119.90
1	A	413	G	C5-C6-N1	-8.05	107.47	111.50
1	A	733	A	OP1-P-OP2	8.05	131.68	119.60
1	A	1125	U	C6-N1-C1'	-8.05	109.93	121.20
1	A	104	G	C4-C5-C6	8.05	123.63	118.80
1	A	1190	G	C5-C6-O6	8.05	133.43	128.60
1	A	1432	G	C4-C5-N7	-8.05	107.58	110.80
1	A	235	C	C4-C5-C6	8.04	121.42	117.40
1	A	942	G	C8-N9-C4	8.04	109.62	106.40
1	A	1505	G	C8-N9-C1'	-8.04	116.55	127.00
1	A	874	G	O5'-P-OP2	-8.04	98.47	105.70
1	A	1139	G	C5-C6-O6	8.04	133.42	128.60
1	A	1335	C	C2-N1-C1'	-8.04	109.96	118.80
1	A	807	A	C5-N7-C8	-8.04	99.88	103.90
1	A	1019	C	C2-N1-C1'	8.03	127.64	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	812	C	P-O3'-C3'	8.03	129.34	119.70
1	A	830	G	N3-C4-N9	-8.03	121.18	126.00
1	A	1483	A	C2-N3-C4	8.03	114.62	110.60
1	A	125	U	OP1-P-OP2	8.03	131.64	119.60
1	A	1087	G	C5-C6-O6	-8.03	123.78	128.60
1	A	657	G	C4-C5-C6	8.03	123.62	118.80
1	A	44	G	C5-C6-N1	-8.02	107.49	111.50
1	A	449	C	O5'-P-OP1	-8.02	98.48	105.70
1	A	1420	C	C5-C6-N1	8.02	125.01	121.00
1	A	1496	C	C5-C4-N4	8.02	125.82	120.20
1	A	176	C	N1-C2-N3	-8.02	113.59	119.20
1	A	1323	G	N3-C4-C5	8.02	132.61	128.60
1	A	1426	C	N1-C2-O2	8.02	123.71	118.90
1	A	243	A	P-O3'-C3'	8.02	129.32	119.70
1	A	319	G	N7-C8-N9	8.01	117.11	113.10
1	A	602	A	N1-C6-N6	-8.01	113.79	118.60
1	A	1451	A	N1-C6-N6	-8.01	113.79	118.60
1	A	26	A	N9-C4-C5	8.01	109.00	105.80
1	A	149	A	N1-C2-N3	8.01	133.31	129.30
1	A	1286	A	N7-C8-N9	8.01	117.80	113.80
1	A	8	A	C5-C6-N1	-8.01	113.70	117.70
1	A	944	G	C5-C6-O6	8.01	133.40	128.60
1	A	1455	G	N1-C2-N3	8.01	128.70	123.90
1	A	872	A	C5-C6-N1	-8.00	113.70	117.70
1	A	279	A	C6-C5-N7	-8.00	126.70	132.30
1	A	1105	A	N1-C2-N3	8.00	133.30	129.30
1	A	1349	A	C2-N3-C4	-8.00	106.60	110.60
1	A	21	G	N9-C4-C5	-8.00	102.20	105.40
1	A	10	A	C6-N1-C2	-8.00	113.80	118.60
1	A	679	C	C6-N1-C2	-8.00	117.10	120.30
1	A	529	G	C5-C6-O6	-7.99	123.80	128.60
1	A	671	G	C2-N3-C4	7.99	115.89	111.90
1	A	361	G	OP1-P-OP2	7.99	131.58	119.60
20	T	62	LEU	CB-CG-CD1	-7.99	97.42	111.00
1	A	790	A	N1-C2-N3	7.98	133.29	129.30
1	A	1499	A	C4-C5-N7	-7.98	106.71	110.70
1	A	782	A	N3-C4-N9	-7.98	121.01	127.40
1	A	1461	G	N3-C4-N9	-7.98	121.21	126.00
1	A	572	A	C2-N3-C4	7.98	114.59	110.60
1	A	482	A	N1-C6-N6	7.98	123.39	118.60
1	A	908	A	N9-C4-C5	7.98	108.99	105.80
1	A	776	G	C4-C5-N7	-7.97	107.61	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1532	U	C4-C5-C6	-7.97	114.92	119.70
1	A	632	A	C4-C5-N7	7.97	114.68	110.70
1	A	985	C	N3-C4-C5	7.97	125.09	121.90
1	A	25	C	N3-C2-O2	7.97	127.48	121.90
1	A	150	C	N1-C2-N3	-7.97	113.62	119.20
1	A	837	G	C6-C5-N7	-7.97	125.62	130.40
1	A	1195	C	P-O3'-C3'	7.96	129.26	119.70
1	A	16	A	C8-N9-C4	7.96	108.98	105.80
1	A	1227	A	C4-N9-C1'	7.96	140.63	126.30
1	A	826	C	C5-C6-N1	7.96	124.98	121.00
1	A	1085	U	O5'-P-OP2	-7.96	98.54	105.70
1	A	579	G	C4-C5-C6	7.96	123.58	118.80
1	A	709	G	C6-C5-N7	-7.96	125.63	130.40
1	A	888	G	C8-N9-C1'	-7.96	116.66	127.00
1	A	320	C	C5-C4-N4	-7.95	114.63	120.20
1	A	858	G	C8-N9-C1'	-7.95	116.66	127.00
1	A	971	G	C6-C5-N7	-7.95	125.63	130.40
1	A	867	G	C5-C6-O6	-7.95	123.83	128.60
1	A	528	C	C5-C4-N4	-7.95	114.64	120.20
1	A	184	G	N1-C2-N3	7.95	128.67	123.90
1	A	963	G	C4-N9-C1'	7.94	136.83	126.50
1	A	710	G	N1-C6-O6	7.94	124.66	119.90
1	A	1526	G	N1-C2-N3	7.94	128.66	123.90
1	A	254	G	N9-C4-C5	-7.94	102.22	105.40
1	A	379	C	C4-C5-C6	7.94	121.37	117.40
1	A	821	G	C8-N9-C1'	-7.94	116.68	127.00
1	A	669	U	N3-C2-O2	7.93	127.75	122.20
1	A	320	C	N3-C2-O2	7.93	127.45	121.90
1	A	491	G	C8-N9-C4	7.93	109.57	106.40
1	A	1346	A	P-O3'-C3'	7.93	129.21	119.70
11	K	48	ILE	CB-CA-C	-7.92	95.75	111.60
1	A	1065	U	N1-C2-N3	-7.92	110.15	114.90
1	A	678	U	C2-N3-C4	-7.92	122.25	127.00
1	A	730	G	N1-C2-N3	7.92	128.65	123.90
1	A	1335	C	C6-N1-C2	7.92	123.47	120.30
1	A	684	A	N1-C6-N6	7.92	123.35	118.60
1	A	44	G	N1-C2-N2	-7.91	109.08	116.20
1	A	204	U	N3-C4-O4	7.91	124.94	119.40
1	A	250	A	N9-C4-C5	-7.91	102.64	105.80
1	A	805	C	C5-C4-N4	-7.91	114.66	120.20
1	A	1531	A	C5-N7-C8	-7.91	99.94	103.90
1	A	427	U	C4-C5-C6	7.91	124.44	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	144	G	C6-N1-C2	7.90	129.84	125.10
1	A	781	A	C5-N7-C8	-7.90	99.95	103.90
1	A	792	A	O4'-C1'-N9	7.90	114.52	108.20
1	A	1397	C	N3-C4-N4	7.90	123.53	118.00
1	A	680	C	N3-C4-C5	7.90	125.06	121.90
1	A	853	G	O5'-P-OP2	-7.90	98.59	105.70
1	A	16	A	C5-N7-C8	7.90	107.85	103.90
1	A	1383	C	C6-N1-C2	7.90	123.46	120.30
1	A	6	G	C8-N9-C4	-7.90	103.24	106.40
3	C	111	LEU	CA-CB-CG	-7.89	97.14	115.30
1	A	167	G	N9-C4-C5	-7.89	102.24	105.40
1	A	499	A	N1-C6-N6	-7.89	113.86	118.60
1	A	1191	A	O4'-C1'-N9	-7.89	101.89	108.20
1	A	782	A	OP1-P-OP2	-7.89	107.77	119.60
1	A	1184	G	N1-C2-N3	7.89	128.63	123.90
1	A	394	G	N3-C4-N9	-7.88	121.27	126.00
1	A	1512	U	C4-C5-C6	7.88	124.43	119.70
1	A	1523	G	N7-C8-N9	7.88	117.04	113.10
1	A	639	G	C5-C6-O6	-7.88	123.87	128.60
1	A	767	A	C6-N1-C2	-7.88	113.87	118.60
1	A	1197	G	N1-C2-N3	7.88	128.63	123.90
1	A	263	A	C5-C6-N1	7.88	121.64	117.70
1	A	757	U	N3-C4-O4	7.88	124.91	119.40
1	A	1109	C	O5'-P-OP1	-7.88	98.61	105.70
1	A	803	G	N9-C4-C5	7.88	108.55	105.40
1	A	908	A	C2-N3-C4	-7.88	106.66	110.60
1	A	217	C	C6-N1-C2	7.87	123.45	120.30
1	A	122	G	C4-C5-C6	7.87	123.52	118.80
1	A	1184	G	C8-N9-C1'	-7.87	116.77	127.00
1	A	324	G	C4-C5-N7	-7.87	107.65	110.80
1	A	1110	A	N1-C2-N3	7.87	133.23	129.30
1	A	484	G	P-O3'-C3'	7.87	129.14	119.70
1	A	413	G	N9-C4-C5	7.86	108.55	105.40
1	A	1506	U	N1-C2-O2	7.86	128.30	122.80
1	A	196	A	N9-C4-C5	-7.86	102.66	105.80
1	A	498	U	N1-C2-O2	-7.86	117.30	122.80
1	A	500	G	N3-C2-N2	-7.86	114.40	119.90
1	A	618	C	N1-C2-N3	-7.85	113.70	119.20
1	A	722	A	C6-C5-N7	-7.85	126.80	132.30
1	A	963	G	N3-C4-N9	7.85	130.71	126.00
5	E	24	ARG	NE-CZ-NH1	7.85	124.23	120.30
1	A	447	G	N1-C6-O6	7.85	124.61	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1305	G	P-O3'-C3'	7.85	129.12	119.70
1	A	347	G	N3-C4-C5	7.85	132.53	128.60
1	A	674	G	N9-C4-C5	-7.85	102.26	105.40
1	A	1211	U	C5-C4-O4	-7.85	121.19	125.90
2	B	11	LEU	CA-CB-CG	7.85	133.35	115.30
1	A	619	U	C5-C4-O4	7.84	130.61	125.90
1	A	1334	G	N3-C4-C5	-7.84	124.68	128.60
1	A	258	G	C8-N9-C4	-7.84	103.26	106.40
1	A	969	A	O4'-C1'-N9	-7.84	101.93	108.20
1	A	835	U	O4'-C1'-N1	-7.84	101.93	108.20
1	A	1361(A)	C	N1-C2-O2	7.84	123.60	118.90
1	A	1314	C	N3-C4-N4	7.83	123.48	118.00
1	A	721	G	C4-C5-C6	7.83	123.50	118.80
1	A	759	A	C5-N7-C8	-7.83	99.98	103.90
1	A	889	A	C4-C5-N7	-7.83	106.78	110.70
1	A	923	A	N1-C6-N6	-7.83	113.90	118.60
1	A	1111	A	O5'-P-OP1	7.83	120.10	110.70
1	A	1484	C	N3-C4-N4	7.83	123.48	118.00
1	A	787	A	N1-C2-N3	7.83	133.21	129.30
1	A	1054	C	N3-C2-O2	-7.83	116.42	121.90
1	A	1507	A	C6-N1-C2	-7.83	113.90	118.60
1	A	81	U	N1-C2-N3	-7.82	110.21	114.90
1	A	1064	G	C8-N9-C4	-7.82	103.27	106.40
1	A	1099	G	C8-N9-C4	-7.82	103.27	106.40
1	A	604	G	C5-C6-O6	-7.82	123.91	128.60
1	A	1190	G	C4-C5-C6	7.81	123.49	118.80
1	A	759	A	C5-C6-N1	7.81	121.61	117.70
1	A	1177	G	C8-N9-C4	-7.81	103.28	106.40
3	C	4	LYS	N-CA-C	7.81	132.09	111.00
1	A	373	A	C5-C6-N6	7.81	129.94	123.70
1	A	437	U	N3-C4-C5	-7.81	109.92	114.60
1	A	725	G	C5-C6-O6	-7.81	123.92	128.60
1	A	1487	G	C8-N9-C1'	-7.81	116.85	127.00
1	A	490	G	N1-C6-O6	7.81	124.58	119.90
1	A	799	G	N1-C2-N3	7.80	128.58	123.90
1	A	1136	U	N3-C4-O4	7.80	124.86	119.40
1	A	1453	G	O4'-C1'-N9	-7.80	101.96	108.20
1	A	22	G	C4-C5-N7	7.80	113.92	110.80
1	A	307	C	N1-C2-N3	-7.80	113.74	119.20
1	A	747	C	C2-N1-C1'	-7.80	110.22	118.80
1	A	533	A	N1-C2-N3	7.80	133.20	129.30
1	A	672	U	N3-C4-O4	7.80	124.86	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	881	G	N1-C6-O6	7.80	124.58	119.90
1	A	1108	G	N3-C4-C5	-7.80	124.70	128.60
1	A	1191	A	C5-C6-N6	-7.80	117.46	123.70
1	A	873	A	C2-N3-C4	7.79	114.50	110.60
1	A	360	A	C5-N7-C8	-7.79	100.00	103.90
1	A	275	G	N9-C4-C5	-7.79	102.28	105.40
1	A	658	G	N3-C4-C5	-7.79	124.70	128.60
1	A	830	G	C8-N9-C1'	7.79	137.13	127.00
1	A	603	U	N3-C4-C5	-7.79	109.93	114.60
1	A	614	A	N9-C4-C5	-7.79	102.69	105.80
1	A	1028	C	C6-N1-C2	-7.79	117.19	120.30
1	A	833	U	N3-C2-O2	-7.79	116.75	122.20
1	A	307	C	C5-C4-N4	-7.79	114.75	120.20
1	A	935	A	N1-C6-N6	7.79	123.27	118.60
1	A	1411	C	C4-C5-C6	7.79	121.29	117.40
1	A	230	G	C4-C5-C6	7.78	123.47	118.80
1	A	24	U	O5'-P-OP1	7.78	120.04	110.70
1	A	260	G	N7-C8-N9	7.78	116.99	113.10
1	A	836	G	C2-N3-C4	-7.78	108.01	111.90
1	A	918	A	N7-C8-N9	-7.78	109.91	113.80
1	A	325	A	N3-C4-N9	-7.77	121.18	127.40
1	A	1283	G	N3-C2-N2	-7.77	114.46	119.90
1	A	687	A	O5'-P-OP2	-7.77	98.70	105.70
1	A	821	G	C6-C5-N7	-7.77	125.74	130.40
1	A	969	A	C5-C6-N6	-7.77	117.48	123.70
1	A	1190	G	C8-N9-C4	-7.77	103.29	106.40
9	I	102	LEU	CA-CB-CG	7.77	133.17	115.30
1	A	515	G	N7-C8-N9	7.77	116.98	113.10
1	A	1387	G	N3-C2-N2	-7.76	114.46	119.90
1	A	1512	U	N3-C4-O4	7.76	124.83	119.40
1	A	48	C	N3-C4-C5	-7.76	118.80	121.90
1	A	386	C	C2-N3-C4	-7.76	116.02	119.90
1	A	423	G	C4-C5-N7	7.76	113.90	110.80
1	A	938	A	N1-C2-N3	7.76	133.18	129.30
1	A	1351	U	N3-C2-O2	-7.76	116.77	122.20
1	A	952	U	C5-C4-O4	-7.76	121.25	125.90
1	A	1276	G	C2-N3-C4	-7.75	108.02	111.90
1	A	316	G	C6-C5-N7	-7.75	125.75	130.40
1	A	148	G	N1-C6-O6	7.75	124.55	119.90
1	A	685	G	N3-C2-N2	-7.75	114.48	119.90
17	Q	38	ARG	NE-CZ-NH1	7.75	124.17	120.30
1	A	817	C	C6-N1-C1'	-7.75	111.51	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	618	C	C2-N1-C1'	-7.74	110.28	118.80
1	A	890	G	C8-N9-C1'	-7.74	116.94	127.00
1	A	1061	G	N1-C6-O6	7.74	124.55	119.90
1	A	398	C	C6-N1-C2	7.74	123.39	120.30
1	A	55	A	N1-C2-N3	7.74	133.17	129.30
1	A	310	G	O5'-P-OP1	-7.74	98.74	105.70
1	A	1126	U	OP1-P-OP2	-7.74	108.00	119.60
1	A	1503	A	N1-C6-N6	-7.74	113.96	118.60
1	A	143	A	N9-C4-C5	-7.73	102.71	105.80
1	A	1167	A	C2-N3-C4	-7.73	106.73	110.60
1	A	220	G	C5-C6-N1	-7.73	107.64	111.50
1	A	531	U	C6-N1-C1'	7.73	132.02	121.20
1	A	1109	C	N3-C4-N4	-7.73	112.59	118.00
1	A	412	A	OP1-P-OP2	-7.72	108.02	119.60
1	A	746	A	C4-C5-N7	-7.72	106.84	110.70
1	A	1333	A	C8-N9-C4	-7.72	102.71	105.80
1	A	869	G	N3-C4-N9	7.72	130.63	126.00
1	A	150	C	N3-C2-O2	7.71	127.30	121.90
1	A	401	C	N3-C4-N4	7.71	123.40	118.00
1	A	9	G	O5'-P-OP1	7.71	119.95	110.70
1	A	1338	G	N7-C8-N9	7.71	116.96	113.10
1	A	190(G)	G	C5-C6-N1	-7.71	107.64	111.50
1	A	1398	A	O5'-P-OP2	-7.71	98.76	105.70
1	A	609	A	N1-C2-N3	7.71	133.15	129.30
1	A	954	G	O5'-P-OP1	7.71	119.95	110.70
1	A	1340	A	N1-C2-N3	7.70	133.15	129.30
1	A	1412	C	N1-C2-O2	-7.70	114.28	118.90
1	A	1280	A	C5-C6-N6	7.70	129.86	123.70
1	A	360	A	C2-N3-C4	-7.70	106.75	110.60
17	Q	76	LEU	CA-CB-CG	-7.70	97.60	115.30
1	A	95	U	C2-N1-C1'	-7.69	108.47	117.70
1	A	814	A	C6-C5-N7	-7.69	126.92	132.30
1	A	1514	C	N3-C2-O2	-7.69	116.52	121.90
1	A	791	G	C4-C5-C6	7.69	123.41	118.80
1	A	801	U	N3-C4-O4	-7.68	114.02	119.40
1	A	1249	C	C6-N1-C2	7.68	123.37	120.30
1	A	1414	U	C5-C4-O4	7.68	130.51	125.90
1	A	1425	U	N3-C4-C5	-7.68	109.99	114.60
1	A	653	A	C2-N3-C4	7.68	114.44	110.60
1	A	662	G	C4-C5-C6	7.68	123.41	118.80
1	A	946	A	N1-C6-N6	7.68	123.21	118.60
1	A	931	C	C6-N1-C2	7.68	123.37	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	235	C	N3-C4-C5	-7.68	118.83	121.90
1	A	1455	G	C2-N3-C4	-7.68	108.06	111.90
1	A	553	A	C6-N1-C2	-7.67	114.00	118.60
1	A	944	G	N3-C2-N2	7.67	125.27	119.90
1	A	1451	A	C6-C5-N7	7.67	137.67	132.30
1	A	276	G	OP1-P-OP2	7.66	131.10	119.60
1	A	887	G	N3-C4-N9	-7.66	121.40	126.00
1	A	256	U	N3-C4-O4	7.66	124.76	119.40
1	A	423	G	C5-C6-O6	-7.66	124.00	128.60
1	A	1474	G	C4-C5-N7	-7.66	107.74	110.80
1	A	285	G	C6-C5-N7	-7.66	125.81	130.40
1	A	414	A	N1-C2-N3	7.66	133.13	129.30
1	A	57	G	C5-C6-N1	-7.66	107.67	111.50
1	A	134	A	N1-C2-N3	7.66	133.13	129.30
1	A	811	C	C5-C6-N1	-7.65	117.17	121.00
1	A	507	C	C6-N1-C2	7.65	123.36	120.30
1	A	1067	A	N9-C4-C5	7.65	108.86	105.80
1	A	118	U	N1-C2-N3	-7.65	110.31	114.90
1	A	1396	A	OP1-P-OP2	7.65	131.07	119.60
1	A	895	G	N7-C8-N9	7.64	116.92	113.10
1	A	243	A	C6-C5-N7	-7.64	126.95	132.30
1	A	81	U	C2-N3-C4	7.64	131.58	127.00
1	A	1530	G	N7-C8-N9	-7.64	109.28	113.10
1	A	15	G	N9-C4-C5	-7.64	102.34	105.40
1	A	517	G	N9-C4-C5	7.64	108.45	105.40
20	T	12	ALA	CB-CA-C	7.64	121.56	110.10
1	A	656	C	OP1-P-O3'	-7.64	88.40	105.20
1	A	836	G	N3-C4-N9	-7.64	121.42	126.00
1	A	1314	C	C5-C4-N4	-7.64	114.86	120.20
1	A	260	G	C4-N9-C1'	7.63	136.42	126.50
1	A	342	C	N3-C4-C5	-7.63	118.85	121.90
1	A	712	A	N1-C6-N6	7.63	123.18	118.60
1	A	945	G	N9-C4-C5	7.63	108.45	105.40
1	A	606	G	N3-C4-N9	7.63	130.58	126.00
1	A	1492	A	N1-C2-N3	-7.63	125.48	129.30
1	A	68	G	N1-C6-O6	7.63	124.48	119.90
1	A	566	G	O5'-P-OP2	7.63	119.85	110.70
1	A	17	U	C2-N3-C4	-7.62	122.42	127.00
1	A	720	C	N3-C4-N4	-7.62	112.66	118.00
1	A	1463	C	C6-N1-C2	7.62	123.35	120.30
1	A	740	U	C6-N1-C1'	7.62	131.87	121.20
1	A	480	U	N1-C2-N3	7.62	119.47	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	512	U	C5-C4-O4	-7.62	121.33	125.90
1	A	529	G	C8-N9-C4	-7.62	103.35	106.40
1	A	840	C	C2-N3-C4	7.62	123.71	119.90
1	A	668	G	C4-C5-C6	7.62	123.37	118.80
1	A	964	A	C5-C6-N1	-7.62	113.89	117.70
1	A	780	A	C5-C6-N6	-7.62	117.61	123.70
1	A	113	G	C4-C5-C6	7.61	123.37	118.80
1	A	773	G	C6-C5-N7	-7.61	125.83	130.40
1	A	894	G	N1-C6-O6	7.61	124.47	119.90
1	A	929	G	C8-N9-C4	7.61	109.45	106.40
1	A	350	G	N3-C2-N2	-7.61	114.57	119.90
1	A	372	C	C6-N1-C1'	-7.61	111.67	120.80
1	A	776	G	C5-C6-O6	7.61	133.17	128.60
1	A	1056	U	N3-C2-O2	7.61	127.53	122.20
1	A	1193	G	N1-C2-N3	7.61	128.46	123.90
1	A	1527	C	OP1-P-O3'	-7.61	88.47	105.20
1	A	499	A	C8-N9-C4	-7.60	102.76	105.80
1	A	251	G	OP2-P-O3'	-7.60	88.47	105.20
1	A	15	G	C5-N7-C8	-7.60	100.50	104.30
1	A	410	G	N3-C4-C5	-7.60	124.80	128.60
1	A	500	G	C5-C6-N1	-7.60	107.70	111.50
1	A	1301	U	C6-N1-C2	-7.60	116.44	121.00
1	A	1217	C	OP1-P-OP2	7.59	130.99	119.60
1	A	818	G	OP1-P-OP2	7.59	130.98	119.60
1	A	331	G	N1-C6-O6	7.59	124.45	119.90
1	A	1414	U	C6-N1-C2	-7.59	116.45	121.00
1	A	1194	U	C4-C5-C6	7.58	124.25	119.70
1	A	46	G	C8-N9-C4	-7.58	103.37	106.40
1	A	658	G	C6-C5-N7	-7.58	125.85	130.40
1	A	723	U	C2-N3-C4	7.58	131.55	127.00
1	A	1250	A	C6-C5-N7	-7.58	126.99	132.30
1	A	83	U	C5-C6-N1	7.58	126.49	122.70
1	A	108	G	C8-N9-C4	-7.58	103.37	106.40
1	A	774	G	C6-C5-N7	-7.58	125.85	130.40
1	A	498	U	O5'-P-OP2	-7.58	98.88	105.70
1	A	500	G	C5-C6-O6	-7.58	124.05	128.60
1	A	7	G	C4-N9-C1'	-7.58	116.65	126.50
1	A	419	C	N3-C4-C5	7.58	124.93	121.90
1	A	531	U	N3-C4-C5	-7.57	110.06	114.60
1	A	817	C	N3-C4-N4	7.57	123.30	118.00
1	A	99	C	OP1-P-OP2	-7.57	108.24	119.60
1	A	324	G	N9-C4-C5	7.57	108.43	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1299	A	C2-N3-C4	-7.57	106.82	110.60
1	A	133	U	N3-C2-O2	-7.57	116.91	122.20
1	A	181	G	C5-C6-N1	-7.57	107.72	111.50
1	A	531	U	C5-C4-O4	7.57	130.44	125.90
1	A	755	G	N1-C2-N2	-7.57	109.39	116.20
1	A	1019	C	N1-C2-O2	7.57	123.44	118.90
1	A	437	U	O5'-P-OP2	-7.56	98.89	105.70
1	A	1305	G	OP2-P-O3'	7.56	121.84	105.20
1	A	582	U	C5-C6-N1	-7.56	118.92	122.70
1	A	79	G	C4-C5-C6	7.56	123.33	118.80
1	A	1014	A	N3-C4-C5	-7.56	121.51	126.80
1	A	110	C	C4-C5-C6	7.56	121.18	117.40
1	A	293	G	N3-C4-C5	7.56	132.38	128.60
1	A	559	A	N3-C4-N9	7.56	133.45	127.40
1	A	650	G	C4-C5-N7	-7.56	107.78	110.80
1	A	827	U	N3-C4-C5	-7.56	110.07	114.60
1	A	1495	U	N3-C4-C5	-7.56	110.07	114.60
1	A	281	G	C8-N9-C1'	-7.55	117.18	127.00
1	A	475	G	O5'-P-OP1	-7.55	98.90	105.70
1	A	790	A	C6-C5-N7	-7.55	127.01	132.30
1	A	953	G	N3-C2-N2	7.55	125.19	119.90
1	A	364	A	O5'-P-OP1	-7.55	98.90	105.70
1	A	558	G	N3-C4-N9	-7.55	121.47	126.00
1	A	618	C	C2-N3-C4	7.55	123.68	119.90
1	A	24	U	C6-N1-C2	7.55	125.53	121.00
1	A	259	G	N3-C2-N2	-7.55	114.61	119.90
1	A	46	G	C5-C6-N1	7.55	115.27	111.50
1	A	1329	A	N1-C6-N6	7.55	123.13	118.60
1	A	1364	U	C5-C6-N1	-7.55	118.93	122.70
1	A	823	G	OP2-P-O3'	7.54	121.80	105.20
1	A	249	U	C4-C5-C6	7.54	124.23	119.70
1	A	515	G	C5-C6-N1	-7.54	107.73	111.50
1	A	572	A	C5-C6-N6	7.54	129.74	123.70
1	A	852	G	N1-C2-N3	7.54	128.43	123.90
1	A	893	C	N1-C2-N3	-7.54	113.92	119.20
1	A	1390	U	C4-C5-C6	7.54	124.23	119.70
1	A	1495	U	N3-C4-O4	7.54	124.68	119.40
1	A	106	C	OP2-P-O3'	7.54	121.79	105.20
1	A	123	C	C6-N1-C2	-7.54	117.28	120.30
1	A	266	G	C8-N9-C4	-7.54	103.38	106.40
1	A	484	G	N1-C2-N3	7.54	128.43	123.90
1	A	1312	G	N1-C6-O6	-7.54	115.38	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	314	C	C4-C5-C6	-7.54	113.63	117.40
1	A	572	A	C6-C5-N7	7.53	137.57	132.30
1	A	621	A	C5-N7-C8	-7.53	100.13	103.90
1	A	1308	U	N3-C4-O4	7.53	124.67	119.40
1	A	1532	U	C5-C4-O4	-7.53	121.38	125.90
1	A	289	G	C2-N3-C4	7.53	115.67	111.90
1	A	50	A	N1-C6-N6	-7.53	114.08	118.60
1	A	1415	G	N3-C2-N2	7.53	125.17	119.90
1	A	740	U	C2-N1-C1'	-7.53	108.67	117.70
1	A	1401	G	C6-N1-C2	-7.53	120.58	125.10
1	A	36	C	C6-N1-C2	-7.53	117.29	120.30
1	A	295	C	C5-C6-N1	7.53	124.76	121.00
1	A	855	G	N1-C6-O6	7.53	124.42	119.90
1	A	1316	G	N3-C4-C5	7.53	132.36	128.60
1	A	1197	G	C2-N3-C4	-7.52	108.14	111.90
1	A	260	G	N1-C2-N3	7.52	128.41	123.90
1	A	154	C	C2-N3-C4	-7.52	116.14	119.90
1	A	766	A	C8-N9-C4	7.52	108.81	105.80
1	A	499	A	N9-C4-C5	7.51	108.81	105.80
1	A	1385	G	O5'-P-OP2	-7.51	98.94	105.70
1	A	120	A	C2-N3-C4	-7.51	106.84	110.60
1	A	252	U	C6-N1-C2	-7.51	116.49	121.00
1	A	818	G	N9-C4-C5	7.51	108.40	105.40
1	A	1346	A	C2-N3-C4	-7.51	106.85	110.60
1	A	814	A	C4-C5-C6	7.50	120.75	117.00
1	A	1248	A	N1-C6-N6	7.50	123.10	118.60
1	A	276	G	C8-N9-C1'	-7.50	117.25	127.00
1	A	657	G	C5-C6-O6	-7.50	124.10	128.60
1	A	308	C	N3-C4-N4	7.50	123.25	118.00
1	A	1326	C	N3-C4-C5	-7.50	118.90	121.90
1	A	89	C	N3-C4-C5	-7.50	118.90	121.90
1	A	482	A	C6-C5-N7	-7.50	127.05	132.30
1	A	1322	C	N1-C2-N3	-7.50	113.95	119.20
1	A	712	A	C6-N1-C2	-7.50	114.10	118.60
1	A	1165	C	N3-C4-C5	-7.50	118.90	121.90
1	A	1212	U	C5-C4-O4	-7.50	121.40	125.90
1	A	1058	G	N3-C2-N2	7.50	125.15	119.90
1	A	518	C	C6-N1-C2	-7.49	117.30	120.30
1	A	1024	G	N1-C6-O6	-7.49	115.40	119.90
1	A	1339	A	C6-N1-C2	-7.49	114.10	118.60
1	A	348	G	N7-C8-N9	7.49	116.85	113.10
1	A	77	G	O5'-P-OP2	-7.49	98.96	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1148	U	N1-C2-N3	7.49	119.39	114.90
1	A	40	C	N3-C2-O2	7.49	127.14	121.90
1	A	248	C	O5'-P-OP2	-7.49	98.96	105.70
1	A	520	A	C2-N3-C4	-7.49	106.86	110.60
1	A	1366	C	N3-C2-O2	-7.49	116.66	121.90
1	A	1396	A	C5-C6-N1	-7.49	113.96	117.70
1	A	1531	A	N7-C8-N9	7.49	117.54	113.80
1	A	62	U	C2-N3-C4	7.49	131.49	127.00
1	A	321	A	C5-C6-N1	7.49	121.44	117.70
1	A	1462	G	C8-N9-C4	7.49	109.39	106.40
1	A	26	A	O5'-P-OP1	-7.48	98.97	105.70
1	A	1251	A	C4-C5-C6	7.48	120.74	117.00
1	A	147	G	N1-C2-N3	7.48	128.39	123.90
1	A	800	G	O5'-P-OP2	-7.48	98.97	105.70
1	A	840	C	N1-C2-N3	-7.48	113.97	119.20
1	A	930	C	N3-C2-O2	-7.48	116.67	121.90
1	A	24	U	P-O3'-C3'	-7.48	110.73	119.70
1	A	598	U	C6-N1-C2	7.47	125.48	121.00
1	A	1178	G	N9-C4-C5	7.47	108.39	105.40
1	A	42	G	N1-C6-O6	7.47	124.38	119.90
1	A	1023	G	N3-C4-C5	-7.47	124.86	128.60
1	A	957	U	N1-C2-N3	7.47	119.38	114.90
1	A	864	A	C8-N9-C4	-7.47	102.81	105.80
1	A	22	G	N9-C4-C5	-7.46	102.41	105.40
1	A	42	G	C5-C6-O6	-7.46	124.12	128.60
1	A	668	G	C5-C6-N1	-7.46	107.77	111.50
1	A	890	G	N1-C2-N2	-7.46	109.48	116.20
1	A	929	G	C6-N1-C2	-7.46	120.62	125.10
1	A	394	G	C8-N9-C1'	7.46	136.70	127.00
1	A	61	G	N3-C2-N2	-7.46	114.68	119.90
1	A	79	G	C5-C6-O6	-7.46	124.12	128.60
1	A	1163	C	C6-N1-C2	-7.46	117.32	120.30
1	A	1341	U	C5-C4-O4	7.46	130.38	125.90
1	A	955	U	N3-C2-O2	-7.46	116.98	122.20
1	A	8	A	C2-N3-C4	-7.45	106.87	110.60
1	A	484	G	C5-C6-O6	7.45	133.07	128.60
1	A	546	G	C5-C6-O6	7.45	133.07	128.60
1	A	293	G	O5'-P-OP1	7.45	119.64	110.70
1	A	270	A	C5-N7-C8	-7.45	100.18	103.90
1	A	622	A	C8-N9-C4	7.45	108.78	105.80
1	A	1434	A	N1-C6-N6	7.45	123.07	118.60
1	A	119	A	C8-N9-C4	-7.44	102.82	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	963	G	C8-N9-C1'	-7.44	117.32	127.00
1	A	1450	U	O5'-P-OP1	7.44	119.63	110.70
1	A	1199	U	C4-C5-C6	7.44	124.16	119.70
1	A	568	G	OP1-P-OP2	7.44	130.76	119.60
1	A	1125	U	C5'-C4'-C3'	7.44	127.90	116.00
1	A	664	G	N3-C4-C5	-7.44	124.88	128.60
1	A	1171	G	N9-C4-C5	7.44	108.37	105.40
1	A	193	C	OP2-P-O3'	7.43	121.56	105.20
1	A	512	U	C5-C6-N1	7.43	126.42	122.70
1	A	553	A	C8-N9-C4	7.43	108.77	105.80
1	A	1157	A	C8-N9-C4	-7.43	102.83	105.80
1	A	947	G	N1-C2-N3	7.43	128.36	123.90
1	A	229	U	C2-N3-C4	-7.43	122.54	127.00
1	A	352	C	N3-C4-C5	-7.43	118.93	121.90
1	A	1010	G	N1-C6-O6	7.43	124.36	119.90
1	A	1414	U	C2-N3-C4	7.43	131.46	127.00
1	A	432	A	C6-C5-N7	7.43	137.50	132.30
1	A	623	C	N1-C2-O2	-7.43	114.44	118.90
1	A	839	U	N3-C2-O2	-7.43	117.00	122.20
1	A	901	A	N3-C4-C5	7.43	132.00	126.80
1	A	1441	G	C5-C6-N1	-7.42	107.79	111.50
1	A	1405	G	C5-N7-C8	-7.42	100.59	104.30
1	A	500	G	C8-N9-C4	7.42	109.37	106.40
1	A	1281	U	C2-N3-C4	7.42	131.45	127.00
1	A	1530	G	C6-N1-C2	7.42	129.55	125.10
1	A	331	G	C6-C5-N7	-7.42	125.95	130.40
1	A	860	A	C2-N3-C4	-7.42	106.89	110.60
1	A	1363	A	C5-C6-N1	7.42	121.41	117.70
1	A	234	C	N3-C4-C5	7.42	124.87	121.90
1	A	1047	G	C5-C6-N1	-7.41	107.79	111.50
1	A	216	G	N1-C6-O6	7.41	124.35	119.90
1	A	926	G	O5'-P-OP1	-7.41	99.03	105.70
1	A	761	G	C5-N7-C8	-7.40	100.60	104.30
1	A	964	A	C5-C6-N6	7.40	129.62	123.70
1	A	890	G	C5-C6-N1	-7.40	107.80	111.50
1	A	1446	A	C5-C6-N6	7.40	129.62	123.70
1	A	236	G	N9-C4-C5	-7.40	102.44	105.40
1	A	864	A	OP1-P-OP2	-7.40	108.50	119.60
1	A	251	G	N1-C2-N2	-7.40	109.54	116.20
1	A	329	A	N1-C6-N6	7.40	123.04	118.60
1	A	1532	U	C5-C6-N1	7.40	126.40	122.70
1	A	480	U	C4-C5-C6	7.40	124.14	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	498	U	N1-C2-N3	7.40	119.34	114.90
1	A	1393	U	C2-N1-C1'	7.40	126.58	117.70
1	A	862	C	N1-C2-N3	-7.40	114.02	119.20
1	A	918	A	C5-N7-C8	7.40	107.60	103.90
1	A	189	G	N7-C8-N9	-7.39	109.40	113.10
1	A	560	U	N3-C4-C5	-7.39	110.16	114.60
1	A	762	C	O5'-P-OP1	-7.39	99.04	105.70
1	A	460	A	N1-C6-N6	-7.39	114.17	118.60
1	A	756	C	O5'-P-OP2	-7.39	99.05	105.70
1	A	763	G	N1-C6-O6	7.39	124.33	119.90
1	A	774	G	C5-C6-N1	-7.39	107.81	111.50
1	A	1340	A	C6-N1-C2	-7.39	114.17	118.60
1	A	66	G	C5-C6-O6	-7.39	124.17	128.60
1	A	781	A	N7-C8-N9	7.38	117.49	113.80
1	A	1075	C	C4-C5-C6	7.38	121.09	117.40
1	A	1307	U	N3-C2-O2	-7.38	117.03	122.20
1	A	1191	A	C5-N7-C8	-7.38	100.21	103.90
1	A	1529	G	C4-C5-C6	7.38	123.23	118.80
1	A	1100	C	C2-N1-C1'	7.38	126.92	118.80
1	A	1173	G	N3-C4-C5	7.38	132.29	128.60
1	A	232	G	N1-C6-O6	7.38	124.33	119.90
1	A	376	G	O5'-P-OP2	-7.37	99.06	105.70
1	A	250	A	O4'-C1'-N9	-7.37	102.30	108.20
1	A	93	G	C8-N9-C4	7.37	109.35	106.40
1	A	319	G	C4-C5-C6	7.37	123.22	118.80
1	A	322	C	OP2-P-O3'	7.37	121.41	105.20
1	A	707	C	O5'-P-OP2	-7.37	99.07	105.70
1	A	35	G	C8-N9-C4	7.37	109.35	106.40
1	A	755	G	C2-N3-C4	-7.37	108.22	111.90
1	A	1433	A	OP1-P-O3'	-7.37	88.99	105.20
1	A	1385	G	N3-C2-N2	-7.37	114.74	119.90
1	A	1390	U	N3-C4-C5	-7.37	110.18	114.60
1	A	530	G	C4-N9-C1'	7.37	136.07	126.50
1	A	791	G	C2-N3-C4	-7.37	108.22	111.90
1	A	1429	C	C6-N1-C2	-7.37	117.35	120.30
1	A	328	C	C6-N1-C1'	-7.36	111.96	120.80
1	A	339	C	N1-C2-O2	-7.36	114.48	118.90
1	A	161	A	N1-C6-N6	-7.36	114.18	118.60
1	A	552	U	C5-C4-O4	-7.36	121.48	125.90
1	A	1103	C	N3-C4-C5	7.36	124.84	121.90
1	A	1117	G	C8-N9-C4	7.36	109.34	106.40
1	A	1379	G	C2-N3-C4	-7.36	108.22	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1117	G	N3-C2-N2	7.35	125.05	119.90
1	A	389	A	C8-N9-C4	-7.35	102.86	105.80
1	A	1129	C	N1-C2-O2	7.35	123.31	118.90
1	A	1487	G	C4-C5-N7	-7.35	107.86	110.80
1	A	1492	A	C5-C6-N1	7.35	121.37	117.70
1	A	75	G	O5'-P-OP1	7.35	119.52	110.70
1	A	1065	U	N3-C4-C5	7.35	119.01	114.60
1	A	1079	G	C5-C6-O6	-7.35	124.19	128.60
1	A	1499	A	O5'-P-OP1	7.35	119.52	110.70
1	A	376	G	C2-N3-C4	7.34	115.57	111.90
1	A	530	G	C8-N9-C4	-7.34	103.47	106.40
1	A	70	G	C5-N7-C8	-7.34	100.63	104.30
1	A	285	G	C5-C6-N1	-7.34	107.83	111.50
1	A	1124	G	N3-C4-C5	-7.34	124.93	128.60
1	A	144	G	C5-N7-C8	-7.33	100.63	104.30
1	A	927	G	N3-C4-N9	-7.33	121.60	126.00
1	A	378	G	N3-C2-N2	-7.33	114.77	119.90
1	A	398	C	N3-C4-C5	7.33	124.83	121.90
1	A	279	A	N1-C6-N6	7.33	123.00	118.60
1	A	723	U	N3-C2-O2	-7.33	117.07	122.20
1	A	580	U	N3-C4-O4	7.33	124.53	119.40
1	A	133	U	C5-C4-O4	7.33	130.30	125.90
1	A	358	U	C5-C4-O4	-7.33	121.50	125.90
1	A	1151	A	C5-N7-C8	7.33	107.56	103.90
1	A	1278	U	C5-C6-N1	7.33	126.36	122.70
1	A	1331	G	N7-C8-N9	7.33	116.76	113.10
1	A	5	U	N1-C2-O2	7.33	127.93	122.80
1	A	724	G	C2-N3-C4	7.32	115.56	111.90
1	A	1300	G	C4-C5-N7	7.32	113.73	110.80
1	A	372	C	C4-C5-C6	7.32	121.06	117.40
1	A	396	G	C4-N9-C1'	7.32	136.02	126.50
1	A	517	G	C4-C5-N7	-7.32	107.87	110.80
1	A	953	G	N7-C8-N9	-7.32	109.44	113.10
1	A	1380	U	N3-C4-O4	-7.32	114.28	119.40
1	A	292	G	C8-N9-C4	-7.32	103.47	106.40
1	A	345	C	N1-C2-O2	7.32	123.29	118.90
1	A	229	U	C5-C6-N1	-7.31	119.04	122.70
1	A	376	G	C5-N7-C8	7.31	107.96	104.30
1	A	778	G	N1-C2-N3	7.31	128.29	123.90
1	A	1058	G	C8-N9-C1'	-7.31	117.49	127.00
1	A	567	G	O5'-P-OP1	-7.31	99.12	105.70
1	A	1499	A	N7-C8-N9	-7.31	110.14	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1110	A	C6-N1-C2	-7.31	114.22	118.60
1	A	1274	G	C8-N9-C4	7.31	109.32	106.40
1	A	1424	C	C6-N1-C2	7.30	123.22	120.30
1	A	264	U	N1-C2-N3	7.30	119.28	114.90
1	A	523	A	C5-C6-N6	7.30	129.54	123.70
1	A	887	G	N1-C2-N2	7.30	122.77	116.20
1	A	1485	U	C2-N3-C4	7.30	131.38	127.00
1	A	321	A	C6-N1-C2	-7.30	114.22	118.60
1	A	1099	G	N3-C4-C5	7.30	132.25	128.60
1	A	32	A	OP1-P-O3'	7.29	121.25	105.20
1	A	1003	G	C2-N3-C4	7.29	115.55	111.90
1	A	220	G	C4-C5-C6	7.29	123.18	118.80
1	A	390	C	O5'-P-OP2	-7.29	99.14	105.70
1	A	8	A	N3-C4-N9	-7.29	121.57	127.40
1	A	452	A	N7-C8-N9	7.29	117.44	113.80
1	A	620	C	N3-C4-C5	7.29	124.81	121.90
1	A	1168	A	C8-N9-C4	-7.29	102.88	105.80
1	A	97	G	N1-C2-N3	7.29	128.27	123.90
1	A	61	G	C5-N7-C8	-7.28	100.66	104.30
1	A	675	A	O5'-P-OP1	-7.28	99.14	105.70
1	A	728	A	OP1-P-O3'	7.28	121.22	105.20
1	A	1485	U	N1-C2-O2	7.28	127.90	122.80
1	A	1062	U	C2-N3-C4	7.28	131.37	127.00
1	A	1220	G	N3-C4-N9	7.28	130.37	126.00
1	A	122	G	C5-C6-O6	-7.28	124.23	128.60
1	A	705	U	N1-C2-N3	7.28	119.27	114.90
1	A	722	A	N1-C6-N6	7.28	122.97	118.60
1	A	164	U	C6-N1-C2	7.28	125.36	121.00
1	A	768	A	C2-N3-C4	7.27	114.24	110.60
1	A	255	G	C8-N9-C1'	-7.27	117.55	127.00
1	A	568	G	O5'-P-OP1	-7.27	99.16	105.70
1	A	623	C	C6-N1-C2	7.27	123.21	120.30
1	A	61	G	C2-N3-C4	-7.27	108.26	111.90
1	A	949	A	O5'-P-OP2	-7.27	99.16	105.70
1	A	778	G	N1-C2-N2	-7.27	109.66	116.20
1	A	885	G	C6-C5-N7	-7.27	126.04	130.40
1	A	141	A	C5-C6-N6	-7.26	117.89	123.70
1	A	783	C	N1-C2-N3	-7.26	114.11	119.20
1	A	1080	A	C5-N7-C8	7.26	107.53	103.90
1	A	1323	G	C6-C5-N7	-7.26	126.04	130.40
1	A	51	A	C4-C5-N7	7.26	114.33	110.70
1	A	148	G	C6-C5-N7	-7.26	126.04	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	325	A	OP1-P-O3'	7.26	121.17	105.20
1	A	888	G	C4-N9-C1'	7.26	135.93	126.50
1	A	239	U	C6-N1-C1'	7.25	131.36	121.20
1	A	10	A	OP1-P-OP2	7.25	130.48	119.60
1	A	822	C	N3-C4-N4	7.25	123.08	118.00
1	A	1339	A	N9-C4-C5	7.25	108.70	105.80
1	A	190(E)	U	N1-C2-N3	-7.25	110.55	114.90
1	A	401	C	N1-C2-O2	-7.25	114.55	118.90
1	A	581	G	C5-C6-O6	7.25	132.95	128.60
1	A	6	G	N1-C2-N2	7.25	122.72	116.20
1	A	198	G	N3-C4-N9	7.25	130.35	126.00
1	A	525	C	N3-C2-O2	7.25	126.97	121.90
1	A	1020	U	N3-C2-O2	-7.25	117.13	122.20
1	A	1508	G	C8-N9-C4	-7.25	103.50	106.40
15	O	57	LEU	CA-CB-CG	-7.25	98.63	115.30
1	A	44	G	C4-C5-C6	7.25	123.15	118.80
1	A	830	G	C6-C5-N7	7.24	134.75	130.40
1	A	984	C	O5'-P-OP2	7.24	119.39	110.70
1	A	1290	G	C5-C6-N1	-7.24	107.88	111.50
1	A	1256	A	O4'-C1'-N9	-7.24	102.41	108.20
1	A	44	G	C8-N9-C1'	-7.24	117.59	127.00
1	A	1098	C	N3-C2-O2	7.24	126.97	121.90
1	A	112	G	OP1-P-OP2	7.24	130.45	119.60
1	A	332	G	N3-C2-N2	-7.24	114.83	119.90
1	A	712	A	C6-C5-N7	-7.24	127.23	132.30
1	A	530	G	C4-C5-C6	7.23	123.14	118.80
1	A	782	A	C2-N3-C4	-7.23	106.99	110.60
1	A	380	G	C5-C6-N1	-7.23	107.89	111.50
1	A	250	A	O5'-P-OP1	7.23	119.37	110.70
1	A	1433	A	O5'-P-OP1	-7.23	99.20	105.70
1	A	286	G	C5-C6-O6	-7.22	124.27	128.60
1	A	354	G	O5'-P-OP2	7.22	119.37	110.70
1	A	402	G	N1-C2-N2	-7.22	109.70	116.20
1	A	965	A	C4-C5-C6	-7.22	113.39	117.00
1	A	1529	G	C6-C5-N7	-7.22	126.06	130.40
1	A	5	U	N3-C2-O2	-7.22	117.14	122.20
1	A	723	U	C5-C6-N1	7.22	126.31	122.70
1	A	734	G	N9-C4-C5	-7.22	102.51	105.40
1	A	74	C	C6-N1-C2	7.22	123.19	120.30
1	A	944	G	C4-N9-C1'	7.21	135.88	126.50
1	A	1183	A	P-O3'-C3'	7.21	128.36	119.70
1	A	1337	G	N1-C6-O6	7.21	124.23	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1230	C	N3-C2-O2	7.21	126.95	121.90
1	A	74	C	O5'-P-OP1	7.21	119.35	110.70
1	A	413	G	O5'-P-OP1	-7.21	99.21	105.70
1	A	729	A	N3-C4-C5	-7.21	121.75	126.80
1	A	1240	U	N3-C4-O4	-7.21	114.35	119.40
1	A	978	A	C8-N9-C4	-7.21	102.92	105.80
1	A	1391	U	C4-C5-C6	7.21	124.03	119.70
1	A	259	G	C5-C6-O6	-7.21	124.28	128.60
1	A	856	C	OP2-P-O3'	7.21	121.06	105.20
1	A	581	G	N1-C6-O6	-7.21	115.58	119.90
1	A	1019	C	C5-C6-N1	7.21	124.60	121.00
1	A	1388	C	C2-N3-C4	-7.21	116.30	119.90
5	E	140	ARG	NE-CZ-NH2	-7.21	116.70	120.30
1	A	789	U	C2-N3-C4	7.21	131.32	127.00
1	A	548	G	N3-C2-N2	-7.20	114.86	119.90
1	A	560	U	C2-N1-C1'	7.20	126.34	117.70
1	A	557	G	O4'-C1'-N9	7.20	113.96	108.20
1	A	115	G	P-O3'-C3'	7.20	128.34	119.70
1	A	234	C	C2-N3-C4	-7.20	116.30	119.90
1	A	372	C	C2-N3-C4	-7.20	116.30	119.90
1	A	666	G	C5-C6-N1	-7.20	107.90	111.50
1	A	935	A	C4-C5-C6	7.20	120.60	117.00
1	A	161	A	N9-C4-C5	7.20	108.68	105.80
1	A	763	G	N3-C4-N9	7.20	130.32	126.00
1	A	901	A	C5-C6-N6	7.20	129.46	123.70
1	A	953	G	C5-C6-O6	7.20	132.92	128.60
1	A	1177	G	C5-N7-C8	-7.20	100.70	104.30
1	A	1504	G	N9-C4-C5	7.20	108.28	105.40
1	A	1515	C	C5-C4-N4	-7.20	115.16	120.20
1	A	1239	A	C2-N3-C4	-7.20	107.00	110.60
1	A	76	C	N3-C4-N4	7.19	123.03	118.00
1	A	881	G	C8-N9-C1'	-7.19	117.65	127.00
1	A	964	A	C2-N3-C4	-7.19	107.01	110.60
1	A	1509	C	N1-C2-N3	7.19	124.23	119.20
1	A	780	A	N1-C6-N6	7.19	122.91	118.60
1	A	839	U	O5'-P-OP2	-7.19	99.23	105.70
1	A	736	C	N3-C2-O2	-7.18	116.87	121.90
1	A	325	A	N1-C6-N6	-7.18	114.29	118.60
1	A	834	C	O5'-P-OP1	7.18	119.32	110.70
1	A	1506	U	C6-N1-C1'	-7.18	111.15	121.20
1	A	815	A	C4-C5-C6	7.18	120.59	117.00
1	A	821	G	N1-C6-O6	7.18	124.21	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	896	C	N1-C2-O2	-7.18	114.59	118.90
1	A	510	A	N9-C4-C5	7.18	108.67	105.80
1	A	976	G	N7-C8-N9	-7.18	109.51	113.10
1	A	21	G	C8-N9-C4	7.18	109.27	106.40
1	A	586	C	OP2-P-O3'	7.18	120.99	105.20
1	A	592	G	C2-N3-C4	-7.17	108.31	111.90
1	A	368	U	N1-C2-N3	7.17	119.20	114.90
1	A	461	C	OP2-P-O3'	7.17	120.97	105.20
1	A	1279	A	N7-C8-N9	7.17	117.39	113.80
1	A	1139	G	C5-C6-N1	-7.17	107.92	111.50
1	A	700	G	N1-C6-O6	7.16	124.20	119.90
1	A	912	C	N3-C4-C5	-7.16	119.03	121.90
1	A	243	A	C4-C5-C6	7.16	120.58	117.00
1	A	285	G	C5-C6-O6	-7.16	124.30	128.60
1	A	422	C	N1-C2-O2	7.16	123.20	118.90
1	A	841	U	C6-N1-C2	-7.16	116.70	121.00
1	A	1064	G	C6-C5-N7	7.16	134.70	130.40
1	A	1504	G	C4-C5-C6	7.16	123.10	118.80
1	A	284	G	N3-C4-C5	7.16	132.18	128.60
1	A	356	A	N1-C6-N6	-7.16	114.31	118.60
1	A	372	C	N3-C4-N4	7.16	123.01	118.00
1	A	285	G	C2-N3-C4	-7.16	108.32	111.90
1	A	1081	G	C5-C6-N1	7.16	115.08	111.50
4	D	10	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	A	1108	G	C4-N9-C1'	7.16	135.80	126.50
1	A	1449	C	C6-N1-C2	7.16	123.16	120.30
1	A	196	A	N1-C2-N3	-7.15	125.72	129.30
1	A	45	U	OP2-P-O3'	7.15	120.94	105.20
1	A	281	G	C8-N9-C4	7.15	109.26	106.40
1	A	319	G	N1-C2-N3	7.15	128.19	123.90
1	A	1531	A	C4-C5-N7	7.15	114.28	110.70
1	A	121	C	N1-C2-N3	-7.15	114.19	119.20
1	A	954	G	C8-N9-C4	7.15	109.26	106.40
1	A	1227	A	C8-N9-C1'	-7.15	114.83	127.70
1	A	240	C	C6-N1-C2	7.15	123.16	120.30
1	A	1079	G	C4-C5-C6	7.15	123.09	118.80
1	A	690	G	C2-N3-C4	-7.15	108.33	111.90
1	A	1322	C	N3-C2-O2	7.15	126.90	121.90
1	A	1377	A	N3-C4-C5	7.15	131.80	126.80
1	A	1379	G	C5-N7-C8	-7.15	100.73	104.30
1	A	329	A	C4-C5-N7	7.15	114.27	110.70
1	A	396	G	N9-C4-C5	7.14	108.26	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	806	C	N3-C4-N4	7.14	123.00	118.00
1	A	1070	U	C5-C4-O4	-7.14	121.61	125.90
1	A	136	C	C5-C4-N4	-7.14	115.20	120.20
1	A	1442	G	N3-C2-N2	7.14	124.90	119.90
1	A	421	U	C6-N1-C2	7.14	125.28	121.00
1	A	436	C	N3-C4-C5	7.14	124.76	121.90
1	A	710	G	C6-C5-N7	-7.14	126.12	130.40
1	A	764	C	O5'-P-OP1	-7.14	99.27	105.70
1	A	486	U	C6-N1-C2	7.14	125.28	121.00
1	A	190(L)	U	N3-C2-O2	7.13	127.19	122.20
1	A	1091	U	N3-C4-C5	-7.13	110.32	114.60
1	A	1186	G	N3-C4-C5	7.13	132.17	128.60
1	A	1050	G	N1-C2-N3	7.13	128.18	123.90
1	A	222	U	O5'-P-OP2	-7.13	99.28	105.70
1	A	36	C	N1-C2-N3	7.13	124.19	119.20
1	A	423	G	C6-C5-N7	-7.13	126.12	130.40
1	A	701	C	P-O3'-C3'	7.13	128.25	119.70
1	A	620	C	O5'-P-OP2	-7.12	99.29	105.70
1	A	800	G	C5-C6-O6	7.12	132.87	128.60
1	A	1095	U	N1-C2-O2	-7.12	117.81	122.80
1	A	237	C	OP1-P-O3'	-7.12	89.53	105.20
1	A	639	G	N1-C2-N2	7.12	122.61	116.20
1	A	1414	U	N3-C4-O4	7.12	124.39	119.40
1	A	398	C	N1-C2-N3	-7.12	114.22	119.20
1	A	1448	C	C6-N1-C2	7.12	123.15	120.30
1	A	80	G	OP2-P-O3'	-7.12	89.54	105.20
1	A	111	G	C6-N1-C2	7.12	129.37	125.10
19	S	5	LEU	CA-CB-CG	7.12	131.67	115.30
1	A	836	G	O5'-P-OP2	7.12	119.24	110.70
1	A	597	G	N1-C6-O6	7.11	124.17	119.90
1	A	1530	G	N3-C4-N9	-7.11	121.73	126.00
1	A	639	G	N3-C2-N2	-7.11	114.92	119.90
1	A	694	A	C2-N3-C4	-7.11	107.04	110.60
1	A	971	G	C2-N3-C4	-7.11	108.35	111.90
1	A	21	G	N3-C2-N2	7.11	124.88	119.90
1	A	290	C	O5'-P-OP1	7.11	119.23	110.70
1	A	542	G	N1-C2-N3	7.11	128.16	123.90
1	A	703	G	N3-C2-N2	7.11	124.87	119.90
1	A	1289	A	C4-C5-C6	7.11	120.55	117.00
1	A	569	C	N3-C4-N4	-7.10	113.03	118.00
1	A	1079	G	N1-C6-O6	7.10	124.16	119.90
1	A	144	G	N1-C2-N2	7.10	122.59	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	U	C2-N3-C4	7.10	131.26	127.00
1	A	813	U	O5'-P-OP1	-7.10	99.31	105.70
1	A	1455	G	N1-C6-O6	7.10	124.16	119.90
1	A	504	C	N3-C2-O2	-7.10	116.93	121.90
1	A	1239	A	N1-C6-N6	7.10	122.86	118.60
1	A	793	U	C5-C4-O4	7.10	130.16	125.90
1	A	715	A	N1-C2-N3	7.10	132.85	129.30
1	A	799	G	N1-C2-N2	-7.10	109.81	116.20
1	A	1305	G	OP1-P-O3'	-7.10	89.58	105.20
1	A	407	G	N1-C2-N3	7.09	128.16	123.90
1	A	649	G	N9-C4-C5	-7.09	102.56	105.40
1	A	1507	A	C5-C6-N1	7.09	121.25	117.70
1	A	693	G	C6-C5-N7	7.09	134.66	130.40
1	A	768	A	C6-N1-C2	-7.09	114.34	118.60
1	A	238	G	C4-C5-C6	7.09	123.05	118.80
1	A	792	A	O5'-P-OP1	-7.09	99.32	105.70
1	A	1067	A	C5-C6-N6	7.09	129.37	123.70
1	A	356	A	N9-C4-C5	7.09	108.64	105.80
1	A	583	A	C8-N9-C4	7.09	108.64	105.80
1	A	790	A	N9-C4-C5	-7.09	102.97	105.80
17	Q	31	LEU	CA-CB-CG	-7.09	99.00	115.30
1	A	438	G	C6-C5-N7	7.08	134.65	130.40
1	A	832	C	C4-C5-C6	7.08	120.94	117.40
1	A	796	C	N3-C4-N4	7.08	122.96	118.00
1	A	1210	C	C4-C5-C6	7.08	120.94	117.40
1	A	614	A	C5-N7-C8	-7.08	100.36	103.90
1	A	664	G	N3-C2-N2	7.08	124.86	119.90
1	A	769	G	O5'-P-OP1	7.08	119.19	110.70
1	A	295	C	C5-C4-N4	-7.08	115.25	120.20
1	A	761	G	C6-C5-N7	-7.08	126.15	130.40
1	A	286	G	N3-C2-N2	-7.08	114.95	119.90
1	A	552	U	N1-C2-O2	-7.08	117.85	122.80
1	A	168	G	N1-C6-O6	7.07	124.14	119.90
1	A	266	G	N3-C4-N9	-7.07	121.76	126.00
1	A	794	A	OP1-P-OP2	-7.07	108.99	119.60
1	A	904	C	C2-N3-C4	-7.07	116.36	119.90
1	A	1206	G	C2-N3-C4	-7.07	108.36	111.90
1	A	154	C	N3-C4-C5	7.07	124.73	121.90
1	A	689	C	N1-C2-O2	-7.07	114.66	118.90
1	A	802	A	N1-C2-N3	7.07	132.84	129.30
1	A	198	G	N9-C4-C5	-7.07	102.57	105.40
1	A	1409	C	N3-C4-N4	7.07	122.95	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1469	G	C6-N1-C2	-7.07	120.86	125.10
3	C	30	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	A	1080	A	C4-C5-N7	-7.07	107.17	110.70
1	A	405	U	OP1-P-O3'	7.07	120.74	105.20
1	A	413	G	C5-C6-O6	7.07	132.84	128.60
1	A	685	G	N9-C4-C5	7.07	108.23	105.40
1	A	1053	G	N3-C4-N9	-7.07	121.76	126.00
1	A	1231	G	N3-C4-C5	7.06	132.13	128.60
1	A	1530	G	O5'-P-OP2	-7.06	99.34	105.70
17	Q	67	LYS	N-CA-C	-7.06	91.93	111.00
1	A	1186	G	C5-C6-N1	-7.06	107.97	111.50
1	A	1509	C	C5-C6-N1	-7.06	117.47	121.00
1	A	564	C	N1-C2-O2	-7.06	114.67	118.90
1	A	568	G	C5-C6-O6	7.06	132.83	128.60
1	A	823	G	C4-C5-N7	7.06	113.62	110.80
1	A	266	G	C5-C6-O6	-7.06	124.37	128.60
1	A	1474	G	N9-C4-C5	7.06	108.22	105.40
1	A	1129	C	C6-N1-C2	-7.05	117.48	120.30
1	A	1177	G	N7-C8-N9	7.05	116.63	113.10
1	A	413	G	C8-N9-C1'	7.05	136.16	127.00
1	A	141	A	C6-C5-N7	-7.05	127.37	132.30
1	A	562	C	OP1-P-O3'	7.05	120.70	105.20
1	A	293	G	C5-C6-N1	-7.04	107.98	111.50
1	A	654	G	N3-C4-N9	-7.04	121.77	126.00
1	A	344	A	O4'-C1'-N9	-7.04	102.57	108.20
1	A	590	C	N3-C4-C5	7.04	124.72	121.90
1	A	1344	C	N3-C4-C5	7.04	124.72	121.90
1	A	1485	U	O5'-P-OP2	-7.04	99.36	105.70
1	A	555	C	OP2-P-O3'	7.04	120.69	105.20
1	A	609	A	N7-C8-N9	7.04	117.32	113.80
1	A	596	C	C5-C6-N1	-7.04	117.48	121.00
1	A	964	A	N1-C2-N3	7.04	132.82	129.30
1	A	313	A	O5'-P-OP1	-7.04	99.37	105.70
1	A	490	G	C2-N3-C4	-7.04	108.38	111.90
1	A	66	G	N3-C4-C5	7.04	132.12	128.60
1	A	484	G	C6-N1-C2	-7.04	120.88	125.10
1	A	1452	C	C6-N1-C1'	-7.04	112.36	120.80
11	K	125	PHE	N-CA-C	7.04	130.00	111.00
1	A	945	G	N7-C8-N9	7.03	116.62	113.10
1	A	1455	G	C5-C6-N1	-7.03	107.98	111.50
1	A	1526	G	C4-C5-C6	7.03	123.02	118.80
1	A	1528	U	C6-N1-C2	7.03	125.22	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	353	A	N1-C2-N3	-7.03	125.78	129.30
1	A	1087	G	OP1-P-O3'	-7.03	89.73	105.20
1	A	30	U	N1-C2-O2	-7.03	117.88	122.80
1	A	576	G	C6-C5-N7	-7.03	126.19	130.40
1	A	867	G	C5-C6-N1	-7.03	107.99	111.50
1	A	1195	C	OP1-P-O3'	7.03	120.66	105.20
8	H	18	ARG	NE-CZ-NH1	7.03	123.81	120.30
1	A	429	U	O5'-P-OP2	7.02	119.13	110.70
1	A	1414	U	O4'-C1'-N1	7.02	113.82	108.20
1	A	577	G	N1-C2-N3	7.02	128.11	123.90
1	A	39	G	C6-C5-N7	7.02	134.61	130.40
1	A	771	G	OP1-P-OP2	7.02	130.13	119.60
1	A	1020	U	N1-C2-N3	7.02	119.11	114.90
1	A	726	C	O5'-P-OP1	-7.02	99.38	105.70
1	A	260	G	C6-C5-N7	-7.02	126.19	130.40
1	A	1155	G	O5'-P-OP1	-7.02	99.38	105.70
1	A	787	A	OP1-P-OP2	7.02	130.12	119.60
1	A	112	G	C6-N1-C2	-7.01	120.89	125.10
1	A	1121	U	C5-C6-N1	-7.01	119.19	122.70
1	A	898	G	C6-C5-N7	-7.01	126.19	130.40
1	A	1502	A	C5-C6-N6	-7.01	118.09	123.70
1	A	144	G	C8-N9-C4	-7.01	103.60	106.40
1	A	745	C	N3-C4-C5	7.01	124.70	121.90
1	A	770	C	OP1-P-O3'	-7.01	89.78	105.20
1	A	108	G	N9-C1'-C2'	-7.01	104.29	112.00
1	A	918	A	N3-C4-C5	-7.00	121.90	126.80
1	A	856	C	OP1-P-O3'	-7.00	89.79	105.20
1	A	1091	U	N1-C2-N3	7.00	119.10	114.90
1	A	299	G	C6-C5-N7	-7.00	126.20	130.40
1	A	554	C	C5-C4-N4	7.00	125.10	120.20
1	A	485	G	N3-C2-N2	7.00	124.80	119.90
1	A	792	A	C8-N9-C4	-7.00	103.00	105.80
1	A	907	A	OP1-P-OP2	7.00	130.10	119.60
1	A	962	C	N3-C4-C5	7.00	124.70	121.90
1	A	307	C	C4-C5-C6	-7.00	113.90	117.40
1	A	623	C	C5-C6-N1	-7.00	117.50	121.00
1	A	1521	G	C6-N1-C2	-7.00	120.90	125.10
1	A	103	C	OP1-P-OP2	6.99	130.09	119.60
1	A	113	G	O4'-C1'-N9	-6.99	102.61	108.20
1	A	656	C	C5-C4-N4	-6.99	115.30	120.20
1	A	99	C	N3-C4-N4	6.99	122.89	118.00
1	A	151	A	C8-N9-C4	6.99	108.60	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1331	G	O5'-P-OP1	6.99	119.08	110.70
1	A	1424	C	C5-C6-N1	-6.99	117.50	121.00
1	A	907	A	N9-C4-C5	6.99	108.59	105.80
1	A	37	U	N3-C4-C5	-6.99	110.41	114.60
1	A	44	G	C4-N9-C1'	6.99	135.58	126.50
1	A	120	A	N9-C4-C5	6.99	108.59	105.80
1	A	360	A	O4'-C1'-N9	-6.99	102.61	108.20
1	A	989	C	C6-N1-C2	-6.99	117.51	120.30
1	A	825	G	N3-C2-N2	-6.98	115.01	119.90
1	A	152	A	O5'-P-OP1	-6.98	99.42	105.70
1	A	405	U	N1-C2-N3	6.98	119.09	114.90
1	A	1505	G	N1-C6-O6	6.98	124.09	119.90
1	A	478	A	C5-C6-N1	-6.98	114.21	117.70
1	A	706	A	N7-C8-N9	-6.98	110.31	113.80
1	A	273	A	C2-N3-C4	-6.98	107.11	110.60
1	A	632	A	C6-C5-N7	-6.98	127.42	132.30
1	A	771	G	N3-C4-N9	-6.98	121.81	126.00
1	A	977	A	C2-N3-C4	6.98	114.09	110.60
1	A	30	U	C4-C5-C6	6.97	123.89	119.70
1	A	387	U	N3-C4-O4	6.97	124.28	119.40
1	A	1339	A	C5-N7-C8	6.97	107.39	103.90
10	J	99	LYS	CD-CE-NZ	6.97	127.74	111.70
1	A	511	C	C2-N1-C1'	-6.97	111.13	118.80
14	N	47	LEU	CA-CB-CG	-6.97	99.26	115.30
1	A	746	A	C5-C6-N6	6.97	129.28	123.70
1	A	1447	G	C5-C6-O6	-6.97	124.42	128.60
1	A	1499	A	C6-N1-C2	-6.97	114.42	118.60
1	A	61	G	C5-C6-N1	-6.97	108.02	111.50
1	A	1491	G	C2-N3-C4	6.97	115.38	111.90
1	A	1228	C	N1-C2-N3	-6.96	114.33	119.20
1	A	1321	C	C4-C5-C6	6.96	120.88	117.40
1	A	908	A	C4-C5-N7	-6.96	107.22	110.70
1	A	376	G	N7-C8-N9	-6.96	109.62	113.10
1	A	494	G	C4-C5-C6	6.96	122.97	118.80
1	A	768	A	C5-C6-N6	-6.96	118.13	123.70
1	A	782	A	C5-C6-N6	6.96	129.27	123.70
1	A	560	U	C6-N1-C2	-6.96	116.83	121.00
1	A	662	G	C8-N9-C1'	-6.96	117.96	127.00
1	A	789	U	N1-C2-N3	6.96	119.07	114.90
1	A	555	C	O5'-P-OP1	6.96	119.05	110.70
1	A	175	C	O5'-P-OP2	-6.95	99.44	105.70
1	A	1065	U	OP2-P-O3'	6.95	120.50	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1151	A	C4-C5-N7	-6.95	107.22	110.70
1	A	58	C	O5'-P-OP1	-6.95	99.45	105.70
1	A	292	G	C6-C5-N7	-6.95	126.23	130.40
1	A	833	U	C5-C6-N1	-6.95	119.23	122.70
1	A	910	C	C2-N3-C4	-6.95	116.43	119.90
1	A	299	G	N1-C6-O6	6.95	124.07	119.90
1	A	168	G	C5-C6-N1	-6.94	108.03	111.50
1	A	236	G	C5-C6-N1	6.94	114.97	111.50
1	A	356	A	O5'-P-OP1	-6.94	99.45	105.70
1	A	379	C	C5-C6-N1	-6.94	117.53	121.00
1	A	399	G	N3-C4-C5	6.94	132.07	128.60
1	A	1236	A	N1-C6-N6	6.94	122.76	118.60
1	A	1342	C	N3-C4-N4	6.94	122.86	118.00
1	A	386	C	C5-C4-N4	-6.94	115.34	120.20
1	A	51	A	N9-C4-C5	-6.94	103.03	105.80
1	A	388	G	C5-C6-O6	-6.94	124.44	128.60
15	O	77	ARG	NE-CZ-NH2	-6.93	116.83	120.30
1	A	27	G	C5-N7-C8	-6.93	100.83	104.30
1	A	251	G	C2-N3-C4	-6.93	108.43	111.90
1	A	190(D)	U	C5-C6-N1	-6.93	119.23	122.70
1	A	1474	G	C5-C6-O6	6.93	132.76	128.60
1	A	32	A	C6-N1-C2	-6.93	114.44	118.60
1	A	60	A	N9-C4-C5	6.93	108.57	105.80
1	A	935	A	O4'-C1'-N9	-6.93	102.66	108.20
1	A	289	G	O5'-P-OP2	-6.93	99.47	105.70
1	A	190(E)	U	N3-C2-O2	-6.93	117.35	122.20
1	A	1202	G	N9-C4-C5	6.93	108.17	105.40
1	A	33	A	C4-C5-N7	6.92	114.16	110.70
1	A	113	G	C4-N9-C1'	6.92	135.50	126.50
1	A	804	U	OP1-P-O3'	-6.92	89.97	105.20
1	A	1346	A	C8-N9-C4	6.92	108.57	105.80
1	A	1446	A	C4-C5-N7	-6.92	107.24	110.70
1	A	1373	G	C8-N9-C4	-6.92	103.63	106.40
1	A	136	C	N3-C2-O2	6.92	126.75	121.90
1	A	662	G	N1-C6-O6	6.92	124.05	119.90
1	A	933	G	C5-C6-O6	-6.92	124.45	128.60
1	A	1151	A	C8-N9-C4	6.92	108.57	105.80
1	A	890	G	N1-C2-N3	6.92	128.05	123.90
1	A	14	U	C2-N1-C1'	-6.92	109.40	117.70
1	A	223	U	OP1-P-OP2	6.92	129.97	119.60
1	A	1126	U	C6-N1-C2	-6.92	116.85	121.00
1	A	59	A	N1-C6-N6	-6.91	114.45	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	194	C	C5-C6-N1	-6.91	117.54	121.00
1	A	252	U	N1-C2-O2	-6.91	117.96	122.80
1	A	759	A	N7-C8-N9	6.91	117.26	113.80
1	A	306	G	C5-C6-O6	-6.91	124.45	128.60
1	A	836	G	O4'-C1'-N9	-6.91	102.67	108.20
1	A	899	C	N1-C2-O2	-6.91	114.75	118.90
1	A	288	A	C5-C6-N6	6.91	129.23	123.70
1	A	444	C	C5-C4-N4	-6.91	115.36	120.20
1	A	975	A	O5'-P-OP2	6.91	118.99	110.70
1	A	1159	U	C5-C6-N1	-6.91	119.25	122.70
1	A	719	C	C2-N3-C4	-6.91	116.45	119.90
1	A	807	A	C6-C5-N7	-6.91	127.47	132.30
1	A	898	G	OP1-P-OP2	6.91	129.96	119.60
1	A	1405	G	N9-C4-C5	-6.91	102.64	105.40
1	A	741	G	N9-C4-C5	6.91	108.16	105.40
1	A	318	G	C8-N9-C4	6.90	109.16	106.40
1	A	752	G	N9-C4-C5	6.90	108.16	105.40
1	A	24	U	N1-C2-O2	-6.90	117.97	122.80
1	A	307	C	C5-C6-N1	6.90	124.45	121.00
1	A	485	G	N3-C4-C5	-6.90	125.15	128.60
1	A	942	G	N9-C4-C5	-6.90	102.64	105.40
1	A	24	U	C2-N3-C4	-6.90	122.86	127.00
1	A	519	C	C4-C5-C6	6.90	120.85	117.40
1	A	578	C	C5-C4-N4	6.90	125.03	120.20
1	A	821	G	O5'-P-OP2	-6.90	99.49	105.70
1	A	387	U	N1-C2-O2	-6.90	117.97	122.80
1	A	1285	A	P-O3'-C3'	6.90	127.98	119.70
1	A	685	G	C6-C5-N7	6.90	134.54	130.40
1	A	108	G	N3-C2-N2	-6.89	115.07	119.90
1	A	1332	A	C2-N3-C4	-6.89	107.15	110.60
1	A	792	A	C5-C6-N1	-6.89	114.25	117.70
1	A	291	C	N3-C2-O2	-6.89	117.08	121.90
1	A	1348	U	C6-N1-C2	-6.89	116.87	121.00
4	D	70	ILE	CB-CA-C	-6.89	97.83	111.60
1	A	1189	C	N3-C2-O2	-6.88	117.08	121.90
1	A	1139	G	P-O3'-C3'	6.88	127.96	119.70
1	A	1117	G	N3-C4-N9	6.88	130.13	126.00
1	A	1385	G	OP1-P-OP2	6.88	129.92	119.60
1	A	1533	C	C5-C6-N1	6.88	124.44	121.00
1	A	1425	U	C5-C4-O4	6.88	130.03	125.90
1	A	1438	G	C5-C6-N1	-6.88	108.06	111.50
1	A	523	A	N9-C4-C5	6.88	108.55	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1443	G	N3-C4-N9	-6.88	121.88	126.00
1	A	257	G	O5'-P-OP1	6.88	118.95	110.70
1	A	632	A	C5-C6-N6	-6.88	118.20	123.70
1	A	228	A	N9-C4-C5	6.87	108.55	105.80
1	A	1092	A	O5'-P-OP2	-6.87	99.52	105.70
1	A	316	G	N9-C4-C5	-6.87	102.65	105.40
1	A	368	U	N3-C2-O2	-6.87	117.39	122.20
1	A	1269	A	C5-C6-N6	6.87	129.20	123.70
1	A	915	A	OP2-P-O3'	6.87	120.31	105.20
1	A	759	A	C6-N1-C2	-6.87	114.48	118.60
1	A	968	A	C2-N3-C4	6.87	114.03	110.60
1	A	898	G	N1-C6-O6	6.87	124.02	119.90
1	A	625	G	N9-C4-C5	-6.86	102.66	105.40
1	A	817	C	C4-C5-C6	6.86	120.83	117.40
1	A	509	A	C5-N7-C8	-6.86	100.47	103.90
1	A	653	A	C5-C6-N1	6.86	121.13	117.70
1	A	656	C	N1-C2-N3	-6.86	114.40	119.20
1	A	399	G	C4-C5-C6	-6.86	114.68	118.80
1	A	780	A	O5'-P-OP2	6.86	118.93	110.70
1	A	176	C	C2-N3-C4	6.86	123.33	119.90
1	A	561	U	C5-C6-N1	6.86	126.13	122.70
1	A	821	G	C4-C5-C6	6.86	122.92	118.80
1	A	1300	G	C5-N7-C8	-6.86	100.87	104.30
1	A	1516	G	N3-C2-N2	-6.86	115.10	119.90
1	A	386	C	N3-C4-C5	6.85	124.64	121.90
1	A	430	A	N1-C6-N6	6.85	122.71	118.60
1	A	780	A	C6-N1-C2	-6.85	114.49	118.60
1	A	749	C	C5-C6-N1	6.85	124.43	121.00
1	A	762	C	C6-N1-C1'	-6.85	112.58	120.80
1	A	45	U	C5-C6-N1	-6.85	119.28	122.70
1	A	972	C	N1-C2-O2	-6.85	114.79	118.90
1	A	60	A	OP1-P-O3'	6.85	120.27	105.20
1	A	778	G	N3-C4-C5	-6.85	125.17	128.60
1	A	338	A	N1-C2-N3	6.85	132.72	129.30
1	A	1064	G	C4-N9-C1'	-6.85	117.60	126.50
1	A	1163	C	C5-C6-N1	6.85	124.42	121.00
1	A	336	C	N1-C2-O2	-6.85	114.79	118.90
1	A	93	G	N3-C4-C5	6.84	132.02	128.60
1	A	317	G	N1-C2-N3	6.84	128.01	123.90
1	A	719	C	C5-C6-N1	-6.84	117.58	121.00
1	A	1197	G	N3-C2-N2	-6.84	115.11	119.90
1	A	1331	G	C5-C6-N1	-6.84	108.08	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	193	C	O5'-P-OP2	-6.84	99.54	105.70
1	A	1380	U	C5-C4-O4	6.84	130.00	125.90
1	A	1401	G	C2-N3-C4	6.84	115.32	111.90
1	A	118	U	C6-N1-C2	6.84	125.10	121.00
15	O	45	VAL	CB-CA-C	-6.84	98.41	111.40
1	A	625	G	C8-N9-C1'	-6.84	118.11	127.00
1	A	907	A	C2-N3-C4	-6.84	107.18	110.60
1	A	1195	C	C6-N1-C2	-6.84	117.56	120.30
1	A	1353	G	N3-C4-C5	-6.84	125.18	128.60
1	A	523	A	N1-C6-N6	-6.84	114.50	118.60
1	A	529	G	N7-C8-N9	6.84	116.52	113.10
1	A	971	G	C4-C5-C6	6.84	122.90	118.80
1	A	1094	G	N3-C2-N2	6.84	124.69	119.90
1	A	1221	G	C5-C6-N1	-6.84	108.08	111.50
1	A	766	A	N9-C4-C5	-6.83	103.07	105.80
1	A	1439	C	C5-C4-N4	-6.83	115.42	120.20
1	A	1450	U	N3-C4-O4	6.83	124.18	119.40
1	A	750	G	N1-C6-O6	-6.83	115.80	119.90
1	A	1264	C	C4-C5-C6	6.83	120.82	117.40
1	A	1530	G	N9-C4-C5	-6.83	102.67	105.40
1	A	1532	U	N3-C4-C5	6.83	118.70	114.60
1	A	324	G	C5-C6-N1	-6.83	108.08	111.50
1	A	383	A	C8-N9-C4	-6.83	103.07	105.80
1	A	1116	C	C5-C6-N1	-6.83	117.58	121.00
1	A	643	C	C6-N1-C2	6.83	123.03	120.30
1	A	684	A	C5-C6-N1	-6.83	114.28	117.70
1	A	929	G	N7-C8-N9	-6.83	109.69	113.10
1	A	1194	U	N3-C4-C5	-6.83	110.50	114.60
1	A	610	G	O5'-P-OP2	-6.83	99.55	105.70
1	A	860	A	O5'-P-OP1	6.83	118.89	110.70
1	A	633	G	C2-N3-C4	-6.83	108.49	111.90
1	A	848	C	C5-C6-N1	6.83	124.41	121.00
1	A	135	C	N3-C4-N4	6.82	122.78	118.00
17	Q	5	VAL	CB-CA-C	-6.82	98.44	111.40
1	A	406	G	C6-C5-N7	-6.82	126.31	130.40
1	A	659	U	C2-N3-C4	-6.82	122.91	127.00
1	A	692	U	N1-C2-O2	6.82	127.58	122.80
1	A	895	G	C5-N7-C8	-6.82	100.89	104.30
1	A	1131	G	C6-C5-N7	-6.82	126.31	130.40
1	A	612	C	N1-C2-O2	-6.81	114.81	118.90
1	A	1486	G	N3-C4-C5	-6.81	125.19	128.60
1	A	561	U	C2-N1-C1'	6.81	125.87	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	768	A	C8-N9-C4	-6.81	103.08	105.80
1	A	1521	G	N3-C4-C5	-6.81	125.20	128.60
1	A	1083	U	C5-C4-O4	6.81	129.98	125.90
1	A	1066	C	N3-C4-C5	-6.81	119.18	121.90
1	A	270	A	N7-C8-N9	6.80	117.20	113.80
1	A	911	U	N3-C4-C5	-6.80	110.52	114.60
1	A	969	A	N1-C6-N6	6.80	122.68	118.60
10	J	99	LYS	N-CA-C	-6.80	92.63	111.00
1	A	1442	G	N1-C6-O6	-6.80	115.82	119.90
1	A	229	U	C4-C5-C6	6.80	123.78	119.70
1	A	1168	A	N3-C4-C5	-6.80	122.04	126.80
1	A	521	G	N1-C6-O6	-6.80	115.82	119.90
1	A	1054	C	C5-C6-N1	6.80	124.40	121.00
1	A	278	G	N1-C2-N3	6.80	127.98	123.90
1	A	860	A	N9-C4-C5	-6.80	103.08	105.80
1	A	1020	U	C6-N1-C1'	6.80	130.72	121.20
1	A	1372	U	C5-C4-O4	-6.80	121.82	125.90
1	A	566	G	C4-C5-N7	6.79	113.52	110.80
1	A	833	U	O5'-P-OP2	-6.79	99.58	105.70
1	A	1435	G	N1-C2-N3	6.79	127.98	123.90
1	A	486	U	C5-C6-N1	-6.79	119.30	122.70
1	A	791	G	O5'-P-OP1	-6.79	99.59	105.70
1	A	1003(A)	G	N3-C2-N2	-6.79	115.14	119.90
1	A	483	C	C5-C6-N1	-6.79	117.60	121.00
1	A	753	A	C5-N7-C8	6.79	107.30	103.90
1	A	1231	G	C8-N9-C1'	6.79	135.83	127.00
1	A	1375	A	C5-C6-N6	-6.79	118.27	123.70
1	A	1499	A	C5-C6-N6	6.79	129.13	123.70
1	A	1063	C	C2-N3-C4	-6.79	116.50	119.90
1	A	1087	G	OP2-P-O3'	6.79	120.13	105.20
1	A	1533	C	N3-C4-N4	6.79	122.75	118.00
1	A	42	G	N1-C2-N2	6.78	122.31	116.20
1	A	1432	G	C5-N7-C8	6.78	107.69	104.30
1	A	309	G	N7-C8-N9	6.78	116.49	113.10
1	A	1053	G	C4-N9-C1'	-6.78	117.69	126.50
1	A	43	C	N3-C4-C5	6.78	124.61	121.90
17	Q	98	LEU	CA-CB-CG	6.78	130.88	115.30
20	T	94	ALA	N-CA-C	-6.77	92.71	111.00
1	A	43	C	N1-C2-N3	-6.77	114.46	119.20
1	A	236	G	C4-N9-C1'	6.77	135.30	126.50
1	A	570	G	C2-N3-C4	6.77	115.28	111.90
1	A	1054	C	C2-N1-C1'	6.77	126.25	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	589	C	OP1-P-OP2	6.77	129.75	119.60
1	A	809	G	C6-C5-N7	6.77	134.46	130.40
1	A	1335	C	C5-C6-N1	-6.77	117.62	121.00
1	A	1387	G	O5'-P-OP2	-6.77	99.61	105.70
1	A	369	C	OP2-P-O3'	6.76	120.08	105.20
1	A	806	C	C5-C6-N1	6.76	124.38	121.00
1	A	293	G	O5'-P-OP2	-6.76	99.61	105.70
1	A	1060	C	N1-C2-N3	6.76	123.93	119.20
1	A	65	U	C4-C5-C6	6.76	123.76	119.70
1	A	164	U	O5'-P-OP1	-6.76	99.62	105.70
1	A	406	G	N1-C6-O6	6.76	123.96	119.90
1	A	886	G	N1-C2-N3	6.76	127.95	123.90
1	A	79	G	C8-N9-C1'	-6.76	118.22	127.00
1	A	613	C	N3-C4-C5	6.76	124.60	121.90
1	A	841	U	N1-C2-O2	6.76	127.53	122.80
1	A	19	C	O5'-P-OP2	-6.75	99.62	105.70
1	A	1069	C	O5'-P-OP2	-6.75	99.62	105.70
1	A	252	U	C4-C5-C6	6.75	123.75	119.70
1	A	61	G	C4-C5-N7	6.75	113.50	110.80
1	A	181	G	N1-C6-O6	6.75	123.95	119.90
1	A	889	A	C8-N9-C4	-6.75	103.10	105.80
1	A	953	G	N1-C6-O6	-6.75	115.85	119.90
1	A	1186	G	N3-C4-N9	-6.75	121.95	126.00
1	A	888	G	N3-C4-N9	6.75	130.05	126.00
1	A	40	C	OP2-P-O3'	6.75	120.05	105.20
1	A	1216	G	OP2-P-O3'	6.75	120.05	105.20
1	A	617	G	N1-C2-N3	6.75	127.95	123.90
1	A	1099	G	N7-C8-N9	6.75	116.47	113.10
1	A	1471	G	N3-C2-N2	-6.74	115.18	119.90
1	A	288	A	C2-N3-C4	-6.74	107.23	110.60
1	A	293	G	N3-C2-N2	-6.74	115.18	119.90
1	A	867	G	C6-C5-N7	-6.74	126.36	130.40
1	A	1304	G	C4-C5-N7	-6.74	108.10	110.80
1	A	1068	G	C5-N7-C8	-6.74	100.93	104.30
17	Q	99	SER	N-CA-C	6.74	129.20	111.00
1	A	141	A	C4-C5-N7	6.74	114.07	110.70
1	A	588	G	C5-C6-N1	-6.74	108.13	111.50
1	A	1487	G	N1-C6-O6	-6.74	115.86	119.90
1	A	145	G	N1-C6-O6	6.73	123.94	119.90
1	A	573	A	C8-N9-C4	-6.73	103.11	105.80
1	A	27	G	N1-C6-O6	6.73	123.94	119.90
1	A	108	G	C8-N9-C1'	-6.73	118.25	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	819	A	C5-N7-C8	-6.73	100.53	103.90
1	A	949	A	C8-N9-C4	6.73	108.49	105.80
1	A	1047	G	N3-C2-N2	-6.73	115.19	119.90
1	A	238	G	C6-C5-N7	-6.73	126.36	130.40
1	A	1386	G	N3-C2-N2	-6.73	115.19	119.90
1	A	1302	U	C2-N1-C1'	6.73	125.78	117.70
4	D	76	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	A	157	G	OP2-P-O3'	6.73	120.00	105.20
1	A	276	G	C5-C6-N1	-6.73	108.14	111.50
1	A	797	C	N3-C4-C5	-6.73	119.21	121.90
1	A	1203	C	C2-N3-C4	-6.73	116.54	119.90
1	A	1542	U	N1-C2-N3	-6.73	110.86	114.90
1	A	1055	A	N3-C4-N9	6.73	132.78	127.40
1	A	811	C	OP1-P-OP2	6.72	129.69	119.60
1	A	1094	G	C4-N9-C1'	6.72	135.24	126.50
1	A	1379	G	C6-C5-N7	-6.72	126.36	130.40
1	A	869	G	N9-C4-C5	-6.72	102.71	105.40
1	A	22	G	OP2-P-O3'	6.72	119.98	105.20
1	A	264	U	C2-N3-C4	-6.72	122.97	127.00
1	A	1395	C	N3-C2-O2	6.72	126.60	121.90
1	A	1441	G	C4-C5-N7	-6.72	108.11	110.80
1	A	38	G	C4-N9-C1'	-6.72	117.77	126.50
1	A	1411	C	N3-C4-C5	-6.72	119.21	121.90
1	A	220	G	C2-N3-C4	-6.72	108.54	111.90
1	A	834	C	O5'-P-OP2	-6.71	99.66	105.70
1	A	1192	C	N3-C4-C5	6.71	124.59	121.90
1	A	1205	U	C5-C6-N1	-6.71	119.34	122.70
1	A	863	U	N1-C2-N3	6.71	118.93	114.90
1	A	1250	A	N7-C8-N9	6.71	117.16	113.80
1	A	123	C	N3-C4-C5	-6.71	119.22	121.90
1	A	1066	C	C5-C4-N4	-6.71	115.50	120.20
1	A	1076	C	N3-C4-N4	6.71	122.70	118.00
1	A	1078	U	N1-C2-O2	6.71	127.50	122.80
1	A	1214	C	N3-C4-N4	-6.71	113.30	118.00
1	A	1023	G	C4-N9-C1'	6.71	135.22	126.50
1	A	1502	A	C4-C5-C6	6.71	120.36	117.00
1	A	251	G	OP1-P-O3'	6.71	119.96	105.20
1	A	389	A	P-O3'-C3'	6.71	127.75	119.70
1	A	714	G	C4-C5-N7	-6.71	108.12	110.80
1	A	1203	C	O5'-P-OP1	-6.71	99.66	105.70
1	A	1356	G	O5'-P-OP1	6.71	118.75	110.70
1	A	751	U	O5'-P-OP1	-6.71	99.66	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1464	G	C5-C6-N1	-6.71	108.15	111.50
1	A	1392	G	C5-C6-O6	6.71	132.62	128.60
1	A	333	G	N1-C2-N2	6.70	122.23	116.20
1	A	546	G	C4-C5-N7	-6.70	108.12	110.80
1	A	1131	G	C8-N9-C4	-6.70	103.72	106.40
1	A	368	U	C4-C5-C6	6.70	123.72	119.70
1	A	446	G	OP2-P-O3'	6.70	119.94	105.20
1	A	655	A	C5-C6-N1	6.70	121.05	117.70
1	A	509	A	C6-C5-N7	-6.70	127.61	132.30
1	A	572	A	C5-N7-C8	6.70	107.25	103.90
1	A	953	G	C5-N7-C8	6.70	107.65	104.30
1	A	1080	A	C5-C6-N1	6.70	121.05	117.70
1	A	239	U	C5-C6-N1	6.70	126.05	122.70
1	A	289	G	C4-N9-C1'	6.70	135.20	126.50
1	A	407	G	O5'-P-OP1	-6.70	99.67	105.70
1	A	1109	C	N1-C2-N3	6.70	123.89	119.20
1	A	230	G	C4-C5-N7	-6.69	108.12	110.80
1	A	762	C	O5'-P-OP2	6.69	118.73	110.70
1	A	484	G	O4'-C1'-N9	-6.69	102.85	108.20
1	A	621	A	C4-C5-N7	6.69	114.05	110.70
1	A	1396	A	OP2-P-O3'	-6.69	90.48	105.20
1	A	230	G	C8-N9-C1'	-6.69	118.30	127.00
1	A	306	G	N1-C2-N2	6.69	122.22	116.20
1	A	381	C	C5-C6-N1	6.69	124.34	121.00
1	A	930	C	N3-C4-C5	6.69	124.58	121.90
1	A	1125	U	C4'-C3'-O3'	6.69	126.38	113.00
1	A	1524	C	OP2-P-O3'	6.69	119.92	105.20
12	L	115	LYS	C-N-CA	-6.69	104.98	121.70
1	A	297	G	C5-C6-N1	-6.69	108.16	111.50
1	A	1360	A	O5'-P-OP2	-6.69	99.68	105.70
1	A	786	G	C4-C5-N7	6.68	113.47	110.80
1	A	485	G	N1-C2-N2	-6.68	110.19	116.20
1	A	814	A	N3-C4-N9	-6.68	122.05	127.40
5	E	139	LEU	CB-CG-CD2	-6.68	99.64	111.00
1	A	774	G	OP1-P-OP2	6.68	129.62	119.60
1	A	521	G	C6-C5-N7	6.68	134.41	130.40
1	A	933	G	C6-C5-N7	-6.68	126.39	130.40
1	A	1307	U	C5-C4-O4	6.68	129.91	125.90
1	A	1516	G	C5-C6-O6	-6.68	124.59	128.60
1	A	1090	U	N1-C2-N3	6.68	118.91	114.90
1	A	483	C	C5-C4-N4	6.67	124.87	120.20
1	A	99	C	C6-N1-C2	-6.67	117.63	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	339	C	N3-C2-O2	6.67	126.57	121.90
1	A	506	G	C6-C5-N7	-6.67	126.40	130.40
1	A	510	A	N1-C6-N6	-6.67	114.60	118.60
1	A	601	C	N3-C4-C5	-6.67	119.23	121.90
1	A	606	G	N3-C4-C5	-6.67	125.26	128.60
1	A	676	A	C6-N1-C2	-6.67	114.60	118.60
1	A	992	U	C5-C4-O4	6.67	129.90	125.90
1	A	1218	C	C6-N1-C2	-6.67	117.63	120.30
1	A	1478	C	N3-C4-C5	-6.67	119.23	121.90
2	B	53	ARG	NE-CZ-NH1	-6.67	116.97	120.30
1	A	288	A	O5'-P-OP1	-6.67	99.70	105.70
10	J	66	ARG	NE-CZ-NH1	6.67	123.63	120.30
1	A	111	G	OP2-P-O3'	6.67	119.87	105.20
1	A	198	G	N1-C2-N2	-6.67	110.20	116.20
1	A	309	G	C6-C5-N7	-6.67	126.40	130.40
1	A	1384	C	C2-N1-C1'	-6.67	111.47	118.80
1	A	521	G	C6-N1-C2	-6.67	121.10	125.10
1	A	684	A	C2-N3-C4	-6.67	107.27	110.60
1	A	703	G	N3-C4-N9	6.67	130.00	126.00
1	A	1074	G	N3-C2-N2	6.67	124.56	119.90
1	A	699	C	C5-C6-N1	-6.66	117.67	121.00
1	A	758	G	OP2-P-O3'	6.66	119.86	105.20
1	A	722	A	C5-C6-N1	-6.66	114.37	117.70
1	A	506	G	C5-N7-C8	-6.66	100.97	104.30
1	A	769	G	C4-C5-C6	6.66	122.80	118.80
1	A	1311	G	C5-C6-N1	-6.66	108.17	111.50
1	A	296	U	N1-C2-N3	6.66	118.89	114.90
1	A	307	C	C6-N1-C1'	-6.66	112.81	120.80
1	A	523	A	C2-N3-C4	-6.66	107.27	110.60
1	A	880	C	N3-C4-N4	-6.66	113.34	118.00
1	A	1478	C	N3-C4-N4	6.66	122.66	118.00
1	A	1502	A	O4'-C1'-N9	6.66	113.53	108.20
1	A	380	G	O5'-P-OP1	6.66	118.69	110.70
1	A	669	U	C6-N1-C2	6.66	124.99	121.00
1	A	878	G	C8-N9-C4	6.66	109.06	106.40
1	A	296	U	C4-C5-C6	6.66	123.69	119.70
1	A	315	A	C6-N1-C2	-6.66	114.61	118.60
1	A	684	A	C6-C5-N7	-6.66	127.64	132.30
1	A	231	G	N3-C2-N2	-6.65	115.24	119.90
1	A	1065	U	C6-N1-C2	6.65	124.99	121.00
1	A	232	G	C5-N7-C8	-6.65	100.97	104.30
1	A	271	C	N3-C2-O2	6.65	126.56	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	497	A	N1-C2-N3	6.65	132.63	129.30
1	A	658	G	C4-C5-C6	6.65	122.79	118.80
1	A	1175	G	N7-C8-N9	6.65	116.42	113.10
1	A	1475	G	N1-C6-O6	6.65	123.89	119.90
1	A	809	G	C5-C6-N1	6.65	114.82	111.50
1	A	43	C	O5'-P-OP1	-6.65	99.72	105.70
1	A	170	U	N1-C2-O2	-6.65	118.15	122.80
1	A	900	A	C2-N3-C4	-6.65	107.28	110.60
12	L	41	ARG	NE-CZ-NH2	-6.65	116.98	120.30
1	A	776	G	N3-C4-N9	-6.65	122.01	126.00
1	A	1409	C	N1-C2-N3	-6.65	114.55	119.20
1	A	136	C	N3-C4-N4	6.64	122.65	118.00
1	A	105	G	OP2-P-O3'	6.64	119.81	105.20
1	A	586	C	C2-N1-C1'	-6.64	111.49	118.80
1	A	674	G	C4-N9-C1'	6.64	135.14	126.50
1	A	854	G	C4-C5-N7	6.64	113.46	110.80
1	A	1233	G	C4-C5-N7	6.64	113.46	110.80
1	A	1184	G	C5-C6-N1	-6.64	108.18	111.50
1	A	1391	U	C5-C6-N1	-6.64	119.38	122.70
1	A	70	G	C4-N9-C1'	-6.64	117.87	126.50
1	A	110	C	C6-N1-C2	-6.64	117.64	120.30
1	A	439	A	OP1-P-OP2	-6.64	109.64	119.60
1	A	605	U	OP2-P-O3'	6.64	119.80	105.20
1	A	618	C	C6-N1-C2	6.63	122.95	120.30
1	A	786	G	C6-C5-N7	-6.63	126.42	130.40
1	A	795	C	OP2-P-O3'	6.63	119.80	105.20
1	A	1136	U	C2-N1-C1'	6.63	125.66	117.70
1	A	318	G	N1-C2-N2	6.63	122.17	116.20
1	A	1485	U	C2-N1-C1'	6.63	125.66	117.70
1	A	97	G	C2-N3-C4	-6.63	108.58	111.90
1	A	376	G	N1-C6-O6	-6.63	115.92	119.90
1	A	770	C	C4-C5-C6	-6.63	114.08	117.40
1	A	887	G	N9-C4-C5	6.63	108.05	105.40
1	A	960	U	N3-C4-C5	-6.63	110.62	114.60
1	A	1178	G	N3-C4-C5	-6.63	125.28	128.60
1	A	148	G	C4-C5-C6	6.63	122.78	118.80
1	A	413	G	N3-C2-N2	-6.63	115.26	119.90
1	A	34	C	N3-C4-N4	6.63	122.64	118.00
1	A	1365	G	C5-C6-N1	6.63	114.81	111.50
1	A	63	C	C6-N1-C2	6.63	122.95	120.30
1	A	1329	A	OP1-P-O3'	6.63	119.78	105.20
1	A	1501	C	C2-N3-C4	-6.63	116.59	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	123	LEU	CB-CG-CD2	-6.63	99.73	111.00
1	A	284	G	N1-C2-N3	6.62	127.87	123.90
1	A	651	C	N1-C2-N3	-6.62	114.56	119.20
1	A	1395	C	OP2-P-O3'	6.62	119.77	105.20
1	A	1082	G	N3-C4-C5	6.62	131.91	128.60
1	A	805	C	C4-C5-C6	-6.62	114.09	117.40
1	A	1158	C	C6-N1-C1'	-6.62	112.86	120.80
1	A	276	G	N3-C4-N9	6.62	129.97	126.00
1	A	1068	G	O5'-P-OP2	-6.62	99.74	105.70
1	A	1057	G	C8-N9-C4	-6.62	103.75	106.40
1	A	497	A	O5'-P-OP1	-6.62	99.75	105.70
1	A	323	U	C6-N1-C2	-6.61	117.03	121.00
1	A	507	C	C5-C6-N1	-6.61	117.69	121.00
1	A	973	G	N3-C4-N9	-6.61	122.03	126.00
1	A	187	C	N3-C4-N4	6.61	122.63	118.00
1	A	792	A	C2-N3-C4	-6.61	107.30	110.60
1	A	654	G	N3-C2-N2	-6.61	115.28	119.90
1	A	703	G	C5-C6-O6	6.61	132.56	128.60
1	A	224	C	N3-C2-O2	-6.61	117.28	121.90
1	A	968	A	C6-N1-C2	6.61	122.56	118.60
1	A	1316	G	C4-N9-C1'	-6.61	117.91	126.50
1	A	1517	G	O5'-P-OP2	-6.61	99.75	105.70
1	A	190(I)	G	C8-N9-C4	-6.60	103.76	106.40
1	A	244	U	N3-C4-O4	6.60	124.02	119.40
1	A	1343	G	N3-C2-N2	-6.60	115.28	119.90
1	A	649	G	N7-C8-N9	-6.60	109.80	113.10
1	A	935	A	C8-N9-C1'	-6.60	115.81	127.70
1	A	1050	G	C8-N9-C1'	-6.60	118.42	127.00
4	D	202	LEU	CB-CG-CD2	-6.60	99.78	111.00
1	A	70	G	C8-N9-C1'	6.60	135.58	127.00
1	A	284	G	C4-C5-N7	6.60	113.44	110.80
1	A	319	G	C5-N7-C8	-6.60	101.00	104.30
1	A	902	G	O5'-P-OP1	6.60	118.62	110.70
1	A	586	C	O5'-P-OP1	6.60	118.62	110.70
1	A	780	A	OP1-P-OP2	-6.60	109.70	119.60
1	A	1152	A	C5-C6-N1	6.60	121.00	117.70
1	A	1233	G	C5-C6-O6	-6.60	124.64	128.60
1	A	1416	G	C5-C6-N1	6.60	114.80	111.50
1	A	1054	C	C2-N3-C4	6.60	123.20	119.90
1	A	494	G	OP1-P-O3'	6.59	119.71	105.20
1	A	1235	U	N3-C2-O2	-6.59	117.58	122.20
1	A	1485	U	O4'-C1'-N1	6.59	113.48	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	719	C	N3-C4-C5	6.59	124.54	121.90
1	A	576	G	C4-N9-C1'	6.59	135.07	126.50
1	A	755	G	N9-C4-C5	-6.59	102.76	105.40
1	A	837	G	C5-C6-O6	-6.59	124.65	128.60
1	A	483	C	C6-N1-C2	6.59	122.94	120.30
1	A	9	G	N1-C6-O6	6.59	123.85	119.90
1	A	258	G	N7-C8-N9	6.58	116.39	113.10
1	A	312	C	N1-C2-O2	6.58	122.85	118.90
1	A	801	U	C6-N1-C2	6.58	124.95	121.00
1	A	984	C	N1-C2-O2	6.58	122.85	118.90
1	A	135	C	C6-N1-C2	-6.58	117.67	120.30
1	A	488	C	N3-C4-C5	-6.58	119.27	121.90
1	A	856	C	N3-C4-N4	6.58	122.61	118.00
1	A	874	G	C4-C5-N7	-6.58	108.17	110.80
1	A	1435	G	C2-N3-C4	-6.58	108.61	111.90
1	A	1452	C	N1-C2-O2	6.58	122.85	118.90
1	A	1368	G	N3-C4-C5	-6.58	125.31	128.60
1	A	1375	A	N1-C6-N6	6.58	122.55	118.60
1	A	1388	C	N1-C2-N3	6.58	123.80	119.20
1	A	913	A	C8-N9-C4	-6.58	103.17	105.80
1	A	24	U	N3-C2-O2	6.57	126.80	122.20
1	A	81	U	N3-C4-O4	6.57	124.00	119.40
1	A	365	U	C5-C4-O4	-6.57	121.96	125.90
1	A	15	G	OP1-P-OP2	6.57	129.46	119.60
1	A	1064	G	N1-C2-N2	6.57	122.11	116.20
1	A	1186	G	C2-N3-C4	-6.57	108.61	111.90
1	A	512	U	OP2-P-O3'	6.57	119.65	105.20
1	A	1403	C	O5'-P-OP2	6.57	118.58	110.70
19	S	31	ILE	N-CA-C	-6.57	93.26	111.00
1	A	91	C	N3-C4-C5	-6.57	119.27	121.90
1	A	1378	C	C2-N1-C1'	6.57	126.02	118.80
1	A	39	G	C4-C5-C6	-6.56	114.86	118.80
1	A	782	A	C8-N9-C4	-6.56	103.17	105.80
1	A	886	G	C5-C6-N1	-6.56	108.22	111.50
1	A	791	G	C4-N9-C1'	6.56	135.03	126.50
1	A	800	G	OP2-P-O3'	6.56	119.64	105.20
1	A	1091	U	C5-C4-O4	6.56	129.84	125.90
1	A	900	A	OP1-P-OP2	-6.56	109.76	119.60
2	B	16	HIS	N-CA-C	6.56	128.72	111.00
1	A	400	C	C6-N1-C2	6.56	122.92	120.30
1	A	641	U	C2-N1-C1'	6.56	125.57	117.70
1	A	448	A	C5-N7-C8	-6.56	100.62	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1393	U	O5'-P-OP2	-6.56	99.80	105.70
1	A	499	A	N3-C4-C5	-6.56	122.21	126.80
1	A	706	A	O5'-P-OP1	6.56	118.57	110.70
1	A	646	U	C2-N1-C1'	-6.55	109.83	117.70
1	A	569	C	N3-C2-O2	-6.55	117.31	121.90
1	A	699	C	OP1-P-OP2	6.55	129.43	119.60
1	A	292	G	C4-C5-C6	6.55	122.73	118.80
1	A	801	U	C2-N3-C4	-6.55	123.07	127.00
1	A	827	U	C4-C5-C6	6.55	123.63	119.70
1	A	291	C	C2-N1-C1'	6.55	126.00	118.80
1	A	676	A	N1-C2-N3	6.55	132.57	129.30
1	A	11	G	P-O3'-C3'	-6.55	111.84	119.70
1	A	250	A	C8-N9-C4	6.55	108.42	105.80
1	A	251	G	N1-C6-O6	6.55	123.83	119.90
1	A	819	A	C2-N3-C4	-6.55	107.33	110.60
1	A	1016	A	C5-C6-N1	6.55	120.97	117.70
1	A	14	U	C6-N1-C1'	6.54	130.36	121.20
1	A	47	C	C6-N1-C1'	-6.54	112.95	120.80
1	A	277	C	C5-C6-N1	-6.54	117.73	121.00
1	A	1539	C	N3-C4-C5	-6.54	119.28	121.90
1	A	112	G	C5-C6-O6	-6.54	124.67	128.60
17	Q	92	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	A	267	C	OP1-P-OP2	-6.54	109.79	119.60
1	A	271	C	C6-N1-C2	6.54	122.92	120.30
1	A	316	G	C2-N3-C4	-6.54	108.63	111.90
1	A	1158	C	N3-C2-O2	-6.54	117.32	121.90
1	A	1172	C	N3-C4-C5	-6.54	119.28	121.90
1	A	17	U	C4-C5-C6	6.54	123.62	119.70
1	A	139	G	N1-C2-N3	6.54	127.82	123.90
1	A	182	U	C6-N1-C2	-6.54	117.08	121.00
1	A	624	C	C5-C4-N4	-6.54	115.62	120.20
1	A	654	G	C5-N7-C8	-6.54	101.03	104.30
1	A	742	G	C8-N9-C1'	-6.54	118.50	127.00
1	A	791	G	C6-C5-N7	-6.54	126.48	130.40
1	A	1526	G	C2-N3-C4	-6.54	108.63	111.90
1	A	147	G	C4-C5-N7	-6.54	108.19	110.80
1	A	227	G	C2-N3-C4	-6.54	108.63	111.90
1	A	229	U	N1-C2-N3	6.54	118.82	114.90
1	A	576	G	C8-N9-C4	-6.54	103.78	106.40
1	A	190(F)	G	N9-C4-C5	6.53	108.01	105.40
1	A	410	G	C5-C6-O6	6.53	132.52	128.60
1	A	895	G	C4-C5-N7	6.53	113.41	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	569	C	N1-C2-N3	6.53	123.77	119.20
1	A	1078	U	C5-C4-O4	-6.53	121.98	125.90
1	A	73	C	N3-C2-O2	6.53	126.47	121.90
1	A	309	G	C5-C6-O6	-6.53	124.68	128.60
1	A	804	U	OP2-P-O3'	6.53	119.57	105.20
1	A	109	A	O5'-P-OP1	-6.53	99.83	105.70
1	A	260	G	C2-N3-C4	-6.53	108.64	111.90
1	A	485	G	N3-C4-N9	6.53	129.92	126.00
1	A	837	G	N9-C4-C5	-6.53	102.79	105.40
1	A	9	G	C5-C6-O6	-6.53	124.69	128.60
1	A	103	C	N1-C2-O2	6.53	122.81	118.90
1	A	133	U	C2-N3-C4	6.53	130.92	127.00
1	A	950	U	C5-C4-O4	6.53	129.81	125.90
1	A	1211	U	N3-C4-O4	6.53	123.97	119.40
1	A	144	G	N1-C2-N3	6.52	127.81	123.90
1	A	1252	A	C5-C6-N6	6.52	128.92	123.70
1	A	1345	U	O5'-P-OP1	-6.52	99.83	105.70
1	A	22	G	N3-C4-N9	6.52	129.91	126.00
1	A	115	G	N7-C8-N9	-6.52	109.84	113.10
1	A	1441	G	C5-C6-O6	6.52	132.51	128.60
1	A	337	C	C2-N3-C4	-6.52	116.64	119.90
1	A	1477	C	C2-N3-C4	6.52	123.16	119.90
1	A	1463	C	C5-C6-N1	-6.52	117.74	121.00
1	A	105	G	C4-C5-N7	6.51	113.41	110.80
1	A	122	G	N7-C8-N9	-6.51	109.84	113.10
1	A	370	C	N1-C2-N3	-6.51	114.64	119.20
1	A	557	G	C5-C6-N1	6.51	114.76	111.50
1	A	664	G	N1-C2-N2	-6.51	110.34	116.20
1	A	839	U	C4-C5-C6	6.51	123.61	119.70
1	A	219	C	OP1-P-OP2	6.51	129.37	119.60
1	A	1506	U	C6-N1-C2	6.51	124.91	121.00
1	A	431	A	OP2-P-O3'	6.51	119.52	105.20
1	A	735	C	N3-C4-C5	6.51	124.50	121.90
1	A	791	G	OP2-P-O3'	6.51	119.52	105.20
1	A	1279	A	OP1-P-O3'	6.51	119.52	105.20
1	A	230	G	C2-N3-C4	-6.51	108.65	111.90
1	A	670	G	C5-C6-O6	-6.51	124.70	128.60
1	A	1248	A	C5-C6-N6	-6.51	118.50	123.70
1	A	650	G	C5-N7-C8	6.50	107.55	104.30
1	A	805	C	N3-C4-N4	6.50	122.55	118.00
1	A	915	A	N1-C6-N6	-6.50	114.70	118.60
1	A	177	C	C4-C5-C6	6.50	120.65	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	248	C	N3-C4-C5	6.50	124.50	121.90
1	A	1409	C	C6-N1-C2	6.50	122.90	120.30
1	A	1436	U	OP2-P-O3'	6.50	119.51	105.20
1	A	332	G	N1-C2-N2	6.50	122.05	116.20
1	A	351	G	O5'-P-OP2	-6.50	99.85	105.70
1	A	597	G	N9-C4-C5	-6.50	102.80	105.40
1	A	821	G	C5-C6-N1	-6.50	108.25	111.50
1	A	841	U	C2-N1-C1'	6.50	125.50	117.70
1	A	1190	G	N9-C4-C5	6.50	108.00	105.40
1	A	47	C	C2-N3-C4	-6.50	116.65	119.90
1	A	317	G	C5-C6-O6	-6.50	124.70	128.60
1	A	1237	C	N3-C2-O2	-6.50	117.35	121.90
1	A	1311	G	N3-C2-N2	-6.50	115.35	119.90
1	A	1435	G	OP2-P-O3'	6.50	119.50	105.20
1	A	274	A	OP1-P-OP2	6.50	129.35	119.60
1	A	635	G	C8-N9-C1'	-6.50	118.56	127.00
1	A	703	G	C4-N9-C1'	6.50	134.94	126.50
1	A	1397	C	C5-C4-N4	-6.50	115.65	120.20
1	A	450	G	C5-C6-O6	-6.50	124.70	128.60
1	A	46	G	C2-N3-C4	6.49	115.15	111.90
1	A	1212	U	N1-C2-O2	6.49	127.34	122.80
1	A	1215	G	C6-C5-N7	-6.49	126.50	130.40
1	A	853	G	N3-C4-C5	-6.49	125.35	128.60
1	A	947	G	N1-C2-N2	-6.49	110.36	116.20
1	A	1269	A	C4-C5-N7	-6.49	107.45	110.70
1	A	1515	C	N1-C2-O2	-6.49	115.01	118.90
1	A	332	G	C5-N7-C8	-6.49	101.06	104.30
1	A	692	U	C6-N1-C2	6.49	124.89	121.00
1	A	743	U	C5-C6-N1	-6.49	119.46	122.70
1	A	1269	A	N7-C8-N9	-6.48	110.56	113.80
1	A	247	G	O5'-P-OP1	6.48	118.48	110.70
1	A	272	C	N3-C4-N4	6.48	122.54	118.00
1	A	450	G	N1-C2-N2	6.48	122.03	116.20
1	A	982	U	N3-C2-O2	-6.48	117.66	122.20
1	A	1203	C	C2-N1-C1'	-6.48	111.67	118.80
1	A	367	U	OP2-P-O3'	6.48	119.45	105.20
1	A	933	G	N1-C6-O6	6.48	123.79	119.90
1	A	994	A	C5-N7-C8	-6.48	100.66	103.90
1	A	1366	C	N1-C2-N3	6.48	123.74	119.20
1	A	653	A	N3-C4-C5	-6.48	122.27	126.80
1	A	35	G	N3-C2-N2	-6.48	115.37	119.90
1	A	350	G	C8-N9-C4	-6.48	103.81	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	368	U	C2-N3-C4	-6.48	123.11	127.00
1	A	115	G	C5-C6-O6	-6.48	124.71	128.60
1	A	662	G	C4-N9-C1'	6.48	134.92	126.50
1	A	1460	A	C5-C6-N6	-6.48	118.52	123.70
1	A	68	G	C5-C6-N1	-6.47	108.26	111.50
1	A	1429	C	N1-C2-O2	-6.47	115.02	118.90
1	A	125	U	C6-N1-C2	-6.47	117.12	121.00
1	A	190(A)	C	O5'-P-OP2	6.47	118.47	110.70
1	A	494	G	C4-N9-C1'	6.47	134.91	126.50
1	A	576	G	C6-N1-C2	-6.47	121.22	125.10
1	A	251	G	N1-C2-N3	6.47	127.78	123.90
1	A	871	U	O5'-P-OP1	-6.47	99.88	105.70
1	A	836	G	C5-C6-N1	-6.47	108.27	111.50
1	A	885	G	C4-C5-C6	6.47	122.68	118.80
1	A	564	C	C6-N1-C2	-6.47	117.71	120.30
1	A	878	G	C2-N3-C4	-6.46	108.67	111.90
1	A	1515	C	O5'-P-OP2	-6.46	99.88	105.70
1	A	1529	G	C8-N9-C4	-6.46	103.81	106.40
1	A	494	G	N3-C4-C5	-6.46	125.37	128.60
1	A	300	A	C4-C5-N7	-6.46	107.47	110.70
1	A	307	C	N3-C4-N4	6.46	122.52	118.00
1	A	1045	C	C6-N1-C2	6.46	122.89	120.30
1	A	1083	U	N3-C4-O4	-6.46	114.88	119.40
1	A	1505	G	P-O3'-C3'	6.46	127.45	119.70
1	A	679	C	OP2-P-O3'	6.46	119.41	105.20
1	A	879	C	O5'-P-OP1	6.46	118.45	110.70
1	A	647	C	C6-N1-C2	-6.46	117.72	120.30
1	A	763	G	N9-C4-C5	-6.46	102.82	105.40
1	A	1093	A	C4-C5-C6	-6.46	113.77	117.00
1	A	1103	C	C2-N3-C4	-6.46	116.67	119.90
1	A	515	G	C4-C5-C6	6.46	122.67	118.80
1	A	902	G	C5-C6-O6	-6.46	124.73	128.60
1	A	1502	A	N9-C1'-C2'	6.46	122.39	114.00
1	A	93	G	C5-C6-O6	-6.46	124.73	128.60
1	A	404	U	OP1-P-OP2	-6.46	109.92	119.60
1	A	1455	G	C6-C5-N7	-6.46	126.53	130.40
1	A	248	C	N1-C2-O2	-6.45	115.03	118.90
1	A	541	G	C5-C6-N1	-6.45	108.27	111.50
1	A	771	G	N3-C4-C5	6.45	131.83	128.60
1	A	190(E)	U	N3-C4-O4	6.45	123.92	119.40
1	A	604	G	N3-C4-N9	-6.45	122.13	126.00
1	A	988	G	C8-N9-C4	-6.45	103.82	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1067	A	C4-C5-C6	6.45	120.23	117.00
1	A	528	C	OP1-P-OP2	6.45	129.28	119.60
1	A	108	G	O4'-C1'-N9	6.45	113.36	108.20
1	A	181	G	N3-C4-C5	-6.45	125.38	128.60
1	A	1508	G	OP2-P-O3'	6.45	119.39	105.20
1	A	804	U	N1-C2-N3	6.45	118.77	114.90
1	A	1373	G	C8-N9-C1'	-6.45	118.62	127.00
1	A	782	A	N1-C2-N3	6.44	132.52	129.30
1	A	406	G	C5-C6-O6	-6.44	124.73	128.60
1	A	414	A	C4-C5-C6	6.44	120.22	117.00
1	A	1124	G	N3-C4-N9	6.44	129.87	126.00
1	A	1244	C	C6-N1-C2	6.44	122.88	120.30
1	A	149	A	N1-C6-N6	-6.44	114.74	118.60
1	A	904	C	C6-N1-C2	6.44	122.88	120.30
1	A	54	C	N1-C2-N3	-6.44	114.69	119.20
1	A	507	C	C4-C5-C6	6.44	120.62	117.40
1	A	275	G	C6-N1-C2	6.44	128.96	125.10
1	A	1222	G	C4-C5-C6	6.44	122.66	118.80
1	A	462	G	O5'-P-OP1	6.43	118.42	110.70
1	A	1285	A	O4'-C1'-N9	-6.43	103.05	108.20
1	A	129	U	C2-N1-C1'	-6.43	109.98	117.70
1	A	499	A	P-O3'-C3'	6.43	127.42	119.70
1	A	1050	G	C4-N9-C1'	6.43	134.86	126.50
1	A	1494	G	C4-C5-N7	-6.43	108.23	110.80
1	A	907	A	C4-C5-N7	-6.43	107.48	110.70
1	A	944	G	C8-N9-C1'	-6.43	118.64	127.00
1	A	1024	G	C5-C6-N1	6.43	114.72	111.50
1	A	1139	G	C4-C5-C6	6.43	122.66	118.80
1	A	1233	G	N1-C6-O6	6.43	123.76	119.90
1	A	1511	G	N1-C2-N3	6.43	127.76	123.90
1	A	1182	G	N3-C4-N9	6.43	129.86	126.00
1	A	1366	C	C6-N1-C2	-6.43	117.73	120.30
1	A	108	G	OP1-P-O3'	6.42	119.33	105.20
1	A	573	A	OP1-P-O3'	6.42	119.33	105.20
1	A	1438	G	C8-N9-C4	6.42	108.97	106.40
1	A	1235	U	C6-N1-C2	-6.42	117.15	121.00
1	A	755	G	C8-N9-C1'	-6.42	118.65	127.00
1	A	1080	A	N7-C8-N9	-6.42	110.59	113.80
1	A	1485	U	OP2-P-O3'	6.42	119.33	105.20
1	A	147	G	C8-N9-C4	-6.42	103.83	106.40
1	A	150	C	O4'-C1'-N1	-6.42	103.07	108.20
1	A	297	G	N1-C2-N3	6.42	127.75	123.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	305	G	C5-C6-N1	-6.42	108.29	111.50
1	A	961	U	N3-C4-O4	6.42	123.89	119.40
1	A	965	A	C4-N9-C1'	-6.42	114.75	126.30
1	A	193	C	C5-C4-N4	6.41	124.69	120.20
1	A	742	G	C5-C6-O6	6.41	132.45	128.60
1	A	1497	G	N7-C8-N9	6.41	116.31	113.10
1	A	849	C	C5-C6-N1	6.41	124.21	121.00
1	A	721	G	C5-C6-N1	-6.41	108.29	111.50
1	A	840	C	C4-C5-C6	-6.41	114.19	117.40
1	A	1251	A	OP2-P-O3'	6.41	119.30	105.20
1	A	255	G	N7-C8-N9	-6.41	109.90	113.10
1	A	625	G	C5-C6-O6	-6.41	124.76	128.60
15	O	57	LEU	CB-CG-CD2	-6.41	100.11	111.00
1	A	190(I)	G	N7-C8-N9	6.40	116.30	113.10
1	A	436	C	C6-N1-C2	6.40	122.86	120.30
1	A	190(H)	G	C5-C6-N1	-6.40	108.30	111.50
1	A	364	A	O5'-P-OP2	6.40	118.38	110.70
1	A	504	C	C5-C6-N1	6.40	124.20	121.00
1	A	657	G	C5-C6-N1	-6.40	108.30	111.50
1	A	1108	G	N3-C4-N9	6.40	129.84	126.00
1	A	1110	A	OP1-P-OP2	-6.40	110.00	119.60
1	A	23	C	N3-C4-C5	6.40	124.46	121.90
1	A	27	G	N9-C4-C5	-6.40	102.84	105.40
1	A	413	G	O4'-C1'-N9	6.40	113.32	108.20
1	A	1384	C	N3-C4-N4	-6.40	113.52	118.00
12	L	101	VAL	CB-CA-C	-6.40	99.24	111.40
1	A	69	G	N3-C2-N2	-6.40	115.42	119.90
1	A	483	C	C2-N1-C1'	-6.40	111.76	118.80
1	A	14	U	N3-C4-O4	-6.40	114.92	119.40
1	A	265	G	C6-C5-N7	-6.40	126.56	130.40
1	A	458	C	C5-C4-N4	-6.40	115.72	120.20
1	A	1124	G	C8-N9-C4	-6.40	103.84	106.40
1	A	654	G	N7-C8-N9	6.39	116.30	113.10
1	A	1102	A	C8-N9-C4	-6.39	103.24	105.80
1	A	1511	G	C8-N9-C1'	-6.39	118.69	127.00
1	A	193	C	C5-C6-N1	-6.39	117.81	121.00
1	A	326	G	C6-N1-C2	6.39	128.93	125.10
1	A	946	A	C8-N9-C4	6.39	108.36	105.80
1	A	1028	C	C2-N3-C4	6.39	123.09	119.90
1	A	1033	G	C8-N9-C4	-6.39	103.84	106.40
12	L	24	VAL	N-CA-CB	-6.39	97.44	111.50
1	A	425	G	C2-N3-C4	-6.39	108.71	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	686	U	N1-C2-N3	6.39	118.73	114.90
1	A	562	C	C6-N1-C1'	-6.39	113.14	120.80
1	A	1071	C	N3-C4-C5	6.39	124.45	121.90
1	A	1258	G	N3-C4-C5	-6.39	125.41	128.60
1	A	323	U	N3-C4-C5	-6.38	110.77	114.60
1	A	325	A	C2-N3-C4	-6.38	107.41	110.60
1	A	759	A	N1-C6-N6	-6.38	114.77	118.60
1	A	893	C	C5-C6-N1	6.38	124.19	121.00
1	A	391	G	N7-C8-N9	-6.38	109.91	113.10
1	A	484	G	C6-C5-N7	-6.38	126.57	130.40
1	A	109	A	N7-C8-N9	6.38	116.99	113.80
1	A	113	G	C4-C5-N7	6.38	113.35	110.80
1	A	635	G	N1-C2-N3	6.38	127.73	123.90
1	A	524	G	N3-C4-C5	-6.38	125.41	128.60
1	A	780	A	C8-N9-C4	-6.38	103.25	105.80
1	A	1329	A	C4-C5-C6	6.38	120.19	117.00
1	A	307	C	OP2-P-O3'	6.38	119.23	105.20
1	A	821	G	N1-C2-N2	-6.38	110.46	116.20
1	A	1396	A	C2-N3-C4	-6.38	107.41	110.60
1	A	840	C	N3-C4-N4	6.37	122.46	118.00
1	A	1068	G	C6-C5-N7	-6.37	126.58	130.40
1	A	718	G	C5-C6-O6	-6.37	124.78	128.60
1	A	1084	G	C4-C5-N7	-6.37	108.25	110.80
1	A	1167	A	C5-C6-N1	-6.37	114.52	117.70
1	A	289	G	N9-C4-C5	6.37	107.95	105.40
1	A	886	G	C4-C5-C6	6.37	122.62	118.80
1	A	190(J)	U	N3-C4-O4	6.37	123.86	119.40
1	A	252	U	N1-C2-N3	6.37	118.72	114.90
1	A	325	A	N3-C4-C5	6.37	131.25	126.80
1	A	735	C	C6-N1-C2	6.37	122.85	120.30
1	A	1473	A	OP2-P-O3'	6.37	119.21	105.20
2	B	102	LEU	CA-CB-CG	-6.37	100.66	115.30
2	B	154	LEU	CA-CB-CG	-6.37	100.66	115.30
1	A	8	A	C8-N9-C4	-6.36	103.25	105.80
1	A	83	U	OP1-P-OP2	-6.36	110.05	119.60
1	A	405	U	N3-C4-O4	6.36	123.85	119.40
1	A	1494	G	N3-C4-C5	-6.36	125.42	128.60
1	A	293	G	C6-C5-N7	-6.36	126.58	130.40
1	A	916	G	C6-N1-C2	-6.36	121.28	125.10
1	A	451	A	N1-C2-N3	6.36	132.48	129.30
1	A	452	A	C5-N7-C8	-6.36	100.72	103.90
1	A	504	C	N3-C4-C5	-6.36	119.36	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	534	U	C5-C4-O4	6.36	129.72	125.90
1	A	1483	A	C4-C5-C6	-6.36	113.82	117.00
1	A	1505	G	C5-C6-N1	-6.36	108.32	111.50
1	A	161	A	C5-C6-N6	6.36	128.79	123.70
1	A	1057	G	C4-C5-C6	-6.36	114.98	118.80
1	A	39	G	C2-N3-C4	6.36	115.08	111.90
1	A	46	G	C8-N9-C1'	6.36	135.26	127.00
1	A	576	G	C4-C5-C6	6.36	122.61	118.80
1	A	582	U	N1-C2-N3	6.36	118.72	114.90
1	A	937	A	C6-N1-C2	-6.36	114.78	118.60
1	A	981	U	C6-N1-C2	-6.36	117.19	121.00
1	A	113	G	C8-N9-C4	6.36	108.94	106.40
1	A	863	U	N3-C2-O2	-6.36	117.75	122.20
1	A	887	G	C6-N1-C2	-6.36	121.29	125.10
1	A	1217	C	C5-C4-N4	6.36	124.65	120.20
1	A	14	U	C5-C6-N1	-6.35	119.52	122.70
1	A	190(A)	C	N3-C4-N4	6.35	122.45	118.00
1	A	952	U	O5'-P-OP2	6.35	118.32	110.70
1	A	1052	U	C6-N1-C2	6.35	124.81	121.00
1	A	1497	G	C6-C5-N7	-6.35	126.59	130.40
1	A	691	G	N3-C4-C5	-6.35	125.42	128.60
1	A	952	U	N3-C2-O2	6.35	126.65	122.20
1	A	48	C	C2-N3-C4	6.35	123.08	119.90
1	A	243	A	C5-C6-N6	-6.35	118.62	123.70
1	A	673	G	C5-N7-C8	-6.35	101.12	104.30
1	A	867	G	N3-C2-N2	-6.35	115.46	119.90
1	A	930	C	OP1-P-OP2	6.35	129.12	119.60
1	A	410	G	C5-N7-C8	6.35	107.47	104.30
1	A	428	G	P-O3'-C3'	6.35	127.32	119.70
1	A	1193	G	N7-C8-N9	6.35	116.27	113.10
1	A	731	G	N7-C8-N9	6.35	116.27	113.10
1	A	775	G	N3-C4-C5	-6.35	125.43	128.60
1	A	878	G	O5'-P-OP1	-6.35	99.99	105.70
1	A	1491	G	N1-C2-N3	-6.35	120.09	123.90
1	A	222	U	C5-C6-N1	-6.34	119.53	122.70
1	A	926	G	OP1-P-OP2	6.34	129.12	119.60
1	A	1305	G	N7-C8-N9	6.34	116.27	113.10
1	A	792	A	N9-C4-C5	6.34	108.34	105.80
1	A	1421	G	O5'-P-OP1	6.34	118.31	110.70
1	A	354	G	O5'-P-OP1	-6.34	99.99	105.70
1	A	524	G	N1-C2-N3	-6.34	120.09	123.90
1	A	1042	G	C8-N9-C4	6.34	108.94	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	956	U	C4-C5-C6	6.34	123.50	119.70
1	A	1322	C	C2-N3-C4	6.34	123.07	119.90
1	A	1432	G	C5-C6-N1	-6.34	108.33	111.50
1	A	414	A	OP1-P-OP2	-6.34	110.09	119.60
1	A	949	A	N3-C4-C5	6.34	131.24	126.80
1	A	199	G	C5-C6-O6	-6.33	124.80	128.60
1	A	219	C	N3-C4-N4	-6.33	113.56	118.00
1	A	286	G	N3-C4-C5	6.33	131.77	128.60
1	A	584	G	N7-C8-N9	-6.33	109.93	113.10
1	A	588	G	C4-C5-C6	6.33	122.60	118.80
1	A	57	G	N1-C6-O6	6.33	123.70	119.90
1	A	1425	U	C4-C5-C6	6.33	123.50	119.70
1	A	612	C	C2-N3-C4	-6.33	116.73	119.90
1	A	254	G	C6-C5-N7	-6.33	126.60	130.40
1	A	816	A	C5-C6-N6	6.33	128.76	123.70
1	A	681	C	C5-C4-N4	-6.33	115.77	120.20
1	A	737	A	C5-C6-N1	-6.33	114.54	117.70
1	A	518	C	O5'-P-OP1	-6.33	100.01	105.70
1	A	852	G	N3-C2-N2	-6.32	115.47	119.90
1	A	1294	G	O5'-P-OP1	6.32	118.29	110.70
1	A	1300	G	N3-C4-C5	6.32	131.76	128.60
12	L	39	VAL	CB-CA-C	-6.32	99.39	111.40
1	A	1120	G	OP2-P-O3'	6.32	119.11	105.20
1	A	35	G	N7-C8-N9	-6.32	109.94	113.10
1	A	1057	G	N3-C4-C5	6.32	131.76	128.60
1	A	1286	A	C6-C5-N7	-6.32	127.88	132.30
1	A	338	A	C2-N3-C4	-6.32	107.44	110.60
1	A	167	G	C4-C5-C6	6.32	122.59	118.80
1	A	521	G	C4-C5-C6	-6.32	115.01	118.80
1	A	650	G	N7-C8-N9	-6.32	109.94	113.10
1	A	1442	G	C4-N9-C1'	6.32	134.71	126.50
1	A	1484	C	N1-C2-O2	-6.32	115.11	118.90
1	A	181	G	C6-C5-N7	-6.32	126.61	130.40
1	A	328	C	C6-N1-C2	-6.32	117.77	120.30
1	A	1493	A	C2-N3-C4	6.32	113.76	110.60
1	A	1243	C	N3-C4-C5	-6.31	119.37	121.90
1	A	821	G	C4-N9-C1'	6.31	134.71	126.50
1	A	891	U	C6-N1-C2	6.31	124.79	121.00
1	A	918	A	O5'-P-OP2	6.31	118.28	110.70
1	A	1125	U	P-O5'-C5'	6.31	131.00	120.90
1	A	1127	G	C5-C6-O6	-6.31	124.81	128.60
1	A	1392	G	C4-N9-C1'	6.31	134.71	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	C	O5'-P-OP1	-6.31	100.02	105.70
1	A	277	C	C2-N1-C1'	-6.31	111.86	118.80
1	A	824	C	C4-C5-C6	6.31	120.56	117.40
1	A	1464	G	N1-C2-N3	6.31	127.68	123.90
1	A	815	A	N1-C2-N3	6.31	132.45	129.30
1	A	889	A	C5-C6-N6	6.31	128.75	123.70
17	Q	95	TYR	CB-CG-CD1	-6.31	117.22	121.00
1	A	7	G	C8-N9-C1'	6.30	135.20	127.00
1	A	77	G	C5-C6-O6	-6.30	124.82	128.60
1	A	408	A	OP2-P-O3'	6.30	119.07	105.20
1	A	1499	A	C8-N9-C4	6.30	108.32	105.80
20	T	83	ARG	NE-CZ-NH1	-6.30	117.15	120.30
1	A	232	G	C6-C5-N7	-6.30	126.62	130.40
1	A	255	G	N1-C6-O6	6.30	123.68	119.90
1	A	1259	C	C6-N1-C2	6.30	122.82	120.30
1	A	1520	G	C8-N9-C4	6.30	108.92	106.40
1	A	480	U	N3-C4-O4	6.30	123.81	119.40
1	A	1228	C	C4-C5-C6	-6.30	114.25	117.40
1	A	388	G	C6-C5-N7	-6.30	126.62	130.40
1	A	500	G	N3-C4-N9	-6.30	122.22	126.00
1	A	670	G	N3-C4-N9	6.30	129.78	126.00
1	A	721	G	N1-C2-N2	-6.30	110.53	116.20
1	A	4	U	O5'-P-OP1	-6.30	100.03	105.70
1	A	19	C	OP1-P-OP2	6.30	129.04	119.60
1	A	288	A	C5-C6-N1	-6.30	114.55	117.70
1	A	356	A	C5-C6-N6	6.30	128.74	123.70
1	A	1301	U	N1-C2-N3	6.30	118.68	114.90
1	A	258	G	N1-C6-O6	6.29	123.68	119.90
1	A	728	A	C5-C6-N6	6.29	128.74	123.70
1	A	1159	U	C5-C4-O4	6.29	129.68	125.90
1	A	25	C	N1-C2-O2	-6.29	115.12	118.90
1	A	161	A	C8-N9-C4	-6.29	103.28	105.80
1	A	902	G	N7-C8-N9	-6.29	109.95	113.10
1	A	582	U	N3-C2-O2	-6.29	117.80	122.20
1	A	823	G	C6-C5-N7	-6.29	126.63	130.40
1	A	949	A	C2-N3-C4	-6.29	107.45	110.60
11	K	120	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	A	275	G	C4-C5-N7	6.29	113.31	110.80
1	A	703	G	N1-C2-N2	-6.29	110.54	116.20
1	A	1127	G	O5'-P-OP2	-6.29	100.04	105.70
1	A	1276	G	C6-C5-N7	-6.29	126.63	130.40
1	A	1280	A	N1-C2-N3	6.29	132.44	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	308	C	N1-C2-N3	-6.28	114.80	119.20
1	A	569	C	C4-C5-C6	6.28	120.54	117.40
1	A	721	G	N3-C2-N2	6.28	124.30	119.90
1	A	148	G	C5-C6-N1	-6.28	108.36	111.50
1	A	438	G	C5-C6-N1	-6.28	108.36	111.50
1	A	1128	C	N1-C2-O2	6.28	122.67	118.90
1	A	561	U	C6-N1-C2	-6.28	117.23	121.00
1	A	423	G	N9-C4-C5	-6.28	102.89	105.40
1	A	622	A	N3-C4-C5	6.28	131.19	126.80
1	A	1080	A	C6-N1-C2	-6.28	114.83	118.60
1	A	244	U	N3-C4-C5	-6.27	110.84	114.60
1	A	945	G	N3-C4-C5	-6.27	125.46	128.60
1	A	367	U	C5-C6-N1	-6.27	119.56	122.70
1	A	568	G	N9-C4-C5	6.27	107.91	105.40
1	A	1406	U	N3-C4-C5	-6.27	110.84	114.60
1	A	1521	G	N3-C4-N9	6.27	129.76	126.00
1	A	549	C	C6-N1-C2	6.27	122.81	120.30
1	A	1322	C	C6-N1-C2	6.27	122.81	120.30
1	A	522	C	N1-C2-N3	-6.27	114.81	119.20
1	A	1212	U	C4-C5-C6	-6.27	115.94	119.70
1	A	397	A	OP1-P-O3'	6.27	118.99	105.20
1	A	649	G	C5-C6-N1	6.27	114.63	111.50
1	A	1086	U	C2-N1-C1'	6.27	125.22	117.70
1	A	940	C	N3-C2-O2	6.27	126.29	121.90
1	A	1269	A	C5-N7-C8	6.27	107.03	103.90
1	A	176	C	C5-C6-N1	6.26	124.13	121.00
1	A	233	C	OP2-P-O3'	6.26	118.98	105.20
1	A	788	U	N3-C2-O2	6.26	126.58	122.20
1	A	1163	C	C2-N3-C4	6.26	123.03	119.90
1	A	706	A	N9-C4-C5	-6.26	103.30	105.80
1	A	43	C	N3-C4-N4	-6.26	113.62	118.00
1	A	321	A	C5-C6-N6	-6.26	118.69	123.70
1	A	584	G	C4-C5-N7	-6.26	108.30	110.80
1	A	774	G	C4-C5-C6	6.26	122.56	118.80
1	A	1379	G	N3-C4-C5	6.26	131.73	128.60
1	A	399	G	C5-C6-N1	6.26	114.63	111.50
1	A	1387	G	C5-C6-O6	-6.26	124.84	128.60
1	A	507	C	O5'-P-OP2	6.26	118.21	110.70
1	A	1379	G	N1-C6-O6	6.26	123.66	119.90
1	A	951	G	N1-C6-O6	6.26	123.65	119.90
1	A	1385	G	N1-C2-N3	6.26	127.65	123.90
1	A	99	C	C5-C4-N4	-6.25	115.82	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	326	G	N1-C2-N3	-6.25	120.15	123.90
1	A	407	G	N3-C2-N2	-6.25	115.52	119.90
1	A	440	A	N1-C2-N3	6.25	132.43	129.30
1	A	899	C	C6-N1-C2	6.25	122.80	120.30
1	A	1108	G	C4-C5-C6	6.25	122.55	118.80
1	A	1331	G	N3-C2-N2	-6.25	115.52	119.90
1	A	501	C	OP2-P-O3'	6.25	118.95	105.20
1	A	1140	C	N1-C2-O2	6.25	122.65	118.90
1	A	1460	A	N1-C6-N6	6.25	122.35	118.60
1	A	395	C	N3-C4-N4	6.25	122.38	118.00
1	A	373	A	C4-C5-N7	-6.25	107.58	110.70
1	A	578	C	N3-C4-C5	6.25	124.40	121.90
1	A	624	C	N1-C2-O2	-6.25	115.15	118.90
1	A	652	U	N3-C2-O2	6.25	126.57	122.20
1	A	890	G	C5-C6-O6	6.25	132.35	128.60
1	A	894	G	C5-N7-C8	-6.25	101.18	104.30
1	A	930	C	N3-C4-N4	-6.25	113.63	118.00
1	A	105	G	C5-C6-O6	-6.25	124.85	128.60
1	A	1333	A	C5-C6-N1	6.25	120.82	117.70
1	A	1361(A)	C	N3-C2-O2	-6.25	117.53	121.90
1	A	1466	C	OP1-P-O3'	-6.25	91.46	105.20
1	A	869	G	C2-N3-C4	6.25	115.02	111.90
1	A	1195	C	C2'-C3'-O3'	6.24	123.69	113.70
1	A	1423	G	OP1-P-OP2	6.24	128.96	119.60
1	A	1498	UR3	OP2-P-O3'	6.24	118.94	105.20
1	A	386	C	N1-C2-O2	-6.24	115.16	118.90
1	A	639	G	N3-C4-C5	6.24	131.72	128.60
1	A	1199	U	N3-C4-C5	-6.24	110.86	114.60
1	A	1501	C	C5-C6-N1	-6.24	117.88	121.00
1	A	437	U	N3-C2-O2	-6.24	117.83	122.20
1	A	546	G	N7-C8-N9	6.24	116.22	113.10
1	A	661	G	O5'-P-OP1	-6.24	100.09	105.70
1	A	726	C	OP1-P-O3'	6.24	118.92	105.20
1	A	766	A	C4-N9-C1'	-6.24	115.07	126.30
19	S	79	THR	N-CA-C	6.24	127.84	111.00
1	A	1439	C	N3-C4-C5	6.24	124.39	121.90
1	A	1459	C	C2-N3-C4	-6.24	116.78	119.90
1	A	149	A	C4-C5-N7	-6.23	107.58	110.70
1	A	609	A	C2-N3-C4	-6.23	107.48	110.60
1	A	435	C	C5-C6-N1	6.23	124.12	121.00
1	A	570	G	N3-C4-C5	-6.23	125.48	128.60
1	A	888	G	C4-C5-C6	6.23	122.54	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1075	C	C5-C4-N4	6.23	124.56	120.20
1	A	1224	G	N9-C1'-C2'	6.23	122.10	114.00
1	A	1265	G	N3-C2-N2	-6.23	115.54	119.90
1	A	360	A	N1-C2-N3	6.23	132.41	129.30
1	A	766	A	O4'-C1'-N9	6.23	113.19	108.20
1	A	1397	C	C6-N1-C1'	-6.23	113.32	120.80
1	A	1182	G	N1-C6-O6	-6.23	116.16	119.90
1	A	364	A	C5-C6-N1	-6.23	114.59	117.70
1	A	1508	G	O5'-P-OP2	-6.23	100.09	105.70
1	A	44	G	C2-N3-C4	-6.23	108.79	111.90
1	A	947	G	C2-N3-C4	-6.23	108.79	111.90
1	A	51	A	C6-C5-N7	-6.22	127.94	132.30
1	A	175	C	N3-C2-O2	6.22	126.26	121.90
1	A	324	G	C5-C6-O6	6.22	132.34	128.60
1	A	540	G	N1-C2-N2	-6.22	110.60	116.20
1	A	881	G	C8-N9-C4	6.22	108.89	106.40
1	A	938	A	C6-N1-C2	-6.22	114.86	118.60
1	A	1280	A	C5-N7-C8	6.22	107.01	103.90
1	A	193	C	N3-C2-O2	-6.22	117.54	121.90
1	A	413	G	C4-N9-C1'	-6.22	118.41	126.50
1	A	898	G	C4-C5-N7	6.22	113.29	110.80
1	A	1421	G	N1-C2-N3	-6.22	120.17	123.90
1	A	243	A	O4'-C1'-N9	-6.22	103.22	108.20
1	A	281	G	C5-C6-O6	-6.22	124.87	128.60
1	A	729	A	OP1-P-O3'	6.22	118.88	105.20
1	A	1385	G	C2-N3-C4	-6.22	108.79	111.90
1	A	635	G	C4-N9-C1'	6.22	134.58	126.50
1	A	142	G	C8-N9-C4	6.22	108.89	106.40
1	A	243	A	N1-C2-N3	6.22	132.41	129.30
1	A	1092	A	C5-N7-C8	-6.22	100.79	103.90
20	T	74	LYS	CA-C-N	-6.22	103.52	117.20
1	A	311	C	OP1-P-OP2	6.21	128.92	119.60
1	A	396	G	C5-C6-N1	-6.21	108.39	111.50
1	A	487	A	C5-C6-N1	6.21	120.81	117.70
1	A	810	C	OP1-P-O3'	6.21	118.87	105.20
1	A	586	C	N3-C2-O2	6.21	126.25	121.90
1	A	292	G	C5-C6-N1	-6.21	108.39	111.50
1	A	1037	C	C5-C4-N4	-6.21	115.85	120.20
1	A	1394	A	O4'-C1'-N9	-6.21	103.23	108.20
1	A	182	U	N3-C4-O4	6.21	123.75	119.40
1	A	232	G	N7-C8-N9	6.21	116.20	113.10
1	A	432	A	C4-C5-N7	-6.21	107.60	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1530	G	N1-C6-O6	6.21	123.63	119.90
1	A	1105	A	C6-N1-C2	-6.21	114.88	118.60
1	A	1451	A	C4-C5-C6	-6.21	113.90	117.00
1	A	1539	C	C2-N3-C4	6.21	123.00	119.90
1	A	181	G	N3-C4-N9	6.21	129.72	126.00
1	A	970	C	N3-C2-O2	-6.21	117.56	121.90
1	A	1283	G	C5-C6-O6	-6.21	124.88	128.60
1	A	505	G	C8-N9-C4	6.20	108.88	106.40
1	A	748	C	C6-N1-C2	-6.20	117.82	120.30
1	A	765	G	C5-N7-C8	-6.20	101.20	104.30
1	A	1193	G	C2-N3-C4	-6.20	108.80	111.90
1	A	1528	U	C2-N3-C4	-6.20	123.28	127.00
1	A	408	A	N9-C4-C5	6.20	108.28	105.80
1	A	515	G	N1-C2-N3	6.20	127.62	123.90
1	A	656	C	C5-C6-N1	6.20	124.10	121.00
1	A	852	G	C5-C6-N1	-6.20	108.40	111.50
1	A	1286	A	C2-N3-C4	-6.20	107.50	110.60
1	A	320	C	C4-C5-C6	6.20	120.50	117.40
1	A	453	A	N9-C4-C5	6.20	108.28	105.80
1	A	593	G	C6-N1-C2	6.20	128.82	125.10
1	A	823	G	C5-N7-C8	-6.20	101.20	104.30
1	A	1014	A	C8-N9-C4	-6.20	103.32	105.80
1	A	1303	C	OP1-P-OP2	-6.20	110.30	119.60
1	A	204	U	N3-C4-C5	-6.20	110.88	114.60
1	A	920	U	C2-N1-C1'	-6.20	110.26	117.70
1	A	28	G	C5-C6-N1	-6.20	108.40	111.50
1	A	750	G	C8-N9-C4	6.20	108.88	106.40
1	A	944	G	N3-C4-C5	-6.20	125.50	128.60
1	A	1126	U	N3-C2-O2	-6.20	117.86	122.20
1	A	1148	U	C4-C5-C6	6.20	123.42	119.70
17	Q	69	LYS	N-CA-C	-6.20	94.27	111.00
1	A	61	G	OP1-P-OP2	6.19	128.89	119.60
1	A	553	A	OP2-P-O3'	6.19	118.83	105.20
1	A	688	G	O5'-P-OP1	-6.19	100.13	105.70
1	A	186	C	C2-N3-C4	6.19	123.00	119.90
1	A	976	G	O5'-P-OP1	-6.19	100.13	105.70
1	A	1024	G	C2-N3-C4	6.19	115.00	111.90
1	A	1074	G	C6-C5-N7	-6.19	126.69	130.40
1	A	1460	A	N7-C8-N9	-6.19	110.70	113.80
1	A	660	G	C8-N9-C4	6.19	108.88	106.40
1	A	1108	G	C8-N9-C1'	-6.19	118.95	127.00
1	A	277	C	N3-C2-O2	6.19	126.23	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	588	G	N1-C2-N3	6.19	127.61	123.90
1	A	1336	C	C6-N1-C2	6.19	122.78	120.30
1	A	16	A	C6-C5-N7	6.19	136.63	132.30
1	A	921	U	N3-C2-O2	6.19	126.53	122.20
1	A	1191	A	C6-C5-N7	-6.18	127.97	132.30
1	A	153	C	OP1-P-O3'	-6.18	91.60	105.20
1	A	60	A	N1-C2-N3	6.18	132.39	129.30
1	A	1055	A	C2-N3-C4	6.18	113.69	110.60
1	A	482	A	C5-C6-N1	-6.18	114.61	117.70
1	A	1452	C	C5-C4-N4	-6.18	115.87	120.20
1	A	260	G	N1-C6-O6	6.18	123.61	119.90
1	A	631	G	N1-C2-N3	-6.18	120.19	123.90
1	A	1142	G	C2-N3-C4	6.18	114.99	111.90
1	A	264	U	N3-C4-O4	-6.18	115.08	119.40
1	A	797	C	C2-N1-C1'	6.18	125.59	118.80
1	A	963	G	C4-C5-C6	6.18	122.51	118.80
16	P	68	ASP	CB-CG-OD1	-6.18	112.74	118.30
1	A	294	U	C5-C6-N1	-6.17	119.61	122.70
1	A	322	C	N3-C4-C5	-6.17	119.43	121.90
1	A	840	C	C5-C4-N4	-6.17	115.88	120.20
1	A	711	G	C5-C6-O6	-6.17	124.90	128.60
1	A	916	G	C5-N7-C8	-6.17	101.21	104.30
1	A	1003(A)	G	C8-N9-C4	-6.17	103.93	106.40
1	A	1052	U	OP2-P-O3'	6.17	118.78	105.20
1	A	1323	G	C5-N7-C8	-6.17	101.21	104.30
1	A	297	G	C5-C6-O6	6.17	132.30	128.60
1	A	676	A	N7-C8-N9	-6.17	110.72	113.80
1	A	1203	C	N1-C2-O2	-6.17	115.20	118.90
1	A	66	G	C5-N7-C8	-6.17	101.22	104.30
1	A	187	C	OP2-P-O3'	6.17	118.77	105.20
1	A	994	A	N1-C6-N6	6.17	122.30	118.60
1	A	1358	U	C5-C4-O4	-6.17	122.20	125.90
1	A	319	G	N3-C2-N2	-6.17	115.58	119.90
1	A	935	A	C6-C5-N7	-6.17	127.98	132.30
1	A	1101	A	N1-C6-N6	6.17	122.30	118.60
1	A	523	A	OP2-P-O3'	6.16	118.76	105.20
1	A	851	G	C5-C6-O6	-6.16	124.90	128.60
1	A	34	C	C5-C4-N4	-6.16	115.89	120.20
1	A	779	C	C6-N1-C2	6.16	122.77	120.30
1	A	47	C	O5'-P-OP2	-6.16	100.16	105.70
1	A	104	G	C6-C5-N7	-6.16	126.70	130.40
1	A	609	A	C4-C5-C6	6.16	120.08	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	755	G	N1-C6-O6	6.16	123.60	119.90
1	A	1468	A	N3-C4-C5	6.16	131.11	126.80
1	A	499	A	O5'-P-OP1	-6.16	100.16	105.70
1	A	567	G	OP1-P-OP2	6.16	128.83	119.60
1	A	1337	G	C5-C6-N1	-6.16	108.42	111.50
3	C	188	LEU	CB-CG-CD2	6.16	121.47	111.00
9	I	66	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	A	742	G	O4'-C1'-N9	-6.15	103.28	108.20
1	A	1488	G	C4-C5-C6	6.15	122.49	118.80
8	H	8	ASP	CB-CG-OD1	-6.15	112.76	118.30
1	A	73	C	N1-C2-O2	-6.15	115.21	118.90
1	A	501	C	C2-N1-C1'	-6.15	112.03	118.80
1	A	915	A	C5-C6-N6	6.15	128.62	123.70
1	A	1013	G	C4-C5-N7	-6.15	108.34	110.80
1	A	783	C	O5'-P-OP1	-6.15	100.16	105.70
1	A	955	U	C5-C6-N1	-6.15	119.62	122.70
1	A	1292	U	C6-N1-C2	6.15	124.69	121.00
1	A	1348	U	O5'-P-OP2	-6.15	100.17	105.70
2	B	155	LEU	CB-CG-CD1	-6.15	100.55	111.00
12	L	27	LEU	CB-CG-CD2	6.15	121.45	111.00
1	A	1082	G	C4-C5-N7	6.15	113.26	110.80
1	A	238	G	O5'-P-OP2	-6.15	100.17	105.70
1	A	289	G	C4-C5-C6	6.15	122.49	118.80
1	A	368	U	C5-C6-N1	-6.15	119.63	122.70
1	A	644	G	C5-C6-O6	-6.15	124.91	128.60
1	A	811	C	OP2-P-O3'	6.15	118.72	105.20
1	A	196	A	N3-C4-C5	6.15	131.10	126.80
1	A	686	U	O5'-P-OP2	-6.15	100.17	105.70
1	A	65	U	N3-C4-C5	-6.14	110.91	114.60
1	A	448	A	N7-C8-N9	6.14	116.87	113.80
1	A	629	G	C6-C5-N7	6.14	134.09	130.40
1	A	1342	C	C4-C5-C6	-6.14	114.33	117.40
1	A	20	U	C5-C4-O4	-6.14	122.21	125.90
1	A	255	G	O4'-C1'-N9	-6.14	103.29	108.20
1	A	279	A	C4-C5-N7	6.14	113.77	110.70
1	A	336	C	C6-N1-C2	6.14	122.76	120.30
1	A	453	A	N1-C6-N6	-6.14	114.91	118.60
1	A	481	G	OP1-P-OP2	6.14	128.81	119.60
1	A	613	C	C2-N3-C4	-6.14	116.83	119.90
1	A	1171	G	N7-C8-N9	6.14	116.17	113.10
1	A	899	C	N1-C2-N3	-6.14	114.90	119.20
1	A	1339	A	C5-C6-N6	6.14	128.61	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	G	C8-N9-C4	6.14	108.86	106.40
1	A	1286	A	O5'-P-OP2	6.14	118.07	110.70
1	A	809	G	C4-C5-C6	-6.14	115.12	118.80
1	A	1168	A	N1-C2-N3	6.14	132.37	129.30
1	A	1380	U	P-O3'-C3'	6.13	127.06	119.70
1	A	248	C	C2-N3-C4	-6.13	116.83	119.90
1	A	1079	G	C4-N9-C1'	6.13	134.47	126.50
1	A	1415	G	OP1-P-O3'	6.13	118.69	105.20
13	M	74	VAL	CB-CA-C	-6.13	99.75	111.40
16	P	25	ARG	NE-CZ-NH1	-6.13	117.23	120.30
1	A	236	G	C8-N9-C4	6.13	108.85	106.40
1	A	658	G	N9-C4-C5	-6.13	102.95	105.40
1	A	1087	G	C6-C5-N7	-6.13	126.72	130.40
1	A	121	C	N3-C2-O2	6.13	126.19	121.90
1	A	647	C	N3-C4-C5	-6.13	119.45	121.90
1	A	854	G	O5'-P-OP1	-6.13	100.18	105.70
1	A	1378	C	C6-N1-C1'	-6.13	113.44	120.80
1	A	1383	C	C4-C5-C6	-6.13	114.33	117.40
1	A	653	A	C6-N1-C2	-6.13	114.92	118.60
1	A	540	G	C5-C6-N1	-6.12	108.44	111.50
1	A	609	A	C6-C5-N7	-6.12	128.01	132.30
1	A	1223	C	C5-C6-N1	6.12	124.06	121.00
1	A	45	U	C5-C4-O4	6.12	129.57	125.90
1	A	446	G	N1-C6-O6	6.12	123.57	119.90
1	A	537	G	OP1-P-OP2	6.12	128.78	119.60
1	A	744	C	N1-C2-O2	6.12	122.57	118.90
1	A	768	A	N3-C4-C5	-6.12	122.51	126.80
1	A	1142	G	N3-C4-C5	-6.12	125.54	128.60
1	A	747	C	C4-C5-C6	6.12	120.46	117.40
1	A	916	G	N3-C2-N2	-6.12	115.62	119.90
1	A	1369	C	C5-C6-N1	-6.12	117.94	121.00
1	A	1486	G	C5-C6-O6	-6.12	124.93	128.60
20	T	20	LEU	CA-CB-CG	-6.12	101.22	115.30
1	A	236	G	OP2-P-O3'	6.12	118.66	105.20
1	A	1419	G	C6-C5-N7	-6.12	126.73	130.40
1	A	324	G	N3-C4-N9	-6.12	122.33	126.00
1	A	373	A	OP1-P-O3'	6.12	118.66	105.20
1	A	1182	G	N3-C4-C5	-6.12	125.54	128.60
1	A	1438	G	N1-C6-O6	6.12	123.57	119.90
10	J	72	VAL	N-CA-C	6.12	127.52	111.00
1	A	853	G	N3-C4-N9	6.12	129.67	126.00
1	A	925	G	N1-C6-O6	6.12	123.57	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	G	O4'-C1'-N9	-6.11	103.31	108.20
1	A	41	G	N1-C2-N2	6.11	121.70	116.20
1	A	562	C	N3-C4-C5	6.11	124.34	121.90
1	A	634	C	N3-C4-C5	-6.11	119.45	121.90
1	A	1015	A	O5'-P-OP1	-6.11	100.20	105.70
1	A	1514	C	O5'-P-OP1	6.11	118.03	110.70
2	B	208	ILE	CB-CA-C	-6.11	99.38	111.60
1	A	547	A	OP1-P-O3'	6.11	118.64	105.20
1	A	736	C	OP2-P-O3'	6.11	118.64	105.20
1	A	888	G	N1-C2-N2	-6.11	110.70	116.20
1	A	696	A	O4'-C1'-N9	-6.11	103.31	108.20
1	A	994	A	N7-C8-N9	6.11	116.86	113.80
1	A	203	U	C2-N1-C1'	6.11	125.03	117.70
1	A	503	C	N1-C2-O2	-6.11	115.23	118.90
1	A	1152	A	C6-N1-C2	-6.11	114.94	118.60
1	A	1220	G	N3-C4-C5	-6.11	125.55	128.60
1	A	1405	G	C8-N9-C4	6.11	108.84	106.40
1	A	298	A	C6-N1-C2	-6.11	114.94	118.60
1	A	1149	C	C2-N1-C1'	-6.11	112.08	118.80
1	A	1392	G	C4-C5-C6	6.11	122.46	118.80
1	A	1512	U	C6-N1-C2	-6.11	117.34	121.00
1	A	424	G	OP1-P-OP2	6.10	128.76	119.60
1	A	414	A	N9-C4-C5	6.10	108.24	105.80
1	A	432	A	N7-C8-N9	-6.10	110.75	113.80
1	A	580	U	N1-C2-N3	6.10	118.56	114.90
1	A	864	A	C5-C6-N6	6.10	128.58	123.70
1	A	1187	G	N1-C2-N3	6.10	127.56	123.90
15	O	77	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	A	106	C	OP1-P-O3'	-6.10	91.78	105.20
1	A	969	A	OP1-P-OP2	-6.10	110.45	119.60
1	A	1507	A	OP1-P-OP2	6.10	128.75	119.60
10	J	50	ILE	N-CA-C	-6.10	94.53	111.00
1	A	20	U	N1-C2-N3	-6.10	111.24	114.90
1	A	1023	G	C8-N9-C4	-6.10	103.96	106.40
1	A	15	G	C5-C6-O6	-6.10	124.94	128.60
1	A	126	G	N9-C4-C5	6.10	107.84	105.40
1	A	238	G	N3-C2-N2	-6.10	115.63	119.90
1	A	276	G	C5-C6-O6	-6.10	124.94	128.60
1	A	363	A	N3-C4-N9	-6.10	122.52	127.40
1	A	1053	G	N1-C2-N2	6.10	121.69	116.20
1	A	1106	G	C8-N9-C4	-6.10	103.96	106.40
1	A	1406	U	C6-N1-C2	-6.10	117.34	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1449	C	N3-C4-C5	6.10	124.34	121.90
1	A	54	C	N3-C2-O2	6.10	126.17	121.90
1	A	394	G	N9-C4-C5	6.09	107.84	105.40
1	A	734	G	C4-C5-C6	6.09	122.46	118.80
1	A	1316	G	C8-N9-C1'	6.09	134.92	127.00
1	A	1195	C	N1-C2-O2	-6.09	115.24	118.90
1	A	628	G	C6-N1-C2	-6.09	121.44	125.10
1	A	657	G	N3-C4-N9	6.09	129.66	126.00
1	A	896	C	N3-C2-O2	6.09	126.16	121.90
1	A	1433	A	OP2-P-O3'	6.09	118.60	105.20
1	A	1485	U	C5-C6-N1	6.09	125.75	122.70
1	A	1533	C	C2-N3-C4	6.09	122.95	119.90
1	A	126	G	C4-C5-N7	-6.09	108.36	110.80
1	A	147	G	N3-C4-N9	-6.09	122.35	126.00
1	A	372	C	C6-N1-C2	-6.09	117.86	120.30
1	A	720	C	O5'-P-OP1	6.09	118.01	110.70
2	B	98	LEU	CB-CG-CD1	-6.09	100.65	111.00
1	A	916	G	C4-N9-C1'	6.09	134.41	126.50
1	A	1075	C	N3-C2-O2	6.09	126.16	121.90
1	A	320	C	OP1-P-OP2	6.09	128.73	119.60
1	A	326	G	C5-C6-N1	-6.09	108.46	111.50
1	A	848	C	C6-N1-C2	-6.09	117.87	120.30
1	A	1338	G	N9-C4-C5	6.09	107.83	105.40
1	A	265	G	N3-C4-N9	6.08	129.65	126.00
1	A	333	G	C2-N3-C4	-6.08	108.86	111.90
1	A	376	G	N3-C2-N2	6.08	124.16	119.90
1	A	642	A	N1-C2-N3	6.08	132.34	129.30
1	A	189	G	C5-N7-C8	6.08	107.34	104.30
1	A	231	G	C8-N9-C4	6.08	108.83	106.40
1	A	1080	A	C2-N3-C4	6.08	113.64	110.60
1	A	1415	G	C6-N1-C2	-6.08	121.45	125.10
1	A	1486	G	C5-C6-N1	6.08	114.54	111.50
1	A	226	G	C6-C5-N7	-6.08	126.75	130.40
1	A	957	U	N3-C2-O2	-6.08	117.94	122.20
1	A	1151	A	OP1-P-OP2	6.08	128.72	119.60
1	A	880	C	C5-C6-N1	-6.08	117.96	121.00
1	A	314	C	N3-C2-O2	6.08	126.16	121.90
1	A	1125	U	O4'-C1'-N1	6.08	113.06	108.20
1	A	1417	G	O4'-C1'-N9	6.08	113.06	108.20
1	A	928	G	C8-N9-C4	6.08	108.83	106.40
1	A	374	A	O5'-P-OP2	-6.08	100.23	105.70
1	A	447	G	C8-N9-C1'	-6.08	119.10	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	534	U	C2-N1-C1'	-6.08	110.41	117.70
1	A	1083	U	C5-C6-N1	-6.08	119.66	122.70
1	A	1102	A	C6-C5-N7	-6.08	128.05	132.30
1	A	1427	U	C5-C6-N1	-6.08	119.66	122.70
1	A	562	C	O5'-P-OP1	-6.07	100.23	105.70
1	A	917	G	C6-N1-C2	-6.07	121.46	125.10
1	A	1179	A	C2-N3-C4	-6.07	107.56	110.60
1	A	111	G	N1-C2-N2	6.07	121.66	116.20
1	A	149	A	C2-N3-C4	-6.07	107.56	110.60
1	A	390	C	C2-N3-C4	6.07	122.94	119.90
1	A	499	A	C4-C5-N7	-6.07	107.67	110.70
1	A	767	A	C2-N3-C4	-6.07	107.56	110.60
1	A	854	G	N1-C6-O6	6.07	123.54	119.90
1	A	1063	C	C5-C4-N4	-6.07	115.95	120.20
5	E	140	ARG	NE-CZ-NH1	6.07	123.34	120.30
1	A	219	C	C2-N3-C4	-6.07	116.87	119.90
1	A	263	A	C5-N7-C8	-6.07	100.87	103.90
1	A	637	G	N1-C2-N3	6.07	127.54	123.90
1	A	656	C	C4-C5-C6	-6.07	114.37	117.40
1	A	1063	C	N1-C2-N3	6.07	123.45	119.20
1	A	1308	U	C4-C5-C6	6.07	123.34	119.70
1	A	979	C	OP2-P-O3'	6.06	118.54	105.20
1	A	1392	G	N3-C4-C5	-6.06	125.57	128.60
1	A	1411	C	N1-C2-N3	6.06	123.44	119.20
12	L	97	ARG	NE-CZ-NH1	-6.06	117.27	120.30
1	A	1053	G	OP1-P-OP2	-6.06	110.51	119.60
1	A	773	G	OP1-P-OP2	6.06	128.69	119.60
1	A	115	G	N9-C4-C5	-6.06	102.98	105.40
1	A	671	G	N1-C2-N3	-6.06	120.27	123.90
1	A	910	C	N3-C4-N4	6.06	122.24	118.00
1	A	912	C	N3-C4-N4	6.06	122.24	118.00
1	A	328	C	C5-C6-N1	6.05	124.03	121.00
1	A	495	U	P-O3'-C3'	6.05	126.97	119.70
1	A	910	C	N1-C2-N3	6.05	123.44	119.20
1	A	10	A	N9-C4-C5	6.05	108.22	105.80
1	A	306	G	O5'-P-OP1	-6.05	100.25	105.70
1	A	375	U	N1-C2-N3	6.05	118.53	114.90
1	A	650	G	N3-C2-N2	-6.05	115.66	119.90
1	A	443	C	C5-C6-N1	-6.05	117.97	121.00
1	A	693	G	C4-N9-C1'	-6.05	118.64	126.50
1	A	849	C	C6-N1-C2	-6.05	117.88	120.30
1	A	53	A	O5'-P-OP2	-6.05	100.26	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	687	A	C5-N7-C8	6.05	106.92	103.90
1	A	654	G	OP2-P-O3'	6.05	118.50	105.20
1	A	1278	U	N1-C2-O2	6.05	127.03	122.80
1	A	308	C	N3-C2-O2	6.04	126.13	121.90
1	A	1203	C	C4-C5-C6	6.04	120.42	117.40
1	A	250	A	N1-C2-N3	6.04	132.32	129.30
1	A	792	A	C4-C5-C6	6.04	120.02	117.00
1	A	988	G	N9-C4-C5	6.04	107.82	105.40
1	A	1203	C	O5'-P-OP2	6.04	117.95	110.70
1	A	1265	G	C2-N3-C4	-6.04	108.88	111.90
1	A	68	G	N3-C2-N2	-6.04	115.67	119.90
1	A	680	C	C5-C4-N4	-6.04	115.97	120.20
1	A	67	C	C6-N1-C1'	-6.04	113.55	120.80
1	A	1437	C	OP1-P-OP2	6.04	128.66	119.60
1	A	37	U	N3-C4-O4	6.04	123.63	119.40
1	A	258	G	O5'-P-OP1	6.04	117.95	110.70
1	A	1070	U	N3-C2-O2	6.04	126.43	122.20
1	A	1190	G	C2-N3-C4	-6.04	108.88	111.90
1	A	1343	G	C2-N3-C4	-6.04	108.88	111.90
1	A	1487	G	C5-C6-O6	6.04	132.22	128.60
1	A	1139	G	N3-C4-C5	-6.04	125.58	128.60
1	A	105	G	C5-N7-C8	-6.04	101.28	104.30
1	A	440	A	C2-N3-C4	-6.04	107.58	110.60
1	A	578	C	C4-C5-C6	6.04	120.42	117.40
1	A	1465	C	N1-C2-O2	6.04	122.52	118.90
1	A	237	C	O5'-P-OP2	-6.03	100.27	105.70
1	A	402	G	C8-N9-C4	6.03	108.81	106.40
1	A	884	U	P-O5'-C5'	-6.03	111.25	120.90
1	A	1055	A	C6-C5-N7	-6.03	128.08	132.30
1	A	1504	G	N3-C4-C5	-6.03	125.58	128.60
1	A	273	A	OP2-P-O3'	6.03	118.47	105.20
1	A	558	G	O5'-P-OP1	-6.03	100.27	105.70
1	A	806	C	C6-N1-C2	-6.03	117.89	120.30
1	A	1052	U	C5-C6-N1	-6.03	119.69	122.70
10	J	66	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	A	1473	A	C8-N9-C4	-6.03	103.39	105.80
1	A	1499	A	C5-N7-C8	6.03	106.91	103.90
1	A	255	G	C4-C5-C6	6.03	122.42	118.80
1	A	382	A	C5-N7-C8	6.03	106.91	103.90
1	A	919	A	N1-C2-N3	-6.03	126.29	129.30
1	A	1245	A	C6-C5-N7	6.03	136.52	132.30
2	B	44	LEU	CA-CB-CG	6.03	129.16	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	747	C	N3-C4-N4	-6.03	113.78	118.00
1	A	953	G	N3-C4-N9	6.03	129.62	126.00
1	A	1231	G	C4-N9-C1'	-6.03	118.67	126.50
1	A	1287	A	N1-C2-N3	6.03	132.31	129.30
1	A	865	A	N9-C4-C5	-6.02	103.39	105.80
1	A	921	U	N1-C2-O2	-6.02	118.58	122.80
1	A	219	C	N3-C4-C5	6.02	124.31	121.90
1	A	244	U	C2-N3-C4	6.02	130.61	127.00
1	A	788	U	N3-C4-C5	-6.02	110.99	114.60
1	A	479	C	C5-C6-N1	6.02	124.01	121.00
1	A	76	C	C5-C4-N4	-6.02	115.99	120.20
1	A	161	A	C4-C5-N7	-6.02	107.69	110.70
1	A	336	C	C2-N3-C4	-6.02	116.89	119.90
1	A	385	C	C6-N1-C2	6.02	122.71	120.30
1	A	517	G	C8-N9-C4	-6.02	103.99	106.40
1	A	592	G	OP1-P-OP2	-6.02	110.57	119.60
1	A	625	G	C4-C5-N7	6.02	113.21	110.80
1	A	509	A	N3-C4-C5	-6.02	122.59	126.80
1	A	875	C	C2-N3-C4	-6.02	116.89	119.90
1	A	1253	G	OP2-P-O3'	6.02	118.44	105.20
1	A	546	G	N1-C2-N3	6.01	127.51	123.90
1	A	764	C	C2-N1-C1'	6.01	125.42	118.80
1	A	1531	A	C8-N9-C4	-6.01	103.39	105.80
1	A	190(D)	U	N3-C2-O2	-6.01	117.99	122.20
1	A	1055	A	N3-C4-C5	-6.01	122.59	126.80
1	A	267	C	N3-C4-C5	6.01	124.31	121.90
1	A	929	G	C5-C6-O6	-6.01	124.99	128.60
1	A	1173	G	N1-C6-O6	6.01	123.51	119.90
1	A	1414	U	C6-N1-C1'	6.01	129.62	121.20
1	A	29	G	OP2-P-O3'	6.01	118.42	105.20
1	A	550	G	N3-C2-N2	-6.01	115.69	119.90
1	A	724	G	OP1-P-OP2	-6.01	110.59	119.60
1	A	529	G	C5-N7-C8	-6.01	101.30	104.30
1	A	789	U	C4-C5-C6	6.01	123.31	119.70
1	A	369	C	C6-N1-C2	6.01	122.70	120.30
1	A	654	G	N9-C4-C5	6.01	107.80	105.40
1	A	55	A	N9-C4-C5	6.00	108.20	105.80
1	A	646	U	C6-N1-C1'	6.00	129.61	121.20
1	A	328	C	N1-C2-O2	6.00	122.50	118.90
1	A	409	G	N1-C2-N3	6.00	127.50	123.90
1	A	693	G	O4'-C1'-N9	6.00	113.00	108.20
1	A	694	A	C8-N9-C4	6.00	108.20	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1339	A	N1-C2-N3	6.00	132.30	129.30
1	A	708	C	OP1-P-OP2	-6.00	110.60	119.60
1	A	578	C	N3-C2-O2	-6.00	117.70	121.90
1	A	190(K)	G	C5-C6-N1	-6.00	108.50	111.50
1	A	674	G	C8-N9-C4	6.00	108.80	106.40
1	A	853	G	N3-C2-N2	6.00	124.10	119.90
1	A	1051	C	N3-C4-C5	6.00	124.30	121.90
1	A	628	G	OP2-P-O3'	5.99	118.39	105.20
1	A	938	A	N1-C6-N6	-5.99	115.00	118.60
1	A	1019	C	C6-N1-C2	-5.99	117.90	120.30
1	A	1239	A	C8-N9-C4	5.99	108.20	105.80
1	A	134	A	C4-C5-C6	5.99	120.00	117.00
1	A	511	C	C6-N1-C1'	5.99	127.99	120.80
1	A	670	G	N1-C6-O6	5.99	123.50	119.90
1	A	759	A	OP2-P-O3'	5.99	118.38	105.20
1	A	1505	G	N7-C8-N9	5.99	116.09	113.10
1	A	133	U	C6-N1-C2	-5.99	117.41	121.00
1	A	1399	C	C6-N1-C2	-5.99	117.91	120.30
1	A	147	G	N9-C4-C5	5.99	107.79	105.40
1	A	700	G	N1-C2-N3	5.99	127.49	123.90
1	A	809	G	C2-N3-C4	5.99	114.89	111.90
1	A	1236	A	C4-C5-N7	5.99	113.69	110.70
1	A	1379	G	N7-C8-N9	5.99	116.09	113.10
1	A	111	G	N9-C4-C5	5.98	107.79	105.40
1	A	124	G	N3-C4-N9	-5.98	122.41	126.00
1	A	453	A	C6-N1-C2	-5.98	115.01	118.60
1	A	1493	A	N1-C2-N3	-5.98	126.31	129.30
1	A	122	G	C5'-C4'-O4'	-5.98	101.92	109.10
1	A	654	G	C2-N3-C4	-5.98	108.91	111.90
1	A	780	A	C6-C5-N7	-5.98	128.11	132.30
1	A	884	U	N3-C4-O4	5.98	123.59	119.40
1	A	803	G	C6-N1-C2	-5.98	121.51	125.10
1	A	1166	G	C4-C5-C6	5.98	122.39	118.80
1	A	1322	C	C6-N1-C1'	-5.98	113.62	120.80
1	A	190(F)	G	C4-C5-N7	-5.98	108.41	110.80
1	A	536	C	N1-C2-N3	5.98	123.38	119.20
1	A	621	A	OP1-P-OP2	-5.98	110.63	119.60
1	A	691	G	N7-C8-N9	5.98	116.09	113.10
1	A	757	U	N3-C2-O2	-5.98	118.02	122.20
1	A	1337	G	C6-C5-N7	-5.98	126.81	130.40
4	D	56	VAL	CB-CA-C	-5.98	100.04	111.40
8	H	85	ARG	NE-CZ-NH2	5.98	123.29	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	135	C	C4-C5-C6	5.97	120.39	117.40
1	A	347	G	C4-C5-N7	5.97	113.19	110.80
1	A	1529	G	N9-C4-C5	5.97	107.79	105.40
1	A	231	G	O5'-P-OP1	5.97	117.87	110.70
1	A	485	G	OP1-P-OP2	-5.97	110.64	119.60
1	A	984	C	N1-C2-N3	-5.97	115.02	119.20
1	A	1327	C	N3-C4-N4	-5.97	113.82	118.00
1	A	1378	C	N1-C2-O2	5.97	122.48	118.90
19	S	77	THR	N-CA-C	5.97	127.13	111.00
1	A	129(A)	G	P-O3'-C3'	5.97	126.86	119.70
1	A	230	G	C4-N9-C1'	5.97	134.26	126.50
1	A	342	C	O5'-P-OP2	-5.97	100.33	105.70
1	A	861	G	O5'-P-OP1	-5.97	100.33	105.70
1	A	149	A	C5-C6-N6	5.97	128.48	123.70
1	A	1214	C	C4-C5-C6	5.97	120.39	117.40
8	H	100	ILE	CB-CA-C	-5.97	99.66	111.60
1	A	111	G	N3-C2-N2	-5.97	115.72	119.90
1	A	729	A	C8-N9-C4	-5.97	103.41	105.80
1	A	783	C	C2-N1-C1'	-5.97	112.23	118.80
1	A	795	C	N3-C4-C5	5.97	124.29	121.90
1	A	125	U	N1-C2-O2	-5.97	118.62	122.80
1	A	187	C	O5'-P-OP1	-5.97	100.33	105.70
1	A	518	C	OP1-P-OP2	5.97	128.55	119.60
1	A	637	G	C2-N3-C4	-5.97	108.92	111.90
1	A	805	C	OP2-P-O3'	5.97	118.33	105.20
1	A	909	A	N1-C2-N3	5.97	132.28	129.30
12	L	57	LYS	N-CA-C	-5.97	94.89	111.00
1	A	21	G	N7-C8-N9	-5.96	110.12	113.10
1	A	28	G	OP1-P-OP2	5.96	128.55	119.60
1	A	699	C	C2-N1-C1'	-5.96	112.24	118.80
1	A	254	G	N1-C2-N3	5.96	127.48	123.90
1	A	1539	C	N3-C2-O2	-5.96	117.73	121.90
20	T	17	ARG	NE-CZ-NH1	-5.96	117.32	120.30
1	A	244	U	C5-C6-N1	5.96	125.68	122.70
1	A	299	G	C2-N3-C4	-5.96	108.92	111.90
1	A	791	G	N1-C6-O6	5.96	123.48	119.90
16	P	12	LYS	CD-CE-NZ	5.96	125.41	111.70
1	A	129	U	C5-C6-N1	-5.96	119.72	122.70
1	A	241	C	C2-N3-C4	-5.96	116.92	119.90
1	A	1250	A	C4-C5-C6	5.96	119.98	117.00
1	A	110	C	C2-N1-C1'	5.96	125.35	118.80
1	A	317	G	C6-C5-N7	-5.96	126.83	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	773	G	N1-C2-N2	-5.96	110.84	116.20
1	A	232	G	C4-C5-N7	5.96	113.18	110.80
1	A	351	G	C5-C6-N1	5.96	114.48	111.50
1	A	1075	C	C6-N1-C1'	5.96	127.95	120.80
1	A	326	G	OP2-P-O3'	5.96	118.30	105.20
1	A	507	C	OP1-P-OP2	-5.96	110.67	119.60
1	A	560	U	C4-C5-C6	5.96	123.27	119.70
1	A	625	G	C4-N9-C1'	5.96	134.24	126.50
1	A	131	C	N1-C2-N3	5.95	123.37	119.20
1	A	319	G	C5-C6-N1	-5.95	108.52	111.50
1	A	779	C	N1-C2-O2	-5.95	115.33	118.90
1	A	781	A	C2-N3-C4	-5.95	107.62	110.60
1	A	1147	C	N3-C4-N4	-5.95	113.83	118.00
1	A	1202	G	N3-C4-C5	5.95	131.57	128.60
1	A	597	G	C4-C5-N7	5.95	113.18	110.80
1	A	111	G	C2-N3-C4	-5.94	108.93	111.90
1	A	201	C	C6-N1-C1'	-5.94	113.67	120.80
1	A	381	C	C2-N1-C1'	5.94	125.33	118.80
1	A	726	C	N3-C4-C5	-5.94	119.52	121.90
1	A	979	C	P-O3'-C3'	5.94	126.83	119.70
9	I	105	ASP	CA-C-N	-5.94	104.13	117.20
1	A	41	G	C6-C5-N7	-5.94	126.84	130.40
1	A	310	G	C5-C6-N1	5.94	114.47	111.50
1	A	759	A	O5'-P-OP2	-5.94	100.36	105.70
1	A	770	C	N3-C4-N4	-5.94	113.84	118.00
1	A	1168	A	C4-N9-C1'	5.94	136.99	126.30
1	A	1280	A	N1-C6-N6	-5.94	115.04	118.60
1	A	1450	U	C5-C4-O4	5.94	129.46	125.90
1	A	1497	G	C4-C5-C6	5.94	122.36	118.80
1	A	80	G	OP1-P-O3'	5.94	118.26	105.20
1	A	859	A	C8-N9-C4	5.94	108.17	105.80
1	A	1084	G	N7-C8-N9	-5.94	110.13	113.10
1	A	198	G	N7-C8-N9	-5.93	110.13	113.10
1	A	515	G	C5-N7-C8	-5.93	101.33	104.30
1	A	804	U	C4-C5-C6	5.93	123.26	119.70
1	A	851	G	N3-C2-N2	-5.93	115.75	119.90
1	A	1055	A	C4-C5-C6	5.93	119.97	117.00
1	A	306	G	O5'-P-OP2	5.93	117.82	110.70
1	A	693	G	C4-C5-N7	-5.93	108.43	110.80
1	A	822	C	C5-C4-N4	-5.93	116.05	120.20
1	A	782	A	N1-C6-N6	-5.93	115.04	118.60
1	A	1392	G	O4'-C1'-N9	-5.93	103.45	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	851	G	C4-N9-C1'	5.93	134.21	126.50
1	A	1507	A	O5'-P-OP2	-5.93	100.36	105.70
6	F	72	VAL	CB-CA-C	-5.93	100.13	111.40
14	N	31	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	A	1413	A	C4-C5-C6	5.93	119.96	117.00
19	S	33	THR	CB-CA-C	-5.93	95.59	111.60
1	A	484	G	C5-C6-N1	5.93	114.46	111.50
1	A	661	G	N3-C4-C5	5.93	131.56	128.60
1	A	672	U	N1-C2-N3	5.93	118.46	114.90
1	A	879	C	C6-N1-C2	-5.93	117.93	120.30
1	A	1487	G	C4-C5-C6	5.93	122.36	118.80
1	A	954	G	N7-C8-N9	-5.92	110.14	113.10
1	A	1082	G	OP1-P-O3'	5.92	118.24	105.20
1	A	137	C	N1-C2-O2	5.92	122.45	118.90
1	A	1419	G	N7-C8-N9	5.92	116.06	113.10
1	A	499	A	C6-N1-C2	-5.92	115.05	118.60
1	A	534	U	N3-C4-O4	-5.92	115.25	119.40
1	A	735	C	N3-C4-N4	5.92	122.14	118.00
1	A	1346	A	N3-C4-N9	-5.92	122.66	127.40
1	A	1480	G	C5-C6-O6	-5.92	125.05	128.60
2	B	23	ARG	N-CA-C	-5.92	95.02	111.00
1	A	736	C	C6-N1-C2	-5.92	117.93	120.30
1	A	740	U	P-O3'-C3'	-5.92	112.60	119.70
1	A	1284	C	C5-C6-N1	-5.92	118.04	121.00
1	A	1416	G	C4-N9-C1'	5.92	134.19	126.50
16	P	73	LEU	CA-CB-CG	-5.92	101.69	115.30
18	R	35	ARG	NE-CZ-NH2	5.92	123.26	120.30
1	A	329	A	OP2-P-O3'	5.92	118.22	105.20
1	A	711	G	C5-C6-N1	-5.92	108.54	111.50
1	A	1065	U	C4-C5-C6	-5.92	116.15	119.70
20	T	102	GLY	N-CA-C	-5.92	98.31	113.10
1	A	193	C	N1-C2-N3	5.92	123.34	119.20
1	A	285	G	N3-C2-N2	-5.92	115.76	119.90
1	A	564	C	OP1-P-OP2	5.91	128.47	119.60
1	A	568	G	N1-C2-N3	5.91	127.45	123.90
1	A	1068	G	O5'-P-OP1	5.91	117.80	110.70
1	A	116	A	N1-C2-N3	5.91	132.26	129.30
1	A	230	G	C5-N7-C8	5.91	107.26	104.30
1	A	431	A	C2-N3-C4	-5.91	107.64	110.60
1	A	917	G	C8-N9-C4	5.91	108.77	106.40
1	A	234	C	C5-C4-N4	5.91	124.34	120.20
1	A	318	G	C5-C6-N1	-5.91	108.55	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	927	G	OP2-P-O3'	5.91	118.20	105.20
1	A	1250	A	C8-N9-C4	-5.91	103.44	105.80
1	A	188	C	C5-C6-N1	-5.91	118.05	121.00
1	A	554	C	C2-N1-C1'	-5.91	112.30	118.80
1	A	687	A	C4-C5-C6	5.91	119.95	117.00
1	A	915	A	N9-C4-C5	5.91	108.16	105.80
1	A	1179	A	C4-C5-C6	-5.91	114.05	117.00
1	A	1179	A	N3-C4-N9	-5.91	122.67	127.40
1	A	1411	C	N3-C2-O2	-5.91	117.77	121.90
1	A	1516	G	OP2-P-O3'	5.91	118.20	105.20
9	I	56	LEU	N-CA-C	-5.91	95.05	111.00
1	A	1168	A	N9-C4-C5	5.91	108.16	105.80
1	A	1502	A	OP2-P-O3'	5.91	118.20	105.20
1	A	549	C	C5-C6-N1	-5.91	118.05	121.00
1	A	801	U	C5-C6-N1	-5.91	119.75	122.70
1	A	887	G	N1-C2-N3	5.91	127.44	123.90
1	A	1211	U	N3-C2-O2	-5.91	118.07	122.20
6	F	48	LEU	CB-CG-CD1	-5.91	100.96	111.00
1	A	512	U	OP1-P-O3'	-5.90	92.21	105.20
1	A	789	U	C5-C6-N1	5.90	125.65	122.70
1	A	1233	G	O5'-P-OP2	-5.90	100.39	105.70
1	A	453	A	N1-C2-N3	5.90	132.25	129.30
1	A	509	A	OP2-P-O3'	5.90	118.18	105.20
1	A	709	G	C4-C5-N7	5.90	113.16	110.80
1	A	1065	U	N3-C2-O2	5.90	126.33	122.20
1	A	1346	A	OP2-P-O3'	5.90	118.18	105.20
1	A	554	C	C5-C6-N1	-5.90	118.05	121.00
1	A	930	C	C4-C5-C6	5.90	120.35	117.40
1	A	1448	C	C5-C6-N1	-5.90	118.05	121.00
1	A	278	G	N3-C2-N2	5.90	124.03	119.90
1	A	432	A	C5-C6-N6	5.90	128.42	123.70
1	A	662	G	O5'-P-OP1	5.90	117.78	110.70
1	A	1165	C	C6-N1-C2	-5.90	117.94	120.30
1	A	339	C	N3-C4-N4	5.89	122.12	118.00
1	A	371	G	O5'-P-OP1	-5.89	100.40	105.70
1	A	674	G	N1-C6-O6	5.89	123.44	119.90
1	A	1437	C	C6-N1-C2	5.89	122.66	120.30
1	A	1508	G	C4-C5-N7	-5.89	108.44	110.80
1	A	737	A	C6-C5-N7	-5.89	128.18	132.30
1	A	766	A	N3-C4-C5	5.89	130.93	126.80
1	A	890	G	C4-N9-C1'	5.89	134.16	126.50
1	A	981	U	N3-C2-O2	5.89	126.33	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1074	G	N3-C4-N9	5.89	129.54	126.00
1	A	345	C	C5-C4-N4	-5.89	116.08	120.20
1	A	700	G	C5-C6-N1	-5.89	108.56	111.50
1	A	44	G	N3-C2-N2	5.89	124.02	119.90
1	A	97	G	OP2-P-O3'	5.89	118.15	105.20
1	A	705	U	C2-N3-C4	-5.89	123.47	127.00
1	A	734	G	C5-C6-N1	-5.89	108.56	111.50
1	A	1520	G	C6-N1-C2	-5.89	121.57	125.10
1	A	30	U	N1-C2-N3	5.88	118.43	114.90
1	A	118	U	N1-C2-O2	5.88	126.92	122.80
1	A	316	G	N1-C2-N3	5.88	127.43	123.90
1	A	446	G	N9-C4-C5	5.88	107.75	105.40
1	A	793	U	OP2-P-O3'	5.88	118.15	105.20
1	A	297	G	OP1-P-OP2	-5.88	110.78	119.60
1	A	980	C	N3-C2-O2	-5.88	117.78	121.90
1	A	552	U	OP2-P-O3'	5.88	118.14	105.20
1	A	1114	C	N1-C2-O2	5.88	122.43	118.90
1	A	1183	A	N1-C6-N6	5.88	122.13	118.60
1	A	579	G	C8-N9-C4	-5.88	104.05	106.40
1	A	233	C	C6-N1-C2	5.87	122.65	120.30
1	A	628	G	OP1-P-O3'	-5.87	92.28	105.20
1	A	711	G	C2-N3-C4	-5.87	108.96	111.90
1	A	722	A	C4-C5-C6	5.87	119.94	117.00
1	A	1363	A	C6-C5-N7	5.87	136.41	132.30
1	A	462	G	OP2-P-O3'	5.87	118.11	105.20
1	A	937	A	N1-C2-N3	5.87	132.24	129.30
1	A	323	U	C4-C5-C6	5.87	123.22	119.70
1	A	114	U	N1-C2-O2	-5.87	118.69	122.80
1	A	122	G	N3-C2-N2	5.87	124.01	119.90
1	A	600	C	C4-C5-C6	5.87	120.33	117.40
1	A	797	C	C6-N1-C1'	-5.87	113.76	120.80
1	A	38	G	C8-N9-C1'	5.87	134.63	127.00
1	A	361	G	C2-N3-C4	-5.87	108.97	111.90
1	A	50	A	OP1-P-OP2	5.87	128.40	119.60
1	A	58	C	C5-C6-N1	5.87	123.93	121.00
1	A	781	A	C8-N9-C4	-5.87	103.45	105.80
1	A	1166	G	N1-C2-N3	5.87	127.42	123.90
1	A	1278	U	C2-N3-C4	5.87	130.52	127.00
1	A	1387	G	C6-N1-C2	-5.87	121.58	125.10
1	A	675	A	C5-N7-C8	-5.86	100.97	103.90
1	A	1338	G	C6-N1-C2	-5.86	121.58	125.10
1	A	1464	G	N3-C2-N2	-5.86	115.80	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	446	G	C4-N9-C1'	5.86	134.12	126.50
1	A	970	C	C6-N1-C1'	-5.86	113.77	120.80
1	A	1503	A	C5-C6-N6	5.86	128.39	123.70
1	A	297	G	C4-C5-N7	-5.86	108.46	110.80
1	A	390	C	O5'-P-OP1	5.86	117.73	110.70
1	A	435	C	C6-N1-C2	-5.86	117.96	120.30
1	A	768	A	C4-C5-C6	5.86	119.93	117.00
1	A	1133	G	C4-C5-N7	-5.86	108.45	110.80
1	A	551	U	N3-C4-C5	5.86	118.12	114.60
1	A	806	C	OP2-P-O3'	5.86	118.09	105.20
1	A	903	G	N9-C4-C5	5.86	107.74	105.40
1	A	946	A	C4-C5-N7	5.86	113.63	110.70
1	A	1432	G	N1-C2-N3	5.86	127.42	123.90
1	A	513	C	N3-C4-C5	5.86	124.24	121.90
1	A	508	C	C2-N1-C1'	5.85	125.24	118.80
1	A	1322	C	N3-C4-N4	5.85	122.10	118.00
1	A	63	C	OP2-P-O3'	5.85	118.08	105.20
1	A	906	G	C4-C5-N7	5.85	113.14	110.80
1	A	1530	G	O4'-C1'-N9	5.85	112.88	108.20
1	A	147	G	OP1-P-OP2	5.85	128.38	119.60
1	A	280	C	N1-C2-O2	5.85	122.41	118.90
1	A	435	C	N1-C2-O2	-5.85	115.39	118.90
1	A	1189	C	N1-C2-O2	5.85	122.41	118.90
1	A	1063	C	N3-C4-N4	5.85	122.09	118.00
5	E	53	LEU	CB-CG-CD2	-5.85	101.06	111.00
1	A	249	U	OP1-P-OP2	5.85	128.37	119.60
1	A	251	G	N3-C4-N9	5.85	129.51	126.00
1	A	350	G	O4'-C1'-N9	-5.85	103.52	108.20
1	A	771	G	N3-C2-N2	-5.85	115.81	119.90
1	A	1292	U	O5'-P-OP1	5.85	117.72	110.70
1	A	439	A	N3-C4-N9	-5.84	122.72	127.40
1	A	59	A	O5'-P-OP2	-5.84	100.44	105.70
1	A	130	A	C6-N1-C2	-5.84	115.10	118.60
1	A	227	G	C4-C5-C6	5.84	122.31	118.80
1	A	651	C	C2-N3-C4	5.84	122.82	119.90
1	A	1116	C	C2-N1-C1'	-5.84	112.38	118.80
1	A	1175	G	C8-N9-C4	-5.84	104.06	106.40
1	A	1215	G	C5-C6-O6	-5.84	125.09	128.60
1	A	1316	G	C6-C5-N7	5.84	133.91	130.40
1	A	1465	C	C5-C6-N1	5.84	123.92	121.00
1	A	190(H)	G	C2-N3-C4	-5.84	108.98	111.90
1	A	267	C	C2-N3-C4	-5.84	116.98	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	643	C	OP2-P-O3'	5.84	118.05	105.20
1	A	975	A	C4-C5-N7	5.84	113.62	110.70
12	L	98	TYR	CD1-CE1-CZ	5.84	125.06	119.80
1	A	1319	A	C6-N1-C2	5.84	122.10	118.60
1	A	1335	C	C5-C4-N4	5.84	124.29	120.20
1	A	1496	C	P-O3'-C3'	-5.84	112.69	119.70
1	A	512	U	O5'-P-OP2	-5.84	100.45	105.70
1	A	321	A	C8-N9-C4	-5.83	103.47	105.80
1	A	494	G	N7-C8-N9	5.83	116.02	113.10
1	A	1338	G	C4-N9-C1'	5.83	134.09	126.50
1	A	6	G	N7-C8-N9	5.83	116.02	113.10
1	A	822	C	O5'-P-OP1	5.83	117.70	110.70
1	A	18	C	N1-C2-N3	5.83	123.28	119.20
1	A	315	A	O4'-C1'-N9	-5.83	103.53	108.20
1	A	583	A	C4-C5-C6	5.83	119.92	117.00
1	A	740	U	N1-C2-N3	5.83	118.40	114.90
1	A	1401	G	C5-C6-O6	-5.83	125.10	128.60
1	A	1252	A	C6-C5-N7	5.83	136.38	132.30
1	A	488	C	N3-C4-N4	5.83	122.08	118.00
1	A	773	G	C4-C5-C6	5.83	122.30	118.80
1	A	935	A	N1-C2-N3	5.83	132.21	129.30
1	A	953	G	C8-N9-C1'	-5.83	119.42	127.00
1	A	1125	U	C4'-C3'-C2'	-5.83	96.77	102.60
1	A	1173	G	N9-C4-C5	-5.83	103.07	105.40
1	A	223	U	N3-C2-O2	-5.83	118.12	122.20
1	A	894	G	C6-C5-N7	-5.83	126.90	130.40
1	A	1484	C	N3-C4-C5	-5.83	119.57	121.90
1	A	276	G	O5'-P-OP2	-5.83	100.46	105.70
1	A	1087	G	N3-C2-N2	-5.83	115.82	119.90
1	A	1285	A	C5-C6-N1	5.83	120.61	117.70
1	A	779	C	O5'-P-OP1	5.82	117.69	110.70
1	A	1110	A	O4'-C1'-N9	-5.82	103.54	108.20
1	A	1193	G	C6-C5-N7	-5.82	126.91	130.40
1	A	780	A	C4-C5-N7	5.82	113.61	110.70
1	A	1134	G	C4-C5-N7	-5.82	108.47	110.80
1	A	1504	G	C4-C5-N7	-5.82	108.47	110.80
1	A	351	G	C4-C5-N7	-5.82	108.47	110.80
1	A	590	C	C6-N1-C1'	-5.82	113.82	120.80
1	A	739	C	N3-C4-C5	-5.82	119.57	121.90
1	A	760	G	C4-N9-C1'	-5.82	118.94	126.50
1	A	995	C	N3-C4-N4	5.82	122.07	118.00
1	A	1224	G	N3-C4-C5	-5.82	125.69	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1232	U	N1-C2-N3	5.82	118.39	114.90
1	A	88	A	C5-C6-N1	-5.82	114.79	117.70
1	A	286	G	C8-N9-C4	5.82	108.73	106.40
1	A	375	U	OP1-P-OP2	5.82	128.32	119.60
1	A	1166	G	C4-C5-N7	-5.82	108.47	110.80
1	A	1265	G	N1-C6-O6	5.82	123.39	119.90
1	A	374	A	C5-C6-N1	-5.81	114.79	117.70
1	A	227	G	C5-C6-N1	-5.81	108.59	111.50
1	A	394	G	N1-C2-N2	5.81	121.43	116.20
1	A	709	G	N1-C6-O6	5.81	123.39	119.90
1	A	835	U	O5'-P-OP2	5.81	117.67	110.70
1	A	1327	C	N1-C2-O2	-5.81	115.41	118.90
1	A	1496	C	C5'-C4'-C3'	-5.81	106.70	116.00
6	F	43	LEU	CB-CG-CD2	5.81	120.88	111.00
1	A	280	C	OP1-P-OP2	5.81	128.31	119.60
1	A	583	A	N9-C4-C5	-5.81	103.48	105.80
1	A	1131	G	C5-N7-C8	-5.81	101.40	104.30
1	A	51	A	C8-N9-C4	5.81	108.12	105.80
1	A	1099	G	N9-C4-C5	5.81	107.72	105.40
1	A	1359	C	C5-C4-N4	-5.81	116.14	120.20
1	A	458	C	N3-C4-N4	5.80	122.06	118.00
1	A	491	G	N7-C8-N9	-5.80	110.20	113.10
1	A	910	C	C5-C4-N4	-5.80	116.14	120.20
1	A	957	U	C5-C4-O4	5.80	129.38	125.90
1	A	1228	C	C6-N1-C2	5.80	122.62	120.30
1	A	939	G	OP2-P-O3'	5.80	117.97	105.20
1	A	533	A	C5-C6-N1	-5.80	114.80	117.70
1	A	919	A	C8-N9-C4	-5.80	103.48	105.80
1	A	968	A	C4-C5-C6	-5.80	114.10	117.00
1	A	1427	U	N3-C2-O2	-5.80	118.14	122.20
7	G	3	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	A	484	G	C4-C5-C6	5.80	122.28	118.80
1	A	1237	C	N3-C4-C5	-5.80	119.58	121.90
1	A	1226	C	C6-N1-C2	-5.80	117.98	120.30
1	A	255	G	N3-C2-N2	-5.80	115.84	119.90
1	A	258	G	C6-C5-N7	-5.80	126.92	130.40
1	A	480	U	O5'-P-OP1	-5.79	100.48	105.70
1	A	858	G	OP2-P-O3'	5.79	117.95	105.20
1	A	1510	U	N3-C4-O4	5.79	123.46	119.40
1	A	31	G	C4-C5-N7	-5.79	108.48	110.80
1	A	1321	C	OP2-P-O3'	5.79	117.95	105.20
1	A	1361	G	N1-C6-O6	-5.79	116.42	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1460	A	C6-N1-C2	-5.79	115.12	118.60
1	A	329	A	N9-C4-C5	-5.79	103.48	105.80
1	A	523	A	N3-C4-N9	-5.79	122.77	127.40
1	A	1336	C	N1-C2-O2	5.79	122.38	118.90
19	S	6	LYS	N-CA-C	5.79	126.63	111.00
1	A	262	A	C5-C6-N6	5.79	128.33	123.70
1	A	894	G	N3-C4-C5	5.79	131.49	128.60
1	A	1176	A	OP2-P-O3'	5.79	117.94	105.20
1	A	1514	C	OP2-P-O3'	5.79	117.94	105.20
5	E	60	TYR	CA-CB-CG	5.79	124.40	113.40
1	A	29	G	C6-N1-C2	5.79	128.57	125.10
1	A	50	A	N9-C4-C5	5.79	108.11	105.80
1	A	394	G	N3-C2-N2	-5.79	115.85	119.90
1	A	55	A	C4-C5-N7	-5.78	107.81	110.70
1	A	134	A	OP2-P-O3'	5.78	117.92	105.20
1	A	823	G	O5'-P-OP1	5.78	117.64	110.70
1	A	394	G	C4-N9-C1'	-5.78	118.98	126.50
1	A	1299	A	C5-C6-N1	-5.78	114.81	117.70
1	A	1513	A	C8-N9-C4	5.78	108.11	105.80
1	A	130	A	O4'-C1'-N9	-5.78	103.58	108.20
1	A	687	A	P-O3'-C3'	5.78	126.64	119.70
8	H	119	LEU	CB-CG-CD2	-5.78	101.18	111.00
1	A	304	U	N3-C4-C5	5.78	118.06	114.60
1	A	664	G	N7-C8-N9	-5.78	110.21	113.10
1	A	1104	G	C8-N9-C4	-5.78	104.09	106.40
1	A	1388	C	C5-C4-N4	-5.78	116.16	120.20
1	A	21	G	C8-N9-C1'	-5.77	119.49	127.00
1	A	351	G	C6-C5-N7	5.77	133.86	130.40
1	A	248	C	N3-C4-N4	-5.77	113.96	118.00
1	A	300	A	N3-C4-N9	-5.77	122.78	127.40
1	A	833	U	N1-C2-N3	5.77	118.36	114.90
1	A	1188	A	C5-C6-N1	-5.77	114.81	117.70
1	A	1237	C	C2-N3-C4	-5.77	117.01	119.90
1	A	1377	A	C6-N1-C2	5.77	122.06	118.60
1	A	1452	C	C2-N1-C1'	5.77	125.15	118.80
1	A	1517	G	C4-C5-N7	-5.77	108.49	110.80
1	A	402	G	C2-N3-C4	-5.77	109.01	111.90
1	A	61	G	C6-C5-N7	-5.77	126.94	130.40
1	A	432	A	C8-N9-C4	5.77	108.11	105.80
1	A	901	A	OP1-P-O3'	-5.77	92.51	105.20
1	A	1511	G	C4-N9-C1'	5.77	134.00	126.50
1	A	60	A	OP2-P-O3'	-5.77	92.51	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	307	C	C6-N1-C2	5.77	122.61	120.30
1	A	740	U	N3-C4-C5	-5.77	111.14	114.60
1	A	815	A	O5'-P-OP2	5.77	117.62	110.70
1	A	866	C	C6-N1-C2	-5.77	117.99	120.30
1	A	1343	G	N3-C4-C5	5.77	131.48	128.60
1	A	1383	C	C2-N3-C4	5.77	122.78	119.90
1	A	1430	C	C6-N1-C2	5.77	122.61	120.30
1	A	246	A	C5-C6-N6	-5.77	119.09	123.70
1	A	509	A	C2'-C3'-O3'	5.77	122.93	113.70
1	A	663	A	C5-C6-N1	-5.77	114.82	117.70
1	A	95	U	C5-C4-O4	5.76	129.36	125.90
1	A	908	A	N3-C4-N9	-5.76	122.79	127.40
1	A	1485	U	OP1-P-OP2	5.76	128.25	119.60
1	A	786	G	OP1-P-OP2	5.76	128.24	119.60
1	A	521	G	C8-N9-C4	5.76	108.70	106.40
1	A	804	U	N3-C4-O4	-5.76	115.37	119.40
1	A	899	C	C2-N3-C4	5.76	122.78	119.90
1	A	1281	U	N3-C4-O4	5.76	123.43	119.40
1	A	1446	A	N9-C4-C5	5.76	108.11	105.80
1	A	235	C	OP2-P-O3'	5.76	117.87	105.20
1	A	249	U	N3-C4-C5	-5.76	111.14	114.60
1	A	1129	C	C5-C6-N1	5.76	123.88	121.00
15	O	60	VAL	CB-CA-C	-5.76	100.46	111.40
1	A	262	A	N3-C4-N9	-5.76	122.79	127.40
1	A	672	U	OP1-P-OP2	5.76	128.24	119.60
1	A	944	G	C5-C6-N1	-5.76	108.62	111.50
1	A	387	U	C4-C5-C6	5.76	123.15	119.70
1	A	916	G	C5-C6-N1	5.76	114.38	111.50
1	A	1487	G	C2-N3-C4	5.76	114.78	111.90
1	A	775	G	O5'-P-OP2	-5.75	100.52	105.70
1	A	1065	U	P-O3'-C3'	5.75	126.61	119.70
1	A	1383	C	C5-C4-N4	-5.75	116.17	120.20
1	A	232	G	C6-N1-C2	5.75	128.55	125.10
1	A	408	A	N7-C8-N9	5.75	116.67	113.80
1	A	1157	A	N9-C4-C5	5.75	108.10	105.80
1	A	1216	G	N1-C6-O6	5.75	123.35	119.90
1	A	1516	G	O5'-P-OP1	5.75	117.60	110.70
1	A	161	A	N1-C2-N3	5.75	132.18	129.30
1	A	363	A	N7-C8-N9	5.75	116.67	113.80
1	A	858	G	C4-C5-C6	5.75	122.25	118.80
1	A	1196	U	N1-C2-N3	-5.75	111.45	114.90
1	A	22	G	C5-C6-N1	-5.75	108.63	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	277	C	OP1-P-OP2	5.75	128.22	119.60
1	A	900	A	C8-N9-C4	-5.75	103.50	105.80
1	A	917	G	C8-N9-C1'	-5.75	119.53	127.00
1	A	1062	U	N3-C4-C5	-5.75	111.15	114.60
1	A	1100	C	O5'-P-OP1	-5.75	100.53	105.70
8	H	2	LEU	CA-CB-CG	5.75	128.51	115.30
1	A	927	G	C8-N9-C4	-5.74	104.10	106.40
1	A	1182	G	N3-C2-N2	5.74	123.92	119.90
1	A	1191	A	N9-C4-C5	-5.74	103.50	105.80
1	A	1492	A	N1-C6-N6	-5.74	115.15	118.60
1	A	51	A	C5-C6-N1	5.74	120.57	117.70
1	A	864	A	N3-C4-N9	-5.74	122.81	127.40
1	A	869	G	C4-C5-N7	5.74	113.10	110.80
1	A	1322	C	OP1-P-O3'	5.74	117.83	105.20
1	A	323	U	N1-C2-O2	-5.74	118.78	122.80
1	A	396	G	C6-C5-N7	-5.74	126.96	130.40
1	A	579	G	N1-C2-N3	5.74	127.34	123.90
1	A	33	A	N9-C4-C5	-5.74	103.50	105.80
1	A	81	U	N3-C2-O2	5.74	126.22	122.20
1	A	654	G	N1-C2-N3	5.74	127.34	123.90
1	A	994	A	C4-C5-N7	5.74	113.57	110.70
1	A	829	G	N3-C4-C5	5.74	131.47	128.60
1	A	1326	C	N3-C4-N4	5.74	122.02	118.00
1	A	1446	A	C6-C5-N7	5.74	136.32	132.30
1	A	739	C	C4-C5-C6	5.74	120.27	117.40
1	A	919	A	O5'-P-OP2	-5.74	100.54	105.70
1	A	1030	C	C6-N1-C2	-5.74	118.01	120.30
1	A	1339	A	C5-C6-N1	5.74	120.57	117.70
1	A	1501	C	C6-N1-C2	5.74	122.59	120.30
1	A	487	A	O5'-P-OP2	-5.73	100.54	105.70
1	A	807	A	N1-C6-N6	5.73	122.04	118.60
1	A	1095	U	OP1-P-OP2	-5.73	111.00	119.60
1	A	1190	G	OP2-P-O3'	5.73	117.82	105.20
1	A	194	C	N1-C2-O2	5.73	122.34	118.90
1	A	817	C	N3-C4-C5	-5.73	119.61	121.90
1	A	826	C	C6-N1-C2	-5.73	118.01	120.30
1	A	1460	A	N1-C2-N3	5.73	132.17	129.30
1	A	43	C	OP1-P-OP2	5.73	128.19	119.60
1	A	113	G	N3-C2-N2	-5.73	115.89	119.90
1	A	234	C	C2-N1-C1'	-5.73	112.50	118.80
1	A	444	C	N3-C4-C5	5.73	124.19	121.90
1	A	965	A	O5'-P-OP2	-5.73	100.54	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1376	U	N3-C2-O2	-5.73	118.19	122.20
1	A	1425	U	O4'-C1'-N1	5.73	112.78	108.20
1	A	1469	G	C2-N3-C4	-5.73	109.03	111.90
1	A	165	C	N3-C2-O2	5.73	125.91	121.90
1	A	21	G	N3-C4-C5	-5.73	125.74	128.60
1	A	324	G	C8-N9-C4	-5.73	104.11	106.40
1	A	446	G	N3-C2-N2	-5.73	115.89	119.90
1	A	521	G	O4'-C1'-N9	-5.73	103.62	108.20
1	A	666	G	N1-C6-O6	5.73	123.34	119.90
1	A	737	A	C2-N3-C4	-5.73	107.74	110.60
1	A	741	G	O5'-P-OP2	-5.73	100.54	105.70
1	A	1048	G	N1-C6-O6	-5.73	116.46	119.90
13	M	63	THR	N-CA-C	-5.73	95.54	111.00
1	A	75	G	C8-N9-C4	5.73	108.69	106.40
1	A	853	G	C2-N3-C4	5.73	114.76	111.90
1	A	1276	G	N3-C4-N9	-5.73	122.56	126.00
1	A	1331	G	C8-N9-C1'	5.73	134.44	127.00
1	A	1499	A	C2-N3-C4	-5.73	107.74	110.60
1	A	8	A	N1-C6-N6	-5.72	115.17	118.60
1	A	1050	G	N3-C2-N2	-5.72	115.89	119.90
1	A	127	G	C8-N9-C4	5.72	108.69	106.40
1	A	447	G	C6-C5-N7	-5.72	126.97	130.40
1	A	808	C	C5-C4-N4	-5.72	116.19	120.20
1	A	1148	U	C5-C6-N1	-5.72	119.84	122.70
1	A	1379	G	N3-C4-N9	-5.72	122.57	126.00
8	H	109	ILE	CB-CA-C	-5.72	100.16	111.60
1	A	1127	G	C4-C5-N7	5.72	113.09	110.80
1	A	1417	G	C4-C5-N7	5.72	113.09	110.80
1	A	116	A	OP1-P-O3'	5.72	117.78	105.20
1	A	190(G)	G	C6-C5-N7	-5.72	126.97	130.40
1	A	731	G	N3-C2-N2	-5.72	115.90	119.90
1	A	1165	C	C2-N3-C4	5.72	122.76	119.90
1	A	700	G	C6-C5-N7	-5.72	126.97	130.40
1	A	1331	G	O4'-C1'-N9	5.72	112.77	108.20
1	A	298	A	O5'-P-OP2	-5.72	100.55	105.70
1	A	681	C	C6-N1-C2	5.72	122.59	120.30
1	A	734	G	N7-C8-N9	5.72	115.96	113.10
1	A	742	G	C4-C5-N7	-5.72	108.51	110.80
1	A	743	U	C2-N1-C1'	-5.72	110.84	117.70
1	A	707	C	C4-C5-C6	5.71	120.26	117.40
1	A	730	G	C8-N9-C1'	-5.71	119.57	127.00
1	A	799	G	C8-N9-C4	5.71	108.69	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1061	G	C4-C5-C6	5.71	122.23	118.80
1	A	1106	G	O5'-P-OP1	-5.71	100.56	105.70
1	A	276	G	C2-N3-C4	-5.71	109.04	111.90
1	A	487	A	C5-C6-N6	-5.71	119.13	123.70
1	A	1501	C	OP2-P-O3'	5.71	117.77	105.20
1	A	394	G	O4'-C1'-N9	5.71	112.77	108.20
14	N	41	ARG	NE-CZ-NH1	-5.71	117.44	120.30
1	A	73	C	C6-N1-C2	5.71	122.58	120.30
1	A	131	C	OP2-P-O3'	5.71	117.75	105.20
1	A	268	C	O5'-P-OP1	-5.71	100.56	105.70
1	A	536	C	OP1-P-O3'	-5.71	92.65	105.20
1	A	829	G	OP1-P-OP2	5.71	128.16	119.60
1	A	59	A	N1-C2-N3	-5.71	126.45	129.30
1	A	488	C	C5-C6-N1	5.71	123.85	121.00
1	A	531	U	O5'-P-OP2	5.70	117.54	110.70
1	A	692	U	C6-N1-C1'	-5.70	113.22	121.20
1	A	918	A	C5-C6-N6	-5.70	119.14	123.70
1	A	1094	G	N3-C4-C5	-5.70	125.75	128.60
1	A	1324	A	C8-N9-C4	-5.70	103.52	105.80
1	A	825	G	N3-C4-C5	5.70	131.45	128.60
1	A	255	G	C4-C5-N7	-5.70	108.52	110.80
1	A	489	C	OP2-P-O3'	5.70	117.74	105.20
1	A	716	A	N1-C2-N3	5.70	132.15	129.30
1	A	894	G	C5-C6-O6	-5.70	125.18	128.60
1	A	959	A	N1-C6-N6	5.70	122.02	118.60
1	A	1045	C	N3-C4-C5	5.70	124.18	121.90
1	A	1167	A	N3-C4-N9	-5.70	122.84	127.40
1	A	1229	A	N1-C2-N3	5.70	132.15	129.30
1	A	1321	C	N3-C2-O2	-5.70	117.91	121.90
1	A	1505	G	C2-N3-C4	5.70	114.75	111.90
16	P	74	LEU	CA-CB-CG	-5.70	102.19	115.30
1	A	726	C	N1-C2-N3	5.70	123.19	119.20
1	A	965	A	N3-C4-C5	5.70	130.79	126.80
1	A	1144	G	C5-C6-O6	-5.70	125.18	128.60
1	A	1463	C	O5'-P-OP2	-5.70	100.57	105.70
1	A	35	G	C5-N7-C8	5.70	107.15	104.30
1	A	443	C	C6-N1-C2	5.70	122.58	120.30
1	A	759	A	N9-C4-C5	5.70	108.08	105.80
1	A	883	C	P-O3'-C3'	5.70	126.53	119.70
1	A	1031	G	N3-C4-N9	5.70	129.42	126.00
1	A	1224	G	P-O3'-C3'	5.70	126.53	119.70
8	H	83	ILE	CG1-CB-CG2	-5.70	98.87	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	883	C	C6-N1-C2	-5.69	118.02	120.30
1	A	1241	G	C8-N9-C1'	-5.69	119.60	127.00
1	A	1525	G	N9-C1'-C2'	-5.69	105.74	112.00
1	A	65	U	OP1-P-O3'	5.69	117.72	105.20
1	A	242	C	N3-C4-N4	-5.69	114.02	118.00
1	A	360	A	C4-C5-N7	5.69	113.55	110.70
1	A	594	G	C8-N9-C1'	-5.69	119.60	127.00
1	A	871	U	N1-C2-O2	5.69	126.78	122.80
1	A	900	A	C5-N7-C8	-5.69	101.05	103.90
1	A	1397	C	C2-N1-C1'	5.69	125.06	118.80
1	A	176	C	OP2-P-O3'	5.69	117.72	105.20
1	A	1094	G	N1-C2-N2	-5.69	111.08	116.20
1	A	1228	C	C6-N1-C1'	-5.69	113.97	120.80
1	A	389	A	N3-C4-N9	5.69	131.95	127.40
1	A	425	G	N1-C6-O6	5.69	123.31	119.90
1	A	837	G	OP1-P-O3'	-5.69	92.69	105.20
1	A	1383	C	N1-C2-O2	5.69	122.31	118.90
1	A	1460	A	N9-C4-C5	-5.69	103.52	105.80
1	A	21	G	C2-N3-C4	5.69	114.74	111.90
1	A	438	G	OP2-P-O3'	5.69	117.71	105.20
1	A	579	G	C4-C5-N7	5.69	113.08	110.80
1	A	778	G	N7-C8-N9	-5.69	110.26	113.10
1	A	1449	C	C2-N3-C4	-5.69	117.06	119.90
1	A	902	G	C6-N1-C2	-5.69	121.69	125.10
1	A	583	A	C6-C5-N7	-5.68	128.32	132.30
1	A	680	C	C4-C5-C6	-5.68	114.56	117.40
2	B	44	LEU	CB-CG-CD1	5.68	120.66	111.00
1	A	266	G	OP2-P-O3'	5.68	117.70	105.20
1	A	387	U	N3-C4-C5	-5.68	111.19	114.60
1	A	573	A	N7-C8-N9	5.68	116.64	113.80
1	A	590	C	C5-C4-N4	-5.68	116.22	120.20
1	A	920	U	C6-N1-C2	5.68	124.41	121.00
1	A	1030(D)	A	O4'-C1'-N9	5.68	112.75	108.20
1	A	1235	U	C2-N3-C4	-5.68	123.59	127.00
17	Q	96	GLU	CB-CA-C	5.68	121.76	110.40
1	A	111	G	N1-C6-O6	5.68	123.31	119.90
1	A	1169	A	O5'-P-OP1	-5.68	100.59	105.70
1	A	11	G	OP1-P-O3'	5.68	117.70	105.20
1	A	409	G	C2-N3-C4	-5.68	109.06	111.90
1	A	627	G	C8-N9-C4	-5.68	104.13	106.40
1	A	676	A	C8-N9-C4	5.68	108.07	105.80
1	A	689	C	N3-C2-O2	5.68	125.88	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	429	U	OP1-P-OP2	-5.68	111.08	119.60
1	A	1131	G	C5-C6-O6	-5.68	125.19	128.60
6	F	82	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	A	322	C	C5-C6-N1	5.68	123.84	121.00
1	A	363	A	C8-N9-C4	-5.68	103.53	105.80
1	A	373	A	C2-N3-C4	-5.68	107.76	110.60
1	A	537	G	N1-C2-N2	-5.68	111.09	116.20
1	A	1013	G	N3-C4-C5	-5.68	125.76	128.60
1	A	114	U	N1-C2-N3	5.67	118.31	114.90
1	A	274	A	N7-C8-N9	-5.67	110.96	113.80
1	A	1103	C	OP2-P-O3'	5.67	117.68	105.20
1	A	1376	U	OP2-P-O3'	5.67	117.68	105.20
1	A	883	C	N1-C2-O2	-5.67	115.50	118.90
1	A	786	G	N1-C6-O6	5.67	123.30	119.90
1	A	827	U	N3-C4-O4	5.67	123.37	119.40
1	A	940	C	C6-N1-C2	5.67	122.57	120.30
1	A	1152	A	C4-C5-N7	-5.67	107.87	110.70
1	A	79	G	C4-N9-C1'	5.67	133.87	126.50
1	A	885	G	N1-C2-N3	5.67	127.30	123.90
1	A	1251	A	C5-C6-N1	-5.67	114.87	117.70
1	A	1281	U	C5-C6-N1	5.67	125.53	122.70
2	B	21	ARG	N-CA-C	5.67	126.30	111.00
1	A	849	C	N3-C4-N4	5.67	121.97	118.00
1	A	1100	C	C6-N1-C2	5.67	122.57	120.30
1	A	275	G	C8-N9-C1'	-5.66	119.64	127.00
1	A	623	C	N3-C2-O2	5.66	125.86	121.90
1	A	661	G	C5-C6-O6	5.66	132.00	128.60
1	A	698	G	C5-C6-O6	-5.66	125.20	128.60
1	A	1149	C	C6-N1-C2	5.66	122.56	120.30
1	A	1204	A	OP2-P-O3'	5.66	117.65	105.20
1	A	1363	A	C4-C5-C6	-5.66	114.17	117.00
1	A	328	C	OP1-P-O3'	5.66	117.65	105.20
1	A	170	U	N3-C4-O4	5.66	123.36	119.40
1	A	351	G	N7-C8-N9	-5.66	110.27	113.10
1	A	893	C	C4-C5-C6	-5.66	114.57	117.40
1	A	1055	A	OP1-P-O3'	5.66	117.64	105.20
1	A	1369	C	C2-N3-C4	-5.66	117.07	119.90
1	A	388	G	N9-C4-C5	-5.66	103.14	105.40
1	A	892	A	N1-C2-N3	5.66	132.13	129.30
1	A	1053	G	C8-N9-C1'	5.66	134.35	127.00
1	A	1133	G	C8-N9-C4	5.66	108.66	106.40
1	A	1222	G	N1-C2-N3	5.66	127.29	123.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	278	G	N3-C4-C5	-5.65	125.77	128.60
1	A	527	7MG	OP2-P-O3'	5.65	117.64	105.20
1	A	1224	G	C8-N9-C4	-5.65	104.14	106.40
1	A	1279	A	C5-N7-C8	-5.65	101.07	103.90
1	A	1337	G	C4-C5-C6	5.65	122.19	118.80
1	A	1403	C	C6-N1-C1'	-5.65	114.02	120.80
1	A	253	U	N1-C2-O2	-5.65	118.84	122.80
1	A	431	A	C6-N1-C2	-5.65	115.21	118.60
1	A	547	A	N7-C8-N9	5.65	116.63	113.80
1	A	783	C	C4-C5-C6	-5.65	114.58	117.40
1	A	933	G	N3-C4-N9	5.65	129.39	126.00
1	A	1413	A	N7-C8-N9	5.65	116.63	113.80
1	A	603	U	OP1-P-OP2	-5.65	111.13	119.60
1	A	377	G	C2-N3-C4	-5.65	109.08	111.90
1	A	649	G	N3-C4-N9	5.65	129.39	126.00
1	A	715	A	C2-N3-C4	-5.65	107.78	110.60
1	A	979	C	N3-C4-N4	5.65	121.95	118.00
1	A	1211	U	C6-N1-C1'	-5.65	113.29	121.20
1	A	1465	C	N3-C4-N4	5.65	121.95	118.00
1	A	1503	A	N9-C4-C5	5.64	108.06	105.80
1	A	150	C	C2-N3-C4	5.64	122.72	119.90
1	A	363	A	C5-C6-N1	-5.64	114.88	117.70
1	A	382	A	C4-C5-N7	-5.64	107.88	110.70
1	A	435	C	O5'-P-OP2	5.64	117.47	110.70
1	A	926	G	N9-C1'-C2'	-5.64	105.79	112.00
1	A	964	A	OP1-P-O3'	5.64	117.61	105.20
1	A	1494	G	C4-C5-C6	5.64	122.19	118.80
1	A	965	A	N7-C8-N9	-5.64	110.98	113.80
1	A	1124	G	O4'-C1'-N9	-5.64	103.69	108.20
1	A	66	G	C2-N3-C4	-5.64	109.08	111.90
1	A	176	C	C5-C4-N4	-5.64	116.25	120.20
1	A	397	A	C5-N7-C8	-5.64	101.08	103.90
1	A	722	A	C5-N7-C8	-5.64	101.08	103.90
1	A	815	A	N9-C4-C5	5.64	108.06	105.80
1	A	881	G	C4-C5-C6	5.64	122.18	118.80
1	A	945	G	O4'-C1'-N9	5.64	112.71	108.20
1	A	1058	G	N7-C8-N9	-5.64	110.28	113.10
1	A	700	G	C2-N3-C4	-5.64	109.08	111.90
1	A	529	G	C4-C5-N7	5.64	113.06	110.80
1	A	532	A	N7-C8-N9	5.64	116.62	113.80
1	A	618	C	O5'-P-OP2	-5.64	100.63	105.70
1	A	859	A	C6-C5-N7	-5.64	128.35	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1187	G	C6-N1-C2	-5.64	121.72	125.10
1	A	1203	C	N1-C1'-C2'	-5.64	105.80	112.00
1	A	1274	G	C4-C5-N7	-5.64	108.55	110.80
4	D	22	LYS	CD-CE-NZ	5.64	124.66	111.70
1	A	184	G	C6-N1-C2	-5.63	121.72	125.10
1	A	344	A	O5'-P-OP2	-5.63	100.63	105.70
1	A	691	G	C4-C5-C6	5.63	122.18	118.80
1	A	784	C	N3-C2-O2	-5.63	117.96	121.90
1	A	1276	G	N3-C4-C5	5.63	131.42	128.60
1	A	1410	G	C5-C6-O6	-5.63	125.22	128.60
1	A	46	G	N9-C4-C5	5.63	107.65	105.40
1	A	644	G	C8-N9-C4	-5.63	104.15	106.40
1	A	850	U	O5'-P-OP1	-5.63	100.63	105.70
1	A	1076	C	N3-C4-C5	5.63	124.15	121.90
1	A	43	C	C2-N1-C1'	-5.63	112.61	118.80
1	A	239	U	O5'-P-OP2	-5.63	100.63	105.70
1	A	670	G	C8-N9-C1'	-5.63	119.68	127.00
1	A	906	G	C4-C5-C6	5.63	122.18	118.80
1	A	1471	G	N3-C4-N9	-5.63	122.62	126.00
1	A	1492	A	N3-C4-C5	-5.63	122.86	126.80
1	A	148	G	N1-C2-N3	5.63	127.28	123.90
1	A	423	G	N1-C6-O6	5.63	123.28	119.90
1	A	601	C	C2-N3-C4	-5.63	117.08	119.90
1	A	1438	G	N1-C2-N3	5.63	127.28	123.90
1	A	1517	G	C8-N9-C1'	-5.63	119.68	127.00
1	A	157	G	OP1-P-O3'	-5.63	92.82	105.20
1	A	525	C	C2-N1-C1'	-5.63	112.61	118.80
1	A	1339	A	C6-C5-N7	5.63	136.24	132.30
1	A	311	C	C5-C6-N1	-5.62	118.19	121.00
1	A	688	G	N3-C4-C5	-5.62	125.79	128.60
1	A	1194	U	OP1-P-OP2	5.62	128.04	119.60
1	A	1212	U	C2-N3-C4	5.62	130.38	127.00
1	A	415	A	C2-N3-C4	-5.62	107.79	110.60
1	A	610	G	N3-C2-N2	-5.62	115.96	119.90
1	A	881	G	N3-C4-N9	5.62	129.37	126.00
1	A	1166	G	C5-C6-O6	5.62	131.97	128.60
20	T	13	LEU	CB-CA-C	-5.62	99.52	110.20
1	A	21	G	C5-N7-C8	5.62	107.11	104.30
1	A	745	C	C5-C4-N4	5.62	124.14	120.20
1	A	765	G	N7-C8-N9	5.62	115.91	113.10
4	D	94	LEU	CA-CB-CG	-5.62	102.37	115.30
1	A	1018	C	C6-N1-C2	-5.62	118.05	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	780	A	C5-N7-C8	-5.62	101.09	103.90
1	A	981	U	C5-C6-N1	5.62	125.51	122.70
1	A	989	C	C5-C6-N1	5.62	123.81	121.00
1	A	1066	C	C2-N3-C4	5.62	122.71	119.90
1	A	1178	G	C5-C6-O6	5.62	131.97	128.60
1	A	1524	C	N1-C2-O2	-5.62	115.53	118.90
1	A	590	C	N3-C2-O2	-5.62	117.97	121.90
1	A	79	G	N3-C4-C5	5.62	131.41	128.60
1	A	513	C	C2-N3-C4	-5.62	117.09	119.90
1	A	796	C	C2-N1-C1'	5.62	124.98	118.80
1	A	1490	C	C4-C5-C6	-5.62	114.59	117.40
1	A	173	U	C5-C6-N1	5.61	125.51	122.70
1	A	553	A	C4-C5-C6	5.61	119.81	117.00
1	A	882	C	O5'-P-OP1	5.61	117.44	110.70
1	A	874	G	C5-N7-C8	5.61	107.11	104.30
3	C	196	LEU	CB-CG-CD1	-5.61	101.46	111.00
1	A	251	G	C8-N9-C1'	-5.61	119.71	127.00
1	A	681	C	N1-C2-N3	-5.61	115.27	119.20
1	A	975	A	C6-C5-N7	-5.61	128.37	132.30
1	A	124	G	O5'-P-OP2	5.61	117.43	110.70
19	S	5	LEU	N-CA-C	5.61	126.14	111.00
1	A	52	G	N3-C4-N9	-5.61	122.64	126.00
4	D	36	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	A	1431	C	N1-C2-O2	-5.61	115.54	118.90
1	A	43	C	N1-C2-O2	5.60	122.26	118.90
1	A	1117	G	C8-N9-C1'	-5.60	119.72	127.00
1	A	891	U	N3-C2-O2	5.60	126.12	122.20
1	A	955	U	N1-C2-O2	5.60	126.72	122.80
1	A	1128	C	O5'-P-OP1	5.60	117.42	110.70
1	A	1221	G	C8-N9-C1'	-5.60	119.72	127.00
4	D	36	ARG	N-CA-C	5.60	126.13	111.00
1	A	292	G	N1-C6-O6	5.60	123.26	119.90
1	A	924	C	N3-C4-N4	-5.60	114.08	118.00
1	A	396	G	N3-C4-C5	-5.60	125.80	128.60
1	A	508	C	C6-N1-C2	-5.60	118.06	120.30
1	A	1129	C	N3-C2-O2	-5.60	117.98	121.90
1	A	1370	G	N9-C4-C5	5.60	107.64	105.40
1	A	139	G	C6-N1-C2	-5.60	121.74	125.10
1	A	352	C	OP1-P-OP2	5.60	128.00	119.60
1	A	431	A	O5'-P-OP2	5.60	117.42	110.70
1	A	802	A	C4-C5-C6	5.60	119.80	117.00
16	P	6	LEU	CA-CB-CG	-5.60	102.42	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	664	G	C6-C5-N7	5.60	133.76	130.40
1	A	833	U	O5'-P-OP1	5.60	117.42	110.70
1	A	867	G	N1-C2-N2	5.59	121.23	116.20
1	A	101	A	C2-N3-C4	-5.59	107.80	110.60
1	A	1181	G	P-O3'-C3'	5.59	126.41	119.70
1	A	1442	G	C8-N9-C1'	-5.59	119.73	127.00
1	A	33	A	O5'-P-OP1	5.59	117.41	110.70
1	A	299	G	N1-C2-N3	5.59	127.25	123.90
1	A	915	A	N3-C4-N9	-5.59	122.93	127.40
1	A	998	G	C5-C6-N1	-5.59	108.70	111.50
1	A	1054	C	C6-N1-C2	-5.59	118.06	120.30
1	A	1248	A	C4-C5-N7	5.59	113.50	110.70
1	A	1530	G	C2-N3-C4	5.59	114.70	111.90
1	A	355	C	C5-C6-N1	5.59	123.80	121.00
1	A	896	C	C5-C4-N4	-5.59	116.29	120.20
1	A	1269	A	C4-C5-C6	-5.59	114.20	117.00
1	A	1348	U	C2-N1-C1'	5.59	124.41	117.70
1	A	1231	G	N1-C2-N2	5.59	121.23	116.20
1	A	701	C	N1-C2-O2	-5.59	115.55	118.90
1	A	862	C	N3-C2-O2	5.59	125.81	121.90
1	A	1037	C	N3-C4-N4	5.59	121.91	118.00
1	A	1163	C	N3-C4-C5	-5.59	119.67	121.90
1	A	126	G	C5-C6-N1	-5.58	108.71	111.50
1	A	324	G	N3-C2-N2	-5.58	115.99	119.90
1	A	1276	G	C4-C5-C6	5.58	122.15	118.80
1	A	1290	G	N9-C4-C5	-5.58	103.17	105.40
1	A	59	A	C5-C6-N1	5.58	120.49	117.70
1	A	120	A	C8-N9-C4	-5.58	103.57	105.80
1	A	122	G	N3-C4-N9	5.58	129.35	126.00
1	A	620	C	O5'-P-OP1	5.58	117.40	110.70
1	A	636	U	C4-C5-C6	5.58	123.05	119.70
1	A	759	A	N1-C2-N3	5.58	132.09	129.30
1	A	1241	G	C5-C6-N1	-5.58	108.71	111.50
1	A	1524	C	OP1-P-O3'	-5.58	92.92	105.20
11	K	108	ILE	CB-CA-C	-5.58	100.44	111.60
1	A	154	C	N1-C2-O2	5.58	122.25	118.90
1	A	429	U	C5-C6-N1	-5.58	119.91	122.70
1	A	509	A	P-O3'-C3'	5.58	126.39	119.70
1	A	730	G	C4-N9-C1'	5.58	133.75	126.50
1	A	814	A	C5-N7-C8	-5.58	101.11	103.90
1	A	1258	G	N7-C8-N9	5.58	115.89	113.10
11	K	80	VAL	CB-CA-C	-5.58	100.80	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	432	A	C5-N7-C8	5.58	106.69	103.90
1	A	591	U	C5-C6-N1	-5.58	119.91	122.70
1	A	683	G	OP2-P-O3'	5.58	117.47	105.20
1	A	852	G	OP1-P-OP2	5.58	127.96	119.60
1	A	1127	G	C6-C5-N7	-5.58	127.06	130.40
18	R	68	LYS	CD-CE-NZ	5.58	124.53	111.70
1	A	883	C	N1-C2-N3	5.57	123.10	119.20
12	L	36	VAL	CG1-CB-CG2	5.57	119.81	110.90
1	A	39	G	N9-C1'-C2'	-5.57	105.87	112.00
1	A	198	G	O4'-C1'-N9	-5.57	103.74	108.20
1	A	247	G	OP1-P-OP2	-5.57	111.24	119.60
1	A	559	A	C8-N9-C4	-5.57	103.57	105.80
1	A	628	G	C5-C6-N1	5.57	114.28	111.50
1	A	1149	C	N3-C2-O2	5.57	125.80	121.90
1	A	1179	A	C5-C6-N6	5.57	128.16	123.70
11	K	48	ILE	CG1-CB-CG2	5.57	123.66	111.40
1	A	531	U	N1-C2-O2	-5.57	118.90	122.80
1	A	864	A	N9-C4-C5	5.57	108.03	105.80
1	A	1269	A	C5-C6-N1	5.57	120.48	117.70
5	E	16	THR	CA-CB-CG2	5.57	120.20	112.40
1	A	454	C	C6-N1-C2	5.57	122.53	120.30
1	A	785	G	N3-C4-C5	5.57	131.38	128.60
1	A	91	C	OP2-P-O3'	5.57	117.44	105.20
1	A	925	G	C5-C6-N1	-5.57	108.72	111.50
1	A	557	G	N3-C4-C5	-5.56	125.82	128.60
1	A	676	A	C5-C6-N1	5.56	120.48	117.70
1	A	792	A	N7-C8-N9	5.56	116.58	113.80
1	A	891	U	C5-C6-N1	-5.56	119.92	122.70
15	O	63	ARG	NE-CZ-NH1	-5.56	117.52	120.30
1	A	1076	C	C6-N1-C1'	-5.56	114.13	120.80
1	A	597	G	C6-C5-N7	-5.56	127.06	130.40
1	A	881	G	OP2-P-O3'	5.56	117.43	105.20
1	A	1275	A	N3-C4-C5	5.56	130.69	126.80
1	A	1290	G	C2-N3-C4	-5.56	109.12	111.90
1	A	509	A	C4-C5-C6	5.56	119.78	117.00
1	A	577	G	C5-N7-C8	-5.56	101.52	104.30
1	A	726	C	C4-C5-C6	5.56	120.18	117.40
1	A	786	G	C5-C6-O6	-5.56	125.27	128.60
1	A	1278	U	N3-C4-O4	5.56	123.29	119.40
1	A	96	G	N1-C6-O6	5.56	123.23	119.90
1	A	914	A	O5'-P-OP2	5.56	117.37	110.70
1	A	91	C	N3-C4-N4	5.55	121.89	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	167	G	C8-N9-C4	5.55	108.62	106.40
1	A	203	U	C6-N1-C2	-5.55	117.67	121.00
1	A	620	C	N1-C2-N3	-5.55	115.31	119.20
1	A	705	U	N3-C4-O4	-5.55	115.51	119.40
1	A	885	G	O5'-P-OP1	-5.55	100.70	105.70
1	A	1057	G	C4-C5-N7	-5.55	108.58	110.80
1	A	1127	G	C5-C6-N1	-5.55	108.72	111.50
1	A	1449	C	N1-C2-O2	-5.55	115.57	118.90
1	A	1471	G	OP2-P-O3'	5.55	117.42	105.20
9	I	100	GLY	N-CA-C	5.55	126.98	113.10
1	A	510	A	C5-C6-N6	5.55	128.14	123.70
1	A	622	A	C2-N3-C4	-5.55	107.82	110.60
1	A	1082	G	O5'-P-OP1	5.55	117.36	110.70
1	A	573	A	C4-C5-C6	5.55	119.78	117.00
1	A	131	C	C2-N3-C4	-5.55	117.12	119.90
1	A	657	G	N1-C2-N3	5.55	127.23	123.90
1	A	771	G	C2-N3-C4	-5.55	109.12	111.90
1	A	1201	A	N1-C2-N3	5.55	132.07	129.30
1	A	184	G	N1-C2-N2	-5.55	111.21	116.20
1	A	253	U	O5'-P-OP2	-5.55	100.71	105.70
1	A	1490	C	OP1-P-OP2	5.55	127.92	119.60
1	A	649	G	C5-C6-O6	-5.55	125.27	128.60
1	A	654	G	O5'-P-OP1	-5.55	100.71	105.70
1	A	903	G	C6-N1-C2	-5.55	121.77	125.10
1	A	1467	G	O5'-P-OP2	-5.55	100.71	105.70
1	A	142	G	N7-C8-N9	-5.54	110.33	113.10
1	A	1388	C	N3-C4-C5	5.54	124.12	121.90
1	A	56	U	N1-C2-O2	5.54	126.68	122.80
1	A	306	G	C8-N9-C1'	5.54	134.21	127.00
1	A	403	C	O5'-P-OP1	5.54	117.35	110.70
1	A	851	G	C2-N3-C4	-5.54	109.13	111.90
1	A	1116	C	N3-C4-N4	-5.54	114.12	118.00
1	A	343	U	N3-C4-O4	5.54	123.28	119.40
1	A	381	C	N1-C2-O2	5.54	122.22	118.90
1	A	536	C	OP2-P-O3'	5.54	117.39	105.20
1	A	562	C	C2-N1-C1'	5.54	124.89	118.80
1	A	854	G	C4-N9-C1'	5.54	133.70	126.50
1	A	1164	G	C8-N9-C4	5.54	108.62	106.40
1	A	708	C	N3-C4-N4	5.54	121.88	118.00
1	A	274	A	C8-N9-C4	5.54	108.02	105.80
1	A	566	G	N1-C6-O6	5.54	123.22	119.90
1	A	798	G	O5'-P-OP2	-5.54	100.71	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	802	A	C6-C5-N7	-5.54	128.42	132.30
1	A	1446	A	O5'-P-OP2	-5.54	100.72	105.70
1	A	93	G	C2-N3-C4	-5.54	109.13	111.90
1	A	307	C	O5'-P-OP2	-5.54	100.72	105.70
1	A	637	G	N9-C4-C5	-5.54	103.19	105.40
1	A	429	U	N1-C2-O2	-5.54	118.92	122.80
1	A	624	C	C5-C6-N1	-5.54	118.23	121.00
1	A	727	G	N1-C2-N3	5.54	127.22	123.90
1	A	1168	A	OP1-P-O3'	5.54	117.38	105.20
1	A	1214	C	N1-C2-N3	5.54	123.08	119.20
1	A	1520	G	C4-C5-N7	5.54	113.01	110.80
1	A	33	A	C5-C6-N1	5.53	120.47	117.70
1	A	188	C	C6-N1-C2	5.53	122.51	120.30
1	A	705	U	C5-C6-N1	-5.53	119.93	122.70
1	A	781	A	N3-C4-N9	-5.53	122.97	127.40
1	A	1095	U	N3-C4-C5	-5.53	111.28	114.60
5	E	86	ALA	N-CA-CB	-5.53	102.35	110.10
1	A	767	A	OP2-P-O3'	5.53	117.37	105.20
1	A	826	C	C4-C5-C6	-5.53	114.64	117.40
1	A	881	G	N9-C4-C5	-5.53	103.19	105.40
1	A	950	U	C5-C6-N1	-5.53	119.93	122.70
1	A	963	G	N1-C2-N2	-5.53	111.22	116.20
1	A	1190	G	N7-C8-N9	5.53	115.86	113.10
1	A	545	C	OP1-P-OP2	5.53	127.89	119.60
1	A	895	G	C6-C5-N7	-5.53	127.08	130.40
1	A	659	U	C4-C5-C6	5.53	123.02	119.70
1	A	676	A	OP1-P-O3'	5.53	117.36	105.20
1	A	748	C	C2-N1-C1'	5.53	124.88	118.80
1	A	254	G	N3-C4-C5	5.52	131.36	128.60
1	A	773	G	C4-N9-C1'	5.52	133.68	126.50
1	A	755	G	C4-N9-C1'	5.52	133.68	126.50
1	A	837	G	C4-C5-N7	5.52	113.01	110.80
1	A	1292	U	C5-C6-N1	-5.52	119.94	122.70
1	A	1379	G	OP2-P-O3'	5.52	117.35	105.20
1	A	229	U	O5'-P-OP2	-5.52	100.73	105.70
1	A	101	A	C5-N7-C8	-5.52	101.14	103.90
1	A	526	C	O5'-P-OP2	-5.52	100.73	105.70
1	A	623	C	O5'-P-OP1	5.52	117.32	110.70
1	A	681	C	N3-C4-N4	5.52	121.86	118.00
1	A	1304	G	C4-C5-C6	5.52	122.11	118.80
1	A	1306	A	C4-C5-N7	-5.52	107.94	110.70
1	A	1410	G	C8-N9-C4	5.52	108.61	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	832	C	OP2-P-O3'	5.52	117.34	105.20
1	A	1520	G	C5-C6-N1	5.52	114.26	111.50
1	A	403	C	N1-C2-O2	-5.52	115.59	118.90
1	A	659	U	C2-N1-C1'	5.52	124.32	117.70
1	A	255	G	OP2-P-O3'	5.51	117.33	105.20
1	A	916	G	N3-C4-C5	-5.51	125.84	128.60
1	A	1076	C	C2-N1-C1'	5.51	124.86	118.80
1	A	1507	A	OP1-P-O3'	5.51	117.33	105.20
1	A	729	A	C4-C5-C6	5.51	119.76	117.00
1	A	1360	A	OP2-P-O3'	5.51	117.33	105.20
1	A	274	A	C4-C5-C6	-5.51	114.24	117.00
1	A	302	G	N1-C6-O6	-5.51	116.59	119.90
1	A	372	C	O5'-P-OP1	5.51	117.31	110.70
1	A	1369	C	C4-C5-C6	5.51	120.16	117.40
1	A	37	U	N1-C2-N3	5.51	118.20	114.90
1	A	252	U	O5'-P-OP2	5.51	117.31	110.70
1	A	1119	C	C2-N3-C4	5.51	122.66	119.90
1	A	1521	G	C5-C6-N1	5.51	114.25	111.50
1	A	42	G	C8-N9-C4	-5.51	104.20	106.40
1	A	880	C	N3-C4-C5	5.51	124.10	121.90
1	A	1003	G	N3-C4-N9	5.51	129.31	126.00
1	A	1099	G	C5-N7-C8	-5.51	101.55	104.30
1	A	1327	C	C2-N1-C1'	-5.51	112.74	118.80
1	A	1486	G	C2-N3-C4	5.51	114.65	111.90
1	A	1500	A	OP1-P-OP2	5.51	127.86	119.60
1	A	545	C	N1-C2-N3	5.51	123.06	119.20
1	A	599	C	C6-N1-C2	5.51	122.50	120.30
1	A	673	G	N7-C8-N9	5.51	115.85	113.10
1	A	855	G	N3-C4-C5	5.51	131.35	128.60
12	L	25	PRO	CA-C-N	-5.50	105.09	117.20
1	A	190(C)	C	C5-C4-N4	5.50	124.05	120.20
1	A	762	C	C5-C4-N4	-5.50	116.35	120.20
1	A	1267	C	C5-C6-N1	5.50	123.75	121.00
1	A	223	U	C4-C5-C6	5.50	123.00	119.70
1	A	730	G	N3-C4-C5	-5.50	125.85	128.60
1	A	1151	A	O5'-P-OP1	-5.50	100.75	105.70
1	A	1184	G	C2-N3-C4	-5.50	109.15	111.90
1	A	1441	G	OP1-P-OP2	5.50	127.85	119.60
1	A	427	U	C5-C6-N1	-5.50	119.95	122.70
1	A	488	C	N1-C2-O2	-5.50	115.60	118.90
1	A	512	U	C2-N1-C1'	5.50	124.30	117.70
1	A	728	A	OP2-P-O3'	-5.50	93.10	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1095	U	C6-N1-C2	-5.50	117.70	121.00
1	A	1282	C	OP1-P-OP2	-5.50	111.35	119.60
1	A	1387	G	C5-C6-N1	5.50	114.25	111.50
1	A	879	C	N3-C4-N4	5.50	121.85	118.00
2	B	71	VAL	CB-CA-C	-5.50	100.96	111.40
1	A	128	G	C5-C6-N1	-5.50	108.75	111.50
1	A	147	G	C6-C5-N7	-5.50	127.10	130.40
1	A	294	U	C4-C5-C6	5.50	123.00	119.70
1	A	39	G	OP1-P-OP2	5.49	127.84	119.60
1	A	257	G	C2-N3-C4	-5.49	109.15	111.90
1	A	684	A	C4-C5-N7	5.49	113.45	110.70
1	A	738	C	N1-C2-O2	5.49	122.20	118.90
1	A	850	U	N3-C4-C5	-5.49	111.30	114.60
1	A	1160	G	N3-C2-N2	5.49	123.75	119.90
1	A	1356	G	N1-C2-N3	5.49	127.20	123.90
1	A	1061	G	C8-N9-C1'	-5.49	119.86	127.00
1	A	1239	A	N9-C4-C5	-5.49	103.60	105.80
1	A	1470	G	C4-C5-N7	-5.49	108.60	110.80
1	A	226	G	C2-N3-C4	-5.49	109.16	111.90
1	A	370	C	C6-N1-C2	5.49	122.50	120.30
1	A	392	G	N1-C6-O6	5.49	123.19	119.90
1	A	555	C	N3-C4-C5	-5.49	119.70	121.90
3	C	27	LYS	CD-CE-NZ	5.49	124.33	111.70
1	A	724	G	N1-C6-O6	-5.49	116.61	119.90
1	A	732	C	N3-C2-O2	-5.49	118.06	121.90
1	A	749	C	C2-N3-C4	5.49	122.64	119.90
1	A	841	U	N3-C4-O4	5.49	123.24	119.40
1	A	850	U	N3-C4-O4	5.49	123.24	119.40
1	A	1032	G	O4'-C1'-N9	5.49	112.59	108.20
1	A	1090	U	N3-C2-O2	-5.49	118.36	122.20
1	A	1157	A	N1-C6-N6	-5.49	115.31	118.60
1	A	79	G	C5-N7-C8	-5.49	101.56	104.30
1	A	662	G	N9-C4-C5	-5.49	103.20	105.40
1	A	825	G	N1-C6-O6	5.49	123.19	119.90
1	A	1106	G	C5-C6-O6	-5.49	125.31	128.60
1	A	404	U	O5'-P-OP2	-5.49	100.76	105.70
1	A	780	A	N7-C8-N9	5.49	116.54	113.80
1	A	935	A	N9-C4-C5	-5.49	103.61	105.80
1	A	1048	G	OP2-P-O3'	5.49	117.27	105.20
1	A	1384	C	OP2-P-O3'	5.49	117.27	105.20
1	A	329	A	N1-C2-N3	-5.48	126.56	129.30
1	A	436	C	OP1-P-O3'	5.48	117.27	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	992	U	P-O3'-C3'	5.48	126.28	119.70
1	A	1060	C	C4-C5-C6	5.48	120.14	117.40
1	A	1394	A	C2-N3-C4	-5.48	107.86	110.60
1	A	188	C	O5'-P-OP2	-5.48	100.77	105.70
1	A	397	A	N1-C2-N3	5.48	132.04	129.30
1	A	1058	G	C6-C5-N7	-5.48	127.11	130.40
1	A	1102	A	N7-C8-N9	5.48	116.54	113.80
1	A	22	G	C8-N9-C1'	-5.48	119.88	127.00
1	A	190(G)	G	C4-C5-C6	5.48	122.09	118.80
1	A	841	U	C2-N3-C4	5.48	130.29	127.00
1	A	973	G	N9-C4-C5	5.48	107.59	105.40
1	A	1351	U	N1-C2-N3	5.48	118.19	114.90
17	Q	73	VAL	CB-CA-C	-5.48	100.99	111.40
1	A	1178	G	C8-N9-C4	-5.48	104.21	106.40
1	A	1452	C	C6-N1-C2	5.48	122.49	120.30
1	A	35	G	C5-C6-N1	-5.48	108.76	111.50
1	A	431	A	N1-C6-N6	-5.48	115.31	118.60
1	A	704	A	O4'-C1'-N9	-5.48	103.82	108.20
1	A	890	G	C5'-C4'-O4'	5.48	115.67	109.10
1	A	890	G	C4-C5-N7	-5.48	108.61	110.80
1	A	1143	G	C5-C6-N1	-5.48	108.76	111.50
1	A	1289	A	C8-N9-C1'	-5.48	117.84	127.70
1	A	1443	G	C2-N3-C4	-5.48	109.16	111.90
1	A	113	G	OP2-P-O3'	5.47	117.25	105.20
1	A	1429	C	C4-C5-C6	5.47	120.14	117.40
12	L	20	LYS	CD-CE-NZ	5.47	124.29	111.70
1	A	129(A)	G	C8-N9-C4	-5.47	104.21	106.40
1	A	886	G	C5-N7-C8	-5.47	101.56	104.30
1	A	1377	A	C8-N9-C4	5.47	107.99	105.80
1	A	1520	G	N9-C4-C5	-5.47	103.21	105.40
1	A	299	G	C4-C5-C6	5.47	122.08	118.80
1	A	548	G	N1-C6-O6	5.47	123.18	119.90
1	A	596	C	C4-C5-C6	5.47	120.14	117.40
1	A	1544	U	N3-C4-C5	-5.47	111.32	114.60
12	L	18	VAL	N-CA-C	5.47	125.77	111.00
1	A	7	G	C5-C6-O6	-5.47	125.32	128.60
1	A	168	G	C4-C5-C6	5.47	122.08	118.80
1	A	1395	C	N1-C2-O2	-5.47	115.62	118.90
1	A	1436	U	N3-C4-O4	5.47	123.23	119.40
1	A	595	G	N1-C2-N2	-5.47	111.28	116.20
1	A	604	G	C8-N9-C1'	5.47	134.11	127.00
1	A	739	C	N3-C4-N4	5.47	121.83	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1541	PSU	OP2-P-O3'	5.47	117.23	105.20
1	A	615	C	N3-C2-O2	5.46	125.72	121.90
1	A	1360	A	N1-C6-N6	5.46	121.88	118.60
1	A	18	C	O5'-P-OP2	-5.46	100.78	105.70
1	A	35	G	N1-C6-O6	5.46	123.18	119.90
1	A	314	C	C5-C6-N1	-5.46	118.27	121.00
1	A	615	C	C5-C6-N1	5.46	123.73	121.00
1	A	1406	U	N1-C2-N3	5.46	118.18	114.90
1	A	41	G	N7-C8-N9	5.46	115.83	113.10
1	A	715	A	N9-C4-C5	5.46	107.98	105.80
1	A	899	C	C6-N1-C1'	5.46	127.35	120.80
1	A	921	U	C4-C5-C6	5.46	122.97	119.70
1	A	1073	U	N1-C2-N3	5.46	118.17	114.90
1	A	1424	C	C2-N1-C1'	-5.46	112.80	118.80
1	A	32	A	C4-N9-C1'	5.46	136.12	126.30
1	A	532	A	P-O3'-C3'	5.46	126.25	119.70
1	A	1455	G	N1-C2-N2	-5.46	111.29	116.20
1	A	691	G	N9-C4-C5	5.46	107.58	105.40
1	A	70	G	N3-C2-N2	-5.45	116.08	119.90
1	A	189	G	C8-N9-C1'	-5.45	119.91	127.00
1	A	225	C	C5-C6-N1	-5.45	118.27	121.00
1	A	317	G	N1-C6-O6	5.45	123.17	119.90
1	A	816	A	OP1-P-O3'	5.45	117.20	105.20
1	A	706	A	N1-C6-N6	5.45	121.87	118.60
1	A	305	G	O5'-P-OP2	-5.45	100.79	105.70
1	A	317	G	C6-N1-C2	-5.45	121.83	125.10
1	A	792	A	N3-C4-N9	-5.45	123.04	127.40
1	A	935	A	C4-N9-C1'	5.45	136.11	126.30
1	A	1243	C	C4-C5-C6	5.45	120.12	117.40
5	E	90	VAL	CB-CA-C	-5.45	101.04	111.40
1	A	28	G	N1-C2-N3	5.45	127.17	123.90
1	A	75	G	N1-C6-O6	5.45	123.17	119.90
1	A	228	A	C5-C6-N6	5.45	128.06	123.70
1	A	231	G	N1-C6-O6	5.45	123.17	119.90
1	A	363	A	C5-N7-C8	-5.45	101.17	103.90
1	A	457	C	O5'-P-OP1	5.45	117.24	110.70
1	A	911	U	O5'-P-OP1	5.45	117.24	110.70
1	A	1058	G	C4-C5-N7	5.45	112.98	110.80
1	A	1094	G	C8-N9-C4	5.45	108.58	106.40
1	A	1338	G	C5-C6-N1	5.45	114.22	111.50
1	A	448	A	C8-N9-C4	-5.45	103.62	105.80
1	A	537	G	N1-C2-N3	5.45	127.17	123.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116	A	N9-C4-C5	-5.45	103.62	105.80
1	A	162	A	N1-C6-N6	-5.45	115.33	118.60
1	A	803	G	C6-C5-N7	5.45	133.67	130.40
1	A	895	G	C5-C6-O6	-5.45	125.33	128.60
1	A	975	A	N9-C1'-C2'	-5.45	106.01	112.00
1	A	1104	G	N7-C8-N9	5.45	115.82	113.10
1	A	1266	G	N3-C4-C5	5.45	131.32	128.60
12	L	58	VAL	CB-CA-C	-5.45	101.05	111.40
1	A	922	G	N1-C2-N2	5.44	121.10	116.20
1	A	1252	A	OP1-P-OP2	-5.44	111.43	119.60
1	A	538	G	N1-C6-O6	-5.44	116.63	119.90
1	A	679	C	OP1-P-O3'	-5.44	93.23	105.20
1	A	40	C	C6-N1-C2	5.44	122.48	120.30
1	A	124	G	N3-C2-N2	-5.44	116.09	119.90
1	A	329	A	C2-N3-C4	-5.44	107.88	110.60
1	A	435	C	N3-C4-N4	5.44	121.81	118.00
1	A	530	G	C4-C5-N7	5.44	112.98	110.80
1	A	973	G	N1-C6-O6	-5.44	116.64	119.90
1	A	304	U	N3-C4-O4	-5.44	115.59	119.40
1	A	1523	G	N9-C4-C5	5.44	107.58	105.40
1	A	545	C	N3-C2-O2	-5.44	118.09	121.90
1	A	978	A	N1-C6-N6	5.44	121.86	118.60
1	A	1151	A	N1-C6-N6	-5.44	115.34	118.60
1	A	67	C	C6-N1-C2	5.43	122.47	120.30
1	A	311	C	C6-N1-C2	5.43	122.47	120.30
1	A	530	G	C8-N9-C1'	-5.43	119.94	127.00
1	A	1361(A)	C	C2-N1-C1'	5.43	124.78	118.80
1	A	550	G	OP1-P-OP2	5.43	127.75	119.60
1	A	557	G	C5-N7-C8	5.43	107.02	104.30
1	A	652	U	O5'-P-OP1	-5.43	100.81	105.70
1	A	810	C	OP2-P-O3'	-5.43	93.25	105.20
1	A	973	G	C5-C6-N1	5.43	114.22	111.50
1	A	1375	A	C6-C5-N7	-5.43	128.50	132.30
1	A	356	A	N3-C4-N9	-5.43	123.06	127.40
1	A	1346	A	C4-C5-C6	-5.43	114.28	117.00
1	A	1432	G	OP1-P-OP2	5.43	127.74	119.60
1	A	39	G	C4-N9-C1'	-5.43	119.44	126.50
1	A	133	U	C4-C5-C6	5.43	122.96	119.70
1	A	135	C	OP1-P-OP2	-5.43	111.46	119.60
1	A	839	U	N1-C2-O2	5.43	126.60	122.80
1	A	131	C	C5-C6-N1	-5.43	118.29	121.00
1	A	373	A	OP2-P-O3'	-5.43	93.26	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	724	G	O4'-C1'-N9	5.43	112.54	108.20
1	A	743	U	C6-N1-C2	5.43	124.26	121.00
1	A	803	G	N1-C2-N3	5.43	127.16	123.90
1	A	53	A	C6-C5-N7	-5.42	128.50	132.30
1	A	255	G	C5-N7-C8	5.42	107.01	104.30
1	A	644	G	C5-C6-N1	5.42	114.21	111.50
1	A	1271	G	C8-N9-C4	5.42	108.57	106.40
1	A	1305	G	C5-C6-N1	-5.42	108.79	111.50
1	A	1319	A	N3-C4-C5	5.42	130.60	126.80
1	A	1399	C	C4-C5-C6	5.42	120.11	117.40
1	A	593	G	C2-N3-C4	-5.42	109.19	111.90
1	A	819	A	N3-C4-N9	-5.42	123.06	127.40
1	A	98	U	N3-C4-C5	5.42	117.85	114.60
1	A	257	G	OP2-P-O3'	5.42	117.12	105.20
1	A	489	C	OP1-P-O3'	-5.42	93.27	105.20
1	A	675	A	C4-C5-N7	5.42	113.41	110.70
1	A	1178	G	C2-N3-C4	5.42	114.61	111.90
1	A	712	A	C4-N9-C1'	5.42	136.06	126.30
1	A	818	G	C6-C5-N7	5.42	133.65	130.40
1	A	1195	C	OP1-P-OP2	5.42	127.73	119.60
1	A	190(F)	G	N3-C4-N9	-5.42	122.75	126.00
1	A	611	A	C2-N3-C4	-5.42	107.89	110.60
1	A	639	G	N3-C4-N9	-5.42	122.75	126.00
1	A	1513	A	OP2-P-O3'	5.42	117.12	105.20
9	I	109	VAL	CB-CA-C	-5.42	101.10	111.40
1	A	238	G	N1-C2-N3	5.42	127.15	123.90
1	A	909	A	OP1-P-O3'	-5.42	93.28	105.20
1	A	1057	G	N1-C2-N3	-5.42	120.65	123.90
1	A	1217	C	C2-N1-C1'	-5.42	112.84	118.80
1	A	1334	G	N3-C4-N9	5.42	129.25	126.00
1	A	1494	G	C4-N9-C1'	5.42	133.54	126.50
1	A	264	U	N3-C2-O2	-5.42	118.41	122.20
1	A	1087	G	C4-C5-N7	5.42	112.97	110.80
1	A	1307	U	C5-C6-N1	-5.42	119.99	122.70
1	A	916	G	OP1-P-OP2	5.41	127.72	119.60
1	A	1386	G	C4-C5-N7	-5.41	108.64	110.80
1	A	982	U	OP1-P-OP2	-5.41	111.48	119.60
1	A	1131	G	C5-C6-N1	-5.41	108.79	111.50
1	A	1227	A	O4'-C1'-N9	-5.41	103.87	108.20
1	A	1365	G	N1-C6-O6	-5.41	116.65	119.90
1	A	190(F)	G	OP2-P-O3'	5.41	117.10	105.20
1	A	1229	A	C8-N9-C4	5.41	107.96	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	283	C	OP1-P-OP2	-5.41	111.49	119.60
1	A	546	G	N3-C2-N2	-5.41	116.11	119.90
1	A	1336	C	C6-N1-C1'	-5.41	114.31	120.80
1	A	224	C	OP1-P-OP2	5.41	127.71	119.60
1	A	406	G	P-O3'-C3'	5.41	126.19	119.70
1	A	1158	C	N3-C4-N4	5.41	121.78	118.00
1	A	32	A	C6-C5-N7	-5.41	128.52	132.30
1	A	197	A	O4'-C1'-N9	-5.41	103.88	108.20
1	A	506	G	C8-N9-C1'	-5.41	119.97	127.00
1	A	626	U	C2-N3-C4	-5.41	123.76	127.00
1	A	897	C	N3-C4-N4	-5.41	114.22	118.00
1	A	14	U	N3-C2-O2	-5.40	118.42	122.20
1	A	834	C	C6-N1-C2	5.40	122.46	120.30
1	A	355	C	C6-N1-C2	-5.40	118.14	120.30
1	A	483	C	N3-C4-N4	-5.40	114.22	118.00
1	A	1364	U	C2-N1-C1'	-5.40	111.22	117.70
9	I	62	TYR	CB-CA-C	-5.40	99.60	110.40
13	M	111	LYS	CD-CE-NZ	5.40	124.12	111.70
1	A	112	G	C5-C6-N1	5.40	114.20	111.50
1	A	176	C	N3-C4-N4	5.40	121.78	118.00
1	A	480	U	N3-C4-C5	-5.40	111.36	114.60
1	A	973	G	C6-C5-N7	5.40	133.64	130.40
1	A	1166	G	C5-C6-N1	-5.40	108.80	111.50
1	A	1196	U	C4-C5-C6	-5.40	116.46	119.70
1	A	1286	A	OP2-P-O3'	5.40	117.08	105.20
1	A	382	A	N1-C2-N3	5.40	132.00	129.30
1	A	760	G	C8-N9-C1'	5.40	134.02	127.00
1	A	63	C	OP1-P-O3'	-5.40	93.33	105.20
1	A	198	G	N1-C2-N3	5.40	127.14	123.90
1	A	319	G	C5-C6-O6	-5.40	125.36	128.60
1	A	327	A	OP1-P-O3'	5.40	117.07	105.20
1	A	885	G	OP1-P-OP2	5.40	127.69	119.60
1	A	1305	G	C5-C6-O6	5.40	131.84	128.60
1	A	1370	G	C2-N3-C4	-5.40	109.20	111.90
12	L	26	ALA	N-CA-C	-5.40	96.42	111.00
1	A	177	C	N3-C2-O2	-5.40	118.12	121.90
1	A	229	U	O5'-P-OP1	5.40	117.18	110.70
1	A	296	U	C5-C6-N1	-5.39	120.00	122.70
1	A	490	G	N1-C2-N3	5.39	127.14	123.90
1	A	690	G	C5-C6-N1	-5.39	108.80	111.50
1	A	1119	C	N3-C4-C5	-5.39	119.74	121.90
1	A	73	C	O4'-C1'-N1	-5.39	103.89	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	618	C	OP2-P-O3'	5.39	117.06	105.20
1	A	623	C	C2-N1-C1'	-5.39	112.87	118.80
1	A	1258	G	C5-C6-O6	5.39	131.84	128.60
1	A	1302	U	C6-N1-C2	-5.39	117.77	121.00
1	A	22	G	C4-C5-C6	5.39	122.03	118.80
1	A	1279	A	C4-C5-N7	5.39	113.39	110.70
1	A	1353	G	C6-N1-C2	-5.39	121.86	125.10
1	A	5	U	C4-C5-C6	5.39	122.93	119.70
1	A	22	G	P-O3'-C3'	5.39	126.17	119.70
1	A	144	G	OP2-P-O3'	5.39	117.06	105.20
1	A	553	A	N1-C6-N6	5.39	121.83	118.60
1	A	716	A	OP2-P-O3'	5.39	117.06	105.20
1	A	333	G	C4-N9-C1'	5.39	133.50	126.50
1	A	678	U	N3-C2-O2	-5.39	118.43	122.20
1	A	1396	A	OP1-P-O3'	5.39	117.05	105.20
11	K	75	TYR	CB-CG-CD1	-5.39	117.77	121.00
17	Q	84	LEU	CA-CB-CG	-5.39	102.91	115.30
1	A	641	U	C5-C4-O4	-5.39	122.67	125.90
1	A	750	G	N3-C4-N9	5.39	129.23	126.00
1	A	975	A	C5-C6-N6	5.39	128.01	123.70
1	A	1033	G	N3-C4-C5	-5.39	125.91	128.60
1	A	1450	U	C5-C6-N1	-5.39	120.01	122.70
1	A	1487	G	N1-C2-N2	-5.39	111.35	116.20
1	A	30	U	N3-C4-O4	5.38	123.17	119.40
1	A	300	A	C2-N3-C4	-5.38	107.91	110.60
1	A	568	G	OP2-P-O3'	5.38	117.04	105.20
1	A	580	U	O4'-C1'-N1	5.38	112.50	108.20
1	A	708	C	O5'-P-OP1	5.38	117.16	110.70
1	A	935	A	C8-N9-C4	5.38	107.95	105.80
1	A	1175	G	C5-N7-C8	-5.38	101.61	104.30
1	A	1394	A	N1-C2-N3	5.38	131.99	129.30
1	A	1405	G	O5'-P-OP1	5.38	117.16	110.70
1	A	1486	G	N3-C4-N9	5.38	129.23	126.00
1	A	166	G	C8-N9-C4	5.38	108.55	106.40
1	A	194	C	OP1-P-OP2	-5.38	111.53	119.60
1	A	357	G	C5-N7-C8	5.38	106.99	104.30
1	A	309	G	C4-C5-C6	5.38	122.03	118.80
1	A	403	C	N1-C2-N3	5.37	122.96	119.20
1	A	1425	U	C6-N1-C1'	5.37	128.72	121.20
1	A	333	G	C5-N7-C8	5.37	106.99	104.30
1	A	1420	C	C2-N3-C4	5.37	122.59	119.90
1	A	1533	C	OP1-P-OP2	-5.37	111.54	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	53	LEU	CB-CG-CD1	-5.37	101.87	111.00
1	A	28	G	N3-C2-N2	-5.37	116.14	119.90
1	A	574	A	OP2-P-O3'	5.37	117.01	105.20
1	A	918	A	N1-C2-N3	5.37	131.99	129.30
1	A	1031	G	C2-N3-C4	5.37	114.58	111.90
1	A	1104	G	C2-N3-C4	-5.37	109.22	111.90
1	A	24	U	C5-C4-O4	-5.37	122.68	125.90
1	A	1187	G	N7-C8-N9	5.37	115.78	113.10
1	A	396	G	N7-C8-N9	5.37	115.78	113.10
1	A	422	C	N3-C2-O2	-5.37	118.14	121.90
1	A	1002	G	C8-N9-C4	-5.37	104.25	106.40
1	A	246	A	C6-N1-C2	-5.36	115.38	118.60
1	A	499	A	C2-N3-C4	5.36	113.28	110.60
1	A	627	G	OP2-P-O3'	5.36	117.00	105.20
1	A	883	C	OP1-P-O3'	-5.36	93.40	105.20
1	A	988	G	C4-C5-N7	-5.36	108.66	110.80
1	A	1290	G	C4-C5-N7	5.36	112.95	110.80
1	A	1533	C	C6-N1-C2	-5.36	118.16	120.30
1	A	167	G	N9-C1'-C2'	-5.36	106.10	112.00
1	A	319	G	C4-N9-C1'	5.36	133.47	126.50
1	A	1222	G	C5-N7-C8	5.36	106.98	104.30
1	A	173	U	C5-C4-O4	5.36	129.12	125.90
1	A	319	G	C4-C5-N7	5.36	112.94	110.80
1	A	752	G	C5-C6-N1	-5.36	108.82	111.50
1	A	770	C	OP2-P-O3'	5.36	116.99	105.20
1	A	816	A	C2-N3-C4	-5.36	107.92	110.60
1	A	1275	A	C8-N9-C4	5.36	107.94	105.80
1	A	668	G	N1-C2-N3	5.36	127.11	123.90
1	A	41	G	N1-C2-N3	5.36	127.11	123.90
1	A	793	U	C4-C5-C6	5.36	122.91	119.70
1	A	1281	U	OP2-P-O3'	5.36	116.99	105.20
1	A	1322	C	C5'-C4'-O4'	-5.36	102.67	109.10
1	A	130	A	OP2-P-O3'	5.36	116.98	105.20
1	A	263	A	C4-C5-C6	-5.36	114.32	117.00
1	A	653	A	OP1-P-OP2	-5.36	111.57	119.60
1	A	705	U	N3-C2-O2	-5.36	118.45	122.20
1	A	779	C	C2-N3-C4	-5.36	117.22	119.90
1	A	553	A	O5'-P-OP2	-5.35	100.88	105.70
1	A	943	U	N1-C2-N3	5.35	118.11	114.90
1	A	552	U	N3-C2-O2	5.35	125.95	122.20
4	D	2	GLY	N-CA-C	5.35	126.48	113.10
1	A	410	G	N9-C4-C5	5.35	107.54	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	790	A	C4-C5-C6	5.35	119.67	117.00
1	A	821	G	N9-C4-C5	-5.35	103.26	105.40
1	A	1521	G	OP2-P-O3'	5.35	116.97	105.20
1	A	703	G	C8-N9-C4	5.35	108.54	106.40
1	A	1280	A	C8-N9-C4	-5.35	103.66	105.80
1	A	1453	G	N3-C4-N9	5.35	129.21	126.00
1	A	1488	G	C5-N7-C8	5.35	106.97	104.30
1	A	808	C	N3-C2-O2	5.35	125.64	121.90
1	A	16	A	C4-C5-N7	-5.34	108.03	110.70
1	A	32	A	O4'-C1'-N9	-5.34	103.92	108.20
1	A	187	C	OP1-P-O3'	-5.34	93.44	105.20
1	A	423	G	C4-N9-C1'	5.34	133.45	126.50
1	A	415	A	N9-C4-C5	-5.34	103.66	105.80
1	A	1184	G	N1-C6-O6	5.34	123.11	119.90
1	A	134	A	N9-C4-C5	5.34	107.94	105.80
1	A	385	C	C4-C5-C6	-5.34	114.73	117.40
1	A	397	A	C6-C5-N7	-5.34	128.56	132.30
1	A	815	A	OP1-P-OP2	-5.34	111.59	119.60
1	A	1279	A	C5-C6-N6	-5.34	119.43	123.70
1	A	1311	G	C8-N9-C4	-5.34	104.26	106.40
1	A	778	G	C5-C6-O6	5.34	131.80	128.60
1	A	818	G	O5'-P-OP2	5.34	117.11	110.70
1	A	828	A	C2-N3-C4	-5.34	107.93	110.60
18	R	82	THR	N-CA-C	-5.34	96.58	111.00
1	A	282	A	N1-C6-N6	5.34	121.80	118.60
1	A	336	C	C5-C6-N1	-5.34	118.33	121.00
1	A	756	C	C5-C6-N1	5.34	123.67	121.00
1	A	830	G	OP2-P-O3'	5.34	116.94	105.20
1	A	287	U	OP2-P-O3'	5.34	116.94	105.20
1	A	694	A	N7-C8-N9	-5.34	111.13	113.80
1	A	1403	C	N3-C4-C5	-5.34	119.77	121.90
1	A	1466	C	C2-N3-C4	-5.34	117.23	119.90
1	A	514	C	C4-C5-C6	5.33	120.07	117.40
1	A	630	G	C6-C5-N7	5.33	133.60	130.40
1	A	653	A	N1-C6-N6	-5.33	115.40	118.60
1	A	259	G	N3-C4-C5	5.33	131.27	128.60
1	A	830	G	C4-C5-C6	-5.33	115.60	118.80
1	A	1464	G	N1-C6-O6	5.33	123.10	119.90
1	A	398	C	O5'-P-OP2	5.33	117.10	110.70
1	A	74	C	OP2-P-O3'	5.33	116.92	105.20
1	A	753	A	OP1-P-O3'	5.33	116.92	105.20
1	A	821	G	C8-N9-C4	5.33	108.53	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	445	G	C8-N9-C4	-5.33	104.27	106.40
1	A	12	U	N1-C2-N3	-5.33	111.70	114.90
1	A	764	C	C6-N1-C1'	-5.33	114.41	120.80
1	A	1349	A	N1-C6-N6	-5.33	115.40	118.60
1	A	1353	G	C5-C6-N1	5.33	114.16	111.50
1	A	1539	C	N1-C2-O2	5.33	122.10	118.90
2	B	205	ASP	CB-CG-OD1	5.33	123.09	118.30
1	A	222	U	OP1-P-OP2	5.32	127.59	119.60
1	A	330	C	P-O3'-C3'	-5.32	113.31	119.70
1	A	684	A	O5'-P-OP1	-5.32	100.91	105.70
1	A	1074	G	C8-N9-C1'	-5.32	120.08	127.00
1	A	732	C	N1-C2-O2	5.32	122.09	118.90
1	A	740	U	C4-C5-C6	5.32	122.89	119.70
1	A	830	G	N3-C2-N2	-5.32	116.17	119.90
1	A	145	G	N3-C2-N2	-5.32	116.17	119.90
1	A	204	U	C6-N1-C1'	-5.32	113.75	121.20
1	A	509	A	OP1-P-OP2	5.32	127.58	119.60
1	A	1222	G	N3-C4-N9	-5.32	122.81	126.00
1	A	1476	G	N1-C6-O6	5.32	123.09	119.90
1	A	219	C	C5-C6-N1	-5.32	118.34	121.00
1	A	271	C	N1-C2-N3	-5.32	115.48	119.20
1	A	626	U	C5-C6-N1	-5.32	120.04	122.70
1	A	825	G	C2-N3-C4	-5.32	109.24	111.90
1	A	34	C	OP1-P-OP2	5.32	127.58	119.60
1	A	551	U	C2-N3-C4	-5.32	123.81	127.00
1	A	1218	C	O4'-C1'-N1	5.32	112.45	108.20
1	A	1426	C	O5'-P-OP1	5.32	117.08	110.70
1	A	1452	C	N1-C2-N3	-5.32	115.48	119.20
1	A	1523	G	C6-C5-N7	-5.32	127.21	130.40
18	R	64	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	130	A	N1-C2-N3	5.32	131.96	129.30
1	A	458	C	C5-C6-N1	5.32	123.66	121.00
1	A	629	G	C8-N9-C4	-5.32	104.27	106.40
1	A	803	G	C5-C6-O6	5.32	131.79	128.60
1	A	1121	U	N3-C4-C5	5.32	117.79	114.60
1	A	1524	C	O4'-C1'-N1	-5.32	103.95	108.20
1	A	280	C	C4-C5-C6	5.31	120.06	117.40
1	A	838	G	OP2-P-O3'	5.31	116.89	105.20
1	A	1179	A	N3-C4-C5	5.31	130.52	126.80
1	A	520	A	P-O3'-C3'	-5.31	113.33	119.70
1	A	1150	U	C6-N1-C2	-5.31	117.81	121.00
1	A	1306	A	C5-C6-N6	5.31	127.95	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	U	C6-N1-C2	5.31	124.19	121.00
1	A	687	A	N3-C4-C5	-5.31	123.08	126.80
1	A	797	C	C5-C4-N4	-5.31	116.48	120.20
1	A	811	C	N3-C4-C5	5.31	124.02	121.90
1	A	1485	U	N1-C2-N3	5.31	118.08	114.90
1	A	399	G	C4-N9-C1'	-5.31	119.60	126.50
1	A	423	G	N3-C4-C5	-5.31	125.95	128.60
1	A	733	A	O4'-C1'-N9	5.31	112.45	108.20
1	A	1524	C	N3-C4-N4	5.31	121.72	118.00
1	A	1376	U	N3-C4-C5	-5.31	111.42	114.60
1	A	388	G	C8-N9-C4	5.30	108.52	106.40
1	A	1383	C	C6-N1-C1'	-5.30	114.43	120.80
14	N	27	CYS	CA-CB-SG	-5.30	104.45	114.00
1	A	339	C	C5-C4-N4	-5.30	116.49	120.20
1	A	350	G	N7-C8-N9	5.30	115.75	113.10
1	A	1357	A	OP2-P-O3'	5.30	116.87	105.20
1	A	89	C	C2-N3-C4	5.30	122.55	119.90
1	A	275	G	C4-C5-C6	5.30	121.98	118.80
1	A	307	C	C2-N3-C4	5.30	122.55	119.90
1	A	331	G	C4-N9-C1'	5.30	133.39	126.50
1	A	812	C	N3-C4-C5	-5.30	119.78	121.90
1	A	1031	G	N3-C4-C5	-5.30	125.95	128.60
1	A	1488	G	C8-N9-C4	5.30	108.52	106.40
1	A	1503	A	OP1-P-O3'	5.30	116.86	105.20
1	A	1515	C	C2-N1-C1'	-5.30	112.97	118.80
1	A	709	G	C8-N9-C4	-5.30	104.28	106.40
1	A	669	U	C2-N3-C4	5.30	130.18	127.00
1	A	944	G	C4-C5-C6	5.30	121.98	118.80
1	A	57	G	N1-C2-N3	5.30	127.08	123.90
1	A	773	G	N3-C4-N9	5.30	129.18	126.00
1	A	1359	C	N3-C4-C5	5.30	124.02	121.90
1	A	566	G	C6-C5-N7	-5.29	127.22	130.40
1	A	1542	U	C2-N3-C4	5.29	130.18	127.00
1	A	166	G	N1-C6-O6	5.29	123.08	119.90
1	A	256	U	N1-C2-O2	-5.29	119.09	122.80
1	A	418	C	C2-N3-C4	-5.29	117.25	119.90
1	A	719	C	C6-N1-C2	5.29	122.42	120.30
1	A	1083	U	C2-N1-C1'	-5.29	111.35	117.70
1	A	1276	G	N1-C2-N2	5.29	120.97	116.20
1	A	23	C	OP2-P-O3'	5.29	116.84	105.20
1	A	437	U	N1-C2-N3	5.29	118.08	114.90
1	A	739	C	P-O5'-C5'	-5.29	112.43	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1096	C	OP2-P-O3'	5.29	116.84	105.20
11	K	25	TYR	CA-CB-CG	-5.29	103.34	113.40
1	A	331	G	C8-N9-C1'	-5.29	120.12	127.00
1	A	488	C	N3-C2-O2	5.29	125.60	121.90
1	A	976	G	C5-N7-C8	5.29	106.94	104.30
1	A	637	G	O4'-C1'-N9	-5.29	103.97	108.20
1	A	1495	U	N1-C2-O2	-5.29	119.10	122.80
1	A	1503	A	O4'-C1'-N9	5.29	112.43	108.20
1	A	331	G	OP1-P-OP2	-5.29	111.67	119.60
1	A	529	G	C4-C5-C6	5.29	121.97	118.80
1	A	1190	G	N3-C4-N9	-5.29	122.83	126.00
1	A	246	A	C5-C6-N1	5.29	120.34	117.70
1	A	633	G	N1-C6-O6	5.29	123.07	119.90
1	A	877	C	N3-C4-C5	5.29	124.01	121.90
1	A	1196	U	OP1-P-OP2	-5.29	111.67	119.60
1	A	637	G	OP2-P-O3'	5.28	116.82	105.20
1	A	650	G	N1-C2-N2	5.28	120.95	116.20
1	A	941	G	C5-C6-O6	-5.28	125.43	128.60
1	A	1019	C	C6-N1-C1'	-5.28	114.46	120.80
1	A	51	A	C6-N1-C2	-5.28	115.43	118.60
1	A	315	A	OP2-P-O3'	-5.28	93.58	105.20
1	A	1303	C	C5-C4-N4	5.28	123.90	120.20
1	A	352	C	OP1-P-O3'	5.28	116.82	105.20
1	A	589	C	O5'-P-OP2	-5.28	100.95	105.70
1	A	986	A	C2-N3-C4	-5.28	107.96	110.60
1	A	1075	C	C6-N1-C2	-5.28	118.19	120.30
1	A	1135	U	C5-C6-N1	5.28	125.34	122.70
1	A	416	G	OP2-P-O3'	5.28	116.81	105.20
1	A	773	G	N1-C6-O6	5.28	123.07	119.90
1	A	1241	G	C4-N9-C1'	5.28	133.36	126.50
1	A	117	G	N3-C4-N9	5.28	129.17	126.00
1	A	900	A	C6-N1-C2	-5.28	115.43	118.60
1	A	960	U	C6-N1-C2	-5.28	117.83	121.00
1	A	1152	A	C5-N7-C8	5.28	106.54	103.90
1	A	228	A	N1-C2-N3	5.28	131.94	129.30
1	A	322	C	OP1-P-O3'	-5.28	93.59	105.20
1	A	577	G	N3-C4-N9	-5.28	122.83	126.00
1	A	811	C	C4-C5-C6	5.28	120.04	117.40
1	A	870	U	N3-C2-O2	5.28	125.89	122.20
1	A	910	C	C2-N1-C1'	5.28	124.60	118.80
1	A	912	C	OP2-P-O3'	5.28	116.81	105.20
1	A	1077	G	C5-C6-O6	5.28	131.76	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1405	G	O5'-P-OP2	-5.28	100.95	105.70
1	A	1474	G	N3-C4-N9	-5.28	122.83	126.00
9	I	96	LEU	CA-CB-CG	5.28	127.43	115.30
1	A	16	A	C5-C6-N6	5.27	127.92	123.70
1	A	172	A	C2-N3-C4	-5.27	107.96	110.60
1	A	1232	U	C5-C4-O4	-5.27	122.74	125.90
1	A	730	G	N9-C4-C5	5.27	107.51	105.40
1	A	1313	U	C5-C4-O4	-5.27	122.74	125.90
1	A	254	G	C4-C5-N7	5.27	112.91	110.80
1	A	394	G	C8-N9-C4	-5.27	104.29	106.40
1	A	905	U	N3-C4-O4	5.27	123.09	119.40
1	A	1090	U	N3-C4-C5	-5.27	111.44	114.60
1	A	1182	G	N1-C2-N2	-5.27	111.46	116.20
1	A	1214	C	C6-N1-C1'	5.27	127.12	120.80
11	K	117	ASN	N-CA-C	5.27	125.23	111.00
1	A	415	A	N3-C4-C5	5.27	130.49	126.80
1	A	1074	G	N9-C4-C5	-5.27	103.29	105.40
1	A	32	A	C5-N7-C8	-5.27	101.27	103.90
1	A	389	A	C4-C5-C6	5.27	119.63	117.00
1	A	835	U	C2-N1-C1'	5.27	124.02	117.70
1	A	408	A	C4-C5-C6	5.26	119.63	117.00
1	A	594	G	C8-N9-C4	5.26	108.51	106.40
1	A	638	G	O5'-P-OP2	-5.26	100.96	105.70
1	A	26	A	C4-C5-C6	5.26	119.63	117.00
1	A	43	C	OP2-P-O3'	5.26	116.78	105.20
1	A	408	A	OP1-P-O3'	-5.26	93.62	105.20
1	A	970	C	C5-C4-N4	-5.26	116.52	120.20
1	A	64	G	N1-C2-N2	-5.26	111.47	116.20
1	A	171	A	O4'-C1'-N9	-5.26	103.99	108.20
1	A	481	G	N1-C6-O6	5.26	123.06	119.90
1	A	619	U	C4-C5-C6	5.26	122.86	119.70
1	A	1082	G	C5-C6-O6	-5.26	125.44	128.60
1	A	1124	G	N7-C8-N9	5.26	115.73	113.10
1	A	1166	G	C4-N9-C1'	5.26	133.34	126.50
1	A	170	U	N3-C2-O2	5.26	125.88	122.20
1	A	241	C	C2-N1-C1'	-5.26	113.02	118.80
1	A	975	A	C8-N9-C4	-5.26	103.70	105.80
1	A	1335	C	N3-C4-C5	5.26	124.00	121.90
1	A	1341	U	C4-C5-C6	5.26	122.86	119.70
1	A	980	C	C5-C6-N1	5.26	123.63	121.00
1	A	576	G	N3-C4-N9	5.26	129.15	126.00
1	A	591	U	C4-C5-C6	5.26	122.85	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	733	A	C4-C5-C6	5.26	119.63	117.00
1	A	892	A	C8-N9-C4	-5.26	103.70	105.80
1	A	1211	U	C2-N1-C1'	5.26	124.01	117.70
1	A	1483	A	O4'-C1'-N9	5.26	112.40	108.20
1	A	103	C	C2-N1-C1'	5.25	124.58	118.80
1	A	697	U	O5'-P-OP2	-5.25	100.97	105.70
1	A	149	A	N7-C8-N9	-5.25	111.17	113.80
1	A	909	A	N3-C4-C5	-5.25	123.12	126.80
1	A	1136	U	O4'-C1'-N1	5.25	112.40	108.20
1	A	1173	G	C4-N9-C1'	-5.25	119.67	126.50
9	I	53	VAL	CB-CA-C	5.25	121.38	111.40
1	A	374	A	C2-N3-C4	-5.25	107.97	110.60
1	A	588	G	N1-C6-O6	5.25	123.05	119.90
1	A	601	C	OP1-P-OP2	-5.25	111.72	119.60
1	A	641	U	C4-C5-C6	5.25	122.85	119.70
1	A	755	G	C4-C5-N7	5.25	112.90	110.80
1	A	962	C	C2-N1-C1'	-5.25	113.02	118.80
1	A	982	U	C2-N1-C1'	5.25	124.00	117.70
1	A	1205	U	C6-N1-C2	5.25	124.15	121.00
1	A	603	U	O5'-P-OP1	5.25	117.00	110.70
1	A	1474	G	N3-C2-N2	-5.25	116.22	119.90
14	N	43	CYS	CA-CB-SG	-5.25	104.55	114.00
1	A	101	A	N9-C4-C5	5.25	107.90	105.80
1	A	230	G	N1-C2-N3	5.25	127.05	123.90
1	A	496	A	C8-N9-C4	5.25	107.90	105.80
1	A	685	G	N1-C2-N2	5.25	120.92	116.20
1	A	1077	G	C4-C5-N7	-5.25	108.70	110.80
1	A	1465	C	C2-N1-C1'	5.25	124.57	118.80
1	A	1514	C	C5-C6-N1	-5.25	118.38	121.00
1	A	342	C	N1-C2-N3	5.25	122.87	119.20
1	A	500	G	C4-N9-C1'	-5.25	119.68	126.50
1	A	539	A	C5-C6-N1	5.25	120.32	117.70
1	A	817	C	N1-C1'-C2'	5.25	120.82	114.00
1	A	760	G	C6-N1-C2	-5.25	121.95	125.10
1	A	1067	A	N7-C8-N9	5.25	116.42	113.80
1	A	332	G	OP1-P-OP2	5.24	127.46	119.60
1	A	557	G	C6-C5-N7	5.24	133.54	130.40
1	A	909	A	C5-C6-N6	-5.24	119.51	123.70
1	A	987	G	N3-C2-N2	-5.24	116.23	119.90
1	A	541	G	OP1-P-O3'	5.24	116.73	105.20
1	A	635	G	C6-N1-C2	5.24	128.24	125.10
1	A	854	G	C8-N9-C1'	-5.24	120.19	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	952	U	OP2-P-O3'	5.24	116.72	105.20
1	A	1379	G	C4-C5-N7	5.24	112.89	110.80
1	A	293	G	C8-N9-C4	5.24	108.50	106.40
1	A	1337	G	C8-N9-C4	-5.24	104.31	106.40
9	I	14	VAL	CB-CA-C	-5.24	101.45	111.40
1	A	13	U	OP1-P-OP2	-5.24	111.75	119.60
1	A	299	G	C8-N9-C1'	-5.24	120.19	127.00
1	A	305	G	C6-C5-N7	-5.24	127.26	130.40
1	A	720	C	O5'-P-OP2	-5.24	100.99	105.70
1	A	1311	G	N7-C8-N9	5.24	115.72	113.10
1	A	1338	G	C2-N3-C4	5.24	114.52	111.90
1	A	58	C	C5-C4-N4	-5.23	116.54	120.20
1	A	275	G	OP1-P-O3'	5.23	116.72	105.20
1	A	310	G	C2-N3-C4	5.23	114.52	111.90
1	A	357	G	C8-N9-C1'	-5.23	120.20	127.00
1	A	398	C	OP1-P-OP2	5.23	127.45	119.60
1	A	476	G	O5'-P-OP1	-5.23	100.99	105.70
1	A	536	C	C5-C6-N1	5.23	123.61	121.00
1	A	831	U	N1-C2-O2	-5.23	119.14	122.80
1	A	1003	G	C4-N9-C1'	5.23	133.30	126.50
1	A	1449	C	N3-C2-O2	5.23	125.56	121.90
1	A	970	C	C2-N1-C1'	5.23	124.55	118.80
1	A	790	A	C4-C5-N7	5.23	113.31	110.70
1	A	875	C	C4-C5-C6	5.23	120.01	117.40
1	A	1147	C	C5-C4-N4	5.23	123.86	120.20
1	A	1367	C	N3-C4-N4	5.23	121.66	118.00
3	C	83	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	A	365	U	OP1-P-O3'	5.23	116.70	105.20
1	A	1127	G	P-O3'-C3'	-5.23	113.43	119.70
1	A	145	G	N3-C4-C5	5.22	131.21	128.60
1	A	259	G	OP2-P-O3'	5.22	116.69	105.20
1	A	872	A	C6-N1-C2	5.22	121.73	118.60
1	A	1199	U	C5-C6-N1	-5.22	120.09	122.70
1	A	1356	G	C2-N3-C4	-5.22	109.29	111.90
1	A	1395	C	OP1-P-O3'	-5.22	93.71	105.20
1	A	745	C	C6-N1-C1'	5.22	127.06	120.80
1	A	975	A	N1-C6-N6	5.22	121.73	118.60
1	A	174	C	N1-C2-O2	-5.22	115.77	118.90
1	A	325	A	C4-C5-C6	-5.22	114.39	117.00
1	A	530	G	C6-N1-C2	5.22	128.23	125.10
1	A	684	A	C5-N7-C8	-5.22	101.29	103.90
1	A	824	C	N1-C2-O2	-5.22	115.77	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	960	U	C2-N1-C1'	5.22	123.96	117.70
1	A	962	C	C5-C6-N1	-5.22	118.39	121.00
1	A	1198	G	OP1-P-OP2	5.22	127.43	119.60
1	A	1297	C	OP2-P-O3'	5.22	116.68	105.20
1	A	1409	C	C6-N1-C1'	-5.22	114.54	120.80
1	A	33	A	C6-N1-C2	-5.22	115.47	118.60
1	A	69	G	C8-N9-C1'	5.22	133.78	127.00
1	A	132	C	C5-C4-N4	5.22	123.85	120.20
1	A	35	G	C4-C5-N7	-5.22	108.71	110.80
1	A	70	G	OP2-P-O3'	5.22	116.68	105.20
1	A	84	U	O5'-P-OP2	5.22	116.96	110.70
1	A	131	C	N1-C2-O2	-5.22	115.77	118.90
1	A	179	A	C2-N3-C4	-5.22	107.99	110.60
1	A	254	G	N3-C2-N2	-5.22	116.25	119.90
1	A	818	G	OP2-P-O3'	5.21	116.67	105.20
1	A	1094	G	O5'-P-OP1	-5.21	101.01	105.70
1	A	1289	A	C4-N9-C1'	5.21	135.68	126.30
1	A	105	G	N3-C4-C5	5.21	131.21	128.60
1	A	148	G	C2-N3-C4	-5.21	109.29	111.90
1	A	175	C	OP2-P-O3'	5.21	116.67	105.20
1	A	397	A	C6-N1-C2	-5.21	115.47	118.60
1	A	116	A	N3-C4-C5	5.21	130.45	126.80
1	A	223	U	C5-C4-O4	5.21	129.03	125.90
1	A	736	C	N1-C2-O2	5.21	122.03	118.90
1	A	1291	G	C8-N9-C4	5.21	108.48	106.40
1	A	1524	C	C5-C6-N1	5.21	123.61	121.00
1	A	790	A	C8-N9-C4	5.21	107.88	105.80
1	A	61	G	C8-N9-C4	5.21	108.48	106.40
1	A	535	A	OP2-P-O3'	5.21	116.66	105.20
1	A	687	A	C4-C5-N7	-5.21	108.10	110.70
1	A	814	A	OP1-P-O3'	5.21	116.66	105.20
1	A	1354	C	C2-N3-C4	5.21	122.50	119.90
1	A	1070	U	C2-N3-C4	-5.21	123.88	127.00
1	A	1506	U	C2-N1-C1'	5.21	123.95	117.70
9	I	61	ALA	N-CA-C	5.21	125.06	111.00
1	A	31	G	C5-C6-N1	-5.21	108.90	111.50
1	A	125	U	N3-C4-C5	-5.21	111.48	114.60
1	A	281	G	O4'-C1'-N9	5.21	112.36	108.20
1	A	653	A	O5'-P-OP2	5.21	116.95	110.70
1	A	819	A	O5'-P-OP2	-5.21	101.02	105.70
1	A	1096	C	C2-N3-C4	5.21	122.50	119.90
2	B	17	PHE	CB-CA-C	5.21	120.81	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	53	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	A	5	U	C6-N1-C2	5.20	124.12	121.00
1	A	376	G	N3-C4-C5	-5.20	126.00	128.60
1	A	1090	U	C6-N1-C2	-5.20	117.88	121.00
1	A	1137	C	O5'-P-OP1	-5.20	101.02	105.70
1	A	1168	A	C4-C5-N7	-5.20	108.10	110.70
1	A	1230	C	C5-C4-N4	-5.20	116.56	120.20
1	A	1309	G	N1-C6-O6	-5.20	116.78	119.90
1	A	1403	C	O4'-C1'-N1	-5.20	104.04	108.20
1	A	300	A	OP2-P-O3'	5.20	116.64	105.20
1	A	506	G	O4'-C1'-N9	-5.20	104.04	108.20
1	A	1080	A	OP1-P-O3'	5.20	116.64	105.20
3	C	172	ARG	NE-CZ-NH2	-5.20	117.70	120.30
7	G	115	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	A	141	A	C5-N7-C8	-5.20	101.30	103.90
1	A	701	C	C5-C6-N1	-5.20	118.40	121.00
1	A	1368	G	C5-C6-N1	5.20	114.10	111.50
1	A	851	G	C8-N9-C1'	-5.20	120.25	127.00
1	A	1067	A	C4-C5-N7	-5.20	108.10	110.70
1	A	1160	G	N1-C2-N2	-5.20	111.52	116.20
1	A	1217	C	C6-N1-C1'	5.20	127.03	120.80
1	A	1509	C	OP2-P-O3'	5.20	116.63	105.20
15	O	48	LYS	CD-CE-NZ	5.20	123.65	111.70
1	A	449	C	OP1-P-OP2	5.19	127.39	119.60
1	A	494	G	O5'-P-OP1	-5.19	101.03	105.70
1	A	518	C	N3-C4-C5	5.19	123.98	121.90
1	A	757	U	C5-C4-O4	5.19	129.01	125.90
1	A	837	G	OP1-P-OP2	-5.19	111.81	119.60
1	A	859	A	C4-C5-C6	5.19	119.60	117.00
1	A	1280	A	C5-C6-N1	-5.19	115.10	117.70
1	A	1364	U	C2-N3-C4	-5.19	123.88	127.00
1	A	36	C	C4-C5-C6	5.19	120.00	117.40
1	A	452	A	N9-C4-C5	5.19	107.88	105.80
1	A	565	U	OP1-P-OP2	-5.19	111.81	119.60
1	A	708	C	C5-C4-N4	-5.19	116.57	120.20
1	A	907	A	C6-N1-C2	-5.19	115.48	118.60
1	A	1299	A	N9-C1'-C2'	5.19	120.75	114.00
1	A	1465	C	C5-C4-N4	-5.19	116.57	120.20
1	A	1515	C	N1-C2-N3	-5.19	115.57	119.20
1	A	22	G	C5-N7-C8	-5.19	101.70	104.30
1	A	217	C	C5-C6-N1	-5.19	118.41	121.00
1	A	521	G	OP2-P-O3'	5.19	116.62	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	G	OP1-P-OP2	5.19	127.38	119.60
1	A	1074	G	C4-N9-C1'	5.19	133.25	126.50
1	A	1386	G	C5-N7-C8	5.19	106.89	104.30
1	A	1415	G	C8-N9-C1'	-5.19	120.26	127.00
1	A	337	C	OP2-P-O3'	5.19	116.61	105.20
1	A	530	G	N3-C4-C5	5.19	131.19	128.60
1	A	745	C	C4-C5-C6	-5.19	114.81	117.40
4	D	68	TYR	CB-CG-CD2	-5.19	117.89	121.00
1	A	40	C	N1-C2-O2	-5.18	115.79	118.90
1	A	216	G	C8-N9-C4	5.18	108.47	106.40
1	A	998	G	C8-N9-C4	5.18	108.47	106.40
1	A	1070	U	N3-C4-C5	5.18	117.71	114.60
1	A	1082	G	C4-C5-C6	5.18	121.91	118.80
1	A	298	A	N9-C4-C5	5.18	107.87	105.80
1	A	881	G	C6-C5-N7	-5.18	127.29	130.40
1	A	886	G	N7-C8-N9	5.18	115.69	113.10
1	A	960	U	N3-C2-O2	-5.18	118.57	122.20
1	A	1020	U	N3-C4-O4	-5.18	115.77	119.40
1	A	1080	A	N9-C4-C5	5.18	107.87	105.80
1	A	477	G	O4'-C1'-N9	5.18	112.34	108.20
1	A	568	G	C4-C5-N7	-5.18	108.73	110.80
1	A	705	U	OP2-P-O3'	5.18	116.59	105.20
1	A	755	G	N3-C4-N9	5.18	129.11	126.00
1	A	768	A	C5-C6-N1	5.18	120.29	117.70
1	A	805	C	N1-C2-N3	-5.18	115.57	119.20
1	A	1181	G	N1-C2-N3	5.18	127.01	123.90
1	A	1372	U	N3-C4-O4	5.18	123.03	119.40
1	A	1543	C	OP2-P-O3'	5.18	116.59	105.20
19	S	80	TYR	N-CA-C	-5.18	97.01	111.00
1	A	1279	A	C8-N9-C4	-5.18	103.73	105.80
1	A	1333	A	N3-C4-C5	-5.18	123.17	126.80
1	A	550	G	C6-N1-C2	-5.18	121.99	125.10
1	A	691	G	O5'-P-OP1	-5.18	101.04	105.70
1	A	858	G	OP1-P-O3'	-5.18	93.81	105.20
1	A	983	A	N7-C8-N9	5.18	116.39	113.80
1	A	1099	G	C5-C6-N1	-5.18	108.91	111.50
1	A	1311	G	C2-N3-C4	-5.18	109.31	111.90
1	A	1392	G	N1-C6-O6	-5.18	116.79	119.90
1	A	1398	A	OP1-P-OP2	5.18	127.37	119.60
5	E	24	ARG	N-CA-C	-5.18	97.02	111.00
19	S	80	TYR	CG-CD1-CE1	5.18	125.44	121.30
1	A	281	G	O5'-P-OP1	-5.17	101.04	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	405	U	N1-C2-O2	-5.17	119.18	122.80
1	A	1080	A	C6-C5-N7	5.17	135.92	132.30
1	A	1261	A	C8-N9-C4	5.17	107.87	105.80
1	A	546	G	N1-C6-O6	-5.17	116.80	119.90
1	A	1392	G	C8-N9-C1'	-5.17	120.28	127.00
1	A	76	C	N1-C2-O2	-5.17	115.80	118.90
1	A	500	G	C6-C5-N7	-5.17	127.30	130.40
1	A	545	C	C2-N1-C1'	5.17	124.49	118.80
1	A	881	G	C4-N9-C1'	5.17	133.22	126.50
1	A	918	A	N3-C4-N9	5.17	131.54	127.40
1	A	1090	U	C4-C5-C6	5.17	122.80	119.70
1	A	1470	G	C5-C6-O6	5.17	131.70	128.60
1	A	347	G	C2-N3-C4	-5.17	109.31	111.90
1	A	1413	A	C4-N9-C1'	5.17	135.61	126.30
1	A	919	A	N9-C4-C5	5.17	107.87	105.80
1	A	983	A	C8-N9-C4	-5.17	103.73	105.80
1	A	984	C	C2-N3-C4	5.17	122.48	119.90
1	A	1064	G	N3-C4-C5	5.17	131.18	128.60
1	A	1127	G	N3-C4-N9	-5.17	122.90	126.00
1	A	1343	G	N3-C4-N9	-5.17	122.90	126.00
1	A	1443	G	N1-C6-O6	5.17	123.00	119.90
1	A	1499	A	N9-C4-C5	5.17	107.87	105.80
1	A	378	G	N1-C2-N2	5.17	120.85	116.20
1	A	545	C	C4-C5-C6	5.17	119.98	117.40
1	A	712	A	N3-C4-C5	-5.17	123.18	126.80
1	A	766	A	OP1-P-OP2	5.17	127.35	119.60
1	A	791	G	N1-C2-N3	5.17	127.00	123.90
1	A	849	C	C5-C4-N4	-5.17	116.58	120.20
1	A	1057	G	O5'-P-OP2	-5.17	101.05	105.70
1	A	1299	A	C5-N7-C8	-5.17	101.32	103.90
20	T	33	ILE	CG1-CB-CG2	5.17	122.76	111.40
1	A	616	G	C4-C5-C6	5.16	121.90	118.80
1	A	721	G	C6-C5-N7	-5.16	127.30	130.40
1	A	906	G	C5-C6-O6	-5.16	125.50	128.60
1	A	1220	G	C5-C6-N1	5.16	114.08	111.50
12	L	92	ASP	CB-CG-OD1	5.16	122.94	118.30
1	A	83	U	N1-C2-N3	-5.16	111.80	114.90
1	A	124	G	OP1-P-O3'	-5.16	93.85	105.20
1	A	497	A	C6-N1-C2	-5.16	115.50	118.60
1	A	517	G	C5-C6-O6	5.16	131.70	128.60
1	A	88	A	N1-C6-N6	5.16	121.69	118.60
1	A	707	C	O5'-P-OP1	5.16	116.89	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1345	U	C5-C6-N1	-5.16	120.12	122.70
9	I	32	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	A	555	C	N3-C4-N4	5.16	121.61	118.00
1	A	661	G	C2-N3-C4	-5.16	109.32	111.90
1	A	1376	U	C6-N1-C2	-5.16	117.91	121.00
1	A	42	G	O5'-P-OP1	-5.16	101.06	105.70
1	A	550	G	N7-C8-N9	-5.16	110.52	113.10
1	A	805	C	N3-C2-O2	5.16	125.51	121.90
1	A	884	U	C2-N3-C4	-5.16	123.91	127.00
1	A	1093	A	P-O3'-C3'	5.16	125.89	119.70
1	A	1251	A	N1-C2-N3	5.16	131.88	129.30
1	A	1531	A	N1-C6-N6	5.16	121.69	118.60
1	A	1408	A	C8-N9-C4	5.15	107.86	105.80
1	A	1543	C	C6-N1-C2	5.15	122.36	120.30
1	A	624	C	N3-C4-N4	5.15	121.61	118.00
1	A	1160	G	N9-C4-C5	-5.15	103.34	105.40
1	A	1215	G	C5-N7-C8	-5.15	101.72	104.30
1	A	1248	A	C5-N7-C8	-5.15	101.32	103.90
1	A	1291	G	N3-C4-C5	5.15	131.18	128.60
1	A	1479	C	C6-N1-C2	-5.15	118.24	120.30
3	C	2	GLY	N-CA-C	5.15	125.98	113.10
1	A	200	G	OP1-P-OP2	5.15	127.33	119.60
1	A	400	C	OP1-P-O3'	-5.15	93.87	105.20
1	A	525	C	C5-C6-N1	5.15	123.58	121.00
1	A	740	U	O4'-C1'-N1	5.15	112.32	108.20
15	O	57	LEU	CB-CG-CD1	-5.15	102.24	111.00
17	Q	4	LYS	CD-CE-NZ	5.15	123.55	111.70
1	A	363	A	OP1-P-OP2	-5.15	111.88	119.60
9	I	27	THR	CB-CA-C	-5.15	97.70	111.60
1	A	5	U	OP2-P-O3'	-5.15	93.88	105.20
1	A	457	C	C5-C6-N1	5.15	123.57	121.00
1	A	1066	C	C5-C6-N1	5.15	123.57	121.00
17	Q	38	ARG	NE-CZ-NH2	-5.15	117.73	120.30
1	A	150	C	OP2-P-O3'	5.14	116.52	105.20
1	A	625	G	C2-N3-C4	-5.14	109.33	111.90
1	A	633	G	N7-C8-N9	5.14	115.67	113.10
1	A	1505	G	N1-C2-N3	5.14	126.99	123.90
1	A	1517	G	OP1-P-OP2	5.14	127.32	119.60
8	H	102	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	78	G	C8-N9-C4	-5.14	104.34	106.40
1	A	831	U	N3-C2-O2	5.14	125.80	122.20
1	A	927	G	C6-N1-C2	5.14	128.19	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	964	A	C4-C5-N7	-5.14	108.13	110.70
1	A	982	U	N1-C2-O2	5.14	126.40	122.80
1	A	1380	U	C5-C6-N1	-5.14	120.13	122.70
12	L	79	GLU	C-N-CA	-5.14	108.84	121.70
1	A	111	G	C8-N9-C1'	5.14	133.68	127.00
1	A	896	C	OP1-P-OP2	5.14	127.31	119.60
1	A	1069	C	O5'-P-OP1	5.14	116.87	110.70
1	A	39	G	C8-N9-C1'	5.14	133.68	127.00
1	A	791	G	OP1-P-O3'	-5.14	93.89	105.20
1	A	1024	G	C6-C5-N7	5.14	133.48	130.40
1	A	1258	G	N9-C4-C5	5.14	107.45	105.40
1	A	1386	G	N1-C6-O6	5.14	122.98	119.90
1	A	292	G	N7-C8-N9	5.14	115.67	113.10
1	A	307	C	C2-N1-C1'	5.14	124.45	118.80
1	A	404	U	O5'-P-OP1	5.14	116.86	110.70
1	A	108	G	C1'-O4'-C4'	-5.14	105.79	109.90
1	A	407	G	C8-N9-C4	-5.14	104.34	106.40
1	A	662	G	O4'-C1'-N9	-5.14	104.09	108.20
1	A	753	A	C2-N3-C4	5.14	113.17	110.60
1	A	775	G	OP1-P-O3'	5.14	116.50	105.20
1	A	21	G	C5-C6-N1	5.13	114.07	111.50
1	A	248	C	C2-N1-C1'	-5.13	113.15	118.80
1	A	529	G	N3-C2-N2	-5.13	116.31	119.90
1	A	1095	U	C4-C5-C6	5.13	122.78	119.70
2	B	18	GLY	N-CA-C	5.13	125.94	113.10
1	A	533	A	C8-N9-C4	-5.13	103.75	105.80
1	A	791	G	C8-N9-C4	5.13	108.45	106.40
1	A	81	U	OP1-P-OP2	-5.13	111.90	119.60
1	A	141	A	C2-N3-C4	-5.13	108.03	110.60
1	A	352	C	O3'-P-O5'	-5.13	94.25	104.00
1	A	813	U	N3-C4-C5	5.13	117.68	114.60
1	A	850	U	O5'-P-OP2	5.13	116.86	110.70
1	A	476	G	N1-C6-O6	5.13	122.98	119.90
1	A	365	U	C2-N1-C1'	5.13	123.85	117.70
1	A	1273	G	O5'-P-OP2	-5.13	101.08	105.70
1	A	1305	G	C4-C5-N7	-5.13	108.75	110.80
1	A	1384	C	C6-N1-C2	5.13	122.35	120.30
1	A	678	U	P-O3'-C3'	5.13	125.85	119.70
1	A	815	A	C8-N9-C4	-5.13	103.75	105.80
1	A	879	C	OP1-P-O3'	-5.13	93.92	105.20
1	A	1293	G	C5-C6-N1	5.13	114.06	111.50
1	A	558	G	N3-C4-C5	5.12	131.16	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	63	C	C5-C6-N1	-5.12	118.44	121.00
1	A	485	G	C4-N9-C1'	5.12	133.16	126.50
1	A	938	A	N9-C4-C5	5.12	107.85	105.80
1	A	957	U	C4-C5-C6	5.12	122.77	119.70
1	A	1159	U	N3-C4-O4	-5.12	115.81	119.40
1	A	42	G	N3-C2-N2	-5.12	116.31	119.90
1	A	990	C	C6-N1-C2	-5.12	118.25	120.30
4	D	202	LEU	CA-CB-CG	-5.12	103.52	115.30
1	A	1319	A	C8-N9-C4	5.12	107.85	105.80
1	A	429	U	C4-C5-C6	5.12	122.77	119.70
1	A	506	G	C4-C5-C6	5.12	121.87	118.80
1	A	542	G	C6-C5-N7	-5.12	127.33	130.40
1	A	682	G	N3-C4-C5	-5.12	126.04	128.60
1	A	329	A	C5-C6-N1	-5.12	115.14	117.70
1	A	601	C	N1-C2-O2	-5.12	115.83	118.90
1	A	973	G	C8-N9-C1'	5.12	133.65	127.00
10	J	96	ILE	CB-CA-C	-5.12	101.37	111.60
12	L	98	TYR	CE1-CZ-CE2	-5.12	111.61	119.80
1	A	194	C	N1-C2-N3	-5.12	115.62	119.20
1	A	323	U	OP1-P-O3'	5.12	116.45	105.20
1	A	1341	U	N3-C4-O4	-5.12	115.82	119.40
1	A	5	U	OP1-P-O3'	5.11	116.45	105.20
1	A	446	G	C5-N7-C8	-5.11	101.74	104.30
1	A	546	G	N3-C4-N9	-5.11	122.93	126.00
1	A	607	A	C2-N3-C4	-5.11	108.04	110.60
1	A	727	G	O5'-P-OP1	-5.11	101.10	105.70
1	A	1233	G	C5-N7-C8	-5.11	101.74	104.30
1	A	1401	G	N3-C4-N9	5.11	129.07	126.00
1	A	1523	G	OP2-P-O3'	5.11	116.45	105.20
1	A	612	C	C5-C6-N1	-5.11	118.44	121.00
1	A	1451	A	C4-N9-C1'	-5.11	117.10	126.30
1	A	1504	G	O4'-C1'-N9	-5.11	104.11	108.20
20	T	25	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	A	6	G	C5-N7-C8	-5.11	101.75	104.30
1	A	451	A	C4-C5-C6	5.11	119.56	117.00
1	A	944	G	N1-C2-N3	5.11	126.97	123.90
1	A	1368	G	C6-N1-C2	-5.11	122.03	125.10
1	A	901	A	N3-C4-N9	-5.11	123.31	127.40
1	A	1432	G	C2-N3-C4	-5.11	109.35	111.90
1	A	328	C	N1-C1'-C2'	5.11	120.64	114.00
1	A	722	A	C4-C5-N7	5.11	113.25	110.70
1	A	722	A	OP1-P-OP2	5.11	127.26	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	765	G	C8-N9-C4	-5.11	104.36	106.40
1	A	1045	C	C4-C5-C6	-5.11	114.85	117.40
1	A	1047	G	O4'-C1'-N9	-5.11	104.11	108.20
1	A	1306	A	N1-C6-N6	-5.11	115.54	118.60
21	U	3	LYS	CD-CE-NZ	5.11	123.45	111.70
1	A	651	C	O5'-P-OP1	-5.11	101.11	105.70
1	A	761	G	N7-C8-N9	5.11	115.65	113.10
1	A	860	A	N7-C8-N9	-5.11	111.25	113.80
1	A	866	C	C4-C5-C6	5.11	119.95	117.40
1	A	1284	C	C2-N1-C1'	-5.11	113.18	118.80
1	A	1352	C	N1-C2-O2	-5.11	115.84	118.90
2	B	39	ILE	CB-CA-C	-5.11	101.39	111.60
1	A	601	C	OP2-P-O3'	5.10	116.43	105.20
1	A	803	G	N3-C4-N9	-5.10	122.94	126.00
1	A	809	G	OP2-P-O3'	5.10	116.43	105.20
1	A	1341	U	C2-N1-C1'	-5.10	111.58	117.70
1	A	1388	C	N1-C2-O2	5.10	121.96	118.90
1	A	578	C	C2-N1-C1'	-5.10	113.19	118.80
1	A	853	G	N1-C6-O6	-5.10	116.84	119.90
1	A	864	A	C6-N1-C2	5.10	121.66	118.60
1	A	917	G	C5-C6-N1	5.10	114.05	111.50
1	A	1104	G	C5-N7-C8	-5.10	101.75	104.30
1	A	1137	C	N3-C4-N4	-5.10	114.43	118.00
1	A	1212	U	N3-C4-O4	5.10	122.97	119.40
1	A	1237	C	OP2-P-O3'	5.10	116.42	105.20
1	A	1343	G	N1-C6-O6	5.10	122.96	119.90
1	A	551	U	O5'-P-OP1	-5.10	101.11	105.70
1	A	869	G	C5-C6-O6	-5.10	125.54	128.60
1	A	330	C	N3-C4-N4	-5.10	114.43	118.00
1	A	462	G	OP1-P-O3'	-5.10	93.98	105.20
1	A	539	A	OP2-P-O3'	5.10	116.42	105.20
1	A	1265	G	N3-C4-N9	-5.10	122.94	126.00
1	A	65	U	OP1-P-OP2	5.10	127.25	119.60
1	A	388	G	OP1-P-OP2	-5.10	111.95	119.60
1	A	579	G	N3-C4-C5	-5.10	126.05	128.60
1	A	646	U	N1-C2-O2	-5.10	119.23	122.80
1	A	860	A	N1-C6-N6	5.10	121.66	118.60
1	A	1178	G	N1-C6-O6	-5.10	116.84	119.90
17	Q	63	ARG	NE-CZ-NH1	-5.10	117.75	120.30
1	A	199	G	N1-C2-N3	5.10	126.96	123.90
1	A	600	C	N1-C2-O2	-5.10	115.84	118.90
1	A	737	A	C5-N7-C8	-5.10	101.35	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	190(D)	U	C6-N1-C2	5.09	124.06	121.00
1	A	260	G	C8-N9-C1'	-5.09	120.38	127.00
1	A	406	G	C4-C5-N7	5.09	112.84	110.80
1	A	951	G	C8-N9-C4	5.09	108.44	106.40
1	A	1136	U	C6-N1-C2	-5.09	117.94	121.00
1	A	1351	U	C6-N1-C1'	5.09	128.33	121.20
1	A	55	A	C5-C6-N1	5.09	120.25	117.70
1	A	97	G	N1-C2-N2	-5.09	111.62	116.20
1	A	309	G	C5-C6-N1	-5.09	108.95	111.50
1	A	934	C	OP1-P-O3'	5.09	116.40	105.20
4	D	155	LEU	CA-CB-CG	5.09	127.01	115.30
1	A	280	C	O5'-P-OP2	-5.09	101.12	105.70
1	A	425	G	N9-C1'-C2'	-5.09	106.40	112.00
20	T	100	ILE	CB-CA-C	-5.09	101.42	111.60
1	A	45	U	C4-C5-C6	5.09	122.75	119.70
1	A	351	G	C5-N7-C8	5.09	106.84	104.30
1	A	688	G	C4-N9-C1'	5.09	133.11	126.50
1	A	116	A	O4'-C1'-N9	-5.08	104.13	108.20
1	A	577	G	N3-C4-C5	5.08	131.14	128.60
1	A	825	G	N3-C4-N9	-5.08	122.95	126.00
1	A	167	G	C5-C6-O6	-5.08	125.55	128.60
1	A	1162	C	C4-C5-C6	5.08	119.94	117.40
1	A	1311	G	C5-N7-C8	-5.08	101.76	104.30
1	A	89	C	N3-C4-N4	5.08	121.56	118.00
1	A	122	G	C8-N9-C1'	-5.08	120.39	127.00
1	A	328	C	C4-C5-C6	-5.08	114.86	117.40
1	A	711	G	C4-C5-C6	5.08	121.85	118.80
1	A	942	G	OP2-P-O3'	5.08	116.38	105.20
12	L	115	LYS	CD-CE-NZ	5.08	123.39	111.70
1	A	562	C	C5'-C4'-O4'	-5.08	103.00	109.10
1	A	1094	G	N9-C4-C5	-5.08	103.37	105.40
1	A	1321	C	C5-C4-N4	5.08	123.76	120.20
1	A	1350	A	C2-N3-C4	5.08	113.14	110.60
1	A	874	G	C4-C5-C6	5.08	121.85	118.80
1	A	928	G	N1-C2-N3	5.08	126.95	123.90
1	A	1066	C	C2-N1-C1'	5.08	124.39	118.80
1	A	1416	G	N1-C2-N2	-5.08	111.63	116.20
1	A	1467	G	C8-N9-C1'	-5.08	120.40	127.00
1	A	102	G	C5-C6-O6	-5.08	125.56	128.60
1	A	228	A	O5'-P-OP2	-5.08	101.13	105.70
1	A	703	G	N3-C4-C5	-5.08	126.06	128.60
1	A	922	G	C5-N7-C8	5.08	106.84	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	254	G	OP2-P-O3'	5.07	116.36	105.20
1	A	664	G	OP1-P-OP2	5.07	127.21	119.60
1	A	860	A	O5'-P-OP2	-5.07	101.13	105.70
1	A	954	G	C4-N9-C1'	-5.07	119.91	126.50
1	A	417	C	N3-C4-N4	5.07	121.55	118.00
1	A	838	G	C5-C6-N1	-5.07	108.96	111.50
1	A	850	U	N3-C2-O2	5.07	125.75	122.20
1	A	1460	A	C2-N3-C4	-5.07	108.06	110.60
1	A	44	G	C5-C6-O6	5.07	131.64	128.60
1	A	101	A	N1-C2-N3	5.07	131.84	129.30
1	A	1102	A	C4-C5-C6	5.07	119.53	117.00
1	A	1229	A	OP1-P-O3'	5.07	116.36	105.20
1	A	66	G	C4-C5-N7	5.07	112.83	110.80
1	A	74	C	N1-C2-O2	-5.07	115.86	118.90
1	A	196	A	C6-N1-C2	5.07	121.64	118.60
1	A	570	G	OP1-P-OP2	5.07	127.20	119.60
1	A	732	C	C6-N1-C2	-5.07	118.27	120.30
1	A	1492	A	N3-C4-N9	5.07	131.45	127.40
1	A	190	C	N3-C4-C5	-5.06	119.87	121.90
1	A	723	U	N1-C2-O2	5.06	126.34	122.80
1	A	772	U	C5-C4-O4	-5.06	122.86	125.90
9	I	59	PHE	N-CA-C	5.06	124.67	111.00
14	N	53	LEU	CB-CG-CD1	-5.06	102.39	111.00
1	A	235	C	C5-C6-N1	-5.06	118.47	121.00
1	A	869	G	C5-C6-N1	5.06	114.03	111.50
1	A	1368	G	C2-N3-C4	5.06	114.43	111.90
1	A	199	G	N9-C4-C5	-5.06	103.38	105.40
1	A	760	G	C5-N7-C8	5.06	106.83	104.30
1	A	1224	G	C2-N3-C4	5.06	114.43	111.90
1	A	279	A	C4-C5-C6	5.06	119.53	117.00
1	A	624	C	N1-C2-N3	-5.06	115.66	119.20
1	A	812	C	C2'-C3'-O3'	5.06	121.80	113.70
1	A	863	U	C2-N3-C4	-5.06	123.97	127.00
1	A	1180	A	N9-C4-C5	5.06	107.82	105.80
1	A	1184	G	N3-C4-N9	5.06	129.03	126.00
1	A	1206	G	N1-C2-N3	5.06	126.93	123.90
1	A	1262	C	C5-C6-N1	-5.06	118.47	121.00
1	A	404	U	N1-C2-N3	5.06	117.93	114.90
12	L	73	GLU	C-N-CA	-5.06	111.68	122.30
1	A	257	G	C5-C6-O6	5.05	131.63	128.60
1	A	645	C	N3-C4-C5	5.05	123.92	121.90
1	A	728	A	N7-C8-N9	5.05	116.33	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1354	C	OP1-P-OP2	-5.05	112.02	119.60
1	A	343	U	OP1-P-OP2	5.05	127.18	119.60
1	A	565	U	C5-C6-N1	5.05	125.23	122.70
1	A	979	C	N3-C2-O2	5.05	125.44	121.90
1	A	1066	C	O4'-C1'-N1	-5.05	104.16	108.20
12	L	44	THR	CB-CA-C	-5.05	97.96	111.60
1	A	375	U	N1-C2-O2	-5.05	119.27	122.80
1	A	420	U	C5-C4-O4	5.05	128.93	125.90
1	A	559	A	OP1-P-OP2	5.05	127.17	119.60
1	A	1413	A	C6-C5-N7	-5.05	128.77	132.30
1	A	1503	A	N1-C2-N3	5.05	131.82	129.30
1	A	347	G	C5-N7-C8	-5.05	101.78	104.30
1	A	670	G	C6-C5-N7	-5.05	127.37	130.40
1	A	900	A	N1-C2-N3	5.05	131.82	129.30
1	A	1525	G	C4-C5-N7	5.05	112.82	110.80
3	C	183	ASP	N-CA-C	-5.05	97.38	111.00
1	A	255	G	OP1-P-O3'	-5.04	94.10	105.20
1	A	292	G	P-O3'-C3'	5.04	125.75	119.70
1	A	707	C	OP2-P-O3'	5.04	116.30	105.20
1	A	812	C	OP2-P-O3'	5.04	116.30	105.20
1	A	921	U	C5-C6-N1	5.04	125.22	122.70
1	A	1443	G	P-O3'-C3'	5.04	125.75	119.70
10	J	40	LEU	CA-CB-CG	5.04	126.90	115.30
1	A	494	G	C6-C5-N7	-5.04	127.38	130.40
1	A	501	C	N1-C2-O2	-5.04	115.88	118.90
1	A	737	A	C4-C5-N7	5.04	113.22	110.70
1	A	775	G	C5-N7-C8	5.04	106.82	104.30
1	A	201	C	N1-C2-O2	5.04	121.92	118.90
1	A	115	G	O4'-C1'-N9	-5.04	104.17	108.20
1	A	506	G	OP1-P-OP2	5.04	127.16	119.60
1	A	1230	C	OP2-P-O3'	5.04	116.28	105.20
1	A	1349	A	OP1-P-OP2	-5.04	112.05	119.60
15	O	34	LEU	CB-CA-C	5.04	119.77	110.20
1	A	224	C	C6-N1-C2	5.04	122.31	120.30
1	A	485	G	O4'-C1'-N9	5.04	112.23	108.20
1	A	501	C	C6-N1-C2	5.04	122.31	120.30
1	A	534	U	C5-C6-N1	-5.04	120.18	122.70
1	A	584	G	C5-N7-C8	5.04	106.82	104.30
1	A	712	A	C5-C6-N6	-5.04	119.67	123.70
1	A	1241	G	OP1-P-O3'	5.04	116.28	105.20
1	A	1311	G	N3-C4-N9	-5.04	122.98	126.00
10	J	54	PHE	N-CA-C	5.04	124.59	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	327	A	C5-C6-N1	5.03	120.22	117.70
1	A	456	C	O5'-P-OP1	5.03	116.74	110.70
1	A	559	A	P-O3'-C3'	5.03	125.74	119.70
1	A	644	G	C2-N3-C4	5.03	114.42	111.90
1	A	666	G	C6-N1-C2	5.03	128.12	125.10
1	A	690	G	N1-C2-N3	5.03	126.92	123.90
1	A	939	G	N3-C4-C5	5.03	131.12	128.60
1	A	1013	G	C5-N7-C8	5.03	106.82	104.30
1	A	1384	C	C5-C6-N1	-5.03	118.48	121.00
1	A	49	U	N1-C2-O2	-5.03	119.28	122.80
1	A	111	G	C5-N7-C8	-5.03	101.78	104.30
1	A	175	C	C2-N1-C1'	-5.03	113.27	118.80
1	A	284	G	C8-N9-C1'	-5.03	120.46	127.00
1	A	376	G	N1-C2-N3	-5.03	120.88	123.90
1	A	983	A	N1-C2-N3	5.03	131.81	129.30
1	A	1341	U	C6-N1-C2	5.03	124.02	121.00
1	A	525	C	C4-C5-C6	-5.03	114.89	117.40
1	A	536	C	C6-N1-C1'	5.03	126.83	120.80
1	A	853	G	C4-N9-C1'	5.03	133.04	126.50
1	A	1526	G	C6-C5-N7	-5.03	127.38	130.40
4	D	198	VAL	CB-CA-C	-5.03	101.84	111.40
1	A	593	G	C5-C6-O6	5.03	131.62	128.60
1	A	724	G	C5-C6-N1	5.03	114.01	111.50
1	A	746	A	C6-C5-N7	5.03	135.82	132.30
1	A	926	G	OP1-P-O3'	5.03	116.26	105.20
1	A	1256	A	O5'-P-OP2	-5.03	101.17	105.70
1	A	565	U	OP1-P-O3'	5.03	116.25	105.20
1	A	724	G	N9-C4-C5	5.03	107.41	105.40
1	A	1180	A	C2-N3-C4	5.03	113.11	110.60
1	A	1300	G	N1-C2-N3	-5.03	120.89	123.90
1	A	875	C	C6-N1-C2	5.02	122.31	120.30
1	A	907	A	OP2-P-O3'	5.02	116.25	105.20
1	A	295	C	O5'-P-OP1	-5.02	101.18	105.70
1	A	333	G	C8-N9-C1'	-5.02	120.47	127.00
1	A	625	G	N3-C4-N9	5.02	129.01	126.00
1	A	839	U	C2-N1-C1'	-5.02	111.67	117.70
1	A	1139	G	C5-N7-C8	5.02	106.81	104.30
1	A	1361	G	C5-C6-O6	5.02	131.61	128.60
1	A	1401	G	N3-C4-C5	-5.02	126.09	128.60
1	A	203	U	C5-C4-O4	-5.02	122.89	125.90
1	A	630	G	C4-N9-C1'	-5.02	119.97	126.50
1	A	167	G	C4-C5-N7	5.02	112.81	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	496	A	O5'-P-OP2	5.02	116.72	110.70
1	A	1178	G	C5-N7-C8	5.02	106.81	104.30
1	A	261	U	N1-C2-N3	5.02	117.91	114.90
1	A	611	A	N1-C2-N3	5.02	131.81	129.30
1	A	1001	A	C8-N9-C4	-5.02	103.79	105.80
1	A	1079	G	C4-C5-N7	5.02	112.81	110.80
1	A	1443	G	C5-C6-N1	-5.02	108.99	111.50
1	A	1521	G	C5-C6-O6	-5.02	125.59	128.60
6	F	14	LEU	CA-CB-CG	5.02	126.84	115.30
1	A	37	U	OP2-P-O3'	5.02	116.23	105.20
1	A	642	A	C2-N3-C4	-5.02	108.09	110.60
1	A	888	G	N3-C4-C5	-5.02	126.09	128.60
1	A	17	U	C5-C4-O4	-5.01	122.89	125.90
1	A	363	A	O5'-P-OP1	5.01	116.72	110.70
1	A	553	A	C6-C5-N7	-5.01	128.79	132.30
1	A	731	G	C5-C6-O6	-5.01	125.59	128.60
1	A	1140	C	C2-N3-C4	5.01	122.41	119.90
1	A	1190	G	C4-C5-N7	-5.01	108.79	110.80
9	I	105	ASP	O-C-N	5.01	130.72	122.70
1	A	912	C	N1-C2-N3	5.01	122.71	119.20
1	A	1494	G	N1-C2-N3	5.01	126.91	123.90
8	H	44	PHE	N-CA-C	5.01	124.53	111.00
1	A	115	G	OP1-P-OP2	-5.01	112.08	119.60
1	A	258	G	C4-C5-N7	5.01	112.81	110.80
1	A	528	C	N3-C2-O2	5.01	125.41	121.90
1	A	542	G	C5-C6-O6	-5.01	125.59	128.60
1	A	601	C	N1-C2-N3	5.01	122.71	119.20
1	A	838	G	N1-C6-O6	5.01	122.91	119.90
1	A	1336	C	O5'-P-OP2	5.01	116.72	110.70
1	A	1503	A	C4-C5-N7	-5.01	108.19	110.70
1	A	880	C	OP1-P-OP2	5.01	127.11	119.60
1	A	886	G	OP2-P-O3'	5.01	116.22	105.20
1	A	920	U	N3-C2-O2	-5.01	118.69	122.20
1	A	1220	G	C2-N3-C4	5.01	114.40	111.90
1	A	1279	A	P-O3'-C3'	5.01	125.71	119.70
1	A	1477	C	C5-C6-N1	5.01	123.50	121.00
1	A	240	C	C5-C4-N4	-5.01	116.69	120.20
1	A	531	U	N3-C2-O2	5.01	125.70	122.20
1	A	618	C	OP1-P-OP2	5.01	127.11	119.60
1	A	919	A	C2-N3-C4	5.01	113.10	110.60
1	A	1143	G	N1-C6-O6	5.01	122.90	119.90
1	A	1229	A	O5'-P-OP2	-5.00	101.19	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	582	U	C2-N1-C1'	5.00	123.70	117.70
1	A	674	G	N3-C4-N9	5.00	129.00	126.00
1	A	880	C	N1-C2-O2	5.00	121.90	118.90
1	A	1056	U	C6-N1-C2	5.00	124.00	121.00
1	A	1461	G	C5-N7-C8	-5.00	101.80	104.30
1	A	265	G	N3-C4-C5	-5.00	126.10	128.60
1	A	592	G	C5-C6-N1	-5.00	109.00	111.50
1	A	680	C	OP2-P-O3'	5.00	116.20	105.20
1	A	964	A	C4-C5-C6	5.00	119.50	117.00
1	A	1075	C	OP2-P-O3'	5.00	116.20	105.20
16	P	52	ASP	N-CA-CB	5.00	119.60	110.60

There are no chirality outliers.

All (40) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	11	LEU	Peptide
2	B	21	ARG	Peptide
2	B	34	ALA	Peptide
2	B	8	LYS	Peptide
3	C	166	GLU	Peptide
3	C	206	GLU	Peptide
3	C	24	ALA	Peptide
3	C	96	GLY	Peptide
4	D	11	LEU	Peptide
4	D	195	ALA	Peptide
4	D	28	SER	Peptide
4	D	29	PRO	Peptide
4	D	3	ARG	Peptide
5	E	11	ILE	Peptide
5	E	24	ARG	Peptide
6	F	100	ASN	Peptide
8	H	90	GLY	Peptide
9	I	57	GLY	Peptide
10	J	88	LEU	Peptide
10	J	89	ASP	Peptide
11	K	49	GLY	Peptide
11	K	87	THR	Peptide
12	L	24	VAL	Peptide
12	L	28	LYS	Peptide
12	L	46	LYS	Peptide
12	L	87	GLY	Peptide

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Mol	Chain	Res	Type	Group
12	L	92	ASP	Peptide
13	M	105	THR	Peptide
13	M	11	ARG	Peptide
13	M	62	ASN	Peptide
14	N	30	ALA	Peptide
17	Q	13	ASP	Peptide
17	Q	96	GLU	Peptide
18	R	24	ALA	Peptide
18	R	48	GLY	Peptide
18	R	86	VAL	Peptide
19	S	47	HIS	Peptide
20	T	12	ALA	Peptide
20	T	92	LEU	Peptide
20	T	93	GLU	Peptide

## 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	A	32550	0	16439	1131	1
2	B	1900	0	1951	132	0
3	C	1612	0	1677	116	0
4	D	1703	0	1763	120	0
5	E	1146	0	1207	120	0
6	F	843	0	857	75	0
7	G	1257	0	1296	98	0
8	H	1116	0	1177	116	0
9	I	1010	0	1037	101	0
10	J	792	0	835	82	0
11	K	864	0	881	75	0
12	L	977	0	1060	82	0
13	M	937	0	995	89	0
14	N	492	0	528	55	0
15	O	729	0	768	55	0
16	P	700	0	720	44	0
17	Q	823	0	891	84	0
18	R	574	0	644	72	0
19	S	647	0	673	75	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	T	763	0	861	67	0
21	U	208	0	221	18	0
22	A	40	0	38	6	0
23	A	389	0	0	0	0
23	B	3	0	0	0	0
23	C	4	0	0	0	0
23	D	6	0	0	0	0
23	E	3	0	0	0	0
23	F	1	0	0	0	0
23	H	1	0	0	0	0
23	L	1	0	0	0	0
23	N	1	0	0	0	0
23	O	1	0	0	0	0
23	P	1	0	0	0	0
23	Q	2	0	0	0	0
23	S	1	0	0	0	0
24	D	1	0	0	0	0
24	N	1	0	0	0	0
25	A	1371	0	0	60	1
25	C	16	0	0	0	0
25	D	24	0	0	2	0
25	E	8	0	0	0	0
25	F	6	0	0	0	0
25	G	6	0	0	0	0
25	H	5	0	0	1	0
25	I	1	0	0	0	0
25	L	7	0	0	0	0
25	M	4	0	0	2	0
25	N	4	0	0	0	0
25	O	2	0	0	0	0
25	P	1	0	0	0	0
25	Q	8	0	0	0	0
25	T	1	0	0	0	0
All	All	53563	0	36519	2556	1

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 29.

All (2556) 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)
15:O:34:LEU:CG	15:O:34:LEU:CD1	1.77	1.63
4:D:12:CYS:SG	4:D:12:CYS:CB	2.02	1.46
18:R:53:ARG:HA	18:R:56:THR:HG22	1.41	1.02
3:C:14:ILE:HB	3:C:15:THR:HG23	1.36	1.02
12:L:27:LEU:O	12:L:29:GLY:N	1.94	1.00
2:B:31:TYR:HD2	2:B:202:PRO:HG3	1.24	0.99
1:A:7:G:H5'	1:A:298:A:H5'	1.45	0.98
1:A:598:U:H4'	8:H:94:TYR:CD1	1.99	0.97
5:E:15:ARG:HH11	5:E:15:ARG:HG2	1.24	0.97
4:D:38:TYR:HD2	4:D:38:TYR:H	1.11	0.96
17:Q:40:LYS:HG3	17:Q:42:TYR:HE1	1.31	0.95
1:A:975:A:H5'	1:A:975:A:H8	1.31	0.94
1:A:53:A:N6	25:A:2540:HOH:O	2.00	0.94
1:A:1052:U:O2'	25:A:3070:HOH:O	1.85	0.94
21:U:10:ARG:HG3	21:U:13:ILE:HD12	1.46	0.94
1:A:1425:U:H2'	1:A:1426:C:C6	2.02	0.94
1:A:966:M2G:HM13	1:A:967:5MC:H1'	1.49	0.94
1:A:1256:A:H4'	1:A:1257:U:O5'	1.68	0.92
10:J:34:VAL:HG22	10:J:74:ILE:HA	1.49	0.92
12:L:27:LEU:C	12:L:29:GLY:H	1.72	0.91
1:A:1211:U:O2'	1:A:1213:A:N3	2.03	0.91
1:A:1442:G:N2	1:A:1447:G:N7	2.18	0.91
11:K:18:ARG:HB3	11:K:33:THR:HG23	1.51	0.90
1:A:598:U:H4'	8:H:94:TYR:HD1	1.36	0.90
1:A:717:C:H6	1:A:717:C:H5''	1.36	0.90
9:I:97:LYS:HE2	9:I:97:LYS:HA	1.52	0.89
17:Q:29:HIS:HB2	17:Q:36:ILE:HD13	1.54	0.89
18:R:56:THR:HG23	18:R:58:LEU:H	1.38	0.88
1:A:1004:A:N1	1:A:1037:C:N4	2.21	0.88
9:I:114:TYR:HE1	10:J:60:ARG:H	1.21	0.88
11:K:101:SER:OG	11:K:103:LEU:N	2.07	0.88
1:A:279:A:OP2	17:Q:95:TYR:OH	1.91	0.88
1:A:1488:G:H2'	1:A:1489:G:C8	2.08	0.87
1:A:1417:G:O2'	1:A:1483:A:N6	2.07	0.87
1:A:527:7MG:OP2	22:A:1601:SRY:O32	1.92	0.87
11:K:15:ALA:HA	11:K:77:MET:HA	1.56	0.86
1:A:1178:G:N2	1:A:1181:G:OP2	2.08	0.86
1:A:1412:C:H2'	1:A:1413:A:H8	1.41	0.86
1:A:1415:G:H1'	1:A:1486:G:N2	1.91	0.85
12:L:20:LYS:HE2	12:L:20:LYS:H	1.41	0.85
12:L:27:LEU:HG	12:L:28:LYS:H	1.41	0.85
15:O:34:LEU:CD1	15:O:34:LEU:HG	2.04	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1420:C:O2	1:A:1480:G:N2	2.09	0.85
1:A:372:C:O2'	25:A:3344:HOH:O	1.91	0.85
5:E:86:ALA:HB1	5:E:125:SER:HB3	1.56	0.85
1:A:838:G:N2	1:A:848:C:O2	2.10	0.84
3:C:6:HIS:HE1	3:C:8:ILE:HB	1.42	0.84
1:A:227:G:O2'	25:A:2712:HOH:O	1.95	0.83
3:C:6:HIS:CE1	3:C:8:ILE:HB	2.11	0.83
12:L:25:PRO:HB2	12:L:64:TYR:HE2	1.42	0.83
16:P:34:GLU:OE1	16:P:55:ARG:NH1	2.12	0.83
4:D:188:LEU:HD22	4:D:189:PRO:HD2	1.61	0.83
1:A:1057:G:H5''	3:C:154:SER:HB2	1.59	0.83
1:A:1488:G:H2'	1:A:1489:G:H8	1.44	0.82
3:C:67:THR:HA	3:C:102:ASN:HB2	1.62	0.82
18:R:21:LYS:HB2	18:R:24:ALA:HB3	1.61	0.82
1:A:1223:C:OP1	19:S:78:ARG:NH1	2.12	0.81
1:A:1320:C:O2	19:S:36:ARG:NH2	2.14	0.81
20:T:89:ARG:HH21	20:T:104:LEU:HD12	1.46	0.81
1:A:939:G:H5''	7:G:102:ARG:NH2	1.95	0.81
16:P:40:ASP:OD1	16:P:44:THR:OG1	1.97	0.81
3:C:25:GLY:HA3	3:C:28:GLN:HB2	1.62	0.81
1:A:1412:C:H2'	1:A:1413:A:C8	2.16	0.81
1:A:350:G:H5''	1:A:350:G:H8	1.46	0.80
1:A:413:G:H8	1:A:428:G:H21	1.29	0.80
1:A:403:C:OP1	4:D:137:SER:OG	1.97	0.80
20:T:57:ARG:HH12	20:T:100:ILE:HD12	1.46	0.80
1:A:975:A:H5'	1:A:975:A:C8	2.16	0.80
3:C:14:ILE:O	3:C:16:ARG:N	2.15	0.80
2:B:31:TYR:CD2	2:B:202:PRO:HG3	2.13	0.80
18:R:84:LYS:H	18:R:84:LYS:HD2	1.46	0.80
1:A:1030:C:N4	1:A:1033:G:O6	2.14	0.80
1:A:1402:4OC:HM22	1:A:1403:C:H5'	1.64	0.79
8:H:4:ASP:OD2	8:H:85:ARG:NH1	2.15	0.79
1:A:1286:A:H2'	1:A:1287:A:H4'	1.63	0.79
1:A:1366:C:O2'	10:J:60:ARG:NH2	2.14	0.79
12:L:89:ARG:HD3	12:L:97:ARG:HA	1.64	0.79
7:G:46:ALA:HB1	7:G:121:ALA:HB2	1.63	0.79
1:A:301:G:H2'	1:A:302:G:H5'	1.65	0.78
4:D:64:LEU:HD23	4:D:198:VAL:HG11	1.65	0.78
1:A:776:G:N2	1:A:803:G:O6	2.16	0.78
18:R:46:GLU:OE2	18:R:46:GLU:N	2.14	0.78
10:J:96:ILE:H	10:J:96:ILE:HD12	1.45	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:23:GLY:HA3	4:D:112:VAL:HG13	1.65	0.78
1:A:677:U:H3	1:A:713:G:H22	1.29	0.78
1:A:939:G:H5''	7:G:102:ARG:HH22	1.47	0.78
4:D:22:LYS:HG3	4:D:26:CYS:SG	2.23	0.78
1:A:1125:U:H5'	25:A:3142:HOH:O	1.84	0.78
2:B:171:ALA:HA	2:B:174:VAL:HB	1.66	0.77
9:I:17:VAL:HG13	9:I:63:ILE:HD13	1.67	0.77
1:A:1416:G:N2	1:A:1417:G:H1'	1.99	0.77
1:A:1350:A:OP2	9:I:118:LYS:NZ	2.17	0.77
11:K:93:GLN:HG2	11:K:96:ARG:HH21	1.49	0.77
4:D:68:TYR:OH	4:D:98:GLU:OE1	2.01	0.77
17:Q:40:LYS:HG3	17:Q:42:TYR:CE1	2.18	0.77
1:A:1367:C:H5'	10:J:60:ARG:NH2	2.00	0.76
13:M:23:TYR:CD2	13:M:70:LEU:HD13	2.20	0.76
16:P:19:ILE:HG22	16:P:36:ILE:HG13	1.68	0.76
1:A:974:A:OP2	14:N:41:ARG:NH1	2.17	0.76
4:D:31:CYS:SG	4:D:31:CYS:O	2.43	0.76
4:D:54:TYR:HE1	4:D:206:PHE:HE1	1.34	0.76
4:D:25:ARG:HA	4:D:28:SER:HB2	1.65	0.76
1:A:1190:G:H5'	3:C:176:HIS:NE2	2.00	0.76
9:I:97:LYS:HE3	9:I:102:LEU:H	1.51	0.76
17:Q:91:ARG:O	17:Q:94:ASN:HB2	1.86	0.76
20:T:10:LEU:HD13	20:T:13:LEU:H	1.50	0.76
3:C:155:GLY:HA3	3:C:163:ALA:HB1	1.65	0.76
9:I:112:LYS:HG2	9:I:119:ALA:H	1.50	0.76
3:C:34:LEU:HD21	3:C:38:ARG:HH11	1.50	0.76
6:F:2:ARG:HD2	6:F:69:GLU:HG3	1.68	0.76
12:L:25:PRO:C	12:L:27:LEU:H	1.89	0.76
1:A:1075:C:H5''	2:B:179:LYS:HE3	1.68	0.75
1:A:1291:G:OP1	7:G:37:ASN:ND2	2.19	0.75
1:A:927:G:O2'	1:A:1503:A:N7	2.17	0.75
5:E:27:ARG:HB2	5:E:27:ARG:NH1	2.01	0.75
17:Q:6:LEU:H	17:Q:59:ILE:HG22	1.51	0.75
7:G:27:ILE:HD13	7:G:40:ALA:HA	1.67	0.75
20:T:74:LYS:HB2	20:T:76:ALA:H	1.51	0.75
1:A:1256:A:H8	1:A:1256:A:H5''	1.51	0.75
19:S:80:TYR:HD1	19:S:81:ARG:N	1.84	0.75
7:G:85:TYR:CD1	7:G:154:TYR:HE1	2.04	0.75
1:A:1226:C:H5'	19:S:80:TYR:HD2	1.50	0.75
1:A:1496:C:H2'	1:A:1496:C:O2	1.86	0.75
1:A:1279:A:O2'	1:A:1281:U:OP2	2.05	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:49:THR:HG22	13:M:51:ALA:H	1.52	0.74
1:A:658:G:H1	1:A:747:C:H42	1.34	0.74
1:A:567:G:O2'	25:A:2033:HOH:O	2.05	0.74
4:D:78:LEU:HD11	4:D:96:LEU:HB3	1.69	0.74
1:A:1397:C:O2'	1:A:1398:A:OP1	2.06	0.74
2:B:19:HIS:HE1	2:B:206:ASP:HB3	1.53	0.74
5:E:121:LYS:HG3	5:E:122:GLU:O	1.88	0.74
1:A:668:G:H1'	15:O:46:HIS:HD2	1.52	0.73
1:A:923:A:OP1	5:E:21:ALA:HB2	1.88	0.73
1:A:992:U:H3	1:A:1044:A:H62	1.36	0.73
1:A:1219:U:OP1	14:N:19:ARG:NH2	2.21	0.73
18:R:61:LYS:O	18:R:65:ILE:HG12	1.89	0.73
1:A:1405:G:H22	1:A:1496:C:H5	1.35	0.73
1:A:298:A:N6	25:A:2126:HOH:O	2.20	0.73
1:A:737:A:H1'	6:F:73:ASN:OD1	1.89	0.73
10:J:78:ASN:OD1	10:J:81:THR:N	2.20	0.73
1:A:1085:U:N3	25:A:2271:HOH:O	2.22	0.73
4:D:11:LEU:HD13	4:D:66:ARG:HD2	1.69	0.73
4:D:66:ARG:HH11	4:D:66:ARG:HG3	1.52	0.73
5:E:27:ARG:HH11	5:E:27:ARG:HB2	1.53	0.73
9:I:8:GLY:HA2	9:I:79:LEU:HD13	1.68	0.73
19:S:44:MET:HB2	19:S:62:ILE:HD11	1.71	0.73
1:A:1057:G:O6	1:A:1203:C:N4	2.17	0.73
1:A:1327:C:OP2	21:U:12:LYS:NZ	2.20	0.73
5:E:105:VAL:HG23	5:E:106:PRO:HD3	1.70	0.72
8:H:18:ARG:HG2	8:H:18:ARG:HH11	1.55	0.72
11:K:120:ARG:HH22	11:K:126:ARG:HH12	1.37	0.72
19:S:64:GLU:O	19:S:67:VAL:HG23	1.89	0.72
1:A:869:G:O6	25:A:3263:HOH:O	2.06	0.72
5:E:116:THR:OG1	5:E:117:ASP:OD2	2.06	0.72
1:A:933:G:H1	1:A:1384:C:H42	1.38	0.72
3:C:134:ILE:HD11	3:C:153:VAL:HG22	1.71	0.72
1:A:833:U:H2'	1:A:834:C:C6	2.25	0.72
2:B:10:LEU:O	2:B:12:GLU:HG3	1.89	0.72
18:R:87:ARG:HG2	18:R:88:LYS:H	1.55	0.72
1:A:1051:C:N4	25:A:3086:HOH:O	2.12	0.72
1:A:1314:C:N4	19:S:4:SER:O	2.22	0.72
1:A:672:U:H2'	1:A:673:G:C8	2.25	0.72
7:G:70:LYS:HG2	7:G:96:GLN:HB3	1.70	0.72
9:I:50:LEU:HD13	9:I:56:LEU:HG	1.72	0.72
17:Q:66:SER:O	17:Q:70:ARG:NH1	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:50:GLU:HG2	20:T:99:LEU:HD22	1.70	0.72
1:A:1415:G:N2	1:A:1485:U:O4	2.22	0.72
13:M:11:ARG:HE	13:M:12:ASN:N	1.88	0.72
1:A:1112:C:N3	3:C:178:LEU:HB2	2.05	0.71
3:C:43:LEU:HD21	3:C:91:LEU:HD13	1.71	0.71
5:E:15:ARG:HG2	5:E:15:ARG:NH1	2.03	0.71
1:A:382:A:H2'	1:A:383:A:C8	2.24	0.71
20:T:46:GLU:HB2	20:T:48:LYS:HD3	1.72	0.71
1:A:664:G:OP1	18:R:64:ARG:HD2	1.91	0.71
1:A:91:C:H2'	1:A:92:C:H6	1.54	0.71
1:A:1053:G:H4'	1:A:1054:C:H5'	1.72	0.71
2:B:18:GLY:H	2:B:41:ILE:HG23	1.55	0.71
7:G:85:TYR:HD1	7:G:154:TYR:HE1	1.38	0.71
15:O:26:GLU:CD	15:O:26:GLU:H	1.94	0.71
1:A:1399:C:H4'	1:A:1400:5MC:H5''	1.73	0.71
1:A:390:C:O3'	16:P:28:ARG:NH2	2.24	0.71
15:O:34:LEU:CD2	15:O:34:LEU:CD1	2.67	0.71
1:A:1126:U:H5''	25:A:3119:HOH:O	1.89	0.71
1:A:797:C:OP1	11:K:124:LYS:HD3	1.91	0.71
4:D:13:ARG:HG2	4:D:38:TYR:O	1.91	0.71
18:R:54:ARG:HB2	18:R:54:ARG:HH11	1.56	0.71
1:A:1415:G:H1'	1:A:1486:G:H22	1.56	0.71
20:T:65:LYS:O	20:T:68:LYS:HB2	1.90	0.71
18:R:84:LYS:H	18:R:84:LYS:CD	2.01	0.70
9:I:97:LYS:O	9:I:100:GLY:N	2.24	0.70
13:M:23:TYR:HD2	13:M:70:LEU:HD13	1.54	0.70
1:A:1330:U:H2'	1:A:1331:G:H5'	1.73	0.70
5:E:51:VAL:N	5:E:52:PRO:HD2	2.05	0.70
8:H:17:THR:HB	8:H:78:GLN:HE22	1.56	0.70
13:M:114:ARG:NE	25:M:202:HOH:O	2.23	0.70
3:C:77:ILE:HG23	3:C:81:GLY:HA2	1.74	0.70
1:A:1226:C:H3'	13:M:96:LEU:HD11	1.73	0.70
14:N:23:ARG:HG2	14:N:28:GLY:O	1.91	0.70
1:A:758:G:N7	25:A:3363:HOH:O	2.25	0.70
7:G:140:ASP:HA	7:G:143:ARG:NH1	2.06	0.70
1:A:376:G:H5''	16:P:5:ARG:HD2	1.73	0.70
1:A:975:A:H4'	1:A:976:G:H5''	1.74	0.70
1:A:691:G:H2'	1:A:692:U:H6	1.56	0.70
4:D:150:GLU:N	4:D:150:GLU:OE2	2.24	0.70
12:L:8:ASN:O	12:L:12:ARG:HB2	1.92	0.70
4:D:30:LYS:HG2	4:D:35:ARG:HH21	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:A:OP1	12:L:52:LEU:HD12	1.91	0.69
18:R:45:SER:OG	18:R:49:LYS:HB2	1.91	0.69
19:S:6:LYS:HB2	19:S:7:LYS:NZ	2.06	0.69
1:A:297:G:N2	25:A:3188:HOH:O	2.24	0.69
11:K:20:TYR:CE2	11:K:83:ILE:HD12	2.27	0.69
1:A:144:G:H1	1:A:178:C:H42	1.40	0.69
2:B:68:ILE:H	2:B:90:MET:HG2	1.56	0.69
6:F:14:LEU:HD22	6:F:18:GLN:HB3	1.74	0.69
14:N:37:PHE:HE2	14:N:53:LEU:HD13	1.57	0.69
3:C:150:LYS:HA	3:C:169:ALA:HB2	1.73	0.69
13:M:66:LEU:HA	13:M:70:LEU:HD12	1.74	0.69
1:A:412:A:O2'	1:A:413:G:OP2	2.10	0.69
2:B:118:LEU:O	2:B:122:PHE:HB2	1.91	0.69
1:A:1004:A:N6	1:A:1035:A:N7	2.41	0.69
1:A:1427:U:H2'	1:A:1428:A:C8	2.27	0.69
7:G:38:LEU:O	7:G:42:ILE:HG13	1.92	0.69
17:Q:29:HIS:HB2	17:Q:36:ILE:CD1	2.21	0.69
2:B:16:HIS:HB3	2:B:210:SER:HB2	1.74	0.69
1:A:1108:G:H2'	1:A:1109:C:H5'	1.74	0.69
1:A:1497:G:C2'	1:A:1498:UR3:H5'	2.22	0.69
8:H:82:HIS:HD1	8:H:138:TRP:HE1	1.39	0.69
8:H:82:HIS:ND1	8:H:138:TRP:NE1	2.41	0.69
18:R:53:ARG:HA	18:R:56:THR:CG2	2.21	0.69
1:A:99:C:H2'	1:A:101:A:C8	2.28	0.69
5:E:118:ILE:C	5:E:119:LEU:HD23	2.13	0.69
11:K:122:LYS:O	11:K:125:PHE:N	2.18	0.69
1:A:413:G:H22	4:D:35:ARG:HD3	1.58	0.68
1:A:962:C:O2'	25:A:2695:HOH:O	2.10	0.68
2:B:90:MET:H	2:B:90:MET:HE2	1.56	0.68
6:F:82:ARG:HB2	6:F:85:VAL:HG23	1.75	0.68
8:H:86:ILE:HG21	8:H:133:LEU:HD13	1.73	0.68
19:S:22:LEU:HD22	19:S:28:LYS:HG3	1.75	0.68
1:A:1316:G:N1	1:A:1319:A:OP2	2.25	0.68
4:D:12:CYS:HA	4:D:19:LEU:HD12	1.75	0.68
10:J:87:THR:O	10:J:87:THR:OG1	2.07	0.68
4:D:12:CYS:HA	4:D:19:LEU:CD1	2.24	0.68
5:E:95:ALA:HB1	5:E:96:PRO:HD2	1.73	0.68
18:R:54:ARG:NH1	18:R:54:ARG:HB2	2.08	0.68
1:A:1226:C:H4'	1:A:1227:A:OP1	1.93	0.68
1:A:1228:C:OP2	13:M:111:LYS:HE2	1.93	0.68
1:A:717:C:H5''	1:A:717:C:C6	2.25	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:23:TYR:HE2	13:M:70:LEU:HD22	1.57	0.68
1:A:1378:C:H5''	1:A:1379:G:OP2	1.93	0.68
9:I:97:LYS:HA	9:I:97:LYS:CE	2.17	0.68
11:K:25:TYR:HE1	11:K:87:THR:HB	1.59	0.68
11:K:57:THR:HG22	11:K:59:TYR:N	2.08	0.68
1:A:1002:G:H1	1:A:1003(A):G:H22	1.40	0.68
4:D:13:ARG:HH11	4:D:13:ARG:HG2	1.58	0.68
6:F:98:LEU:H	6:F:98:LEU:HD12	1.58	0.68
8:H:85:ARG:HG3	8:H:86:ILE:H	1.57	0.68
14:N:21:TYR:HE2	14:N:23:ARG:HE	1.41	0.68
18:R:46:GLU:CD	18:R:46:GLU:H	1.97	0.68
1:A:113:G:H1	1:A:314:C:H42	1.39	0.67
1:A:190(A):C:O2	1:A:190(H):G:N2	2.24	0.67
1:A:1518:MA6:H93	1:A:1519:MA6:N6	2.09	0.67
1:A:291:C:H2'	1:A:292:G:H5'	1.77	0.67
4:D:22:LYS:HB2	4:D:26:CYS:SG	2.35	0.67
13:M:48:LEU:HD12	13:M:53:VAL:HG22	1.76	0.67
17:Q:75:ARG:HB2	17:Q:75:ARG:HH11	1.58	0.67
1:A:737:A:H2'	1:A:738:C:H6	1.58	0.67
19:S:80:TYR:CD1	19:S:81:ARG:N	2.63	0.67
5:E:12:LEU:HD22	5:E:12:LEU:O	1.95	0.67
8:H:43:GLY:O	8:H:64:LYS:NZ	2.24	0.67
12:L:25:PRO:HA	12:L:27:LEU:H	1.60	0.67
1:A:1003(A):G:H2'	1:A:1004:A:H4'	1.77	0.67
17:Q:38:ARG:HG2	17:Q:38:ARG:HH11	1.59	0.67
1:A:277:C:H5''	17:Q:68:ARG:HH21	1.58	0.67
20:T:39:LYS:HD3	20:T:55:ILE:HG13	1.76	0.67
3:C:177:THR:HG22	3:C:180:ALA:HB2	1.77	0.67
13:M:3:ARG:NH1	13:M:57:ARG:HH21	1.92	0.67
1:A:187:C:O2	20:T:105:SER:HB3	1.93	0.67
1:A:450:G:H1	1:A:483:C:H42	1.42	0.67
1:A:581:G:C8	25:A:3364:HOH:O	2.46	0.67
11:K:120:ARG:NH2	11:K:126:ARG:HH12	1.92	0.67
1:A:1034:G:N2	1:A:1035:A:N1	2.42	0.67
9:I:112:LYS:HG2	9:I:119:ALA:N	2.10	0.67
10:J:76:ASN:OD1	10:J:76:ASN:N	2.27	0.67
5:E:106:PRO:O	5:E:110:LEU:HG	1.95	0.66
8:H:26:VAL:HG23	8:H:27:PRO:HD2	1.77	0.66
12:L:25:PRO:C	12:L:27:LEU:N	2.48	0.66
2:B:189:ASP:OD2	2:B:190:THR:N	2.23	0.66
18:R:47:THR:HG22	18:R:48:GLY:H	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1223:C:H3'	1:A:1224:G:H5''	1.77	0.66
1:A:1415:G:H3'	1:A:1415:G:H8	1.60	0.66
1:A:301:G:C2'	1:A:302:G:H5'	2.26	0.66
14:N:29:ARG:HG3	14:N:31:ARG:H	1.60	0.66
1:A:1220:G:N2	19:S:54:GLY:O	2.19	0.66
1:A:254:G:H2'	1:A:255:G:H8	1.59	0.66
9:I:40:LEU:HD11	9:I:70:LYS:HD2	1.76	0.66
11:K:33:THR:OG1	11:K:34:ASP:N	2.27	0.66
8:H:20:TYR:CE1	8:H:76:PRO:HG2	2.31	0.66
3:C:53:ALA:HB2	3:C:115:LEU:HD21	1.76	0.66
3:C:153:VAL:HG23	3:C:166:GLU:HB3	1.77	0.66
9:I:49:PRO:HB3	9:I:82:ALA:HB2	1.76	0.66
1:A:1005:A:N1	1:A:1025:U:O2'	2.28	0.66
1:A:410:G:OP1	4:D:30:LYS:NZ	2.28	0.66
1:A:263:A:OP2	20:T:79:ARG:NH1	2.28	0.66
1:A:1015:A:H2'	1:A:1016:A:C8	2.30	0.66
2:B:212:GLN:NE2	2:B:236:TYR:HB2	2.10	0.66
7:G:85:TYR:HD1	7:G:154:TYR:CE1	2.14	0.66
2:B:194:PRO:HA	2:B:197:VAL:HG23	1.77	0.66
1:A:1127:G:N2	1:A:1145:C:N3	2.44	0.65
4:D:108:LEU:HD22	4:D:176:LEU:HD22	1.77	0.65
5:E:6:PHE:HE2	5:E:36:ASP:HB3	1.61	0.65
5:E:32:VAL:HG23	5:E:58:ALA:HB3	1.78	0.65
9:I:17:VAL:HG21	9:I:80:GLY:HA3	1.77	0.65
1:A:1496:C:O2'	1:A:1497:G:H5''	1.96	0.65
1:A:1505:G:O2'	1:A:1506:U:OP2	2.14	0.65
1:A:770:C:N4	25:A:2519:HOH:O	2.29	0.65
10:J:61:GLU:OE2	14:N:49:HIS:NE2	2.28	0.65
1:A:1279:A:H5''	1:A:1280:A:OP1	1.97	0.65
1:A:260:G:H2'	1:A:261:U:H6	1.60	0.65
9:I:10:ARG:HG2	9:I:10:ARG:HH11	1.62	0.65
10:J:16:LEU:HD21	10:J:70:ARG:HB2	1.78	0.65
19:S:41:VAL:HB	19:S:43:GLU:HG2	1.77	0.65
1:A:1442:G:N2	25:A:3044:HOH:O	2.08	0.65
8:H:61:VAL:HG12	8:H:63:LEU:HD12	1.77	0.65
14:N:24:CYS:O	14:N:28:GLY:N	2.27	0.65
20:T:56:MET:HE1	20:T:104:LEU:HD23	1.78	0.65
1:A:1416:G:H21	1:A:1417:G:H1'	1.61	0.65
1:A:1452:C:H4'	1:A:1453:G:H5''	1.78	0.65
1:A:940:C:OP1	7:G:29:LYS:NZ	2.29	0.65
17:Q:7:THR:O	17:Q:23:VAL:HG13	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:57:THR:HG22	11:K:59:TYR:H	1.61	0.65
1:A:1196:U:H4'	1:A:1197:G:OP2	1.96	0.65
1:A:547:A:H4'	1:A:548:G:O5'	1.96	0.65
10:J:38:ILE:HD12	10:J:71:LEU:HG	1.77	0.65
1:A:1028:C:N3	1:A:1029:C:N4	2.44	0.65
1:A:392:G:H2'	1:A:393:A:H8	1.62	0.65
5:E:52:PRO:HG2	5:E:53:LEU:H	1.61	0.65
12:L:27:LEU:C	12:L:29:GLY:N	2.40	0.65
13:M:12:ASN:ND2	13:M:12:ASN:O	2.26	0.65
1:A:182:U:H5'	1:A:182:U:H6	1.62	0.65
5:E:109:ILE:HG22	5:E:110:LEU:HD23	1.79	0.65
7:G:143:ARG:HH11	7:G:143:ARG:HB2	1.61	0.65
7:G:15:ASP:HB3	7:G:19:GLY:N	2.12	0.65
16:P:45:THR:OG1	16:P:47:ASP:N	2.29	0.65
1:A:1345:U:C4	1:A:1377:A:C2	2.85	0.65
1:A:664:G:H22	1:A:741:G:H1	1.42	0.65
1:A:932:C:H5'	7:G:4:ARG:HG2	1.79	0.65
3:C:174:PRO:HB2	3:C:177:THR:HB	1.79	0.64
4:D:187:ARG:NH2	4:D:188:LEU:HB2	2.12	0.64
1:A:1127:G:H5'	9:I:66:ARG:HH12	1.62	0.64
1:A:673:G:H2'	1:A:674:G:C8	2.32	0.64
1:A:1148:U:H2'	1:A:1149:C:O4'	1.98	0.64
7:G:113:GLU:HG2	7:G:119:ARG:HG2	1.79	0.64
1:A:242:C:H2'	1:A:243:A:H5'	1.79	0.64
17:Q:29:HIS:CE1	17:Q:32:TYR:H	2.16	0.64
1:A:489:C:H2'	1:A:490:G:C8	2.33	0.64
1:A:853:G:H2'	1:A:854:G:H5'	1.80	0.64
2:B:101:MET:HA	2:B:108:ILE:HG13	1.79	0.64
1:A:110:C:H2'	1:A:111:G:O4'	1.96	0.64
2:B:60:ASP:O	2:B:64:ARG:HB2	1.96	0.64
3:C:108:ASN:ND2	3:C:111:LEU:HD12	2.12	0.64
9:I:50:LEU:HB3	9:I:85:LEU:HD21	1.78	0.64
10:J:23:ILE:HG21	10:J:72:VAL:HG11	1.80	0.64
13:M:54:VAL:HA	13:M:57:ARG:HB2	1.79	0.64
14:N:8:GLU:HA	14:N:11:LYS:CG	2.27	0.64
11:K:33:THR:HB	11:K:39:PRO:HA	1.79	0.64
1:A:149:A:H2'	1:A:150:C:C6	2.33	0.64
1:A:869:G:N7	25:A:3263:HOH:O	2.30	0.64
4:D:191:ARG:O	4:D:194:LEU:HD12	1.98	0.64
8:H:10:LEU:HB3	8:H:83:ILE:HD11	1.80	0.64
1:A:942:G:H21	9:I:124:GLN:HE22	1.46	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:671:G:C2	1:A:672:U:H1'	2.33	0.64
1:A:1030(A):G:H1	1:A:1032:G:H1	1.45	0.64
1:A:658:G:H2'	1:A:659:U:H6	1.63	0.64
10:J:38:ILE:H	10:J:71:LEU:HB2	1.63	0.64
14:N:47:LEU:O	14:N:50:LYS:N	2.30	0.64
18:R:44:LEU:HD11	18:R:79:LEU:HD22	1.80	0.64
1:A:1370:G:H5''	9:I:109:VAL:HG21	1.80	0.63
11:K:77:MET:HE1	11:K:80:VAL:HG13	1.81	0.63
12:L:41:ARG:HG2	12:L:42:THR:H	1.62	0.63
21:U:8:THR:OG1	21:U:9:ARG:N	2.30	0.63
1:A:21:G:H2'	1:A:22:G:C8	2.34	0.63
1:A:352:C:O2'	1:A:354:G:OP1	2.13	0.63
1:A:967:5MC:O2'	9:I:128:ARG:NH1	2.31	0.63
1:A:243:A:C2	1:A:246:A:C8	2.87	0.63
1:A:767:A:H2'	1:A:768:A:O4'	1.99	0.63
4:D:30:LYS:O	4:D:32:ALA:N	2.31	0.63
15:O:15:PHE:HE2	15:O:84:LYS:HB3	1.62	0.63
18:R:34:TYR:CE1	18:R:35:ARG:HD3	2.33	0.63
19:S:40:ILE:HD13	19:S:62:ILE:HD12	1.80	0.63
1:A:202:U:H4'	1:A:203:U:OP2	1.98	0.63
4:D:155:LEU:HD22	4:D:156:GLU:N	2.13	0.63
19:S:50:ALA:HB1	19:S:57:HIS:HB3	1.81	0.63
1:A:1203:C:OP1	14:N:2:ALA:HB3	1.98	0.63
1:A:527:7MG:C2'	1:A:528:C:H5'	2.29	0.63
12:L:20:LYS:N	12:L:20:LYS:HE2	2.11	0.63
14:N:8:GLU:HA	14:N:11:LYS:CD	2.28	0.63
19:S:31:ILE:HG22	19:S:49:ILE:HA	1.81	0.63
1:A:1233:G:OP2	9:I:124:GLN:HB3	1.99	0.63
4:D:66:ARG:NH1	4:D:66:ARG:HG3	2.13	0.63
5:E:10:MET:HG3	5:E:11:ILE:N	2.13	0.63
15:O:63:ARG:O	15:O:67:LEU:HB2	1.97	0.63
1:A:695:A:H2'	1:A:696:A:C8	2.33	0.63
3:C:58:GLU:HB3	10:J:92:THR:HG21	1.81	0.63
5:E:31:LEU:HD21	5:E:45:PHE:HD1	1.63	0.63
8:H:10:LEU:H	8:H:10:LEU:HD12	1.62	0.63
1:A:1031:G:N7	1:A:1032:G:N2	2.43	0.63
3:C:111:LEU:HD11	3:C:144:SER:O	1.99	0.63
5:E:79:GLU:HG3	8:H:105:ARG:HG2	1.79	0.63
1:A:572:A:H5'	1:A:573:A:OP2	1.98	0.62
3:C:22:TRP:CD1	3:C:59:ARG:HD2	2.34	0.62
6:F:62:TRP:CH2	6:F:64:GLN:HB2	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:42:ILE:HG22	7:G:120:ILE:HD11	1.80	0.62
10:J:17:ASP:OD1	10:J:70:ARG:NH1	2.31	0.62
10:J:96:ILE:H	10:J:96:ILE:CD1	2.10	0.62
1:A:922:G:H5''	1:A:922:G:H8	1.65	0.62
1:A:1057:G:H5''	3:C:154:SER:CB	2.29	0.62
1:A:503:C:OP2	12:L:116:SER:OG	2.17	0.62
2:B:16:HIS:CB	2:B:210:SER:HB2	2.29	0.62
3:C:155:GLY:HA2	3:C:164:ARG:O	1.99	0.62
9:I:4:TYR:CE2	9:I:88:TYR:HA	2.34	0.62
18:R:87:ARG:HB2	18:R:87:ARG:CZ	2.28	0.62
1:A:254:G:H2'	1:A:255:G:C8	2.35	0.62
3:C:149:ALA:O	3:C:169:ALA:HB1	2.00	0.62
4:D:43:HIS:HD2	4:D:46:LYS:HD2	1.63	0.62
11:K:57:THR:O	11:K:60:ALA:HB3	1.99	0.62
20:T:67:ALA:O	20:T:73:HIS:ND1	2.31	0.62
1:A:262:A:C6	1:A:263:A:C6	2.88	0.62
1:A:459:G:H8	1:A:459:G:O5'	1.83	0.62
5:E:146:ALA:O	5:E:150:ARG:HG3	2.00	0.62
9:I:114:TYR:CE1	10:J:60:ARG:N	2.66	0.62
19:S:62:ILE:HA	19:S:66:MET:SD	2.40	0.62
1:A:946:A:H2'	1:A:947:G:C8	2.35	0.62
5:E:26:PHE:N	5:E:26:PHE:CD1	2.66	0.62
5:E:76:ILE:HD13	5:E:118:ILE:HD11	1.81	0.62
19:S:40:ILE:HB	19:S:67:VAL:O	1.99	0.62
1:A:1201:A:H5''	25:A:3077:HOH:O	1.98	0.62
1:A:975:A:H4'	1:A:976:G:C5'	2.30	0.62
8:H:87:SER:HA	8:H:93:VAL:HG23	1.82	0.62
1:A:382:A:H2'	1:A:383:A:H8	1.64	0.62
6:F:39:LYS:HB3	6:F:62:TRP:HZ3	1.65	0.62
1:A:235:C:N4	25:A:2070:HOH:O	2.33	0.61
1:A:737:A:H2'	1:A:738:C:O4'	1.99	0.61
1:A:827:U:H5''	1:A:828:A:OP2	1.99	0.61
5:E:78:HIS:HE1	5:E:142:LEU:HD23	1.65	0.61
6:F:69:GLU:CD	6:F:69:GLU:H	2.03	0.61
14:N:37:PHE:CE2	14:N:53:LEU:HD13	2.34	0.61
1:A:1421:G:N2	1:A:1480:G:H1'	2.16	0.61
1:A:300:A:H2'	1:A:301:G:O4'	1.99	0.61
1:A:1251:A:H5'	9:I:12:GLU:HG2	1.81	0.61
1:A:37:U:O2'	1:A:500:G:H4'	2.00	0.61
1:A:646:U:H2'	1:A:647:C:C6	2.36	0.61
1:A:515:G:H2'	1:A:516:PSU:O4'	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:806:C:H2'	1:A:807:A:H8	1.65	0.61
8:H:11:THR:O	8:H:15:ASN:ND2	2.34	0.61
1:A:1179:A:OP2	9:I:93:ARG:NH1	2.34	0.61
7:G:99:LEU:HB3	7:G:103:TRP:CZ3	2.35	0.61
12:L:6:THR:N	12:L:9:GLN:OE1	2.31	0.61
17:Q:87:LYS:O	17:Q:90:ILE:HG22	2.00	0.61
1:A:447:G:H2'	1:A:485:G:N2	2.16	0.61
3:C:121:ALA:O	3:C:124:ILE:HB	2.00	0.61
10:J:35:SER:OG	10:J:73:ASP:HB2	2.01	0.61
1:A:490:G:H2'	1:A:491:G:H8	1.66	0.61
1:A:589:C:N4	25:A:2337:HOH:O	2.23	0.61
14:N:21:TYR:HE2	14:N:23:ARG:NE	1.98	0.61
1:A:1126:U:H5''	25:A:3121:HOH:O	1.99	0.61
1:A:1482:G:H2'	1:A:1483:A:H8	1.66	0.61
1:A:606:G:H1'	1:A:632:A:H61	1.65	0.61
1:A:652:U:O4	1:A:752:G:O2'	2.17	0.61
11:K:40:ILE:HG23	11:K:75:TYR:CD1	2.35	0.61
1:A:135:C:O2	16:P:1:MET:HB3	1.99	0.61
1:A:439:A:C4	1:A:497:A:C2	2.89	0.61
2:B:20:GLU:HB2	2:B:190:THR:HB	1.83	0.61
8:H:33:GLU:HG2	8:H:48:TYR:OH	2.01	0.61
17:Q:48:GLU:HG2	17:Q:50:LYS:HB3	1.82	0.61
1:A:141:A:H1'	1:A:182:U:O2	2.01	0.60
1:A:1484:C:C4	1:A:1485:U:H5	2.19	0.60
1:A:414:A:H2'	1:A:415:A:C8	2.35	0.60
2:B:150:SER:HA	2:B:153:ARG:HG3	1.83	0.60
2:B:77:ALA:HB2	2:B:211:ILE:HD12	1.81	0.60
2:B:68:ILE:H	2:B:90:MET:CG	2.14	0.60
4:D:49:ARG:HA	4:D:49:ARG:HE	1.66	0.60
13:M:5:ALA:N	13:M:8:GLU:OE2	2.33	0.60
16:P:49:LEU:HD22	16:P:73:LEU:HD22	1.83	0.60
1:A:1124:G:HO2'	1:A:1145:C:N4	1.99	0.60
2:B:19:HIS:CE1	2:B:206:ASP:HB3	2.35	0.60
3:C:179:ARG:HD2	3:C:206:GLU:OE1	2.01	0.60
19:S:41:VAL:HG12	19:S:42:PRO:HD2	1.82	0.60
1:A:1443:G:H4'	1:A:1446:A:H5'	1.83	0.60
17:Q:92:ARG:HH11	17:Q:92:ARG:HB3	1.65	0.60
1:A:1343:G:H2'	1:A:1344:C:C6	2.37	0.60
1:A:1352:C:H2'	1:A:1353:G:C8	2.37	0.60
1:A:731:G:OP1	1:A:766:A:H1'	2.01	0.60
2:B:42:ILE:HG13	2:B:203:GLY:HA2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:118:LYS:O	9:I:120:ARG:N	2.33	0.60
12:L:89:ARG:HD3	12:L:97:ARG:CA	2.31	0.60
1:A:1442:G:C2	1:A:1446:A:N7	2.69	0.60
7:G:15:ASP:HB2	7:G:20:ASP:O	2.02	0.60
7:G:73:MET:SD	7:G:90:GLU:HA	2.41	0.60
14:N:8:GLU:O	14:N:11:LYS:HB2	2.01	0.60
1:A:532:A:O2'	1:A:533:A:OP1	2.14	0.60
1:A:853:G:C2'	1:A:854:G:H5'	2.30	0.60
7:G:26:PHE:CD2	7:G:62:PHE:HE1	2.20	0.60
10:J:25:GLU:HA	10:J:28:ARG:HB2	1.82	0.60
10:J:4:ILE:O	10:J:74:ILE:HG13	2.00	0.60
1:A:1100:C:N4	25:A:3039:HOH:O	2.20	0.60
1:A:1251:A:H2'	1:A:1252:A:O4'	2.01	0.60
1:A:248:C:N4	1:A:276:G:H1	2.00	0.60
2:B:22:LYS:HD2	2:B:35:GLU:OE1	2.00	0.60
1:A:1497:G:H2'	1:A:1498:UR3:H5'	1.84	0.60
1:A:291:C:C2'	1:A:292:G:H5'	2.31	0.60
1:A:737:A:H2'	1:A:738:C:C6	2.37	0.60
8:H:121:ASP:OD2	8:H:122:ARG:HG2	2.02	0.60
13:M:80:ARG:CZ	13:M:80:ARG:HB3	2.31	0.60
16:P:9:PHE:CE2	16:P:18:ARG:HD2	2.37	0.60
17:Q:67:LYS:HA	17:Q:70:ARG:HH12	1.67	0.60
20:T:89:ARG:NH2	20:T:104:LEU:HD12	2.15	0.60
1:A:1305:G:H3'	21:U:4:GLY:O	2.00	0.60
1:A:527:7MG:O2'	1:A:535:A:N1	2.28	0.60
1:A:598:U:H4'	8:H:94:TYR:CE1	2.37	0.60
1:A:267:C:OP2	17:Q:67:LYS:HE3	2.02	0.59
5:E:78:HIS:HB2	8:H:104:ARG:HG2	1.83	0.59
10:J:38:ILE:HB	10:J:71:LEU:HD23	1.83	0.59
13:M:4:ILE:HG22	13:M:57:ARG:HA	1.84	0.59
21:U:19:GLY:N	21:U:22:ARG:O	2.25	0.59
1:A:1309:G:OP1	13:M:88:ARG:NH2	2.33	0.59
4:D:52:SER:O	4:D:56:VAL:HG23	2.02	0.59
9:I:79:LEU:HD22	9:I:83:ARG:NE	2.18	0.59
1:A:1016:A:H2'	1:A:1017:G:O4'	2.03	0.59
1:A:1321:C:H3'	1:A:1322:C:H5''	1.84	0.59
1:A:332:G:H2'	1:A:333:G:H8	1.65	0.59
1:A:393:A:N6	25:A:2839:HOH:O	2.34	0.59
1:A:881:G:H2'	1:A:882:C:O4'	2.02	0.59
1:A:1038:C:H2'	1:A:1039:C:H6	1.67	0.59
1:A:924:C:O2'	1:A:925:G:H5'	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:148:GLY:HA3	3:C:172:ARG:O	2.03	0.59
11:K:120:ARG:HB3	11:K:120:ARG:HH11	1.66	0.59
14:N:44:LEU:O	14:N:44:LEU:HD12	2.02	0.59
15:O:70:LEU:HD12	15:O:78:TYR:HB2	1.84	0.59
1:A:1171:G:O2'	1:A:1172:C:H5'	2.02	0.59
1:A:411:A:C8	1:A:413:G:H1'	2.37	0.59
3:C:5:ILE:HD12	3:C:6:HIS:N	2.16	0.59
6:F:7:ASN:HD21	18:R:34:TYR:HE1	1.49	0.59
11:K:20:TYR:CZ	11:K:83:ILE:HD12	2.37	0.59
1:A:1234:C:H1'	1:A:1364:U:O2	2.03	0.59
1:A:586:C:C2'	1:A:587:G:H5'	2.33	0.59
4:D:31:CYS:C	4:D:33:MET:H	2.05	0.59
11:K:62:GLN:O	11:K:66:LEU:HG	2.02	0.59
16:P:9:PHE:N	16:P:16:HIS:O	2.30	0.59
12:L:11:VAL:HG23	17:Q:29:HIS:CD2	2.37	0.59
17:Q:68:ARG:H	17:Q:70:ARG:NH1	2.00	0.59
19:S:7:LYS:H	19:S:7:LYS:HZ3	1.49	0.59
1:A:1072:G:H2'	1:A:1073:U:C6	2.38	0.59
9:I:5:TYR:HE2	9:I:16:ARG:HG2	1.68	0.59
1:A:148:G:H2'	1:A:149:A:H8	1.67	0.59
1:A:833:U:O2	1:A:854:G:C2	2.55	0.59
9:I:19:LEU:HB2	9:I:59:PHE:HE2	1.68	0.59
11:K:109:VAL:HG12	11:K:110:ASP:N	2.18	0.59
13:M:37:THR:HB	13:M:39:ILE:HD11	1.84	0.59
1:A:1085:U:C2	25:A:2271:HOH:O	2.53	0.59
1:A:1151:A:C4	1:A:1152:A:N7	2.70	0.59
1:A:427:U:OP1	4:D:13:ARG:NH2	2.35	0.59
5:E:84:PHE:HB3	5:E:134:ALA:HB2	1.85	0.59
1:A:1314:C:C5	19:S:6:LYS:HE2	2.38	0.58
1:A:1314:C:OP2	19:S:6:LYS:HD3	2.03	0.58
1:A:941:G:H2'	1:A:942:G:O5'	2.02	0.58
10:J:38:ILE:N	10:J:71:LEU:HB2	2.18	0.58
1:A:530:G:O2'	1:A:531:U:OP2	2.21	0.58
1:A:677:U:O2	1:A:777:A:O2'	2.18	0.58
1:A:734:G:H21	18:R:75:ILE:HD11	1.68	0.58
8:H:6:ILE:HD11	8:H:31:PHE:CE2	2.38	0.58
1:A:187:C:C2	20:T:105:SER:HB3	2.39	0.58
3:C:116:VAL:HG21	3:C:202:ILE:HD11	1.85	0.58
9:I:84:ALA:O	9:I:87:GLN:HB3	2.02	0.58
16:P:1:MET:HG2	16:P:2:VAL:N	2.18	0.58
19:S:53:ASN:HB2	19:S:56:GLN:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:49:ALA:HB2	20:T:92:LEU:HG	1.85	0.58
1:A:189:G:H2'	1:A:190:C:C6	2.39	0.58
1:A:519:C:OP2	12:L:50:SER:HB3	2.03	0.58
3:C:157:ILE:HD12	3:C:164:ARG:NH1	2.18	0.58
7:G:54:THR:HB	7:G:56:GLN:OE1	2.03	0.58
19:S:7:LYS:HD2	19:S:7:LYS:O	2.02	0.58
1:A:1397:C:HO2'	1:A:1398:A:P	2.26	0.58
17:Q:68:ARG:H	17:Q:70:ARG:HH11	1.52	0.58
20:T:10:LEU:O	20:T:13:LEU:HD23	2.03	0.58
1:A:1357:A:H5''	1:A:1358:U:OP2	2.03	0.58
1:A:222:U:H2'	1:A:223:U:C6	2.38	0.58
2:B:97:TRP:HH2	2:B:176:GLU:CD	2.06	0.58
4:D:150:GLU:HA	4:D:153:ARG:HG3	1.86	0.58
4:D:9:CYS:SG	4:D:31:CYS:O	2.62	0.58
4:D:35:ARG:O	4:D:36:ARG:HG3	2.03	0.58
6:F:48:LEU:HB2	6:F:56:PRO:O	2.03	0.58
16:P:53:VAL:HG12	16:P:79:VAL:HG22	1.86	0.58
2:B:167:PRO:O	2:B:171:ALA:HB2	2.04	0.58
20:T:64:ASP:OD2	20:T:81:LYS:NZ	2.32	0.58
1:A:1145:C:H4'	1:A:1146:A:OP1	2.02	0.58
1:A:1182:G:H4'	1:A:1183:A:H5''	1.86	0.58
2:B:92:TYR:CD1	2:B:151:GLY:HA3	2.39	0.58
1:A:1121:U:H2'	1:A:1122:U:C6	2.39	0.58
1:A:929:G:N2	1:A:1388:C:O2	2.24	0.58
7:G:149:ARG:HD2	11:K:59:TYR:CD1	2.38	0.58
8:H:109:ILE:HD12	8:H:111:ILE:HG13	1.86	0.58
9:I:19:LEU:HD11	9:I:85:LEU:HD12	1.86	0.58
19:S:6:LYS:HB2	19:S:7:LYS:HZ3	1.68	0.58
1:A:1096:C:H6	1:A:1096:C:H5''	1.69	0.57
1:A:1213:A:C8	1:A:1215:G:C5	2.92	0.57
1:A:11:G:C5	1:A:12:U:C5	2.92	0.57
1:A:1526:G:O2'	1:A:1527:C:H5'	2.03	0.57
1:A:229:U:C2'	1:A:230:G:H5'	2.33	0.57
5:E:144:THR:HG22	5:E:146:ALA:H	1.69	0.57
6:F:3:ARG:O	6:F:93:SER:HB2	2.03	0.57
7:G:111:ARG:NH2	7:G:122:HIS:HB3	2.19	0.57
1:A:750:G:N3	15:O:23:GLY:HA3	2.19	0.57
2:B:131:PRO:HB2	2:B:133:LYS:HD2	1.84	0.57
2:B:97:TRP:HH2	2:B:176:GLU:OE1	1.86	0.57
6:F:98:LEU:N	6:F:98:LEU:HD12	2.18	0.57
15:O:25:THR:HG21	15:O:70:LEU:HD23	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:38:TYR:O	16:P:49:LEU:HD12	2.04	0.57
1:A:1314:C:H5	19:S:6:LYS:HE2	1.69	0.57
1:A:953:G:H5''	1:A:965:A:H61	1.67	0.57
1:A:986:A:C2	1:A:1220:G:C2	2.92	0.57
5:E:65:ASN:CG	5:E:65:ASN:O	2.43	0.57
8:H:118:VAL:O	8:H:119:LEU:HD23	2.04	0.57
13:M:49:THR:HG22	13:M:51:ALA:N	2.20	0.57
18:R:47:THR:HG22	18:R:48:GLY:N	2.20	0.57
20:T:10:LEU:HD22	20:T:11:SER:N	2.19	0.57
1:A:1213:A:C5	1:A:1215:G:C4	2.93	0.57
1:A:1328:C:H2'	1:A:1329:A:H8	1.69	0.57
1:A:1329:A:H2'	1:A:1330:U:O4'	2.03	0.57
6:F:43:LEU:HD13	6:F:46:ARG:HG3	1.85	0.57
1:A:1348:U:H4'	9:I:120:ARG:HD2	1.86	0.57
10:J:45:ARG:HB3	10:J:47:PHE:HE1	1.69	0.57
20:T:99:LEU:HD23	20:T:100:ILE:N	2.18	0.57
1:A:1135:U:O2'	1:A:1138:G:O6	2.21	0.57
1:A:1448:C:H42	1:A:1455:G:H1	1.51	0.57
1:A:392:G:H2'	1:A:393:A:C8	2.40	0.57
1:A:45:U:H2'	1:A:46:G:C8	2.39	0.57
3:C:59:ARG:HH11	3:C:59:ARG:HG2	1.68	0.57
7:G:15:ASP:HB3	7:G:19:GLY:H	1.68	0.57
7:G:16:LEU:HD11	9:I:42:ARG:HA	1.84	0.57
13:M:96:LEU:HB3	13:M:97:PRO:HD2	1.87	0.57
1:A:1216:G:H5''	14:N:5:ALA:HB2	1.87	0.57
1:A:977:A:H2'	1:A:978:A:H5''	1.86	0.57
7:G:69:VAL:HG21	7:G:104:LEU:HD21	1.85	0.57
9:I:38:GLN:HG2	9:I:39:GLY:N	2.18	0.57
13:M:29:ARG:HD3	13:M:64:TRP:CE2	2.40	0.57
1:A:1505:G:H4'	1:A:1506:U:H5''	1.85	0.57
1:A:109:A:C4	1:A:327:A:C2	2.93	0.57
1:A:610:G:H2'	1:A:611:A:H5'	1.87	0.57
1:A:683:G:H5''	1:A:684:A:OP2	2.04	0.57
8:H:71:GLY:O	8:H:74:PRO:HD3	2.05	0.57
1:A:878:G:H5'	8:H:89:PRO:HG2	1.85	0.57
15:O:56:LEU:O	15:O:60:VAL:HG23	2.04	0.57
18:R:26:LEU:HG	18:R:27:GLY:H	1.70	0.57
1:A:1329:A:OP1	13:M:29:ARG:HG3	2.04	0.57
1:A:344:A:H5''	1:A:345:C:H5	1.69	0.57
1:A:350:G:H5''	1:A:350:G:C8	2.35	0.57
1:A:518:C:H2'	1:A:530:G:C8	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:U:O2'	1:A:99:C:H5'	2.04	0.57
5:E:17:ALA:HB2	5:E:26:PHE:HD2	1.70	0.57
1:A:1267:C:O2	21:U:20:LYS:HD2	2.04	0.57
1:A:1496:C:H6	1:A:1517:G:H1	1.53	0.57
1:A:344:A:C5'	1:A:345:C:H5	2.17	0.57
3:C:9:GLY:HA2	3:C:12:LEU:HD12	1.86	0.57
5:E:43:LEU:N	5:E:136:MET:HE1	2.20	0.57
5:E:78:HIS:CE1	5:E:142:LEU:HD23	2.40	0.57
18:R:56:THR:HG23	18:R:58:LEU:N	2.13	0.57
1:A:1122:U:O4	1:A:1123:A:N6	2.37	0.56
1:A:1387:G:C6	1:A:1388:C:N4	2.73	0.56
1:A:56:U:O2'	1:A:57:G:H5'	2.04	0.56
20:T:10:LEU:CD1	20:T:13:LEU:H	2.16	0.56
1:A:1269:A:H2	1:A:1312:G:N3	2.02	0.56
1:A:1415:G:H3'	1:A:1415:G:C8	2.39	0.56
1:A:924:C:C2'	1:A:925:G:H5'	2.34	0.56
4:D:88:VAL:O	4:D:92:VAL:HG23	2.04	0.56
15:O:57:LEU:O	15:O:60:VAL:N	2.38	0.56
1:A:561:U:H5'	25:A:2992:HOH:O	2.05	0.56
8:H:120:THR:N	8:H:123:GLU:OE1	2.32	0.56
1:A:1065:U:H5''	1:A:1190:G:N2	2.19	0.56
2:B:97:TRP:CH2	2:B:176:GLU:CD	2.79	0.56
4:D:95:GLY:O	4:D:99:SER:HB2	2.06	0.56
10:J:47:PHE:HD2	14:N:44:LEU:HD21	1.70	0.56
1:A:735:C:H1'	18:R:75:ILE:HD11	1.87	0.56
2:B:10:LEU:O	2:B:12:GLU:N	2.38	0.56
8:H:105:ARG:NH1	25:H:305:HOH:O	2.38	0.56
1:A:1149:C:OP1	9:I:9:ARG:NH1	2.39	0.56
17:Q:15:MET:CE	17:Q:43:LEU:HD11	2.35	0.56
1:A:1027:C:N4	1:A:1034:G:H22	2.04	0.56
2:B:189:ASP:HB2	2:B:205:ASP:HB3	1.88	0.56
5:E:14:ARG:HG3	5:E:16:THR:HG23	1.88	0.56
12:L:53:ARG:HG3	12:L:93:LEU:CD2	2.35	0.56
13:M:23:TYR:CE2	13:M:70:LEU:HD22	2.39	0.56
18:R:66:LEU:HD11	18:R:70:ILE:HD11	1.88	0.56
13:M:99:ARG:NH2	19:S:2:PRO:HG3	2.20	0.56
20:T:49:ALA:HA	20:T:52:ALA:HB3	1.88	0.56
1:A:1256:A:H5''	1:A:1256:A:C8	2.38	0.56
1:A:1305:G:H5''	21:U:4:GLY:O	2.05	0.56
1:A:1316:G:H2'	1:A:1317:C:H5''	1.88	0.56
1:A:324:G:OP1	20:T:22:ARG:HD2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:G:C8	1:A:506:G:H5'	2.40	0.56
4:D:98:GLU:OE2	4:D:107:ARG:HG3	2.04	0.56
13:M:74:VAL:O	13:M:77:ASN:HB2	2.05	0.56
1:A:1074:G:C4'	2:B:104:ASN:HB2	2.35	0.56
1:A:1405:G:N2	1:A:1496:C:H5	2.02	0.56
1:A:414:A:H2'	1:A:415:A:H8	1.71	0.56
1:A:964:A:N6	25:A:2709:HOH:O	2.31	0.56
12:L:25:PRO:HB2	12:L:64:TYR:CE2	2.32	0.56
1:A:1166:G:N2	1:A:1169:A:OP2	2.39	0.56
3:C:92:ALA:HB2	3:C:99:VAL:HG22	1.88	0.56
1:A:1124:G:O2'	1:A:1145:C:N4	2.38	0.56
1:A:1504:G:C3'	1:A:1505:G:H5'	2.36	0.56
6:F:95:GLU:O	18:R:32:ARG:NH1	2.39	0.56
12:L:90:VAL:HG11	12:L:93:LEU:HG	1.88	0.56
1:A:1293:G:H2'	1:A:1294:G:O4'	2.07	0.55
1:A:671:G:H2'	1:A:672:U:O4'	2.06	0.55
19:S:53:ASN:HB3	19:S:55:LYS:H	1.69	0.55
1:A:1010:G:O2'	1:A:1011:G:H5'	2.07	0.55
1:A:1194:U:C2'	1:A:1195:C:H5'	2.36	0.55
1:A:1219:U:C4	1:A:1220:G:N7	2.74	0.55
1:A:1413:A:H2	1:A:1487:G:H22	1.54	0.55
1:A:452:A:C2	1:A:453:A:C4	2.94	0.55
1:A:132:C:O3'	20:T:74:LYS:NZ	2.39	0.55
1:A:1123:A:O2'	10:J:38:ILE:HG12	2.05	0.55
1:A:517:G:N1	1:A:533:A:OP2	2.22	0.55
1:A:778:G:H2'	1:A:779:C:H6	1.69	0.55
12:L:34:ARG:HB2	12:L:105:TYR:HE1	1.71	0.55
13:M:108:ARG:HD3	13:M:114:ARG:NH2	2.21	0.55
13:M:11:ARG:HH21	13:M:12:ASN:HA	1.70	0.55
1:A:1411:C:H42	1:A:1489:G:H1	1.54	0.55
5:E:78:HIS:HE1	5:E:142:LEU:HA	1.72	0.55
9:I:111:ARG:O	9:I:111:ARG:HG3	2.06	0.55
14:N:29:ARG:HE	14:N:31:ARG:HB2	1.72	0.55
8:H:61:VAL:CG1	8:H:63:LEU:HD12	2.35	0.55
1:A:975:A:N6	10:J:60:ARG:HH21	2.04	0.55
1:A:506:G:C5'	1:A:506:G:H8	2.20	0.55
1:A:580:U:H2'	1:A:581:G:C8	2.40	0.55
1:A:758:G:O2'	1:A:759:A:H5'	2.07	0.55
1:A:763:G:N2	1:A:764:C:C2	2.75	0.55
1:A:745:C:H5''	1:A:851:G:O2'	2.06	0.55
2:B:208:ILE:H	2:B:208:ILE:HD12	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1303:C:H2'	1:A:1304:G:H5'	1.88	0.55
1:A:192:U:H2'	1:A:193:C:H6	1.71	0.55
1:A:806:C:H2'	1:A:807:A:C8	2.41	0.55
2:B:16:HIS:ND1	2:B:17:PHE:O	2.39	0.55
2:B:92:TYR:HD1	2:B:92:TYR:C	2.10	0.55
11:K:29:ILE:HG22	11:K:44:SER:HB2	1.88	0.55
13:M:114:ARG:CZ	25:M:202:HOH:O	2.53	0.55
18:R:73:ALA:HB3	18:R:79:LEU:HD12	1.88	0.55
20:T:43:LEU:HA	20:T:46:GLU:HG3	1.88	0.55
1:A:1062:U:H2'	1:A:1063:C:C6	2.41	0.55
1:A:1259:C:H5''	1:A:1260:C:OP2	2.07	0.55
1:A:1442:G:N7	1:A:1446:A:N6	2.54	0.55
1:A:672:U:H2'	1:A:673:G:H8	1.72	0.55
3:C:5:ILE:HD12	3:C:6:HIS:H	1.72	0.55
3:C:76:VAL:O	3:C:83:ARG:HG2	2.06	0.55
4:D:7:PRO:HB2	4:D:10:ARG:HG2	1.89	0.55
6:F:44:GLY:HA2	6:F:60:PHE:H	1.72	0.55
1:A:1018:C:H2'	1:A:1019:C:O4'	2.07	0.55
1:A:1130:A:C2	1:A:1146:A:C4	2.94	0.55
1:A:1410:G:H2'	1:A:1411:C:H6	1.71	0.55
2:B:84:GLU:HG3	2:B:215:LEU:HB3	1.89	0.55
5:E:45:PHE:HE2	5:E:47:LYS:HE3	1.72	0.55
6:F:1:MET:HB2	6:F:67:MET:O	2.07	0.55
13:M:105:THR:O	13:M:107:ALA:N	2.40	0.55
19:S:2:PRO:N	19:S:3:ARG:HG3	2.21	0.55
21:U:13:ILE:HA	21:U:22:ARG:NH1	2.22	0.55
1:A:987:G:N2	1:A:1219:U:O2	2.40	0.54
1:A:1346:A:C5	7:G:10:ARG:NH2	2.76	0.54
1:A:109:A:C6	1:A:326:G:C6	2.95	0.54
2:B:97:TRP:CG	2:B:173:ALA:HB2	2.42	0.54
10:J:8:LEU:HD23	10:J:96:ILE:HA	1.89	0.54
1:A:949:A:C2	1:A:1233:G:N3	2.75	0.54
1:A:1298:C:C4	7:G:114:ARG:HD2	2.42	0.54
13:M:49:THR:O	13:M:53:VAL:HG23	2.07	0.54
1:A:981:U:H5'	14:N:21:TYR:CE1	2.42	0.54
1:A:1484:C:C2	1:A:1485:U:H6	2.26	0.54
3:C:156:ARG:H	3:C:163:ALA:HA	1.71	0.54
7:G:121:ALA:O	7:G:125:MET:HG3	2.07	0.54
1:A:1539:C:H5''	7:G:82:GLY:HA2	1.90	0.54
8:H:104:ARG:NH1	8:H:138:TRP:CE2	2.76	0.54
18:R:39:VAL:O	18:R:42:ARG:HG2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:53:ARG:CA	18:R:56:THR:HG22	2.26	0.54
1:A:1368:G:H2'	1:A:1369:C:H5'	1.89	0.54
1:A:1443:G:H5'	1:A:1443:G:H8	1.72	0.54
1:A:642:A:C8	8:H:115:SER:HA	2.42	0.54
8:H:104:ARG:CZ	8:H:138:TRP:CZ2	2.90	0.54
18:R:74:ARG:HB3	18:R:81:PHE:CZ	2.43	0.54
1:A:1002:G:H22	1:A:1003(A):G:N2	2.05	0.54
1:A:937:A:N6	1:A:1345:U:O4	2.36	0.54
6:F:71:ARG:HH11	6:F:71:ARG:HB2	1.71	0.54
1:A:689:C:P	11:K:46:GLY:HA3	2.48	0.54
12:L:19:ARG:HB3	12:L:20:LYS:NZ	2.22	0.54
16:P:6:LEU:HD12	16:P:6:LEU:N	2.22	0.54
1:A:496:A:H4'	1:A:497:A:OP1	2.07	0.54
1:A:966:M2G:HM13	1:A:967:5MC:C1'	2.33	0.54
6:F:2:ARG:HD2	6:F:69:GLU:CG	2.38	0.54
13:M:108:ARG:NH2	13:M:114:ARG:HA	2.23	0.54
21:U:13:ILE:HG12	21:U:22:ARG:NH1	2.22	0.54
1:A:277:C:OP2	17:Q:41:LYS:HE3	2.07	0.54
5:E:18:ARG:HG2	5:E:19:MET:N	2.23	0.54
1:A:1227:A:H5''	1:A:1228:C:OP2	2.08	0.54
1:A:1415:G:N2	1:A:1485:U:C4	2.75	0.54
3:C:155:GLY:O	3:C:156:ARG:HB2	2.08	0.54
3:C:15:THR:HB	3:C:181:ASN:HB2	1.90	0.54
4:D:10:ARG:O	4:D:13:ARG:HB2	2.08	0.54
4:D:54:TYR:HE1	4:D:206:PHE:CE1	2.19	0.54
5:E:78:HIS:CE1	5:E:142:LEU:HA	2.43	0.54
6:F:80:ARG:HH11	6:F:80:ARG:HG2	1.73	0.54
7:G:9:VAL:HG22	7:G:10:ARG:N	2.23	0.54
9:I:81:ILE:O	9:I:85:LEU:HD13	2.08	0.54
12:L:93:LEU:N	12:L:93:LEU:HD23	2.22	0.54
13:M:51:ALA:HA	13:M:54:VAL:HG12	1.89	0.54
1:A:1525:G:O2'	1:A:1526:G:H5'	2.08	0.54
1:A:261:U:O2	1:A:263:A:C8	2.61	0.54
1:A:526:C:C5	1:A:527:7MG:H1'	2.43	0.54
1:A:527:7MG:H2'	1:A:528:C:H5'	1.88	0.54
1:A:538:G:P	12:L:115:LYS:HB2	2.48	0.54
2:B:21:ARG:HA	2:B:39:ILE:HA	1.90	0.54
2:B:92:TYR:C	2:B:92:TYR:CD1	2.80	0.54
13:M:12:ASN:O	13:M:44:ARG:HG3	2.08	0.54
1:A:1004:A:C6	1:A:1037:C:N4	2.76	0.54
1:A:1352:C:H2'	1:A:1353:G:H8	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1379:G:N2	1:A:1381:U:O4	2.40	0.54
1:A:1442:G:C8	1:A:1446:A:N6	2.75	0.54
1:A:1497:G:O2'	1:A:1498:UR3:H5'	2.08	0.54
1:A:216:G:O2'	1:A:217:C:OP2	2.21	0.54
1:A:639:G:O2'	1:A:640:A:H5'	2.08	0.54
1:A:735:C:H1'	18:R:75:ILE:CD1	2.38	0.54
1:A:778:G:O5'	1:A:778:G:H8	1.91	0.54
3:C:111:LEU:HD21	3:C:146:ALA:HB2	1.90	0.54
1:A:421:U:H3	3:C:127:ARG:HH12	1.56	0.54
5:E:52:PRO:HG2	5:E:53:LEU:N	2.23	0.54
5:E:83:GLU:HG2	5:E:88:LYS:HG3	1.90	0.54
15:O:30:ALA:HA	15:O:85:LEU:HD11	1.89	0.54
16:P:53:VAL:HG23	16:P:54:GLU:N	2.22	0.54
20:T:100:ILE:HB	20:T:102:GLY:H	1.73	0.54
1:A:1527:C:H2'	1:A:1528:U:C6	2.42	0.53
1:A:965:A:C2	1:A:969:A:C2	2.96	0.53
6:F:62:TRP:HB2	18:R:35:ARG:HH12	1.73	0.53
1:A:1373:G:H5''	7:G:36:LYS:HD2	1.89	0.53
15:O:56:LEU:O	15:O:56:LEU:HD13	2.08	0.53
17:Q:15:MET:HB3	17:Q:18:THR:HB	1.90	0.53
1:A:657:G:H2'	1:A:658:G:H5'	1.90	0.53
1:A:735:C:H2'	1:A:736:C:H6	1.73	0.53
2:B:158:LEU:H	2:B:158:LEU:HD12	1.73	0.53
4:D:170:VAL:HG22	4:D:171:GLY:N	2.23	0.53
4:D:126:ILE:HG22	4:D:127:THR:N	2.24	0.53
13:M:9:ILE:O	13:M:11:ARG:N	2.41	0.53
13:M:48:LEU:CD1	13:M:53:VAL:HG22	2.38	0.53
15:O:33:THR:HG21	15:O:85:LEU:HD22	1.90	0.53
1:A:1125:U:C5	1:A:1281:U:O2	2.61	0.53
5:E:6:PHE:CE2	5:E:36:ASP:HB3	2.41	0.53
7:G:111:ARG:HH21	7:G:123:GLU:HA	1.73	0.53
1:A:1376:U:OP1	7:G:98:SER:OG	2.25	0.53
12:L:60:LEU:HB2	12:L:64:TYR:O	2.08	0.53
17:Q:5:VAL:C	17:Q:6:LEU:HD23	2.28	0.53
18:R:53:ARG:NH1	18:R:59:SER:HA	2.22	0.53
1:A:11:G:C6	1:A:12:U:C4	2.97	0.53
1:A:690:G:C6	1:A:691:G:C6	2.96	0.53
1:A:77:G:C4	1:A:93:G:N2	2.77	0.53
1:A:1112:C:H1'	3:C:179:ARG:HH21	1.73	0.53
5:E:14:ARG:HE	5:E:16:THR:CG2	2.21	0.53
7:G:99:LEU:O	7:G:103:TRP:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:10:LEU:HD23	8:H:83:ILE:HD11	1.89	0.53
12:L:25:PRO:CA	12:L:27:LEU:H	2.21	0.53
16:P:6:LEU:HD23	16:P:17:TYR:CG	2.43	0.53
20:T:56:MET:HG3	20:T:88:VAL:HG21	1.90	0.53
1:A:432:A:C8	1:A:433:C:C5	2.96	0.53
1:A:502:G:H2'	1:A:503:C:O4'	2.08	0.53
10:J:8:LEU:HD21	10:J:96:ILE:HG23	1.91	0.53
1:A:1106:G:C6	1:A:1107:C:C4	2.96	0.53
1:A:1245:A:C2	1:A:1293:G:C2	2.97	0.53
1:A:158:G:H2'	1:A:159:G:H5'	1.91	0.53
1:A:587:G:O2'	1:A:588:G:OP2	2.23	0.53
1:A:734:G:N2	18:R:75:ILE:HD11	2.23	0.53
2:B:57:PHE:CG	2:B:199:TYR:CE1	2.97	0.53
4:D:187:ARG:CZ	4:D:188:LEU:H	2.21	0.53
8:H:25:ASP:OD1	8:H:25:ASP:N	2.41	0.53
8:H:7:ALA:O	8:H:10:LEU:N	2.41	0.53
11:K:81:ASP:HB3	11:K:107:SER:OG	2.09	0.53
19:S:11:VAL:HG12	19:S:12:ASP:O	2.08	0.53
1:A:1118:C:H1'	1:A:1179:A:C4	2.44	0.53
1:A:1280:A:H3'	1:A:1281:U:H5'	1.91	0.53
1:A:299:G:C6	1:A:300:A:C6	2.96	0.53
1:A:449:C:N4	1:A:450:G:C2	2.77	0.53
2:B:197:VAL:HG21	2:B:200:ILE:HD12	1.90	0.53
1:A:409:G:OP1	4:D:24:GLU:O	2.26	0.53
5:E:139:LEU:HD23	5:E:139:LEU:N	2.22	0.53
5:E:9:LYS:HD3	5:E:108:ALA:HB1	1.91	0.53
8:H:29:SER:HB3	8:H:32:LYS:HG3	1.90	0.53
1:A:1251:A:H4'	9:I:12:GLU:OE2	2.08	0.53
17:Q:26:GLN:O	17:Q:27:PHE:HB3	2.06	0.53
1:A:1437:C:H2'	1:A:1438:G:H5'	1.89	0.53
1:A:1492:A:H2'	1:A:1492:A:N3	2.23	0.53
1:A:929:G:H2'	1:A:930:C:H6	1.74	0.53
16:P:12:LYS:O	16:P:13:HIS:HB2	2.07	0.53
1:A:1007:C:H2'	1:A:1008:C:H6	1.73	0.53
1:A:1288:A:H2'	1:A:1289:A:O4'	2.08	0.53
1:A:390:C:H2'	1:A:391:G:C8	2.44	0.53
1:A:39:G:O2'	1:A:40:C:H5'	2.09	0.53
10:J:26:ALA:HA	10:J:84:GLN:HG2	1.91	0.53
17:Q:51:TYR:N	17:Q:51:TYR:CD1	2.77	0.53
19:S:7:LYS:NZ	19:S:7:LYS:H	2.07	0.53
1:A:1121:U:O2'	1:A:1122:U:H5'	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1125:U:C3'	1:A:1125:U:C6	2.89	0.52
1:A:658:G:C4	1:A:659:U:C5	2.97	0.52
1:A:814:A:N7	1:A:816:A:C4	2.77	0.52
6:F:2:ARG:CD	6:F:69:GLU:HG3	2.38	0.52
7:G:12:LEU:H	7:G:12:LEU:HD12	1.73	0.52
7:G:51:GLN:HB2	7:G:58:PRO:HD3	1.89	0.52
13:M:12:ASN:H	13:M:45:VAL:CG1	2.23	0.52
15:O:30:ALA:CB	15:O:85:LEU:HD11	2.39	0.52
19:S:60:VAL:HG12	19:S:62:ILE:HG22	1.91	0.52
19:S:79:THR:HG22	19:S:80:TYR:O	2.09	0.52
1:A:1214:C:H4'	25:A:2356:HOH:O	2.08	0.52
1:A:31:G:N2	1:A:48:C:OP1	2.39	0.52
1:A:701:C:O5'	1:A:703:G:H5'	2.08	0.52
8:H:137:VAL:HG12	8:H:138:TRP:N	2.25	0.52
10:J:65:LEU:O	10:J:65:LEU:HD12	2.08	0.52
15:O:29:VAL:HG12	15:O:30:ALA:N	2.24	0.52
15:O:36:ILE:HG13	15:O:59:MET:HE2	1.90	0.52
15:O:36:ILE:HG13	15:O:59:MET:CE	2.39	0.52
1:A:1492:A:C8	1:A:1493:A:C2	2.97	0.52
3:C:179:ARG:HG3	3:C:206:GLU:HG2	1.91	0.52
1:A:1060:C:C4	3:C:2:GLY:HA2	2.45	0.52
13:M:34:LEU:CD1	13:M:41:PRO:HA	2.40	0.52
1:A:1145:C:H1'	1:A:1146:A:C8	2.44	0.52
1:A:1502:A:H2	1:A:1505:G:H1	1.57	0.52
1:A:203:U:OP1	1:A:203:U:H4'	2.09	0.52
1:A:3:G:O6	4:D:87:GLY:N	2.43	0.52
1:A:923:A:H8	1:A:923:A:O5'	1.92	0.52
1:A:878:G:C5'	8:H:89:PRO:HG2	2.38	0.52
13:M:78:ILE:HD13	13:M:92:HIS:CE1	2.45	0.52
18:R:55:ARG:HG2	18:R:55:ARG:HH11	1.75	0.52
19:S:70:LYS:H	19:S:73:GLU:HG3	1.74	0.52
20:T:56:MET:HG2	20:T:84:LEU:HD21	1.90	0.52
1:A:1415:G:C1'	1:A:1486:G:H22	2.23	0.52
1:A:1486:G:H2'	1:A:1487:G:O4'	2.08	0.52
1:A:691:G:H2'	1:A:692:U:C6	2.41	0.52
1:A:91:C:H2'	1:A:92:C:C6	2.41	0.52
2:B:112:VAL:O	2:B:115:LEU:HB3	2.09	0.52
2:B:18:GLY:CA	2:B:42:ILE:HG12	2.40	0.52
3:C:56:ASP:HB2	3:C:67:THR:HB	1.90	0.52
11:K:67:ASP:OD1	11:K:71:LYS:HE3	2.10	0.52
11:K:84:VAL:HG21	11:K:95:ILE:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:16:ASP:OD1	13:M:16:ASP:N	2.43	0.52
18:R:74:ARG:HB3	18:R:81:PHE:CE2	2.44	0.52
19:S:35:SER:O	19:S:35:SER:OG	2.23	0.52
1:A:1126:U:H6	1:A:1126:U:H3'	1.73	0.52
1:A:1321:C:H3'	1:A:1322:C:C5'	2.39	0.52
1:A:518:C:H4'	1:A:519:C:H5''	1.90	0.52
1:A:524:G:O2'	1:A:525:C:H5'	2.10	0.52
1:A:556:C:C2'	1:A:557:G:H5'	2.39	0.52
7:G:75:VAL:HA	7:G:87:VAL:O	2.10	0.52
1:A:1054:C:H3'	25:A:3065:HOH:O	2.09	0.52
1:A:1074:G:H4'	2:B:104:ASN:HB2	1.92	0.52
1:A:1112:C:H5''	1:A:1113:C:OP2	2.09	0.52
1:A:299:G:N1	25:A:2126:HOH:O	2.32	0.52
1:A:377:G:C2	1:A:387:U:O2	2.63	0.52
1:A:521:G:OP1	12:L:54:LYS:HE2	2.09	0.52
1:A:660:G:H1	1:A:745:C:H42	1.58	0.52
1:A:837:G:N2	1:A:849:C:O2	2.43	0.52
1:A:591:U:OP1	8:H:30:ARG:NH1	2.43	0.52
8:H:6:ILE:O	8:H:10:LEU:HD12	2.10	0.52
17:Q:15:MET:HE2	17:Q:43:LEU:HD11	1.92	0.52
18:R:56:THR:HG21	18:R:63:GLN:OE1	2.10	0.52
20:T:37:SER:HB2	20:T:84:LEU:HD13	1.91	0.52
1:A:1130:A:H4'	9:I:18:PHE:CE1	2.45	0.52
1:A:1287:A:C6	1:A:1288:A:N6	2.77	0.52
1:A:259:G:H2'	1:A:260:G:C8	2.44	0.52
1:A:429:U:H4'	1:A:430:A:O5'	2.08	0.52
1:A:581:G:N7	25:A:3364:HOH:O	2.42	0.52
1:A:699:C:H1'	25:A:3282:HOH:O	2.10	0.52
1:A:943:U:C2'	1:A:944:G:H5'	2.40	0.52
13:M:11:ARG:HE	13:M:12:ASN:HB2	1.75	0.52
1:A:129:U:O3'	1:A:129(A):G:H3'	2.10	0.52
1:A:1402:4OC:C5	1:A:1403:C:C5	2.93	0.52
1:A:331:G:OP1	1:A:332:G:H8	1.92	0.52
1:A:436:C:O2'	1:A:437:U:H5'	2.09	0.52
1:A:826:C:H2'	1:A:827:U:H6	1.74	0.52
2:B:24:TRP:HA	2:B:190:THR:HG22	1.92	0.52
4:D:17:VAL:HG22	4:D:18:LYS:N	2.25	0.52
4:D:92:VAL:HG12	4:D:96:LEU:HD13	1.91	0.52
13:M:4:ILE:HD12	13:M:8:GLU:OE2	2.10	0.52
15:O:17:ARG:NH1	15:O:77:ARG:NH1	2.58	0.52
17:Q:76:LEU:HD23	17:Q:77:VAL:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:38:LYS:O	20:T:41:ILE:HG12	2.09	0.52
1:A:1298:C:H4'	1:A:1299:A:O4'	2.10	0.52
1:A:258:G:H2'	1:A:259:G:H8	1.75	0.52
1:A:902:G:O2'	1:A:903:G:H5'	2.10	0.52
7:G:115:ARG:HB2	7:G:118:VAL:HG23	1.92	0.52
11:K:30:VAL:HG21	11:K:65:ALA:HA	1.91	0.52
1:A:1092:A:N3	1:A:1183:A:N6	2.59	0.51
1:A:1296:C:H4'	1:A:1302:U:C5	2.45	0.51
1:A:1328:C:H2'	1:A:1329:A:C8	2.45	0.51
1:A:1435:G:H2'	1:A:1436:U:C6	2.44	0.51
1:A:275:G:C8	1:A:275:G:H5''	2.45	0.51
1:A:451:A:O2'	25:A:2737:HOH:O	2.19	0.51
1:A:514:C:O2'	1:A:515:G:H5'	2.10	0.51
1:A:762:C:H2'	1:A:763:G:H8	1.74	0.51
1:A:96:G:C2'	1:A:97:G:H5'	2.40	0.51
2:B:32:ILE:HD11	2:B:190:THR:HG23	1.92	0.51
13:M:40:ASN:HB3	13:M:43:THR:HG23	1.90	0.51
1:A:1151:A:H1'	1:A:1152:A:C8	2.45	0.51
1:A:597:G:H1'	1:A:644:G:N2	2.25	0.51
2:B:42:ILE:HG21	2:B:202:PRO:HB2	1.93	0.51
3:C:138:VAL:HG21	3:C:169:ALA:HA	1.91	0.51
3:C:58:GLU:H	3:C:65:ALA:HB3	1.75	0.51
6:F:4:TYR:HB3	6:F:91:VAL:O	2.10	0.51
7:G:16:LEU:HG	9:I:41:VAL:HG12	1.92	0.51
3:C:69:HIS:N	3:C:69:HIS:ND1	2.58	0.51
9:I:97:LYS:HD3	9:I:102:LEU:HD12	1.92	0.51
1:A:1305:G:N2	1:A:1331:G:H1'	2.25	0.51
1:A:1499:A:C1'	1:A:1520:G:H5'	2.41	0.51
1:A:452:A:HO2'	1:A:453:A:H8	1.56	0.51
1:A:721:G:N1	1:A:733:A:C2	2.78	0.51
2:B:82:ARG:NH1	2:B:86:GLU:OE2	2.42	0.51
3:C:150:LYS:HG3	3:C:169:ALA:HB2	1.91	0.51
3:C:174:PRO:O	3:C:176:HIS:N	2.43	0.51
4:D:174:LEU:HD23	4:D:185:PHE:HA	1.93	0.51
4:D:62:GLN:HA	4:D:62:GLN:OE1	2.10	0.51
7:G:15:ASP:HB3	7:G:20:ASP:H	1.75	0.51
12:L:83:VAL:HG21	12:L:100:ILE:HD13	1.92	0.51
13:M:56:LEU:O	13:M:60:VAL:HG23	2.11	0.51
1:A:933:G:H1	1:A:1384:C:N4	2.05	0.51
5:E:151:LEU:HD13	8:H:79:VAL:HG23	1.93	0.51
6:F:23:LYS:NZ	6:F:42:GLU:OE1	2.34	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:6:ILE:HG22	10:J:97:GLU:O	2.10	0.51
11:K:18:ARG:CB	11:K:33:THR:HG23	2.32	0.51
1:A:1228:C:H5'	13:M:115:LYS:O	2.10	0.51
14:N:7:ILE:O	14:N:11:LYS:HD3	2.10	0.51
18:R:40:LEU:O	18:R:42:ARG:N	2.44	0.51
1:A:1237:C:H3'	1:A:1336:C:H41	1.75	0.51
1:A:248:C:N3	1:A:276:G:N2	2.59	0.51
1:A:260:G:C4	1:A:261:U:C5	2.99	0.51
1:A:414:A:OP2	1:A:428:G:N2	2.43	0.51
3:C:131:ARG:NH2	3:C:166:GLU:OE2	2.38	0.51
4:D:187:ARG:HA	4:D:187:ARG:HH11	1.76	0.51
6:F:23:LYS:O	6:F:27:GLN:HG3	2.11	0.51
9:I:22:GLY:HA3	9:I:60:ASP:HB2	1.93	0.51
18:R:58:LEU:HD22	18:R:62:GLU:HB3	1.92	0.51
1:A:106:C:O2	1:A:379:C:H4'	2.11	0.51
1:A:12:U:H3	1:A:22:G:H1	1.59	0.51
1:A:539:A:H2'	1:A:540:G:C8	2.46	0.51
1:A:989:C:O2'	1:A:1017:G:O2'	2.20	0.51
3:C:112:SER:O	3:C:116:VAL:HG23	2.11	0.51
10:J:47:PHE:CD2	14:N:44:LEU:HD21	2.45	0.51
3:C:23:TYR:CE2	10:J:9:ARG:HD2	2.46	0.51
17:Q:95:TYR:O	17:Q:98:LEU:HD12	2.10	0.51
1:A:1254:C:H42	1:A:1283:G:H1	1.59	0.51
1:A:1487:G:C4	1:A:1488:G:C8	2.99	0.51
1:A:627:G:O2'	1:A:628:G:H5'	2.10	0.51
1:A:657:G:C2'	1:A:658:G:H5'	2.41	0.51
1:A:81:U:H3'	1:A:82:U:H5''	1.93	0.51
3:C:120:VAL:HG12	3:C:121:ALA:N	2.25	0.51
4:D:28:SER:CB	4:D:30:LYS:H	2.23	0.51
9:I:114:TYR:CD1	10:J:60:ARG:HB2	2.46	0.51
12:L:89:ARG:NE	12:L:97:ARG:HG2	2.25	0.51
13:M:11:ARG:HG3	13:M:12:ASN:HB2	1.93	0.51
13:M:48:LEU:HB2	13:M:53:VAL:HG22	1.92	0.51
18:R:36:ASN:O	18:R:40:LEU:HG	2.11	0.51
1:A:617:G:O6	1:A:623:C:N4	2.42	0.51
1:A:620:C:H2'	1:A:621:A:O4'	2.11	0.51
3:C:166:GLU:HA	3:C:166:GLU:OE1	2.11	0.51
5:E:150:ARG:HH11	5:E:150:ARG:HG2	1.75	0.51
8:H:62:TYR:N	8:H:62:TYR:CD2	2.79	0.51
15:O:70:LEU:O	15:O:73:GLU:N	2.44	0.51
17:Q:3:LYS:HB3	17:Q:61:GLU:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:38:GLU:HA	18:R:41:LYS:HD3	1.91	0.51
1:A:1125:U:H5	1:A:1281:U:O2	1.94	0.51
1:A:512:U:H2'	1:A:513:C:H6	1.76	0.51
2:B:201:ILE:HG21	2:B:214:ILE:HG21	1.93	0.51
8:H:137:VAL:O	8:H:138:TRP:HB3	2.10	0.51
8:H:85:ARG:HG3	8:H:86:ILE:N	2.23	0.51
16:P:43:LYS:HG2	16:P:48:TRP:CD2	2.46	0.51
1:A:1052:U:H5''	1:A:1053:G:OP2	2.11	0.50
1:A:1504:G:H4'	1:A:1505:G:H5'	1.93	0.50
1:A:725:G:O2'	1:A:726:C:H5'	2.12	0.50
1:A:899:C:H2'	1:A:900:A:O4'	2.11	0.50
2:B:178:ARG:HA	2:B:178:ARG:HH11	1.76	0.50
4:D:30:LYS:C	4:D:32:ALA:H	2.14	0.50
1:A:1116:C:H5''	25:A:3034:HOH:O	2.10	0.50
1:A:1145:C:H1'	1:A:1146:A:H8	1.76	0.50
1:A:1215:G:C2	1:A:1216:G:C8	3.00	0.50
1:A:556:C:H2'	1:A:557:G:H5'	1.93	0.50
1:A:938:A:C6	1:A:939:G:C5	3.00	0.50
2:B:183:PRO:HA	2:B:198:ASP:OD2	2.12	0.50
9:I:112:LYS:HA	9:I:119:ALA:HB2	1.93	0.50
10:J:40:LEU:O	10:J:69:ASN:HB2	2.11	0.50
17:Q:88:TYR:CD2	17:Q:89:LEU:N	2.79	0.50
18:R:38:GLU:OE2	18:R:38:GLU:N	2.44	0.50
1:A:1133:G:H1	1:A:1141:C:H42	1.59	0.50
1:A:1150:U:C2'	1:A:1151:A:H5'	2.42	0.50
1:A:692:U:H1'	1:A:695:A:N7	2.26	0.50
1:A:918:A:H2'	1:A:919:A:C8	2.46	0.50
1:A:948:C:H42	1:A:1233:G:H1	1.59	0.50
5:E:119:LEU:HD23	5:E:119:LEU:N	2.25	0.50
7:G:102:ARG:O	7:G:106:GLN:HG2	2.11	0.50
8:H:77:GLU:HG3	8:H:78:GLN:N	2.25	0.50
18:R:87:ARG:CG	18:R:88:LYS:H	2.21	0.50
1:A:250:A:H4'	1:A:251:G:O5'	2.11	0.50
1:A:312:C:H2'	1:A:313:A:C8	2.47	0.50
1:A:505:G:C2'	1:A:506:G:H5''	2.42	0.50
1:A:578:C:H42	1:A:763:G:H1	1.58	0.50
1:A:660:G:H2'	1:A:661:G:H8	1.76	0.50
1:A:791:G:N2	1:A:1497:G:O3'	2.45	0.50
1:A:977:A:O2'	1:A:979:C:OP2	2.28	0.50
2:B:30:ARG:HD2	2:B:31:TYR:CE1	2.46	0.50
5:E:121:LYS:HZ2	5:E:126:ARG:HH12	1.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:20:TYR:HE1	8:H:76:PRO:HG2	1.75	0.50
9:I:97:LYS:CE	9:I:102:LEU:H	2.22	0.50
12:L:36:VAL:HG12	12:L:37:CYS:N	2.26	0.50
12:L:90:VAL:HG12	12:L:90:VAL:O	2.11	0.50
18:R:54:ARG:H	18:R:54:ARG:HD3	1.76	0.50
1:A:1136:U:H5''	1:A:1137:C:OP2	2.11	0.50
1:A:1346:A:H5'	1:A:1348:U:H1'	1.93	0.50
1:A:1426:C:H42	1:A:1474:G:H1	1.60	0.50
1:A:1505:G:C3'	1:A:1505:G:C8	2.95	0.50
1:A:1504:G:C4'	1:A:1505:G:H5'	2.42	0.50
1:A:237:C:OP2	17:Q:40:LYS:NZ	2.35	0.50
1:A:434:U:H2'	1:A:435:C:C6	2.47	0.50
1:A:658:G:H1	1:A:747:C:N4	2.05	0.50
2:B:204:ASN:HD22	2:B:207:ALA:HB3	1.76	0.50
4:D:21:LEU:HD12	4:D:21:LEU:H	1.75	0.50
9:I:7:THR:H	9:I:83:ARG:HD3	1.76	0.50
15:O:70:LEU:O	15:O:72:ARG:N	2.44	0.50
17:Q:67:LYS:O	17:Q:68:ARG:HB2	2.11	0.50
20:T:43:LEU:HB2	20:T:52:ALA:HB2	1.94	0.50
1:A:1256:A:C2	1:A:1277:C:N4	2.80	0.50
1:A:229:U:H5''	16:P:33:ILE:HD13	1.92	0.50
1:A:684:A:H5''	1:A:685:G:OP2	2.11	0.50
4:D:150:GLU:OE1	4:D:151:LYS:HG3	2.12	0.50
8:H:120:THR:O	8:H:123:GLU:HB2	2.11	0.50
8:H:17:THR:CB	8:H:78:GLN:HE22	2.22	0.50
13:M:105:THR:CB	13:M:106:ASN:HB2	2.42	0.50
15:O:24:SER:O	15:O:28:GLN:N	2.41	0.50
20:T:30:LYS:O	20:T:33:ILE:HB	2.12	0.50
1:A:1124:G:H5''	10:J:35:SER:O	2.11	0.50
1:A:1518:MA6:H5''	1:A:1519:MA6:OP2	2.12	0.50
1:A:277:C:OP1	17:Q:68:ARG:NH2	2.45	0.50
1:A:487:A:H2'	1:A:488:C:O4'	2.12	0.50
1:A:530:G:HO2'	1:A:531:U:P	2.35	0.50
1:A:563:A:H2'	1:A:567:G:C8	2.46	0.50
1:A:683:G:H21	11:K:38:ASN:HD22	1.59	0.50
1:A:758:G:C8	25:A:3365:HOH:O	2.63	0.50
1:A:819:A:H4'	1:A:820:U:OP2	2.11	0.50
2:B:148:TYR:N	2:B:148:TYR:HD2	2.09	0.50
11:K:48:ILE:HG22	11:K:49:GLY:H	1.76	0.50
16:P:11:SER:N	16:P:14:ASN:O	2.41	0.50
16:P:22:THR:HA	16:P:33:ILE:HG13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:31:ILE:CG2	19:S:49:ILE:HA	2.42	0.50
1:A:1202:G:N2	14:N:43:CYS:SG	2.84	0.50
1:A:976:G:H5'	1:A:1358:U:O2'	2.12	0.50
1:A:1437:C:C2'	1:A:1438:G:H5'	2.42	0.50
1:A:412:A:N7	4:D:35:ARG:NH1	2.59	0.50
1:A:664:G:N2	1:A:741:G:H1	2.10	0.50
2:B:109:SER:O	2:B:112:VAL:HG12	2.12	0.50
2:B:161:ALA:O	2:B:162:ILE:HD13	2.11	0.50
5:E:109:ILE:HG22	5:E:110:LEU:N	2.25	0.50
6:F:33:TYR:O	6:F:71:ARG:NH1	2.45	0.50
7:G:15:ASP:CB	7:G:20:ASP:H	2.25	0.50
9:I:37:PHE:CD2	9:I:74:ILE:HD11	2.45	0.50
11:K:84:VAL:HG11	11:K:91:ARG:HD3	1.94	0.50
1:A:252:U:H6	1:A:252:U:H5''	1.77	0.50
1:A:562:C:H6	1:A:562:C:H5'	1.75	0.50
1:A:902:G:H2'	1:A:903:G:H8	1.76	0.50
2:B:148:TYR:N	2:B:148:TYR:CD2	2.79	0.50
17:Q:15:MET:HG2	17:Q:18:THR:HB	1.93	0.50
19:S:36:ARG:O	19:S:71:LEU:HB2	2.11	0.50
1:A:1127:G:H3'	1:A:1127:G:C8	2.47	0.49
1:A:1127:G:H5''	1:A:1128:C:OP2	2.12	0.49
1:A:1191:A:O2'	1:A:1192:C:H5'	2.12	0.49
1:A:1411:C:O2	1:A:1411:C:H2'	2.12	0.49
1:A:192:U:O2'	20:T:57:ARG:HG3	2.12	0.49
1:A:352:C:H5'	25:A:3093:HOH:O	2.12	0.49
1:A:460:A:O2'	1:A:461:C:H5'	2.11	0.49
18:R:44:LEU:CD1	18:R:79:LEU:HD22	2.41	0.49
1:A:1310:G:O6	19:S:2:PRO:HG2	2.12	0.49
20:T:23:ARG:HH11	20:T:23:ARG:HB3	1.76	0.49
1:A:103:C:OP1	20:T:17:ARG:NH1	2.45	0.49
1:A:1505:G:H3'	1:A:1505:G:C8	2.47	0.49
1:A:457:C:H2'	1:A:458:C:H6	1.76	0.49
4:D:190:ASP:N	4:D:193:ASP:HB2	2.27	0.49
4:D:25:ARG:HA	4:D:28:SER:CB	2.37	0.49
5:E:84:PHE:CB	5:E:134:ALA:HB2	2.42	0.49
6:F:44:GLY:HA2	6:F:60:PHE:N	2.27	0.49
8:H:110:ALA:N	8:H:121:ASP:OD1	2.44	0.49
12:L:53:ARG:HG3	12:L:93:LEU:HD21	1.94	0.49
15:O:25:THR:CG2	15:O:70:LEU:HD23	2.42	0.49
15:O:39:LEU:HB3	15:O:56:LEU:HD23	1.93	0.49
1:A:1172:C:H2'	1:A:1173:G:C8	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:663:A:H2'	1:A:664:G:O4'	2.12	0.49
2:B:139:LYS:HD3	2:B:142:LEU:HD12	1.93	0.49
3:C:50:ALA:HB2	3:C:75:VAL:HB	1.94	0.49
1:A:542:G:OP1	4:D:10:ARG:NH2	2.45	0.49
4:D:168:ARG:NH1	25:D:424:HOH:O	2.38	0.49
8:H:97:VAL:HG13	8:H:98:LYS:HG2	1.94	0.49
9:I:114:TYR:HE1	10:J:60:ARG:N	1.98	0.49
18:R:63:GLN:O	18:R:66:LEU:HB3	2.12	0.49
1:A:1315:U:H2'	1:A:1316:G:O4'	2.12	0.49
5:E:90:VAL:O	5:E:120:THR:HA	2.12	0.49
1:A:1292:U:H5'	9:I:38:GLN:NE2	2.27	0.49
19:S:18:LYS:HB3	19:S:31:ILE:HD11	1.94	0.49
19:S:53:ASN:HB2	19:S:56:GLN:H	1.77	0.49
5:E:32:VAL:HG23	5:E:58:ALA:CB	2.40	0.49
1:A:737:A:OP1	6:F:92:LYS:HB2	2.12	0.49
1:A:1298:C:H2'	7:G:114:ARG:HH12	1.77	0.49
8:H:41:ARG:HH22	8:H:123:GLU:CD	2.15	0.49
10:J:11:PHE:HE2	10:J:67:THR:HG23	1.77	0.49
17:Q:29:HIS:C	17:Q:29:HIS:ND1	2.65	0.49
1:A:1303:C:C2'	1:A:1304:G:H5'	2.43	0.49
1:A:1253:G:H1'	1:A:1355:G:O2'	2.13	0.49
1:A:190(J):U:H2'	1:A:190(K):G:C8	2.47	0.49
1:A:552:U:H2'	1:A:553:A:C8	2.48	0.49
1:A:676:A:H1'	11:K:115:PRO:HB3	1.94	0.49
2:B:130:ARG:NH2	2:B:134:GLU:OE1	2.44	0.49
3:C:33:LEU:O	3:C:33:LEU:HD22	2.11	0.49
4:D:13:ARG:NH1	4:D:13:ARG:HG2	2.26	0.49
6:F:23:LYS:O	6:F:26:ILE:HB	2.13	0.49
8:H:91:ARG:NH1	17:Q:33:GLY:HA3	2.27	0.49
9:I:91:ASP:N	9:I:91:ASP:OD2	2.45	0.49
1:A:1207:2MG:CM2	1:A:1208:C:H1'	2.42	0.49
1:A:1417:G:N2	1:A:1484:C:N4	2.60	0.49
1:A:1510:U:H2'	1:A:1511:G:C8	2.47	0.49
1:A:1532:U:H2'	1:A:1533:C:C5	2.47	0.49
1:A:573:A:H5'	1:A:573:A:H8	1.77	0.49
1:A:742:G:OP2	15:O:35:ARG:NH2	2.44	0.49
1:A:869:G:C8	25:A:3262:HOH:O	2.66	0.49
1:A:953:G:C5'	1:A:965:A:H61	2.26	0.49
4:D:131:ARG:O	4:D:133:VAL:HG23	2.13	0.49
13:M:12:ASN:H	13:M:45:VAL:HG11	1.78	0.49
13:M:86:CYS:HA	19:S:73:GLU:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:C:P	20:T:17:ARG:HH12	2.35	0.49
1:A:1113:C:H6	1:A:1113:C:O5'	1.96	0.49
1:A:114:U:O2'	1:A:115:G:H5'	2.12	0.49
1:A:1256:A:C6	1:A:1277:C:C5	3.01	0.49
1:A:1368:G:H5''	9:I:112:LYS:HB3	1.95	0.49
1:A:1484:C:C4	1:A:1485:U:C5	3.01	0.49
1:A:1405:G:H1	1:A:1496:C:H41	1.61	0.49
1:A:656:C:H4'	15:O:62:GLN:HE22	1.77	0.49
1:A:806:C:O2'	1:A:807:A:H5'	2.12	0.49
1:A:975:A:H4'	1:A:976:G:O5'	2.13	0.49
3:C:108:ASN:HD21	3:C:144:SER:CB	2.26	0.49
4:D:111:ALA:HA	4:D:161:ASN:ND2	2.28	0.49
5:E:14:ARG:O	5:E:28:PHE:HD2	1.95	0.49
1:A:107:G:C2'	1:A:108:G:H5'	2.43	0.49
1:A:1541:PSU:H5''	1:A:1542:U:OP1	2.12	0.49
1:A:787:A:N6	25:A:3170:HOH:O	2.46	0.49
2:B:166:ASP:HA	2:B:167:PRO:HD2	1.69	0.49
2:B:68:ILE:N	2:B:90:MET:HG2	2.26	0.49
3:C:77:ILE:HG22	3:C:78:GLY:O	2.13	0.49
4:D:101:LEU:HD12	4:D:101:LEU:O	2.13	0.49
5:E:81:GLU:OE1	5:E:88:LYS:HD3	2.12	0.49
9:I:16:ARG:HB3	9:I:64:THR:HG22	1.94	0.49
12:L:27:LEU:CG	12:L:28:LYS:H	2.09	0.49
1:A:1345:U:N3	1:A:1377:A:C2	2.81	0.49
1:A:725:G:C5	1:A:726:C:C5	3.01	0.49
1:A:954:G:H2'	1:A:955:U:C6	2.48	0.49
4:D:191:ARG:O	4:D:191:ARG:HD2	2.13	0.49
7:G:54:THR:HG22	7:G:55:GLY:H	1.78	0.49
1:A:588:G:H5'	8:H:1:MET:HG3	1.94	0.49
8:H:3:THR:OG1	8:H:4:ASP:N	2.46	0.49
8:H:73:ASP:OD2	8:H:75:ARG:HB2	2.13	0.49
9:I:36:TYR:CD2	9:I:37:PHE:CE1	3.01	0.49
25:A:3147:HOH:O	10:J:38:ILE:HB	2.11	0.49
10:J:8:LEU:CD2	10:J:96:ILE:HA	2.42	0.49
15:O:25:THR:O	15:O:29:VAL:HB	2.13	0.49
18:R:52:PRO:HG2	18:R:54:ARG:NH2	2.27	0.49
21:U:5:ASP:O	21:U:11:GLY:HA3	2.13	0.49
1:A:429:U:H1'	1:A:430:A:H5''	1.95	0.48
1:A:779:C:C2'	1:A:780:A:H5'	2.42	0.48
7:G:43:PHE:O	7:G:46:ALA:HB3	2.13	0.48
8:H:13:ILE:O	8:H:17:THR:HG23	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:17:ARG:HH12	15:O:77:ARG:NH1	2.11	0.48
1:A:113:G:H1	1:A:314:C:N4	2.08	0.48
1:A:1236:A:H2'	1:A:1237:C:C6	2.48	0.48
1:A:1305:G:OP2	21:U:2:GLY:N	2.46	0.48
1:A:1360:A:H2'	1:A:1361:G:O4'	2.13	0.48
2:B:17:PHE:CE1	2:B:18:GLY:O	2.66	0.48
2:B:69:LEU:HB3	2:B:162:ILE:HD12	1.94	0.48
14:N:22:THR:HB	14:N:33:VAL:HG11	1.94	0.48
19:S:30:LEU:HD23	19:S:48:THR:HG22	1.94	0.48
1:A:1125:U:H5	1:A:1281:U:C2	2.31	0.48
1:A:17:U:H2'	1:A:18:C:C6	2.48	0.48
1:A:357:G:H1'	1:A:368:U:O2	2.14	0.48
1:A:403:C:H2'	1:A:404:U:H6	1.78	0.48
1:A:836:G:C6	1:A:851:G:C6	3.02	0.48
2:B:71:VAL:HG13	2:B:93:VAL:HB	1.95	0.48
1:A:1060:C:N4	3:C:2:GLY:HA2	2.27	0.48
13:M:19:LEU:HD11	13:M:34:LEU:HD21	1.95	0.48
19:S:63:THR:H	19:S:66:MET:HG3	1.77	0.48
1:A:1002:G:H1	1:A:1003(A):G:N2	2.08	0.48
1:A:115:G:H1'	1:A:116:A:N7	2.28	0.48
1:A:1517:G:H3'	1:A:1518:MA6:H8	1.94	0.48
1:A:974:A:P	14:N:41:ARG:HH12	2.36	0.48
20:T:50:GLU:HA	20:T:99:LEU:HD22	1.95	0.48
1:A:1124:G:H4'	10:J:38:ILE:CD1	2.43	0.48
1:A:1509:C:H2'	1:A:1510:U:O4'	2.13	0.48
1:A:369:C:O2'	1:A:370:C:H5'	2.14	0.48
1:A:412:A:C8	4:D:35:ARG:NH1	2.81	0.48
1:A:98:U:H6	1:A:98:U:O5'	1.96	0.48
4:D:174:LEU:HA	4:D:186:LEU:HD13	1.95	0.48
8:H:28:ALA:HB3	8:H:57:PRO:HB2	1.96	0.48
9:I:62:TYR:C	9:I:62:TYR:CD1	2.85	0.48
9:I:9:ARG:HB3	9:I:14:VAL:HG13	1.95	0.48
11:K:21:ILE:HG12	11:K:30:VAL:HG12	1.95	0.48
15:O:68:ARG:O	15:O:71:GLN:N	2.46	0.48
19:S:33:THR:CG2	19:S:35:SER:H	2.26	0.48
20:T:89:ARG:HH21	20:T:104:LEU:CD1	2.22	0.48
1:A:257:G:C2	1:A:270:A:C2	3.01	0.48
1:A:261:U:O2	1:A:263:A:H8	1.96	0.48
1:A:55:A:H2'	1:A:56:U:H5'	1.96	0.48
2:B:18:GLY:HA2	2:B:42:ILE:HG12	1.95	0.48
2:B:92:TYR:CE1	2:B:151:GLY:HA3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:11:ARG:NH1	3:C:177:THR:O	2.47	0.48
3:C:95:THR:OG1	3:C:97:LYS:HB2	2.13	0.48
10:J:81:THR:HG22	10:J:82:ILE:N	2.28	0.48
15:O:71:GLN:O	15:O:75:PRO:HD3	2.13	0.48
16:P:14:ASN:HA	16:P:15:PRO:HD3	1.56	0.48
1:A:1241:G:H2'	1:A:1242:C:H6	1.79	0.48
1:A:516:PSU:C2	1:A:517:G:C6	3.01	0.48
1:A:610:G:C2'	1:A:611:A:H5'	2.43	0.48
4:D:61:LYS:HD2	4:D:207:TYR:OH	2.14	0.48
10:J:38:ILE:CD1	10:J:71:LEU:HG	2.41	0.48
11:K:18:ARG:HB3	11:K:33:THR:CG2	2.35	0.48
18:R:53:ARG:HG2	18:R:63:GLN:OE1	2.14	0.48
20:T:63:ILE:HD13	20:T:80:ARG:HB3	1.96	0.48
1:A:1106:G:C6	1:A:1107:C:N4	2.82	0.48
1:A:981:U:O4	1:A:1222:G:O6	2.31	0.48
1:A:151:A:H2'	1:A:152:A:O4'	2.14	0.48
1:A:506:G:C8	1:A:506:G:C5'	2.96	0.48
1:A:622:A:C8	1:A:623:C:C5	3.02	0.48
1:A:569:C:H42	1:A:881:G:H1	1.61	0.48
1:A:977:A:C2'	1:A:978:A:H5''	2.44	0.48
2:B:236:TYR:HE2	2:B:239:VAL:HG11	1.78	0.48
3:C:205:GLY:O	3:C:206:GLU:HG3	2.14	0.48
5:E:28:PHE:O	5:E:47:LYS:HA	2.14	0.48
6:F:52:ILE:HD13	6:F:87:ARG:NH2	2.29	0.48
8:H:14:ARG:HH11	8:H:14:ARG:HG2	1.79	0.48
14:N:47:LEU:O	14:N:49:HIS:N	2.47	0.48
16:P:82:GLN:O	16:P:83:GLU:HB2	2.14	0.48
17:Q:27:PHE:CZ	17:Q:36:ILE:HD11	2.49	0.48
20:T:72:LEU:HD23	20:T:72:LEU:HA	1.67	0.48
1:A:383:A:H5''	1:A:384:G:OP2	2.14	0.48
1:A:499:A:C6	1:A:547:A:C8	3.02	0.48
1:A:770:C:H1'	1:A:899:C:H42	1.79	0.48
1:A:939:G:H2'	1:A:940:C:C6	2.49	0.48
2:B:208:ILE:HD12	2:B:208:ILE:N	2.29	0.48
3:C:40:ARG:O	3:C:44:GLU:HG3	2.14	0.48
3:C:43:LEU:HD23	3:C:43:LEU:N	2.29	0.48
4:D:22:LYS:CG	4:D:26:CYS:SG	2.98	0.48
6:F:75:LEU:O	6:F:79:LEU:HG	2.13	0.48
7:G:79:ARG:HA	7:G:84:ASN:HA	1.95	0.48
9:I:38:GLN:O	9:I:40:LEU:HD23	2.13	0.48
10:J:38:ILE:H	10:J:71:LEU:CB	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:48:ILE:HG22	11:K:49:GLY:N	2.29	0.48
11:K:59:TYR:O	11:K:63:LEU:HG	2.14	0.48
1:A:1286:A:C8	1:A:1287:A:H4'	2.49	0.48
1:A:1539:C:C4	1:A:1540:PSU:C6	3.02	0.48
1:A:652:U:C2	1:A:752:G:N2	2.81	0.48
6:F:16:GLN:HA	6:F:16:GLN:OE1	2.13	0.48
7:G:57:GLU:O	7:G:61:VAL:HG23	2.13	0.48
10:J:53:PRO:HA	14:N:41:ARG:HH21	1.78	0.48
12:L:24:VAL:HG22	12:L:98:TYR:CE2	2.49	0.48
13:M:105:THR:OG1	13:M:106:ASN:HB2	2.13	0.48
1:A:1075:C:OP1	2:B:179:LYS:NZ	2.45	0.47
1:A:1410:G:C4	1:A:1411:C:C5	3.02	0.47
1:A:260:G:H2'	1:A:261:U:C6	2.45	0.47
1:A:292:G:H3'	1:A:292:G:C8	2.49	0.47
1:A:527:7MG:H81	1:A:527:7MG:C5'	2.44	0.47
1:A:922:G:N3	1:A:1398:A:H2	2.12	0.47
3:C:108:ASN:HD21	3:C:144:SER:HB2	1.79	0.47
3:C:66:VAL:HG11	3:C:91:LEU:HD21	1.95	0.47
6:F:14:LEU:HB2	6:F:19:LEU:HD22	1.95	0.47
8:H:124:ALA:O	8:H:128:GLY:N	2.41	0.47
2:B:178:ARG:HH21	8:H:74:PRO:HG3	1.78	0.47
13:M:49:THR:O	13:M:52:GLU:HB2	2.14	0.47
1:A:463:A:P	16:P:75:ARG:HH22	2.37	0.47
3:C:182:ILE:HG22	3:C:183:ASP:O	2.14	0.47
6:F:14:LEU:HD12	6:F:19:LEU:HD13	1.96	0.47
1:A:673:G:H5''	6:F:87:ARG:CZ	2.44	0.47
8:H:116:LYS:HG2	8:H:127:LEU:HD12	1.97	0.47
9:I:40:LEU:CD1	9:I:70:LYS:HD2	2.43	0.47
10:J:29:ARG:HD3	10:J:29:ARG:O	2.14	0.47
10:J:65:LEU:C	10:J:65:LEU:HD12	2.35	0.47
11:K:91:ARG:HB3	11:K:91:ARG:HH11	1.78	0.47
1:A:1270:C:H2'	1:A:1271:G:H8	1.79	0.47
1:A:1417:G:N2	1:A:1484:C:H42	2.13	0.47
1:A:200:G:H2'	1:A:201:C:O4'	2.15	0.47
1:A:259:G:OP2	20:T:83:ARG:NE	2.47	0.47
1:A:375:U:O3'	16:P:6:LEU:HB2	2.14	0.47
1:A:44:G:N2	1:A:399:G:C4	2.82	0.47
2:B:149:LEU:HD22	2:B:152:PHE:HB3	1.96	0.47
4:D:108:LEU:HA	4:D:108:LEU:HD23	1.71	0.47
7:G:120:ILE:O	7:G:124:LEU:HD12	2.14	0.47
5:E:152:ARG:HB3	8:H:43:GLY:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1226:C:H5'	19:S:80:TYR:CD2	2.41	0.47
1:A:1343:G:C6	1:A:1344:C:N4	2.82	0.47
1:A:1540:PSU:O4	1:A:1540:PSU:H2'	2.14	0.47
1:A:332:G:H2'	1:A:333:G:C8	2.47	0.47
1:A:654:G:H2'	1:A:655:A:H5'	1.96	0.47
1:A:858:G:N7	25:A:3261:HOH:O	2.35	0.47
3:C:34:LEU:HD13	3:C:35:GLU:N	2.30	0.47
5:E:15:ARG:HH11	5:E:15:ARG:CG	2.11	0.47
1:A:1375:A:P	7:G:28:ASN:HD22	2.37	0.47
17:Q:68:ARG:HH11	17:Q:68:ARG:CG	2.27	0.47
18:R:72:ARG:O	18:R:76:LEU:HB2	2.14	0.47
1:A:1270:C:H2'	1:A:1271:G:C8	2.49	0.47
1:A:148:G:H2'	1:A:149:A:C8	2.50	0.47
1:A:758:G:N7	25:A:3364:HOH:O	2.35	0.47
2:B:170:GLU:O	2:B:173:ALA:N	2.48	0.47
5:E:123:LEU:HA	5:E:123:LEU:HD23	1.47	0.47
6:F:43:LEU:HD22	6:F:45:LEU:O	2.14	0.47
8:H:10:LEU:CB	8:H:83:ILE:HD11	2.44	0.47
10:J:59:SER:C	10:J:60:ARG:HG2	2.35	0.47
14:N:8:GLU:C	14:N:11:LYS:HB2	2.34	0.47
20:T:104:LEU:HD22	20:T:104:LEU:HA	1.69	0.47
1:A:1330:U:C2'	1:A:1331:G:H5'	2.44	0.47
3:C:29:TYR:OH	14:N:54:PRO:HD2	2.15	0.47
4:D:194:LEU:HB2	4:D:196:LEU:HD13	1.96	0.47
5:E:115:VAL:HG12	5:E:117:ASP:H	1.80	0.47
5:E:46:GLY:N	5:E:58:ALA:HB2	2.30	0.47
1:A:1351:U:O4'	7:G:33:ASP:HB3	2.14	0.47
7:G:53:LYS:O	7:G:54:THR:OG1	2.30	0.47
9:I:10:ARG:NH1	9:I:10:ARG:HG2	2.28	0.47
11:K:122:LYS:O	11:K:123:LYS:C	2.53	0.47
18:R:45:SER:HA	18:R:51:LEU:HD11	1.96	0.47
1:A:1459:C:H2'	1:A:1460:A:O4'	2.14	0.47
1:A:725:G:H2'	1:A:726:C:H6	1.78	0.47
4:D:206:PHE:CD2	4:D:207:TYR:CE2	3.03	0.47
4:D:24:GLU:O	4:D:25:ARG:HB3	2.14	0.47
1:A:1150:U:O2'	10:J:41:PRO:HG3	2.13	0.47
11:K:124:LYS:HG2	11:K:125:PHE:CE2	2.49	0.47
11:K:13:GLN:HA	11:K:13:GLN:OE1	2.15	0.47
15:O:39:LEU:HD22	15:O:43:LEU:HG	1.95	0.47
1:A:1014:A:H4'	19:S:14:HIS:CE1	2.50	0.47
1:A:192:U:H4'	20:T:57:ARG:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1129:C:OP1	9:I:62:TYR:OH	2.21	0.47
1:A:1375:A:C4	1:A:1376:U:C6	3.03	0.47
1:A:1473:A:H8	1:A:1473:A:O5'	1.98	0.47
1:A:408:A:H2'	1:A:409:G:O5'	2.15	0.47
2:B:84:GLU:HB3	2:B:219:VAL:HG21	1.97	0.47
7:G:140:ASP:HA	7:G:143:ARG:HH11	1.78	0.47
8:H:4:ASP:HA	8:H:5:PRO:HD2	1.64	0.47
12:L:69:TYR:HE2	12:L:71:PRO:HA	1.80	0.47
1:A:1358:U:OP1	14:N:35:ARG:HB2	2.14	0.47
1:A:1191:A:H5''	3:C:4:LYS:HE3	1.97	0.47
1:A:1366:C:H2'	1:A:1367:C:C6	2.50	0.47
1:A:1491:G:H5''	1:A:1492:A:P	2.55	0.47
3:C:5:ILE:O	3:C:5:ILE:HG23	2.15	0.47
5:E:31:LEU:HA	5:E:31:LEU:HD23	1.10	0.47
7:G:71:PRO:HG2	7:G:103:TRP:HZ3	1.79	0.47
10:J:47:PHE:CE2	14:N:37:PHE:CE1	3.02	0.47
1:A:1124:G:H22	1:A:1149:C:H42	1.62	0.47
1:A:370:C:O2'	1:A:371:G:H5'	2.15	0.47
3:C:59:ARG:NH1	3:C:97:LYS:HE2	2.29	0.47
6:F:2:ARG:HD3	6:F:4:TYR:OH	2.15	0.47
8:H:97:VAL:HG13	8:H:98:LYS:N	2.30	0.47
9:I:16:ARG:CB	9:I:64:THR:HG22	2.44	0.47
12:L:33:ARG:NH1	12:L:61:THR:HB	2.30	0.47
6:F:7:ASN:HD22	18:R:76:LEU:HD11	1.79	0.47
1:A:1124:G:H4'	10:J:38:ILE:HD13	1.97	0.47
1:A:1213:A:C8	1:A:1215:G:C6	3.02	0.47
1:A:1236:A:OP1	21:U:2:GLY:HA3	2.15	0.47
1:A:1465:C:H2'	1:A:1466:C:O4'	2.15	0.47
1:A:788:U:O3'	1:A:1539:C:N4	2.47	0.47
3:C:120:VAL:O	3:C:123:GLN:HB2	2.15	0.47
4:D:12:CYS:HA	4:D:19:LEU:HD11	1.97	0.47
5:E:35:GLY:HA3	5:E:112:LEU:HB3	1.95	0.47
7:G:115:ARG:HB2	7:G:118:VAL:CG2	2.45	0.47
8:H:65:TYR:CD1	8:H:65:TYR:N	2.83	0.47
10:J:38:ILE:HG13	10:J:38:ILE:H	1.51	0.47
10:J:70:ARG:HA	10:J:70:ARG:HD3	1.67	0.47
11:K:15:ALA:HA	11:K:77:MET:CA	2.37	0.47
17:Q:20:THR:HG21	17:Q:41:LYS:HD2	1.97	0.47
21:U:10:ARG:NH1	21:U:10:ARG:HB3	2.30	0.47
1:A:1058:G:H2'	1:A:1059:C:C6	2.50	0.46
1:A:1489:G:N2	1:A:1490:C:C2	2.82	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:941:G:C2'	1:A:942:G:O5'	2.63	0.46
1:A:945:G:N2	1:A:1334:G:O3'	2.47	0.46
2:B:146:GLN:O	2:B:150:SER:HB3	2.14	0.46
2:B:39:ILE:HD12	2:B:39:ILE:N	2.30	0.46
3:C:135:LYS:O	3:C:138:VAL:HG12	2.15	0.46
3:C:175:LEU:HD21	3:C:201:TYR:HE2	1.80	0.46
7:G:5:ARG:HG3	7:G:7:ALA:H	1.80	0.46
8:H:87:SER:HA	8:H:93:VAL:CG2	2.44	0.46
8:H:89:PRO:HA	8:H:92:ARG:NH1	2.29	0.46
9:I:108:VAL:HG12	9:I:109:VAL:HG23	1.96	0.46
9:I:124:GLN:HG3	9:I:125:TYR:N	2.31	0.46
12:L:27:LEU:CG	12:L:28:LYS:N	2.78	0.46
12:L:27:LEU:O	12:L:30:ALA:N	2.48	0.46
13:M:66:LEU:O	13:M:69:GLU:HB3	2.15	0.46
15:O:54:ARG:O	15:O:55:GLY:C	2.52	0.46
18:R:52:PRO:HG2	18:R:54:ARG:CZ	2.45	0.46
1:A:1004:A:N6	1:A:1035:A:C8	2.84	0.46
1:A:1112:C:C4	3:C:178:LEU:HB2	2.50	0.46
1:A:1212:U:O2'	1:A:1213:A:O5'	2.33	0.46
1:A:1531:A:O5'	1:A:1531:A:H8	1.97	0.46
1:A:914:A:OP1	22:A:1601:SRY:HI33	2.14	0.46
1:A:494:G:O2'	1:A:495:U:H5'	2.15	0.46
1:A:642:A:H1'	8:H:114:THR:O	2.15	0.46
1:A:657:G:O5'	1:A:657:G:H8	1.98	0.46
1:A:945:G:O6	1:A:1236:A:N1	2.48	0.46
2:B:114:ARG:HG3	2:B:114:ARG:O	2.16	0.46
9:I:40:LEU:N	9:I:40:LEU:HD23	2.31	0.46
1:A:1126:U:C6	1:A:1126:U:H3'	2.51	0.46
1:A:117:G:P	25:A:2007:HOH:O	2.73	0.46
1:A:234:C:H2'	1:A:235:C:H6	1.80	0.46
1:A:838:G:H2'	1:A:840:C:C5	2.50	0.46
3:C:142:MET:HE1	3:C:148:GLY:HA2	1.97	0.46
5:E:98:THR:HG21	5:E:119:LEU:HD21	1.96	0.46
6:F:37:VAL:HG12	6:F:38:GLU:N	2.30	0.46
9:I:46:ALA:HB2	9:I:74:ILE:HD12	1.98	0.46
10:J:49:VAL:O	10:J:60:ARG:HD2	2.15	0.46
15:O:36:ILE:HG22	15:O:37:ASN:N	2.29	0.46
18:R:33:ASP:OD1	18:R:35:ARG:N	2.45	0.46
20:T:31:SER:HA	20:T:34:LYS:HD3	1.97	0.46
1:A:1125:U:C3'	1:A:1125:U:H6	2.17	0.46
1:A:1234:C:C2'	1:A:1235:U:H5'	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:43:LEU:HB2	5:E:136:MET:CE	2.45	0.46
6:F:45:LEU:HA	6:F:45:LEU:HD22	1.54	0.46
11:K:115:PRO:C	11:K:117:ASN:H	2.19	0.46
13:M:37:THR:CG2	13:M:39:ILE:HD11	2.45	0.46
13:M:64:TRP:HB2	13:M:66:LEU:HD11	1.97	0.46
20:T:40:ALA:HB2	20:T:55:ILE:HG22	1.96	0.46
1:A:1240:U:C2	7:G:32:ARG:HG3	2.51	0.46
1:A:1285:A:H4'	1:A:1286:A:O5'	2.16	0.46
1:A:923:A:H61	1:A:1393:U:H3	1.62	0.46
1:A:961:U:H2'	1:A:962:C:O4'	2.15	0.46
4:D:165:MET:HG2	4:D:168:ARG:HD3	1.97	0.46
1:A:1006:C:N3	1:A:1023:G:N2	2.64	0.46
1:A:236:G:H1'	17:Q:4:LYS:NZ	2.30	0.46
1:A:520:A:N1	1:A:536:C:H1'	2.30	0.46
1:A:778:G:H1	1:A:804:U:H3	1.64	0.46
2:B:208:ILE:H	2:B:208:ILE:CD1	2.26	0.46
5:E:17:ALA:HA	5:E:26:PHE:HB3	1.97	0.46
8:H:10:LEU:HD23	8:H:83:ILE:CG1	2.45	0.46
11:K:114:VAL:CG2	11:K:115:PRO:HD2	2.45	0.46
14:N:25:VAL:HG12	14:N:38:GLY:O	2.16	0.46
1:A:1353:G:N2	1:A:1354:C:C2	2.84	0.46
1:A:1402:4OC:C4	1:A:1403:C:C5	2.98	0.46
1:A:181:G:H4'	1:A:182:U:C5'	2.45	0.46
1:A:405:U:O4	4:D:2:GLY:HA3	2.16	0.46
1:A:631:G:H1'	25:A:2849:HOH:O	2.16	0.46
1:A:748:C:O5'	1:A:748:C:H6	1.99	0.46
4:D:105:VAL:HG13	4:D:110:PHE:HB2	1.98	0.46
4:D:142:PRO:HA	4:D:185:PHE:HD2	1.81	0.46
8:H:119:LEU:HA	8:H:123:GLU:OE1	2.15	0.46
13:M:15:VAL:O	13:M:18:ALA:HB3	2.16	0.46
16:P:48:TRP:CD1	16:P:48:TRP:N	2.84	0.46
1:A:1036:G:N2	1:A:1037:C:C2	2.84	0.46
1:A:1375:A:C5	1:A:1376:U:C5	3.04	0.46
1:A:1436:U:H2'	1:A:1437:C:C6	2.50	0.46
1:A:725:G:C4	1:A:726:C:C5	3.04	0.46
1:A:756:C:H2'	1:A:757:U:O4'	2.16	0.46
1:A:936:C:H2'	1:A:937:A:O4'	2.15	0.46
2:B:184:VAL:O	2:B:198:ASP:HB2	2.16	0.46
5:E:11:ILE:HB	5:E:31:LEU:HB3	1.96	0.46
6:F:71:ARG:HH11	6:F:71:ARG:CB	2.29	0.46
7:G:21:VAL:HG23	7:G:22:LEU:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:35:ILE:HG22	8:H:36:LEU:N	2.30	0.46
8:H:82:HIS:HD2	8:H:83:ILE:N	2.13	0.46
11:K:40:ILE:HA	11:K:40:ILE:HD13	1.64	0.46
12:L:33:ARG:HB3	12:L:60:LEU:HD13	1.98	0.46
1:A:112:G:C2'	1:A:113:G:H5'	2.46	0.46
1:A:1196:U:H1'	25:A:2957:HOH:O	2.15	0.46
1:A:1515:C:C2'	1:A:1516:G:H5'	2.45	0.46
1:A:325:A:H2'	1:A:326:G:O4'	2.16	0.46
1:A:409:G:H1	1:A:433:C:H42	1.63	0.46
1:A:44:G:C6	1:A:45:U:C2	3.04	0.46
1:A:660:G:H2'	1:A:661:G:C8	2.51	0.46
1:A:679:C:O2'	1:A:680:C:H5'	2.15	0.46
1:A:949:A:H2'	1:A:950:U:O4'	2.15	0.46
2:B:77:ALA:O	2:B:81:VAL:HG23	2.16	0.46
5:E:37:ARG:O	5:E:114:GLY:HA3	2.15	0.46
5:E:144:THR:HB	5:E:146:ALA:HB3	1.98	0.46
6:F:22:GLU:O	6:F:26:ILE:HG13	2.15	0.46
9:I:24:GLY:HA2	9:I:59:PHE:O	2.15	0.46
9:I:53:VAL:HG11	9:I:85:LEU:HD23	1.97	0.46
11:K:27:ASN:OD1	11:K:55:LYS:HB3	2.16	0.46
13:M:29:ARG:HD3	13:M:64:TRP:CZ2	2.50	0.46
14:N:3:ARG:H	14:N:3:ARG:HG2	1.32	0.46
16:P:58:TYR:CD1	16:P:58:TYR:C	2.89	0.46
16:P:74:LEU:O	16:P:79:VAL:HG23	2.15	0.46
17:Q:12:SER:HB3	17:Q:20:THR:H	1.80	0.46
13:M:84:ILE:HB	19:S:74:PHE:HE2	1.81	0.46
20:T:16:HIS:HA	20:T:19:SER:HB3	1.96	0.46
1:A:1084:G:H5'	1:A:1102:A:OP2	2.16	0.46
1:A:1317:C:C6	14:N:16:PHE:CD2	3.04	0.46
22:A:1601:SRY:H12	22:A:1601:SRY:HN31	1.81	0.46
1:A:170:U:O2'	1:A:171:A:H5'	2.15	0.46
1:A:30:U:H1'	25:A:3124:HOH:O	2.16	0.46
1:A:578:C:H2'	1:A:579:G:O4'	2.16	0.46
1:A:723:U:H2'	1:A:723:U:O2	2.15	0.46
1:A:901:A:C5	1:A:902:G:H1'	2.50	0.46
1:A:924:C:H2'	1:A:925:G:H5'	1.97	0.46
3:C:72:LYS:O	3:C:75:VAL:HG23	2.16	0.46
7:G:26:PHE:HB2	7:G:101:LEU:HD23	1.97	0.46
7:G:22:LEU:HD21	7:G:66:VAL:HG11	1.98	0.46
11:K:44:SER:O	11:K:47:VAL:HG12	2.16	0.46
12:L:84:LEU:O	12:L:101:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:14:PRO:HB3	14:N:20:ALA:HB2	1.97	0.46
15:O:26:GLU:CD	15:O:26:GLU:N	2.67	0.46
15:O:82:ILE:HD11	15:O:87:ILE:HD11	1.96	0.46
17:Q:27:PHE:O	17:Q:36:ILE:HG12	2.16	0.46
17:Q:59:ILE:HA	17:Q:59:ILE:HD12	1.53	0.46
6:F:48:LEU:HD22	18:R:77:GLY:O	2.15	0.46
19:S:25:LYS:HB2	19:S:25:LYS:NZ	2.31	0.46
1:A:1128:C:O2'	1:A:1129:C:O5'	2.33	0.45
1:A:1484:C:H6	1:A:1484:C:O5'	1.99	0.45
1:A:189:G:H2'	1:A:190:C:H6	1.79	0.45
1:A:268:C:O2'	1:A:269:C:H5'	2.16	0.45
1:A:116:A:H61	1:A:313:A:H1'	1.81	0.45
1:A:603:U:H3	1:A:635:G:H1	1.62	0.45
1:A:925:G:O2'	1:A:927:G:OP1	2.27	0.45
1:A:951:G:OP2	13:M:102:ARG:NH2	2.48	0.45
2:B:10:LEU:HD23	2:B:10:LEU:O	2.16	0.45
2:B:92:TYR:HD1	2:B:92:TYR:O	1.99	0.45
12:L:33:ARG:O	12:L:85:ILE:HB	2.16	0.45
17:Q:74:LEU:HA	17:Q:74:LEU:HD12	1.33	0.45
1:A:1256:A:HO2'	1:A:1257:U:P	2.40	0.45
1:A:1238:A:N7	1:A:1303:C:H1'	2.32	0.45
1:A:526:C:O3'	22:A:1601:SRV:HI31	2.16	0.45
1:A:55:A:C2'	1:A:56:U:H5'	2.46	0.45
1:A:671:G:C6	1:A:672:U:C2	3.03	0.45
1:A:919:A:O2'	1:A:920:U:H5'	2.16	0.45
2:B:10:LEU:HD23	2:B:10:LEU:C	2.37	0.45
2:B:117:GLU:HG2	2:B:121:LEU:HG	1.98	0.45
2:B:24:TRP:HA	2:B:190:THR:O	2.16	0.45
6:F:52:ILE:HD13	6:F:87:ARG:CZ	2.45	0.45
6:F:72:VAL:HG13	6:F:90:VAL:HG11	1.97	0.45
7:G:91:VAL:HG12	7:G:96:GLN:HG3	1.97	0.45
12:L:111:LYS:HB3	12:L:111:LYS:HE2	1.54	0.45
1:A:1490:C:O2'	12:L:94:TRP:CZ3	2.67	0.45
13:M:80:ARG:NH1	13:M:80:ARG:HB3	2.30	0.45
14:N:8:GLU:HA	14:N:11:LYS:HD3	1.99	0.45
1:A:1473:A:H2'	1:A:1474:G:O4'	2.16	0.45
1:A:793:U:O2	1:A:1516:G:H4'	2.16	0.45
1:A:160:A:N6	1:A:346:G:C6	2.85	0.45
1:A:254:G:OP1	17:Q:67:LYS:O	2.33	0.45
1:A:576:G:H3'	1:A:577:G:H5''	1.98	0.45
1:A:584:G:H2'	1:A:585:G:C8	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:665:A:C2	1:A:732:C:C2	3.04	0.45
1:A:841:U:C6	1:A:848:C:O4'	2.69	0.45
2:B:131:PRO:HG2	2:B:134:GLU:HB2	1.98	0.45
2:B:24:TRP:CG	2:B:25:ASN:N	2.85	0.45
5:E:10:MET:SD	5:E:13:ILE:HG23	2.56	0.45
7:G:22:LEU:HD23	7:G:63:LYS:HG2	1.97	0.45
10:J:5:ARG:O	10:J:6:ILE:HG23	2.16	0.45
1:A:35:G:O2'	12:L:118:SER:O	2.31	0.45
1:A:1226:C:P	13:M:91:ARG:HH22	2.38	0.45
15:O:26:GLU:OE1	15:O:77:ARG:HD2	2.16	0.45
1:A:1108:G:H5''	1:A:1108:G:H8	1.81	0.45
1:A:586:C:H2'	1:A:587:G:H5'	1.97	0.45
2:B:28:PHE:O	2:B:32:ILE:HG13	2.16	0.45
5:E:69:VAL:HG13	5:E:70:PRO:HD2	1.99	0.45
6:F:39:LYS:O	6:F:40:VAL:HG12	2.16	0.45
6:F:4:TYR:CE1	6:F:92:LYS:HG2	2.51	0.45
6:F:76:ALA:O	6:F:80:ARG:HG3	2.15	0.45
9:I:22:GLY:CA	9:I:60:ASP:HB2	2.46	0.45
10:J:27:ALA:O	10:J:31:GLY:N	2.43	0.45
11:K:39:PRO:O	11:K:40:ILE:HD13	2.16	0.45
11:K:48:ILE:HG13	11:K:48:ILE:H	1.43	0.45
16:P:53:VAL:O	16:P:54:GLU:C	2.54	0.45
17:Q:65:ILE:HB	17:Q:69:LYS:HB2	1.98	0.45
1:A:1485:U:O2	1:A:1485:U:H2'	2.17	0.45
1:A:228:A:H2'	1:A:229:U:C6	2.52	0.45
1:A:267:C:O2'	1:A:268:C:H5'	2.17	0.45
1:A:934:C:P	25:A:2844:HOH:O	2.74	0.45
2:B:43:ASP:CG	2:B:46:LYS:HG2	2.37	0.45
5:E:137:GLU:O	5:E:141:GLN:HG3	2.15	0.45
8:H:85:ARG:NE	8:H:87:SER:O	2.48	0.45
13:M:20:THR:HG22	13:M:20:THR:O	2.17	0.45
18:R:56:THR:OG1	18:R:58:LEU:HD12	2.15	0.45
1:A:985:C:C2	1:A:1221:G:N2	2.85	0.45
1:A:1327:C:H2'	1:A:1328:C:C6	2.52	0.45
1:A:1387:G:C6	1:A:1388:C:C4	3.05	0.45
1:A:285:G:O2'	1:A:286:G:H5'	2.16	0.45
1:A:36:C:H2'	1:A:37:U:O4'	2.17	0.45
2:B:17:PHE:HD1	2:B:18:GLY:N	2.14	0.45
4:D:36:ARG:HG2	4:D:38:TYR:CE2	2.51	0.45
8:H:10:LEU:HD12	8:H:10:LEU:N	2.29	0.45
12:L:6:THR:HG23	12:L:9:GLN:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:29:HIS:CE1	17:Q:31:LEU:H	2.35	0.45
17:Q:6:LEU:HD23	17:Q:6:LEU:N	2.32	0.45
18:R:33:ASP:OD1	18:R:33:ASP:C	2.55	0.45
1:A:1442:G:N2	1:A:1447:G:C8	2.82	0.45
1:A:450:G:O5'	1:A:450:G:H8	1.98	0.45
1:A:855:G:H5''	1:A:871:U:O4	2.17	0.45
4:D:171:GLY:HA2	4:D:172:PRO:HD3	1.49	0.45
4:D:72:GLU:O	4:D:73:ARG:C	2.55	0.45
4:D:9:CYS:SG	4:D:22:LYS:HD2	2.56	0.45
12:L:53:ARG:NH1	12:L:92:ASP:OD1	2.48	0.45
13:M:15:VAL:HG12	13:M:34:LEU:HD11	1.98	0.45
17:Q:22:LEU:HD12	17:Q:23:VAL:N	2.32	0.45
17:Q:51:TYR:CE2	17:Q:73:VAL:HG11	2.52	0.45
6:F:100:ASN:HA	18:R:23:LYS:HE3	1.97	0.45
19:S:39:THR:HG23	19:S:70:LYS:HD3	1.98	0.45
1:A:1050:G:C2	1:A:1051:C:C5	3.05	0.45
1:A:1379:G:C2'	1:A:1380:U:H5'	2.47	0.45
2:B:91:PRO:HG3	2:B:155:LEU:HG	1.98	0.45
2:B:28:PHE:CD2	2:B:190:THR:HA	2.52	0.45
2:B:74:LYS:HE3	2:B:74:LYS:HB3	1.45	0.45
3:C:157:ILE:HD13	3:C:166:GLU:HB2	1.99	0.45
3:C:47:LEU:HD23	3:C:68:VAL:HG11	1.98	0.45
5:E:45:PHE:HE2	5:E:47:LYS:CE	2.29	0.45
6:F:62:TRP:HB2	18:R:35:ARG:NH1	2.32	0.45
7:G:65:ALA:HB2	7:G:124:LEU:O	2.17	0.45
8:H:100:ILE:HA	8:H:101:PRO:HD2	1.55	0.45
8:H:9:MET:HE2	8:H:32:LYS:HD3	1.98	0.45
12:L:41:ARG:CG	12:L:42:THR:H	2.29	0.45
13:M:40:ASN:HA	13:M:41:PRO:HD2	1.83	0.45
15:O:60:VAL:HG23	15:O:60:VAL:H	1.46	0.45
17:Q:66:SER:O	17:Q:67:LYS:C	2.54	0.45
18:R:26:LEU:HA	18:R:26:LEU:HD12	1.75	0.45
1:A:1074:G:O4'	2:B:104:ASN:HB2	2.16	0.45
1:A:1127:G:H1	1:A:1145:C:H42	1.65	0.45
1:A:1213:A:N1	1:A:1215:G:H1'	2.32	0.45
1:A:1332:A:O2'	1:A:1333:A:H5'	2.17	0.45
1:A:1497:G:O2'	1:A:1518:MA6:H92	2.17	0.45
3:C:43:LEU:C	3:C:45:LYS:N	2.68	0.45
3:C:53:ALA:HB2	3:C:115:LEU:CD2	2.46	0.45
4:D:22:LYS:CB	4:D:26:CYS:SG	3.04	0.45
6:F:2:ARG:CG	6:F:69:GLU:HG3	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:12:LEU:HD22	7:G:24:THR:CG2	2.47	0.45
7:G:152:ALA:O	7:G:155:ARG:HG3	2.17	0.45
9:I:46:ALA:HB1	9:I:77:ILE:HG21	1.99	0.45
9:I:47:LEU:HD13	9:I:47:LEU:HA	1.68	0.45
7:G:149:ARG:HD2	11:K:59:TYR:CE1	2.51	0.45
16:P:53:VAL:HG23	16:P:54:GLU:H	1.80	0.45
18:R:54:ARG:CB	18:R:54:ARG:HH11	2.28	0.45
1:A:613:C:C2	1:A:628:G:N2	2.84	0.45
1:A:801:U:H2'	1:A:802:A:C8	2.52	0.45
1:A:869:G:N7	25:A:3262:HOH:O	2.35	0.45
6:F:47:ARG:HH11	6:F:47:ARG:HG3	1.81	0.45
11:K:40:ILE:HG23	11:K:75:TYR:HD1	1.78	0.45
15:O:30:ALA:HB2	15:O:85:LEU:HD11	1.99	0.45
20:T:56:MET:SD	20:T:85:MET:HG2	2.57	0.45
20:T:88:VAL:HG12	20:T:89:ARG:N	2.32	0.45
1:A:1033:G:N2	1:A:1034:G:O4'	2.50	0.44
1:A:1128:C:O2'	1:A:1130:A:C8	2.65	0.44
1:A:1190:G:HO2'	1:A:1191:A:P	2.40	0.44
1:A:1309:G:C6	1:A:1329:A:C2	3.05	0.44
1:A:1379:G:H2'	1:A:1380:U:H5'	2.00	0.44
1:A:1499:A:H1'	1:A:1520:G:H5'	1.99	0.44
1:A:273:A:N6	1:A:274:A:C6	2.85	0.44
1:A:419:C:N4	25:A:3051:HOH:O	2.18	0.44
1:A:41:G:O2'	1:A:42:G:H5'	2.16	0.44
1:A:658:G:C4	1:A:659:U:C6	3.05	0.44
1:A:9:G:OP2	5:E:121:LYS:HD2	2.17	0.44
2:B:172:ILE:H	2:B:172:ILE:HD12	1.82	0.44
3:C:30:ARG:HB3	3:C:30:ARG:NH1	2.31	0.44
4:D:38:TYR:N	4:D:38:TYR:CD2	2.68	0.44
5:E:18:ARG:HG2	5:E:19:MET:H	1.82	0.44
12:L:41:ARG:HD3	12:L:42:THR:O	2.16	0.44
12:L:53:ARG:HG3	12:L:93:LEU:HD22	1.98	0.44
13:M:37:THR:HB	13:M:39:ILE:CD1	2.47	0.44
16:P:10:GLY:HA3	16:P:14:ASN:O	2.17	0.44
1:A:1162:C:C2	1:A:1175:G:N2	2.86	0.44
1:A:130:A:H1'	1:A:263:A:O2'	2.18	0.44
1:A:689:C:N4	1:A:690:G:C6	2.85	0.44
1:A:81:U:OP1	1:A:81:U:H4'	2.17	0.44
1:A:949:A:N1	1:A:1233:G:C4	2.85	0.44
1:A:978:A:C2'	1:A:979:C:H5'	2.47	0.44
2:B:64:ARG:NH1	2:B:64:ARG:HG3	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:G:H4'	4:D:123:HIS:CD2	2.52	0.44
5:E:117:ASP:O	5:E:118:ILE:HB	2.17	0.44
5:E:148:VAL:O	5:E:152:ARG:HG3	2.17	0.44
8:H:11:THR:HG23	8:H:15:ASN:HD21	1.82	0.44
12:L:42:THR:HA	12:L:53:ARG:O	2.17	0.44
13:M:21:TYR:N	13:M:21:TYR:CD2	2.85	0.44
1:A:1003(A):G:N2	1:A:1039:C:C2	2.85	0.44
1:A:1405:G:H1	1:A:1496:C:N4	2.15	0.44
1:A:273:A:N6	1:A:274:A:N6	2.65	0.44
1:A:90:U:O2'	1:A:91:C:H5'	2.17	0.44
1:A:985:C:H2'	1:A:986:A:C8	2.52	0.44
1:A:9:G:OP1	5:E:122:GLU:HG3	2.16	0.44
2:B:175:ARG:O	2:B:179:LYS:HB2	2.17	0.44
5:E:121:LYS:NZ	5:E:126:ARG:HH12	2.15	0.44
5:E:36:ASP:C	5:E:38:GLN:H	2.21	0.44
7:G:91:VAL:CG1	7:G:96:GLN:HG3	2.48	0.44
8:H:118:VAL:C	8:H:119:LEU:HD23	2.37	0.44
11:K:21:ILE:HB	11:K:84:VAL:HG22	1.99	0.44
12:L:60:LEU:HD21	12:L:85:ILE:HD12	2.00	0.44
12:L:69:TYR:CE2	12:L:71:PRO:HA	2.51	0.44
13:M:36:LYS:HB2	13:M:36:LYS:HE2	1.75	0.44
15:O:4:THR:HB	15:O:6:GLU:H	1.82	0.44
20:T:50:GLU:HG2	20:T:99:LEU:CD2	2.43	0.44
1:A:179:A:H2'	1:A:180:U:C6	2.53	0.44
1:A:242:C:C2'	1:A:243:A:H5'	2.46	0.44
1:A:255:G:H4'	17:Q:17:LYS:HD2	1.99	0.44
1:A:373:A:H1'	1:A:481:G:N3	2.32	0.44
2:B:18:GLY:HA3	2:B:42:ILE:H	1.83	0.44
1:A:620:C:C2	4:D:135:LEU:HD22	2.53	0.44
4:D:150:GLU:N	4:D:150:GLU:CD	2.71	0.44
7:G:103:TRP:HA	7:G:106:GLN:HG3	1.99	0.44
7:G:11:GLN:NE2	7:G:11:GLN:HA	2.29	0.44
7:G:154:TYR:N	7:G:154:TYR:CD2	2.83	0.44
1:A:4:U:H5	8:H:105:ARG:CZ	2.30	0.44
8:H:82:HIS:NE2	8:H:84:ARG:HB2	2.33	0.44
8:H:82:HIS:CD2	8:H:83:ILE:N	2.86	0.44
10:J:38:ILE:CG2	10:J:39:PRO:HD2	2.47	0.44
10:J:85:LEU:HD12	10:J:85:LEU:HA	1.69	0.44
11:K:20:TYR:HB2	11:K:31:THR:O	2.18	0.44
14:N:39:LEU:HA	14:N:39:LEU:HD23	1.66	0.44
20:T:88:VAL:HG13	20:T:92:LEU:HD23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1091:U:O2	1:A:1093:A:C8	2.70	0.44
1:A:1241:G:H2'	1:A:1242:C:C6	2.52	0.44
1:A:1277:C:C6	1:A:1277:C:H3'	2.52	0.44
1:A:1492:A:C8	1:A:1493:A:H2	2.36	0.44
1:A:434:U:H2'	1:A:435:C:H6	1.81	0.44
1:A:512:U:H2'	1:A:513:C:C6	2.52	0.44
1:A:693:G:H2'	1:A:694:A:C8	2.53	0.44
1:A:838:G:C2	1:A:849:C:C2	3.05	0.44
1:A:909:A:H2'	1:A:910:C:O4'	2.17	0.44
1:A:865:A:C2	1:A:918:A:H4'	2.52	0.44
6:F:68:PRO:HG2	6:F:71:ARG:HH12	1.82	0.44
10:J:69:ASN:O	10:J:70:ARG:NE	2.50	0.44
10:J:47:PHE:CZ	14:N:37:PHE:HE1	2.34	0.44
1:A:1072:G:C5	1:A:1073:U:C4	3.06	0.44
1:A:1130:A:C4'	9:I:18:PHE:HE1	2.31	0.44
1:A:1190:G:O2'	1:A:1191:A:P	2.76	0.44
1:A:1353:G:C2	1:A:1354:C:C2	3.06	0.44
1:A:1478:C:H6	1:A:1478:C:O5'	2.00	0.44
1:A:22:G:O2'	1:A:23:C:H5'	2.18	0.44
1:A:414:A:C5	1:A:431:A:C2	3.06	0.44
1:A:421:U:H4'	1:A:422:C:OP2	2.17	0.44
1:A:538:G:OP1	12:L:115:LYS:HB2	2.17	0.44
1:A:615:C:O5'	1:A:615:C:H6	2.01	0.44
2:B:171:ALA:CA	2:B:174:VAL:HB	2.43	0.44
3:C:35:GLU:OE2	3:C:59:ARG:NH2	2.46	0.44
5:E:82:VAL:HG21	5:E:138:ALA:HA	2.00	0.44
8:H:17:THR:OG1	8:H:18:ARG:NH1	2.51	0.44
8:H:51:VAL:HG23	8:H:52:ASP:N	2.33	0.44
11:K:48:ILE:HD11	11:K:64:ALA:N	2.33	0.44
15:O:15:PHE:CE2	15:O:84:LYS:HB3	2.49	0.44
1:A:564:C:C6	17:Q:31:LEU:HD21	2.52	0.44
19:S:80:TYR:CE1	19:S:81:ARG:HB3	2.51	0.44
1:A:229:U:O2'	16:P:23:ASP:HB2	2.18	0.44
1:A:294:U:H2'	1:A:295:C:C6	2.52	0.44
1:A:942:G:H21	9:I:124:GLN:NE2	2.13	0.44
2:B:149:LEU:HD23	2:B:149:LEU:HA	1.45	0.44
3:C:58:GLU:N	3:C:65:ALA:HB3	2.33	0.44
3:C:72:LYS:HA	3:C:73:PRO:HD2	1.76	0.44
5:E:20:GLN:O	5:E:23:GLY:N	2.43	0.44
5:E:61:TYR:HA	5:E:61:TYR:HD1	1.73	0.44
6:F:15:ASP:OD2	6:F:15:ASP:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:148:VAL:HG21	8:H:107:LEU:HD13	2.00	0.44
1:A:825:G:O2'	8:H:8:ASP:OD1	2.31	0.44
9:I:118:LYS:C	9:I:120:ARG:H	2.21	0.44
9:I:75:ASP:O	9:I:78:LYS:HB2	2.18	0.44
9:I:89:ASN:HA	9:I:90:PRO:HD2	1.86	0.44
10:J:79:ARG:H	10:J:79:ARG:HG3	1.52	0.44
13:M:48:LEU:HB2	13:M:53:VAL:CG2	2.48	0.44
14:N:18:VAL:HG23	14:N:19:ARG:N	2.32	0.44
19:S:53:ASN:N	19:S:56:GLN:O	2.45	0.44
1:A:1039:C:H2'	1:A:1040:U:C6	2.53	0.44
1:A:1060:C:H5''	10:J:51:ARG:HB3	2.00	0.44
1:A:1103:C:H2'	1:A:1104:G:O4'	2.18	0.44
1:A:1167:A:C6	1:A:1168:A:C6	3.06	0.44
1:A:1443:G:H5'	1:A:1443:G:C8	2.53	0.44
1:A:1488:G:C2'	1:A:1489:G:H8	2.23	0.44
1:A:178:C:OP2	20:T:65:LYS:NZ	2.51	0.44
1:A:376:G:C4	1:A:389:A:C2	3.06	0.44
1:A:539:A:N7	12:L:115:LYS:HE3	2.33	0.44
1:A:674:G:H8	1:A:674:G:O5'	2.00	0.44
1:A:674:G:OP1	6:F:87:ARG:NH2	2.50	0.44
2:B:19:HIS:HB3	2:B:189:ASP:OD1	2.17	0.44
2:B:97:TRP:CD1	2:B:173:ALA:HB2	2.53	0.44
3:C:23:TYR:HD1	10:J:11:PHE:CE2	2.36	0.44
4:D:53:ASP:O	4:D:57:ARG:HD2	2.17	0.44
4:D:8:VAL:O	4:D:11:LEU:N	2.51	0.44
7:G:95:ARG:HA	7:G:95:ARG:HD2	1.73	0.44
8:H:31:PHE:O	8:H:34:GLU:HB2	2.17	0.44
13:M:44:ARG:HA	13:M:44:ARG:HD2	1.75	0.44
14:N:8:GLU:N	14:N:11:LYS:HE2	2.33	0.44
1:A:1367:C:H2'	1:A:1368:G:O4'	2.18	0.44
1:A:491:G:O2'	1:A:492:G:H5'	2.18	0.44
1:A:645:C:H2'	1:A:645:C:O2	2.17	0.44
3:C:53:ALA:O	3:C:54:ARG:HB2	2.18	0.44
4:D:158:ILE:HD13	4:D:158:ILE:N	2.33	0.44
8:H:18:ARG:HG2	8:H:18:ARG:NH1	2.25	0.44
8:H:82:HIS:C	8:H:82:HIS:CD2	2.90	0.44
8:H:85:ARG:CG	8:H:86:ILE:N	2.81	0.44
8:H:86:ILE:HG22	8:H:87:SER:N	2.33	0.44
9:I:50:LEU:HD12	9:I:51:ARG:N	2.32	0.44
9:I:97:LYS:NZ	9:I:100:GLY:HA2	2.33	0.44
10:J:50:ILE:HG12	10:J:60:ARG:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:19:ARG:H	12:L:19:ARG:HH11	1.65	0.44
1:A:1036:G:H5''	1:A:1037:C:OP2	2.18	0.43
1:A:1345:U:C2	1:A:1377:A:N1	2.85	0.43
1:A:1387:G:C4	1:A:1388:C:C5	3.06	0.43
1:A:1389:C:H2'	1:A:1390:U:O4'	2.17	0.43
1:A:143:A:H8	1:A:143:A:O5'	2.00	0.43
1:A:925:G:O4'	1:A:1502:A:C5	2.71	0.43
1:A:530:G:O2'	1:A:531:U:P	2.76	0.43
1:A:750:G:C2	1:A:751:U:C6	3.05	0.43
5:E:148:VAL:H	5:E:148:VAL:HG23	1.32	0.43
7:G:87:VAL:HG13	7:G:88:PRO:HD2	2.00	0.43
8:H:29:SER:OG	8:H:30:ARG:N	2.50	0.43
17:Q:38:ARG:HG2	17:Q:38:ARG:NH1	2.29	0.43
17:Q:83:ASP:N	17:Q:83:ASP:OD2	2.49	0.43
19:S:71:LEU:HD23	19:S:71:LEU:HA	1.85	0.43
1:A:1108:G:H2'	1:A:1109:C:C5'	2.46	0.43
1:A:1110:A:H8	1:A:1110:A:O5'	2.01	0.43
1:A:1171:G:H2'	1:A:1172:C:C6	2.53	0.43
1:A:1172:C:H2'	1:A:1173:G:H8	1.82	0.43
1:A:1211:U:H6	1:A:1211:U:H3'	1.83	0.43
1:A:1299:A:C8	1:A:1301:U:H1'	2.52	0.43
1:A:1388:C:O2'	1:A:1389:C:H5'	2.17	0.43
1:A:1518:MA6:H93	1:A:1519:MA6:C9	2.48	0.43
1:A:253:U:H2'	1:A:254:G:C8	2.54	0.43
1:A:509:A:H3'	1:A:509:A:C8	2.53	0.43
1:A:730:G:N2	1:A:765:G:H5''	2.32	0.43
2:B:18:GLY:N	2:B:41:ILE:HG23	2.27	0.43
9:I:80:GLY:HA2	9:I:83:ARG:HG3	1.98	0.43
11:K:82:VAL:O	11:K:108:ILE:HA	2.18	0.43
16:P:53:VAL:O	16:P:57:ARG:HG3	2.18	0.43
16:P:59:TRP:HB3	16:P:64:ALA:HB2	1.99	0.43
18:R:49:LYS:O	18:R:50:ILE:HG13	2.18	0.43
18:R:73:ALA:CB	18:R:79:LEU:HD12	2.49	0.43
19:S:22:LEU:HD13	19:S:28:LYS:HB2	2.00	0.43
1:A:1028:C:C4	1:A:1029:C:N4	2.85	0.43
1:A:1104:G:C6	1:A:1105:A:C5	3.06	0.43
1:A:1300:G:C5	1:A:1334:G:C5	3.06	0.43
1:A:1488:G:C2	1:A:1489:G:C5	3.06	0.43
1:A:560:U:H5'	25:A:3354:HOH:O	2.19	0.43
2:B:154:LEU:HA	2:B:154:LEU:HD23	1.71	0.43
3:C:92:ALA:HA	3:C:95:THR:HG23	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:737:A:OP1	6:F:92:LYS:N	2.50	0.43
7:G:97:GLN:O	7:G:101:LEU:HD12	2.18	0.43
7:G:25:ALA:O	7:G:28:ASN:HB2	2.18	0.43
8:H:74:PRO:O	8:H:75:ARG:C	2.55	0.43
17:Q:9:VAL:HG11	17:Q:84:LEU:HB2	1.99	0.43
1:A:1212:U:O2'	1:A:1213:A:P	2.76	0.43
1:A:1229:A:OP2	13:M:114:ARG:HD3	2.18	0.43
1:A:1323:G:H2'	1:A:1324:A:C8	2.53	0.43
1:A:1327:C:OP1	21:U:20:LYS:N	2.47	0.43
1:A:1441:G:H4'	1:A:1442:G:C5	2.54	0.43
1:A:163:C:H2'	1:A:164:U:O4'	2.19	0.43
1:A:229:U:H2'	1:A:230:G:H5'	2.00	0.43
1:A:355:C:C4	1:A:356:A:N7	2.86	0.43
1:A:665:A:C5	1:A:733:A:C5	3.06	0.43
1:A:961:U:OP1	1:A:1223:C:H4'	2.16	0.43
1:A:978:A:H1'	1:A:1322:C:O2	2.18	0.43
3:C:48:TYR:C	3:C:48:TYR:CD1	2.91	0.43
1:A:620:C:N3	4:D:135:LEU:HD22	2.32	0.43
5:E:112:LEU:HD23	5:E:112:LEU:HA	1.63	0.43
5:E:14:ARG:HE	5:E:16:THR:HG22	1.83	0.43
6:F:19:LEU:HD13	6:F:19:LEU:HA	1.58	0.43
6:F:12:PRO:HD3	6:F:58:GLY:HA2	2.00	0.43
6:F:69:GLU:O	6:F:72:VAL:HG23	2.19	0.43
7:G:118:VAL:O	7:G:122:HIS:HB2	2.19	0.43
9:I:28:VAL:HG13	9:I:63:ILE:HB	2.00	0.43
10:J:38:ILE:HA	10:J:39:PRO:HD2	1.57	0.43
10:J:72:VAL:O	10:J:72:VAL:HG12	2.17	0.43
13:M:76:ALA:O	13:M:80:ARG:HB2	2.17	0.43
15:O:45:VAL:HG23	15:O:45:VAL:H	1.49	0.43
19:S:70:LYS:N	19:S:73:GLU:HG3	2.32	0.43
1:A:191:G:N3	20:T:105:SER:HB2	2.33	0.43
1:A:1329:A:OP1	13:M:28:ALA:HB3	2.18	0.43
1:A:409:G:H1'	25:A:2605:HOH:O	2.18	0.43
1:A:632:A:H2'	1:A:633:G:O4'	2.18	0.43
1:A:710:G:N1	1:A:711:G:C5	2.87	0.43
1:A:749:C:O2'	1:A:750:G:H5'	2.18	0.43
2:B:69:LEU:HG	2:B:155:LEU:HD11	2.01	0.43
3:C:6:HIS:ND1	3:C:7:PRO:HD2	2.34	0.43
4:D:107:ARG:NH1	4:D:114:ARG:NH2	2.66	0.43
4:D:206:PHE:CD2	4:D:207:TYR:HE2	2.36	0.43
5:E:15:ARG:O	5:E:17:ALA:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:47:CYS:HB3	7:G:58:PRO:CB	2.49	0.43
10:J:62:HIS:HB3	14:N:59:ALA:HB3	1.99	0.43
11:K:114:VAL:HG23	11:K:115:PRO:HD2	1.99	0.43
1:A:523:A:H61	12:L:53:ARG:NH1	2.17	0.43
13:M:15:VAL:O	13:M:19:LEU:HD12	2.18	0.43
17:Q:29:HIS:HA	17:Q:30:PRO:HD3	1.24	0.43
17:Q:76:LEU:HD21	17:Q:78:GLU:O	2.19	0.43
1:A:1319:A:OP1	19:S:5:LEU:HD13	2.18	0.43
19:S:7:LYS:HZ2	19:S:7:LYS:HG3	1.61	0.43
1:A:1005:A:OP2	1:A:1006:C:N4	2.52	0.43
1:A:109:A:H4'	1:A:110:C:OP2	2.19	0.43
1:A:1126:U:C4	1:A:1127:G:N1	2.87	0.43
1:A:1126:U:H2'	1:A:1127:G:O5'	2.18	0.43
1:A:1378:C:H3'	1:A:1379:G:H5''	2.01	0.43
1:A:1454:G:O2'	1:A:1455:G:H5'	2.19	0.43
1:A:833:U:H2'	1:A:834:C:C5	2.53	0.43
4:D:190:ASP:C	4:D:190:ASP:OD2	2.57	0.43
7:G:127:ALA:C	7:G:130:GLY:H	2.22	0.43
1:A:1378:C:OP2	7:G:7:ALA:HB3	2.19	0.43
12:L:24:VAL:O	12:L:24:VAL:HG12	2.19	0.43
13:M:46:LYS:HG3	13:M:46:LYS:H	1.41	0.43
14:N:61:TRP:N	14:N:61:TRP:CE3	2.87	0.43
16:P:73:LEU:HD23	16:P:73:LEU:HA	1.56	0.43
18:R:76:LEU:HA	18:R:76:LEU:HD23	1.65	0.43
1:A:1002:G:C2	1:A:1003:G:H1'	2.54	0.43
1:A:1036:G:N2	1:A:1037:C:N1	2.67	0.43
1:A:1079:G:C6	1:A:1080:A:N6	2.86	0.43
1:A:1126:U:C5'	25:A:3121:HOH:O	2.60	0.43
1:A:1133:G:H2'	1:A:1134:G:C8	2.53	0.43
1:A:179:A:O2'	1:A:180:U:H5'	2.19	0.43
1:A:370:C:C2'	1:A:371:G:H5'	2.49	0.43
1:A:778:G:C5	1:A:779:C:C5	3.07	0.43
1:A:804:U:H5''	1:A:805:C:OP2	2.18	0.43
2:B:145:LEU:O	2:B:149:LEU:HB2	2.19	0.43
2:B:236:TYR:O	2:B:236:TYR:CD2	2.72	0.43
3:C:196:LEU:HA	3:C:196:LEU:HD13	1.60	0.43
4:D:30:LYS:C	4:D:32:ALA:N	2.71	0.43
6:F:75:LEU:HD23	6:F:75:LEU:HA	1.89	0.43
10:J:46:ARG:C	10:J:47:PHE:CD1	2.92	0.43
12:L:110:VAL:O	12:L:122:THR:HG21	2.19	0.43
13:M:89:GLY:O	13:M:92:HIS:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:31:LEU:HA	17:Q:31:LEU:HD12	1.67	0.43
18:R:42:ARG:HH11	18:R:42:ARG:HB3	1.83	0.43
1:A:1064:G:OP1	1:A:1386:G:H4'	2.19	0.43
1:A:1215:G:P	25:A:2356:HOH:O	2.75	0.43
1:A:1257:U:H4'	1:A:1258:G:OP2	2.17	0.43
1:A:1442:G:H5''	25:A:2899:HOH:O	2.18	0.43
22:A:1601:SRY:H11	22:A:1601:SRY:HB11	1.38	0.43
1:A:182:U:C5'	1:A:182:U:H6	2.28	0.43
1:A:773:G:C6	1:A:774:G:N7	2.87	0.43
1:A:794:A:OP1	25:A:2165:HOH:O	2.21	0.43
1:A:803:G:C6	1:A:804:U:C4	3.07	0.43
2:B:90:MET:HE1	2:B:222:ILE:HD13	2.01	0.43
4:D:13:ARG:HB3	4:D:40:PRO:HD3	2.01	0.43
4:D:187:ARG:HD2	4:D:187:ARG:HA	1.47	0.43
6:F:82:ARG:HB2	6:F:85:VAL:CG2	2.47	0.43
11:K:20:TYR:O	11:K:30:VAL:HA	2.19	0.43
13:M:11:ARG:HE	13:M:12:ASN:CA	2.32	0.43
14:N:37:PHE:N	14:N:37:PHE:CD1	2.87	0.43
15:O:63:ARG:HH12	15:O:87:ILE:HG21	1.84	0.43
15:O:67:LEU:HD13	15:O:78:TYR:HE1	1.84	0.43
17:Q:56:VAL:HB	17:Q:78:GLU:HB3	2.00	0.43
1:A:278:G:C6	17:Q:95:TYR:HD2	2.37	0.43
20:T:83:ARG:O	20:T:87:LYS:HG3	2.19	0.43
1:A:1014:A:O5'	1:A:1014:A:H8	2.02	0.43
1:A:1053:G:C4'	1:A:1054:C:H5'	2.46	0.43
1:A:1349:A:H1'	1:A:1374:A:N6	2.33	0.43
1:A:246:A:N1	1:A:279:A:N7	2.67	0.43
1:A:289:G:P	25:A:2004:HOH:O	2.76	0.43
1:A:43:C:H2'	1:A:44:G:O5'	2.19	0.43
1:A:562:C:H5'	1:A:562:C:C6	2.54	0.43
1:A:244:U:C6	1:A:894:G:N2	2.87	0.43
1:A:912:C:H2'	1:A:913:A:C8	2.53	0.43
5:E:47:LYS:HE3	5:E:47:LYS:HB3	1.87	0.43
8:H:103:VAL:HG12	8:H:108:GLY:HA3	2.00	0.43
8:H:48:TYR:O	8:H:48:TYR:CG	2.71	0.43
8:H:20:TYR:CE2	8:H:75:ARG:HD2	2.54	0.43
9:I:27:THR:HG22	9:I:28:VAL:N	2.33	0.43
13:M:50:GLU:O	13:M:53:VAL:HB	2.19	0.43
1:A:1164:G:C6	1:A:1165:C:C4	3.07	0.43
1:A:1487:G:C5	1:A:1488:G:N7	2.87	0.43
1:A:333:G:H2'	1:A:334:C:H6	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:665:A:N3	1:A:732:C:H2'	2.34	0.43
1:A:774:G:N2	1:A:775:G:H1'	2.34	0.43
6:F:40:VAL:HG23	6:F:41:GLU:N	2.34	0.43
7:G:148:ASN:O	7:G:150:ALA:N	2.52	0.43
8:H:103:VAL:O	8:H:106:GLY:N	2.50	0.43
8:H:29:SER:CB	8:H:32:LYS:HG3	2.49	0.43
9:I:97:LYS:HZ3	9:I:100:GLY:HA2	1.84	0.43
1:A:1343:G:H4'	9:I:122:ALA:HB3	2.01	0.43
10:J:49:VAL:HG23	10:J:60:ARG:O	2.19	0.43
10:J:34:VAL:CG2	10:J:74:ILE:HA	2.35	0.43
13:M:8:GLU:N	13:M:8:GLU:CD	2.72	0.43
14:N:43:CYS:O	14:N:46:GLU:N	2.52	0.43
15:O:67:LEU:HA	15:O:67:LEU:HD23	1.72	0.43
21:U:2:GLY:C	21:U:4:GLY:N	2.72	0.43
1:A:1407:5MC:H2'	1:A:1408:A:O4'	2.19	0.42
1:A:1453:G:H2'	1:A:1454:G:O4'	2.19	0.42
1:A:445:G:C4	1:A:490:G:N2	2.87	0.42
1:A:502:G:OP1	12:L:118:SER:N	2.40	0.42
1:A:841:U:H6	1:A:848:C:O4'	2.01	0.42
2:B:189:ASP:HB2	2:B:205:ASP:CB	2.49	0.42
2:B:41:ILE:HG22	2:B:42:ILE:O	2.19	0.42
3:C:20:SER:HA	3:C:57:ILE:O	2.18	0.42
5:E:105:VAL:O	5:E:106:PRO:C	2.56	0.42
6:F:14:LEU:HB3	6:F:18:GLN:HB3	2.01	0.42
6:F:2:ARG:HG3	6:F:69:GLU:HG3	2.01	0.42
7:G:113:GLU:O	7:G:119:ARG:HD3	2.19	0.42
12:L:113:ARG:HH11	12:L:116:SER:H	1.66	0.42
12:L:33:ARG:HH12	12:L:61:THR:HB	1.82	0.42
1:A:1491:G:H5'	12:L:94:TRP:CZ2	2.54	0.42
17:Q:18:THR:HA	17:Q:44:ALA:O	2.18	0.42
18:R:42:ARG:HH11	18:R:42:ARG:CG	2.31	0.42
20:T:24:LEU:HD22	20:T:24:LEU:HA	1.75	0.42
1:A:1127:G:C3'	1:A:1127:G:C8	3.03	0.42
1:A:1127:G:H8	1:A:1127:G:H3'	1.84	0.42
1:A:1212:U:HO2'	1:A:1213:A:P	2.42	0.42
1:A:1344:C:O5'	1:A:1344:C:H6	2.02	0.42
1:A:12:U:H5''	1:A:13:U:OP2	2.20	0.42
1:A:241:C:H42	1:A:285:G:H1	1.65	0.42
1:A:292:G:C8	1:A:292:G:C3'	3.02	0.42
1:A:360:A:H2'	1:A:361:G:O4'	2.19	0.42
1:A:448:A:P	1:A:485:G:H22	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:563:A:H5''	1:A:564:C:OP1	2.18	0.42
1:A:689:C:O5'	1:A:689:C:H6	2.00	0.42
1:A:735:C:O2'	1:A:736:C:H5'	2.20	0.42
1:A:778:G:H2'	1:A:779:C:O4'	2.18	0.42
1:A:811:C:H4'	1:A:900:A:N6	2.34	0.42
6:F:10:LEU:HD12	6:F:59:TYR:HB3	2.01	0.42
7:G:59:LEU:HD21	7:G:63:LYS:NZ	2.34	0.42
9:I:53:VAL:O	9:I:55:ALA:N	2.52	0.42
10:J:38:ILE:HG22	10:J:39:PRO:HD2	2.00	0.42
11:K:124:LYS:O	11:K:125:PHE:HD2	2.02	0.42
11:K:48:ILE:HD13	11:K:63:LEU:HB2	2.01	0.42
12:L:33:ARG:HH11	12:L:33:ARG:HG3	1.84	0.42
12:L:60:LEU:HA	12:L:60:LEU:HD22	1.74	0.42
12:L:6:THR:HG23	12:L:9:GLN:CD	2.39	0.42
14:N:53:LEU:HA	14:N:53:LEU:HD23	1.50	0.42
19:S:30:LEU:HB3	19:S:31:ILE:H	1.49	0.42
19:S:58:VAL:HA	19:S:59:PRO:HD3	1.64	0.42
19:S:80:TYR:CD1	19:S:81:ARG:HG2	2.54	0.42
20:T:46:GLU:HB2	20:T:48:LYS:CD	2.45	0.42
1:A:1316:G:N2	1:A:1319:A:OP2	2.52	0.42
1:A:1330:U:OP1	13:M:23:TYR:O	2.37	0.42
1:A:1369:C:H2'	1:A:1370:G:O4'	2.19	0.42
1:A:335:C:H2'	1:A:336:C:C6	2.54	0.42
3:C:11:ARG:HH11	3:C:180:ALA:HB3	1.83	0.42
4:D:6:GLY:O	4:D:8:VAL:HG22	2.18	0.42
6:F:33:TYR:CE1	6:F:75:LEU:HA	2.54	0.42
7:G:114:ARG:O	7:G:119:ARG:NH1	2.52	0.42
9:I:112:LYS:HG3	9:I:118:LYS:HA	2.00	0.42
9:I:23:ASN:HB3	9:I:25:LYS:HD2	2.01	0.42
9:I:97:LYS:O	9:I:98:PRO:C	2.56	0.42
11:K:101:SER:OG	11:K:102:GLY:N	2.52	0.42
13:M:11:ARG:NE	13:M:12:ASN:N	2.64	0.42
13:M:79:LYS:HG3	13:M:80:ARG:N	2.34	0.42
15:O:67:LEU:HD13	15:O:78:TYR:CE1	2.54	0.42
16:P:36:ILE:HG21	16:P:36:ILE:HD13	1.79	0.42
19:S:37:ARG:HB3	19:S:37:ARG:CZ	2.49	0.42
21:U:5:ASP:O	21:U:7:ARG:N	2.52	0.42
1:A:1050:G:H4'	25:A:2357:HOH:O	2.19	0.42
1:A:1054:C:P	25:A:2132:HOH:O	2.78	0.42
1:A:1183:A:O2'	1:A:1185:G:OP2	2.38	0.42
1:A:1194:U:O2'	1:A:1195:C:H5'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1052:U:O4	1:A:1200:C:C2	2.73	0.42
1:A:173:U:C6	1:A:198:G:H1'	2.55	0.42
1:A:229:U:O2'	1:A:230:G:H5'	2.20	0.42
1:A:403:C:C2	1:A:404:U:C5	3.07	0.42
1:A:408:A:C8	1:A:408:A:H3'	2.55	0.42
1:A:938:A:N6	1:A:939:G:C6	2.88	0.42
2:B:111:ARG:HD3	2:B:111:ARG:HH11	1.70	0.42
2:B:221:LEU:HD23	2:B:221:LEU:HA	1.74	0.42
3:C:137:ALA:HA	3:C:140:ARG:HH21	1.84	0.42
3:C:32:LEU:O	3:C:35:GLU:N	2.52	0.42
5:E:45:PHE:CE2	5:E:47:LYS:HE3	2.53	0.42
9:I:4:TYR:CD2	9:I:88:TYR:HA	2.54	0.42
9:I:6:GLY:HA3	9:I:83:ARG:HB2	2.02	0.42
11:K:101:SER:CB	11:K:103:LEU:H	2.30	0.42
12:L:34:ARG:CB	12:L:105:TYR:HE1	2.31	0.42
12:L:82:VAL:O	12:L:106:ASP:HB2	2.20	0.42
12:L:90:VAL:CG1	12:L:93:LEU:HG	2.48	0.42
14:N:11:LYS:O	14:N:12:ARG:C	2.58	0.42
10:J:50:ILE:HB	14:N:41:ARG:HD2	2.01	0.42
17:Q:68:ARG:HG2	17:Q:68:ARG:NH1	2.33	0.42
1:A:1033:G:N3	1:A:1033:G:H2'	2.34	0.42
1:A:109:A:C6	1:A:327:A:C6	3.08	0.42
1:A:1442:G:N3	1:A:1446:A:N7	2.66	0.42
1:A:32:A:H2'	1:A:33:A:O4'	2.20	0.42
1:A:65:U:C5	1:A:381:C:C4	3.07	0.42
1:A:749:C:H2'	1:A:750:G:H8	1.84	0.42
4:D:18:LYS:HD3	4:D:20:TYR:OH	2.20	0.42
4:D:57:ARG:HA	4:D:202:LEU:HD23	2.00	0.42
5:E:137:GLU:OE2	5:E:140:ARG:HD2	2.19	0.42
5:E:53:LEU:HD13	5:E:53:LEU:HA	1.75	0.42
5:E:32:VAL:CG2	5:E:58:ALA:HB3	2.47	0.42
5:E:75:THR:HG23	5:E:76:ILE:N	2.35	0.42
7:G:9:VAL:CG2	7:G:10:ARG:N	2.83	0.42
11:K:122:LYS:O	11:K:124:LYS:N	2.52	0.42
11:K:98:LEU:O	11:K:101:SER:HB3	2.19	0.42
16:P:75:ARG:HH21	16:P:80:PHE:HD1	1.67	0.42
1:A:1354:C:H6	1:A:1354:C:O5'	2.03	0.42
1:A:1532:U:H2'	1:A:1533:C:C6	2.54	0.42
1:A:168:G:C2	1:A:169:C:C6	3.07	0.42
1:A:236:G:H2'	1:A:237:C:O4'	2.19	0.42
1:A:247:G:OP2	17:Q:100:LYS:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:748:C:H4'	1:A:749:C:O5'	2.18	0.42
1:A:855:G:C6	1:A:856:C:C4	3.08	0.42
5:E:11:ILE:HA	5:E:11:ILE:HD13	1.43	0.42
9:I:107:ARG:HH11	9:I:107:ARG:HG2	1.83	0.42
15:O:62:GLN:HA	15:O:65:ARG:NH1	2.34	0.42
16:P:74:LEU:CD2	16:P:79:VAL:HG21	2.49	0.42
17:Q:68:ARG:HG2	17:Q:68:ARG:HH11	1.85	0.42
1:A:1065:U:O2'	1:A:1066:C:OP2	2.32	0.42
1:A:1110:A:OP2	25:A:2090:HOH:O	2.22	0.42
1:A:1283:G:O2'	1:A:1284:C:H5'	2.19	0.42
1:A:310:G:H2'	1:A:311:C:H6	1.84	0.42
1:A:602:A:H2'	1:A:603:U:O4'	2.20	0.42
1:A:686:U:HO2'	1:A:687:A:H8	1.63	0.42
1:A:686:U:O2'	1:A:687:A:H8	2.03	0.42
1:A:690:G:H2'	1:A:691:G:O4'	2.19	0.42
2:B:215:LEU:HD23	2:B:215:LEU:HA	1.79	0.42
3:C:73:PRO:HG3	3:C:105:GLU:HG3	2.01	0.42
3:C:32:LEU:HD13	3:C:32:LEU:HA	1.76	0.42
5:E:100:VAL:HG22	5:E:118:ILE:HG22	2.01	0.42
7:G:146:GLU:HA	7:G:149:ARG:HB2	2.01	0.42
8:H:40:ALA:HB3	8:H:41:ARG:H	1.66	0.42
11:K:109:VAL:HG13	18:R:85:LEU:O	2.19	0.42
1:A:716:A:H2'	11:K:117:ASN:O	2.19	0.42
1:A:708:C:OP1	11:K:85:ARG:NH2	2.52	0.42
15:O:45:VAL:HG12	15:O:46:HIS:ND1	2.34	0.42
17:Q:59:ILE:HG23	17:Q:71:PHE:CD1	2.55	0.42
19:S:36:ARG:HD2	19:S:52:TYR:O	2.19	0.42
21:U:12:LYS:HB3	21:U:22:ARG:HD3	2.00	0.42
1:A:112:G:H2'	1:A:113:G:H5'	2.01	0.42
1:A:1415:G:C2	1:A:1416:G:O6	2.72	0.42
1:A:262:A:N6	1:A:263:A:C6	2.88	0.42
1:A:276:G:O2'	1:A:277:C:H5'	2.20	0.42
1:A:862:C:C2'	1:A:863:U:H5'	2.49	0.42
3:C:142:MET:CE	3:C:171:GLY:HA3	2.49	0.42
4:D:54:TYR:O	4:D:55:ALA:C	2.58	0.42
1:A:401:C:OP2	4:D:73:ARG:NH2	2.53	0.42
7:G:115:ARG:HG3	7:G:115:ARG:H	1.70	0.42
8:H:104:ARG:NH1	8:H:138:TRP:NE1	2.67	0.42
13:M:30:ALA:O	13:M:31:LYS:C	2.58	0.42
14:N:26:ARG:HH11	14:N:26:ARG:HG2	1.85	0.42
14:N:47:LEU:HD23	14:N:47:LEU:HA	1.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:30:LEU:O	19:S:31:ILE:HB	2.20	0.42
19:S:72:GLY:HA2	19:S:75:ALA:H	1.85	0.42
1:A:1077:G:H5''	1:A:1078:U:OP2	2.20	0.42
1:A:1167:A:H2'	1:A:1168:A:C8	2.55	0.42
1:A:1225:A:N6	25:A:3278:HOH:O	2.52	0.42
1:A:1342:C:H2'	1:A:1343:G:C8	2.55	0.42
1:A:1402:4OC:C6	1:A:1403:C:H5	2.31	0.42
1:A:294:U:H2'	1:A:295:C:H6	1.84	0.42
1:A:569:C:H5''	1:A:570:G:OP1	2.19	0.42
1:A:772:U:C4	1:A:773:G:N7	2.88	0.42
1:A:773:G:N2	1:A:806:C:O2	2.51	0.42
3:C:34:LEU:O	3:C:38:ARG:HG3	2.19	0.42
5:E:33:VAL:HG11	5:E:109:ILE:HA	2.02	0.42
7:G:143:ARG:O	7:G:145:ALA:O	2.38	0.42
8:H:20:TYR:HE2	8:H:75:ARG:HD2	1.84	0.42
11:K:70:LYS:HA	11:K:73:MET:HG3	2.02	0.42
12:L:85:ILE:HG21	12:L:85:ILE:HD13	1.50	0.42
13:M:11:ARG:NH2	13:M:45:VAL:HG12	2.34	0.42
19:S:36:ARG:HG2	19:S:51:VAL:CG1	2.49	0.42
1:A:1150:U:H2'	1:A:1151:A:H5'	2.01	0.42
1:A:1217:C:H2'	1:A:1218:C:O4'	2.20	0.42
1:A:1277:C:H2'	1:A:1279:A:C8	2.55	0.42
1:A:1319:A:H4'	1:A:1320:C:OP1	2.20	0.42
1:A:1451:A:C5'	1:A:1452:C:H5	2.33	0.42
1:A:181:G:H8	1:A:181:G:H2'	1.57	0.42
1:A:505:G:H2'	1:A:506:G:C8	2.55	0.42
1:A:561:U:O2'	1:A:562:C:P	2.78	0.42
1:A:620:C:H2'	1:A:621:A:C8	2.55	0.42
2:B:139:LYS:O	2:B:143:GLU:HB2	2.20	0.42
2:B:16:HIS:O	2:B:17:PHE:C	2.59	0.42
3:C:112:SER:OG	3:C:114:PRO:HG2	2.20	0.42
3:C:28:GLN:HB3	3:C:32:LEU:HD23	2.02	0.42
4:D:3:ARG:HD3	4:D:3:ARG:HA	1.52	0.42
6:F:19:LEU:O	6:F:23:LYS:HB2	2.20	0.42
7:G:103:TRP:HE1	7:G:137:LYS:CD	2.33	0.42
8:H:64:LYS:C	8:H:65:TYR:CD1	2.93	0.42
9:I:50:LEU:HB2	9:I:55:ALA:O	2.19	0.42
9:I:5:TYR:HD2	9:I:18:PHE:CD2	2.38	0.42
11:K:22:HIS:O	11:K:28:THR:HA	2.20	0.42
13:M:2:ALA:O	13:M:10:PRO:HD2	2.20	0.42
14:N:27:CYS:SG	14:N:29:ARG:HB2	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:31:LYS:HG2	16:P:32:TYR:N	2.34	0.42
17:Q:22:LEU:C	17:Q:22:LEU:HD12	2.38	0.42
19:S:11:VAL:HG11	19:S:16:LEU:HB2	2.01	0.42
19:S:19:VAL:HG13	19:S:20:LEU:N	2.35	0.42
19:S:71:LEU:O	19:S:74:PHE:N	2.43	0.42
1:A:1247:U:H1'	1:A:1291:G:N2	2.35	0.41
1:A:293:G:C6	1:A:294:U:C4	3.08	0.41
1:A:826:C:H2'	1:A:827:U:C6	2.54	0.41
4:D:126:ILE:CG2	4:D:127:THR:N	2.83	0.41
4:D:163:GLU:OE2	4:D:166:LYS:HD3	2.20	0.41
5:E:42:GLY:HA2	5:E:136:MET:HE1	2.02	0.41
6:F:4:TYR:CZ	6:F:72:VAL:HG21	2.55	0.41
10:J:50:ILE:HG12	10:J:60:ARG:CD	2.50	0.41
11:K:109:VAL:CG1	11:K:110:ASP:N	2.83	0.41
12:L:102:ARG:HH11	12:L:102:ARG:HD2	1.63	0.41
15:O:30:ALA:CA	15:O:85:LEU:HD11	2.49	0.41
16:P:41:PRO:O	16:P:43:LYS:HG3	2.20	0.41
19:S:22:LEU:HD13	19:S:28:LYS:CB	2.49	0.41
20:T:91:LEU:HA	20:T:91:LEU:HD23	1.67	0.41
1:A:412:A:HO2'	1:A:413:G:P	2.38	0.41
1:A:644:G:C5	1:A:645:C:C6	3.07	0.41
2:B:17:PHE:CD1	2:B:18:GLY:N	2.88	0.41
3:C:155:GLY:HA2	3:C:164:ARG:H	1.84	0.41
3:C:50:ALA:HA	3:C:75:VAL:HG21	2.00	0.41
5:E:124:GLY:O	5:E:125:SER:C	2.55	0.41
5:E:12:LEU:H	5:E:31:LEU:HB2	1.85	0.41
9:I:125:TYR:CD1	9:I:125:TYR:C	2.94	0.41
10:J:71:LEU:HB3	10:J:72:VAL:H	1.48	0.41
11:K:87:THR:HG22	11:K:88:GLY:N	2.35	0.41
12:L:66:VAL:HG11	12:L:98:TYR:CE1	2.56	0.41
17:Q:50:LYS:HG3	17:Q:51:TYR:CE1	2.55	0.41
18:R:58:LEU:CD2	18:R:62:GLU:HB3	2.51	0.41
19:S:40:ILE:HG23	19:S:44:MET:SD	2.60	0.41
19:S:80:TYR:HE1	19:S:81:ARG:HB3	1.85	0.41
1:A:101:A:O2'	1:A:102:G:H5'	2.21	0.41
1:A:1126:U:C6	1:A:1126:U:C3'	3.03	0.41
1:A:1241:G:C4	1:A:1242:C:C5	3.08	0.41
1:A:290:C:H2'	1:A:291:C:O4'	2.20	0.41
1:A:407:G:H4'	4:D:116:GLN:HA	2.02	0.41
1:A:448:A:C4	1:A:487:A:C2	3.09	0.41
1:A:496:A:H4'	1:A:497:A:H5''	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:634:C:O2'	1:A:635:G:H5'	2.20	0.41
1:A:737:A:C2'	1:A:738:C:O4'	2.65	0.41
2:B:152:PHE:C	2:B:154:LEU:N	2.73	0.41
2:B:167:PRO:HD3	2:B:186:ALA:HB1	2.02	0.41
4:D:2:GLY:O	4:D:3:ARG:NE	2.51	0.41
1:A:1397:C:OP2	5:E:24:ARG:NH2	2.52	0.41
5:E:44:GLY:N	5:E:62:ALA:HB2	2.35	0.41
1:A:4:U:C5	8:H:105:ARG:NE	2.88	0.41
9:I:15:ALA:CB	9:I:77:ILE:HD12	2.50	0.41
10:J:75:ILE:HA	10:J:77:PRO:HG3	2.02	0.41
11:K:124:LYS:O	11:K:125:PHE:CD2	2.73	0.41
12:L:84:LEU:HB3	12:L:104:VAL:HG21	2.02	0.41
13:M:21:TYR:N	13:M:21:TYR:HD2	2.18	0.41
20:T:28:ALA:HA	20:T:31:SER:OG	2.20	0.41
1:A:1226:C:OP1	13:M:91:ARG:NH1	2.42	0.41
1:A:1526:G:C2'	1:A:1527:C:H5'	2.50	0.41
1:A:193:C:O2'	20:T:61:SER:HA	2.20	0.41
1:A:234:C:H2'	1:A:235:C:C6	2.55	0.41
1:A:358:U:H2'	1:A:359:U:O4'	2.20	0.41
1:A:357:G:OP1	1:A:367:U:H2'	2.20	0.41
2:B:171:ALA:HA	2:B:174:VAL:CB	2.44	0.41
3:C:26:LYS:H	3:C:26:LYS:HG3	1.26	0.41
4:D:174:LEU:CA	4:D:186:LEU:HD13	2.50	0.41
4:D:88:VAL:O	4:D:89:THR:C	2.59	0.41
1:A:1080:A:H5''	5:E:16:THR:HB	2.02	0.41
6:F:39:LYS:HD2	6:F:39:LYS:HA	1.77	0.41
8:H:40:ALA:O	8:H:41:ARG:C	2.58	0.41
8:H:60:ARG:HG2	8:H:62:TYR:CZ	2.55	0.41
8:H:20:TYR:HA	8:H:65:TYR:CE2	2.56	0.41
10:J:9:ARG:HA	10:J:68:HIS:O	2.21	0.41
16:P:25:ARG:HG3	16:P:25:ARG:H	1.66	0.41
1:A:187:C:N3	20:T:105:SER:HB3	2.34	0.41
1:A:1048:G:H2'	1:A:1050:G:C8	2.55	0.41
1:A:1211:U:C3'	1:A:1211:U:H6	2.33	0.41
1:A:1300:G:C4	1:A:1334:G:C6	3.09	0.41
1:A:1415:G:C3'	1:A:1415:G:C8	3.03	0.41
1:A:1399:C:C2	1:A:1502:A:N6	2.89	0.41
1:A:235:C:O2'	1:A:236:G:H5'	2.19	0.41
1:A:259:G:C2	1:A:260:G:C4	3.08	0.41
1:A:275:G:H8	1:A:275:G:H5''	1.86	0.41
5:E:13:ILE:HD13	5:E:13:ILE:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:17:ALA:CA	5:E:26:PHE:HB3	2.49	0.41
5:E:79:GLU:HB3	5:E:93:PRO:HD2	2.01	0.41
5:E:89:ILE:HD11	5:E:91:LEU:HD21	2.01	0.41
5:E:78:HIS:HA	8:H:105:ARG:CG	2.51	0.41
8:H:112:LEU:H	8:H:112:LEU:HD23	1.86	0.41
1:A:1250:A:H4'	9:I:68:GLY:N	2.35	0.41
10:J:4:ILE:HD12	10:J:74:ILE:HD12	2.01	0.41
10:J:80:LYS:HA	10:J:83:GLU:HB2	2.02	0.41
12:L:102:ARG:HB3	12:L:102:ARG:HE	1.69	0.41
12:L:69:TYR:HB3	12:L:99:HIS:ND1	2.35	0.41
16:P:38:TYR:O	16:P:49:LEU:HA	2.21	0.41
20:T:20:LEU:HD23	20:T:20:LEU:HA	1.40	0.41
20:T:74:LYS:HB2	20:T:76:ALA:N	2.29	0.41
1:A:1061:G:C5	1:A:1062:U:C5	3.09	0.41
1:A:1514:C:H5'	25:A:2510:HOH:O	2.21	0.41
1:A:166:G:O2'	1:A:167:G:H5'	2.20	0.41
1:A:42:G:H2'	1:A:43:C:O4'	2.20	0.41
1:A:455:C:H6	1:A:455:C:O5'	2.03	0.41
1:A:550:G:C5	1:A:551:U:C5	3.09	0.41
2:B:97:TRP:CZ3	2:B:176:GLU:OE2	2.73	0.41
4:D:168:ARG:HB3	4:D:168:ARG:CZ	2.50	0.41
4:D:60:GLU:OE1	4:D:60:GLU:CA	2.68	0.41
5:E:148:VAL:HG12	5:E:152:ARG:HE	1.85	0.41
6:F:26:ILE:O	6:F:30:LEU:HD23	2.19	0.41
12:L:6:THR:HG23	12:L:9:GLN:OE1	2.20	0.41
15:O:43:LEU:HA	15:O:43:LEU:HD23	1.69	0.41
15:O:70:LEU:HD22	15:O:70:LEU:HA	1.82	0.41
16:P:67:THR:O	16:P:70:ALA:HB3	2.21	0.41
17:Q:12:SER:HB2	17:Q:20:THR:HB	2.02	0.41
17:Q:3:LYS:HD3	17:Q:61:GLU:O	2.21	0.41
17:Q:59:ILE:HG23	17:Q:71:PHE:HD1	1.84	0.41
18:R:35:ARG:HD2	18:R:35:ARG:HH11	1.62	0.41
19:S:72:GLY:HA2	19:S:75:ALA:HB3	2.03	0.41
1:A:1134:G:H2'	1:A:1135:U:H5'	2.03	0.41
1:A:1309:G:O2'	13:M:74:VAL:HG13	2.21	0.41
1:A:1332:A:C2	1:A:1333:A:C4	3.09	0.41
1:A:1415:G:H1'	1:A:1486:G:C2	2.51	0.41
1:A:1516:G:H2'	1:A:1518:MA6:OP2	2.20	0.41
1:A:444:C:C2'	1:A:445:G:H5'	2.50	0.41
1:A:630:G:H2'	1:A:631:G:O4'	2.21	0.41
1:A:986:A:N6	1:A:987:G:C6	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:17:ALA:CB	5:E:26:PHE:HD2	2.33	0.41
7:G:53:LYS:HA	7:G:53:LYS:HE3	2.03	0.41
5:E:79:GLU:CG	8:H:105:ARG:HG2	2.48	0.41
9:I:10:ARG:O	9:I:11:LYS:C	2.58	0.41
1:A:689:C:OP2	11:K:46:GLY:HA3	2.20	0.41
17:Q:83:ASP:OD2	17:Q:84:LEU:HG	2.21	0.41
17:Q:88:TYR:C	17:Q:88:TYR:CD2	2.93	0.41
20:T:55:ILE:HD13	20:T:55:ILE:HA	1.66	0.41
21:U:5:ASP:O	21:U:8:THR:HG23	2.20	0.41
1:A:1120:G:H2'	1:A:1121:U:H6	1.86	0.41
1:A:1181:G:H1'	1:A:1182:G:C5	2.56	0.41
1:A:1256:A:N1	1:A:1277:C:C5	2.88	0.41
1:A:1281:U:O2	1:A:1281:U:O4'	2.39	0.41
1:A:345:C:OP2	1:A:345:C:H6	2.03	0.41
1:A:44:G:C2	1:A:399:G:C5	3.09	0.41
1:A:699:C:C2'	1:A:700:G:H5'	2.51	0.41
1:A:1074:G:O3'	2:B:103:THR:HG21	2.21	0.41
2:B:132:LYS:HZ2	2:B:136:VAL:HG23	1.85	0.41
5:E:105:VAL:O	5:E:108:ALA:N	2.54	0.41
1:A:1073:U:OP2	5:E:57:LYS:HE3	2.20	0.41
7:G:57:GLU:O	7:G:58:PRO:C	2.59	0.41
7:G:58:PRO:O	7:G:61:VAL:HB	2.21	0.41
8:H:28:ALA:HA	8:H:59:LEU:HG	2.03	0.41
8:H:61:VAL:HG23	8:H:61:VAL:H	1.61	0.41
12:L:86:ARG:HH22	12:L:99:HIS:CD2	2.38	0.41
3:C:29:TYR:CZ	14:N:54:PRO:HD2	2.56	0.41
18:R:64:ARG:O	18:R:68:LYS:HD3	2.19	0.41
20:T:50:GLU:O	20:T:100:ILE:HD11	2.21	0.41
1:A:1007:C:H2'	1:A:1008:C:C6	2.54	0.41
1:A:1378:C:H3'	1:A:1379:G:C5'	2.51	0.41
1:A:1424:C:O2'	1:A:1425:U:H5'	2.20	0.41
1:A:651:C:O2'	1:A:652:U:H5'	2.20	0.41
1:A:681:C:C2	1:A:710:G:C2	3.09	0.41
3:C:119:ARG:O	3:C:119:ARG:HG3	2.21	0.41
3:C:202:ILE:HG22	3:C:204:LEU:HD23	2.03	0.41
4:D:78:LEU:HB3	4:D:93:PHE:HE2	1.85	0.41
4:D:8:VAL:HG21	4:D:115:ARG:NH1	2.36	0.41
5:E:101:ILE:O	5:E:120:THR:HB	2.20	0.41
6:F:10:LEU:CD1	6:F:59:TYR:HB3	2.50	0.41
1:A:642:A:C4	8:H:114:THR:O	2.73	0.41
8:H:21:LYS:O	8:H:63:LEU:CD2	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:49:ASN:ND2	12:L:92:ASP:OD2	2.54	0.41
17:Q:78:GLU:HG3	17:Q:79:SER:N	2.36	0.41
1:A:134:A:H2'	1:A:135:C:O4'	2.20	0.41
1:A:1508:G:O2'	1:A:1509:C:H5'	2.21	0.41
22:A:1601:SRY:H12	22:A:1601:SRY:N31	2.35	0.41
1:A:421:U:H5'	1:A:422:C:C5	2.56	0.41
1:A:452:A:O2'	1:A:453:A:H8	2.03	0.41
1:A:519:C:N4	1:A:533:A:N6	2.68	0.41
1:A:581:G:O2'	1:A:582:U:H5'	2.21	0.41
1:A:771:G:C2'	1:A:772:U:H5'	2.51	0.41
1:A:828:A:OP1	1:A:828:A:H4'	2.19	0.41
4:D:17:VAL:HG22	4:D:18:LYS:H	1.86	0.41
6:F:78:GLU:O	6:F:81:ILE:HG13	2.21	0.41
6:F:82:ARG:HE	6:F:82:ARG:HA	1.85	0.41
7:G:127:ALA:HB1	7:G:135:VAL:HG22	2.02	0.41
9:I:112:LYS:CG	9:I:118:LYS:HA	2.51	0.41
9:I:83:ARG:O	9:I:86:VAL:HG12	2.21	0.41
14:N:6:LEU:HA	14:N:6:LEU:HD13	1.50	0.41
15:O:36:ILE:HG22	15:O:37:ASN:OD1	2.20	0.41
16:P:19:ILE:C	16:P:20:VAL:HG23	2.42	0.41
1:A:664:G:P	18:R:64:ARG:HH11	2.43	0.41
1:A:1121:U:H2'	1:A:1122:U:H6	1.83	0.41
1:A:1312:G:O6	19:S:3:ARG:HB3	2.21	0.41
1:A:1402:4OC:CM2	1:A:1403:C:H5'	2.43	0.41
1:A:1404:5MC:H1'	1:A:1499:A:C2	2.56	0.41
1:A:1410:G:H2'	1:A:1411:C:C6	2.55	0.41
1:A:796:C:H5''	1:A:797:C:OP2	2.20	0.41
2:B:95:GLN:HG3	2:B:147:LYS:HE2	2.03	0.41
2:B:47:THR:OG1	2:B:202:PRO:HG2	2.21	0.41
3:C:124:ILE:HD13	3:C:124:ILE:HG21	1.93	0.41
3:C:97:LYS:HB3	3:C:97:LYS:HE3	1.82	0.41
4:D:20:TYR:HD1	25:D:414:HOH:O	2.04	0.41
5:E:43:LEU:HD11	5:E:132:ALA:HB1	2.03	0.41
6:F:79:LEU:HB2	6:F:88:VAL:HG21	2.02	0.41
9:I:79:LEU:HD22	9:I:83:ARG:CD	2.51	0.41
10:J:26:ALA:CA	10:J:84:GLN:HG2	2.50	0.41
12:L:86:ARG:HG2	12:L:87:GLY:O	2.21	0.41
13:M:37:THR:CB	13:M:39:ILE:HD11	2.50	0.41
1:A:277:C:C5'	17:Q:68:ARG:HH21	2.27	0.41
17:Q:95:TYR:HD1	17:Q:95:TYR:HA	1.36	0.41
19:S:3:ARG:O	19:S:4:SER:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:10:LEU:CD1	20:T:13:LEU:N	2.82	0.41
20:T:97:ALA:O	20:T:99:LEU:N	2.54	0.41
1:A:1025:U:O2'	1:A:1026:G:N7	2.35	0.40
1:A:1408:A:C4	1:A:1494:G:N2	2.89	0.40
1:A:404:U:O2'	1:A:405:U:H5'	2.21	0.40
1:A:490:G:H8	1:A:490:G:O5'	2.04	0.40
1:A:593:G:O2'	1:A:594:G:H5'	2.21	0.40
1:A:658:G:C5	1:A:659:U:C5	3.09	0.40
1:A:64:G:N2	1:A:67:C:C4	2.90	0.40
3:C:152:ILE:HA	3:C:166:GLU:O	2.21	0.40
3:C:35:GLU:O	3:C:38:ARG:N	2.54	0.40
5:E:129:ILE:O	5:E:132:ALA:HB3	2.20	0.40
7:G:21:VAL:HG22	7:G:21:VAL:H	1.67	0.40
9:I:108:VAL:HG12	9:I:109:VAL:H	1.86	0.40
11:K:79:SER:HB2	11:K:106:LYS:HD3	2.03	0.40
13:M:23:TYR:CB	13:M:67:GLU:HA	2.51	0.40
15:O:45:VAL:HG12	15:O:46:HIS:N	2.36	0.40
17:Q:27:PHE:CE1	17:Q:36:ILE:HD11	2.56	0.40
18:R:43:PHE:O	18:R:51:LEU:HD12	2.21	0.40
1:A:1125:U:H2'	1:A:1126:U:OP2	2.21	0.40
1:A:1164:G:C2	1:A:1173:G:C2	3.10	0.40
1:A:1427:U:H2'	1:A:1428:A:H8	1.77	0.40
1:A:1432:G:O5'	1:A:1432:G:H8	2.04	0.40
1:A:1443:G:C4'	1:A:1446:A:H5'	2.48	0.40
1:A:254:G:O4'	17:Q:15:MET:HE3	2.21	0.40
1:A:682:G:C6	1:A:683:G:N7	2.89	0.40
1:A:839:U:H5''	1:A:840:C:H5	1.86	0.40
2:B:54:THR:HG21	2:B:201:ILE:HD11	2.03	0.40
2:B:235:SER:O	2:B:238:LEU:HG	2.20	0.40
2:B:18:GLY:HA3	2:B:42:ILE:HG12	2.03	0.40
4:D:9:CYS:O	4:D:12:CYS:HB2	2.22	0.40
7:G:145:ALA:C	7:G:147:ALA:H	2.25	0.40
1:A:1375:A:H4'	7:G:29:LYS:HE2	2.03	0.40
14:N:18:VAL:O	14:N:20:ALA:N	2.54	0.40
14:N:47:LEU:O	14:N:48:ALA:C	2.59	0.40
14:N:8:GLU:HA	14:N:11:LYS:HG2	2.03	0.40
15:O:36:ILE:HA	15:O:59:MET:CE	2.51	0.40
19:S:63:THR:O	19:S:66:MET:HB2	2.21	0.40
1:A:1420:C:H6	1:A:1420:C:O5'	2.05	0.40
1:A:189:G:H2'	1:A:190:C:O4'	2.21	0.40
1:A:763:G:N3	1:A:764:C:C6	2.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:767:A:H8	1:A:767:A:O5'	2.05	0.40
1:A:791:G:C2'	1:A:792:A:H5'	2.52	0.40
1:A:800:G:H2'	1:A:801:U:C5	2.56	0.40
1:A:570:G:H1'	1:A:820:U:C4	2.57	0.40
1:A:997:U:O2	1:A:1044:A:H2	2.04	0.40
4:D:56:VAL:H	4:D:56:VAL:HG23	1.61	0.40
1:A:613:C:P	4:D:84:LYS:HE2	2.62	0.40
5:E:128:PRO:HG2	5:E:129:ILE:H	1.87	0.40
5:E:55:VAL:HG12	5:E:56:GLN:N	2.36	0.40
7:G:84:ASN:O	7:G:85:TYR:HD2	2.03	0.40
8:H:104:ARG:HD2	8:H:138:TRP:CE3	2.57	0.40
12:L:11:VAL:CG2	17:Q:29:HIS:CD2	3.04	0.40
17:Q:97:SER:O	17:Q:98:LEU:HB2	2.21	0.40
1:A:101:A:C2	1:A:102:G:C8	3.10	0.40
1:A:226:G:C2	1:A:227:G:C8	3.10	0.40
1:A:77:G:O2'	1:A:78:G:H5'	2.21	0.40
1:A:577:G:H1'	1:A:816:A:C4	2.56	0.40
1:A:937:A:H5''	1:A:938:A:OP2	2.21	0.40
3:C:166:GLU:HG3	3:C:167:TRP:H	1.86	0.40
3:C:84:ILE:O	3:C:87:LEU:HB2	2.22	0.40
5:E:32:VAL:HG12	5:E:33:VAL:N	2.36	0.40
1:A:19:C:H5''	5:E:86:ALA:HB2	2.03	0.40
8:H:104:ARG:O	8:H:105:ARG:HB2	2.22	0.40
9:I:108:VAL:HG12	9:I:109:VAL:CG2	2.52	0.40
10:J:15:THR:HG23	10:J:15:THR:H	1.55	0.40
12:L:41:ARG:CG	12:L:42:THR:N	2.83	0.40
17:Q:76:LEU:HD23	17:Q:77:VAL:C	2.41	0.40
19:S:63:THR:H	19:S:66:MET:CG	2.34	0.40
20:T:74:LYS:HE2	20:T:74:LYS:HA	2.02	0.40
1:A:1022:G:C2	1:A:1023:G:C8	3.08	0.40
1:A:1453:G:O3'	20:T:39:LYS:NZ	2.52	0.40
1:A:392:G:N3	1:A:393:A:C8	2.89	0.40
1:A:457:C:C2	1:A:476:G:C2	3.09	0.40
1:A:654:G:C2'	1:A:655:A:H5'	2.51	0.40
1:A:740:U:O2'	1:A:741:G:H5'	2.21	0.40
2:B:169:LYS:HE2	2:B:169:LYS:HB2	1.73	0.40
2:B:211:ILE:O	2:B:215:LEU:HB2	2.21	0.40
2:B:31:TYR:HE2	2:B:50:GLU:HG3	1.86	0.40
2:B:52:GLU:HG2	2:B:56:ARG:NH2	2.37	0.40
5:E:151:LEU:HD23	5:E:151:LEU:HA	1.52	0.40
6:F:11:ASN:O	6:F:13:ASN:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1298:C:N4	7:G:114:ARG:HD2	2.36	0.40
7:G:70:LYS:HA	7:G:71:PRO:HD3	1.60	0.40
9:I:46:ALA:HB1	9:I:77:ILE:CG2	2.51	0.40
9:I:89:ASN:O	9:I:92:TYR:HB2	2.21	0.40
10:J:14:LYS:O	10:J:17:ASP:HB2	2.22	0.40
10:J:48:THR:HG1	10:J:62:HIS:CE1	2.40	0.40
1:A:1523:G:P	11:K:123:LYS:HZ3	2.45	0.40
11:K:58:PRO:HA	11:K:90:GLY:HA3	2.03	0.40
15:O:10:LYS:HB2	15:O:10:LYS:HE3	1.80	0.40
1:A:236:G:H1'	17:Q:4:LYS:HZ3	1.86	0.40
6:F:100:ASN:CG	18:R:23:LYS:HG3	2.42	0.40
19:S:6:LYS:HB2	19:S:7:LYS:H	1.48	0.40
20:T:49:ALA:HB1	20:T:53:LEU:HD13	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1443:G:N2	25:A:2379:HOH:O[4_554]	2.19	0.01

## 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	
2	B	232/256 (91%)	197 (85%)	31 (13%)	4 (2%)	9	43
3	C	204/239 (85%)	166 (81%)	37 (18%)	1 (0%)	29	65
4	D	206/209 (99%)	184 (89%)	22 (11%)	0	100	100
5	E	148/162 (91%)	134 (90%)	12 (8%)	2 (1%)	11	46
6	F	99/101 (98%)	90 (91%)	8 (8%)	1 (1%)	15	51
7	G	153/156 (98%)	142 (93%)	11 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	136/138 (99%)	125 (92%)	10 (7%)	1 (1%)	22	59
9	I	125/128 (98%)	111 (89%)	13 (10%)	1 (1%)	19	56
10	J	96/105 (91%)	74 (77%)	17 (18%)	5 (5%)	2	22
11	K	114/129 (88%)	97 (85%)	17 (15%)	0	100	100
12	L	122/135 (90%)	104 (85%)	15 (12%)	3 (2%)	5	36
13	M	116/126 (92%)	96 (83%)	17 (15%)	3 (3%)	5	36
14	N	58/61 (95%)	43 (74%)	14 (24%)	1 (2%)	9	43
15	O	85/89 (96%)	73 (86%)	12 (14%)	0	100	100
16	P	81/88 (92%)	70 (86%)	11 (14%)	0	100	100
17	Q	97/105 (92%)	86 (89%)	11 (11%)	0	100	100
18	R	68/88 (77%)	57 (84%)	7 (10%)	4 (6%)	1	20
19	S	78/93 (84%)	67 (86%)	10 (13%)	1 (1%)	12	48
20	T	97/106 (92%)	80 (82%)	13 (13%)	4 (4%)	3	26
21	U	22/27 (82%)	21 (96%)	1 (4%)	0	100	100
All	All	2337/2541 (92%)	2017 (86%)	289 (12%)	31 (1%)	12	48

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	9	GLU
2	B	21	ARG
3	C	15	THR
12	L	28	LYS
19	S	31	ILE
2	B	11	LEU
10	J	35	SER
5	E	65	ASN
12	L	25	PRO
14	N	8	GLU
18	R	49	LYS
20	T	13	LEU
20	T	50	GLU
12	L	27	LEU
18	R	60	ALA
20	T	98	PRO
6	F	96	PRO
9	I	119	ALA

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Mol	Chain	Res	Type
10	J	34	VAL
10	J	83	GLU
13	M	7	VAL
18	R	41	LYS
18	R	45	SER
20	T	73	HIS
5	E	118	ILE
13	M	28	ALA
10	J	49	VAL
10	J	72	VAL
2	B	229	VAL
8	H	74	PRO
13	M	60	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	
2	B	202/220 (92%)	150 (74%)	52 (26%)	0	4
3	C	160/188 (85%)	103 (64%)	57 (36%)	0	0
4	D	180/181 (99%)	128 (71%)	52 (29%)	0	2
5	E	115/123 (94%)	83 (72%)	32 (28%)	0	2
6	F	90/90 (100%)	63 (70%)	27 (30%)	0	2
7	G	126/127 (99%)	81 (64%)	45 (36%)	0	0
8	H	119/119 (100%)	82 (69%)	37 (31%)	0	2
9	I	98/99 (99%)	65 (66%)	33 (34%)	0	1
10	J	87/92 (95%)	63 (72%)	24 (28%)	0	3
11	K	88/99 (89%)	56 (64%)	32 (36%)	0	0
12	L	104/111 (94%)	78 (75%)	26 (25%)	0	4
13	M	94/101 (93%)	65 (69%)	29 (31%)	0	2
14	N	49/50 (98%)	37 (76%)	12 (24%)	0	5
15	O	79/80 (99%)	51 (65%)	28 (35%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	P	72/74 (97%)	53 (74%)	19 (26%)	0	3
17	Q	94/97 (97%)	69 (73%)	25 (27%)	0	3
18	R	61/77 (79%)	43 (70%)	18 (30%)	0	2
19	S	71/80 (89%)	49 (69%)	22 (31%)	0	2
20	T	76/82 (93%)	50 (66%)	26 (34%)	0	1
21	U	19/22 (86%)	14 (74%)	5 (26%)	0	3
All	All	1984/2112 (94%)	1383 (70%)	601 (30%)	0	2

All (601) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	7	VAL
2	B	9	GLU
2	B	11	LEU
2	B	12	GLU
2	B	21	ARG
2	B	24	TRP
2	B	30	ARG
2	B	31	TYR
2	B	44	LEU
2	B	48	MET
2	B	51	LEU
2	B	53	ARG
2	B	64	ARG
2	B	67	THR
2	B	69	LEU
2	B	73	THR
2	B	74	LYS
2	B	75	LYS
2	B	86	GLU
2	B	87	ARG
2	B	92	TYR
2	B	95	GLN
2	B	106	LYS
2	B	110	GLN
2	B	112	VAL
2	B	122	PHE
2	B	127	ILE
2	B	133	LYS
2	B	135	GLN

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Mol	Chain	Res	Type
2	B	140	HIS
2	B	142	LEU
2	B	144	ARG
2	B	145	LEU
2	B	153	ARG
2	B	162	ILE
2	B	163	PHE
2	B	165	VAL
2	B	169	LYS
2	B	170	GLU
2	B	172	ILE
2	B	175	ARG
2	B	178	ARG
2	B	184	VAL
2	B	187	LEU
2	B	196	LEU
2	B	208	ILE
2	B	211	ILE
2	B	217	ARG
2	B	221	LEU
2	B	223	ILE
2	B	226	ARG
2	B	233	SER
3	C	3	ASN
3	C	4	LYS
3	C	5	ILE
3	C	7	PRO
3	C	11	ARG
3	C	12	LEU
3	C	14	ILE
3	C	15	THR
3	C	16	ARG
3	C	26	LYS
3	C	29	TYR
3	C	32	LEU
3	C	34	LEU
3	C	36	ASP
3	C	45	LYS
3	C	47	LEU
3	C	48	TYR
3	C	55	VAL
3	C	59	ARG

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Mol	Chain	Res	Type
3	C	62	ASP
3	C	69	HIS
3	C	77	ILE
3	C	79	ARG
3	C	82	GLU
3	C	83	ARG
3	C	85	ARG
3	C	87	LEU
3	C	88	ARG
3	C	89	GLU
3	C	94	LEU
3	C	95	THR
3	C	99	VAL
3	C	101	LEU
3	C	103	VAL
3	C	119	ARG
3	C	120	VAL
3	C	138	VAL
3	C	142	MET
3	C	144	SER
3	C	147	LYS
3	C	151	VAL
3	C	153	VAL
3	C	157	ILE
3	C	162	GLN
3	C	164	ARG
3	C	165	THR
3	C	167	TRP
3	C	170	GLN
3	C	175	LEU
3	C	177	THR
3	C	188	LEU
3	C	191	THR
3	C	192	THR
3	C	193	TYR
3	C	195	VAL
3	C	196	LEU
3	C	204	LEU
4	D	3	ARG
4	D	8	VAL
4	D	9	CYS
4	D	10	ARG

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Mol	Chain	Res	Type
4	D	13	ARG
4	D	19	LEU
4	D	21	LEU
4	D	25	ARG
4	D	26	CYS
4	D	38	TYR
4	D	47	ARG
4	D	49	ARG
4	D	58	LEU
4	D	59	ARG
4	D	64	LEU
4	D	66	ARG
4	D	76	ARG
4	D	78	LEU
4	D	81	GLU
4	D	85	LYS
4	D	97	LEU
4	D	99	SER
4	D	100	ARG
4	D	103	ASN
4	D	114	ARG
4	D	120	LEU
4	D	122	ARG
4	D	132	ARG
4	D	135	LEU
4	D	137	SER
4	D	142	PRO
4	D	146	ILE
4	D	150	GLU
4	D	152	SER
4	D	155	LEU
4	D	158	ILE
4	D	160	GLN
4	D	162	LEU
4	D	163	GLU
4	D	165	MET
4	D	168	ARG
4	D	176	LEU
4	D	184	LYS
4	D	187	ARG
4	D	188	LEU
4	D	191	ARG

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Mol	Chain	Res	Type
4	D	192	GLU
4	D	194	LEU
4	D	201	GLN
4	D	202	LEU
4	D	208	SER
4	D	209	ARG
5	E	6	PHE
5	E	7	GLU
5	E	10	MET
5	E	11	ILE
5	E	12	LEU
5	E	13	ILE
5	E	15	ARG
5	E	18	ARG
5	E	19	MET
5	E	24	ARG
5	E	25	ARG
5	E	26	PHE
5	E	27	ARG
5	E	41	VAL
5	E	43	LEU
5	E	47	LYS
5	E	55	VAL
5	E	56	GLN
5	E	60	TYR
5	E	63	ARG
5	E	65	ASN
5	E	68	GLU
5	E	70	PRO
5	E	76	ILE
5	E	78	HIS
5	E	79	GLU
5	E	87	SER
5	E	89	ILE
5	E	100	VAL
5	E	105	VAL
5	E	125	SER
5	E	148	VAL
6	F	1	MET
6	F	10	LEU
6	F	16	GLN
6	F	17	SER

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Mol	Chain	Res	Type
6	F	18	GLN
6	F	19	LEU
6	F	21	LEU
6	F	24	GLU
6	F	30	LEU
6	F	36	ARG
6	F	39	LYS
6	F	40	VAL
6	F	45	LEU
6	F	46	ARG
6	F	47	ARG
6	F	48	LEU
6	F	55	ASP
6	F	60	PHE
6	F	61	LEU
6	F	67	MET
6	F	71	ARG
6	F	75	LEU
6	F	82	ARG
6	F	91	VAL
6	F	92	LYS
6	F	93	SER
6	F	98	LEU
7	G	5	ARG
7	G	6	ARG
7	G	8	GLU
7	G	12	LEU
7	G	16	LEU
7	G	17	VAL
7	G	21	VAL
7	G	24	THR
7	G	33	ASP
7	G	38	LEU
7	G	41	ARG
7	G	45	ASP
7	G	49	ILE
7	G	52	GLU
7	G	53	LYS
7	G	54	THR
7	G	56	GLN
7	G	59	LEU
7	G	72	ARG

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Mol	Chain	Res	Type
7	G	75	VAL
7	G	77	SER
7	G	79	ARG
7	G	80	VAL
7	G	90	GLU
7	G	92	SER
7	G	94	ARG
7	G	98	SER
7	G	103	TRP
7	G	104	LEU
7	G	106	GLN
7	G	114	ARG
7	G	120	ILE
7	G	122	HIS
7	G	124	LEU
7	G	125	MET
7	G	126	ASP
7	G	131	LYS
7	G	135	VAL
7	G	136	LYS
7	G	138	LYS
7	G	139	GLU
7	G	142	GLU
7	G	143	ARG
7	G	153	HIS
7	G	155	ARG
8	H	1	MET
8	H	6	ILE
8	H	8	ASP
8	H	9	MET
8	H	12	ARG
8	H	14	ARG
8	H	18	ARG
8	H	19	VAL
8	H	23	SER
8	H	25	ASP
8	H	26	VAL
8	H	29	SER
8	H	35	ILE
8	H	37	ARG
8	H	39	LEU
8	H	52	ASP

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Mol	Chain	Res	Type
8	H	53	VAL
8	H	60	ARG
8	H	63	LEU
8	H	65	TYR
8	H	68	ARG
8	H	74	PRO
8	H	79	VAL
8	H	82	HIS
8	H	83	ILE
8	H	84	ARG
8	H	88	LYS
8	H	91	ARG
8	H	92	ARG
8	H	94	TYR
8	H	104	ARG
8	H	112	LEU
8	H	116	LYS
8	H	121	ASP
8	H	122	ARG
8	H	127	LEU
8	H	133	LEU
9	I	3	GLN
9	I	12	GLU
9	I	14	VAL
9	I	19	LEU
9	I	29	ASN
9	I	31	GLN
9	I	40	LEU
9	I	42	ARG
9	I	48	GLU
9	I	50	LEU
9	I	53	VAL
9	I	54	ASP
9	I	59	PHE
9	I	62	TYR
9	I	63	ILE
9	I	64	THR
9	I	65	VAL
9	I	71	SER
9	I	79	LEU
9	I	90	PRO
9	I	93	ARG

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Mol	Chain	Res	Type
9	I	97	LYS
9	I	104	ARG
9	I	107	ARG
9	I	108	VAL
9	I	109	VAL
9	I	112	LYS
9	I	113	LYS
9	I	114	TYR
9	I	117	HIS
9	I	118	LYS
9	I	121	ARG
9	I	127	LYS
10	J	5	ARG
10	J	6	ILE
10	J	7	LYS
10	J	19	SER
10	J	33	GLN
10	J	38	ILE
10	J	44	VAL
10	J	45	ARG
10	J	46	ARG
10	J	49	VAL
10	J	61	GLU
10	J	65	LEU
10	J	66	ARG
10	J	67	THR
10	J	70	ARG
10	J	71	LEU
10	J	74	ILE
10	J	76	ASN
10	J	79	ARG
10	J	81	THR
10	J	85	LEU
10	J	87	THR
10	J	88	LEU
10	J	96	ILE
11	K	11	LYS
11	K	12	ARG
11	K	13	GLN
11	K	16	SER
11	K	18	ARG
11	K	29	ILE

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Mol	Chain	Res	Type
11	K	33	THR
11	K	36	ASP
11	K	40	ILE
11	K	48	ILE
11	K	53	SER
11	K	75	TYR
11	K	78	GLN
11	K	80	VAL
11	K	81	ASP
11	K	83	ILE
11	K	87	THR
11	K	91	ARG
11	K	92	GLU
11	K	93	GLN
11	K	96	ARG
11	K	98	LEU
11	K	101	SER
11	K	104	GLN
11	K	105	VAL
11	K	113	PRO
11	K	115	PRO
11	K	119	CYS
11	K	120	ARG
11	K	121	PRO
11	K	122	LYS
11	K	126	ARG
12	L	11	VAL
12	L	13	LYS
12	L	17	LYS
12	L	18	VAL
12	L	19	ARG
12	L	20	LYS
12	L	21	LYS
12	L	24	VAL
12	L	33	ARG
12	L	38	THR
12	L	41	ARG
12	L	43	VAL
12	L	44	THR
12	L	60	LEU
12	L	61	THR
12	L	76	ASN

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Mol	Chain	Res	Type
12	L	82	VAL
12	L	85	ILE
12	L	89	ARG
12	L	93	LEU
12	L	96	VAL
12	L	101	VAL
12	L	111	LYS
12	L	114	LYS
12	L	118	SER
12	L	122	THR
13	M	4	ILE
13	M	7	VAL
13	M	9	ILE
13	M	12	ASN
13	M	31	LYS
13	M	32	GLU
13	M	34	LEU
13	M	39	ILE
13	M	44	ARG
13	M	45	VAL
13	M	46	LYS
13	M	48	LEU
13	M	56	LEU
13	M	57	ARG
13	M	63	THR
13	M	66	LEU
13	M	79	LYS
13	M	80	ARG
13	M	83	ASP
13	M	84	ILE
13	M	93	ARG
13	M	94	ARG
13	M	96	LEU
13	M	99	ARG
13	M	106	ASN
13	M	109	THR
13	M	110	ARG
13	M	111	LYS
13	M	117	VAL
14	N	3	ARG
14	N	6	LEU
14	N	9	LYS

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Mol	Chain	Res	Type
14	N	19	ARG
14	N	22	THR
14	N	23	ARG
14	N	24	CYS
14	N	26	ARG
14	N	35	ARG
14	N	41	ARG
14	N	42	ILE
14	N	45	ARG
15	O	3	ILE
15	O	4	THR
15	O	5	LYS
15	O	6	GLU
15	O	9	GLN
15	O	10	LYS
15	O	13	GLN
15	O	22	THR
15	O	28	GLN
15	O	29	VAL
15	O	36	ILE
15	O	39	LEU
15	O	40	SER
15	O	41	GLU
15	O	47	LYS
15	O	53	HIS
15	O	57	LEU
15	O	63	ARG
15	O	65	ARG
15	O	67	LEU
15	O	70	LEU
15	O	71	GLN
15	O	72	ARG
15	O	75	PRO
15	O	81	LEU
15	O	82	ILE
15	O	83	GLU
15	O	84	LYS
16	P	1	MET
16	P	3	LYS
16	P	8	ARG
16	P	11	SER
16	P	18	ARG

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Mol	Chain	Res	Type
16	P	27	LYS
16	P	31	LYS
16	P	34	GLU
16	P	42	ARG
16	P	44	THR
16	P	54	GLU
16	P	55	ARG
16	P	61	SER
16	P	62	VAL
16	P	67	THR
16	P	71	ARG
16	P	75	ARG
16	P	76	GLN
16	P	81	ARG
17	Q	4	LYS
17	Q	6	LEU
17	Q	13	ASP
17	Q	15	MET
17	Q	22	LEU
17	Q	25	ARG
17	Q	29	HIS
17	Q	35	VAL
17	Q	36	ILE
17	Q	38	ARG
17	Q	43	LEU
17	Q	48	GLU
17	Q	50	LYS
17	Q	53	LEU
17	Q	59	ILE
17	Q	60	ILE
17	Q	63	ARG
17	Q	67	LYS
17	Q	68	ARG
17	Q	75	ARG
17	Q	77	VAL
17	Q	86	GLU
17	Q	88	TYR
17	Q	92	ARG
17	Q	95	TYR
18	R	22	VAL
18	R	35	ARG
18	R	42	ARG

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Mol	Chain	Res	Type
18	R	46	GLU
18	R	50	ILE
18	R	51	LEU
18	R	53	ARG
18	R	54	ARG
18	R	59	SER
18	R	64	ARG
18	R	69	THR
18	R	78	LEU
18	R	82	THR
18	R	84	LYS
18	R	85	LEU
18	R	86	VAL
18	R	87	ARG
18	R	88	LYS
19	S	3	ARG
19	S	5	LEU
19	S	6	LYS
19	S	7	LYS
19	S	15	LEU
19	S	16	LEU
19	S	17	GLU
19	S	20	LEU
19	S	22	LEU
19	S	33	THR
19	S	35	SER
19	S	39	THR
19	S	41	VAL
19	S	43	GLU
19	S	44	MET
19	S	58	VAL
19	S	64	GLU
19	S	65	ASN
19	S	71	LEU
19	S	77	THR
19	S	79	THR
19	S	80	TYR
20	T	10	LEU
20	T	11	SER
20	T	19	SER
20	T	22	ARG
20	T	23	ARG

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Mol	Chain	Res	Type
20	T	24	LEU
20	T	27	LYS
20	T	29	LYS
20	T	33	ILE
20	T	34	LYS
20	T	36	LEU
20	T	41	ILE
20	T	42	GLN
20	T	46	GLU
20	T	48	LYS
20	T	50	GLU
20	T	56	MET
20	T	57	ARG
20	T	62	LEU
20	T	68	LYS
20	T	72	LEU
20	T	75	ASN
20	T	80	ARG
20	T	83	ARG
20	T	91	LEU
20	T	104	LEU
21	U	6	ARG
21	U	8	THR
21	U	10	ARG
21	U	17	THR
21	U	24	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	108	ASN
4	D	43	HIS
5	E	78	HIS
8	H	78	GLN
9	I	124	GLN
10	J	68	HIS
11	K	38	ASN
13	M	106	ASN
15	O	28	GLN
20	T	16	HIS

## 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1509/1522 (99%)	443 (29%)	63 (4%)

All (443) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	4	U
1	A	9	G
1	A	12	U
1	A	16	A
1	A	30	U
1	A	31	G
1	A	32	A
1	A	33	A
1	A	39	G
1	A	44	G
1	A	45	U
1	A	47	C
1	A	48	C
1	A	50	A
1	A	51	A
1	A	54	C
1	A	58	C
1	A	73	C
1	A	81	U
1	A	82	U
1	A	83	U
1	A	97	G
1	A	101	A
1	A	105	G
1	A	108	G
1	A	116	A
1	A	121	C
1	A	122	G
1	A	123	C
1	A	127	G
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	163	C
1	A	176	C
1	A	182	U

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Mol	Chain	Res	Type
1	A	183	G
1	A	190	C
1	A	190(E)	U
1	A	190(I)	G
1	A	195	A
1	A	197	A
1	A	201	C
1	A	202	U
1	A	203	U
1	A	204	U
1	A	216	G
1	A	217	C
1	A	240	C
1	A	244	U
1	A	245	C
1	A	247	G
1	A	251	G
1	A	252	U
1	A	254	G
1	A	266	G
1	A	267	C
1	A	270	A
1	A	279	A
1	A	289	G
1	A	291	C
1	A	292	G
1	A	293	G
1	A	299	G
1	A	301	G
1	A	302	G
1	A	303	A
1	A	308	C
1	A	314	C
1	A	319	G
1	A	321	A
1	A	325	A
1	A	327	A
1	A	328	C
1	A	329	A
1	A	330	C
1	A	331	G
1	A	344	A

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Mol	Chain	Res	Type
1	A	345	C
1	A	350	G
1	A	351	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	355	C
1	A	356	A
1	A	367	U
1	A	372	C
1	A	373	A
1	A	381	C
1	A	383	A
1	A	384	G
1	A	390	C
1	A	397	A
1	A	398	C
1	A	406	G
1	A	409	G
1	A	412	A
1	A	413	G
1	A	421	U
1	A	423	G
1	A	424	G
1	A	429	U
1	A	430	A
1	A	433	C
1	A	434	U
1	A	439	A
1	A	446	G
1	A	452	A
1	A	453	A
1	A	454	C
1	A	458	C
1	A	460	A
1	A	462	G
1	A	484	G
1	A	485	G
1	A	496	A
1	A	497	A
1	A	498	U
1	A	500	G

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Mol	Chain	Res	Type
1	A	503	C
1	A	506	G
1	A	507	C
1	A	508	C
1	A	509	A
1	A	510	A
1	A	511	C
1	A	516	PSU
1	A	518	C
1	A	519	C
1	A	520	A
1	A	521	G
1	A	527	7MG
1	A	528	C
1	A	531	U
1	A	532	A
1	A	533	A
1	A	536	C
1	A	539	A
1	A	545	C
1	A	547	A
1	A	557	G
1	A	558	G
1	A	559	A
1	A	560	U
1	A	561	U
1	A	562	C
1	A	563	A
1	A	564	C
1	A	565	U
1	A	566	G
1	A	572	A
1	A	573	A
1	A	576	G
1	A	577	G
1	A	581	G
1	A	587	G
1	A	588	G
1	A	595	G
1	A	611	A
1	A	615	C
1	A	618	C

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Mol	Chain	Res	Type
1	A	642	A
1	A	645	C
1	A	653	A
1	A	658	G
1	A	662	G
1	A	664	G
1	A	665	A
1	A	666	G
1	A	682	G
1	A	684	A
1	A	686	U
1	A	687	A
1	A	688	G
1	A	695	A
1	A	700	G
1	A	701	C
1	A	702	A
1	A	705	U
1	A	715	A
1	A	716	A
1	A	717	C
1	A	720	C
1	A	721	G
1	A	722	A
1	A	723	U
1	A	724	G
1	A	731	G
1	A	733	A
1	A	742	G
1	A	744	C
1	A	749	C
1	A	753	A
1	A	755	G
1	A	759	A
1	A	760	G
1	A	764	C
1	A	765	G
1	A	775	G
1	A	777	A
1	A	779	C
1	A	781	A
1	A	787	A

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Mol	Chain	Res	Type
1	A	792	A
1	A	793	U
1	A	794	A
1	A	795	C
1	A	796	C
1	A	798	G
1	A	801	U
1	A	802	A
1	A	804	U
1	A	805	C
1	A	810	C
1	A	811	C
1	A	812	C
1	A	813	U
1	A	815	A
1	A	817	C
1	A	818	G
1	A	819	A
1	A	827	U
1	A	828	A
1	A	837	G
1	A	839	U
1	A	840	C
1	A	841	U
1	A	848	C
1	A	858	G
1	A	870	U
1	A	872	A
1	A	873	A
1	A	876	G
1	A	889	A
1	A	902	G
1	A	914	A
1	A	922	G
1	A	925	G
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	937	A
1	A	942	G
1	A	944	G

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Mol	Chain	Res	Type
1	A	960	U
1	A	963	G
1	A	966	M2G
1	A	969	A
1	A	971	G
1	A	972	C
1	A	973	G
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	980	C
1	A	992	U
1	A	993	G
1	A	994	A
1	A	1001	A
1	A	1003(A)	G
1	A	1004	A
1	A	1005	A
1	A	1011	G
1	A	1016	A
1	A	1020	U
1	A	1021	G
1	A	1024	G
1	A	1025	U
1	A	1026	G
1	A	1029	C
1	A	1031	G
1	A	1032	G
1	A	1034	G
1	A	1036	G
1	A	1037	C
1	A	1042	G
1	A	1043	C
1	A	1045	C
1	A	1046	A
1	A	1047	G
1	A	1050	G
1	A	1052	U
1	A	1055	A
1	A	1065	U
1	A	1066	C

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Mol	Chain	Res	Type
1	A	1070	U
1	A	1073	U
1	A	1077	G
1	A	1078	U
1	A	1094	G
1	A	1095	U
1	A	1096	C
1	A	1099	G
1	A	1101	A
1	A	1108	G
1	A	1109	C
1	A	1112	C
1	A	1118	C
1	A	1125	U
1	A	1126	U
1	A	1127	G
1	A	1129	C
1	A	1130	A
1	A	1131	G
1	A	1134	G
1	A	1135	U
1	A	1136	U
1	A	1137	C
1	A	1139	G
1	A	1140	C
1	A	1141	C
1	A	1145	C
1	A	1146	A
1	A	1147	C
1	A	1151	A
1	A	1152	A
1	A	1159	U
1	A	1162	C
1	A	1165	C
1	A	1168	A
1	A	1171	G
1	A	1172	C
1	A	1177	G
1	A	1178	G
1	A	1182	G
1	A	1183	A
1	A	1184	G

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Mol	Chain	Res	Type
1	A	1188	A
1	A	1189	C
1	A	1190	G
1	A	1191	A
1	A	1192	C
1	A	1195	C
1	A	1196	U
1	A	1197	G
1	A	1201	A
1	A	1202	G
1	A	1205	U
1	A	1211	U
1	A	1212	U
1	A	1213	A
1	A	1214	C
1	A	1217	C
1	A	1220	G
1	A	1224	G
1	A	1225	A
1	A	1226	C
1	A	1227	A
1	A	1228	C
1	A	1233	G
1	A	1238	A
1	A	1241	G
1	A	1246	C
1	A	1256	A
1	A	1257	U
1	A	1258	G
1	A	1259	C
1	A	1260	C
1	A	1266	G
1	A	1270	C
1	A	1278	U
1	A	1279	A
1	A	1280	A
1	A	1281	U
1	A	1285	A
1	A	1286	A
1	A	1287	A
1	A	1289	A
1	A	1300	G

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Mol	Chain	Res	Type
1	A	1301	U
1	A	1302	U
1	A	1303	C
1	A	1304	G
1	A	1305	G
1	A	1306	A
1	A	1312	G
1	A	1317	C
1	A	1319	A
1	A	1320	C
1	A	1322	C
1	A	1335	C
1	A	1336	C
1	A	1338	G
1	A	1340	A
1	A	1346	A
1	A	1347	G
1	A	1353	G
1	A	1355	G
1	A	1362	C
1	A	1363	A
1	A	1364	U
1	A	1368	G
1	A	1370	G
1	A	1377	A
1	A	1378	C
1	A	1379	G
1	A	1381	U
1	A	1382	C
1	A	1394	A
1	A	1397	C
1	A	1398	A
1	A	1400	5MC
1	A	1405	G
1	A	1411	C
1	A	1413	A
1	A	1417	G
1	A	1428	A
1	A	1437	C
1	A	1439	C
1	A	1442	G
1	A	1443	G

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Mol	Chain	Res	Type
1	A	1446	A
1	A	1447	G
1	A	1451	A
1	A	1453	G
1	A	1479	C
1	A	1483	A
1	A	1490	C
1	A	1491	G
1	A	1492	A
1	A	1493	A
1	A	1496	C
1	A	1497	G
1	A	1498	UR3
1	A	1499	A
1	A	1502	A
1	A	1503	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1510	U
1	A	1517	G
1	A	1520	G
1	A	1529	G
1	A	1530	G
1	A	1532	U
1	A	1533	C
1	A	1541	PSU
1	A	1542	U
1	A	1543	C

All (63) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	80	G
1	A	81	U
1	A	115	G
1	A	129(A)	G
1	A	181	G
1	A	190(E)	U
1	A	202	U
1	A	243	A
1	A	292	G

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Mol	Chain	Res	Type
1	A	330	C
1	A	372	C
1	A	428	G
1	A	429	U
1	A	484	G
1	A	497	A
1	A	506	G
1	A	509	A
1	A	518	C
1	A	530	G
1	A	531	U
1	A	532	A
1	A	559	A
1	A	560	U
1	A	641	U
1	A	686	U
1	A	687	A
1	A	701	C
1	A	748	C
1	A	793	U
1	A	812	C
1	A	913	A
1	A	992	U
1	A	1048	G
1	A	1054	C
1	A	1065	U
1	A	1125	U
1	A	1129	C
1	A	1139	G
1	A	1145	C
1	A	1181	G
1	A	1183	A
1	A	1189	C
1	A	1190	G
1	A	1195	C
1	A	1201	A
1	A	1212	U
1	A	1240	U
1	A	1256	A
1	A	1257	U
1	A	1285	A
1	A	1305	G

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Mol	Chain	Res	Type
1	A	1319	A
1	A	1335	C
1	A	1346	A
1	A	1380	U
1	A	1394	A
1	A	1443	G
1	A	1492	A
1	A	1496	C
1	A	1502	A
1	A	1505	G
1	A	1529	G
1	A	1532	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
1	5MC	A	967	1	15,22,23	1.44	2 (13%)	19,32,35	1.34	2 (10%)
1	5MC	A	1404	1	15,22,23	1.35	4 (26%)	19,32,35	1.14	2 (10%)
1	M2G	A	966	1	20,27,28	1.80	4 (20%)	22,40,43	3.80	9 (40%)
1	7MG	A	527	1	22,26,27	2.89	8 (36%)	28,39,42	2.00	9 (32%)
1	UR3	A	1498	1	14,22,23	2.38	5 (35%)	15,32,35	1.42	2 (13%)
1	PSU	A	1541	1	17,21,22	1.49	4 (23%)	20,30,33	3.33	7 (35%)
1	PSU	A	1540	1	17,21,22	1.22	1 (5%)	20,30,33	3.81	6 (30%)
1	MA6	A	1519	1	19,26,27	1.84	5 (26%)	18,38,41	1.55	1 (5%)
1	5MC	A	1407	1	15,22,23	2.68	5 (33%)	19,32,35	1.59	3 (15%)
1	PSU	A	516	1,23	17,21,22	1.73	5 (29%)	20,30,33	4.67	4 (20%)
1	MA6	A	1518	1	19,26,27	1.50	2 (10%)	18,38,41	1.91	3 (16%)
1	5MC	A	1400	1	15,22,23	1.72	4 (26%)	19,32,35	1.25	2 (10%)
1	4OC	A	1402	1	16,23,24	1.05	1 (6%)	17,32,35	1.13	1 (5%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	2MG	A	1207	1	19,26,27	2.01	4 (21%)	21,38,41	2.44	6 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	A	967	1	-	0/5/25/26	0/2/2/2
1	5MC	A	1404	1	-	0/5/25/26	0/2/2/2
1	M2G	A	966	1	-	6/7/29/30	0/3/3/3
1	7MG	A	527	1	-	2/7/37/38	0/3/3/3
1	UR3	A	1498	1	-	0/5/25/26	0/2/2/2
1	PSU	A	1541	1	-	0/7/25/26	0/2/2/2
1	PSU	A	1540	1	-	2/7/25/26	0/2/2/2
1	MA6	A	1519	1	-	3/7/29/30	0/3/3/3
1	5MC	A	1407	1	-	0/5/25/26	0/2/2/2
1	PSU	A	516	1,23	-	0/7/25/26	0/2/2/2
1	MA6	A	1518	1	-	3/7/29/30	0/3/3/3
1	5MC	A	1400	1	-	2/5/25/26	0/2/2/2
1	4OC	A	1402	1	-	4/9/29/30	0/2/2/2
1	2MG	A	1207	1	-	2/5/27/28	0/3/3/3

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1407	5MC	C5-C4	7.68	1.53	1.41
1	A	527	7MG	C2-N3	-6.43	1.24	1.35
1	A	527	7MG	C5-N7	6.42	1.50	1.39
1	A	1498	UR3	C4-N3	-5.90	1.29	1.38
1	A	1207	2MG	C6-C5	-5.86	1.31	1.41
1	A	527	7MG	C8-N9	-4.81	1.34	1.45
1	A	1400	5MC	C4-N3	-4.78	1.28	1.35
1	A	527	7MG	C6-C5	4.55	1.47	1.41
1	A	1498	UR3	C6-N1	-4.47	1.30	1.35
1	A	966	M2G	C2-N2	-4.43	1.27	1.34
1	A	1407	5MC	C4-N4	4.14	1.44	1.34
1	A	1540	PSU	C4-N3	4.05	1.40	1.33
1	A	516	PSU	C4-N3	3.90	1.39	1.33
1	A	527	7MG	C2-N1	-3.71	1.28	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1407	5MC	C6-C5	-3.55	1.30	1.40
1	A	1207	2MG	O6-C6	-3.53	1.15	1.24
1	A	967	5MC	C6-C5	-3.52	1.30	1.40
1	A	1541	PSU	C5-C1'	-3.43	1.49	1.52
1	A	966	M2G	C6-C5	3.42	1.47	1.41
1	A	527	7MG	C2-N2	3.39	1.40	1.33
1	A	516	PSU	C5-C1'	-3.34	1.49	1.52
1	A	516	PSU	O4'-C1'	-3.27	1.39	1.44
1	A	966	M2G	C4-N3	-3.27	1.30	1.35
1	A	1407	5MC	C4-N3	3.10	1.39	1.35
1	A	1519	MA6	C2'-C1'	-3.09	1.49	1.53
1	A	1207	2MG	CM2-N2	3.06	1.50	1.45
1	A	527	7MG	CM7-N7	-3.04	1.40	1.46
1	A	1498	UR3	O4-C4	-2.99	1.17	1.24
1	A	1541	PSU	C4-N3	2.94	1.38	1.33
1	A	1207	2MG	C2-N2	2.86	1.36	1.34
1	A	1541	PSU	O4'-C1'	-2.78	1.40	1.44
1	A	1400	5MC	C6-C5	-2.74	1.32	1.40
1	A	1541	PSU	C2'-C1'	-2.71	1.50	1.54
1	A	1407	5MC	C2-N3	2.71	1.43	1.38
1	A	1518	MA6	C2'-C1'	-2.69	1.49	1.53
1	A	1404	5MC	C6-C5	-2.65	1.32	1.40
1	A	1519	MA6	C2-N3	2.62	1.36	1.32
1	A	1519	MA6	C8-N7	2.52	1.39	1.34
1	A	516	PSU	C4-C5	-2.51	1.36	1.41
1	A	527	7MG	C4-N3	2.49	1.37	1.34
1	A	1400	5MC	C5-C4	2.41	1.45	1.41
1	A	1519	MA6	C2-N1	2.41	1.38	1.33
1	A	1518	MA6	C9-N6	-2.40	1.40	1.45
1	A	1404	5MC	CM5-C5	-2.40	1.46	1.51
1	A	1404	5MC	C4-N3	-2.31	1.31	1.35
1	A	1519	MA6	C9-N6	2.30	1.51	1.45
1	A	1498	UR3	C3U-N3	-2.15	1.42	1.47
1	A	1404	5MC	O5'-C5'	-2.13	1.39	1.44
1	A	1498	UR3	C6-C5	-2.12	1.33	1.38
1	A	967	5MC	C4-N3	2.11	1.38	1.35
1	A	966	M2G	C2-N1	2.11	1.38	1.34
1	A	1400	5MC	C4-N4	2.04	1.39	1.34
1	A	516	PSU	C6-N1	2.03	1.38	1.34
1	A	1402	4OC	O5'-C5'	-2.02	1.39	1.44

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	516	PSU	N1-C2-N3	-16.18	115.57	128.43
1	A	1540	PSU	N1-C2-N3	-11.86	119.00	128.43
1	A	1541	PSU	N1-C2-N3	-11.26	119.48	128.43
1	A	516	PSU	C4-N3-C2	11.19	124.59	115.14
1	A	966	M2G	C5-C6-N1	-10.70	108.80	123.43
1	A	966	M2G	N1-C2-N2	-9.43	107.64	117.19
1	A	1540	PSU	C4-N3-C2	8.97	122.72	115.14
1	A	1518	MA6	N1-C6-N6	-6.57	110.14	117.06
1	A	1540	PSU	C5-C4-N3	-6.17	117.41	125.36
1	A	1541	PSU	C4-N3-C2	5.90	120.12	115.14
1	A	1207	2MG	C5-C6-N1	-5.89	115.38	123.43
1	A	527	7MG	N7-C8-N9	5.15	110.75	103.38
1	A	966	M2G	C1'-N9-C4	5.03	135.48	126.64
1	A	1207	2MG	C4-C5-N7	4.86	114.46	109.40
1	A	1519	MA6	N1-C6-N6	-4.75	112.05	117.06
1	A	1407	5MC	CM5-C5-C4	4.69	126.47	121.72
1	A	966	M2G	C2-N3-C4	-4.67	109.97	115.28
1	A	966	M2G	C6-N1-C2	4.67	121.74	116.18
1	A	516	PSU	C5-C4-N3	-4.66	119.35	125.36
1	A	1207	2MG	N2-C2-N1	-4.60	112.55	116.96
1	A	1541	PSU	C5-C4-N3	-4.36	119.75	125.36
1	A	1207	2MG	N2-C2-N3	4.35	121.14	116.96
1	A	527	7MG	C6-C5-C4	-3.94	110.97	115.20
1	A	1400	5MC	N4-C4-N3	-3.87	111.56	117.03
1	A	1498	UR3	O3'-C3'-C2'	3.72	123.84	111.82
1	A	1402	4OC	CM4-N4-C4	-3.56	119.91	122.97
1	A	527	7MG	CM7-N7-C5	3.51	137.48	124.01
1	A	1518	MA6	C1'-N9-C4	-3.38	120.69	126.64
1	A	527	7MG	C6-N1-C2	3.32	121.20	115.93
1	A	1207	2MG	C6-N1-C2	3.20	120.92	115.18
1	A	966	M2G	C6-C5-C4	3.19	123.84	120.80
1	A	966	M2G	CM2-N2-C2	-3.16	118.28	121.29
1	A	527	7MG	C2-N3-C4	3.15	122.59	113.89
1	A	967	5MC	C5-C4-N3	3.09	126.14	121.26
1	A	1541	PSU	C6-N1-C2	3.09	120.46	115.36
1	A	1540	PSU	C4-C5-C1'	3.05	126.87	121.12
1	A	966	M2G	N3-C2-N2	2.99	120.22	117.18
1	A	1407	5MC	N4-C4-N3	-2.95	112.87	117.03
1	A	527	7MG	N2-C2-N1	2.92	121.79	117.25
1	A	1207	2MG	C2-N3-C4	-2.89	111.99	115.28
1	A	1498	UR3	O2'-C2'-C3'	2.83	120.98	111.82
1	A	1541	PSU	O2'-C2'-C1'	-2.77	105.35	111.94
1	A	516	PSU	C6-N1-C2	2.72	119.85	115.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1404	5MC	C5-C6-N1	-2.69	119.30	122.19
1	A	1541	PSU	C5-C6-N1	-2.66	121.17	124.44
1	A	527	7MG	N1-C2-N3	-2.41	121.63	125.42
1	A	1540	PSU	C6-N1-C2	2.40	119.33	115.36
1	A	527	7MG	O4'-C1'-N9	-2.38	106.14	109.35
1	A	1407	5MC	C6-N1-C1'	-2.36	113.94	119.24
1	A	1541	PSU	O4'-C1'-C5	-2.20	106.53	109.93
1	A	967	5MC	N4-C4-N3	-2.19	113.94	117.03
1	A	1540	PSU	O4'-C1'-C5	2.18	113.30	109.93
1	A	966	M2G	CM1-N2-C2	-2.14	119.25	121.29
1	A	1400	5MC	C2-N3-C4	2.06	118.51	116.02
1	A	527	7MG	C5-C4-N3	-2.06	123.13	126.49
1	A	1404	5MC	CM5-C5-C4	-2.04	119.66	121.72
1	A	1518	MA6	O2'-C2'-C1'	-2.02	103.40	110.85

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	527	7MG	O4'-C4'-C5'-O5'
1	A	527	7MG	C3'-C4'-C5'-O5'
1	A	1540	PSU	C2'-C1'-C5-C4
1	A	1540	PSU	C2'-C1'-C5-C6
1	A	1519	MA6	O4'-C4'-C5'-O5'
1	A	1519	MA6	C3'-C4'-C5'-O5'
1	A	1518	MA6	O4'-C4'-C5'-O5'
1	A	1518	MA6	C5-C6-N6-C10
1	A	1400	5MC	O4'-C4'-C5'-O5'
1	A	1402	4OC	C5-C4-N4-CM4
1	A	1207	2MG	N1-C2-N2-CM2
1	A	1207	2MG	N3-C2-N2-CM2
1	A	966	M2G	N1-C2-N2-CM1
1	A	966	M2G	O4'-C4'-C5'-O5'
1	A	966	M2G	C3'-C4'-C5'-O5'
1	A	1518	MA6	C3'-C4'-C5'-O5'
1	A	1400	5MC	C3'-C4'-C5'-O5'
1	A	1402	4OC	O4'-C4'-C5'-O5'
1	A	1402	4OC	C3'-C4'-C5'-O5'
1	A	966	M2G	N3-C2-N2-CM1
1	A	966	M2G	N1-C2-N2-CM2
1	A	1519	MA6	C4'-C5'-O5'-P
1	A	1402	4OC	N3-C4-N4-CM4

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Mol	Chain	Res	Type	Atoms
1	A	966	M2G	N3-C2-N2-CM2

There are no ring outliers.

14 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	967	5MC	3	0
1	A	1404	5MC	1	0
1	A	966	M2G	2	0
1	A	527	7MG	6	0
1	A	1498	UR3	3	0
1	A	1541	PSU	1	0
1	A	1540	PSU	2	0
1	A	1519	MA6	3	0
1	A	1407	5MC	1	0
1	A	516	PSU	2	0
1	A	1518	MA6	6	0
1	A	1400	5MC	1	0
1	A	1402	4OC	5	0
1	A	1207	2MG	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 417 ligands modelled in this entry, 416 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	$\# Z  > 2$
22	SRY	A	1601	-	40,42,42	2.32	10 (25%)	49,63,63	3.05	23 (46%)

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
22	SRY	A	1601	-	-	2/20/87/87	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	1601	SRY	CD1-N31	9.07	1.49	1.33
22	A	1601	SRY	CA1-N11	5.68	1.43	1.33
22	A	1601	SRY	C21-C11	-3.76	1.46	1.53
22	A	1601	SRY	C32-CG2	-3.75	1.46	1.52
22	A	1601	SRY	O53-C53	-3.19	1.36	1.44
22	A	1601	SRY	CD1-NE1	2.75	1.46	1.34
22	A	1601	SRY	CA1-NB1	2.74	1.46	1.34
22	A	1601	SRY	C23-N23	-2.72	1.42	1.47
22	A	1601	SRY	O32-C32	-2.46	1.40	1.44
22	A	1601	SRY	C11-N11	-2.36	1.42	1.45

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1601	SRY	O42-C42-C32	7.22	114.65	104.33
22	A	1601	SRY	O13-C13-C23	5.73	118.13	108.24
22	A	1601	SRY	O21-C21-C31	5.50	120.77	109.66
22	A	1601	SRY	CH2-C42-C32	-5.40	107.08	116.65
22	A	1601	SRY	O53-C13-C23	-5.02	100.78	110.58
22	A	1601	SRY	O41-C12-O42	-4.98	106.04	111.43
22	A	1601	SRY	O42-C12-C22	4.70	112.38	107.30
22	A	1601	SRY	C61-C51-C41	-4.53	99.35	109.68
22	A	1601	SRY	C12-O42-C42	-4.37	101.50	108.38
22	A	1601	SRY	C61-C11-C21	-4.37	102.02	110.78
22	A	1601	SRY	O61-C61-C11	4.26	118.26	109.66
22	A	1601	SRY	O32-C32-C22	4.20	121.35	111.62
22	A	1601	SRY	OG2-CG2-C32	-4.08	114.85	124.27
22	A	1601	SRY	O61-C61-C51	3.97	119.54	110.35
22	A	1601	SRY	C33-C43-C53	-3.92	103.25	110.24
22	A	1601	SRY	O41-C41-C51	3.82	117.43	107.28
22	A	1601	SRY	C13-C23-N23	3.41	117.11	111.00
22	A	1601	SRY	O43-C43-C33	3.29	117.94	110.35
22	A	1601	SRY	C21-C11-N11	-3.28	104.41	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1601	SRY	O33-C33-C43	2.60	116.36	110.35
22	A	1601	SRY	C13-O53-C53	-2.17	109.44	113.69
22	A	1601	SRY	C12-O41-C41	-2.08	112.81	117.96
22	A	1601	SRY	N31-CD1-NF1	2.06	124.19	120.59

There are no chirality outliers.

All (2) torsion outliers are listed below:

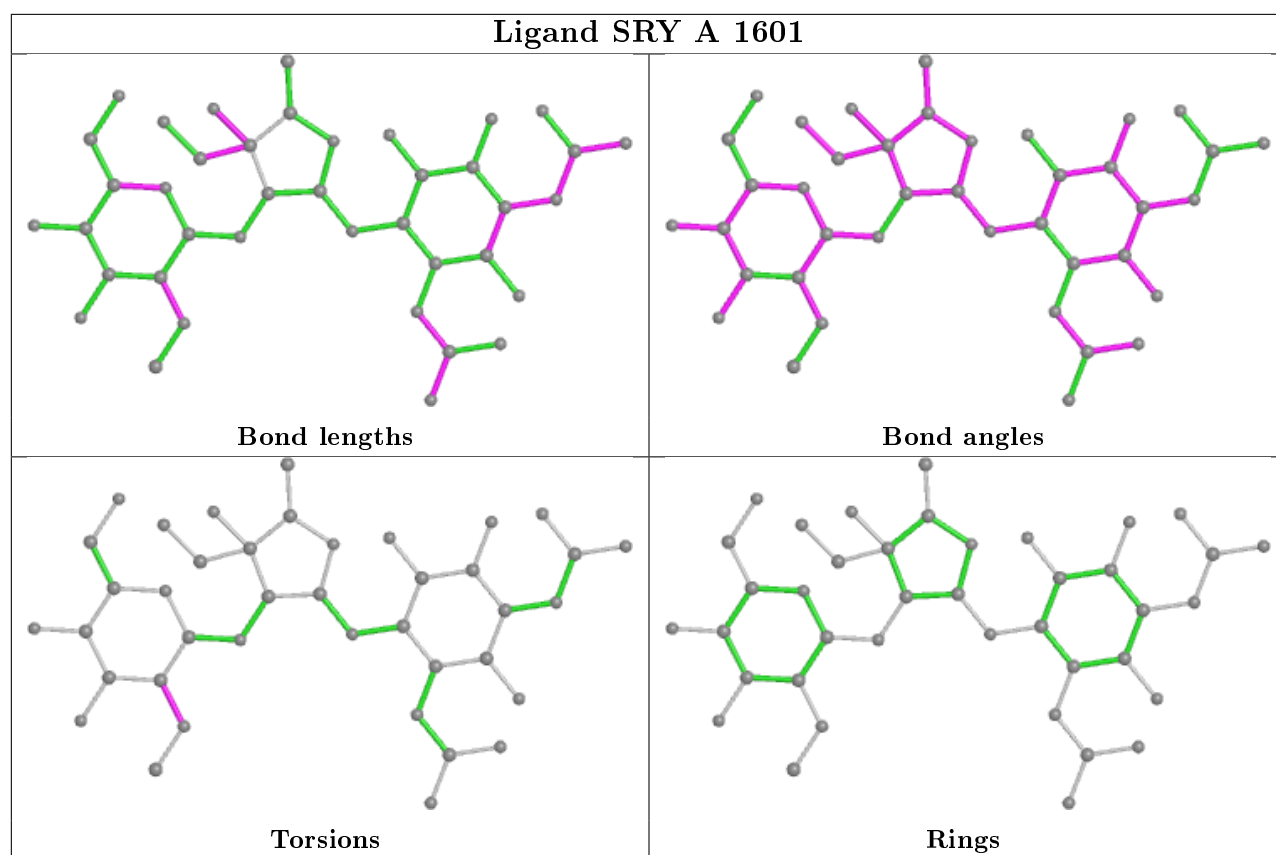
Mol	Chain	Res	Type	Atoms
22	A	1601	SRY	C13-C23-N23-CI3
22	A	1601	SRY	C33-C23-N23-CI3

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	1601	SRY	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	1500/1522 (98%)	-0.31	0 <b>100</b> <b>100</b>	98, 142, 223, 347	0
2	B	234/256 (91%)	-0.22	5 (2%) 63 57	114, 162, 231, 270	0
3	C	206/239 (86%)	-0.44	0 <b>100</b> <b>100</b>	124, 157, 201, 231	0
4	D	208/209 (99%)	-0.40	1 (0%) 91 89	103, 138, 185, 204	0
5	E	150/162 (92%)	-0.34	0 <b>100</b> <b>100</b>	89, 123, 168, 198	0
6	F	101/101 (100%)	-0.28	2 (1%) 65 59	119, 157, 191, 255	0
7	G	155/156 (99%)	-0.36	1 (0%) 89 87	134, 171, 213, 252	0
8	H	138/138 (100%)	-0.35	2 (1%) 75 70	98, 133, 174, 204	0
9	I	127/128 (99%)	-0.20	1 (0%) 86 83	138, 172, 220, 235	0
10	J	98/105 (93%)	0.03	0 <b>100</b> <b>100</b>	129, 177, 209, 245	0
11	K	116/129 (89%)	-0.16	2 (1%) 70 64	122, 156, 198, 213	0
12	L	124/135 (91%)	-0.08	1 (0%) 86 83	99, 120, 160, 208	0
13	M	118/126 (93%)	-0.03	2 (1%) 70 64	143, 181, 214, 246	0
14	N	60/61 (98%)	-0.24	0 <b>100</b> <b>100</b>	120, 158, 192, 261	0
15	O	87/89 (97%)	-0.42	0 <b>100</b> <b>100</b>	121, 156, 184, 221	0
16	P	83/88 (94%)	0.08	0 <b>100</b> <b>100</b>	113, 136, 172, 197	0
17	Q	99/105 (94%)	-0.10	1 (1%) 82 78	110, 137, 165, 179	0
18	R	70/88 (79%)	-0.30	0 <b>100</b> <b>100</b>	106, 162, 228, 315	0
19	S	80/93 (86%)	0.21	3 (3%) 40 34	153, 192, 236, 258	0
20	T	99/106 (93%)	-0.21	1 (1%) 82 78	104, 143, 190, 217	0
21	U	24/27 (88%)	0.25	1 (4%) 36 31	154, 187, 221, 234	0
All	All	3877/4063 (95%)	-0.26	23 (0%) <b>89</b> <b>87</b>	89, 149, 211, 347	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	M	7	VAL	3.5
2	B	134	GLU	3.2
2	B	132	LYS	3.2
19	S	32	LYS	2.9
20	T	106	ALA	2.8
2	B	122	PHE	2.6
19	S	33	THR	2.6
2	B	131	PRO	2.5
21	U	18	TYR	2.4
8	H	131	GLY	2.4
9	I	15	ALA	2.3
12	L	128	ALA	2.3
6	F	6	VAL	2.3
6	F	63	TYR	2.3
19	S	29	ARG	2.2
8	H	130	GLY	2.2
11	K	50	TYR	2.2
17	Q	43	LEU	2.1
11	K	19	ALA	2.1
2	B	125	PRO	2.1
7	G	78	ARG	2.1
13	M	4	ILE	2.0
4	D	36	ARG	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	PSU	A	1540	20/21	0.82	0.32	260,269,276,281	0
1	PSU	A	1541	20/21	0.86	0.19	232,239,263,263	0
1	MA6	A	1519	24/25	0.87	0.33	115,132,140,141	0
1	MA6	A	1518	24/25	0.88	0.26	125,140,146,183	0
1	5MC	A	1404	21/22	0.90	0.26	118,130,148,152	0
1	4OC	A	1402	22/23	0.93	0.26	124,133,143,146	0
1	2MG	A	1207	24/25	0.94	0.14	139,147,158,160	0
1	PSU	A	516	20/21	0.95	0.11	106,116,150,153	0
1	UR3	A	1498	21/22	0.95	0.27	120,127,140,141	0
1	5MC	A	1400	21/22	0.95	0.17	99,126,158,159	0
1	M2G	A	966	25/26	0.95	0.17	127,141,177,180	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	5MC	A	1407	21/22	0.95	0.14	122,135,143,146	0
1	5MC	A	967	21/22	0.96	0.19	134,151,163,167	0
1	7MG	A	527	24/25	0.97	0.18	105,114,120,122	0

## 6.3 Carbohydrates

There are no carbohydrates in this entry.

## 6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1986	1/1	0.08	0.80	156,156,156,156	0
23	MG	A	1988	1/1	0.09	0.35	141,141,141,141	0
23	MG	A	1745	1/1	0.12	0.36	119,119,119,119	0
23	MG	A	1739	1/1	0.12	0.77	150,150,150,150	0
23	MG	A	1925	1/1	0.15	0.38	493,493,493,493	0
23	MG	A	1717	1/1	0.20	0.96	112,112,112,112	0
23	MG	A	1889	1/1	0.24	0.23	463,463,463,463	0
23	MG	A	1795	1/1	0.27	1.55	538,538,538,538	0
23	MG	A	1860	1/1	0.36	0.25	507,507,507,507	0
23	MG	A	1663	1/1	0.38	0.36	114,114,114,114	0
23	MG	A	1987	1/1	0.42	0.73	134,134,134,134	0
23	MG	A	1602	1/1	0.43	0.62	138,138,138,138	0
23	MG	A	1733	1/1	0.48	0.28	134,134,134,134	0
23	MG	A	1919	1/1	0.48	0.24	501,501,501,501	0
23	MG	A	1989	1/1	0.50	0.49	123,123,123,123	0
23	MG	A	1648	1/1	0.52	0.18	133,133,133,133	0
23	MG	A	1798	1/1	0.53	0.12	501,501,501,501	0
23	MG	A	1653	1/1	0.55	0.38	193,193,193,193	0
23	MG	A	1843	1/1	0.56	0.14	464,464,464,464	0
23	MG	A	1891	1/1	0.56	0.22	449,449,449,449	0
23	MG	A	1815	1/1	0.58	0.88	535,535,535,535	0
23	MG	A	1857	1/1	0.59	0.27	550,550,550,550	0
23	MG	A	1947	1/1	0.59	0.71	484,484,484,484	0
23	MG	A	1681	1/1	0.59	0.71	122,122,122,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	D	302	1/1	0.60	0.30	103,103,103,103	0
23	MG	E	201	1/1	0.60	0.32	163,163,163,163	0
23	MG	Q	202	1/1	0.60	0.23	454,454,454,454	0
23	MG	A	1984	1/1	0.61	0.34	128,128,128,128	0
23	MG	A	1800	1/1	0.61	0.44	547,547,547,547	0
23	MG	A	1966	1/1	0.62	0.47	480,480,480,480	0
23	MG	A	1911	1/1	0.63	0.31	472,472,472,472	0
23	MG	A	1763	1/1	0.64	0.69	149,149,149,149	0
23	MG	A	1752	1/1	0.64	0.62	124,124,124,124	0
23	MG	A	1701	1/1	0.64	0.16	150,150,150,150	0
23	MG	A	1627	1/1	0.65	0.39	333,333,333,333	0
23	MG	A	1719	1/1	0.65	0.17	101,101,101,101	0
23	MG	A	1932	1/1	0.66	0.22	505,505,505,505	0
23	MG	A	1728	1/1	0.66	0.97	115,115,115,115	0
23	MG	A	1657	1/1	0.66	0.98	145,145,145,145	0
23	MG	A	1819	1/1	0.66	0.66	511,511,511,511	0
23	MG	A	1844	1/1	0.67	0.34	498,498,498,498	0
23	MG	A	1666	1/1	0.67	0.30	129,129,129,129	0
23	MG	A	1769	1/1	0.67	0.69	129,129,129,129	0
23	MG	A	1962	1/1	0.67	0.86	482,482,482,482	0
23	MG	A	1834	1/1	0.67	0.81	498,498,498,498	0
23	MG	A	1773	1/1	0.68	0.27	122,122,122,122	0
23	MG	A	1786	1/1	0.68	0.32	550,550,550,550	0
23	MG	A	1759	1/1	0.69	0.37	119,119,119,119	0
23	MG	A	1785	1/1	0.69	0.29	533,533,533,533	0
23	MG	E	203	1/1	0.70	0.56	116,116,116,116	0
23	MG	A	1702	1/1	0.70	1.13	112,112,112,112	0
23	MG	A	1983	1/1	0.70	0.31	153,153,153,153	0
23	MG	A	1787	1/1	0.71	0.25	508,508,508,508	0
23	MG	A	1776	1/1	0.71	0.41	550,550,550,550	0
23	MG	A	1814	1/1	0.71	1.03	550,550,550,550	0
23	MG	A	1828	1/1	0.72	0.39	542,542,542,542	0
23	MG	A	1923	1/1	0.72	0.47	550,550,550,550	0
23	MG	A	1961	1/1	0.72	0.42	473,473,473,473	0
23	MG	A	1624	1/1	0.73	0.38	120,120,120,120	0
23	MG	A	1697	1/1	0.73	0.97	121,121,121,121	0
23	MG	A	1718	1/1	0.73	0.63	140,140,140,140	0
23	MG	A	1829	1/1	0.73	0.37	438,438,438,438	0
23	MG	A	1691	1/1	0.74	1.23	130,130,130,130	0
23	MG	A	1772	1/1	0.74	0.69	174,174,174,174	0
23	MG	A	1732	1/1	0.74	0.37	138,138,138,138	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1855	1/1	0.74	0.55	467,467,467,467	0
23	MG	A	1704	1/1	0.75	0.71	121,121,121,121	0
23	MG	A	1824	1/1	0.75	0.41	446,446,446,446	0
23	MG	A	1943	1/1	0.75	0.63	476,476,476,476	0
23	MG	A	1664	1/1	0.75	0.47	118,118,118,118	0
23	MG	A	1784	1/1	0.76	0.14	501,501,501,501	0
23	MG	C	302	1/1	0.76	0.37	128,128,128,128	0
23	MG	A	1821	1/1	0.76	0.22	513,513,513,513	0
23	MG	A	1890	1/1	0.76	0.13	466,466,466,466	0
23	MG	A	1895	1/1	0.76	0.17	483,483,483,483	0
23	MG	A	1846	1/1	0.77	0.37	550,550,550,550	0
23	MG	A	1665	1/1	0.77	0.29	246,246,246,246	0
23	MG	A	1856	1/1	0.77	0.87	530,530,530,530	0
23	MG	A	1942	1/1	0.77	1.10	550,550,550,550	0
23	MG	Q	201	1/1	0.77	0.55	81,81,81,81	0
23	MG	A	1936	1/1	0.77	0.86	502,502,502,502	0
23	MG	A	1868	1/1	0.77	0.38	510,510,510,510	0
23	MG	A	1802	1/1	0.77	0.29	469,469,469,469	0
23	MG	A	1659	1/1	0.78	0.52	117,117,117,117	0
23	MG	A	1971	1/1	0.78	0.09	278,278,278,278	0
23	MG	A	1944	1/1	0.78	0.61	488,488,488,488	0
23	MG	A	1770	1/1	0.78	0.71	112,112,112,112	0
23	MG	A	1638	1/1	0.78	0.40	321,321,321,321	0
23	MG	A	1637	1/1	0.78	0.45	126,126,126,126	0
23	MG	A	1647	1/1	0.79	0.33	101,101,101,101	0
23	MG	A	1894	1/1	0.79	0.21	420,420,420,420	0
23	MG	A	1774	1/1	0.80	0.56	129,129,129,129	0
23	MG	A	1779	1/1	0.80	0.07	416,416,416,416	0
23	MG	A	1731	1/1	0.80	0.46	107,107,107,107	0
23	MG	A	1905	1/1	0.80	0.29	523,523,523,523	0
23	MG	A	1813	1/1	0.80	0.11	368,368,368,368	0
23	MG	A	1896	1/1	0.80	0.21	507,507,507,507	0
23	MG	A	1922	1/1	0.80	0.47	501,501,501,501	0
23	MG	A	1812	1/1	0.80	0.05	445,445,445,445	0
23	MG	A	1783	1/1	0.80	0.28	490,490,490,490	0
23	MG	A	1678	1/1	0.80	0.32	138,138,138,138	0
23	MG	A	1714	1/1	0.80	0.35	131,131,131,131	0
23	MG	A	1623	1/1	0.80	0.38	171,171,171,171	0
23	MG	A	1764	1/1	0.81	0.58	158,158,158,158	0
23	MG	A	1958	1/1	0.81	0.37	508,508,508,508	0
23	MG	A	1741	1/1	0.81	0.13	140,140,140,140	0
23	MG	A	1792	1/1	0.82	0.23	383,383,383,383	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1849	1/1	0.82	0.21	482,482,482,482	0
23	MG	A	1690	1/1	0.82	0.13	244,244,244,244	0
23	MG	A	1836	1/1	0.83	0.63	475,475,475,475	0
23	MG	S	101	1/1	0.83	0.29	123,123,123,123	0
23	MG	A	1830	1/1	0.83	0.31	439,439,439,439	0
23	MG	A	1679	1/1	0.83	0.07	170,170,170,170	0
23	MG	A	1618	1/1	0.83	0.19	104,104,104,104	0
23	MG	A	1893	1/1	0.83	0.36	319,319,319,319	0
23	MG	A	1699	1/1	0.83	0.44	119,119,119,119	0
23	MG	A	1696	1/1	0.83	0.84	157,157,157,157	0
23	MG	A	1655	1/1	0.84	0.22	155,155,155,155	0
23	MG	A	1809	1/1	0.84	0.18	492,492,492,492	0
23	MG	A	1721	1/1	0.84	0.55	125,125,125,125	0
23	MG	A	1683	1/1	0.84	0.41	145,145,145,145	0
23	MG	A	1751	1/1	0.84	0.41	80,80,80,80	0
23	MG	A	1801	1/1	0.84	1.43	550,550,550,550	0
23	MG	A	1794	1/1	0.84	0.20	458,458,458,458	0
23	MG	A	1768	1/1	0.84	0.44	152,152,152,152	0
23	MG	A	1823	1/1	0.85	0.09	334,334,334,334	0
23	MG	A	1850	1/1	0.85	0.41	416,416,416,416	0
23	MG	A	1970	1/1	0.85	0.48	354,354,354,354	0
23	MG	A	1724	1/1	0.85	0.30	107,107,107,107	0
23	MG	A	1737	1/1	0.85	0.38	142,142,142,142	0
23	MG	A	1976	1/1	0.85	1.33	124,124,124,124	0
23	MG	A	1827	1/1	0.85	0.18	533,533,533,533	0
23	MG	A	1952	1/1	0.85	0.24	475,475,475,475	0
23	MG	A	1788	1/1	0.85	0.42	550,550,550,550	0
23	MG	A	1825	1/1	0.85	0.45	506,506,506,506	0
23	MG	D	303	1/1	0.85	0.16	136,136,136,136	0
23	MG	P	101	1/1	0.86	0.36	104,104,104,104	0
23	MG	D	307	1/1	0.86	0.25	511,511,511,511	0
23	MG	A	1630	1/1	0.86	0.24	112,112,112,112	0
23	MG	A	1668	1/1	0.86	0.33	177,177,177,177	0
23	MG	A	1903	1/1	0.86	0.19	480,480,480,480	0
23	MG	N	102	1/1	0.87	0.57	127,127,127,127	0
23	MG	A	1883	1/1	0.87	0.20	512,512,512,512	0
23	MG	A	1610	1/1	0.87	0.16	136,136,136,136	0
23	MG	A	1937	1/1	0.87	0.68	438,438,438,438	0
23	MG	A	1933	1/1	0.87	0.08	451,451,451,451	0
23	MG	A	1680	1/1	0.87	0.26	118,118,118,118	0
23	MG	A	1662	1/1	0.87	0.27	158,158,158,158	0
23	MG	A	1743	1/1	0.87	0.27	128,128,128,128	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1924	1/1	0.87	0.21	496,496,496,496	0
23	MG	A	1626	1/1	0.87	1.80	125,125,125,125	0
23	MG	A	1867	1/1	0.87	0.15	411,411,411,411	0
23	MG	A	1622	1/1	0.87	0.76	86,86,86,86	0
23	MG	A	1634	1/1	0.87	0.18	141,141,141,141	0
23	MG	A	1700	1/1	0.87	0.39	114,114,114,114	0
23	MG	A	1673	1/1	0.88	0.23	89,89,89,89	0
23	MG	A	1740	1/1	0.88	0.36	128,128,128,128	0
23	MG	A	1693	1/1	0.88	0.26	143,143,143,143	0
23	MG	A	1837	1/1	0.88	1.25	550,550,550,550	0
23	MG	A	1847	1/1	0.88	0.19	457,457,457,457	0
23	MG	A	1606	1/1	0.88	0.34	105,105,105,105	0
23	MG	A	1938	1/1	0.88	0.13	433,433,433,433	0
23	MG	A	1804	1/1	0.88	0.13	314,314,314,314	0
23	MG	A	1845	1/1	0.88	0.42	458,458,458,458	0
23	MG	A	1756	1/1	0.88	0.46	165,165,165,165	0
23	MG	A	1880	1/1	0.88	0.14	541,541,541,541	0
23	MG	A	1735	1/1	0.88	0.63	132,132,132,132	0
23	MG	A	1675	1/1	0.89	0.36	141,141,141,141	0
23	MG	A	1884	1/1	0.89	0.48	504,504,504,504	0
23	MG	A	1730	1/1	0.89	0.30	95,95,95,95	0
23	MG	A	1899	1/1	0.89	0.09	453,453,453,453	0
23	MG	A	1807	1/1	0.89	0.10	451,451,451,451	0
23	MG	A	1793	1/1	0.89	0.20	508,508,508,508	0
23	MG	A	1608	1/1	0.89	0.18	316,316,316,316	0
23	MG	A	1755	1/1	0.89	0.21	161,161,161,161	0
23	MG	A	1949	1/1	0.89	0.50	474,474,474,474	0
23	MG	A	1940	1/1	0.89	0.78	499,499,499,499	0
23	MG	A	1981	1/1	0.89	0.23	118,118,118,118	0
23	MG	A	1914	1/1	0.89	0.64	525,525,525,525	0
23	MG	C	301	1/1	0.89	0.26	125,125,125,125	0
23	MG	A	1709	1/1	0.89	0.66	107,107,107,107	0
23	MG	A	1854	1/1	0.89	0.45	541,541,541,541	0
23	MG	A	1985	1/1	0.89	0.54	107,107,107,107	0
23	MG	A	1960	1/1	0.89	0.41	404,404,404,404	0
23	MG	A	1688	1/1	0.90	0.18	114,114,114,114	0
23	MG	D	305	1/1	0.90	0.11	437,437,437,437	0
23	MG	A	1969	1/1	0.90	0.63	456,456,456,456	0
23	MG	A	1865	1/1	0.90	0.19	358,358,358,358	0
23	MG	A	1650	1/1	0.90	0.35	155,155,155,155	0
23	MG	B	303	1/1	0.90	0.18	111,111,111,111	0
23	MG	A	1839	1/1	0.90	0.24	484,484,484,484	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1727	1/1	0.90	0.24	91,91,91,91	0
23	MG	A	1886	1/1	0.90	0.35	461,461,461,461	0
23	MG	A	1863	1/1	0.90	0.27	514,514,514,514	0
23	MG	A	1873	1/1	0.90	0.26	509,509,509,509	0
23	MG	A	1660	1/1	0.90	0.23	118,118,118,118	0
23	MG	C	303	1/1	0.90	0.06	495,495,495,495	0
23	MG	A	1851	1/1	0.90	0.23	475,475,475,475	0
23	MG	A	1980	1/1	0.90	0.16	419,419,419,419	0
23	MG	A	1736	1/1	0.90	0.11	120,120,120,120	0
23	MG	A	1871	1/1	0.90	0.38	401,401,401,401	0
23	MG	A	1791	1/1	0.90	0.14	472,472,472,472	0
23	MG	A	1975	1/1	0.91	0.64	138,138,138,138	0
23	MG	A	1918	1/1	0.91	0.22	446,446,446,446	0
23	MG	A	1780	1/1	0.91	0.17	522,522,522,522	0
23	MG	A	1782	1/1	0.91	0.16	471,471,471,471	0
23	MG	A	1698	1/1	0.91	0.07	281,281,281,281	0
23	MG	A	1835	1/1	0.91	0.75	517,517,517,517	0
23	MG	A	1861	1/1	0.91	0.46	534,534,534,534	0
23	MG	A	1881	1/1	0.91	0.28	466,466,466,466	0
23	MG	A	1742	1/1	0.91	0.34	134,134,134,134	0
23	MG	A	1870	1/1	0.91	0.28	497,497,497,497	0
23	MG	A	1826	1/1	0.91	0.21	456,456,456,456	0
23	MG	A	1799	1/1	0.91	0.20	440,440,440,440	0
23	MG	A	1902	1/1	0.91	0.11	452,452,452,452	0
23	MG	A	1892	1/1	0.91	0.22	450,450,450,450	0
23	MG	A	1621	1/1	0.91	0.24	143,143,143,143	0
23	MG	D	306	1/1	0.91	0.26	421,421,421,421	0
23	MG	A	1910	1/1	0.91	0.39	398,398,398,398	0
23	MG	A	1803	1/1	0.92	0.79	507,507,507,507	0
23	MG	A	1760	1/1	0.92	0.07	261,261,261,261	0
23	MG	B	302	1/1	0.92	0.10	136,136,136,136	0
23	MG	A	1906	1/1	0.92	0.23	449,449,449,449	0
23	MG	A	1716	1/1	0.92	0.29	110,110,110,110	0
23	MG	A	1757	1/1	0.92	0.31	136,136,136,136	0
23	MG	A	1642	1/1	0.92	0.16	98,98,98,98	0
23	MG	A	1874	1/1	0.92	0.81	422,422,422,422	0
23	MG	A	1876	1/1	0.92	0.45	512,512,512,512	0
23	MG	A	1885	1/1	0.92	0.23	498,498,498,498	0
23	MG	A	1862	1/1	0.92	0.15	412,412,412,412	0
23	MG	A	1818	1/1	0.92	0.46	467,467,467,467	0
23	MG	A	1671	1/1	0.92	1.04	217,217,217,217	0
23	MG	A	1636	1/1	0.92	0.07	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1661	1/1	0.92	0.18	157,157,157,157	0
23	MG	A	1744	1/1	0.92	0.10	137,137,137,137	0
23	MG	A	1864	1/1	0.92	0.17	393,393,393,393	0
23	MG	A	1898	1/1	0.92	0.85	512,512,512,512	0
23	MG	A	1921	1/1	0.92	0.19	502,502,502,502	0
23	MG	A	1790	1/1	0.92	0.32	499,499,499,499	0
23	MG	A	1753	1/1	0.93	0.15	104,104,104,104	0
23	MG	A	1972	1/1	0.93	0.16	336,336,336,336	0
23	MG	A	1878	1/1	0.93	0.19	437,437,437,437	0
23	MG	L	201	1/1	0.93	0.24	405,405,405,405	0
23	MG	A	1811	1/1	0.93	0.24	509,509,509,509	0
23	MG	A	1692	1/1	0.93	0.28	132,132,132,132	0
23	MG	O	1001	1/1	0.93	0.23	298,298,298,298	0
23	MG	A	1956	1/1	0.93	0.12	384,384,384,384	0
23	MG	A	1852	1/1	0.93	0.25	462,462,462,462	0
23	MG	A	1820	1/1	0.93	0.49	469,469,469,469	0
23	MG	A	1816	1/1	0.93	0.09	418,418,418,418	0
23	MG	E	202	1/1	0.93	0.12	146,146,146,146	0
23	MG	A	1729	1/1	0.93	0.24	100,100,100,100	0
23	MG	A	1806	1/1	0.93	0.11	432,432,432,432	0
23	MG	A	1754	1/1	0.93	0.26	125,125,125,125	0
23	MG	A	1950	1/1	0.93	0.28	222,222,222,222	0
23	MG	A	1916	1/1	0.94	0.26	503,503,503,503	0
23	MG	A	1838	1/1	0.94	0.16	449,449,449,449	0
23	MG	A	1619	1/1	0.94	0.09	100,100,100,100	0
23	MG	A	1897	1/1	0.94	0.28	505,505,505,505	0
22	SRY	A	1601	40/40	0.94	0.21	90,115,122,132	0
23	MG	A	1734	1/1	0.94	0.45	118,118,118,118	0
23	MG	H	201	1/1	0.94	0.32	465,465,465,465	0
23	MG	C	304	1/1	0.94	0.10	533,533,533,533	0
23	MG	A	1900	1/1	0.94	0.17	404,404,404,404	0
23	MG	A	1904	1/1	0.94	0.11	421,421,421,421	0
23	MG	A	1631	1/1	0.94	0.51	290,290,290,290	0
23	MG	A	1667	1/1	0.94	0.20	152,152,152,152	0
23	MG	A	1877	1/1	0.94	0.16	465,465,465,465	0
23	MG	A	1797	1/1	0.94	0.37	472,472,472,472	0
23	MG	A	1982	1/1	0.94	0.28	150,150,150,150	0
23	MG	A	1926	1/1	0.94	0.29	537,537,537,537	0
23	MG	A	1853	1/1	0.94	0.18	407,407,407,407	0
23	MG	A	1833	1/1	0.94	0.15	409,409,409,409	0
23	MG	A	1639	1/1	0.94	0.42	125,125,125,125	0
23	MG	D	304	1/1	0.94	0.14	550,550,550,550	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1808	1/1	0.94	0.17	510,510,510,510	0
23	MG	A	1810	1/1	0.94	0.24	514,514,514,514	0
23	MG	A	1771	1/1	0.94	0.50	124,124,124,124	0
23	MG	A	1908	1/1	0.94	0.19	442,442,442,442	0
23	MG	B	301	1/1	0.94	0.33	103,103,103,103	0
23	MG	A	1703	1/1	0.94	0.22	152,152,152,152	0
23	MG	A	1723	1/1	0.94	0.09	95,95,95,95	0
23	MG	A	1765	1/1	0.94	0.33	111,111,111,111	0
23	MG	A	1617	1/1	0.94	0.26	122,122,122,122	0
23	MG	A	1945	1/1	0.94	0.12	446,446,446,446	0
23	MG	A	1625	1/1	0.94	0.20	135,135,135,135	0
23	MG	A	1990	1/1	0.94	0.14	116,116,116,116	0
23	MG	A	1640	1/1	0.94	0.29	87,87,87,87	0
23	MG	A	1789	1/1	0.94	0.20	425,425,425,425	0
23	MG	A	1927	1/1	0.94	0.10	460,460,460,460	0
23	MG	A	1887	1/1	0.95	0.52	376,376,376,376	0
23	MG	A	1738	1/1	0.95	0.11	143,143,143,143	0
23	MG	A	1682	1/1	0.95	0.23	147,147,147,147	0
23	MG	A	1609	1/1	0.95	0.23	138,138,138,138	0
23	MG	A	1762	1/1	0.95	0.18	453,453,453,453	0
23	MG	A	1707	1/1	0.95	0.30	113,113,113,113	0
23	MG	A	1614	1/1	0.95	0.59	195,195,195,195	0
23	MG	A	1750	1/1	0.95	0.26	109,109,109,109	0
23	MG	A	1651	1/1	0.95	0.23	149,149,149,149	0
23	MG	A	1613	1/1	0.95	0.24	85,85,85,85	0
23	MG	A	1674	1/1	0.95	0.16	159,159,159,159	0
23	MG	A	1832	1/1	0.95	0.09	178,178,178,178	0
23	MG	A	1615	1/1	0.95	0.12	123,123,123,123	0
23	MG	A	1796	1/1	0.95	0.34	536,536,536,536	0
23	MG	A	1954	1/1	0.95	0.26	509,509,509,509	0
23	MG	A	1635	1/1	0.95	0.25	99,99,99,99	0
23	MG	A	1777	1/1	0.95	0.20	459,459,459,459	0
23	MG	A	1948	1/1	0.95	0.14	266,266,266,266	0
23	MG	A	1953	1/1	0.95	0.28	430,430,430,430	0
23	MG	A	1963	1/1	0.95	0.86	361,361,361,361	0
23	MG	A	1917	1/1	0.96	0.39	506,506,506,506	0
23	MG	A	1934	1/1	0.96	0.54	462,462,462,462	0
23	MG	A	1715	1/1	0.96	0.35	118,118,118,118	0
23	MG	A	1841	1/1	0.96	0.24	463,463,463,463	0
23	MG	A	1712	1/1	0.96	0.27	127,127,127,127	0
23	MG	A	1641	1/1	0.96	0.09	104,104,104,104	0
23	MG	A	1620	1/1	0.96	1.06	118,118,118,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1920	1/1	0.96	0.10	498,498,498,498	0
23	MG	A	1875	1/1	0.96	0.08	336,336,336,336	0
23	MG	A	1842	1/1	0.96	0.15	448,448,448,448	0
23	MG	A	1935	1/1	0.96	0.04	306,306,306,306	0
23	MG	A	1761	1/1	0.96	0.14	234,234,234,234	0
23	MG	A	1711	1/1	0.96	0.18	122,122,122,122	0
23	MG	A	1817	1/1	0.96	0.05	549,549,549,549	0
23	MG	A	1882	1/1	0.96	0.87	508,508,508,508	0
23	MG	A	1689	1/1	0.96	0.12	282,282,282,282	0
23	MG	A	1866	1/1	0.96	0.15	408,408,408,408	0
23	MG	A	1708	1/1	0.96	0.19	102,102,102,102	0
23	MG	A	1831	1/1	0.96	0.51	490,490,490,490	0
23	MG	A	1965	1/1	0.96	0.19	467,467,467,467	0
23	MG	A	1633	1/1	0.96	0.36	149,149,149,149	0
23	MG	A	1901	1/1	0.97	0.18	468,468,468,468	0
23	MG	A	1955	1/1	0.97	0.07	364,364,364,364	0
23	MG	A	1669	1/1	0.97	0.05	109,109,109,109	0
23	MG	A	1951	1/1	0.97	0.09	222,222,222,222	0
23	MG	A	1748	1/1	0.97	0.24	120,120,120,120	0
23	MG	A	1912	1/1	0.97	0.22	477,477,477,477	0
23	MG	A	1767	1/1	0.97	0.21	107,107,107,107	0
23	MG	A	1968	1/1	0.97	0.19	433,433,433,433	0
23	MG	A	1781	1/1	0.97	0.05	237,237,237,237	0
23	MG	A	1646	1/1	0.97	0.26	127,127,127,127	0
23	MG	A	1778	1/1	0.97	0.21	499,499,499,499	0
23	MG	A	1859	1/1	0.97	0.17	467,467,467,467	0
23	MG	A	1977	1/1	0.97	0.10	159,159,159,159	0
23	MG	A	1967	1/1	0.97	0.15	309,309,309,309	0
23	MG	A	1706	1/1	0.97	0.08	78,78,78,78	0
23	MG	A	1964	1/1	0.97	0.36	492,492,492,492	0
23	MG	A	1931	1/1	0.97	0.62	510,510,510,510	0
23	MG	A	1930	1/1	0.97	0.38	404,404,404,404	0
23	MG	A	1720	1/1	0.97	0.45	162,162,162,162	0
23	MG	A	1915	1/1	0.97	0.60	492,492,492,492	0
23	MG	A	1725	1/1	0.97	0.28	118,118,118,118	0
23	MG	A	1644	1/1	0.97	0.36	116,116,116,116	0
23	MG	A	1946	1/1	0.97	0.16	525,525,525,525	0
23	MG	A	1749	1/1	0.97	0.13	173,173,173,173	0
23	MG	A	1879	1/1	0.97	0.20	451,451,451,451	0
23	MG	A	1684	1/1	0.97	0.37	130,130,130,130	0
23	MG	A	1941	1/1	0.98	1.71	549,549,549,549	0
23	MG	A	1909	1/1	0.98	0.32	400,400,400,400	0

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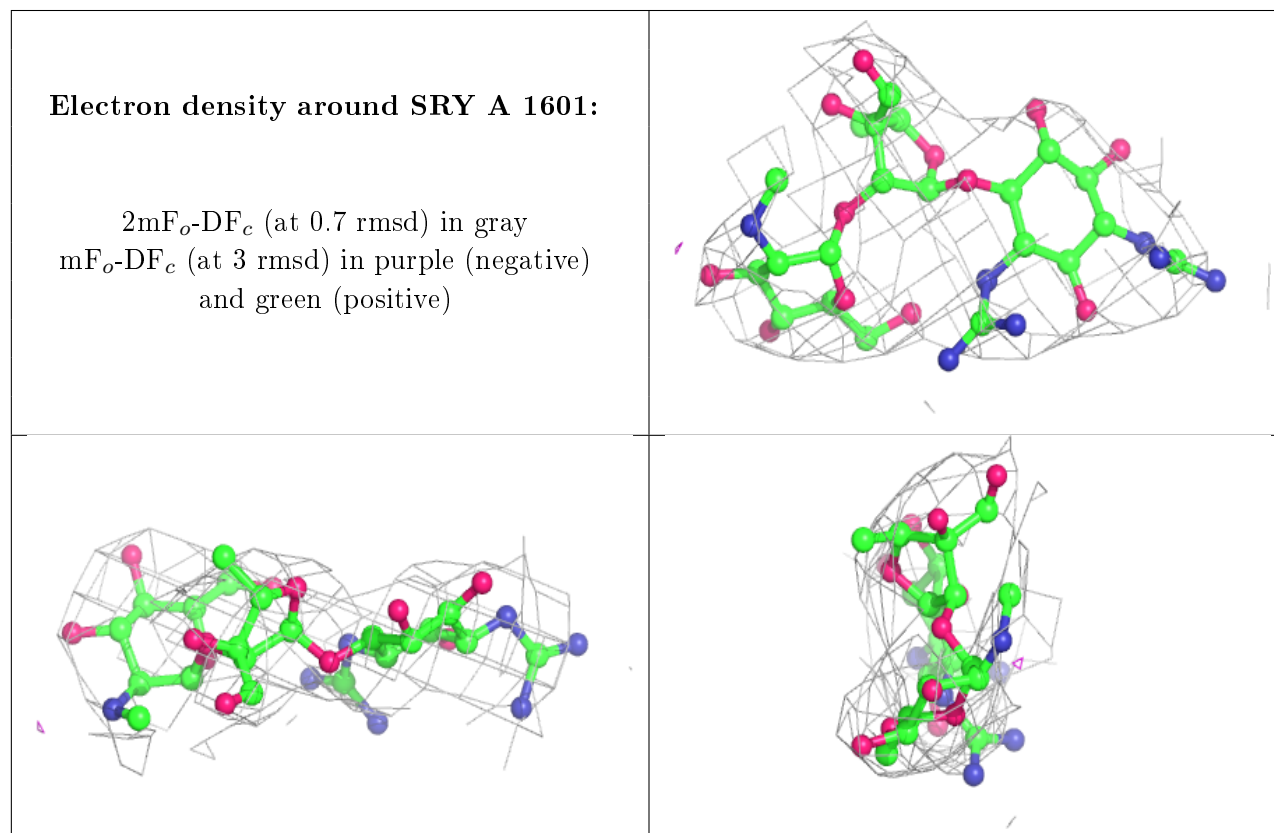
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1822	1/1	0.98	0.09	541,541,541,541	0
23	MG	A	1722	1/1	0.98	0.24	115,115,115,115	0
23	MG	A	1888	1/1	0.98	0.21	264,264,264,264	0
23	MG	A	1649	1/1	0.98	0.15	117,117,117,117	0
23	MG	A	1676	1/1	0.98	0.13	142,142,142,142	0
23	MG	A	1974	1/1	0.98	0.25	136,136,136,136	0
23	MG	A	1605	1/1	0.98	0.03	169,169,169,169	0
23	MG	A	1840	1/1	0.98	0.09	247,247,247,247	0
23	MG	A	1616	1/1	0.98	0.12	168,168,168,168	0
23	MG	A	1645	1/1	0.98	0.22	107,107,107,107	0
23	MG	F	201	1/1	0.98	0.13	438,438,438,438	0
23	MG	A	1913	1/1	0.98	0.55	550,550,550,550	0
23	MG	A	1705	1/1	0.98	0.16	151,151,151,151	0
23	MG	A	1858	1/1	0.98	0.41	459,459,459,459	0
23	MG	A	1848	1/1	0.98	0.14	418,418,418,418	0
23	MG	A	1805	1/1	0.98	0.22	316,316,316,316	0
23	MG	A	1710	1/1	0.98	0.13	89,89,89,89	0
23	MG	A	1747	1/1	0.98	0.08	103,103,103,103	0
23	MG	A	1654	1/1	0.98	0.10	113,113,113,113	0
23	MG	A	1907	1/1	0.98	0.24	475,475,475,475	0
23	MG	A	1775	1/1	0.98	0.29	152,152,152,152	0
23	MG	A	1656	1/1	0.98	0.16	163,163,163,163	0
23	MG	A	1766	1/1	0.98	0.09	118,118,118,118	0
23	MG	A	1632	1/1	0.98	0.15	119,119,119,119	0
23	MG	A	1726	1/1	0.98	0.21	106,106,106,106	0
23	MG	A	1672	1/1	0.98	0.14	160,160,160,160	0
23	MG	A	1713	1/1	0.99	0.26	129,129,129,129	0
23	MG	A	1686	1/1	0.99	0.19	194,194,194,194	0
23	MG	A	1929	1/1	0.99	0.52	458,458,458,458	0
23	MG	A	1957	1/1	0.99	0.15	379,379,379,379	0
23	MG	A	1612	1/1	0.99	0.15	145,145,145,145	0
23	MG	A	1978	1/1	0.99	0.16	229,229,229,229	0
23	MG	A	1643	1/1	0.99	0.13	90,90,90,90	0
23	MG	A	1928	1/1	0.99	0.25	455,455,455,455	0
23	MG	A	1869	1/1	0.99	0.07	414,414,414,414	0
23	MG	A	1973	1/1	0.99	0.35	442,442,442,442	0
23	MG	A	1694	1/1	0.99	0.88	413,413,413,413	0
23	MG	A	1758	1/1	0.99	0.14	95,95,95,95	0
23	MG	A	1677	1/1	0.99	0.14	93,93,93,93	0
23	MG	A	1746	1/1	0.99	0.65	74,74,74,74	0
23	MG	A	1695	1/1	0.99	0.17	113,113,113,113	0
23	MG	A	1872	1/1	0.99	0.17	325,325,325,325	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1611	1/1	0.99	0.12	184,184,184,184	0
23	MG	A	1687	1/1	0.99	0.27	136,136,136,136	0
23	MG	A	1652	1/1	0.99	0.24	114,114,114,114	0
23	MG	A	1603	1/1	0.99	0.05	163,163,163,163	0
23	MG	A	1685	1/1	0.99	0.09	209,209,209,209	0
23	MG	A	1607	1/1	0.99	0.13	74,74,74,74	0
23	MG	A	1629	1/1	0.99	0.19	91,91,91,91	0
23	MG	A	1658	1/1	0.99	0.05	225,225,225,225	0
23	MG	A	1670	1/1	0.99	0.46	196,196,196,196	0
23	MG	A	1628	1/1	0.99	0.15	149,149,149,149	0
23	MG	A	1979	1/1	0.99	0.21	133,133,133,133	0
23	MG	A	1604	1/1	1.00	0.12	137,137,137,137	0
23	MG	A	1939	1/1	1.00	0.37	506,506,506,506	0
24	ZN	N	101	1/1	1.00	0.21	147,147,147,147	0
23	MG	A	1959	1/1	1.00	0.14	106,106,106,106	0
24	ZN	D	301	1/1	1.00	0.31	114,114,114,114	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers

There are no such residues in this entry.